



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:47 PM UTC

PDB ID : 9FIA / pdb_00009fia
EMDB ID : EMD-50470
Title : SSU(body) structure derived from the SSU sample of the mitoribosome from *T. gondii*.
Authors : Rocha, R.E.O.; Barua, S.; Boissier, F.; Nguyen, T.T.; Hashem, Y.
Deposited on : 2024-05-28
Resolution : 3.29 Å(reported)

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:

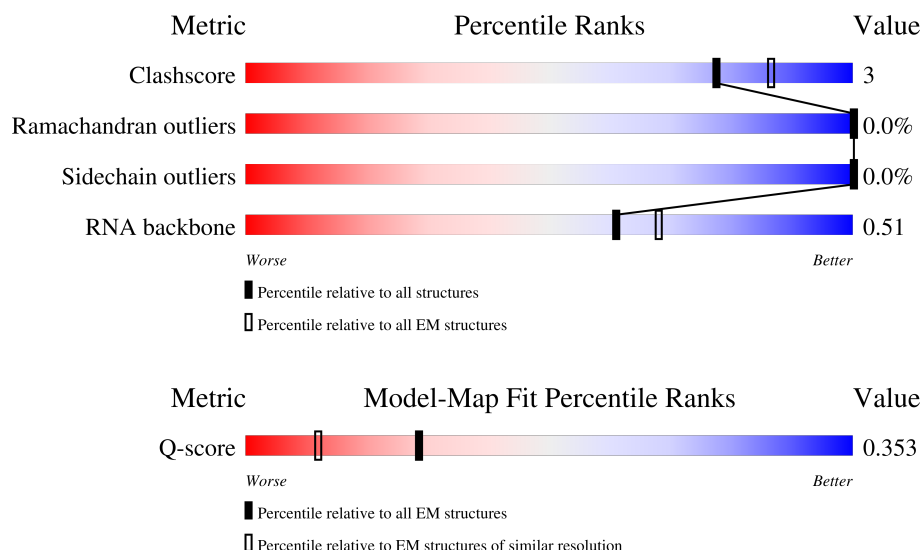
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.29 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.







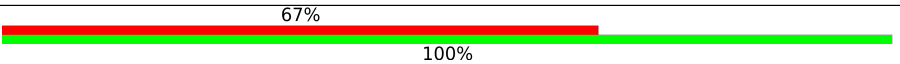
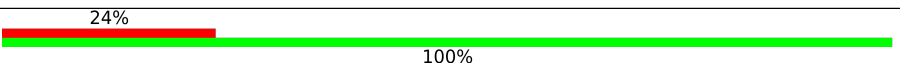
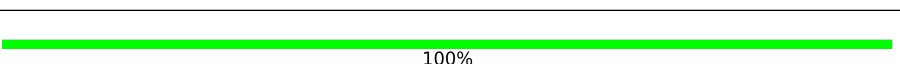
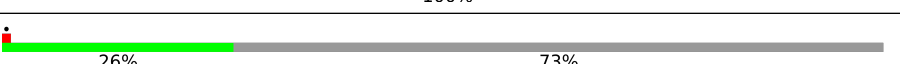

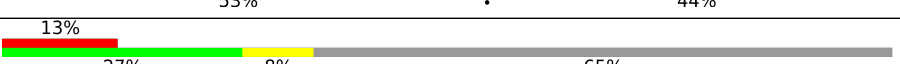


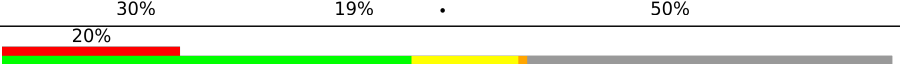
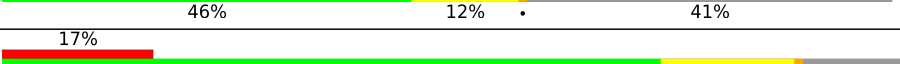



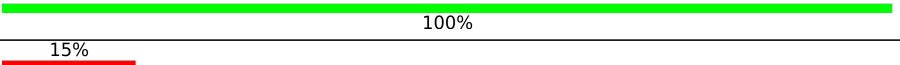
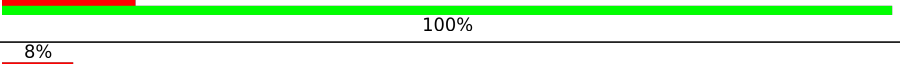
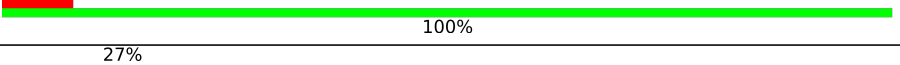
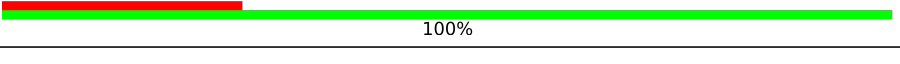


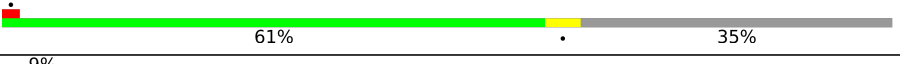
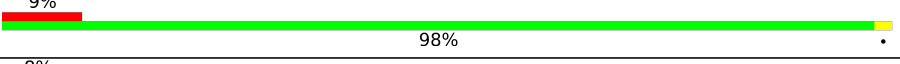
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14466 (2.79 - 3.79)

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	B0	680	
2	B1	17	
3	B2	738	

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Mol	Chain	Length	Quality of chain
4	B3	377	
5	B4	138	
6	B5	393	
7	B6	163	
8	B7	12	
9	B8	21	
9	Bj	21	
10	B9	233	
11	BA	939	
12	BB	1547	
13	BC	421	
14	BD	686	
15	BE	1053	
16	BF	304	
17	BG	160	
18	BH	129	
19	BI	13	
19	BN	13	
19	BX	13	
20	BJ	26	
21	BK	530	
22	BL	116	
23	BO	395	
24	BP	47	
25	BQ	698	

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Mol	Chain	Length	Quality of chain
26	BS	243	
27	BT	280	
28	BU	14	
29	BV	597	
30	BW	547	
31	BY	11	
32	Ba	10	
33	Bb	8	
34	Bc	716	
35	Bd	33	
36	Be	18	
37	Bg	302	
38	Bh	167	
39	Bi	268	
40	Bk	447	
41	Bl	593	
42	HJ	1140	
43	HS	235	
44	b1	8	
45	b2	48	
46	b3	5	
47	b4	34	
48	bA	34	
49	bD	27	
50	bE	107	

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Mol	Chain	Length	Quality of chain
51	bG	4	
52	bH	2	
53	bI	3	
54	bJ	71	
55	bK	83	
56	bL	48	
57	bN	122	
58	bO	115	
59	bP	15	
60	bQ	14	
61	bR	31	
62	bS	31	
63	bT	60	
64	bU	25	
65	bV	6	
66	bY	11	

2 Entry composition [i](#)

There are 66 unique types of molecules in this entry. The entry contains 80775 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 Mitochondrial ribosomal protein, mS145.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B0	278	Total	C	N	O	S	0	0
			2311	1461	428	414	8		

- Molecule 2 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B1	17	Total	C	N	O	0	0
			68	34	17	17		

- Molecule 3 is a protein called Ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B2	335	Total	C	N	O	S	0	0
			2790	1755	522	502	11		

- Molecule 4 is a protein called Mitochondrial ribosomal protein, mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B3	218	Total	C	N	O	S	0	0
			1735	1092	329	303	11		

- Molecule 5 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B4	80	Total	C	N	O	S	0	0
			663	434	120	106	3		

- Molecule 6 is a protein called Ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B5	140	Total	C	N	O	S	0	0
			1109	692	229	184	4		

- Molecule 7 is a protein called Putative mitochondrial ribosomal protein s6-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B6	113	Total	C	N	O	S	0	0
			943	606	183	150	4		

- Molecule 8 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	B7	12	Total	C	N	O	0	0
			48	24	12	12		

- Molecule 9 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	B8	21	Total	C	N	O	0	0
			84	42	21	21		
9	Bj	21	Total	C	N	O	0	0
			84	42	21	21		

- Molecule 10 is a protein called DnaJ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B9	62	Total	C	N	O	S	0	0
			531	340	99	91	1		

- Molecule 11 is a protein called Mitochondrial ribosomal protein, mS137.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BA	526	Total	C	N	O	S	0	0
			4093	2596	723	759	15		

- Molecule 12 is a protein called RAP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BB	546	Total	C	N	O	S	0	0
			4313	2744	793	755	21		

- Molecule 13 is a protein called Mitochondrial ribosomal protein, mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BC	204	Total	C	N	O	S	0	0
			1581	1014	292	269	6		

- Molecule 14 is a protein called Pentatricopeptide repeat domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BD	341	Total	C	N	O	S	0	0
			2682	1693	498	484	7		

- Molecule 15 is a protein called Mitochondrial ribosomal protein, mS140.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	624	Total	C	N	O	S	0	0
			5085	3236	940	887	22		

- Molecule 16 is a protein called Mitochondrial ribosomal protein, mS147.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BF	271	Total	C	N	O	S	0	0
			2195	1391	428	370	6		

- Molecule 17 is a protein called Ribosomal protein, uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BG	148	Total	C	N	O	S	0	0
			1187	765	210	204	8		

- Molecule 18 is a protein called Putative ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BH	125	Total	C	N	O	S	0	0
			998	636	188	166	8		

- Molecule 19 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	BI	13	Total	C	N	O	0	0
			52	26	13	13		
19	BN	13	Total	C	N	O	0	0
			52	26	13	13		
19	BX	13	Total	C	N	O	0	0
			52	26	13	13		

- Molecule 20 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	BJ	26	Total	C	N	O	0	0
			104	52	26	26		

- Molecule 21 is a protein called Mitochondrial ribosomal protein, mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	198	Total	C	N	O	S	0	0
			1673	1068	307	292	6		

- Molecule 22 is a protein called Putative ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BL	103	Total	C	N	O	S	0	0
			887	570	168	144	5		

- Molecule 23 is a protein called Putative 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BO	257	Total	C	N	O	S	0	0
			2150	1371	419	350	10		

- Molecule 24 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	BP	47	Total	C	N	O	0	0
			188	94	47	47		

- Molecule 25 is a protein called Macro domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BQ	455	Total	C	N	O	S	0	0
			3588	2295	657	628	8		

- Molecule 26 is a protein called Ribosomal protein, bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BS	156	Total	C	N	O	S	0	0
			1305	825	253	225	2		

- Molecule 27 is a protein called Mitochondrial ribosomal protein, mS156.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	100	Total	C	N	O	S	0	0
			801	519	148	132	2		

- Molecule 28 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BU	14	Total	C	N	O	0	0
			56	28	14	14		

- Molecule 29 is a protein called Putative homeodomain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BV	262	Total	C	N	O	S	0	0
			2181	1410	370	395	6		

- Molecule 30 is a protein called Mitochondrial ribosomal protein, mS144.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BW	339	Total	C	N	O	S	0	0
			2716	1714	489	503	10		

- Molecule 31 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	BY	11	Total	C	N	O	0	0
			44	22	11	11		

- Molecule 32 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Ba	10	Total	C	N	O	0	0
			40	20	10	10		

- Molecule 33 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Bb	8	Total	C	N	O	0	0
			32	16	8	8		

- Molecule 34 is a protein called Enoyl-CoA hydratase/isomerase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bc	537	Total	C	N	O	S	0	0
			4276	2717	763	779	17		

- Molecule 35 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Bd	33	Total	C	N	O	0	0
			132	66	33	33		

- Molecule 36 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Be	18	Total	C	N	O	0	0
			72	36	18	18		

- Molecule 37 is a protein called Ribosomal protein, uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bg	187	Total	C	N	O	S	0	0
			1543	997	294	249	3		

- Molecule 38 is a protein called Putative 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bh	153	Total	C	N	O	S	0	0
			1242	791	229	215	7		

- Molecule 39 is a protein called Mitochondrial ribosomal protein, mS153.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bi	119	Total	C	N	O	S	0	0
			928	595	163	167	3		

- Molecule 40 is a protein called Mitochondrial ribosomal protein, mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bk	415	Total	C	N	O	S	0	0
			3394	2130	645	612	7		

- Molecule 41 is a protein called 30S ribosomal protein S12, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	200	Total	C	N	O	S	0	0
			1660	1044	334	276	6		

- Molecule 42 is a protein called 30S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	HJ	355	Total	C	N	O	S	0	0
			2916	1851	550	505	10		

- Molecule 43 is a protein called Acylphosphatase-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	HS	90	Total	C	N	O	S	0	0
			720	450	141	127	2		

- Molecule 44 is a RNA chain called ulr11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	b1	8	Total	C	N	O	P	0	0
			160	72	16	64	8		

- Molecule 45 is a RNA chain called SSUE.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	b2	30	Total	C	N	O	P	0	0
			632	284	112	206	30		

- Molecule 46 is a RNA chain called ulr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	b3	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

- Molecule 47 is a RNA chain called RNA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	b4	27	Total	C	N	O	P	0	0
			585	260	108	190	27		

- Molecule 48 is a RNA chain called RNA19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	bA	27	Total	C	N	O	P	0	0
			571	255	93	196	27		

- Molecule 49 is a RNA chain called RNA15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	bD	25	Total	C	N	O	P	0	0
			546	243	106	172	25		

- Molecule 50 is a RNA chain called RNA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	bE	92	Total	C	N	O	P	0	0
			1965	879	355	639	92		

- Molecule 51 is a RNA chain called ulr13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	bG	4	Total	C	N	O	P	0	0
			80	36	8	32	4		

- Molecule 52 is a RNA chain called ulr14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	bH	2	Total	C	N	O	P	0	0
			40	18	4	16	2		

- Molecule 53 is a RNA chain called ulr15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	bI	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 54 is a RNA chain called RNA33.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	bJ	58	Total	C	N	O	P	0	0
			1220	548	203	411	58		

- Molecule 55 is a RNA chain called RNA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	bK	66	Total	C	N	O	P	0	0
			1397	628	246	457	66		

- Molecule 56 is a RNA chain called RNA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	bL	48	Total	C	N	O	P	0	0
			1019	456	176	339	48		

- Molecule 57 is a RNA chain called SSUB.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	bN	50	Total	C	N	O	P	0	0
			1069	477	187	355	50		

- Molecule 58 is a RNA chain called SSUA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	bO	115	Total	C	N	O	P	0	0
			2451	1099	445	792	115		

- Molecule 59 is a RNA chain called ulr16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	bP	15	Total	C	N	O	P	0	0
			300	135	30	120	15		

- Molecule 60 is a RNA chain called ulr17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	bQ	14	Total	C	N	O	P	0	0
			280	126	28	112	14		

- Molecule 61 is a RNA chain called RNA30.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	bR	19	Total	C	N	O	P	0	0
			408	183	77	129	19		

- Molecule 62 is a RNA chain called url18.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	bS	31	Total	C	N	O	P	0	0
			620	279	62	248	31		

- Molecule 63 is a RNA chain called SSUF.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	bT	52	Total	C	N	O	P	0	0
			1128	504	219	353	52		

- Molecule 64 is a RNA chain called ulr19.

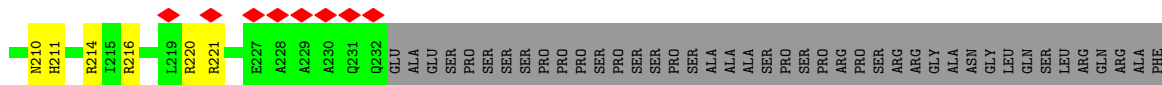
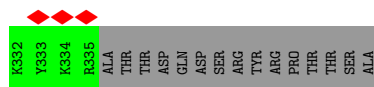
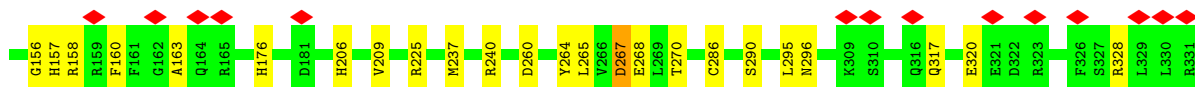
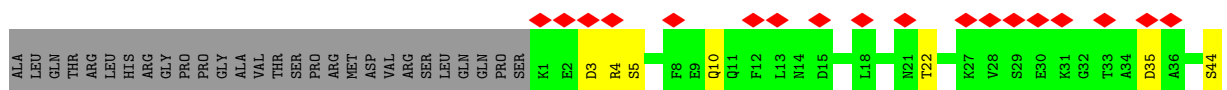
Mol	Chain	Residues	Atoms					AltConf	Trace
64	bU	25	Total	C	N	O	P	0	0
			500	225	50	200	25		

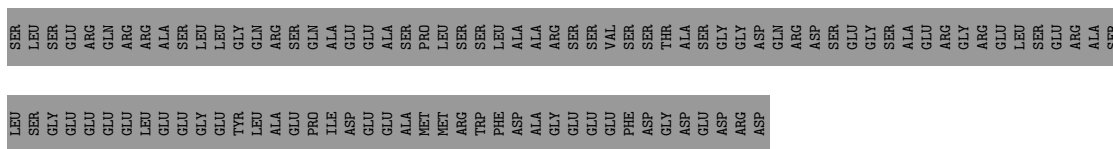
- Molecule 65 is a RNA chain called ulr20.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	bV	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

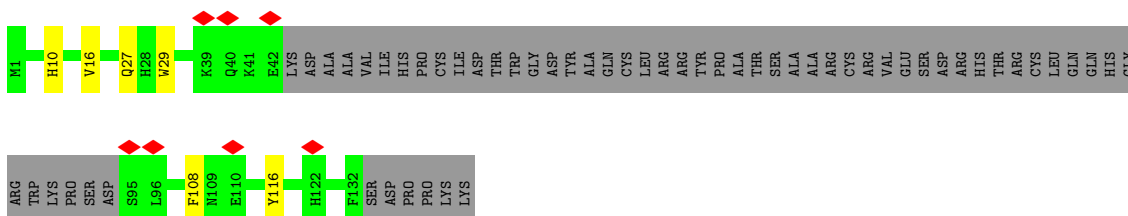
- Molecule 66 is a RNA chain called ulr21.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	bY	11	Total	C	N	O	P	0	0
			220	99	22	88	11		

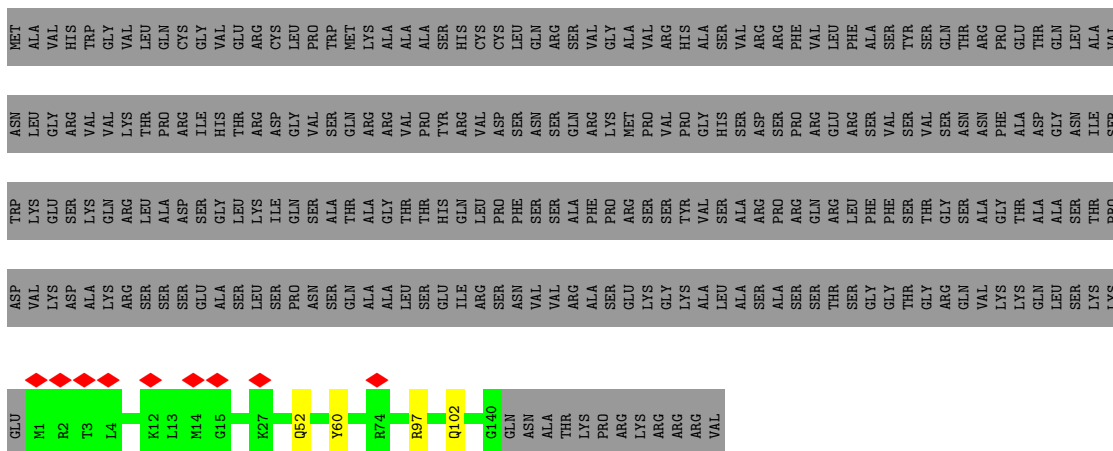




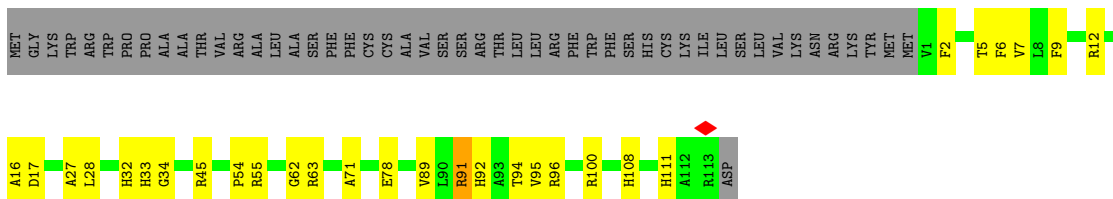
- Molecule 5: CHCH domain-containing protein



- Molecule 6: Ribosomal protein S11, putative

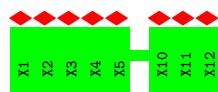


- Molecule 7: Putative mitochondrial ribosomal protein s6-2

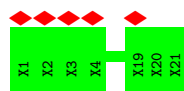


- Molecule 8: unidentified peptide





- Molecule 9: unidentified peptide

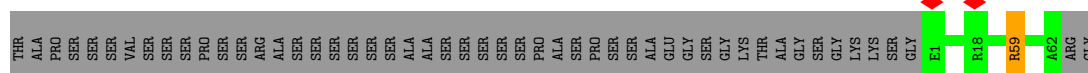
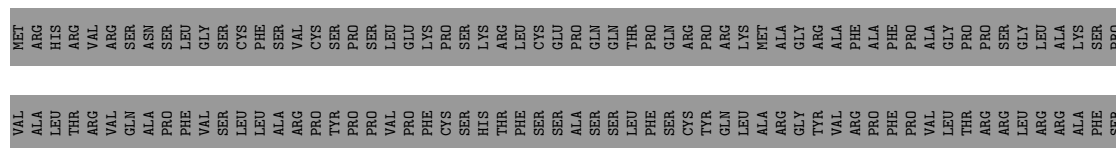


- Molecule 9: unidentified peptide

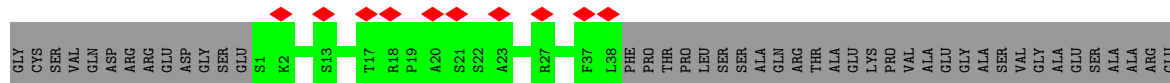
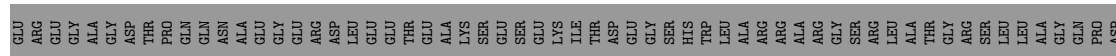
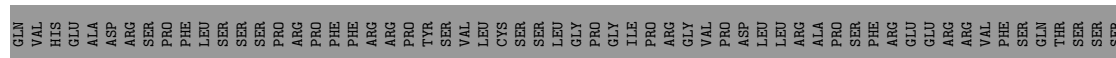


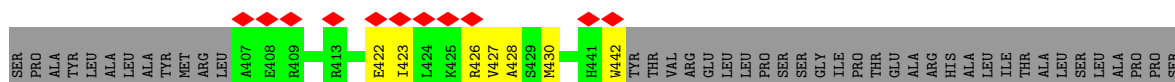
There are no outlier residues recorded for this chain.

- Molecule 10: DnaJ domain-containing protein

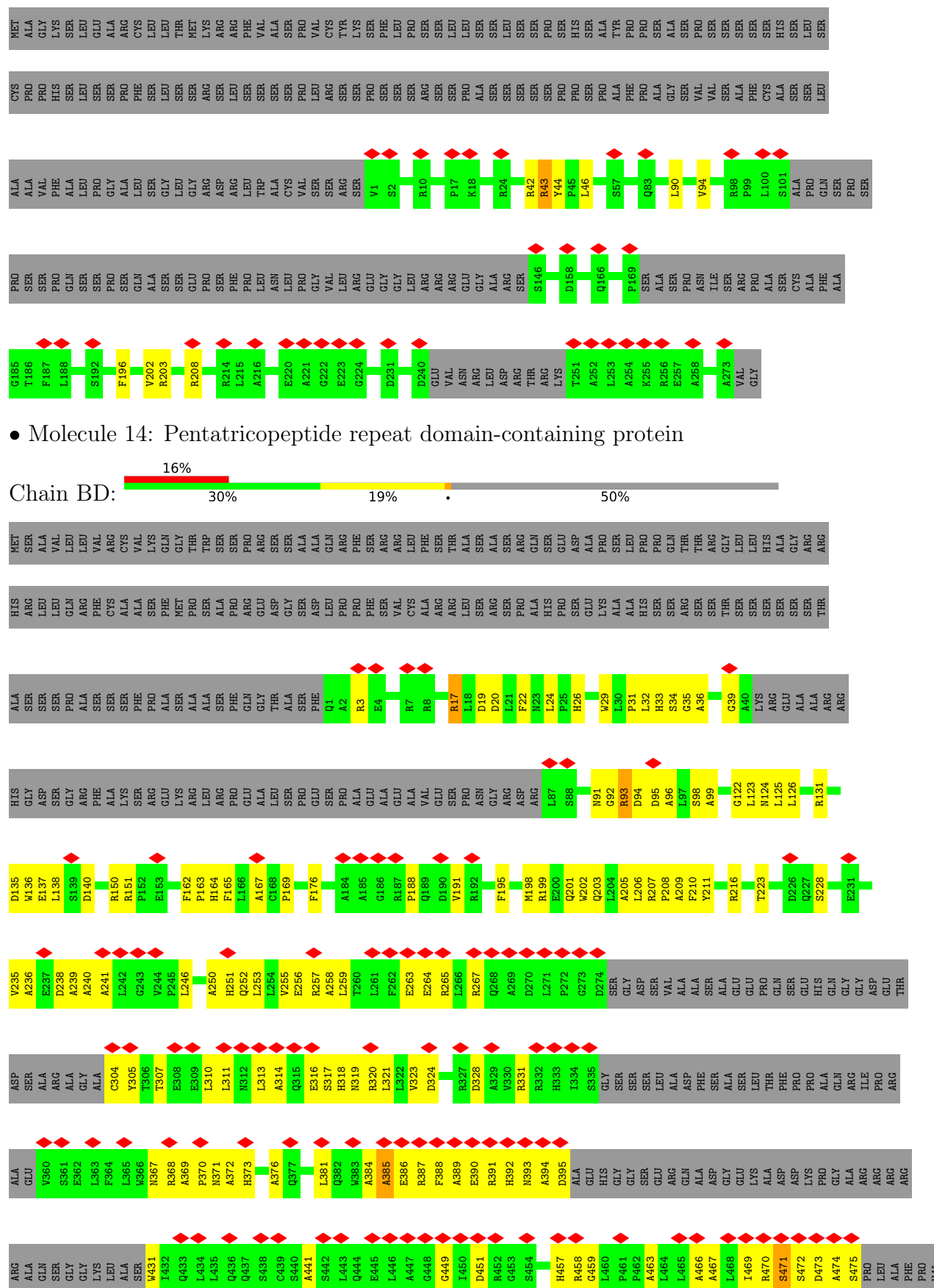


- Molecule 11: Mitochondrial ribosomal protein, mS137



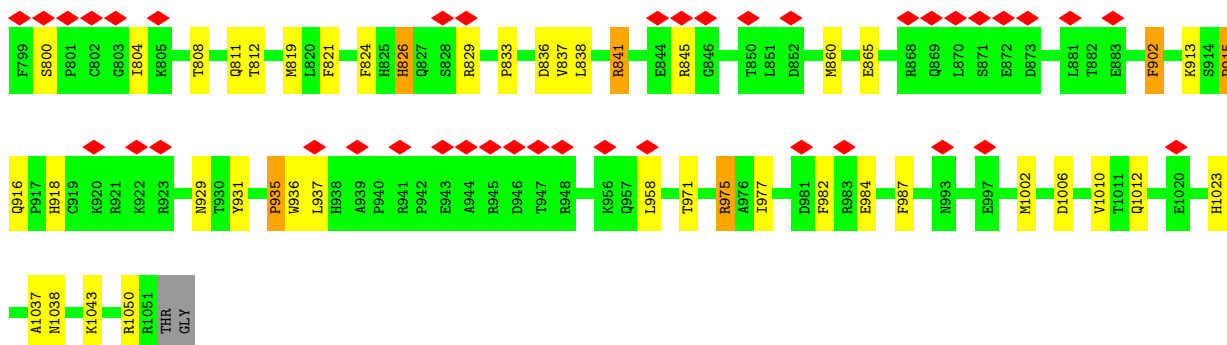




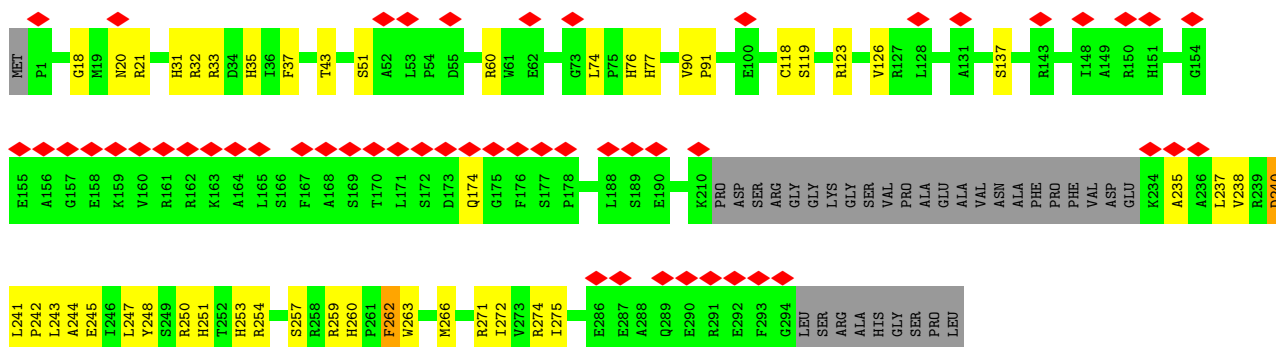
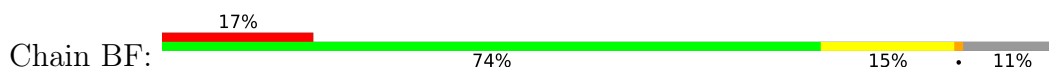


- Molecule 15: Mitochondrial ribosomal protein, mS140

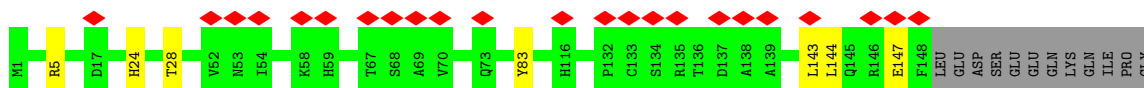
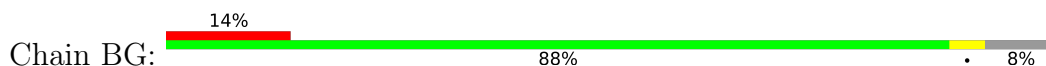
M732	G733	L734	E737	K738	D739	G744	G745	L746	L747	Q748	Q749	E750	L751	L754	R757	E758	K759	E762	L763	R764	G765	G766	L767	R768	G769	SER	LEU	PRO	PRO	VAL	SER	SER	VAL	GLN	LEU	ASP	ASP	ALA	LYS	ALA	GLY	GLU	S786	F787	D788	A789	Q790	E791	T792	F793	G794	R795	S796	E797	T798
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------



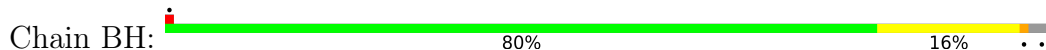
- Molecule 16: Mitochondrial ribosomal protein, mS147



- Molecule 17: Ribosomal protein, uS2m



- Molecule 18: Putative ribosomal protein S8



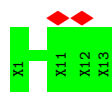
- Molecule 19: unidentified peptide



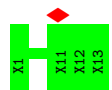
There are no outlier residues recorded for this chain.

