



Full wwPDB EM Validation Report ⓘ

Jul 4, 2026 – 08:51 PM EDT

PDB ID : 9OM3 / pdb_00009om3
EMDB ID : EMD-70605
Title : Two Component Protein Nano-Particle (T=3). De Novo Design, Computationally Relaxed into Low Resolution Single Particle CryoEM Map with Icosahedral Symmetry Applied
Authors : DiMaio, F.; Weidle, C.
Deposited on : 2025-05-13
Resolution : 17.45 Å (reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

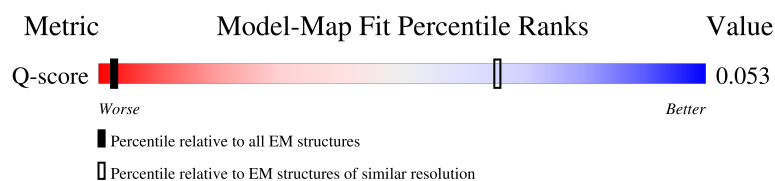
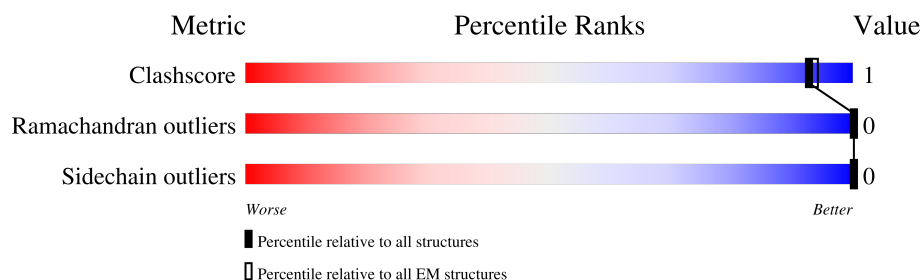
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	29 (17.00 - 17.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	114	 84% 8% 7%
1	AA	114	 82% 11% 7%
1	AC	114	 81% 11% 7%
1	AE	114	 86% 7% 7%

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Mol	Chain	Length	Quality of chain
1	AG	114	
1	AI	114	
1	AK	114	
1	AM	114	
1	AO	114	
1	AQ	114	
1	AS	114	
1	AU	114	
1	AW	114	
1	AY	114	
1	Aa	114	
1	Ac	114	
1	Ae	114	
1	Ag	114	
1	Ai	114	
1	Ak	114	
1	Am	114	
1	Ao	114	
1	Aq	114	
1	As	114	
1	Au	114	
1	Aw	114	
1	Ay	114	
1	BA	114	
1	BC	114	

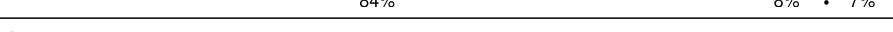
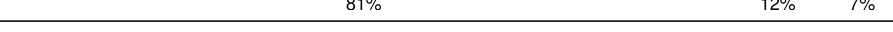
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Mol	Chain	Length	Quality of chain
1	BE	114	
1	BG	114	
1	BI	114	
1	BK	114	
1	BM	114	
1	BO	114	
1	BQ	114	
1	BS	114	
1	BU	114	
1	BW	114	
1	BY	114	
1	Ba	114	
1	Bc	114	
1	Be	114	
1	Bg	114	
1	Bi	114	
1	Bk	114	
1	Bm	114	
1	Bo	114	
1	Bq	114	
1	Bs	114	
1	Bu	114	
1	Bw	114	
1	By	114	
1	C	114	

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Mol	Chain	Length	Quality of chain
1	CA	114	 84% 8% 7%
1	CC	114	 81% 12% 7%
1	CE	114	 82% 10% 7%
1	CG	114	 84% 8% 7%
1	CI	114	 84% 9% 7%
1	CK	114	 82% 10% 7%
1	CM	114	 85% 8% 7%
1	CO	114	 18% 82% 11% 7%
1	CQ	114	 82% 10% 7%
1	CS	114	 85% 8% 7%
1	CU	114	 9% 82% 11% 7%
1	CW	114	 82% 10% 7%
1	CY	114	 83% 9% 7%
1	Ca	114	 15% 82% 11% 7%
1	Cc	114	 82% 10% 7%
1	Ce	114	 84% 8% 7%
1	Cg	114	 81% 12% 7%
1	Ci	114	 82% 10% 7%
1	Ck	114	 84% 8% 7%
1	Cm	114	 6% 82% 11% 7%
1	Co	114	 82% 10% 7%
1	Cq	114	 85% 8% 7%
1	Cs	114	 15% 82% 11% 7%
1	Cu	114	 82% 10% 7%
1	Cw	114	 86% 7% 7%

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Mol	Chain	Length	Quality of chain
1	Cy	114	
1	DA	114	
1	DC	114	
1	DE	114	
1	DG	114	
1	DI	114	
1	DK	114	
1	DM	114	
1	DO	114	
1	DQ	114	
1	DS	114	
1	DU	114	
1	DW	114	
1	DY	114	
1	Da	114	
1	Dc	114	
1	De	114	
1	Dg	114	
1	Di	114	
1	Dk	114	
1	Dm	114	
1	Do	114	
1	Dq	114	
1	Ds	114	
1	Du	114	

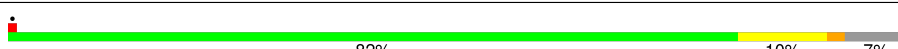
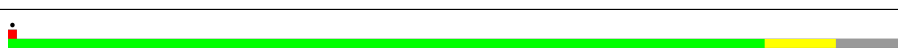
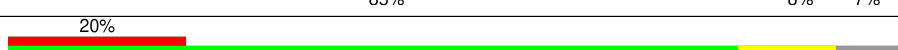
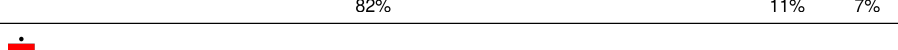
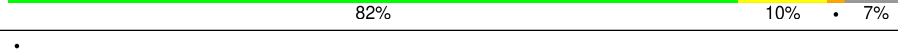
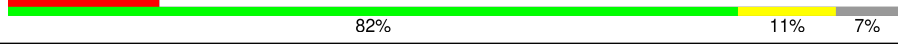
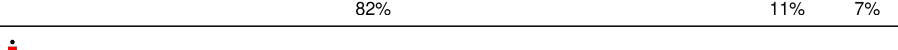
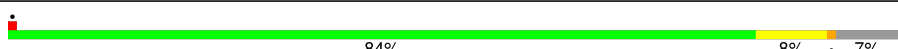
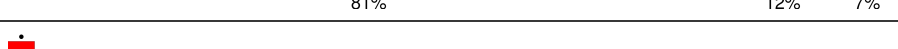
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Mol	Chain	Length	Quality of chain
1	Dw	114	 6% 82% 11% 7%
1	Dy	114	 82% 10% 7%
1	E	114	 82% 10% 7%
1	EA	114	 82% 10% 7%
1	EC	114	 85% 8% 7%
1	EE	114	 9% 82% 11% 7%
1	EG	114	 80% 11% 7%
1	EI	114	 86% 7% 7%
1	EK	114	 82% 11% 7%
1	EM	114	 82% 10% 7%
1	EO	114	 84% 8% 7%
1	EQ	114	 14% 82% 11% 7%
1	ES	114	 82% 10% 7%
1	EU	114	 85% 7% 7%
1	EW	114	 82% 11% 7%
1	EY	114	 82% 10% 7%
1	Ea	114	 85% 8% 7%
1	Ec	114	 6% 82% 11% 7%
1	Ee	114	 82% 10% 7%
1	Eg	114	 84% 8% 7%
1	Ei	114	 7% 82% 11% 7%
1	Ek	114	 82% 10% 7%
1	Em	114	 86% 7% 7%
1	Eo	114	 82% 11% 7%
1	Eq	114	 82% 10% 7%

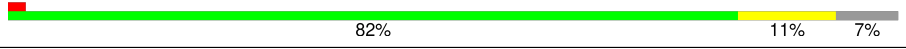
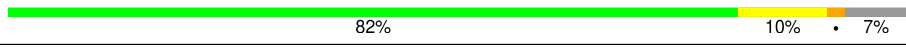
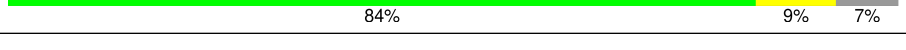
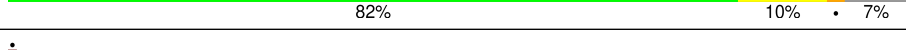
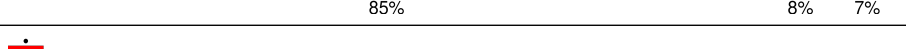
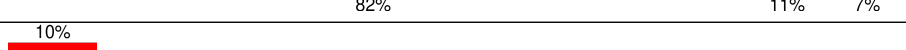
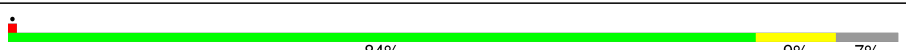
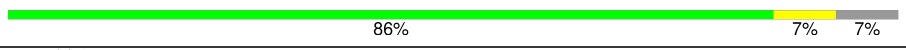
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Mol	Chain	Length	Quality of chain
1	Es	114	
1	Eu	114	
1	Ew	114	
1	G	114	
1	I	114	
1	K	114	
1	M	114	
1	O	114	
1	Q	114	
1	S	114	
1	U	114	
1	W	114	
1	Y	114	
1	YA	114	
1	YC	114	
1	YE	114	
1	YG	114	
1	YI	114	
1	YK	114	
1	YM	114	
1	YO	114	
1	YQ	114	
1	YS	114	
1	YU	114	
1	YW	114	

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Mol	Chain	Length	Quality of chain
1	ZA	114	
1	ZC	114	
1	ZE	114	
1	ZG	114	
1	ZI	114	
1	ZK	114	
1	ZM	114	
1	ZO	114	
1	ZQ	114	
1	ZS	114	
1	ZU	114	
1	ZW	114	
1	ZY	114	
1	a	114	
1	c	114	
1	e	114	
1	g	114	
1	i	114	
1	k	114	
1	m	114	
1	o	114	
1	q	114	
1	s	114	
1	u	114	
1	w	114	

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Mol	Chain	Length	Quality of chain
1	y	114	9% 82% 11% 7%
2	AB	300	12% 94%
2	AD	300	11% 93% 5%
2	AF	300	10% 94%
2	AH	300	11% 94%
2	AJ	300	6% 93% 5%
2	AL	300	94%
2	AN	300	9% 94%
2	AP	300	7% 93%
2	AR	300	6% 94%
2	AT	300	10% 93%
2	AV	300	7% 93% 5%
2	AX	300	9% 95%
2	AZ	300	11% 94%
2	Ab	300	8% 93%
2	Ad	300	9% 94%
2	Af	300	11% 94%
2	Ah	300	93%
2	Aj	300	12% 94%
2	Al	300	12% 94%
2	An	300	7% 93%
2	Ap	300	7% 94%
2	Ar	300	10% 94%
2	At	300	5% 93%
2	Av	300	7% 94%

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Mol	Chain	Length	Quality of chain
2	Ax	300	11% 94% 5%
2	Az	300	12% 93% 5%
2	B	300	8% 94% 5%
2	BB	300	10% 93% 5%
2	BD	300	9% 94% 5%
2	BF	300	11% 93% 5%
2	BH	300	6% 93% 5%
2	BJ	300	11% 95% 5%
2	BL	300	13% 93% 5%
2	BN	300	8% 93% 5%
2	BP	300	5% 94% 5%
2	BR	300	9% 93% 5%
2	BT	300	9% 93% 5%
2	BV	300	9% 94% 5%
2	BX	300	13% 94% 5%
2	BZ	300	12% 93% 5%
2	Bb	300	8% 94% 5%
2	Bd	300	10% 93% 5%
2	Bf	300	10% 93% 5%
2	Bh	300	7% 94% 5%
2	Bj	300	11% 94% 5%
2	Bl	300	12% 93% 5%
2	Bn	300	10% 94% 5%
2	Bp	300	12% 93% 5%
2	Br	300	11% 93% 5%

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Mol	Chain	Length	Quality of chain
2	Bt	300	8% 94% • •
2	Bv	300	10% 93% • •
2	Bx	300	10% 93% • •
2	Bz	300	7% 94% • •
2	CB	300	7% 94% • •
2	CD	300	11% 93% • •
2	CF	300	10% 93% • •
2	CH	300	12% 95% • •
2	CJ	300	13% 93% • •
2	CL	300	7% 93% • •
2	CN	300	5% 94% • •
2	CP	300	10% 94% • •
2	CR	300	5% 93% • •
2	CT	300	9% 94% • •
2	CV	300	11% 93% 5% •
2	CX	300	• 93% 5% •
2	CZ	300	6% 94% • •
2	C'b	300	10% 92% 5% •
2	Cd	300	7% 93% 5% •
2	Cf	300	9% 94% • •
2	Ch	300	11% 93% • •
2	Cj	300	8% 93% 5% •
2	Cl	300	9% 94% • •
2	Cn	300	13% 93% • •
2	Cp	300	12% 93% • •

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Mol	Chain	Length	Quality of chain
2	Cr	300	11% 95% • •
2	Ct	300	13% 93% 5% •
2	Cv	300	8% 93% • •
2	Cx	300	5% 94% • •
2	Cz	300	9% 94% • •
2	D	300	11% 93% • •
2	DB	300	11% 94% • •
2	DD	300	12% 92% 5% •
2	DF	300	12% 94% • •
2	DH	300	12% 92% 5% •
2	DJ	300	7% 93% • •
2	DL	300	12% 94% • •
2	DN	300	12% 93% • •
2	DP	300	10% 93% 5% •
2	DR	300	7% 94% • •
2	DT	300	10% 93% 5% •
2	DV	300	7% 92% 5% •
2	DX	300	7% 94% • •
2	DZ	300	12% 93% • •
2	Db	300	13% 92% 5% •
2	Dd	300	• 94% • •
2	Df	300	9% 93% • •
2	Dh	300	7% 93% • •
2	Dj	300	11% 94% • •
2	DI	300	12% 93% 5% •

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Mol	Chain	Length	Quality of chain
2	Dn	300	
2	Dp	300	
2	Dr	300	
2	Dt	300	
2	Dv	300	
2	Dx	300	
2	Dz	300	
2	EB	300	
2	ED	300	
2	EF	300	
2	EH	300	
2	EJ	300	
2	EL	300	
2	EN	300	
2	EP	300	
2	ER	300	
2	ET	300	
2	EV	300	
2	EX	300	
2	EZ	300	
2	Eb	300	
2	Ed	300	
2	Ef	300	
2	Eh	300	
2	Ej	300	

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Mol	Chain	Length	Quality of chain
2	El	300	
2	En	300	
2	Ep	300	
2	Er	300	
2	Et	300	
2	Ev	300	
2	Ex	300	
2	F	300	
2	H	300	
2	J	300	
2	L	300	
2	N	300	
2	P	300	
2	R	300	
2	T	300	
2	V	300	
2	X	300	
2	YB	300	
2	YD	300	
2	YF	300	
2	YH	300	
2	YJ	300	
2	YL	300	
2	YN	300	
2	YP	300	

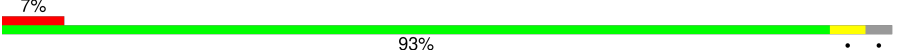
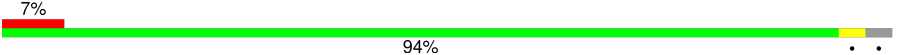
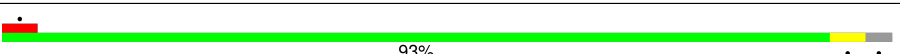
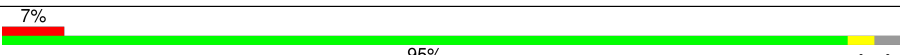
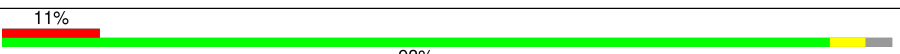
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Mol	Chain	Length	Quality of chain
2	YR	300	
2	YT	300	
2	YV	300	
2	YX	300	
2	Z	300	
2	ZB	300	
2	ZD	300	
2	ZF	300	
2	ZH	300	
2	ZJ	300	
2	ZL	300	
2	ZN	300	
2	ZP	300	
2	ZR	300	
2	ZT	300	
2	ZV	300	
2	ZX	300	
2	ZZ	300	
2	b	300	
2	d	300	
2	f	300	
2	h	300	
2	j	300	
2	l	300	
2	n	300	

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Mol	Chain	Length	Quality of chain
2	p	300	
2	r	300	
2	t	300	
2	v	300	
2	x	300	
2	z	300	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 553500 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called C2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	C	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	E	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	G	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	I	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	K	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	M	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	O	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Q	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	S	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	U	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	W	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Y	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	a	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	c	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	e	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	g	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	k	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	m	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	o	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	q	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	s	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	u	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	w	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	y	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AM	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Aa	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ac	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ae	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ag	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ai	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ak	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Am	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ao	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Aq	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	As	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Au	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Aw	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ay	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZM	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ba	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bc	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Be	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bg	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bi	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bk	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bm	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bo	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bq	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bs	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bu	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Bw	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	By	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CO	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ca	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cc	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ce	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cg	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ci	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ck	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cm	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Co	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cq	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cs	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cu	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cw	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Cy	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YI	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	YK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Da	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Dc	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	De	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Dg	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Di	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Dk	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Dm	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Do	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Dq	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Ds	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Du	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Dw	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	Dy	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EQ	106	Total 808	C 506	N 149	O 152	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ES	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	EU	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	EW	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	EY	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Ea	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Ec	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Ee	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Eg	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Ei	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Ek	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Em	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Eo	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Eq	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Es	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Eu	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	Ew	106	Total	C	N	O	S	0	0
			808	506	149	152	1		

- Molecule 2 is a protein called C3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	292	Total	C	N	O	S	0	0
			2267	1421	413	430	3		
2	D	292	Total	C	N	O	S	0	0
			2267	1421	413	430	3		
2	F	292	Total	C	N	O	S	0	0
			2267	1421	413	430	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	J	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	L	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	N	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	P	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	R	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	T	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	V	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	X	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Z	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	b	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	d	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	f	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	h	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	j	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	l	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	n	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	p	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	r	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	t	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	v	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	x	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	z	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ab	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ad	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Af	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ah	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Aj	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Al	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	An	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ap	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ar	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	At	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Av	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ax	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Az	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bb	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bd	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bf	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bh	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bj	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bl	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bn	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bp	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Br	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bt	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bv	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Bx	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bz	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cb	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cd	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cf	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ch	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cj	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cl	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cn	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cp	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cr	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ct	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cv	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cx	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Cz	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Db	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dd	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Df	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dh	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dj	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Di	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dn	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dp	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dr	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dt	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dv	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dx	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Dz	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	YP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ED	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ER	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ET	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Eb	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ed	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ef	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

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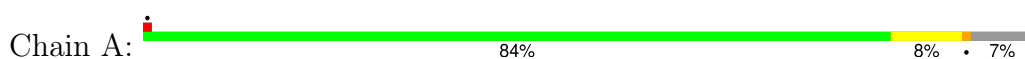
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Mol	Chain	Residues	Atoms					AltConf	Trace
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2	Ej	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	El	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	En	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ep	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Er	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Et	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ev	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	Ex	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

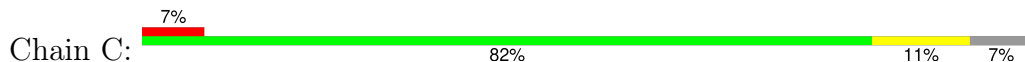
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

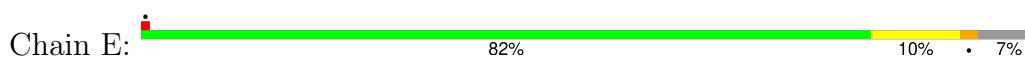
- Molecule 1: C2-B



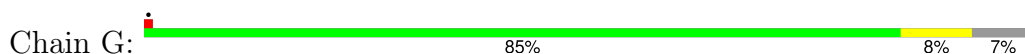
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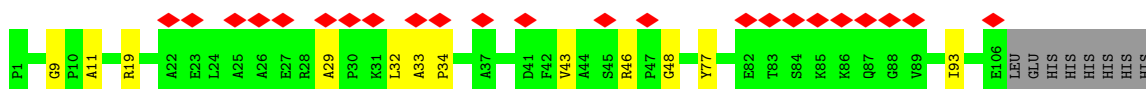
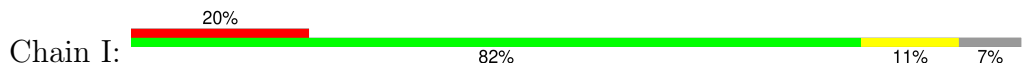
- Molecule 1: C2-B



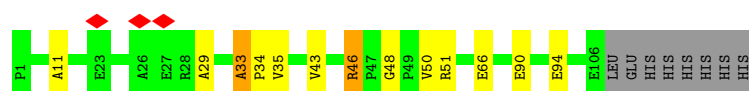
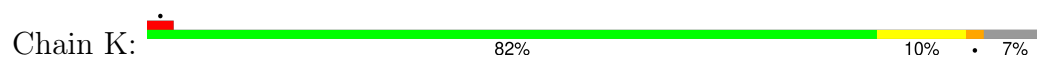
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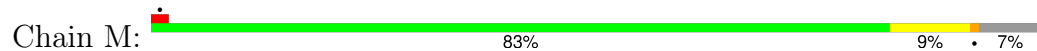
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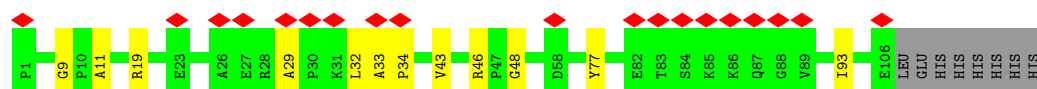
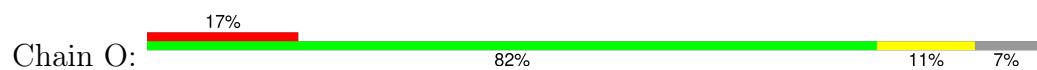
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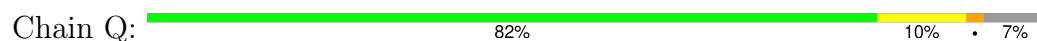
- Molecule 1: C2-B



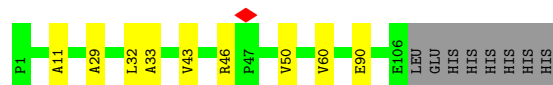
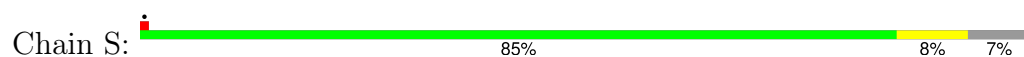
- Molecule 1: C2-B



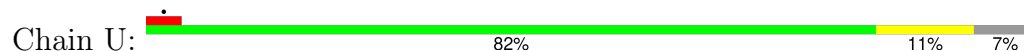
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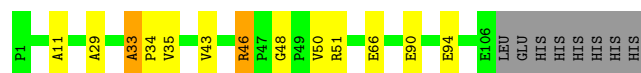
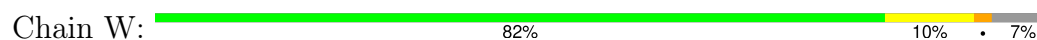
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B

Chain Y:  83% 9% • 7%



• Molecule 1: C2-B

Chain a:  9% 80% 13% 7%



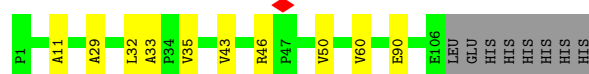
• Molecule 1: C2-B

Chain c:  82% 10% • 7%



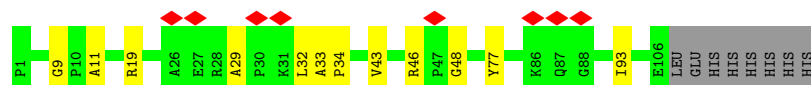
• Molecule 1: C2-B

Chain e:  84% 9% 7%



• Molecule 1: C2-B

Chain g:  7% 82% 11% 7%



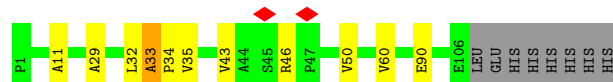
• Molecule 1: C2-B

Chain i:  82% 10% • 7%

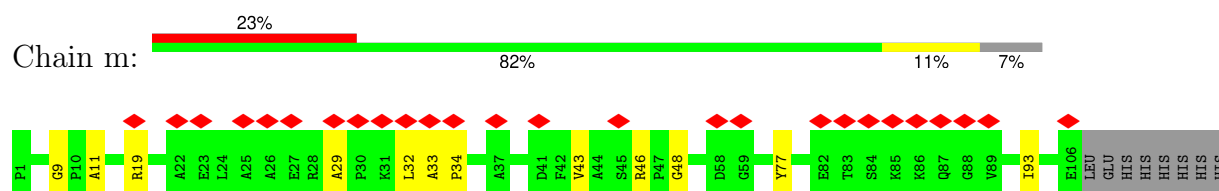


• Molecule 1: C2-B

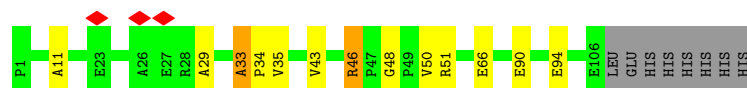
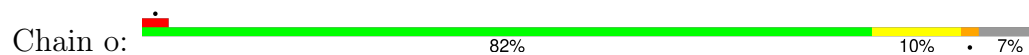
Chain k:  83% 9% • 7%



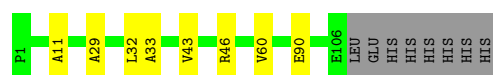
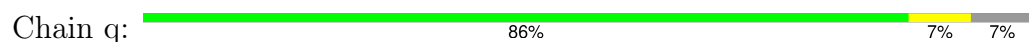
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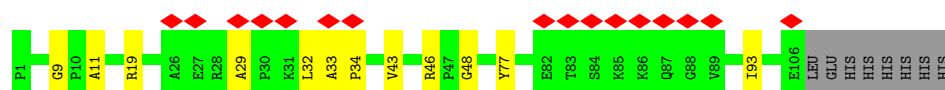
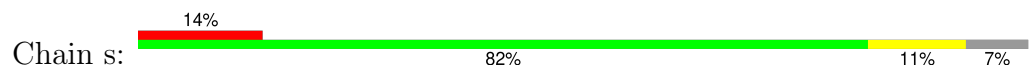
- Molecule 1: C2-B



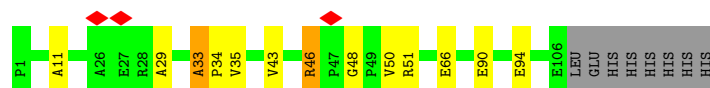
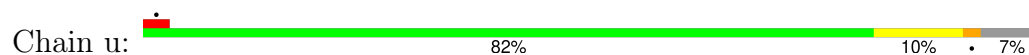
- Molecule 1: C2-B



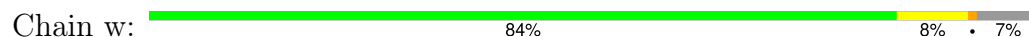
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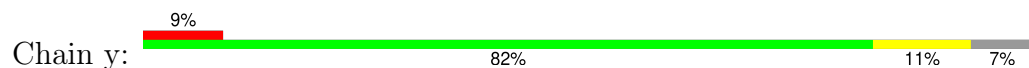
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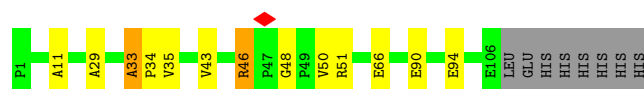
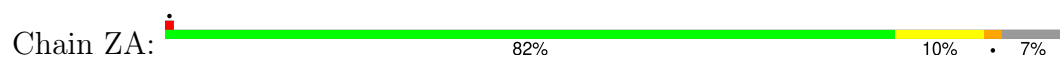
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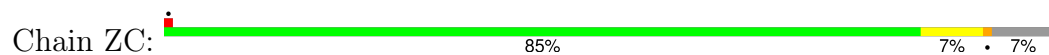
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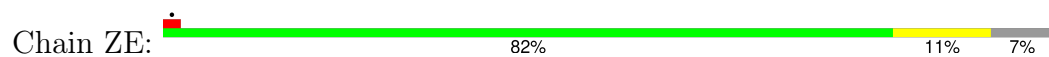
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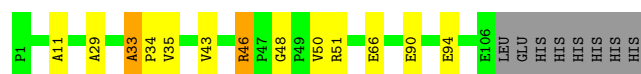
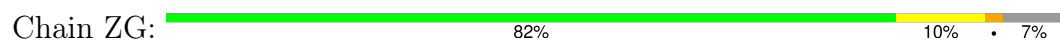
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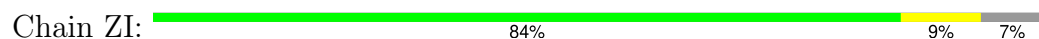
- Molecule 1: C2-B



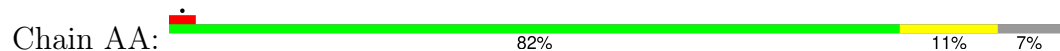
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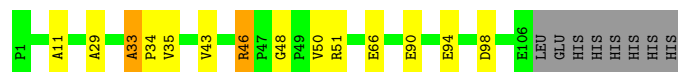
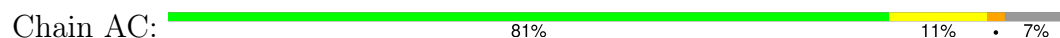
- Molecule 1: C2-B



- Molecule 1: C2-B

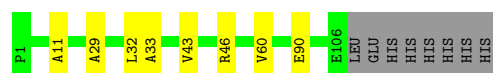


- Molecule 1: C2-B



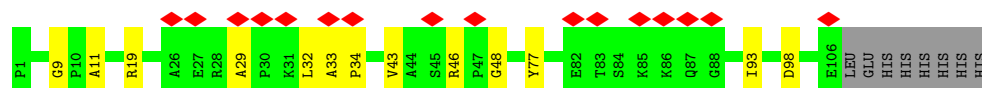
- Molecule 1: C2-B

Chain AE:  86% 7% 7%



• Molecule 1: C2-B

Chain AG:  14% 82% 11% 7%



• Molecule 1: C2-B

Chain AI:  82% 10% 7%



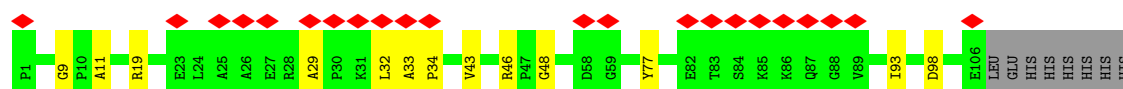
• Molecule 1: C2-B

Chain AK:  86% 7% 7%



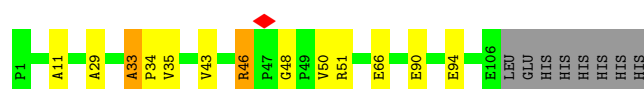
• Molecule 1: C2-B

Chain AM:  19% 82% 11% 7%



• Molecule 1: C2-B

Chain AO:  82% 10% 7%

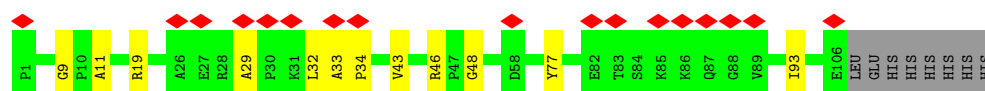
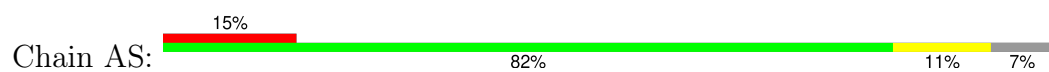


• Molecule 1: C2-B

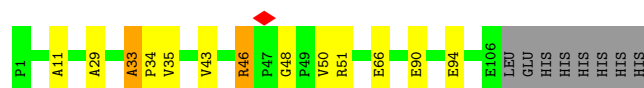
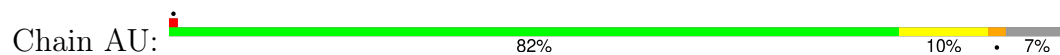
Chain AQ:  85% 8% 7%



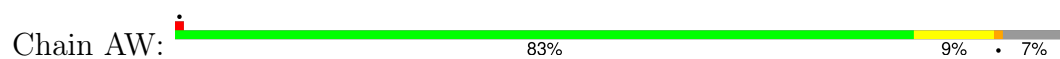
• Molecule 1: C2-B



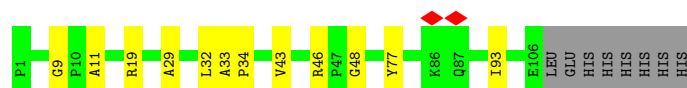
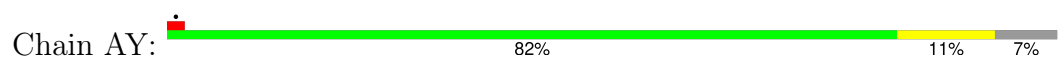
- Molecule 1: C2-B



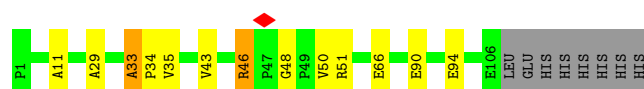
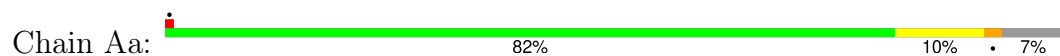
- Molecule 1: C2-B



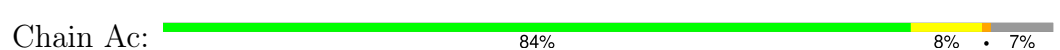
- Molecule 1: C2-B



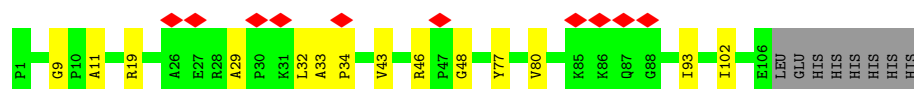
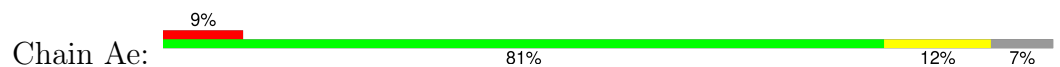
- Molecule 1: C2-B



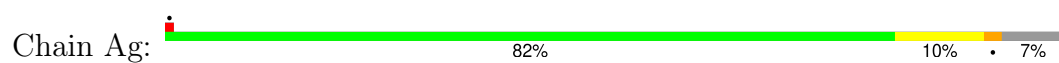
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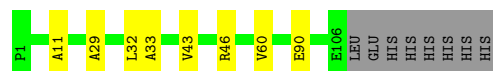
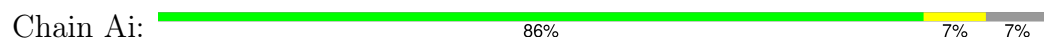
- Molecule 1: C2-B



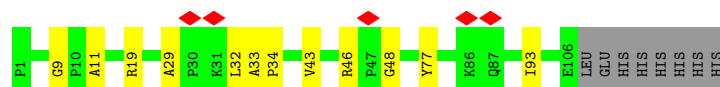
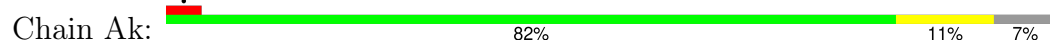
- Molecule 1: C2-B



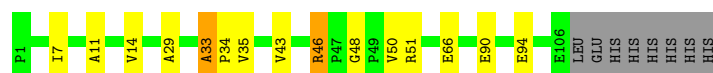
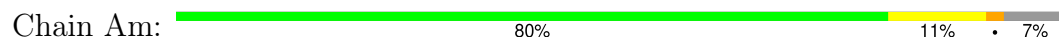
- Molecule 1: C2-B



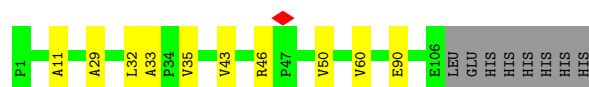
- Molecule 1: C2-B



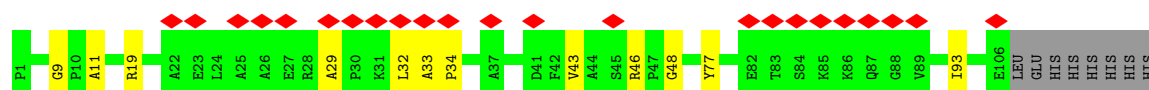
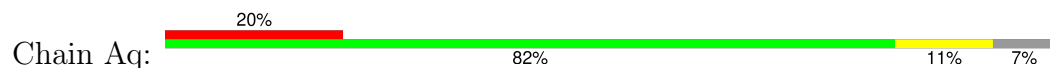
- Molecule 1: C2-B



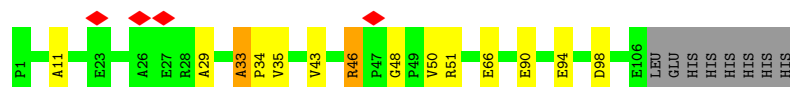
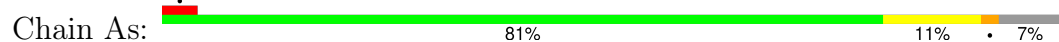
- Molecule 1: C2-B



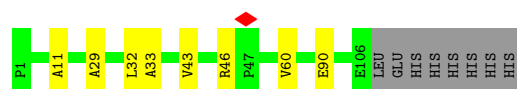
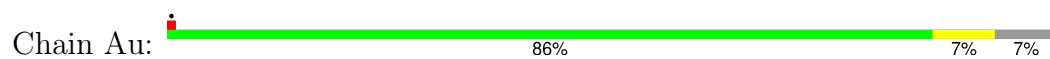
- Molecule 1: C2-B



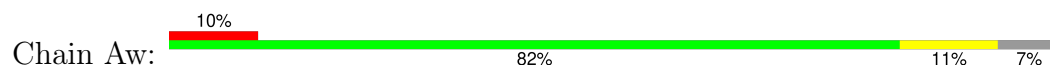
- Molecule 1: C2-B



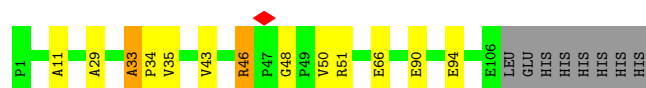
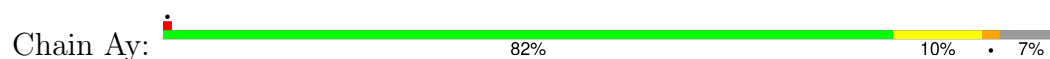
- Molecule 1: C2-B



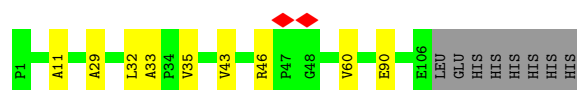
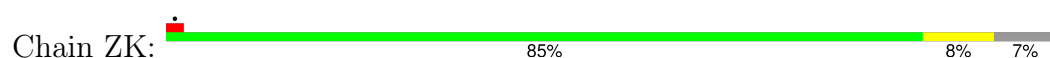
- Molecule 1: C2-B



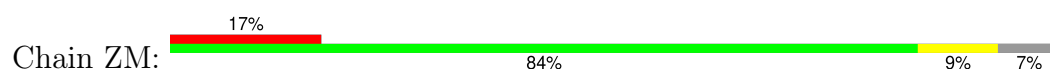
- Molecule 1: C2-B



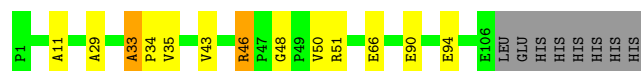
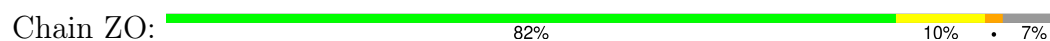
- Molecule 1: C2-B



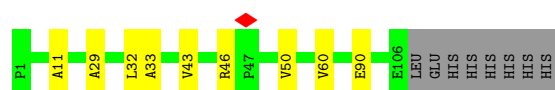
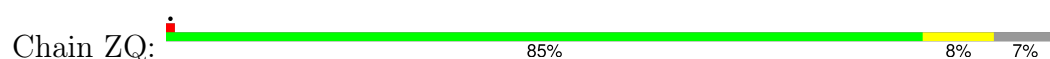
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B



• Molecule 1: C2-B

Chain ZS:  82% 11% 7%



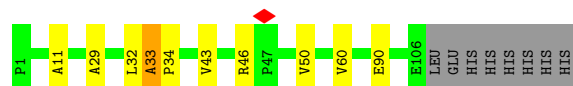
• Molecule 1: C2-B

Chain BA:  82% 10% 7%



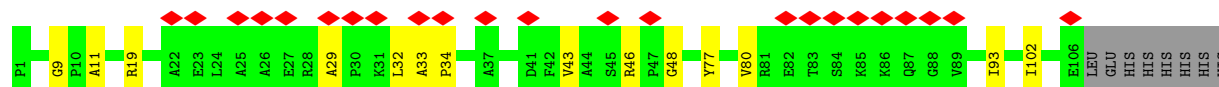
• Molecule 1: C2-B

Chain BC:  84% 8% 7%



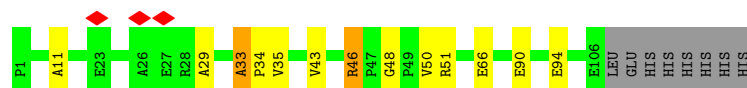
• Molecule 1: C2-B

Chain BE:  20% 81% 12% 7%



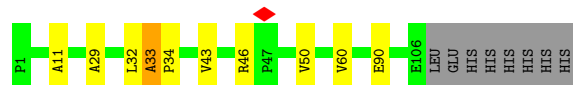
• Molecule 1: C2-B

Chain BG:  82% 10% 7%



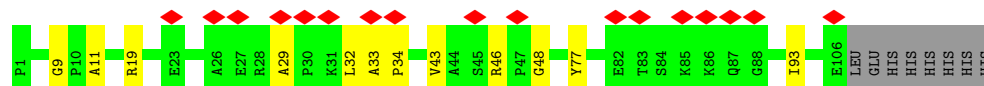
• Molecule 1: C2-B

Chain BI:  84% 8% 7%

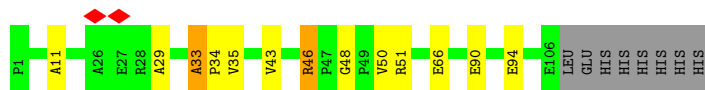


• Molecule 1: C2-B

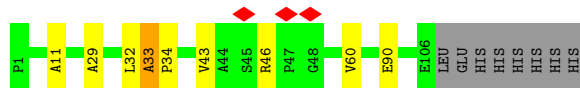
Chain BK:  15% 82% 11% 7%



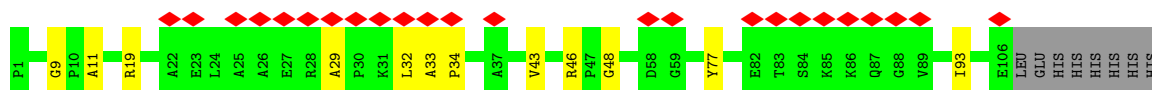
● Molecule 1: C2-B

Chain BM:  82% 10% 7%

● Molecule 1: C2-B

Chain BO:  85% 7% 7%

● Molecule 1: C2-B

Chain BQ:  21% 82% 11% 7%

● Molecule 1: C2-B

Chain BS:  81% 11% 7%

● Molecule 1: C2-B

Chain BU:  86% 7% 7%

● Molecule 1: C2-B

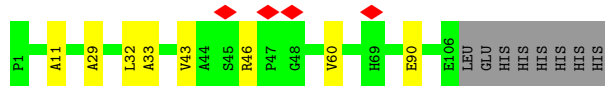
Chain BW:  6% 82% 11% 7%

● Molecule 1: C2-B

Chain BY:  82% 10% 7%

• Molecule 1: C2-B

Chain Ba:  86% 7% 7%



• Molecule 1: C2-B

Chain Bc:  18% 82% 11% 7%



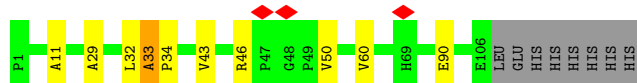
• Molecule 1: C2-B

Chain Be:  82% 10% 7%



• Molecule 1: C2-B

Chain Bg:  84% 8% 7%



• Molecule 1: C2-B

Chain Bi:  10% 82% 11% 7%



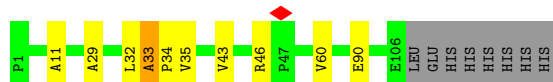
• Molecule 1: C2-B

Chain Bk:  82% 10% 7%

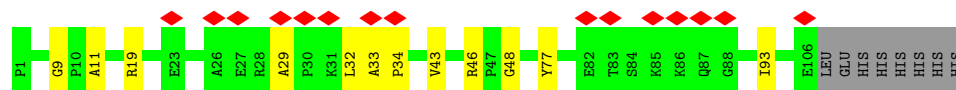
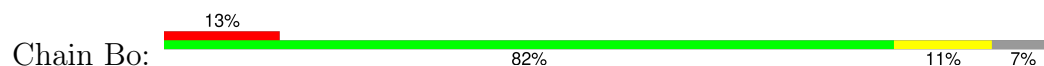


• Molecule 1: C2-B

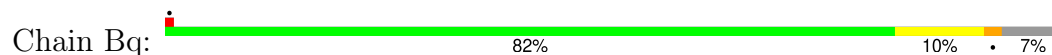
Chain Bm:  84% 8% 7%



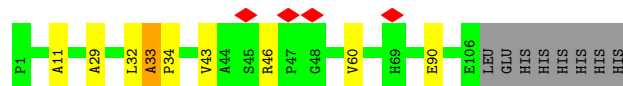
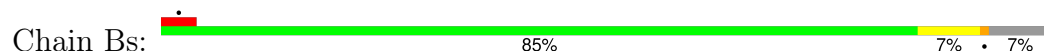
• Molecule 1: C2-B



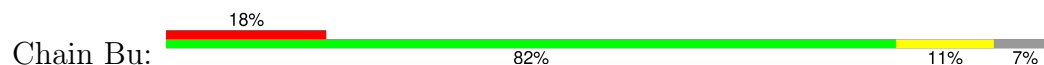
• Molecule 1: C2-B



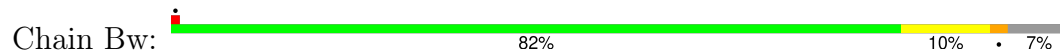
• Molecule 1: C2-B



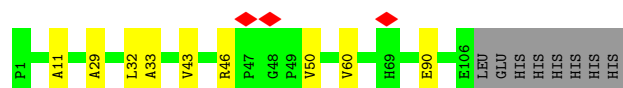
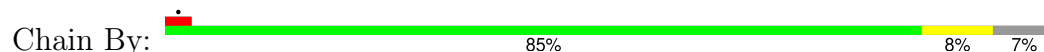
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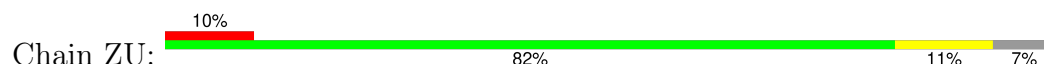
• Molecule 1: C2-B



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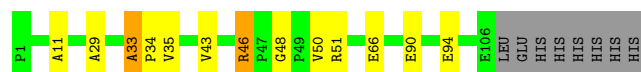
• Molecule 1: C2-B





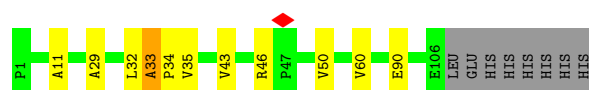
- Molecule 1: C2-B

Chain ZW: 82% 10% 7%



- Molecule 1: C2-B

Chain ZY: 83% 9% 7%



- Molecule 1: C2-B

Chain YA: 13% 82% 11% 7%



- Molecule 1: C2-B

Chain YC: 82% 10% 7%



- Molecule 1: C2-B

Chain CA: 84% 8% 7%



- Molecule 1: C2-B

Chain CC: 81% 12% 7%

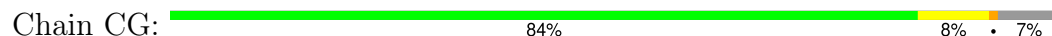


- Molecule 1: C2-B

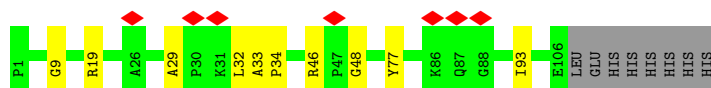
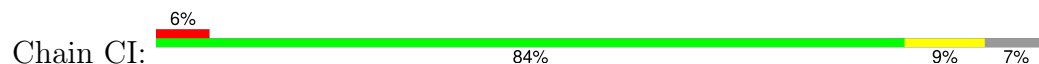
Chain CE: 82% 10% 7%



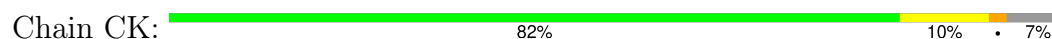
- Molecule 1: C2-B



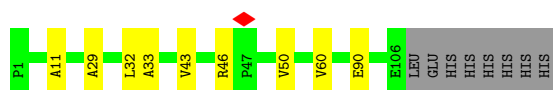
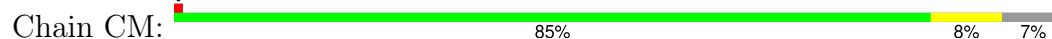
- Molecule 1: C2-B



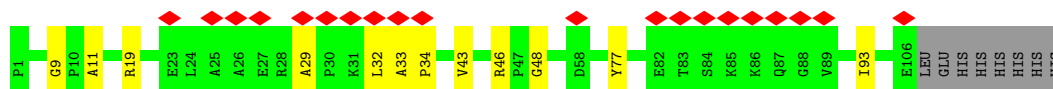
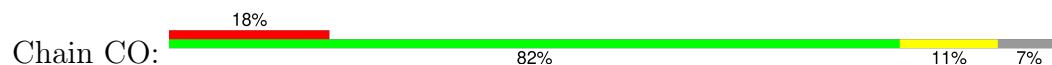
- Molecule 1: C2-B



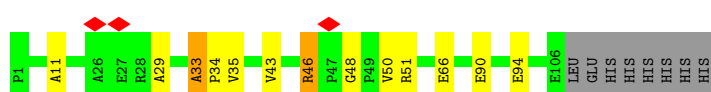
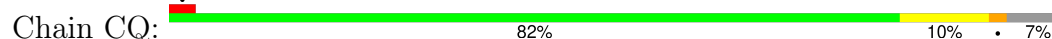
- Molecule 1: C2-B



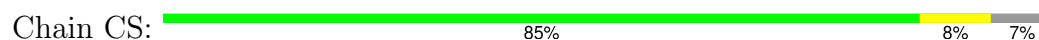
- Molecule 1: C2-B



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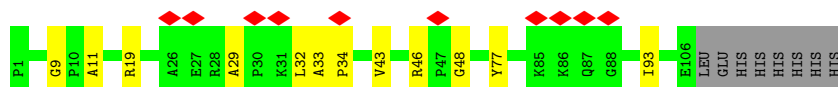
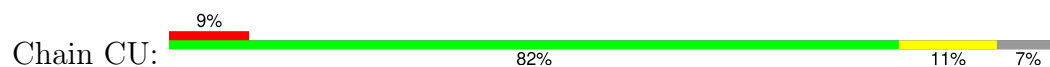


- Molecule 1: C2-B

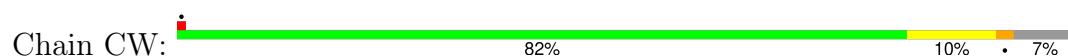




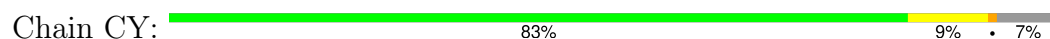
- Molecule 1: C2-B



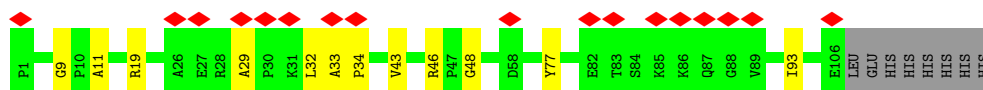
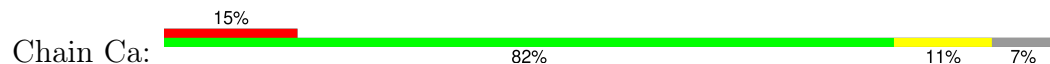
- Molecule 1: C2-B



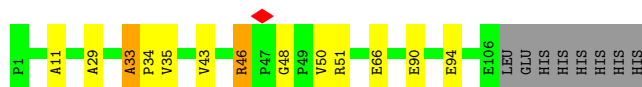
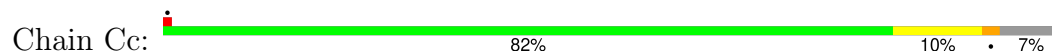
- Molecule 1: C2-B



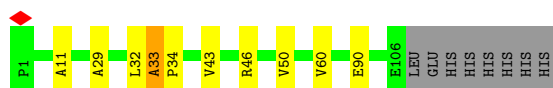
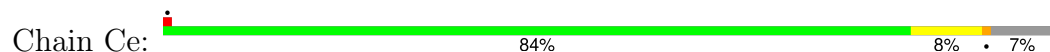
- Molecule 1: C2-B



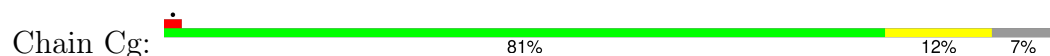
- Molecule 1: C2-B

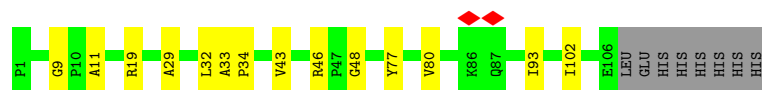


- Molecule 1: C2-B

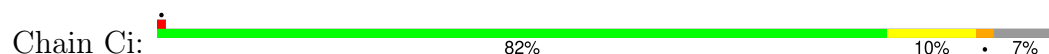


- Molecule 1: C2-B

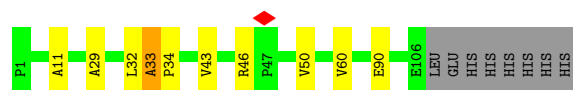
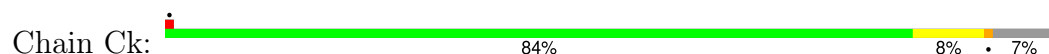




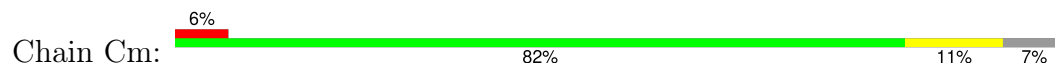
- Molecule 1: C2-B



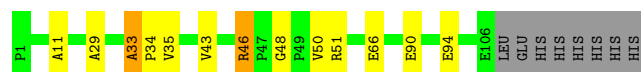
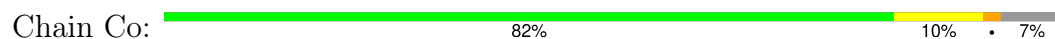
- Molecule 1: C2-B



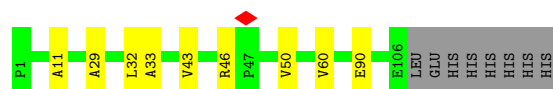
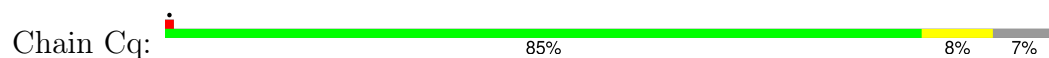
- Molecule 1: C2-B



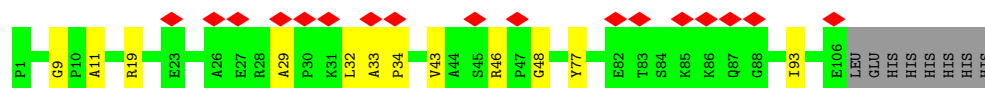
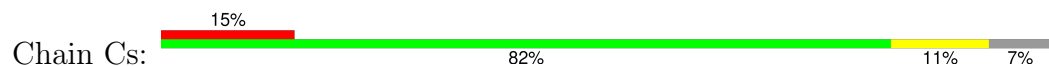
- Molecule 1: C2-B



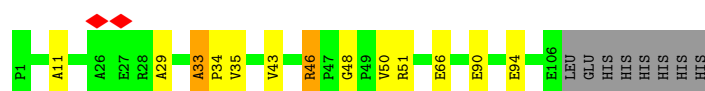
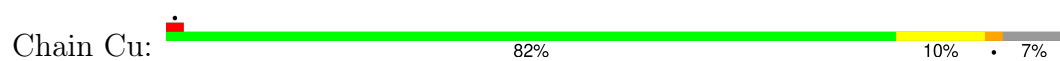
- Molecule 1: C2-B



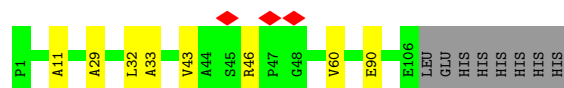
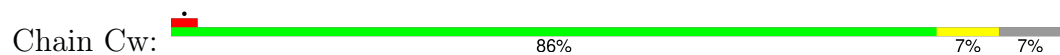
- Molecule 1: C2-B



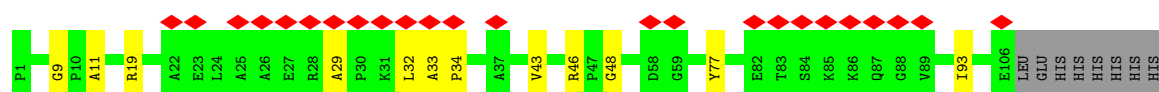
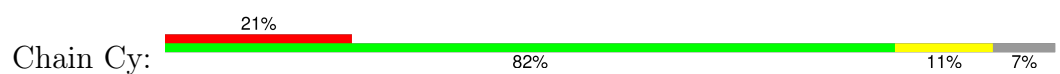
- Molecule 1: C2-B



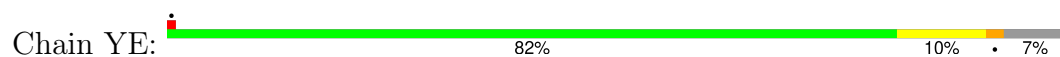
- Molecule 1: C2-B



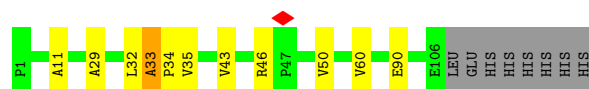
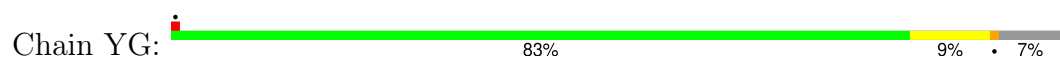
- Molecule 1: C2-B



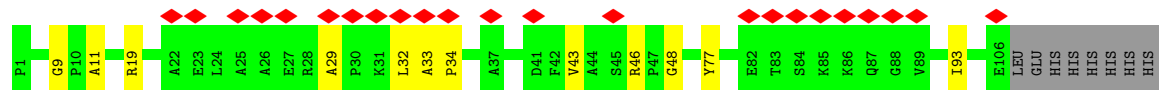
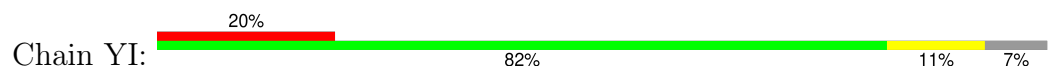
- Molecule 1: C2-B



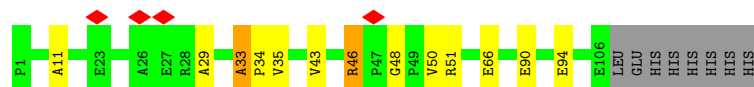
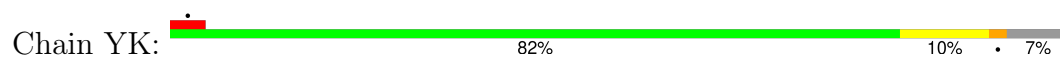
- Molecule 1: C2-B



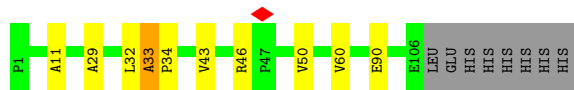
- Molecule 1: C2-B



- Molecule 1: C2-B



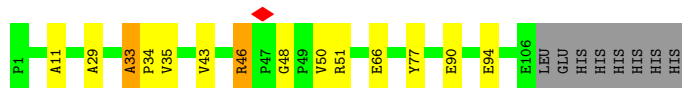
● Molecule 1: C2-B

Chain YM:  84% 8% 7%

● Molecule 1: C2-B

Chain DA:  10% 82% 11% 7%

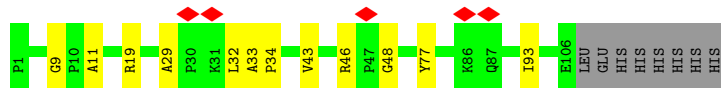
● Molecule 1: C2-B

Chain DC:  81% 11% 7%

● Molecule 1: C2-B

Chain DE:  85% 7% 7%

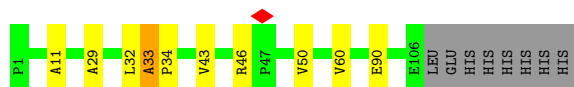
● Molecule 1: C2-B

Chain DG:  82% 11% 7%

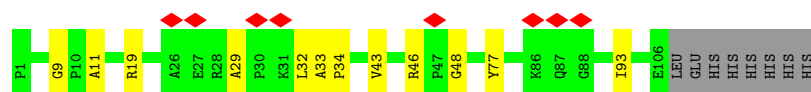
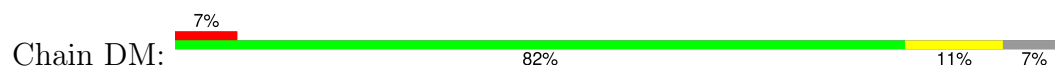
● Molecule 1: C2-B

Chain DI:  79% 12% 7%

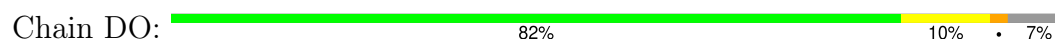
● Molecule 1: C2-B

Chain DK:  84% 8% 7%

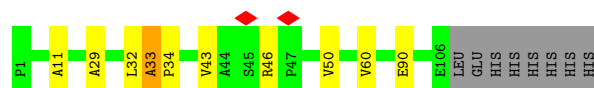
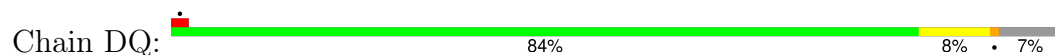
• Molecule 1: C2-B



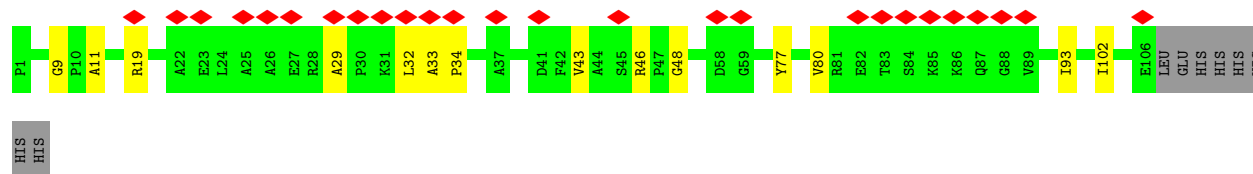
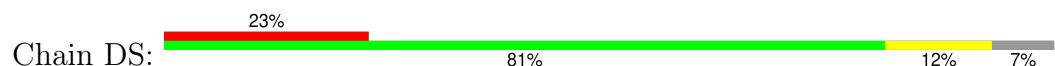
• Molecule 1: C2-B



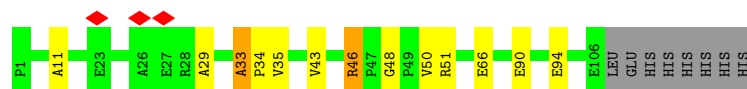
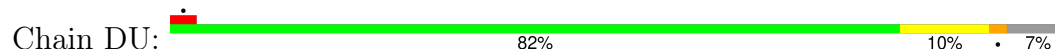
• Molecule 1: C2-B



• Molecule 1: C2-B



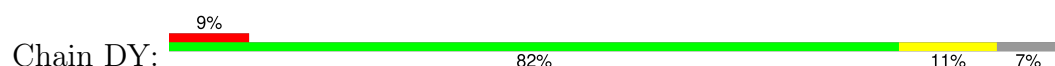
• Molecule 1: C2-B



• Molecule 1: C2-B

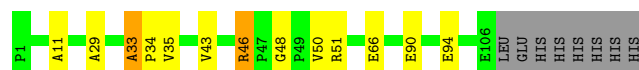
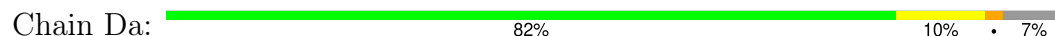


• Molecule 1: C2-B

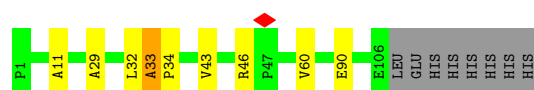
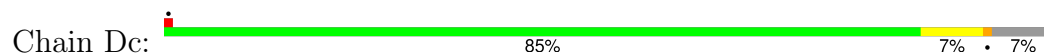




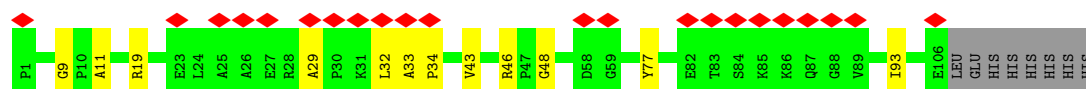
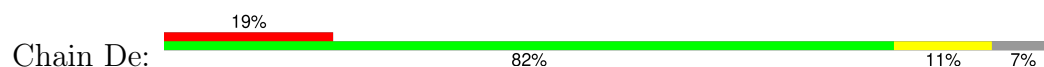
- Molecule 1: C2-B



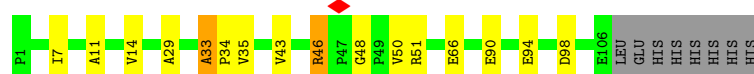
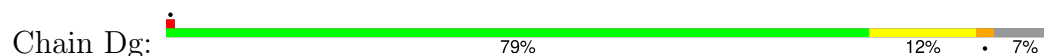
- Molecule 1: C2-B



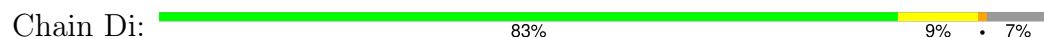
- Molecule 1: C2-B



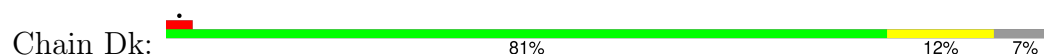
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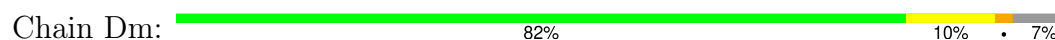
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B





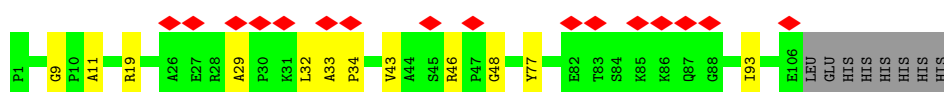
- Molecule 1: C2-B

Chain Do: 84% 8% 7%



- Molecule 1: C2-B

Chain Dq: 14% 82% 11% 7%



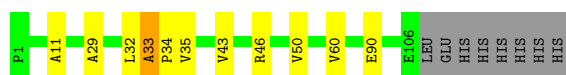
- Molecule 1: C2-B

Chain Ds: 82% 10% 7%



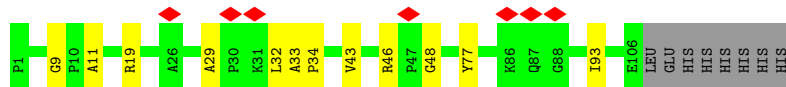
- Molecule 1: C2-B

Chain Du: 83% 9% 7%



- Molecule 1: C2-B

Chain Dw: 6% 82% 11% 7%



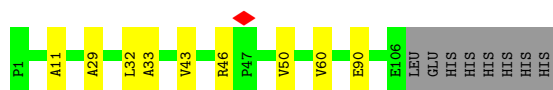
- Molecule 1: C2-B

Chain Dy: 82% 10% 7%

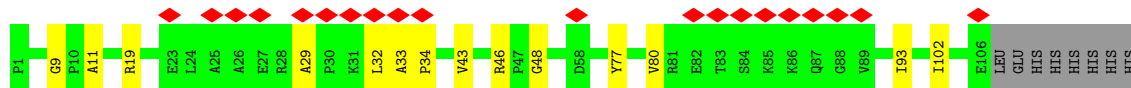
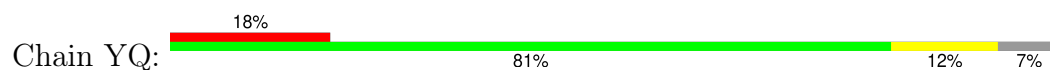


- Molecule 1: C2-B

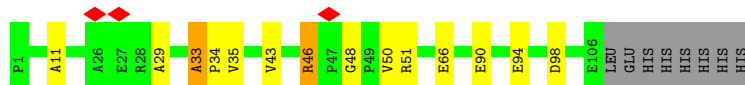
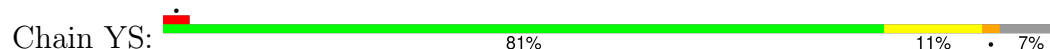
Chain YO: 85% 8% 7%



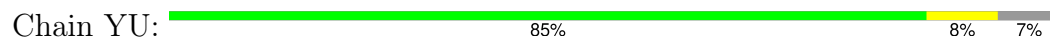
- Molecule 1: C2-B



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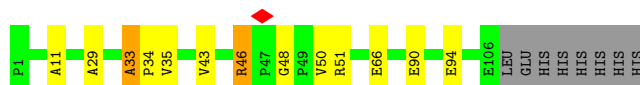
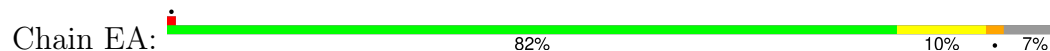
- Molecule 1: C2-B



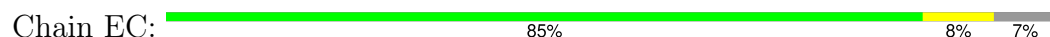
- Molecule 1: C2-B



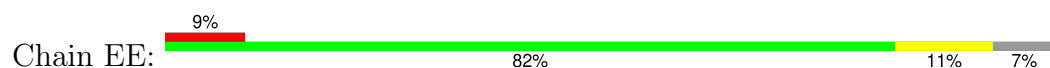
- Molecule 1: C2-B



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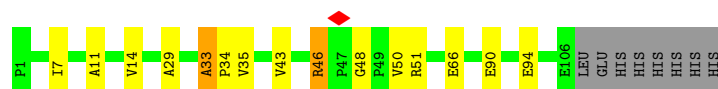
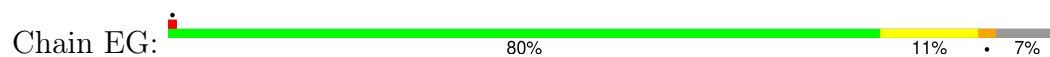


- Molecule 1: C2-B

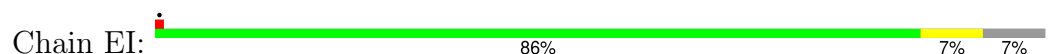




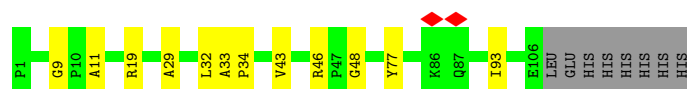
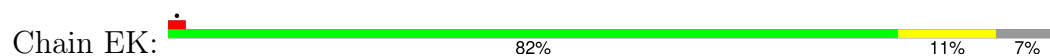
- Molecule 1: C2-B



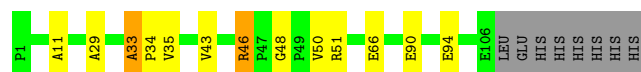
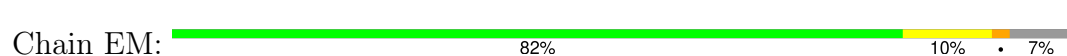
- Molecule 1: C2-B



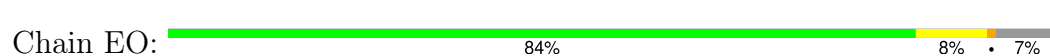
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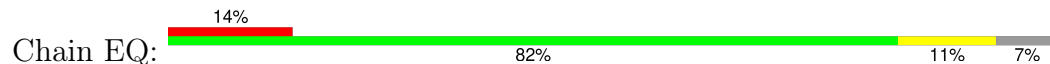
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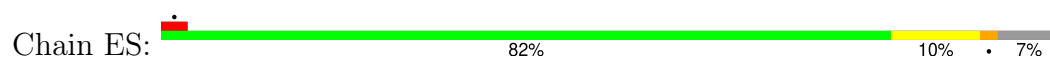
- Molecule 1: C2-B

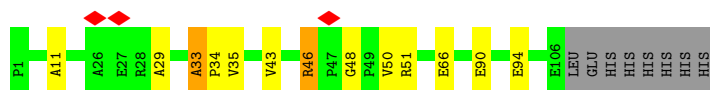


- Molecule 1: C2-B

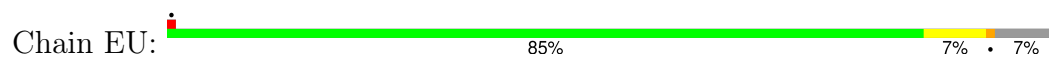


- Molecule 1: C2-B

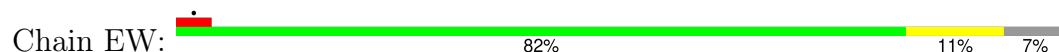




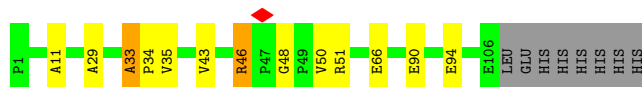
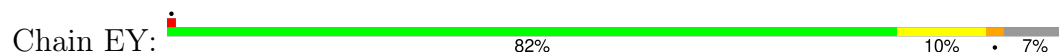
- Molecule 1: C2-B



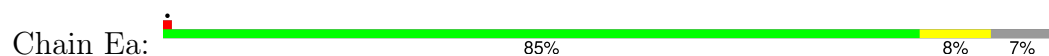
- Molecule 1: C2-B



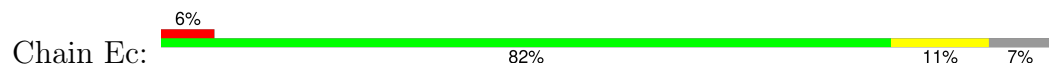
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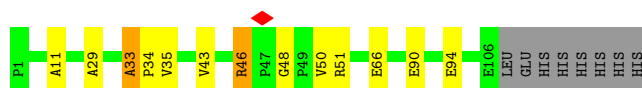
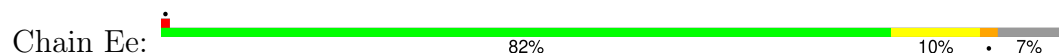
- Molecule 1: C2-B



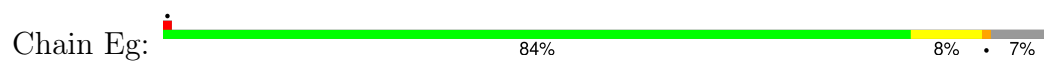
- Molecule 1: C2-B



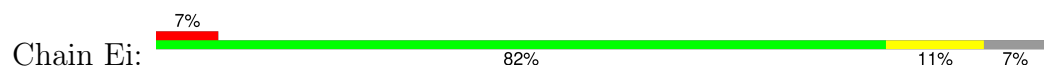
- Molecule 1: C2-B



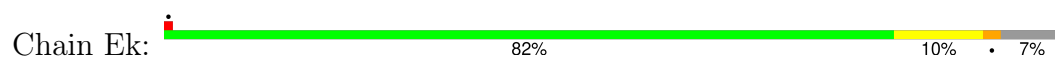
- Molecule 1: C2-B



• Molecule 1: C2-B



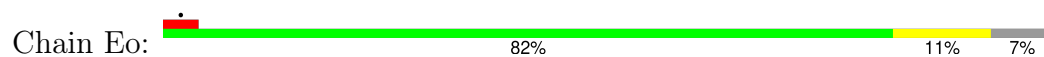
• Molecule 1: C2-B



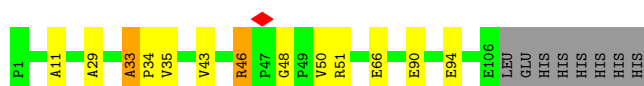
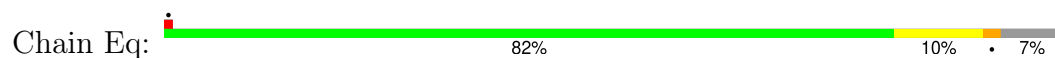
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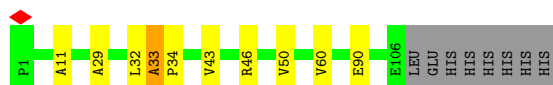
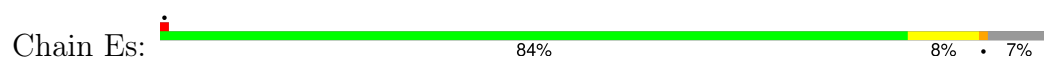
• Molecule 1: C2-B



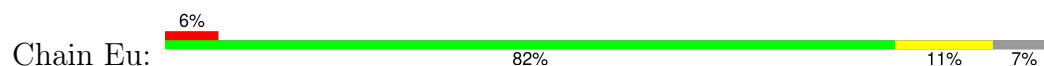
• Molecule 1: C2-B



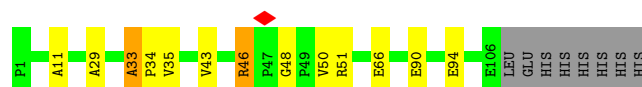
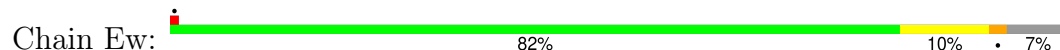
• Molecule 1: C2-B



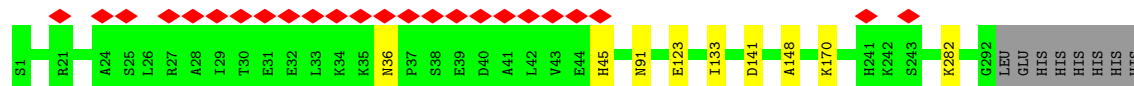
• Molecule 1: C2-B



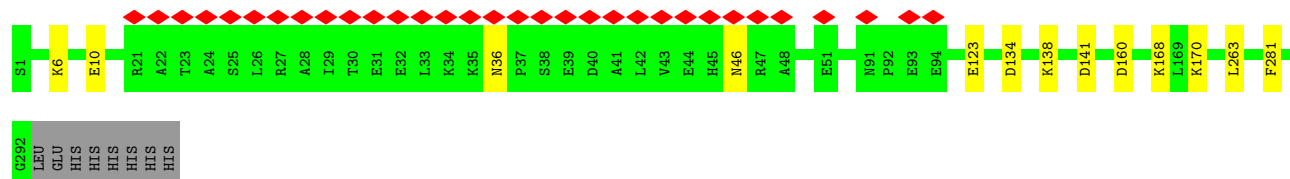
• Molecule 1: C2-B



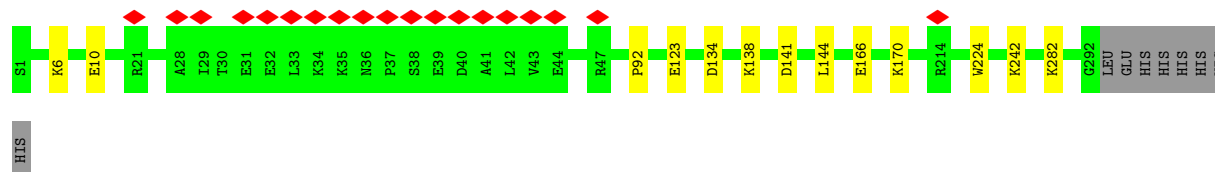
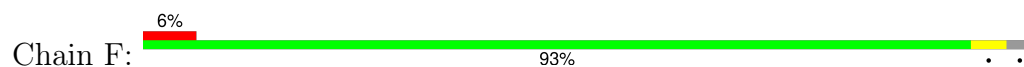
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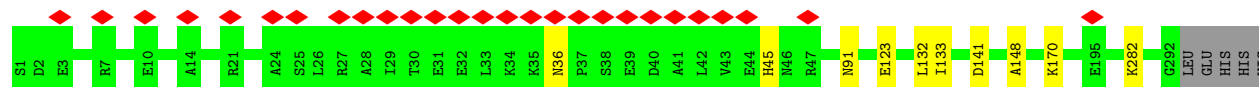
• Molecule 2: C3-A



• Molecule 2: C3-A



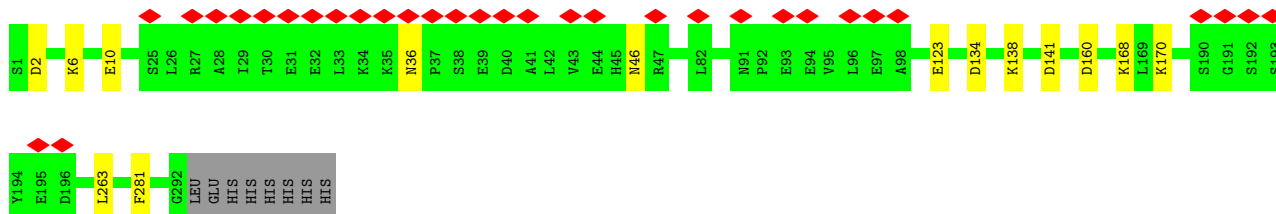
• Molecule 2: C3-A



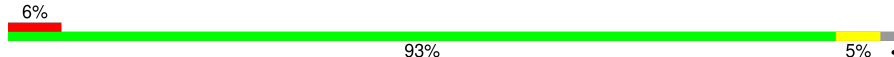
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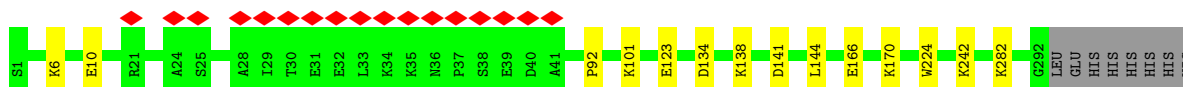
• Molecule 2: C3-A

Chain J:  11% 93% 5% .

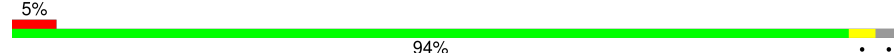


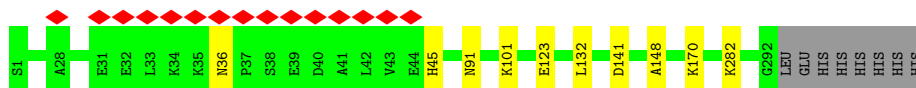
• Molecule 2: C3-A

Chain L:  6% 93% 5% .