- Molecule 19: unidentified peptide

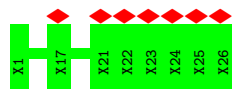




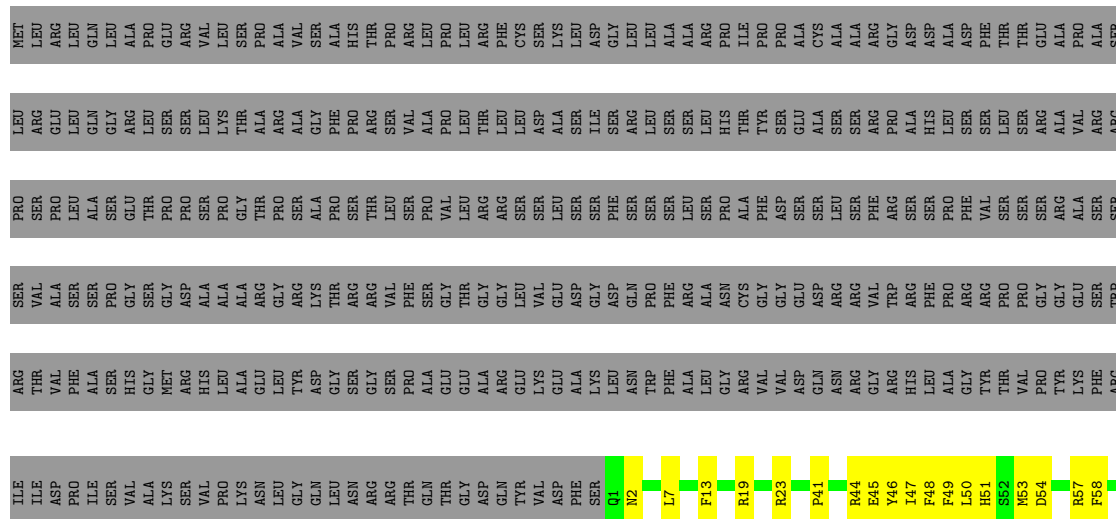
- Molecule 19: unidentified peptide



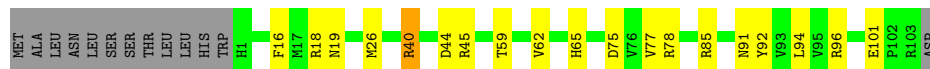
- Molecule 20: unidentified peptide



- Molecule 21: Mitochondrial ribosomal protein, mS26

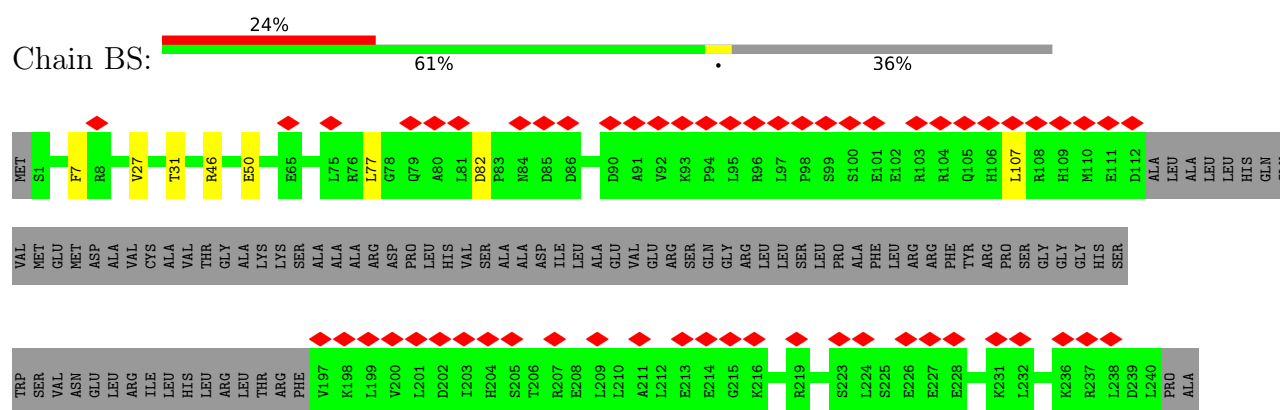


- Molecule 22: Putative ribosomal protein S17

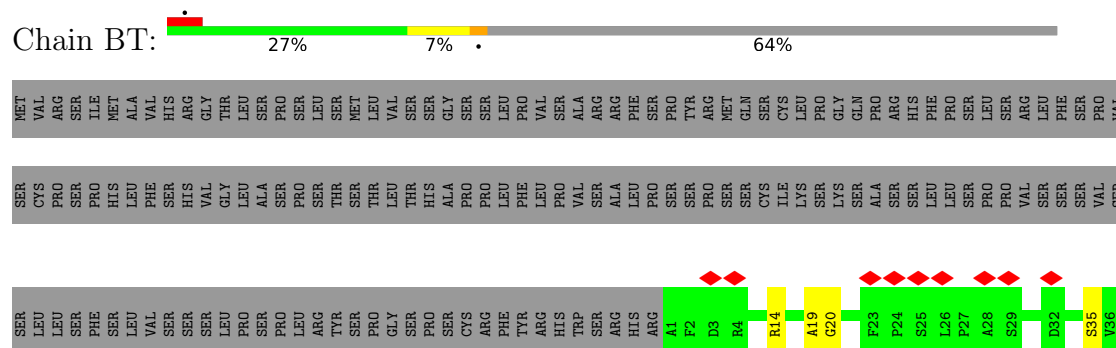


- Molecule 23: Putative 30S ribosomal protein S15

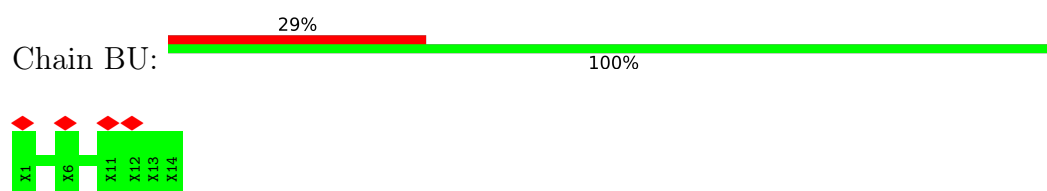
Frequency	Percentage
Daily	61%
Weekly	35%
Monthly	4%



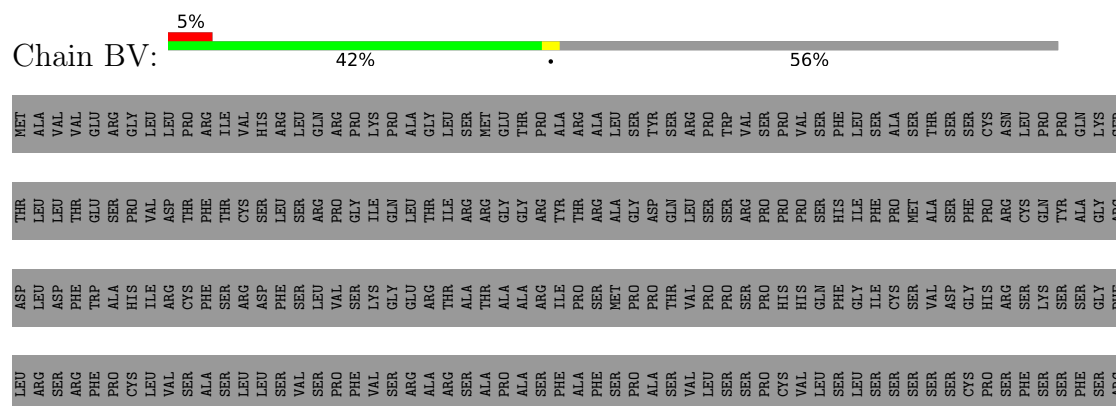
- Molecule 27: Mitochondrial ribosomal protein, mS156

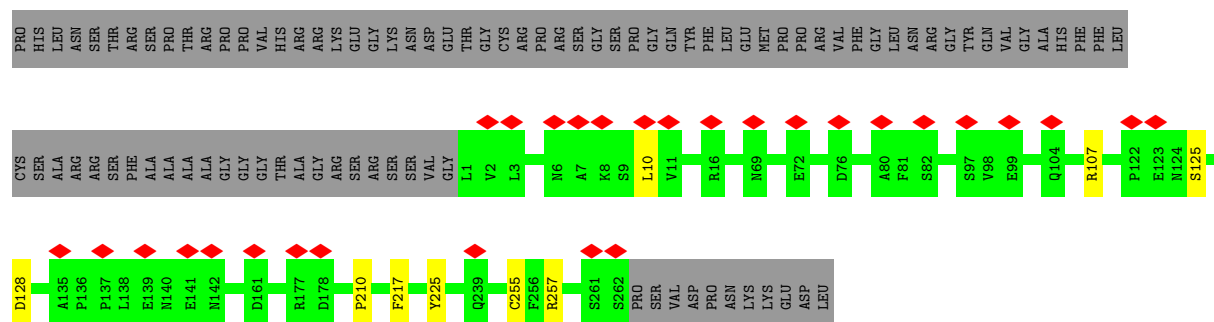


- Molecule 28: unidentified peptide

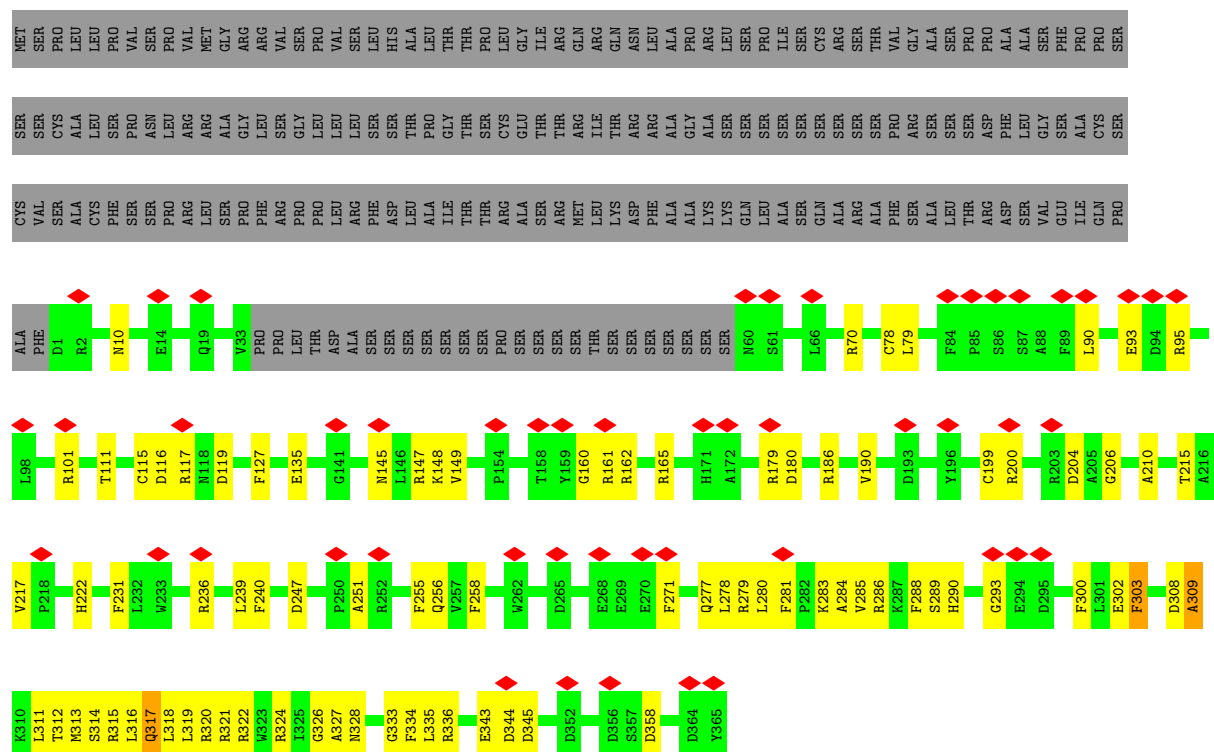


- Molecule 29: Putative homeodomain containing protein

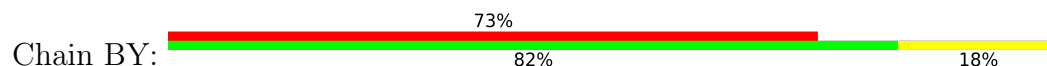




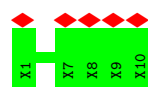
- Molecule 30: Mitochondrial ribosomal protein, mS144



- Molecule 31: unidentified peptide



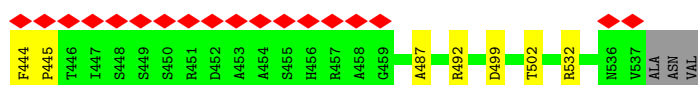
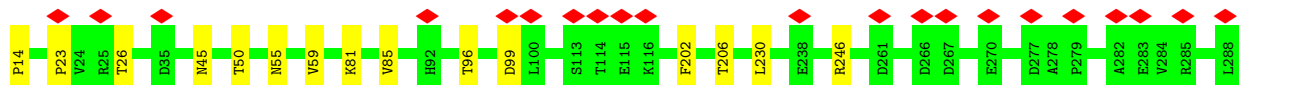
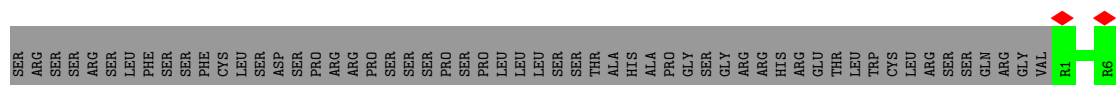
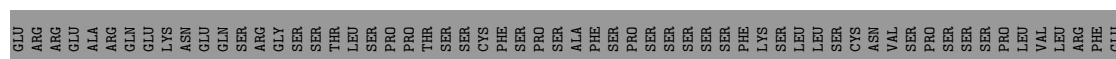
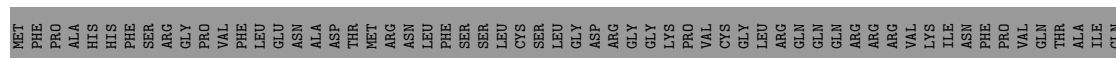
- Molecule 32: unidentified peptide



- Molecule 33: unidentified peptide



- Molecule 34: Enoyl-CoA hydratase/isomerase family protein



- Molecule 35: unidentified peptide

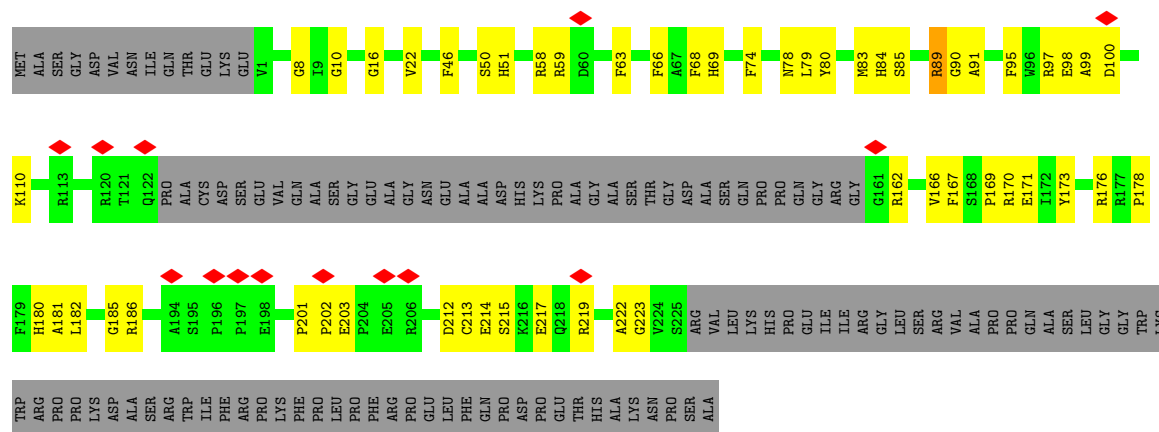


- Molecule 36: unidentified peptide

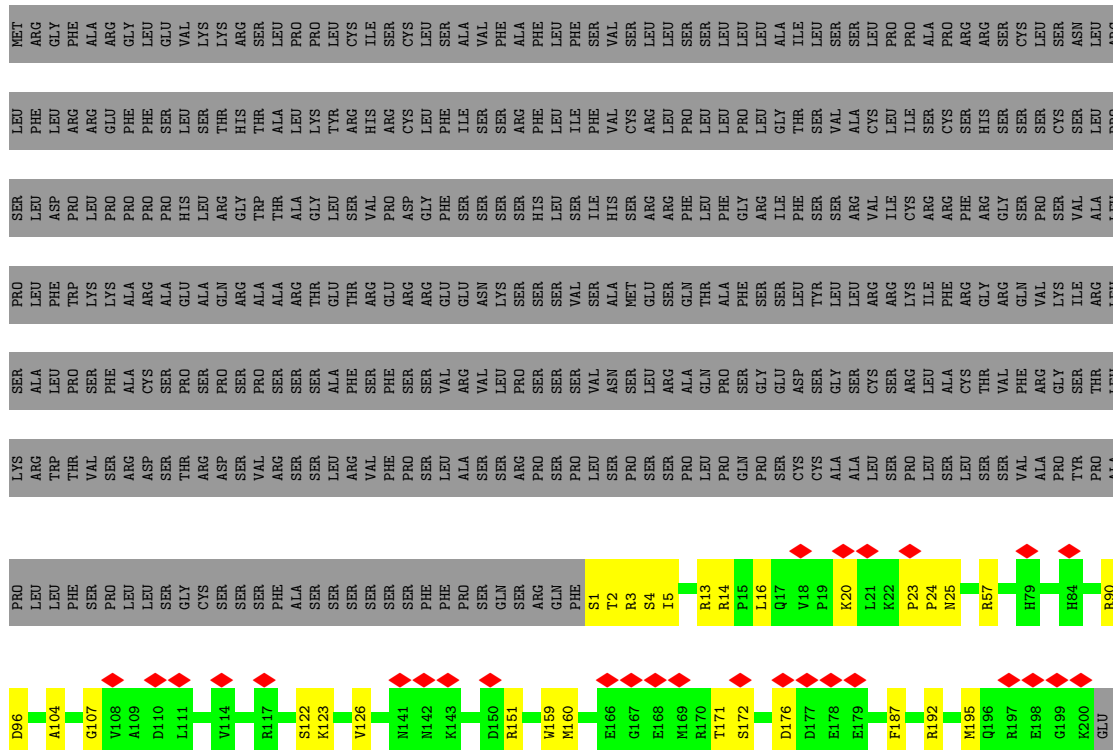


- Molecule 37: Ribosomal protein, uS2m

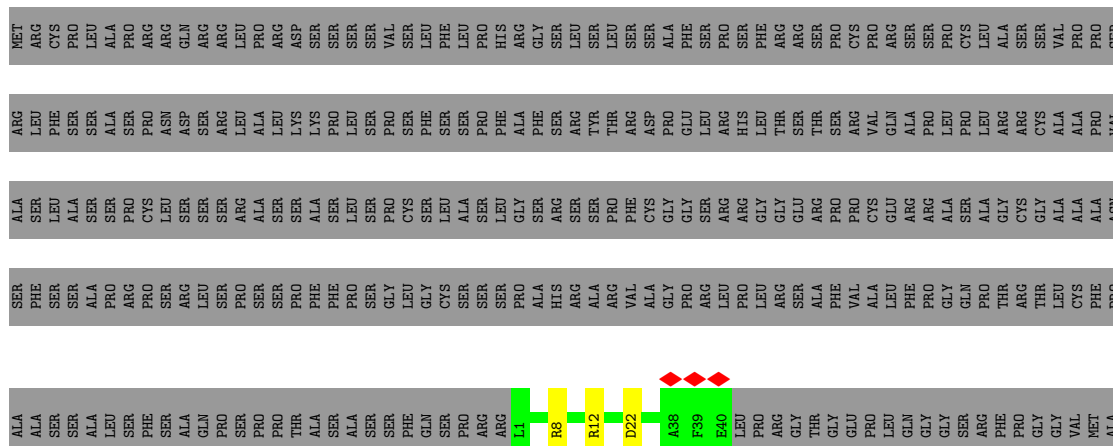




- Molecule 41: 30S ribosomal protein S12, putative



- Molecule 42: 30S ribosomal protein S5, putative







• Molecule 44: ulr11



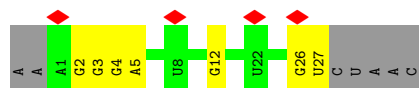
• Molecule 45: SSUE



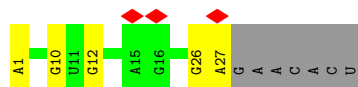
• Molecule 46: ulr12



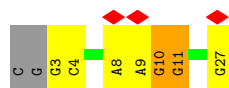
• Molecule 47: RNA13



• Molecule 48: RNA19

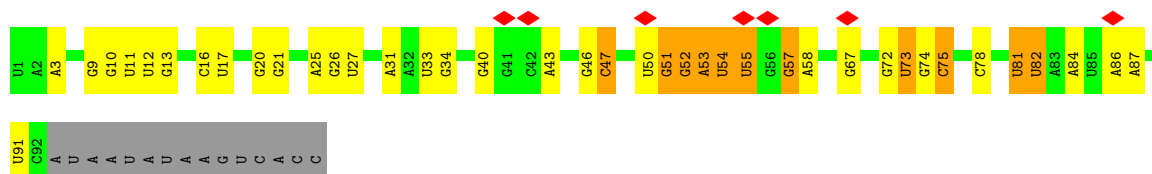


• Molecule 49: RNA15

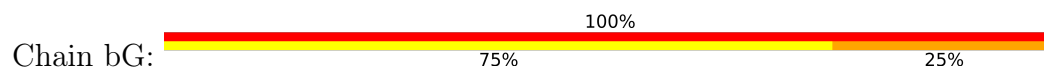


• Molecule 50: RNA8





• Molecule 51: ulr13



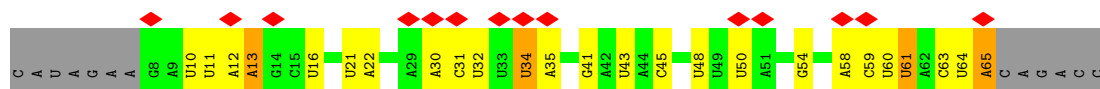
• Molecule 52: ulr14



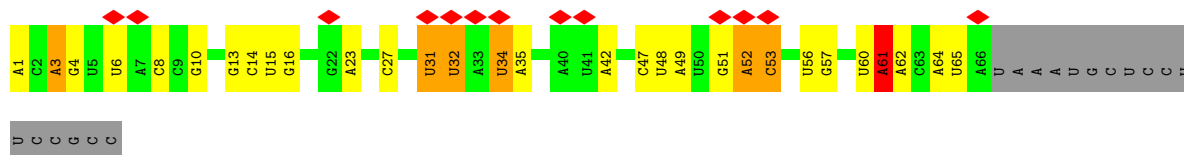
• Molecule 53: ulr15



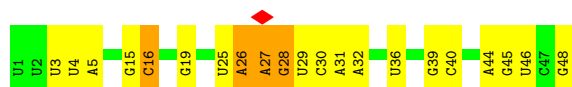
• Molecule 54: RNA33



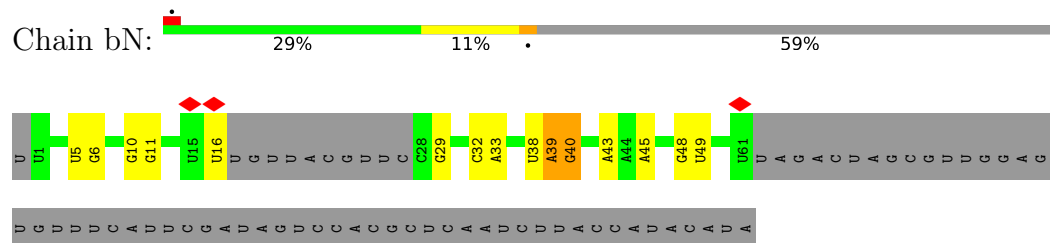
• Molecule 55: RNA5



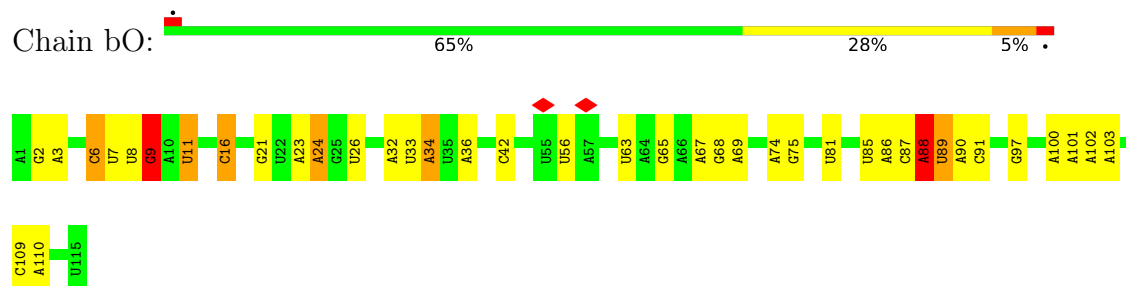
• Molecule 56: RNA17



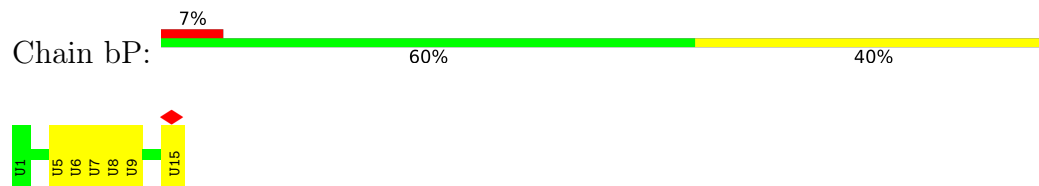
- Molecule 57: SSUB



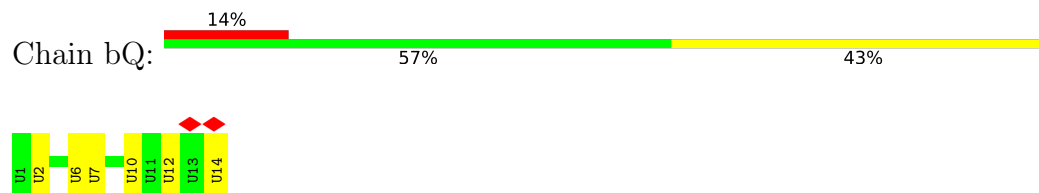
- Molecule 58: SSUA



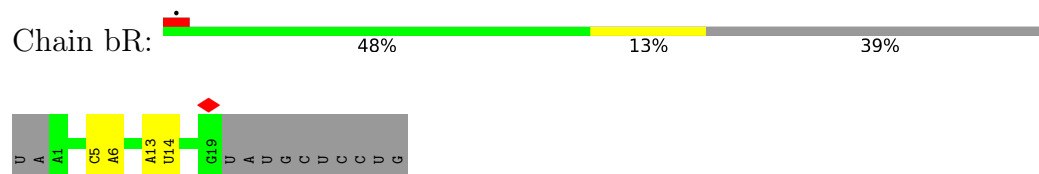
- Molecule 59: ulr16



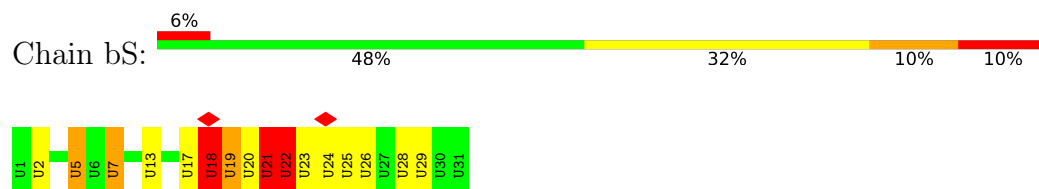
- Molecule 60: ulr17



- Molecule 61: RNA30

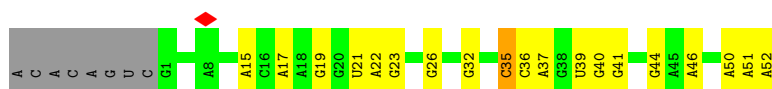


- Molecule 62: url18



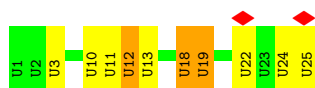
- Molecule 63: SSUF

Chain bT:  55% 30% 13%



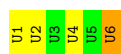
- Molecule 64: ulr19

Chain bU:  8% 60% 28% 12%



- Molecule 65: ulr20

Chain bV:  33% 50% 17%



- Molecule 66: ulr21

Chain bY:  9% 45% 55%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.159	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	632.394, 632.394, 632.394	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5057, 1.5057, 1.5057	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	B0	2.03	69/2369 (2.9%)	1.92	127/3204 (4.0%)
3	B2	1.41	23/2853 (0.8%)	1.46	48/3844 (1.2%)
4	B3	1.28	15/1767 (0.8%)	1.26	9/2381 (0.4%)
5	B4	0.66	2/682 (0.3%)	0.65	0/914
6	B5	0.28	0/1129	0.50	0/1513
7	B6	2.11	22/967 (2.3%)	1.98	34/1298 (2.6%)
10	B9	0.75	3/546 (0.5%)	0.70	1/730 (0.1%)
11	BA	0.83	11/4190 (0.3%)	0.87	3/5693 (0.1%)
12	BB	1.94	95/4388 (2.2%)	1.83	168/5925 (2.8%)
13	BC	0.81	13/1617 (0.8%)	0.73	6/2196 (0.3%)
14	BD	2.28	91/2738 (3.3%)	2.11	168/3720 (4.5%)
15	BE	1.58	58/5196 (1.1%)	1.64	136/7021 (1.9%)
16	BF	1.50	44/2259 (1.9%)	1.32	47/3058 (1.5%)
17	BG	0.37	0/1217	0.55	0/1657
18	BH	1.34	14/1015 (1.4%)	1.25	27/1365 (2.0%)
21	BK	0.97	6/1713 (0.4%)	1.07	40/2311 (1.7%)
22	BL	1.47	7/912 (0.8%)	1.53	29/1228 (2.4%)
23	BO	0.40	1/2206 (0.0%)	0.56	2/2975 (0.1%)
25	BQ	1.44	39/3683 (1.1%)	1.45	117/5001 (2.3%)
26	BS	0.59	0/1334	0.74	0/1796
27	BT	1.93	21/830 (2.5%)	1.81	30/1131 (2.7%)
29	BV	0.58	1/2242 (0.0%)	0.66	5/3045 (0.2%)
30	BW	1.72	51/2773 (1.8%)	1.67	91/3752 (2.4%)
34	Bc	0.25	0/4386	0.43	0/5958
37	Bg	1.91	45/1602 (2.8%)	1.73	62/2164 (2.9%)
38	Bh	1.02	6/1272 (0.5%)	1.05	21/1710 (1.2%)
39	Bi	1.23	9/947 (1.0%)	1.17	25/1278 (2.0%)
40	Bk	1.30	27/3445 (0.8%)	1.35	73/4624 (1.6%)
41	Bl	0.97	11/1696 (0.6%)	0.99	19/2277 (0.8%)
42	HJ	1.45	35/2987 (1.2%)	1.44	66/4027 (1.6%)
43	HS	0.80	2/733 (0.3%)	0.89	1/986 (0.1%)
44	b1	0.95	0/175	0.63	0/268
45	b2	0.15	0/705	0.22	0/1094
46	b3	1.18	2/109 (1.8%)	0.77	0/166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
47	b4	1.57	3/655 (0.5%)	1.04	0/1021
48	bA	0.21	0/636	0.22	0/988
49	bD	0.81	0/613	0.59	0/956
50	bE	0.16	0/2199	0.26	0/3425
51	bG	0.80	0/87	0.45	0/132
52	bH	0.98	0/43	0.97	0/64
53	bI	0.78	0/65	0.53	0/98
54	bJ	0.37	0/1361	0.51	4/2114 (0.2%)
55	bK	1.20	6/1562 (0.4%)	0.87	0/2428
56	bL	0.90	2/1138 (0.2%)	0.67	3/1770 (0.2%)
57	bN	0.99	3/1194 (0.3%)	0.74	1/1857 (0.1%)
58	bO	1.29	10/2744 (0.4%)	0.92	1/4272 (0.0%)
59	bP	0.76	0/329	0.36	0/506
60	bQ	1.62	0/307	1.07	0/472
61	bR	0.59	0/457	0.44	0/710
62	bS	0.87	0/681	1.14	11/1050 (1.0%)
63	bT	0.35	0/1267	0.37	0/1976
64	bU	0.87	0/549	0.74	0/846
65	bV	1.36	2/131 (1.5%)	0.89	1/200 (0.5%)
66	bY	1.08	0/241	0.62	0/370
All	All	1.30	749/82942 (0.9%)	1.24	1376/115565 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	BE	0	1
42	HJ	0	1
52	bH	0	1
62	bS	0	4
63	bT	0	2
All	All	0	9