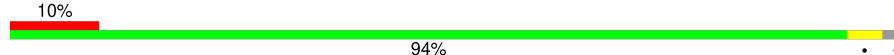


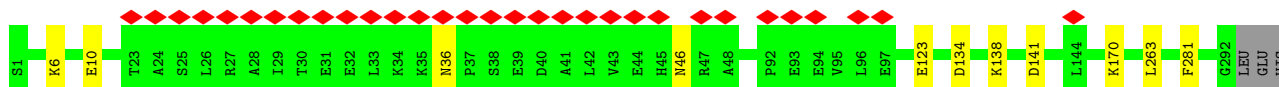
• Molecule 2: C3-A

Chain N:  5% 94% . .



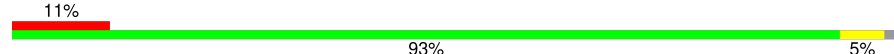
• Molecule 2: C3-A

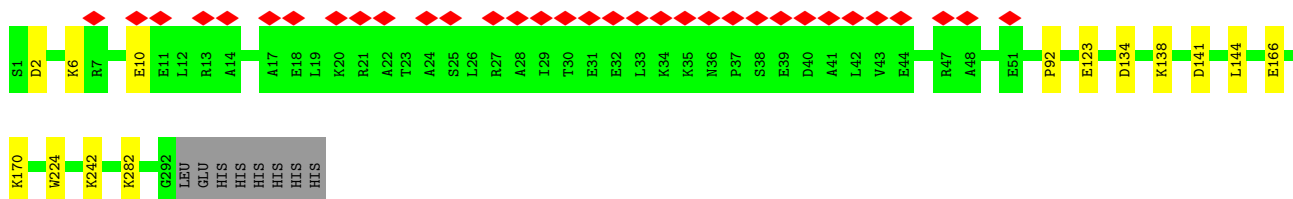
Chain P:  10% 94% . .



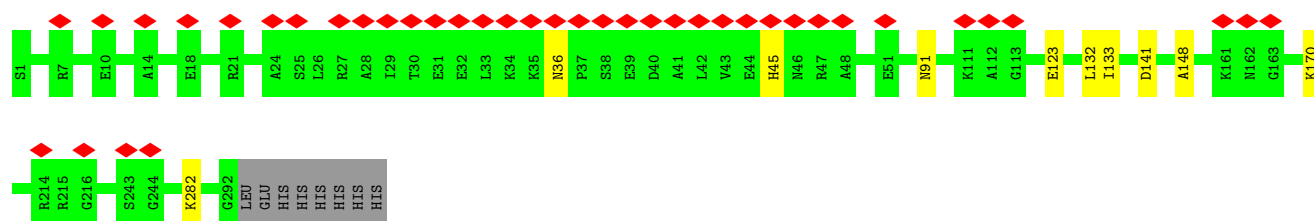
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• Molecule 2: C3-A

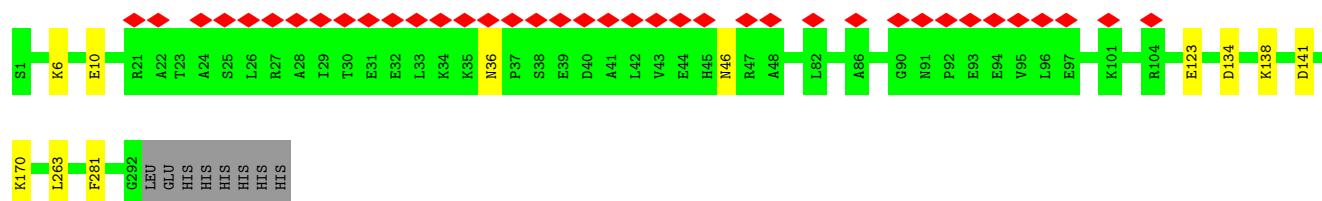
Chain R:  11% 93% 5% .



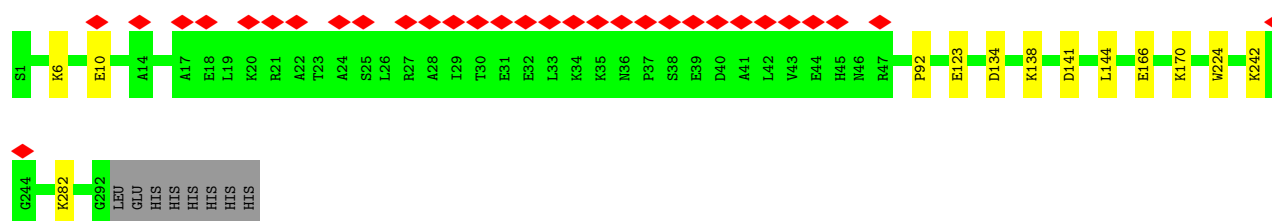
• Molecule 2: C3-A



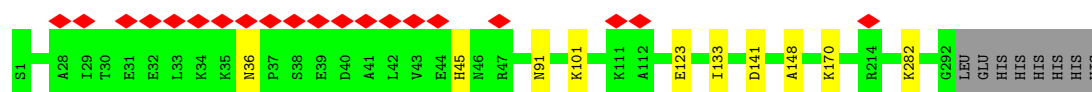
- Molecule 2: C3-A



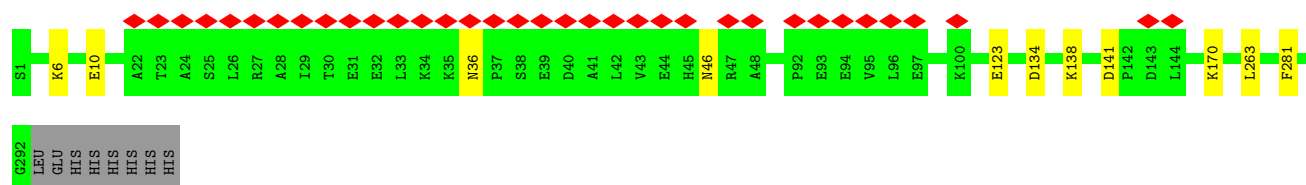
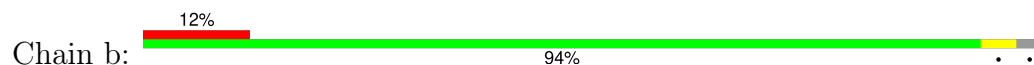
- Molecule 2: C3-A



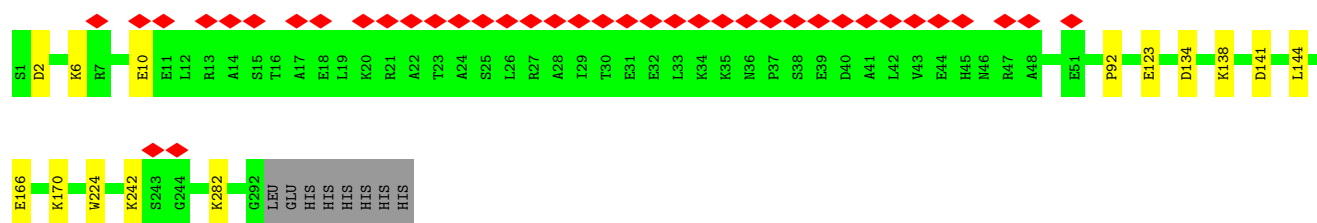
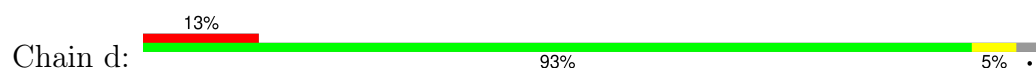
- Molecule 2: C3-A



- Molecule 2: C3-A



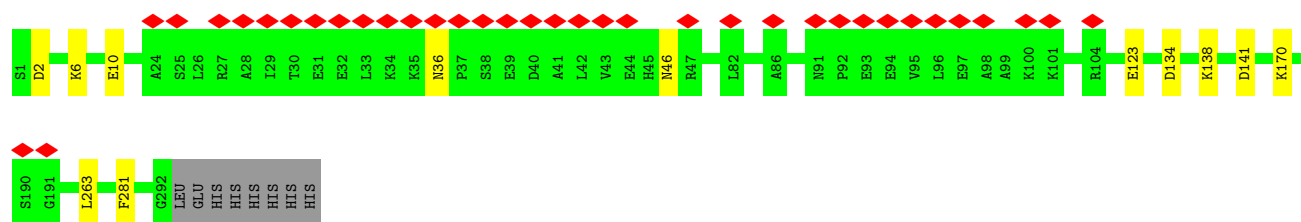
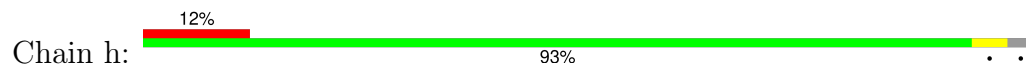
- Molecule 2: C3-A



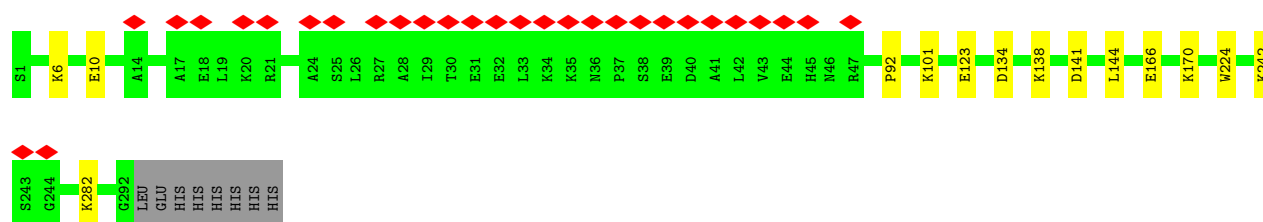
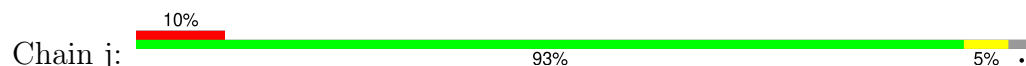
• Molecule 2: C3-A



• Molecule 2: C3-A



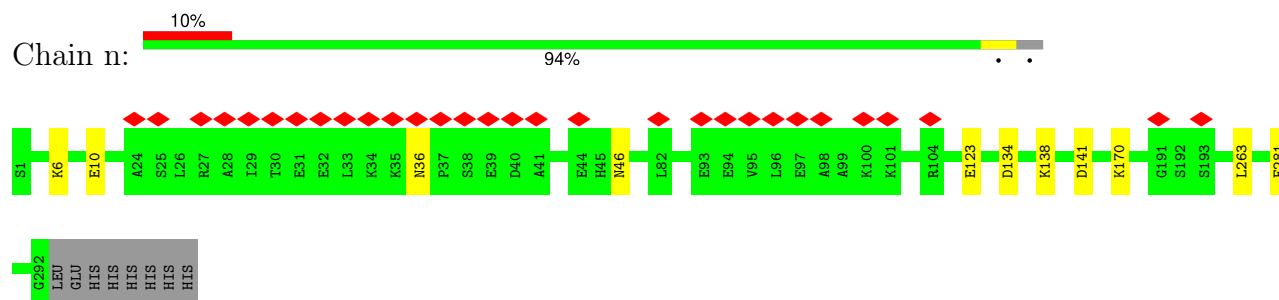
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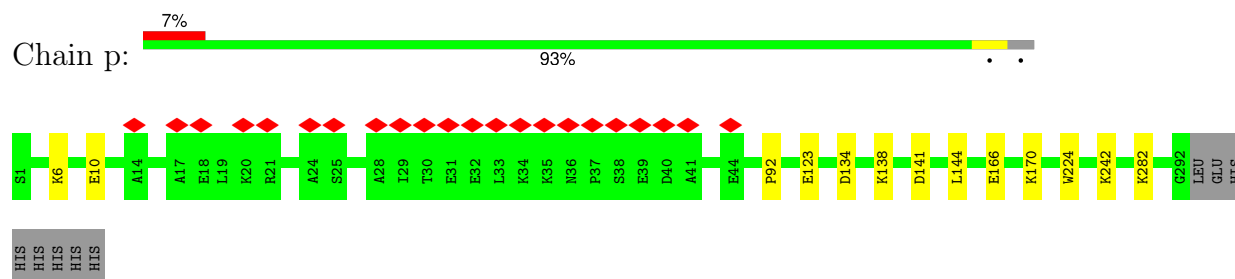
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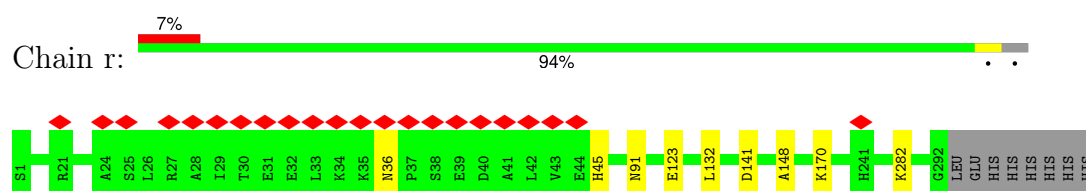
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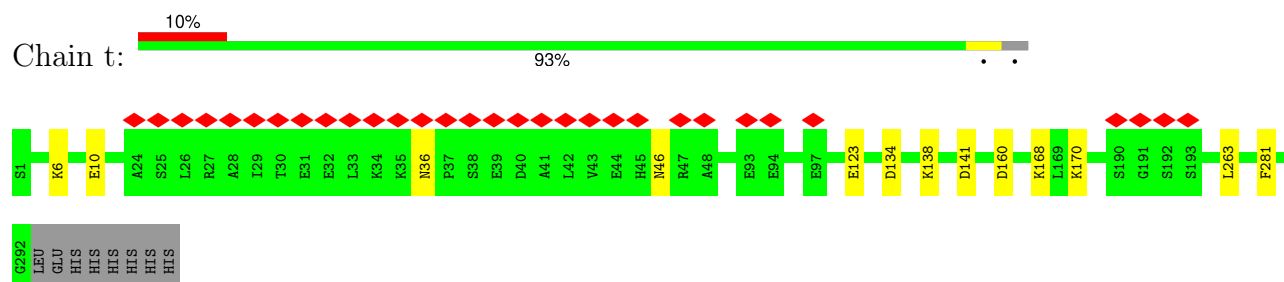
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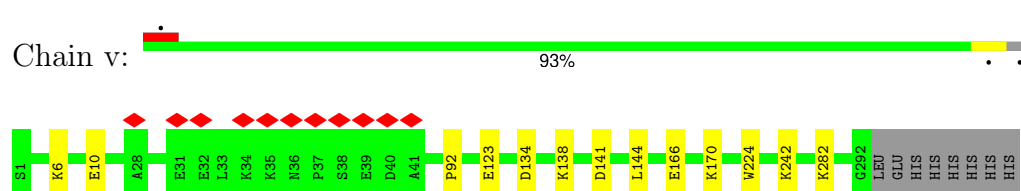
• Molecule 2: C3-A



• Molecule 2: C3-A

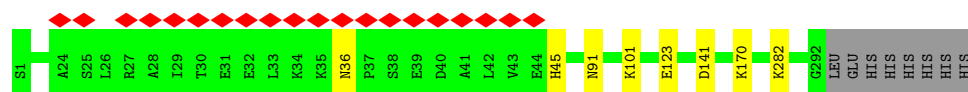


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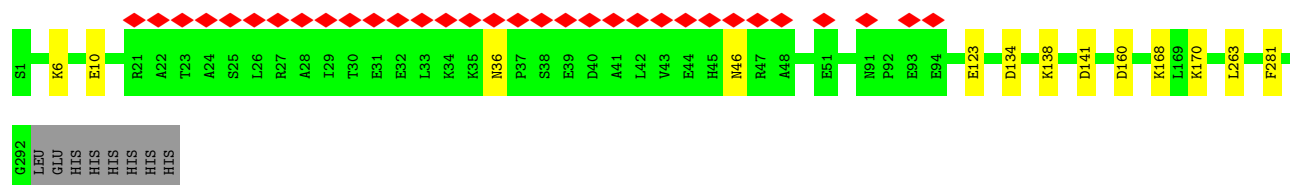


• Molecule 2: C3-A

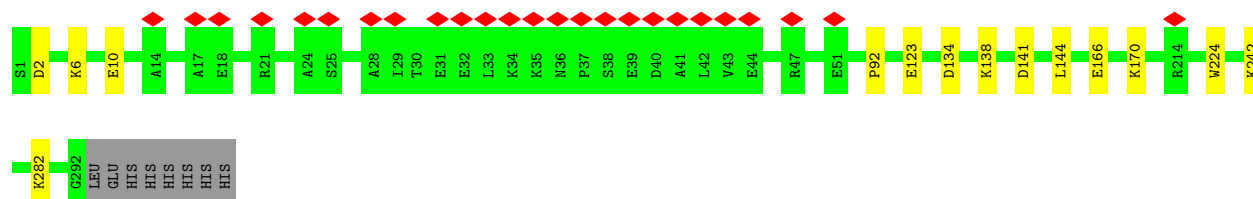




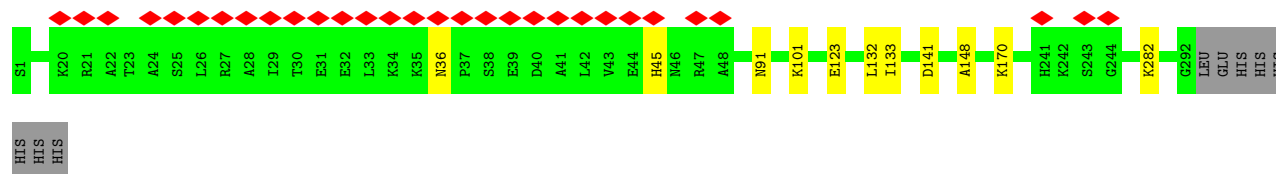
• Molecule 2: C3-A



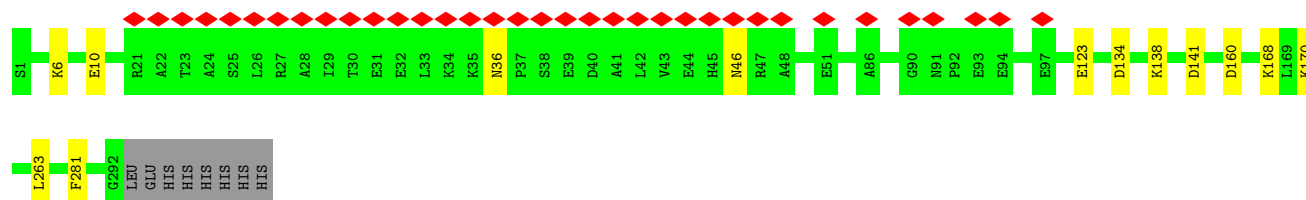
• Molecule 2: C3-A



• Molecule 2: C3-A

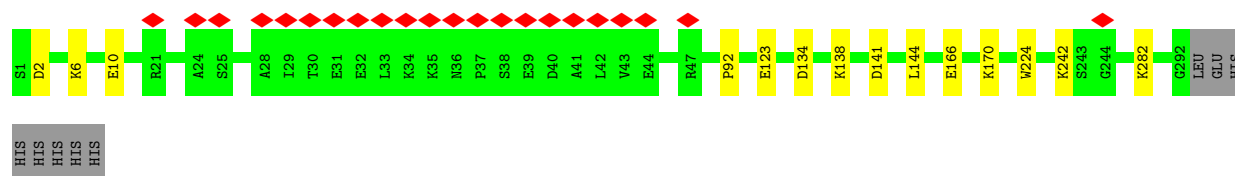


• Molecule 2: C3-A



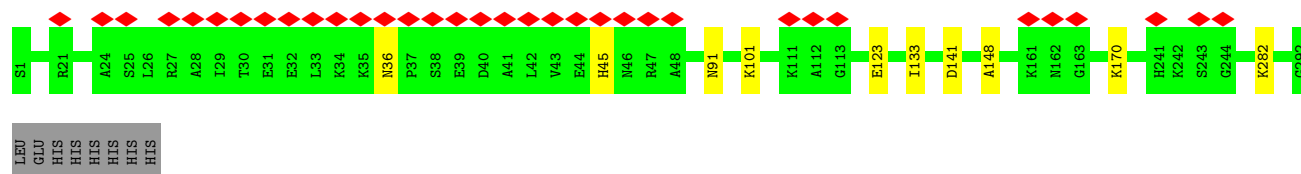
• Molecule 2: C3-A





● Molecule 2: C3-A

Chain ZJ: 11% 94%



● Molecule 2: C3-A

Chain AB: 12% 94%



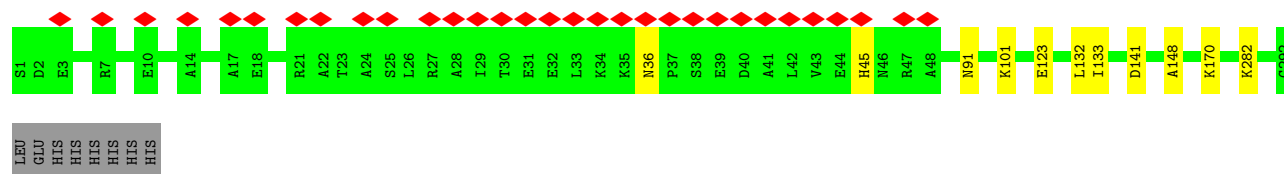
● Molecule 2: C3-A

Chain AD: 11% 93% 5%



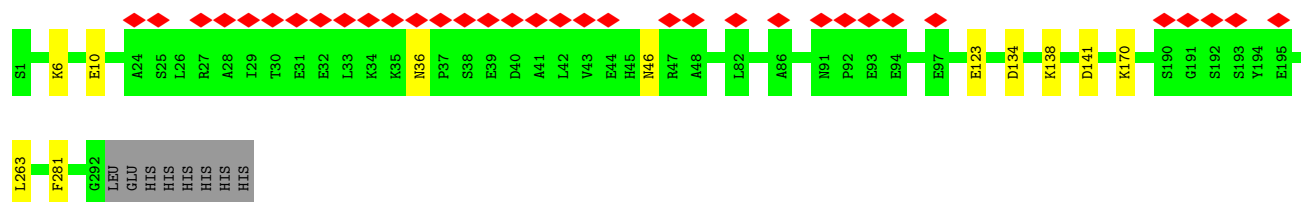
● Molecule 2: C3-A

Chain AF: 10% 94%

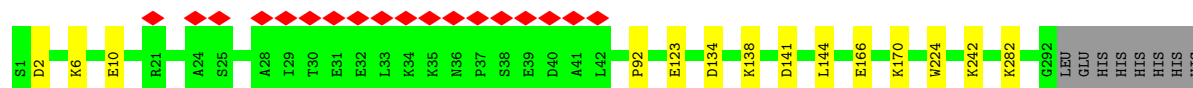


● Molecule 2: C3-A

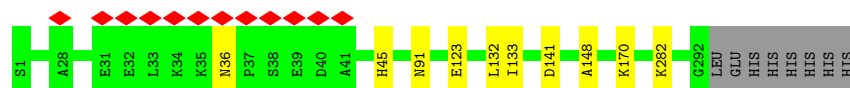
Chain AH: 11% 94%



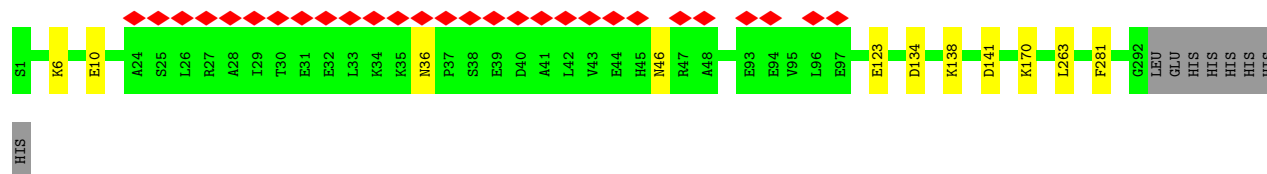
- Molecule 2: C3-A



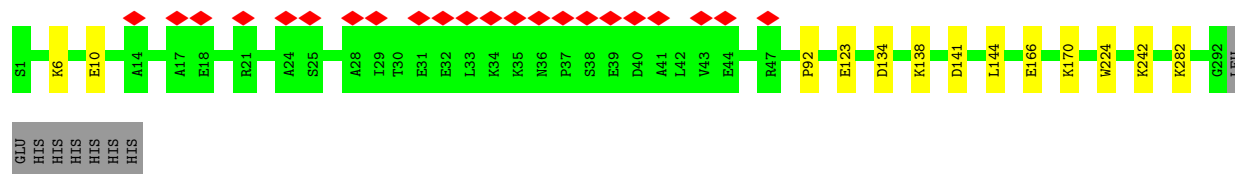
- Molecule 2: C3-A



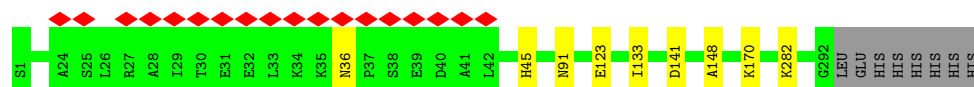
- Molecule 2: C3-A



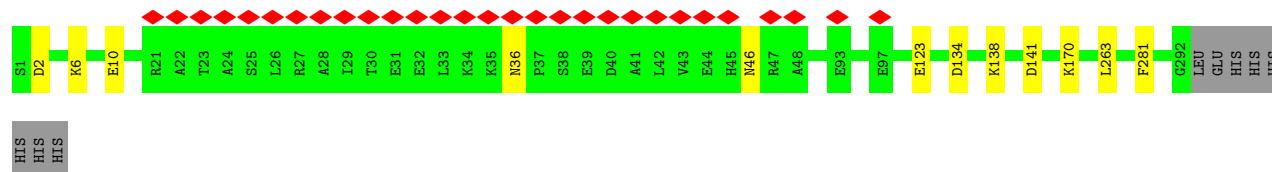
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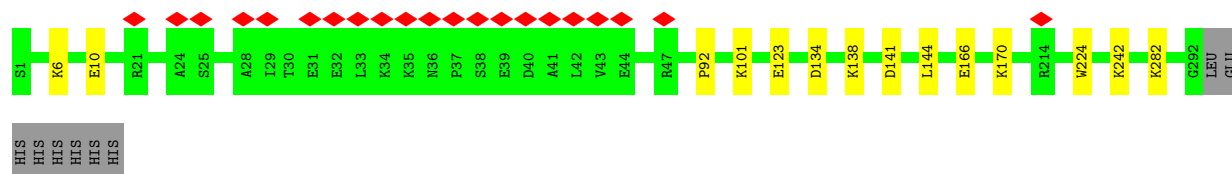
- Molecule 2: C3-A



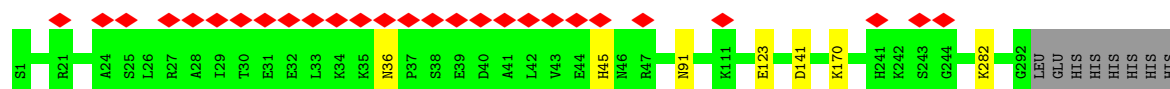
- Molecule 2: C3-A



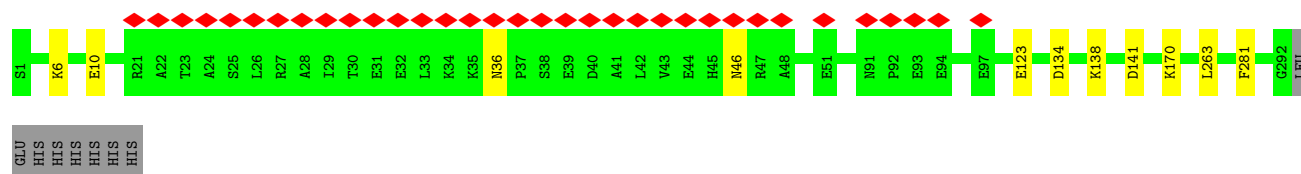
- Molecule 2: C3-A



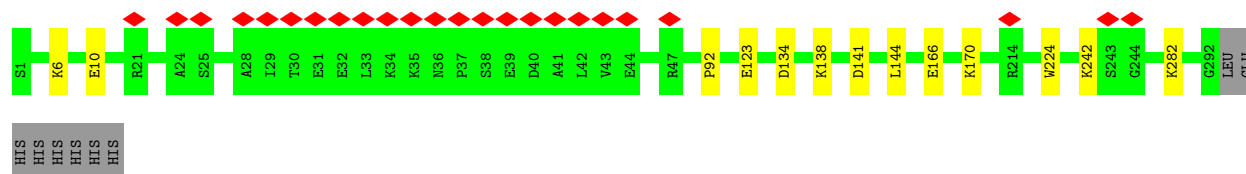
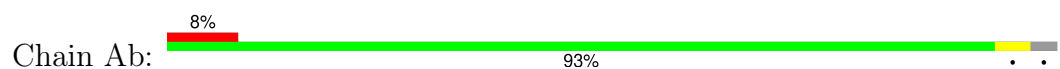
- Molecule 2: C3-A



- Molecule 2: C3-A

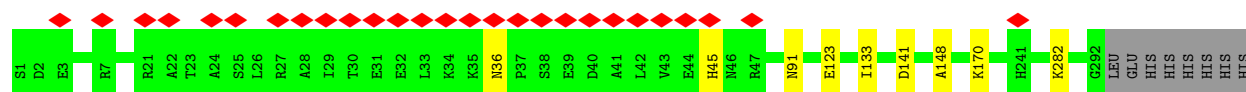


- Molecule 2: C3-A

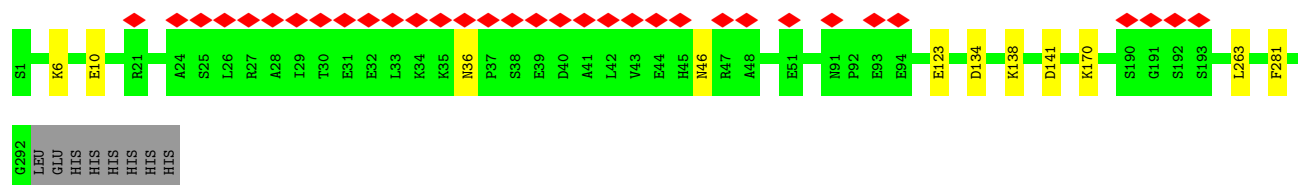


- Molecule 2: C3-A





- Molecule 2: C3-A



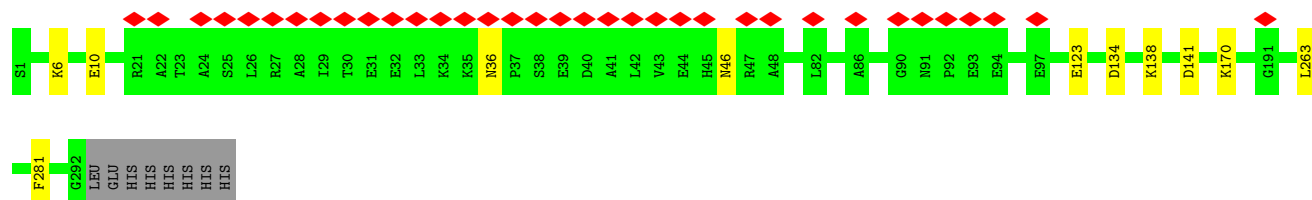
- Molecule 2: C3-A



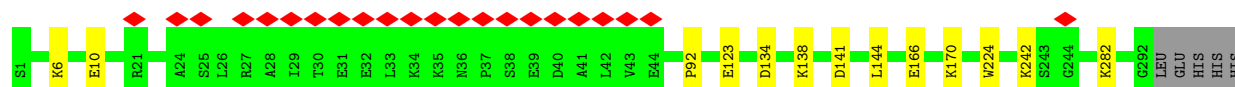
- Molecule 2: C3-A



- Molecule 2: C3-A

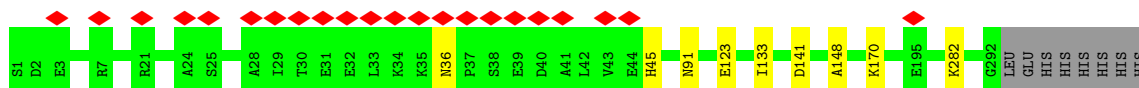


- Molecule 2: C3-A

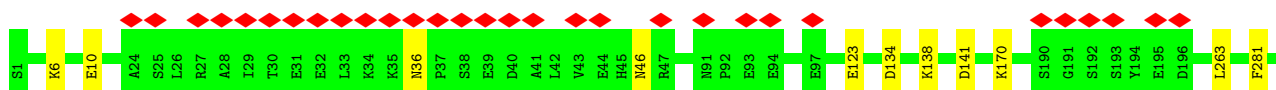


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• Molecule 2: C3-A



• Molecule 2: C3-A

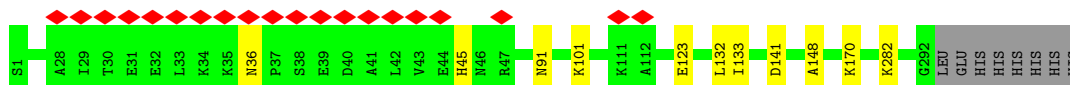


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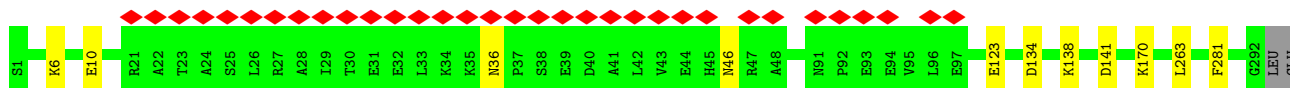
• Molecule 2: C3-A



• Molecule 2: C3-A



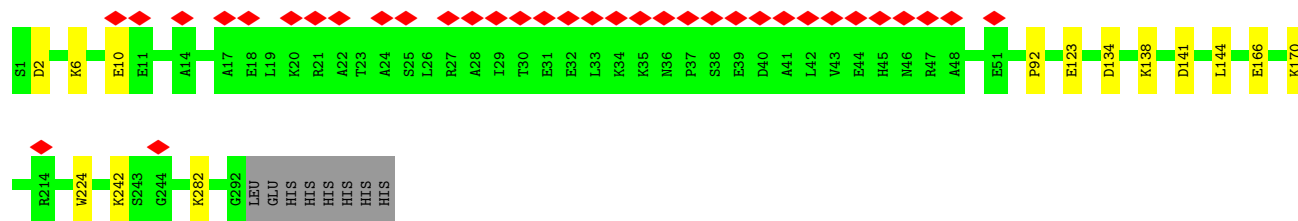
• Molecule 2: C3-A



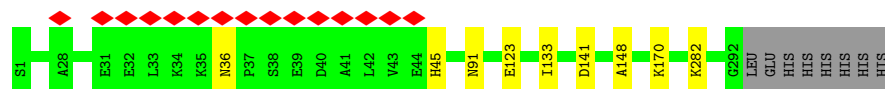
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• Molecule 2: C3-A

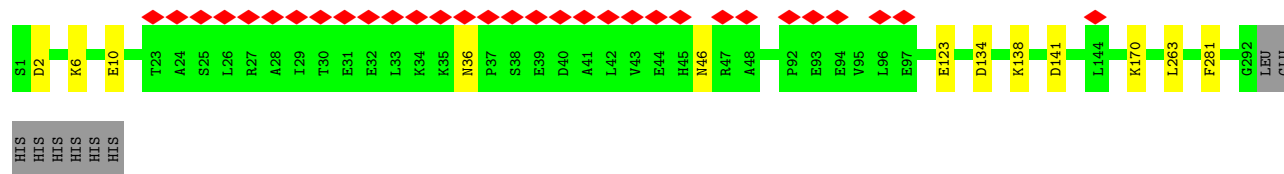




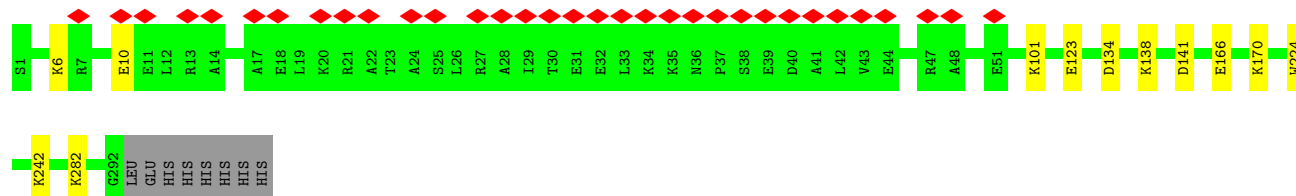
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A

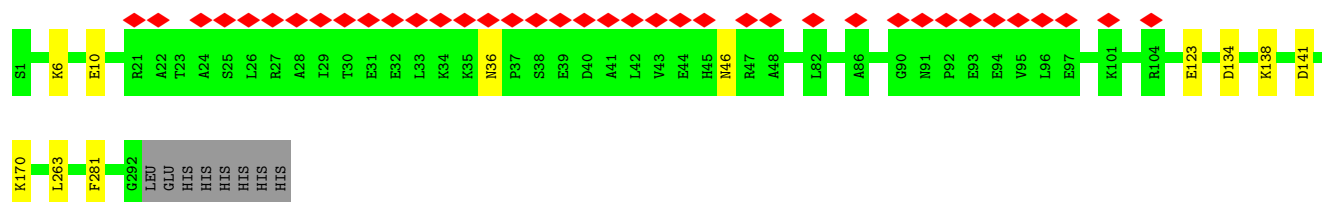


• Molecule 2: C3-A

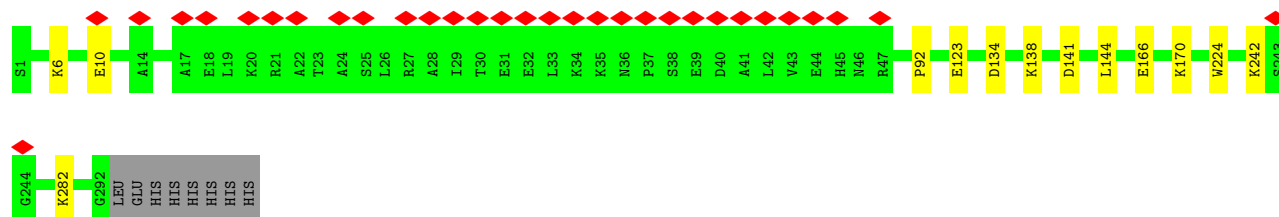


• Molecule 2: C3-A

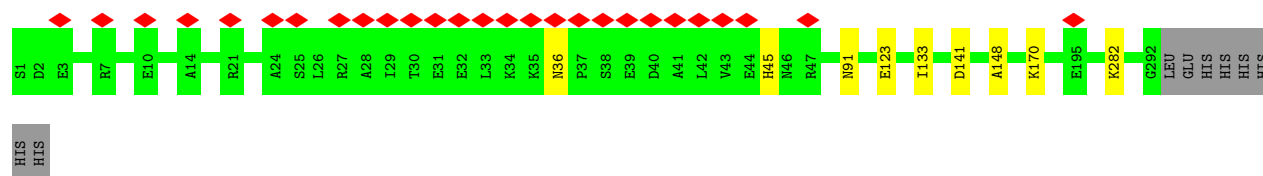




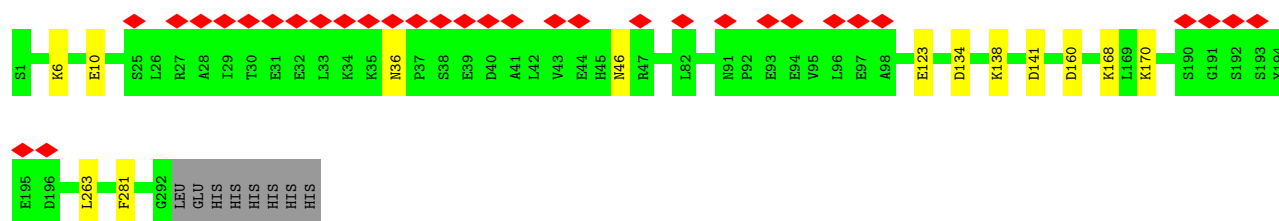
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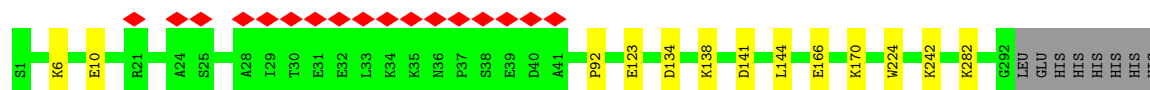
• Molecule 2: C3-A



• Molecule 2: C3-A

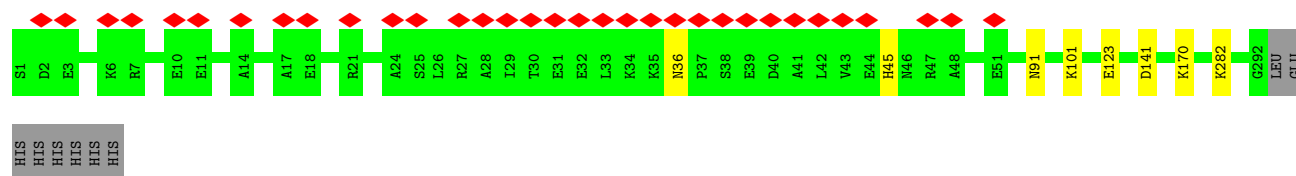


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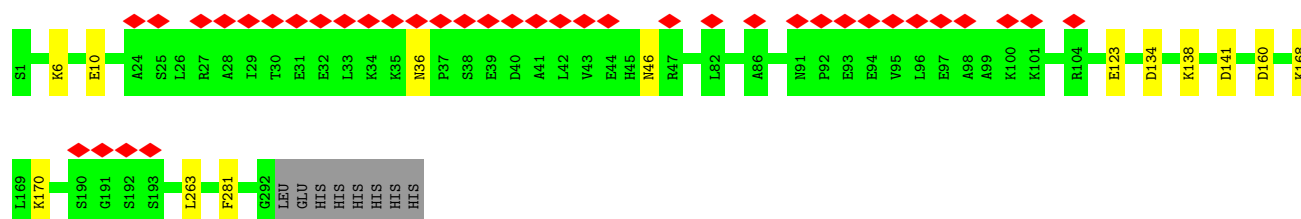


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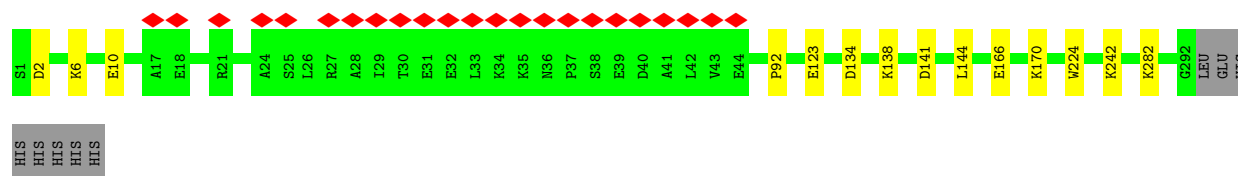




- Molecule 2: C3-A



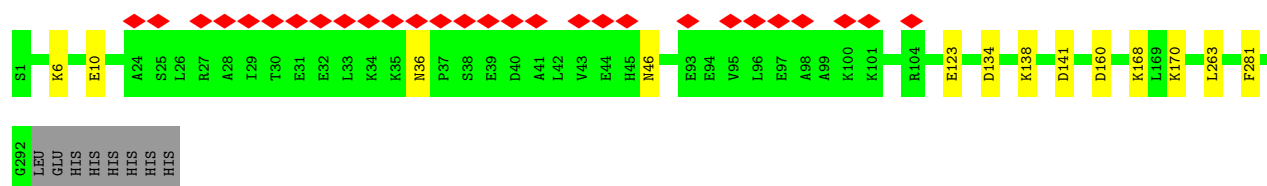
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- Molecule 2: C3-A

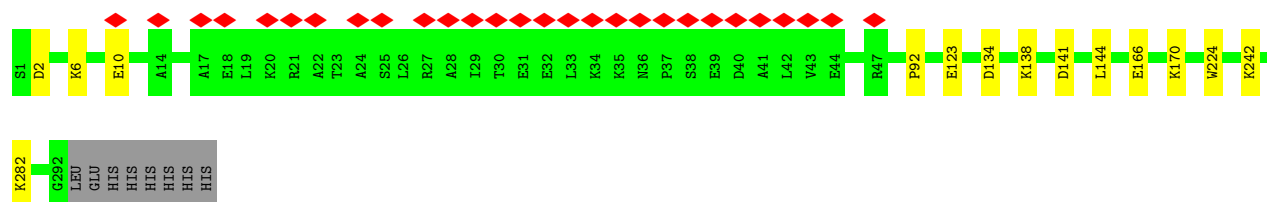


- Molecule 2: C3-A



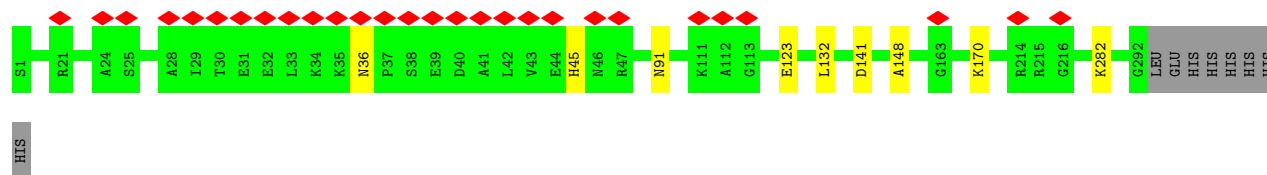
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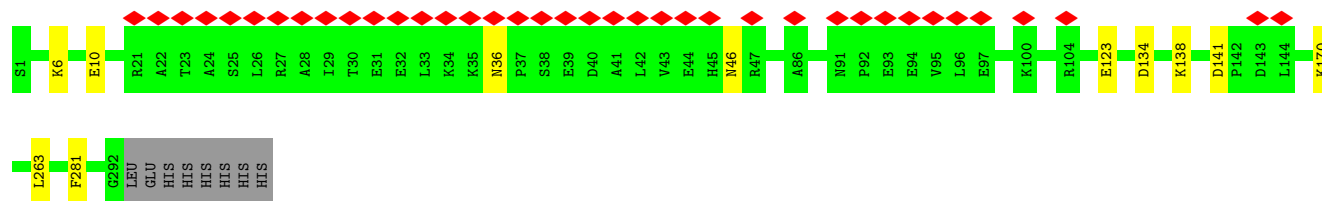
- Molecule 2: C3-A

Chain BV: 9% 94%



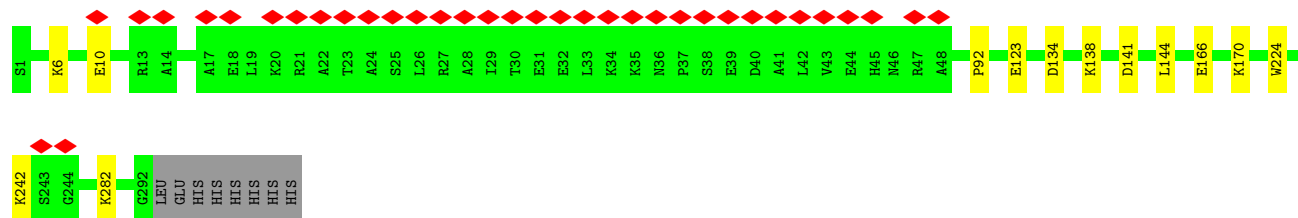
- Molecule 2: C3-A

Chain BX: 13% 94%



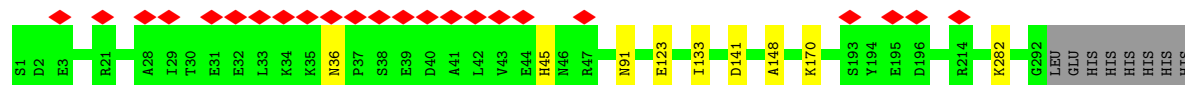
- Molecule 2: C3-A

Chain BZ: 12% 93%



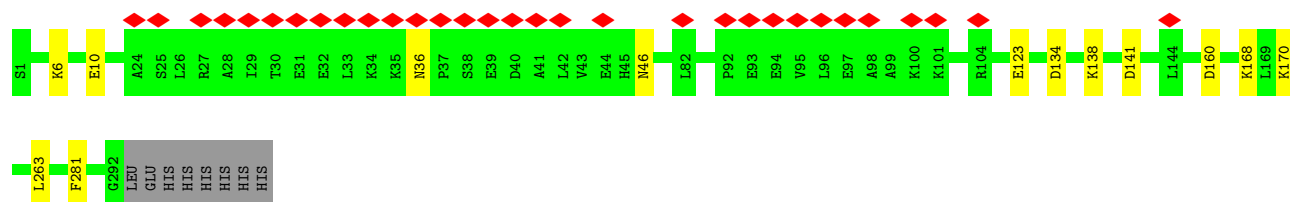
- Molecule 2: C3-A

Chain Bb: 8% 94%

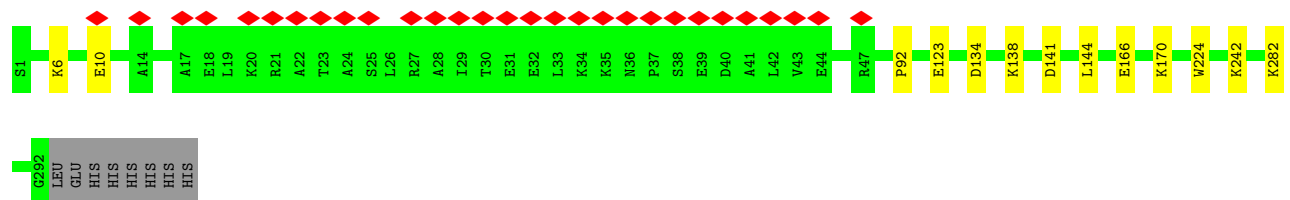


- Molecule 2: C3-A

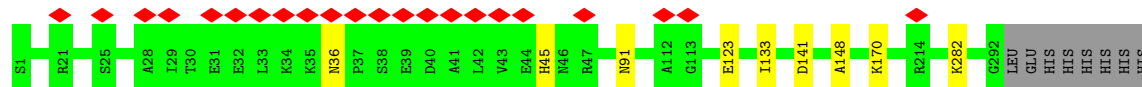
Chain Bd: 10% 93%



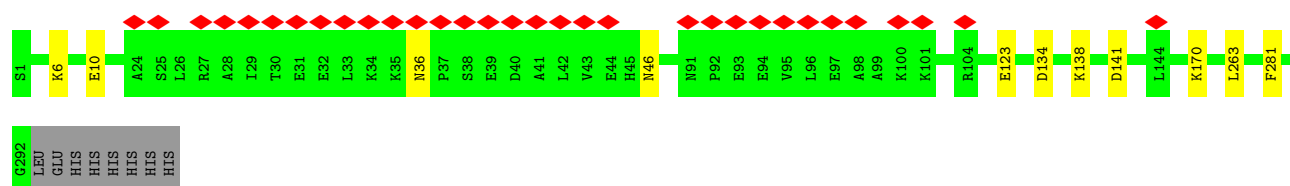
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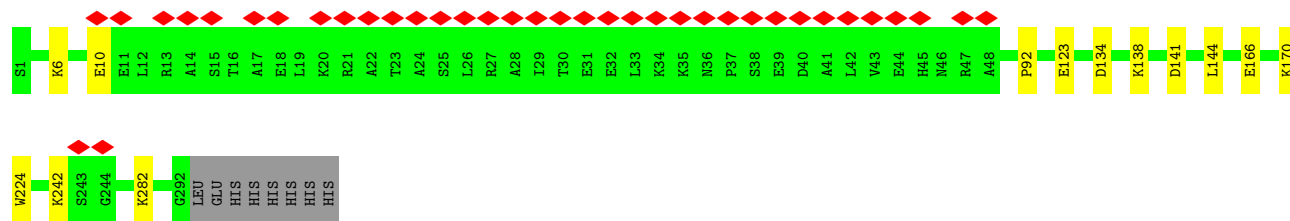
• Molecule 2: C3-A



• Molecule 2: C3-A

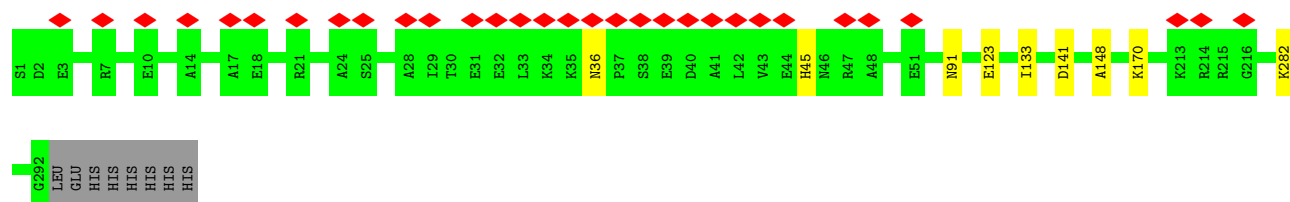


• Molecule 2: C3-A

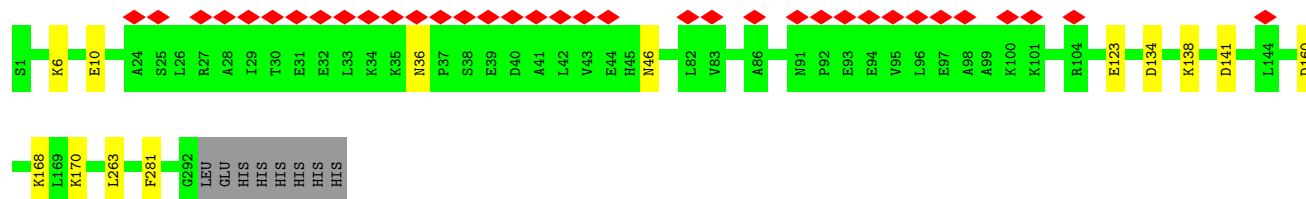


• Molecule 2: C3-A

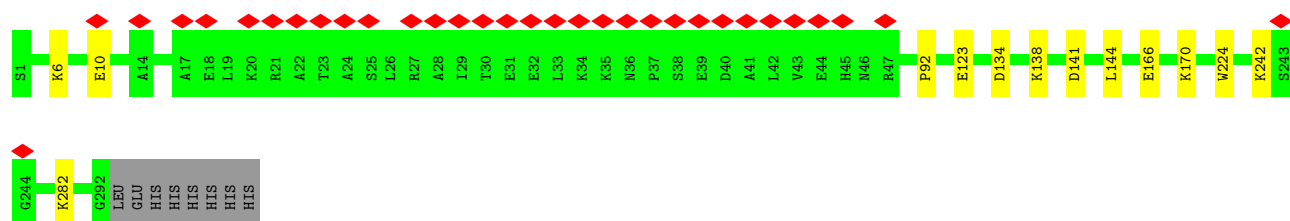




• Molecule 2: C3-A



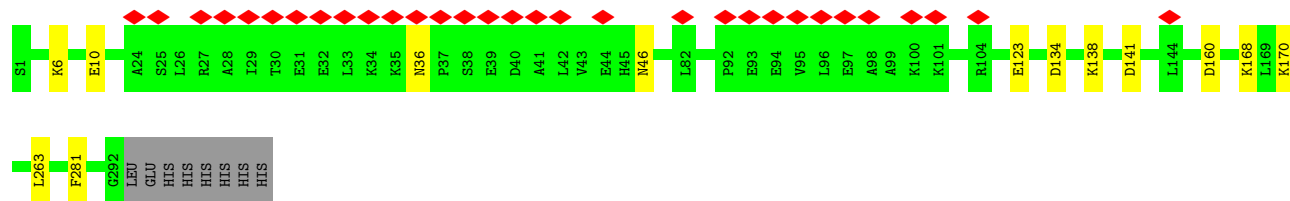
• Molecule 2: C3-A



• Molecule 2: C3-A

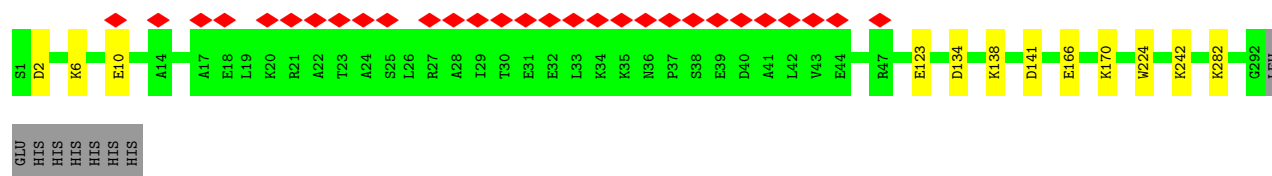


• Molecule 2: C3-A

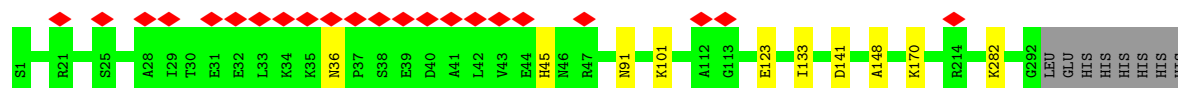


• Molecule 2: C3-A

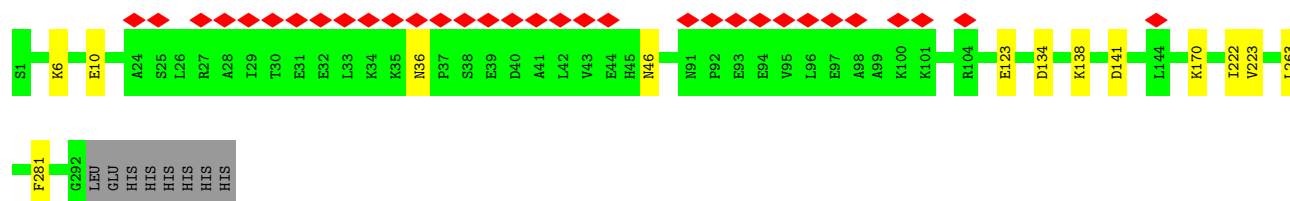




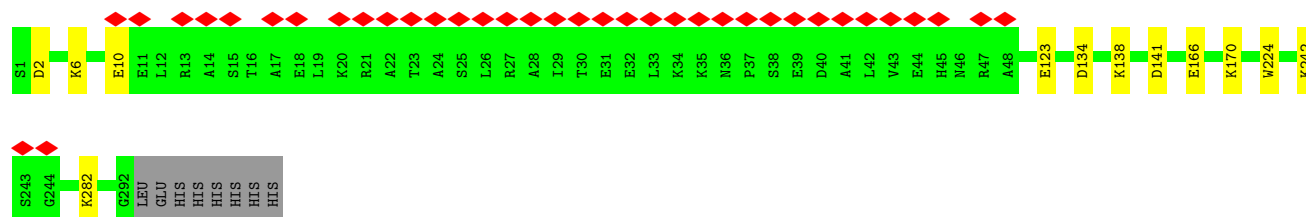
- Molecule 2: C3-A



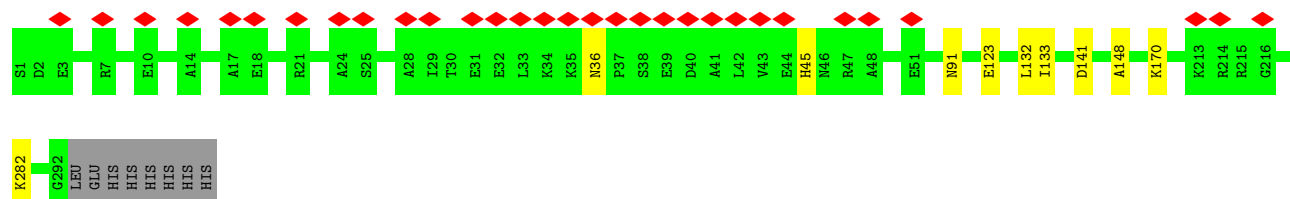
- Molecule 2: C3-A



- Molecule 2: C3-A

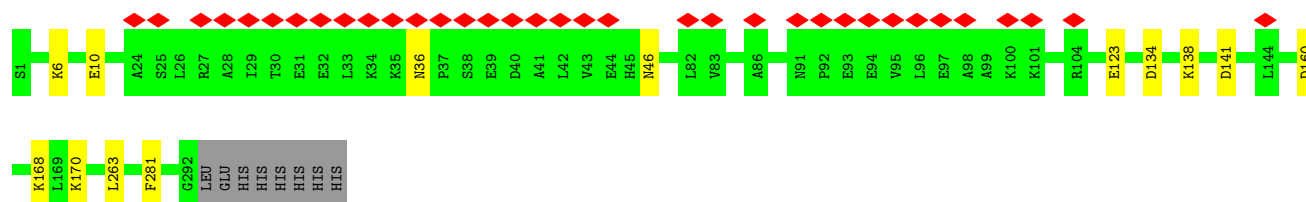


- Molecule 2: C3-A

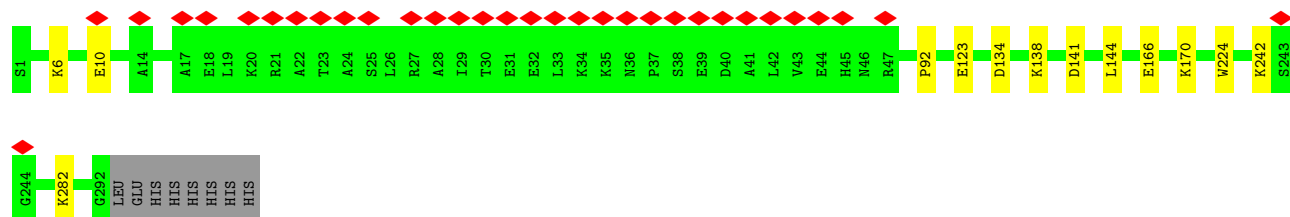


- Molecule 2: C3-A

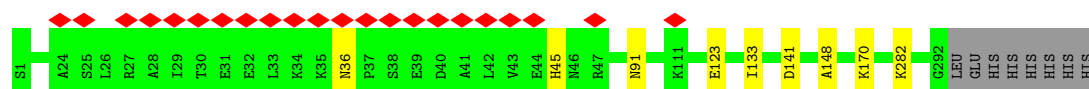




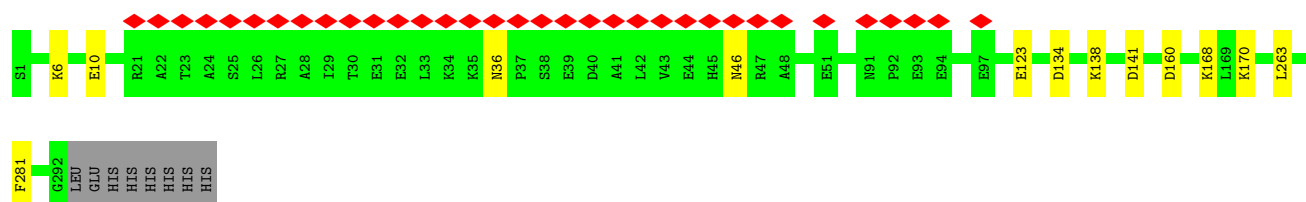
• Molecule 2: C3-A



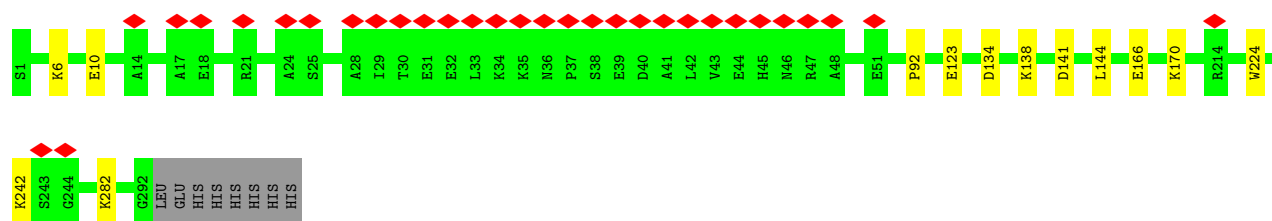
• Molecule 2: C3-A



• Molecule 2: C3-A

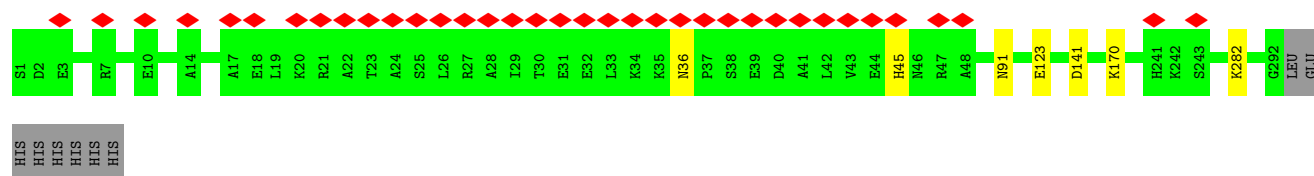


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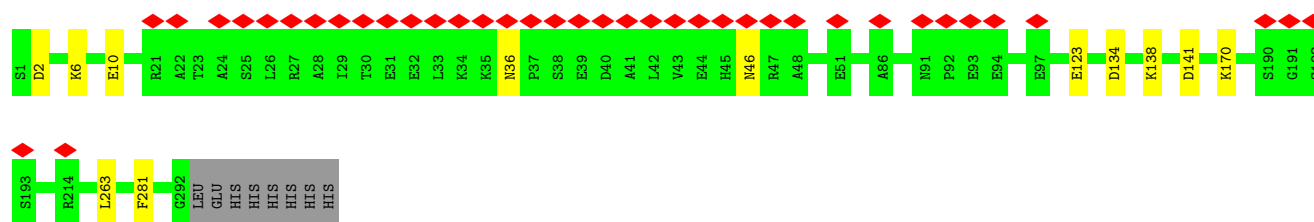


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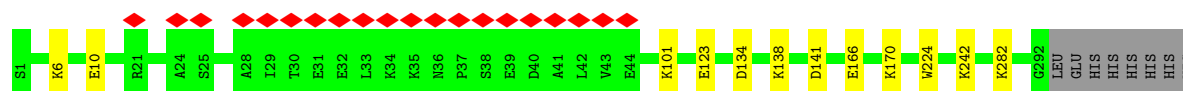




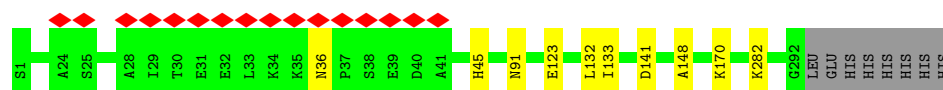
- Molecule 2: C3-A



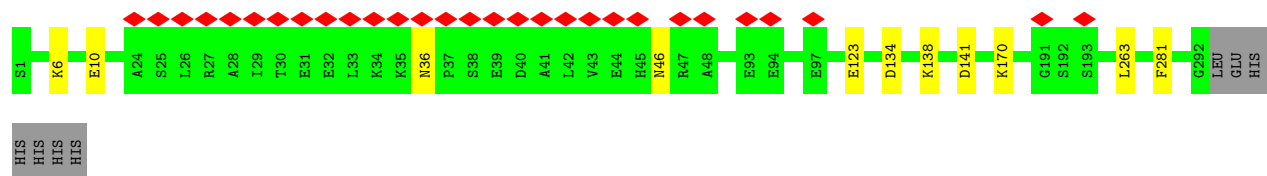
- Molecule 2: C3-A



- Molecule 2: C3-A



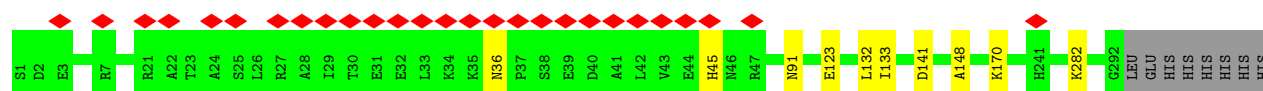
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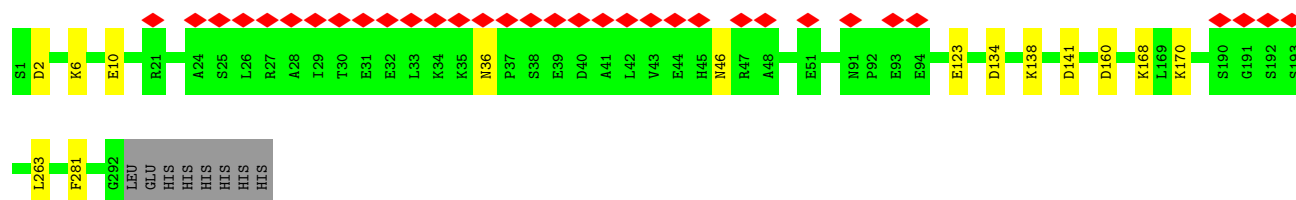
- Molecule 2: C3-A



- Molecule 2: C3-A



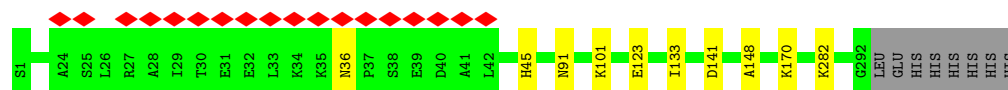
- Molecule 2: C3-A



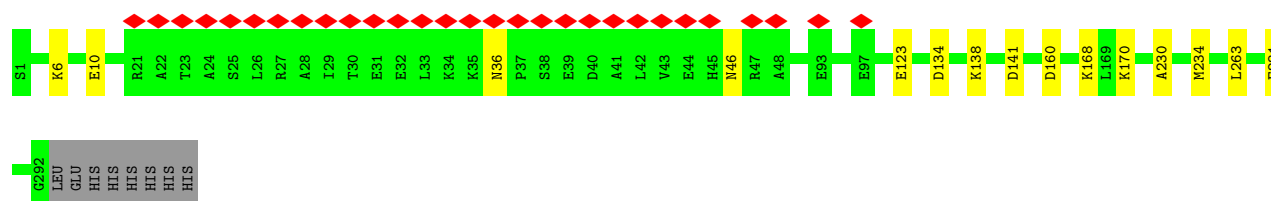
- Molecule 2: C3-A



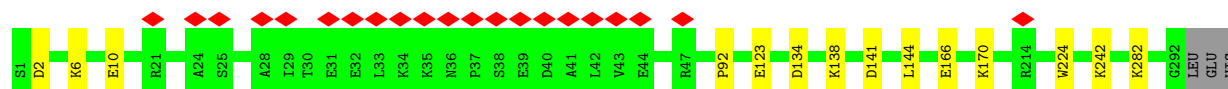
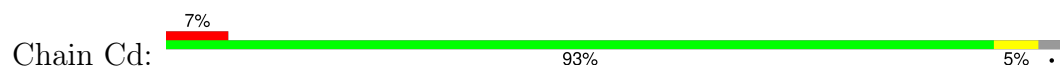
- Molecule 2: C3-A



- Molecule 2: C3-A



- Molecule 2: C3-A



HIS
HIS
HIS
HIS
HIS

• Molecule 2: C3-A

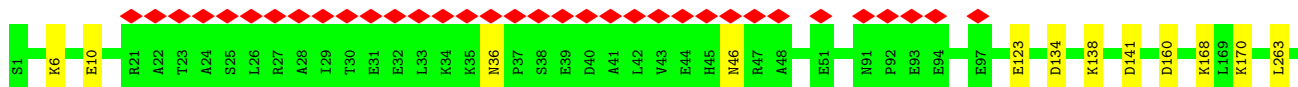
Chain Cf: 9% 94% . .



HIS
HIS

• Molecule 2: C3-A

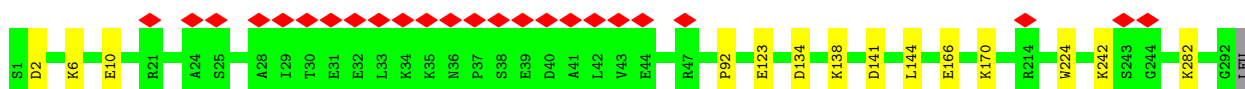
Chain Ch: 11% 93% . .



F281
G292
LEU
HIS
HIS
HIS
HIS
HIS

• Molecule 2: C3-A

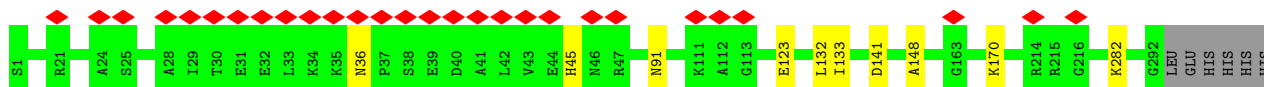
Chain Cj: 8% 93% 5% .



GLU
HIS
HIS
HIS
HIS
HIS

• Molecule 2: C3-A

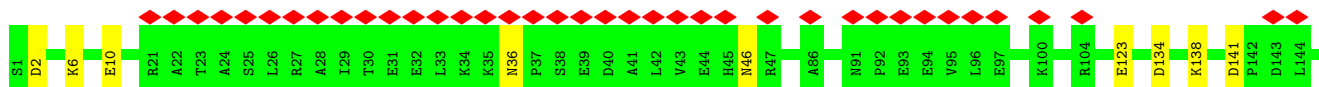
Chain Cl: 9% 94% . .

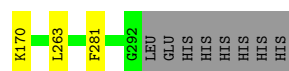


HIS
HIS

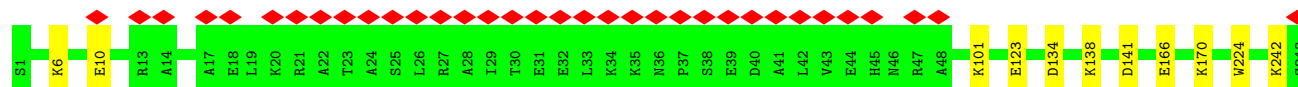
• Molecule 2: C3-A

Chain Cn: 13% 93% . .

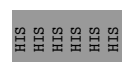
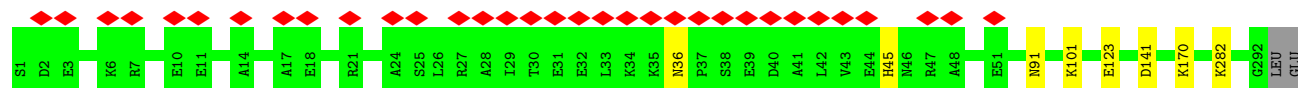




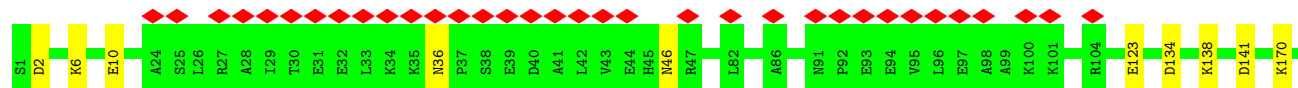
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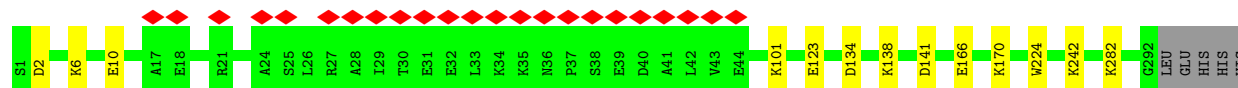
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A

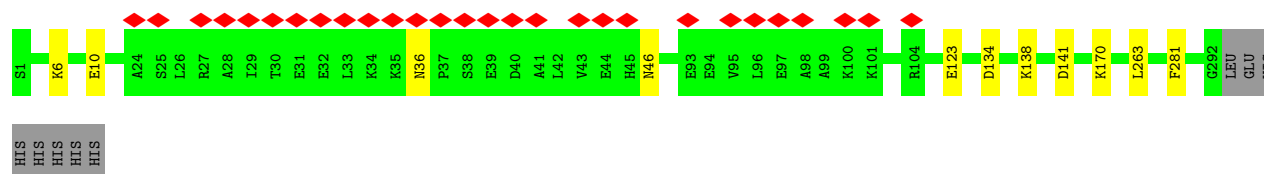


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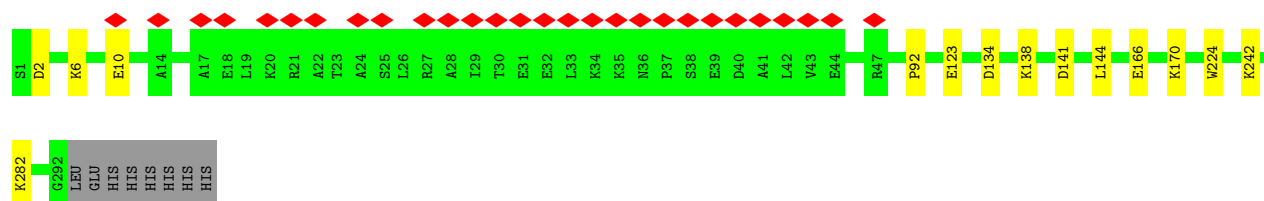




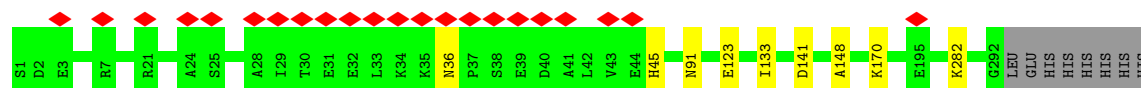
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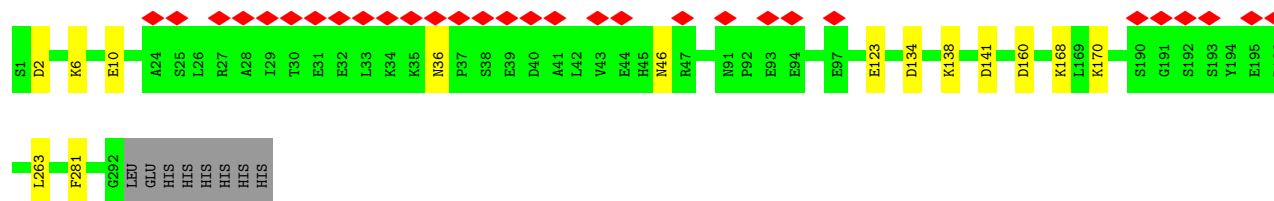
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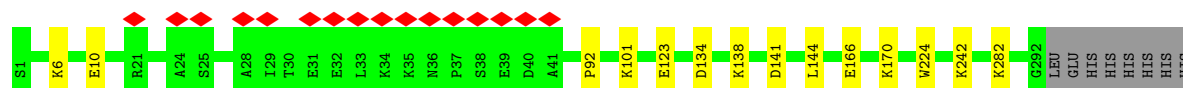
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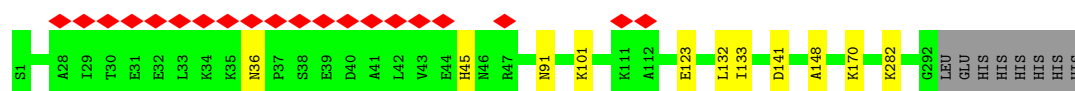
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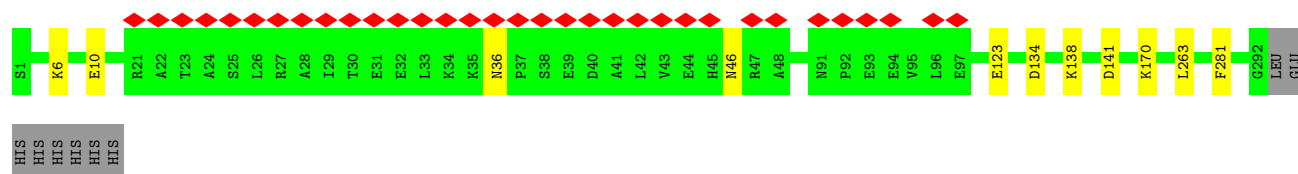
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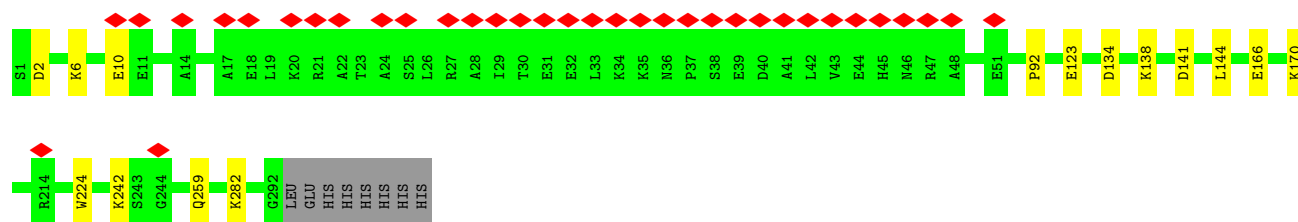
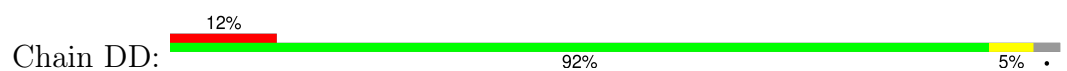
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A



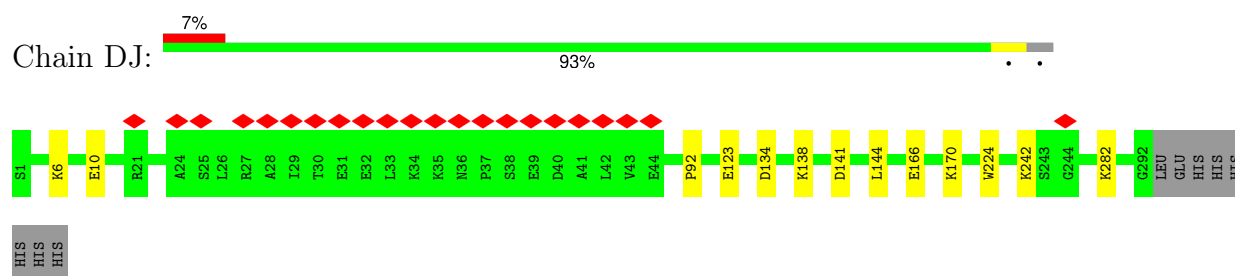
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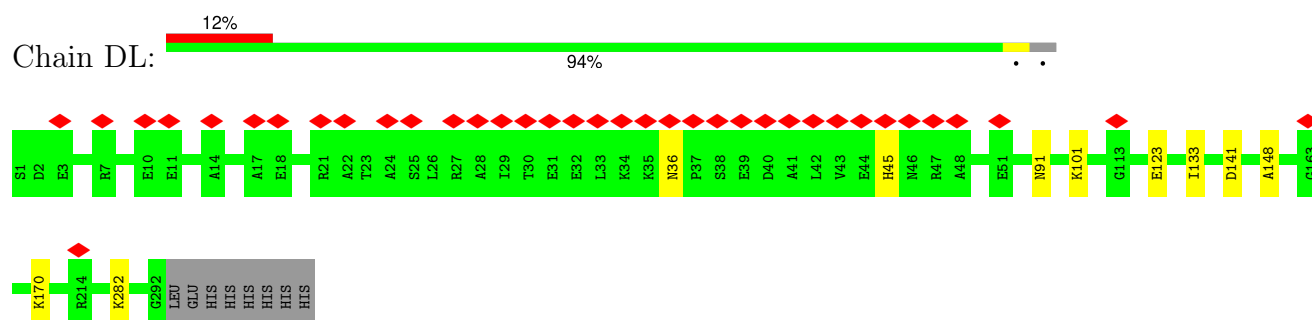
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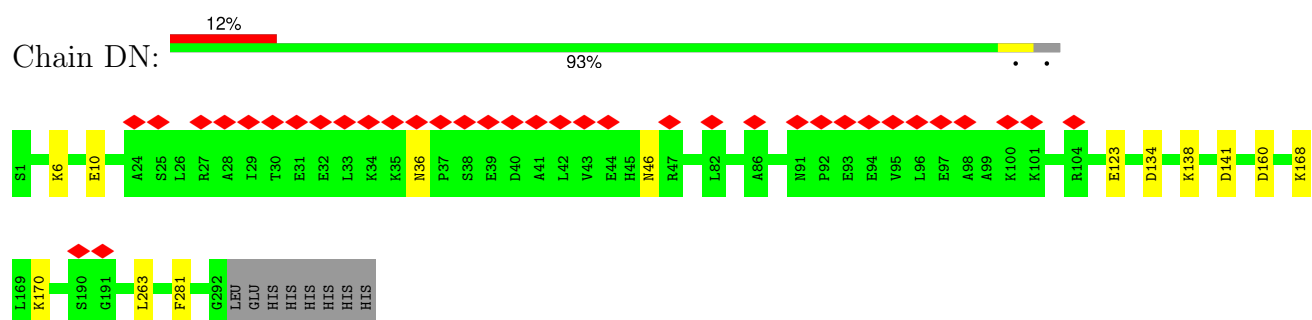
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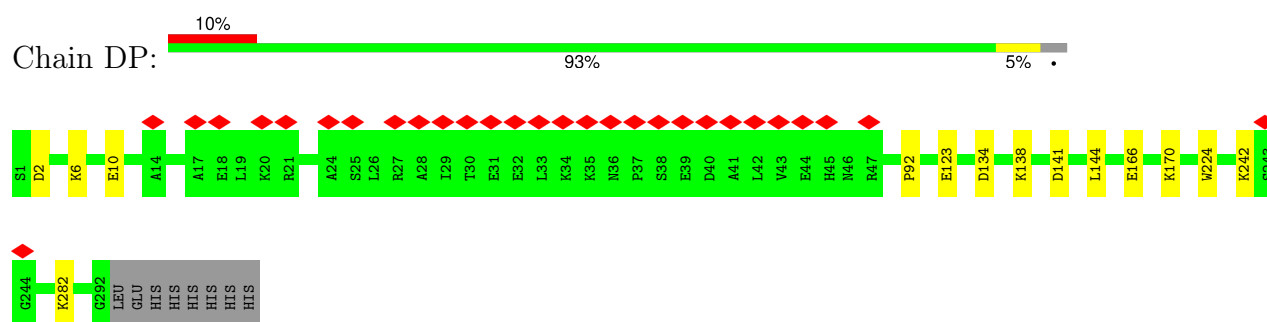
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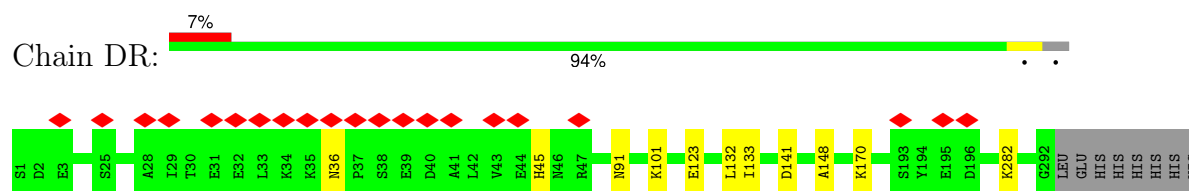
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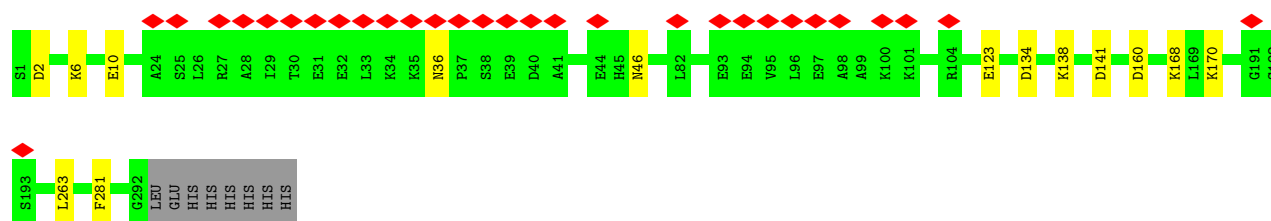
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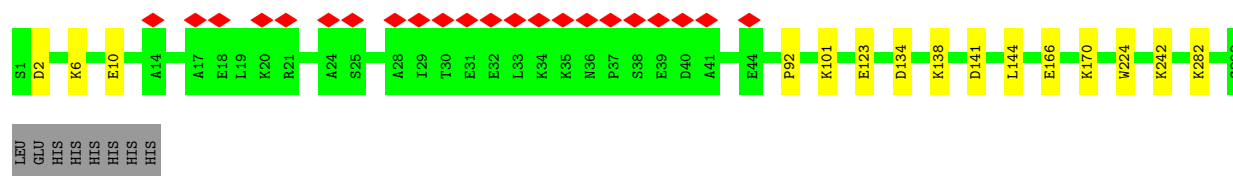
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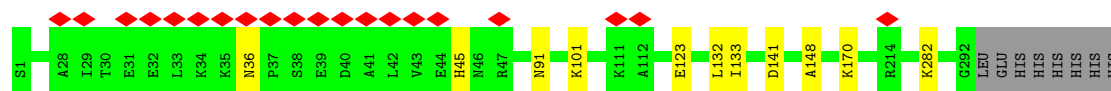
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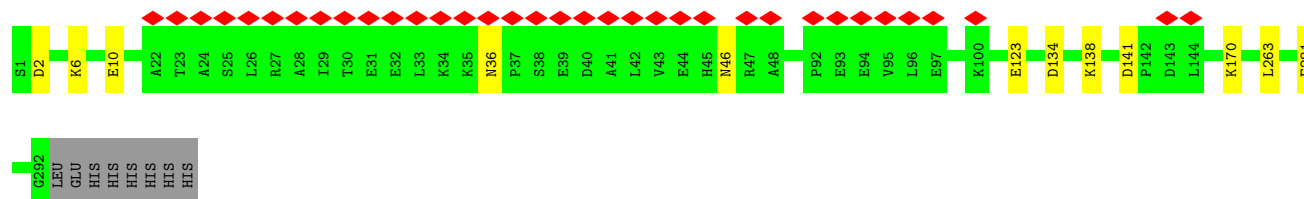
- Molecule 2: C3-A



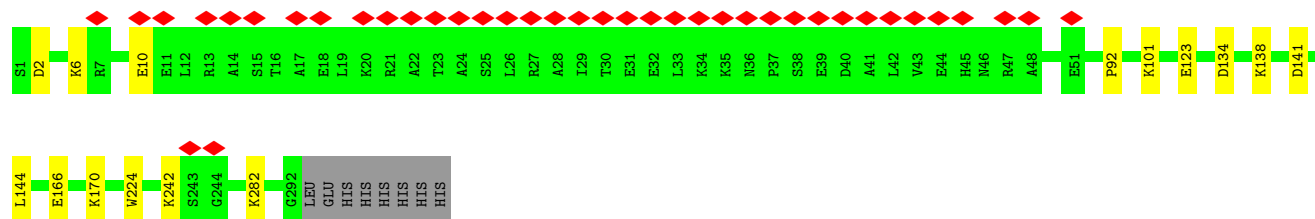
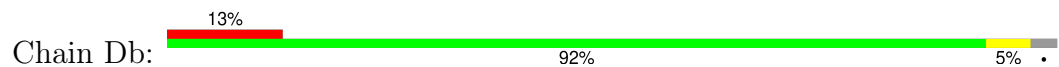
- Molecule 2: C3-A



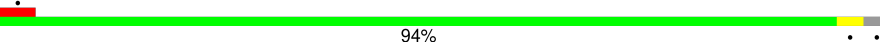
- Molecule 2: C3-A



- Molecule 2: C3-A

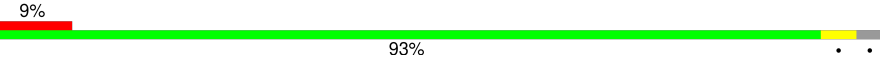


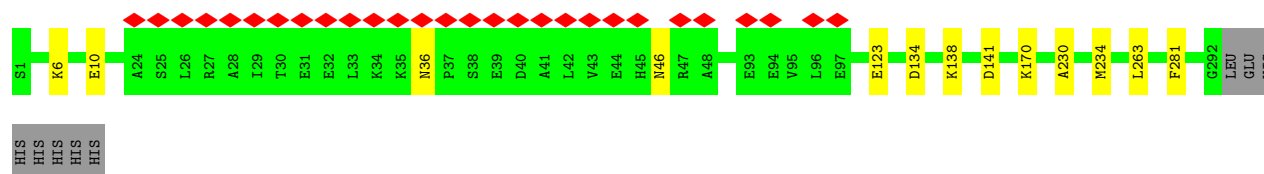
- Molecule 2: C3-A

Chain Dd:  94%

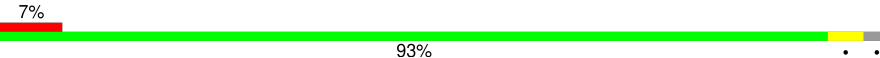


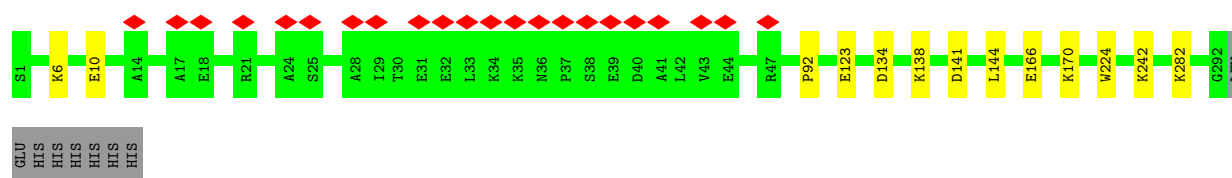
• Molecule 2: C3-A

Chain Df:  93%

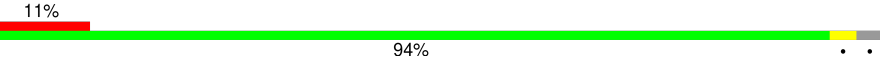


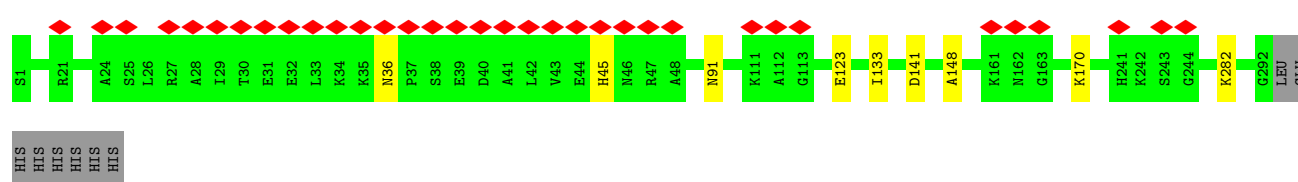
• Molecule 2: C3-A

Chain Dh:  93%

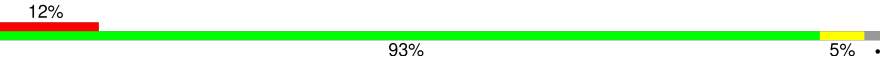


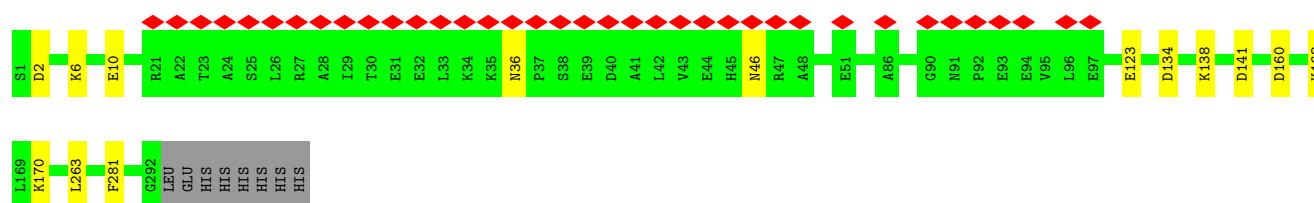
• Molecule 2: C3-A

Chain Dj:  94%

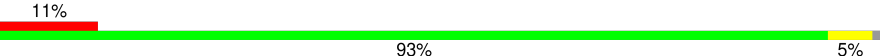


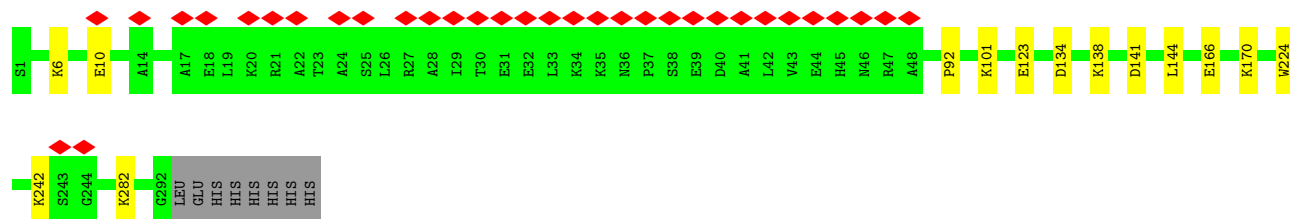
• Molecule 2: C3-A

Chain Dl:  93% 5%

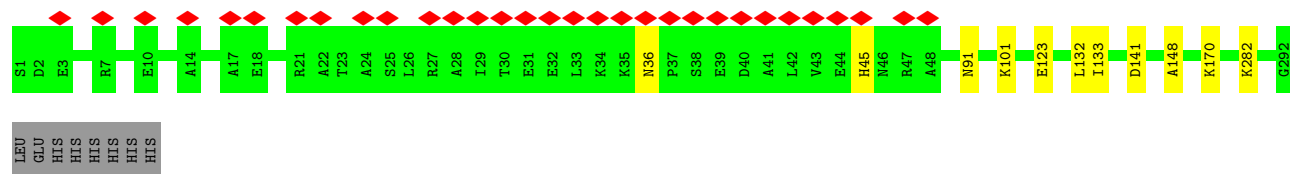


• Molecule 2: C3-A

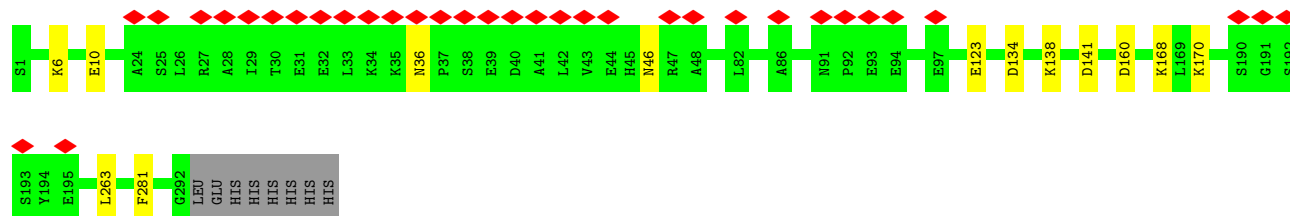
Chain Dn:  93% 5%



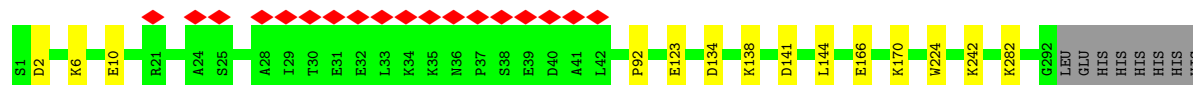
- Molecule 2: C3-A



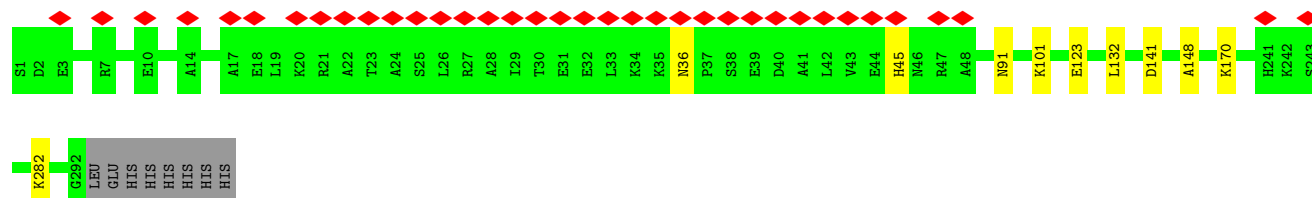
- Molecule 2: C3-A



- Molecule 2: C3-A

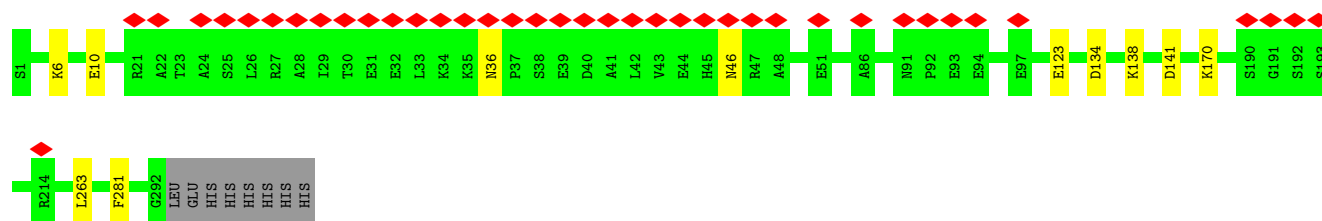


- Molecule 2: C3-A

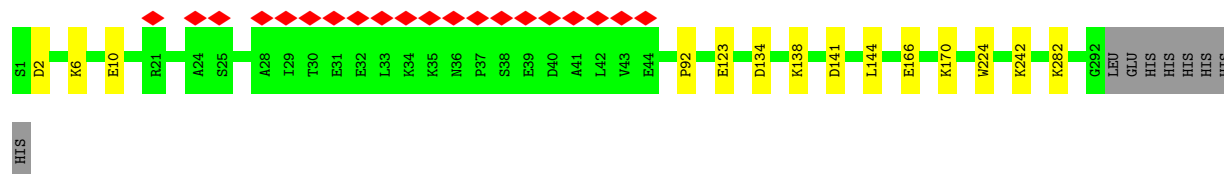


- Molecule 2: C3-A

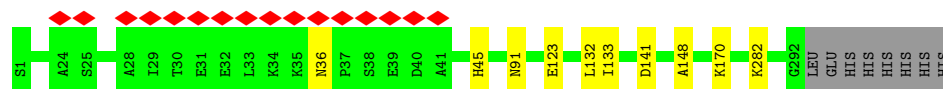




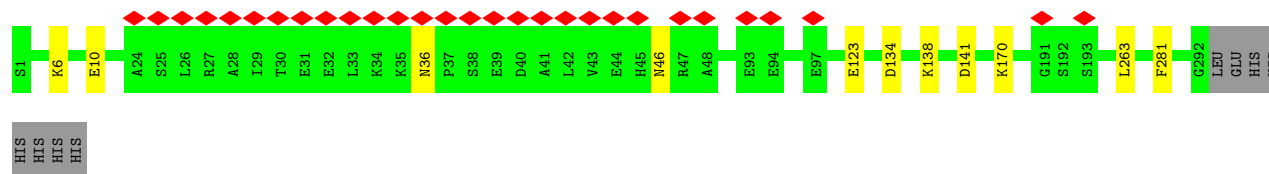
- Molecule 2: C3-A



- Molecule 2: C3-A



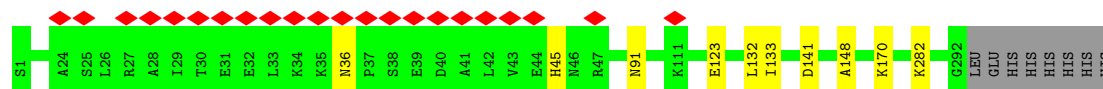
- Molecule 2: C3-A



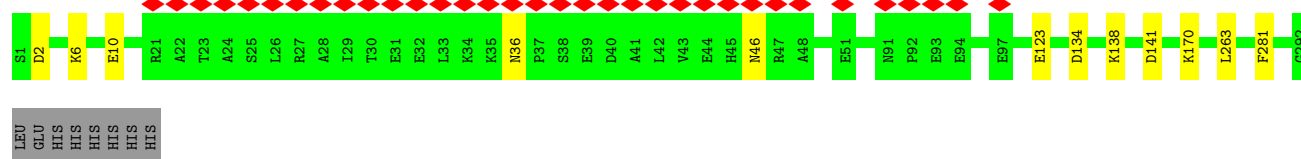
- Molecule 2: C3-A



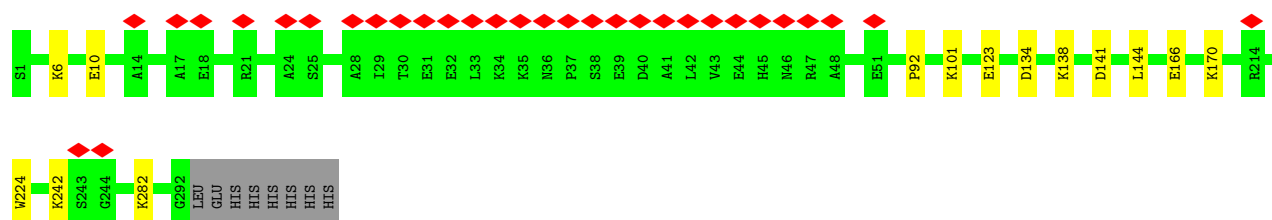
- Molecule 2: C3-A



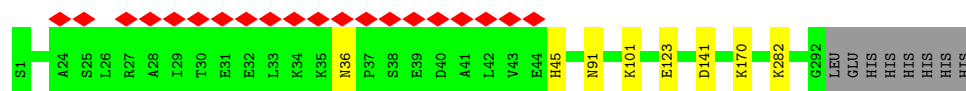
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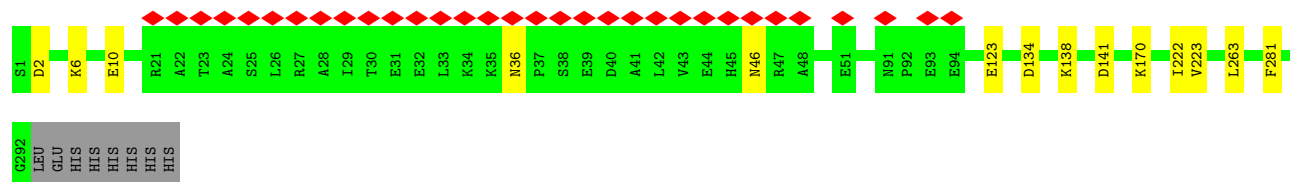
- Molecule 2: C3-A



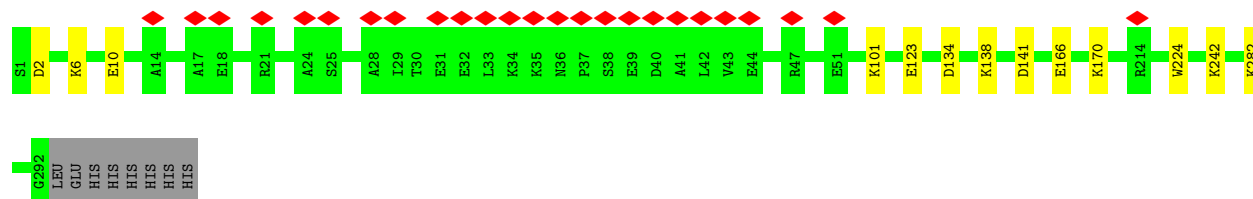
- Molecule 2: C3-A



- Molecule 2: C3-A

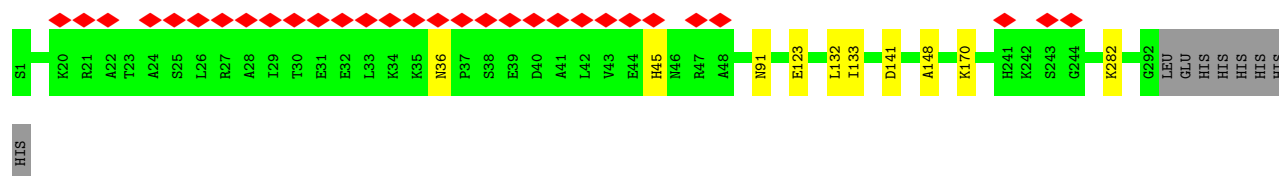


- Molecule 2: C3-A

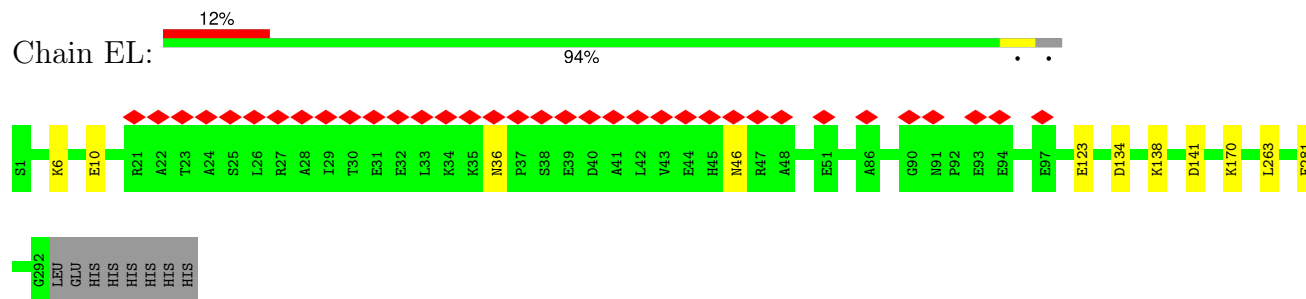


- Molecule 2: C3-A

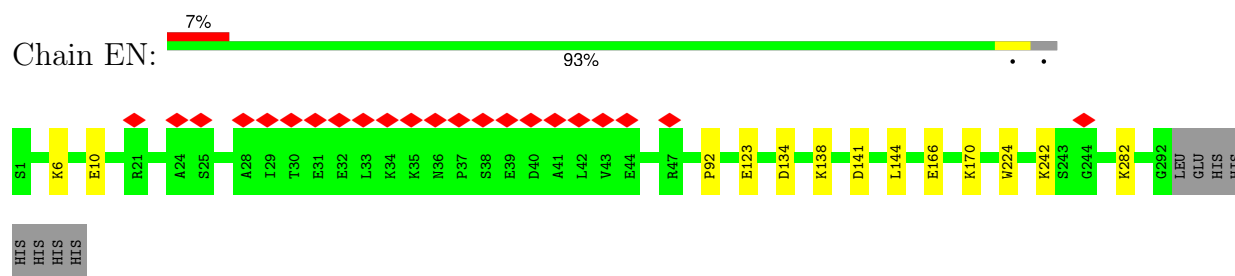




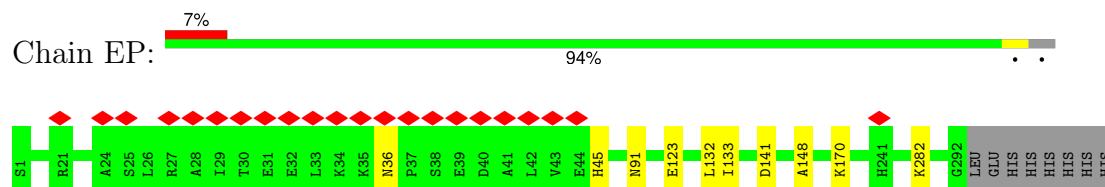
- Molecule 2: C3-A



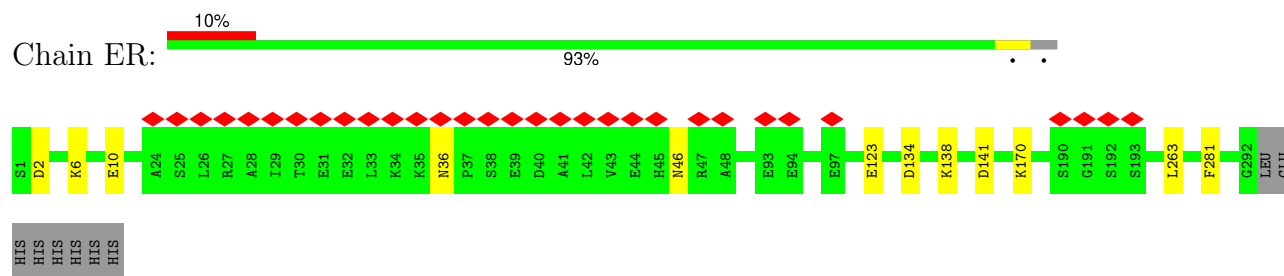
- Molecule 2: C3-A



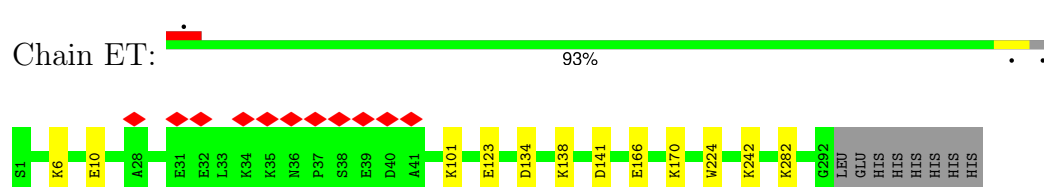
- Molecule 2: C3-A



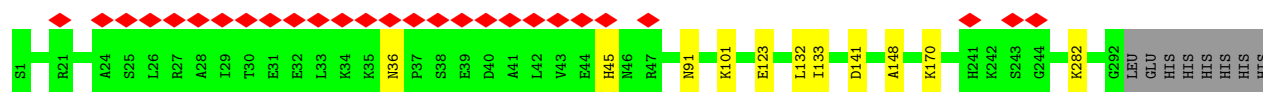
- Molecule 2: C3-A



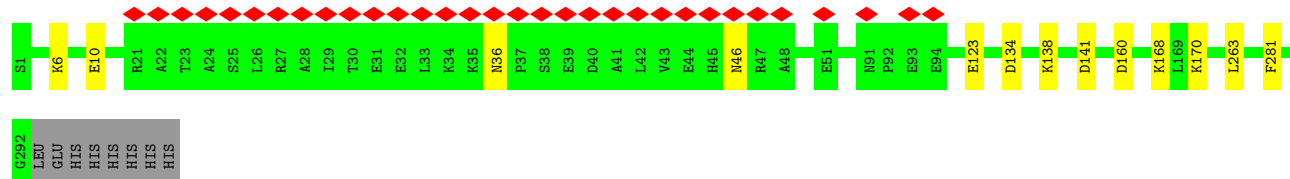
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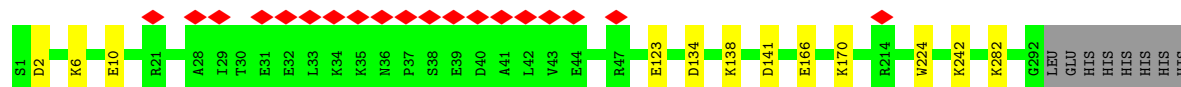
● Molecule 2: C3-A



● Molecule 2: C3-A



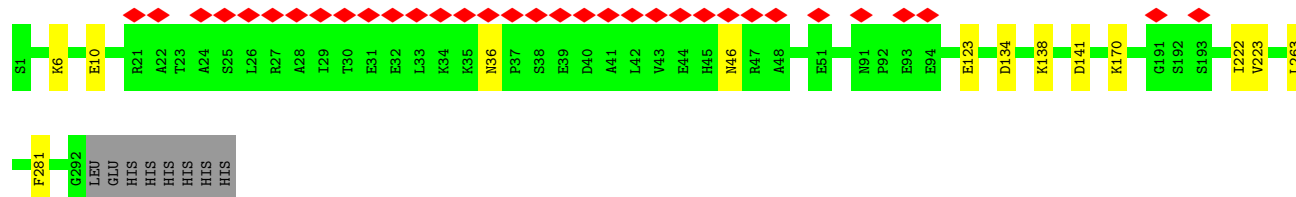
● Molecule 2: C3-A



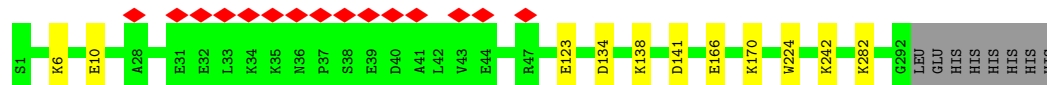
● Molecule 2: C3-A



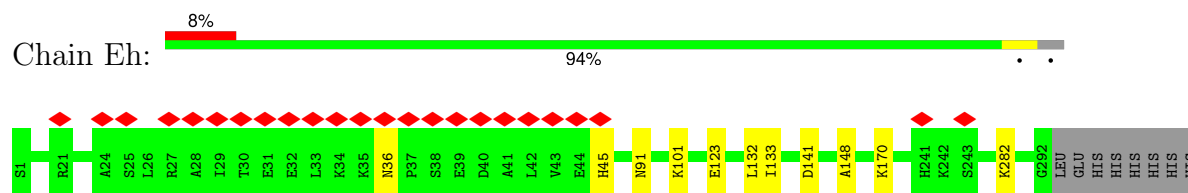
● Molecule 2: C3-A



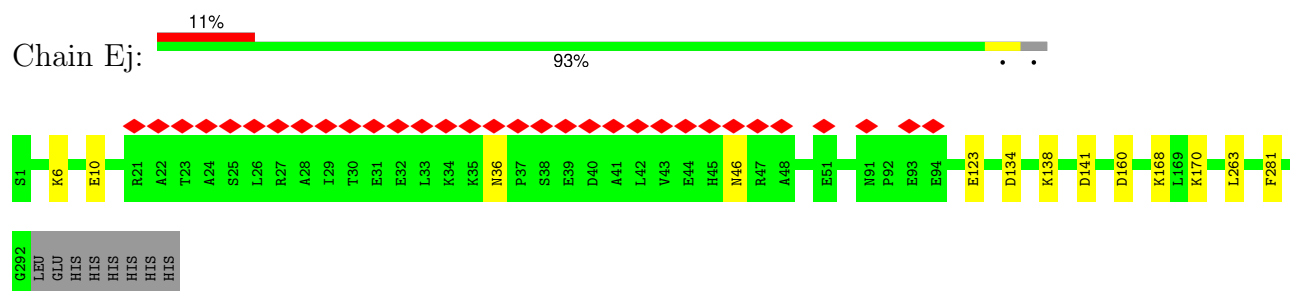
● Molecule 2: C3-A



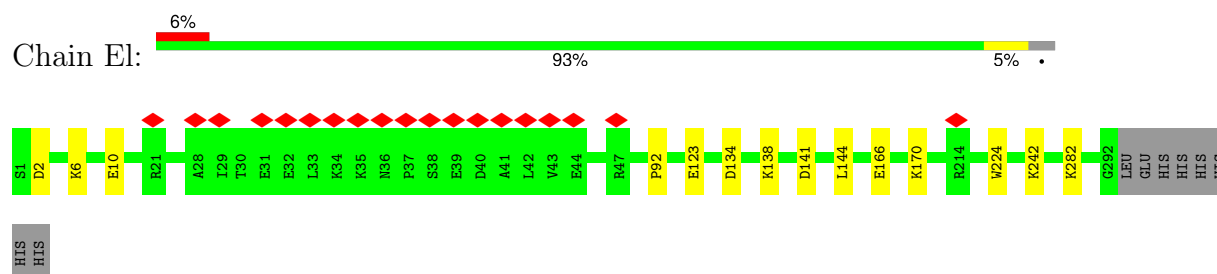
• Molecule 2: C3-A



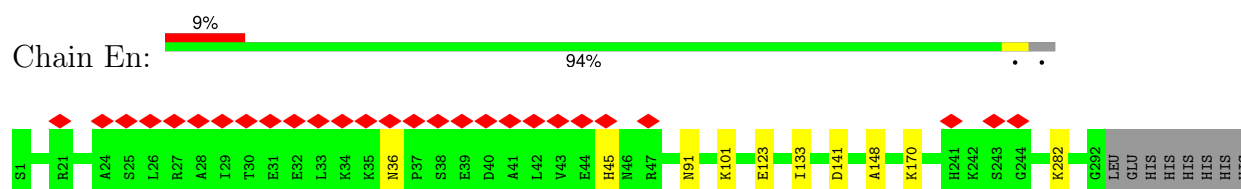
• Molecule 2: C3-A



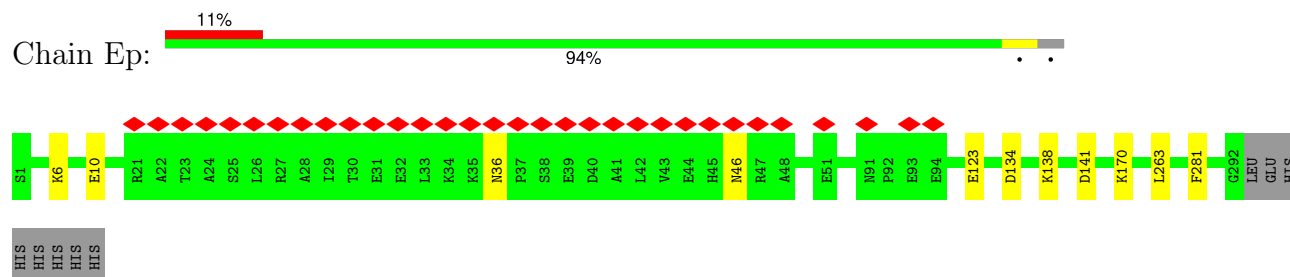
• Molecule 2: C3-A



• Molecule 2: C3-A

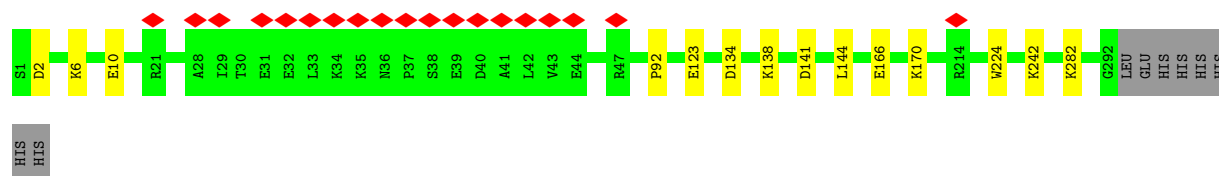


• Molecule 2: C3-A

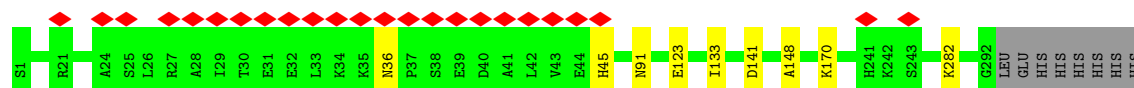


• Molecule 2: C3-A

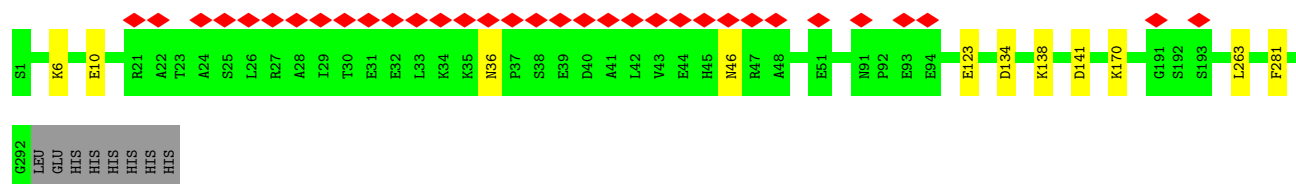




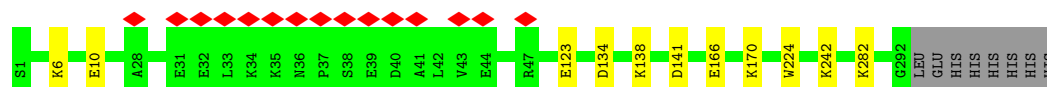
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.507	Depositor
Minimum map value	-0.126	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.221	Depositor
Map size (Å)	1180.2, 1180.2, 1180.2	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.372, 3.372, 3.372	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	0/816	1.29	9/1106 (0.8%)
1	AA	0.97	0/816	1.37	10/1106 (0.9%)
1	AC	0.97	0/816	1.31	11/1106 (1.0%)
1	AE	0.97	0/816	1.29	8/1106 (0.7%)
1	AG	0.97	0/816	1.37	10/1106 (0.9%)
1	AI	0.97	0/816	1.31	11/1106 (1.0%)
1	AK	0.97	0/816	1.29	8/1106 (0.7%)
1	AM	0.97	0/816	1.37	10/1106 (0.9%)
1	AO	0.97	0/816	1.31	11/1106 (1.0%)
1	AQ	0.97	0/816	1.29	8/1106 (0.7%)
1	AS	0.97	0/816	1.37	10/1106 (0.9%)
1	AU	0.97	0/816	1.31	11/1106 (1.0%)
1	AW	0.97	0/816	1.29	9/1106 (0.8%)
1	AY	0.97	0/816	1.37	10/1106 (0.9%)
1	Aa	0.97	0/816	1.31	11/1106 (1.0%)
1	Ac	0.97	0/816	1.29	8/1106 (0.7%)
1	Ae	0.97	0/816	1.37	10/1106 (0.9%)
1	Ag	0.97	0/816	1.31	11/1106 (1.0%)
1	Ai	0.97	0/816	1.29	8/1106 (0.7%)
1	Ak	0.97	0/816	1.37	10/1106 (0.9%)
1	Am	0.97	0/816	1.31	11/1106 (1.0%)
1	Ao	0.97	0/816	1.29	9/1106 (0.8%)
1	Aq	0.97	0/816	1.37	10/1106 (0.9%)
1	As	0.97	0/816	1.31	11/1106 (1.0%)
1	Au	0.97	0/816	1.29	8/1106 (0.7%)
1	Aw	0.97	0/816	1.37	10/1106 (0.9%)
1	Ay	0.97	0/816	1.31	11/1106 (1.0%)
1	BA	0.97	0/816	1.31	11/1106 (1.0%)
1	BC	0.97	0/816	1.29	8/1106 (0.7%)
1	BE	0.97	0/816	1.37	10/1106 (0.9%)
1	BG	0.97	0/816	1.31	11/1106 (1.0%)
1	BI	0.97	0/816	1.29	8/1106 (0.7%)
1	BK	0.97	0/816	1.37	10/1106 (0.9%)
1	BM	0.98	0/816	1.31	11/1106 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BO	0.97	0/816	1.29	8/1106 (0.7%)
1	BQ	0.97	0/816	1.37	10/1106 (0.9%)
1	BS	0.98	0/816	1.31	11/1106 (1.0%)
1	BU	0.97	0/816	1.29	8/1106 (0.7%)
1	BW	0.97	0/816	1.37	10/1106 (0.9%)
1	BY	0.98	0/816	1.31	11/1106 (1.0%)
1	Ba	0.97	0/816	1.29	8/1106 (0.7%)
1	Bc	0.97	0/816	1.37	10/1106 (0.9%)
1	Be	0.97	0/816	1.31	11/1106 (1.0%)
1	Bg	0.97	0/816	1.29	8/1106 (0.7%)
1	Bi	0.97	0/816	1.37	10/1106 (0.9%)
1	Bk	0.97	0/816	1.31	11/1106 (1.0%)
1	Bm	0.97	0/816	1.29	9/1106 (0.8%)
1	Bo	0.97	0/816	1.37	10/1106 (0.9%)
1	Bq	0.97	0/816	1.31	11/1106 (1.0%)
1	Bs	0.97	0/816	1.29	8/1106 (0.7%)
1	Bu	0.97	0/816	1.37	10/1106 (0.9%)
1	Bw	0.97	0/816	1.31	11/1106 (1.0%)
1	By	0.97	0/816	1.29	8/1106 (0.7%)
1	C	0.97	0/816	1.37	10/1106 (0.9%)
1	CA	0.97	0/816	1.29	8/1106 (0.7%)
1	CC	0.97	0/816	1.37	10/1106 (0.9%)
1	CE	0.97	0/816	1.31	11/1106 (1.0%)
1	CG	0.97	0/816	1.29	9/1106 (0.8%)
1	CI	0.97	0/816	1.37	10/1106 (0.9%)
1	CK	0.97	0/816	1.31	11/1106 (1.0%)
1	CM	0.97	0/816	1.29	8/1106 (0.7%)
1	CO	0.97	0/816	1.37	10/1106 (0.9%)
1	CQ	0.97	0/816	1.31	11/1106 (1.0%)
1	CS	0.97	0/816	1.29	8/1106 (0.7%)
1	CU	0.97	0/816	1.37	10/1106 (0.9%)
1	CW	0.97	0/816	1.31	11/1106 (1.0%)
1	CY	0.97	0/816	1.29	9/1106 (0.8%)
1	Ca	0.97	0/816	1.37	10/1106 (0.9%)
1	Cc	0.97	0/816	1.31	11/1106 (1.0%)
1	Ce	0.97	0/816	1.29	8/1106 (0.7%)
1	Cg	0.97	0/816	1.37	10/1106 (0.9%)
1	Ci	0.97	0/816	1.31	11/1106 (1.0%)
1	Ck	0.97	0/816	1.29	8/1106 (0.7%)
1	Cm	0.97	0/816	1.37	10/1106 (0.9%)
1	Co	0.98	0/816	1.31	11/1106 (1.0%)
1	Cq	0.97	0/816	1.29	8/1106 (0.7%)
1	Cs	0.97	0/816	1.37	10/1106 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Cu	0.98	0/816	1.31	11/1106 (1.0%)
1	Cw	0.97	0/816	1.29	8/1106 (0.7%)
1	Cy	0.97	0/816	1.37	10/1106 (0.9%)
1	DA	0.97	0/816	1.37	10/1106 (0.9%)
1	DC	0.97	0/816	1.31	11/1106 (1.0%)
1	DE	0.97	0/816	1.29	8/1106 (0.7%)
1	DG	0.97	0/816	1.37	10/1106 (0.9%)
1	DI	0.97	0/816	1.31	11/1106 (1.0%)
1	DK	0.97	0/816	1.29	8/1106 (0.7%)
1	DM	0.97	0/816	1.37	10/1106 (0.9%)
1	DO	0.97	0/816	1.31	11/1106 (1.0%)
1	DQ	0.97	0/816	1.29	8/1106 (0.7%)
1	DS	0.97	0/816	1.37	10/1106 (0.9%)
1	DU	0.97	0/816	1.31	11/1106 (1.0%)
1	DW	0.97	0/816	1.29	9/1106 (0.8%)
1	DY	0.97	0/816	1.37	10/1106 (0.9%)
1	Da	0.97	0/816	1.31	11/1106 (1.0%)
1	Dc	0.97	0/816	1.29	8/1106 (0.7%)
1	De	0.97	0/816	1.37	10/1106 (0.9%)
1	Dg	0.97	0/816	1.31	11/1106 (1.0%)
1	Di	0.97	0/816	1.29	9/1106 (0.8%)
1	Dk	0.97	0/816	1.37	10/1106 (0.9%)
1	Dm	0.97	0/816	1.31	11/1106 (1.0%)
1	Do	0.97	0/816	1.29	8/1106 (0.7%)
1	Dq	0.97	0/816	1.37	10/1106 (0.9%)
1	Ds	0.97	0/816	1.31	11/1106 (1.0%)
1	Du	0.97	0/816	1.29	9/1106 (0.8%)
1	Dw	0.97	0/816	1.37	10/1106 (0.9%)
1	Dy	0.97	0/816	1.31	11/1106 (1.0%)
1	E	0.97	0/816	1.31	11/1106 (1.0%)
1	EA	0.97	0/816	1.31	11/1106 (1.0%)
1	EC	0.97	0/816	1.29	8/1106 (0.7%)
1	EE	0.97	0/816	1.37	10/1106 (0.9%)
1	EG	0.98	0/816	1.31	11/1106 (1.0%)
1	EI	0.97	0/816	1.29	8/1106 (0.7%)
1	EK	0.97	0/816	1.37	10/1106 (0.9%)
1	EM	0.98	0/816	1.31	11/1106 (1.0%)
1	EO	0.97	0/816	1.29	8/1106 (0.7%)
1	EQ	0.97	0/816	1.37	10/1106 (0.9%)
1	ES	0.98	0/816	1.31	11/1106 (1.0%)
1	EU	0.97	0/816	1.29	8/1106 (0.7%)
1	EW	0.97	0/816	1.37	10/1106 (0.9%)
1	EY	0.97	0/816	1.31	11/1106 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ea	0.97	0/816	1.29	8/1106 (0.7%)
1	Ec	0.97	0/816	1.37	10/1106 (0.9%)
1	Ee	0.97	0/816	1.31	11/1106 (1.0%)
1	Eg	0.97	0/816	1.29	9/1106 (0.8%)
1	Ei	0.97	0/816	1.37	10/1106 (0.9%)
1	Ek	0.97	0/816	1.31	11/1106 (1.0%)
1	Em	0.97	0/816	1.29	8/1106 (0.7%)
1	Eo	0.97	0/816	1.37	10/1106 (0.9%)
1	Eq	0.97	0/816	1.31	11/1106 (1.0%)
1	Es	0.97	0/816	1.29	8/1106 (0.7%)
1	Eu	0.97	0/816	1.37	10/1106 (0.9%)
1	Ew	0.97	0/816	1.31	11/1106 (1.0%)
1	G	0.97	0/816	1.29	8/1106 (0.7%)
1	I	0.97	0/816	1.37	10/1106 (0.9%)
1	K	0.97	0/816	1.31	11/1106 (1.0%)
1	M	0.97	0/816	1.29	9/1106 (0.8%)
1	O	0.97	0/816	1.37	10/1106 (0.9%)
1	Q	0.97	0/816	1.31	11/1106 (1.0%)
1	S	0.97	0/816	1.29	8/1106 (0.7%)
1	U	0.97	0/816	1.37	10/1106 (0.9%)
1	W	0.97	0/816	1.31	11/1106 (1.0%)
1	Y	0.97	0/816	1.29	9/1106 (0.8%)
1	YA	0.97	0/816	1.37	10/1106 (0.9%)
1	YC	0.97	0/816	1.31	11/1106 (1.0%)
1	YE	0.98	0/816	1.31	11/1106 (1.0%)
1	YG	0.97	0/816	1.29	9/1106 (0.8%)
1	YI	0.97	0/816	1.37	10/1106 (0.9%)
1	YK	0.97	0/816	1.31	11/1106 (1.0%)
1	YM	0.97	0/816	1.29	8/1106 (0.7%)
1	YO	0.97	0/816	1.29	8/1106 (0.7%)
1	YQ	0.97	0/816	1.37	10/1106 (0.9%)
1	YS	0.97	0/816	1.31	11/1106 (1.0%)
1	YU	0.97	0/816	1.29	8/1106 (0.7%)
1	YW	0.97	0/816	1.37	10/1106 (0.9%)
1	ZA	0.98	0/816	1.31	11/1106 (1.0%)
1	ZC	0.97	0/816	1.29	8/1106 (0.7%)
1	ZE	0.97	0/816	1.37	10/1106 (0.9%)
1	ZG	0.98	0/816	1.31	11/1106 (1.0%)
1	ZI	0.97	0/816	1.29	9/1106 (0.8%)
1	ZK	0.97	0/816	1.29	9/1106 (0.8%)
1	ZM	0.97	0/816	1.37	10/1106 (0.9%)
1	ZO	0.97	0/816	1.31	11/1106 (1.0%)
1	ZQ	0.97	0/816	1.29	8/1106 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ZS	0.97	0/816	1.37	10/1106 (0.9%)
1	ZU	0.97	0/816	1.37	10/1106 (0.9%)
1	ZW	0.97	0/816	1.31	11/1106 (1.0%)
1	ZY	0.97	0/816	1.29	9/1106 (0.8%)
1	a	0.97	0/816	1.37	10/1106 (0.9%)
1	c	0.97	0/816	1.31	11/1106 (1.0%)
1	e	0.97	0/816	1.29	9/1106 (0.8%)
1	g	0.97	0/816	1.37	10/1106 (0.9%)
1	i	0.97	0/816	1.31	11/1106 (1.0%)
1	k	0.97	0/816	1.29	9/1106 (0.8%)
1	m	0.97	0/816	1.37	10/1106 (0.9%)
1	o	0.97	0/816	1.31	11/1106 (1.0%)
1	q	0.97	0/816	1.29	8/1106 (0.7%)
1	s	0.97	0/816	1.37	10/1106 (0.9%)
1	u	0.98	0/816	1.31	11/1106 (1.0%)
1	w	0.97	0/816	1.29	8/1106 (0.7%)
1	y	0.97	0/816	1.37	10/1106 (0.9%)
2	AB	0.92	0/2283	0.99	4/3073 (0.1%)
2	AD	0.89	0/2283	1.00	2/3073 (0.1%)
2	AF	0.89	0/2283	1.00	6/3073 (0.2%)
2	AH	0.92	0/2283	0.99	4/3073 (0.1%)
2	AJ	0.89	0/2283	1.00	2/3073 (0.1%)
2	AL	0.89	0/2283	1.00	6/3073 (0.2%)
2	AN	0.92	0/2283	1.00	4/3073 (0.1%)
2	AP	0.89	0/2283	1.00	2/3073 (0.1%)
2	AR	0.89	0/2283	1.00	6/3073 (0.2%)
2	AT	0.92	0/2283	0.99	4/3073 (0.1%)
2	AV	0.89	0/2283	1.00	2/3073 (0.1%)
2	AX	0.89	0/2283	1.00	6/3073 (0.2%)
2	AZ	0.92	0/2283	0.99	4/3073 (0.1%)
2	Ab	0.89	0/2283	1.00	2/3073 (0.1%)
2	Ad	0.89	0/2283	1.00	6/3073 (0.2%)
2	Af	0.92	0/2283	0.99	4/3073 (0.1%)
2	Ah	0.89	0/2283	1.00	2/3073 (0.1%)
2	Aj	0.89	0/2283	1.00	6/3073 (0.2%)
2	Al	0.92	0/2283	1.00	4/3073 (0.1%)
2	An	0.89	0/2283	1.00	2/3073 (0.1%)
2	Ap	0.89	0/2283	1.00	6/3073 (0.2%)
2	Ar	0.92	0/2283	0.99	4/3073 (0.1%)
2	At	0.89	0/2283	1.00	2/3073 (0.1%)
2	Av	0.89	0/2283	1.00	6/3073 (0.2%)
2	Ax	0.92	0/2283	0.99	4/3073 (0.1%)
2	Az	0.89	0/2283	1.00	2/3073 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	B	0.89	0/2283	1.00	6/3073 (0.2%)
2	BB	0.89	0/2283	1.00	2/3073 (0.1%)
2	BD	0.89	0/2283	1.00	6/3073 (0.2%)
2	BF	0.92	0/2283	0.99	4/3073 (0.1%)
2	BH	0.89	0/2283	1.00	2/3073 (0.1%)
2	BJ	0.89	0/2283	1.00	6/3073 (0.2%)
2	BL	0.92	0/2283	1.00	4/3073 (0.1%)
2	BN	0.89	0/2283	1.00	2/3073 (0.1%)
2	BP	0.89	0/2283	1.00	6/3073 (0.2%)
2	BR	0.92	0/2283	1.00	4/3073 (0.1%)
2	BT	0.89	0/2283	1.00	2/3073 (0.1%)
2	BV	0.89	0/2283	1.00	6/3073 (0.2%)
2	BX	0.92	0/2283	1.00	4/3073 (0.1%)
2	BZ	0.89	0/2283	1.00	2/3073 (0.1%)
2	Bb	0.89	0/2283	1.00	6/3073 (0.2%)
2	Bd	0.92	0/2283	0.99	4/3073 (0.1%)
2	Bf	0.89	0/2283	1.00	2/3073 (0.1%)
2	Bh	0.89	0/2283	1.00	6/3073 (0.2%)
2	Bj	0.92	0/2283	1.00	4/3073 (0.1%)
2	Bl	0.89	0/2283	1.00	2/3073 (0.1%)
2	Bn	0.89	0/2283	1.00	6/3073 (0.2%)
2	Bp	0.92	0/2283	0.99	4/3073 (0.1%)
2	Br	0.89	0/2283	1.00	2/3073 (0.1%)
2	Bt	0.89	0/2283	1.00	6/3073 (0.2%)
2	Bv	0.92	0/2283	0.99	4/3073 (0.1%)
2	Bx	0.89	0/2283	1.00	2/3073 (0.1%)
2	Bz	0.89	0/2283	1.00	6/3073 (0.2%)
2	CB	0.89	0/2283	1.00	6/3073 (0.2%)
2	CD	0.92	0/2283	1.00	4/3073 (0.1%)
2	CF	0.89	0/2283	1.00	2/3073 (0.1%)
2	CH	0.89	0/2283	1.00	6/3073 (0.2%)
2	CJ	0.92	0/2283	0.99	4/3073 (0.1%)
2	CL	0.89	0/2283	1.00	2/3073 (0.1%)
2	CN	0.89	0/2283	1.00	6/3073 (0.2%)
2	CP	0.92	0/2283	0.99	4/3073 (0.1%)
2	CR	0.89	0/2283	1.00	2/3073 (0.1%)
2	CT	0.89	0/2283	1.00	6/3073 (0.2%)
2	CV	0.92	0/2283	0.99	4/3073 (0.1%)
2	CX	0.89	0/2283	1.00	2/3073 (0.1%)
2	CZ	0.89	0/2283	1.00	6/3073 (0.2%)
2	Cb	0.92	0/2283	0.99	4/3073 (0.1%)
2	Cd	0.89	0/2283	1.00	2/3073 (0.1%)
2	Cf	0.89	0/2283	1.00	6/3073 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Ch	0.92	0/2283	0.99	4/3073 (0.1%)
2	Cj	0.89	0/2283	1.00	2/3073 (0.1%)
2	Cl	0.89	0/2283	1.00	6/3073 (0.2%)
2	Cn	0.92	0/2283	1.00	4/3073 (0.1%)
2	Cp	0.89	0/2283	1.00	2/3073 (0.1%)
2	Cr	0.89	0/2283	1.00	6/3073 (0.2%)
2	Ct	0.92	0/2283	1.00	4/3073 (0.1%)
2	Cv	0.89	0/2283	1.00	2/3073 (0.1%)
2	Cx	0.89	0/2283	1.00	6/3073 (0.2%)
2	Cz	0.92	0/2283	1.00	4/3073 (0.1%)
2	D	0.92	0/2283	0.99	4/3073 (0.1%)
2	DB	0.92	0/2283	1.00	4/3073 (0.1%)
2	DD	0.89	0/2283	1.00	2/3073 (0.1%)
2	DF	0.89	0/2283	1.00	6/3073 (0.2%)
2	DH	0.92	0/2283	0.99	4/3073 (0.1%)
2	DJ	0.89	0/2283	1.00	2/3073 (0.1%)
2	DL	0.89	0/2283	1.00	6/3073 (0.2%)
2	DN	0.92	0/2283	0.99	4/3073 (0.1%)
2	DP	0.89	0/2283	1.00	2/3073 (0.1%)
2	DR	0.89	0/2283	1.00	6/3073 (0.2%)
2	DT	0.92	0/2283	0.99	4/3073 (0.1%)
2	DV	0.89	0/2283	1.00	2/3073 (0.1%)
2	DX	0.89	0/2283	1.00	6/3073 (0.2%)
2	DZ	0.92	0/2283	0.99	4/3073 (0.1%)
2	Db	0.89	0/2283	1.00	2/3073 (0.1%)
2	Dd	0.89	0/2283	1.00	6/3073 (0.2%)
2	Df	0.92	0/2283	0.99	4/3073 (0.1%)
2	Dh	0.89	0/2283	1.00	2/3073 (0.1%)
2	Dj	0.89	0/2283	1.00	6/3073 (0.2%)
2	Di	0.92	0/2283	0.99	4/3073 (0.1%)
2	Dn	0.89	0/2283	1.00	2/3073 (0.1%)
2	Dp	0.89	0/2283	1.00	6/3073 (0.2%)
2	Dr	0.92	0/2283	0.99	4/3073 (0.1%)
2	Dt	0.89	0/2283	1.00	2/3073 (0.1%)
2	Dv	0.89	0/2283	1.00	6/3073 (0.2%)
2	Dx	0.92	0/2283	0.99	4/3073 (0.1%)
2	Dz	0.89	0/2283	1.00	2/3073 (0.1%)
2	EB	0.89	0/2283	1.00	2/3073 (0.1%)
2	ED	0.89	0/2283	1.00	6/3073 (0.2%)
2	EF	0.92	0/2283	1.00	4/3073 (0.1%)
2	EH	0.89	0/2283	1.00	2/3073 (0.1%)
2	EJ	0.89	0/2283	1.00	6/3073 (0.2%)
2	EL	0.92	0/2283	1.00	4/3073 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	EN	0.89	0/2283	1.00	2/3073 (0.1%)
2	EP	0.89	0/2283	1.00	6/3073 (0.2%)
2	ER	0.92	0/2283	1.00	4/3073 (0.1%)
2	ET	0.89	0/2283	1.00	2/3073 (0.1%)
2	EV	0.89	0/2283	1.00	6/3073 (0.2%)
2	EX	0.92	0/2283	1.00	4/3073 (0.1%)
2	EZ	0.89	0/2283	1.00	2/3073 (0.1%)
2	Eb	0.89	0/2283	1.00	6/3073 (0.2%)
2	Ed	0.92	0/2283	0.99	4/3073 (0.1%)
2	Ef	0.89	0/2283	1.00	2/3073 (0.1%)
2	Eh	0.89	0/2283	1.00	6/3073 (0.2%)
2	Ej	0.92	0/2283	0.99	4/3073 (0.1%)
2	El	0.89	0/2283	1.00	2/3073 (0.1%)
2	En	0.89	0/2283	1.00	6/3073 (0.2%)
2	Ep	0.92	0/2283	0.99	4/3073 (0.1%)
2	Er	0.89	0/2283	1.00	2/3073 (0.1%)
2	Et	0.89	0/2283	1.00	6/3073 (0.2%)
2	Ev	0.92	0/2283	0.99	4/3073 (0.1%)
2	Ex	0.89	0/2283	1.00	2/3073 (0.1%)
2	F	0.89	0/2283	1.00	2/3073 (0.1%)
2	H	0.89	0/2283	1.00	6/3073 (0.2%)
2	J	0.92	0/2283	1.00	4/3073 (0.1%)
2	L	0.89	0/2283	1.00	2/3073 (0.1%)
2	N	0.89	0/2283	1.00	6/3073 (0.2%)
2	P	0.92	0/2283	0.99	4/3073 (0.1%)
2	R	0.89	0/2283	1.00	2/3073 (0.1%)
2	T	0.89	0/2283	1.00	6/3073 (0.2%)
2	V	0.92	0/2283	0.99	4/3073 (0.1%)
2	X	0.89	0/2283	1.00	2/3073 (0.1%)
2	YB	0.92	0/2283	0.99	4/3073 (0.1%)
2	YD	0.89	0/2283	1.00	2/3073 (0.1%)
2	YF	0.89	0/2283	1.00	2/3073 (0.1%)
2	YH	0.89	0/2283	1.00	6/3073 (0.2%)
2	YJ	0.92	0/2283	0.99	4/3073 (0.1%)
2	YL	0.89	0/2283	1.00	2/3073 (0.1%)
2	YN	0.89	0/2283	1.00	6/3073 (0.2%)
2	YP	0.89	0/2283	1.00	6/3073 (0.2%)
2	YR	0.92	0/2283	0.99	4/3073 (0.1%)
2	YT	0.89	0/2283	1.00	2/3073 (0.1%)
2	YV	0.89	0/2283	1.00	6/3073 (0.2%)
2	YX	0.92	0/2283	0.99	4/3073 (0.1%)
2	Z	0.89	0/2283	1.00	6/3073 (0.2%)
2	ZB	0.89	0/2283	1.00	2/3073 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	ZD	0.89	0/2283	1.00	6/3073 (0.2%)
2	ZF	0.92	0/2283	1.00	4/3073 (0.1%)
2	ZH	0.89	0/2283	1.00	2/3073 (0.1%)
2	ZJ	0.89	0/2283	1.00	6/3073 (0.2%)
2	ZL	0.89	0/2283	1.00	6/3073 (0.2%)
2	ZN	0.92	0/2283	0.99	4/3073 (0.1%)
2	ZP	0.89	0/2283	1.00	2/3073 (0.1%)
2	ZR	0.89	0/2283	1.00	6/3073 (0.2%)
2	ZT	0.92	0/2283	1.00	4/3073 (0.1%)
2	ZV	0.92	0/2283	1.00	4/3073 (0.1%)
2	ZX	0.89	0/2283	1.00	2/3073 (0.1%)
2	ZZ	0.89	0/2283	1.00	6/3073 (0.2%)
2	b	0.92	0/2283	1.00	4/3073 (0.1%)
2	d	0.89	0/2283	1.00	2/3073 (0.1%)
2	f	0.89	0/2283	1.00	6/3073 (0.2%)
2	h	0.92	0/2283	1.00	4/3073 (0.1%)
2	j	0.89	0/2283	1.00	2/3073 (0.1%)
2	l	0.89	0/2283	1.00	6/3073 (0.2%)
2	n	0.92	0/2283	1.00	4/3073 (0.1%)
2	p	0.89	0/2283	1.00	2/3073 (0.1%)
2	r	0.89	0/2283	1.00	6/3073 (0.2%)
2	t	0.92	0/2283	1.00	4/3073 (0.1%)
2	v	0.89	0/2283	1.00	2/3073 (0.1%)
2	x	0.89	0/2283	1.00	6/3073 (0.2%)
2	z	0.92	0/2283	1.00	4/3073 (0.1%)
All	All	0.92	0/557820	1.09	2478/752220 (0.3%)

There are no bond length outliers.