All (749) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BE	935	PRO	N-CD	-13.04	1.29	1.47
14	BD	369	ALA	CA-CB	-9.51	1.42	1.53
40	Bk	32	HIS	CE1-NE2	-9.16	1.23	1.32
39	Bi	132	HIS	CE1-NE2	-9.14	1.23	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BT	51	HIS	ND1-CE1	-9.12	1.23	1.32
27	BT	51	HIS	CE1-NE2	-9.06	1.23	1.32
39	Bi	132	HIS	ND1-CE1	-9.02	1.23	1.32
40	Bk	32	HIS	ND1-CE1	-8.98	1.23	1.32
12	BB	170	HIS	CE1-NE2	-8.84	1.23	1.32
12	BB	153	HIS	CE1-NE2	-8.80	1.23	1.32
12	BB	339	HIS	ND1-CE1	-8.80	1.23	1.32
14	BD	318	HIS	CE1-NE2	-8.79	1.23	1.32
16	BF	31	HIS	CE1-NE2	-8.79	1.23	1.32
14	BD	251	HIS	CE1-NE2	-8.79	1.23	1.32
15	BE	508	HIS	CE1-NE2	-8.79	1.23	1.32
14	BD	373	HIS	CE1-NE2	-8.79	1.23	1.32
15	BE	478	HIS	CE1-NE2	-8.79	1.23	1.32
30	BW	290	HIS	CE1-NE2	-8.79	1.23	1.32
12	BB	151	HIS	CE1-NE2	-8.78	1.23	1.32
16	BF	253	HIS	CE1-NE2	-8.78	1.23	1.32
16	BF	35	HIS	CE1-NE2	-8.76	1.23	1.32
14	BD	392	HIS	ND1-CE1	-8.76	1.23	1.32
16	BF	35	HIS	ND1-CE1	-8.76	1.23	1.32
12	BB	339	HIS	CE1-NE2	-8.75	1.23	1.32
12	BB	39	HIS	CE1-NE2	-8.74	1.23	1.32
14	BD	33	HIS	CE1-NE2	-8.74	1.23	1.32
12	BB	150	HIS	ND1-CE1	-8.73	1.23	1.32
12	BB	151	HIS	ND1-CE1	-8.73	1.23	1.32
14	BD	33	HIS	ND1-CE1	-8.73	1.23	1.32
14	BD	251	HIS	ND1-CE1	-8.72	1.23	1.32
42	HJ	678	HIS	CE1-NE2	-8.72	1.23	1.32
42	HJ	678	HIS	ND1-CE1	-8.72	1.23	1.32
15	BE	478	HIS	ND1-CE1	-8.71	1.23	1.32
15	BE	508	HIS	ND1-CE1	-8.71	1.23	1.32
12	BB	150	HIS	CE1-NE2	-8.71	1.23	1.32
12	BB	170	HIS	ND1-CE1	-8.71	1.23	1.32
16	BF	251	HIS	CE1-NE2	-8.70	1.23	1.32
16	BF	260	HIS	CE1-NE2	-8.70	1.23	1.32
30	BW	290	HIS	ND1-CE1	-8.70	1.23	1.32
14	BD	318	HIS	ND1-CE1	-8.70	1.23	1.32
12	BB	309	HIS	CE1-NE2	-8.69	1.23	1.32
14	BD	373	HIS	ND1-CE1	-8.69	1.23	1.32
1	B0	47	HIS	CE1-NE2	-8.68	1.23	1.32
14	BD	392	HIS	CE1-NE2	-8.68	1.23	1.32
16	BF	260	HIS	ND1-CE1	-8.68	1.23	1.32
12	BB	153	HIS	ND1-CE1	-8.67	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	BF	253	HIS	ND1-CE1	-8.67	1.23	1.32
21	BK	51	HIS	CE1-NE2	-8.67	1.23	1.32
37	Bg	69	HIS	CE1-NE2	-8.67	1.23	1.32
12	BB	309	HIS	ND1-CE1	-8.65	1.23	1.32
12	BB	39	HIS	ND1-CE1	-8.65	1.23	1.32
16	BF	251	HIS	ND1-CE1	-8.64	1.24	1.32
16	BF	31	HIS	ND1-CE1	-8.64	1.24	1.32
1	B0	47	HIS	ND1-CE1	-8.63	1.24	1.32
37	Bg	84	HIS	ND1-CE1	-8.61	1.24	1.32
14	BD	164	HIS	CE1-NE2	-8.61	1.24	1.32
40	Bk	309	HIS	CE1-NE2	-8.58	1.24	1.32
37	Bg	69	HIS	ND1-CE1	-8.58	1.24	1.32
37	Bg	180	HIS	CE1-NE2	-8.58	1.24	1.32
21	BK	51	HIS	ND1-CE1	-8.57	1.24	1.32
37	Bg	51	HIS	CE1-NE2	-8.56	1.24	1.32
37	Bg	84	HIS	CE1-NE2	-8.56	1.24	1.32
37	Bg	180	HIS	ND1-CE1	-8.56	1.24	1.32
14	BD	164	HIS	ND1-CE1	-8.54	1.24	1.32
37	Bg	51	HIS	ND1-CE1	-8.54	1.24	1.32
15	BE	826	HIS	ND1-CE1	-8.49	1.24	1.32
15	BE	826	HIS	CE1-NE2	-8.47	1.24	1.32
40	Bk	309	HIS	ND1-CE1	-8.47	1.24	1.32
37	Bg	99	ALA	CA-CB	-8.46	1.42	1.52
27	BT	51	HIS	CD2-NE2	-8.35	1.28	1.37
7	B6	33	HIS	CE1-NE2	-8.34	1.24	1.32
39	Bi	132	HIS	CD2-NE2	-8.34	1.28	1.37
14	BD	199	ARG	CZ-NH2	-8.32	1.22	1.33
7	B6	92	HIS	CE1-NE2	-8.31	1.24	1.32
14	BD	458	ARG	CZ-NH2	-8.31	1.22	1.33
14	BD	391	ARG	CZ-NH2	-8.31	1.22	1.33
14	BD	257	ARG	CZ-NH2	-8.31	1.22	1.33
40	Bk	32	HIS	CD2-NE2	-8.30	1.28	1.37
7	B6	108	HIS	CE1-NE2	-8.30	1.24	1.32
40	Bk	76	HIS	CE1-NE2	-8.30	1.24	1.32
1	B0	54	ALA	CA-CB	-8.29	1.43	1.53
22	BL	65	HIS	CE1-NE2	-8.28	1.24	1.32
12	BB	282	ARG	CZ-NH2	-8.28	1.22	1.33
7	B6	32	HIS	ND1-CE1	-8.28	1.24	1.32
14	BD	387	ARG	CZ-NH2	-8.27	1.22	1.33
1	B0	34	ARG	CZ-NH2	-8.27	1.22	1.33
1	B0	268	ARG	CZ-NH2	-8.27	1.22	1.33
42	HJ	759	ARG	CZ-NH2	-8.27	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B6	111	HIS	CE1-NE2	-8.26	1.24	1.32
12	BB	230	ARG	CZ-NH2	-8.26	1.22	1.33
40	Bk	114	ARG	CZ-NH2	-8.26	1.22	1.33
1	B0	42	ARG	CZ-NH2	-8.25	1.22	1.33
14	BD	265	ARG	CZ-NH2	-8.25	1.22	1.33
42	HJ	639	ARG	CZ-NH2	-8.25	1.22	1.33
1	B0	273	ARG	CZ-NH2	-8.25	1.22	1.33
12	BB	670	ARG	CZ-NH2	-8.25	1.22	1.33
42	HJ	751	ARG	CZ-NH2	-8.25	1.22	1.33
14	BD	368	ARG	CZ-NH2	-8.24	1.22	1.33
14	BD	470	ARG	CZ-NH2	-8.24	1.22	1.33
30	BW	286	ARG	CZ-NH2	-8.24	1.22	1.33
38	Bh	3	HIS	ND1-CE1	-8.23	1.24	1.32
14	BD	207	ARG	CZ-NH2	-8.23	1.22	1.33
15	BE	492	ARG	CZ-NH2	-8.23	1.22	1.33
25	BQ	410	ARG	CZ-NH2	-8.23	1.22	1.33
7	B6	33	HIS	ND1-CE1	-8.23	1.24	1.32
15	BE	500	ALA	CA-CB	-8.23	1.42	1.53
18	BH	88	ARG	CZ-NH2	-8.23	1.22	1.33
7	B6	111	HIS	ND1-CE1	-8.23	1.24	1.32
1	B0	271	ARG	CZ-NH2	-8.22	1.22	1.33
38	Bh	129	ARG	CZ-NH2	-8.22	1.22	1.33
42	HJ	705	ARG	CZ-NH2	-8.22	1.22	1.33
4	B3	12	ARG	CZ-NH2	-8.22	1.22	1.33
12	BB	160	ARG	CZ-NH2	-8.22	1.22	1.33
1	B0	68	ALA	CA-CB	-8.22	1.42	1.53
1	B0	150	ARG	CZ-NH2	-8.22	1.22	1.33
42	HJ	741	ARG	CZ-NH2	-8.22	1.22	1.33
25	BQ	411	ARG	CZ-NH2	-8.22	1.22	1.33
41	Bl	3	ARG	CZ-NH2	-8.22	1.22	1.33
41	Bl	90	ARG	CZ-NH2	-8.22	1.22	1.33
42	HJ	685	ARG	CZ-NH2	-8.21	1.22	1.33
18	BH	67	ARG	CZ-NH2	-8.21	1.22	1.33
7	B6	108	HIS	ND1-CE1	-8.21	1.24	1.32
30	BW	322	ARG	CZ-NH2	-8.21	1.22	1.33
7	B6	32	HIS	CE1-NE2	-8.20	1.24	1.32
16	BF	21	ARG	CZ-NH2	-8.20	1.22	1.33
18	BH	86	ARG	CZ-NH2	-8.20	1.22	1.33
25	BQ	469	ARG	CZ-NH2	-8.20	1.22	1.33
42	HJ	730	ARG	CZ-NH2	-8.20	1.22	1.33
4	B3	13	ARG	CZ-NH2	-8.20	1.22	1.33
10	B9	59	ARG	CZ-NH2	-8.20	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	BH	64	ARG	CZ-NH2	-8.20	1.22	1.33
37	Bg	170	ARG	CZ-NH2	-8.20	1.22	1.33
14	BD	320	ARG	CZ-NH2	-8.19	1.22	1.33
16	BF	271	ARG	CZ-NH2	-8.20	1.22	1.33
16	BF	274	ARG	CZ-NH2	-8.20	1.22	1.33
37	Bg	97	ARG	CZ-NH2	-8.20	1.22	1.33
15	BE	394	ARG	CZ-NH2	-8.19	1.22	1.33
27	BT	37	HIS	CE1-NE2	-8.19	1.24	1.32
37	Bg	162	ARG	CZ-NH2	-8.19	1.22	1.33
16	BF	254	ARG	CZ-NH2	-8.19	1.22	1.33
7	B6	92	HIS	ND1-CE1	-8.19	1.24	1.32
15	BE	475	ARG	CZ-NH2	-8.19	1.22	1.33
37	Bg	219	ARG	CZ-NH2	-8.19	1.22	1.33
42	HJ	760	ARG	CZ-NH2	-8.19	1.22	1.33
38	Bh	3	HIS	CE1-NE2	-8.19	1.24	1.32
1	B0	264	ARG	CZ-NH2	-8.18	1.22	1.33
13	BC	43	ARG	CZ-NH2	-8.18	1.22	1.33
37	Bg	186	ARG	CZ-NH2	-8.17	1.22	1.33
30	BW	279	ARG	CZ-NH2	-8.16	1.22	1.33
13	BC	42	ARG	CZ-NH2	-8.15	1.22	1.33
1	B0	66	ALA	CA-CB	-8.15	1.41	1.52
16	BF	250	ARG	CZ-NH2	-8.15	1.22	1.33
3	B2	134	ARG	CZ-NH2	-8.15	1.22	1.33
40	Bk	76	HIS	ND1-CE1	-8.14	1.24	1.32
16	BF	33	ARG	CZ-NH2	-8.14	1.22	1.33
41	Bl	14	ARG	CZ-NH2	-8.14	1.22	1.33
16	BF	32	ARG	CZ-NH2	-8.13	1.22	1.33
30	BW	321	ARG	CZ-NH2	-8.13	1.22	1.33
1	B0	36	ARG	CZ-NH2	-8.12	1.22	1.33
12	BB	1125	ARG	CZ-NH2	-8.12	1.22	1.33
12	BB	340	ALA	CA-CB	-8.12	1.43	1.53
1	B0	43	ARG	CZ-NH2	-8.12	1.22	1.33
16	BF	259	ARG	CZ-NH2	-8.12	1.22	1.33
3	B2	47	HIS	ND1-CE1	-8.11	1.24	1.32
30	BW	324	ARG	CZ-NH2	-8.11	1.23	1.33
12	BB	309	HIS	CD2-NE2	-8.10	1.28	1.37
21	BK	89	ARG	CZ-NH2	-8.10	1.23	1.33
12	BB	1124	ARG	CZ-NH2	-8.09	1.23	1.33
3	B2	150	HIS	CE1-NE2	-8.08	1.24	1.32
1	B0	305	ARG	CZ-NH2	-8.08	1.23	1.33
12	BB	153	HIS	CD2-NE2	-8.08	1.28	1.37
30	BW	236	ARG	CZ-NH2	-8.08	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B3	211	HIS	ND1-CE1	-8.07	1.24	1.32
12	BB	151	HIS	CD2-NE2	-8.07	1.28	1.37
3	B2	47	HIS	CE1-NE2	-8.07	1.24	1.32
3	B2	157	HIS	CE1-NE2	-8.07	1.24	1.32
14	BD	33	HIS	CD2-NE2	-8.06	1.28	1.37
15	BE	478	HIS	CD2-NE2	-8.06	1.28	1.37
16	BF	35	HIS	CD2-NE2	-8.06	1.28	1.37
4	B3	211	HIS	CE1-NE2	-8.05	1.24	1.32
12	BB	426	ARG	CZ-NH2	-8.05	1.23	1.33
16	BF	260	HIS	CD2-NE2	-8.05	1.28	1.37
15	BE	327	ARG	CZ-NH2	-8.05	1.23	1.33
27	BT	37	HIS	ND1-CE1	-8.05	1.24	1.32
3	B2	150	HIS	ND1-CE1	-8.04	1.24	1.32
22	BL	65	HIS	ND1-CE1	-8.04	1.24	1.32
15	BE	508	HIS	CD2-NE2	-8.04	1.29	1.37
14	BD	131	ARG	CZ-NH2	-8.03	1.23	1.33
12	BB	170	HIS	CD2-NE2	-8.03	1.29	1.37
14	BD	251	HIS	CD2-NE2	-8.03	1.29	1.37
14	BD	373	HIS	CD2-NE2	-8.03	1.29	1.37
30	BW	290	HIS	CD2-NE2	-8.02	1.29	1.37
42	HJ	678	HIS	CD2-NE2	-8.02	1.29	1.37
12	BB	339	HIS	CD2-NE2	-8.02	1.29	1.37
16	BF	253	HIS	CD2-NE2	-8.02	1.29	1.37
3	B2	157	HIS	ND1-CE1	-8.01	1.24	1.32
12	BB	68	ARG	CZ-NH2	-8.01	1.23	1.33
25	BQ	204	ARG	CZ-NH2	-8.01	1.23	1.33
14	BD	392	HIS	CD2-NE2	-8.00	1.29	1.37
13	BC	203	ARG	CZ-NH2	-7.99	1.23	1.33
16	BF	251	HIS	CD2-NE2	-7.99	1.29	1.37
12	BB	39	HIS	CD2-NE2	-7.98	1.29	1.37
13	BC	208	ARG	CZ-NH2	-7.98	1.23	1.33
14	BD	318	HIS	CD2-NE2	-7.98	1.29	1.37
30	BW	210	ALA	CA-CB	-7.98	1.42	1.53
12	BB	150	HIS	CD2-NE2	-7.97	1.29	1.37
1	B0	47	HIS	CD2-NE2	-7.97	1.29	1.37
25	BQ	373	ARG	CZ-NH2	-7.96	1.23	1.33
37	Bg	51	HIS	CD2-NE2	-7.96	1.29	1.37
16	BF	31	HIS	CD2-NE2	-7.96	1.29	1.37
25	BQ	366	ARG	CZ-NH2	-7.94	1.23	1.33
30	BW	320	ARG	CZ-NH2	-7.92	1.23	1.33
21	BK	51	HIS	CD2-NE2	-7.91	1.29	1.37
14	BD	164	HIS	CD2-NE2	-7.91	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Bg	69	HIS	CD2-NE2	-7.88	1.29	1.37
12	BB	984	HIS	ND1-CE1	-7.86	1.24	1.32
30	BW	315	ARG	CZ-NH2	-7.86	1.23	1.33
37	Bg	180	HIS	CD2-NE2	-7.85	1.29	1.37
30	BW	336	ARG	CZ-NH2	-7.84	1.23	1.33
40	Bk	309	HIS	CD2-NE2	-7.84	1.29	1.37
15	BE	826	HIS	CD2-NE2	-7.83	1.29	1.37
37	Bg	84	HIS	CD2-NE2	-7.83	1.29	1.37
14	BD	93	ARG	CZ-NH2	-7.81	1.23	1.33
30	BW	147	ARG	CZ-NH2	-7.81	1.23	1.33
12	BB	984	HIS	CE1-NE2	-7.80	1.24	1.32
37	Bg	89	ARG	CZ-NH2	-7.78	1.23	1.33
37	Bg	176	ARG	CZ-NH2	-7.76	1.23	1.33
12	BB	32	ARG	CZ-NH2	-7.75	1.23	1.33
12	BB	61	ARG	CZ-NH2	-7.75	1.23	1.33
14	BD	457	HIS	CE1-NE2	-7.70	1.24	1.32
7	B6	111	HIS	CD2-NE2	-7.65	1.29	1.37
12	BB	1153	ARG	CZ-NH2	-7.65	1.23	1.33
12	BB	839	HIS	ND1-CE1	-7.64	1.25	1.32
7	B6	108	HIS	CD2-NE2	-7.62	1.29	1.37
12	BB	839	HIS	CE1-NE2	-7.62	1.25	1.32
12	BB	1019	HIS	CE1-NE2	-7.61	1.25	1.32
7	B6	32	HIS	CD2-NE2	-7.60	1.29	1.37
27	BT	44	ARG	CZ-NH2	-7.59	1.23	1.33
7	B6	92	HIS	CD2-NE2	-7.59	1.29	1.37
14	BD	457	HIS	ND1-CE1	-7.58	1.25	1.32
12	BB	1019	HIS	ND1-CE1	-7.57	1.25	1.32
37	Bg	222	ALA	CA-CB	-7.56	1.42	1.53
7	B6	33	HIS	CD2-NE2	-7.54	1.29	1.37
43	HS	34	ALA	CA-CB	-7.52	1.43	1.54
3	B2	157	HIS	CD2-NE2	-7.51	1.29	1.37
3	B2	150	HIS	CD2-NE2	-7.48	1.29	1.37
22	BL	65	HIS	CD2-NE2	-7.48	1.29	1.37
14	BD	463	ALA	CA-CB	-7.48	1.43	1.54
27	BT	37	HIS	CD2-NE2	-7.47	1.29	1.37
16	BF	18	GLY	N-CA	-7.47	1.37	1.45
12	BB	428	ALA	CA-CB	-7.45	1.43	1.52
14	BD	239	ALA	CA-CB	-7.44	1.42	1.53
40	Bk	76	HIS	CD2-NE2	-7.43	1.29	1.37
38	Bh	3	HIS	CD2-NE2	-7.43	1.29	1.37
3	B2	47	HIS	CD2-NE2	-7.43	1.29	1.37
37	Bg	223	GLY	N-CA	-7.42	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B3	211	HIS	CD2-NE2	-7.41	1.29	1.37
30	BW	251	ALA	CA-CB	-7.37	1.43	1.52
18	BH	60	ALA	CA-CB	-7.27	1.42	1.53
12	BB	984	HIS	CD2-NE2	-7.23	1.29	1.37
15	BE	829	ARG	CZ-NH2	-7.22	1.24	1.33
37	Bg	185	GLY	N-CA	-7.19	1.38	1.45
15	BE	841	ARG	CZ-NH2	-7.18	1.24	1.33
14	BD	441	ALA	CA-CB	-7.16	1.42	1.53
14	BD	394	ALA	CA-CB	-7.15	1.42	1.53
14	BD	236	ALA	CA-CB	-7.12	1.42	1.53
12	BB	231	ALA	CA-CB	-7.11	1.42	1.53
12	BB	1153	ARG	CZ-NH1	-7.10	1.22	1.32
1	B0	149	ALA	CA-CB	-7.09	1.42	1.53
12	BB	312	ALA	CA-CB	-7.08	1.42	1.53
1	B0	39	ALA	CA-CB	-7.08	1.42	1.53
15	BE	765	ARG	CZ-NH2	-7.06	1.24	1.33
12	BB	164	ALA	CA-CB	-7.04	1.42	1.53
15	BE	497	ALA	CA-CB	-7.04	1.42	1.53
14	BD	376	ALA	CA-CB	-7.04	1.42	1.53
12	BB	1019	HIS	CD2-NE2	-7.04	1.30	1.37
15	BE	560	ARG	CZ-NH2	-7.03	1.24	1.33
30	BW	284	ALA	CA-CB	-7.03	1.42	1.53
15	BE	472	ALA	CA-CB	-7.02	1.42	1.53
12	BB	167	ALA	CA-CB	-7.02	1.42	1.53
15	BE	509	ALA	CA-CB	-7.01	1.42	1.53
14	BD	457	HIS	CD2-NE2	-7.01	1.30	1.37
15	BE	504	ALA	CA-CB	-7.01	1.42	1.53
7	B6	34	GLY	N-CA	-7.00	1.38	1.45
15	BE	393	ALA	CA-CB	-6.98	1.42	1.53
14	BD	209	ALA	CA-CB	-6.98	1.42	1.53
25	BQ	182	ALA	CA-CB	-6.98	1.43	1.53
15	BE	503	ALA	CA-CB	-6.97	1.42	1.53
12	BB	839	HIS	CD2-NE2	-6.97	1.30	1.37
15	BE	491	ALA	CA-CB	-6.96	1.42	1.53
14	BD	167	ALA	CA-CB	-6.95	1.43	1.53
12	BB	310	ALA	CA-CB	-6.93	1.42	1.53
30	BW	333	GLY	N-CA	-6.91	1.38	1.45
15	BE	473	ALA	CA-CB	-6.91	1.42	1.53
27	BT	20	GLY	N-CA	-6.90	1.38	1.44
15	BE	412	ALA	CA-CB	-6.90	1.42	1.53
16	BF	244	ALA	CA-CB	-6.89	1.42	1.53
1	B0	56	ALA	CA-CB	-6.86	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	HS	42	PRO	CA-CB	-6.85	1.47	1.53
14	BD	314	ALA	CA-CB	-6.84	1.42	1.53
14	BD	205	ALA	CA-CB	-6.81	1.42	1.53
14	BD	99	ALA	CA-CB	-6.80	1.42	1.53
12	BB	266	ALA	CA-CB	-6.74	1.42	1.53
40	Bk	51	ARG	CZ-NH2	-6.74	1.24	1.33
12	BB	230	ARG	CZ-NH1	-6.74	1.23	1.32
27	BT	59	ARG	CZ-NH2	-6.74	1.24	1.33
14	BD	467	ALA	CA-CB	-6.74	1.42	1.53
40	Bk	34	ARG	CZ-NH2	-6.72	1.24	1.33
12	BB	282	ARG	CZ-NH1	-6.72	1.23	1.32
39	Bi	128	ARG	CZ-NH2	-6.71	1.24	1.33
12	BB	338	ALA	CA-CB	-6.71	1.42	1.52
27	BT	79	ARG	CZ-NH2	-6.71	1.24	1.33
1	B0	42	ARG	CZ-NH1	-6.70	1.23	1.32
14	BD	391	ARG	CZ-NH1	-6.70	1.23	1.32
14	BD	250	ALA	CA-CB	-6.70	1.42	1.53
42	HJ	705	ARG	CZ-NH1	-6.70	1.23	1.32
40	Bk	30	ARG	CZ-NH2	-6.69	1.24	1.33
25	BQ	411	ARG	CZ-NH1	-6.69	1.23	1.32
37	Bg	219	ARG	CZ-NH1	-6.69	1.23	1.32
14	BD	387	ARG	CZ-NH1	-6.68	1.23	1.32
25	BQ	375	ALA	CA-CB	-6.68	1.43	1.53
18	BH	64	ARG	CZ-NH1	-6.68	1.23	1.32
14	BD	458	ARG	CZ-NH1	-6.68	1.23	1.32
11	BA	509	HIS	ND1-CE1	-6.68	1.25	1.32
4	B3	12	ARG	CZ-NH1	-6.67	1.23	1.32
14	BD	199	ARG	CZ-NH1	-6.67	1.23	1.32
11	BA	509	HIS	CE1-NE2	-6.67	1.25	1.32
12	BB	670	ARG	CZ-NH1	-6.67	1.23	1.32
18	BH	86	ARG	CZ-NH1	-6.67	1.23	1.32
25	BQ	379	ALA	CA-CB	-6.67	1.43	1.53
25	BQ	410	ARG	CZ-NH1	-6.67	1.23	1.32
15	BE	394	ARG	CZ-NH1	-6.66	1.23	1.32
25	BQ	378	ALA	CA-CB	-6.66	1.43	1.53
14	BD	265	ARG	CZ-NH1	-6.66	1.23	1.32
13	BC	42	ARG	CZ-NH1	-6.66	1.23	1.32
42	HJ	759	ARG	CZ-NH1	-6.66	1.23	1.32
14	BD	470	ARG	CZ-NH1	-6.65	1.23	1.32
25	BQ	388	ALA	CA-CB	-6.65	1.43	1.53
30	BW	279	ARG	CZ-NH1	-6.65	1.23	1.32
30	BW	321	ARG	CZ-NH1	-6.65	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	Bl	3	ARG	CZ-NH1	-6.65	1.23	1.32
12	BB	160	ARG	CZ-NH1	-6.65	1.23	1.32
25	BQ	469	ARG	CZ-NH1	-6.65	1.23	1.32
41	Bl	14	ARG	CZ-NH1	-6.65	1.23	1.32
16	BF	21	ARG	CZ-NH1	-6.65	1.23	1.32
42	HJ	730	ARG	CZ-NH1	-6.65	1.23	1.32
1	B0	273	ARG	CZ-NH1	-6.65	1.23	1.32
1	B0	150	ARG	CZ-NH1	-6.64	1.23	1.32
27	BT	62	ARG	CZ-NH2	-6.64	1.24	1.33
42	HJ	751	ARG	CZ-NH1	-6.64	1.23	1.32
1	B0	268	ARG	CZ-NH1	-6.64	1.23	1.32
1	B0	271	ARG	CZ-NH1	-6.64	1.23	1.32
14	BD	257	ARG	CZ-NH1	-6.64	1.23	1.32
12	BB	1139	ALA	CA-CB	-6.64	1.43	1.53
3	B2	134	ARG	CZ-NH1	-6.64	1.23	1.32
15	BE	475	ARG	CZ-NH1	-6.64	1.23	1.32
15	BE	492	ARG	CZ-NH1	-6.64	1.23	1.32
16	BF	33	ARG	CZ-NH1	-6.64	1.23	1.32
18	BH	67	ARG	CZ-NH1	-6.64	1.23	1.32
25	BQ	385	ALA	CA-CB	-6.63	1.43	1.53
38	Bh	129	ARG	CZ-NH1	-6.63	1.23	1.32
42	HJ	639	ARG	CZ-NH1	-6.63	1.23	1.32
4	B3	13	ARG	CZ-NH1	-6.63	1.23	1.32
42	HJ	760	ARG	CZ-NH1	-6.63	1.23	1.32
16	BF	254	ARG	CZ-NH1	-6.63	1.23	1.32
21	BK	89	ARG	CZ-NH1	-6.63	1.23	1.32
1	B0	305	ARG	CZ-NH1	-6.62	1.23	1.32
14	BD	320	ARG	CZ-NH1	-6.62	1.23	1.32
25	BQ	312	ALA	CA-CB	-6.62	1.43	1.53
10	B9	59	ARG	CZ-NH1	-6.62	1.23	1.32
37	Bg	186	ARG	CZ-NH1	-6.62	1.23	1.32
42	HJ	685	ARG	CZ-NH1	-6.62	1.23	1.32
42	HJ	741	ARG	CZ-NH1	-6.62	1.23	1.32
30	BW	322	ARG	CZ-NH1	-6.62	1.23	1.32
14	BD	207	ARG	CZ-NH1	-6.61	1.23	1.32
16	BF	271	ARG	CZ-NH1	-6.61	1.23	1.32
37	Bg	170	ARG	CZ-NH1	-6.61	1.23	1.32
16	BF	32	ARG	CZ-NH1	-6.61	1.23	1.32
41	Bl	90	ARG	CZ-NH1	-6.61	1.23	1.32
37	Bg	97	ARG	CZ-NH1	-6.61	1.23	1.32
37	Bg	162	ARG	CZ-NH1	-6.61	1.23	1.32
16	BF	259	ARG	CZ-NH1	-6.61	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BQ	342	ALA	CA-CB	-6.61	1.43	1.53
1	B0	34	ARG	CZ-NH1	-6.59	1.23	1.32
37	Bg	91	ALA	CA-CB	-6.59	1.42	1.53
40	Bk	114	ARG	CZ-NH1	-6.59	1.23	1.32
14	BD	368	ARG	CZ-NH1	-6.59	1.23	1.32
18	BH	88	ARG	CZ-NH1	-6.59	1.23	1.32
16	BF	274	ARG	CZ-NH1	-6.59	1.23	1.32
1	B0	36	ARG	CZ-NH1	-6.59	1.23	1.32
1	B0	171	ARG	CZ-NH2	-6.59	1.24	1.33
15	BE	511	ALA	CA-CB	-6.59	1.42	1.53
25	BQ	384	ALA	CA-CB	-6.58	1.43	1.53
16	BF	250	ARG	CZ-NH1	-6.57	1.23	1.32
13	BC	43	ARG	CZ-NH1	-6.57	1.23	1.32
25	BQ	349	ALA	CA-CB	-6.57	1.43	1.53
30	BW	309	ALA	CA-CB	-6.57	1.43	1.53
1	B0	43	ARG	CZ-NH1	-6.56	1.23	1.32
30	BW	222	HIS	CE1-NE2	-6.56	1.25	1.32
30	BW	324	ARG	CZ-NH1	-6.55	1.23	1.32
42	HJ	746	ALA	CA-CB	-6.55	1.42	1.53
12	BB	163	ALA	CA-CB	-6.55	1.43	1.53
30	BW	286	ARG	CZ-NH1	-6.55	1.23	1.32
25	BQ	382	ALA	CA-CB	-6.54	1.43	1.53
1	B0	242	ARG	CZ-NH2	-6.54	1.25	1.33
1	B0	249	ARG	CZ-NH2	-6.54	1.25	1.33
1	B0	264	ARG	CZ-NH1	-6.53	1.23	1.32
30	BW	222	HIS	ND1-CE1	-6.53	1.26	1.32
25	BQ	341	ALA	CA-CB	-6.53	1.43	1.53
1	B0	165	ARG	CZ-NH2	-6.53	1.25	1.33
1	B0	181	ARG	CZ-NH2	-6.52	1.25	1.33
30	BW	236	ARG	CZ-NH1	-6.52	1.23	1.32
30	BW	327	ALA	CA-CB	-6.52	1.43	1.53
1	B0	294	ARG	CZ-NH2	-6.52	1.25	1.33
12	BB	157	ALA	CA-CB	-6.52	1.42	1.53
1	B0	241	ARG	CZ-NH2	-6.50	1.25	1.33
12	BB	77	ALA	CA-CB	-6.49	1.42	1.53
14	BD	241	ALA	CA-CB	-6.49	1.43	1.53
14	BD	474	ALA	CA-CB	-6.48	1.42	1.53
12	BB	426	ARG	CZ-NH1	-6.46	1.23	1.32
15	BE	327	ARG	CZ-NH1	-6.46	1.23	1.32
12	BB	68	ARG	CZ-NH1	-6.46	1.23	1.32
12	BB	1125	ARG	CZ-NH1	-6.46	1.23	1.32
14	BD	131	ARG	CZ-NH1	-6.46	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BB	1124	ARG	CZ-NH1	-6.44	1.23	1.32
1	B0	60	ALA	CA-CB	-6.44	1.42	1.53
25	BQ	366	ARG	CZ-NH1	-6.43	1.23	1.32
15	BE	495	LEU	N-CA	-6.42	1.41	1.46
25	BQ	138	GLY	CA-C	-6.42	1.47	1.52
25	BQ	286	ALA	CA-CB	-6.42	1.43	1.53
25	BQ	204	ARG	CZ-NH1	-6.42	1.23	1.32
13	BC	203	ARG	CZ-NH1	-6.41	1.23	1.32
13	BC	208	ARG	CZ-NH1	-6.41	1.23	1.32
25	BQ	373	ARG	CZ-NH1	-6.38	1.23	1.32
30	BW	336	ARG	CZ-NH1	-6.35	1.23	1.32
14	BD	258	ALA	CA-CB	-6.35	1.42	1.53
14	BD	385	ALA	CA-CB	-6.35	1.42	1.53
14	BD	36	ALA	CA-CB	-6.34	1.43	1.53
30	BW	147	ARG	CZ-NH1	-6.33	1.23	1.32
12	BB	1143	ALA	CA-CB	-6.33	1.43	1.53
14	BD	35	GLY	N-CA	-6.32	1.38	1.45
1	B0	2	PRO	CA-CB	-6.31	1.48	1.53
42	HJ	703	VAL	N-CA	-6.30	1.41	1.46
30	BW	315	ARG	CZ-NH1	-6.29	1.24	1.32
1	B0	259	ALA	CA-CB	-6.29	1.42	1.53
30	BW	320	ARG	CZ-NH1	-6.28	1.24	1.32
37	Bg	89	ARG	CZ-NH1	-6.26	1.24	1.32
40	Bk	38	GLY	N-CA	-6.26	1.38	1.45
15	BE	544	ALA	CA-CB	-6.25	1.43	1.53
15	BE	409	GLY	N-CA	-6.25	1.38	1.45
46	b3	3	U	P-OP1	6.25	1.61	1.49
65	bV	1	U	P-OP1	6.24	1.61	1.49
42	HJ	604	ARG	CZ-NH2	-6.24	1.25	1.33
12	BB	61	ARG	CZ-NH1	-6.23	1.24	1.32
14	BD	93	ARG	CZ-NH1	-6.23	1.24	1.32
37	Bg	176	ARG	CZ-NH1	-6.23	1.24	1.32
46	b3	4	U	P-OP1	6.22	1.61	1.49
15	BE	845	ARG	CZ-NH2	-6.22	1.25	1.33
65	bV	6	U	P-OP1	6.22	1.61	1.49
30	BW	206	GLY	N-CA	-6.19	1.38	1.45
37	Bg	181	ALA	CA-CB	-6.17	1.43	1.53
12	BB	32	ARG	CZ-NH1	-6.16	1.24	1.32
11	BA	509	HIS	CD2-NE2	-6.16	1.31	1.37
7	B6	45	ARG	CZ-NH2	-6.15	1.25	1.33
14	BD	389	ALA	CA-CB	-6.15	1.42	1.53
14	BD	372	ALA	CA-CB	-6.15	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BB	279	ALA	CA-CB	-6.13	1.42	1.53
23	BO	49	ARG	CZ-NH2	-6.11	1.25	1.33
7	B6	91	ARG	CZ-NH2	-6.11	1.25	1.33
7	B6	12	ARG	CZ-NH2	-6.11	1.25	1.33
40	Bk	236	ARG	CZ-NH2	-6.10	1.25	1.33
15	BE	397	ALA	CA-CB	-6.10	1.42	1.53
12	BB	281	ALA	CA-CB	-6.09	1.42	1.53
11	BA	129	ARG	CZ-NH2	-6.09	1.25	1.33
7	B6	63	ARG	CZ-NH2	-6.07	1.25	1.33
27	BT	44	ARG	CZ-NH1	-6.06	1.24	1.32
16	BF	275	ILE	CA-CB	-6.06	1.51	1.54
14	BD	466	ALA	CA-CB	-6.04	1.42	1.53
15	BE	483	GLY	N-CA	-6.01	1.38	1.45
39	Bi	86	ARG	CZ-NH2	-5.99	1.25	1.33
25	BQ	506	ARG	CZ-NH2	-5.98	1.25	1.33
30	BW	101	ARG	CZ-NH2	-5.98	1.25	1.33
25	BQ	499	ARG	CZ-NH2	-5.98	1.25	1.33
30	BW	222	HIS	CD2-NE2	-5.97	1.31	1.37
1	B0	35	GLY	N-CA	-5.97	1.38	1.45
22	BL	45	ARG	CZ-NH2	-5.96	1.25	1.33
40	Bk	16	ARG	CZ-NH2	-5.95	1.25	1.33
25	BQ	68	ARG	CZ-NH2	-5.95	1.25	1.33
4	B3	220	ARG	CZ-NH2	-5.94	1.25	1.33
39	Bi	83	ARG	CZ-NH2	-5.93	1.25	1.33
27	BT	14	ARG	CZ-NH2	-5.93	1.25	1.33
22	BL	78	ARG	CZ-NH2	-5.92	1.25	1.33
22	BL	96	ARG	CZ-NH2	-5.92	1.25	1.33
15	BE	606	ALA	CA-CB	-5.91	1.44	1.53
3	B2	148	ARG	CZ-NH2	-5.89	1.25	1.33
4	B3	214	ARG	CZ-NH2	-5.89	1.25	1.33
3	B2	95	ARG	CZ-NH2	-5.89	1.25	1.33
14	BD	240	ALA	CA-CB	-5.89	1.43	1.54
14	BD	39	GLY	N-CA	-5.89	1.38	1.45
22	BL	85	ARG	CZ-NH2	-5.88	1.25	1.33
4	B3	221	ARG	CZ-NH2	-5.88	1.25	1.33
3	B2	108	ARG	CZ-NH2	-5.88	1.25	1.33
4	B3	216	ARG	CZ-NH2	-5.88	1.25	1.33
15	BE	523	ARG	CZ-NH2	-5.87	1.25	1.33
3	B2	4	ARG	CZ-NH2	-5.87	1.25	1.33
27	BT	19	ALA	CA-CB	-5.86	1.45	1.52
12	BB	1152	ALA	CA-CB	-5.85	1.43	1.53
3	B2	46	ARG	CZ-NH2	-5.84	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B2	91	ARG	CZ-NH2	-5.84	1.25	1.33
15	BE	534	ARG	CZ-NH2	-5.83	1.25	1.33
3	B2	145	ARG	CZ-NH2	-5.83	1.25	1.33
3	B2	133	ARG	CZ-NH2	-5.83	1.25	1.33
12	BB	948	ARG	CZ-NH2	-5.81	1.25	1.33
14	BD	17	ARG	CZ-NH2	-5.80	1.25	1.33
12	BB	1108	ARG	CZ-NH2	-5.79	1.25	1.33
12	BB	952	ARG	CZ-NH2	-5.79	1.25	1.33
14	BD	151	ARG	CZ-NH2	-5.79	1.25	1.33
1	B0	57	GLU	N-CA	-5.77	1.41	1.46
37	Bg	58	ARG	CZ-NH2	-5.77	1.25	1.33
12	BB	1111	ARG	CZ-NH2	-5.77	1.25	1.33
14	BD	3	ARG	CZ-NH2	-5.76	1.25	1.33
12	BB	947	ARG	CZ-NH2	-5.76	1.25	1.33
12	BB	981	ARG	CZ-NH2	-5.76	1.25	1.33
12	BB	963	ARG	CZ-NH2	-5.75	1.25	1.33
14	BD	459	GLY	N-CA	-5.75	1.38	1.45
37	Bg	59	ARG	CZ-NH2	-5.75	1.25	1.33
12	BB	1007	ARG	CZ-NH2	-5.75	1.25	1.33
12	BB	1112	ARG	CZ-NH2	-5.74	1.25	1.33
15	BE	829	ARG	CZ-NH1	-5.74	1.24	1.32
15	BE	841	ARG	CZ-NH1	-5.73	1.24	1.32
42	HJ	614	HIS	ND1-CE1	-5.70	1.26	1.32
12	BB	983	ARG	CZ-NH2	-5.69	1.26	1.33
12	BB	1011	ALA	CA-CB	-5.67	1.44	1.53
18	BH	92	GLY	N-CA	-5.67	1.37	1.45
42	HJ	614	HIS	CE1-NE2	-5.65	1.26	1.32
58	bO	11	U	C2'-O2'	-5.62	1.34	1.42
12	BB	1022	ARG	CZ-NH2	-5.58	1.26	1.33
15	BE	560	ARG	CZ-NH1	-5.57	1.25	1.32
12	BB	230	ARG	CD-NE	-5.56	1.38	1.46
18	BH	86	ARG	CD-NE	-5.56	1.38	1.46
15	BE	765	ARG	CZ-NH1	-5.55	1.25	1.32
40	Bk	279	VAL	N-CA	-5.55	1.42	1.46
40	Bk	114	ARG	CD-NE	-5.54	1.38	1.46
14	BD	265	ARG	CD-NE	-5.54	1.38	1.46
16	BF	250	ARG	CD-NE	-5.54	1.38	1.46
41	Bl	91	GLY	N-CA	-5.53	1.37	1.45
14	BD	458	ARG	CD-NE	-5.52	1.38	1.46
4	B3	13	ARG	CD-NE	-5.51	1.38	1.46
14	BD	216	ARG	CZ-NH2	-5.51	1.26	1.33
16	BF	32	ARG	CD-NE	-5.51	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B0	264	ARG	CD-NE	-5.51	1.38	1.46
41	Bl	3	ARG	CD-NE	-5.50	1.38	1.46
42	HJ	710	GLY	N-CA	-5.50	1.37	1.45
42	HJ	741	ARG	CD-NE	-5.49	1.38	1.46
18	BH	67	ARG	CD-NE	-5.49	1.38	1.46
25	BQ	204	ARG	CD-NE	-5.49	1.38	1.46
30	BW	160	GLY	N-CA	-5.49	1.40	1.45
4	B3	12	ARG	CD-NE	-5.48	1.38	1.46
15	BE	475	ARG	CD-NE	-5.48	1.38	1.46
12	BB	1125	ARG	CD-NE	-5.46	1.38	1.46
15	BE	327	ARG	CD-NE	-5.46	1.38	1.46
41	Bl	90	ARG	CD-NE	-5.46	1.38	1.46
16	BF	21	ARG	CD-NE	-5.45	1.38	1.46
18	BH	88	ARG	CD-NE	-5.45	1.38	1.46
30	BW	236	ARG	CD-NE	-5.45	1.38	1.46
42	HJ	705	ARG	CD-NE	-5.45	1.38	1.46
1	B0	34	ARG	CD-NE	-5.44	1.38	1.46
21	BK	89	ARG	CD-NE	-5.44	1.38	1.46
37	Bg	97	ARG	CD-NE	-5.44	1.38	1.46
37	Bg	219	ARG	CD-NE	-5.44	1.38	1.46
1	B0	42	ARG	CD-NE	-5.43	1.38	1.46
15	BE	415	ASP	CA-CB	-5.43	1.47	1.53
12	BB	1124	ARG	CD-NE	-5.43	1.38	1.46
39	Bi	89	ALA	CA-CB	-5.43	1.45	1.53
14	BD	131	ARG	CD-NE	-5.43	1.38	1.46
1	B0	43	ARG	CD-NE	-5.42	1.38	1.46
7	B6	71	ALA	CA-CB	-5.42	1.46	1.53
30	BW	293	GLY	N-CA	-5.42	1.38	1.45
7	B6	62	GLY	N-CA	-5.42	1.39	1.45
14	BD	470	ARG	CD-NE	-5.42	1.38	1.46
15	BE	500	ALA	N-CA	-5.42	1.41	1.46
30	BW	336	ARG	CD-NE	-5.41	1.38	1.46
25	BQ	411	ARG	CD-NE	-5.41	1.38	1.46
3	B2	134	ARG	CD-NE	-5.40	1.38	1.46
30	BW	324	ARG	CD-NE	-5.39	1.38	1.46
16	BF	271	ARG	CD-NE	-5.39	1.38	1.46
37	Bg	51	HIS	CA-CB	-5.39	1.47	1.53
14	BD	320	ARG	CD-NE	-5.38	1.38	1.46
37	Bg	186	ARG	CD-NE	-5.38	1.38	1.46
42	HJ	760	ARG	CD-NE	-5.38	1.38	1.46
13	BC	44	TYR	CA-CB	-5.38	1.47	1.53
40	Bk	237	GLY	N-CA	-5.38	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	BF	254	ARG	CD-NE	-5.37	1.38	1.46
30	BW	147	ARG	CD-NE	-5.37	1.38	1.46
38	Bh	129	ARG	CD-NE	-5.37	1.38	1.46
12	BB	302	GLY	N-CA	-5.35	1.38	1.45
14	BD	384	ALA	CA-CB	-5.35	1.43	1.53
1	B0	305	ARG	CD-NE	-5.34	1.38	1.46
15	BE	598	HIS	CE1-NE2	-5.33	1.27	1.32
12	BB	968	LEU	N-CA	-5.33	1.42	1.46
30	BW	321	ARG	CD-NE	-5.30	1.38	1.46
3	B2	90	PRO	CA-CB	-5.29	1.48	1.53
15	BE	598	HIS	ND1-CE1	-5.29	1.27	1.32
13	BC	43	ARG	CD-NE	-5.29	1.38	1.46
25	BQ	366	ARG	CD-NE	-5.29	1.38	1.46
41	Bl	14	ARG	CD-NE	-5.29	1.38	1.46
27	BT	46	ALA	CA-CB	-5.29	1.45	1.53
37	Bg	89	ARG	CD-NE	-5.29	1.38	1.46
1	B0	273	ARG	CD-NE	-5.28	1.38	1.46
40	Bk	41	ALA	CA-CB	-5.28	1.45	1.53
41	Bl	14	ARG	N-CA	-5.27	1.41	1.46
42	HJ	639	ARG	CD-NE	-5.26	1.38	1.46
27	BT	62	ARG	CZ-NH1	-5.26	1.25	1.32
4	B3	100	HIS	ND1-CE1	-5.26	1.27	1.32
40	Bk	30	ARG	CZ-NH1	-5.26	1.25	1.32
12	BB	32	ARG	CD-NE	-5.25	1.39	1.46
14	BD	199	ARG	CD-NE	-5.25	1.39	1.46
16	BF	259	ARG	CD-NE	-5.24	1.39	1.46
30	BW	322	ARG	CD-NE	-5.24	1.39	1.46
1	B0	70	GLY	N-CA	-5.24	1.37	1.45
40	Bk	34	ARG	CZ-NH1	-5.24	1.25	1.32
5	B4	10	HIS	CE1-NE2	-5.24	1.27	1.32
12	BB	670	ARG	CD-NE	-5.24	1.39	1.46
14	BD	207	ARG	CD-NE	-5.23	1.39	1.46
25	BQ	469	ARG	CD-NE	-5.23	1.39	1.46
39	Bi	128	ARG	CZ-NH1	-5.23	1.25	1.32
13	BC	42	ARG	CD-NE	-5.23	1.39	1.46
15	BE	394	ARG	CD-NE	-5.23	1.39	1.46
42	HJ	685	ARG	CD-NE	-5.23	1.39	1.46
1	B0	36	ARG	CD-NE	-5.22	1.39	1.46
1	B0	268	ARG	CD-NE	-5.22	1.39	1.46
14	BD	387	ARG	CD-NE	-5.22	1.39	1.46
16	BF	33	ARG	CD-NE	-5.22	1.39	1.46
1	B0	271	ARG	CD-NE	-5.21	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B9	59	ARG	CD-NE	-5.21	1.39	1.46
14	BD	368	ARG	CD-NE	-5.21	1.39	1.46
27	BT	79	ARG	CZ-NH1	-5.21	1.25	1.32
37	Bg	170	ARG	CD-NE	-5.21	1.39	1.46
14	BD	391	ARG	CD-NE	-5.21	1.39	1.46
12	BB	160	ARG	CD-NE	-5.21	1.39	1.46
25	BQ	322	GLY	N-CA	-5.21	1.37	1.45
25	BQ	205	GLY	N-CA	-5.21	1.38	1.45
40	Bk	56	ALA	CA-CB	-5.21	1.45	1.53
42	HJ	751	ARG	CD-NE	-5.21	1.39	1.46
11	BA	442	ARG	CZ-NH2	-5.20	1.26	1.33
16	BF	241	LEU	CA-CB	-5.20	1.47	1.53
25	BQ	373	ARG	CD-NE	-5.20	1.39	1.46
40	Bk	51	ARG	CZ-NH1	-5.20	1.25	1.32
12	BB	1153	ARG	CD-NE	-5.20	1.39	1.46
15	BE	829	ARG	CD-NE	-5.20	1.39	1.46
40	Bk	30	ARG	CD-NE	-5.20	1.39	1.46
30	BW	286	ARG	CD-NE	-5.20	1.39	1.46
15	BE	492	ARG	CD-NE	-5.20	1.39	1.46
15	BE	841	ARG	CD-NE	-5.20	1.39	1.46
42	HJ	730	ARG	CD-NE	-5.20	1.39	1.46
42	HJ	614	HIS	CD2-NE2	-5.19	1.32	1.37
25	BQ	410	ARG	CD-NE	-5.19	1.39	1.46
12	BB	282	ARG	CD-NE	-5.19	1.39	1.46
30	BW	165	ARG	CZ-NH2	-5.19	1.26	1.33
3	B2	89	ALA	CA-CB	-5.18	1.46	1.54
37	Bg	90	GLY	N-CA	-5.18	1.38	1.45
1	B0	175	ALA	CA-CB	-5.18	1.45	1.53
4	B3	100	HIS	CE1-NE2	-5.18	1.27	1.32
27	BT	59	ARG	CZ-NH1	-5.18	1.25	1.32
37	Bg	162	ARG	CD-NE	-5.18	1.39	1.46
16	BF	274	ARG	CD-NE	-5.18	1.39	1.46
18	BH	64	ARG	CD-NE	-5.17	1.39	1.46
42	HJ	759	ARG	CD-NE	-5.17	1.39	1.46
12	BB	426	ARG	CD-NE	-5.17	1.39	1.46
1	B0	294	ARG	CD-NE	-5.17	1.39	1.46
5	B4	10	HIS	ND1-CE1	-5.17	1.27	1.32
30	BW	279	ARG	CD-NE	-5.17	1.39	1.46
12	BB	280	GLY	N-CA	-5.17	1.37	1.45
15	BE	389	GLY	N-CA	-5.16	1.37	1.45
14	BD	257	ARG	CD-NE	-5.16	1.39	1.46
27	BT	59	ARG	CD-NE	-5.16	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BC	203	ARG	CD-NE	-5.15	1.39	1.46
11	BA	448	ARG	CZ-NH2	-5.15	1.26	1.33
1	B0	179	ALA	CA-CB	-5.15	1.45	1.53
27	BT	48	GLY	N-CA	-5.15	1.38	1.45
1	B0	150	ARG	CD-NE	-5.15	1.39	1.46
13	BC	208	ARG	CD-NE	-5.15	1.39	1.46
11	BA	449	ARG	CZ-NH2	-5.14	1.26	1.33
30	BW	162	ARG	CZ-NH2	-5.14	1.26	1.33
11	BA	425	ARG	CZ-NH2	-5.14	1.26	1.33
1	B0	181	ARG	CD-NE	-5.14	1.39	1.46
55	bK	3	A	C6-N6	-5.14	1.23	1.33
30	BW	161	ARG	CZ-NH2	-5.13	1.26	1.33
30	BW	290	HIS	CA-CB	-5.13	1.47	1.53
25	BQ	138	GLY	N-CA	-5.13	1.38	1.45
30	BW	320	ARG	CD-NE	-5.13	1.39	1.46
27	BT	44	ARG	CD-NE	-5.13	1.39	1.46
11	BA	446	ARG	CZ-NH2	-5.12	1.26	1.33
1	B0	249	ARG	CZ-NH1	-5.12	1.25	1.32
30	BW	179	ARG	CZ-NH2	-5.12	1.26	1.33
1	B0	294	ARG	CZ-NH1	-5.12	1.25	1.32
29	BV	257	ARG	CZ-NH2	-5.12	1.26	1.33
11	BA	483	ARG	CZ-NH2	-5.12	1.26	1.33
30	BW	315	ARG	CD-NE	-5.11	1.39	1.46
37	Bg	169	PRO	CA-CB	-5.11	1.46	1.53
12	BB	68	ARG	CD-NE	-5.11	1.39	1.46
1	B0	251	GLY	N-CA	-5.11	1.38	1.45
11	BA	473	ARG	CZ-NH2	-5.10	1.26	1.33
15	BE	560	ARG	CD-NE	-5.10	1.39	1.46
16	BF	235	ALA	CA-CB	-5.09	1.45	1.53
1	B0	165	ARG	CD-NE	-5.09	1.39	1.46
40	Bk	39	ALA	CA-CB	-5.09	1.45	1.53
37	Bg	176	ARG	CD-NE	-5.09	1.39	1.46
1	B0	241	ARG	CD-NE	-5.08	1.39	1.46
1	B0	181	ARG	CZ-NH1	-5.08	1.25	1.32
12	BB	61	ARG	CD-NE	-5.08	1.39	1.46
42	HJ	718	LEU	N-CA	-5.08	1.41	1.46
37	Bg	10	GLY	N-CA	-5.08	1.38	1.45
3	B2	156	GLY	N-CA	-5.08	1.39	1.45
58	bO	6	C	C4-N4	-5.07	1.23	1.33
1	B0	242	ARG	CZ-NH1	-5.07	1.25	1.32
1	B0	165	ARG	CZ-NH1	-5.07	1.25	1.32
1	B0	241	ARG	CZ-NH1	-5.07	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B0	153	GLY	N-CA	-5.06	1.38	1.45
58	bO	9	G	C2-N2	-5.06	1.24	1.34
56	bL	27	A	C6-N6	-5.05	1.23	1.33
1	B0	89	PRO	CA-CB	-5.05	1.46	1.53
56	bL	26	A	C6-N6	-5.04	1.23	1.33
14	BD	93	ARG	CD-NE	-5.04	1.39	1.46
55	bK	16	G	C2-N2	-5.04	1.24	1.34
57	bN	11	G	C2-N2	-5.04	1.24	1.34
1	B0	171	ARG	CZ-NH1	-5.04	1.25	1.32
14	BD	31	PRO	CA-CB	-5.04	1.47	1.53
47	b4	4	G	C2-N2	-5.04	1.24	1.34
25	BQ	320	GLY	N-CA	-5.03	1.37	1.44
14	BD	169	PRO	CA-CB	-5.03	1.47	1.54
55	bK	13	G	C2-N2	-5.03	1.24	1.34
55	bK	27	C	C4-N4	-5.03	1.23	1.33
47	b4	3	G	C2-N2	-5.03	1.24	1.34
47	b4	5	A	C6-N6	-5.03	1.23	1.33
1	B0	249	ARG	CA-CB	-5.02	1.48	1.53
58	bO	88	A	C6-N6	-5.02	1.24	1.33
58	bO	90	A	C6-N6	-5.02	1.24	1.33
55	bK	61	A	C6-N6	-5.01	1.24	1.33
14	BD	92	GLY	N-CA	-5.01	1.38	1.45
58	bO	87	C	C4-N4	-5.01	1.24	1.33
58	bO	102	A	C6-N6	-5.01	1.24	1.33
57	bN	43	A	C6-N6	-5.01	1.24	1.33
58	bO	32	A	C6-N6	-5.01	1.24	1.33
57	bN	45	A	C6-N6	-5.00	1.24	1.33
39	Bi	128	ARG	CD-NE	-5.00	1.39	1.46
58	bO	16	C	C4-N4	-5.00	1.24	1.33
58	bO	101	A	C6-N6	-5.00	1.24	1.33
55	bK	4	G	C2-N2	-5.00	1.24	1.34