All (2478) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	s	46	ARG	CA-C-N	8.13	128.33	119.87
1	s	46	ARG	C-N-CA	8.13	128.33	119.87
1	ZE	46	ARG	CA-C-N	8.13	128.33	119.87
1	ZE	46	ARG	C-N-CA	8.13	128.33	119.87
1	BK	46	ARG	CA-C-N	8.13	128.33	119.87
1	BK	46	ARG	C-N-CA	8.13	128.33	119.87
1	BQ	46	ARG	CA-C-N	8.13	128.33	119.87
1	BQ	46	ARG	C-N-CA	8.13	128.33	119.87
1	Cm	46	ARG	CA-C-N	8.13	128.33	119.87
1	Cm	46	ARG	C-N-CA	8.13	128.33	119.87
1	Cs	46	ARG	CA-C-N	8.13	128.33	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cs	46	ARG	C-N-CA	8.13	128.33	119.87
1	y	46	ARG	CA-C-N	8.13	128.33	119.87
1	y	46	ARG	C-N-CA	8.13	128.33	119.87
1	BW	46	ARG	CA-C-N	8.13	128.33	119.87
1	BW	46	ARG	C-N-CA	8.13	128.33	119.87
1	Cy	46	ARG	CA-C-N	8.13	128.33	119.87
1	Cy	46	ARG	C-N-CA	8.13	128.33	119.87
1	EE	46	ARG	CA-C-N	8.13	128.33	119.87
1	EE	46	ARG	C-N-CA	8.13	128.33	119.87
1	EK	46	ARG	CA-C-N	8.13	128.33	119.87
1	EK	46	ARG	C-N-CA	8.13	128.33	119.87
1	EQ	46	ARG	CA-C-N	8.13	128.33	119.87
1	EQ	46	ARG	C-N-CA	8.13	128.33	119.87
1	U	46	ARG	CA-C-N	8.11	128.31	119.87
1	U	46	ARG	C-N-CA	8.11	128.31	119.87
1	AG	46	ARG	CA-C-N	8.11	128.31	119.87
1	AG	46	ARG	C-N-CA	8.11	128.31	119.87
1	Aw	46	ARG	CA-C-N	8.11	128.31	119.87
1	Aw	46	ARG	C-N-CA	8.11	128.31	119.87
1	Bc	46	ARG	CA-C-N	8.11	128.31	119.87
1	Bc	46	ARG	C-N-CA	8.11	128.31	119.87
1	Bu	46	ARG	CA-C-N	8.11	128.31	119.87
1	Bu	46	ARG	C-N-CA	8.11	128.31	119.87
1	CO	46	ARG	CA-C-N	8.11	128.31	119.87
1	CO	46	ARG	C-N-CA	8.11	128.31	119.87
1	C	46	ARG	CA-C-N	8.11	128.30	119.87
1	C	46	ARG	C-N-CA	8.11	128.30	119.87
1	O	46	ARG	CA-C-N	8.11	128.30	119.87
1	O	46	ARG	C-N-CA	8.11	128.30	119.87
1	AA	46	ARG	CA-C-N	8.11	128.30	119.87
1	AA	46	ARG	C-N-CA	8.11	128.30	119.87
1	Aq	46	ARG	CA-C-N	8.11	128.30	119.87
1	Aq	46	ARG	C-N-CA	8.11	128.30	119.87
1	ZM	46	ARG	CA-C-N	8.11	128.30	119.87
1	ZM	46	ARG	C-N-CA	8.11	128.30	119.87
1	Bo	46	ARG	CA-C-N	8.11	128.30	119.87
1	Bo	46	ARG	C-N-CA	8.11	128.30	119.87
1	YA	46	ARG	CA-C-N	8.11	128.30	119.87
1	YA	46	ARG	C-N-CA	8.11	128.30	119.87
1	CI	46	ARG	CA-C-N	8.11	128.30	119.87
1	CI	46	ARG	C-N-CA	8.11	128.30	119.87
1	YI	46	ARG	CA-C-N	8.11	128.30	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YI	46	ARG	C-N-CA	8.11	128.30	119.87
1	Dk	46	ARG	CA-C-N	8.11	128.30	119.87
1	Dk	46	ARG	C-N-CA	8.11	128.30	119.87
1	Dw	46	ARG	CA-C-N	8.11	128.30	119.87
1	Dw	46	ARG	C-N-CA	8.11	128.30	119.87
1	Ei	46	ARG	CA-C-N	8.11	128.30	119.87
1	Ei	46	ARG	C-N-CA	8.11	128.30	119.87
1	ZS	46	ARG	CA-C-N	8.10	128.30	119.87
1	ZS	46	ARG	C-N-CA	8.10	128.30	119.87
1	DA	46	ARG	CA-C-N	8.10	128.30	119.87
1	DA	46	ARG	C-N-CA	8.10	128.30	119.87
1	Dq	46	ARG	CA-C-N	8.10	128.30	119.87
1	Dq	46	ARG	C-N-CA	8.10	128.30	119.87
1	YQ	46	ARG	CA-C-N	8.10	128.30	119.87
1	YQ	46	ARG	C-N-CA	8.10	128.30	119.87
1	EW	46	ARG	CA-C-N	8.10	128.30	119.87
1	EW	46	ARG	C-N-CA	8.10	128.30	119.87
1	Eo	46	ARG	CA-C-N	8.10	128.30	119.87
1	Eo	46	ARG	C-N-CA	8.10	128.30	119.87
1	I	46	ARG	CA-C-N	8.09	128.28	119.87
1	I	46	ARG	C-N-CA	8.09	128.28	119.87
1	AM	46	ARG	CA-C-N	8.09	128.28	119.87
1	AM	46	ARG	C-N-CA	8.09	128.28	119.87
1	Ak	46	ARG	CA-C-N	8.09	128.28	119.87
1	Ak	46	ARG	C-N-CA	8.09	128.28	119.87
1	BE	46	ARG	CA-C-N	8.09	128.28	119.87
1	BE	46	ARG	C-N-CA	8.09	128.28	119.87
1	Bi	46	ARG	CA-C-N	8.09	128.28	119.87
1	Bi	46	ARG	C-N-CA	8.09	128.28	119.87
1	ZU	46	ARG	CA-C-N	8.09	128.28	119.87
1	ZU	46	ARG	C-N-CA	8.09	128.28	119.87
1	CC	46	ARG	CA-C-N	8.09	128.28	119.87
1	CC	46	ARG	C-N-CA	8.09	128.28	119.87
1	DG	46	ARG	CA-C-N	8.09	128.28	119.87
1	DG	46	ARG	C-N-CA	8.09	128.28	119.87
1	De	46	ARG	CA-C-N	8.09	128.28	119.87
1	De	46	ARG	C-N-CA	8.09	128.28	119.87
1	YW	46	ARG	CA-C-N	8.09	128.28	119.87
1	YW	46	ARG	C-N-CA	8.09	128.28	119.87
1	Ec	46	ARG	CA-C-N	8.09	128.28	119.87
1	Ec	46	ARG	C-N-CA	8.09	128.28	119.87
1	Eu	46	ARG	CA-C-N	8.09	128.28	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Eu	46	ARG	C-N-CA	8.09	128.28	119.87
1	a	46	ARG	CA-C-N	8.08	128.28	119.87
1	a	46	ARG	C-N-CA	8.08	128.28	119.87
1	g	46	ARG	CA-C-N	8.08	128.28	119.87
1	g	46	ARG	C-N-CA	8.08	128.28	119.87
1	m	46	ARG	CA-C-N	8.08	128.28	119.87
1	m	46	ARG	C-N-CA	8.08	128.28	119.87
1	AS	46	ARG	CA-C-N	8.08	128.28	119.87
1	AS	46	ARG	C-N-CA	8.08	128.28	119.87
1	AY	46	ARG	CA-C-N	8.08	128.28	119.87
1	AY	46	ARG	C-N-CA	8.08	128.28	119.87
1	Ae	46	ARG	CA-C-N	8.08	128.28	119.87
1	Ae	46	ARG	C-N-CA	8.08	128.28	119.87
1	CU	46	ARG	CA-C-N	8.08	128.28	119.87
1	CU	46	ARG	C-N-CA	8.08	128.28	119.87
1	Ca	46	ARG	CA-C-N	8.08	128.28	119.87
1	Ca	46	ARG	C-N-CA	8.08	128.28	119.87
1	Cg	46	ARG	CA-C-N	8.08	128.28	119.87
1	Cg	46	ARG	C-N-CA	8.08	128.28	119.87
1	DM	46	ARG	CA-C-N	8.08	128.28	119.87
1	DM	46	ARG	C-N-CA	8.08	128.28	119.87
1	DS	46	ARG	CA-C-N	8.08	128.28	119.87
1	DS	46	ARG	C-N-CA	8.08	128.28	119.87
1	DY	46	ARG	CA-C-N	8.08	128.28	119.87
1	DY	46	ARG	C-N-CA	8.08	128.28	119.87
1	I	48	GLY	CA-C-N	7.79	127.81	119.78
1	I	48	GLY	C-N-CA	7.79	127.81	119.78
1	AM	48	GLY	CA-C-N	7.79	127.81	119.78
1	AM	48	GLY	C-N-CA	7.79	127.81	119.78
1	Ak	48	GLY	CA-C-N	7.79	127.81	119.78
1	Ak	48	GLY	C-N-CA	7.79	127.81	119.78
1	Bi	48	GLY	CA-C-N	7.79	127.81	119.78
1	Bi	48	GLY	C-N-CA	7.79	127.81	119.78
1	ZU	48	GLY	CA-C-N	7.79	127.81	119.78
1	ZU	48	GLY	C-N-CA	7.79	127.81	119.78
1	CC	48	GLY	CA-C-N	7.79	127.81	119.78
1	CC	48	GLY	C-N-CA	7.79	127.81	119.78
1	C	48	GLY	CA-C-N	7.79	127.80	119.78
1	C	48	GLY	C-N-CA	7.79	127.80	119.78
1	O	48	GLY	CA-C-N	7.79	127.80	119.78
1	O	48	GLY	C-N-CA	7.79	127.80	119.78
1	AA	48	GLY	CA-C-N	7.79	127.80	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	48	GLY	C-N-CA	7.79	127.80	119.78
1	Aq	48	GLY	CA-C-N	7.79	127.80	119.78
1	Aq	48	GLY	C-N-CA	7.79	127.80	119.78
1	ZM	48	GLY	CA-C-N	7.79	127.80	119.78
1	ZM	48	GLY	C-N-CA	7.79	127.80	119.78
1	Bo	48	GLY	CA-C-N	7.79	127.80	119.78
1	Bo	48	GLY	C-N-CA	7.79	127.80	119.78
1	YA	48	GLY	CA-C-N	7.79	127.80	119.78
1	YA	48	GLY	C-N-CA	7.79	127.80	119.78
1	CI	48	GLY	CA-C-N	7.79	127.80	119.78
1	CI	48	GLY	C-N-CA	7.79	127.80	119.78
1	YI	48	GLY	CA-C-N	7.79	127.80	119.78
1	YI	48	GLY	C-N-CA	7.79	127.80	119.78
1	Dk	48	GLY	CA-C-N	7.79	127.80	119.78
1	Dk	48	GLY	C-N-CA	7.79	127.80	119.78
1	Dw	48	GLY	CA-C-N	7.79	127.80	119.78
1	Dw	48	GLY	C-N-CA	7.79	127.80	119.78
1	Ei	48	GLY	CA-C-N	7.79	127.80	119.78
1	Ei	48	GLY	C-N-CA	7.79	127.80	119.78
1	U	48	GLY	CA-C-N	7.78	127.80	119.78
1	U	48	GLY	C-N-CA	7.78	127.80	119.78
1	AG	48	GLY	CA-C-N	7.78	127.80	119.78
1	AG	48	GLY	C-N-CA	7.78	127.80	119.78
1	Aw	48	GLY	CA-C-N	7.78	127.80	119.78
1	Aw	48	GLY	C-N-CA	7.78	127.80	119.78
1	BE	48	GLY	CA-C-N	7.78	127.80	119.78
1	BE	48	GLY	C-N-CA	7.78	127.80	119.78
1	Bc	48	GLY	CA-C-N	7.78	127.80	119.78
1	Bc	48	GLY	C-N-CA	7.78	127.80	119.78
1	Bu	48	GLY	CA-C-N	7.78	127.80	119.78
1	Bu	48	GLY	C-N-CA	7.78	127.80	119.78
1	CO	48	GLY	CA-C-N	7.78	127.80	119.78
1	CO	48	GLY	C-N-CA	7.78	127.80	119.78
1	DG	48	GLY	CA-C-N	7.78	127.80	119.78
1	DG	48	GLY	C-N-CA	7.78	127.80	119.78
1	De	48	GLY	CA-C-N	7.78	127.80	119.78
1	De	48	GLY	C-N-CA	7.78	127.80	119.78
1	YW	48	GLY	CA-C-N	7.78	127.80	119.78
1	YW	48	GLY	C-N-CA	7.78	127.80	119.78
1	Ec	48	GLY	CA-C-N	7.78	127.80	119.78
1	Ec	48	GLY	C-N-CA	7.78	127.80	119.78
1	Eu	48	GLY	CA-C-N	7.78	127.80	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Eu	48	GLY	C-N-CA	7.78	127.80	119.78
1	y	48	GLY	CA-C-N	7.78	127.79	119.78
1	y	48	GLY	C-N-CA	7.78	127.79	119.78
1	BW	48	GLY	CA-C-N	7.78	127.79	119.78
1	BW	48	GLY	C-N-CA	7.78	127.79	119.78
1	Cy	48	GLY	CA-C-N	7.78	127.79	119.78
1	Cy	48	GLY	C-N-CA	7.78	127.79	119.78
1	EE	48	GLY	CA-C-N	7.78	127.79	119.78
1	EE	48	GLY	C-N-CA	7.78	127.79	119.78
1	EK	48	GLY	CA-C-N	7.78	127.79	119.78
1	EK	48	GLY	C-N-CA	7.78	127.79	119.78
1	EQ	48	GLY	CA-C-N	7.78	127.79	119.78
1	EQ	48	GLY	C-N-CA	7.78	127.79	119.78
1	AS	48	GLY	CA-C-N	7.76	127.77	119.78
1	AS	48	GLY	C-N-CA	7.76	127.77	119.78
1	AY	48	GLY	CA-C-N	7.76	127.77	119.78
1	AY	48	GLY	C-N-CA	7.76	127.77	119.78
1	CU	48	GLY	CA-C-N	7.76	127.77	119.78
1	CU	48	GLY	C-N-CA	7.76	127.77	119.78
1	Ca	48	GLY	CA-C-N	7.76	127.77	119.78
1	Ca	48	GLY	C-N-CA	7.76	127.77	119.78
1	DS	48	GLY	CA-C-N	7.76	127.77	119.78
1	DS	48	GLY	C-N-CA	7.76	127.77	119.78
1	DY	48	GLY	CA-C-N	7.76	127.77	119.78
1	DY	48	GLY	C-N-CA	7.76	127.77	119.78
1	s	48	GLY	CA-C-N	7.75	127.77	119.78
1	s	48	GLY	C-N-CA	7.75	127.77	119.78
1	ZE	48	GLY	CA-C-N	7.75	127.77	119.78
1	ZE	48	GLY	C-N-CA	7.75	127.77	119.78
1	BK	48	GLY	CA-C-N	7.75	127.77	119.78
1	BK	48	GLY	C-N-CA	7.75	127.77	119.78
1	BQ	48	GLY	CA-C-N	7.75	127.77	119.78
1	BQ	48	GLY	C-N-CA	7.75	127.77	119.78
1	Cm	48	GLY	CA-C-N	7.75	127.77	119.78
1	Cm	48	GLY	C-N-CA	7.75	127.77	119.78
1	Cs	48	GLY	CA-C-N	7.75	127.77	119.78
1	Cs	48	GLY	C-N-CA	7.75	127.77	119.78
1	ZS	48	GLY	CA-C-N	7.75	127.76	119.78
1	ZS	48	GLY	C-N-CA	7.75	127.76	119.78
1	DA	48	GLY	CA-C-N	7.75	127.76	119.78
1	DA	48	GLY	C-N-CA	7.75	127.76	119.78
1	Dq	48	GLY	CA-C-N	7.75	127.76	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Dq	48	GLY	C-N-CA	7.75	127.76	119.78
1	YQ	48	GLY	CA-C-N	7.75	127.76	119.78
1	YQ	48	GLY	C-N-CA	7.75	127.76	119.78
1	EW	48	GLY	CA-C-N	7.75	127.76	119.78
1	EW	48	GLY	C-N-CA	7.75	127.76	119.78
1	Eo	48	GLY	CA-C-N	7.75	127.76	119.78
1	Eo	48	GLY	C-N-CA	7.75	127.76	119.78
1	ZA	48	GLY	CA-C-N	7.74	127.73	119.76
1	ZA	48	GLY	C-N-CA	7.74	127.73	119.76
1	BY	48	GLY	CA-C-N	7.74	127.73	119.76
1	BY	48	GLY	C-N-CA	7.74	127.73	119.76
1	YE	48	GLY	CA-C-N	7.74	127.73	119.76
1	YE	48	GLY	C-N-CA	7.74	127.73	119.76
1	EG	48	GLY	CA-C-N	7.74	127.73	119.76
1	EG	48	GLY	C-N-CA	7.74	127.73	119.76
1	EM	48	GLY	CA-C-N	7.74	127.73	119.76
1	EM	48	GLY	C-N-CA	7.74	127.73	119.76
1	ES	48	GLY	CA-C-N	7.74	127.73	119.76
1	ES	48	GLY	C-N-CA	7.74	127.73	119.76
1	K	48	GLY	CA-C-N	7.73	127.73	119.76
1	K	48	GLY	C-N-CA	7.73	127.73	119.76
1	AO	48	GLY	CA-C-N	7.73	127.73	119.76
1	AO	48	GLY	C-N-CA	7.73	127.73	119.76
1	Am	48	GLY	CA-C-N	7.73	127.73	119.76
1	Am	48	GLY	C-N-CA	7.73	127.73	119.76
1	BG	48	GLY	CA-C-N	7.73	127.73	119.76
1	BG	48	GLY	C-N-CA	7.73	127.73	119.76
1	Bk	48	GLY	CA-C-N	7.73	127.73	119.76
1	Bk	48	GLY	C-N-CA	7.73	127.73	119.76
1	ZW	48	GLY	CA-C-N	7.73	127.73	119.76
1	ZW	48	GLY	C-N-CA	7.73	127.73	119.76
1	CE	48	GLY	CA-C-N	7.73	127.73	119.76
1	CE	48	GLY	C-N-CA	7.73	127.73	119.76
1	DI	48	GLY	CA-C-N	7.73	127.73	119.76
1	DI	48	GLY	C-N-CA	7.73	127.73	119.76
1	Dg	48	GLY	CA-C-N	7.73	127.73	119.76
1	Dg	48	GLY	C-N-CA	7.73	127.73	119.76
1	EA	48	GLY	CA-C-N	7.73	127.73	119.76
1	EA	48	GLY	C-N-CA	7.73	127.73	119.76
1	Ee	48	GLY	CA-C-N	7.73	127.73	119.76
1	Ee	48	GLY	C-N-CA	7.73	127.73	119.76
1	Ew	48	GLY	CA-C-N	7.73	127.73	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ew	48	GLY	C-N-CA	7.73	127.73	119.76
1	a	48	GLY	CA-C-N	7.73	127.74	119.78
1	a	48	GLY	C-N-CA	7.73	127.74	119.78
1	g	48	GLY	CA-C-N	7.73	127.74	119.78
1	g	48	GLY	C-N-CA	7.73	127.74	119.78
1	m	48	GLY	CA-C-N	7.73	127.74	119.78
1	m	48	GLY	C-N-CA	7.73	127.74	119.78
1	Ae	48	GLY	CA-C-N	7.73	127.74	119.78
1	Ae	48	GLY	C-N-CA	7.73	127.74	119.78
1	Cg	48	GLY	CA-C-N	7.73	127.74	119.78
1	Cg	48	GLY	C-N-CA	7.73	127.74	119.78
1	DM	48	GLY	CA-C-N	7.73	127.74	119.78
1	DM	48	GLY	C-N-CA	7.73	127.74	119.78
1	BA	48	GLY	CA-C-N	7.72	127.71	119.76
1	BA	48	GLY	C-N-CA	7.72	127.71	119.76
1	DC	48	GLY	CA-C-N	7.72	127.71	119.76
1	DC	48	GLY	C-N-CA	7.72	127.71	119.76
1	Ds	48	GLY	CA-C-N	7.72	127.71	119.76
1	Ds	48	GLY	C-N-CA	7.72	127.71	119.76
1	YS	48	GLY	CA-C-N	7.72	127.71	119.76
1	YS	48	GLY	C-N-CA	7.72	127.71	119.76
1	EY	48	GLY	CA-C-N	7.72	127.71	119.76
1	EY	48	GLY	C-N-CA	7.72	127.71	119.76
1	Eq	48	GLY	CA-C-N	7.72	127.71	119.76
1	Eq	48	GLY	C-N-CA	7.72	127.71	119.76
1	E	48	GLY	CA-C-N	7.71	127.70	119.76
1	E	48	GLY	C-N-CA	7.71	127.70	119.76
1	Q	48	GLY	CA-C-N	7.71	127.70	119.76
1	Q	48	GLY	C-N-CA	7.71	127.70	119.76
1	AC	48	GLY	CA-C-N	7.71	127.70	119.76
1	AC	48	GLY	C-N-CA	7.71	127.70	119.76
1	As	48	GLY	CA-C-N	7.71	127.70	119.76
1	As	48	GLY	C-N-CA	7.71	127.70	119.76
1	ZO	48	GLY	CA-C-N	7.71	127.70	119.76
1	ZO	48	GLY	C-N-CA	7.71	127.70	119.76
1	Bq	48	GLY	CA-C-N	7.71	127.70	119.76
1	Bq	48	GLY	C-N-CA	7.71	127.70	119.76
1	YC	48	GLY	CA-C-N	7.71	127.70	119.76
1	YC	48	GLY	C-N-CA	7.71	127.70	119.76
1	CK	48	GLY	CA-C-N	7.71	127.70	119.76
1	CK	48	GLY	C-N-CA	7.71	127.70	119.76
1	YK	48	GLY	CA-C-N	7.71	127.70	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YK	48	GLY	C-N-CA	7.71	127.70	119.76
1	Dm	48	GLY	CA-C-N	7.71	127.70	119.76
1	Dm	48	GLY	C-N-CA	7.71	127.70	119.76
1	Dy	48	GLY	CA-C-N	7.71	127.70	119.76
1	Dy	48	GLY	C-N-CA	7.71	127.70	119.76
1	Ek	48	GLY	CA-C-N	7.71	127.70	119.76
1	Ek	48	GLY	C-N-CA	7.71	127.70	119.76
1	c	48	GLY	CA-C-N	7.70	127.69	119.76
1	c	48	GLY	C-N-CA	7.70	127.69	119.76
1	i	48	GLY	CA-C-N	7.70	127.69	119.76
1	i	48	GLY	C-N-CA	7.70	127.69	119.76
1	o	48	GLY	CA-C-N	7.70	127.69	119.76
1	o	48	GLY	C-N-CA	7.70	127.69	119.76
1	Aa	48	GLY	CA-C-N	7.70	127.69	119.76
1	Aa	48	GLY	C-N-CA	7.70	127.69	119.76
1	Cc	48	GLY	CA-C-N	7.70	127.69	119.76
1	Cc	48	GLY	C-N-CA	7.70	127.69	119.76
1	Da	48	GLY	CA-C-N	7.70	127.69	119.76
1	Da	48	GLY	C-N-CA	7.70	127.69	119.76
1	AU	48	GLY	CA-C-N	7.69	127.69	119.76
1	AU	48	GLY	C-N-CA	7.69	127.69	119.76
1	Ag	48	GLY	CA-C-N	7.69	127.69	119.76
1	Ag	48	GLY	C-N-CA	7.69	127.69	119.76
1	CW	48	GLY	CA-C-N	7.69	127.69	119.76
1	CW	48	GLY	C-N-CA	7.69	127.69	119.76
1	Ci	48	GLY	CA-C-N	7.69	127.69	119.76
1	Ci	48	GLY	C-N-CA	7.69	127.69	119.76
1	DO	48	GLY	CA-C-N	7.69	127.69	119.76
1	DO	48	GLY	C-N-CA	7.69	127.69	119.76
1	DU	48	GLY	CA-C-N	7.69	127.69	119.76
1	DU	48	GLY	C-N-CA	7.69	127.69	119.76
1	W	48	GLY	CA-C-N	7.68	127.67	119.76
1	W	48	GLY	C-N-CA	7.68	127.67	119.76
1	AI	48	GLY	CA-C-N	7.68	127.67	119.76
1	AI	48	GLY	C-N-CA	7.68	127.67	119.76
1	Ay	48	GLY	CA-C-N	7.68	127.67	119.76
1	Ay	48	GLY	C-N-CA	7.68	127.67	119.76
1	Be	48	GLY	CA-C-N	7.68	127.67	119.76
1	Be	48	GLY	C-N-CA	7.68	127.67	119.76
1	Bw	48	GLY	CA-C-N	7.68	127.67	119.76
1	Bw	48	GLY	C-N-CA	7.68	127.67	119.76
1	CQ	48	GLY	CA-C-N	7.68	127.67	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CQ	48	GLY	C-N-CA	7.68	127.67	119.76
1	u	48	GLY	CA-C-N	7.67	127.66	119.76
1	u	48	GLY	C-N-CA	7.67	127.66	119.76
1	ZG	48	GLY	CA-C-N	7.67	127.66	119.76
1	ZG	48	GLY	C-N-CA	7.67	127.66	119.76
1	BM	48	GLY	CA-C-N	7.67	127.66	119.76
1	BM	48	GLY	C-N-CA	7.67	127.66	119.76
1	BS	48	GLY	CA-C-N	7.67	127.66	119.76
1	BS	48	GLY	C-N-CA	7.67	127.66	119.76
1	Co	48	GLY	CA-C-N	7.67	127.66	119.76
1	Co	48	GLY	C-N-CA	7.67	127.66	119.76
1	Cu	48	GLY	CA-C-N	7.67	127.66	119.76
1	Cu	48	GLY	C-N-CA	7.67	127.66	119.76
1	Ai	29	ALA	CA-C-N	7.18	126.89	119.56
1	Ai	29	ALA	C-N-CA	7.18	126.89	119.56
1	BC	29	ALA	CA-C-N	7.18	126.89	119.56
1	BC	29	ALA	C-N-CA	7.18	126.89	119.56
1	Bg	29	ALA	CA-C-N	7.18	126.89	119.56
1	Bg	29	ALA	C-N-CA	7.18	126.89	119.56
1	CA	29	ALA	CA-C-N	7.18	126.89	119.56
1	CA	29	ALA	C-N-CA	7.18	126.89	119.56
1	DE	29	ALA	CA-C-N	7.18	126.89	119.56
1	DE	29	ALA	C-N-CA	7.18	126.89	119.56
1	Ea	29	ALA	CA-C-N	7.18	126.89	119.56
1	Ea	29	ALA	C-N-CA	7.18	126.89	119.56
1	G	29	ALA	CA-C-N	7.16	126.86	119.56
1	G	29	ALA	C-N-CA	7.16	126.86	119.56
1	AK	29	ALA	CA-C-N	7.16	126.86	119.56
1	AK	29	ALA	C-N-CA	7.16	126.86	119.56
1	By	29	ALA	CA-C-N	7.16	126.86	119.56
1	By	29	ALA	C-N-CA	7.16	126.86	119.56
1	Dc	29	ALA	CA-C-N	7.16	126.86	119.56
1	Dc	29	ALA	C-N-CA	7.16	126.86	119.56
1	YU	29	ALA	CA-C-N	7.16	126.86	119.56
1	YU	29	ALA	C-N-CA	7.16	126.86	119.56
1	Es	29	ALA	CA-C-N	7.16	126.86	119.56
1	Es	29	ALA	C-N-CA	7.16	126.86	119.56
1	A	29	ALA	CA-C-N	7.16	126.86	119.56
1	A	29	ALA	C-N-CA	7.16	126.86	119.56
1	M	29	ALA	CA-C-N	7.16	126.86	119.56
1	M	29	ALA	C-N-CA	7.16	126.86	119.56
1	ZI	29	ALA	CA-C-N	7.16	126.86	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZI	29	ALA	C-N-CA	7.16	126.86	119.56
1	Ao	29	ALA	CA-C-N	7.16	126.86	119.56
1	Ao	29	ALA	C-N-CA	7.16	126.86	119.56
1	ZK	29	ALA	CA-C-N	7.16	126.86	119.56
1	ZK	29	ALA	C-N-CA	7.16	126.86	119.56
1	Bm	29	ALA	CA-C-N	7.16	126.86	119.56
1	Bm	29	ALA	C-N-CA	7.16	126.86	119.56
1	ZY	29	ALA	CA-C-N	7.16	126.86	119.56
1	ZY	29	ALA	C-N-CA	7.16	126.86	119.56
1	CG	29	ALA	CA-C-N	7.16	126.86	119.56
1	CG	29	ALA	C-N-CA	7.16	126.86	119.56
1	YG	29	ALA	CA-C-N	7.16	126.86	119.56
1	YG	29	ALA	C-N-CA	7.16	126.86	119.56
1	Di	29	ALA	CA-C-N	7.16	126.86	119.56
1	Di	29	ALA	C-N-CA	7.16	126.86	119.56
1	Du	29	ALA	CA-C-N	7.16	126.86	119.56
1	Du	29	ALA	C-N-CA	7.16	126.86	119.56
1	Eg	29	ALA	CA-C-N	7.16	126.86	119.56
1	Eg	29	ALA	C-N-CA	7.16	126.86	119.56
1	S	29	ALA	CA-C-N	7.15	126.85	119.56
1	S	29	ALA	C-N-CA	7.15	126.85	119.56
1	AE	29	ALA	CA-C-N	7.15	126.85	119.56
1	AE	29	ALA	C-N-CA	7.15	126.85	119.56
1	Au	29	ALA	CA-C-N	7.15	126.85	119.56
1	Au	29	ALA	C-N-CA	7.15	126.85	119.56
1	ZQ	29	ALA	CA-C-N	7.15	126.85	119.56
1	ZQ	29	ALA	C-N-CA	7.15	126.85	119.56
1	Ba	29	ALA	CA-C-N	7.15	126.85	119.56
1	Ba	29	ALA	C-N-CA	7.15	126.85	119.56
1	Bs	29	ALA	CA-C-N	7.15	126.85	119.56
1	Bs	29	ALA	C-N-CA	7.15	126.85	119.56
1	CM	29	ALA	CA-C-N	7.15	126.85	119.56
1	CM	29	ALA	C-N-CA	7.15	126.85	119.56
1	YM	29	ALA	CA-C-N	7.15	126.85	119.56
1	YM	29	ALA	C-N-CA	7.15	126.85	119.56
1	Do	29	ALA	CA-C-N	7.15	126.85	119.56
1	Do	29	ALA	C-N-CA	7.15	126.85	119.56
1	YO	29	ALA	CA-C-N	7.15	126.85	119.56
1	YO	29	ALA	C-N-CA	7.15	126.85	119.56
1	EU	29	ALA	CA-C-N	7.15	126.85	119.56
1	EU	29	ALA	C-N-CA	7.15	126.85	119.56
1	Em	29	ALA	CA-C-N	7.15	126.85	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Em	29	ALA	C-N-CA	7.15	126.85	119.56
1	Y	29	ALA	CA-C-N	7.12	126.83	119.56
1	Y	29	ALA	C-N-CA	7.12	126.83	119.56
1	e	29	ALA	CA-C-N	7.12	126.83	119.56
1	e	29	ALA	C-N-CA	7.12	126.83	119.56
1	k	29	ALA	CA-C-N	7.12	126.83	119.56
1	k	29	ALA	C-N-CA	7.12	126.83	119.56
1	AQ	29	ALA	CA-C-N	7.12	126.83	119.56
1	AQ	29	ALA	C-N-CA	7.12	126.83	119.56
1	AW	29	ALA	CA-C-N	7.12	126.83	119.56
1	AW	29	ALA	C-N-CA	7.12	126.83	119.56
1	Ac	29	ALA	CA-C-N	7.12	126.83	119.56
1	Ac	29	ALA	C-N-CA	7.12	126.83	119.56
1	CS	29	ALA	CA-C-N	7.12	126.83	119.56
1	CS	29	ALA	C-N-CA	7.12	126.83	119.56
1	CY	29	ALA	CA-C-N	7.12	126.83	119.56
1	CY	29	ALA	C-N-CA	7.12	126.83	119.56
1	Ce	29	ALA	CA-C-N	7.12	126.83	119.56
1	Ce	29	ALA	C-N-CA	7.12	126.83	119.56
1	DK	29	ALA	CA-C-N	7.12	126.83	119.56
1	DK	29	ALA	C-N-CA	7.12	126.83	119.56
1	DQ	29	ALA	CA-C-N	7.12	126.83	119.56
1	DQ	29	ALA	C-N-CA	7.12	126.83	119.56
1	DW	29	ALA	CA-C-N	7.12	126.83	119.56
1	DW	29	ALA	C-N-CA	7.12	126.83	119.56
1	q	29	ALA	CA-C-N	7.09	126.80	119.56
1	q	29	ALA	C-N-CA	7.09	126.80	119.56
1	w	29	ALA	CA-C-N	7.09	126.80	119.56
1	w	29	ALA	C-N-CA	7.09	126.80	119.56
1	ZC	29	ALA	CA-C-N	7.09	126.80	119.56
1	ZC	29	ALA	C-N-CA	7.09	126.80	119.56
1	BI	29	ALA	CA-C-N	7.09	126.80	119.56
1	BI	29	ALA	C-N-CA	7.09	126.80	119.56
1	BO	29	ALA	CA-C-N	7.09	126.80	119.56
1	BO	29	ALA	C-N-CA	7.09	126.80	119.56
1	BU	29	ALA	CA-C-N	7.09	126.80	119.56
1	BU	29	ALA	C-N-CA	7.09	126.80	119.56
1	Ck	29	ALA	CA-C-N	7.09	126.80	119.56
1	Ck	29	ALA	C-N-CA	7.09	126.80	119.56
1	Cq	29	ALA	CA-C-N	7.09	126.80	119.56
1	Cq	29	ALA	C-N-CA	7.09	126.80	119.56
1	Cw	29	ALA	CA-C-N	7.09	126.80	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cw	29	ALA	C-N-CA	7.09	126.80	119.56
1	EC	29	ALA	CA-C-N	7.09	126.80	119.56
1	EC	29	ALA	C-N-CA	7.09	126.80	119.56
1	EI	29	ALA	CA-C-N	7.09	126.80	119.56
1	EI	29	ALA	C-N-CA	7.09	126.80	119.56
1	EO	29	ALA	CA-C-N	7.09	126.80	119.56
1	EO	29	ALA	C-N-CA	7.09	126.80	119.56
1	W	29	ALA	CA-C-N	6.83	126.53	119.56
1	W	29	ALA	C-N-CA	6.83	126.53	119.56
1	u	29	ALA	CA-C-N	6.83	126.53	119.56
1	u	29	ALA	C-N-CA	6.83	126.53	119.56
1	ZA	29	ALA	CA-C-N	6.83	126.53	119.56
1	ZA	29	ALA	C-N-CA	6.83	126.53	119.56
1	ZG	29	ALA	CA-C-N	6.83	126.53	119.56
1	ZG	29	ALA	C-N-CA	6.83	126.53	119.56
1	AI	29	ALA	CA-C-N	6.83	126.53	119.56
1	AI	29	ALA	C-N-CA	6.83	126.53	119.56
1	Ay	29	ALA	CA-C-N	6.83	126.53	119.56
1	Ay	29	ALA	C-N-CA	6.83	126.53	119.56
1	BA	29	ALA	CA-C-N	6.83	126.53	119.56
1	BA	29	ALA	C-N-CA	6.83	126.53	119.56
1	BM	29	ALA	CA-C-N	6.83	126.53	119.56
1	BM	29	ALA	C-N-CA	6.83	126.53	119.56
1	BS	29	ALA	CA-C-N	6.83	126.53	119.56
1	BS	29	ALA	C-N-CA	6.83	126.53	119.56
1	BY	29	ALA	CA-C-N	6.83	126.53	119.56
1	BY	29	ALA	C-N-CA	6.83	126.53	119.56
1	Be	29	ALA	CA-C-N	6.83	126.53	119.56
1	Be	29	ALA	C-N-CA	6.83	126.53	119.56
1	Bw	29	ALA	CA-C-N	6.83	126.53	119.56
1	Bw	29	ALA	C-N-CA	6.83	126.53	119.56
1	CQ	29	ALA	CA-C-N	6.83	126.53	119.56
1	CQ	29	ALA	C-N-CA	6.83	126.53	119.56
1	Co	29	ALA	CA-C-N	6.83	126.53	119.56
1	Co	29	ALA	C-N-CA	6.83	126.53	119.56
1	Cu	29	ALA	CA-C-N	6.83	126.53	119.56
1	Cu	29	ALA	C-N-CA	6.83	126.53	119.56
1	YE	29	ALA	CA-C-N	6.83	126.53	119.56
1	YE	29	ALA	C-N-CA	6.83	126.53	119.56
1	DC	29	ALA	CA-C-N	6.83	126.53	119.56
1	DC	29	ALA	C-N-CA	6.83	126.53	119.56
1	Ds	29	ALA	CA-C-N	6.83	126.53	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ds	29	ALA	C-N-CA	6.83	126.53	119.56
1	YS	29	ALA	CA-C-N	6.83	126.53	119.56
1	YS	29	ALA	C-N-CA	6.83	126.53	119.56
1	EG	29	ALA	CA-C-N	6.83	126.53	119.56
1	EG	29	ALA	C-N-CA	6.83	126.53	119.56
1	EM	29	ALA	CA-C-N	6.83	126.53	119.56
1	EM	29	ALA	C-N-CA	6.83	126.53	119.56
1	ES	29	ALA	CA-C-N	6.83	126.53	119.56
1	ES	29	ALA	C-N-CA	6.83	126.53	119.56
1	EY	29	ALA	CA-C-N	6.83	126.53	119.56
1	EY	29	ALA	C-N-CA	6.83	126.53	119.56
1	Eq	29	ALA	CA-C-N	6.83	126.53	119.56
1	Eq	29	ALA	C-N-CA	6.83	126.53	119.56
1	c	29	ALA	CA-C-N	6.83	126.52	119.56
1	c	29	ALA	C-N-CA	6.83	126.52	119.56
1	i	29	ALA	CA-C-N	6.83	126.52	119.56
1	i	29	ALA	C-N-CA	6.83	126.52	119.56
1	o	29	ALA	CA-C-N	6.83	126.52	119.56
1	o	29	ALA	C-N-CA	6.83	126.52	119.56
1	AU	29	ALA	CA-C-N	6.83	126.52	119.56
1	AU	29	ALA	C-N-CA	6.83	126.52	119.56
1	Aa	29	ALA	CA-C-N	6.83	126.52	119.56
1	Aa	29	ALA	C-N-CA	6.83	126.52	119.56
1	Ag	29	ALA	CA-C-N	6.83	126.52	119.56
1	Ag	29	ALA	C-N-CA	6.83	126.52	119.56
1	CW	29	ALA	CA-C-N	6.83	126.52	119.56
1	CW	29	ALA	C-N-CA	6.83	126.52	119.56
1	Cc	29	ALA	CA-C-N	6.83	126.52	119.56
1	Cc	29	ALA	C-N-CA	6.83	126.52	119.56
1	Ci	29	ALA	CA-C-N	6.83	126.52	119.56
1	Ci	29	ALA	C-N-CA	6.83	126.52	119.56
1	DO	29	ALA	CA-C-N	6.83	126.52	119.56
1	DO	29	ALA	C-N-CA	6.83	126.52	119.56
1	DU	29	ALA	CA-C-N	6.83	126.52	119.56
1	DU	29	ALA	C-N-CA	6.83	126.52	119.56
1	Da	29	ALA	CA-C-N	6.83	126.52	119.56
1	Da	29	ALA	C-N-CA	6.83	126.52	119.56
1	K	29	ALA	CA-C-N	6.82	126.52	119.56
1	K	29	ALA	C-N-CA	6.82	126.52	119.56
1	AO	29	ALA	CA-C-N	6.82	126.52	119.56
1	AO	29	ALA	C-N-CA	6.82	126.52	119.56
1	Am	29	ALA	CA-C-N	6.82	126.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Am	29	ALA	C-N-CA	6.82	126.52	119.56
1	BG	29	ALA	CA-C-N	6.82	126.52	119.56
1	BG	29	ALA	C-N-CA	6.82	126.52	119.56
1	Bk	29	ALA	CA-C-N	6.82	126.52	119.56
1	Bk	29	ALA	C-N-CA	6.82	126.52	119.56
1	ZW	29	ALA	CA-C-N	6.82	126.52	119.56
1	ZW	29	ALA	C-N-CA	6.82	126.52	119.56
1	CE	29	ALA	CA-C-N	6.82	126.52	119.56
1	CE	29	ALA	C-N-CA	6.82	126.52	119.56
1	DI	29	ALA	CA-C-N	6.82	126.52	119.56
1	DI	29	ALA	C-N-CA	6.82	126.52	119.56
1	Dg	29	ALA	CA-C-N	6.82	126.52	119.56
1	Dg	29	ALA	C-N-CA	6.82	126.52	119.56
1	EA	29	ALA	CA-C-N	6.82	126.52	119.56
1	EA	29	ALA	C-N-CA	6.82	126.52	119.56
1	Ee	29	ALA	CA-C-N	6.82	126.52	119.56
1	Ee	29	ALA	C-N-CA	6.82	126.52	119.56
1	Ew	29	ALA	CA-C-N	6.82	126.52	119.56
1	Ew	29	ALA	C-N-CA	6.82	126.52	119.56
1	E	29	ALA	CA-C-N	6.81	126.51	119.56
1	E	29	ALA	C-N-CA	6.81	126.51	119.56
1	Q	29	ALA	CA-C-N	6.81	126.51	119.56
1	Q	29	ALA	C-N-CA	6.81	126.51	119.56
1	AC	29	ALA	CA-C-N	6.81	126.51	119.56
1	AC	29	ALA	C-N-CA	6.81	126.51	119.56
1	As	29	ALA	CA-C-N	6.81	126.51	119.56
1	As	29	ALA	C-N-CA	6.81	126.51	119.56
1	ZO	29	ALA	CA-C-N	6.81	126.51	119.56
1	ZO	29	ALA	C-N-CA	6.81	126.51	119.56
1	Bq	29	ALA	CA-C-N	6.81	126.51	119.56
1	Bq	29	ALA	C-N-CA	6.81	126.51	119.56
1	YC	29	ALA	CA-C-N	6.81	126.51	119.56
1	YC	29	ALA	C-N-CA	6.81	126.51	119.56
1	CK	29	ALA	CA-C-N	6.81	126.51	119.56
1	CK	29	ALA	C-N-CA	6.81	126.51	119.56
1	YK	29	ALA	CA-C-N	6.81	126.51	119.56
1	YK	29	ALA	C-N-CA	6.81	126.51	119.56
1	Dm	29	ALA	CA-C-N	6.81	126.51	119.56
1	Dm	29	ALA	C-N-CA	6.81	126.51	119.56
1	Dy	29	ALA	CA-C-N	6.81	126.51	119.56
1	Dy	29	ALA	C-N-CA	6.81	126.51	119.56
1	Ek	29	ALA	CA-C-N	6.81	126.51	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ek	29	ALA	C-N-CA	6.81	126.51	119.56
1	s	9	GLY	CA-C-N	6.74	126.77	119.90
1	s	9	GLY	C-N-CA	6.74	126.77	119.90
1	y	9	GLY	CA-C-N	6.74	126.77	119.90
1	y	9	GLY	C-N-CA	6.74	126.77	119.90
1	BQ	9	GLY	CA-C-N	6.74	126.77	119.90
1	BQ	9	GLY	C-N-CA	6.74	126.77	119.90
1	BW	9	GLY	CA-C-N	6.74	126.77	119.90
1	BW	9	GLY	C-N-CA	6.74	126.77	119.90
1	Cs	9	GLY	CA-C-N	6.74	126.77	119.90
1	Cs	9	GLY	C-N-CA	6.74	126.77	119.90
1	Cy	9	GLY	CA-C-N	6.74	126.77	119.90
1	Cy	9	GLY	C-N-CA	6.74	126.77	119.90
1	ZE	9	GLY	CA-C-N	6.72	126.75	119.90
1	ZE	9	GLY	C-N-CA	6.72	126.75	119.90
1	BK	9	GLY	CA-C-N	6.72	126.75	119.90
1	BK	9	GLY	C-N-CA	6.72	126.75	119.90
1	Cm	9	GLY	CA-C-N	6.72	126.75	119.90
1	Cm	9	GLY	C-N-CA	6.72	126.75	119.90
1	EE	9	GLY	CA-C-N	6.72	126.75	119.90
1	EE	9	GLY	C-N-CA	6.72	126.75	119.90
1	EK	9	GLY	CA-C-N	6.72	126.75	119.90
1	EK	9	GLY	C-N-CA	6.72	126.75	119.90
1	EQ	9	GLY	CA-C-N	6.72	126.75	119.90
1	EQ	9	GLY	C-N-CA	6.72	126.75	119.90
1	U	9	GLY	CA-C-N	6.70	126.74	119.90
1	U	9	GLY	C-N-CA	6.70	126.74	119.90
1	AG	9	GLY	CA-C-N	6.70	126.74	119.90
1	AG	9	GLY	C-N-CA	6.70	126.74	119.90
1	Aw	9	GLY	CA-C-N	6.70	126.74	119.90
1	Aw	9	GLY	C-N-CA	6.70	126.74	119.90
1	ZS	9	GLY	CA-C-N	6.70	126.74	119.90
1	ZS	9	GLY	C-N-CA	6.70	126.74	119.90
1	Bc	9	GLY	CA-C-N	6.70	126.74	119.90
1	Bc	9	GLY	C-N-CA	6.70	126.74	119.90
1	Bu	9	GLY	CA-C-N	6.70	126.74	119.90
1	Bu	9	GLY	C-N-CA	6.70	126.74	119.90
1	CO	9	GLY	CA-C-N	6.70	126.74	119.90
1	CO	9	GLY	C-N-CA	6.70	126.74	119.90
1	DA	9	GLY	CA-C-N	6.70	126.74	119.90
1	DA	9	GLY	C-N-CA	6.70	126.74	119.90
1	Dq	9	GLY	CA-C-N	6.70	126.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Dq	9	GLY	C-N-CA	6.70	126.74	119.90
1	YQ	9	GLY	CA-C-N	6.70	126.74	119.90
1	YQ	9	GLY	C-N-CA	6.70	126.74	119.90
1	EW	9	GLY	CA-C-N	6.70	126.74	119.90
1	EW	9	GLY	C-N-CA	6.70	126.74	119.90
1	Eo	9	GLY	CA-C-N	6.70	126.74	119.90
1	Eo	9	GLY	C-N-CA	6.70	126.74	119.90
1	C	9	GLY	CA-C-N	6.70	126.73	119.90
1	C	9	GLY	C-N-CA	6.70	126.73	119.90
1	O	9	GLY	CA-C-N	6.70	126.73	119.90
1	O	9	GLY	C-N-CA	6.70	126.73	119.90
1	AA	9	GLY	CA-C-N	6.70	126.73	119.90
1	AA	9	GLY	C-N-CA	6.70	126.73	119.90
1	Aq	9	GLY	CA-C-N	6.70	126.73	119.90
1	Aq	9	GLY	C-N-CA	6.70	126.73	119.90
1	ZM	9	GLY	CA-C-N	6.70	126.73	119.90
1	ZM	9	GLY	C-N-CA	6.70	126.73	119.90
1	Bo	9	GLY	CA-C-N	6.70	126.73	119.90
1	Bo	9	GLY	C-N-CA	6.70	126.73	119.90
1	YA	9	GLY	CA-C-N	6.70	126.73	119.90
1	YA	9	GLY	C-N-CA	6.70	126.73	119.90
1	CI	9	GLY	CA-C-N	6.70	126.73	119.90
1	CI	9	GLY	C-N-CA	6.70	126.73	119.90
1	YI	9	GLY	CA-C-N	6.70	126.73	119.90
1	YI	9	GLY	C-N-CA	6.70	126.73	119.90
1	Dk	9	GLY	CA-C-N	6.70	126.73	119.90
1	Dk	9	GLY	C-N-CA	6.70	126.73	119.90
1	Dw	9	GLY	CA-C-N	6.70	126.73	119.90
1	Dw	9	GLY	C-N-CA	6.70	126.73	119.90
1	Ei	9	GLY	CA-C-N	6.70	126.73	119.90
1	Ei	9	GLY	C-N-CA	6.70	126.73	119.90
1	a	9	GLY	CA-C-N	6.68	126.71	119.90
1	a	9	GLY	C-N-CA	6.68	126.71	119.90
1	g	9	GLY	CA-C-N	6.68	126.71	119.90
1	g	9	GLY	C-N-CA	6.68	126.71	119.90
1	m	9	GLY	CA-C-N	6.68	126.71	119.90
1	m	9	GLY	C-N-CA	6.68	126.71	119.90
1	AS	9	GLY	CA-C-N	6.68	126.71	119.90
1	AS	9	GLY	C-N-CA	6.68	126.71	119.90
1	AY	9	GLY	CA-C-N	6.68	126.71	119.90
1	AY	9	GLY	C-N-CA	6.68	126.71	119.90
1	Ae	9	GLY	CA-C-N	6.68	126.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ae	9	GLY	C-N-CA	6.68	126.71	119.90
1	CU	9	GLY	CA-C-N	6.68	126.71	119.90
1	CU	9	GLY	C-N-CA	6.68	126.71	119.90
1	Ca	9	GLY	CA-C-N	6.68	126.71	119.90
1	Ca	9	GLY	C-N-CA	6.68	126.71	119.90
1	Cg	9	GLY	CA-C-N	6.68	126.71	119.90
1	Cg	9	GLY	C-N-CA	6.68	126.71	119.90
1	DM	9	GLY	CA-C-N	6.68	126.71	119.90
1	DM	9	GLY	C-N-CA	6.68	126.71	119.90
1	DS	9	GLY	CA-C-N	6.68	126.71	119.90
1	DS	9	GLY	C-N-CA	6.68	126.71	119.90
1	DY	9	GLY	CA-C-N	6.68	126.71	119.90
1	DY	9	GLY	C-N-CA	6.68	126.71	119.90
1	I	9	GLY	CA-C-N	6.67	126.70	119.90
1	I	9	GLY	C-N-CA	6.67	126.70	119.90
1	AM	9	GLY	CA-C-N	6.67	126.70	119.90
1	AM	9	GLY	C-N-CA	6.67	126.70	119.90
1	Ak	9	GLY	CA-C-N	6.67	126.70	119.90
1	Ak	9	GLY	C-N-CA	6.67	126.70	119.90
1	BE	9	GLY	CA-C-N	6.67	126.70	119.90
1	BE	9	GLY	C-N-CA	6.67	126.70	119.90
1	Bi	9	GLY	CA-C-N	6.67	126.70	119.90
1	Bi	9	GLY	C-N-CA	6.67	126.70	119.90
1	ZU	9	GLY	CA-C-N	6.67	126.70	119.90
1	ZU	9	GLY	C-N-CA	6.67	126.70	119.90
1	CC	9	GLY	CA-C-N	6.67	126.70	119.90
1	CC	9	GLY	C-N-CA	6.67	126.70	119.90
1	DG	9	GLY	CA-C-N	6.67	126.70	119.90
1	DG	9	GLY	C-N-CA	6.67	126.70	119.90
1	De	9	GLY	CA-C-N	6.67	126.70	119.90
1	De	9	GLY	C-N-CA	6.67	126.70	119.90
1	YW	9	GLY	CA-C-N	6.67	126.70	119.90
1	YW	9	GLY	C-N-CA	6.67	126.70	119.90
1	Ec	9	GLY	CA-C-N	6.67	126.70	119.90
1	Ec	9	GLY	C-N-CA	6.67	126.70	119.90
1	Eu	9	GLY	CA-C-N	6.67	126.70	119.90
1	Eu	9	GLY	C-N-CA	6.67	126.70	119.90
1	I	29	ALA	CA-C-N	6.52	126.21	119.56
1	I	29	ALA	C-N-CA	6.52	126.21	119.56
1	AM	29	ALA	CA-C-N	6.52	126.21	119.56
1	AM	29	ALA	C-N-CA	6.52	126.21	119.56
1	Ak	29	ALA	CA-C-N	6.52	126.21	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ak	29	ALA	C-N-CA	6.52	126.21	119.56
1	BE	29	ALA	CA-C-N	6.52	126.21	119.56
1	BE	29	ALA	C-N-CA	6.52	126.21	119.56
1	Bi	29	ALA	CA-C-N	6.52	126.21	119.56
1	Bi	29	ALA	C-N-CA	6.52	126.21	119.56
1	ZU	29	ALA	CA-C-N	6.52	126.21	119.56
1	ZU	29	ALA	C-N-CA	6.52	126.21	119.56
1	CC	29	ALA	CA-C-N	6.52	126.21	119.56
1	CC	29	ALA	C-N-CA	6.52	126.21	119.56
1	DG	29	ALA	CA-C-N	6.52	126.21	119.56
1	DG	29	ALA	C-N-CA	6.52	126.21	119.56
1	De	29	ALA	CA-C-N	6.52	126.21	119.56
1	De	29	ALA	C-N-CA	6.52	126.21	119.56
1	YW	29	ALA	CA-C-N	6.52	126.21	119.56
1	YW	29	ALA	C-N-CA	6.52	126.21	119.56
1	Ec	29	ALA	CA-C-N	6.52	126.21	119.56
1	Ec	29	ALA	C-N-CA	6.52	126.21	119.56
1	Eu	29	ALA	CA-C-N	6.52	126.21	119.56
1	Eu	29	ALA	C-N-CA	6.52	126.21	119.56
1	s	29	ALA	CA-C-N	6.50	126.19	119.56
1	s	29	ALA	C-N-CA	6.50	126.19	119.56
1	y	29	ALA	CA-C-N	6.50	126.19	119.56
1	y	29	ALA	C-N-CA	6.50	126.19	119.56
1	ZE	29	ALA	CA-C-N	6.50	126.19	119.56
1	ZE	29	ALA	C-N-CA	6.50	126.19	119.56
1	BK	29	ALA	CA-C-N	6.50	126.19	119.56
1	BK	29	ALA	C-N-CA	6.50	126.19	119.56
1	BQ	29	ALA	CA-C-N	6.50	126.19	119.56
1	BQ	29	ALA	C-N-CA	6.50	126.19	119.56
1	BW	29	ALA	CA-C-N	6.50	126.19	119.56
1	BW	29	ALA	C-N-CA	6.50	126.19	119.56
1	Cm	29	ALA	CA-C-N	6.50	126.19	119.56
1	Cm	29	ALA	C-N-CA	6.50	126.19	119.56
1	Cs	29	ALA	CA-C-N	6.50	126.19	119.56
1	Cs	29	ALA	C-N-CA	6.50	126.19	119.56
1	Cy	29	ALA	CA-C-N	6.50	126.19	119.56
1	Cy	29	ALA	C-N-CA	6.50	126.19	119.56
1	EE	29	ALA	CA-C-N	6.50	126.19	119.56
1	EE	29	ALA	C-N-CA	6.50	126.19	119.56
1	EK	29	ALA	CA-C-N	6.50	126.19	119.56
1	EK	29	ALA	C-N-CA	6.50	126.19	119.56
1	EQ	29	ALA	CA-C-N	6.50	126.19	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EQ	29	ALA	C-N-CA	6.50	126.19	119.56
1	Aw	29	ALA	CA-C-N	6.50	126.19	119.56
1	Aw	29	ALA	C-N-CA	6.50	126.19	119.56
1	ZS	29	ALA	CA-C-N	6.50	126.19	119.56
1	ZS	29	ALA	C-N-CA	6.50	126.19	119.56
1	Bc	29	ALA	CA-C-N	6.50	126.19	119.56
1	Bc	29	ALA	C-N-CA	6.50	126.19	119.56
1	CO	29	ALA	CA-C-N	6.50	126.19	119.56
1	CO	29	ALA	C-N-CA	6.50	126.19	119.56
1	DA	29	ALA	CA-C-N	6.50	126.19	119.56
1	DA	29	ALA	C-N-CA	6.50	126.19	119.56
1	EW	29	ALA	CA-C-N	6.50	126.19	119.56
1	EW	29	ALA	C-N-CA	6.50	126.19	119.56
1	C	29	ALA	CA-C-N	6.49	126.18	119.56
1	C	29	ALA	C-N-CA	6.49	126.18	119.56
1	O	29	ALA	CA-C-N	6.49	126.18	119.56
1	O	29	ALA	C-N-CA	6.49	126.18	119.56
1	AA	29	ALA	CA-C-N	6.49	126.18	119.56
1	AA	29	ALA	C-N-CA	6.49	126.18	119.56
1	Aq	29	ALA	CA-C-N	6.49	126.18	119.56
1	Aq	29	ALA	C-N-CA	6.49	126.18	119.56
1	ZM	29	ALA	CA-C-N	6.49	126.18	119.56
1	ZM	29	ALA	C-N-CA	6.49	126.18	119.56
1	Bo	29	ALA	CA-C-N	6.49	126.18	119.56
1	Bo	29	ALA	C-N-CA	6.49	126.18	119.56
1	YA	29	ALA	CA-C-N	6.49	126.18	119.56
1	YA	29	ALA	C-N-CA	6.49	126.18	119.56
1	CI	29	ALA	CA-C-N	6.49	126.18	119.56
1	CI	29	ALA	C-N-CA	6.49	126.18	119.56
1	YI	29	ALA	CA-C-N	6.49	126.18	119.56
1	YI	29	ALA	C-N-CA	6.49	126.18	119.56
1	Dk	29	ALA	CA-C-N	6.49	126.18	119.56
1	Dk	29	ALA	C-N-CA	6.49	126.18	119.56
1	Dw	29	ALA	CA-C-N	6.49	126.18	119.56
1	Dw	29	ALA	C-N-CA	6.49	126.18	119.56
1	Ei	29	ALA	CA-C-N	6.49	126.18	119.56
1	Ei	29	ALA	C-N-CA	6.49	126.18	119.56
1	ZA	46	ARG	CA-C-N	6.47	126.60	119.87
1	ZA	46	ARG	C-N-CA	6.47	126.60	119.87
1	BY	46	ARG	CA-C-N	6.47	126.60	119.87
1	BY	46	ARG	C-N-CA	6.47	126.60	119.87
1	YE	46	ARG	CA-C-N	6.47	126.60	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YE	46	ARG	C-N-CA	6.47	126.60	119.87
1	a	29	ALA	CA-C-N	6.47	126.16	119.56
1	a	29	ALA	C-N-CA	6.47	126.16	119.56
1	g	29	ALA	CA-C-N	6.47	126.16	119.56
1	g	29	ALA	C-N-CA	6.47	126.16	119.56
1	m	29	ALA	CA-C-N	6.47	126.16	119.56
1	m	29	ALA	C-N-CA	6.47	126.16	119.56
1	AS	29	ALA	CA-C-N	6.47	126.16	119.56
1	AS	29	ALA	C-N-CA	6.47	126.16	119.56
1	AY	29	ALA	CA-C-N	6.47	126.16	119.56
1	AY	29	ALA	C-N-CA	6.47	126.16	119.56
1	Ae	29	ALA	CA-C-N	6.47	126.16	119.56
1	Ae	29	ALA	C-N-CA	6.47	126.16	119.56
1	CU	29	ALA	CA-C-N	6.47	126.16	119.56
1	CU	29	ALA	C-N-CA	6.47	126.16	119.56
1	Ca	29	ALA	CA-C-N	6.47	126.16	119.56
1	Ca	29	ALA	C-N-CA	6.47	126.16	119.56
1	Cg	29	ALA	CA-C-N	6.47	126.16	119.56
1	Cg	29	ALA	C-N-CA	6.47	126.16	119.56
1	DM	29	ALA	CA-C-N	6.47	126.16	119.56
1	DM	29	ALA	C-N-CA	6.47	126.16	119.56
1	DS	29	ALA	CA-C-N	6.47	126.16	119.56
1	DS	29	ALA	C-N-CA	6.47	126.16	119.56
1	DY	29	ALA	CA-C-N	6.47	126.16	119.56
1	DY	29	ALA	C-N-CA	6.47	126.16	119.56
1	c	46	ARG	CA-C-N	6.46	126.59	119.87
1	c	46	ARG	C-N-CA	6.46	126.59	119.87
1	i	46	ARG	CA-C-N	6.46	126.59	119.87
1	i	46	ARG	C-N-CA	6.46	126.59	119.87
1	o	46	ARG	CA-C-N	6.46	126.59	119.87
1	o	46	ARG	C-N-CA	6.46	126.59	119.87
1	AU	46	ARG	CA-C-N	6.46	126.59	119.87
1	AU	46	ARG	C-N-CA	6.46	126.59	119.87
1	Aa	46	ARG	CA-C-N	6.46	126.59	119.87
1	Aa	46	ARG	C-N-CA	6.46	126.59	119.87
1	Ag	46	ARG	CA-C-N	6.46	126.59	119.87
1	Ag	46	ARG	C-N-CA	6.46	126.59	119.87
1	CW	46	ARG	CA-C-N	6.46	126.59	119.87
1	CW	46	ARG	C-N-CA	6.46	126.59	119.87
1	Cc	46	ARG	CA-C-N	6.46	126.59	119.87
1	Cc	46	ARG	C-N-CA	6.46	126.59	119.87
1	Ci	46	ARG	CA-C-N	6.46	126.59	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ci	46	ARG	C-N-CA	6.46	126.59	119.87
1	DO	46	ARG	CA-C-N	6.46	126.59	119.87
1	DO	46	ARG	C-N-CA	6.46	126.59	119.87
1	DU	46	ARG	CA-C-N	6.46	126.59	119.87
1	DU	46	ARG	C-N-CA	6.46	126.59	119.87
1	Da	46	ARG	CA-C-N	6.46	126.59	119.87
1	Da	46	ARG	C-N-CA	6.46	126.59	119.87
1	U	29	ALA	CA-C-N	6.46	126.15	119.56
1	U	29	ALA	C-N-CA	6.46	126.15	119.56
1	AG	29	ALA	CA-C-N	6.46	126.15	119.56
1	AG	29	ALA	C-N-CA	6.46	126.15	119.56
1	Bu	29	ALA	CA-C-N	6.46	126.15	119.56
1	Bu	29	ALA	C-N-CA	6.46	126.15	119.56
1	Dq	29	ALA	CA-C-N	6.46	126.15	119.56
1	Dq	29	ALA	C-N-CA	6.46	126.15	119.56
1	YQ	29	ALA	CA-C-N	6.46	126.15	119.56
1	YQ	29	ALA	C-N-CA	6.46	126.15	119.56
1	EG	46	ARG	CA-C-N	6.46	126.59	119.87
1	EG	46	ARG	C-N-CA	6.46	126.59	119.87
1	EM	46	ARG	CA-C-N	6.46	126.59	119.87
1	EM	46	ARG	C-N-CA	6.46	126.59	119.87
1	ES	46	ARG	CA-C-N	6.46	126.59	119.87
1	ES	46	ARG	C-N-CA	6.46	126.59	119.87
1	Eo	29	ALA	CA-C-N	6.46	126.15	119.56
1	Eo	29	ALA	C-N-CA	6.46	126.15	119.56
1	E	46	ARG	CA-C-N	6.46	126.59	119.87
1	E	46	ARG	C-N-CA	6.46	126.59	119.87
1	Q	46	ARG	CA-C-N	6.46	126.59	119.87
1	Q	46	ARG	C-N-CA	6.46	126.59	119.87
1	AC	46	ARG	CA-C-N	6.46	126.59	119.87
1	AC	46	ARG	C-N-CA	6.46	126.59	119.87
1	As	46	ARG	CA-C-N	6.46	126.59	119.87
1	As	46	ARG	C-N-CA	6.46	126.59	119.87
1	ZO	46	ARG	CA-C-N	6.46	126.59	119.87
1	ZO	46	ARG	C-N-CA	6.46	126.59	119.87
1	Bq	46	ARG	CA-C-N	6.46	126.59	119.87
1	Bq	46	ARG	C-N-CA	6.46	126.59	119.87
1	YC	46	ARG	CA-C-N	6.46	126.59	119.87
1	YC	46	ARG	C-N-CA	6.46	126.59	119.87
1	CK	46	ARG	CA-C-N	6.46	126.59	119.87
1	CK	46	ARG	C-N-CA	6.46	126.59	119.87
1	YK	46	ARG	CA-C-N	6.46	126.59	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YK	46	ARG	C-N-CA	6.46	126.59	119.87
1	Dm	46	ARG	CA-C-N	6.46	126.59	119.87
1	Dm	46	ARG	C-N-CA	6.46	126.59	119.87
1	Dy	46	ARG	CA-C-N	6.46	126.59	119.87
1	Dy	46	ARG	C-N-CA	6.46	126.59	119.87
1	Ek	46	ARG	CA-C-N	6.46	126.59	119.87
1	Ek	46	ARG	C-N-CA	6.46	126.59	119.87
1	ZG	46	ARG	CA-C-N	6.45	126.58	119.87
1	ZG	46	ARG	C-N-CA	6.45	126.58	119.87
1	BM	46	ARG	CA-C-N	6.45	126.58	119.87
1	BM	46	ARG	C-N-CA	6.45	126.58	119.87
1	Co	46	ARG	CA-C-N	6.45	126.58	119.87
1	Co	46	ARG	C-N-CA	6.45	126.58	119.87
1	u	46	ARG	CA-C-N	6.44	126.57	119.87
1	u	46	ARG	C-N-CA	6.44	126.57	119.87
1	BS	46	ARG	CA-C-N	6.44	126.57	119.87
1	BS	46	ARG	C-N-CA	6.44	126.57	119.87
1	Cu	46	ARG	CA-C-N	6.44	126.57	119.87
1	Cu	46	ARG	C-N-CA	6.44	126.57	119.87
1	Am	46	ARG	CA-C-N	6.42	126.55	119.87
1	Am	46	ARG	C-N-CA	6.42	126.55	119.87
1	Bk	46	ARG	CA-C-N	6.42	126.55	119.87
1	Bk	46	ARG	C-N-CA	6.42	126.55	119.87
1	CE	46	ARG	CA-C-N	6.42	126.55	119.87
1	CE	46	ARG	C-N-CA	6.42	126.55	119.87
1	Dg	46	ARG	CA-C-N	6.42	126.55	119.87
1	Dg	46	ARG	C-N-CA	6.42	126.55	119.87
1	EA	46	ARG	CA-C-N	6.42	126.55	119.87
1	EA	46	ARG	C-N-CA	6.42	126.55	119.87
1	Ew	46	ARG	CA-C-N	6.42	126.55	119.87
1	Ew	46	ARG	C-N-CA	6.42	126.55	119.87
1	W	46	ARG	CA-C-N	6.42	126.54	119.87
1	W	46	ARG	C-N-CA	6.42	126.54	119.87
1	AI	46	ARG	CA-C-N	6.42	126.54	119.87
1	AI	46	ARG	C-N-CA	6.42	126.54	119.87
1	Ay	46	ARG	CA-C-N	6.42	126.54	119.87
1	Ay	46	ARG	C-N-CA	6.42	126.54	119.87
1	Be	46	ARG	CA-C-N	6.42	126.54	119.87
1	Be	46	ARG	C-N-CA	6.42	126.54	119.87
1	Bw	46	ARG	CA-C-N	6.42	126.54	119.87
1	Bw	46	ARG	C-N-CA	6.42	126.54	119.87
1	CQ	46	ARG	CA-C-N	6.42	126.54	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CQ	46	ARG	C-N-CA	6.42	126.54	119.87
1	BA	46	ARG	CA-C-N	6.40	126.53	119.87
1	BA	46	ARG	C-N-CA	6.40	126.53	119.87
1	DC	46	ARG	CA-C-N	6.40	126.53	119.87
1	DC	46	ARG	C-N-CA	6.40	126.53	119.87
1	Ds	46	ARG	CA-C-N	6.40	126.53	119.87
1	Ds	46	ARG	C-N-CA	6.40	126.53	119.87
1	YS	46	ARG	CA-C-N	6.40	126.53	119.87
1	YS	46	ARG	C-N-CA	6.40	126.53	119.87
1	EY	46	ARG	CA-C-N	6.40	126.53	119.87
1	EY	46	ARG	C-N-CA	6.40	126.53	119.87
1	Eq	46	ARG	CA-C-N	6.40	126.53	119.87
1	Eq	46	ARG	C-N-CA	6.40	126.53	119.87
1	K	46	ARG	CA-C-N	6.40	126.53	119.87
1	K	46	ARG	C-N-CA	6.40	126.53	119.87
1	AO	46	ARG	CA-C-N	6.40	126.53	119.87
1	AO	46	ARG	C-N-CA	6.40	126.53	119.87
1	BG	46	ARG	CA-C-N	6.40	126.53	119.87
1	BG	46	ARG	C-N-CA	6.40	126.53	119.87
1	ZW	46	ARG	CA-C-N	6.40	126.53	119.87
1	ZW	46	ARG	C-N-CA	6.40	126.53	119.87
1	DI	46	ARG	CA-C-N	6.40	126.53	119.87
1	DI	46	ARG	C-N-CA	6.40	126.53	119.87
1	Ee	46	ARG	CA-C-N	6.40	126.53	119.87
1	Ee	46	ARG	C-N-CA	6.40	126.53	119.87
1	q	46	ARG	CA-C-N	6.15	127.11	120.83
1	q	46	ARG	C-N-CA	6.15	127.11	120.83
1	w	46	ARG	CA-C-N	6.15	127.11	120.83
1	w	46	ARG	C-N-CA	6.15	127.11	120.83
1	ZC	46	ARG	CA-C-N	6.15	127.11	120.83
1	ZC	46	ARG	C-N-CA	6.15	127.11	120.83
1	BI	46	ARG	CA-C-N	6.15	127.11	120.83
1	BI	46	ARG	C-N-CA	6.15	127.11	120.83
1	BO	46	ARG	CA-C-N	6.15	127.11	120.83
1	BO	46	ARG	C-N-CA	6.15	127.11	120.83
1	BU	46	ARG	CA-C-N	6.15	127.11	120.83
1	BU	46	ARG	C-N-CA	6.15	127.11	120.83
1	Ck	46	ARG	CA-C-N	6.15	127.11	120.83
1	Ck	46	ARG	C-N-CA	6.15	127.11	120.83
1	Cq	46	ARG	CA-C-N	6.15	127.11	120.83
1	Cq	46	ARG	C-N-CA	6.15	127.11	120.83
1	Cw	46	ARG	CA-C-N	6.15	127.11	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cw	46	ARG	C-N-CA	6.15	127.11	120.83
1	EC	46	ARG	CA-C-N	6.15	127.11	120.83
1	EC	46	ARG	C-N-CA	6.15	127.11	120.83
1	EI	46	ARG	CA-C-N	6.15	127.11	120.83
1	EI	46	ARG	C-N-CA	6.15	127.11	120.83
1	EO	46	ARG	CA-C-N	6.15	127.11	120.83
1	EO	46	ARG	C-N-CA	6.15	127.11	120.83
1	G	46	ARG	CA-C-N	6.14	127.10	120.83
1	G	46	ARG	C-N-CA	6.14	127.10	120.83
1	AK	46	ARG	CA-C-N	6.14	127.10	120.83
1	AK	46	ARG	C-N-CA	6.14	127.10	120.83
1	Ai	46	ARG	CA-C-N	6.14	127.10	120.83
1	Ai	46	ARG	C-N-CA	6.14	127.10	120.83
1	BC	46	ARG	CA-C-N	6.14	127.10	120.83
1	BC	46	ARG	C-N-CA	6.14	127.10	120.83
1	Bg	46	ARG	CA-C-N	6.14	127.10	120.83
1	Bg	46	ARG	C-N-CA	6.14	127.10	120.83
1	By	46	ARG	CA-C-N	6.14	127.10	120.83
1	By	46	ARG	C-N-CA	6.14	127.10	120.83
1	CA	46	ARG	CA-C-N	6.14	127.10	120.83
1	CA	46	ARG	C-N-CA	6.14	127.10	120.83
1	DE	46	ARG	CA-C-N	6.14	127.10	120.83
1	DE	46	ARG	C-N-CA	6.14	127.10	120.83
1	Dc	46	ARG	CA-C-N	6.14	127.10	120.83
1	Dc	46	ARG	C-N-CA	6.14	127.10	120.83
1	YU	46	ARG	CA-C-N	6.14	127.10	120.83
1	YU	46	ARG	C-N-CA	6.14	127.10	120.83
1	Ea	46	ARG	CA-C-N	6.14	127.10	120.83
1	Ea	46	ARG	C-N-CA	6.14	127.10	120.83
1	Es	46	ARG	CA-C-N	6.14	127.10	120.83
1	Es	46	ARG	C-N-CA	6.14	127.10	120.83
1	Y	46	ARG	CA-C-N	6.11	127.06	120.83
1	Y	46	ARG	C-N-CA	6.11	127.06	120.83
1	e	46	ARG	CA-C-N	6.11	127.06	120.83
1	e	46	ARG	C-N-CA	6.11	127.06	120.83
1	k	46	ARG	CA-C-N	6.11	127.06	120.83
1	k	46	ARG	C-N-CA	6.11	127.06	120.83
1	AQ	46	ARG	CA-C-N	6.11	127.06	120.83
1	AQ	46	ARG	C-N-CA	6.11	127.06	120.83
1	AW	46	ARG	CA-C-N	6.11	127.06	120.83
1	AW	46	ARG	C-N-CA	6.11	127.06	120.83
1	Ac	46	ARG	CA-C-N	6.11	127.06	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ac	46	ARG	C-N-CA	6.11	127.06	120.83
1	CS	46	ARG	CA-C-N	6.11	127.06	120.83
1	CS	46	ARG	C-N-CA	6.11	127.06	120.83
1	CY	46	ARG	CA-C-N	6.11	127.06	120.83
1	CY	46	ARG	C-N-CA	6.11	127.06	120.83
1	Ce	46	ARG	CA-C-N	6.11	127.06	120.83
1	Ce	46	ARG	C-N-CA	6.11	127.06	120.83
1	DK	46	ARG	CA-C-N	6.11	127.06	120.83
1	DK	46	ARG	C-N-CA	6.11	127.06	120.83
1	DQ	46	ARG	CA-C-N	6.11	127.06	120.83
1	DQ	46	ARG	C-N-CA	6.11	127.06	120.83
1	DW	46	ARG	CA-C-N	6.11	127.06	120.83
1	DW	46	ARG	C-N-CA	6.11	127.06	120.83
1	A	46	ARG	CA-C-N	6.10	127.05	120.83
1	A	46	ARG	C-N-CA	6.10	127.05	120.83
1	M	46	ARG	CA-C-N	6.10	127.05	120.83
1	M	46	ARG	C-N-CA	6.10	127.05	120.83
1	ZI	46	ARG	CA-C-N	6.10	127.05	120.83
1	ZI	46	ARG	C-N-CA	6.10	127.05	120.83
1	Ao	46	ARG	CA-C-N	6.10	127.05	120.83
1	Ao	46	ARG	C-N-CA	6.10	127.05	120.83
1	ZK	46	ARG	CA-C-N	6.10	127.05	120.83
1	ZK	46	ARG	C-N-CA	6.10	127.05	120.83
1	Bm	46	ARG	CA-C-N	6.10	127.05	120.83
1	Bm	46	ARG	C-N-CA	6.10	127.05	120.83
1	ZY	46	ARG	CA-C-N	6.10	127.05	120.83
1	ZY	46	ARG	C-N-CA	6.10	127.05	120.83
1	CG	46	ARG	CA-C-N	6.10	127.05	120.83
1	CG	46	ARG	C-N-CA	6.10	127.05	120.83
1	YG	46	ARG	CA-C-N	6.10	127.05	120.83
1	YG	46	ARG	C-N-CA	6.10	127.05	120.83
1	Di	46	ARG	CA-C-N	6.10	127.05	120.83
1	Di	46	ARG	C-N-CA	6.10	127.05	120.83
1	Du	46	ARG	CA-C-N	6.10	127.05	120.83
1	Du	46	ARG	C-N-CA	6.10	127.05	120.83
1	Eg	46	ARG	CA-C-N	6.10	127.05	120.83
1	Eg	46	ARG	C-N-CA	6.10	127.05	120.83
1	S	46	ARG	CA-C-N	6.08	127.03	120.83
1	S	46	ARG	C-N-CA	6.08	127.03	120.83
1	AE	46	ARG	CA-C-N	6.08	127.03	120.83
1	AE	46	ARG	C-N-CA	6.08	127.03	120.83
1	Au	46	ARG	CA-C-N	6.08	127.03	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Au	46	ARG	C-N-CA	6.08	127.03	120.83
1	ZQ	46	ARG	CA-C-N	6.08	127.03	120.83
1	ZQ	46	ARG	C-N-CA	6.08	127.03	120.83
1	Ba	46	ARG	CA-C-N	6.08	127.03	120.83
1	Ba	46	ARG	C-N-CA	6.08	127.03	120.83
1	Bs	46	ARG	CA-C-N	6.08	127.03	120.83
1	Bs	46	ARG	C-N-CA	6.08	127.03	120.83
1	CM	46	ARG	CA-C-N	6.08	127.03	120.83
1	CM	46	ARG	C-N-CA	6.08	127.03	120.83
1	YM	46	ARG	CA-C-N	6.08	127.03	120.83
1	YM	46	ARG	C-N-CA	6.08	127.03	120.83
1	Do	46	ARG	CA-C-N	6.08	127.03	120.83
1	Do	46	ARG	C-N-CA	6.08	127.03	120.83
1	YO	46	ARG	CA-C-N	6.08	127.03	120.83
1	YO	46	ARG	C-N-CA	6.08	127.03	120.83
1	EU	46	ARG	CA-C-N	6.08	127.03	120.83
1	EU	46	ARG	C-N-CA	6.08	127.03	120.83
1	Em	46	ARG	CA-C-N	6.08	127.03	120.83
1	Em	46	ARG	C-N-CA	6.08	127.03	120.83
1	K	35	VAL	N-CA-C	-5.92	104.55	111.00
1	c	35	VAL	N-CA-C	-5.92	104.55	111.00
1	i	35	VAL	N-CA-C	-5.92	104.55	111.00
1	o	35	VAL	N-CA-C	-5.92	104.55	111.00
1	ZG	35	VAL	N-CA-C	-5.92	104.55	111.00
1	AO	35	VAL	N-CA-C	-5.92	104.55	111.00
1	AU	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Aa	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Ag	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Am	35	VAL	N-CA-C	-5.92	104.55	111.00
1	BG	35	VAL	N-CA-C	-5.92	104.55	111.00
1	BM	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Bk	35	VAL	N-CA-C	-5.92	104.55	111.00
1	ZW	35	VAL	N-CA-C	-5.92	104.55	111.00
1	CE	35	VAL	N-CA-C	-5.92	104.55	111.00
1	CW	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Cc	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Ci	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Co	35	VAL	N-CA-C	-5.92	104.55	111.00
1	DI	35	VAL	N-CA-C	-5.92	104.55	111.00
1	DO	35	VAL	N-CA-C	-5.92	104.55	111.00
1	DU	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Da	35	VAL	N-CA-C	-5.92	104.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Dg	35	VAL	N-CA-C	-5.92	104.55	111.00
1	EA	35	VAL	N-CA-C	-5.92	104.55	111.00
1	EG	35	VAL	N-CA-C	-5.92	104.55	111.00
1	EM	35	VAL	N-CA-C	-5.92	104.55	111.00
1	ES	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Ee	35	VAL	N-CA-C	-5.92	104.55	111.00
1	Ew	35	VAL	N-CA-C	-5.92	104.55	111.00
1	W	35	VAL	N-CA-C	-5.91	104.56	111.00
1	AI	35	VAL	N-CA-C	-5.91	104.56	111.00
1	Ay	35	VAL	N-CA-C	-5.91	104.56	111.00
1	BA	35	VAL	N-CA-C	-5.91	104.56	111.00
1	Be	35	VAL	N-CA-C	-5.91	104.56	111.00
1	Bw	35	VAL	N-CA-C	-5.91	104.56	111.00
1	CQ	35	VAL	N-CA-C	-5.91	104.56	111.00
1	DC	35	VAL	N-CA-C	-5.91	104.56	111.00
1	Ds	35	VAL	N-CA-C	-5.91	104.56	111.00
1	YS	35	VAL	N-CA-C	-5.91	104.56	111.00
1	EY	35	VAL	N-CA-C	-5.91	104.56	111.00
1	Eq	35	VAL	N-CA-C	-5.91	104.56	111.00
2	H	91	ASN	CA-C-N	5.90	126.01	119.87
2	H	91	ASN	C-N-CA	5.90	126.01	119.87
2	AL	91	ASN	CA-C-N	5.90	126.01	119.87
2	AL	91	ASN	C-N-CA	5.90	126.01	119.87
2	Aj	91	ASN	CA-C-N	5.90	126.01	119.87
2	Aj	91	ASN	C-N-CA	5.90	126.01	119.87
2	BD	91	ASN	CA-C-N	5.90	126.01	119.87
2	BD	91	ASN	C-N-CA	5.90	126.01	119.87
2	Bh	91	ASN	CA-C-N	5.90	126.01	119.87
2	Bh	91	ASN	C-N-CA	5.90	126.01	119.87
2	Bz	91	ASN	CA-C-N	5.90	126.01	119.87
2	Bz	91	ASN	C-N-CA	5.90	126.01	119.87
2	CB	91	ASN	CA-C-N	5.90	126.01	119.87
2	CB	91	ASN	C-N-CA	5.90	126.01	119.87
2	DF	91	ASN	CA-C-N	5.90	126.01	119.87
2	DF	91	ASN	C-N-CA	5.90	126.01	119.87
2	Dd	91	ASN	CA-C-N	5.90	126.01	119.87
2	Dd	91	ASN	C-N-CA	5.90	126.01	119.87
2	YV	91	ASN	CA-C-N	5.90	126.01	119.87
2	YV	91	ASN	C-N-CA	5.90	126.01	119.87
2	Eb	91	ASN	CA-C-N	5.90	126.01	119.87
2	Eb	91	ASN	C-N-CA	5.90	126.01	119.87
2	Et	91	ASN	CA-C-N	5.90	126.01	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Et	91	ASN	C-N-CA	5.90	126.01	119.87
1	E	35	VAL	N-CA-C	-5.90	104.57	111.00
1	Q	35	VAL	N-CA-C	-5.90	104.57	111.00
2	x	91	ASN	CA-C-N	5.90	126.01	119.87
2	x	91	ASN	C-N-CA	5.90	126.01	119.87
2	ZD	91	ASN	CA-C-N	5.90	126.01	119.87
2	ZD	91	ASN	C-N-CA	5.90	126.01	119.87
1	AC	35	VAL	N-CA-C	-5.90	104.57	111.00
1	As	35	VAL	N-CA-C	-5.90	104.57	111.00
1	ZO	35	VAL	N-CA-C	-5.90	104.57	111.00
2	BJ	91	ASN	CA-C-N	5.90	126.01	119.87
2	BJ	91	ASN	C-N-CA	5.90	126.01	119.87
2	BV	91	ASN	CA-C-N	5.90	126.01	119.87
2	BV	91	ASN	C-N-CA	5.90	126.01	119.87
1	Bq	35	VAL	N-CA-C	-5.90	104.57	111.00
1	YC	35	VAL	N-CA-C	-5.90	104.57	111.00
1	CK	35	VAL	N-CA-C	-5.90	104.57	111.00
2	Cl	91	ASN	CA-C-N	5.90	126.01	119.87
2	Cl	91	ASN	C-N-CA	5.90	126.01	119.87
2	Cx	91	ASN	CA-C-N	5.90	126.01	119.87
2	Cx	91	ASN	C-N-CA	5.90	126.01	119.87
1	YK	35	VAL	N-CA-C	-5.90	104.57	111.00
1	Dm	35	VAL	N-CA-C	-5.90	104.57	111.00
1	Dy	35	VAL	N-CA-C	-5.90	104.57	111.00
1	Ek	35	VAL	N-CA-C	-5.90	104.57	111.00
2	r	91	ASN	CA-C-N	5.90	126.00	119.87
2	r	91	ASN	C-N-CA	5.90	126.00	119.87
2	BP	91	ASN	CA-C-N	5.90	126.00	119.87
2	BP	91	ASN	C-N-CA	5.90	126.00	119.87
2	Cr	91	ASN	CA-C-N	5.90	126.00	119.87
2	Cr	91	ASN	C-N-CA	5.90	126.00	119.87
2	ED	91	ASN	CA-C-N	5.90	126.00	119.87
2	ED	91	ASN	C-N-CA	5.90	126.00	119.87
2	EJ	91	ASN	CA-C-N	5.90	126.00	119.87
2	EJ	91	ASN	C-N-CA	5.90	126.00	119.87
2	EP	91	ASN	CA-C-N	5.90	126.00	119.87
2	EP	91	ASN	C-N-CA	5.90	126.00	119.87
1	u	35	VAL	N-CA-C	-5.89	104.58	111.00
1	ZA	35	VAL	N-CA-C	-5.89	104.58	111.00
1	BS	35	VAL	N-CA-C	-5.89	104.58	111.00
1	BY	35	VAL	N-CA-C	-5.89	104.58	111.00
1	Cu	35	VAL	N-CA-C	-5.89	104.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YE	35	VAL	N-CA-C	-5.89	104.58	111.00
2	Z	91	ASN	CA-C-N	5.88	125.99	119.87
2	Z	91	ASN	C-N-CA	5.88	125.99	119.87
2	f	91	ASN	CA-C-N	5.88	125.99	119.87
2	f	91	ASN	C-N-CA	5.88	125.99	119.87
2	l	91	ASN	CA-C-N	5.88	125.99	119.87
2	l	91	ASN	C-N-CA	5.88	125.99	119.87
2	AR	91	ASN	CA-C-N	5.88	125.99	119.87
2	AR	91	ASN	C-N-CA	5.88	125.99	119.87
2	AX	91	ASN	CA-C-N	5.88	125.99	119.87
2	AX	91	ASN	C-N-CA	5.88	125.99	119.87
2	Ad	91	ASN	CA-C-N	5.88	125.99	119.87
2	Ad	91	ASN	C-N-CA	5.88	125.99	119.87
2	CT	91	ASN	CA-C-N	5.88	125.99	119.87
2	CT	91	ASN	C-N-CA	5.88	125.99	119.87
2	CZ	91	ASN	CA-C-N	5.88	125.99	119.87
2	CZ	91	ASN	C-N-CA	5.88	125.99	119.87
2	Cf	91	ASN	CA-C-N	5.88	125.99	119.87
2	Cf	91	ASN	C-N-CA	5.88	125.99	119.87
2	DL	91	ASN	CA-C-N	5.88	125.99	119.87
2	DL	91	ASN	C-N-CA	5.88	125.99	119.87
2	DR	91	ASN	CA-C-N	5.88	125.99	119.87
2	DR	91	ASN	C-N-CA	5.88	125.99	119.87
2	DX	91	ASN	CA-C-N	5.88	125.99	119.87
2	DX	91	ASN	C-N-CA	5.88	125.99	119.87
2	B	91	ASN	CA-C-N	5.88	125.98	119.87
2	B	91	ASN	C-N-CA	5.88	125.98	119.87
2	N	91	ASN	CA-C-N	5.88	125.98	119.87
2	N	91	ASN	C-N-CA	5.88	125.98	119.87
2	ZJ	91	ASN	CA-C-N	5.88	125.98	119.87
2	ZJ	91	ASN	C-N-CA	5.88	125.98	119.87
2	Ap	91	ASN	CA-C-N	5.88	125.98	119.87
2	Ap	91	ASN	C-N-CA	5.88	125.98	119.87
2	ZL	91	ASN	CA-C-N	5.88	125.98	119.87
2	ZL	91	ASN	C-N-CA	5.88	125.98	119.87
2	Bn	91	ASN	CA-C-N	5.88	125.98	119.87
2	Bn	91	ASN	C-N-CA	5.88	125.98	119.87
2	ZZ	91	ASN	CA-C-N	5.88	125.98	119.87
2	ZZ	91	ASN	C-N-CA	5.88	125.98	119.87
2	CH	91	ASN	CA-C-N	5.88	125.98	119.87
2	CH	91	ASN	C-N-CA	5.88	125.98	119.87
2	YH	91	ASN	CA-C-N	5.88	125.98	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YH	91	ASN	C-N-CA	5.88	125.98	119.87
2	Dj	91	ASN	CA-C-N	5.88	125.98	119.87
2	Dj	91	ASN	C-N-CA	5.88	125.98	119.87
2	Dv	91	ASN	CA-C-N	5.88	125.98	119.87
2	Dv	91	ASN	C-N-CA	5.88	125.98	119.87
2	Eh	91	ASN	CA-C-N	5.88	125.98	119.87
2	Eh	91	ASN	C-N-CA	5.88	125.98	119.87
2	T	91	ASN	CA-C-N	5.86	125.97	119.87
2	T	91	ASN	C-N-CA	5.86	125.97	119.87
2	AF	91	ASN	CA-C-N	5.86	125.97	119.87
2	AF	91	ASN	C-N-CA	5.86	125.97	119.87
2	Av	91	ASN	CA-C-N	5.86	125.97	119.87
2	Av	91	ASN	C-N-CA	5.86	125.97	119.87
2	ZR	91	ASN	CA-C-N	5.86	125.97	119.87
2	ZR	91	ASN	C-N-CA	5.86	125.97	119.87
2	Bb	91	ASN	CA-C-N	5.86	125.97	119.87
2	Bb	91	ASN	C-N-CA	5.86	125.97	119.87
2	Bt	91	ASN	CA-C-N	5.86	125.97	119.87
2	Bt	91	ASN	C-N-CA	5.86	125.97	119.87
2	CN	91	ASN	CA-C-N	5.86	125.97	119.87
2	CN	91	ASN	C-N-CA	5.86	125.97	119.87
2	YN	91	ASN	CA-C-N	5.86	125.97	119.87
2	YN	91	ASN	C-N-CA	5.86	125.97	119.87
2	Dp	91	ASN	CA-C-N	5.86	125.97	119.87
2	Dp	91	ASN	C-N-CA	5.86	125.97	119.87
2	YP	91	ASN	CA-C-N	5.86	125.97	119.87
2	YP	91	ASN	C-N-CA	5.86	125.97	119.87
2	EV	91	ASN	CA-C-N	5.86	125.97	119.87
2	EV	91	ASN	C-N-CA	5.86	125.97	119.87
2	En	91	ASN	CA-C-N	5.86	125.97	119.87
2	En	91	ASN	C-N-CA	5.86	125.97	119.87
1	C	32	LEU	N-CA-C	-5.81	106.32	113.41
1	O	32	LEU	N-CA-C	-5.81	106.32	113.41
1	AA	32	LEU	N-CA-C	-5.81	106.32	113.41
1	Aq	32	LEU	N-CA-C	-5.81	106.32	113.41
1	ZM	32	LEU	N-CA-C	-5.81	106.32	113.41
1	Bo	32	LEU	N-CA-C	-5.81	106.32	113.41
1	YA	32	LEU	N-CA-C	-5.81	106.32	113.41
1	CI	32	LEU	N-CA-C	-5.81	106.32	113.41
1	YI	32	LEU	N-CA-C	-5.81	106.32	113.41
1	Dk	32	LEU	N-CA-C	-5.81	106.32	113.41
1	Dw	32	LEU	N-CA-C	-5.81	106.32	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ei	32	LEU	N-CA-C	-5.81	106.32	113.41
2	Z	141	ASP	CA-C-N	5.79	125.90	119.87
2	Z	141	ASP	C-N-CA	5.79	125.90	119.87
2	f	141	ASP	CA-C-N	5.79	125.90	119.87
2	f	141	ASP	C-N-CA	5.79	125.90	119.87
2	l	141	ASP	CA-C-N	5.79	125.90	119.87
2	l	141	ASP	C-N-CA	5.79	125.90	119.87
2	Ad	141	ASP	CA-C-N	5.79	125.90	119.87
2	Ad	141	ASP	C-N-CA	5.79	125.90	119.87
2	Cf	141	ASP	CA-C-N	5.79	125.90	119.87
2	Cf	141	ASP	C-N-CA	5.79	125.90	119.87
2	DL	141	ASP	CA-C-N	5.79	125.90	119.87
2	DL	141	ASP	C-N-CA	5.79	125.90	119.87
1	a	32	LEU	N-CA-C	-5.79	106.34	113.41
1	g	32	LEU	N-CA-C	-5.79	106.34	113.41
1	m	32	LEU	N-CA-C	-5.79	106.34	113.41
1	AS	32	LEU	N-CA-C	-5.79	106.34	113.41
1	AY	32	LEU	N-CA-C	-5.79	106.34	113.41
1	Ae	32	LEU	N-CA-C	-5.79	106.34	113.41
1	CU	32	LEU	N-CA-C	-5.79	106.34	113.41
1	Ca	32	LEU	N-CA-C	-5.79	106.34	113.41
1	Cg	32	LEU	N-CA-C	-5.79	106.34	113.41
1	DM	32	LEU	N-CA-C	-5.79	106.34	113.41
1	DS	32	LEU	N-CA-C	-5.79	106.34	113.41
1	DY	32	LEU	N-CA-C	-5.79	106.34	113.41
1	U	32	LEU	N-CA-C	-5.79	106.35	113.41
1	AG	32	LEU	N-CA-C	-5.79	106.35	113.41
1	Aw	32	LEU	N-CA-C	-5.79	106.35	113.41
1	ZS	32	LEU	N-CA-C	-5.79	106.35	113.41
1	Bc	32	LEU	N-CA-C	-5.79	106.35	113.41
1	Bu	32	LEU	N-CA-C	-5.79	106.35	113.41
1	CO	32	LEU	N-CA-C	-5.79	106.35	113.41
1	DA	32	LEU	N-CA-C	-5.79	106.35	113.41
1	Dq	32	LEU	N-CA-C	-5.79	106.35	113.41
1	YQ	32	LEU	N-CA-C	-5.79	106.35	113.41
1	EW	32	LEU	N-CA-C	-5.79	106.35	113.41
1	Eo	32	LEU	N-CA-C	-5.79	106.35	113.41
1	I	32	LEU	N-CA-C	-5.79	106.35	113.41
1	AM	32	LEU	N-CA-C	-5.79	106.35	113.41
1	Ak	32	LEU	N-CA-C	-5.79	106.35	113.41
2	ZR	141	ASP	CA-C-N	5.79	125.89	119.87
2	ZR	141	ASP	C-N-CA	5.79	125.89	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BE	32	LEU	N-CA-C	-5.79	106.35	113.41
1	Bi	32	LEU	N-CA-C	-5.79	106.35	113.41
1	ZU	32	LEU	N-CA-C	-5.79	106.35	113.41
1	CC	32	LEU	N-CA-C	-5.79	106.35	113.41
2	YN	141	ASP	CA-C-N	5.79	125.89	119.87
2	YN	141	ASP	C-N-CA	5.79	125.89	119.87
1	DG	32	LEU	N-CA-C	-5.79	106.35	113.41
1	De	32	LEU	N-CA-C	-5.79	106.35	113.41
2	Dp	141	ASP	CA-C-N	5.79	125.89	119.87
2	Dp	141	ASP	C-N-CA	5.79	125.89	119.87
2	YP	141	ASP	CA-C-N	5.79	125.89	119.87
2	YP	141	ASP	C-N-CA	5.79	125.89	119.87
1	YW	32	LEU	N-CA-C	-5.79	106.35	113.41
2	EV	141	ASP	CA-C-N	5.79	125.89	119.87
2	EV	141	ASP	C-N-CA	5.79	125.89	119.87
1	Ec	32	LEU	N-CA-C	-5.79	106.35	113.41
2	En	141	ASP	CA-C-N	5.79	125.89	119.87
2	En	141	ASP	C-N-CA	5.79	125.89	119.87
1	Eu	32	LEU	N-CA-C	-5.79	106.35	113.41
1	s	32	LEU	N-CA-C	-5.78	106.36	113.41
1	y	32	LEU	N-CA-C	-5.78	106.36	113.41
1	ZE	32	LEU	N-CA-C	-5.78	106.36	113.41
1	BK	32	LEU	N-CA-C	-5.78	106.36	113.41
1	BQ	32	LEU	N-CA-C	-5.78	106.36	113.41
1	BW	32	LEU	N-CA-C	-5.78	106.36	113.41
1	Cm	32	LEU	N-CA-C	-5.78	106.36	113.41
1	Cs	32	LEU	N-CA-C	-5.78	106.36	113.41
1	Cy	32	LEU	N-CA-C	-5.78	106.36	113.41
1	EE	32	LEU	N-CA-C	-5.78	106.36	113.41
1	EK	32	LEU	N-CA-C	-5.78	106.36	113.41
1	EQ	32	LEU	N-CA-C	-5.78	106.36	113.41
2	B	141	ASP	CA-C-N	5.77	125.87	119.87
2	B	141	ASP	C-N-CA	5.77	125.87	119.87
2	N	141	ASP	CA-C-N	5.77	125.87	119.87
2	N	141	ASP	C-N-CA	5.77	125.87	119.87
2	ZJ	141	ASP	CA-C-N	5.77	125.87	119.87
2	ZJ	141	ASP	C-N-CA	5.77	125.87	119.87
2	Ap	141	ASP	CA-C-N	5.77	125.87	119.87
2	Ap	141	ASP	C-N-CA	5.77	125.87	119.87
2	ZL	141	ASP	CA-C-N	5.77	125.87	119.87
2	ZL	141	ASP	C-N-CA	5.77	125.87	119.87
2	Bn	141	ASP	CA-C-N	5.77	125.87	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Bn	141	ASP	C-N-CA	5.77	125.87	119.87
2	ZZ	141	ASP	CA-C-N	5.77	125.87	119.87
2	ZZ	141	ASP	C-N-CA	5.77	125.87	119.87
2	CH	141	ASP	CA-C-N	5.77	125.87	119.87
2	CH	141	ASP	C-N-CA	5.77	125.87	119.87
2	YH	141	ASP	CA-C-N	5.77	125.87	119.87
2	YH	141	ASP	C-N-CA	5.77	125.87	119.87
2	Dj	141	ASP	CA-C-N	5.77	125.87	119.87
2	Dj	141	ASP	C-N-CA	5.77	125.87	119.87
2	Dv	141	ASP	CA-C-N	5.77	125.87	119.87
2	Dv	141	ASP	C-N-CA	5.77	125.87	119.87
2	Eh	141	ASP	CA-C-N	5.77	125.87	119.87
2	Eh	141	ASP	C-N-CA	5.77	125.87	119.87
2	H	141	ASP	CA-C-N	5.76	125.86	119.87
2	H	141	ASP	C-N-CA	5.76	125.86	119.87
2	AL	141	ASP	CA-C-N	5.76	125.86	119.87
2	AL	141	ASP	C-N-CA	5.76	125.86	119.87
2	Aj	141	ASP	CA-C-N	5.76	125.86	119.87
2	Aj	141	ASP	C-N-CA	5.76	125.86	119.87
2	Bh	141	ASP	CA-C-N	5.76	125.86	119.87
2	Bh	141	ASP	C-N-CA	5.76	125.86	119.87
2	Bz	141	ASP	CA-C-N	5.76	125.86	119.87
2	Bz	141	ASP	C-N-CA	5.76	125.86	119.87
2	CB	141	ASP	CA-C-N	5.76	125.86	119.87
2	CB	141	ASP	C-N-CA	5.76	125.86	119.87
2	r	141	ASP	CA-C-N	5.76	125.86	119.87
2	r	141	ASP	C-N-CA	5.76	125.86	119.87
2	ZD	141	ASP	CA-C-N	5.76	125.86	119.87
2	ZD	141	ASP	C-N-CA	5.76	125.86	119.87
2	BJ	141	ASP	CA-C-N	5.76	125.86	119.87
2	BJ	141	ASP	C-N-CA	5.76	125.86	119.87
2	BP	141	ASP	CA-C-N	5.76	125.86	119.87
2	BP	141	ASP	C-N-CA	5.76	125.86	119.87
2	Cl	141	ASP	CA-C-N	5.76	125.86	119.87
2	Cl	141	ASP	C-N-CA	5.76	125.86	119.87
2	Cr	141	ASP	CA-C-N	5.76	125.86	119.87
2	Cr	141	ASP	C-N-CA	5.76	125.86	119.87
2	T	141	ASP	CA-C-N	5.76	125.86	119.87
2	T	141	ASP	C-N-CA	5.76	125.86	119.87
2	AF	141	ASP	CA-C-N	5.76	125.86	119.87
2	AF	141	ASP	C-N-CA	5.76	125.86	119.87
2	Av	141	ASP	CA-C-N	5.76	125.86	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Av	141	ASP	C-N-CA	5.76	125.86	119.87
2	Bb	141	ASP	CA-C-N	5.76	125.86	119.87
2	Bb	141	ASP	C-N-CA	5.76	125.86	119.87
2	Bt	141	ASP	CA-C-N	5.76	125.86	119.87
2	Bt	141	ASP	C-N-CA	5.76	125.86	119.87
2	CN	141	ASP	CA-C-N	5.76	125.86	119.87
2	CN	141	ASP	C-N-CA	5.76	125.86	119.87
2	AR	141	ASP	CA-C-N	5.76	125.86	119.87
2	AR	141	ASP	C-N-CA	5.76	125.86	119.87
2	AX	141	ASP	CA-C-N	5.76	125.86	119.87
2	AX	141	ASP	C-N-CA	5.76	125.86	119.87
2	CT	141	ASP	CA-C-N	5.76	125.86	119.87
2	CT	141	ASP	C-N-CA	5.76	125.86	119.87
2	CZ	141	ASP	CA-C-N	5.76	125.86	119.87
2	CZ	141	ASP	C-N-CA	5.76	125.86	119.87
2	DR	141	ASP	CA-C-N	5.76	125.86	119.87
2	DR	141	ASP	C-N-CA	5.76	125.86	119.87
2	DX	141	ASP	CA-C-N	5.76	125.86	119.87
2	DX	141	ASP	C-N-CA	5.76	125.86	119.87
2	x	141	ASP	CA-C-N	5.75	125.86	119.87
2	x	141	ASP	C-N-CA	5.75	125.86	119.87
2	BV	141	ASP	CA-C-N	5.75	125.86	119.87
2	BV	141	ASP	C-N-CA	5.75	125.86	119.87
2	Cx	141	ASP	CA-C-N	5.75	125.86	119.87
2	Cx	141	ASP	C-N-CA	5.75	125.86	119.87
2	ED	141	ASP	CA-C-N	5.75	125.86	119.87
2	ED	141	ASP	C-N-CA	5.75	125.86	119.87
2	EJ	141	ASP	CA-C-N	5.75	125.86	119.87
2	EJ	141	ASP	C-N-CA	5.75	125.86	119.87
2	EP	141	ASP	CA-C-N	5.75	125.86	119.87
2	EP	141	ASP	C-N-CA	5.75	125.86	119.87
2	BD	141	ASP	CA-C-N	5.75	125.85	119.87
2	BD	141	ASP	C-N-CA	5.75	125.85	119.87
2	DF	141	ASP	CA-C-N	5.75	125.85	119.87
2	DF	141	ASP	C-N-CA	5.75	125.85	119.87
2	Dd	141	ASP	CA-C-N	5.75	125.85	119.87
2	Dd	141	ASP	C-N-CA	5.75	125.85	119.87
2	YV	141	ASP	CA-C-N	5.75	125.85	119.87
2	YV	141	ASP	C-N-CA	5.75	125.85	119.87
2	Eb	141	ASP	CA-C-N	5.75	125.85	119.87
2	Eb	141	ASP	C-N-CA	5.75	125.85	119.87
2	Et	141	ASP	CA-C-N	5.75	125.85	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Et	141	ASP	C-N-CA	5.75	125.85	119.87
2	b	141	ASP	CA-C-N	5.66	125.76	119.87
2	b	141	ASP	C-N-CA	5.66	125.76	119.87
2	h	141	ASP	CA-C-N	5.66	125.76	119.87
2	h	141	ASP	C-N-CA	5.66	125.76	119.87
2	n	141	ASP	CA-C-N	5.66	125.76	119.87
2	n	141	ASP	C-N-CA	5.66	125.76	119.87
2	Af	141	ASP	CA-C-N	5.66	125.76	119.87
2	Af	141	ASP	C-N-CA	5.66	125.76	119.87
2	Ch	141	ASP	CA-C-N	5.66	125.76	119.87
2	Ch	141	ASP	C-N-CA	5.66	125.76	119.87
2	DN	141	ASP	CA-C-N	5.66	125.76	119.87
2	DN	141	ASP	C-N-CA	5.66	125.76	119.87
1	q	32	LEU	N-CA-C	-5.65	106.52	113.41
1	w	32	LEU	N-CA-C	-5.65	106.52	113.41
1	ZC	32	LEU	N-CA-C	-5.65	106.52	113.41
1	BI	32	LEU	N-CA-C	-5.65	106.52	113.41
1	BO	32	LEU	N-CA-C	-5.65	106.52	113.41
1	BU	32	LEU	N-CA-C	-5.65	106.52	113.41
1	Ck	32	LEU	N-CA-C	-5.65	106.52	113.41
1	Cq	32	LEU	N-CA-C	-5.65	106.52	113.41
1	Cw	32	LEU	N-CA-C	-5.65	106.52	113.41
1	EC	32	LEU	N-CA-C	-5.65	106.52	113.41
1	EI	32	LEU	N-CA-C	-5.65	106.52	113.41
1	EO	32	LEU	N-CA-C	-5.65	106.52	113.41
2	D	141	ASP	CA-C-N	5.64	125.74	119.87
2	D	141	ASP	C-N-CA	5.64	125.74	119.87
2	P	141	ASP	CA-C-N	5.64	125.74	119.87
2	P	141	ASP	C-N-CA	5.64	125.74	119.87
2	AB	141	ASP	CA-C-N	5.64	125.74	119.87
2	AB	141	ASP	C-N-CA	5.64	125.74	119.87
2	Ar	141	ASP	CA-C-N	5.64	125.74	119.87
2	Ar	141	ASP	C-N-CA	5.64	125.74	119.87
2	ZN	141	ASP	CA-C-N	5.64	125.74	119.87
2	ZN	141	ASP	C-N-CA	5.64	125.74	119.87
2	Bp	141	ASP	CA-C-N	5.64	125.74	119.87
2	Bp	141	ASP	C-N-CA	5.64	125.74	119.87
2	YB	141	ASP	CA-C-N	5.64	125.74	119.87
2	YB	141	ASP	C-N-CA	5.64	125.74	119.87
2	CJ	141	ASP	CA-C-N	5.64	125.74	119.87
2	CJ	141	ASP	C-N-CA	5.64	125.74	119.87
2	YJ	141	ASP	CA-C-N	5.64	125.74	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YJ	141	ASP	C-N-CA	5.64	125.74	119.87
2	Dl	141	ASP	CA-C-N	5.64	125.74	119.87
2	Dl	141	ASP	C-N-CA	5.64	125.74	119.87
2	Dx	141	ASP	CA-C-N	5.64	125.74	119.87
2	Dx	141	ASP	C-N-CA	5.64	125.74	119.87
2	Ej	141	ASP	CA-C-N	5.64	125.74	119.87
2	Ej	141	ASP	C-N-CA	5.64	125.74	119.87
2	AT	141	ASP	CA-C-N	5.63	125.73	119.87
2	AT	141	ASP	C-N-CA	5.63	125.73	119.87
2	AZ	141	ASP	CA-C-N	5.63	125.73	119.87
2	AZ	141	ASP	C-N-CA	5.63	125.73	119.87
2	CV	141	ASP	CA-C-N	5.63	125.73	119.87
2	CV	141	ASP	C-N-CA	5.63	125.73	119.87
2	Cb	141	ASP	CA-C-N	5.63	125.73	119.87
2	Cb	141	ASP	C-N-CA	5.63	125.73	119.87
2	DT	141	ASP	CA-C-N	5.63	125.73	119.87
2	DT	141	ASP	C-N-CA	5.63	125.73	119.87
2	DZ	141	ASP	CA-C-N	5.63	125.73	119.87
2	DZ	141	ASP	C-N-CA	5.63	125.73	119.87
1	A	32	LEU	N-CA-C	-5.63	106.54	113.41
1	M	32	LEU	N-CA-C	-5.63	106.54	113.41
1	ZI	32	LEU	N-CA-C	-5.63	106.54	113.41
1	Ao	32	LEU	N-CA-C	-5.63	106.54	113.41
1	ZK	32	LEU	N-CA-C	-5.63	106.54	113.41
1	Bm	32	LEU	N-CA-C	-5.63	106.54	113.41
1	ZY	32	LEU	N-CA-C	-5.63	106.54	113.41
1	CG	32	LEU	N-CA-C	-5.63	106.54	113.41
1	YG	32	LEU	N-CA-C	-5.63	106.54	113.41
1	Di	32	LEU	N-CA-C	-5.63	106.54	113.41
1	Du	32	LEU	N-CA-C	-5.63	106.54	113.41
1	Eg	32	LEU	N-CA-C	-5.63	106.54	113.41
1	G	32	LEU	N-CA-C	-5.62	106.55	113.41
1	AK	32	LEU	N-CA-C	-5.62	106.55	113.41
1	Ai	32	LEU	N-CA-C	-5.62	106.55	113.41
1	BC	32	LEU	N-CA-C	-5.62	106.55	113.41
1	Bg	32	LEU	N-CA-C	-5.62	106.55	113.41
1	By	32	LEU	N-CA-C	-5.62	106.55	113.41
1	CA	32	LEU	N-CA-C	-5.62	106.55	113.41
1	DE	32	LEU	N-CA-C	-5.62	106.55	113.41
1	Dc	32	LEU	N-CA-C	-5.62	106.55	113.41
1	YU	32	LEU	N-CA-C	-5.62	106.55	113.41
1	Ea	32	LEU	N-CA-C	-5.62	106.55	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Es	32	LEU	N-CA-C	-5.62	106.55	113.41
2	V	141	ASP	CA-C-N	5.62	125.72	119.87
2	V	141	ASP	C-N-CA	5.62	125.72	119.87
2	AH	141	ASP	CA-C-N	5.62	125.72	119.87
2	AH	141	ASP	C-N-CA	5.62	125.72	119.87
2	Ax	141	ASP	CA-C-N	5.62	125.72	119.87
2	Ax	141	ASP	C-N-CA	5.62	125.72	119.87
2	ZT	141	ASP	CA-C-N	5.62	125.72	119.87
2	ZT	141	ASP	C-N-CA	5.62	125.72	119.87
2	Bd	141	ASP	CA-C-N	5.62	125.72	119.87
2	Bd	141	ASP	C-N-CA	5.62	125.72	119.87
2	Bv	141	ASP	CA-C-N	5.62	125.72	119.87
2	Bv	141	ASP	C-N-CA	5.62	125.72	119.87
2	CP	141	ASP	CA-C-N	5.62	125.72	119.87
2	CP	141	ASP	C-N-CA	5.62	125.72	119.87
2	DB	141	ASP	CA-C-N	5.62	125.72	119.87
2	DB	141	ASP	C-N-CA	5.62	125.72	119.87
2	Dr	141	ASP	CA-C-N	5.62	125.72	119.87
2	Dr	141	ASP	C-N-CA	5.62	125.72	119.87
2	YR	141	ASP	CA-C-N	5.62	125.72	119.87
2	YR	141	ASP	C-N-CA	5.62	125.72	119.87
2	EX	141	ASP	CA-C-N	5.62	125.72	119.87
2	EX	141	ASP	C-N-CA	5.62	125.72	119.87
2	Ep	141	ASP	CA-C-N	5.62	125.72	119.87
2	Ep	141	ASP	C-N-CA	5.62	125.72	119.87
1	S	32	LEU	N-CA-C	-5.62	106.56	113.41
1	AE	32	LEU	N-CA-C	-5.62	106.56	113.41
1	ZQ	32	LEU	N-CA-C	-5.62	106.56	113.41
1	Bs	32	LEU	N-CA-C	-5.62	106.56	113.41
1	YM	32	LEU	N-CA-C	-5.62	106.56	113.41
1	EU	32	LEU	N-CA-C	-5.62	106.56	113.41
2	J	141	ASP	CA-C-N	5.61	125.71	119.87
2	J	141	ASP	C-N-CA	5.61	125.71	119.87
2	AN	141	ASP	CA-C-N	5.61	125.71	119.87
2	AN	141	ASP	C-N-CA	5.61	125.71	119.87
2	Al	141	ASP	CA-C-N	5.61	125.71	119.87
2	Al	141	ASP	C-N-CA	5.61	125.71	119.87
2	Bj	141	ASP	CA-C-N	5.61	125.71	119.87
2	Bj	141	ASP	C-N-CA	5.61	125.71	119.87
2	ZV	141	ASP	CA-C-N	5.61	125.71	119.87
2	ZV	141	ASP	C-N-CA	5.61	125.71	119.87
2	CD	141	ASP	CA-C-N	5.61	125.71	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CD	141	ASP	C-N-CA	5.61	125.71	119.87
1	AW	32	LEU	N-CA-C	-5.61	106.56	113.41
1	Ac	32	LEU	N-CA-C	-5.61	106.56	113.41
1	CY	32	LEU	N-CA-C	-5.61	106.56	113.41
1	Ce	32	LEU	N-CA-C	-5.61	106.56	113.41
1	DK	32	LEU	N-CA-C	-5.61	106.56	113.41
1	DW	32	LEU	N-CA-C	-5.61	106.56	113.41
2	t	141	ASP	CA-C-N	5.60	125.69	119.87
2	t	141	ASP	C-N-CA	5.60	125.69	119.87
2	z	141	ASP	CA-C-N	5.60	125.69	119.87
2	z	141	ASP	C-N-CA	5.60	125.69	119.87
2	ZF	141	ASP	CA-C-N	5.60	125.69	119.87
2	ZF	141	ASP	C-N-CA	5.60	125.69	119.87
1	Au	32	LEU	N-CA-C	-5.60	106.58	113.41
2	BL	141	ASP	CA-C-N	5.60	125.69	119.87
2	BL	141	ASP	C-N-CA	5.60	125.69	119.87
2	BR	141	ASP	CA-C-N	5.60	125.69	119.87
2	BR	141	ASP	C-N-CA	5.60	125.69	119.87
2	BX	141	ASP	CA-C-N	5.60	125.69	119.87
2	BX	141	ASP	C-N-CA	5.60	125.69	119.87
1	Ba	32	LEU	N-CA-C	-5.60	106.58	113.41
1	CM	32	LEU	N-CA-C	-5.60	106.58	113.41
2	Cn	141	ASP	CA-C-N	5.60	125.69	119.87
2	Cn	141	ASP	C-N-CA	5.60	125.69	119.87
2	Ct	141	ASP	CA-C-N	5.60	125.69	119.87
2	Ct	141	ASP	C-N-CA	5.60	125.69	119.87
2	Cz	141	ASP	CA-C-N	5.60	125.69	119.87
2	Cz	141	ASP	C-N-CA	5.60	125.69	119.87
1	Do	32	LEU	N-CA-C	-5.60	106.58	113.41
1	YO	32	LEU	N-CA-C	-5.60	106.58	113.41
2	EF	141	ASP	CA-C-N	5.60	125.69	119.87
2	EF	141	ASP	C-N-CA	5.60	125.69	119.87
2	EL	141	ASP	CA-C-N	5.60	125.69	119.87
2	EL	141	ASP	C-N-CA	5.60	125.69	119.87
2	ER	141	ASP	CA-C-N	5.60	125.69	119.87
2	ER	141	ASP	C-N-CA	5.60	125.69	119.87
1	Em	32	LEU	N-CA-C	-5.60	106.58	113.41
2	BF	141	ASP	CA-C-N	5.59	125.68	119.87
2	BF	141	ASP	C-N-CA	5.59	125.68	119.87
2	DH	141	ASP	CA-C-N	5.59	125.68	119.87
2	DH	141	ASP	C-N-CA	5.59	125.68	119.87
2	Df	141	ASP	CA-C-N	5.59	125.68	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Df	141	ASP	C-N-CA	5.59	125.68	119.87
2	YX	141	ASP	CA-C-N	5.59	125.68	119.87
2	YX	141	ASP	C-N-CA	5.59	125.68	119.87
2	Ed	141	ASP	CA-C-N	5.59	125.68	119.87
2	Ed	141	ASP	C-N-CA	5.59	125.68	119.87
2	Ev	141	ASP	CA-C-N	5.59	125.68	119.87
2	Ev	141	ASP	C-N-CA	5.59	125.68	119.87
1	Y	32	LEU	N-CA-C	-5.58	106.60	113.41
1	e	32	LEU	N-CA-C	-5.58	106.60	113.41
1	k	32	LEU	N-CA-C	-5.58	106.60	113.41
1	AQ	32	LEU	N-CA-C	-5.58	106.60	113.41
1	CS	32	LEU	N-CA-C	-5.58	106.60	113.41
1	DQ	32	LEU	N-CA-C	-5.58	106.60	113.41
1	I	19	ARG	N-CA-C	-5.47	105.40	111.36
1	AM	19	ARG	N-CA-C	-5.47	105.40	111.36
1	BE	19	ARG	N-CA-C	-5.47	105.40	111.36
1	ZU	19	ARG	N-CA-C	-5.47	105.40	111.36
1	DG	19	ARG	N-CA-C	-5.47	105.40	111.36
1	Ec	19	ARG	N-CA-C	-5.47	105.40	111.36
1	C	19	ARG	N-CA-C	-5.46	105.41	111.36
1	O	19	ARG	N-CA-C	-5.46	105.41	111.36
1	U	19	ARG	N-CA-C	-5.46	105.41	111.36
1	AA	19	ARG	N-CA-C	-5.46	105.41	111.36
1	AG	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Aq	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Aw	19	ARG	N-CA-C	-5.46	105.41	111.36
1	ZM	19	ARG	N-CA-C	-5.46	105.41	111.36
1	ZS	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Bc	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Bo	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Bu	19	ARG	N-CA-C	-5.46	105.41	111.36
1	YA	19	ARG	N-CA-C	-5.46	105.41	111.36
1	CI	19	ARG	N-CA-C	-5.46	105.41	111.36
1	CO	19	ARG	N-CA-C	-5.46	105.41	111.36
1	YI	19	ARG	N-CA-C	-5.46	105.41	111.36
1	DA	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Dk	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Dq	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Dw	19	ARG	N-CA-C	-5.46	105.41	111.36
1	YQ	19	ARG	N-CA-C	-5.46	105.41	111.36
1	EW	19	ARG	N-CA-C	-5.46	105.41	111.36
1	Ei	19	ARG	N-CA-C	-5.46	105.41	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Eo	19	ARG	N-CA-C	-5.46	105.41	111.36
2	Az	141	ASP	CA-C-N	5.45	125.54	119.87
2	Az	141	ASP	C-N-CA	5.45	125.54	119.87
2	Bf	141	ASP	CA-C-N	5.45	125.54	119.87
2	Bf	141	ASP	C-N-CA	5.45	125.54	119.87
2	CR	141	ASP	CA-C-N	5.45	125.54	119.87
2	CR	141	ASP	C-N-CA	5.45	125.54	119.87
2	Dt	141	ASP	CA-C-N	5.45	125.54	119.87
2	Dt	141	ASP	C-N-CA	5.45	125.54	119.87
2	YT	141	ASP	CA-C-N	5.45	125.54	119.87
2	YT	141	ASP	C-N-CA	5.45	125.54	119.87
2	Er	141	ASP	CA-C-N	5.45	125.54	119.87
2	Er	141	ASP	C-N-CA	5.45	125.54	119.87
1	Ak	19	ARG	N-CA-C	-5.44	105.43	111.36
1	Bi	19	ARG	N-CA-C	-5.44	105.43	111.36
1	CC	19	ARG	N-CA-C	-5.44	105.43	111.36
1	De	19	ARG	N-CA-C	-5.44	105.43	111.36
1	YW	19	ARG	N-CA-C	-5.44	105.43	111.36
1	Eu	19	ARG	N-CA-C	-5.44	105.43	111.36
1	a	19	ARG	N-CA-C	-5.43	105.44	111.36
1	g	19	ARG	N-CA-C	-5.43	105.44	111.36
1	m	19	ARG	N-CA-C	-5.43	105.44	111.36
1	AS	19	ARG	N-CA-C	-5.43	105.44	111.36
1	AY	19	ARG	N-CA-C	-5.43	105.44	111.36
1	Ae	19	ARG	N-CA-C	-5.43	105.44	111.36
1	CU	19	ARG	N-CA-C	-5.43	105.44	111.36
1	Ca	19	ARG	N-CA-C	-5.43	105.44	111.36
1	Cg	19	ARG	N-CA-C	-5.43	105.44	111.36
1	DM	19	ARG	N-CA-C	-5.43	105.44	111.36
1	DS	19	ARG	N-CA-C	-5.43	105.44	111.36
1	DY	19	ARG	N-CA-C	-5.43	105.44	111.36
1	s	19	ARG	N-CA-C	-5.43	105.44	111.36
1	y	19	ARG	N-CA-C	-5.43	105.44	111.36
1	ZE	19	ARG	N-CA-C	-5.43	105.44	111.36
1	BK	19	ARG	N-CA-C	-5.43	105.44	111.36
1	BQ	19	ARG	N-CA-C	-5.43	105.44	111.36
1	BW	19	ARG	N-CA-C	-5.43	105.44	111.36
1	Cm	19	ARG	N-CA-C	-5.43	105.44	111.36
1	Cs	19	ARG	N-CA-C	-5.43	105.44	111.36
1	Cy	19	ARG	N-CA-C	-5.43	105.44	111.36
1	EE	19	ARG	N-CA-C	-5.43	105.44	111.36
1	EK	19	ARG	N-CA-C	-5.43	105.44	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EQ	19	ARG	N-CA-C	-5.43	105.44	111.36
2	v	141	ASP	CA-C-N	5.43	125.52	119.87
2	v	141	ASP	C-N-CA	5.43	125.52	119.87
2	ZB	141	ASP	CA-C-N	5.43	125.52	119.87
2	ZB	141	ASP	C-N-CA	5.43	125.52	119.87
2	ZH	141	ASP	CA-C-N	5.43	125.52	119.87
2	ZH	141	ASP	C-N-CA	5.43	125.52	119.87
2	BN	141	ASP	CA-C-N	5.43	125.52	119.87
2	BN	141	ASP	C-N-CA	5.43	125.52	119.87
2	BT	141	ASP	CA-C-N	5.43	125.52	119.87
2	BT	141	ASP	C-N-CA	5.43	125.52	119.87
2	BZ	141	ASP	CA-C-N	5.43	125.52	119.87
2	BZ	141	ASP	C-N-CA	5.43	125.52	119.87
2	Cp	141	ASP	CA-C-N	5.43	125.52	119.87
2	Cp	141	ASP	C-N-CA	5.43	125.52	119.87
2	Cv	141	ASP	CA-C-N	5.43	125.52	119.87
2	Cv	141	ASP	C-N-CA	5.43	125.52	119.87
2	YF	141	ASP	CA-C-N	5.43	125.52	119.87
2	YF	141	ASP	C-N-CA	5.43	125.52	119.87
2	EH	141	ASP	CA-C-N	5.43	125.52	119.87
2	EH	141	ASP	C-N-CA	5.43	125.52	119.87
2	EN	141	ASP	CA-C-N	5.43	125.52	119.87
2	EN	141	ASP	C-N-CA	5.43	125.52	119.87