All (1376) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	bJ	63	C	O4'-C1'-N1	11.81	126.22	108.50
42	HJ	702	ILE	CA-C-N	9.68	129.18	122.60
42	HJ	702	ILE	C-N-CA	9.68	129.18	122.60
62	bS	22	U	O3'-P-O5'	8.65	116.98	104.00
16	BF	274	ARG	CA-C-N	8.39	127.04	120.33
16	BF	274	ARG	C-N-CA	8.39	127.04	120.33
62	bS	28	U	N1-C1'-C2'	8.25	124.37	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	BK	53	MET	CA-C-N	8.05	129.37	122.28
21	BK	53	MET	C-N-CA	8.05	129.37	122.28
62	bS	29	U	N1-C1'-C2'	7.96	125.95	114.00
12	BB	145	ASP	CA-C-N	7.88	129.70	122.37
12	BB	145	ASP	C-N-CA	7.88	129.70	122.37
1	B0	56	ALA	CA-C-N	7.79	129.45	119.78
1	B0	56	ALA	C-N-CA	7.79	129.45	119.78
62	bS	18	U	O5'-C5'-C4'	7.68	123.22	111.70
12	BB	339	HIS	CA-CB-CG	7.55	121.35	113.80
1	B0	47	HIS	CA-CB-CG	7.53	121.33	113.80
30	BW	258	PHE	CA-CB-CG	7.46	121.26	113.80
25	BQ	139	GLU	CA-C-N	7.46	130.46	122.11
25	BQ	139	GLU	C-N-CA	7.46	130.46	122.11
58	bO	11	U	C1'-C2'-O2'	-7.45	97.23	108.40
16	BF	260	HIS	CA-CB-CG	7.43	121.23	113.80
12	BB	151	HIS	CA-CB-CG	7.41	121.21	113.80
30	BW	231	PHE	CA-CB-CG	7.36	121.16	113.80
15	BE	411	PHE	CA-CB-CG	7.32	121.12	113.80
37	Bg	201	PRO	CA-C-N	7.31	128.98	119.84
37	Bg	201	PRO	C-N-CA	7.31	128.98	119.84
12	BB	343	ASP	CA-CB-CG	7.31	119.91	112.60
1	B0	88	ASN	CA-CB-CG	7.29	119.89	112.60
14	BD	210	PHE	CA-CB-CG	7.29	121.08	113.80
30	BW	271	PHE	CA-CB-CG	7.28	121.08	113.80
16	BF	275	ILE	N-CA-CB	7.24	116.10	110.45
14	BD	95	ASP	CA-CB-CG	7.24	119.84	112.60
42	HJ	727	ASP	CA-CB-CG	7.23	119.83	112.60
12	BB	967	SER	CA-C-N	7.23	128.74	119.78
12	BB	967	SER	C-N-CA	7.23	128.74	119.78
15	BE	474	ASN	CA-CB-CG	7.20	119.80	112.60
14	BD	367	ASN	CA-CB-CG	7.18	119.78	112.60
30	BW	290	HIS	CA-CB-CG	7.17	120.97	113.80
42	HJ	714	ASN	CA-CB-CG	7.17	119.77	112.60
42	HJ	677	ASP	CA-CB-CG	7.15	119.75	112.60
14	BD	318	HIS	CA-CB-CG	7.14	120.94	113.80
12	BB	182	ASP	CA-CB-CG	7.12	119.72	112.60
12	BB	309	HIS	CA-CB-CG	7.12	120.92	113.80
12	BB	426	ARG	CA-C-N	7.09	130.39	122.59
12	BB	426	ARG	C-N-CA	7.09	130.39	122.59
12	BB	153	HIS	CA-CB-CG	7.08	120.88	113.80
14	BD	393	ASN	CA-CB-CG	7.08	119.68	112.60
15	BE	478	HIS	CA-CB-CG	7.04	120.84	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BB	1012	LEU	CA-C-N	7.04	130.19	123.08
12	BB	1012	LEU	C-N-CA	7.04	130.19	123.08
21	BK	81	PHE	CA-CB-CG	7.03	120.83	113.80
30	BW	247	ASP	CA-CB-CG	7.01	119.61	112.60
42	HJ	681	PHE	CA-CB-CG	7.01	120.81	113.80
14	BD	373	HIS	CA-CB-CG	7.00	120.80	113.80
14	BD	371	ASN	CA-CB-CG	6.99	119.59	112.60
12	BB	136	PHE	CA-CB-CG	6.97	120.77	113.80
25	BQ	287	PHE	CA-CB-CG	6.97	120.77	113.80
42	HJ	743	PHE	CA-CB-CG	6.97	120.77	113.80
14	BD	395	ASP	CA-CB-CG	6.95	119.55	112.60
15	BE	613	ASN	CA-CB-CG	6.95	119.55	112.60
14	BD	324	ASP	CA-CB-CG	6.95	119.55	112.60
12	BB	181	PHE	CA-CB-CG	6.94	120.74	113.80
37	Bg	84	HIS	CA-CB-CG	6.94	120.74	113.80
30	BW	280	LEU	CA-C-N	6.94	130.66	122.89
30	BW	280	LEU	C-N-CA	6.94	130.66	122.89
42	HJ	680	ASP	CA-CB-CG	6.94	119.54	112.60
40	Bk	305	ASN	CA-CB-CG	6.92	119.52	112.60
12	BB	144	ASP	CA-CB-CG	6.92	119.52	112.60
37	Bg	100	ASP	CA-CB-CG	6.92	119.52	112.60
21	BK	51	HIS	CA-CB-CG	6.90	120.70	113.80
14	BD	319	ASN	CA-CB-CG	6.89	119.50	112.60
4	B3	11	PHE	CA-CB-CG	6.88	120.69	113.80
30	BW	300	PHE	CA-CB-CG	6.88	120.67	113.80
12	BB	66	ASP	CA-CB-CG	6.87	119.47	112.60
42	HJ	682	ASP	CA-CB-CG	6.86	119.46	112.60
54	bJ	64	U	O4'-C1'-N1	6.86	118.79	108.50
16	BF	35	HIS	CA-CB-CG	6.86	120.66	113.80
1	B0	80	PRO	N-CA-C	6.86	122.75	113.84
25	BQ	276	PHE	CA-CB-CG	6.85	120.65	113.80
15	BE	508	HIS	CA-CB-CG	6.84	120.64	113.80
14	BD	238	ASP	CA-CB-CG	6.81	119.41	112.60
15	BE	602	PHE	CA-CB-CG	6.80	120.60	113.80
15	BE	824	PHE	CA-CB-CG	6.79	120.59	113.80
14	BD	392	HIS	CA-CB-CG	6.79	120.59	113.80
21	BK	54	ASP	CA-CB-CG	6.78	119.38	112.60
25	BQ	137	PHE	CA-CB-CG	6.78	120.58	113.80
42	HJ	651	PHE	CA-CB-CG	6.78	120.58	113.80
25	BQ	328	PHE	CA-CB-CG	6.78	120.58	113.80
7	B6	33	HIS	CA-C-N	6.78	128.20	122.17
7	B6	33	HIS	C-N-CA	6.78	128.20	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	BH	65	ASN	CA-CB-CG	6.77	119.37	112.60
21	BK	150	ASN	CA-CB-CG	6.76	119.36	112.60
18	BH	122	ASN	CA-CB-CG	6.74	119.33	112.60
25	BQ	374	ASP	CA-CB-CG	6.72	119.32	112.60
12	BB	333	PHE	CA-CB-CG	6.71	120.51	113.80
30	BW	281	PHE	CA-CB-CG	6.70	120.50	113.80
15	BE	387	ASP	CA-CB-CG	6.68	119.28	112.60
38	Bh	126	ASN	CA-CB-CG	6.67	119.27	112.60
12	BB	139	PHE	CA-CB-CG	6.65	120.45	113.80
54	bJ	63	C	N1-C1'-C2'	-6.64	102.03	112.00
12	BB	39	HIS	CA-CB-CG	6.64	120.44	113.80
30	BW	288	PHE	CA-CB-CG	6.63	120.43	113.80
14	BD	33	HIS	CA-CB-CG	6.63	120.43	113.80
37	Bg	50	SER	CA-C-N	6.62	131.16	123.15
37	Bg	50	SER	C-N-CA	6.62	131.16	123.15
15	BE	381	PRO	CA-C-N	6.61	130.76	122.43
15	BE	381	PRO	C-N-CA	6.61	130.76	122.43
25	BQ	317	ASN	CA-CB-CG	6.61	119.21	112.60
37	Bg	212	ASP	CA-CB-CG	6.61	119.21	112.60
14	BD	473	ASP	CA-CB-CG	6.61	119.21	112.60
30	BW	334	PHE	CA-CB-CG	6.59	120.39	113.80
1	B0	238	PHE	CA-CB-CG	6.58	120.38	113.80
15	BE	415	ASP	CA-CB-CG	6.57	119.17	112.60
27	BT	61	ASN	CA-CB-CG	6.56	119.16	112.60
15	BE	396	PHE	CA-CB-CG	6.56	120.36	113.80
14	BD	388	PHE	CA-CB-CG	6.55	120.35	113.80
37	Bg	180	HIS	CA-CB-CG	6.55	120.35	113.80
40	Bk	278	SER	CA-C-N	6.55	130.32	122.85
40	Bk	278	SER	C-N-CA	6.55	130.32	122.85
40	Bk	42	ASN	CA-CB-CG	6.55	119.15	112.60
16	BF	240	ASP	CA-C-N	6.54	131.06	123.15
16	BF	240	ASP	C-N-CA	6.54	131.06	123.15
39	Bi	132	HIS	CA-CB-CG	6.52	120.32	113.80
16	BF	251	HIS	CA-CB-CG	6.50	120.31	113.80
37	Bg	66	PHE	CA-CB-CG	6.50	120.30	113.80
27	BT	78	ASN	CA-CB-CG	6.49	119.09	112.60
37	Bg	167	PHE	CA-CB-CG	6.48	120.28	113.80
25	BQ	141	ASN	CA-CB-CG	6.47	119.08	112.60
16	BF	37	PHE	CA-CB-CG	6.45	120.25	113.80
12	BB	150	HIS	CA-CB-CG	6.45	120.25	113.80
14	BD	164	HIS	CA-CB-CG	6.44	120.24	113.80
21	BK	49	PHE	CA-CB-CG	6.44	120.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Bk	325	PHE	CA-CB-CG	6.44	120.24	113.80
27	BT	41	CYS	CA-C-N	6.44	131.14	122.90
27	BT	41	CYS	C-N-CA	6.44	131.14	122.90
37	Bg	95	PHE	CA-CB-CG	6.43	120.23	113.80
27	BT	19	ALA	CA-C-N	6.43	128.15	122.43
27	BT	19	ALA	C-N-CA	6.43	128.15	122.43
12	BB	71	ASP	CA-CB-CG	6.40	119.00	112.60
15	BE	599	PHE	CA-CB-CG	6.40	120.20	113.80
62	bS	18	U	O4'-C1'-N1	6.38	117.78	108.20
40	Bk	4	ASN	CA-CB-CG	6.37	118.97	112.60
37	Bg	69	HIS	CA-CB-CG	6.35	120.15	113.80
40	Bk	309	HIS	CA-CB-CG	6.35	120.15	113.80
16	BF	253	HIS	CA-CB-CG	6.35	120.15	113.80
25	BQ	377	ASN	CA-CB-CG	6.34	118.94	112.60
37	Bg	74	PHE	CA-CB-CG	6.34	120.14	113.80
25	BQ	131	GLN	CA-C-N	6.34	130.81	122.95
25	BQ	131	GLN	C-N-CA	6.34	130.81	122.95
30	BW	145	ASN	CA-CB-CG	6.33	118.93	112.60
29	BV	217	PHE	CA-CB-CG	6.32	120.12	113.80
37	Bg	46	PHE	CA-CB-CG	6.31	120.11	113.80
37	Bg	51	HIS	CA-CB-CG	6.30	120.10	113.80
40	Bk	40	PHE	CA-CB-CG	6.30	120.10	113.80
41	Bl	13	ARG	CA-C-N	6.30	128.70	120.26
41	Bl	13	ARG	C-N-CA	6.30	128.70	120.26
30	BW	303	PHE	CA-CB-CG	6.28	120.08	113.80
14	BD	94	ASP	CA-CB-CG	6.28	118.88	112.60
25	BQ	197	PHE	CA-CB-CG	6.27	120.07	113.80
40	Bk	307	PHE	CA-CB-CG	6.25	120.05	113.80
16	BF	35	HIS	CA-C-N	6.22	130.77	122.93
16	BF	35	HIS	C-N-CA	6.22	130.77	122.93
14	BD	199	ARG	CD-NE-CZ	6.22	133.11	124.40
30	BW	322	ARG	CD-NE-CZ	6.21	133.09	124.40
12	BB	147	PRO	CA-C-N	6.19	131.17	123.12
12	BB	147	PRO	C-N-CA	6.19	131.17	123.12
12	BB	312	ALA	CA-C-N	6.19	128.86	120.44
12	BB	312	ALA	C-N-CA	6.19	128.86	120.44
14	BD	391	ARG	CD-NE-CZ	6.19	133.06	124.40
30	BW	256	GLN	CA-C-N	6.19	130.86	123.19
30	BW	256	GLN	C-N-CA	6.19	130.86	123.19
14	BD	368	ARG	CA-C-N	6.18	130.63	123.15
14	BD	368	ARG	C-N-CA	6.18	130.63	123.15
42	HJ	678	HIS	CA-CB-CG	6.18	119.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	HJ	728	ASN	CA-CB-CG	6.18	118.78	112.60
12	BB	282	ARG	CD-NE-CZ	6.18	133.05	124.40
16	BF	259	ARG	CD-NE-CZ	6.17	133.04	124.40
25	BQ	411	ARG	CA-C-N	6.17	130.86	122.84
25	BQ	411	ARG	C-N-CA	6.17	130.86	122.84
30	BW	279	ARG	CD-NE-CZ	6.17	133.04	124.40
12	BB	1153	ARG	CD-NE-CZ	6.17	133.04	124.40
37	Bg	170	ARG	CD-NE-CZ	6.16	133.03	124.40
14	BD	251	HIS	CA-CB-CG	6.16	119.96	113.80
15	BE	394	ARG	CD-NE-CZ	6.15	133.01	124.40
21	BK	150	ASN	CA-C-N	6.15	131.12	123.12
21	BK	150	ASN	C-N-CA	6.15	131.12	123.12
14	BD	207	ARG	CD-NE-CZ	6.14	133.00	124.40
42	HJ	733	PHE	CA-CB-CG	6.14	119.94	113.80
12	BB	160	ARG	CD-NE-CZ	6.14	132.99	124.40
18	BH	64	ARG	CD-NE-CZ	6.14	132.99	124.40
42	HJ	751	ARG	CD-NE-CZ	6.13	132.99	124.40
42	HJ	759	ARG	CD-NE-CZ	6.13	132.99	124.40
16	BF	274	ARG	CD-NE-CZ	6.13	132.98	124.40
42	HJ	685	ARG	CD-NE-CZ	6.13	132.98	124.40
27	BT	62	ARG	CD-NE-CZ	6.13	132.98	124.40
14	BD	257	ARG	CD-NE-CZ	6.12	132.97	124.40
37	Bg	186	ARG	CA-C-N	6.12	130.56	122.30
37	Bg	186	ARG	C-N-CA	6.12	130.56	122.30
37	Bg	162	ARG	CD-NE-CZ	6.11	132.95	124.40
12	BB	670	ARG	CD-NE-CZ	6.11	132.95	124.40
1	B0	36	ARG	CD-NE-CZ	6.10	132.94	124.40
16	BF	33	ARG	CD-NE-CZ	6.10	132.94	124.40
14	BD	368	ARG	CD-NE-CZ	6.10	132.94	124.40
14	BD	387	ARG	CD-NE-CZ	6.10	132.94	124.40
27	BT	40	PHE	CA-CB-CG	6.10	119.90	113.80
1	B0	150	ARG	CD-NE-CZ	6.09	132.93	124.40
13	BC	203	ARG	CD-NE-CZ	6.09	132.93	124.40
27	BT	38	GLY	CA-C-N	6.09	128.93	120.29
27	BT	38	GLY	C-N-CA	6.09	128.93	120.29
42	HJ	639	ARG	CD-NE-CZ	6.08	132.92	124.40
42	HJ	730	ARG	CA-C-N	6.08	129.97	122.37
42	HJ	730	ARG	C-N-CA	6.08	129.97	122.37
10	B9	59	ARG	CD-NE-CZ	6.08	132.91	124.40
15	BE	528	PHE	CA-CB-CG	6.08	119.88	113.80
41	Bl	14	ARG	CD-NE-CZ	6.08	132.91	124.40
40	Bk	34	ARG	CD-NE-CZ	6.07	132.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	HJ	730	ARG	CD-NE-CZ	6.07	132.90	124.40
13	BC	42	ARG	CD-NE-CZ	6.07	132.90	124.40
27	BT	44	ARG	CD-NE-CZ	6.07	132.90	124.40
12	BB	314	PHE	CA-CB-CG	6.07	119.86	113.80
15	BE	492	ARG	CD-NE-CZ	6.06	132.89	124.40
30	BW	328	ASN	CA-CB-CG	6.06	118.66	112.60
1	B0	271	ARG	CD-NE-CZ	6.06	132.88	124.40
12	BB	68	ARG	CD-NE-CZ	6.06	132.88	124.40
25	BQ	66	LEU	CA-C-N	6.06	128.27	120.70
25	BQ	66	LEU	C-N-CA	6.06	128.27	120.70
30	BW	286	ARG	CD-NE-CZ	6.06	132.88	124.40
30	BW	320	ARG	CD-NE-CZ	6.06	132.88	124.40
12	BB	426	ARG	CD-NE-CZ	6.05	132.88	124.40
25	BQ	469	ARG	CD-NE-CZ	6.05	132.88	124.40
1	B0	160	ASP	CA-CB-CG	6.05	118.65	112.60
16	BF	20	ASN	CA-CB-CG	6.05	118.65	112.60
13	BC	43	ARG	CD-NE-CZ	6.04	132.86	124.40
30	BW	315	ARG	CD-NE-CZ	6.04	132.86	124.40
1	B0	268	ARG	CD-NE-CZ	6.04	132.86	124.40
29	BV	225	TYR	CA-C-N	6.04	130.97	123.12
29	BV	225	TYR	C-N-CA	6.04	130.97	123.12
42	HJ	652	GLY	CA-C-N	6.04	131.05	123.14
42	HJ	652	GLY	C-N-CA	6.04	131.05	123.14
13	BC	208	ARG	CD-NE-CZ	6.04	132.85	124.40
25	BQ	410	ARG	CD-NE-CZ	6.03	132.84	124.40
27	BT	79	ARG	CD-NE-CZ	6.03	132.84	124.40
15	BE	499	GLU	CA-C-N	6.02	128.32	120.26
15	BE	499	GLU	C-N-CA	6.02	128.32	120.26
39	Bi	85	TYR	CA-C-N	6.01	128.62	120.44
39	Bi	85	TYR	C-N-CA	6.01	128.62	120.44
21	BK	58	PHE	CA-CB-CG	6.01	119.81	113.80
1	B0	249	ARG	CD-NE-CZ	6.00	132.81	124.40
18	BH	89	PHE	CA-CB-CG	6.00	119.80	113.80
12	BB	61	ARG	CD-NE-CZ	5.99	132.78	124.40
27	BT	94	PRO	CA-C-N	5.99	130.85	122.41
27	BT	94	PRO	C-N-CA	5.99	130.85	122.41
21	BK	48	PHE	CA-CB-CG	5.98	119.78	113.80
18	BH	120	ALA	CA-C-N	5.97	130.96	123.14
18	BH	120	ALA	C-N-CA	5.97	130.96	123.14
42	HJ	732	SER	CA-C-N	5.96	130.59	122.84
42	HJ	732	SER	C-N-CA	5.96	130.59	122.84
14	BD	93	ARG	CD-NE-CZ	5.96	132.75	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	bS	22	U	N1-C1'-C2'	5.96	122.94	114.00
25	BQ	364	THR	CA-C-N	5.96	130.59	122.84
25	BQ	364	THR	C-N-CA	5.96	130.59	122.84
40	Bk	51	ARG	CD-NE-CZ	5.96	132.74	124.40
15	BE	478	HIS	CA-C-N	5.96	130.34	122.30
15	BE	478	HIS	C-N-CA	5.96	130.34	122.30
30	BW	204	ASP	CA-CB-CG	5.95	118.55	112.60
12	BB	260	GLU	CA-C-N	5.95	128.18	120.56
12	BB	260	GLU	C-N-CA	5.95	128.18	120.56
12	BB	1126	LYS	CA-C-N	5.94	129.30	120.87
12	BB	1126	LYS	C-N-CA	5.94	129.30	120.87
4	B3	13	ARG	CA-C-N	5.94	129.06	120.98
4	B3	13	ARG	C-N-CA	5.94	129.06	120.98
14	BD	211	TYR	CA-C-N	5.94	128.16	120.56
14	BD	211	TYR	C-N-CA	5.94	128.16	120.56
7	B6	7	VAL	CA-C-N	5.94	130.56	122.84
7	B6	7	VAL	C-N-CA	5.94	130.56	122.84
42	HJ	725	GLY	CA-C-N	5.93	130.02	122.37
42	HJ	725	GLY	C-N-CA	5.93	130.02	122.37
7	B6	6	PHE	CA-C-N	5.92	130.53	123.19
7	B6	6	PHE	C-N-CA	5.92	130.53	123.19
25	BQ	314	ASP	CA-CB-CG	5.92	118.52	112.60
37	Bg	176	ARG	CD-NE-CZ	5.92	132.68	124.40
39	Bi	149	ASP	CA-CB-CG	5.92	118.52	112.60
15	BE	1023	HIS	CA-CB-CG	-5.91	107.89	113.80
22	BL	91	ASN	CA-CB-CG	5.91	118.51	112.60
40	Bk	223	ASP	CA-CB-CG	5.91	118.51	112.60
41	Bl	104	ALA	CA-C-N	5.91	130.95	123.10
41	Bl	104	ALA	C-N-CA	5.91	130.95	123.10
1	B0	171	ARG	CD-NE-CZ	5.90	132.66	124.40
30	BW	289	SER	CA-C-N	5.90	129.67	122.42
30	BW	289	SER	C-N-CA	5.90	129.67	122.42
15	BE	826	HIS	CA-CB-CG	5.89	119.69	113.80
22	BL	40	ARG	CA-C-N	5.89	129.74	122.37
22	BL	40	ARG	C-N-CA	5.89	129.74	122.37
25	BQ	506	ARG	CA-C-N	5.89	130.36	122.93
25	BQ	506	ARG	C-N-CA	5.89	130.36	122.93
40	Bk	76	HIS	CA-CB-CG	5.88	119.68	113.80
22	BL	94	LEU	CA-C-N	5.88	129.40	123.16
22	BL	94	LEU	C-N-CA	5.88	129.40	123.16
3	B2	260	ASP	CA-CB-CG	5.88	118.48	112.60
12	BB	963	ARG	CA-C-N	5.87	129.39	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BB	963	ARG	C-N-CA	5.87	129.39	123.16
42	HJ	640	ALA	CA-C-N	5.87	131.09	123.10
42	HJ	640	ALA	C-N-CA	5.87	131.09	123.10
30	BW	321	ARG	CD-NE-CZ	5.85	132.59	124.40
1	B0	242	ARG	CD-NE-CZ	5.83	132.57	124.40
1	B0	12	LEU	CA-C-N	5.83	129.08	120.74
1	B0	12	LEU	C-N-CA	5.83	129.08	120.74
16	BF	253	HIS	CA-C-N	5.83	130.41	122.19
16	BF	253	HIS	C-N-CA	5.83	130.41	122.19
3	B2	160	PHE	CA-CB-CG	5.83	119.63	113.80
15	BE	765	ARG	CD-NE-CZ	5.83	132.56	124.40
15	BE	1050	ARG	CB-CA-C	5.83	119.46	110.14
57	bN	48	G	C3'-C2'-O2'	5.83	119.44	110.70
38	Bh	149	ASP	CA-C-N	5.82	130.76	123.14
38	Bh	149	ASP	C-N-CA	5.82	130.76	123.14
37	Bg	171	GLU	CA-C-N	5.81	130.75	123.14
37	Bg	171	GLU	C-N-CA	5.81	130.75	123.14
15	BE	836	ASP	CA-CB-CG	5.80	118.40	112.60
27	BT	39	ASP	CA-CB-CG	5.80	118.40	112.60
38	Bh	126	ASN	CA-C-N	5.79	128.52	120.29
38	Bh	126	ASN	C-N-CA	5.79	128.52	120.29
38	Bh	137	PRO	CA-C-N	5.79	130.65	123.12
38	Bh	137	PRO	C-N-CA	5.79	130.65	123.12
39	Bi	128	ARG	CD-NE-CZ	5.79	132.50	124.40
1	B0	7	ASP	CA-CB-CG	5.79	118.39	112.60
16	BF	245	GLU	CA-C-N	5.78	127.84	120.56
16	BF	245	GLU	C-N-CA	5.78	127.84	120.56
37	Bg	173	TYR	CA-C-N	5.78	130.10	122.30
37	Bg	173	TYR	C-N-CA	5.78	130.10	122.30
62	bS	22	U	C4'-C3'-C2'	-5.78	96.83	102.60
12	BB	145	ASP	CA-CB-CG	5.76	118.36	112.60
30	BW	148	LYS	CA-C-N	5.76	129.26	123.16
30	BW	148	LYS	C-N-CA	5.76	129.26	123.16
25	BQ	373	ARG	CD-NE-CZ	5.76	132.46	124.40
7	B6	12	ARG	CA-C-N	5.75	130.60	123.12
7	B6	12	ARG	C-N-CA	5.75	130.60	123.12
15	BE	494	GLN	CA-C-N	5.75	127.92	120.44
15	BE	494	GLN	C-N-CA	5.75	127.92	120.44
25	BQ	513	PHE	CA-CB-CG	5.75	119.55	113.80
30	BW	283	LYS	CA-C-N	5.75	130.94	123.00
30	BW	283	LYS	C-N-CA	5.75	130.94	123.00
25	BQ	287	PHE	CA-C-N	5.75	130.42	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BQ	287	PHE	C-N-CA	5.75	130.42	122.77
62	bS	21	U	O4'-C1'-C2'	-5.75	100.05	105.80
3	B2	119	ASP	CA-CB-CG	5.73	118.33	112.60
30	BW	240	PHE	CA-CB-CG	5.73	119.53	113.80
22	BL	26	MET	CA-C-N	5.73	130.65	123.14
22	BL	26	MET	C-N-CA	5.73	130.65	123.14
3	B2	106	PHE	CA-CB-CG	5.73	119.53	113.80
27	BT	43	VAL	CA-C-N	5.72	128.96	120.95
27	BT	43	VAL	C-N-CA	5.72	128.96	120.95
3	B2	267	ASP	CA-CB-CG	5.71	118.31	112.60
37	Bg	182	LEU	CA-C-N	5.71	129.51	122.37
37	Bg	182	LEU	C-N-CA	5.71	129.51	122.37
3	B2	151	ASP	CA-CB-CG	5.71	118.31	112.60
40	Bk	58	SER	CA-C-N	5.69	131.03	123.00
40	Bk	58	SER	C-N-CA	5.69	131.03	123.00
30	BW	111	THR	CA-C-N	5.69	130.52	123.12
30	BW	111	THR	C-N-CA	5.69	130.52	123.12
4	B3	210	ASN	CA-CB-CG	5.69	118.29	112.60
25	BQ	409	GLN	CA-C-N	5.68	129.55	121.42
25	BQ	409	GLN	C-N-CA	5.68	129.55	121.42
25	BQ	512	GLN	CA-C-N	5.67	129.96	122.30
25	BQ	512	GLN	C-N-CA	5.67	129.96	122.30
25	BQ	67	VAL	N-CA-CB	5.67	116.80	110.62
40	Bk	57	PHE	CA-CB-CG	5.67	119.47	113.80
25	BQ	199	LEU	CA-C-N	5.66	128.32	120.29
25	BQ	199	LEU	C-N-CA	5.66	128.32	120.29
22	BL	18	ARG	CA-C-N	5.65	128.31	120.29
22	BL	18	ARG	C-N-CA	5.65	128.31	120.29
18	BH	93	LEU	CA-C-N	5.64	130.94	123.05
18	BH	93	LEU	C-N-CA	5.64	130.94	123.05
14	BD	370	PRO	CA-C-N	5.63	129.55	121.50
14	BD	370	PRO	C-N-CA	5.63	129.55	121.50
18	BH	66	ILE	CA-C-N	5.62	130.93	123.00
18	BH	66	ILE	C-N-CA	5.62	130.93	123.00
37	Bg	185	GLY	CA-C-N	5.62	129.87	121.72
37	Bg	185	GLY	C-N-CA	5.62	129.87	121.72
22	BL	85	ARG	CA-C-N	5.62	130.57	123.10
22	BL	85	ARG	C-N-CA	5.62	130.57	123.10
40	Bk	293	VAL	CA-C-N	5.62	130.24	122.77
40	Bk	293	VAL	C-N-CA	5.62	130.24	122.77
40	Bk	235	ALA	CA-C-N	5.62	127.80	120.28
40	Bk	235	ALA	C-N-CA	5.62	127.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BD	19	ASP	CA-CB-CG	5.61	118.21	112.60
1	B0	182	GLY	CA-C-N	5.61	127.73	120.44
1	B0	182	GLY	C-N-CA	5.61	127.73	120.44
3	B2	47	HIS	CA-CB-CG	5.61	119.41	113.80
3	B2	157	HIS	CA-CB-CG	5.61	119.41	113.80
42	HJ	733	PHE	CA-C-N	5.61	129.85	122.06
42	HJ	733	PHE	C-N-CA	5.61	129.85	122.06
15	BE	512	SER	CA-C-N	5.60	131.37	123.30
15	BE	512	SER	C-N-CA	5.60	131.37	123.30
7	B6	6	PHE	CA-CB-CG	5.60	119.40	113.80
14	BD	136	TRP	CA-C-N	5.60	127.78	120.28
14	BD	136	TRP	C-N-CA	5.60	127.78	120.28
54	bJ	61	U	O4'-C1'-N1	5.60	116.90	108.50
25	BQ	437	VAL	N-CA-CB	5.59	116.92	110.49
40	Bk	41	ALA	CA-C-N	5.59	128.71	120.82
40	Bk	41	ALA	C-N-CA	5.59	128.71	120.82
1	B0	183	GLU	CA-C-N	5.59	127.61	120.56
1	B0	183	GLU	C-N-CA	5.59	127.61	120.56
40	Bk	50	LEU	CA-C-N	5.59	127.71	120.44
40	Bk	50	LEU	C-N-CA	5.59	127.71	120.44
14	BD	131	ARG	CA-C-N	5.59	130.87	123.05
14	BD	131	ARG	C-N-CA	5.59	130.87	123.05
18	BH	122	ASN	CA-C-N	5.58	131.03	122.93
18	BH	122	ASN	C-N-CA	5.58	131.03	122.93
27	BT	35	SER	CA-C-N	5.58	127.53	120.72
27	BT	35	SER	C-N-CA	5.58	127.53	120.72
42	HJ	679	ILE	CA-C-N	5.58	131.03	122.77
42	HJ	679	ILE	C-N-CA	5.58	131.03	122.77
15	BE	821	PHE	CA-CB-CG	5.58	119.38	113.80
1	B0	298	GLU	CA-C-N	5.58	127.69	120.44
1	B0	298	GLU	C-N-CA	5.58	127.69	120.44
30	BW	333	GLY	CA-C-N	5.57	130.85	123.05
30	BW	333	GLY	C-N-CA	5.57	130.85	123.05
40	Bk	303	THR	CA-C-N	5.57	130.40	122.72
40	Bk	303	THR	C-N-CA	5.57	130.40	122.72
40	Bk	304	ASP	CA-CB-CG	5.57	118.17	112.60
1	B0	7	ASP	CA-C-N	5.56	128.12	120.67
1	B0	7	ASP	C-N-CA	5.56	128.12	120.67
15	BE	472	ALA	CA-C-N	5.56	127.73	120.28
15	BE	472	ALA	C-N-CA	5.56	127.73	120.28
30	BW	231	PHE	CA-C-N	5.56	129.78	121.72
30	BW	231	PHE	C-N-CA	5.56	129.78	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	BH	86	ARG	CA-C-N	5.56	130.58	122.85
18	BH	86	ARG	C-N-CA	5.56	130.58	122.85
40	Bk	64	ARG	CA-C-N	5.56	130.07	122.84
40	Bk	64	ARG	C-N-CA	5.56	130.07	122.84
27	BT	45	ARG	CA-C-N	5.56	127.73	120.28
27	BT	45	ARG	C-N-CA	5.56	127.73	120.28
15	BE	845	ARG	CD-NE-CZ	5.55	132.18	124.40
25	BQ	517	ASN	CA-CB-CG	5.55	118.15	112.60
42	HJ	726	ILE	CA-C-N	5.55	130.98	122.93
42	HJ	726	ILE	C-N-CA	5.55	130.98	122.93
37	Bg	78	ASN	CA-C-N	5.55	127.71	120.28
37	Bg	78	ASN	C-N-CA	5.55	127.71	120.28
40	Bk	304	ASP	CA-C-N	5.54	129.76	121.72
40	Bk	304	ASP	C-N-CA	5.54	129.76	121.72
30	BW	277	GLN	CA-C-N	5.54	128.26	120.28
30	BW	277	GLN	C-N-CA	5.54	128.26	120.28
12	BB	137	SER	CA-C-N	5.54	128.16	120.29
12	BB	137	SER	C-N-CA	5.54	128.16	120.29
14	BD	390	GLU	CA-C-N	5.54	130.63	121.99
14	BD	390	GLU	C-N-CA	5.54	130.63	121.99
62	bS	18	U	C1'-O4'-C4'	-5.54	104.16	109.70
37	Bg	83	MET	CA-C-N	5.54	128.73	120.31
37	Bg	83	MET	C-N-CA	5.54	128.73	120.31
15	BE	495	LEU	N-CA-CB	5.54	118.08	110.11
41	Bl	16	LEU	CA-C-N	5.54	130.46	122.16
41	Bl	16	LEU	C-N-CA	5.54	130.46	122.16
27	BT	75	TYR	CA-C-N	5.53	130.23	121.99
27	BT	75	TYR	C-N-CA	5.53	130.23	121.99
15	BE	562	PHE	CA-CB-CG	5.53	119.33	113.80
21	BK	57	ARG	CA-C-N	5.53	130.20	122.41
21	BK	57	ARG	C-N-CA	5.53	130.20	122.41
38	Bh	138	VAL	CA-C-N	5.52	130.82	122.98
38	Bh	138	VAL	C-N-CA	5.52	130.82	122.98
15	BE	811	GLN	CA-C-N	5.52	128.12	120.29
15	BE	811	GLN	C-N-CA	5.52	128.12	120.29
27	BT	37	HIS	CA-CB-CG	5.52	119.32	113.80
41	Bl	1	SER	CA-C-N	5.52	131.15	122.49
41	Bl	1	SER	C-N-CA	5.52	131.15	122.49
25	BQ	132	ILE	CA-C-N	5.52	130.61	123.00
25	BQ	132	ILE	C-N-CA	5.52	130.61	123.00
7	B6	9	PHE	CA-CB-CG	5.51	119.31	113.80
25	BQ	348	SER	CA-C-N	5.51	127.60	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BQ	348	SER	C-N-CA	5.51	127.60	120.44
29	BV	210	PRO	CA-C-N	5.51	130.92	122.93
29	BV	210	PRO	C-N-CA	5.51	130.92	122.93
11	BA	424	LEU	CA-C-N	5.51	128.70	122.59
11	BA	424	LEU	C-N-CA	5.51	128.70	122.59
22	BL	19	ASN	CA-CB-CG	5.50	118.10	112.60
42	HJ	841	LYS	CA-C-N	5.50	127.59	120.44
42	HJ	841	LYS	C-N-CA	5.50	127.59	120.44
14	BD	253	LEU	CA-C-N	5.50	127.59	120.44
14	BD	253	LEU	C-N-CA	5.50	127.59	120.44
15	BE	473	ALA	CA-C-N	5.50	127.64	120.28
15	BE	473	ALA	C-N-CA	5.50	127.64	120.28
25	BQ	137	PHE	CA-C-N	5.50	127.84	122.73
25	BQ	137	PHE	C-N-CA	5.50	127.84	122.73
12	BB	136	PHE	CA-C-N	5.49	127.64	120.28
12	BB	136	PHE	C-N-CA	5.49	127.64	120.28
14	BD	150	ARG	CA-C-N	5.49	128.69	122.59
14	BD	150	ARG	C-N-CA	5.49	128.69	122.59
11	BA	129	ARG	CD-NE-CZ	5.48	132.08	124.40
12	BB	309	HIS	CA-C-N	5.48	127.63	120.28
12	BB	309	HIS	C-N-CA	5.48	127.63	120.28
43	HS	229	GLU	N-CA-CB	5.48	118.27	110.16
12	BB	308	LYS	CA-C-N	5.48	128.07	120.29
12	BB	308	LYS	C-N-CA	5.48	128.07	120.29
30	BW	334	PHE	CA-C-N	5.48	128.65	120.87
30	BW	334	PHE	C-N-CA	5.48	128.65	120.87
15	BE	547	GLN	CA-C-N	5.48	127.56	120.44
15	BE	547	GLN	C-N-CA	5.48	127.56	120.44
7	B6	63	ARG	CD-NE-CZ	5.48	132.07	124.40
27	BT	95	LYS	CA-C-N	5.48	130.81	122.65
27	BT	95	LYS	C-N-CA	5.48	130.81	122.65
7	B6	12	ARG	CD-NE-CZ	5.48	132.07	124.40
7	B6	32	HIS	CA-CB-CG	5.47	119.28	113.80
14	BD	22	PHE	CA-CB-CG	5.47	119.28	113.80
12	BB	77	ALA	CA-C-N	5.47	127.45	120.56
12	BB	77	ALA	C-N-CA	5.47	127.45	120.56
15	BE	392	ILE	CA-C-N	5.47	127.55	120.44
15	BE	392	ILE	C-N-CA	5.47	127.55	120.44
7	B6	91	ARG	CD-NE-CZ	5.47	132.05	124.40
14	BD	258	ALA	CA-C-N	5.47	127.55	120.44
14	BD	258	ALA	C-N-CA	5.47	127.55	120.44
16	BF	18	GLY	N-CA-C	5.46	118.94	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BB	971	PHE	CA-CB-CG	5.46	119.26	113.80
40	Bk	226	ASP	CA-CB-CG	5.46	118.06	112.60
15	BE	506	LEU	CA-C-N	5.46	127.59	120.28
15	BE	506	LEU	C-N-CA	5.46	127.59	120.28
39	Bi	132	HIS	ND1-CG-CD2	-5.45	100.65	106.10
27	BT	14	ARG	CD-NE-CZ	5.45	132.03	124.40
12	BB	261	ILE	CA-C-N	5.45	127.43	120.56
12	BB	261	ILE	C-N-CA	5.45	127.43	120.56
7	B6	45	ARG	CD-NE-CZ	5.45	132.02	124.40
14	BD	372	ALA	CA-C-N	5.44	127.57	120.28
14	BD	372	ALA	C-N-CA	5.44	127.57	120.28
15	BE	408	LYS	CA-C-N	5.44	125.98	120.00
15	BE	408	LYS	C-N-CA	5.44	125.98	120.00
1	B0	163	TYR	CA-C-N	5.43	127.41	120.56
1	B0	163	TYR	C-N-CA	5.43	127.41	120.56
40	Bk	32	HIS	ND1-CG-CD2	-5.43	100.67	106.10
18	BH	65	ASN	CA-C-N	5.43	130.69	122.98
18	BH	65	ASN	C-N-CA	5.43	130.69	122.98
27	BT	51	HIS	ND1-CG-CD2	-5.43	100.67	106.10
12	BB	138	LEU	CA-C-N	5.43	127.50	120.44
12	BB	138	LEU	C-N-CA	5.43	127.50	120.44
14	BD	35	GLY	N-CA-C	5.43	118.51	110.42
25	BQ	344	ILE	CA-C-N	5.43	127.50	120.44
25	BQ	344	ILE	C-N-CA	5.43	127.50	120.44
14	BD	125	LEU	CA-C-N	5.42	127.49	120.44
14	BD	125	LEU	C-N-CA	5.42	127.49	120.44
12	BB	54	ALA	CA-C-N	5.42	126.50	119.78
12	BB	54	ALA	C-N-CA	5.42	126.50	119.78
1	B0	35	GLY	CA-C-N	5.42	127.48	120.44
1	B0	35	GLY	C-N-CA	5.42	127.48	120.44
1	B0	190	VAL	CA-C-N	5.42	127.38	120.56
1	B0	190	VAL	C-N-CA	5.42	127.38	120.56
40	Bk	36	LYS	CA-C-N	5.42	129.04	121.24
40	Bk	36	LYS	C-N-CA	5.42	129.04	121.24
40	Bk	16	ARG	CD-NE-CZ	5.41	131.98	124.40
1	B0	272	GLU	CA-C-N	5.41	127.53	120.28
1	B0	272	GLU	C-N-CA	5.41	127.53	120.28
16	BF	244	ALA	CA-C-N	5.41	127.53	120.28
16	BF	244	ALA	C-N-CA	5.41	127.53	120.28
40	Bk	28	GLU	CA-C-N	5.41	127.53	120.28
40	Bk	28	GLU	C-N-CA	5.41	127.53	120.28
39	Bi	125	GLU	CA-C-N	5.41	127.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Bi	125	GLU	C-N-CA	5.41	127.53	120.28
3	B2	225	ARG	NE-CZ-NH2	5.41	124.06	119.20
12	BB	163	ALA	CA-C-N	5.41	127.47	120.44
12	BB	163	ALA	C-N-CA	5.41	127.47	120.44
38	Bh	3	HIS	CA-CB-CG	5.40	119.20	113.80
22	BL	85	ARG	CD-NE-CZ	5.40	131.96	124.40
42	HJ	722	TYR	CA-C-N	5.40	128.06	120.28
42	HJ	722	TYR	C-N-CA	5.40	128.06	120.28
1	B0	9	PRO	CA-C-N	5.40	128.51	120.31
1	B0	9	PRO	C-N-CA	5.40	128.51	120.31
4	B3	14	VAL	CA-C-N	5.40	128.37	120.71
4	B3	14	VAL	C-N-CA	5.40	128.37	120.71
25	BQ	200	GLU	CA-C-N	5.39	127.35	120.56
25	BQ	200	GLU	C-N-CA	5.39	127.35	120.56
14	BD	451	ASP	CA-CB-CG	5.39	117.99	112.60
12	BB	69	VAL	CA-C-N	5.38	127.34	120.56
12	BB	69	VAL	C-N-CA	5.38	127.34	120.56
38	Bh	125	GLU	CA-C-N	5.38	128.03	120.28
38	Bh	125	GLU	C-N-CA	5.38	128.03	120.28
1	B0	162	VAL	CA-C-N	5.38	127.44	120.44
1	B0	162	VAL	C-N-CA	5.38	127.44	120.44
12	BB	305	THR	CA-C-N	5.38	127.34	120.56
12	BB	305	THR	C-N-CA	5.38	127.34	120.56
12	BB	986	ASP	CA-CB-CG	5.38	117.98	112.60
27	BT	42	VAL	CA-C-N	5.38	131.18	122.68
27	BT	42	VAL	C-N-CA	5.38	131.18	122.68
30	BW	101	ARG	CD-NE-CZ	5.38	131.93	124.40
1	B0	33	ASP	CA-C-N	5.38	127.48	120.28
1	B0	33	ASP	C-N-CA	5.38	127.48	120.28
12	BB	984	HIS	CA-CB-CG	5.38	119.17	113.80
15	BE	523	ARG	CD-NE-CZ	5.38	131.93	124.40
12	BB	314	PHE	CA-C-N	5.37	127.48	120.28
12	BB	314	PHE	C-N-CA	5.37	127.48	120.28
22	BL	45	ARG	CD-NE-CZ	5.37	131.92	124.40
15	BE	393	ALA	CA-C-N	5.37	127.48	120.28
15	BE	393	ALA	C-N-CA	5.37	127.48	120.28
22	BL	78	ARG	CD-NE-CZ	5.37	131.92	124.40
7	B6	17	ASP	CA-CB-CG	5.37	117.97	112.60
14	BD	392	HIS	CA-C-N	5.37	130.56	122.99
14	BD	392	HIS	C-N-CA	5.37	130.56	122.99
30	BW	302	GLU	CA-C-N	5.36	131.01	122.59
30	BW	302	GLU	C-N-CA	5.36	131.01	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BB	33	SER	CA-C-N	5.36	127.41	120.44
12	BB	33	SER	C-N-CA	5.36	127.41	120.44
4	B3	221	ARG	CD-NE-CZ	5.36	131.90	124.40
37	Bg	203	GLU	O-C-N	-5.36	118.28	121.71
39	Bi	86	ARG	CD-NE-CZ	5.36	131.90	124.40
3	B2	108	ARG	CD-NE-CZ	5.36	131.90	124.40
22	BL	62	VAL	CA-C-N	5.35	130.01	122.09
22	BL	62	VAL	C-N-CA	5.35	130.01	122.09
3	B2	4	ARG	CD-NE-CZ	5.35	131.89	124.40
14	BD	201	GLN	N-CA-CB	5.35	117.87	109.69
12	BB	135	PRO	CA-C-N	5.34	128.43	120.31
12	BB	135	PRO	C-N-CA	5.34	128.43	120.31
15	BE	391	GLN	CA-C-N	5.34	127.29	120.56
15	BE	391	GLN	C-N-CA	5.34	127.29	120.56
25	BQ	68	ARG	CD-NE-CZ	5.34	131.88	124.40
3	B2	4	ARG	CA-C-N	5.34	130.67	123.46
3	B2	4	ARG	C-N-CA	5.34	130.67	123.46
25	BQ	330	GLY	CA-C-N	5.34	128.78	120.34
25	BQ	330	GLY	C-N-CA	5.34	128.78	120.34
39	Bi	7	LEU	CA-C-N	5.34	127.43	120.28
39	Bi	7	LEU	C-N-CA	5.34	127.43	120.28
40	Bk	37	THR	CA-C-N	5.33	128.12	121.83
40	Bk	37	THR	C-N-CA	5.33	128.12	121.83
1	B0	186	GLN	CA-C-N	5.33	127.37	120.44
1	B0	186	GLN	C-N-CA	5.33	127.37	120.44
12	BB	68	ARG	CA-C-N	5.33	127.28	120.56
12	BB	68	ARG	C-N-CA	5.33	127.28	120.56
14	BD	31	PRO	CA-C-N	5.33	127.37	120.44
14	BD	31	PRO	C-N-CA	5.33	127.37	120.44
14	BD	124	ASN	CA-CB-CG	5.33	117.93	112.60
14	BD	265	ARG	CA-C-N	5.32	128.40	120.31
14	BD	265	ARG	C-N-CA	5.32	128.40	120.31
15	BE	833	PRO	CA-C-N	5.32	127.27	120.56
15	BE	833	PRO	C-N-CA	5.32	127.27	120.56
12	BB	32	ARG	CA-C-N	5.32	127.68	120.44
12	BB	32	ARG	C-N-CA	5.32	127.68	120.44
12	BB	228	GLN	CA-C-N	5.32	127.26	120.56
12	BB	228	GLN	C-N-CA	5.32	127.26	120.56
62	bS	18	U	C5'-C4'-O4'	5.32	117.08	109.10
3	B2	295	LEU	CA-C-N	5.32	129.10	121.50
3	B2	295	LEU	C-N-CA	5.32	129.10	121.50
40	Bk	40	PHE	CA-C-N	5.31	130.72	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Bk	40	PHE	C-N-CA	5.31	130.72	122.49
3	B2	46	ARG	CD-NE-CZ	5.31	131.83	124.40
18	BH	92	GLY	CA-C-N	5.31	130.82	123.07
18	BH	92	GLY	C-N-CA	5.31	130.82	123.07
39	Bi	127	PHE	CA-C-N	5.31	127.34	120.44
39	Bi	127	PHE	C-N-CA	5.31	127.34	120.44
7	B6	63	ARG	CA-C-N	5.31	129.47	122.30
7	B6	63	ARG	C-N-CA	5.31	129.47	122.30
14	BD	458	ARG	CA-C-N	5.31	128.39	122.55
14	BD	458	ARG	C-N-CA	5.31	128.39	122.55
25	BQ	355	GLN	CA-C-N	5.31	127.25	120.56
25	BQ	355	GLN	C-N-CA	5.31	127.25	120.56
40	Bk	300	ILE	N-CA-CB	5.30	116.59	110.49
4	B3	211	HIS	CA-CB-CG	5.30	119.10	113.80
40	Bk	294	LYS	CA-C-N	5.30	127.82	120.29
40	Bk	294	LYS	C-N-CA	5.30	127.82	120.29
25	BQ	374	ASP	CA-C-N	5.30	127.33	120.44
25	BQ	374	ASP	C-N-CA	5.30	127.33	120.44
42	HJ	680	ASP	CA-C-N	5.30	130.62	122.93
42	HJ	680	ASP	C-N-CA	5.30	130.62	122.93
14	BD	140	ASP	CA-CB-CG	5.29	117.89	112.60
39	Bi	124	TYR	CA-C-N	5.29	127.32	120.44
39	Bi	124	TYR	C-N-CA	5.29	127.32	120.44
1	B0	178	GLU	CA-C-N	5.29	127.32	120.44
1	B0	178	GLU	C-N-CA	5.29	127.32	120.44
40	Bk	259	THR	CA-C-N	5.29	127.80	120.29
40	Bk	259	THR	C-N-CA	5.29	127.80	120.29
3	B2	3	ASP	CA-C-N	5.29	130.62	123.11
3	B2	3	ASP	C-N-CA	5.29	130.62	123.11
7	B6	16	ALA	CA-C-N	5.29	127.37	120.28
7	B6	16	ALA	C-N-CA	5.29	127.37	120.28
3	B2	148	ARG	CD-NE-CZ	5.29	131.80	124.40
3	B2	59	ARG	CA-C-N	5.29	129.06	121.50
3	B2	59	ARG	C-N-CA	5.29	129.06	121.50
12	BB	170	HIS	ND1-CG-CD2	-5.29	100.81	106.10
16	BF	257	SER	N-CA-CB	5.29	117.78	110.17
39	Bi	86	ARG	CA-C-N	5.29	127.31	120.44
39	Bi	86	ARG	C-N-CA	5.29	127.31	120.44
12	BB	151	HIS	ND1-CG-CD2	-5.28	100.82	106.10
16	BF	260	HIS	ND1-CG-CD2	-5.28	100.82	106.10
12	BB	153	HIS	ND1-CG-CD2	-5.28	100.82	106.10
1	B0	159	LEU	CA-C-N	5.28	128.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B0	159	LEU	C-N-CA	5.28	128.33	120.31
3	B2	296	ASN	CA-CB-CG	5.28	117.88	112.60
12	BB	178	LEU	CA-C-N	5.28	127.30	120.44
12	BB	178	LEU	C-N-CA	5.28	127.30	120.44
39	Bi	123	SER	CA-C-N	5.28	127.30	120.44
39	Bi	123	SER	C-N-CA	5.28	127.30	120.44