2	ET	141	ASP	CA-C-N	5.43	125.52	119.87
2	ET	141	ASP	C-N-CA	5.43	125.52	119.87
2	F	141	ASP	CA-C-N	5.43	125.52	119.87
2	F	141	ASP	C-N-CA	5.43	125.52	119.87
2	R	141	ASP	CA-C-N	5.43	125.52	119.87
2	R	141	ASP	C-N-CA	5.43	125.52	119.87
2	AD	141	ASP	CA-C-N	5.43	125.52	119.87
2	AD	141	ASP	C-N-CA	5.43	125.52	119.87
2	At	141	ASP	CA-C-N	5.43	125.52	119.87
2	At	141	ASP	C-N-CA	5.43	125.52	119.87
2	ZP	141	ASP	CA-C-N	5.43	125.52	119.87
2	ZP	141	ASP	C-N-CA	5.43	125.52	119.87
2	Br	141	ASP	CA-C-N	5.43	125.52	119.87
2	Br	141	ASP	C-N-CA	5.43	125.52	119.87
2	YD	141	ASP	CA-C-N	5.43	125.52	119.87
2	YD	141	ASP	C-N-CA	5.43	125.52	119.87
2	CL	141	ASP	CA-C-N	5.43	125.52	119.87
2	CL	141	ASP	C-N-CA	5.43	125.52	119.87
2	YL	141	ASP	CA-C-N	5.43	125.52	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YL	141	ASP	C-N-CA	5.43	125.52	119.87
2	Dn	141	ASP	CA-C-N	5.43	125.52	119.87
2	Dn	141	ASP	C-N-CA	5.43	125.52	119.87
2	Dz	141	ASP	CA-C-N	5.43	125.52	119.87
2	Dz	141	ASP	C-N-CA	5.43	125.52	119.87
2	El	141	ASP	CA-C-N	5.43	125.52	119.87
2	El	141	ASP	C-N-CA	5.43	125.52	119.87
2	d	141	ASP	CA-C-N	5.42	125.51	119.87
2	d	141	ASP	C-N-CA	5.42	125.51	119.87
2	j	141	ASP	CA-C-N	5.42	125.51	119.87
2	j	141	ASP	C-N-CA	5.42	125.51	119.87
2	p	141	ASP	CA-C-N	5.42	125.51	119.87
2	p	141	ASP	C-N-CA	5.42	125.51	119.87
2	AV	141	ASP	CA-C-N	5.42	125.51	119.87
2	AV	141	ASP	C-N-CA	5.42	125.51	119.87
2	CX	141	ASP	CA-C-N	5.42	125.51	119.87
2	CX	141	ASP	C-N-CA	5.42	125.51	119.87
2	DV	141	ASP	CA-C-N	5.42	125.51	119.87
2	DV	141	ASP	C-N-CA	5.42	125.51	119.87
2	L	141	ASP	CA-C-N	5.42	125.51	119.87
2	L	141	ASP	C-N-CA	5.42	125.51	119.87
2	AP	141	ASP	CA-C-N	5.42	125.51	119.87
2	AP	141	ASP	C-N-CA	5.42	125.51	119.87
2	An	141	ASP	CA-C-N	5.42	125.51	119.87
2	An	141	ASP	C-N-CA	5.42	125.51	119.87
2	BH	141	ASP	CA-C-N	5.42	125.51	119.87
2	BH	141	ASP	C-N-CA	5.42	125.51	119.87
2	Bl	141	ASP	CA-C-N	5.42	125.51	119.87
2	Bl	141	ASP	C-N-CA	5.42	125.51	119.87
2	ZX	141	ASP	CA-C-N	5.42	125.51	119.87
2	ZX	141	ASP	C-N-CA	5.42	125.51	119.87
2	CF	141	ASP	CA-C-N	5.42	125.51	119.87
2	CF	141	ASP	C-N-CA	5.42	125.51	119.87
2	DJ	141	ASP	CA-C-N	5.42	125.51	119.87
2	DJ	141	ASP	C-N-CA	5.42	125.51	119.87
2	Dh	141	ASP	CA-C-N	5.42	125.51	119.87
2	Dh	141	ASP	C-N-CA	5.42	125.51	119.87
2	EB	141	ASP	CA-C-N	5.42	125.51	119.87
2	EB	141	ASP	C-N-CA	5.42	125.51	119.87
2	Ef	141	ASP	CA-C-N	5.42	125.51	119.87
2	Ef	141	ASP	C-N-CA	5.42	125.51	119.87
2	Ex	141	ASP	CA-C-N	5.42	125.51	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Ex	141	ASP	C-N-CA	5.42	125.51	119.87
2	Ab	141	ASP	CA-C-N	5.41	125.50	119.87
2	Ab	141	ASP	C-N-CA	5.41	125.50	119.87
2	Ah	141	ASP	CA-C-N	5.41	125.50	119.87
2	Ah	141	ASP	C-N-CA	5.41	125.50	119.87
2	Cd	141	ASP	CA-C-N	5.41	125.50	119.87
2	Cd	141	ASP	C-N-CA	5.41	125.50	119.87
2	Cj	141	ASP	CA-C-N	5.41	125.50	119.87
2	Cj	141	ASP	C-N-CA	5.41	125.50	119.87
2	DP	141	ASP	CA-C-N	5.41	125.50	119.87
2	DP	141	ASP	C-N-CA	5.41	125.50	119.87
2	Db	141	ASP	CA-C-N	5.41	125.50	119.87
2	Db	141	ASP	C-N-CA	5.41	125.50	119.87
2	X	141	ASP	CA-C-N	5.40	125.49	119.87
2	X	141	ASP	C-N-CA	5.40	125.49	119.87
2	AJ	141	ASP	CA-C-N	5.40	125.49	119.87
2	AJ	141	ASP	C-N-CA	5.40	125.49	119.87
2	BB	141	ASP	CA-C-N	5.40	125.49	119.87
2	BB	141	ASP	C-N-CA	5.40	125.49	119.87
2	Bx	141	ASP	CA-C-N	5.40	125.49	119.87
2	Bx	141	ASP	C-N-CA	5.40	125.49	119.87
2	DD	141	ASP	CA-C-N	5.40	125.49	119.87
2	DD	141	ASP	C-N-CA	5.40	125.49	119.87
2	EZ	141	ASP	CA-C-N	5.40	125.49	119.87
2	EZ	141	ASP	C-N-CA	5.40	125.49	119.87
1	c	33	ALA	CA-C-N	5.40	125.06	119.56
1	c	33	ALA	C-N-CA	5.40	125.06	119.56
1	i	33	ALA	CA-C-N	5.40	125.06	119.56
1	i	33	ALA	C-N-CA	5.40	125.06	119.56
1	o	33	ALA	CA-C-N	5.40	125.06	119.56
1	o	33	ALA	C-N-CA	5.40	125.06	119.56
1	AU	33	ALA	CA-C-N	5.40	125.06	119.56
1	AU	33	ALA	C-N-CA	5.40	125.06	119.56
1	Aa	33	ALA	CA-C-N	5.40	125.06	119.56
1	Aa	33	ALA	C-N-CA	5.40	125.06	119.56
1	Ag	33	ALA	CA-C-N	5.40	125.06	119.56
1	Ag	33	ALA	C-N-CA	5.40	125.06	119.56
1	CW	33	ALA	CA-C-N	5.40	125.06	119.56
1	CW	33	ALA	C-N-CA	5.40	125.06	119.56
1	Cc	33	ALA	CA-C-N	5.40	125.06	119.56
1	Cc	33	ALA	C-N-CA	5.40	125.06	119.56
1	Ci	33	ALA	CA-C-N	5.40	125.06	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ci	33	ALA	C-N-CA	5.40	125.06	119.56
1	DO	33	ALA	CA-C-N	5.40	125.06	119.56
1	DO	33	ALA	C-N-CA	5.40	125.06	119.56
1	DU	33	ALA	CA-C-N	5.40	125.06	119.56
1	DU	33	ALA	C-N-CA	5.40	125.06	119.56
1	Da	33	ALA	CA-C-N	5.40	125.06	119.56
1	Da	33	ALA	C-N-CA	5.40	125.06	119.56
1	E	33	ALA	CA-C-N	5.39	125.05	119.56
1	E	33	ALA	C-N-CA	5.39	125.05	119.56
1	Q	33	ALA	CA-C-N	5.39	125.05	119.56
1	Q	33	ALA	C-N-CA	5.39	125.05	119.56
1	AC	33	ALA	CA-C-N	5.39	125.05	119.56
1	AC	33	ALA	C-N-CA	5.39	125.05	119.56
1	As	33	ALA	CA-C-N	5.39	125.05	119.56
1	As	33	ALA	C-N-CA	5.39	125.05	119.56
1	ZO	33	ALA	CA-C-N	5.39	125.05	119.56
1	ZO	33	ALA	C-N-CA	5.39	125.05	119.56
1	Bq	33	ALA	CA-C-N	5.39	125.05	119.56
1	Bq	33	ALA	C-N-CA	5.39	125.05	119.56
1	YC	33	ALA	CA-C-N	5.39	125.05	119.56
1	YC	33	ALA	C-N-CA	5.39	125.05	119.56
1	CK	33	ALA	CA-C-N	5.39	125.05	119.56
1	CK	33	ALA	C-N-CA	5.39	125.05	119.56
1	YK	33	ALA	CA-C-N	5.39	125.05	119.56
1	YK	33	ALA	C-N-CA	5.39	125.05	119.56
1	Dm	33	ALA	CA-C-N	5.39	125.05	119.56
1	Dm	33	ALA	C-N-CA	5.39	125.05	119.56
1	Dy	33	ALA	CA-C-N	5.39	125.05	119.56
1	Dy	33	ALA	C-N-CA	5.39	125.05	119.56
1	Ek	33	ALA	CA-C-N	5.39	125.05	119.56
1	Ek	33	ALA	C-N-CA	5.39	125.05	119.56
1	W	33	ALA	CA-C-N	5.37	125.04	119.56
1	W	33	ALA	C-N-CA	5.37	125.04	119.56
1	AI	33	ALA	CA-C-N	5.37	125.04	119.56
1	AI	33	ALA	C-N-CA	5.37	125.04	119.56
1	Ay	33	ALA	CA-C-N	5.37	125.04	119.56
1	Ay	33	ALA	C-N-CA	5.37	125.04	119.56
1	BA	33	ALA	CA-C-N	5.37	125.04	119.56
1	BA	33	ALA	C-N-CA	5.37	125.04	119.56
1	Be	33	ALA	CA-C-N	5.37	125.04	119.56
1	Be	33	ALA	C-N-CA	5.37	125.04	119.56
1	Bw	33	ALA	CA-C-N	5.37	125.04	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bw	33	ALA	C-N-CA	5.37	125.04	119.56
1	CQ	33	ALA	CA-C-N	5.37	125.04	119.56
1	CQ	33	ALA	C-N-CA	5.37	125.04	119.56
1	DC	33	ALA	CA-C-N	5.37	125.04	119.56
1	DC	33	ALA	C-N-CA	5.37	125.04	119.56
1	Ds	33	ALA	CA-C-N	5.37	125.04	119.56
1	Ds	33	ALA	C-N-CA	5.37	125.04	119.56
1	YS	33	ALA	CA-C-N	5.37	125.04	119.56
1	YS	33	ALA	C-N-CA	5.37	125.04	119.56
1	EY	33	ALA	CA-C-N	5.37	125.04	119.56
1	EY	33	ALA	C-N-CA	5.37	125.04	119.56
1	Eq	33	ALA	CA-C-N	5.37	125.04	119.56
1	Eq	33	ALA	C-N-CA	5.37	125.04	119.56
1	K	33	ALA	CA-C-N	5.36	125.02	119.56
1	K	33	ALA	C-N-CA	5.36	125.02	119.56
1	AO	33	ALA	CA-C-N	5.36	125.02	119.56
1	AO	33	ALA	C-N-CA	5.36	125.02	119.56
1	Am	33	ALA	CA-C-N	5.36	125.02	119.56
1	Am	33	ALA	C-N-CA	5.36	125.02	119.56
1	BG	33	ALA	CA-C-N	5.36	125.02	119.56
1	BG	33	ALA	C-N-CA	5.36	125.02	119.56
1	Bk	33	ALA	CA-C-N	5.36	125.02	119.56
1	Bk	33	ALA	C-N-CA	5.36	125.02	119.56
1	ZW	33	ALA	CA-C-N	5.36	125.02	119.56
1	ZW	33	ALA	C-N-CA	5.36	125.02	119.56
1	CE	33	ALA	CA-C-N	5.36	125.02	119.56
1	CE	33	ALA	C-N-CA	5.36	125.02	119.56
1	DI	33	ALA	CA-C-N	5.36	125.02	119.56
1	DI	33	ALA	C-N-CA	5.36	125.02	119.56
1	Dg	33	ALA	CA-C-N	5.36	125.02	119.56
1	Dg	33	ALA	C-N-CA	5.36	125.02	119.56
1	EA	33	ALA	CA-C-N	5.36	125.02	119.56
1	EA	33	ALA	C-N-CA	5.36	125.02	119.56
1	Ee	33	ALA	CA-C-N	5.36	125.02	119.56
1	Ee	33	ALA	C-N-CA	5.36	125.02	119.56
1	Ew	33	ALA	CA-C-N	5.36	125.02	119.56
1	Ew	33	ALA	C-N-CA	5.36	125.02	119.56
1	u	33	ALA	CA-C-N	5.34	125.01	119.56
1	u	33	ALA	C-N-CA	5.34	125.01	119.56
1	ZA	33	ALA	CA-C-N	5.34	125.01	119.56
1	ZA	33	ALA	C-N-CA	5.34	125.01	119.56
1	ZG	33	ALA	CA-C-N	5.34	125.01	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZG	33	ALA	C-N-CA	5.34	125.01	119.56
1	BM	33	ALA	CA-C-N	5.34	125.01	119.56
1	BM	33	ALA	C-N-CA	5.34	125.01	119.56
1	BS	33	ALA	CA-C-N	5.34	125.01	119.56
1	BS	33	ALA	C-N-CA	5.34	125.01	119.56
1	BY	33	ALA	CA-C-N	5.34	125.01	119.56
1	BY	33	ALA	C-N-CA	5.34	125.01	119.56
1	Co	33	ALA	CA-C-N	5.34	125.01	119.56
1	Co	33	ALA	C-N-CA	5.34	125.01	119.56
1	Cu	33	ALA	CA-C-N	5.34	125.01	119.56
1	Cu	33	ALA	C-N-CA	5.34	125.01	119.56
1	YE	33	ALA	CA-C-N	5.34	125.01	119.56
1	YE	33	ALA	C-N-CA	5.34	125.01	119.56
1	EG	33	ALA	CA-C-N	5.34	125.01	119.56
1	EG	33	ALA	C-N-CA	5.34	125.01	119.56
1	EM	33	ALA	CA-C-N	5.34	125.01	119.56
1	EM	33	ALA	C-N-CA	5.34	125.01	119.56
1	ES	33	ALA	CA-C-N	5.34	125.01	119.56
1	ES	33	ALA	C-N-CA	5.34	125.01	119.56
2	Z	36	ASN	CA-C-N	5.22	125.12	119.85
2	Z	36	ASN	C-N-CA	5.22	125.12	119.85
2	f	36	ASN	CA-C-N	5.22	125.12	119.85
2	f	36	ASN	C-N-CA	5.22	125.12	119.85
2	l	36	ASN	CA-C-N	5.22	125.12	119.85
2	l	36	ASN	C-N-CA	5.22	125.12	119.85
2	AR	36	ASN	CA-C-N	5.22	125.12	119.85
2	AR	36	ASN	C-N-CA	5.22	125.12	119.85
2	AX	36	ASN	CA-C-N	5.22	125.12	119.85
2	AX	36	ASN	C-N-CA	5.22	125.12	119.85
2	Ad	36	ASN	CA-C-N	5.22	125.12	119.85
2	Ad	36	ASN	C-N-CA	5.22	125.12	119.85
2	CT	36	ASN	CA-C-N	5.22	125.12	119.85
2	CT	36	ASN	C-N-CA	5.22	125.12	119.85
2	CZ	36	ASN	CA-C-N	5.22	125.12	119.85
2	CZ	36	ASN	C-N-CA	5.22	125.12	119.85
2	Cf	36	ASN	CA-C-N	5.22	125.12	119.85
2	Cf	36	ASN	C-N-CA	5.22	125.12	119.85
2	DL	36	ASN	CA-C-N	5.22	125.12	119.85
2	DL	36	ASN	C-N-CA	5.22	125.12	119.85
2	DR	36	ASN	CA-C-N	5.22	125.12	119.85
2	DR	36	ASN	C-N-CA	5.22	125.12	119.85
2	DX	36	ASN	CA-C-N	5.22	125.12	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DX	36	ASN	C-N-CA	5.22	125.12	119.85
2	H	36	ASN	CA-C-N	5.21	125.11	119.85
2	H	36	ASN	C-N-CA	5.21	125.11	119.85
2	AL	36	ASN	CA-C-N	5.21	125.11	119.85
2	AL	36	ASN	C-N-CA	5.21	125.11	119.85
2	Aj	36	ASN	CA-C-N	5.21	125.11	119.85
2	Aj	36	ASN	C-N-CA	5.21	125.11	119.85
2	BD	36	ASN	CA-C-N	5.21	125.11	119.85
2	BD	36	ASN	C-N-CA	5.21	125.11	119.85
2	Bh	36	ASN	CA-C-N	5.21	125.11	119.85
2	Bh	36	ASN	C-N-CA	5.21	125.11	119.85
2	Bz	36	ASN	CA-C-N	5.21	125.11	119.85
2	Bz	36	ASN	C-N-CA	5.21	125.11	119.85
2	CB	36	ASN	CA-C-N	5.21	125.11	119.85
2	CB	36	ASN	C-N-CA	5.21	125.11	119.85
2	DF	36	ASN	CA-C-N	5.21	125.11	119.85
2	DF	36	ASN	C-N-CA	5.21	125.11	119.85
2	Dd	36	ASN	CA-C-N	5.21	125.11	119.85
2	Dd	36	ASN	C-N-CA	5.21	125.11	119.85
2	YV	36	ASN	CA-C-N	5.21	125.11	119.85
2	YV	36	ASN	C-N-CA	5.21	125.11	119.85
2	Eb	36	ASN	CA-C-N	5.21	125.11	119.85
2	Eb	36	ASN	C-N-CA	5.21	125.11	119.85
2	Et	36	ASN	CA-C-N	5.21	125.11	119.85
2	Et	36	ASN	C-N-CA	5.21	125.11	119.85
2	B	36	ASN	CA-C-N	5.18	125.09	119.85
2	B	36	ASN	C-N-CA	5.18	125.09	119.85
2	N	36	ASN	CA-C-N	5.18	125.09	119.85
2	N	36	ASN	C-N-CA	5.18	125.09	119.85
2	ZJ	36	ASN	CA-C-N	5.18	125.09	119.85
2	ZJ	36	ASN	C-N-CA	5.18	125.09	119.85
2	Ap	36	ASN	CA-C-N	5.18	125.09	119.85
2	Ap	36	ASN	C-N-CA	5.18	125.09	119.85
2	ZL	36	ASN	CA-C-N	5.18	125.09	119.85
2	ZL	36	ASN	C-N-CA	5.18	125.09	119.85
2	Bn	36	ASN	CA-C-N	5.18	125.09	119.85
2	Bn	36	ASN	C-N-CA	5.18	125.09	119.85
2	ZZ	36	ASN	CA-C-N	5.18	125.09	119.85
2	ZZ	36	ASN	C-N-CA	5.18	125.09	119.85
2	CH	36	ASN	CA-C-N	5.18	125.09	119.85
2	CH	36	ASN	C-N-CA	5.18	125.09	119.85
2	YH	36	ASN	CA-C-N	5.18	125.09	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YH	36	ASN	C-N-CA	5.18	125.09	119.85
2	Dj	36	ASN	CA-C-N	5.18	125.09	119.85
2	Dj	36	ASN	C-N-CA	5.18	125.09	119.85
2	Dv	36	ASN	CA-C-N	5.18	125.09	119.85
2	Dv	36	ASN	C-N-CA	5.18	125.09	119.85
2	Eh	36	ASN	CA-C-N	5.18	125.09	119.85
2	Eh	36	ASN	C-N-CA	5.18	125.09	119.85
2	T	36	ASN	CA-C-N	5.17	125.07	119.85
2	T	36	ASN	C-N-CA	5.17	125.07	119.85
2	AF	36	ASN	CA-C-N	5.17	125.07	119.85
2	AF	36	ASN	C-N-CA	5.17	125.07	119.85
2	Av	36	ASN	CA-C-N	5.17	125.07	119.85
2	Av	36	ASN	C-N-CA	5.17	125.07	119.85
2	ZR	36	ASN	CA-C-N	5.17	125.07	119.85
2	ZR	36	ASN	C-N-CA	5.17	125.07	119.85
2	Bb	36	ASN	CA-C-N	5.17	125.07	119.85
2	Bb	36	ASN	C-N-CA	5.17	125.07	119.85
2	Bt	36	ASN	CA-C-N	5.17	125.07	119.85
2	Bt	36	ASN	C-N-CA	5.17	125.07	119.85
2	CN	36	ASN	CA-C-N	5.17	125.07	119.85
2	CN	36	ASN	C-N-CA	5.17	125.07	119.85
2	YN	36	ASN	CA-C-N	5.17	125.07	119.85
2	YN	36	ASN	C-N-CA	5.17	125.07	119.85
2	Dp	36	ASN	CA-C-N	5.17	125.07	119.85
2	Dp	36	ASN	C-N-CA	5.17	125.07	119.85
2	YP	36	ASN	CA-C-N	5.17	125.07	119.85
2	YP	36	ASN	C-N-CA	5.17	125.07	119.85
2	EV	36	ASN	CA-C-N	5.17	125.07	119.85
2	EV	36	ASN	C-N-CA	5.17	125.07	119.85
2	En	36	ASN	CA-C-N	5.17	125.07	119.85
2	En	36	ASN	C-N-CA	5.17	125.07	119.85
2	r	36	ASN	CA-C-N	5.17	125.07	119.85
2	r	36	ASN	C-N-CA	5.17	125.07	119.85
2	x	36	ASN	CA-C-N	5.17	125.07	119.85
2	x	36	ASN	C-N-CA	5.17	125.07	119.85
2	ZD	36	ASN	CA-C-N	5.17	125.07	119.85
2	ZD	36	ASN	C-N-CA	5.17	125.07	119.85
2	BJ	36	ASN	CA-C-N	5.17	125.07	119.85
2	BJ	36	ASN	C-N-CA	5.17	125.07	119.85
2	BP	36	ASN	CA-C-N	5.17	125.07	119.85
2	BP	36	ASN	C-N-CA	5.17	125.07	119.85
2	BV	36	ASN	CA-C-N	5.17	125.07	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BV	36	ASN	C-N-CA	5.17	125.07	119.85
2	Cl	36	ASN	CA-C-N	5.17	125.07	119.85
2	Cl	36	ASN	C-N-CA	5.17	125.07	119.85
2	Cr	36	ASN	CA-C-N	5.17	125.07	119.85
2	Cr	36	ASN	C-N-CA	5.17	125.07	119.85
2	Cx	36	ASN	CA-C-N	5.17	125.07	119.85
2	Cx	36	ASN	C-N-CA	5.17	125.07	119.85
2	ED	36	ASN	CA-C-N	5.17	125.07	119.85
2	ED	36	ASN	C-N-CA	5.17	125.07	119.85
2	EJ	36	ASN	CA-C-N	5.17	125.07	119.85
2	EJ	36	ASN	C-N-CA	5.17	125.07	119.85
2	EP	36	ASN	CA-C-N	5.17	125.07	119.85
2	EP	36	ASN	C-N-CA	5.17	125.07	119.85
1	q	33	ALA	CA-C-N	5.17	124.83	119.56
1	q	33	ALA	C-N-CA	5.17	124.83	119.56
1	w	33	ALA	CA-C-N	5.17	124.83	119.56
1	w	33	ALA	C-N-CA	5.17	124.83	119.56
1	BO	33	ALA	CA-C-N	5.17	124.83	119.56
1	BO	33	ALA	C-N-CA	5.17	124.83	119.56
1	BU	33	ALA	CA-C-N	5.17	124.83	119.56
1	BU	33	ALA	C-N-CA	5.17	124.83	119.56
1	Cq	33	ALA	CA-C-N	5.17	124.83	119.56
1	Cq	33	ALA	C-N-CA	5.17	124.83	119.56
1	Cw	33	ALA	CA-C-N	5.17	124.83	119.56
1	Cw	33	ALA	C-N-CA	5.17	124.83	119.56
2	J	36	ASN	CA-C-N	5.15	124.91	119.76
2	J	36	ASN	C-N-CA	5.15	124.91	119.76
2	AN	36	ASN	CA-C-N	5.15	124.91	119.76
2	AN	36	ASN	C-N-CA	5.15	124.91	119.76
2	Al	36	ASN	CA-C-N	5.15	124.91	119.76
2	Al	36	ASN	C-N-CA	5.15	124.91	119.76
2	BF	36	ASN	CA-C-N	5.15	124.91	119.76
2	BF	36	ASN	C-N-CA	5.15	124.91	119.76
2	Bj	36	ASN	CA-C-N	5.15	124.91	119.76
2	Bj	36	ASN	C-N-CA	5.15	124.91	119.76
2	ZV	36	ASN	CA-C-N	5.15	124.91	119.76
2	ZV	36	ASN	C-N-CA	5.15	124.91	119.76
2	CD	36	ASN	CA-C-N	5.15	124.91	119.76
2	CD	36	ASN	C-N-CA	5.15	124.91	119.76
2	DH	36	ASN	CA-C-N	5.15	124.91	119.76
2	DH	36	ASN	C-N-CA	5.15	124.91	119.76
2	Df	36	ASN	CA-C-N	5.15	124.91	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Df	36	ASN	C-N-CA	5.15	124.91	119.76
2	YX	36	ASN	CA-C-N	5.15	124.91	119.76
2	YX	36	ASN	C-N-CA	5.15	124.91	119.76
2	Ed	36	ASN	CA-C-N	5.15	124.91	119.76
2	Ed	36	ASN	C-N-CA	5.15	124.91	119.76
2	Ev	36	ASN	CA-C-N	5.15	124.91	119.76
2	Ev	36	ASN	C-N-CA	5.15	124.91	119.76
2	D	36	ASN	CA-C-N	5.15	124.91	119.76
2	D	36	ASN	C-N-CA	5.15	124.91	119.76
2	P	36	ASN	CA-C-N	5.15	124.91	119.76
2	P	36	ASN	C-N-CA	5.15	124.91	119.76
2	t	36	ASN	CA-C-N	5.15	124.91	119.76
2	t	36	ASN	C-N-CA	5.15	124.91	119.76
2	z	36	ASN	CA-C-N	5.15	124.91	119.76
2	z	36	ASN	C-N-CA	5.15	124.91	119.76
2	ZF	36	ASN	CA-C-N	5.15	124.91	119.76
2	ZF	36	ASN	C-N-CA	5.15	124.91	119.76
2	AB	36	ASN	CA-C-N	5.15	124.91	119.76
2	AB	36	ASN	C-N-CA	5.15	124.91	119.76
2	Ar	36	ASN	CA-C-N	5.15	124.91	119.76
2	Ar	36	ASN	C-N-CA	5.15	124.91	119.76
2	ZN	36	ASN	CA-C-N	5.15	124.91	119.76
2	ZN	36	ASN	C-N-CA	5.15	124.91	119.76
2	BL	36	ASN	CA-C-N	5.15	124.91	119.76
2	BL	36	ASN	C-N-CA	5.15	124.91	119.76
2	BR	36	ASN	CA-C-N	5.15	124.91	119.76
2	BR	36	ASN	C-N-CA	5.15	124.91	119.76
2	BX	36	ASN	CA-C-N	5.15	124.91	119.76
2	BX	36	ASN	C-N-CA	5.15	124.91	119.76
2	Bp	36	ASN	CA-C-N	5.15	124.91	119.76
2	Bp	36	ASN	C-N-CA	5.15	124.91	119.76
2	YB	36	ASN	CA-C-N	5.15	124.91	119.76
2	YB	36	ASN	C-N-CA	5.15	124.91	119.76
2	CJ	36	ASN	CA-C-N	5.15	124.91	119.76
2	CJ	36	ASN	C-N-CA	5.15	124.91	119.76
2	Cn	36	ASN	CA-C-N	5.15	124.91	119.76
2	Cn	36	ASN	C-N-CA	5.15	124.91	119.76
2	Ct	36	ASN	CA-C-N	5.15	124.91	119.76
2	Ct	36	ASN	C-N-CA	5.15	124.91	119.76
2	Cz	36	ASN	CA-C-N	5.15	124.91	119.76
2	Cz	36	ASN	C-N-CA	5.15	124.91	119.76
2	YJ	36	ASN	CA-C-N	5.15	124.91	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YJ	36	ASN	C-N-CA	5.15	124.91	119.76
2	Dl	36	ASN	CA-C-N	5.15	124.91	119.76
2	Dl	36	ASN	C-N-CA	5.15	124.91	119.76
2	Dx	36	ASN	CA-C-N	5.15	124.91	119.76
2	Dx	36	ASN	C-N-CA	5.15	124.91	119.76
2	EF	36	ASN	CA-C-N	5.15	124.91	119.76
2	EF	36	ASN	C-N-CA	5.15	124.91	119.76
2	EL	36	ASN	CA-C-N	5.15	124.91	119.76
2	EL	36	ASN	C-N-CA	5.15	124.91	119.76
2	ER	36	ASN	CA-C-N	5.15	124.91	119.76
2	ER	36	ASN	C-N-CA	5.15	124.91	119.76
2	Ej	36	ASN	CA-C-N	5.15	124.91	119.76
2	Ej	36	ASN	C-N-CA	5.15	124.91	119.76
1	G	33	ALA	CA-C-N	5.14	124.80	119.56
1	G	33	ALA	C-N-CA	5.14	124.80	119.56
1	AK	33	ALA	CA-C-N	5.14	124.80	119.56
1	AK	33	ALA	C-N-CA	5.14	124.80	119.56
1	Ai	33	ALA	CA-C-N	5.14	124.80	119.56
1	Ai	33	ALA	C-N-CA	5.14	124.80	119.56
1	BC	33	ALA	CA-C-N	5.14	124.80	119.56
1	BC	33	ALA	C-N-CA	5.14	124.80	119.56
1	Bg	33	ALA	CA-C-N	5.14	124.80	119.56
1	Bg	33	ALA	C-N-CA	5.14	124.80	119.56
1	By	33	ALA	CA-C-N	5.14	124.80	119.56
1	By	33	ALA	C-N-CA	5.14	124.80	119.56
1	CA	33	ALA	CA-C-N	5.14	124.80	119.56
1	CA	33	ALA	C-N-CA	5.14	124.80	119.56
1	DE	33	ALA	CA-C-N	5.14	124.80	119.56
1	DE	33	ALA	C-N-CA	5.14	124.80	119.56
1	Dc	33	ALA	CA-C-N	5.14	124.80	119.56
1	Dc	33	ALA	C-N-CA	5.14	124.80	119.56
1	YU	33	ALA	CA-C-N	5.14	124.80	119.56
1	YU	33	ALA	C-N-CA	5.14	124.80	119.56
1	Ea	33	ALA	CA-C-N	5.14	124.80	119.56
1	Ea	33	ALA	C-N-CA	5.14	124.80	119.56
1	Es	33	ALA	CA-C-N	5.14	124.80	119.56
1	Es	33	ALA	C-N-CA	5.14	124.80	119.56
2	V	36	ASN	CA-C-N	5.13	124.89	119.76
2	V	36	ASN	C-N-CA	5.13	124.89	119.76
2	b	36	ASN	CA-C-N	5.13	124.89	119.76
2	b	36	ASN	C-N-CA	5.13	124.89	119.76
2	h	36	ASN	CA-C-N	5.13	124.89	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	36	ASN	C-N-CA	5.13	124.89	119.76
2	n	36	ASN	CA-C-N	5.13	124.89	119.76
2	n	36	ASN	C-N-CA	5.13	124.89	119.76
2	AH	36	ASN	CA-C-N	5.13	124.89	119.76
2	AH	36	ASN	C-N-CA	5.13	124.89	119.76
2	AT	36	ASN	CA-C-N	5.13	124.89	119.76
2	AT	36	ASN	C-N-CA	5.13	124.89	119.76
2	AZ	36	ASN	CA-C-N	5.13	124.89	119.76
2	AZ	36	ASN	C-N-CA	5.13	124.89	119.76
2	Af	36	ASN	CA-C-N	5.13	124.89	119.76
2	Af	36	ASN	C-N-CA	5.13	124.89	119.76
2	Ax	36	ASN	CA-C-N	5.13	124.89	119.76
2	Ax	36	ASN	C-N-CA	5.13	124.89	119.76
2	ZT	36	ASN	CA-C-N	5.13	124.89	119.76
2	ZT	36	ASN	C-N-CA	5.13	124.89	119.76
2	Bd	36	ASN	CA-C-N	5.13	124.89	119.76
2	Bd	36	ASN	C-N-CA	5.13	124.89	119.76
2	Bv	36	ASN	CA-C-N	5.13	124.89	119.76
2	Bv	36	ASN	C-N-CA	5.13	124.89	119.76
2	CP	36	ASN	CA-C-N	5.13	124.89	119.76
2	CP	36	ASN	C-N-CA	5.13	124.89	119.76
2	CV	36	ASN	CA-C-N	5.13	124.89	119.76
2	CV	36	ASN	C-N-CA	5.13	124.89	119.76
2	Cb	36	ASN	CA-C-N	5.13	124.89	119.76
2	Cb	36	ASN	C-N-CA	5.13	124.89	119.76
2	Ch	36	ASN	CA-C-N	5.13	124.89	119.76
2	Ch	36	ASN	C-N-CA	5.13	124.89	119.76
2	DB	36	ASN	CA-C-N	5.13	124.89	119.76
2	DB	36	ASN	C-N-CA	5.13	124.89	119.76
2	DN	36	ASN	CA-C-N	5.13	124.89	119.76
2	DN	36	ASN	C-N-CA	5.13	124.89	119.76
2	DT	36	ASN	CA-C-N	5.13	124.89	119.76
2	DT	36	ASN	C-N-CA	5.13	124.89	119.76
2	DZ	36	ASN	CA-C-N	5.13	124.89	119.76
2	DZ	36	ASN	C-N-CA	5.13	124.89	119.76
2	Dr	36	ASN	CA-C-N	5.13	124.89	119.76
2	Dr	36	ASN	C-N-CA	5.13	124.89	119.76
2	YR	36	ASN	CA-C-N	5.13	124.89	119.76
2	YR	36	ASN	C-N-CA	5.13	124.89	119.76
2	EX	36	ASN	CA-C-N	5.13	124.89	119.76
2	EX	36	ASN	C-N-CA	5.13	124.89	119.76
2	Ep	36	ASN	CA-C-N	5.13	124.89	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Ep	36	ASN	C-N-CA	5.13	124.89	119.76
1	S	33	ALA	CA-C-N	5.13	124.79	119.56
1	S	33	ALA	C-N-CA	5.13	124.79	119.56
1	Y	33	ALA	CA-C-N	5.13	124.79	119.56
1	Y	33	ALA	C-N-CA	5.13	124.79	119.56
1	e	33	ALA	CA-C-N	5.13	124.79	119.56
1	e	33	ALA	C-N-CA	5.13	124.79	119.56
1	k	33	ALA	CA-C-N	5.13	124.79	119.56
1	k	33	ALA	C-N-CA	5.13	124.79	119.56
1	ZC	33	ALA	CA-C-N	5.13	124.79	119.56
1	ZC	33	ALA	C-N-CA	5.13	124.79	119.56
1	AE	33	ALA	CA-C-N	5.13	124.79	119.56
1	AE	33	ALA	C-N-CA	5.13	124.79	119.56
1	AQ	33	ALA	CA-C-N	5.13	124.79	119.56
1	AQ	33	ALA	C-N-CA	5.13	124.79	119.56
1	AW	33	ALA	CA-C-N	5.13	124.79	119.56
1	AW	33	ALA	C-N-CA	5.13	124.79	119.56
1	Ac	33	ALA	CA-C-N	5.13	124.79	119.56
1	Ac	33	ALA	C-N-CA	5.13	124.79	119.56
1	Au	33	ALA	CA-C-N	5.13	124.79	119.56
1	Au	33	ALA	C-N-CA	5.13	124.79	119.56
1	ZQ	33	ALA	CA-C-N	5.13	124.79	119.56
1	ZQ	33	ALA	C-N-CA	5.13	124.79	119.56
1	BI	33	ALA	CA-C-N	5.13	124.79	119.56
1	BI	33	ALA	C-N-CA	5.13	124.79	119.56
1	Ba	33	ALA	CA-C-N	5.13	124.79	119.56
1	Ba	33	ALA	C-N-CA	5.13	124.79	119.56
1	Bs	33	ALA	CA-C-N	5.13	124.79	119.56
1	Bs	33	ALA	C-N-CA	5.13	124.79	119.56
1	CM	33	ALA	CA-C-N	5.13	124.79	119.56
1	CM	33	ALA	C-N-CA	5.13	124.79	119.56
1	CS	33	ALA	CA-C-N	5.13	124.79	119.56
1	CS	33	ALA	C-N-CA	5.13	124.79	119.56
1	CY	33	ALA	CA-C-N	5.13	124.79	119.56
1	CY	33	ALA	C-N-CA	5.13	124.79	119.56
1	Ce	33	ALA	CA-C-N	5.13	124.79	119.56
1	Ce	33	ALA	C-N-CA	5.13	124.79	119.56
1	Ck	33	ALA	CA-C-N	5.13	124.79	119.56
1	Ck	33	ALA	C-N-CA	5.13	124.79	119.56
1	YM	33	ALA	CA-C-N	5.13	124.79	119.56
1	YM	33	ALA	C-N-CA	5.13	124.79	119.56
1	DK	33	ALA	CA-C-N	5.13	124.79	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DK	33	ALA	C-N-CA	5.13	124.79	119.56
1	DQ	33	ALA	CA-C-N	5.13	124.79	119.56
1	DQ	33	ALA	C-N-CA	5.13	124.79	119.56
1	DW	33	ALA	CA-C-N	5.13	124.79	119.56
1	DW	33	ALA	C-N-CA	5.13	124.79	119.56
1	Do	33	ALA	CA-C-N	5.13	124.79	119.56
1	Do	33	ALA	C-N-CA	5.13	124.79	119.56
1	YO	33	ALA	CA-C-N	5.13	124.79	119.56
1	YO	33	ALA	C-N-CA	5.13	124.79	119.56
1	EC	33	ALA	CA-C-N	5.13	124.79	119.56
1	EC	33	ALA	C-N-CA	5.13	124.79	119.56
1	EI	33	ALA	CA-C-N	5.13	124.79	119.56
1	EI	33	ALA	C-N-CA	5.13	124.79	119.56
1	EO	33	ALA	CA-C-N	5.13	124.79	119.56
1	EO	33	ALA	C-N-CA	5.13	124.79	119.56
1	EU	33	ALA	CA-C-N	5.13	124.79	119.56
1	EU	33	ALA	C-N-CA	5.13	124.79	119.56
1	Em	33	ALA	CA-C-N	5.13	124.79	119.56
1	Em	33	ALA	C-N-CA	5.13	124.79	119.56
1	A	33	ALA	CA-C-N	5.13	124.79	119.56
1	A	33	ALA	C-N-CA	5.13	124.79	119.56
1	M	33	ALA	CA-C-N	5.13	124.79	119.56
1	M	33	ALA	C-N-CA	5.13	124.79	119.56
1	ZI	33	ALA	CA-C-N	5.13	124.79	119.56
1	ZI	33	ALA	C-N-CA	5.13	124.79	119.56
1	Ao	33	ALA	CA-C-N	5.13	124.79	119.56
1	Ao	33	ALA	C-N-CA	5.13	124.79	119.56
1	ZK	33	ALA	CA-C-N	5.13	124.79	119.56
1	ZK	33	ALA	C-N-CA	5.13	124.79	119.56
1	Bm	33	ALA	CA-C-N	5.13	124.79	119.56
1	Bm	33	ALA	C-N-CA	5.13	124.79	119.56
1	ZY	33	ALA	CA-C-N	5.13	124.79	119.56
1	ZY	33	ALA	C-N-CA	5.13	124.79	119.56
1	CG	33	ALA	CA-C-N	5.13	124.79	119.56
1	CG	33	ALA	C-N-CA	5.13	124.79	119.56
1	YG	33	ALA	CA-C-N	5.13	124.79	119.56
1	YG	33	ALA	C-N-CA	5.13	124.79	119.56
1	Di	33	ALA	CA-C-N	5.13	124.79	119.56
1	Di	33	ALA	C-N-CA	5.13	124.79	119.56
1	Du	33	ALA	CA-C-N	5.13	124.79	119.56
1	Du	33	ALA	C-N-CA	5.13	124.79	119.56
1	Eg	33	ALA	CA-C-N	5.13	124.79	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Eg	33	ALA	C-N-CA	5.13	124.79	119.56
1	c	94	GLU	CA-C-N	-5.08	116.49	123.14
1	c	94	GLU	C-N-CA	-5.08	116.49	123.14
1	i	94	GLU	CA-C-N	-5.08	116.49	123.14
1	i	94	GLU	C-N-CA	-5.08	116.49	123.14
1	o	94	GLU	CA-C-N	-5.08	116.49	123.14
1	o	94	GLU	C-N-CA	-5.08	116.49	123.14
1	AU	94	GLU	CA-C-N	-5.08	116.49	123.14
1	AU	94	GLU	C-N-CA	-5.08	116.49	123.14
1	Aa	94	GLU	CA-C-N	-5.08	116.49	123.14
1	Aa	94	GLU	C-N-CA	-5.08	116.49	123.14
1	Ag	94	GLU	CA-C-N	-5.08	116.49	123.14
1	Ag	94	GLU	C-N-CA	-5.08	116.49	123.14
1	CW	94	GLU	CA-C-N	-5.08	116.49	123.14
1	CW	94	GLU	C-N-CA	-5.08	116.49	123.14
1	Cc	94	GLU	CA-C-N	-5.08	116.49	123.14
1	Cc	94	GLU	C-N-CA	-5.08	116.49	123.14
1	Ci	94	GLU	CA-C-N	-5.08	116.49	123.14
1	Ci	94	GLU	C-N-CA	-5.08	116.49	123.14
1	DO	94	GLU	CA-C-N	-5.08	116.49	123.14
1	DO	94	GLU	C-N-CA	-5.08	116.49	123.14
1	DU	94	GLU	CA-C-N	-5.08	116.49	123.14
1	DU	94	GLU	C-N-CA	-5.08	116.49	123.14
1	Da	94	GLU	CA-C-N	-5.08	116.49	123.14
1	Da	94	GLU	C-N-CA	-5.08	116.49	123.14
1	G	60	VAL	N-CA-C	5.07	115.28	107.77
1	AK	60	VAL	N-CA-C	5.07	115.28	107.77
1	BC	60	VAL	N-CA-C	5.07	115.28	107.77
1	By	60	VAL	N-CA-C	5.07	115.28	107.77
1	DE	60	VAL	N-CA-C	5.07	115.28	107.77
1	Ea	60	VAL	N-CA-C	5.07	115.28	107.77
1	E	94	GLU	CA-C-N	-5.07	116.50	123.14
1	E	94	GLU	C-N-CA	-5.07	116.50	123.14
1	Q	94	GLU	CA-C-N	-5.07	116.50	123.14
1	Q	94	GLU	C-N-CA	-5.07	116.50	123.14
1	AC	94	GLU	CA-C-N	-5.07	116.50	123.14
1	AC	94	GLU	C-N-CA	-5.07	116.50	123.14
1	As	94	GLU	CA-C-N	-5.07	116.50	123.14
1	As	94	GLU	C-N-CA	-5.07	116.50	123.14
1	ZO	94	GLU	CA-C-N	-5.07	116.50	123.14
1	ZO	94	GLU	C-N-CA	-5.07	116.50	123.14
1	Bq	94	GLU	CA-C-N	-5.07	116.50	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bq	94	GLU	C-N-CA	-5.07	116.50	123.14
1	YC	94	GLU	CA-C-N	-5.07	116.50	123.14
1	YC	94	GLU	C-N-CA	-5.07	116.50	123.14
1	CK	94	GLU	CA-C-N	-5.07	116.50	123.14
1	CK	94	GLU	C-N-CA	-5.07	116.50	123.14
1	YK	94	GLU	CA-C-N	-5.07	116.50	123.14
1	YK	94	GLU	C-N-CA	-5.07	116.50	123.14
1	Dm	94	GLU	CA-C-N	-5.07	116.50	123.14
1	Dm	94	GLU	C-N-CA	-5.07	116.50	123.14
1	Dy	94	GLU	CA-C-N	-5.07	116.50	123.14
1	Dy	94	GLU	C-N-CA	-5.07	116.50	123.14
1	Ek	94	GLU	CA-C-N	-5.07	116.50	123.14
1	Ek	94	GLU	C-N-CA	-5.07	116.50	123.14
1	W	94	GLU	CA-C-N	-5.06	116.51	123.14
1	W	94	GLU	C-N-CA	-5.06	116.51	123.14
1	AI	94	GLU	CA-C-N	-5.06	116.51	123.14
1	AI	94	GLU	C-N-CA	-5.06	116.51	123.14
1	Ay	94	GLU	CA-C-N	-5.06	116.51	123.14
1	Ay	94	GLU	C-N-CA	-5.06	116.51	123.14
1	BA	94	GLU	CA-C-N	-5.06	116.51	123.14
1	BA	94	GLU	C-N-CA	-5.06	116.51	123.14
1	Be	94	GLU	CA-C-N	-5.06	116.51	123.14
1	Be	94	GLU	C-N-CA	-5.06	116.51	123.14
1	Bw	94	GLU	CA-C-N	-5.06	116.51	123.14
1	Bw	94	GLU	C-N-CA	-5.06	116.51	123.14
1	CQ	94	GLU	CA-C-N	-5.06	116.51	123.14
1	CQ	94	GLU	C-N-CA	-5.06	116.51	123.14
1	DC	94	GLU	CA-C-N	-5.06	116.51	123.14
1	DC	94	GLU	C-N-CA	-5.06	116.51	123.14
1	Ds	94	GLU	CA-C-N	-5.06	116.51	123.14
1	Ds	94	GLU	C-N-CA	-5.06	116.51	123.14
1	YS	94	GLU	CA-C-N	-5.06	116.51	123.14
1	YS	94	GLU	C-N-CA	-5.06	116.51	123.14
1	EY	94	GLU	CA-C-N	-5.06	116.51	123.14
1	EY	94	GLU	C-N-CA	-5.06	116.51	123.14
1	Eq	94	GLU	CA-C-N	-5.06	116.51	123.14
1	Eq	94	GLU	C-N-CA	-5.06	116.51	123.14
1	S	60	VAL	N-CA-C	5.05	115.25	107.77
1	q	60	VAL	N-CA-C	5.05	115.25	107.77
1	AE	60	VAL	N-CA-C	5.05	115.25	107.77
1	Au	60	VAL	N-CA-C	5.05	115.25	107.77
1	ZQ	60	VAL	N-CA-C	5.05	115.25	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BO	60	VAL	N-CA-C	5.05	115.25	107.77
1	Ba	60	VAL	N-CA-C	5.05	115.25	107.77
1	Bs	60	VAL	N-CA-C	5.05	115.25	107.77
1	CM	60	VAL	N-CA-C	5.05	115.25	107.77
1	Cq	60	VAL	N-CA-C	5.05	115.25	107.77
1	YM	60	VAL	N-CA-C	5.05	115.25	107.77
1	Do	60	VAL	N-CA-C	5.05	115.25	107.77
1	YO	60	VAL	N-CA-C	5.05	115.25	107.77
1	EC	60	VAL	N-CA-C	5.05	115.25	107.77
1	EI	60	VAL	N-CA-C	5.05	115.25	107.77
1	EO	60	VAL	N-CA-C	5.05	115.25	107.77
1	EU	60	VAL	N-CA-C	5.05	115.25	107.77
1	Em	60	VAL	N-CA-C	5.05	115.25	107.77
1	K	94	GLU	CA-C-N	-5.04	116.54	123.14
1	K	94	GLU	C-N-CA	-5.04	116.54	123.14
1	AO	94	GLU	CA-C-N	-5.04	116.54	123.14
1	AO	94	GLU	C-N-CA	-5.04	116.54	123.14
1	Am	94	GLU	CA-C-N	-5.04	116.54	123.14
1	Am	94	GLU	C-N-CA	-5.04	116.54	123.14
1	BG	94	GLU	CA-C-N	-5.04	116.54	123.14
1	BG	94	GLU	C-N-CA	-5.04	116.54	123.14
1	Bk	94	GLU	CA-C-N	-5.04	116.54	123.14
1	Bk	94	GLU	C-N-CA	-5.04	116.54	123.14
1	ZW	94	GLU	CA-C-N	-5.04	116.54	123.14
1	ZW	94	GLU	C-N-CA	-5.04	116.54	123.14
1	CE	94	GLU	CA-C-N	-5.04	116.54	123.14
1	CE	94	GLU	C-N-CA	-5.04	116.54	123.14
1	DI	94	GLU	CA-C-N	-5.04	116.54	123.14
1	DI	94	GLU	C-N-CA	-5.04	116.54	123.14
1	Dg	94	GLU	CA-C-N	-5.04	116.54	123.14
1	Dg	94	GLU	C-N-CA	-5.04	116.54	123.14
1	EA	94	GLU	CA-C-N	-5.04	116.54	123.14
1	EA	94	GLU	C-N-CA	-5.04	116.54	123.14
1	Ee	94	GLU	CA-C-N	-5.04	116.54	123.14
1	Ee	94	GLU	C-N-CA	-5.04	116.54	123.14
1	Ew	94	GLU	CA-C-N	-5.04	116.54	123.14
1	Ew	94	GLU	C-N-CA	-5.04	116.54	123.14
1	A	60	VAL	N-CA-C	5.03	115.22	107.77
1	M	60	VAL	N-CA-C	5.03	115.22	107.77
1	Y	60	VAL	N-CA-C	5.03	115.22	107.77
1	e	60	VAL	N-CA-C	5.03	115.22	107.77
1	k	60	VAL	N-CA-C	5.03	115.22	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	u	94	GLU	CA-C-N	-5.03	116.55	123.14
1	u	94	GLU	C-N-CA	-5.03	116.55	123.14
1	ZA	94	GLU	CA-C-N	-5.03	116.55	123.14
1	ZA	94	GLU	C-N-CA	-5.03	116.55	123.14
1	ZG	94	GLU	CA-C-N	-5.03	116.55	123.14
1	ZG	94	GLU	C-N-CA	-5.03	116.55	123.14
1	ZI	60	VAL	N-CA-C	5.03	115.22	107.77
1	AQ	60	VAL	N-CA-C	5.03	115.22	107.77
1	AW	60	VAL	N-CA-C	5.03	115.22	107.77
1	Ac	60	VAL	N-CA-C	5.03	115.22	107.77
1	Ai	60	VAL	N-CA-C	5.03	115.21	107.77
1	Ao	60	VAL	N-CA-C	5.03	115.22	107.77
1	ZK	60	VAL	N-CA-C	5.03	115.22	107.77
1	BM	94	GLU	CA-C-N	-5.03	116.55	123.14
1	BM	94	GLU	C-N-CA	-5.03	116.55	123.14
1	BS	94	GLU	CA-C-N	-5.03	116.55	123.14
1	BS	94	GLU	C-N-CA	-5.03	116.55	123.14
1	BY	94	GLU	CA-C-N	-5.03	116.55	123.14
1	BY	94	GLU	C-N-CA	-5.03	116.55	123.14
1	Bg	60	VAL	N-CA-C	5.03	115.21	107.77
1	Bm	60	VAL	N-CA-C	5.03	115.22	107.77
1	ZY	60	VAL	N-CA-C	5.03	115.22	107.77
1	CA	60	VAL	N-CA-C	5.03	115.21	107.77
1	CG	60	VAL	N-CA-C	5.03	115.22	107.77
1	CS	60	VAL	N-CA-C	5.03	115.22	107.77
1	CY	60	VAL	N-CA-C	5.03	115.22	107.77
1	Ce	60	VAL	N-CA-C	5.03	115.22	107.77
1	Co	94	GLU	CA-C-N	-5.03	116.55	123.14
1	Co	94	GLU	C-N-CA	-5.03	116.55	123.14
1	Cu	94	GLU	CA-C-N	-5.03	116.55	123.14
1	Cu	94	GLU	C-N-CA	-5.03	116.55	123.14
1	YE	94	GLU	CA-C-N	-5.03	116.55	123.14
1	YE	94	GLU	C-N-CA	-5.03	116.55	123.14
1	YG	60	VAL	N-CA-C	5.03	115.22	107.77
1	DK	60	VAL	N-CA-C	5.03	115.22	107.77
1	DQ	60	VAL	N-CA-C	5.03	115.22	107.77
1	DW	60	VAL	N-CA-C	5.03	115.22	107.77
1	Dc	60	VAL	N-CA-C	5.03	115.21	107.77
1	Di	60	VAL	N-CA-C	5.03	115.22	107.77
1	Du	60	VAL	N-CA-C	5.03	115.22	107.77
1	YU	60	VAL	N-CA-C	5.03	115.21	107.77
1	EG	94	GLU	CA-C-N	-5.03	116.55	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EG	94	GLU	C-N-CA	-5.03	116.55	123.14
1	EM	94	GLU	CA-C-N	-5.03	116.55	123.14
1	EM	94	GLU	C-N-CA	-5.03	116.55	123.14
1	ES	94	GLU	CA-C-N	-5.03	116.55	123.14
1	ES	94	GLU	C-N-CA	-5.03	116.55	123.14
1	Eg	60	VAL	N-CA-C	5.03	115.22	107.77
1	Es	60	VAL	N-CA-C	5.03	115.21	107.77
1	w	60	VAL	N-CA-C	5.03	115.21	107.77
1	ZC	60	VAL	N-CA-C	5.03	115.21	107.77
1	BI	60	VAL	N-CA-C	5.03	115.21	107.77
1	BU	60	VAL	N-CA-C	5.03	115.21	107.77
1	Ck	60	VAL	N-CA-C	5.03	115.21	107.77
1	Cw	60	VAL	N-CA-C	5.03	115.21	107.77
1	Y	35	VAL	N-CA-C	-5.02	105.53	111.00
1	e	35	VAL	N-CA-C	-5.02	105.53	111.00
1	k	35	VAL	N-CA-C	-5.02	105.53	111.00
1	AW	35	VAL	N-CA-C	-5.02	105.53	111.00
1	CY	35	VAL	N-CA-C	-5.02	105.53	111.00
1	DW	35	VAL	N-CA-C	-5.02	105.53	111.00
1	A	35	VAL	N-CA-C	-5.00	105.55	111.00
1	M	35	VAL	N-CA-C	-5.00	105.55	111.00
1	ZI	35	VAL	N-CA-C	-5.00	105.55	111.00
1	Ao	35	VAL	N-CA-C	-5.00	105.55	111.00
1	ZK	35	VAL	N-CA-C	-5.00	105.55	111.00
1	Bm	35	VAL	N-CA-C	-5.00	105.55	111.00
1	ZY	35	VAL	N-CA-C	-5.00	105.55	111.00
1	CG	35	VAL	N-CA-C	-5.00	105.55	111.00
1	YG	35	VAL	N-CA-C	-5.00	105.55	111.00
1	Di	35	VAL	N-CA-C	-5.00	105.55	111.00
1	Du	35	VAL	N-CA-C	-5.00	105.55	111.00
1	Eg	35	VAL	N-CA-C	-5.00	105.55	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	808	0	851	3	0
1	AA	808	0	851	3	0
1	AC	808	0	851	6	0
1	AE	808	0	851	2	0
1	AG	808	0	851	4	0
1	AI	808	0	851	5	0
1	AK	808	0	851	2	0
1	AM	808	0	851	4	0
1	AO	808	0	851	5	0
1	AQ	808	0	851	3	0
1	AS	808	0	851	3	0
1	AU	808	0	851	6	0
1	AW	808	0	851	4	0
1	AY	808	0	851	3	0
1	Aa	808	0	851	6	0
1	Ac	808	0	851	4	0
1	Ae	808	0	851	4	0
1	Ag	808	0	851	5	0
1	Ai	808	0	851	2	0
1	Ak	808	0	851	3	0
1	Am	808	0	851	6	0
1	Ao	808	0	851	3	0
1	Aq	808	0	851	3	0
1	As	808	0	851	6	0
1	Au	808	0	851	2	0
1	Aw	808	0	851	4	0
1	Ay	808	0	851	5	0
1	BA	808	0	851	5	0
1	BC	808	0	851	4	0
1	BE	808	0	851	4	0
1	BG	808	0	851	5	0
1	BI	808	0	851	4	0
1	BK	808	0	851	3	0
1	BM	808	0	851	5	0
1	BO	808	0	851	3	0
1	BQ	808	0	851	3	0
1	BS	808	0	851	7	0
1	BU	808	0	851	2	0
1	BW	808	0	851	3	0
1	BY	808	0	851	6	0
1	Ba	808	0	851	2	0
1	Bc	808	0	851	3	0
1	Be	808	0	851	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Bg	808	0	851	4	0
1	Bi	808	0	851	3	0
1	Bk	808	0	851	5	0
1	Bm	808	0	851	3	0
1	Bo	808	0	851	3	0
1	Bq	808	0	851	5	0
1	Bs	808	0	851	3	0
1	Bu	808	0	851	3	0
1	Bw	808	0	851	5	0
1	By	808	0	851	3	0
1	C	808	0	851	3	0
1	CA	808	0	851	4	0
1	CC	808	0	851	4	0
1	CE	808	0	851	5	0
1	CG	808	0	851	3	0
1	CI	808	0	851	2	0
1	CK	808	0	851	5	0
1	CM	808	0	851	3	0
1	CO	808	0	851	3	0
1	CQ	808	0	851	5	0
1	CS	808	0	851	3	0
1	CU	808	0	851	3	0
1	CW	808	0	851	5	0
1	CY	808	0	851	4	0
1	Ca	808	0	851	3	0
1	Cc	808	0	851	5	0
1	Ce	808	0	851	4	0
1	Cg	808	0	851	4	0
1	Ci	808	0	851	5	0
1	Ck	808	0	851	5	0
1	Cm	808	0	851	3	0
1	Co	808	0	851	6	0
1	Cq	808	0	851	3	0
1	Cs	808	0	851	3	0
1	Cu	808	0	851	5	0
1	Cw	808	0	851	2	0
1	Cy	808	0	851	3	0
1	DA	808	0	851	3	0
1	DC	808	0	851	7	0
1	DE	808	0	851	4	0
1	DG	808	0	851	3	0
1	DI	808	0	851	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DK	808	0	851	4	0
1	DM	808	0	851	3	0
1	DO	808	0	851	5	0
1	DQ	808	0	851	4	0
1	DS	808	0	851	4	0
1	DU	808	0	851	5	0
1	DW	808	0	851	3	0
1	DY	808	0	851	3	0
1	Da	808	0	851	5	0
1	Dc	808	0	851	4	0
1	De	808	0	851	3	0
1	Dg	808	0	851	8	0
1	Di	808	0	851	4	0
1	Dk	808	0	851	4	0
1	Dm	808	0	851	6	0
1	Do	808	0	851	4	0
1	Dq	808	0	851	3	0
1	Ds	808	0	851	6	0
1	Du	808	0	851	4	0
1	Dw	808	0	851	3	0
1	Dy	808	0	851	5	0
1	E	808	0	851	5	0
1	EA	808	0	851	5	0
1	EC	808	0	851	3	0
1	EE	808	0	851	3	0
1	EG	808	0	851	6	0
1	EI	808	0	851	2	0
1	EK	808	0	851	3	0
1	EM	808	0	851	5	0
1	EO	808	0	851	4	0
1	EQ	808	0	851	3	0
1	ES	808	0	851	6	0
1	EU	808	0	851	3	0
1	EW	808	0	851	3	0
1	EY	808	0	851	5	0
1	Ea	808	0	851	3	0
1	Ec	808	0	851	4	0
1	Ee	808	0	851	5	0
1	Eg	808	0	851	3	0
1	Ei	808	0	851	3	0
1	Ek	808	0	851	5	0
1	Em	808	0	851	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Eo	808	0	851	3	0
1	Eq	808	0	851	6	0
1	Es	808	0	851	4	0
1	Eu	808	0	851	3	0
1	Ew	808	0	851	5	0
1	G	808	0	851	3	0
1	I	808	0	851	3	0
1	K	808	0	851	5	0
1	M	808	0	851	4	0
1	O	808	0	851	3	0
1	Q	808	0	851	5	0
1	S	808	0	851	3	0
1	U	808	0	851	3	0
1	W	808	0	851	5	0
1	Y	808	0	851	4	0
1	YA	808	0	851	3	0
1	YC	808	0	851	5	0
1	YE	808	0	851	5	0
1	YG	808	0	851	4	0
1	YI	808	0	851	3	0
1	YK	808	0	851	6	0
1	YM	808	0	851	4	0
1	YO	808	0	851	3	0
1	YQ	808	0	851	4	0
1	YS	808	0	851	6	0
1	YU	808	0	851	3	0
1	YW	808	0	851	3	0
1	ZA	808	0	851	5	0
1	ZC	808	0	851	3	0
1	ZE	808	0	851	3	0
1	ZG	808	0	851	6	0
1	ZI	808	0	851	3	0
1	ZK	808	0	851	2	0
1	ZM	808	0	851	2	0
1	ZO	808	0	851	5	0
1	ZQ	808	0	851	3	0
1	ZS	808	0	851	3	0
1	ZU	808	0	851	4	0
1	ZW	808	0	851	5	0
1	ZY	808	0	851	4	0
1	a	808	0	851	5	0
1	c	808	0	851	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	808	0	851	3	0
1	g	808	0	851	3	0
1	i	808	0	851	6	0
1	k	808	0	851	4	0
1	m	808	0	851	3	0
1	o	808	0	851	6	0
1	q	808	0	851	2	0
1	s	808	0	851	3	0
1	u	808	0	851	6	0
1	w	808	0	851	4	0
1	y	808	0	851	3	0
2	AB	2267	0	2393	5	0
2	AD	2267	0	2393	8	0
2	AF	2267	0	2393	6	0
2	AH	2267	0	2393	5	0
2	AJ	2267	0	2393	8	0
2	AL	2267	0	2393	5	0
2	AN	2267	0	2393	5	0
2	AP	2267	0	2393	7	0
2	AR	2267	0	2393	4	0
2	AT	2267	0	2393	6	0
2	AV	2267	0	2393	8	0
2	AX	2267	0	2393	3	0
2	AZ	2267	0	2393	5	0
2	Ab	2267	0	2393	7	0
2	Ad	2267	0	2393	4	0
2	Af	2267	0	2393	5	0
2	Ah	2267	0	2393	7	0
2	Aj	2267	0	2393	5	0
2	Al	2267	0	2393	5	0
2	An	2267	0	2393	7	0
2	Ap	2267	0	2393	4	0
2	Ar	2267	0	2393	5	0
2	At	2267	0	2393	7	0
2	Av	2267	0	2393	6	0
2	Ax	2267	0	2393	5	0
2	Az	2267	0	2393	8	0
2	B	2267	0	2393	4	0
2	BB	2267	0	2393	7	0
2	BD	2267	0	2393	4	0
2	BF	2267	0	2393	6	0
2	BH	2267	0	2393	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BJ	2267	0	2393	4	0
2	BL	2267	0	2393	6	0
2	BN	2267	0	2393	8	0
2	BP	2267	0	2393	6	0
2	BR	2267	0	2393	6	0
2	BT	2267	0	2393	8	0
2	BV	2267	0	2393	4	0
2	BX	2267	0	2393	5	0
2	BZ	2267	0	2393	7	0
2	Bb	2267	0	2393	4	0
2	Bd	2267	0	2393	6	0
2	Bf	2267	0	2393	7	0
2	Bh	2267	0	2393	4	0
2	Bj	2267	0	2393	5	0
2	Bl	2267	0	2393	7	0
2	Bn	2267	0	2393	4	0
2	Bp	2267	0	2393	6	0
2	Br	2267	0	2393	7	0
2	Bt	2267	0	2393	6	0
2	Bv	2267	0	2393	6	0
2	Bx	2267	0	2393	7	0
2	Bz	2267	0	2393	5	0
2	CB	2267	0	2393	4	0
2	CD	2267	0	2393	6	0
2	CF	2267	0	2393	7	0
2	CH	2267	0	2393	3	0
2	CJ	2267	0	2393	6	0
2	CL	2267	0	2393	7	0
2	CN	2267	0	2393	5	0
2	CP	2267	0	2393	5	0
2	CR	2267	0	2393	7	0
2	CT	2267	0	2393	5	0
2	CV	2267	0	2393	7	0
2	CX	2267	0	2393	8	0
2	CZ	2267	0	2393	5	0
2	Cb	2267	0	2393	7	0
2	Cd	2267	0	2393	8	0
2	Cf	2267	0	2393	6	0
2	Ch	2267	0	2393	6	0
2	Cj	2267	0	2393	8	0
2	Cl	2267	0	2393	5	0
2	Cn	2267	0	2393	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Cp	2267	0	2393	7	0
2	Cr	2267	0	2393	4	0
2	Ct	2267	0	2393	7	0
2	Cv	2267	0	2393	8	0
2	Cx	2267	0	2393	6	0
2	Cz	2267	0	2393	5	0
2	D	2267	0	2393	6	0
2	DB	2267	0	2393	5	0
2	DD	2267	0	2393	9	0
2	DF	2267	0	2393	4	0
2	DH	2267	0	2393	7	0
2	DJ	2267	0	2393	7	0
2	DL	2267	0	2393	5	0
2	DN	2267	0	2393	6	0
2	DP	2267	0	2393	8	0
2	DR	2267	0	2393	6	0
2	DT	2267	0	2393	7	0
2	DV	2267	0	2393	9	0
2	DX	2267	0	2393	6	0
2	DZ	2267	0	2393	6	0
2	Db	2267	0	2393	9	0
2	Dd	2267	0	2393	4	0
2	Df	2267	0	2393	6	0
2	Dh	2267	0	2393	7	0
2	Dj	2267	0	2393	4	0
2	Di	2267	0	2393	7	0
2	Dn	2267	0	2393	8	0
2	Dp	2267	0	2393	6	0
2	Dr	2267	0	2393	6	0
2	Dt	2267	0	2393	8	0
2	Dv	2267	0	2393	5	0
2	Dx	2267	0	2393	5	0
2	Dz	2267	0	2393	8	0
2	EB	2267	0	2393	8	0
2	ED	2267	0	2393	4	0
2	EF	2267	0	2393	7	0
2	EH	2267	0	2393	8	0
2	EJ	2267	0	2393	5	0
2	EL	2267	0	2393	5	0
2	EN	2267	0	2393	7	0
2	EP	2267	0	2393	5	0
2	ER	2267	0	2393	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	ET	2267	0	2393	7	0
2	EV	2267	0	2393	6	0
2	EX	2267	0	2393	6	0
2	EZ	2267	0	2393	7	0
2	Eb	2267	0	2393	4	0
2	Ed	2267	0	2393	6	0
2	Ef	2267	0	2393	6	0
2	Eh	2267	0	2393	6	0
2	Ej	2267	0	2393	6	0
2	El	2267	0	2393	8	0
2	En	2267	0	2393	5	0
2	Ep	2267	0	2393	5	0
2	Er	2267	0	2393	8	0
2	Et	2267	0	2393	4	0
2	Ev	2267	0	2393	5	0
2	Ex	2267	0	2393	6	0
2	F	2267	0	2393	7	0
2	H	2267	0	2393	5	0
2	J	2267	0	2393	7	0
2	L	2267	0	2393	8	0
2	N	2267	0	2393	5	0
2	P	2267	0	2393	5	0
2	R	2267	0	2393	8	0
2	T	2267	0	2393	5	0
2	V	2267	0	2393	5	0
2	X	2267	0	2393	7	0
2	YB	2267	0	2393	6	0
2	YD	2267	0	2393	7	0
2	YF	2267	0	2393	8	0
2	YH	2267	0	2393	4	0
2	YJ	2267	0	2393	7	0
2	YL	2267	0	2393	8	0
2	YN	2267	0	2393	6	0
2	YP	2267	0	2393	5	0
2	YR	2267	0	2393	5	0
2	YT	2267	0	2393	7	0
2	YV	2267	0	2393	5	0
2	YX	2267	0	2393	6	0
2	Z	2267	0	2393	5	0
2	ZB	2267	0	2393	8	0
2	ZD	2267	0	2393	6	0
2	ZF	2267	0	2393	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	ZH	2267	0	2393	8	0
2	ZJ	2267	0	2393	5	0
2	ZL	2267	0	2393	4	0
2	ZN	2267	0	2393	6	0
2	ZP	2267	0	2393	7	0
2	ZR	2267	0	2393	5	0
2	ZT	2267	0	2393	5	0
2	ZV	2267	0	2393	6	0
2	ZX	2267	0	2393	7	0
2	ZZ	2267	0	2393	5	0
2	b	2267	0	2393	5	0
2	d	2267	0	2393	8	0
2	f	2267	0	2393	4	0
2	h	2267	0	2393	6	0
2	j	2267	0	2393	8	0
2	l	2267	0	2393	3	0
2	n	2267	0	2393	5	0
2	p	2267	0	2393	7	0
2	r	2267	0	2393	4	0
2	t	2267	0	2393	6	0
2	v	2267	0	2393	7	0
2	x	2267	0	2393	4	0
2	z	2267	0	2393	6	0
All	All	553500	0	583920	1575	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (1575) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:123:GLU:OE2	2:d:170:LYS:NZ	2.31	0.64
2:Ah:123:GLU:OE2	2:Ah:170:LYS:NZ	2.31	0.64
2:L:123:GLU:OE2	2:L:170:LYS:NZ	2.31	0.64
2:Cv:123:GLU:OE2	2:Cv:170:LYS:NZ	2.31	0.64
2:EH:123:GLU:OE2	2:EH:170:LYS:NZ	2.31	0.64
2:ZP:123:GLU:OE2	2:ZP:170:LYS:NZ	2.31	0.64
2:Bl:123:GLU:OE2	2:Bl:170:LYS:NZ	2.31	0.64
2:Dh:123:GLU:OE2	2:Dh:170:LYS:NZ	2.31	0.64
2:EB:123:GLU:OE2	2:EB:170:LYS:NZ	2.31	0.64
2:j:123:GLU:OE2	2:j:170:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AV:123:GLU:OE2	2:AV:170:LYS:NZ	2.31	0.63
2:CL:123:GLU:OE2	2:CL:170:LYS:NZ	2.31	0.63
2:Ex:123:GLU:OE2	2:Ex:170:LYS:NZ	2.31	0.63
2:DD:123:GLU:OE2	2:DD:170:LYS:NZ	2.31	0.63
2:BH:123:GLU:OE2	2:BH:170:LYS:NZ	2.31	0.63
2:CF:123:GLU:OE2	2:CF:170:LYS:NZ	2.31	0.63
2:Cp:123:GLU:OE2	2:Cp:170:LYS:NZ	2.31	0.63
2:F:123:GLU:OE2	2:F:170:LYS:NZ	2.31	0.63
2:Dt:123:GLU:OE2	2:Dt:170:LYS:NZ	2.31	0.63
2:AJ:123:GLU:OE2	2:AJ:170:LYS:NZ	2.31	0.63
2:Az:123:GLU:OE2	2:Az:170:LYS:NZ	2.31	0.63
2:Cj:123:GLU:OE2	2:Cj:170:LYS:NZ	2.31	0.63
2:ET:123:GLU:OE2	2:ET:170:LYS:NZ	2.31	0.63
2:El:123:GLU:OE2	2:El:170:LYS:NZ	2.31	0.63
2:DV:123:GLU:OE2	2:DV:170:LYS:NZ	2.31	0.63
2:YD:123:GLU:OE2	2:YD:170:LYS:NZ	2.31	0.63
2:BB:123:GLU:OE2	2:BB:170:LYS:NZ	2.31	0.62
2:CR:123:GLU:OE2	2:CR:170:LYS:NZ	2.31	0.62
2:YL:123:GLU:OE2	2:YL:170:LYS:NZ	2.31	0.62
2:Dn:123:GLU:OE2	2:Dn:170:LYS:NZ	2.31	0.62
2:EZ:123:GLU:OE2	2:EZ:170:LYS:NZ	2.31	0.62
2:BZ:123:GLU:OE2	2:BZ:170:LYS:NZ	2.31	0.62
2:Bx:123:GLU:OE2	2:Bx:170:LYS:NZ	2.31	0.62
2:v:123:GLU:OE2	2:v:170:LYS:NZ	2.31	0.62
2:ZH:123:GLU:OE2	2:ZH:170:LYS:NZ	2.31	0.62
2:R:123:GLU:OE2	2:R:170:LYS:NZ	2.31	0.62
2:Dz:123:GLU:OE2	2:Dz:170:LYS:NZ	2.31	0.62
2:BT:123:GLU:OE2	2:BT:170:LYS:NZ	2.31	0.62
2:Ab:123:GLU:OE2	2:Ab:170:LYS:NZ	2.31	0.62
2:Er:123:GLU:OE2	2:Er:170:LYS:NZ	2.31	0.62
2:Bf:123:GLU:OE2	2:Bf:170:LYS:NZ	2.31	0.62
2:YF:123:GLU:OE2	2:YF:170:LYS:NZ	2.31	0.62
2:p:123:GLU:OE2	2:p:170:LYS:NZ	2.31	0.61
2:ZB:123:GLU:OE2	2:ZB:170:LYS:NZ	2.31	0.61
2:ZX:123:GLU:OE2	2:ZX:170:LYS:NZ	2.31	0.61
2:Cf:123:GLU:OE2	2:Cf:170:LYS:NZ	2.33	0.61
2:YT:123:GLU:OE2	2:YT:170:LYS:NZ	2.31	0.61
2:Ef:123:GLU:OE2	2:Ef:170:LYS:NZ	2.31	0.61
2:B:123:GLU:OE2	2:B:170:LYS:NZ	2.34	0.61
2:X:123:GLU:OE2	2:X:170:LYS:NZ	2.31	0.61
2:l:123:GLU:OE2	2:l:170:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:123:GLU:OE2	2:AD:170:LYS:NZ	2.31	0.61
2:AP:123:GLU:OE2	2:AP:170:LYS:NZ	2.31	0.61
2:An:123:GLU:OE2	2:An:170:LYS:NZ	2.31	0.61
2:BJ:123:GLU:OE2	2:BJ:170:LYS:NZ	2.34	0.61
2:BN:123:GLU:OE2	2:BN:170:LYS:NZ	2.31	0.61
2:Bn:123:GLU:OE2	2:Bn:170:LYS:NZ	2.34	0.61
2:Bt:123:GLU:OE2	2:Bt:170:LYS:NZ	2.34	0.61
2:ZZ:123:GLU:OE2	2:ZZ:170:LYS:NZ	2.34	0.61
2:DR:123:GLU:OE2	2:DR:170:LYS:NZ	2.33	0.61
2:EN:123:GLU:OE2	2:EN:170:LYS:NZ	2.31	0.61
2:EV:123:GLU:OE2	2:EV:170:LYS:NZ	2.34	0.61
2:Eh:123:GLU:OE2	2:Eh:170:LYS:NZ	2.34	0.61
2:x:123:GLU:OE2	2:x:170:LYS:NZ	2.34	0.61
2:AF:123:GLU:OE2	2:AF:170:LYS:NZ	2.34	0.61
2:AX:123:GLU:OE2	2:AX:170:LYS:NZ	2.33	0.61
2:Av:123:GLU:OE2	2:Av:170:LYS:NZ	2.34	0.61
2:CZ:123:GLU:OE2	2:CZ:170:LYS:NZ	2.33	0.61
2:YH:123:GLU:OE2	2:YH:170:LYS:NZ	2.34	0.61
2:Dj:123:GLU:OE2	2:Dj:170:LYS:NZ	2.34	0.61
2:EJ:123:GLU:OE2	2:EJ:170:LYS:NZ	2.34	0.61
2:At:123:GLU:OE2	2:At:170:LYS:NZ	2.31	0.61
2:ZL:123:GLU:OE2	2:ZL:170:LYS:NZ	2.34	0.61
2:Cr:123:GLU:OE2	2:Cr:170:LYS:NZ	2.34	0.61
2:Cx:123:GLU:OE2	2:Cx:170:LYS:NZ	2.34	0.61
2:DH:123:GLU:OE2	2:DH:170:LYS:NZ	2.33	0.61
2:DL:123:GLU:OE2	2:DL:170:LYS:NZ	2.33	0.61
2:DX:123:GLU:OE2	2:DX:170:LYS:NZ	2.33	0.61
2:ED:123:GLU:OE2	2:ED:170:LYS:NZ	2.34	0.61
2:CH:123:GLU:OE2	2:CH:170:LYS:NZ	2.34	0.61
2:CN:123:GLU:OE2	2:CN:170:LYS:NZ	2.34	0.61
2:CT:123:GLU:OE2	2:CT:170:LYS:NZ	2.33	0.61
2:Df:123:GLU:OE2	2:Df:170:LYS:NZ	2.33	0.61
2:ZJ:123:GLU:OE2	2:ZJ:170:LYS:NZ	2.34	0.61
2:ZR:123:GLU:OE2	2:ZR:170:LYS:NZ	2.34	0.61
2:Br:123:GLU:OE2	2:Br:170:LYS:NZ	2.31	0.61
2:YN:123:GLU:OE2	2:YN:170:LYS:NZ	2.34	0.61
2:Dp:123:GLU:OE2	2:Dp:170:LYS:NZ	2.34	0.61
2:T:123:GLU:OE2	2:T:170:LYS:NZ	2.34	0.61
2:ZD:123:GLU:OE2	2:ZD:170:LYS:NZ	2.34	0.61
2:AL:123:GLU:OE2	2:AL:170:LYS:NZ	2.34	0.61
2:Aj:123:GLU:OE2	2:Aj:170:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Al:123:GLU:OE2	2:Al:170:LYS:NZ	2.33	0.61
2:Ap:123:GLU:OE2	2:Ap:170:LYS:NZ	2.34	0.61
2:YP:123:GLU:OE2	2:YP:170:LYS:NZ	2.34	0.61
2:AZ:123:GLU:OE2	2:AZ:170:LYS:NZ	2.33	0.61
2:Bh:123:GLU:OE2	2:Bh:170:LYS:NZ	2.34	0.61
2:Ch:123:GLU:OE2	2:Ch:170:LYS:NZ	2.33	0.61
2:Db:123:GLU:OE2	2:Db:170:LYS:NZ	2.31	0.61
2:Et:123:GLU:OE2	2:Et:170:LYS:NZ	2.33	0.61
2:Z:123:GLU:OE2	2:Z:170:LYS:NZ	2.33	0.61
2:AN:123:GLU:OE2	2:AN:170:LYS:NZ	2.33	0.61
2:BP:123:GLU:OE2	2:BP:170:LYS:NZ	2.34	0.61
2:Cl:123:GLU:OE2	2:Cl:170:LYS:NZ	2.34	0.61
2:DT:123:GLU:OE2	2:DT:170:LYS:NZ	2.33	0.61
2:H:123:GLU:OE2	2:H:170:LYS:NZ	2.34	0.61
2:n:123:GLU:OE2	2:n:170:LYS:NZ	2.33	0.61
2:Ad:123:GLU:OE2	2:Ad:170:LYS:NZ	2.33	0.61
2:Af:123:GLU:OE2	2:Af:170:LYS:NZ	2.33	0.61
2:CX:123:GLU:OE2	2:CX:170:LYS:NZ	2.31	0.61
2:YV:123:GLU:OE2	2:YV:170:LYS:NZ	2.33	0.61
2:EP:123:GLU:OE2	2:EP:170:LYS:NZ	2.34	0.61
2:b:123:GLU:OE2	2:b:170:LYS:NZ	2.33	0.60
2:AR:123:GLU:OE2	2:AR:170:LYS:NZ	2.33	0.60
2:BD:123:GLU:OE2	2:BD:170:LYS:NZ	2.34	0.60
2:Dv:123:GLU:OE2	2:Dv:170:LYS:NZ	2.34	0.60
2:f:123:GLU:OE2	2:f:170:LYS:NZ	2.33	0.60
2:CB:123:GLU:OE2	2:CB:170:LYS:NZ	2.34	0.60
2:Eb:123:GLU:OE2	2:Eb:170:LYS:NZ	2.34	0.60
2:N:123:GLU:OE2	2:N:170:LYS:NZ	2.34	0.60
2:ZT:123:GLU:OE2	2:ZT:170:LYS:NZ	2.33	0.60
2:BX:123:GLU:OE2	2:BX:170:LYS:NZ	2.33	0.60
2:Bz:123:GLU:OE2	2:Bz:170:LYS:NZ	2.34	0.60
2:ZF:123:GLU:OE2	2:ZF:170:LYS:NZ	2.33	0.60
2:EL:123:GLU:OE2	2:EL:170:LYS:NZ	2.33	0.60
2:t:123:GLU:OE2	2:t:170:LYS:NZ	2.33	0.60
2:CP:123:GLU:OE2	2:CP:170:LYS:NZ	2.33	0.60
2:r:123:GLU:OE2	2:r:170:LYS:NZ	2.34	0.60
2:BR:123:GLU:OE2	2:BR:170:LYS:NZ	2.33	0.60
2:BV:123:GLU:OE2	2:BV:170:LYS:NZ	2.34	0.60
2:Cz:123:GLU:OE2	2:Cz:170:LYS:NZ	2.33	0.60
2:CD:123:GLU:OE2	2:CD:170:LYS:NZ	2.33	0.60
2:Dd:123:GLU:OE2	2:Dd:170:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:En:123:GLU:OE2	2:En:170:LYS:NZ	2.34	0.60
2:BF:123:GLU:OE2	2:BF:170:LYS:NZ	2.33	0.60
2:Bb:123:GLU:OE2	2:Bb:170:LYS:NZ	2.34	0.60
2:DF:123:GLU:OE2	2:DF:170:LYS:NZ	2.34	0.60
1:A:90:GLU:OE2	2:B:282:LYS:NZ	2.35	0.59
1:G:90:GLU:OE2	2:H:282:LYS:NZ	2.35	0.59
1:k:90:GLU:OE2	2:l:282:LYS:NZ	2.35	0.59
1:AW:90:GLU:OE2	2:AX:282:LYS:NZ	2.35	0.59
1:BO:90:GLU:OE2	2:BP:282:LYS:NZ	2.35	0.59
1:Bm:90:GLU:OE2	2:Bn:282:LYS:NZ	2.35	0.59
2:Cd:123:GLU:OE2	2:Cd:170:LYS:NZ	2.31	0.59
1:YG:90:GLU:OE2	2:YH:282:LYS:NZ	2.35	0.59
1:Di:90:GLU:OE2	2:Dj:282:LYS:NZ	2.35	0.59
1:ZC:90:GLU:OE2	2:ZD:282:LYS:NZ	2.35	0.59
1:YU:90:GLU:OE2	2:YV:282:LYS:NZ	2.36	0.59
1:ZQ:90:GLU:OE2	2:ZR:282:LYS:NZ	2.35	0.59
1:BC:90:GLU:OE2	2:BD:282:LYS:NZ	2.36	0.59
1:ZY:90:GLU:OE2	2:ZZ:282:LYS:NZ	2.35	0.59
1:CA:90:GLU:OE2	2:CB:282:LYS:NZ	2.35	0.59
1:CM:90:GLU:OE2	2:CN:282:LYS:NZ	2.35	0.59
1:CS:90:GLU:OE2	2:CT:282:LYS:NZ	2.35	0.59
2:DJ:123:GLU:OE2	2:DJ:170:LYS:NZ	2.31	0.59
1:DW:90:GLU:OE2	2:DX:282:LYS:NZ	2.35	0.59
1:Do:90:GLU:OE2	2:Dp:282:LYS:NZ	2.35	0.59
1:YO:90:GLU:OE2	2:YP:282:LYS:NZ	2.35	0.59
1:Eg:90:GLU:OE2	2:Eh:282:LYS:NZ	2.35	0.59
2:Ev:123:GLU:OE2	2:Ev:170:LYS:NZ	2.33	0.59
1:S:90:GLU:OE2	2:T:282:LYS:NZ	2.35	0.59
1:Y:90:GLU:OE2	2:Z:282:LYS:NZ	2.35	0.59
1:AE:90:GLU:OE2	2:AF:282:LYS:NZ	2.35	0.59
1:ZK:90:GLU:OE2	2:ZL:282:LYS:NZ	2.35	0.59
1:CG:90:GLU:OE2	2:CH:282:LYS:NZ	2.35	0.59
1:Ck:90:GLU:OE2	2:Cl:282:LYS:NZ	2.35	0.59
1:YM:90:GLU:OE2	2:YN:282:LYS:NZ	2.35	0.59
1:EO:90:GLU:OE2	2:EP:282:LYS:NZ	2.35	0.59
1:e:90:GLU:OE2	2:f:282:LYS:NZ	2.35	0.59
1:Ac:90:GLU:OE2	2:Ad:282:LYS:NZ	2.35	0.59
1:Au:90:GLU:OE2	2:Av:282:LYS:NZ	2.35	0.59
1:Bs:90:GLU:OE2	2:Bt:282:LYS:NZ	2.35	0.59
2:DP:123:GLU:OE2	2:DP:170:LYS:NZ	2.31	0.59
1:EU:90:GLU:OE2	2:EV:282:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:90:GLU:OE2	2:AR:282:LYS:NZ	2.35	0.59
1:DQ:90:GLU:OE2	2:DR:282:LYS:NZ	2.35	0.59
1:Bg:90:GLU:OE2	2:Bh:282:LYS:NZ	2.35	0.59
1:Ce:90:GLU:OE2	2:Cf:282:LYS:NZ	2.35	0.59
1:Dc:90:GLU:OE2	2:Dd:282:LYS:NZ	2.36	0.59
1:BI:90:GLU:OE2	2:BJ:282:LYS:NZ	2.35	0.59
1:DE:90:GLU:OE2	2:DF:282:LYS:NZ	2.36	0.59
1:DK:90:GLU:OE2	2:DL:282:LYS:NZ	2.35	0.59
1:Ea:90:GLU:OE2	2:Eb:282:LYS:NZ	2.36	0.59
1:w:90:GLU:OE2	2:x:282:LYS:NZ	2.35	0.58
2:Af:134:ASP:OD1	2:Af:138:LYS:NZ	2.36	0.58
2:ZN:134:ASP:OD1	2:ZN:138:LYS:NZ	2.36	0.58
1:Ba:90:GLU:OE2	2:Bb:282:LYS:NZ	2.35	0.58
1:By:90:GLU:OE2	2:Bz:282:LYS:NZ	2.35	0.58
2:CJ:123:GLU:OE2	2:CJ:170:LYS:NZ	2.33	0.58
2:CJ:134:ASP:OD1	2:CJ:138:LYS:NZ	2.36	0.58
1:CY:90:GLU:OE2	2:CZ:282:LYS:NZ	2.35	0.58
2:DN:134:ASP:OD1	2:DN:138:LYS:NZ	2.36	0.58
2:Dl:123:GLU:OE2	2:Dl:170:LYS:NZ	2.33	0.58
1:Du:90:GLU:OE2	2:Dv:282:LYS:NZ	2.35	0.58
1:EC:90:GLU:OE2	2:ED:282:LYS:NZ	2.35	0.58
2:EL:134:ASP:OD1	2:EL:138:LYS:NZ	2.36	0.58
2:Ej:123:GLU:OE2	2:Ej:170:LYS:NZ	2.33	0.58
1:Es:90:GLU:OE2	2:Et:282:LYS:NZ	2.36	0.58
2:b:134:ASP:OD1	2:b:138:LYS:NZ	2.36	0.58
1:AK:90:GLU:OE2	2:AL:282:LYS:NZ	2.35	0.58
1:Ao:90:GLU:OE2	2:Ap:282:LYS:NZ	2.35	0.58
2:Cb:134:ASP:OD1	2:Cb:138:LYS:NZ	2.36	0.58
1:Cq:90:GLU:OE2	2:Cr:282:LYS:NZ	2.35	0.58
2:Cz:134:ASP:OD1	2:Cz:138:LYS:NZ	2.36	0.58
2:YJ:134:ASP:OD1	2:YJ:138:LYS:NZ	2.36	0.58
2:DN:123:GLU:OE2	2:DN:170:LYS:NZ	2.33	0.58
2:Dl:134:ASP:OD1	2:Dl:138:LYS:NZ	2.36	0.58
1:Em:90:GLU:OE2	2:En:282:LYS:NZ	2.35	0.58
1:M:90:GLU:OE2	2:N:282:LYS:NZ	2.35	0.58
2:P:134:ASP:OD1	2:P:138:LYS:NZ	2.36	0.58
2:AB:134:ASP:OD1	2:AB:138:LYS:NZ	2.36	0.58
2:AN:134:ASP:OD1	2:AN:138:LYS:NZ	2.36	0.58
1:Ai:90:GLU:OE2	2:Aj:282:LYS:NZ	2.35	0.58
2:ZN:123:GLU:OE2	2:ZN:170:LYS:NZ	2.33	0.58
2:BF:134:ASP:OD1	2:BF:138:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bp:134:ASP:OD1	2:Bp:138:LYS:NZ	2.36	0.58
2:YB:123:GLU:OE2	2:YB:170:LYS:NZ	2.33	0.58
2:CD:134:ASP:OD1	2:CD:138:LYS:NZ	2.36	0.58
2:Cb:123:GLU:OE2	2:Cb:170:LYS:NZ	2.33	0.58
2:YJ:123:GLU:OE2	2:YJ:170:LYS:NZ	2.33	0.58
2:Dx:134:ASP:OD1	2:Dx:138:LYS:NZ	2.36	0.58
2:D:134:ASP:OD1	2:D:138:LYS:NZ	2.36	0.58
1:q:90:GLU:OE2	2:r:282:LYS:NZ	2.35	0.58
2:z:123:GLU:OE2	2:z:170:LYS:NZ	2.33	0.58
1:ZI:90:GLU:OE2	2:ZJ:282:LYS:NZ	2.35	0.58
2:Al:134:ASP:OD1	2:Al:138:LYS:NZ	2.36	0.58
2:Ar:134:ASP:OD1	2:Ar:138:LYS:NZ	2.36	0.58
2:CP:134:ASP:OD1	2:CP:138:LYS:NZ	2.36	0.58
2:J:134:ASP:OD1	2:J:138:LYS:NZ	2.36	0.58
2:AB:123:GLU:OE2	2:AB:170:LYS:NZ	2.33	0.58
2:ZT:134:ASP:OD1	2:ZT:138:LYS:NZ	2.36	0.58
1:BU:90:GLU:OE2	2:BV:282:LYS:NZ	2.35	0.58
2:Bd:134:ASP:OD1	2:Bd:138:LYS:NZ	2.36	0.58
2:Dr:134:ASP:OD1	2:Dr:138:LYS:NZ	2.36	0.58
1:EI:90:GLU:OE2	2:EJ:282:LYS:NZ	2.35	0.58
2:V:134:ASP:OD1	2:V:138:LYS:NZ	2.36	0.58
2:BL:123:GLU:OE2	2:BL:170:LYS:NZ	2.33	0.58
1:Cw:90:GLU:OE2	2:Cx:282:LYS:NZ	2.35	0.58
2:DB:123:GLU:OE2	2:DB:170:LYS:NZ	2.33	0.58
2:DB:134:ASP:OD1	2:DB:138:LYS:NZ	2.36	0.58
2:YR:134:ASP:OD1	2:YR:138:LYS:NZ	2.36	0.58
2:YX:134:ASP:OD1	2:YX:138:LYS:NZ	2.36	0.58
2:Ar:123:GLU:OE2	2:Ar:170:LYS:NZ	2.33	0.58
2:Bj:134:ASP:OD1	2:Bj:138:LYS:NZ	2.36	0.58
2:YB:134:ASP:OD1	2:YB:138:LYS:NZ	2.36	0.58
2:CV:123:GLU:OE2	2:CV:170:LYS:NZ	2.33	0.58
2:Df:134:ASP:OD1	2:Df:138:LYS:NZ	2.36	0.58
2:Ej:134:ASP:OD1	2:Ej:138:LYS:NZ	2.36	0.58
2:Ep:134:ASP:OD1	2:Ep:138:LYS:NZ	2.36	0.58
2:V:123:GLU:OE2	2:V:170:LYS:NZ	2.33	0.58
2:Ax:134:ASP:OD1	2:Ax:138:LYS:NZ	2.36	0.58
2:BR:134:ASP:OD1	2:BR:138:LYS:NZ	2.36	0.58
2:Ct:123:GLU:OE2	2:Ct:170:LYS:NZ	2.33	0.58
2:EF:123:GLU:OE2	2:EF:170:LYS:NZ	2.33	0.58
2:h:123:GLU:OE2	2:h:170:LYS:NZ	2.33	0.58
2:ZF:134:ASP:OD1	2:ZF:138:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AH:134:ASP:OD1	2:AH:138:LYS:NZ	2.36	0.58
2:BX:134:ASP:OD1	2:BX:138:LYS:NZ	2.36	0.58
2:Bv:134:ASP:OD1	2:Bv:138:LYS:NZ	2.36	0.58
2:Ct:134:ASP:OD1	2:Ct:138:LYS:NZ	2.36	0.58
2:DH:134:ASP:OD1	2:DH:138:LYS:NZ	2.36	0.58
2:Ev:134:ASP:OD1	2:Ev:138:LYS:NZ	2.36	0.58
2:t:134:ASP:OD1	2:t:138:LYS:NZ	2.36	0.58
2:Cn:134:ASP:OD1	2:Cn:138:LYS:NZ	2.36	0.58
2:DZ:123:GLU:OE2	2:DZ:170:LYS:NZ	2.33	0.58
2:EF:134:ASP:OD1	2:EF:138:LYS:NZ	2.36	0.58
2:ER:134:ASP:OD1	2:ER:138:LYS:NZ	2.36	0.58
2:ZV:134:ASP:OD1	2:ZV:138:LYS:NZ	2.36	0.57
2:Dx:123:GLU:OE2	2:Dx:170:LYS:NZ	2.33	0.57
2:YR:123:GLU:OE2	2:YR:170:LYS:NZ	2.33	0.57
2:EX:134:ASP:OD1	2:EX:138:LYS:NZ	2.36	0.57
2:AT:123:GLU:OE2	2:AT:170:LYS:NZ	2.33	0.57
2:AZ:134:ASP:OD1	2:AZ:138:LYS:NZ	2.36	0.57
2:Ed:134:ASP:OD1	2:Ed:138:LYS:NZ	2.36	0.57
2:n:134:ASP:OD1	2:n:138:LYS:NZ	2.36	0.57
2:Bj:123:GLU:OE2	2:Bj:170:LYS:NZ	2.33	0.57
2:Bp:123:GLU:OE2	2:Bp:170:LYS:NZ	2.33	0.57
2:P:123:GLU:OE2	2:P:170:LYS:NZ	2.33	0.57
2:AT:134:ASP:OD1	2:AT:138:LYS:NZ	2.36	0.57
2:D:123:GLU:OE2	2:D:170:LYS:NZ	2.33	0.57
2:h:134:ASP:OD1	2:h:138:LYS:NZ	2.36	0.57
2:z:134:ASP:OD1	2:z:138:LYS:NZ	2.36	0.57
2:AH:123:GLU:OE2	2:AH:170:LYS:NZ	2.33	0.57
2:BL:134:ASP:OD1	2:BL:138:LYS:NZ	2.36	0.57
2:Ch:134:ASP:OD1	2:Ch:138:LYS:NZ	2.36	0.57
2:DT:134:ASP:OD1	2:DT:138:LYS:NZ	2.36	0.57
2:DZ:134:ASP:OD1	2:DZ:138:LYS:NZ	2.36	0.57
2:CV:134:ASP:OD1	2:CV:138:LYS:NZ	2.36	0.57
2:Ep:123:GLU:OE2	2:Ep:170:LYS:NZ	2.33	0.57
2:Dr:123:GLU:OE2	2:Dr:170:LYS:NZ	2.33	0.57
2:Cn:123:GLU:OE2	2:Cn:170:LYS:NZ	2.33	0.57
2:Bd:123:GLU:OE2	2:Bd:170:LYS:NZ	2.33	0.57
2:EX:123:GLU:OE2	2:EX:170:LYS:NZ	2.33	0.57
2:ER:123:GLU:OE2	2:ER:170:LYS:NZ	2.33	0.56
2:Bv:123:GLU:OE2	2:Bv:170:LYS:NZ	2.33	0.56
2:J:123:GLU:OE2	2:J:170:LYS:NZ	2.33	0.56
2:YX:123:GLU:OE2	2:YX:170:LYS:NZ	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:166:GLU:OE2	2:R:242:LYS:NZ	2.38	0.55
2:YD:166:GLU:OE2	2:YD:242:LYS:NZ	2.38	0.55
2:El:166:GLU:OE2	2:El:242:LYS:NZ	2.38	0.55
2:Br:166:GLU:OE2	2:Br:242:LYS:NZ	2.38	0.55
2:YL:166:GLU:OE2	2:YL:242:LYS:NZ	2.38	0.55
2:Dh:166:GLU:OE2	2:Dh:242:LYS:NZ	2.38	0.55
2:Ed:123:GLU:OE2	2:Ed:170:LYS:NZ	2.33	0.55
2:DJ:166:GLU:OE2	2:DJ:242:LYS:NZ	2.38	0.55
2:Dn:166:GLU:OE2	2:Dn:242:LYS:NZ	2.38	0.55
1:K:90:GLU:OE2	2:L:282:LYS:NZ	2.40	0.55
2:L:166:GLU:OE2	2:L:242:LYS:NZ	2.38	0.55
1:Ci:90:GLU:OE2	2:Cj:282:LYS:NZ	2.40	0.55
1:Cu:90:GLU:OE2	2:Cv:282:LYS:NZ	2.40	0.55
1:DU:90:GLU:OE2	2:DV:282:LYS:NZ	2.40	0.55
2:YT:166:GLU:OE2	2:YT:242:LYS:NZ	2.38	0.55
1:EA:90:GLU:OE2	2:EB:282:LYS:NZ	2.40	0.55
2:EB:166:GLU:OE2	2:EB:242:LYS:NZ	2.38	0.55
1:EG:90:GLU:OE2	2:EH:282:LYS:NZ	2.40	0.55
1:c:90:GLU:OE2	2:d:282:LYS:NZ	2.40	0.55
1:Be:90:GLU:OE2	2:Bf:282:LYS:NZ	2.40	0.55
1:o:90:GLU:OE2	2:p:282:LYS:NZ	2.40	0.55
1:AC:90:GLU:OE2	2:AD:282:LYS:NZ	2.40	0.55
1:Aa:90:GLU:OE2	2:Ab:282:LYS:NZ	2.40	0.55
1:Ag:90:GLU:OE2	2:Ah:282:LYS:NZ	2.40	0.55
1:As:90:GLU:OE2	2:At:282:LYS:NZ	2.40	0.55
1:BS:90:GLU:OE2	2:BT:282:LYS:NZ	2.40	0.55
2:ZV:123:GLU:OE2	2:ZV:170:LYS:NZ	2.33	0.55
2:Ef:166:GLU:OE2	2:Ef:242:LYS:NZ	2.38	0.55
1:Eq:90:GLU:OE2	2:Er:282:LYS:NZ	2.40	0.55
2:X:166:GLU:OE2	2:X:242:LYS:NZ	2.38	0.54
1:ZG:90:GLU:OE2	2:ZH:282:LYS:NZ	2.40	0.54
2:Ax:123:GLU:OE2	2:Ax:170:LYS:NZ	2.33	0.54
1:Bw:90:GLU:OE2	2:Bx:282:LYS:NZ	2.40	0.54
1:Co:90:GLU:OE2	2:Cp:282:LYS:NZ	2.40	0.54
1:YK:90:GLU:OE2	2:YL:282:LYS:NZ	2.40	0.54
1:EM:90:GLU:OE2	2:EN:282:LYS:NZ	2.40	0.54
1:ES:90:GLU:OE2	2:ET:282:LYS:NZ	2.40	0.54
1:u:90:GLU:OE2	2:v:282:LYS:NZ	2.40	0.54
1:ZA:90:GLU:OE2	2:ZB:282:LYS:NZ	2.40	0.54
1:ZO:90:GLU:OE2	2:ZP:282:LYS:NZ	2.40	0.54
1:BA:90:GLU:OE2	2:BB:282:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZW:90:GLU:OE2	2:ZX:282:LYS:NZ	2.40	0.54
2:ZX:166:GLU:OE2	2:ZX:242:LYS:NZ	2.38	0.54
1:YE:90:GLU:OE2	2:YF:282:LYS:NZ	2.40	0.54
1:Dm:90:GLU:OE2	2:Dn:282:LYS:NZ	2.40	0.54
1:BM:90:GLU:OE2	2:BN:282:LYS:NZ	2.40	0.54
1:BY:90:GLU:OE2	2:BZ:282:LYS:NZ	2.40	0.54
1:Bq:90:GLU:OE2	2:Br:282:LYS:NZ	2.40	0.54
1:YC:90:GLU:OE2	2:YD:282:LYS:NZ	2.40	0.54
1:CK:90:GLU:OE2	2:CL:282:LYS:NZ	2.40	0.54
1:CQ:90:GLU:OE2	2:CR:282:LYS:NZ	2.40	0.54
1:EY:90:GLU:OE2	2:EZ:282:LYS:NZ	2.40	0.54
1:Ee:90:GLU:OE2	2:Ef:282:LYS:NZ	2.40	0.54
1:E:90:GLU:OE2	2:F:282:LYS:NZ	2.40	0.54
1:Cc:90:GLU:OE2	2:Cd:282:LYS:NZ	2.40	0.54
1:DC:90:GLU:OE2	2:DD:282:LYS:NZ	2.40	0.54
1:DO:90:GLU:OE2	2:DP:282:LYS:NZ	2.40	0.54
1:Da:90:GLU:OE2	2:Db:282:LYS:NZ	2.40	0.54
1:Dy:90:GLU:OE2	2:Dz:282:LYS:NZ	2.40	0.54
1:Ek:90:GLU:OE2	2:El:282:LYS:NZ	2.40	0.54
1:Q:90:GLU:OE2	2:R:282:LYS:NZ	2.40	0.54
1:W:90:GLU:OE2	2:X:282:LYS:NZ	2.40	0.54
1:CW:90:GLU:OE2	2:CX:282:LYS:NZ	2.40	0.54
2:Cv:166:GLU:OE2	2:Cv:242:LYS:NZ	2.38	0.54
1:Ds:90:GLU:OE2	2:Dt:282:LYS:NZ	2.40	0.54
2:EH:166:GLU:OE2	2:EH:242:LYS:NZ	2.38	0.54
1:Ew:90:GLU:OE2	2:Ex:282:LYS:NZ	2.40	0.54
1:Bk:90:GLU:OE2	2:Bl:282:LYS:NZ	2.40	0.54
1:YS:90:GLU:OE2	2:YT:282:LYS:NZ	2.40	0.54
1:BG:90:GLU:OE2	2:BH:282:LYS:NZ	2.40	0.54
2:F:166:GLU:OE2	2:F:242:LYS:NZ	2.38	0.54
1:Am:90:GLU:OE2	2:An:282:LYS:NZ	2.40	0.54
1:CE:90:GLU:OE2	2:CF:282:LYS:NZ	2.40	0.54
2:CX:166:GLU:OE2	2:CX:242:LYS:NZ	2.38	0.54
1:AO:90:GLU:OE2	2:AP:282:LYS:NZ	2.40	0.54
1:DI:90:GLU:OE2	2:DJ:282:LYS:NZ	2.40	0.54
1:Dg:90:GLU:OE2	2:Dh:282:LYS:NZ	2.40	0.54
2:Er:166:GLU:OE2	2:Er:242:LYS:NZ	2.38	0.54
2:Db:166:GLU:OE2	2:Db:242:LYS:NZ	2.38	0.54
2:Bf:166:GLU:OE2	2:Bf:242:LYS:NZ	2.38	0.53
1:i:90:GLU:OE2	2:j:282:LYS:NZ	2.40	0.53
1:AI:90:GLU:OE2	2:AJ:282:LYS:NZ	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AJ:166:GLU:OE2	2:AJ:242:LYS:NZ	2.38	0.53
1:Ay:90:GLU:OE2	2:Az:282:LYS:NZ	2.40	0.53
1:AU:90:GLU:OE2	2:AV:282:LYS:NZ	2.40	0.53
2:Az:166:GLU:OE2	2:Az:242:LYS:NZ	2.38	0.53
2:AB:6:LYS:NZ	2:AB:10:GLU:OE2	2.43	0.52
2:At:166:GLU:OE2	2:At:242:LYS:NZ	2.38	0.52
2:ZV:6:LYS:NZ	2:ZV:10:GLU:OE2	2.43	0.52
2:Cz:6:LYS:NZ	2:Cz:10:GLU:OE2	2.43	0.52
2:EZ:166:GLU:OE2	2:EZ:242:LYS:NZ	2.38	0.52
2:Ed:6:LYS:NZ	2:Ed:10:GLU:OE2	2.43	0.52
2:BF:6:LYS:NZ	2:BF:10:GLU:OE2	2.43	0.52
2:CD:6:LYS:NZ	2:CD:10:GLU:OE2	2.43	0.52
2:YF:166:GLU:OE2	2:YF:242:LYS:NZ	2.38	0.52
2:Dr:6:LYS:NZ	2:Dr:10:GLU:OE2	2.43	0.52
2:AD:166:GLU:OE2	2:AD:242:LYS:NZ	2.38	0.52
2:Bx:166:GLU:OE2	2:Bx:242:LYS:NZ	2.38	0.52
2:DB:6:LYS:NZ	2:DB:10:GLU:OE2	2.43	0.52
2:EX:6:LYS:NZ	2:EX:10:GLU:OE2	2.43	0.52
2:Bv:6:LYS:NZ	2:Bv:10:GLU:OE2	2.43	0.52
2:Cd:166:GLU:OE2	2:Cd:242:LYS:NZ	2.38	0.52
2:Dx:6:LYS:NZ	2:Dx:10:GLU:OE2	2.43	0.52
2:P:6:LYS:NZ	2:P:10:GLU:OE2	2.43	0.52
2:Al:6:LYS:NZ	2:Al:10:GLU:OE2	2.43	0.52
2:Ch:6:LYS:NZ	2:Ch:10:GLU:OE2	2.43	0.52
2:DT:6:LYS:NZ	2:DT:10:GLU:OE2	2.43	0.52
2:Ej:6:LYS:NZ	2:Ej:10:GLU:OE2	2.43	0.52
2:AN:6:LYS:NZ	2:AN:10:GLU:OE2	2.43	0.52
2:BH:166:GLU:OE2	2:BH:242:LYS:NZ	2.38	0.52
2:YB:6:LYS:NZ	2:YB:10:GLU:OE2	2.43	0.52
2:AH:6:LYS:NZ	2:AH:10:GLU:OE2	2.43	0.52
2:Ax:6:LYS:NZ	2:Ax:10:GLU:OE2	2.43	0.52
2:CF:166:GLU:OE2	2:CF:242:LYS:NZ	2.38	0.52
2:DP:166:GLU:OE2	2:DP:242:LYS:NZ	2.38	0.52
2:b:6:LYS:NZ	2:b:10:GLU:OE2	2.43	0.52
2:Af:6:LYS:NZ	2:Af:10:GLU:OE2	2.43	0.52
2:Cj:166:GLU:OE2	2:Cj:242:LYS:NZ	2.38	0.51
2:DV:166:GLU:OE2	2:DV:242:LYS:NZ	2.38	0.51
2:BL:6:LYS:NZ	2:BL:10:GLU:OE2	2.43	0.51
2:Bd:6:LYS:NZ	2:Bd:10:GLU:OE2	2.43	0.51
2:Bj:6:LYS:NZ	2:Bj:10:GLU:OE2	2.43	0.51
2:Cn:6:LYS:NZ	2:Cn:10:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ct:6:LYS:NZ	2:Ct:10:GLU:OE2	2.43	0.51
2:ET:166:GLU:OE2	2:ET:242:LYS:NZ	2.38	0.51
2:Ev:6:LYS:NZ	2:Ev:10:GLU:OE2	2.43	0.51
2:z:6:LYS:NZ	2:z:10:GLU:OE2	2.43	0.51
2:CJ:6:LYS:NZ	2:CJ:10:GLU:OE2	2.43	0.51
2:EF:6:LYS:NZ	2:EF:10:GLU:OE2	2.43	0.51
2:ER:6:LYS:NZ	2:ER:10:GLU:OE2	2.43	0.51
2:Ex:166:GLU:OE2	2:Ex:242:LYS:NZ	2.38	0.51
2:YJ:6:LYS:NZ	2:YJ:10:GLU:OE2	2.43	0.51
2:Dz:166:GLU:OE2	2:Dz:242:LYS:NZ	2.38	0.51
2:Ep:6:LYS:NZ	2:Ep:10:GLU:OE2	2.43	0.51
2:ZN:6:LYS:NZ	2:ZN:10:GLU:OE2	2.43	0.51
2:Dl:6:LYS:NZ	2:Dl:10:GLU:OE2	2.43	0.51
2:V:6:LYS:NZ	2:V:10:GLU:OE2	2.43	0.51
2:BX:6:LYS:NZ	2:BX:10:GLU:OE2	2.43	0.51
2:Bl:166:GLU:OE2	2:Bl:242:LYS:NZ	2.38	0.51
2:Cp:166:GLU:OE2	2:Cp:242:LYS:NZ	2.38	0.51
2:t:6:LYS:NZ	2:t:10:GLU:OE2	2.43	0.51
2:CL:166:GLU:OE2	2:CL:242:LYS:NZ	2.38	0.51
2:YR:6:LYS:NZ	2:YR:10:GLU:OE2	2.43	0.51
2:Ah:166:GLU:OE2	2:Ah:242:LYS:NZ	2.38	0.50
2:ZP:166:GLU:OE2	2:ZP:242:LYS:NZ	2.38	0.50
2:d:166:GLU:OE2	2:d:242:LYS:NZ	2.38	0.50
2:DL:101:LYS:NZ	2:DP:2:ASP:OD2	2.42	0.50
2:EN:166:GLU:OE2	2:EN:242:LYS:NZ	2.38	0.50
2:Ab:166:GLU:OE2	2:Ab:242:LYS:NZ	2.38	0.50
2:p:166:GLU:OE2	2:p:242:LYS:NZ	2.38	0.50
2:ZP:6:LYS:NZ	2:ZP:10:GLU:OE2	2.45	0.50
2:BJ:45:HIS:ND1	2:BL:46:ASN:ND2	2.60	0.50
2:CL:6:LYS:NZ	2:CL:10:GLU:OE2	2.45	0.50
2:CZ:101:LYS:NZ	2:Cd:2:ASP:OD2	2.42	0.50
2:x:45:HIS:ND1	2:z:46:ASN:ND2	2.60	0.50
2:AZ:6:LYS:NZ	2:AZ:10:GLU:OE2	2.43	0.50
2:BR:6:LYS:NZ	2:BR:10:GLU:OE2	2.43	0.50
2:Cl:45:HIS:ND1	2:Cn:46:ASN:ND2	2.60	0.50
2:DN:6:LYS:NZ	2:DN:10:GLU:OE2	2.43	0.50
2:EP:45:HIS:ND1	2:ER:46:ASN:ND2	2.60	0.50
2:Bf:6:LYS:NZ	2:Bf:10:GLU:OE2	2.45	0.49
2:YH:45:HIS:ND1	2:YJ:46:ASN:ND2	2.60	0.49
2:Er:6:LYS:NZ	2:Er:10:GLU:OE2	2.45	0.49
2:ZF:6:LYS:NZ	2:ZF:10:GLU:OE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AL:45:HIS:ND1	2:AN:46:ASN:ND2	2.60	0.49
2:Bt:45:HIS:ND1	2:Bv:46:ASN:ND2	2.60	0.49
2:Cb:6:LYS:NZ	2:Cb:10:GLU:OE2	2.43	0.49
2:Cj:6:LYS:NZ	2:Cj:10:GLU:OE2	2.45	0.49
2:Dj:45:HIS:ND1	2:DI:46:ASN:ND2	2.60	0.49
2:ED:45:HIS:ND1	2:EF:46:ASN:ND2	2.60	0.49
2:Aj:45:HIS:ND1	2:AI:46:ASN:ND2	2.60	0.49
2:Cr:45:HIS:ND1	2:Ct:46:ASN:ND2	2.60	0.49
2:YN:45:HIS:ND1	2:DB:46:ASN:ND2	2.60	0.49
2:DV:6:LYS:NZ	2:DV:10:GLU:OE2	2.45	0.49
2:Dp:45:HIS:ND1	2:Dr:46:ASN:ND2	2.60	0.49
2:ET:6:LYS:NZ	2:ET:10:GLU:OE2	2.45	0.49
2:EV:45:HIS:ND1	2:EX:46:ASN:ND2	2.60	0.49
2:Cp:6:LYS:NZ	2:Cp:10:GLU:OE2	2.45	0.49
2:n:6:LYS:NZ	2:n:10:GLU:OE2	2.43	0.49
2:Bp:6:LYS:NZ	2:Bp:10:GLU:OE2	2.43	0.49
2:CN:45:HIS:ND1	2:CP:46:ASN:ND2	2.60	0.49
2:DR:45:HIS:ND1	2:DT:46:ASN:ND2	2.60	0.49
2:H:45:HIS:ND1	2:J:46:ASN:ND2	2.60	0.49
2:N:45:HIS:ND1	2:P:46:ASN:ND2	2.60	0.49
2:ZR:45:HIS:ND1	2:ZT:46:ASN:ND2	2.60	0.49
2:BP:45:HIS:ND1	2:BR:46:ASN:ND2	2.60	0.49
2:CV:6:LYS:NZ	2:CV:10:GLU:OE2	2.43	0.49
2:DZ:6:LYS:NZ	2:DZ:10:GLU:OE2	2.43	0.49
2:YV:45:HIS:ND1	2:YX:46:ASN:ND2	2.60	0.49
2:D:6:LYS:NZ	2:D:10:GLU:OE2	2.43	0.49
2:Cf:45:HIS:ND1	2:Ch:46:ASN:ND2	2.60	0.49
2:Dv:45:HIS:ND1	2:Dx:46:ASN:ND2	2.60	0.49
2:ZD:45:HIS:ND1	2:ZF:46:ASN:ND2	2.60	0.49
2:J:6:LYS:NZ	2:J:10:GLU:OE2	2.43	0.49
2:l:45:HIS:ND1	2:n:46:ASN:ND2	2.60	0.49
1:Bw:46:ARG:HD3	1:Bw:50:VAL:HB	1.95	0.49
2:CF:6:LYS:NZ	2:CF:10:GLU:OE2	2.45	0.49
2:CT:45:HIS:ND1	2:CV:46:ASN:ND2	2.60	0.49
1:EY:46:ARG:HD3	1:EY:50:VAL:HB	1.95	0.49
2:F:6:LYS:NZ	2:F:10:GLU:OE2	2.45	0.48
1:o:46:ARG:HD3	1:o:50:VAL:HB	1.95	0.48
2:AX:45:HIS:ND1	2:AZ:46:ASN:ND2	2.60	0.48
2:Bz:45:HIS:ND1	2:ZV:46:ASN:ND2	2.60	0.48
2:CZ:45:HIS:ND1	2:Cb:46:ASN:ND2	2.60	0.48
2:Cx:45:HIS:ND1	2:Cz:46:ASN:ND2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YE:46:ARG:HD3	1:YE:50:VAL:HB	1.95	0.48
2:DX:45:HIS:ND1	2:DZ:46:ASN:ND2	2.60	0.48
2:YX:6:LYS:NZ	2:YX:10:GLU:OE2	2.43	0.48
1:EM:46:ARG:HD3	1:EM:50:VAL:HB	1.95	0.48
2:AR:45:HIS:ND1	2:AT:46:ASN:ND2	2.60	0.48
1:Aa:46:ARG:HD3	1:Aa:50:VAL:HB	1.95	0.48
2:ZT:6:LYS:NZ	2:ZT:10:GLU:OE2	2.43	0.48
1:BG:46:ARG:HD3	1:BG:50:VAL:HB	1.95	0.48
2:BH:6:LYS:NZ	2:BH:10:GLU:OE2	2.45	0.48
1:CE:46:ARG:HD3	1:CE:50:VAL:HB	1.95	0.48
1:Cu:46:ARG:HD3	1:Cu:50:VAL:HB	1.95	0.48
2:YL:6:LYS:NZ	2:YL:10:GLU:OE2	2.45	0.48
2:Dn:6:LYS:NZ	2:Dn:10:GLU:OE2	2.45	0.48
1:EG:46:ARG:HD3	1:EG:50:VAL:HB	1.95	0.48
2:Eb:45:HIS:ND1	2:Ed:46:ASN:ND2	2.60	0.48
2:f:45:HIS:ND1	2:h:46:ASN:ND2	2.60	0.48
2:Br:6:LYS:NZ	2:Br:10:GLU:OE2	2.45	0.48
2:DL:45:HIS:ND1	2:DN:46:ASN:ND2	2.60	0.48
2:EJ:45:HIS:ND1	2:EL:46:ASN:ND2	2.60	0.48
1:Ay:46:ARG:HD3	1:Ay:50:VAL:HB	1.95	0.48
2:BT:166:GLU:OE2	2:BT:242:LYS:NZ	2.38	0.48
1:Bq:46:ARG:HD3	1:Bq:50:VAL:HB	1.95	0.48
1:Dm:46:ARG:HD3	1:Dm:50:VAL:HB	1.95	0.48
2:YX:2:ASP:OD2	2:EB:101:LYS:NZ	2.40	0.48
1:E:46:ARG:HD3	1:E:50:VAL:HB	1.95	0.48
1:K:46:ARG:HD3	1:K:50:VAL:HB	1.95	0.48
1:AI:46:ARG:HD3	1:AI:50:VAL:HB	1.95	0.48
2:BN:166:GLU:OE2	2:BN:242:LYS:NZ	2.38	0.48
1:YK:46:ARG:HD3	1:YK:50:VAL:HB	1.95	0.48
1:DU:46:ARG:HD3	1:DU:50:VAL:HB	1.95	0.48
2:R:6:LYS:NZ	2:R:10:GLU:OE2	2.45	0.48
2:d:6:LYS:NZ	2:d:10:GLU:OE2	2.45	0.48
2:Ah:6:LYS:NZ	2:Ah:10:GLU:OE2	2.45	0.48
1:CQ:46:ARG:HD3	1:CQ:50:VAL:HB	1.95	0.48
1:Ci:46:ARG:HD3	1:Ci:50:VAL:HB	1.95	0.48
2:Dz:6:LYS:NZ	2:Dz:10:GLU:OE2	2.45	0.48
1:EA:46:ARG:HD3	1:EA:50:VAL:HB	1.95	0.48
2:EL:6:LYS:NZ	2:EL:10:GLU:OE2	2.43	0.48
2:El:6:LYS:NZ	2:El:10:GLU:OE2	2.45	0.48
2:ZB:166:GLU:OE2	2:ZB:242:LYS:NZ	2.38	0.48
2:ZH:166:GLU:OE2	2:ZH:242:LYS:NZ	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:46:ARG:HD3	1:AO:50:VAL:HB	1.95	0.48
2:Ab:6:LYS:NZ	2:Ab:10:GLU:OE2	2.45	0.48
1:Am:46:ARG:HD3	1:Am:50:VAL:HB	1.95	0.48
1:BA:46:ARG:HD3	1:BA:50:VAL:HB	1.95	0.48
2:BD:45:HIS:ND1	2:BF:46:ASN:ND2	2.60	0.48
2:DD:6:LYS:NZ	2:DD:10:GLU:OE2	2.45	0.48
2:DH:6:LYS:NZ	2:DH:10:GLU:OE2	2.43	0.48
1:Dy:46:ARG:HD3	1:Dy:50:VAL:HB	1.95	0.48
2:YT:6:LYS:NZ	2:YT:10:GLU:OE2	2.45	0.48
2:Eh:101:LYS:NZ	2:El:2:ASP:OD2	2.42	0.48
1:Q:46:ARG:HD3	1:Q:50:VAL:HB	1.95	0.48
1:W:46:ARG:HD3	1:W:50:VAL:HB	1.95	0.48
2:X:6:LYS:NZ	2:X:10:GLU:OE2	2.45	0.48
2:h:6:LYS:NZ	2:h:10:GLU:OE2	2.43	0.48
1:AC:46:ARG:HD3	1:AC:50:VAL:HB	1.95	0.48
2:AP:166:GLU:OE2	2:AP:242:LYS:NZ	2.38	0.48
2:Ad:45:HIS:ND1	2:Af:46:ASN:ND2	2.60	0.48
1:BY:46:ARG:HD3	1:BY:50:VAL:HB	1.95	0.48
2:YD:6:LYS:NZ	2:YD:10:GLU:OE2	2.45	0.48
2:CB:45:HIS:ND1	2:CD:46:ASN:ND2	2.60	0.48
2:CR:166:GLU:OE2	2:CR:242:LYS:NZ	2.38	0.48
1:Cc:46:ARG:HD3	1:Cc:50:VAL:HB	1.95	0.48
1:DO:46:ARG:HD3	1:DO:50:VAL:HB	1.95	0.48
2:Dt:6:LYS:NZ	2:Dt:10:GLU:OE2	2.45	0.48
1:Eq:46:ARG:HD3	1:Eq:50:VAL:HB	1.95	0.48
2:N:101:LYS:NZ	2:R:2:ASP:OD2	2.42	0.48
2:Z:45:HIS:ND1	2:b:46:ASN:ND2	2.60	0.48
1:i:46:ARG:HD3	1:i:50:VAL:HB	1.95	0.48
2:p:6:LYS:NZ	2:p:10:GLU:OE2	2.45	0.48
1:u:46:ARG:HD3	1:u:50:VAL:HB	1.95	0.48
1:AU:46:ARG:HD3	1:AU:50:VAL:HB	1.95	0.48
1:As:46:ARG:HD3	1:As:50:VAL:HB	1.95	0.48
2:Bx:6:LYS:NZ	2:Bx:10:GLU:OE2	2.45	0.48
1:YS:46:ARG:HD3	1:YS:50:VAL:HB	1.95	0.48
2:An:166:GLU:OE2	2:An:242:LYS:NZ	2.38	0.48
2:ZL:45:HIS:ND1	2:ZN:46:ASN:ND2	2.60	0.48
1:Be:46:ARG:HD3	1:Be:50:VAL:HB	1.95	0.48
2:EZ:6:LYS:NZ	2:EZ:10:GLU:OE2	2.45	0.48
2:AF:45:HIS:ND1	2:AH:46:ASN:ND2	2.60	0.47
2:CH:45:HIS:ND1	2:CJ:46:ASN:ND2	2.60	0.47
1:YI:33:ALA:N	1:YI:34:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:46:ARG:HD3	1:DC:50:VAL:HB	1.95	0.47
2:Df:6:LYS:NZ	2:Df:10:GLU:OE2	2.43	0.47
1:Dk:33:ALA:N	1:Dk:34:PRO:HD2	2.29	0.47
1:Ds:46:ARG:HD3	1:Ds:50:VAL:HB	1.95	0.47
2:Dv:101:LYS:NZ	2:Dz:2:ASP:OD2	2.42	0.47
1:O:33:ALA:N	1:O:34:PRO:HD2	2.29	0.47
1:U:33:ALA:N	1:U:34:PRO:HD2	2.30	0.47
1:AA:33:ALA:N	1:AA:34:PRO:HD2	2.29	0.47
2:AT:6:LYS:NZ	2:AT:10:GLU:OE2	2.43	0.47
2:AV:166:GLU:OE2	2:AV:242:LYS:NZ	2.38	0.47
2:BB:166:GLU:OE2	2:BB:242:LYS:NZ	2.38	0.47
2:CP:6:LYS:NZ	2:CP:10:GLU:OE2	2.43	0.47
1:Co:46:ARG:HD3	1:Co:50:VAL:HB	1.95	0.47
1:YQ:33:ALA:N	1:YQ:34:PRO:HD2	2.30	0.47
2:En:45:HIS:ND1	2:Ep:46:ASN:ND2	2.60	0.47
2:ZB:6:LYS:NZ	2:ZB:10:GLU:OE2	2.45	0.47
1:Aq:33:ALA:N	1:Aq:34:PRO:HD2	2.29	0.47
1:ZM:33:ALA:N	1:ZM:34:PRO:HD2	2.29	0.47
2:Bb:45:HIS:ND1	2:Bd:46:ASN:ND2	2.60	0.47
1:Bc:33:ALA:N	1:Bc:34:PRO:HD2	2.30	0.47
1:Bu:33:ALA:N	1:Bu:34:PRO:HD2	2.30	0.47
2:Dh:6:LYS:NZ	2:Dh:10:GLU:OE2	2.45	0.47
1:Dw:33:ALA:N	1:Dw:34:PRO:HD2	2.29	0.47
1:ES:46:ARG:HD3	1:ES:50:VAL:HB	1.95	0.47
1:EW:33:ALA:N	1:EW:34:PRO:HD2	2.30	0.47
1:Eo:33:ALA:N	1:Eo:34:PRO:HD2	2.30	0.47
2:j:166:GLU:OE2	2:j:242:LYS:NZ	2.38	0.47
1:s:33:ALA:N	1:s:34:PRO:HD2	2.30	0.47
1:AG:33:ALA:N	1:AG:34:PRO:HD2	2.30	0.47
2:Av:45:HIS:ND1	2:Ax:46:ASN:ND2	2.60	0.47
1:Aw:33:ALA:N	1:Aw:34:PRO:HD2	2.30	0.47
1:BS:46:ARG:HD3	1:BS:50:VAL:HB	1.95	0.47
1:BW:33:ALA:N	1:BW:34:PRO:HD2	2.30	0.47
1:ZW:46:ARG:HD3	1:ZW:50:VAL:HB	1.95	0.47
1:CI:33:ALA:N	1:CI:34:PRO:HD2	2.29	0.47
1:DI:46:ARG:HD3	1:DI:50:VAL:HB	1.95	0.47
1:Dg:46:ARG:HD3	1:Dg:50:VAL:HB	1.95	0.47
1:Ee:46:ARG:HD3	1:Ee:50:VAL:HB	1.95	0.47
1:Ek:46:ARG:HD3	1:Ek:50:VAL:HB	1.95	0.47
1:ZE:33:ALA:N	1:ZE:34:PRO:HD2	2.30	0.47
1:ZG:46:ARG:HD3	1:ZG:50:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BN:6:LYS:NZ	2:BN:10:GLU:OE2	2.45	0.47
1:YC:46:ARG:HD3	1:YC:50:VAL:HB	1.95	0.47
1:DG:33:ALA:N	1:DG:34:PRO:HD2	2.30	0.47
2:DJ:6:LYS:NZ	2:DJ:10:GLU:OE2	2.45	0.47
1:De:33:ALA:N	1:De:34:PRO:HD2	2.30	0.47
1:g:33:ALA:N	1:g:34:PRO:HD2	2.30	0.47
2:v:166:GLU:OE2	2:v:242:LYS:NZ	2.38	0.47
1:AS:33:ALA:N	1:AS:34:PRO:HD2	2.30	0.47
1:BQ:33:ALA:N	1:BQ:34:PRO:HD2	2.30	0.47
1:EK:33:ALA:N	1:EK:34:PRO:HD2	2.30	0.47
1:y:33:ALA:N	1:y:34:PRO:HD2	2.30	0.47
1:ZA:46:ARG:HD3	1:ZA:50:VAL:HB	1.95	0.47
1:AM:33:ALA:N	1:AM:34:PRO:HD2	2.30	0.47
1:Ak:33:ALA:N	1:Ak:34:PRO:HD2	2.30	0.47
1:BM:46:ARG:HD3	1:BM:50:VAL:HB	1.95	0.47
1:CC:33:ALA:N	1:CC:34:PRO:HD2	2.30	0.47
1:CW:46:ARG:HD3	1:CW:50:VAL:HB	1.95	0.47
1:Cm:33:ALA:N	1:Cm:34:PRO:HD2	2.30	0.47
1:Cy:33:ALA:N	1:Cy:34:PRO:HD2	2.30	0.47
1:DA:33:ALA:N	1:DA:34:PRO:HD2	2.30	0.47
1:Da:46:ARG:HD3	1:Da:50:VAL:HB	1.95	0.47
2:Dl:2:ASP:OD2	2:Dn:101:LYS:NZ	2.40	0.47
1:EQ:33:ALA:N	1:EQ:34:PRO:HD2	2.30	0.47
1:c:46:ARG:HD3	1:c:50:VAL:HB	1.95	0.47
2:v:6:LYS:NZ	2:v:10:GLU:OE2	2.45	0.47
2:AP:6:LYS:NZ	2:AP:10:GLU:OE2	2.45	0.47
2:An:6:LYS:NZ	2:An:10:GLU:OE2	2.45	0.47
2:Ar:6:LYS:NZ	2:Ar:10:GLU:OE2	2.43	0.47
1:BE:33:ALA:N	1:BE:34:PRO:HD2	2.30	0.47
1:BK:33:ALA:N	1:BK:34:PRO:HD2	2.30	0.47
1:CK:46:ARG:HD3	1:CK:50:VAL:HB	1.95	0.47
1:DS:33:ALA:N	1:DS:34:PRO:HD2	2.30	0.47
1:Dq:33:ALA:N	1:Dq:34:PRO:HD2	2.30	0.47
1:Ag:46:ARG:HD3	1:Ag:50:VAL:HB	1.95	0.47
1:ZO:46:ARG:HD3	1:ZO:50:VAL:HB	1.95	0.47
1:Cg:33:ALA:N	1:Cg:34:PRO:HD2	2.30	0.47
2:Eh:45:HIS:ND1	2:Ej:46:ASN:ND2	2.60	0.47
1:Ew:46:ARG:HD3	1:Ew:50:VAL:HB	1.95	0.47
1:C:33:ALA:N	1:C:34:PRO:HD2	2.29	0.47
2:AD:6:LYS:NZ	2:AD:10:GLU:OE2	2.45	0.47
2:AJ:6:LYS:NZ	2:AJ:10:GLU:OE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BZ:166:GLU:OE2	2:BZ:242:LYS:NZ	2.38	0.47
1:Bk:46:ARG:HD3	1:Bk:50:VAL:HB	1.95	0.47
2:ZZ:45:HIS:ND1	2:YB:46:ASN:ND2	2.60	0.47
1:Ca:33:ALA:N	1:Ca:34:PRO:HD2	2.30	0.47
1:Cs:33:ALA:N	1:Cs:34:PRO:HD2	2.30	0.47
2:YJ:2:ASP:OD2	2:YL:101:LYS:NZ	2.40	0.47
1:DY:33:ALA:N	1:DY:34:PRO:HD2	2.30	0.47
1:EE:33:ALA:N	1:EE:34:PRO:HD2	2.30	0.47
1:I:33:ALA:N	1:I:34:PRO:HD2	2.30	0.46
1:AY:33:ALA:N	1:AY:34:PRO:HD2	2.30	0.46
1:Ae:33:ALA:N	1:Ae:34:PRO:HD2	2.30	0.46
2:Az:6:LYS:NZ	2:Az:10:GLU:OE2	2.45	0.46
2:BZ:6:LYS:NZ	2:BZ:10:GLU:OE2	2.45	0.46
2:Bh:45:HIS:ND1	2:Bj:46:ASN:ND2	2.60	0.46
1:Bi:33:ALA:N	1:Bi:34:PRO:HD2	2.30	0.46
2:Bl:6:LYS:NZ	2:Bl:10:GLU:OE2	2.45	0.46
1:Bo:33:ALA:N	1:Bo:34:PRO:HD2	2.29	0.46
1:CU:33:ALA:N	1:CU:34:PRO:HD2	2.30	0.46
1:DM:33:ALA:N	1:DM:34:PRO:HD2	2.30	0.46
1:YW:33:ALA:N	1:YW:34:PRO:HD2	2.30	0.46
2:Et:45:HIS:ND1	2:Ev:46:ASN:ND2	2.60	0.46
1:Eu:33:ALA:N	1:Eu:34:PRO:HD2	2.30	0.46
1:a:33:ALA:N	1:a:34:PRO:HD2	2.30	0.46
1:m:33:ALA:N	1:m:34:PRO:HD2	2.30	0.46
2:Cd:6:LYS:NZ	2:Cd:10:GLU:OE2	2.45	0.46
1:Ec:33:ALA:N	1:Ec:34:PRO:HD2	2.30	0.46
2:Ex:6:LYS:NZ	2:Ex:10:GLU:OE2	2.45	0.46
1:ZU:33:ALA:N	1:ZU:34:PRO:HD2	2.30	0.46
2:YF:6:LYS:NZ	2:YF:10:GLU:OE2	2.45	0.46
1:Ei:33:ALA:N	1:Ei:34:PRO:HD2	2.29	0.46
2:Ap:45:HIS:ND1	2:Ar:46:ASN:ND2	2.60	0.46
2:BV:45:HIS:ND1	2:BX:46:ASN:ND2	2.60	0.46
1:YA:33:ALA:N	1:YA:34:PRO:HD2	2.29	0.46
2:DT:2:ASP:OD2	2:DV:101:LYS:NZ	2.40	0.46
2:Dd:45:HIS:ND1	2:Df:46:ASN:ND2	2.60	0.46
2:EN:6:LYS:NZ	2:EN:10:GLU:OE2	2.45	0.46