42	HJ	682	ASP	CA-C-N	5.28	127.69	120.46
42	HJ	682	ASP	C-N-CA	5.28	127.69	120.46
12	BB	968	LEU	N-CA-CB	5.28	116.64	110.42
14	BD	323	VAL	CA-C-N	5.28	127.61	120.44
14	BD	323	VAL	C-N-CA	5.28	127.61	120.44
30	BW	278	LEU	CA-C-N	5.28	127.61	120.44
30	BW	278	LEU	C-N-CA	5.28	127.61	120.44
14	BD	33	HIS	ND1-CG-CD2	-5.27	100.83	106.10
12	BB	164	ALA	CA-C-N	5.27	127.20	120.56
12	BB	164	ALA	C-N-CA	5.27	127.20	120.56
39	Bi	128	ARG	CA-C-N	5.27	127.29	120.44
39	Bi	128	ARG	C-N-CA	5.27	127.29	120.44
40	Bk	32	HIS	CA-CB-CG	5.27	119.07	113.80
14	BD	240	ALA	CA-C-N	5.27	130.47	122.56
14	BD	240	ALA	C-N-CA	5.27	130.47	122.56
18	BH	119	MET	CA-C-N	5.27	130.85	122.94
18	BH	119	MET	C-N-CA	5.27	130.85	122.94
42	HJ	682	ASP	N-CA-CB	5.27	117.79	109.83
1	B0	164	ILE	CA-C-N	5.27	127.34	120.28
1	B0	164	ILE	C-N-CA	5.27	127.34	120.28
15	BE	508	HIS	ND1-CG-CD2	-5.27	100.83	106.10
37	Bg	98	GLU	CA-C-N	5.27	129.85	122.05
37	Bg	98	GLU	C-N-CA	5.27	129.85	122.05
14	BD	321	LEU	CA-C-N	5.26	127.28	120.44
14	BD	321	LEU	C-N-CA	5.26	127.28	120.44
40	Bk	295	SER	CA-C-N	5.26	127.63	120.63
40	Bk	295	SER	C-N-CA	5.26	127.63	120.63
3	B2	114	GLN	CA-C-N	5.26	127.33	120.28
3	B2	114	GLN	C-N-CA	5.26	127.33	120.28
15	BE	836	ASP	CA-C-N	5.26	127.19	120.56
15	BE	836	ASP	C-N-CA	5.26	127.19	120.56
1	B0	167	VAL	CA-C-N	5.26	127.28	120.44
1	B0	167	VAL	C-N-CA	5.26	127.28	120.44
25	BQ	277	GLY	CA-C-N	5.26	127.19	120.56
25	BQ	277	GLY	C-N-CA	5.26	127.19	120.56
1	B0	175	ALA	CA-C-N	5.26	127.28	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B0	175	ALA	C-N-CA	5.26	127.28	120.44
12	BB	309	HIS	ND1-CG-CD2	-5.26	100.84	106.10
15	BE	561	ASP	CA-C-N	5.26	127.75	120.29
15	BE	561	ASP	C-N-CA	5.26	127.75	120.29
30	BW	215	THR	CA-C-N	5.25	130.82	122.94
30	BW	215	THR	C-N-CA	5.25	130.82	122.94
37	Bg	166	VAL	CA-C-N	5.25	130.25	123.00
37	Bg	166	VAL	C-N-CA	5.25	130.25	123.00
42	HJ	707	LEU	N-CA-CB	5.25	117.72	109.69
42	HJ	678	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	B0	174	GLU	CA-C-N	5.25	127.26	120.44
1	B0	174	GLU	C-N-CA	5.25	127.26	120.44
12	BB	339	HIS	ND1-CG-CD2	-5.25	100.85	106.10
16	BF	263	TRP	CA-C-N	5.25	127.17	120.56
16	BF	263	TRP	C-N-CA	5.25	127.17	120.56
15	BE	478	HIS	ND1-CG-CD2	-5.25	100.85	106.10
16	BF	35	HIS	ND1-CG-CD2	-5.25	100.85	106.10
40	Bk	309	HIS	CA-C-N	5.25	127.17	120.56
40	Bk	309	HIS	C-N-CA	5.25	127.17	120.56
1	B0	160	ASP	CA-C-N	5.25	127.26	120.44
1	B0	160	ASP	C-N-CA	5.25	127.26	120.44
12	BB	230	ARG	CA-C-N	5.25	127.26	120.44
12	BB	230	ARG	C-N-CA	5.25	127.26	120.44
16	BF	242	PRO	CA-C-N	5.24	127.31	120.28
16	BF	242	PRO	C-N-CA	5.24	127.31	120.28
41	Bl	2	THR	CA-C-N	5.24	128.28	120.31
41	Bl	2	THR	C-N-CA	5.24	128.28	120.31
15	BE	496	PRO	CA-C-N	5.24	127.25	120.44
15	BE	496	PRO	C-N-CA	5.24	127.25	120.44
22	BL	77	VAL	CA-C-N	5.24	130.38	122.99
22	BL	77	VAL	C-N-CA	5.24	130.38	122.99
7	B6	2	PHE	CA-CB-CG	5.24	119.04	113.80
14	BD	255	VAL	CA-C-N	5.24	128.28	120.31
14	BD	255	VAL	C-N-CA	5.24	128.28	120.31
14	BD	373	HIS	ND1-CG-CD2	-5.24	100.86	106.10
12	BB	150	HIS	ND1-CG-CD2	-5.24	100.86	106.10
21	BK	80	GLU	CA-C-N	5.24	127.73	120.29
21	BK	80	GLU	C-N-CA	5.24	127.73	120.29
25	BQ	343	GLU	CA-C-N	5.24	127.16	120.56
25	BQ	343	GLU	C-N-CA	5.24	127.16	120.56
14	BD	20	ASP	CA-CB-CG	5.24	117.84	112.60
12	BB	39	HIS	ND1-CG-CD2	-5.23	100.87	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B6	5	THR	CA-C-N	5.23	130.54	123.11
7	B6	5	THR	C-N-CA	5.23	130.54	123.11
14	BD	202	TRP	CA-C-N	5.23	127.24	120.44
14	BD	202	TRP	C-N-CA	5.23	127.24	120.44
14	BD	472	SER	CA-C-N	5.23	127.24	120.44
14	BD	472	SER	C-N-CA	5.23	127.24	120.44
25	BQ	345	LEU	CA-C-N	5.23	127.15	120.56
25	BQ	345	LEU	C-N-CA	5.23	127.15	120.56
30	BW	239	LEU	CA-C-N	5.23	130.80	122.59
30	BW	239	LEU	C-N-CA	5.23	130.80	122.59
37	Bg	51	HIS	ND1-CG-CD2	-5.23	100.87	106.10
14	BD	176	PHE	CA-CB-CG	5.23	119.03	113.80
18	BH	85	PHE	CA-C-N	5.23	127.24	120.44
18	BH	85	PHE	C-N-CA	5.23	127.24	120.44
12	BB	166	CYS	CA-C-N	5.22	127.23	120.44
12	BB	166	CYS	C-N-CA	5.22	127.23	120.44
18	BH	12	LEU	N-CA-CB	5.22	117.03	110.45
25	BQ	319	GLN	CA-C-N	5.22	130.07	121.87
25	BQ	319	GLN	C-N-CA	5.22	130.07	121.87
12	BB	1129	VAL	CA-C-N	5.22	130.07	121.87
12	BB	1129	VAL	C-N-CA	5.22	130.07	121.87
40	Bk	29	LEU	CA-C-N	5.22	129.44	120.72
40	Bk	29	LEU	C-N-CA	5.22	129.44	120.72
1	B0	177	TRP	CA-C-N	5.22	127.23	120.44
1	B0	177	TRP	C-N-CA	5.22	127.23	120.44
14	BD	251	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	B0	176	GLN	CA-C-N	5.22	127.22	120.44
1	B0	176	GLN	C-N-CA	5.22	127.22	120.44
30	BW	335	LEU	N-CA-CB	5.22	117.64	109.97
30	BW	314	SER	CA-C-N	5.22	127.22	120.44
30	BW	314	SER	C-N-CA	5.22	127.22	120.44
12	BB	227	LEU	CA-C-N	5.22	127.22	120.44
12	BB	227	LEU	C-N-CA	5.22	127.22	120.44
12	BB	314	PHE	N-CA-CB	5.21	117.57	110.01
15	BE	484	THR	CA-C-N	5.21	127.22	120.44
15	BE	484	THR	C-N-CA	5.21	127.22	120.44
16	BF	253	HIS	ND1-CG-CD2	-5.21	100.89	106.10
30	BW	149	VAL	N-CA-CB	5.21	115.92	111.64
38	Bh	8	PHE	CA-CB-CG	5.21	119.01	113.80
14	BD	198	MET	CA-C-N	5.21	127.22	120.44
14	BD	198	MET	C-N-CA	5.21	127.22	120.44
30	BW	318	LEU	CA-C-N	5.21	127.27	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BW	318	LEU	C-N-CA	5.21	127.27	120.28
16	BF	31	HIS	ND1-CG-CD2	-5.21	100.89	106.10
30	BW	290	HIS	ND1-CG-CD2	-5.21	100.89	106.10
39	Bi	131	VAL	CA-C-N	5.21	127.26	120.28
39	Bi	131	VAL	C-N-CA	5.21	127.26	120.28
42	HJ	726	ILE	N-CA-CB	5.21	116.40	110.72
1	B0	260	VAL	CA-C-N	5.21	127.60	120.46
1	B0	260	VAL	C-N-CA	5.21	127.60	120.46
12	BB	952	ARG	CD-NE-CZ	5.21	131.69	124.40
15	BE	915	PRO	CA-N-CD	-5.21	104.71	112.00
21	BK	45	GLU	CA-C-N	5.21	127.21	120.44
21	BK	45	GLU	C-N-CA	5.21	127.21	120.44
30	BW	10	ASN	CA-CB-CG	5.21	117.81	112.60
42	HJ	620	LEU	N-CA-CB	5.21	117.73	109.71
7	B6	27	ALA	CA-C-N	5.21	127.26	120.28
7	B6	27	ALA	C-N-CA	5.21	127.26	120.28
14	BD	165	PHE	CA-C-N	5.21	130.74	122.62
14	BD	165	PHE	C-N-CA	5.21	130.74	122.62
4	B3	14	VAL	N-CA-CB	5.21	116.71	110.31
14	BD	392	HIS	ND1-CG-CD2	-5.21	100.89	106.10
30	BW	255	PHE	CA-C-N	5.21	131.25	123.23
30	BW	255	PHE	C-N-CA	5.21	131.25	123.23
12	BB	983	ARG	CD-NE-CZ	5.20	131.69	124.40
12	BB	1007	ARG	CD-NE-CZ	5.20	131.68	124.40
22	BL	19	ASN	CA-C-N	5.20	128.94	121.50
22	BL	19	ASN	C-N-CA	5.20	128.94	121.50
42	HJ	746	ALA	CA-C-N	5.20	127.25	120.28
42	HJ	746	ALA	C-N-CA	5.20	127.25	120.28
7	B6	62	GLY	CA-C-N	5.20	129.68	122.77
7	B6	62	GLY	C-N-CA	5.20	129.68	122.77
16	BF	37	PHE	N-CA-CB	5.20	117.72	109.51
1	B0	47	HIS	ND1-CG-CD2	-5.20	100.90	106.10
15	BE	561	ASP	CA-CB-CG	5.20	117.80	112.60
25	BQ	271	LEU	CA-C-N	5.20	129.78	122.09
25	BQ	271	LEU	C-N-CA	5.20	129.78	122.09
42	HJ	719	PRO	CA-C-N	5.20	127.19	120.44
42	HJ	719	PRO	C-N-CA	5.20	127.19	120.44
21	BK	84	ALA	CA-C-N	5.19	128.20	120.31
21	BK	84	ALA	C-N-CA	5.19	128.20	120.31
1	B0	171	ARG	CA-C-N	5.19	127.19	120.44
1	B0	171	ARG	C-N-CA	5.19	127.19	120.44
7	B6	28	LEU	CA-C-N	5.19	127.10	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B6	28	LEU	C-N-CA	5.19	127.10	120.56
16	BF	251	HIS	ND1-CG-CD2	-5.19	100.91	106.10
18	BH	90	ASN	CA-C-N	5.19	130.70	122.60
18	BH	90	ASN	C-N-CA	5.19	130.70	122.60
25	BQ	379	ALA	CA-C-N	5.19	127.19	120.44
25	BQ	379	ALA	C-N-CA	5.19	127.19	120.44
25	BQ	515	GLY	CA-C-N	5.19	130.40	122.92
25	BQ	515	GLY	C-N-CA	5.19	130.40	122.92
14	BD	33	HIS	CA-C-N	5.19	127.19	120.44
14	BD	33	HIS	C-N-CA	5.19	127.19	120.44
15	BE	412	ALA	CA-C-N	5.19	127.23	120.28
15	BE	412	ALA	C-N-CA	5.19	127.23	120.28
14	BD	318	HIS	ND1-CG-CD2	-5.19	100.91	106.10
30	BW	326	GLY	CA-C-N	5.19	127.18	120.44
30	BW	326	GLY	C-N-CA	5.19	127.18	120.44
12	BB	70	VAL	CA-C-N	5.18	127.18	120.44
12	BB	70	VAL	C-N-CA	5.18	127.18	120.44
3	B2	50	PHE	CA-CB-CG	5.18	118.98	113.80
14	BD	256	GLU	CA-C-N	5.18	127.18	120.44
14	BD	256	GLU	C-N-CA	5.18	127.18	120.44
14	BD	263	GLU	CA-C-N	5.18	127.18	120.44
14	BD	263	GLU	C-N-CA	5.18	127.18	120.44
3	B2	290	SER	CA-C-N	5.18	127.22	120.28
3	B2	290	SER	C-N-CA	5.18	127.22	120.28
14	BD	164	HIS	ND1-CG-CD2	-5.18	100.92	106.10
15	BE	902	PHE	N-CA-CB	-5.18	102.29	110.06
14	BD	318	HIS	CA-C-N	5.18	127.17	120.44
14	BD	318	HIS	C-N-CA	5.18	127.17	120.44
3	B2	134	ARG	N-CA-CB	5.18	117.52	110.01
12	BB	1112	ARG	CD-NE-CZ	5.18	131.65	124.40
37	Bg	63	PHE	CA-CB-CG	5.18	118.98	113.80
3	B2	117	ALA	CA-C-N	5.17	127.21	120.28
3	B2	117	ALA	C-N-CA	5.17	127.21	120.28
3	B2	268	GLU	CA-C-N	5.17	127.22	120.28
3	B2	268	GLU	C-N-CA	5.17	127.22	120.28
30	BW	320	ARG	CA-C-N	5.17	127.17	120.44
30	BW	320	ARG	C-N-CA	5.17	127.17	120.44
15	BE	808	THR	CA-C-N	5.17	127.16	120.44
15	BE	808	THR	C-N-CA	5.17	127.16	120.44
25	BQ	376	THR	CA-C-N	5.17	127.21	120.28
25	BQ	376	THR	C-N-CA	5.17	127.21	120.28
14	BD	151	ARG	CD-NE-CZ	5.17	131.64	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BD	3	ARG	CD-NE-CZ	5.17	131.63	124.40
15	BE	506	LEU	N-CA-CB	5.17	117.50	110.01
15	BE	812	THR	CA-C-N	5.17	127.63	120.29
15	BE	812	THR	C-N-CA	5.17	127.63	120.29
12	BB	1019	HIS	CA-CB-CG	5.17	118.97	113.80
21	BK	44	ARG	CA-C-N	5.16	127.15	120.44
21	BK	44	ARG	C-N-CA	5.16	127.15	120.44
56	bL	45	G	C1'-C2'-O2'	5.16	116.14	108.40
23	BO	43	LEU	CA-C-N	5.16	128.53	120.68
23	BO	43	LEU	C-N-CA	5.16	128.53	120.68
40	Bk	15	ALA	CA-C-N	5.16	130.30	122.56
40	Bk	15	ALA	C-N-CA	5.16	130.30	122.56
1	B0	238	PHE	CA-C-N	5.16	127.14	120.44
1	B0	238	PHE	C-N-CA	5.16	127.14	120.44
21	BK	41	PRO	CA-C-N	5.16	127.15	120.44
21	BK	41	PRO	C-N-CA	5.16	127.15	120.44
30	BW	313	MET	CA-C-N	5.16	127.14	120.44
30	BW	313	MET	C-N-CA	5.16	127.14	120.44
3	B2	267	ASP	CA-C-N	5.16	127.14	120.44
3	B2	267	ASP	C-N-CA	5.16	127.14	120.44
38	Bh	130	GLU	CA-C-N	5.16	127.19	120.28
38	Bh	130	GLU	C-N-CA	5.16	127.19	120.28
42	HJ	759	ARG	CA-C-N	5.16	127.19	120.28
42	HJ	759	ARG	C-N-CA	5.16	127.19	120.28
15	BE	507	LEU	CA-C-N	5.15	127.14	120.44
15	BE	507	LEU	C-N-CA	5.15	127.14	120.44
40	Bk	42	ASN	N-CA-CB	5.15	117.58	109.69
1	B0	296	GLU	CA-C-N	5.15	127.14	120.44
1	B0	296	GLU	C-N-CA	5.15	127.14	120.44
14	BD	122	GLY	CA-C-N	5.15	127.14	120.44
14	BD	122	GLY	C-N-CA	5.15	127.14	120.44
15	BE	411	PHE	CA-C-N	5.15	127.18	120.28
15	BE	411	PHE	C-N-CA	5.15	127.18	120.28
30	BW	311	LEU	CA-C-N	5.15	127.18	120.28
30	BW	311	LEU	C-N-CA	5.15	127.18	120.28
41	Bl	20	LYS	CA-CB-CG	5.15	124.41	114.10
1	B0	38	GLU	CA-C-N	5.15	127.14	120.44
1	B0	38	GLU	C-N-CA	5.15	127.14	120.44
12	BB	64	VAL	N-CA-CB	5.15	116.41	110.49
12	BB	342	GLU	CA-C-N	5.15	127.18	120.28
12	BB	342	GLU	C-N-CA	5.15	127.18	120.28
21	BK	51	HIS	ND1-CG-CD2	-5.15	100.95	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BB	165	ILE	CA-C-N	5.15	127.13	120.44
12	BB	165	ILE	C-N-CA	5.15	127.13	120.44
14	BD	470	ARG	N-CA-CB	5.15	117.48	110.01
40	Bk	309	HIS	ND1-CG-CD2	-5.15	100.95	106.10
42	HJ	681	PHE	CA-C-N	5.15	128.02	120.71
42	HJ	681	PHE	C-N-CA	5.15	128.02	120.71
1	B0	158	ALA	CA-C-N	5.15	127.18	120.28
1	B0	158	ALA	C-N-CA	5.15	127.18	120.28
1	B0	166	PHE	CA-C-N	5.15	127.15	120.56
1	B0	166	PHE	C-N-CA	5.15	127.15	120.56
3	B2	286	CYS	CA-C-N	5.15	127.15	120.56
3	B2	286	CYS	C-N-CA	5.15	127.15	120.56
14	BD	441	ALA	CA-C-N	5.15	130.19	122.47
14	BD	441	ALA	C-N-CA	5.15	130.19	122.47
15	BE	483	GLY	CA-C-N	5.15	127.44	120.44
15	BE	483	GLY	C-N-CA	5.15	127.44	120.44
37	Bg	215	SER	CA-C-N	5.15	130.65	122.62
37	Bg	215	SER	C-N-CA	5.15	130.65	122.62
15	BE	509	ALA	CA-C-N	5.15	127.13	120.44
15	BE	509	ALA	C-N-CA	5.15	127.13	120.44
1	B0	294	ARG	CA-C-N	5.14	127.13	120.44
1	B0	294	ARG	C-N-CA	5.14	127.13	120.44
30	BW	321	ARG	CA-C-N	5.14	127.13	120.44
30	BW	321	ARG	C-N-CA	5.14	127.13	120.44
38	Bh	129	ARG	CA-C-N	5.14	128.13	120.31
38	Bh	129	ARG	C-N-CA	5.14	128.13	120.31
42	HJ	676	LEU	CA-C-N	5.14	130.66	122.94
42	HJ	676	LEU	C-N-CA	5.14	130.66	122.94
7	B6	78	GLU	CA-C-N	5.14	127.17	120.28
7	B6	78	GLU	C-N-CA	5.14	127.17	120.28
12	BB	1126	LYS	CA-CB-CG	5.14	124.38	114.10
13	BC	202	VAL	CA-C-N	5.14	127.12	120.44
13	BC	202	VAL	C-N-CA	5.14	127.12	120.44
25	BQ	374	ASP	N-CA-CB	5.14	117.55	109.69
1	B0	268	ARG	N-CA-CB	5.14	117.46	110.01
25	BQ	387	ALA	CA-C-N	5.14	127.12	120.44
25	BQ	387	ALA	C-N-CA	5.14	127.12	120.44
3	B2	264	TYR	CA-C-N	5.14	127.12	120.44
3	B2	264	TYR	C-N-CA	5.14	127.12	120.44
12	BB	264	ARG	CA-C-N	5.14	127.13	120.56
12	BB	264	ARG	C-N-CA	5.14	127.13	120.56
14	BD	235	VAL	CA-C-N	5.14	127.12	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BD	235	VAL	C-N-CA	5.14	127.12	120.44
14	BD	449	GLY	CA-C-N	5.14	129.93	123.10
14	BD	449	GLY	C-N-CA	5.14	129.93	123.10
15	BE	488	MET	CA-C-N	5.14	127.12	120.44
15	BE	488	MET	C-N-CA	5.14	127.12	120.44
15	BE	550	GLU	CA-C-N	5.14	127.12	120.44
15	BE	550	GLU	C-N-CA	5.14	127.12	120.44
12	BB	71	ASP	N-CA-CB	5.13	117.45	110.01
12	BB	987	PHE	CA-CB-CG	5.13	118.93	113.80
1	B0	295	LEU	CA-C-N	5.13	127.16	120.28
1	B0	295	LEU	C-N-CA	5.13	127.16	120.28
12	BB	1139	ALA	CA-C-N	5.13	127.11	120.44
12	BB	1139	ALA	C-N-CA	5.13	127.11	120.44
14	BD	252	GLN	CA-C-N	5.13	127.58	120.29
14	BD	252	GLN	C-N-CA	5.13	127.58	120.29
14	BD	311	LEU	N-CA-CB	5.13	117.45	110.01
15	BE	609	LEU	CA-C-N	5.13	127.11	120.44
15	BE	609	LEU	C-N-CA	5.13	127.11	120.44
22	BL	92	TYR	CA-C-N	5.13	130.07	122.94
22	BL	92	TYR	C-N-CA	5.13	130.07	122.94
25	BQ	375	ALA	CA-C-N	5.13	127.11	120.44
25	BQ	375	ALA	C-N-CA	5.13	127.11	120.44
15	BE	826	HIS	ND1-CG-CD2	-5.13	100.97	106.10
1	B0	270	THR	CA-C-N	5.13	127.15	120.28
1	B0	270	THR	C-N-CA	5.13	127.15	120.28
3	B2	58	ASN	CA-CB-CG	5.13	117.73	112.60
12	BB	948	ARG	CD-NE-CZ	5.13	131.58	124.40
14	BD	317	SER	CA-C-N	5.13	127.11	120.44
14	BD	317	SER	C-N-CA	5.13	127.11	120.44
21	BK	47	ILE	CA-C-N	5.13	127.15	120.28
21	BK	47	ILE	C-N-CA	5.13	127.15	120.28
30	BW	317	GLN	CA-C-N	5.13	127.11	120.44
30	BW	317	GLN	C-N-CA	5.13	127.11	120.44
37	Bg	68	PHE	CA-C-N	5.13	127.11	120.44
37	Bg	68	PHE	C-N-CA	5.13	127.11	120.44
3	B2	22	THR	CA-C-N	5.13	128.13	120.95
3	B2	22	THR	C-N-CA	5.13	128.13	120.95
12	BB	260	GLU	N-CA-CB	5.13	117.44	110.01
14	BD	99	ALA	CA-C-N	5.13	127.15	120.28
14	BD	99	ALA	C-N-CA	5.13	127.15	120.28
14	BD	206	LEU	N-CA-CB	5.13	117.57	109.83
21	BK	50	LEU	CA-C-N	5.13	127.11	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	BK	50	LEU	C-N-CA	5.13	127.11	120.44
12	BB	38	LEU	CA-C-N	5.12	127.10	120.44
12	BB	38	LEU	C-N-CA	5.12	127.10	120.44
15	BE	521	VAL	CA-C-N	5.12	127.10	120.44
15	BE	521	VAL	C-N-CA	5.12	127.10	120.44
1	B0	180	LYS	CA-C-N	5.12	127.10	120.44
1	B0	180	LYS	C-N-CA	5.12	127.10	120.44
14	BD	138	LEU	N-CA-CB	5.12	117.44	110.01
14	BD	313	LEU	CA-C-N	5.12	127.41	120.65
14	BD	313	LEU	C-N-CA	5.12	127.41	120.65
14	BD	320	ARG	CA-C-N	5.12	127.57	120.29
14	BD	320	ARG	C-N-CA	5.12	127.57	120.29
15	BE	410	LEU	CA-C-N	5.12	127.10	120.44
15	BE	410	LEU	C-N-CA	5.12	127.10	120.44
37	Bg	80	TYR	CA-C-N	5.12	128.10	120.31
37	Bg	80	TYR	C-N-CA	5.12	128.10	120.31
40	Bk	76	HIS	CA-C-N	5.12	128.15	120.87
40	Bk	76	HIS	C-N-CA	5.12	128.15	120.87
1	B0	239	GLU	CA-C-N	5.12	127.66	120.28
1	B0	239	GLU	C-N-CA	5.12	127.66	120.28
12	BB	61	ARG	CA-C-N	5.12	127.59	120.63
12	BB	61	ARG	C-N-CA	5.12	127.59	120.63
15	BE	394	ARG	CA-C-N	5.12	127.10	120.44
15	BE	394	ARG	C-N-CA	5.12	127.10	120.44
15	BE	535	ASP	CA-CB-CG	5.12	117.72	112.60
1	B0	6	TRP	CA-C-N	5.12	130.84	122.65
1	B0	6	TRP	C-N-CA	5.12	130.84	122.65
1	B0	144	HIS	CA-C-N	5.12	127.09	120.44
1	B0	144	HIS	C-N-CA	5.12	127.09	120.44
12	BB	52	LEU	N-CA-CB	5.12	117.43	110.01
12	BB	259	TYR	CA-C-N	5.12	127.09	120.44
12	BB	259	TYR	C-N-CA	5.12	127.09	120.44
12	BB	1108	ARG	CD-NE-CZ	5.12	131.57	124.40
14	BD	195	PHE	CA-CB-CG	5.12	118.92	113.80
22	BL	16	PHE	CA-CB-CG	5.12	118.92	113.80
41	Bl	122	SER	CA-C-N	5.12	127.14	120.28
41	Bl	122	SER	C-N-CA	5.12	127.14	120.28
14	BD	316	GLU	CA-C-N	5.12	127.09	120.44
14	BD	316	GLU	C-N-CA	5.12	127.09	120.44
37	Bg	69	HIS	ND1-CG-CD2	-5.12	100.98	106.10
21	BK	81	PHE	CA-C-N	5.12	127.09	120.44
21	BK	81	PHE	C-N-CA	5.12	127.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	BK	88	ARG	CA-C-N	5.12	127.09	120.44
21	BK	88	ARG	C-N-CA	5.12	127.09	120.44
22	BL	78	ARG	CA-C-N	5.12	129.82	122.45
22	BL	78	ARG	C-N-CA	5.12	129.82	122.45
7	B6	89	VAL	N-CA-CB	5.11	116.93	111.46
16	BF	259	ARG	N-CA-CB	5.11	117.56	110.04
25	BQ	203	GLU	CA-C-N	5.11	127.09	120.44
25	BQ	203	GLU	C-N-CA	5.11	127.09	120.44
41	Bl	14	ARG	N-CA-CB	5.11	117.92	110.30
30	BW	204	ASP	N-CA-CB	5.11	117.42	110.01
1	B0	297	GLU	CA-C-N	5.11	127.08	120.44
1	B0	297	GLU	C-N-CA	5.11	127.08	120.44
12	BB	216	GLU	CA-C-N	5.11	127.13	120.28
12	BB	216	GLU	C-N-CA	5.11	127.13	120.28
14	BD	126	LEU	CA-C-N	5.11	127.00	120.56
14	BD	126	LEU	C-N-CA	5.11	127.00	120.56
15	BE	471	GLU	CA-C-N	5.11	127.08	120.44
15	BE	471	GLU	C-N-CA	5.11	127.08	120.44
21	BK	48	PHE	CA-C-N	5.11	127.08	120.44
21	BK	48	PHE	C-N-CA	5.11	127.08	120.44
25	BQ	312	ALA	CA-C-N	5.11	127.08	120.44
25	BQ	312	ALA	C-N-CA	5.11	127.08	120.44
12	BB	225	LEU	CA-C-N	5.11	127.12	120.28
12	BB	225	LEU	C-N-CA	5.11	127.12	120.28
38	Bh	124	ARG	CA-C-N	5.11	127.08	120.44
38	Bh	124	ARG	C-N-CA	5.11	127.08	120.44
12	BB	310	ALA	CA-C-N	5.11	127.08	120.44
12	BB	310	ALA	C-N-CA	5.11	127.08	120.44
15	BE	395	LEU	CA-C-N	5.11	127.08	120.44
15	BE	395	LEU	C-N-CA	5.11	127.08	120.44
15	BE	527	ALA	CA-C-N	5.11	127.08	120.44
15	BE	527	ALA	C-N-CA	5.11	127.08	120.44
37	Bg	84	HIS	ND1-CG-CD2	-5.10	101.00	106.10
40	Bk	38	GLY	CA-C-N	5.10	128.02	120.82
40	Bk	38	GLY	C-N-CA	5.10	128.02	120.82
1	B0	142	LEU	N-CA-CB	5.10	117.41	110.01
1	B0	247	PRO	CA-C-N	5.10	129.19	122.30
1	B0	247	PRO	C-N-CA	5.10	129.19	122.30
1	B0	268	ARG	CA-C-N	5.10	127.07	120.44
1	B0	268	ARG	C-N-CA	5.10	127.07	120.44
12	BB	427	VAL	CA-C-N	5.10	129.81	122.16
12	BB	427	VAL	C-N-CA	5.10	129.81	122.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BD	208	PRO	CA-C-N	5.10	127.12	120.28
14	BD	208	PRO	C-N-CA	5.10	127.12	120.28
16	BF	33	ARG	CA-C-N	5.10	127.12	120.28
16	BF	33	ARG	C-N-CA	5.10	127.12	120.28
3	B2	111	GLU	CA-C-N	5.10	127.12	120.28
3	B2	111	GLU	C-N-CA	5.10	127.12	120.28
1	B0	267	GLN	CA-C-N	5.10	127.07	120.44
1	B0	267	GLN	C-N-CA	5.10	127.07	120.44
14	BD	236	ALA	CA-C-N	5.10	127.11	120.28
14	BD	236	ALA	C-N-CA	5.10	127.11	120.28
15	BE	470	CYS	CA-C-N	5.10	127.07	120.44
15	BE	470	CYS	C-N-CA	5.10	127.07	120.44
15	BE	508	HIS	N-CA-CB	5.10	117.41	110.01
22	BL	65	HIS	CA-CB-CG	5.10	118.90	113.80
1	B0	269	GLU	CA-C-N	5.10	127.07	120.44
1	B0	269	GLU	C-N-CA	5.10	127.07	120.44
15	BE	489	LEU	N-CA-CB	5.10	117.40	110.01
15	BE	508	HIS	CA-C-N	5.10	127.07	120.44
15	BE	508	HIS	C-N-CA	5.10	127.07	120.44
37	Bg	180	HIS	ND1-CG-CD2	-5.10	101.00	106.10
40	Bk	281	ASP	CA-C-N	5.10	127.53	120.29
40	Bk	281	ASP	C-N-CA	5.10	127.53	120.29
62	bS	19	U	C4'-C3'-O3'	-5.10	105.35	113.00
16	BF	262	PHE	CA-C-N	5.10	127.11	120.28
16	BF	262	PHE	C-N-CA	5.10	127.11	120.28
14	BD	199	ARG	N-CA-CB	5.09	117.40	110.01
14	BD	386	GLU	CA-C-N	5.09	127.06	120.44
14	BD	386	GLU	C-N-CA	5.09	127.06	120.44
12	BB	35	LEU	N-CA-CB	5.09	117.39	110.01
14	BD	203	GLN	N-CA-CB	5.09	117.39	110.01
21	BK	49	PHE	N-CA-CB	5.09	117.39	110.01
25	BQ	311	ARG	CA-C-N	5.09	127.06	120.44
25	BQ	311	ARG	C-N-CA	5.09	127.06	120.44
30	BW	308	ASP	CA-C-N	5.09	127.06	120.44
30	BW	308	ASP	C-N-CA	5.09	127.06	120.44
40	Bk	74	LYS	CA-C-N	5.09	128.10	120.87
40	Bk	74	LYS	C-N-CA	5.09	128.10	120.87
30	BW	149	VAL	CA-C-N	5.09	127.51	120.49
30	BW	149	VAL	C-N-CA	5.09	127.51	120.49
42	HJ	741	ARG	CA-C-N	5.09	129.85	123.03
42	HJ	741	ARG	C-N-CA	5.09	129.85	123.03
12	BB	177	LEU	CA-C-N	5.09	127.60	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BB	177	LEU	C-N-CA	5.09	127.60	120.28
25	BQ	327	PRO	CA-C-N	5.09	129.13	121.40
25	BQ	327	PRO	C-N-CA	5.09	129.13	121.40
25	BQ	366	ARG	CD-NE-CZ	5.09	131.52	124.40
37	Bg	178	PRO	CA-C-N	5.09	130.20	122.37
37	Bg	178	PRO	C-N-CA	5.09	130.20	122.37
1	B0	297	GLU	N-CA-CB	5.08	117.38	110.01
14	BD	98	SER	CA-C-N	5.08	127.05	120.44
14	BD	98	SER	C-N-CA	5.08	127.05	120.44
15	BE	395	LEU	N-CA-CB	5.08	117.38	110.01
1	B0	145	LEU	N-CA-CB	5.08	117.38	110.01
1	B0	305	ARG	CA-C-N	5.08	131.07	123.24
1	B0	305	ARG	C-N-CA	5.08	131.07	123.24
12	BB	51	ASP	CA-C-N	5.08	127.05	120.44
12	BB	51	ASP	C-N-CA	5.08	127.05	120.44
14	BD	123	LEU	N-CA-CB	5.08	117.38	110.01
14	BD	138	LEU	CA-C-N	5.08	128.04	120.31
14	BD	138	LEU	C-N-CA	5.08	128.04	120.31
22	BL	59	THR	CA-C-N	5.08	130.27	122.95
22	BL	59	THR	C-N-CA	5.08	130.27	122.95
40	Bk	45	LYS	CA-C-N	5.08	127.60	120.28
40	Bk	45	LYS	C-N-CA	5.08	127.60	120.28
15	BE	837	VAL	CA-C-N	5.08	127.05	120.44
15	BE	837	VAL	C-N-CA	5.08	127.05	120.44
15	BE	916	GLN	N-CA-CB	-5.08	102.36	110.03
14	BD	203	GLN	CA-C-N	5.08	128.06	120.95
14	BD	203	GLN	C-N-CA	5.08	128.06	120.95
12	BB	428	ALA	CA-C-N	5.08	127.08	120.28
12	BB	428	ALA	C-N-CA	5.08	127.08	120.28
25	BQ	382	ALA	CA-C-N	5.08	127.04	120.44
25	BQ	382	ALA	C-N-CA	5.08	127.04	120.44
41	Bl	4	SER	CA-C-N	5.08	128.69	121.02
41	Bl	4	SER	C-N-CA	5.08	128.69	121.02
14	BD	257	ARG	CG-CD-NE	5.07	123.16	112.00
41	Bl	123	LYS	CA-C-N	5.07	127.04	120.44
41	Bl	123	LYS	C-N-CA	5.07	127.04	120.44
65	bV	6	U	C2'-C3'-O3'	5.07	117.11	109.50
1	B0	302	LEU	N-CA-CB	5.07	117.31	109.91
21	BK	46	TYR	N-CA-CB	5.07	117.36	110.01
25	BQ	377	ASN	CA-C-N	5.07	127.03	120.44
25	BQ	377	ASN	C-N-CA	5.07	127.03	120.44
30	BW	277	GLN	CA-CB-CG	5.07	124.24	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BD	473	ASP	N-CA-CB	5.07	117.36	110.01
30	BW	309	ALA	CA-C-N	5.07	127.03	120.44
30	BW	309	ALA	C-N-CA	5.07	127.03	120.44
37	Bg	85	SER	CA-C-N	5.07	128.38	120.68
37	Bg	85	SER	C-N-CA	5.07	128.38	120.68
1	B0	150	ARG	CA-C-N	5.07	130.07	122.47
1	B0	150	ARG	C-N-CA	5.07	130.07	122.47
12	BB	37	VAL	CA-C-N	5.07	127.58	120.28
12	BB	37	VAL	C-N-CA	5.07	127.58	120.28
25	BQ	381	LEU	CA-C-N	5.07	127.07	120.28
25	BQ	381	LEU	C-N-CA	5.07	127.07	120.28
37	Bg	169	PRO	CA-C-N	5.07	130.27	122.42
37	Bg	169	PRO	C-N-CA	5.07	130.27	122.42
14	BD	96	ALA	CA-C-N	5.07	129.14	122.30
14	BD	96	ALA	C-N-CA	5.07	129.14	122.30
37	Bg	213	CYS	N-CA-CB	5.07	117.50	110.26
37	Bg	170	ARG	CA-CB-CG	5.06	124.23	114.10
1	B0	141	ARG	CA-C-N	5.06	127.02	120.44
1	B0	141	ARG	C-N-CA	5.06	127.02	120.44
3	B2	150	HIS	CA-CB-CG	5.06	118.86	113.80
12	BB	59	CYS	CA-C-N	5.06	127.02	120.44
12	BB	59	CYS	C-N-CA	5.06	127.02	120.44
14	BD	471	SER	CA-C-N	5.06	130.27	122.42
14	BD	471	SER	C-N-CA	5.06	130.27	122.42
16	BF	243	LEU	CA-C-N	5.06	127.06	120.28
16	BF	243	LEU	C-N-CA	5.06	127.06	120.28
25	BQ	313	LEU	CA-C-N	5.06	127.02	120.44
25	BQ	313	LEU	C-N-CA	5.06	127.02	120.44
12	BB	34	LEU	CA-C-N	5.06	127.02	120.44
12	BB	34	LEU	C-N-CA	5.06	127.02	120.44
14	BD	257	ARG	CA-CB-CG	5.06	124.22	114.10
1	B0	139	LYS	N-CA-CB	5.06	117.34	110.01
12	BB	1022	ARG	CD-NE-CZ	5.06	131.48	124.40
25	BQ	351	GLU	CA-C-N	5.06	127.01	120.44
25	BQ	351	GLU	C-N-CA	5.06	127.01	120.44
38	Bh	125	GLU	N-CA-CB	5.06	117.34	110.01
14	BD	469	ILE	CA-C-N	5.06	127.01	120.44
14	BD	469	ILE	C-N-CA	5.06	127.01	120.44
25	BQ	385	ALA	CA-C-N	5.06	127.01	120.44
25	BQ	385	ALA	C-N-CA	5.06	127.01	120.44
39	Bi	128	ARG	N-CA-CB	5.06	117.34	110.01
30	BW	316	LEU	CA-C-N	5.05	127.01	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BW	316	LEU	C-N-CA	5.05	127.01	120.44
56	bL	46	U	C1'-C2'-O2'	5.05	115.98	108.40
14	BD	207	ARG	CG-CD-NE	5.05	123.12	112.00
15	BE	528	PHE	N-CA-CB	5.05	117.34	110.01
39	Bi	124	TYR	N-CA-CB	5.05	117.34	110.01
1	B0	42	ARG	CA-C-N	5.05	127.56	120.28
1	B0	42	ARG	C-N-CA	5.05	127.56	120.28
12	BB	58	VAL	CA-C-N	5.05	127.05	120.28
12	BB	58	VAL	C-N-CA	5.05	127.05	120.28
14	BD	32	LEU	N-CA-CB	5.05	117.33	110.01
14	BD	205	ALA	CA-C-N	5.05	127.88	120.71
14	BD	205	ALA	C-N-CA	5.05	127.88	120.71
25	BQ	352	GLN	N-CA-CB	5.05	117.33	110.01
42	HJ	604	ARG	CD-NE-CZ	5.05	131.47	124.40
1	B0	142	LEU	CA-C-N	5.05	127.00	120.44
1	B0	142	LEU	C-N-CA	5.05	127.00	120.44
12	BB	265	VAL	CA-C-N	5.05	127.94	120.82
12	BB	265	VAL	C-N-CA	5.05	127.94	120.82
16	BF	248	TYR	N-CA-CB	5.05	117.28	109.91
16	BF	250	ARG	CA-C-N	5.05	130.32	122.49
16	BF	250	ARG	C-N-CA	5.05	130.32	122.49
25	BQ	378	ALA	CA-C-N	5.05	127.00	120.44
25	BQ	378	ALA	C-N-CA	5.05	127.00	120.44
14	BD	209	ALA	CA-C-N	5.05	127.55	120.28
14	BD	209	ALA	C-N-CA	5.05	127.55	120.28
25	BQ	274	PRO	CA-C-N	5.05	127.88	120.71
25	BQ	274	PRO	C-N-CA	5.05	127.88	120.71
3	B2	133	ARG	CA-C-N	5.05	127.00	120.44
3	B2	133	ARG	C-N-CA	5.05	127.00	120.44
12	BB	67	PHE	CA-C-N	5.05	129.14	120.71
12	BB	67	PHE	C-N-CA	5.05	129.14	120.71
25	BQ	383	GLU	CA-C-N	5.05	127.04	120.28
25	BQ	383	GLU	C-N-CA	5.05	127.04	120.28
25	BQ	384	ALA	CA-C-N	5.05	127.00	120.44
25	BQ	384	ALA	C-N-CA	5.05	127.00	120.44
42	HJ	759	ARG	CG-CD-NE	5.05	123.10	112.00
16	BF	247	LEU	CA-C-N	5.04	127.31	120.65
16	BF	247	LEU	C-N-CA	5.04	127.31	120.65
30	BW	319	LEU	CA-C-N	5.04	127.00	120.44
30	BW	319	LEU	C-N-CA	5.04	127.00	120.44
56	bL	44	A	C1'-C2'-O2'	5.04	115.97	108.40
1	B0	253	LEU	CA-C-N	5.04	127.54	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B0	253	LEU	C-N-CA	5.04	127.54	120.28
12	BB	139	PHE	N-CA-CB	5.04	117.32	110.01
14	BD	259	LEU	N-CA-CB	5.04	117.32	110.01
14	BD	319	ASN	CA-C-N	5.04	127.03	120.28
14	BD	319	ASN	C-N-CA	5.04	127.03	120.28
15	BE	559	GLU	CA-C-N	5.04	127.04	120.28
15	BE	559	GLU	C-N-CA	5.04	127.04	120.28
15	BE	918	HIS	CA-CB-CG	5.04	118.84	113.80
25	BQ	196	GLY	CA-C-N	5.04	127.03	120.28
25	BQ	196	GLY	C-N-CA	5.04	127.03	120.28
42	HJ	721	LEU	CA-C-N	5.04	127.04	120.28
42	HJ	721	LEU	C-N-CA	5.04	127.04	120.28
14	BD	264	GLU	CA-C-N	5.04	127.45	120.29
14	BD	264	GLU	C-N-CA	5.04	127.45	120.29
1	B0	268	ARG	CG-CD-NE	5.04	123.08	112.00
15	BE	409	GLY	CA-C-N	5.04	127.29	120.44
15	BE	409	GLY	C-N-CA	5.04	127.29	120.44
21	BK	82	SER	N-CA-CB	5.04	117.32	110.01
30	BW	320	ARG	N-CA-CB	5.04	117.32	110.01
12	BB	166	CYS	N-CA-CB	5.04	117.31	110.01
25	BQ	315	ASP	CA-C-N	5.04	127.53	120.28
25	BQ	315	ASP	C-N-CA	5.04	127.53	120.28
18	BH	63	ILE	CA-C-N	5.04	130.14	122.23
18	BH	63	ILE	C-N-CA	5.04	130.14	122.23
25	BQ	346	VAL	CA-C-N	5.04	127.53	120.28
25	BQ	346	VAL	C-N-CA	5.04	127.53	120.28
14	BD	310	LEU	CA-C-N	5.03	126.98	120.44
14	BD	310	LEU	C-N-CA	5.03	126.98	120.44
15	BE	410	LEU	N-CA-CB	5.03	117.37	110.07
15	BE	523	ARG	CA-C-N	5.03	127.02	120.28
15	BE	523	ARG	C-N-CA	5.03	127.02	120.28
15	BE	838	LEU	N-CA-CB	5.03	117.31	110.01
37	Bg	97	ARG	CA-C-N	5.03	131.13	123.23
37	Bg	97	ARG	C-N-CA	5.03	131.13	123.23
7	B6	96	ARG	CA-C-N	5.03	128.48	121.24
7	B6	96	ARG	C-N-CA	5.03	128.48	121.24
12	BB	229	ILE	CA-C-N	5.03	126.98	120.44
12	BB	229	ILE	C-N-CA	5.03	126.98	120.44
12	BB	300	THR	CA-C-N	5.03	128.84	120.94
12	BB	300	THR	C-N-CA	5.03	128.84	120.94
30	BW	285	VAL	CA-C-N	5.03	130.41	122.36
30	BW	285	VAL	C-N-CA	5.03	130.41	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BE	423	GLN	N-CA-CB	5.03	117.30	110.01
15	BE	497	ALA	CA-C-N	5.03	127.85	120.71
15	BE	497	ALA	C-N-CA	5.03	127.85	120.71
15	BE	519	SER	CA-C-N	5.03	127.00	120.56
15	BE	519	SER	C-N-CA	5.03	127.00	120.56
14	BD	216	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B0	67	SER	CA-C-N	5.02	130.57	122.83
1	B0	67	SER	C-N-CA	5.02	130.57	122.83
1	B0	301	THR	CA-C-N	5.02	127.28	120.65
1	B0	301	THR	C-N-CA	5.02	127.28	120.65
1	B0	172	SER	N-CA-CB	5.02	117.29	110.01
3	B2	265	LEU	CA-C-N	5.02	126.89	120.56
3	B2	265	LEU	C-N-CA	5.02	126.89	120.56
12	BB	34	LEU	N-CA-CB	5.02	117.29	110.01
16	BF	259	ARG	CG-CD-NE	5.02	123.05	112.00
40	Bk	306	VAL	CA-C-N	5.02	126.97	120.44
40	Bk	306	VAL	C-N-CA	5.02	126.97	120.44
12	BB	73	LEU	CA-C-N	5.02	127.00	120.28
12	BB	73	LEU	C-N-CA	5.02	127.00	120.28
15	BE	485	GLU	N-CA-CB	5.02	117.29	110.01
15	BE	514	PRO	CA-C-N	5.02	127.01	120.28
15	BE	514	PRO	C-N-CA	5.02	127.01	120.28
15	BE	764	ARG	CA-C-N	5.02	127.51	120.28
15	BE	764	ARG	C-N-CA	5.02	127.51	120.28
30	BW	315	ARG	CA-C-N	5.02	126.97	120.44
30	BW	315	ARG	C-N-CA	5.02	126.97	120.44
30	BW	317	GLN	N-CA-CB	5.02	117.29	110.01
14	BD	135	ASP	CA-C-N	5.02	127.00	120.28
14	BD	135	ASP	C-N-CA	5.02	127.00	120.28
25	BQ	380	LEU	CA-C-N	5.02	127.00	120.28
25	BQ	380	LEU	C-N-CA	5.02	127.00	120.28
42	HJ	720	LEU	CA-C-N	5.02	126.96	120.44
42	HJ	720	LEU	C-N-CA	5.02	126.96	120.44
14	BD	368	ARG	CG-CD-NE	5.02	123.03	112.00
37	Bg	222	ALA	CA-C-N	5.02	129.95	121.47
37	Bg	222	ALA	C-N-CA	5.02	129.95	121.47
25	BQ	314	ASP	N-CA-CB	5.01	117.28	110.01
25	BQ	383	GLU	N-CA-CB	5.01	117.28	110.01
40	Bk	114	ARG	N-CA-CB	5.01	117.36	109.69
1	B0	269	GLU	N-CA-CB	5.01	117.28	110.01
15	BE	819	MET	CA-C-N	5.01	126.95	120.44
15	BE	819	MET	C-N-CA	5.01	126.95	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BW	314	SER	N-CA-CB	5.01	117.28	110.01
12	BB	228	GLN	N-CA-CB	5.01	117.27	110.01
14	BD	137	GLU	CA-C-N	5.01	126.95	120.44
14	BD	137	GLU	C-N-CA	5.01	126.95	120.44
21	BK	49	PHE	CA-C-N	5.01	126.95	120.44
21	BK	49	PHE	C-N-CA	5.01	126.95	120.44
21	BK	51	HIS	N-CA-CB	5.01	117.27	110.01
15	BE	503	ALA	CA-C-N	5.01	126.95	120.44
15	BE	503	ALA	C-N-CA	5.01	126.95	120.44
30	BW	322	ARG	CG-CD-NE	5.01	123.01	112.00
42	HJ	720	LEU	N-CA-CB	5.01	117.27	110.01
1	B0	138	ASN	CA-C-N	5.00	126.95	120.44
1	B0	138	ASN	C-N-CA	5.00	126.95	120.44
1	B0	46	THR	CA-C-N	5.00	126.98	120.28
1	B0	46	THR	C-N-CA	5.00	126.98	120.28
14	BD	34	SER	CA-C-N	5.00	128.97	120.86
14	BD	34	SER	C-N-CA	5.00	128.97	120.86
25	BQ	308	THR	CA-C-N	5.00	126.94	120.44
25	BQ	308	THR	C-N-CA	5.00	126.94	120.44
37	Bg	8	GLY	CA-C-N	5.00	127.21	120.50
37	Bg	8	GLY	C-N-CA	5.00	127.21	120.50
38	Bh	129	ARG	N-CA-CB	5.00	117.27	110.01
12	BB	39	HIS	N-CA-CB	5.00	117.26	110.01
40	Bk	3	PRO	CA-C-N	5.00	130.95	122.65
40	Bk	3	PRO	C-N-CA	5.00	130.95	122.65