2:r:45:HIS:ND1	2:t:46:ASN:ND2	2.60	0.46
2:DP:6:LYS:NZ	2:DP:10:GLU:OE2	2.45	0.46
2:x:101:LYS:NZ	2:ZB:2:ASP:OD2	2.42	0.46
2:AV:6:LYS:NZ	2:AV:10:GLU:OE2	2.45	0.46
2:Dt:166:GLU:OE2	2:Dt:242:LYS:NZ	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:LYS:NZ	2:L:10:GLU:OE2	2.45	0.46
2:ZJ:45:HIS:ND1	2:AB:46:ASN:ND2	2.60	0.46
2:BJ:101:LYS:NZ	2:BN:2:ASP:OD2	2.42	0.46
2:DF:45:HIS:ND1	2:DH:46:ASN:ND2	2.60	0.46
2:EB:6:LYS:NZ	2:EB:10:GLU:OE2	2.45	0.46
2:CR:6:LYS:NZ	2:CR:10:GLU:OE2	2.45	0.46
2:YP:45:HIS:ND1	2:YR:46:ASN:ND2	2.60	0.46
2:B:45:HIS:ND1	2:D:46:ASN:ND2	2.60	0.46
2:j:6:LYS:NZ	2:j:10:GLU:OE2	2.45	0.46
2:CX:6:LYS:NZ	2:CX:10:GLU:OE2	2.45	0.46
2:Cv:6:LYS:NZ	2:Cv:10:GLU:OE2	2.45	0.46
2:T:45:HIS:ND1	2:V:46:ASN:ND2	2.60	0.45
2:h:2:ASP:OD2	2:j:101:LYS:NZ	2.40	0.45
2:BB:6:LYS:NZ	2:BB:10:GLU:OE2	2.45	0.45
2:DD:166:GLU:OE2	2:DD:242:LYS:NZ	2.38	0.45
2:Bn:45:HIS:ND1	2:Bp:46:ASN:ND2	2.60	0.45
1:W:33:ALA:N	1:W:34:PRO:CD	2.80	0.45
1:u:33:ALA:N	1:u:34:PRO:CD	2.80	0.45
2:z:160:ASP:OD1	2:z:168:LYS:NZ	2.44	0.45
2:ZN:2:ASP:OD2	2:ZP:101:LYS:NZ	2.40	0.45
1:BY:33:ALA:N	1:BY:34:PRO:CD	2.80	0.45
1:Bk:33:ALA:N	1:Bk:34:PRO:CD	2.80	0.45
1:CW:33:ALA:N	1:CW:34:PRO:CD	2.80	0.45
2:DX:101:LYS:NZ	2:Db:2:ASP:OD2	2.42	0.45
1:Da:33:ALA:N	1:Da:34:PRO:CD	2.80	0.45
2:Db:6:LYS:NZ	2:Db:10:GLU:OE2	2.45	0.45
1:YS:33:ALA:N	1:YS:34:PRO:CD	2.80	0.45
2:At:6:LYS:NZ	2:At:10:GLU:OE2	2.45	0.45
1:ZS:33:ALA:N	1:ZS:34:PRO:HD2	2.30	0.45
1:BA:33:ALA:N	1:BA:34:PRO:CD	2.80	0.45
1:YK:33:ALA:N	1:YK:34:PRO:CD	2.80	0.45
1:Dm:33:ALA:N	1:Dm:34:PRO:CD	2.80	0.45
1:Ew:33:ALA:N	1:Ew:34:PRO:CD	2.80	0.45
1:K:33:ALA:N	1:K:34:PRO:CD	2.80	0.45
1:AI:33:ALA:N	1:AI:34:PRO:CD	2.80	0.45
2:AT:2:ASP:OD2	2:AV:101:LYS:NZ	2.40	0.45
1:CQ:33:ALA:N	1:CQ:34:PRO:CD	2.80	0.45
1:YE:33:ALA:N	1:YE:34:PRO:CD	2.80	0.45
1:DC:33:ALA:N	1:DC:34:PRO:CD	2.80	0.45
1:EA:33:ALA:N	1:EA:34:PRO:CD	2.80	0.45
1:ZA:33:ALA:N	1:ZA:34:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:33:ALA:N	1:Ay:34:PRO:CD	2.80	0.45
1:BM:33:ALA:N	1:BM:34:PRO:CD	2.80	0.45
2:ZX:6:LYS:NZ	2:ZX:10:GLU:OE2	2.45	0.45
1:CO:33:ALA:N	1:CO:34:PRO:HD2	2.30	0.45
1:Ds:33:ALA:N	1:Ds:34:PRO:CD	2.80	0.45
1:EM:33:ALA:N	1:EM:34:PRO:CD	2.80	0.45
2:Ef:6:LYS:NZ	2:Ef:10:GLU:OE2	2.45	0.45
1:E:33:ALA:N	1:E:34:PRO:CD	2.80	0.45
1:o:33:ALA:N	1:o:34:PRO:CD	2.80	0.45
1:AU:33:ALA:N	1:AU:34:PRO:CD	2.80	0.45
2:BL:160:ASP:OD1	2:BL:168:LYS:NZ	2.44	0.45
1:Ci:33:ALA:N	1:Ci:34:PRO:CD	2.80	0.45
2:EF:2:ASP:OD2	2:EH:101:LYS:NZ	2.40	0.45
1:Ee:33:ALA:N	1:Ee:34:PRO:CD	2.80	0.45
1:i:33:ALA:N	1:i:34:PRO:CD	2.80	0.45
2:ZF:263:LEU:HD13	2:ZF:281:PHE:CE1	2.52	0.45
1:Aa:33:ALA:N	1:Aa:34:PRO:CD	2.80	0.45
2:Af:263:LEU:HD13	2:Af:281:PHE:CE1	2.52	0.45
2:ZN:263:LEU:HD13	2:ZN:281:PHE:CE1	2.52	0.45
2:BR:263:LEU:HD13	2:BR:281:PHE:CE1	2.52	0.45
1:Be:33:ALA:N	1:Be:34:PRO:CD	2.80	0.45
1:Bq:33:ALA:N	1:Bq:34:PRO:CD	2.80	0.45
1:ZW:33:ALA:N	1:ZW:34:PRO:CD	2.80	0.45
2:CJ:263:LEU:HD13	2:CJ:281:PHE:CE1	2.52	0.45
2:CV:263:LEU:HD13	2:CV:281:PHE:CE1	2.52	0.45
1:Cc:33:ALA:N	1:Cc:34:PRO:CD	2.80	0.45
2:YJ:263:LEU:HD13	2:YJ:281:PHE:CE1	2.52	0.45
1:DO:33:ALA:N	1:DO:34:PRO:CD	2.80	0.45
1:DU:33:ALA:N	1:DU:34:PRO:CD	2.80	0.45
2:DZ:263:LEU:HD13	2:DZ:281:PHE:CE1	2.52	0.45
1:Eq:33:ALA:N	1:Eq:34:PRO:CD	2.80	0.45
2:b:263:LEU:HD13	2:b:281:PHE:CE1	2.52	0.45
2:AN:263:LEU:HD13	2:AN:281:PHE:CE1	2.52	0.45
2:Al:263:LEU:HD13	2:Al:281:PHE:CE1	2.52	0.45
2:Cx:101:LYS:NZ	2:YF:2:ASP:OD2	2.42	0.45
2:Dl:263:LEU:HD13	2:Dl:281:PHE:CE1	2.52	0.45
1:Dy:33:ALA:N	1:Dy:34:PRO:CD	2.80	0.45
1:Q:33:ALA:N	1:Q:34:PRO:CD	2.80	0.45
2:Ev:263:LEU:HD13	2:Ev:281:PHE:CE1	2.52	0.45
2:Bj:263:LEU:HD13	2:Bj:281:PHE:CE1	2.52	0.44
2:Bv:263:LEU:HD13	2:Bv:281:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ZV:263:LEU:HD13	2:ZV:281:PHE:CE1	2.52	0.44
2:Cb:263:LEU:HD13	2:Cb:281:PHE:CE1	2.52	0.44
2:Ct:2:ASP:OD2	2:Cv:101:LYS:NZ	2.40	0.44
2:Cz:263:LEU:HD13	2:Cz:281:PHE:CE1	2.52	0.44
2:DN:263:LEU:HD13	2:DN:281:PHE:CE1	2.52	0.44
2:EL:263:LEU:HD13	2:EL:281:PHE:CE1	2.52	0.44
1:ES:33:ALA:N	1:ES:34:PRO:CD	2.80	0.44
2:EX:263:LEU:HD13	2:EX:281:PHE:CE1	2.52	0.44
2:Ed:263:LEU:HD13	2:Ed:281:PHE:CE1	2.52	0.44
2:ZT:263:LEU:HD13	2:ZT:281:PHE:CE1	2.52	0.44
2:CP:263:LEU:HD13	2:CP:281:PHE:CE1	2.52	0.44
2:Ch:263:LEU:HD13	2:Ch:281:PHE:CE1	2.52	0.44
2:Cn:2:ASP:OD2	2:Cp:101:LYS:NZ	2.40	0.44
1:Cu:33:ALA:N	1:Cu:34:PRO:CD	2.80	0.44
1:DI:33:ALA:N	1:DI:34:PRO:CD	2.80	0.44
2:DT:263:LEU:HD13	2:DT:281:PHE:CE1	2.52	0.44
1:Dg:33:ALA:N	1:Dg:34:PRO:CD	2.80	0.44
2:EF:263:LEU:HD13	2:EF:281:PHE:CE1	2.52	0.44
1:EG:33:ALA:N	1:EG:34:PRO:CD	2.80	0.44
1:Ek:33:ALA:N	1:Ek:34:PRO:CD	2.80	0.44
2:Bp:263:LEU:HD13	2:Bp:281:PHE:CE1	2.52	0.44
2:CD:263:LEU:HD13	2:CD:281:PHE:CE1	2.52	0.44
1:Co:33:ALA:N	1:Co:34:PRO:CD	2.80	0.44
2:Ct:263:LEU:HD13	2:Ct:281:PHE:CE1	2.52	0.44
2:Dr:263:LEU:HD13	2:Dr:281:PHE:CE1	2.52	0.44
2:EH:6:LYS:NZ	2:EH:10:GLU:OE2	2.45	0.44
2:D:263:LEU:HD13	2:D:281:PHE:CE1	2.52	0.44
1:i:51:ARG:HD2	1:i:66:GLU:OE1	2.18	0.44
1:ZG:33:ALA:N	1:ZG:34:PRO:CD	2.80	0.44
1:AC:51:ARG:HD2	1:AC:66:GLU:OE1	2.18	0.44
1:AU:51:ARG:HD2	1:AU:66:GLU:OE1	2.18	0.44
1:As:51:ARG:HD2	1:As:66:GLU:OE1	2.18	0.44
2:BF:263:LEU:HD13	2:BF:281:PHE:CE1	2.52	0.44
1:BS:33:ALA:N	1:BS:34:PRO:CD	2.80	0.44
2:Bd:263:LEU:HD13	2:Bd:281:PHE:CE1	2.52	0.44
1:Bw:33:ALA:N	1:Bw:34:PRO:CD	2.80	0.44
1:YC:33:ALA:N	1:YC:34:PRO:CD	2.80	0.44
1:YE:51:ARG:HD2	1:YE:66:GLU:OE1	2.18	0.44
2:DB:263:LEU:HD13	2:DB:281:PHE:CE1	2.52	0.44
1:EM:51:ARG:HD2	1:EM:66:GLU:OE1	2.18	0.44
2:Ep:263:LEU:HD13	2:Ep:281:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:263:LEU:HD13	2:n:281:PHE:CE1	2.52	0.44
2:AZ:263:LEU:HD13	2:AZ:281:PHE:CE1	2.52	0.44
1:Ag:33:ALA:N	1:Ag:34:PRO:CD	2.80	0.44
1:BG:33:ALA:N	1:BG:34:PRO:CD	2.80	0.44
2:Bd:160:ASP:OD1	2:Bd:168:LYS:NZ	2.44	0.44
1:Bw:51:ARG:HD2	1:Bw:66:GLU:OE1	2.18	0.44
1:CK:33:ALA:N	1:CK:34:PRO:CD	2.80	0.44
2:Cn:263:LEU:HD13	2:Cn:281:PHE:CE1	2.52	0.44
2:ER:2:ASP:OD2	2:ET:101:LYS:NZ	2.40	0.44
2:ER:263:LEU:HD13	2:ER:281:PHE:CE1	2.52	0.44
1:EY:33:ALA:N	1:EY:34:PRO:CD	2.80	0.44
1:c:33:ALA:N	1:c:34:PRO:CD	2.80	0.44
1:c:51:ARG:HD2	1:c:66:GLU:OE1	2.18	0.44
1:o:51:ARG:HD2	1:o:66:GLU:OE1	2.18	0.44
2:t:263:LEU:HD13	2:t:281:PHE:CE1	2.52	0.44
1:Aa:51:ARG:HD2	1:Aa:66:GLU:OE1	2.18	0.44
1:Ag:51:ARG:HD2	1:Ag:66:GLU:OE1	2.18	0.44
1:ZO:33:ALA:N	1:ZO:34:PRO:CD	2.80	0.44
1:Bq:51:ARG:HD2	1:Bq:66:GLU:OE1	2.18	0.44
1:EY:51:ARG:HD2	1:EY:66:GLU:OE1	2.18	0.44
2:Ej:263:LEU:HD13	2:Ej:281:PHE:CE1	2.52	0.44
1:E:51:ARG:HD2	1:E:66:GLU:OE1	2.18	0.44
1:W:51:ARG:HD2	1:W:66:GLU:OE1	2.18	0.44
2:BX:263:LEU:HD13	2:BX:281:PHE:CE1	2.52	0.44
2:YB:263:LEU:HD13	2:YB:281:PHE:CE1	2.52	0.44
1:CE:33:ALA:N	1:CE:34:PRO:CD	2.80	0.44
1:CQ:51:ARG:HD2	1:CQ:66:GLU:OE1	2.18	0.44
2:J:263:LEU:HD13	2:J:281:PHE:CE1	2.52	0.44
2:h:263:LEU:HD13	2:h:281:PHE:CE1	2.52	0.44
2:z:263:LEU:HD13	2:z:281:PHE:CE1	2.52	0.44
1:AO:33:ALA:N	1:AO:34:PRO:CD	2.80	0.44
1:Am:33:ALA:N	1:Am:34:PRO:CD	2.80	0.44
1:BA:51:ARG:HD2	1:BA:66:GLU:OE1	2.18	0.44
2:BT:6:LYS:NZ	2:BT:10:GLU:OE2	2.45	0.44
2:DH:263:LEU:HD13	2:DH:281:PHE:CE1	2.52	0.44
1:YS:51:ARG:HD2	1:YS:66:GLU:OE1	2.18	0.44
1:EG:51:ARG:HD2	1:EG:66:GLU:OE1	2.18	0.44
1:Ew:51:ARG:HD2	1:Ew:66:GLU:OE1	2.18	0.44
2:BL:263:LEU:HD13	2:BL:281:PHE:CE1	2.52	0.44
1:Bk:51:ARG:HD2	1:Bk:66:GLU:OE1	2.18	0.44
1:Cu:51:ARG:HD2	1:Cu:66:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Df:263:LEU:HD13	2:Df:281:PHE:CE1	2.52	0.44
2:YX:263:LEU:HD13	2:YX:281:PHE:CE1	2.52	0.44
2:V:263:LEU:HD13	2:V:281:PHE:CE1	2.52	0.43
2:AH:263:LEU:HD13	2:AH:281:PHE:CE1	2.52	0.43
2:AT:263:LEU:HD13	2:AT:281:PHE:CE1	2.52	0.43
2:Ar:263:LEU:HD13	2:Ar:281:PHE:CE1	2.52	0.43
1:Ay:51:ARG:HD2	1:Ay:66:GLU:OE1	2.18	0.43
1:ZO:51:ARG:HD2	1:ZO:66:GLU:OE1	2.18	0.43
1:BG:51:ARG:HD2	1:BG:66:GLU:OE1	2.18	0.43
2:YR:263:LEU:HD13	2:YR:281:PHE:CE1	2.52	0.43
2:ZH:6:LYS:NZ	2:ZH:10:GLU:OE2	2.45	0.43
2:AB:263:LEU:HD13	2:AB:281:PHE:CE1	2.52	0.43
1:AC:33:ALA:N	1:AC:34:PRO:CD	2.80	0.43
1:AI:51:ARG:HD2	1:AI:66:GLU:OE1	2.18	0.43
1:As:33:ALA:N	1:As:34:PRO:CD	2.80	0.43
2:Ax:263:LEU:HD13	2:Ax:281:PHE:CE1	2.52	0.43
1:YC:51:ARG:HD2	1:YC:66:GLU:OE1	2.18	0.43
1:CE:51:ARG:HD2	1:CE:66:GLU:OE1	2.18	0.43
1:CK:51:ARG:HD2	1:CK:66:GLU:OE1	2.18	0.43
1:Co:51:ARG:HD2	1:Co:66:GLU:OE1	2.18	0.43
1:DU:51:ARG:HD2	1:DU:66:GLU:OE1	2.18	0.43
1:Ds:51:ARG:HD2	1:Ds:66:GLU:OE1	2.18	0.43
1:ES:51:ARG:HD2	1:ES:66:GLU:OE1	2.18	0.43
2:P:263:LEU:HD13	2:P:281:PHE:CE1	2.52	0.43
1:Am:51:ARG:HD2	1:Am:66:GLU:OE1	2.18	0.43
1:BM:51:ARG:HD2	1:BM:66:GLU:OE1	2.18	0.43
1:Cc:51:ARG:HD2	1:Cc:66:GLU:OE1	2.18	0.43
1:ZA:51:ARG:HD2	1:ZA:66:GLU:OE1	2.18	0.43
1:ZG:51:ARG:HD2	1:ZG:66:GLU:OE1	2.18	0.43
1:AO:51:ARG:HD2	1:AO:66:GLU:OE1	2.18	0.43
1:Ci:51:ARG:HD2	1:Ci:66:GLU:OE1	2.18	0.43
1:DC:51:ARG:HD2	1:DC:66:GLU:OE1	2.18	0.43
2:Dx:263:LEU:HD13	2:Dx:281:PHE:CE1	2.52	0.43
1:Dy:51:ARG:HD2	1:Dy:66:GLU:OE1	2.18	0.43
1:EA:51:ARG:HD2	1:EA:66:GLU:OE1	2.18	0.43
1:Ek:51:ARG:HD2	1:Ek:66:GLU:OE1	2.18	0.43
1:K:51:ARG:HD2	1:K:66:GLU:OE1	2.18	0.43
1:BS:51:ARG:HD2	1:BS:66:GLU:OE1	2.18	0.43
1:Be:51:ARG:HD2	1:Be:66:GLU:OE1	2.18	0.43
1:YK:51:ARG:HD2	1:YK:66:GLU:OE1	2.18	0.43
1:DI:51:ARG:HD2	1:DI:66:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DO:51:ARG:HD2	1:DO:66:GLU:OE1	2.18	0.43
1:Q:51:ARG:HD2	1:Q:66:GLU:OE1	2.18	0.43
2:Av:101:LYS:NZ	2:Az:2:ASP:OD2	2.42	0.43
1:ZW:51:ARG:HD2	1:ZW:66:GLU:OE1	2.18	0.43
1:Dg:51:ARG:HD2	1:Dg:66:GLU:OE1	2.18	0.43
1:Dm:51:ARG:HD2	1:Dm:66:GLU:OE1	2.18	0.43
2:Dl:160:ASP:OD1	2:Dl:168:LYS:NZ	2.44	0.43
1:Ee:51:ARG:HD2	1:Ee:66:GLU:OE1	2.18	0.43
1:Eq:51:ARG:HD2	1:Eq:66:GLU:OE1	2.18	0.43
1:CW:51:ARG:HD2	1:CW:66:GLU:OE1	2.18	0.43
1:Da:51:ARG:HD2	1:Da:66:GLU:OE1	2.18	0.43
2:Ej:160:ASP:OD1	2:Ej:168:LYS:NZ	2.44	0.43
2:CV:160:ASP:OD1	2:CV:168:LYS:NZ	2.44	0.43
2:YJ:160:ASP:OD1	2:YJ:168:LYS:NZ	2.44	0.43
2:t:160:ASP:OD1	2:t:168:LYS:NZ	2.44	0.42
2:AF:101:LYS:NZ	2:AJ:2:ASP:OD2	2.42	0.42
1:BY:51:ARG:HD2	1:BY:66:GLU:OE1	2.18	0.42
2:Dr:160:ASP:OD1	2:Dr:168:LYS:NZ	2.44	0.42
1:ZG:11:ALA:HB1	1:ZG:43:VAL:O	2.20	0.42
1:BS:11:ALA:HB1	1:BS:43:VAL:O	2.20	0.42
2:YB:160:ASP:OD1	2:YB:168:LYS:NZ	2.44	0.42
1:Cc:11:ALA:HB1	1:Cc:43:VAL:O	2.20	0.42
2:EV:101:LYS:NZ	2:EZ:2:ASP:OD2	2.42	0.42
2:J:160:ASP:OD1	2:J:168:LYS:NZ	2.44	0.42
1:Q:11:ALA:HB1	1:Q:43:VAL:O	2.20	0.42
1:u:51:ARG:HD2	1:u:66:GLU:OE1	2.18	0.42
2:Bt:101:LYS:NZ	2:Bx:2:ASP:OD2	2.42	0.42
1:DO:11:ALA:HB1	1:DO:43:VAL:O	2.20	0.42
1:Dg:11:ALA:HB1	1:Dg:43:VAL:O	2.20	0.42
1:Dy:11:ALA:HB1	1:Dy:43:VAL:O	2.20	0.42
1:E:11:ALA:HB1	1:E:43:VAL:O	2.20	0.42
1:i:11:ALA:HB1	1:i:43:VAL:O	2.20	0.42
1:Bq:11:ALA:HB1	1:Bq:43:VAL:O	2.20	0.42
1:ZU:77:TYR:CE2	1:ZU:93:ILE:HD13	2.55	0.42
1:DI:11:ALA:HB1	1:DI:43:VAL:O	2.20	0.42
1:Ek:11:ALA:HB1	1:Ek:43:VAL:O	2.20	0.42
1:U:77:TYR:CE2	1:U:93:ILE:HD13	2.55	0.42
2:AD:134:ASP:OD1	2:AD:138:LYS:NZ	2.53	0.42
1:AU:11:ALA:HB1	1:AU:43:VAL:O	2.20	0.42
1:Aa:11:ALA:HB1	1:Aa:43:VAL:O	2.20	0.42
2:At:134:ASP:OD1	2:At:138:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZM:77:TYR:CE2	1:ZM:93:ILE:HD13	2.55	0.42
2:BZ:134:ASP:OD1	2:BZ:138:LYS:NZ	2.53	0.42
1:Bu:77:TYR:CE2	1:Bu:93:ILE:HD13	2.55	0.42
1:YC:11:ALA:HB1	1:YC:43:VAL:O	2.20	0.42
1:CI:77:TYR:CE2	1:CI:93:ILE:HD13	2.55	0.42
1:Cu:11:ALA:HB1	1:Cu:43:VAL:O	2.20	0.42
1:DU:11:ALA:HB1	1:DU:43:VAL:O	2.20	0.42
1:De:77:TYR:CE2	1:De:93:ILE:HD13	2.55	0.42
1:YQ:77:TYR:CE2	1:YQ:93:ILE:HD13	2.55	0.42
1:EM:11:ALA:HB1	1:EM:43:VAL:O	2.20	0.42
1:EW:77:TYR:CE2	1:EW:93:ILE:HD13	2.55	0.42
1:K:11:ALA:HB1	1:K:43:VAL:O	2.20	0.42
2:d:134:ASP:OD1	2:d:138:LYS:NZ	2.53	0.42
1:o:11:ALA:HB1	1:o:43:VAL:O	2.20	0.42
2:v:134:ASP:OD1	2:v:138:LYS:NZ	2.53	0.42
1:AC:11:ALA:HB1	1:AC:43:VAL:O	2.20	0.42
2:AP:134:ASP:OD1	2:AP:138:LYS:NZ	2.53	0.42
2:Ah:134:ASP:OD1	2:Ah:138:LYS:NZ	2.53	0.42
2:An:134:ASP:OD1	2:An:138:LYS:NZ	2.53	0.42
1:As:11:ALA:HB1	1:As:43:VAL:O	2.20	0.42
2:ZP:134:ASP:OD1	2:ZP:138:LYS:NZ	2.53	0.42
2:BB:134:ASP:OD1	2:BB:138:LYS:NZ	2.53	0.42
1:BG:11:ALA:HB1	1:BG:43:VAL:O	2.20	0.42
2:BH:134:ASP:OD1	2:BH:138:LYS:NZ	2.53	0.42
1:BS:98:ASP:OD1	1:BS:98:ASP:N	2.51	0.42
1:BY:11:ALA:HB1	1:BY:43:VAL:O	2.20	0.42
2:Bf:134:ASP:OD1	2:Bf:138:LYS:NZ	2.53	0.42
2:YD:134:ASP:OD1	2:YD:138:LYS:NZ	2.53	0.42
2:CF:134:ASP:OD1	2:CF:138:LYS:NZ	2.53	0.42
2:CL:134:ASP:OD1	2:CL:138:LYS:NZ	2.53	0.42
2:CR:134:ASP:OD1	2:CR:138:LYS:NZ	2.53	0.42
1:Ci:11:ALA:HB1	1:Ci:43:VAL:O	2.20	0.42
1:Cs:77:TYR:CE2	1:Cs:93:ILE:HD13	2.55	0.42
1:YE:11:ALA:HB1	1:YE:43:VAL:O	2.20	0.42
1:EA:11:ALA:HB1	1:EA:43:VAL:O	2.20	0.42
1:EE:77:TYR:CE2	1:EE:93:ILE:HD13	2.55	0.42
1:EG:11:ALA:HB1	1:EG:43:VAL:O	2.20	0.42
1:Ec:77:TYR:CE2	1:Ec:93:ILE:HD13	2.55	0.42
2:El:134:ASP:OD1	2:El:138:LYS:NZ	2.53	0.42
1:Eq:11:ALA:HB1	1:Eq:43:VAL:O	2.20	0.42
2:Er:134:ASP:OD1	2:Er:138:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ew:11:ALA:HB1	1:Ew:43:VAL:O	2.20	0.42
1:S:11:ALA:HB1	1:S:43:VAL:O	2.20	0.42
1:u:11:ALA:HB1	1:u:43:VAL:O	2.20	0.42
1:Bk:11:ALA:HB1	1:Bk:43:VAL:O	2.20	0.42
1:CE:11:ALA:HB1	1:CE:43:VAL:O	2.20	0.42
1:Ds:11:ALA:HB1	1:Ds:43:VAL:O	2.20	0.42
1:YO:11:ALA:HB1	1:YO:43:VAL:O	2.20	0.42
1:s:77:TYR:CE2	1:s:93:ILE:HD13	2.55	0.42
2:ZB:134:ASP:OD1	2:ZB:138:LYS:NZ	2.53	0.42
2:ZH:134:ASP:OD1	2:ZH:138:LYS:NZ	2.53	0.42
1:Am:11:ALA:HB1	1:Am:43:VAL:O	2.20	0.42
1:Au:11:ALA:HB1	1:Au:43:VAL:O	2.20	0.42
2:BN:134:ASP:OD1	2:BN:138:LYS:NZ	2.53	0.42
2:BT:134:ASP:OD1	2:BT:138:LYS:NZ	2.53	0.42
1:BW:77:TYR:CE2	1:BW:93:ILE:HD13	2.55	0.42
1:Be:11:ALA:HB1	1:Be:43:VAL:O	2.20	0.42
1:Bw:11:ALA:HB1	1:Bw:43:VAL:O	2.20	0.42
1:YA:77:TYR:CE2	1:YA:93:ILE:HD13	2.55	0.42
1:Cw:11:ALA:HB1	1:Cw:43:VAL:O	2.20	0.42
2:YL:170:LYS:HG2	2:YL:224:TRP:CH2	2.55	0.42
1:DG:77:TYR:CE2	1:DG:93:ILE:HD13	2.55	0.42
1:Da:11:ALA:HB1	1:Da:43:VAL:O	2.20	0.42
1:Dk:77:TYR:CE2	1:Dk:93:ILE:HD13	2.55	0.42
2:Dn:170:LYS:HG2	2:Dn:224:TRP:CH2	2.55	0.42
2:EH:134:ASP:OD1	2:EH:138:LYS:NZ	2.53	0.42
1:EU:11:ALA:HB1	1:EU:43:VAL:O	2.20	0.42
1:Ei:77:TYR:CE2	1:Ei:93:ILE:HD13	2.55	0.42
2:R:170:LYS:HG2	2:R:224:TRP:CH2	2.55	0.42
1:W:11:ALA:HB1	1:W:43:VAL:O	2.20	0.42
1:m:77:TYR:CE2	1:m:93:ILE:HD13	2.55	0.42
1:s:11:ALA:HB1	1:s:43:VAL:O	2.20	0.42
1:AA:77:TYR:CE2	1:AA:93:ILE:HD13	2.55	0.42
1:AE:11:ALA:HB1	1:AE:43:VAL:O	2.20	0.42
1:AG:77:TYR:CE2	1:AG:93:ILE:HD13	2.55	0.42
1:AO:11:ALA:HB1	1:AO:43:VAL:O	2.20	0.42
1:AY:77:TYR:CE2	1:AY:93:ILE:HD13	2.55	0.42
2:Ab:134:ASP:OD1	2:Ab:138:LYS:NZ	2.53	0.42
2:ZP:170:LYS:HG2	2:ZP:224:TRP:CH2	2.55	0.42
2:BN:170:LYS:HG2	2:BN:224:TRP:CH2	2.55	0.42
1:BQ:77:TYR:CE2	1:BQ:93:ILE:HD13	2.55	0.42
1:BW:11:ALA:HB1	1:BW:43:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BZ:170:LYS:HG2	2:BZ:224:TRP:CH2	2.55	0.42
1:Bs:11:ALA:HB1	1:Bs:43:VAL:O	2.20	0.42
2:Bx:134:ASP:OD1	2:Bx:138:LYS:NZ	2.53	0.42
1:CC:77:TYR:CE2	1:CC:93:ILE:HD13	2.55	0.42
2:CL:170:LYS:HG2	2:CL:224:TRP:CH2	2.55	0.42
1:CQ:11:ALA:HB1	1:CQ:43:VAL:O	2.20	0.42
2:CX:134:ASP:OD1	2:CX:138:LYS:NZ	2.53	0.42
2:Cv:134:ASP:OD1	2:Cv:138:LYS:NZ	2.53	0.42
1:Cy:11:ALA:HB1	1:Cy:43:VAL:O	2.20	0.42
2:YF:134:ASP:OD1	2:YF:138:LYS:NZ	2.53	0.42
1:YI:77:TYR:CE2	1:YI:93:ILE:HD13	2.55	0.42
1:DC:11:ALA:HB1	1:DC:43:VAL:O	2.20	0.42
2:Db:134:ASP:OD1	2:Db:138:LYS:NZ	2.53	0.42
2:Dz:170:LYS:HG2	2:Dz:224:TRP:CH2	2.55	0.42
1:YS:11:ALA:HB1	1:YS:43:VAL:O	2.20	0.42
1:EI:11:ALA:HB1	1:EI:43:VAL:O	2.20	0.42
1:EK:11:ALA:HB1	1:EK:43:VAL:O	2.20	0.42
2:EN:134:ASP:OD1	2:EN:138:LYS:NZ	2.53	0.42
1:ES:11:ALA:HB1	1:ES:43:VAL:O	2.20	0.42
1:G:11:ALA:HB1	1:G:43:VAL:O	2.20	0.42
1:O:11:ALA:HB1	1:O:43:VAL:O	2.20	0.42
2:R:134:ASP:OD1	2:R:138:LYS:NZ	2.53	0.42
1:U:11:ALA:HB1	1:U:43:VAL:O	2.20	0.42
2:j:170:LYS:HG2	2:j:224:TRP:CH2	2.55	0.42
1:m:11:ALA:HB1	1:m:43:VAL:O	2.20	0.42
2:p:134:ASP:OD1	2:p:138:LYS:NZ	2.53	0.42
2:v:170:LYS:HG2	2:v:224:TRP:CH2	2.55	0.42
1:y:11:ALA:HB1	1:y:43:VAL:O	2.20	0.42
2:ZB:170:LYS:HG2	2:ZB:224:TRP:CH2	2.55	0.42
1:ZE:77:TYR:CE2	1:ZE:93:ILE:HD13	2.55	0.42
1:AS:77:TYR:CE2	1:AS:93:ILE:HD13	2.55	0.42
2:AV:170:LYS:HG2	2:AV:224:TRP:CH2	2.55	0.42
1:AY:11:ALA:HB1	1:AY:43:VAL:O	2.20	0.42
1:Aw:77:TYR:CE2	1:Aw:93:ILE:HD13	2.55	0.42
1:BA:11:ALA:HB1	1:BA:43:VAL:O	2.20	0.42
1:BE:77:TYR:CE2	1:BE:93:ILE:HD13	2.55	0.42
1:BK:11:ALA:HB1	1:BK:43:VAL:O	2.20	0.42
1:Bi:11:ALA:HB1	1:Bi:43:VAL:O	2.20	0.42
2:ZX:134:ASP:OD1	2:ZX:138:LYS:NZ	2.53	0.42
2:YD:170:LYS:HG2	2:YD:224:TRP:CH2	2.55	0.42
1:CW:11:ALA:HB1	1:CW:43:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cd:134:ASP:OD1	2:Cd:138:LYS:NZ	2.53	0.42
2:Cd:170:LYS:HG2	2:Cd:224:TRP:CH2	2.55	0.42
1:Cm:77:TYR:CE2	1:Cm:93:ILE:HD13	2.55	0.42
1:Co:11:ALA:HB1	1:Co:43:VAL:O	2.20	0.42
2:Cp:134:ASP:OD1	2:Cp:138:LYS:NZ	2.53	0.42
2:DD:170:LYS:HG2	2:DD:224:TRP:CH2	2.55	0.42
1:DG:11:ALA:HB1	1:DG:43:VAL:O	2.20	0.42
2:DP:170:LYS:HG2	2:DP:224:TRP:CH2	2.55	0.42
1:De:11:ALA:HB1	1:De:43:VAL:O	2.20	0.42
2:Dt:170:LYS:HG2	2:Dt:224:TRP:CH2	2.55	0.42
1:Dw:11:ALA:HB1	1:Dw:43:VAL:O	2.20	0.42
2:Dz:134:ASP:OD1	2:Dz:138:LYS:NZ	2.53	0.42
1:EQ:77:TYR:CE2	1:EQ:93:ILE:HD13	2.55	0.42
1:EY:11:ALA:HB1	1:EY:43:VAL:O	2.20	0.42
2:Ef:134:ASP:OD1	2:Ef:138:LYS:NZ	2.53	0.42
1:Eu:11:ALA:HB1	1:Eu:43:VAL:O	2.20	0.42
2:Ex:134:ASP:OD1	2:Ex:138:LYS:NZ	2.53	0.42
2:J:2:ASP:OD2	2:L:101:LYS:NZ	2.40	0.41
2:d:170:LYS:HG2	2:d:224:TRP:CH2	2.55	0.41
1:g:77:TYR:CE2	1:g:93:ILE:HD13	2.55	0.41
1:q:11:ALA:HB1	1:q:43:VAL:O	2.20	0.41
1:ZE:11:ALA:HB1	1:ZE:43:VAL:O	2.20	0.41
2:AJ:134:ASP:OD1	2:AJ:138:LYS:NZ	2.53	0.41
2:Ah:170:LYS:HG2	2:Ah:224:TRP:CH2	2.55	0.41
1:Aq:77:TYR:CE2	1:Aq:93:ILE:HD13	2.55	0.41
1:Ay:11:ALA:HB1	1:Ay:43:VAL:O	2.20	0.41
2:Az:134:ASP:OD1	2:Az:138:LYS:NZ	2.53	0.41
2:BB:170:LYS:HG2	2:BB:224:TRP:CH2	2.55	0.41
1:BU:11:ALA:HB1	1:BU:43:VAL:O	2.20	0.41
1:Bc:77:TYR:CE2	1:Bc:93:ILE:HD13	2.55	0.41
2:Bl:134:ASP:OD1	2:Bl:138:LYS:NZ	2.53	0.41
2:Bx:170:LYS:HG2	2:Bx:224:TRP:CH2	2.55	0.41
2:CR:170:LYS:HG2	2:CR:224:TRP:CH2	2.55	0.41
2:Cp:170:LYS:HG2	2:Cp:224:TRP:CH2	2.55	0.41
1:YK:11:ALA:HB1	1:YK:43:VAL:O	2.20	0.41
1:DA:11:ALA:HB1	1:DA:43:VAL:O	2.20	0.41
2:DD:134:ASP:OD1	2:DD:138:LYS:NZ	2.53	0.41
2:DP:134:ASP:OD1	2:DP:138:LYS:NZ	2.53	0.41
1:Dc:11:ALA:HB1	1:Dc:43:VAL:O	2.20	0.41
1:Dk:11:ALA:HB1	1:Dk:43:VAL:O	2.20	0.41
1:Dq:11:ALA:HB1	1:Dq:43:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Dt:134:ASP:OD1	2:Dt:138:LYS:NZ	2.53	0.41
1:YQ:11:ALA:HB1	1:YQ:43:VAL:O	2.20	0.41
1:YU:11:ALA:HB1	1:YU:43:VAL:O	2.20	0.41
2:ET:134:ASP:OD1	2:ET:138:LYS:NZ	2.53	0.41
2:ET:170:LYS:HG2	2:ET:224:TRP:CH2	2.55	0.41
2:El:170:LYS:HG2	2:El:224:TRP:CH2	2.55	0.41
1:Es:11:ALA:HB1	1:Es:43:VAL:O	2.20	0.41
2:F:134:ASP:OD1	2:F:138:LYS:NZ	2.53	0.41
1:w:11:ALA:HB1	1:w:43:VAL:O	2.20	0.41
1:AG:98:ASP:OD1	1:AG:98:ASP:N	2.52	0.41
1:AI:11:ALA:HB1	1:AI:43:VAL:O	2.20	0.41
1:AK:11:ALA:HB1	1:AK:43:VAL:O	2.20	0.41
1:AW:11:ALA:HB1	1:AW:43:VAL:O	2.20	0.41
1:Ai:11:ALA:HB1	1:Ai:43:VAL:O	2.20	0.41
1:ZK:11:ALA:HB1	1:ZK:43:VAL:O	2.20	0.41
1:BQ:11:ALA:HB1	1:BQ:43:VAL:O	2.20	0.41
1:Bc:11:ALA:HB1	1:Bc:43:VAL:O	2.20	0.41
1:Bg:11:ALA:HB1	1:Bg:43:VAL:O	2.20	0.41
1:CG:11:ALA:HB1	1:CG:43:VAL:O	2.20	0.41
1:Cs:11:ALA:HB1	1:Cs:43:VAL:O	2.20	0.41
1:YI:11:ALA:HB1	1:YI:43:VAL:O	2.20	0.41
1:DE:11:ALA:HB1	1:DE:43:VAL:O	2.20	0.41
2:Dh:134:ASP:OD1	2:Dh:138:LYS:NZ	2.53	0.41
1:Dm:11:ALA:HB1	1:Dm:43:VAL:O	2.20	0.41
1:YW:11:ALA:HB1	1:YW:43:VAL:O	2.20	0.41
1:EE:11:ALA:HB1	1:EE:43:VAL:O	2.20	0.41
2:EZ:134:ASP:OD1	2:EZ:138:LYS:NZ	2.53	0.41
2:EZ:170:LYS:HG2	2:EZ:224:TRP:CH2	2.55	0.41
1:Eo:77:TYR:CE2	1:Eo:93:ILE:HD13	2.55	0.41
1:I:11:ALA:HB1	1:I:43:VAL:O	2.20	0.41
1:k:11:ALA:HB1	1:k:43:VAL:O	2.20	0.41
1:ZA:11:ALA:HB1	1:ZA:43:VAL:O	2.20	0.41
1:AM:77:TYR:CE2	1:AM:93:ILE:HD13	2.55	0.41
1:Aw:98:ASP:OD1	1:Aw:98:ASP:N	2.52	0.41
1:BM:11:ALA:HB1	1:BM:43:VAL:O	2.20	0.41
2:Br:134:ASP:OD1	2:Br:138:LYS:NZ	2.53	0.41
1:CU:11:ALA:HB1	1:CU:43:VAL:O	2.20	0.41
1:Ca:77:TYR:CE2	1:Ca:93:ILE:HD13	2.55	0.41
2:Cv:170:LYS:HG2	2:Cv:224:TRP:CH2	2.55	0.41
2:YF:170:LYS:HG2	2:YF:224:TRP:CH2	2.55	0.41
2:DJ:134:ASP:OD1	2:DJ:138:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DV:170:LYS:HG2	2:DV:224:TRP:CH2	2.55	0.41
2:EH:170:LYS:HG2	2:EH:224:TRP:CH2	2.55	0.41
2:EN:170:LYS:HG2	2:EN:224:TRP:CH2	2.55	0.41
1:Eo:11:ALA:HB1	1:Eo:43:VAL:O	2.20	0.41
2:F:92:PRO:HB2	2:F:144:LEU:HD13	2.03	0.41
2:L:134:ASP:OD1	2:L:138:LYS:NZ	2.53	0.41
1:M:11:ALA:HB1	1:M:43:VAL:O	2.20	0.41
2:X:134:ASP:OD1	2:X:138:LYS:NZ	2.53	0.41
1:Y:11:ALA:HB1	1:Y:43:VAL:O	2.20	0.41
1:a:11:ALA:HB1	1:a:43:VAL:O	2.20	0.41
1:e:11:ALA:HB1	1:e:43:VAL:O	2.20	0.41
1:g:11:ALA:HB1	1:g:43:VAL:O	2.20	0.41
2:j:92:PRO:HB2	2:j:144:LEU:HD13	2.03	0.41
2:p:92:PRO:HB2	2:p:144:LEU:HD13	2.03	0.41
1:y:77:TYR:CE2	1:y:93:ILE:HD13	2.55	0.41
2:AV:92:PRO:HB2	2:AV:144:LEU:HD13	2.03	0.41
2:Ab:92:PRO:HB2	2:Ab:144:LEU:HD13	2.03	0.41
1:Ac:11:ALA:HB1	1:Ac:43:VAL:O	2.20	0.41
1:ZQ:11:ALA:HB1	1:ZQ:43:VAL:O	2.20	0.41
1:BI:11:ALA:HB1	1:BI:43:VAL:O	2.20	0.41
1:BK:77:TYR:CE2	1:BK:93:ILE:HD13	2.55	0.41
1:Bo:11:ALA:HB1	1:Bo:43:VAL:O	2.20	0.41
2:Br:92:PRO:HB2	2:Br:144:LEU:HD13	2.03	0.41
2:ZX:170:LYS:HG2	2:ZX:224:TRP:CH2	2.55	0.41
2:CF:170:LYS:HG2	2:CF:224:TRP:CH2	2.55	0.41
1:CY:11:ALA:HB1	1:CY:43:VAL:O	2.20	0.41
2:Cf:101:LYS:NZ	2:Cj:2:ASP:OD2	2.42	0.41
2:Cj:170:LYS:HG2	2:Cj:224:TRP:CH2	2.55	0.41
1:Cm:11:ALA:HB1	1:Cm:43:VAL:O	2.20	0.41
2:YL:134:ASP:OD1	2:YL:138:LYS:NZ	2.53	0.41
1:DK:11:ALA:HB1	1:DK:43:VAL:O	2.20	0.41
1:DM:77:TYR:CE2	1:DM:93:ILE:HD13	2.55	0.41
1:DY:11:ALA:HB1	1:DY:43:VAL:O	2.20	0.41
2:Dn:134:ASP:OD1	2:Dn:138:LYS:NZ	2.53	0.41
2:Ef:170:LYS:HG2	2:Ef:224:TRP:CH2	2.55	0.41
1:Em:11:ALA:HB1	1:Em:43:VAL:O	2.20	0.41
1:C:11:ALA:HB1	1:C:43:VAL:O	2.20	0.41
2:X:170:LYS:HG2	2:X:224:TRP:CH2	2.55	0.41
2:ZD:101:LYS:NZ	2:ZH:2:ASP:OD2	2.42	0.41
2:ZH:92:PRO:HB2	2:ZH:144:LEU:HD13	2.03	0.41
1:AQ:11:ALA:HB1	1:AQ:43:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:11:ALA:HB1	1:Ae:43:VAL:O	2.20	0.41
1:Ak:77:TYR:CE2	1:Ak:93:ILE:HD13	2.55	0.41
1:BC:11:ALA:HB1	1:BC:43:VAL:O	2.20	0.41
2:BH:170:LYS:HG2	2:BH:224:TRP:CH2	2.55	0.41
2:BT:92:PRO:HB2	2:BT:144:LEU:HD13	2.03	0.41
1:Ba:11:ALA:HB1	1:Ba:43:VAL:O	2.20	0.41
2:Br:170:LYS:HG2	2:Br:224:TRP:CH2	2.55	0.41
1:CM:11:ALA:HB1	1:CM:43:VAL:O	2.20	0.41
2:CX:170:LYS:HG2	2:CX:224:TRP:CH2	2.55	0.41
1:Ce:11:ALA:HB1	1:Ce:43:VAL:O	2.20	0.41
1:Cg:11:ALA:HB1	1:Cg:43:VAL:O	2.20	0.41
2:Cj:134:ASP:OD1	2:Cj:138:LYS:NZ	2.53	0.41
1:Cy:77:TYR:CE2	1:Cy:93:ILE:HD13	2.55	0.41
1:DA:77:TYR:CE2	1:DA:93:ILE:HD13	2.55	0.41
2:DD:92:PRO:HB2	2:DD:144:LEU:HD13	2.03	0.41
1:DQ:11:ALA:HB1	1:DQ:43:VAL:O	2.20	0.41
2:Db:170:LYS:HG2	2:Db:224:TRP:CH2	2.55	0.41
1:Do:11:ALA:HB1	1:Do:43:VAL:O	2.20	0.41
2:Dt:92:PRO:HB2	2:Dt:144:LEU:HD13	2.03	0.41
1:YW:77:TYR:CE2	1:YW:93:ILE:HD13	2.55	0.41
2:EB:134:ASP:OD1	2:EB:138:LYS:NZ	2.53	0.41
1:EQ:11:ALA:HB1	1:EQ:43:VAL:O	2.20	0.41
2:EX:160:ASP:OD1	2:EX:168:LYS:NZ	2.44	0.41
2:D:160:ASP:OD1	2:D:168:LYS:NZ	2.44	0.41
1:I:77:TYR:CE2	1:I:93:ILE:HD13	2.55	0.41
2:v:92:PRO:HB2	2:v:144:LEU:HD13	2.03	0.41
1:ZC:11:ALA:HB1	1:ZC:43:VAL:O	2.20	0.41
1:AS:11:ALA:HB1	1:AS:43:VAL:O	2.20	0.41
1:Aw:11:ALA:HB1	1:Aw:43:VAL:O	2.20	0.41
2:BZ:92:PRO:HB2	2:BZ:144:LEU:HD13	2.03	0.41
2:Bl:170:LYS:HG2	2:Bl:224:TRP:CH2	2.55	0.41
1:CA:11:ALA:HB1	1:CA:43:VAL:O	2.20	0.41
2:CF:92:PRO:HB2	2:CF:144:LEU:HD13	2.03	0.41
1:CO:77:TYR:CE2	1:CO:93:ILE:HD13	2.55	0.41
1:CU:77:TYR:CE2	1:CU:93:ILE:HD13	2.55	0.41
2:CX:92:PRO:HB2	2:CX:144:LEU:HD13	2.03	0.41
1:Ce:43:VAL:HG13	1:Ce:50:VAL:HG11	2.03	0.41
1:Cg:77:TYR:CE2	1:Cg:93:ILE:HD13	2.55	0.41
2:Ch:160:ASP:OD1	2:Ch:168:LYS:NZ	2.44	0.41
1:DS:11:ALA:HB1	1:DS:43:VAL:O	2.20	0.41
1:DS:77:TYR:CE2	1:DS:93:ILE:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DV:134:ASP:OD1	2:DV:138:LYS:NZ	2.53	0.41
1:DY:77:TYR:CE2	1:DY:93:ILE:HD13	2.55	0.41
2:Db:92:PRO:HB2	2:Db:144:LEU:HD13	2.03	0.41
2:Dp:101:LYS:NZ	2:Dt:2:ASP:OD2	2.42	0.41
1:Dq:77:TYR:CE2	1:Dq:93:ILE:HD13	2.55	0.41
1:Du:11:ALA:HB1	1:Du:43:VAL:O	2.20	0.41
2:YT:134:ASP:OD1	2:YT:138:LYS:NZ	2.53	0.41
2:YT:170:LYS:HG2	2:YT:224:TRP:CH2	2.55	0.41
1:EK:77:TYR:CE2	1:EK:93:ILE:HD13	2.55	0.41
1:Ec:98:ASP:OD1	1:Ec:98:ASP:N	2.52	0.41
1:C:77:TYR:CE2	1:C:93:ILE:HD13	2.55	0.41
2:F:170:LYS:HG2	2:F:224:TRP:CH2	2.55	0.41
1:G:43:VAL:HG13	1:G:50:VAL:HG11	2.03	0.41
1:ZI:43:VAL:HG13	1:ZI:50:VAL:HG11	2.03	0.41
2:AJ:92:PRO:HB2	2:AJ:144:LEU:HD13	2.03	0.41
1:Ag:11:ALA:HB1	1:Ag:43:VAL:O	2.20	0.41
1:Ao:43:VAL:HG13	1:Ao:50:VAL:HG11	2.03	0.41
1:ZO:11:ALA:HB1	1:ZO:43:VAL:O	2.20	0.41
1:ZS:77:TYR:CE2	1:ZS:93:ILE:HD13	2.55	0.41
2:BH:92:PRO:HB2	2:BH:144:LEU:HD13	2.03	0.41
1:BO:11:ALA:HB1	1:BO:43:VAL:O	2.20	0.41
2:Bf:92:PRO:HB2	2:Bf:144:LEU:HD13	2.03	0.41
1:CK:11:ALA:HB1	1:CK:43:VAL:O	2.20	0.41
2:CT:133:ILE:CD1	2:CT:148:ALA:HB3	2.51	0.41
2:Cl:133:ILE:CD1	2:Cl:148:ALA:HB3	2.51	0.41
1:Cq:11:ALA:HB1	1:Cq:43:VAL:O	2.20	0.41
1:YG:11:ALA:HB1	1:YG:43:VAL:O	2.20	0.41
1:YM:11:ALA:HB1	1:YM:43:VAL:O	2.20	0.41
1:YM:43:VAL:HG13	1:YM:50:VAL:HG11	2.03	0.41
2:DJ:92:PRO:HB2	2:DJ:144:LEU:HD13	2.03	0.41
2:DJ:170:LYS:HG2	2:DJ:224:TRP:CH2	2.55	0.41
1:DQ:43:VAL:HG13	1:DQ:50:VAL:HG11	2.03	0.41
2:DX:133:ILE:CD1	2:DX:148:ALA:HB3	2.51	0.41
2:Dh:170:LYS:HG2	2:Dh:224:TRP:CH2	2.55	0.41
1:Di:11:ALA:HB1	1:Di:43:VAL:O	2.20	0.41
2:Dn:92:PRO:HB2	2:Dn:144:LEU:HD13	2.03	0.41
1:YU:43:VAL:HG13	1:YU:50:VAL:HG11	2.03	0.41
1:EO:11:ALA:HB1	1:EO:43:VAL:O	2.20	0.41
2:EP:133:ILE:CD1	2:EP:148:ALA:HB3	2.51	0.41
1:Ee:11:ALA:HB1	1:Ee:43:VAL:O	2.20	0.41
1:Eg:11:ALA:HB1	1:Eg:43:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ex:170:LYS:HG2	2:Ex:224:TRP:CH2	2.55	0.41
1:a:98:ASP:OD1	1:a:98:ASP:N	2.52	0.41
2:j:134:ASP:OD1	2:j:138:LYS:NZ	2.53	0.41
2:ZJ:101:LYS:NZ	2:AD:2:ASP:OD2	2.42	0.41
2:ZJ:133:ILE:CD1	2:ZJ:148:ALA:HB3	2.51	0.41
1:AG:11:ALA:HB1	1:AG:43:VAL:O	2.20	0.41
2:AV:134:ASP:OD1	2:AV:138:LYS:NZ	2.53	0.41
2:Ap:133:ILE:CD1	2:Ap:148:ALA:HB3	2.51	0.41
2:Az:92:PRO:HB2	2:Az:144:LEU:HD13	2.03	0.41
2:ZR:133:ILE:CD1	2:ZR:148:ALA:HB3	2.51	0.41
2:BR:160:ASP:OD1	2:BR:168:LYS:NZ	2.44	0.41
2:Bf:170:LYS:HG2	2:Bf:224:TRP:CH2	2.55	0.41
2:Bh:133:ILE:CD1	2:Bh:148:ALA:HB3	2.51	0.41
1:Bo:77:TYR:CE2	1:Bo:93:ILE:HD13	2.55	0.41
2:Bv:160:ASP:OD1	2:Bv:168:LYS:NZ	2.44	0.41
1:ZU:98:ASP:OD1	1:ZU:98:ASP:N	2.52	0.41
1:Ck:11:ALA:HB1	1:Ck:43:VAL:O	2.20	0.41
2:YH:133:ILE:CD1	2:YH:148:ALA:HB3	2.51	0.41
2:YL:92:PRO:HB2	2:YL:144:LEU:HD13	2.03	0.41
2:DR:101:LYS:NZ	2:DV:2:ASP:OD2	2.42	0.41
2:Dj:133:ILE:CD1	2:Dj:148:ALA:HB3	2.51	0.41
1:Do:43:VAL:HG13	1:Do:50:VAL:HG11	2.03	0.41
2:Dz:92:PRO:HB2	2:Dz:144:LEU:HD13	2.03	0.41
1:EC:11:ALA:HB1	1:EC:43:VAL:O	2.20	0.41
2:Er:92:PRO:HB2	2:Er:144:LEU:HD13	2.03	0.41
2:Et:133:ILE:CD1	2:Et:148:ALA:HB3	2.51	0.41
2:B:133:ILE:CD1	2:B:148:ALA:HB3	2.51	0.41
2:H:133:ILE:CD1	2:H:148:ALA:HB3	2.51	0.41
1:M:33:ALA:N	1:M:34:PRO:CD	2.84	0.41
1:O:77:TYR:CE2	1:O:93:ILE:HD13	2.55	0.41
2:R:92:PRO:HB2	2:R:144:LEU:HD13	2.03	0.41
1:c:11:ALA:HB1	1:c:43:VAL:O	2.20	0.41
2:d:92:PRO:HB2	2:d:144:LEU:HD13	2.03	0.41
2:f:133:ILE:CD1	2:f:148:ALA:HB3	2.51	0.41
1:i:43:VAL:HG13	1:i:50:VAL:HG11	2.03	0.41
2:r:132:LEU:HD23	2:r:148:ALA:HB2	2.03	0.41
1:w:43:VAL:HG13	1:w:50:VAL:HG11	2.03	0.41
2:ZF:160:ASP:OD1	2:ZF:168:LYS:NZ	2.44	0.41
2:ZH:170:LYS:HG2	2:ZH:224:TRP:CH2	2.55	0.41
1:AA:11:ALA:HB1	1:AA:43:VAL:O	2.20	0.41
2:AF:133:ILE:CD1	2:AF:148:ALA:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AL:133:ILE:CD1	2:AL:148:ALA:HB3	2.51	0.41
2:AP:170:LYS:HG2	2:AP:224:TRP:CH2	2.55	0.41
2:AR:133:ILE:CD1	2:AR:148:ALA:HB3	2.51	0.41
1:AU:43:VAL:HG13	1:AU:50:VAL:HG11	2.03	0.41
1:Ac:43:VAL:HG13	1:Ac:50:VAL:HG11	2.03	0.41
2:Aj:133:ILE:CD1	2:Aj:148:ALA:HB3	2.51	0.41
2:An:170:LYS:HG2	2:An:224:TRP:CH2	2.55	0.41
1:Aq:11:ALA:HB1	1:Aq:43:VAL:O	2.20	0.41
1:As:98:ASP:OD1	1:As:98:ASP:N	2.51	0.41
2:Av:133:ILE:CD1	2:Av:148:ALA:HB3	2.51	0.41
1:ZQ:43:VAL:HG13	1:ZQ:50:VAL:HG11	2.03	0.41
1:BC:33:ALA:N	1:BC:34:PRO:CD	2.84	0.41
1:BI:43:VAL:HG13	1:BI:50:VAL:HG11	2.03	0.41
2:BP:101:LYS:NZ	2:BT:2:ASP:OD2	2.42	0.41
2:BT:170:LYS:HG2	2:BT:224:TRP:CH2	2.55	0.41
2:BV:132:LEU:HD23	2:BV:148:ALA:HB2	2.03	0.41
1:Bm:11:ALA:HB1	1:Bm:43:VAL:O	2.20	0.41
2:Bn:133:ILE:CD1	2:Bn:148:ALA:HB3	2.51	0.41
2:Bp:160:ASP:OD1	2:Bp:168:LYS:NZ	2.44	0.41
1:By:11:ALA:HB1	1:By:43:VAL:O	2.20	0.41
2:Bz:133:ILE:CD1	2:Bz:148:ALA:HB3	2.51	0.41
1:ZU:11:ALA:HB1	1:ZU:43:VAL:O	2.20	0.41
1:ZW:11:ALA:HB1	1:ZW:43:VAL:O	2.20	0.41
1:ZY:11:ALA:HB1	1:ZY:43:VAL:O	2.20	0.41
1:ZY:33:ALA:N	1:ZY:34:PRO:CD	2.84	0.41
1:CA:33:ALA:N	1:CA:34:PRO:CD	2.84	0.41
1:CM:43:VAL:HG13	1:CM:50:VAL:HG11	2.03	0.41
2:CN:133:ILE:CD1	2:CN:148:ALA:HB3	2.51	0.41
1:CS:43:VAL:HG13	1:CS:50:VAL:HG11	2.03	0.41
1:Ca:11:ALA:HB1	1:Ca:43:VAL:O	2.20	0.41
2:Cb:160:ASP:OD1	2:Cb:168:LYS:NZ	2.44	0.41
2:Cd:92:PRO:HB2	2:Cd:144:LEU:HD13	2.03	0.41
2:Cf:133:ILE:CD1	2:Cf:148:ALA:HB3	2.51	0.41
1:Cq:43:VAL:HG13	1:Cq:50:VAL:HG11	2.03	0.41
2:Ct:222:ILE:O	2:Ct:223:VAL:C	2.63	0.41
1:YG:43:VAL:HG13	1:YG:50:VAL:HG11	2.03	0.41
2:YN:101:LYS:NZ	2:DD:2:ASP:OD2	2.42	0.41
2:DL:133:ILE:CD1	2:DL:148:ALA:HB3	2.51	0.41
1:DM:11:ALA:HB1	1:DM:43:VAL:O	2.20	0.41
2:DP:92:PRO:HB2	2:DP:144:LEU:HD13	2.03	0.41
2:DT:160:ASP:OD1	2:DT:168:LYS:NZ	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DW:43:VAL:HG13	1:DW:50:VAL:HG11	2.03	0.41
2:Dh:92:PRO:HB2	2:Dh:144:LEU:HD13	2.03	0.41
1:Di:43:VAL:HG13	1:Di:50:VAL:HG11	2.03	0.41
2:Dp:133:ILE:CD1	2:Dp:148:ALA:HB3	2.51	0.41
1:Du:33:ALA:N	1:Du:34:PRO:CD	2.84	0.41
2:YV:133:ILE:CD1	2:YV:148:ALA:HB3	2.51	0.41
2:EB:170:LYS:HG2	2:EB:224:TRP:CH2	2.55	0.41
1:EC:43:VAL:HG13	1:EC:50:VAL:HG11	2.03	0.41
2:EF:222:ILE:O	2:EF:223:VAL:C	2.63	0.41
1:Ea:11:ALA:HB1	1:Ea:43:VAL:O	2.20	0.41
1:Ec:11:ALA:HB1	1:Ec:43:VAL:O	2.20	0.41
1:Eg:33:ALA:N	1:Eg:34:PRO:CD	2.84	0.41
2:Er:170:LYS:HG2	2:Er:224:TRP:CH2	2.55	0.41
1:Eu:77:TYR:CE2	1:Eu:93:ILE:HD13	2.55	0.41
1:A:11:ALA:HB1	1:A:43:VAL:O	2.20	0.41
2:L:170:LYS:HG2	2:L:224:TRP:CH2	2.55	0.41
1:M:43:VAL:HG13	1:M:50:VAL:HG11	2.03	0.41
1:S:43:VAL:HG13	1:S:50:VAL:HG11	2.03	0.41
2:T:132:LEU:HD23	2:T:148:ALA:HB2	2.03	0.41
1:Y:43:VAL:HG13	1:Y:50:VAL:HG11	2.03	0.41
1:u:43:VAL:HG13	1:u:50:VAL:HG11	2.03	0.41
1:w:33:ALA:N	1:w:34:PRO:CD	2.84	0.41
2:ZB:92:PRO:HB2	2:ZB:144:LEU:HD13	2.03	0.41
2:AD:92:PRO:HB2	2:AD:144:LEU:HD13	2.03	0.41
2:AF:132:LEU:HD23	2:AF:148:ALA:HB2	2.03	0.41
1:AM:98:ASP:OD1	1:AM:98:ASP:N	2.52	0.41
1:Ae:77:TYR:CE2	1:Ae:93:ILE:HD13	2.55	0.41
2:Ah:92:PRO:HB2	2:Ah:144:LEU:HD13	2.03	0.41
1:Ak:11:ALA:HB1	1:Ak:43:VAL:O	2.20	0.41
2:Av:132:LEU:HD23	2:Av:148:ALA:HB2	2.03	0.41
1:ZS:11:ALA:HB1	1:ZS:43:VAL:O	2.20	0.41
1:BC:43:VAL:HG13	1:BC:50:VAL:HG11	2.03	0.41
1:BI:33:ALA:N	1:BI:34:PRO:CD	2.84	0.41
1:BY:43:VAL:HG13	1:BY:50:VAL:HG11	2.03	0.41
1:Be:43:VAL:HG13	1:Be:50:VAL:HG11	2.03	0.41
1:Bi:77:TYR:CE2	1:Bi:93:ILE:HD13	2.55	0.41
2:Bt:132:LEU:HD23	2:Bt:148:ALA:HB2	2.03	0.41
1:CA:43:VAL:HG13	1:CA:50:VAL:HG11	2.03	0.41
2:CD:160:ASP:OD1	2:CD:168:LYS:NZ	2.44	0.41
2:CZ:133:ILE:CD1	2:CZ:148:ALA:HB3	2.51	0.41
1:Ck:43:VAL:HG13	1:Ck:50:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YM:33:ALA:N	1:YM:34:PRO:CD	2.84	0.41
2:YN:132:LEU:HD23	2:YN:148:ALA:HB2	2.03	0.41
2:YN:133:ILE:CD1	2:YN:148:ALA:HB3	2.51	0.41
2:DR:133:ILE:CD1	2:DR:148:ALA:HB3	2.51	0.41
2:DZ:2:ASP:OD2	2:Db:101:LYS:NZ	2.40	0.41
1:Do:33:ALA:N	1:Do:34:PRO:CD	2.84	0.41
2:Dp:132:LEU:HD23	2:Dp:148:ALA:HB2	2.03	0.41
1:Du:43:VAL:HG13	1:Du:50:VAL:HG11	2.03	0.41
1:Dw:77:TYR:CE2	1:Dw:93:ILE:HD13	2.55	0.41
1:YO:43:VAL:HG13	1:YO:50:VAL:HG11	2.03	0.41
1:EO:43:VAL:HG13	1:EO:50:VAL:HG11	2.03	0.41
2:Eb:133:ILE:CD1	2:Eb:148:ALA:HB3	2.51	0.41
2:En:133:ILE:CD1	2:En:148:ALA:HB3	2.51	0.41
1:Eq:43:VAL:HG13	1:Eq:50:VAL:HG11	2.03	0.41
2:T:133:ILE:CD1	2:T:148:ALA:HB3	2.51	0.40
1:Y:33:ALA:N	1:Y:34:PRO:CD	2.84	0.40
1:a:77:TYR:CE2	1:a:93:ILE:HD13	2.55	0.40
2:p:170:LYS:HG2	2:p:224:TRP:CH2	2.55	0.40
1:ZG:43:VAL:HG13	1:ZG:50:VAL:HG11	2.03	0.40
2:AD:170:LYS:HG2	2:AD:224:TRP:CH2	2.55	0.40
1:AM:11:ALA:HB1	1:AM:43:VAL:O	2.20	0.40
2:AP:92:PRO:HB2	2:AP:144:LEU:HD13	2.03	0.40
1:Ac:33:ALA:N	1:Ac:34:PRO:CD	2.84	0.40
2:Aj:132:LEU:HD23	2:Aj:148:ALA:HB2	2.03	0.40
2:An:92:PRO:HB2	2:An:144:LEU:HD13	2.03	0.40
2:At:92:PRO:HB2	2:At:144:LEU:HD13	2.03	0.40
2:At:170:LYS:HG2	2:At:224:TRP:CH2	2.55	0.40
1:BS:43:VAL:HG13	1:BS:50:VAL:HG11	2.03	0.40
2:Bb:133:ILE:CD1	2:Bb:148:ALA:HB3	2.51	0.40
1:Bg:43:VAL:HG13	1:Bg:50:VAL:HG11	2.03	0.40
1:Bs:33:ALA:N	1:Bs:34:PRO:CD	2.84	0.40
2:Bz:101:LYS:NZ	2:ZX:2:ASP:OD2	2.42	0.40
2:ZV:222:ILE:O	2:ZV:223:VAL:C	2.63	0.40
1:YA:11:ALA:HB1	1:YA:43:VAL:O	2.20	0.40
2:CJ:2:ASP:OD2	2:CL:101:LYS:NZ	2.40	0.40
1:CO:11:ALA:HB1	1:CO:43:VAL:O	2.20	0.40
1:Ce:33:ALA:N	1:Ce:34:PRO:CD	2.84	0.40
1:Ck:33:ALA:HB3	1:Ck:34:PRO:HD3	2.04	0.40
1:DE:33:ALA:N	1:DE:34:PRO:CD	2.84	0.40
2:DH:160:ASP:OD1	2:DH:168:LYS:NZ	2.44	0.40
1:DQ:33:ALA:N	1:DQ:34:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DR:132:LEU:HD23	2:DR:148:ALA:HB2	2.04	0.40
1:Dc:33:ALA:N	1:Dc:34:PRO:CD	2.84	0.40
2:YP:132:LEU:HD23	2:YP:148:ALA:HB2	2.03	0.40
1:EO:33:ALA:HB3	1:EO:34:PRO:HD3	2.04	0.40
2:EV:132:LEU:HD23	2:EV:148:ALA:HB2	2.03	0.40
1:EW:11:ALA:HB1	1:EW:43:VAL:O	2.20	0.40
1:Es:43:VAL:HG13	1:Es:50:VAL:HG11	2.03	0.40
2:L:92:PRO:HB2	2:L:144:LEU:HD13	2.03	0.40
1:ZI:11:ALA:HB1	1:ZI:43:VAL:O	2.20	0.40
1:AC:98:ASP:OD1	1:AC:98:ASP:N	2.51	0.40
2:AL:132:LEU:HD23	2:AL:148:ALA:HB2	2.03	0.40
2:Ab:170:LYS:HG2	2:Ab:224:TRP:CH2	2.55	0.40
2:Ad:133:ILE:CD1	2:Ad:148:ALA:HB3	2.51	0.40
1:Ao:11:ALA:HB1	1:Ao:43:VAL:O	2.20	0.40
1:BE:11:ALA:HB1	1:BE:43:VAL:O	2.20	0.40
2:BN:92:PRO:HB2	2:BN:144:LEU:HD13	2.03	0.40
2:BP:132:LEU:HD23	2:BP:148:ALA:HB2	2.03	0.40
1:Bg:33:ALA:N	1:Bg:34:PRO:CD	2.84	0.40
1:Bm:33:ALA:N	1:Bm:34:PRO:CD	2.84	0.40
2:Bt:133:ILE:CD1	2:Bt:148:ALA:HB3	2.51	0.40
1:Bu:11:ALA:HB1	1:Bu:43:VAL:O	2.20	0.40
1:CS:11:ALA:HB1	1:CS:43:VAL:O	2.20	0.40
2:Cf:132:LEU:HD23	2:Cf:148:ALA:HB2	2.04	0.40
2:Cx:132:LEU:HD23	2:Cx:148:ALA:HB2	2.03	0.40
1:YG:33:ALA:N	1:YG:34:PRO:CD	2.84	0.40
1:YK:43:VAL:HG13	1:YK:50:VAL:HG11	2.03	0.40
2:DN:160:ASP:OD1	2:DN:168:LYS:NZ	2.44	0.40
1:Dg:98:ASP:OD1	1:Dg:98:ASP:N	2.51	0.40
1:Di:33:ALA:N	1:Di:34:PRO:CD	2.84	0.40
1:Dm:43:VAL:HG13	1:Dm:50:VAL:HG11	2.03	0.40
2:Dv:132:LEU:HD23	2:Dv:148:ALA:HB2	2.03	0.40
2:YP:133:ILE:CD1	2:YP:148:ALA:HB3	2.51	0.40
2:EB:92:PRO:HB2	2:EB:144:LEU:HD13	2.03	0.40
2:EJ:132:LEU:HD23	2:EJ:148:ALA:HB2	2.03	0.40
1:EU:33:ALA:N	1:EU:34:PRO:CD	2.84	0.40
2:Ed:222:ILE:O	2:Ed:223:VAL:C	2.63	0.40
2:Eh:132:LEU:HD23	2:Eh:148:ALA:HB2	2.03	0.40
1:Es:33:ALA:N	1:Es:34:PRO:CD	2.84	0.40
1:A:33:ALA:N	1:A:34:PRO:CD	2.84	0.40
2:N:132:LEU:HD23	2:N:148:ALA:HB2	2.03	0.40
2:Z:133:ILE:CD1	2:Z:148:ALA:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:43:VAL:HG13	1:o:50:VAL:HG11	2.03	0.40
2:ZD:132:LEU:HD23	2:ZD:148:ALA:HB2	2.03	0.40
2:ZD:133:ILE:CD1	2:ZD:148:ALA:HB3	2.51	0.40
2:AJ:170:LYS:HG2	2:AJ:224:TRP:CH2	2.55	0.40
2:ZR:132:LEU:HD23	2:ZR:148:ALA:HB2	2.03	0.40
2:BP:133:ILE:CD1	2:BP:148:ALA:HB3	2.51	0.40
2:ZZ:132:LEU:HD23	2:ZZ:148:ALA:HB2	2.03	0.40
1:CY:43:VAL:HG13	1:CY:50:VAL:HG11	2.03	0.40
2:Cj:92:PRO:HB2	2:Cj:144:LEU:HD13	2.03	0.40
2:Cl:132:LEU:HD23	2:Cl:148:ALA:HB2	2.03	0.40
1:Co:43:VAL:HG13	1:Co:50:VAL:HG11	2.03	0.40
1:DC:77:TYR:OH	2:DD:259:GLN:OE1	2.38	0.40
2:DF:132:LEU:HD23	2:DF:148:ALA:HB2	2.03	0.40
1:DK:43:VAL:HG13	1:DK:50:VAL:HG11	2.03	0.40
1:DS:80:VAL:HG11	1:DS:102:ILE:HG21	2.04	0.40
2:DV:92:PRO:HB2	2:DV:144:LEU:HD13	2.03	0.40
1:DW:11:ALA:HB1	1:DW:43:VAL:O	2.20	0.40
2:EN:92:PRO:HB2	2:EN:144:LEU:HD13	2.03	0.40
2:EP:132:LEU:HD23	2:EP:148:ALA:HB2	2.03	0.40
1:ES:43:VAL:HG13	1:ES:50:VAL:HG11	2.03	0.40
2:EV:133:ILE:CD1	2:EV:148:ALA:HB3	2.51	0.40
1:Ei:11:ALA:HB1	1:Ei:43:VAL:O	2.20	0.40
2:H:132:LEU:HD23	2:H:148:ALA:HB2	2.03	0.40
1:e:43:VAL:HG13	1:e:50:VAL:HG11	2.03	0.40
1:AQ:43:VAL:HG13	1:AQ:50:VAL:HG11	2.03	0.40
1:Aa:43:VAL:HG13	1:Aa:50:VAL:HG11	2.03	0.40
1:Ae:80:VAL:HG11	1:Ae:102:ILE:HG21	2.04	0.40
2:Az:170:LYS:HG2	2:Az:224:TRP:CH2	2.55	0.40
2:BD:133:ILE:CD1	2:BD:148:ALA:HB3	2.51	0.40
2:BF:160:ASP:OD1	2:BF:168:LYS:NZ	2.44	0.40
2:ZZ:133:ILE:CD1	2:ZZ:148:ALA:HB3	2.51	0.40
2:YD:92:PRO:HB2	2:YD:144:LEU:HD13	2.03	0.40
1:CC:11:ALA:HB1	1:CC:43:VAL:O	2.20	0.40
1:CC:80:VAL:HG11	1:CC:102:ILE:HG21	2.04	0.40
2:CN:132:LEU:HD23	2:CN:148:ALA:HB2	2.03	0.40
2:CR:92:PRO:HB2	2:CR:144:LEU:HD13	2.03	0.40
1:CY:33:ALA:N	1:CY:34:PRO:CD	2.84	0.40
1:Cg:80:VAL:HG11	1:Cg:102:ILE:HG21	2.04	0.40
2:Cr:101:LYS:NZ	2:Cr:2:ASP:OD2	2.42	0.40
2:Cx:133:ILE:CD1	2:Cx:148:ALA:HB3	2.51	0.40
2:YF:92:PRO:HB2	2:YF:144:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:43:VAL:HG13	1:DC:50:VAL:HG11	2.03	0.40
1:DE:33:ALA:HB3	1:DE:34:PRO:HD3	2.04	0.40
1:DI:43:VAL:HG13	1:DI:50:VAL:HG11	2.03	0.40
1:DK:33:ALA:N	1:DK:34:PRO:CD	2.84	0.40
2:Dd:132:LEU:HD23	2:Dd:148:ALA:HB2	2.03	0.40
1:Ds:43:VAL:HG13	1:Ds:50:VAL:HG11	2.03	0.40
2:YV:132:LEU:HD23	2:YV:148:ALA:HB2	2.03	0.40
2:EJ:133:ILE:CD1	2:EJ:148:ALA:HB3	2.51	0.40
2:Eh:133:ILE:CD1	2:Eh:148:ALA:HB3	2.51	0.40
2:X:92:PRO:HB2	2:X:144:LEU:HD13	2.03	0.40
2:Z:101:LYS:NZ	2:d:2:ASP:OD2	2.42	0.40
1:a:80:VAL:HG11	1:a:102:ILE:HG21	2.04	0.40
1:k:33:ALA:N	1:k:34:PRO:CD	2.84	0.40
1:k:43:VAL:HG13	1:k:50:VAL:HG11	2.03	0.40
1:ZC:33:ALA:N	1:ZC:34:PRO:CD	2.84	0.40
1:AW:33:ALA:N	1:AW:34:PRO:CD	2.84	0.40
1:AW:43:VAL:HG13	1:AW:50:VAL:HG11	2.03	0.40
1:Am:7:ILE:HG22	1:Am:14:VAL:HG22	2.04	0.40
2:ZL:133:ILE:CD1	2:ZL:148:ALA:HB3	2.51	0.40
2:BB:92:PRO:HB2	2:BB:144:LEU:HD13	2.03	0.40
1:BE:80:VAL:HG11	1:BE:102:ILE:HG21	2.04	0.40
1:BO:33:ALA:N	1:BO:34:PRO:CD	2.84	0.40
2:Bl:92:PRO:HB2	2:Bl:144:LEU:HD13	2.03	0.40
1:By:43:VAL:HG13	1:By:50:VAL:HG11	2.03	0.40
1:ZY:43:VAL:HG13	1:ZY:50:VAL:HG11	2.03	0.40
2:CB:133:ILE:CD1	2:CB:148:ALA:HB3	2.51	0.40
1:CG:33:ALA:N	1:CG:34:PRO:CD	2.84	0.40
2:CT:132:LEU:HD23	2:CT:148:ALA:HB2	2.04	0.40
2:CV:2:ASP:OD2	2:CX:101:LYS:NZ	2.40	0.40
2:Cb:230:ALA:O	2:Cb:234:MET:HG3	2.22	0.40
1:Ck:33:ALA:N	1:Ck:34:PRO:CD	2.84	0.40
2:DH:230:ALA:O	2:DH:234:MET:HG3	2.22	0.40
1:DI:7:ILE:HG22	1:DI:14:VAL:HG22	2.04	0.40
1:DI:98:ASP:OD1	1:DI:98:ASP:N	2.51	0.40
2:DX:132:LEU:HD23	2:DX:148:ALA:HB2	2.04	0.40
1:Dc:33:ALA:HB3	1:Dc:34:PRO:HD3	2.04	0.40
2:Df:230:ALA:O	2:Df:234:MET:HG3	2.22	0.40
1:Dg:7:ILE:HG22	1:Dg:14:VAL:HG22	2.04	0.40
1:Dg:43:VAL:HG13	1:Dg:50:VAL:HG11	2.03	0.40
1:Dk:80:VAL:HG11	1:Dk:102:ILE:HG21	2.04	0.40
1:YQ:80:VAL:HG11	1:YQ:102:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YS:98:ASP:OD1	1:YS:98:ASP:N	2.51	0.40
2:YT:92:PRO:HB2	2:YT:144:LEU:HD13	2.03	0.40
2:ED:101:LYS:NZ	2:EH:2:ASP:OD2	2.42	0.40
1:EG:7:ILE:HG22	1:EG:14:VAL:HG22	2.04	0.40
1:Ea:43:VAL:HG13	1:Ea:50:VAL:HG11	2.03	0.40
2:El:92:PRO:HB2	2:El:144:LEU:HD13	2.03	0.40
2:En:101:LYS:NZ	2:Er:2:ASP:OD2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	104/114 (91%)	104 (100%)	0	0	100	100
1	AA	104/114 (91%)	104 (100%)	0	0	100	100
1	AC	104/114 (91%)	104 (100%)	0	0	100	100
1	AE	104/114 (91%)	104 (100%)	0	0	100	100
1	AG	104/114 (91%)	104 (100%)	0	0	100	100
1	AI	104/114 (91%)	104 (100%)	0	0	100	100
1	AK	104/114 (91%)	104 (100%)	0	0	100	100
1	AM	104/114 (91%)	104 (100%)	0	0	100	100
1	AO	104/114 (91%)	104 (100%)	0	0	100	100
1	AQ	104/114 (91%)	104 (100%)	0	0	100	100
1	AS	104/114 (91%)	104 (100%)	0	0	100	100
1	AU	104/114 (91%)	104 (100%)	0	0	100	100
1	AW	104/114 (91%)	104 (100%)	0	0	100	100
1	AY	104/114 (91%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	104/114 (91%)	104 (100%)	0	0	100	100
1	Ac	104/114 (91%)	104 (100%)	0	0	100	100
1	Ae	104/114 (91%)	104 (100%)	0	0	100	100
1	Ag	104/114 (91%)	104 (100%)	0	0	100	100
1	Ai	104/114 (91%)	104 (100%)	0	0	100	100
1	Ak	104/114 (91%)	104 (100%)	0	0	100	100
1	Am	104/114 (91%)	104 (100%)	0	0	100	100
1	Ao	104/114 (91%)	104 (100%)	0	0	100	100
1	Aq	104/114 (91%)	104 (100%)	0	0	100	100
1	As	104/114 (91%)	104 (100%)	0	0	100	100
1	Au	104/114 (91%)	104 (100%)	0	0	100	100
1	Aw	104/114 (91%)	104 (100%)	0	0	100	100
1	Ay	104/114 (91%)	104 (100%)	0	0	100	100
1	BA	104/114 (91%)	104 (100%)	0	0	100	100
1	BC	104/114 (91%)	104 (100%)	0	0	100	100
1	BE	104/114 (91%)	104 (100%)	0	0	100	100
1	BG	104/114 (91%)	104 (100%)	0	0	100	100
1	BI	104/114 (91%)	104 (100%)	0	0	100	100
1	BK	104/114 (91%)	104 (100%)	0	0	100	100
1	BM	104/114 (91%)	104 (100%)	0	0	100	100
1	BO	104/114 (91%)	104 (100%)	0	0	100	100
1	BQ	104/114 (91%)	104 (100%)	0	0	100	100
1	BS	104/114 (91%)	104 (100%)	0	0	100	100
1	BU	104/114 (91%)	104 (100%)	0	0	100	100
1	BW	104/114 (91%)	104 (100%)	0	0	100	100
1	BY	104/114 (91%)	104 (100%)	0	0	100	100
1	Ba	104/114 (91%)	104 (100%)	0	0	100	100
1	Bc	104/114 (91%)	104 (100%)	0	0	100	100
1	Be	104/114 (91%)	104 (100%)	0	0	100	100
1	Bg	104/114 (91%)	104 (100%)	0	0	100	100
1	Bi	104/114 (91%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bk	104/114 (91%)	104 (100%)	0	0	100	100
1	Bm	104/114 (91%)	104 (100%)	0	0	100	100
1	Bo	104/114 (91%)	104 (100%)	0	0	100	100
1	Bq	104/114 (91%)	104 (100%)	0	0	100	100
1	Bs	104/114 (91%)	104 (100%)	0	0	100	100
1	Bu	104/114 (91%)	104 (100%)	0	0	100	100
1	Bw	104/114 (91%)	104 (100%)	0	0	100	100
1	By	104/114 (91%)	104 (100%)	0	0	100	100
1	C	104/114 (91%)	104 (100%)	0	0	100	100
1	CA	104/114 (91%)	104 (100%)	0	0	100	100
1	CC	104/114 (91%)	104 (100%)	0	0	100	100
1	CE	104/114 (91%)	104 (100%)	0	0	100	100
1	CG	104/114 (91%)	104 (100%)	0	0	100	100
1	CI	104/114 (91%)	104 (100%)	0	0	100	100
1	CK	104/114 (91%)	104 (100%)	0	0	100	100
1	CM	104/114 (91%)	104 (100%)	0	0	100	100
1	CO	104/114 (91%)	104 (100%)	0	0	100	100
1	CQ	104/114 (91%)	104 (100%)	0	0	100	100
1	CS	104/114 (91%)	104 (100%)	0	0	100	100
1	CU	104/114 (91%)	104 (100%)	0	0	100	100
1	CW	104/114 (91%)	104 (100%)	0	0	100	100
1	CY	104/114 (91%)	104 (100%)	0	0	100	100
1	Ca	104/114 (91%)	104 (100%)	0	0	100	100
1	Cc	104/114 (91%)	104 (100%)	0	0	100	100
1	Ce	104/114 (91%)	104 (100%)	0	0	100	100
1	Cg	104/114 (91%)	104 (100%)	0	0	100	100
1	Ci	104/114 (91%)	104 (100%)	0	0	100	100
1	Ck	104/114 (91%)	104 (100%)	0	0	100	100
1	Cm	104/114 (91%)	104 (100%)	0	0	100	100
1	Co	104/114 (91%)	104 (100%)	0	0	100	100
1	Cq	104/114 (91%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Cs	104/114 (91%)	104 (100%)	0	0	100	100
1	Cu	104/114 (91%)	104 (100%)	0	0	100	100
1	Cw	104/114 (91%)	104 (100%)	0	0	100	100
1	Cy	104/114 (91%)	104 (100%)	0	0	100	100
1	DA	104/114 (91%)	104 (100%)	0	0	100	100
1	DC	104/114 (91%)	104 (100%)	0	0	100	100
1	DE	104/114 (91%)	104 (100%)	0	0	100	100
1	DG	104/114 (91%)	104 (100%)	0	0	100	100
1	DI	104/114 (91%)	104 (100%)	0	0	100	100
1	DK	104/114 (91%)	104 (100%)	0	0	100	100
1	DM	104/114 (91%)	104 (100%)	0	0	100	100
1	DO	104/114 (91%)	104 (100%)	0	0	100	100
1	DQ	104/114 (91%)	104 (100%)	0	0	100	100
1	DS	104/114 (91%)	104 (100%)	0	0	100	100
1	DU	104/114 (91%)	104 (100%)	0	0	100	100
1	DW	104/114 (91%)	104 (100%)	0	0	100	100
1	DY	104/114 (91%)	104 (100%)	0	0	100	100
1	Da	104/114 (91%)	104 (100%)	0	0	100	100
1	Dc	104/114 (91%)	104 (100%)	0	0	100	100
1	De	104/114 (91%)	104 (100%)	0	0	100	100
1	Dg	104/114 (91%)	104 (100%)	0	0	100	100
1	Di	104/114 (91%)	104 (100%)	0	0	100	100
1	Dk	104/114 (91%)	104 (100%)	0	0	100	100
1	Dm	104/114 (91%)	104 (100%)	0	0	100	100
1	Do	104/114 (91%)	104 (100%)	0	0	100	100
1	Dq	104/114 (91%)	104 (100%)	0	0	100	100
1	Ds	104/114 (91%)	104 (100%)	0	0	100	100
1	Du	104/114 (91%)	104 (100%)	0	0	100	100
1	Dw	104/114 (91%)	104 (100%)	0	0	100	100
1	Dy	104/114 (91%)	104 (100%)	0	0	100	100
1	E	104/114 (91%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EA	104/114 (91%)	104 (100%)	0	0	100	100
1	EC	104/114 (91%)	104 (100%)	0	0	100	100
1	EE	104/114 (91%)	104 (100%)	0	0	100	100
1	EG	104/114 (91%)	104 (100%)	0	0	100	100
1	EI	104/114 (91%)	104 (100%)	0	0	100	100
1	EK	104/114 (91%)	104 (100%)	0	0	100	100
1	EM	104/114 (91%)	104 (100%)	0	0	100	100
1	EO	104/114 (91%)	104 (100%)	0	0	100	100
1	EQ	104/114 (91%)	104 (100%)	0	0	100	100
1	ES	104/114 (91%)	104 (100%)	0	0	100	100
1	EU	104/114 (91%)	104 (100%)	0	0	100	100
1	EW	104/114 (91%)	104 (100%)	0	0	100	100
1	EY	104/114 (91%)	104 (100%)	0	0	100	100
1	Ea	104/114 (91%)	104 (100%)	0	0	100	100
1	Ec	104/114 (91%)	104 (100%)	0	0	100	100
1	Ee	104/114 (91%)	104 (100%)	0	0	100	100
1	Eg	104/114 (91%)	104 (100%)	0	0	100	100
1	Ei	104/114 (91%)	104 (100%)	0	0	100	100
1	Ek	104/114 (91%)	104 (100%)	0	0	100	100
1	Em	104/114 (91%)	104 (100%)	0	0	100	100
1	Eo	104/114 (91%)	104 (100%)	0	0	100	100
1	Eq	104/114 (91%)	104 (100%)	0	0	100	100
1	Es	104/114 (91%)	104 (100%)	0	0	100	100
1	Eu	104/114 (91%)	104 (100%)	0	0	100	100
1	Ew	104/114 (91%)	104 (100%)	0	0	100	100
1	G	104/114 (91%)	104 (100%)	0	0	100	100
1	I	104/114 (91%)	104 (100%)	0	0	100	100
1	K	104/114 (91%)	104 (100%)	0	0	100	100
1	M	104/114 (91%)	104 (100%)	0	0	100	100
1	O	104/114 (91%)	104 (100%)	0	0	100	100
1	Q	104/114 (91%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	104/114 (91%)	104 (100%)	0	0	100	100
1	U	104/114 (91%)	104 (100%)	0	0	100	100
1	W	104/114 (91%)	104 (100%)	0	0	100	100
1	Y	104/114 (91%)	104 (100%)	0	0	100	100
1	YA	104/114 (91%)	104 (100%)	0	0	100	100
1	YC	104/114 (91%)	104 (100%)	0	0	100	100
1	YE	104/114 (91%)	104 (100%)	0	0	100	100
1	YG	104/114 (91%)	104 (100%)	0	0	100	100
1	YI	104/114 (91%)	104 (100%)	0	0	100	100
1	YK	104/114 (91%)	104 (100%)	0	0	100	100
1	YM	104/114 (91%)	104 (100%)	0	0	100	100
1	YO	104/114 (91%)	104 (100%)	0	0	100	100
1	YQ	104/114 (91%)	104 (100%)	0	0	100	100
1	YS	104/114 (91%)	104 (100%)	0	0	100	100
1	YU	104/114 (91%)	104 (100%)	0	0	100	100
1	YW	104/114 (91%)	104 (100%)	0	0	100	100
1	ZA	104/114 (91%)	104 (100%)	0	0	100	100
1	ZC	104/114 (91%)	104 (100%)	0	0	100	100
1	ZE	104/114 (91%)	104 (100%)	0	0	100	100
1	ZG	104/114 (91%)	104 (100%)	0	0	100	100
1	ZI	104/114 (91%)	104 (100%)	0	0	100	100
1	ZK	104/114 (91%)	104 (100%)	0	0	100	100
1	ZM	104/114 (91%)	104 (100%)	0	0	100	100
1	ZO	104/114 (91%)	104 (100%)	0	0	100	100
1	ZQ	104/114 (91%)	104 (100%)	0	0	100	100
1	ZS	104/114 (91%)	104 (100%)	0	0	100	100
1	ZU	104/114 (91%)	104 (100%)	0	0	100	100
1	ZW	104/114 (91%)	104 (100%)	0	0	100	100
1	ZY	104/114 (91%)	104 (100%)	0	0	100	100
1	a	104/114 (91%)	104 (100%)	0	0	100	100
1	c	104/114 (91%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	104/114 (91%)	104 (100%)	0	0	100	100
1	g	104/114 (91%)	104 (100%)	0	0	100	100
1	i	104/114 (91%)	104 (100%)	0	0	100	100
1	k	104/114 (91%)	104 (100%)	0	0	100	100
1	m	104/114 (91%)	104 (100%)	0	0	100	100
1	o	104/114 (91%)	104 (100%)	0	0	100	100
1	q	104/114 (91%)	104 (100%)	0	0	100	100
1	s	104/114 (91%)	104 (100%)	0	0	100	100
1	u	104/114 (91%)	104 (100%)	0	0	100	100
1	w	104/114 (91%)	104 (100%)	0	0	100	100
1	y	104/114 (91%)	104 (100%)	0	0	100	100
2	AB	290/300 (97%)	290 (100%)	0	0	100	100
2	AD	290/300 (97%)	290 (100%)	0	0	100	100
2	AF	290/300 (97%)	290 (100%)	0	0	100	100
2	AH	290/300 (97%)	290 (100%)	0	0	100	100
2	AJ	290/300 (97%)	290 (100%)	0	0	100	100
2	AL	290/300 (97%)	290 (100%)	0	0	100	100
2	AN	290/300 (97%)	290 (100%)	0	0	100	100
2	AP	290/300 (97%)	290 (100%)	0	0	100	100
2	AR	290/300 (97%)	290 (100%)	0	0	100	100
2	AT	290/300 (97%)	290 (100%)	0	0	100	100
2	AV	290/300 (97%)	290 (100%)	0	0	100	100
2	AX	290/300 (97%)	290 (100%)	0	0	100	100
2	AZ	290/300 (97%)	290 (100%)	0	0	100	100
2	Ab	290/300 (97%)	290 (100%)	0	0	100	100
2	Ad	290/300 (97%)	290 (100%)	0	0	100	100
2	Af	290/300 (97%)	290 (100%)	0	0	100	100
2	Ah	290/300 (97%)	290 (100%)	0	0	100	100
2	Aj	290/300 (97%)	290 (100%)	0	0	100	100
2	Al	290/300 (97%)	290 (100%)	0	0	100	100
2	An	290/300 (97%)	290 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ap	290/300 (97%)	290 (100%)	0	0	100	100
2	Ar	290/300 (97%)	290 (100%)	0	0	100	100
2	At	290/300 (97%)	290 (100%)	0	0	100	100
2	Av	290/300 (97%)	290 (100%)	0	0	100	100
2	Ax	290/300 (97%)	290 (100%)	0	0	100	100
2	Az	290/300 (97%)	290 (100%)	0	0	100	100
2	B	290/300 (97%)	290 (100%)	0	0	100	100
2	BB	290/300 (97%)	290 (100%)	0	0	100	100
2	BD	290/300 (97%)	290 (100%)	0	0	100	100
2	BF	290/300 (97%)	290 (100%)	0	0	100	100
2	BH	290/300 (97%)	290 (100%)	0	0	100	100
2	BJ	290/300 (97%)	290 (100%)	0	0	100	100
2	BL	290/300 (97%)	290 (100%)	0	0	100	100
2	BN	290/300 (97%)	290 (100%)	0	0	100	100
2	BP	290/300 (97%)	290 (100%)	0	0	100	100
2	BR	290/300 (97%)	290 (100%)	0	0	100	100
2	BT	290/300 (97%)	290 (100%)	0	0	100	100
2	BV	290/300 (97%)	290 (100%)	0	0	100	100
2	BX	290/300 (97%)	290 (100%)	0	0	100	100
2	BZ	290/300 (97%)	290 (100%)	0	0	100	100
2	Bb	290/300 (97%)	290 (100%)	0	0	100	100
2	Bd	290/300 (97%)	290 (100%)	0	0	100	100
2	Bf	290/300 (97%)	290 (100%)	0	0	100	100
2	Bh	290/300 (97%)	290 (100%)	0	0	100	100
2	Bj	290/300 (97%)	290 (100%)	0	0	100	100
2	Bl	290/300 (97%)	290 (100%)	0	0	100	100
2	Bn	290/300 (97%)	290 (100%)	0	0	100	100
2	Bp	290/300 (97%)	290 (100%)	0	0	100	100
2	Br	290/300 (97%)	290 (100%)	0	0	100	100
2	Bt	290/300 (97%)	290 (100%)	0	0	100	100
2	Bv	290/300 (97%)	290 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bx	290/300 (97%)	290 (100%)	0	0	100	100
2	Bz	290/300 (97%)	290 (100%)	0	0	100	100
2	CB	290/300 (97%)	290 (100%)	0	0	100	100
2	CD	290/300 (97%)	290 (100%)	0	0	100	100
2	CF	290/300 (97%)	290 (100%)	0	0	100	100
2	CH	290/300 (97%)	290 (100%)	0	0	100	100
2	CJ	290/300 (97%)	290 (100%)	0	0	100	100
2	CL	290/300 (97%)	290 (100%)	0	0	100	100
2	CN	290/300 (97%)	290 (100%)	0	0	100	100
2	CP	290/300 (97%)	290 (100%)	0	0	100	100
2	CR	290/300 (97%)	290 (100%)	0	0	100	100
2	CT	290/300 (97%)	290 (100%)	0	0	100	100
2	CV	290/300 (97%)	290 (100%)	0	0	100	100
2	CX	290/300 (97%)	290 (100%)	0	0	100	100
2	CZ	290/300 (97%)	290 (100%)	0	0	100	100
2	Cb	290/300 (97%)	290 (100%)	0	0	100	100
2	Cd	290/300 (97%)	290 (100%)	0	0	100	100
2	Cf	290/300 (97%)	290 (100%)	0	0	100	100
2	Ch	290/300 (97%)	290 (100%)	0	0	100	100
2	Cj	290/300 (97%)	290 (100%)	0	0	100	100
2	Cl	290/300 (97%)	290 (100%)	0	0	100	100
2	Cn	290/300 (97%)	290 (100%)	0	0	100	100
2	Cp	290/300 (97%)	290 (100%)	0	0	100	100
2	Cr	290/300 (97%)	290 (100%)	0	0	100	100
2	Ct	290/300 (97%)	290 (100%)	0	0	100	100
2	Cv	290/300 (97%)	290 (100%)	0	0	100	100
2	Cx	290/300 (97%)	290 (100%)	0	0	100	100
2	Cz	290/300 (97%)	290 (100%)	0	0	100	100
2	D	290/300 (97%)	290 (100%)	0	0	100	100
2	DB	290/300 (97%)	290 (100%)	0	0	100	100
2	DD	290/300 (97%)	290 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DF	290/300 (97%)	290 (100%)	0	0	100	100
2	DH	290/300 (97%)	290 (100%)	0	0	100	100
2	DJ	290/300 (97%)	290 (100%)	0	0	100	100
2	DL	290/300 (97%)	290 (100%)	0	0	100	100
2	DN	290/300 (97%)	290 (100%)	0	0	100	100
2	DP	290/300 (97%)	290 (100%)	0	0	100	100
2	DR	290/300 (97%)	290 (100%)	0	0	100	100
2	DT	290/300 (97%)	290 (100%)	0	0	100	100
2	DV	290/300 (97%)	290 (100%)	0	0	100	100
2	DX	290/300 (97%)	290 (100%)	0	0	100	100
2	DZ	290/300 (97%)	290 (100%)	0	0	100	100
2	Db	290/300 (97%)	290 (100%)	0	0	100	100
2	Dd	290/300 (97%)	290 (100%)	0	0	100	100
2	Df	290/300 (97%)	290 (100%)	0	0	100	100
2	Dh	290/300 (97%)	290 (100%)	0	0	100	100
2	Dj	290/300 (97%)	290 (100%)	0	0	100	100
2	Di	290/300 (97%)	290 (100%)	0	0	100	100
2	Dn	290/300 (97%)	290 (100%)	0	0	100	100
2	Dp	290/300 (97%)	290 (100%)	0	0	100	100
2	Dr	290/300 (97%)	290 (100%)	0	0	100	100
2	Dt	290/300 (97%)	290 (100%)	0	0	100	100
2	Dv	290/300 (97%)	290 (100%)	0	0	100	100
2	Dx	290/300 (97%)	290 (100%)	0	0	100	100
2	Dz	290/300 (97%)	290 (100%)	0	0	100	100
2	EB	290/300 (97%)	290 (100%)	0	0	100	100
2	ED	290/300 (97%)	290 (100%)	0	0	100	100
2	EF	290/300 (97%)	290 (100%)	0	0	100	100
2	EH	290/300 (97%)	290 (100%)	0	0	100	100
2	EJ	290/300 (97%)	290 (100%)	0	0	100	100
2	EL	290/300 (97%)	290 (100%)	0	0	100	100
2	EN	290/300 (97%)	290 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	EP	290/300 (97%)	290 (100%)	0	0	100	100
2	ER	290/300 (97%)	290 (100%)	0	0	100	100
2	ET	290/300 (97%)	290 (100%)	0	0	100	100
2	EV	290/300 (97%)	290 (100%)	0	0	100	100
2	EX	290/300 (97%)	290 (100%)	0	0	100	100
2	EZ	290/300 (97%)	290 (100%)	0	0	100	100
2	Eb	290/300 (97%)	290 (100%)	0	0	100	100
2	Ed	290/300 (97%)	290 (100%)	0	0	100	100
2	Ef	290/300 (97%)	290 (100%)	0	0	100	100
2	Eh	290/300 (97%)	290 (100%)	0	0	100	100
2	Ej	290/300 (97%)	290 (100%)	0	0	100	100
2	El	290/300 (97%)	290 (100%)	0	0	100	100
2	En	290/300 (97%)	290 (100%)	0	0	100	100
2	Ep	290/300 (97%)	290 (100%)	0	0	100	100
2	Er	290/300 (97%)	290 (100%)	0	0	100	100
2	Et	290/300 (97%)	290 (100%)	0	0	100	100
2	Ev	290/300 (97%)	290 (100%)	0	0	100	100
2	Ex	290/300 (97%)	290 (100%)	0	0	100	100
2	F	290/300 (97%)	290 (100%)	0	0	100	100
2	H	290/300 (97%)	290 (100%)	0	0	100	100
2	J	290/300 (97%)	290 (100%)	0	0	100	100
2	L	290/300 (97%)	290 (100%)	0	0	100	100
2	N	290/300 (97%)	290 (100%)	0	0	100	100
2	P	290/300 (97%)	290 (100%)	0	0	100	100
2	R	290/300 (97%)	290 (100%)	0	0	100	100
2	T	290/300 (97%)	290 (100%)	0	0	100	100
2	V	290/300 (97%)	290 (100%)	0	0	100	100
2	X	290/300 (97%)	290 (100%)	0	0	100	100
2	YB	290/300 (97%)	290 (100%)	0	0	100	100
2	YD	290/300 (97%)	290 (100%)	0	0	100	100
2	YF	290/300 (97%)	290 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	YH	290/300 (97%)	290 (100%)	0	0	100	100
2	YJ	290/300 (97%)	290 (100%)	0	0	100	100
2	YL	290/300 (97%)	290 (100%)	0	0	100	100
2	YN	290/300 (97%)	290 (100%)	0	0	100	100
2	YP	290/300 (97%)	290 (100%)	0	0	100	100
2	YR	290/300 (97%)	290 (100%)	0	0	100	100
2	YT	290/300 (97%)	290 (100%)	0	0	100	100
2	YV	290/300 (97%)	290 (100%)	0	0	100	100
2	YX	290/300 (97%)	290 (100%)	0	0	100	100
2	Z	290/300 (97%)	290 (100%)	0	0	100	100
2	ZB	290/300 (97%)	290 (100%)	0	0	100	100
2	ZD	290/300 (97%)	290 (100%)	0	0	100	100
2	ZF	290/300 (97%)	290 (100%)	0	0	100	100
2	ZH	290/300 (97%)	290 (100%)	0	0	100	100
2	ZJ	290/300 (97%)	290 (100%)	0	0	100	100
2	ZL	290/300 (97%)	290 (100%)	0	0	100	100
2	ZN	290/300 (97%)	290 (100%)	0	0	100	100
2	ZP	290/300 (97%)	290 (100%)	0	0	100	100
2	ZR	290/300 (97%)	290 (100%)	0	0	100	100
2	ZT	290/300 (97%)	290 (100%)	0	0	100	100
2	ZV	290/300 (97%)	290 (100%)	0	0	100	100
2	ZX	290/300 (97%)	290 (100%)	0	0	100	100
2	ZZ	290/300 (97%)	290 (100%)	0	0	100	100
2	b	290/300 (97%)	290 (100%)	0	0	100	100
2	d	290/300 (97%)	290 (100%)	0	0	100	100
2	f	290/300 (97%)	290 (100%)	0	0	100	100
2	h	290/300 (97%)	290 (100%)	0	0	100	100
2	j	290/300 (97%)	290 (100%)	0	0	100	100
2	l	290/300 (97%)	290 (100%)	0	0	100	100
2	n	290/300 (97%)	290 (100%)	0	0	100	100
2	p	290/300 (97%)	290 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	r	290/300 (97%)	290 (100%)	0	0	100	100
2	t	290/300 (97%)	290 (100%)	0	0	100	100
2	v	290/300 (97%)	290 (100%)	0	0	100	100
2	x	290/300 (97%)	290 (100%)	0	0	100	100
2	z	290/300 (97%)	290 (100%)	0	0	100	100
All	All	70920/74520 (95%)	70920 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/94 (92%)	86 (100%)	0	100	100
1	AA	86/94 (92%)	86 (100%)	0	100	100
1	AC	86/94 (92%)	86 (100%)	0	100	100
1	AE	86/94 (92%)	86 (100%)	0	100	100
1	AG	86/94 (92%)	86 (100%)	0	100	100
1	AI	86/94 (92%)	86 (100%)	0	100	100
1	AK	86/94 (92%)	86 (100%)	0	100	100
1	AM	86/94 (92%)	86 (100%)	0	100	100
1	AO	86/94 (92%)	86 (100%)	0	100	100
1	AQ	86/94 (92%)	86 (100%)	0	100	100
1	AS	86/94 (92%)	86 (100%)	0	100	100
1	AU	86/94 (92%)	86 (100%)	0	100	100
1	AW	86/94 (92%)	86 (100%)	0	100	100
1	AY	86/94 (92%)	86 (100%)	0	100	100
1	Aa	86/94 (92%)	86 (100%)	0	100	100
1	Ac	86/94 (92%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ae	86/94 (92%)	86 (100%)	0	100	100
1	Ag	86/94 (92%)	86 (100%)	0	100	100
1	Ai	86/94 (92%)	86 (100%)	0	100	100
1	Ak	86/94 (92%)	86 (100%)	0	100	100
1	Am	86/94 (92%)	86 (100%)	0	100	100
1	Ao	86/94 (92%)	86 (100%)	0	100	100
1	Aq	86/94 (92%)	86 (100%)	0	100	100
1	As	86/94 (92%)	86 (100%)	0	100	100
1	Au	86/94 (92%)	86 (100%)	0	100	100
1	Aw	86/94 (92%)	86 (100%)	0	100	100
1	Ay	86/94 (92%)	86 (100%)	0	100	100
1	BA	86/94 (92%)	86 (100%)	0	100	100
1	BC	86/94 (92%)	86 (100%)	0	100	100
1	BE	86/94 (92%)	86 (100%)	0	100	100
1	BG	86/94 (92%)	86 (100%)	0	100	100
1	BI	86/94 (92%)	86 (100%)	0	100	100
1	BK	86/94 (92%)	86 (100%)	0	100	100
1	BM	86/94 (92%)	86 (100%)	0	100	100
1	BO	86/94 (92%)	86 (100%)	0	100	100
1	BQ	86/94 (92%)	86 (100%)	0	100	100
1	BS	86/94 (92%)	86 (100%)	0	100	100
1	BU	86/94 (92%)	86 (100%)	0	100	100
1	BW	86/94 (92%)	86 (100%)	0	100	100
1	BY	86/94 (92%)	86 (100%)	0	100	100
1	Ba	86/94 (92%)	86 (100%)	0	100	100
1	Bc	86/94 (92%)	86 (100%)	0	100	100
1	Be	86/94 (92%)	86 (100%)	0	100	100
1	Bg	86/94 (92%)	86 (100%)	0	100	100
1	Bi	86/94 (92%)	86 (100%)	0	100	100
1	Bk	86/94 (92%)	86 (100%)	0	100	100
1	Bm	86/94 (92%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bo	86/94 (92%)	86 (100%)	0	100	100
1	Bq	86/94 (92%)	86 (100%)	0	100	100
1	Bs	86/94 (92%)	86 (100%)	0	100	100
1	Bu	86/94 (92%)	86 (100%)	0	100	100
1	Bw	86/94 (92%)	86 (100%)	0	100	100
1	By	86/94 (92%)	86 (100%)	0	100	100
1	C	86/94 (92%)	86 (100%)	0	100	100
1	CA	86/94 (92%)	86 (100%)	0	100	100
1	CC	86/94 (92%)	86 (100%)	0	100	100
1	CE	86/94 (92%)	86 (100%)	0	100	100
1	CG	86/94 (92%)	86 (100%)	0	100	100
1	CI	86/94 (92%)	86 (100%)	0	100	100
1	CK	86/94 (92%)	86 (100%)	0	100	100
1	CM	86/94 (92%)	86 (100%)	0	100	100
1	CO	86/94 (92%)	86 (100%)	0	100	100
1	CQ	86/94 (92%)	86 (100%)	0	100	100
1	CS	86/94 (92%)	86 (100%)	0	100	100
1	CU	86/94 (92%)	86 (100%)	0	100	100
1	CW	86/94 (92%)	86 (100%)	0	100	100
1	CY	86/94 (92%)	86 (100%)	0	100	100
1	Ca	86/94 (92%)	86 (100%)	0	100	100
1	Cc	86/94 (92%)	86 (100%)	0	100	100
1	Ce	86/94 (92%)	86 (100%)	0	100	100
1	Cg	86/94 (92%)	86 (100%)	0	100	100
1	Ci	86/94 (92%)	86 (100%)	0	100	100
1	Ck	86/94 (92%)	86 (100%)	0	100	100
1	Cm	86/94 (92%)	86 (100%)	0	100	100
1	Co	86/94 (92%)	86 (100%)	0	100	100
1	Cq	86/94 (92%)	86 (100%)	0	100	100
1	Cs	86/94 (92%)	86 (100%)	0	100	100
1	Cu	86/94 (92%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cw	86/94 (92%)	86 (100%)	0	100	100
1	Cy	86/94 (92%)	86 (100%)	0	100	100
1	DA	86/94 (92%)	86 (100%)	0	100	100
1	DC	86/94 (92%)	86 (100%)	0	100	100
1	DE	86/94 (92%)	86 (100%)	0	100	100
1	DG	86/94 (92%)	86 (100%)	0	100	100
1	DI	86/94 (92%)	86 (100%)	0	100	100
1	DK	86/94 (92%)	86 (100%)	0	100	100
1	DM	86/94 (92%)	86 (100%)	0	100	100
1	DO	86/94 (92%)	86 (100%)	0	100	100
1	DQ	86/94 (92%)	86 (100%)	0	100	100
1	DS	86/94 (92%)	86 (100%)	0	100	100
1	DU	86/94 (92%)	86 (100%)	0	100	100
1	DW	86/94 (92%)	86 (100%)	0	100	100
1	DY	86/94 (92%)	86 (100%)	0	100	100
1	Da	86/94 (92%)	86 (100%)	0	100	100
1	Dc	86/94 (92%)	86 (100%)	0	100	100
1	De	86/94 (92%)	86 (100%)	0	100	100
1	Dg	86/94 (92%)	86 (100%)	0	100	100
1	Di	86/94 (92%)	86 (100%)	0	100	100
1	Dk	86/94 (92%)	86 (100%)	0	100	100
1	Dm	86/94 (92%)	86 (100%)	0	100	100
1	Do	86/94 (92%)	86 (100%)	0	100	100
1	Dq	86/94 (92%)	86 (100%)	0	100	100
1	Ds	86/94 (92%)	86 (100%)	0	100	100
1	Du	86/94 (92%)	86 (100%)	0	100	100
1	Dw	86/94 (92%)	86 (100%)	0	100	100
1	Dy	86/94 (92%)	86 (100%)	0	100	100
1	E	86/94 (92%)	86 (100%)	0	100	100
1	EA	86/94 (92%)	86 (100%)	0	100	100
1	EC	86/94 (92%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EE	86/94 (92%)	86 (100%)	0	100	100
1	EG	86/94 (92%)	86 (100%)	0	100	100
1	EI	86/94 (92%)	86 (100%)	0	100	100
1	EK	86/94 (92%)	86 (100%)	0	100	100
1	EM	86/94 (92%)	86 (100%)	0	100	100
1	EO	86/94 (92%)	86 (100%)	0	100	100
1	EQ	86/94 (92%)	86 (100%)	0	100	100
1	ES	86/94 (92%)	86 (100%)	0	100	100
1	EU	86/94 (92%)	86 (100%)	0	100	100
1	EW	86/94 (92%)	86 (100%)	0	100	100
1	EY	86/94 (92%)	86 (100%)	0	100	100
1	Ea	86/94 (92%)	86 (100%)	0	100	100
1	Ec	86/94 (92%)	86 (100%)	0	100	100
1	Ee	86/94 (92%)	86 (100%)	0	100	100
1	Eg	86/94 (92%)	86 (100%)	0	100	100
1	Ei	86/94 (92%)	86 (100%)	0	100	100
1	Ek	86/94 (92%)	86 (100%)	0	100	100
1	Em	86/94 (92%)	86 (100%)	0	100	100
1	Eo	86/94 (92%)	86 (100%)	0	100	100
1	Eq	86/94 (92%)	86 (100%)	0	100	100
1	Es	86/94 (92%)	86 (100%)	0	100	100
1	Eu	86/94 (92%)	86 (100%)	0	100	100
1	Ew	86/94 (92%)	86 (100%)	0	100	100
1	G	86/94 (92%)	86 (100%)	0	100	100
1	I	86/94 (92%)	86 (100%)	0	100	100
1	K	86/94 (92%)	86 (100%)	0	100	100
1	M	86/94 (92%)	86 (100%)	0	100	100
1	O	86/94 (92%)	86 (100%)	0	100	100
1	Q	86/94 (92%)	86 (100%)	0	100	100
1	S	86/94 (92%)	86 (100%)	0	100	100
1	U	86/94 (92%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	86/94 (92%)	86 (100%)	0	100	100
1	Y	86/94 (92%)	86 (100%)	0	100	100
1	YA	86/94 (92%)	86 (100%)	0	100	100
1	YC	86/94 (92%)	86 (100%)	0	100	100
1	YE	86/94 (92%)	86 (100%)	0	100	100
1	YG	86/94 (92%)	86 (100%)	0	100	100
1	YI	86/94 (92%)	86 (100%)	0	100	100
1	YK	86/94 (92%)	86 (100%)	0	100	100
1	YM	86/94 (92%)	86 (100%)	0	100	100
1	YO	86/94 (92%)	86 (100%)	0	100	100
1	YQ	86/94 (92%)	86 (100%)	0	100	100
1	YS	86/94 (92%)	86 (100%)	0	100	100
1	YU	86/94 (92%)	86 (100%)	0	100	100
1	YW	86/94 (92%)	86 (100%)	0	100	100
1	ZA	86/94 (92%)	86 (100%)	0	100	100
1	ZC	86/94 (92%)	86 (100%)	0	100	100
1	ZE	86/94 (92%)	86 (100%)	0	100	100
1	ZG	86/94 (92%)	86 (100%)	0	100	100
1	ZI	86/94 (92%)	86 (100%)	0	100	100
1	ZK	86/94 (92%)	86 (100%)	0	100	100
1	ZM	86/94 (92%)	86 (100%)	0	100	100
1	ZO	86/94 (92%)	86 (100%)	0	100	100
1	ZQ	86/94 (92%)	86 (100%)	0	100	100
1	ZS	86/94 (92%)	86 (100%)	0	100	100
1	ZU	86/94 (92%)	86 (100%)	0	100	100
1	ZW	86/94 (92%)	86 (100%)	0	100	100
1	ZY	86/94 (92%)	86 (100%)	0	100	100
1	a	86/94 (92%)	86 (100%)	0	100	100
1	c	86/94 (92%)	86 (100%)	0	100	100
1	e	86/94 (92%)	86 (100%)	0	100	100
1	g	86/94 (92%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	86/94 (92%)	86 (100%)	0	100	100
1	k	86/94 (92%)	86 (100%)	0	100	100
1	m	86/94 (92%)	86 (100%)	0	100	100
1	o	86/94 (92%)	86 (100%)	0	100	100
1	q	86/94 (92%)	86 (100%)	0	100	100
1	s	86/94 (92%)	86 (100%)	0	100	100
1	u	86/94 (92%)	86 (100%)	0	100	100
1	w	86/94 (92%)	86 (100%)	0	100	100
1	y	86/94 (92%)	86 (100%)	0	100	100
2	AB	233/241 (97%)	233 (100%)	0	100	100
2	AD	233/241 (97%)	233 (100%)	0	100	100
2	AF	233/241 (97%)	233 (100%)	0	100	100
2	AH	233/241 (97%)	233 (100%)	0	100	100
2	AJ	233/241 (97%)	233 (100%)	0	100	100
2	AL	233/241 (97%)	233 (100%)	0	100	100
2	AN	233/241 (97%)	233 (100%)	0	100	100
2	AP	233/241 (97%)	233 (100%)	0	100	100
2	AR	233/241 (97%)	233 (100%)	0	100	100
2	AT	233/241 (97%)	233 (100%)	0	100	100
2	AV	233/241 (97%)	233 (100%)	0	100	100
2	AX	233/241 (97%)	233 (100%)	0	100	100
2	AZ	233/241 (97%)	233 (100%)	0	100	100
2	Ab	233/241 (97%)	233 (100%)	0	100	100
2	Ad	233/241 (97%)	233 (100%)	0	100	100
2	Af	233/241 (97%)	233 (100%)	0	100	100
2	Ah	233/241 (97%)	233 (100%)	0	100	100
2	Aj	233/241 (97%)	233 (100%)	0	100	100
2	Al	233/241 (97%)	233 (100%)	0	100	100
2	An	233/241 (97%)	233 (100%)	0	100	100
2	Ap	233/241 (97%)	233 (100%)	0	100	100
2	Ar	233/241 (97%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	At	233/241 (97%)	233 (100%)	0	100	100
2	Av	233/241 (97%)	233 (100%)	0	100	100
2	Ax	233/241 (97%)	233 (100%)	0	100	100
2	Az	233/241 (97%)	233 (100%)	0	100	100
2	B	233/241 (97%)	233 (100%)	0	100	100
2	BB	233/241 (97%)	233 (100%)	0	100	100
2	BD	233/241 (97%)	233 (100%)	0	100	100
2	BF	233/241 (97%)	233 (100%)	0	100	100
2	BH	233/241 (97%)	233 (100%)	0	100	100
2	BJ	233/241 (97%)	233 (100%)	0	100	100
2	BL	233/241 (97%)	233 (100%)	0	100	100
2	BN	233/241 (97%)	233 (100%)	0	100	100
2	BP	233/241 (97%)	233 (100%)	0	100	100
2	BR	233/241 (97%)	233 (100%)	0	100	100
2	BT	233/241 (97%)	233 (100%)	0	100	100
2	BV	233/241 (97%)	233 (100%)	0	100	100
2	BX	233/241 (97%)	233 (100%)	0	100	100
2	BZ	233/241 (97%)	233 (100%)	0	100	100
2	Bb	233/241 (97%)	233 (100%)	0	100	100
2	Bd	233/241 (97%)	233 (100%)	0	100	100
2	Bf	233/241 (97%)	233 (100%)	0	100	100
2	Bh	233/241 (97%)	233 (100%)	0	100	100
2	Bj	233/241 (97%)	233 (100%)	0	100	100
2	Bl	233/241 (97%)	233 (100%)	0	100	100
2	Bn	233/241 (97%)	233 (100%)	0	100	100
2	Bp	233/241 (97%)	233 (100%)	0	100	100
2	Br	233/241 (97%)	233 (100%)	0	100	100
2	Bt	233/241 (97%)	233 (100%)	0	100	100
2	Bv	233/241 (97%)	233 (100%)	0	100	100
2	Bx	233/241 (97%)	233 (100%)	0	100	100
2	Bz	233/241 (97%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CB	233/241 (97%)	233 (100%)	0	100	100
2	CD	233/241 (97%)	233 (100%)	0	100	100
2	CF	233/241 (97%)	233 (100%)	0	100	100
2	CH	233/241 (97%)	233 (100%)	0	100	100
2	CJ	233/241 (97%)	233 (100%)	0	100	100
2	CL	233/241 (97%)	233 (100%)	0	100	100
2	CN	233/241 (97%)	233 (100%)	0	100	100
2	CP	233/241 (97%)	233 (100%)	0	100	100
2	CR	233/241 (97%)	233 (100%)	0	100	100
2	CT	233/241 (97%)	233 (100%)	0	100	100
2	CV	233/241 (97%)	233 (100%)	0	100	100
2	CX	233/241 (97%)	233 (100%)	0	100	100
2	CZ	233/241 (97%)	233 (100%)	0	100	100
2	Cb	233/241 (97%)	233 (100%)	0	100	100
2	Cd	233/241 (97%)	233 (100%)	0	100	100
2	Cf	233/241 (97%)	233 (100%)	0	100	100
2	Ch	233/241 (97%)	233 (100%)	0	100	100
2	Cj	233/241 (97%)	233 (100%)	0	100	100
2	Cl	233/241 (97%)	233 (100%)	0	100	100
2	Cn	233/241 (97%)	233 (100%)	0	100	100
2	Cp	233/241 (97%)	233 (100%)	0	100	100
2	Cr	233/241 (97%)	233 (100%)	0	100	100
2	Ct	233/241 (97%)	233 (100%)	0	100	100
2	Cv	233/241 (97%)	233 (100%)	0	100	100
2	Cx	233/241 (97%)	233 (100%)	0	100	100
2	Cz	233/241 (97%)	233 (100%)	0	100	100
2	D	233/241 (97%)	233 (100%)	0	100	100
2	DB	233/241 (97%)	233 (100%)	0	100	100
2	DD	233/241 (97%)	233 (100%)	0	100	100
2	DF	233/241 (97%)	233 (100%)	0	100	100
2	DH	233/241 (97%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DJ	233/241 (97%)	233 (100%)	0	100	100
2	DL	233/241 (97%)	233 (100%)	0	100	100
2	DN	233/241 (97%)	233 (100%)	0	100	100
2	DP	233/241 (97%)	233 (100%)	0	100	100
2	DR	233/241 (97%)	233 (100%)	0	100	100
2	DT	233/241 (97%)	233 (100%)	0	100	100
2	DV	233/241 (97%)	233 (100%)	0	100	100
2	DX	233/241 (97%)	233 (100%)	0	100	100
2	DZ	233/241 (97%)	233 (100%)	0	100	100
2	Db	233/241 (97%)	233 (100%)	0	100	100
2	Dd	233/241 (97%)	233 (100%)	0	100	100
2	Df	233/241 (97%)	233 (100%)	0	100	100
2	Dh	233/241 (97%)	233 (100%)	0	100	100
2	Dj	233/241 (97%)	233 (100%)	0	100	100
2	Di	233/241 (97%)	233 (100%)	0	100	100
2	Dn	233/241 (97%)	233 (100%)	0	100	100
2	Dp	233/241 (97%)	233 (100%)	0	100	100
2	Dr	233/241 (97%)	233 (100%)	0	100	100
2	Dt	233/241 (97%)	233 (100%)	0	100	100
2	Dv	233/241 (97%)	233 (100%)	0	100	100
2	Dx	233/241 (97%)	233 (100%)	0	100	100
2	Dz	233/241 (97%)	233 (100%)	0	100	100
2	EB	233/241 (97%)	233 (100%)	0	100	100
2	ED	233/241 (97%)	233 (100%)	0	100	100
2	EF	233/241 (97%)	233 (100%)	0	100	100
2	EH	233/241 (97%)	233 (100%)	0	100	100
2	EJ	233/241 (97%)	233 (100%)	0	100	100
2	EL	233/241 (97%)	233 (100%)	0	100	100
2	EN	233/241 (97%)	233 (100%)	0	100	100
2	EP	233/241 (97%)	233 (100%)	0	100	100
2	ER	233/241 (97%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	ET	233/241 (97%)	233 (100%)	0	100	100
2	EV	233/241 (97%)	233 (100%)	0	100	100
2	EX	233/241 (97%)	233 (100%)	0	100	100
2	EZ	233/241 (97%)	233 (100%)	0	100	100
2	Eb	233/241 (97%)	233 (100%)	0	100	100
2	Ed	233/241 (97%)	233 (100%)	0	100	100
2	Ef	233/241 (97%)	233 (100%)	0	100	100
2	Eh	233/241 (97%)	233 (100%)	0	100	100
2	Ej	233/241 (97%)	233 (100%)	0	100	100
2	El	233/241 (97%)	233 (100%)	0	100	100
2	En	233/241 (97%)	233 (100%)	0	100	100
2	Ep	233/241 (97%)	233 (100%)	0	100	100
2	Er	233/241 (97%)	233 (100%)	0	100	100
2	Et	233/241 (97%)	233 (100%)	0	100	100
2	Ev	233/241 (97%)	233 (100%)	0	100	100
2	Ex	233/241 (97%)	233 (100%)	0	100	100
2	F	233/241 (97%)	233 (100%)	0	100	100
2	H	233/241 (97%)	233 (100%)	0	100	100
2	J	233/241 (97%)	233 (100%)	0	100	100
2	L	233/241 (97%)	233 (100%)	0	100	100
2	N	233/241 (97%)	233 (100%)	0	100	100
2	P	233/241 (97%)	233 (100%)	0	100	100
2	R	233/241 (97%)	233 (100%)	0	100	100
2	T	233/241 (97%)	233 (100%)	0	100	100
2	V	233/241 (97%)	233 (100%)	0	100	100
2	X	233/241 (97%)	233 (100%)	0	100	100
2	YB	233/241 (97%)	233 (100%)	0	100	100
2	YD	233/241 (97%)	233 (100%)	0	100	100
2	YF	233/241 (97%)	233 (100%)	0	100	100
2	YH	233/241 (97%)	233 (100%)	0	100	100
2	YJ	233/241 (97%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	YL	233/241 (97%)	233 (100%)	0	100	100
2	YN	233/241 (97%)	233 (100%)	0	100	100
2	YP	233/241 (97%)	233 (100%)	0	100	100
2	YR	233/241 (97%)	233 (100%)	0	100	100
2	YT	233/241 (97%)	233 (100%)	0	100	100
2	YV	233/241 (97%)	233 (100%)	0	100	100
2	YX	233/241 (97%)	233 (100%)	0	100	100
2	Z	233/241 (97%)	233 (100%)	0	100	100
2	ZB	233/241 (97%)	233 (100%)	0	100	100
2	ZD	233/241 (97%)	233 (100%)	0	100	100
2	ZF	233/241 (97%)	233 (100%)	0	100	100
2	ZH	233/241 (97%)	233 (100%)	0	100	100
2	ZJ	233/241 (97%)	233 (100%)	0	100	100
2	ZL	233/241 (97%)	233 (100%)	0	100	100
2	ZN	233/241 (97%)	233 (100%)	0	100	100
2	ZP	233/241 (97%)	233 (100%)	0	100	100
2	ZR	233/241 (97%)	233 (100%)	0	100	100
2	ZT	233/241 (97%)	233 (100%)	0	100	100
2	ZV	233/241 (97%)	233 (100%)	0	100	100
2	ZX	233/241 (97%)	233 (100%)	0	100	100
2	ZZ	233/241 (97%)	233 (100%)	0	100	100
2	b	233/241 (97%)	233 (100%)	0	100	100
2	d	233/241 (97%)	233 (100%)	0	100	100
2	f	233/241 (97%)	233 (100%)	0	100	100
2	h	233/241 (97%)	233 (100%)	0	100	100
2	j	233/241 (97%)	233 (100%)	0	100	100
2	l	233/241 (97%)	233 (100%)	0	100	100
2	n	233/241 (97%)	233 (100%)	0	100	100
2	p	233/241 (97%)	233 (100%)	0	100	100
2	r	233/241 (97%)	233 (100%)	0	100	100
2	t	233/241 (97%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	v	233/241 (97%)	233 (100%)	0	100	100
2	x	233/241 (97%)	233 (100%)	0	100	100
2	z	233/241 (97%)	233 (100%)	0	100	100
All	All	57420/60300 (95%)	57420 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
2	D	46	ASN
2	F	59	ASN
1	G	87	GLN
2	J	46	ASN
2	L	59	ASN
1	M	87	GLN
2	P	46	ASN
2	R	59	ASN
1	S	87	GLN
2	X	59	ASN
1	Y	87	GLN
2	b	46	ASN
2	d	59	ASN
1	e	87	GLN
2	h	46	ASN
2	j	59	ASN
1	k	87	GLN
2	n	46	ASN
2	p	59	ASN
1	q	87	GLN
2	v	59	ASN
1	w	87	GLN
2	z	46	ASN
2	ZB	59	ASN
1	ZC	87	GLN
2	ZH	59	ASN
1	ZI	87	GLN
2	AB	46	ASN
2	AD	59	ASN
1	AE	87	GLN

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Mol	Chain	Res	Type
2	AH	46	ASN
2	AJ	59	ASN
1	AK	87	GLN
2	AN	46	ASN
2	AP	59	ASN
1	AQ	87	GLN
2	AT	46	ASN
2	AV	59	ASN
1	AW	87	GLN
2	Ab	59	ASN
1	Ac	87	GLN
2	Af	46	ASN
2	Ah	59	ASN
1	Ai	87	GLN
2	Al	46	ASN
2	An	59	ASN
1	Ao	87	GLN
2	Ar	46	ASN
2	At	59	ASN
1	Au	87	GLN
2	Ax	46	ASN
2	Az	59	ASN
1	ZK	87	GLN
2	ZP	59	ASN
1	ZQ	87	GLN
2	ZT	46	ASN
2	BB	59	ASN
1	BC	87	GLN
2	BF	46	ASN
2	BH	59	ASN
1	BI	87	GLN
2	BL	46	ASN
2	BN	59	ASN
1	BO	87	GLN
2	BT	59	ASN
1	BU	87	GLN
2	BZ	59	ASN
1	Ba	87	GLN
2	Bd	46	ASN
2	Bf	59	ASN
1	Bg	87	GLN
2	Bj	46	ASN

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Mol	Chain	Res	Type
2	Bl	59	ASN
1	Bm	87	GLN
2	Bp	46	ASN
2	Br	59	ASN
1	Bs	87	GLN
2	Bv	46	ASN
2	Bx	59	ASN
1	By	87	GLN
2	ZV	46	ASN
2	ZX	59	ASN
1	ZY	87	GLN
2	YB	46	ASN
2	YD	59	ASN
1	CA	87	GLN
2	CD	46	ASN
2	CF	59	ASN
1	CG	87	GLN
2	CL	59	ASN
1	CM	87	GLN
2	CP	46	ASN
2	CR	59	ASN
1	CS	87	GLN
2	CX	59	ASN
1	CY	87	GLN
2	Cd	59	ASN
1	Ce	87	GLN
2	Ch	46	ASN
2	Cj	59	ASN
1	Ck	87	GLN
2	Cn	46	ASN
2	Cp	59	ASN
1	Cq	87	GLN
2	Cv	59	ASN
1	Cw	87	GLN
2	YF	59	ASN
1	YG	87	GLN
2	YJ	46	ASN
2	YL	59	ASN
1	YM	87	GLN
2	DB	46	ASN
2	DD	59	ASN
1	DE	87	GLN