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	BE	931	TYR	Sidechain
42	HJ	745	ARG	Sidechain
52	bH	1	U	Sidechain
62	bS	18	U	Sidechain
62	bS	21	U	Sidechain
62	bS	22	U	Sidechain
62	bS	5	U	Sidechain
63	bT	51	A	Sidechain
63	bT	52	A	Sidechain

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	B0	2311	0	2283	9	0
2	B1	68	0	3	0	0
3	B2	2790	0	2770	16	0
4	B3	1735	0	1758	5	0
5	B4	663	0	684	3	0
6	B5	1109	0	1144	9	0
7	B6	943	0	963	6	0
8	B7	48	0	2	0	0
9	B8	84	0	2	0	0
9	Bj	84	0	3	0	0
10	B9	531	0	533	1	0
11	BA	4093	0	4060	11	0
12	BB	4313	0	4430	18	0
13	BC	1581	0	1643	3	0
14	BD	2682	0	2667	15	0
15	BE	5085	0	5150	54	0
16	BF	2195	0	2198	16	0
17	BG	1187	0	1220	5	0
18	BH	998	0	1050	4	0
19	BI	52	0	3	0	0
19	BN	52	0	2	0	0
19	BX	52	0	3	0	0
20	BJ	104	0	3	0	0
21	BK	1673	0	1689	6	0
22	BL	887	0	901	3	0
23	BO	2150	0	2220	16	0
24	BP	188	0	3	1	0
25	BQ	3588	0	3626	16	0
26	BS	1305	0	1320	6	0
27	BT	801	0	804	16	0
28	BU	56	0	2	0	0
29	BV	2181	0	2158	6	0
30	BW	2716	0	2681	23	0
31	BY	44	0	4	3	0
32	Ba	40	0	3	0	0
33	Bb	32	0	2	0	0
34	Bc	4276	0	4207	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	Bd	132	0	5	0	0
36	Be	72	0	2	0	0
37	Bg	1543	0	1534	8	0
38	Bh	1242	0	1259	6	0
39	Bi	928	0	936	2	0
40	Bk	3394	0	3540	14	0
41	Bl	1660	0	1739	13	0
42	HJ	2916	0	2948	19	0
43	HS	720	0	753	2	0
44	b1	160	0	81	14	0
45	b2	632	0	325	1	0
46	b3	100	0	51	7	0
47	b4	585	0	254	4	0
48	bA	571	0	286	4	0
49	bD	546	0	263	3	0
50	bE	1965	0	990	28	0
51	bG	80	0	41	9	0
52	bH	40	0	21	6	0
53	bI	60	0	31	6	0
54	bJ	1220	0	614	10	0
55	bK	1397	0	665	22	0
56	bL	1019	0	493	9	0
57	bN	1069	0	510	5	0
58	bO	2451	0	1152	14	0
59	bP	300	0	151	12	0
60	bQ	280	0	141	6	0
61	bR	408	0	202	0	0
62	bS	620	0	311	8	0
63	bT	1128	0	564	5	0
64	bU	500	0	251	7	0
65	bV	120	0	61	3	0
66	bY	220	0	111	18	0
All	All	80775	0	72479	442	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 3.

All (442) 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)
27:BT:45:ARG:HG3	27:BT:51:HIS:CE1	1.46	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:bP:5:U:O2	59:bP:8:U:C5	1.94	1.20
27:BT:45:ARG:CG	27:BT:51:HIS:CE1	2.26	1.17
66:bY:5:U:N3	66:bY:7:U:N3	1.96	1.14
15:BE:971:THR:HG22	15:BE:1010:VAL:CG2	1.81	1.11
15:BE:971:THR:CG2	15:BE:1010:VAL:CG2	2.32	1.07
53:bI:3:U:H5	55:bK:32:U:C2	1.74	1.06
53:bI:3:U:C5	55:bK:32:U:N3	2.24	1.06
66:bY:2:U:N3	66:bY:8:U:C4	2.28	1.01
14:BD:246:LEU:HD12	14:BD:246:LEU:O	1.60	1.00
66:bY:5:U:C2	66:bY:7:U:N3	2.31	0.97
66:bY:5:U:N3	66:bY:7:U:C2	2.31	0.97
41:Bl:159:TRP:CD1	41:Bl:160:MET:SD	2.58	0.96
59:bP:5:U:O2'	59:bP:7:U:H5	1.48	0.95
25:BQ:144:HIS:HB3	25:BQ:176:ASN:OD1	1.65	0.95
41:Bl:159:TRP:NE1	41:Bl:160:MET:SD	2.44	0.91
27:BT:45:ARG:HG3	27:BT:51:HIS:HE1	1.14	0.89
59:bP:5:U:O2	59:bP:8:U:H5	1.48	0.88
53:bI:3:U:C5	55:bK:32:U:C2	2.61	0.88
59:bP:5:U:O2'	59:bP:7:U:C5	2.24	0.88
66:bY:5:U:C2	66:bY:7:U:C4	2.61	0.88
53:bI:3:U:H5	55:bK:32:U:N3	1.65	0.87
42:HJ:773:LEU:HG	42:HJ:774:VAL:H	1.39	0.86
59:bP:5:U:HO2'	59:bP:7:U:H5	0.92	0.85
46:b3:5:U:C6	46:b3:5:U:OP1	2.30	0.84
15:BE:913:LYS:NZ	64:bU:12:U:OP2	2.11	0.83
15:BE:982:PHE:CZ	15:BE:984:GLU:OE1	2.31	0.83
15:BE:971:THR:HG22	15:BE:1010:VAL:HG21	1.61	0.83
56:bL:15:G:O2'	56:bL:16:C:OP1	1.96	0.83
66:bY:5:U:C2	66:bY:7:U:C2	2.67	0.82
11:BA:336:GLU:O	11:BA:340:SER:OG	2.00	0.80
6:B5:60:TYR:OH	15:BE:1043:LYS:HD2	1.80	0.80
46:b3:4:U:O2'	46:b3:5:U:P	2.38	0.80
23:BO:79:ASP:OD1	50:bE:16:C:O2'	1.98	0.79
50:bE:31:A:O2'	50:bE:82:U:O4	1.99	0.79
15:BE:971:THR:HG22	15:BE:1010:VAL:HG22	1.63	0.79
25:BQ:144:HIS:CB	25:BQ:176:ASN:OD1	2.29	0.79
47:b4:12:G:N2	60:bQ:10:U:O2	2.15	0.79
55:bK:60:U:O2'	55:bK:61:A:OP1	2.00	0.79
15:BE:971:THR:CG2	15:BE:1010:VAL:HG23	2.11	0.78
56:bL:19:G:N2	56:bL:19:G:OP2	2.16	0.78
40:Bk:42:ASN:O	40:Bk:46:THR:OG1	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B5:60:TYR:OH	15:BE:1043:LYS:CD	2.32	0.78
51:bG:2:U:O4	52:bH:2:U:H1'	1.84	0.78
50:bE:46:G:O2'	50:bE:47:C:O5'	2.02	0.75
50:bE:81:U:OP2	63:bT:41:G:O2'	2.04	0.75
46:b3:5:U:OP1	46:b3:5:U:H6	1.70	0.75
15:BE:971:THR:CG2	15:BE:1010:VAL:HG21	2.13	0.74
17:BG:143:LEU:HD23	17:BG:147:GLU:OE2	1.86	0.74
15:BE:971:THR:HG21	15:BE:1010:VAL:CG2	2.16	0.74
15:BE:936:TRP:CZ3	15:BE:937:LEU:HD21	2.22	0.74
34:Bc:23:PRO:O	34:Bc:26:THR:OG1	2.06	0.73
27:BT:45:ARG:CD	27:BT:51:HIS:ND1	2.49	0.73
6:B5:102:GLN:HE22	15:BE:1037:ALA:HB2	1.52	0.73
23:BO:41:SER:HA	23:BO:48:ARG:NH1	2.04	0.73
27:BT:45:ARG:CG	27:BT:51:HIS:ND1	2.51	0.73
38:Bh:53:TYR:OH	38:Bh:62:GLU:OE1	2.06	0.72
7:B6:55:ARG:N	62:bS:7:U:O2	2.21	0.72
23:BO:212:TRP:O	23:BO:214:LEU:HD12	1.89	0.72
14:BD:471:SER:O	14:BD:475:SER:OG	2.08	0.72
34:Bc:499:ASP:OD1	34:Bc:502:THR:OG1	2.07	0.72
14:BD:304:CYS:SG	14:BD:305:TYR:N	2.63	0.71
66:bY:2:U:C2	66:bY:8:U:C4	2.78	0.71
53:bI:3:U:C5	55:bK:32:U:C4	2.78	0.71
34:Bc:45:ASN:O	34:Bc:81:LYS:NZ	2.23	0.71
41:Bl:25:ASN:ND2	58:bO:81:U:OP2	2.23	0.71
13:BC:43:ARG:O	13:BC:46:LEU:HG	1.89	0.71
46:b3:5:U:P	46:b3:5:U:H6	2.14	0.70
50:bE:46:G:HO2'	50:bE:47:C:P	2.13	0.70
58:bO:88:A:O2'	58:bO:89:U:O5'	2.10	0.70
55:bK:31:U:O2'	55:bK:32:U:OP1	2.09	0.70
59:bP:5:U:C2'	59:bP:7:U:H5	2.03	0.70
54:bJ:12:A:O2'	54:bJ:13:A:OP1	2.07	0.70
50:bE:78:C:O2	63:bT:26:G:O2'	2.09	0.70
59:bP:5:U:C2	59:bP:8:U:H5	2.09	0.70
66:bY:5:U:O2	66:bY:7:U:C2	2.45	0.69
30:BW:70:ARG:NH2	30:BW:135:GLU:OE1	2.25	0.69
15:BE:798:ASP:OD2	15:BE:800:SER:OG	2.09	0.69
15:BE:971:THR:HG21	15:BE:1010:VAL:HG23	1.75	0.69
11:BA:465:LEU:HD23	11:BA:540:MET:CE	2.23	0.69
34:Bc:96:THR:OG1	34:Bc:99:ASP:OD1	2.03	0.69
21:BK:19:ARG:O	42:HJ:648:ARG:NH2	2.26	0.68
25:BQ:144:HIS:HB3	25:BQ:176:ASN:CG	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BW:309:ALA:O	30:BW:312:THR:HG22	1.93	0.68
50:bE:52:G:O2'	59:bP:9:U:O2	2.10	0.68
27:BT:45:ARG:HD3	27:BT:51:HIS:ND1	2.09	0.68
6:B5:52:GLN:NE2	62:bS:2:U:O2	2.26	0.68
50:bE:53:A:O2'	50:bE:54:U:OP1	2.11	0.68
30:BW:303:PHE:CZ	30:BW:312:THR:HG21	2.28	0.68
15:BE:723:GLN:OE1	15:BE:727:ARG:NH1	2.27	0.68
14:BD:223:THR:HG1	14:BD:228:SER:HG	1.42	0.68
51:bG:1:U:O4	55:bK:34:U:C5	2.48	0.67
22:BL:40:ARG:NH2	56:bL:3:U:OP1	2.27	0.67
54:bJ:34:U:O2'	54:bJ:54:G:N2	2.27	0.67
27:BT:75:TYR:OH	37:Bg:22:VAL:O	2.07	0.67
1:B0:230:ARG:NH2	65:bV:4:U:OP1	2.27	0.67
49:bD:10:G:O2'	49:bD:11:G:OP1	2.12	0.66
21:BK:23:ARG:O	58:bO:21:G:N2	2.29	0.66
42:HJ:773:LEU:HG	42:HJ:774:VAL:N	2.09	0.66
15:BE:982:PHE:CE2	15:BE:984:GLU:OE1	2.49	0.66
54:bJ:41:G:N2	54:bJ:41:G:OP2	2.29	0.65
16:BF:272:ILE:CD1	44:b1:7:U:O2	2.43	0.65
39:Bi:9:SER:O	39:Bi:12:THR:OG1	2.13	0.65
40:Bk:120:GLN:NE2	54:bJ:43:U:O2	2.28	0.65
11:BA:465:LEU:HD23	11:BA:540:MET:HE2	1.78	0.65
27:BT:45:ARG:HA	27:BT:51:HIS:HE1	1.62	0.64
51:bG:1:U:O2'	51:bG:3:U:O3'	2.16	0.64
15:BE:323:SER:O	15:BE:327:ARG:NE	2.31	0.63
16:BF:137:SER:OG	16:BF:174:GLN:OE1	2.13	0.63
46:b3:5:U:OP1	46:b3:5:U:C5	2.51	0.63
48:bA:26:G:N2	62:bS:5:U:O2	2.31	0.63
7:B6:94:THR:O	50:bE:3:A:O2'	2.14	0.63
11:BA:465:LEU:CD2	11:BA:540:MET:HE2	2.28	0.63
58:bO:24:A:O2'	58:bO:26:U:OP1	2.13	0.63
5:B4:108:PHE:O	5:B4:116:TYR:OH	2.16	0.63
37:Bg:214:GLU:OE1	37:Bg:217:GLU:OE2	2.17	0.63
27:BT:45:ARG:CG	27:BT:51:HIS:HE1	1.92	0.62
15:BE:421:LEU:HD23	15:BE:461:ARG:HG2	1.79	0.62
66:bY:5:U:O2	66:bY:7:U:C6	2.52	0.62
30:BW:343:GLU:HG2	30:BW:344:ASP:N	2.15	0.62
13:BC:90:LEU:O	13:BC:94:VAL:HG23	1.99	0.61
30:BW:343:GLU:HG2	30:BW:344:ASP:H	1.64	0.61
16:BF:74:LEU:HD11	16:BF:77:HIS:CD2	2.35	0.61
23:BO:212:TRP:O	23:BO:214:LEU:CD1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BT:45:ARG:CB	27:BT:51:HIS:CE1	2.83	0.61
1:B0:227:SER:OG	65:bV:2:U:OP1	2.17	0.61
15:BE:975:ARG:HD3	15:BE:1012:GLN:OE1	2.01	0.61
55:bK:3:A:HO2'	58:bO:11:U:HO2'	1.43	0.61
34:Bc:354:ILE:O	34:Bc:357:THR:OG1	2.18	0.61
34:Bc:246:ARG:NH1	34:Bc:362:PRO:O	2.34	0.60
12:BB:1011:ALA:O	12:BB:1014:LYS:NZ	2.30	0.60
41:Bl:151:ARG:NH2	41:Bl:176:ASP:OD1	2.34	0.60
34:Bc:202:PHE:O	34:Bc:206:THR:OG1	2.19	0.60
46:b3:4:U:O2'	46:b3:5:U:OP2	2.19	0.60
21:BK:2:ASN:ND2	42:HJ:780:TRP:O	2.35	0.60
59:bP:5:U:N3	59:bP:8:U:OP2	2.31	0.60
27:BT:47:ASP:O	30:BW:317:GLN:NE2	2.36	0.59
58:bO:8:U:OP1	58:bO:9:G:N2	2.35	0.59
47:b4:12:G:C2	60:bQ:10:U:O2	2.56	0.59
15:BE:860:MET:SD	15:BE:902:PHE:CE2	2.97	0.58
16:BF:43:THR:OG1	16:BF:60:ARG:O	2.19	0.58
23:BO:107:ASP:OD1	48:bA:12:G:O2'	2.19	0.58
30:BW:199:CYS:SG	30:BW:200:ARG:N	2.76	0.58
15:BE:936:TRP:HZ3	15:BE:937:LEU:HD21	1.68	0.58
44:b1:2:U:O4	44:b1:4:U:O4'	2.22	0.58
23:BO:41:SER:HA	23:BO:48:ARG:HH11	1.68	0.57
3:B2:48:ARG:NH1	40:Bk:391:GLN:OE1	2.37	0.57
25:BQ:144:HIS:CG	25:BQ:176:ASN:OD1	2.57	0.57
29:BV:255:CYS:C	30:BW:180:ASP:OD1	2.47	0.57
58:bO:88:A:HO2'	58:bO:89:U:C5'	2.17	0.57
34:Bc:55:ASN:ND2	34:Bc:59:VAL:O	2.38	0.57
12:BB:843:LEU:HD12	12:BB:846:GLN:HE21	1.68	0.57
27:BT:45:ARG:CD	27:BT:51:HIS:CE1	2.86	0.57
30:BW:78:CYS:SG	30:BW:79:LEU:N	2.78	0.56
66:bY:2:U:N3	66:bY:8:U:N3	2.51	0.56
44:b1:2:U:C4	44:b1:4:U:O4'	2.58	0.56
16:BF:262:PHE:O	16:BF:266:MET:HG2	2.06	0.56
23:BO:160:ARG:NH2	56:bL:4:U:O4	2.38	0.56
3:B2:81:ARG:NH2	4:B3:89:TRP:O	2.38	0.56
11:BA:488:PRO:O	11:BA:490:HIS:CD2	2.58	0.56
46:b3:5:U:C6	46:b3:5:U:P	2.98	0.56
16:BF:272:ILE:HD11	44:b1:7:U:O2	2.06	0.56
12:BB:430:MET:HG2	37:Bg:89:ARG:NH2	2.20	0.56
40:Bk:106:GLN:OE1	40:Bk:129:GLN:NE2	2.39	0.56
15:BE:826:HIS:NE2	64:bU:11:U:C4	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:bD:3:G:N2	54:bJ:41:G:O3'	2.39	0.55
55:bK:57:G:O2'	55:bK:60:U:OP1	2.18	0.55
42:HJ:773:LEU:CG	42:HJ:774:VAL:H	2.15	0.55
41:Bl:107:GLY:HA3	41:Bl:126:VAL:HG21	1.88	0.55
56:bL:27:A:O2'	56:bL:28:G:OP1	2.23	0.55
21:BK:135:GLU:OE1	21:BK:137:ARG:NH1	2.39	0.55
66:bY:5:U:O2	66:bY:7:U:N1	2.40	0.55
30:BW:309:ALA:O	30:BW:312:THR:CG2	2.55	0.54
27:BT:79:ARG:NH1	56:bL:48:G:N7	2.55	0.54
45:b2:45:A:N1	45:b2:46:A:N6	2.55	0.54
66:bY:2:U:O2	66:bY:8:U:N3	2.40	0.54
21:BK:13:PHE:O	21:BK:19:ARG:NH1	2.40	0.54
23:BO:213:ASN:C	23:BO:214:LEU:HD12	2.33	0.54
50:bE:74:G:O2'	50:bE:75:C:OP1	2.25	0.54
1:B0:284:ARG:NH2	1:B0:287:GLU:OE2	2.41	0.54
50:bE:72:G:O2'	50:bE:73:U:OP1	2.24	0.54
6:B5:60:TYR:OH	15:BE:1043:LYS:CG	2.56	0.54
42:HJ:8:ARG:O	42:HJ:12:ARG:NH2	2.40	0.54
59:bP:5:U:C2	59:bP:8:U:C5	2.86	0.54
23:BO:212:TRP:N	23:BO:214:LEU:HD13	2.23	0.54
40:Bk:208:SER:O	40:Bk:212:VAL:HG23	2.07	0.54
66:bY:2:U:N3	66:bY:8:U:C5	2.75	0.54
55:bK:62:A:OP2	55:bK:64:A:N6	2.41	0.53
6:B5:102:GLN:HE22	15:BE:1037:ALA:CB	2.20	0.53
14:BD:267:ARG:HG2	14:BD:267:ARG:O	2.09	0.53
3:B2:320:GLU:OE1	3:B2:328:ARG:NH2	2.42	0.53
37:Bg:79:LEU:HD23	37:Bg:214:GLU:CD	2.33	0.53
66:bY:2:U:C2	66:bY:8:U:N3	2.76	0.53
14:BD:246:LEU:O	14:BD:246:LEU:CD1	2.47	0.53
15:BE:860:MET:SD	15:BE:902:PHE:CD2	3.02	0.53
42:HJ:856:VAL:O	42:HJ:859:THR:OG1	2.26	0.53
58:bO:33:U:O2'	58:bO:34:A:P	2.67	0.53
5:B4:16:VAL:HG21	26:BS:77:LEU:HD13	1.90	0.53
11:BA:264:ASP:OD1	11:BA:265:SER:N	2.41	0.53
15:BE:865:GLU:OE2	64:bU:10:U:C5	2.62	0.53
37:Bg:16:GLY:O	54:bJ:12:A:N6	2.42	0.52
40:Bk:94:ARG:NH1	40:Bk:132:GLU:OE1	2.41	0.52
59:bP:5:U:O2	59:bP:8:U:C6	2.58	0.52
3:B2:176:HIS:CE1	62:bS:21:U:C2	2.97	0.52
11:BA:503:LEU:O	34:Bc:532:ARG:NH1	2.43	0.52
57:bN:39:A:H1'	57:bN:40:G:OP1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BB:1132:CYS:SG	12:BB:1133:GLN:N	2.83	0.52
51:bG:1:U:O4	55:bK:34:U:C6	2.62	0.52
1:B0:204:ILE:O	1:B0:208:GLY:N	2.42	0.52
15:BE:421:LEU:HG	15:BE:421:LEU:O	2.09	0.52
15:BE:613:ASN:OD1	15:BE:841:ARG:NH1	2.42	0.52
29:BV:10:LEU:CD1	41:Bl:195:MET:HG3	2.39	0.52
17:BG:5:ARG:HG2	62:bS:21:U:C2	2.45	0.52
12:BB:430:MET:HG2	37:Bg:89:ARG:HH21	1.75	0.51
15:BE:346:GLU:O	15:BE:349:TRP:NE1	2.43	0.51
30:BW:115:CYS:SG	30:BW:116:ASP:N	2.83	0.51
38:Bh:19:ARG:NH1	38:Bh:41:PRO:O	2.43	0.51
44:b1:6:U:O4'	44:b1:7:U:C5	2.64	0.51
63:bT:36:C:O2	63:bT:37:A:C8	2.63	0.51
13:BC:196:PHE:CE2	25:BQ:203:GLU:HG3	2.46	0.51
14:BD:26:HIS:HD1	60:bQ:2:U:HO2'	1.59	0.51
16:BF:272:ILE:HD13	44:b1:7:U:O2	2.10	0.51
38:Bh:143:VAL:HG23	38:Bh:144:SER:H	1.76	0.51
1:B0:155:SER:OG	25:BQ:357:ASP:OD1	2.16	0.51
7:B6:54:PRO:HA	62:bS:7:U:O2	2.11	0.51
14:BD:24:LEU:O	14:BD:29:TRP:NE1	2.44	0.51
15:BE:290:ARG:NH2	15:BE:347:GLU:OE1	2.44	0.51
16:BF:237:LEU:HD21	42:HJ:605:GLU:OE2	2.11	0.50
42:HJ:775:ALA:HB3	42:HJ:776:PRO:HD3	1.93	0.50
50:bE:74:G:O2'	50:bE:75:C:P	2.69	0.50
51:bG:2:U:C4	52:bH:2:U:H1'	2.44	0.50
41:Bl:187:PHE:O	41:Bl:192:ARG:NH1	2.44	0.50
25:BQ:144:HIS:ND1	25:BQ:176:ASN:OD1	2.44	0.50
58:bO:88:A:O2'	58:bO:89:U:P	2.69	0.50
22:BL:75:ASP:OD1	22:BL:101:GLU:N	2.45	0.50
30:BW:343:GLU:CG	30:BW:344:ASP:H	2.25	0.50
1:B0:238:PHE:CZ	44:b1:1:U:C4	2.99	0.50
16:BF:118:CYS:SG	16:BF:119:SER:N	2.85	0.50
44:b1:2:U:N3	44:b1:4:U:O4'	2.45	0.50
57:bN:39:A:O2'	57:bN:40:G:OP1	2.24	0.50
15:BE:792:THR:O	15:BE:795:ARG:NH1	2.45	0.49
14:BD:91:ASN:O	14:BD:93:ARG:NH1	2.45	0.49
18:BH:75:ASP:N	18:BH:75:ASP:OD1	2.44	0.49
40:Bk:114:ARG:NH2	55:bK:65:U:H5	2.08	0.49
3:B2:91:ARG:O	4:B3:201:GLN:NE2	2.46	0.49
44:b1:2:U:O4	44:b1:4:U:C1'	2.60	0.49
16:BF:240:ASP:O	42:HJ:617:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BQ:508:ASN:OD1	25:BQ:512:GLN:N	2.46	0.49
14:BD:188:PRO:O	14:BD:191:VAL:HG22	2.12	0.49
15:BE:290:ARG:NH1	15:BE:301:PRO:O	2.44	0.49
16:BF:90:VAL:N	16:BF:91:PRO:CD	2.76	0.49
42:HJ:604:ARG:O	42:HJ:607:VAL:N	2.42	0.49
51:bG:2:U:O4	52:bH:2:U:C1'	2.59	0.49
25:BQ:187:VAL:HG12	25:BQ:334:TYR:HE1	1.78	0.48
43:HS:2:ALA:N	62:bS:17:U:OP2	2.45	0.48
1:B0:256:LEU:O	1:B0:260:VAL:HG23	2.12	0.48
25:BQ:185:VAL:HG13	25:BQ:290:THR:CG2	2.42	0.48
34:Bc:395:ARG:NH1	34:Bc:438:THR:OG1	2.46	0.48
15:BE:356:LEU:O	15:BE:358:ALA:N	2.47	0.48
26:BS:46:ARG:NH2	26:BS:50:GLU:OE2	2.46	0.48
51:bG:1:U:O2	51:bG:3:U:OP1	2.31	0.48
52:bH:1:U:O4	53:bI:3:U:O3'	2.31	0.48
51:bG:2:U:C4	52:bH:2:U:C1'	2.96	0.48
34:Bc:85:VAL:HG21	34:Bc:230:LEU:HD13	1.96	0.48
38:Bh:13:ARG:NE	38:Bh:40:ASP:OD1	2.43	0.48
41:Bl:126:VAL:HG22	41:Bl:126:VAL:O	2.14	0.48
66:bY:5:U:O2	66:bY:7:U:C5	2.67	0.48
15:BE:573:TYR:OH	15:BE:792:THR:N	2.47	0.48
15:BE:958:LEU:HD23	15:BE:958:LEU:C	2.39	0.47
29:BV:107:ARG:NH1	54:bJ:48:U:OP1	2.44	0.47
6:B5:97:ARG:NH2	64:bU:24:U:OP2	2.47	0.47
12:BB:248:SER:O	12:BB:254:ASN:ND2	2.45	0.47
34:Bc:487:ALA:O	34:Bc:492:ARG:NH2	2.47	0.47
31:BY:8:UNK:C	31:BY:9:UNK:O	2.61	0.47
44:b1:5:U:H3	65:bV:4:U:H3	1.61	0.47
15:BE:1012:GLN:NE2	64:bU:13:U:O2'	2.47	0.47
27:BT:45:ARG:CA	27:BT:51:HIS:HE1	2.26	0.47
50:bE:46:G:H4'	50:bE:47:C:OP1	2.14	0.47
3:B2:35:ASP:OD2	3:B2:317:GLN:NE2	2.46	0.47
3:B2:267:ASP:O	3:B2:270:THR:OG1	2.33	0.47
30:BW:345:ASP:N	30:BW:345:ASP:OD1	2.48	0.47
40:Bk:114:ARG:CZ	55:bK:65:U:H5	2.28	0.47
15:BE:580:THR:OG1	15:BE:583:GLU:OE1	2.33	0.47
16:BF:123:ARG:O	16:BF:126:VAL:HG12	2.15	0.47
23:BO:156:ARG:NH2	56:bL:5:A:O2'	2.47	0.46
47:b4:12:G:N2	60:bQ:10:U:C2	2.83	0.46
40:Bk:409:VAL:HG13	40:Bk:410:ARG:H	1.81	0.46
47:b4:12:G:N1	60:bQ:10:U:N3	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:bE:46:G:HO2'	50:bE:47:C:C5'	2.19	0.46
30:BW:343:GLU:CG	30:BW:344:ASP:N	2.79	0.46
42:HJ:745:ARG:HH22	55:bK:10:G:H5'	1.81	0.46
44:b1:2:U:H3	44:b1:4:U:C4'	2.28	0.46
56:bL:15:G:HO2'	56:bL:16:C:P	2.30	0.46
31:BY:8:UNK:O	31:BY:9:UNK:C	2.63	0.46
16:BF:240:ASP:OD2	42:HJ:665:ARG:NH1	2.49	0.46
11:BA:578:ARG:NH1	48:bA:1:A:OP2	2.49	0.45
16:BF:238:VAL:O	42:HJ:618:GLN:NE2	2.47	0.45
14:BD:381:LEU:HD22	14:BD:431:TRP:CE2	2.52	0.45
4:B3:63:TYR:OH	34:Bc:14:PRO:O	2.34	0.45
16:BF:74:LEU:HD13	16:BF:76:HIS:CE1	2.51	0.45
23:BO:211:ALA:C	23:BO:214:LEU:HD13	2.41	0.45
50:bE:53:A:HO2'	50:bE:54:U:P	2.38	0.45
25:BQ:35:SER:N	25:BQ:36:PRO:CD	2.80	0.45
51:bG:2:U:C4	52:bH:2:U:O4'	2.70	0.45
63:bT:39:U:C2	63:bT:40:G:C8	3.04	0.45
15:BE:636:ARG:NH2	15:BE:739:ASP:OD1	2.49	0.45
21:BK:7:LEU:O	21:BK:7:LEU:HD23	2.16	0.45
30:BW:127:PHE:O	30:BW:186:ARG:NH1	2.49	0.45
18:BH:96:MET:HE3	18:BH:115:GLY:HA3	1.98	0.45
26:BS:82:ASP:OD1	26:BS:82:ASP:N	2.46	0.45
15:BE:513:SER:O	15:BE:516:THR:OG1	2.31	0.45
23:BO:212:TRP:C	23:BO:214:LEU:HD12	2.41	0.45
26:BS:107:LEU:HD23	26:BS:107:LEU:O	2.17	0.45
27:BT:62:ARG:NH1	27:BT:79:ARG:O	2.50	0.45
63:bT:35:C:C2	63:bT:36:C:C5	3.05	0.45
6:B5:60:TYR:OH	15:BE:1043:LYS:HG2	2.16	0.45
12:BB:442:TRP:O	60:bQ:12:U:O4	2.35	0.45
12:BB:679:LEU:HD23	12:BB:679:LEU:O	2.17	0.45
34:Bc:444:PHE:N	34:Bc:445:PRO:CD	2.80	0.45
3:B2:102:LEU:O	40:Bk:346:ARG:NH1	2.50	0.44
57:bN:39:A:O2'	57:bN:40:G:P	2.75	0.44
25:BQ:143:VAL:HG12	25:BQ:143:VAL:O	2.17	0.44
29:BV:10:LEU:HD11	41:Bl:195:MET:HG3	1.99	0.44
56:bL:39:G:C2	56:bL:40:C:C5	3.05	0.44
37:Bg:110:LYS:NZ	55:bK:56:U:OP2	2.46	0.44
3:B2:122:GLU:O	3:B2:122:GLU:HG2	2.16	0.44
25:BQ:139:GLU:O	25:BQ:140:ILE:HG23	2.17	0.44
48:bA:26:G:C2	62:bS:5:U:O2	2.71	0.44
30:BW:217:VAL:O	30:BW:217:VAL:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BQ:266:ASP:OD1	42:HJ:834:THR:OG1	2.30	0.44
41:Bl:171:THR:OG1	41:Bl:172:SER:N	2.48	0.44
15:BE:792:THR:OG1	15:BE:795:ARG:NH2	2.44	0.44
64:bU:18:U:O2	64:bU:19:U:O4'	2.36	0.44
4:B3:199:TYR:OH	24:BP:42:UNK:O	2.31	0.43
58:bO:6:C:C2	58:bO:7:U:C5	3.05	0.43
4:B3:4:VAL:O	10:B9:59:ARG:NH1	2.52	0.43
6:B5:60:TYR:CZ	15:BE:1043:LYS:HE3	2.52	0.43
29:BV:125:SER:OG	29:BV:128:ASP:OD2	2.29	0.43
42:HJ:775:ALA:HB3	42:HJ:776:PRO:CD	2.47	0.43
57:bN:32:C:C2	57:bN:33:A:C8	3.06	0.43
59:bP:6:U:C5	59:bP:7:U:C4	3.07	0.43
17:BG:83:TYR:OH	42:HJ:604:ARG:NH1	2.51	0.43
26:BS:27:VAL:O	26:BS:31:THR:OG1	2.35	0.43
50:bE:74:G:HO2'	50:bE:75:C:P	2.42	0.43
3:B2:240:ARG:O	7:B6:91:ARG:NH2	2.51	0.43
15:BE:476:VAL:HG12	15:BE:476:VAL:O	2.17	0.43
12:BB:422:GLU:HG2	12:BB:423:ILE:N	2.34	0.43
17:BG:24:HIS:O	17:BG:28:THR:OG1	2.30	0.43
18:BH:62:VAL:HG13	18:BH:63:ILE:HG13	1.99	0.43
55:bK:52:A:O2'	55:bK:53:C:OP2	2.30	0.43
3:B2:44:SER:O	3:B2:48:ARG:NH2	2.52	0.43
5:B4:27:GLN:OE1	5:B4:29:TRP:NE1	2.49	0.43
7:B6:100:ARG:NH2	11:BA:623:ASP:OD2	2.51	0.43
31:BY:8:UNK:O	31:BY:9:UNK:O	2.37	0.43
43:HS:224:GLU:O	43:HS:229:GLU:HB2	2.18	0.43
3:B2:5:SER:O	3:B2:10:GLN:NE2	2.52	0.43
14:BD:162:PHE:N	14:BD:163:PRO:CD	2.82	0.43
30:BW:190:VAL:HG22	30:BW:190:VAL:O	2.19	0.43
44:b1:2:U:C2	44:b1:4:U:H5'	2.54	0.43
49:bD:4:C:O2'	54:bJ:41:G:OP1	2.37	0.43
15:BE:913:LYS:HG2	15:BE:929:ASN:ND2	2.34	0.43
15:BE:971:THR:HG21	15:BE:1010:VAL:HG21	1.91	0.43
18:BH:19:GLN:OE1	50:bE:91:U:O2'	2.37	0.43
50:bE:9:G:C2	50:bE:10:G:C8	3.06	0.43
55:bK:48:U:C2	55:bK:49:A:C8	3.07	0.43
12:BB:169:LEU:O	12:BB:228:GLN:NE2	2.48	0.42
34:Bc:400:SER:OG	34:Bc:402:ASP:OD1	2.37	0.42
3:B2:46:ARG:O	3:B2:47:HIS:HB2	2.18	0.42
3:B2:158:ARG:NH2	3:B2:163:ALA:O	2.49	0.42
29:BV:255:CYS:O	30:BW:180:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Bc:45:ASN:ND2	34:Bc:50:THR:OG1	2.51	0.42
41:Bl:5:ILE:O	41:Bl:5:ILE:HG22	2.19	0.42
41:Bl:57:ARG:NH2	41:Bl:96:ASP:OD2	2.50	0.42
50:bE:33:U:C2	50:bE:34:G:C8	3.06	0.42
50:bE:51:G:O2'	50:bE:52:G:OP2	2.27	0.42
15:BE:826:HIS:NE2	64:bU:11:U:O4	2.53	0.42
15:BE:902:PHE:CD1	15:BE:902:PHE:C	2.98	0.42
42:HJ:702:ILE:HG12	42:HJ:731:VAL:HG22	2.01	0.42
66:bY:2:U:C2	66:bY:8:U:O4	2.72	0.42
66:bY:2:U:C4	66:bY:8:U:C5	3.08	0.42
3:B2:237:MET:HE1	7:B6:95:VAL:HG22	2.01	0.42
12:BB:988:SER:N	12:BB:989:PRO:CD	2.82	0.42
17:BG:144:LEU:O	17:BG:147:GLU:HG2	2.20	0.42
38:Bh:141:ARG:NE	38:Bh:148:ASP:OD2	2.53	0.42
40:Bk:409:VAL:HG13	40:Bk:410:ARG:N	2.35	0.42
30:BW:93:GLU:OE1	39:Bi:143:SER:N	2.53	0.42
55:bK:14:C:C2	55:bK:15:U:C5	3.08	0.42
23:BO:76:ARG:NH1	50:bE:17:U:OP1	2.52	0.42
23:BO:182:LYS:NZ	50:bE:27:U:OP1	2.52	0.42
40:Bk:272:LEU:HB2	40:Bk:273:PRO:HA	2.02	0.42
50:bE:55:U:OP1	50:bE:57:G:N2	2.49	0.42
41:Bl:23:PRO:N	41:Bl:24:PRO:CD	2.83	0.41
30:BW:309:ALA:C	30:BW:312:THR:HG22	2.46	0.41
12:BB:656:GLU:O	12:BB:659:VAL:HG22	2.20	0.41
50:bE:12:U:O2	50:bE:13:G:C8	2.74	0.41
11:BA:107:VAL:HG13	11:BA:117:VAL:HG22	2.02	0.41
50:bE:11:U:N3	50:bE:12:U:C5	2.89	0.41
57:bN:5:U:C2	57:bN:6:G:C8	3.08	0.41
15:BE:984:GLU:CD	15:BE:987:PHE:HB2	2.46	0.41
40:Bk:272:LEU:HD23	40:Bk:272:LEU:H	1.85	0.41
50:bE:25:A:O2'	50:bE:27:U:OP2	2.38	0.41
55:bK:60:U:HO2'	55:bK:61:A:P	2.34	0.41
58:bO:109:C:C2	58:bO:110:A:C8	3.08	0.41
15:BE:639:GLN:OE1	15:BE:639:GLN:HA	2.21	0.41
15:BE:786:SER:N	15:BE:787:PRO:CD	2.83	0.41
30:BW:90:LEU:O	30:BW:95:ARG:NH2	2.53	0.41
15:BE:739:ASP:O	15:BE:804:ILE:HG22	2.21	0.41
15:BE:1038:ASN:OD1	26:BS:7:PHE:HD1	2.03	0.41
22:BL:44:ASP:OD1	22:BL:44:ASP:N	2.46	0.41
11:BA:234:ASN:O	11:BA:237:VAL:HG22	2.19	0.41
12:BB:964:VAL:O	14:BD:17:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:bK:47:C:N3	55:bK:48:U:C5	2.88	0.41
3:B2:206:HIS:O	3:B2:209:VAL:HG12	2.21	0.41
25:BQ:427:THR:HG21	54:bJ:65:A:C2	2.56	0.41
30:BW:358:ASP:OD1	30:BW:358:ASP:N	2.54	0.41
58:bO:26:U:O2	58:bO:26:U:H2'	2.20	0.41
58:bO:33:U:O2'	58:bO:34:A:O5'	2.39	0.41
12:BB:174:THR:CG2	12:BB:175:PRO:HD3	2.51	0.41
12:BB:340:ALA:O	12:BB:342:GLU:N	2.50	0.41
14:BD:328:ASP:OD1	14:BD:331:ARG:NH2	2.54	0.41
37:Bg:79:LEU:HD23	37:Bg:214:GLU:OE2	2.21	0.41
55:bK:1:A:N6	58:bO:85:U:O2'	2.54	0.41
12:BB:318:SER:N	12:BB:319:PRO:CD	2.85	0.40
15:BE:1002:MET:HG3	15:BE:1006:ASP:HB3	2.03	0.40
23:BO:212:TRP:C	23:BO:214:LEU:CD1	2.94	0.40
27:BT:45:ARG:CB	27:BT:51:HIS:HE1	2.29	0.40
38:Bh:143:VAL:HG23	38:Bh:144:SER:N	2.36	0.40
1:B0:230:ARG:NH1	16:BF:51:SER:O	2.55	0.40
25:BQ:360:ASP:OD1	25:BQ:360:ASP:N	2.51	0.40
30:BW:117:ARG:NH2	30:BW:119:ASP:OD2	2.54	0.40
40:Bk:185:ARG:NH2	42:HJ:22:ASP:OD1	2.48	0.40
44:b1:2:U:O2	44:b1:4:U:H5'	2.20	0.40
50:bE:11:U:C2	50:bE:12:U:C5	3.09	0.40
54:bJ:21:U:C2	54:bJ:22:A:C8	3.10	0.40
66:bY:5:U:O2	66:bY:7:U:C4	2.73	0.40
1:B0:211:LEU:O	1:B0:214:VAL:HG12	2.21	0.40
12:BB:173:THR:HG23	12:BB:175:PRO:HD2	2.04	0.40
23:BO:80:THR:HA	23:BO:85:VAL:HG11	2.02	0.40
44:b1:5:U:H2'	44:b1:6:U:C5	2.56	0.40
50:bE:72:G:HO2'	50:bE:73:U:P	2.44	0.40
12:BB:27:PRO:O	12:BB:28:TYR:HB2	2.22	0.40
14:BD:307:THR:OG1	14:BD:385:ALA:O	2.31	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	B0	274/680 (40%)	259 (94%)	15 (6%)	0	100	100
3	B2	333/738 (45%)	321 (96%)	12 (4%)	0	100	100
4	B3	212/377 (56%)	208 (98%)	4 (2%)	0	100	100
5	B4	76/138 (55%)	75 (99%)	1 (1%)	0	100	100
6	B5	138/393 (35%)	133 (96%)	5 (4%)	0	100	100
7	B6	111/163 (68%)	105 (95%)	6 (5%)	0	100	100
10	B9	60/233 (26%)	60 (100%)	0	0	100	100
11	BA	516/939 (55%)	503 (98%)	13 (2%)	0	100	100
12	BB	518/1547 (34%)	490 (95%)	28 (5%)	0	100	100
13	BC	196/421 (47%)	191 (97%)	5 (3%)	0	100	100
14	BD	331/686 (48%)	312 (94%)	19 (6%)	0	100	100
15	BE	612/1053 (58%)	580 (95%)	30 (5%)	2 (0%)	36	65
16	BF	267/304 (88%)	262 (98%)	5 (2%)	0	100	100
17	BG	146/160 (91%)	141 (97%)	5 (3%)	0	100	100
18	BH	123/129 (95%)	122 (99%)	1 (1%)	0	100	100
21	BK	196/530 (37%)	190 (97%)	6 (3%)	0	100	100
22	BL	101/116 (87%)	101 (100%)	0	0	100	100
23	BO	255/395 (65%)	248 (97%)	7 (3%)	0	100	100
25	BQ	447/698 (64%)	433 (97%)	14 (3%)	0	100	100
26	BS	152/243 (63%)	144 (95%)	8 (5%)	0	100	100
27	BT	98/280 (35%)	88 (90%)	10 (10%)	0	100	100
29	BV	260/597 (44%)	248 (95%)	12 (5%)	0	100	100
30	BW	335/547 (61%)	307 (92%)	28 (8%)	0	100	100
34	Bc	535/716 (75%)	522 (98%)	13 (2%)	0	100	100
37	Bg	183/302 (61%)	164 (90%)	18 (10%)	1 (0%)	24	55
38	Bh	151/167 (90%)	149 (99%)	2 (1%)	0	100	100
39	Bi	111/268 (41%)	109 (98%)	2 (2%)	0	100	100
40	Bk	413/447 (92%)	404 (98%)	9 (2%)	0	100	100
41	Bl	198/593 (33%)	184 (93%)	14 (7%)	0	100	100
42	HJ	349/1140 (31%)	325 (93%)	24 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	HS	86/235 (37%)	83 (96%)	3 (4%)	0	100	100
All	All	7783/15235 (51%)	7461 (96%)	319 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BE	915	PRO
37	Bg	202	PRO
15	BE	935	PRO