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Mol	Chain	Res	Type
2	DH	46	ASN
2	DJ	59	ASN
1	DK	87	GLN
2	DP	59	ASN
1	DQ	87	GLN
2	DT	46	ASN
2	DV	59	ASN
1	DW	87	GLN
2	Db	59	ASN
1	Dc	87	GLN
2	Dh	59	ASN
1	Di	87	GLN
2	Dl	46	ASN
2	Dn	59	ASN
1	Do	87	GLN
2	Dt	59	ASN
1	Du	87	GLN
2	Dx	46	ASN
2	Dz	59	ASN
1	YO	87	GLN
2	YT	59	ASN
1	YU	87	GLN
2	YX	46	ASN
2	EB	59	ASN
1	EC	87	GLN
2	EH	59	ASN
1	EI	87	GLN
2	EN	59	ASN
1	EO	87	GLN
2	ER	46	ASN
2	ET	59	ASN
1	EU	87	GLN
2	EZ	59	ASN
1	Ea	87	GLN
2	Ed	46	ASN
2	Ef	59	ASN
1	Eg	87	GLN
2	Ej	46	ASN
2	El	59	ASN
1	Em	87	GLN
2	Ep	46	ASN
2	Er	59	ASN

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Mol	Chain	Res	Type
1	Es	87	GLN
2	Ev	46	ASN
2	Ex	59	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

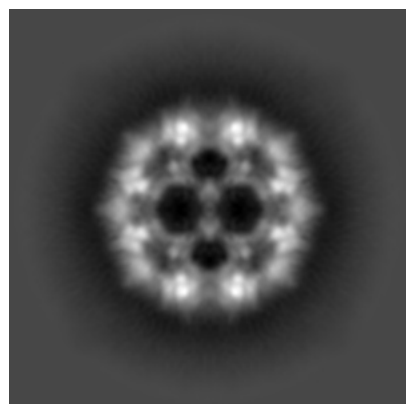
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70605. These allow visual inspection of the internal detail of the map and identification of artifacts.

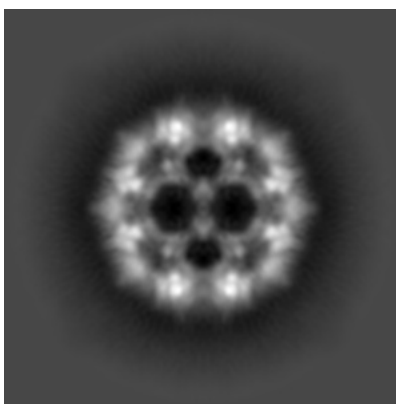
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

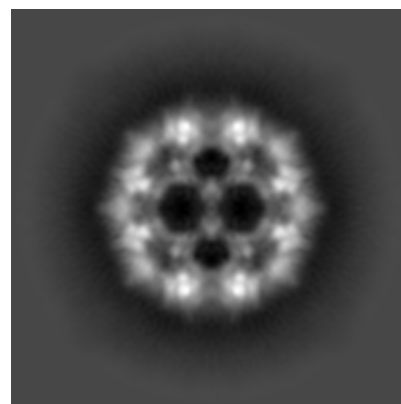
6.1.1 Primary map



X

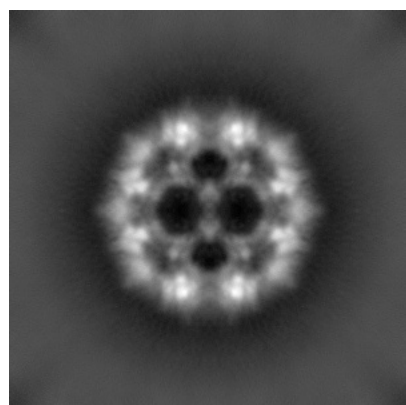


Y

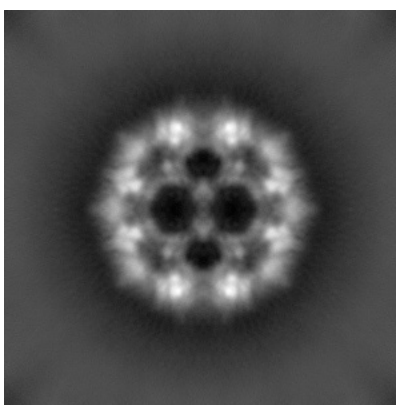


Z

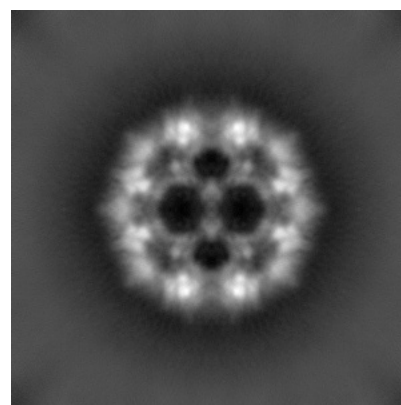
6.1.2 Raw map



X



Y

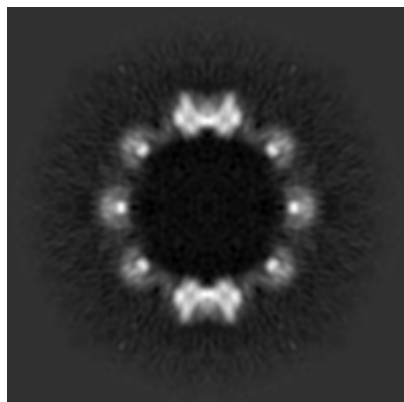


Z

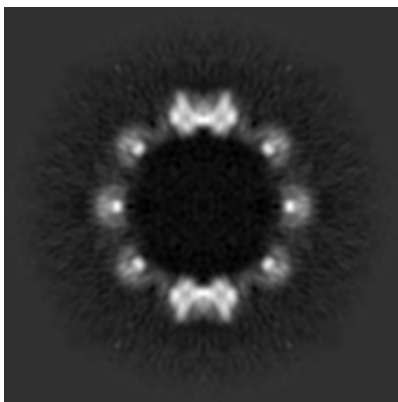
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

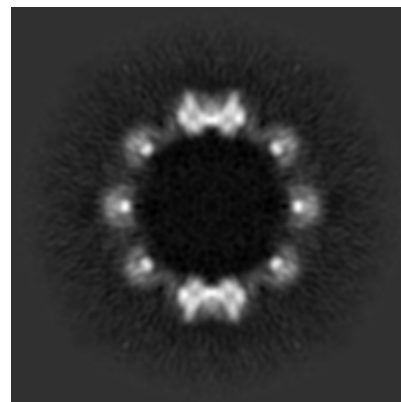
6.2.1 Primary map



X Index: 175

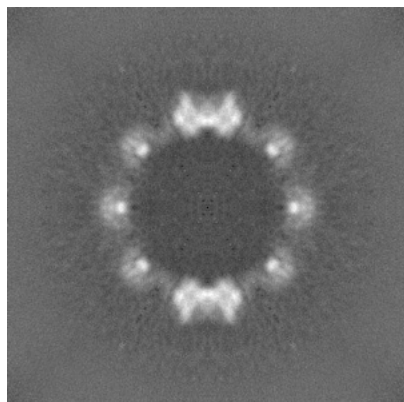


Y Index: 175

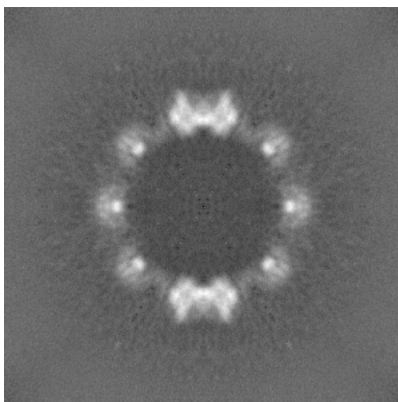


Z Index: 175

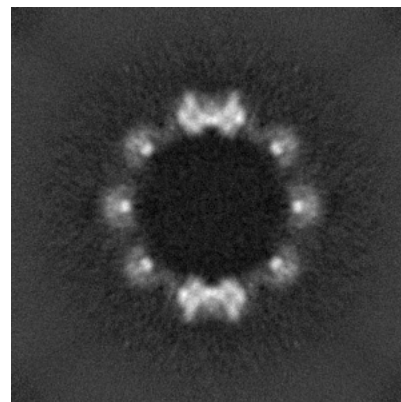
6.2.2 Raw map



X Index: 175



Y Index: 175

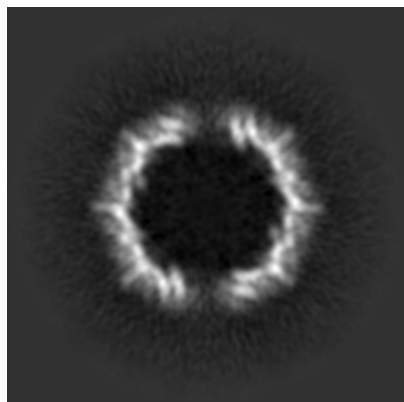


Z Index: 175

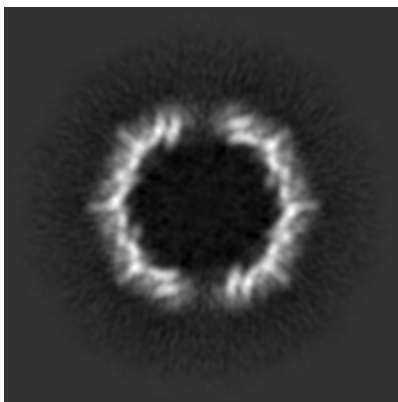
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

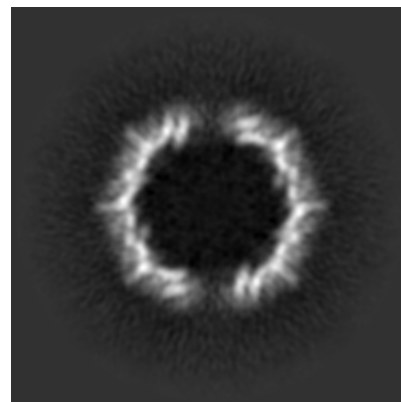
6.3.1 Primary map



X Index: 198

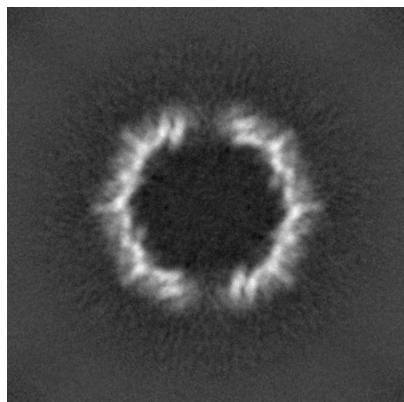


Y Index: 152

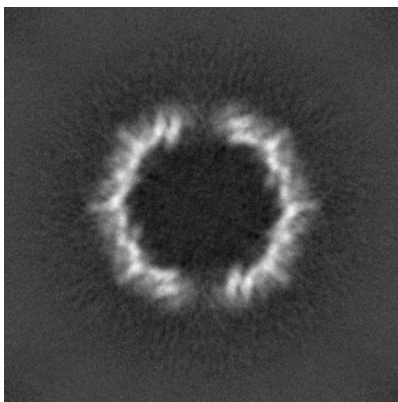


Z Index: 151

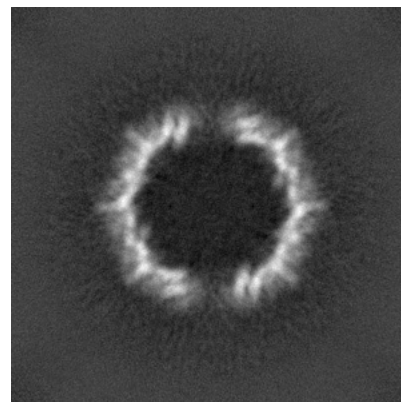
6.3.2 Raw map



X Index: 152



Y Index: 152

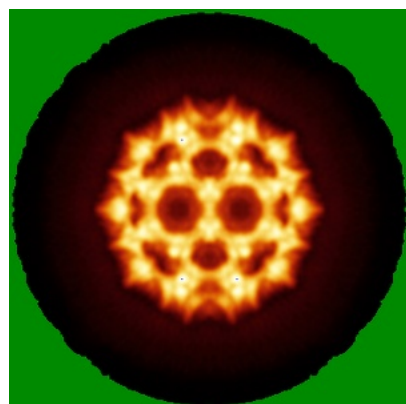


Z Index: 151

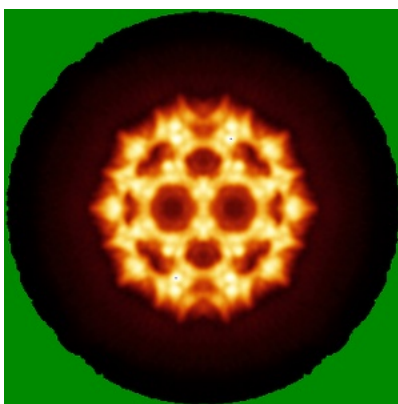
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

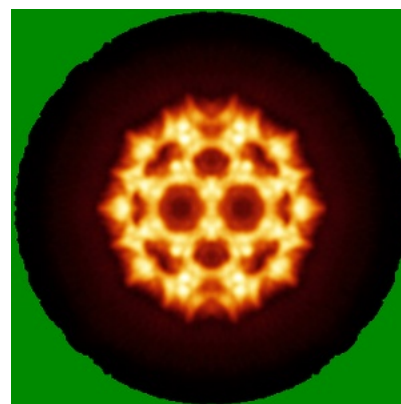
6.4.1 Primary map



X

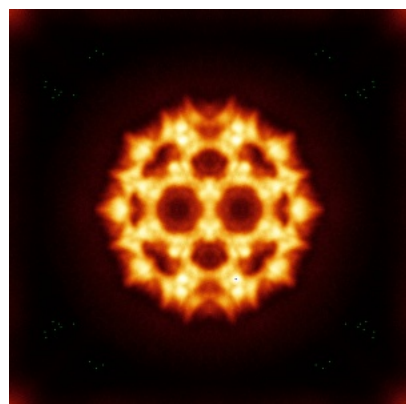


Y

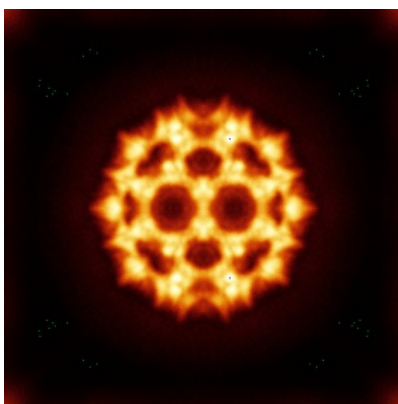


Z

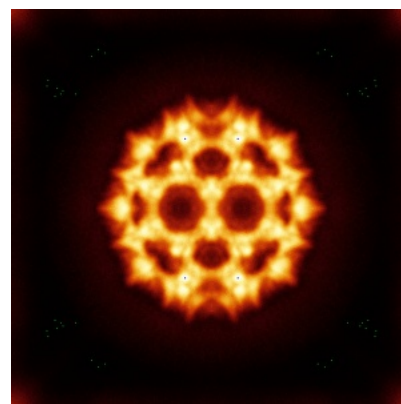
6.4.2 Raw map



X



Y

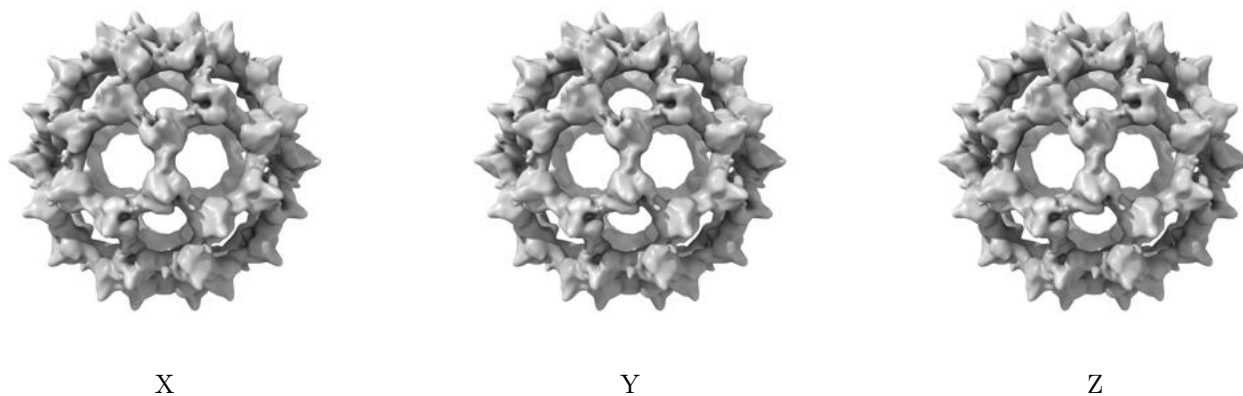


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

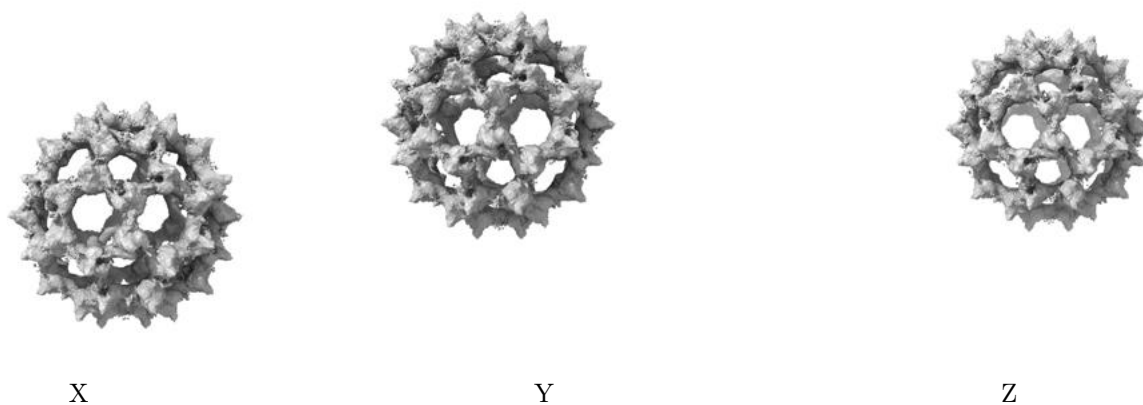
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.221. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

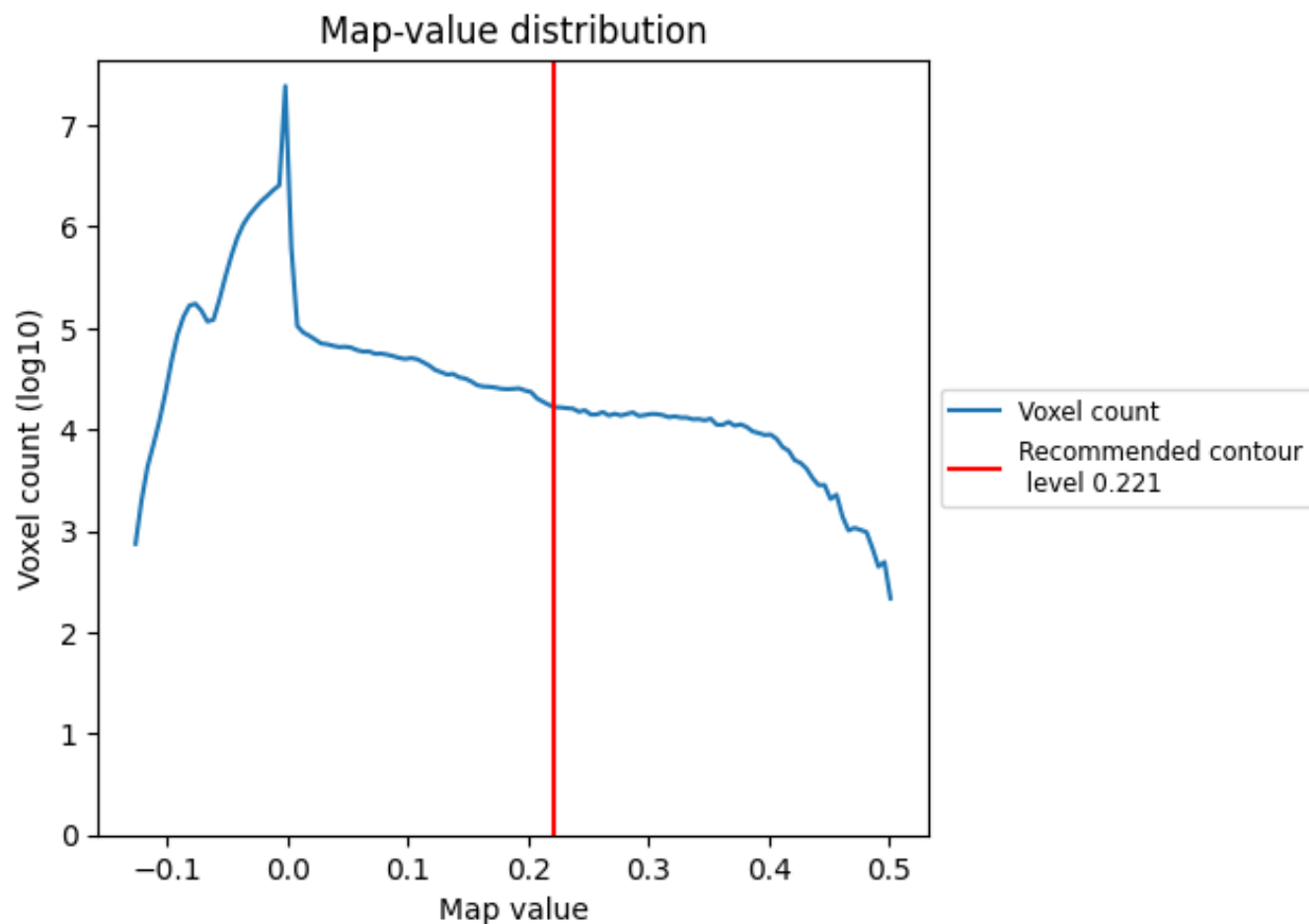
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

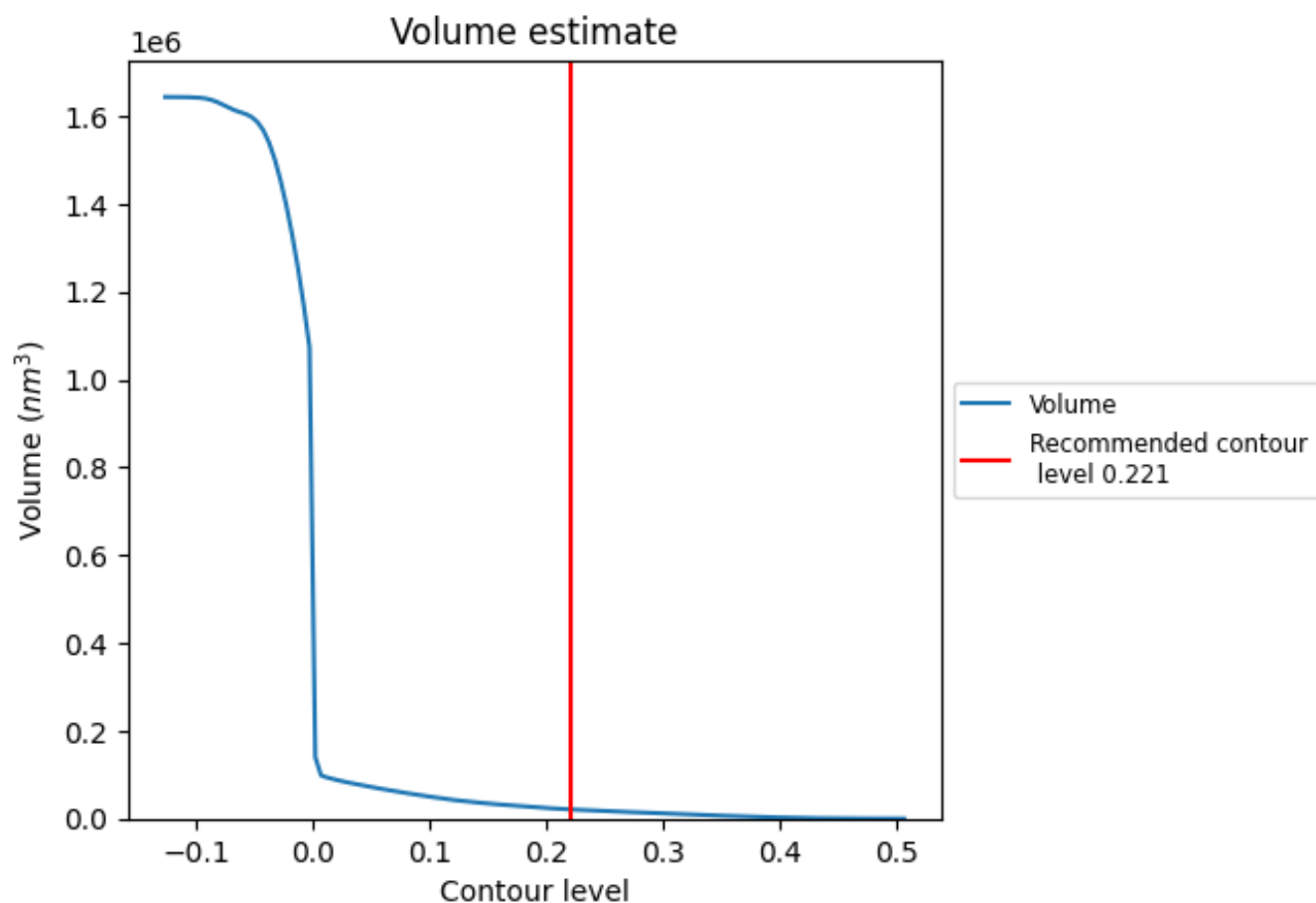
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

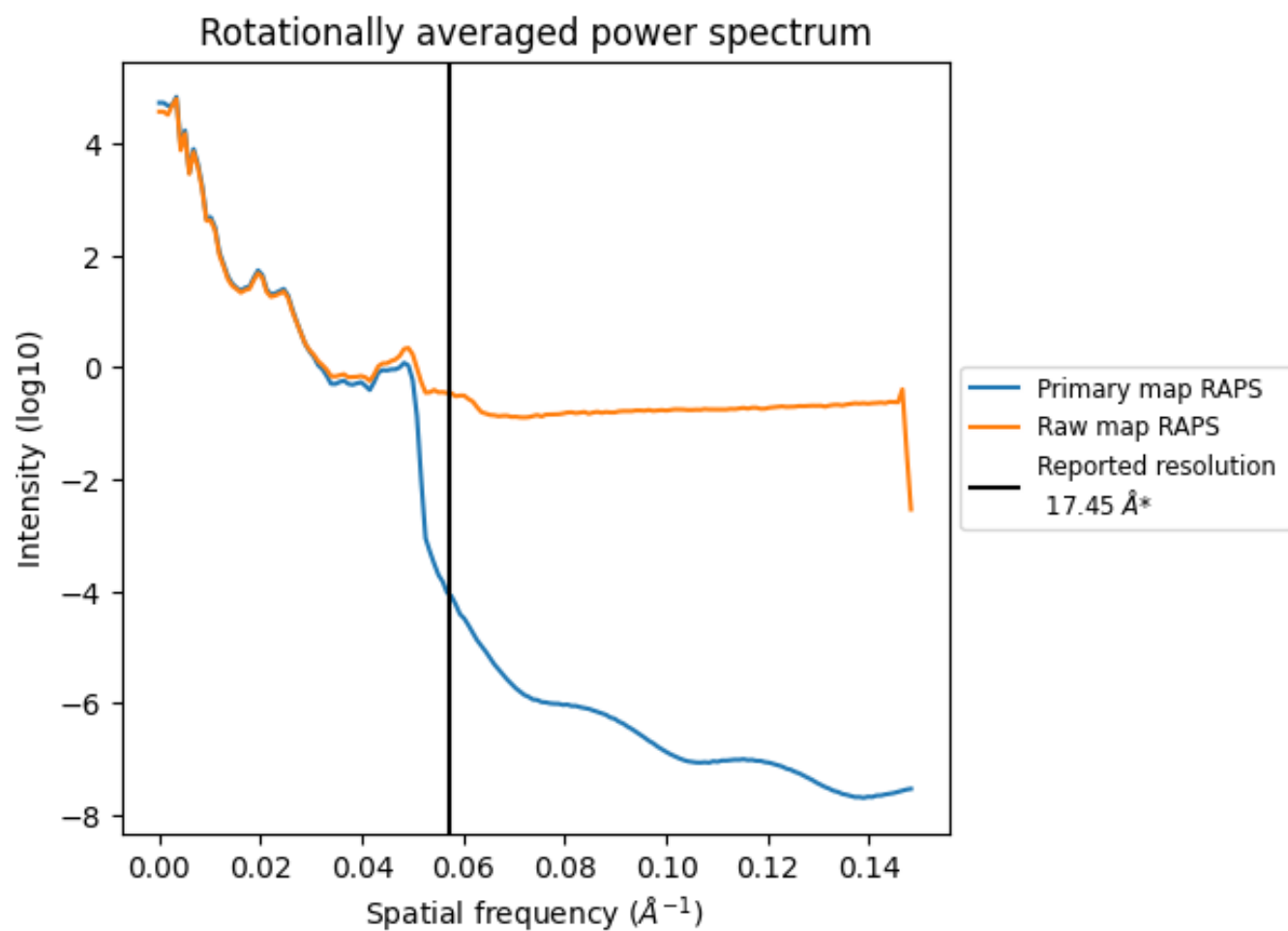
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20911 nm^3 ; this corresponds to an approximate mass of 18890 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

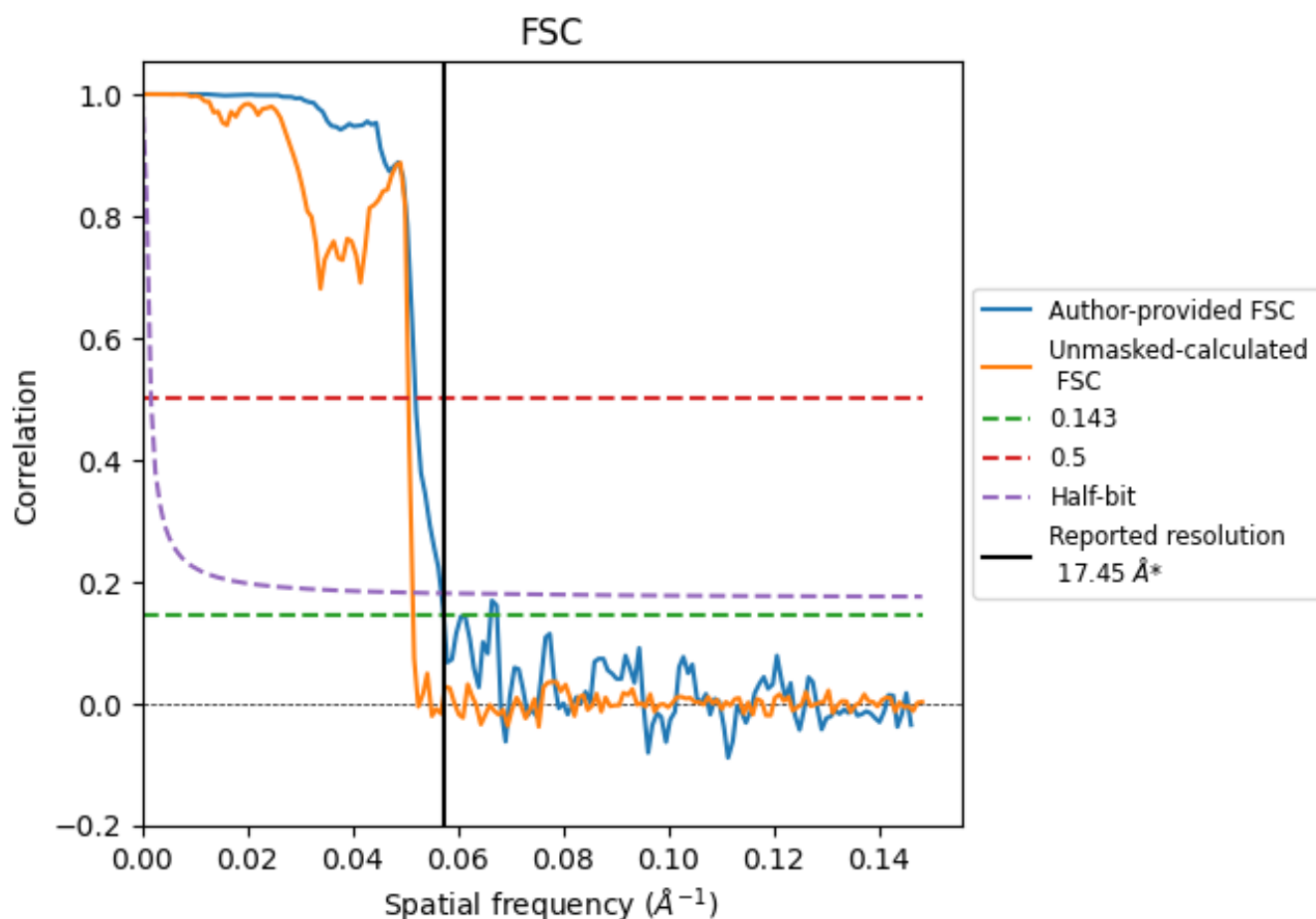


*Reported resolution corresponds to spatial frequency of 0.057 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.057 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

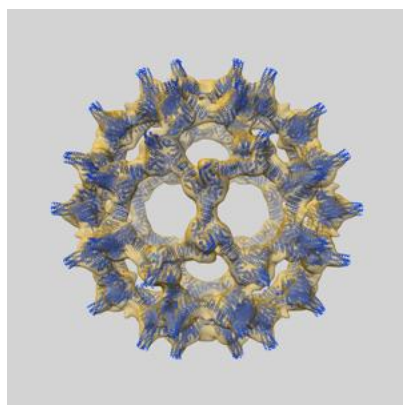
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	17.45	-	-
Author-provided FSC curve	17.45	19.23	17.57
Unmasked-calculated*	19.42	19.72	19.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 19.42 differs from the reported value 17.45 by more than 10 %

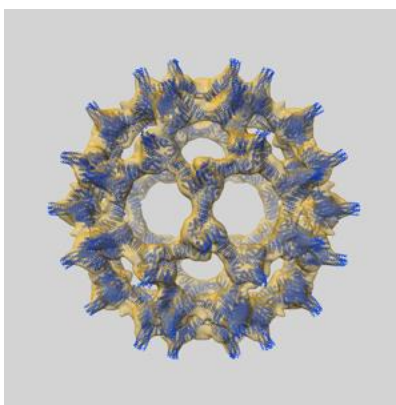
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70605 and PDB model 9OM3. Per-residue inclusion information can be found in section 3 on page 36.

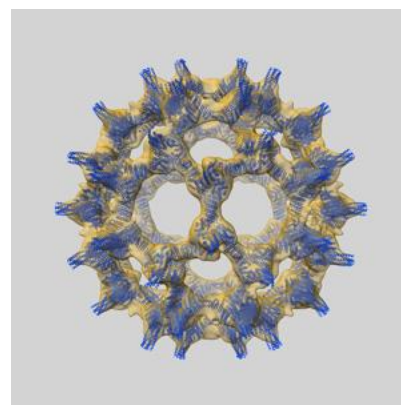
9.1 Map-model overlay [i](#)



X



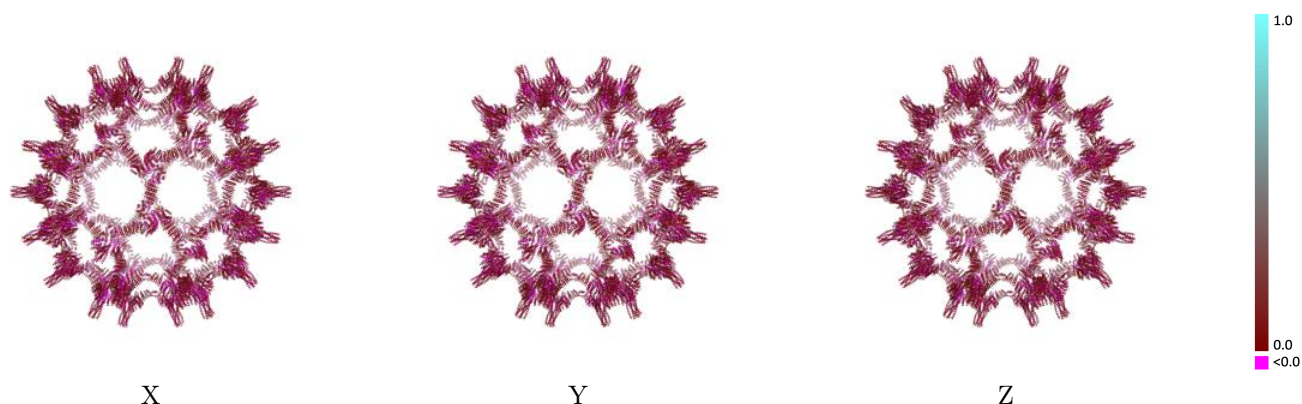
Y



Z

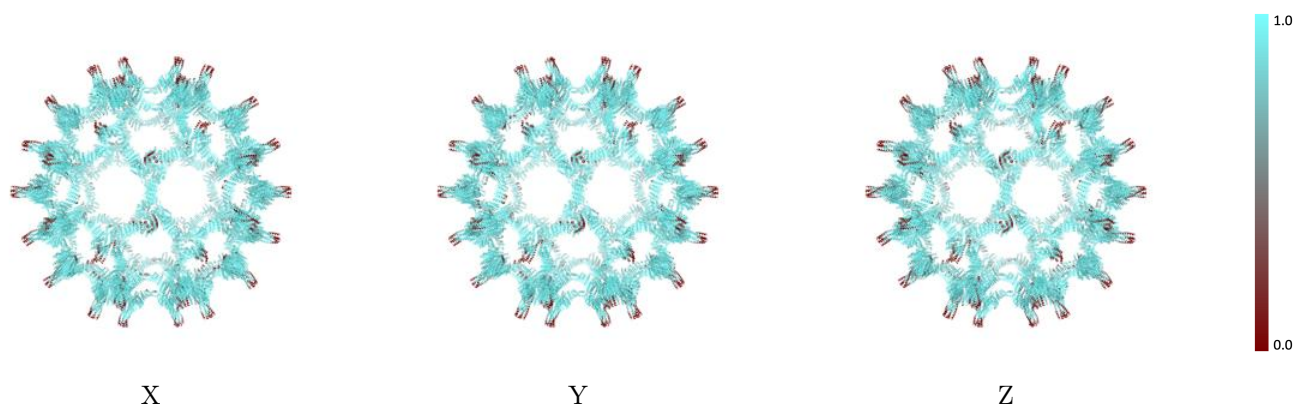
The images above show the 3D surface view of the map at the recommended contour level 0.221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



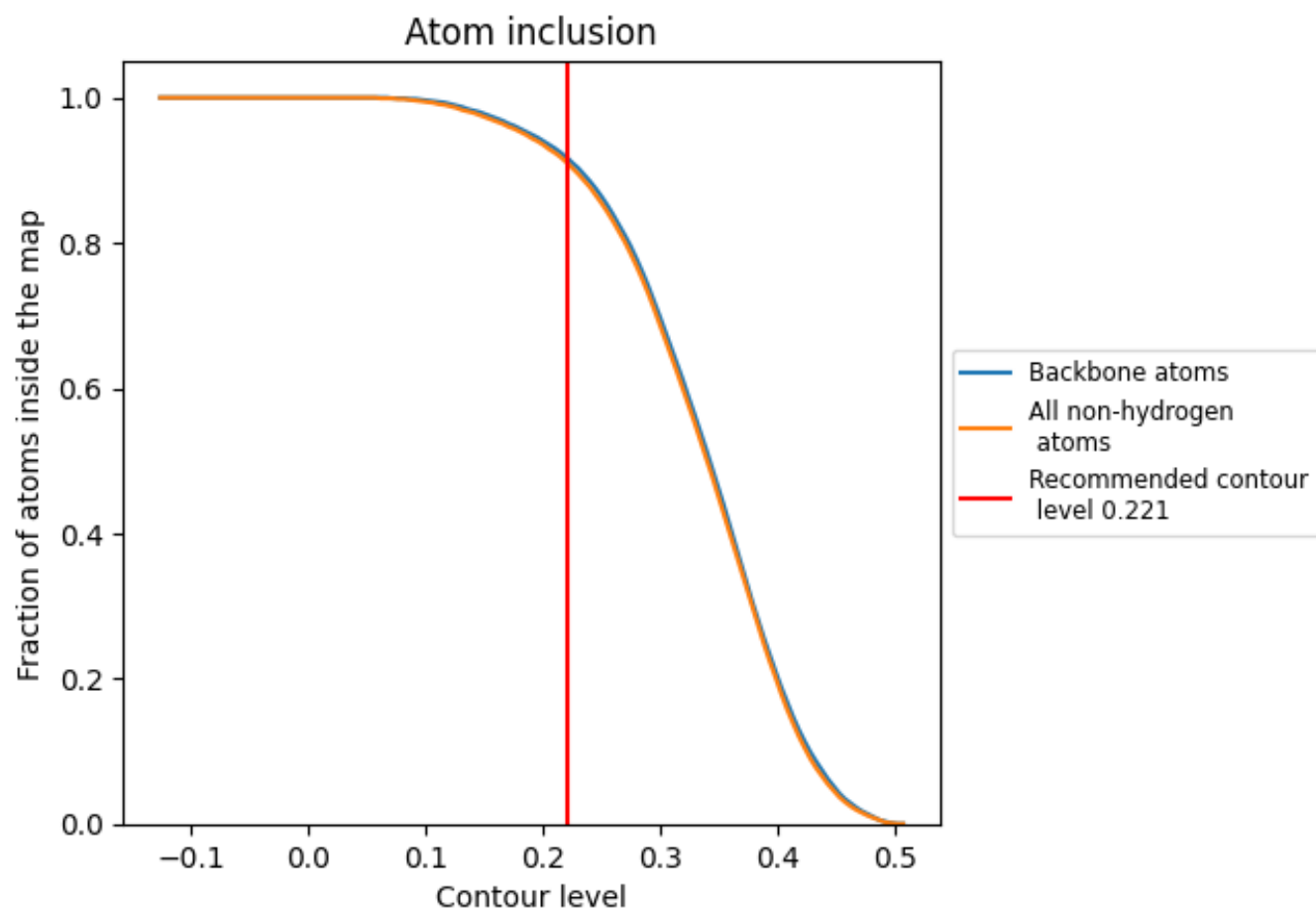
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.221).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.0530
A	 0.9920	 0.0620
AA	 0.9610	 0.0540
AB	 0.8610	 0.0430
AC	 1.0000	 0.0700
AD	 0.8740	 0.0600
AE	 0.9910	 0.0730
AF	 0.8780	 0.0390
AG	 0.8330	 0.0550
AH	 0.8750	 0.0460
AI	 0.9800	 0.0750
AJ	 0.9350	 0.0570
AK	 0.9800	 0.0650
AL	 0.9440	 0.0470
AM	 0.7850	 0.0580
AN	 0.8940	 0.0370
AO	 0.9810	 0.0750
AP	 0.9150	 0.0550
AQ	 0.9940	 0.0620
AR	 0.9340	 0.0460
AS	 0.8400	 0.0550
AT	 0.8940	 0.0410
AU	 0.9800	 0.0710
AV	 0.9200	 0.0610
AW	 0.9910	 0.0650
AX	 0.8900	 0.0460
AY	 0.9750	 0.0570
AZ	 0.8740	 0.0490
Aa	 0.9940	 0.0710
Ab	 0.9080	 0.0600
Ac	 0.9850	 0.0680
Ad	 0.8940	 0.0330
Ae	 0.8840	 0.0630
Af	 0.8780	 0.0430
Ag	 0.9850	 0.0770



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Chain	Atom inclusion	Q-score
Ah	 0.9480	 0.0600
Ai	 0.9910	 0.0670
Aj	 0.8680	 0.0440
Ak	 0.9500	 0.0550
Al	 0.8680	 0.0460
Am	 1.0000	 0.0640
An	 0.9160	 0.0560
Ao	 0.9850	 0.0730
Ap	 0.9130	 0.0370
Aq	 0.7530	 0.0610
Ar	 0.8870	 0.0340
As	 0.9630	 0.0730
At	 0.9350	 0.0560
Au	 0.9900	 0.0620
Av	 0.9310	 0.0550
Aw	 0.8760	 0.0520
Ax	 0.8770	 0.0400
Ay	 0.9940	 0.0680
Az	 0.8710	 0.0600
B	 0.9100	 0.0390
BA	 1.0000	 0.0730
BB	 0.8880	 0.0590
BC	 0.9850	 0.0750
BD	 0.8960	 0.0390
BE	 0.7640	 0.0600
BF	 0.8850	 0.0390
BG	 0.9660	 0.0780
BH	 0.9330	 0.0570
BI	 0.9890	 0.0720
BJ	 0.8720	 0.0420
BK	 0.8190	 0.0580
BL	 0.8720	 0.0420
BM	 0.9770	 0.0740
BN	 0.9180	 0.0540
BO	 0.9610	 0.0780
BP	 0.9330	 0.0470
BQ	 0.7620	 0.0510
BR	 0.8910	 0.0370
BS	 0.9810	 0.0660
BT	 0.9020	 0.0580
BU	 0.9820	 0.0740
BV	 0.8920	 0.0540

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Chain	Atom inclusion	Q-score
BW	 0.9180	 0.0440
BX	 0.8640	 0.0450
BY	 1.0000	 0.0680
BZ	 0.8680	 0.0600
Ba	 0.9550	 0.0730
Bb	 0.9010	 0.0570
Bc	 0.7870	 0.0510
Bd	 0.8830	 0.0420
Be	 0.9800	 0.0720
Bf	 0.8920	 0.0540
Bg	 0.9640	 0.0720
Bh	 0.8950	 0.0510
Bi	 0.8600	 0.0520
Bj	 0.8720	 0.0390
Bk	 0.9980	 0.0650
Bl	 0.8720	 0.0550
Bm	 0.9720	 0.0690
Bn	 0.8680	 0.0500
Bo	 0.8380	 0.0460
Bp	 0.8620	 0.0380
Bq	 0.9810	 0.0680
Br	 0.8880	 0.0590
Bs	 0.9550	 0.0740
Bt	 0.9010	 0.0470
Bu	 0.7870	 0.0580
Bv	 0.8830	 0.0370
Bw	 0.9800	 0.0760
Bx	 0.8920	 0.0560
By	 0.9640	 0.0740
Bz	 0.8950	 0.0550
C	 0.9080	 0.0590
CA	 0.9950	 0.0600
CB	 0.9150	 0.0420
CC	 0.9380	 0.0610
CD	 0.8740	 0.0420
CE	 0.9940	 0.0650
CF	 0.8850	 0.0640
CG	 0.9910	 0.0690
CH	 0.8640	 0.0400
CI	 0.9220	 0.0550
CJ	 0.8620	 0.0490
CK	 0.9990	 0.0650

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Chain	Atom inclusion	Q-score
CL	 0.9320	 0.0620
CM	 0.9910	 0.0730
CN	 0.9300	 0.0440
CO	 0.7950	 0.0620
CP	 0.8940	 0.0390
CQ	 0.9640	 0.0780
CR	 0.9370	 0.0540
CS	 0.9850	 0.0740
CT	 0.8940	 0.0420
CU	 0.8840	 0.0550
CV	 0.8780	 0.0510
CW	 0.9850	 0.0720
CX	 0.9480	 0.0610
CY	 0.9940	 0.0590
CZ	 0.9340	 0.0450
Ca	 0.8400	 0.0620
Cb	 0.8940	 0.0370
Cc	 0.9800	 0.0800
Cd	 0.9200	 0.0610
Ce	 0.9910	 0.0690
Cf	 0.8900	 0.0430
Cg	 0.9750	 0.0560
Ch	 0.8740	 0.0460
Ci	 0.9940	 0.0640
Cj	 0.9080	 0.0670
Ck	 0.9820	 0.0720
Cl	 0.8920	 0.0480
Cm	 0.9180	 0.0520
Cn	 0.8640	 0.0390
Co	 1.0000	 0.0660
Cp	 0.8680	 0.0610
Cq	 0.9890	 0.0740
Cr	 0.8720	 0.0480
Cs	 0.8190	 0.0520
Ct	 0.8720	 0.0470
Cu	 0.9770	 0.0660
Cv	 0.9180	 0.0570
Cw	 0.9610	 0.0750
Cx	 0.9330	 0.0490
Cy	 0.7620	 0.0600
Cz	 0.8910	 0.0350
D	 0.8830	 0.0400

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Chain	Atom inclusion	Q-score
DA	 0.8760	 0.0610
DB	 0.8770	 0.0390
DC	 0.9940	 0.0670
DD	 0.8710	 0.0630
DE	 0.9910	 0.0780
DF	 0.8680	 0.0460
DG	 0.9500	 0.0530
DH	 0.8680	 0.0510
DI	 1.0000	 0.0590
DJ	 0.9160	 0.0630
DK	 0.9890	 0.0690
DL	 0.8550	 0.0470
DM	 0.9150	 0.0510
DN	 0.8630	 0.0440
DO	 0.9950	 0.0690
DP	 0.8990	 0.0580
DQ	 0.9660	 0.0740
DR	 0.9100	 0.0480
DS	 0.7390	 0.0540
DT	 0.8900	 0.0410
DU	 0.9670	 0.0750
DV	 0.9190	 0.0550
DW	 0.9750	 0.0650
DX	 0.9200	 0.0570
DY	 0.8730	 0.0500
DZ	 0.8700	 0.0430
Da	 1.0000	 0.0650
Db	 0.8630	 0.0570
Dc	 0.9800	 0.0700
Dd	 0.9440	 0.0460
De	 0.7850	 0.0590
Df	 0.8940	 0.0380
Dg	 0.9810	 0.0700
Dh	 0.9150	 0.0590
Di	 0.9940	 0.0690
Dj	 0.8780	 0.0490
Dk	 0.9610	 0.0550
Dl	 0.8610	 0.0440
Dm	 1.0000	 0.0650
Dn	 0.8740	 0.0640
Do	 0.9910	 0.0760
Dp	 0.8780	 0.0390

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Chain	Atom inclusion	Q-score
Dq	 0.8330	 0.0580
Dr	 0.8750	 0.0470
Ds	 0.9800	 0.0700
Dt	 0.9350	 0.0600
Du	 0.9910	 0.0690
Dv	 0.8640	 0.0390
Dw	 0.9220	 0.0610
Dx	 0.8620	 0.0460
Dy	 0.9990	 0.0710
Dz	 0.9320	 0.0600
E	 0.9830	 0.0720
EA	 0.9940	 0.0610
EB	 0.8850	 0.0610
EC	 0.9960	 0.0670
ED	 0.9290	 0.0450
EE	 0.8930	 0.0550
EF	 0.8860	 0.0420
EG	 0.9890	 0.0650
EH	 0.9030	 0.0660
EI	 0.9890	 0.0810
EJ	 0.8740	 0.0430
EK	 0.9660	 0.0580
EL	 0.8680	 0.0510
EM	 0.9980	 0.0630
EN	 0.9280	 0.0630
EO	 0.9860	 0.0770
EP	 0.9150	 0.0330
EQ	 0.8280	 0.0660
ER	 0.8890	 0.0420
ES	 0.9660	 0.0740
ET	 0.9520	 0.0610
EU	 0.9890	 0.0680
EV	 0.8920	 0.0370
EW	 0.9570	 0.0630
EX	 0.8760	 0.0470
EY	 0.9900	 0.0690
EZ	 0.9290	 0.0620
Ea	 0.9830	 0.0700
Eb	 0.9020	 0.0380
Ec	 0.9120	 0.0500
Ed	 0.8820	 0.0470
Ee	 0.9860	 0.0690

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Chain	Atom inclusion	Q-score
Ef	 0.9460	 0.0660
Eg	 0.9920	 0.0640
Eh	 0.9100	 0.0440
Ei	 0.9080	 0.0510
Ej	 0.8830	 0.0460
Ek	 0.9830	 0.0700
El	 0.9250	 0.0630
Em	 0.9890	 0.0720
En	 0.8920	 0.0440
Eo	 0.9570	 0.0550
Ep	 0.8760	 0.0490
Eq	 0.9900	 0.0660
Er	 0.9290	 0.0660
Es	 0.9830	 0.0690
Et	 0.9020	 0.0400
Eu	 0.9120	 0.0590
Ev	 0.8820	 0.0470
Ew	 0.9860	 0.0720
Ex	 0.9460	 0.0620
F	 0.9250	 0.0680
G	 0.9850	 0.0740
H	 0.8960	 0.0480
I	 0.7640	 0.0570
J	 0.8850	 0.0440
K	 0.9660	 0.0750
L	 0.9330	 0.0540
M	 0.9730	 0.0610
N	 0.9370	 0.0490
O	 0.8040	 0.0590
P	 0.8810	 0.0320
Q	 0.9980	 0.0670
R	 0.8770	 0.0580
S	 0.9920	 0.0770
T	 0.8560	 0.0460
U	 0.9520	 0.0480
V	 0.8580	 0.0450
W	 1.0000	 0.0650
X	 0.8880	 0.0610
Y	 0.9750	 0.0620
YA	 0.8380	 0.0510
YB	 0.8620	 0.0420
YC	 0.9810	 0.0740

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Chain	Atom inclusion	Q-score
YD	 0.8880	 0.0520
YE	 0.9810	 0.0710
YF	 0.9020	 0.0530
YG	 0.9850	 0.0770
YH	 0.9130	 0.0420
YI	 0.7530	 0.0580
YJ	 0.8870	 0.0410
YK	 0.9630	 0.0720
YL	 0.9350	 0.0580
YM	 0.9900	 0.0610
YN	 0.9310	 0.0500
YO	 0.9910	 0.0780
YP	 0.9300	 0.0390
YQ	 0.7950	 0.0590
YR	 0.8940	 0.0390
YS	 0.9640	 0.0720
YT	 0.9370	 0.0610
YU	 0.9950	 0.0620
YV	 0.9150	 0.0530
YW	 0.9380	 0.0530
YX	 0.8740	 0.0460
Z	 0.9200	 0.0500
ZA	 0.9890	 0.0680
ZB	 0.9030	 0.0610
ZC	 0.9890	 0.0750
ZD	 0.8740	 0.0350
ZE	 0.9660	 0.0570
ZF	 0.8680	 0.0460
ZG	 0.9980	 0.0640
ZH	 0.9280	 0.0620
ZI	 0.9940	 0.0640
ZJ	 0.8780	 0.0480
ZK	 0.9730	 0.0680
ZL	 0.9370	 0.0560
ZM	 0.8040	 0.0550
ZN	 0.8810	 0.0390
ZO	 0.9980	 0.0640
ZP	 0.8770	 0.0610
ZQ	 0.9920	 0.0760
ZR	 0.8560	 0.0510
ZS	 0.9520	 0.0510
ZT	 0.8580	 0.0460

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Chain	Atom inclusion	Q-score
ZU	 0.8600	 0.0400
ZV	 0.8720	 0.0430
ZW	 0.9980	 0.0620
ZX	 0.8720	 0.0570
ZY	 0.9720	 0.0730
ZZ	 0.8680	 0.0530
a	 0.8730	 0.0530
b	 0.8700	 0.0370
c	 1.0000	 0.0690
d	 0.8630	 0.0580
e	 0.9890	 0.0690
f	 0.8550	 0.0500
g	 0.9150	 0.0480
h	 0.8630	 0.0490
i	 0.9950	 0.0690
j	 0.8990	 0.0550
k	 0.9660	 0.0730
l	 0.9100	 0.0450
m	 0.7390	 0.0600
n	 0.8900	 0.0380
o	 0.9670	 0.0810
p	 0.9190	 0.0490
q	 0.9860	 0.0750
r	 0.9150	 0.0370
s	 0.8280	 0.0530
t	 0.8890	 0.0430
u	 0.9660	 0.0710
v	 0.9520	 0.0600
w	 0.9960	 0.0630
x	 0.9290	 0.0440
y	 0.8930	 0.0600
z	 0.8860	 0.0390