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	B0	238/558 (43%)	238 (100%)	0	100	100
3	B2	297/648 (46%)	297 (100%)	0	100	100
4	B3	177/302 (59%)	177 (100%)	0	100	100
5	B4	72/123 (58%)	72 (100%)	0	100	100
6	B5	114/328 (35%)	114 (100%)	0	100	100
7	B6	98/142 (69%)	98 (100%)	0	100	100
10	B9	55/197 (28%)	55 (100%)	0	100	100
11	BA	429/769 (56%)	429 (100%)	0	100	100
12	BB	465/1261 (37%)	464 (100%)	1 (0%)	87	88
13	BC	166/351 (47%)	166 (100%)	0	100	100
14	BD	276/548 (50%)	276 (100%)	0	100	100
15	BE	541/908 (60%)	539 (100%)	2 (0%)	84	84
16	BF	227/252 (90%)	227 (100%)	0	100	100
17	BG	134/145 (92%)	134 (100%)	0	100	100
18	BH	109/115 (95%)	109 (100%)	0	100	100
21	BK	183/456 (40%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	BL	94/106 (89%)	94 (100%)	0	100	100
23	BO	230/346 (66%)	230 (100%)	0	100	100
25	BQ	376/572 (66%)	376 (100%)	0	100	100
26	BS	137/207 (66%)	137 (100%)	0	100	100
27	BT	86/249 (34%)	86 (100%)	0	100	100
29	BV	238/525 (45%)	238 (100%)	0	100	100
30	BW	296/475 (62%)	296 (100%)	0	100	100
34	Bc	458/620 (74%)	458 (100%)	0	100	100
37	Bg	160/251 (64%)	160 (100%)	0	100	100
38	Bh	130/143 (91%)	130 (100%)	0	100	100
39	Bi	99/221 (45%)	99 (100%)	0	100	100
40	Bk	360/385 (94%)	360 (100%)	0	100	100
41	Bl	181/534 (34%)	181 (100%)	0	100	100
42	HJ	307/968 (32%)	307 (100%)	0	100	100
43	HS	78/207 (38%)	78 (100%)	0	100	100
All	All	6811/12912 (53%)	6808 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	BB	151	HIS
15	BE	975	ARG
15	BE	977	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	B0	176	GLN
1	B0	215	GLN
3	B2	10	GLN
3	B2	14	ASN
3	B2	176	HIS
3	B2	194	ASN
4	B3	80	GLN
4	B3	210	ASN
6	B5	22	HIS

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Mol	Chain	Res	Type
6	B5	39	GLN
6	B5	47	ASN
6	B5	102	GLN
7	B6	111	HIS
11	BA	158	ASN
11	BA	230	GLN
11	BA	357	HIS
11	BA	509	HIS
12	BB	846	GLN
13	BC	64	GLN
14	BD	227	GLN
14	BD	318	HIS
15	BE	478	HIS
15	BE	748	GLN
15	BE	827	GLN
15	BE	929	ASN
15	BE	1023	HIS
21	BK	12	ASN
21	BK	122	GLN
21	BK	131	GLN
22	BL	24	ASN
23	BO	26	GLN
23	BO	86	GLN
23	BO	109	GLN
25	BQ	434	HIS
26	BS	26	ASN
27	BT	61	ASN
29	BV	89	ASN
29	BV	105	GLN
30	BW	10	ASN
30	BW	290	HIS
34	Bc	45	ASN
34	Bc	54	ASN
34	Bc	342	GLN
34	Bc	507	ASN
34	Bc	525	GLN
37	Bg	36	GLN
37	Bg	49	HIS
38	Bh	3	HIS
40	Bk	222	GLN
40	Bk	285	GLN
40	Bk	345	GLN

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Mol	Chain	Res	Type
41	Bl	80	ASN
41	Bl	84	HIS
42	HJ	675	ASN
42	HJ	678	HIS
42	HJ	768	GLN
43	HS	207	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	b1	7/8 (87%)	0	0
45	b2	29/48 (60%)	2 (6%)	0
46	b3	4/5 (80%)	2 (50%)	0
47	b4	26/34 (76%)	3 (11%)	0
48	bA	26/34 (76%)	2 (7%)	0
49	bD	24/27 (88%)	5 (20%)	0
50	bE	90/107 (84%)	22 (24%)	0
51	bG	3/4 (75%)	2 (66%)	0
52	bH	1/2 (50%)	1 (100%)	0
53	bI	2/3 (66%)	2 (100%)	0
54	bJ	57/71 (80%)	16 (28%)	0
55	bK	62/83 (74%)	12 (19%)	0
56	bL	47/48 (97%)	9 (19%)	0
57	bN	48/122 (39%)	7 (14%)	0
58	bO	114/115 (99%)	24 (21%)	0
59	bP	14/15 (93%)	1 (7%)	0
60	bQ	13/14 (92%)	3 (23%)	0
61	bR	18/31 (58%)	4 (22%)	0
62	bS	30/31 (96%)	11 (36%)	0
63	bT	51/60 (85%)	11 (21%)	0
64	bU	24/25 (96%)	6 (25%)	0
65	bV	5/6 (83%)	1 (20%)	0
66	bY	10/11 (90%)	2 (20%)	0
All	All	705/904 (77%)	148 (20%)	0

All (148) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	b2	31	A
45	b2	48	A
46	b3	4	U

Continued on next page...

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Mol	Chain	Res	Type
46	b3	5	U
47	b4	2	G
47	b4	26	G
47	b4	27	U
48	bA	10	G
48	bA	27	A
49	bD	8	A
49	bD	9	A
49	bD	10	G
49	bD	11	G
49	bD	27	G
50	bE	20	G
50	bE	21	G
50	bE	26	G
50	bE	40	G
50	bE	43	A
50	bE	47	C
50	bE	50	U
50	bE	51	G
50	bE	52	G
50	bE	53	A
50	bE	54	U
50	bE	55	U
50	bE	57	G
50	bE	58	A
50	bE	67	G
50	bE	73	U
50	bE	75	C
50	bE	81	U
50	bE	82	U
50	bE	84	A
50	bE	86	A
50	bE	87	A
51	bG	3	U
51	bG	4	U
52	bH	2	U
53	bI	2	U
53	bI	3	U
54	bJ	10	U
54	bJ	11	U
54	bJ	13	A
54	bJ	16	U

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Mol	Chain	Res	Type
54	bJ	30	A
54	bJ	31	C
54	bJ	32	U
54	bJ	34	U
54	bJ	35	A
54	bJ	45	C
54	bJ	50	U
54	bJ	58	A
54	bJ	59	C
54	bJ	60	U
54	bJ	61	U
54	bJ	65	A
55	bK	6	U
55	bK	8	C
55	bK	23	A
55	bK	31	U
55	bK	32	U
55	bK	34	U
55	bK	35	A
55	bK	42	A
55	bK	51	G
55	bK	52	A
55	bK	53	C
55	bK	61	A
56	bL	16	C
56	bL	25	U
56	bL	26	A
56	bL	28	G
56	bL	29	U
56	bL	30	C
56	bL	31	A
56	bL	32	A
56	bL	36	U
57	bN	10	G
57	bN	16	U
57	bN	29	G
57	bN	38	U
57	bN	39	A
57	bN	40	G
57	bN	49	U
58	bO	2	G
58	bO	3	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	bO	9	G
58	bO	16	C
58	bO	23	A
58	bO	24	A
58	bO	34	A
58	bO	36	A
58	bO	42	C
58	bO	56	U
58	bO	63	U
58	bO	65	G
58	bO	67	A
58	bO	68	G
58	bO	69	A
58	bO	74	A
58	bO	75	G
58	bO	86	A
58	bO	88	A
58	bO	89	U
58	bO	91	C
58	bO	97	G
58	bO	100	A
58	bO	103	A
59	bP	15	U
60	bQ	6	U
60	bQ	7	U
60	bQ	14	U
61	bR	5	C
61	bR	6	A
61	bR	13	A
61	bR	14	U
62	bS	7	U
62	bS	13	U
62	bS	18	U
62	bS	19	U
62	bS	20	U
62	bS	21	U
62	bS	22	U
62	bS	23	U
62	bS	24	U
62	bS	25	U
62	bS	26	U
63	bT	15	A

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Mol	Chain	Res	Type
63	bT	17	A
63	bT	19	G
63	bT	21	U
63	bT	22	A
63	bT	23	G
63	bT	32	G
63	bT	35	C
63	bT	44	G
63	bT	46	A
63	bT	50	A
64	bU	3	U
64	bU	12	U
64	bU	18	U
64	bU	19	U
64	bU	22	U
64	bU	25	U
65	bV	6	U
66	bY	6	U
66	bY	9	U

There are no RNA pucker outliers to report.

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 ⓘ

There are no chain breaks in this entry.

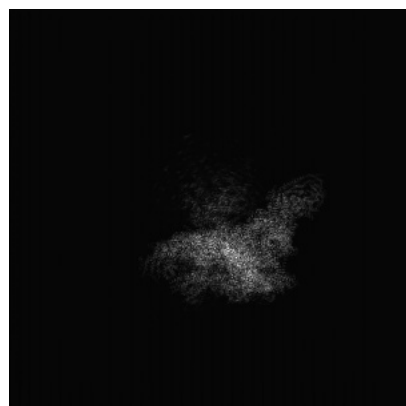
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50470. These allow visual inspection of the internal detail of the map and identification of artifacts.

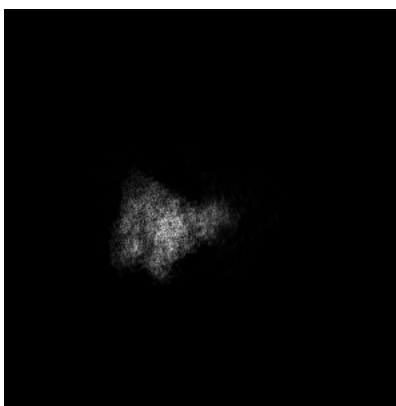
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

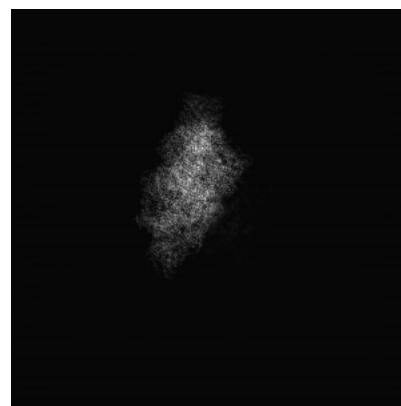
6.1.1 Primary map



X

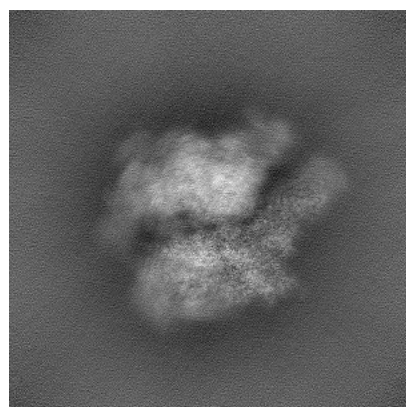


Y

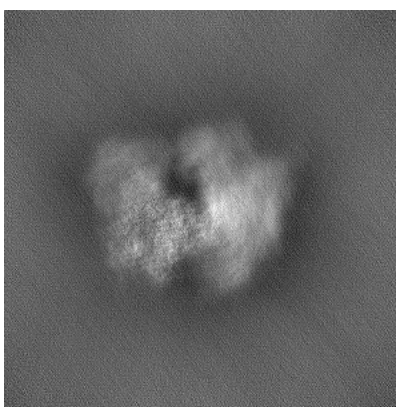


Z

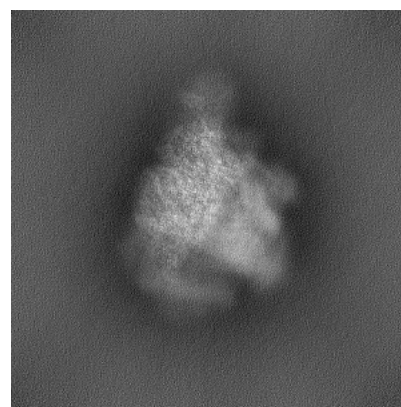
6.1.2 Raw map



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: 210

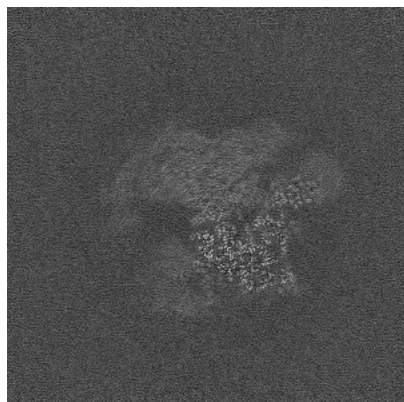


Y Index: 210

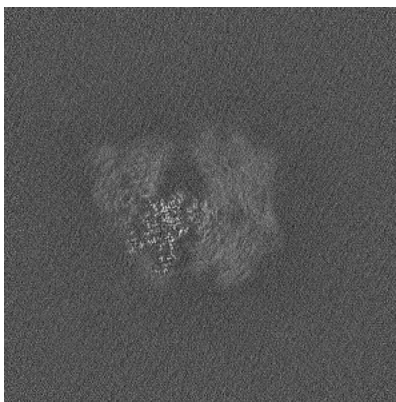


Z Index: 210

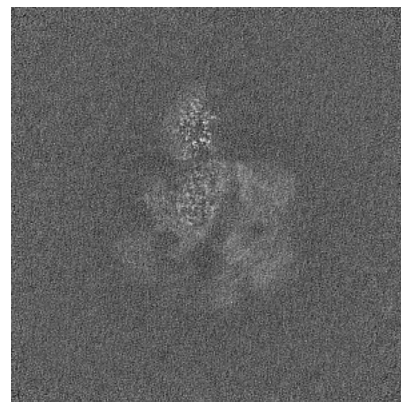
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

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: 196

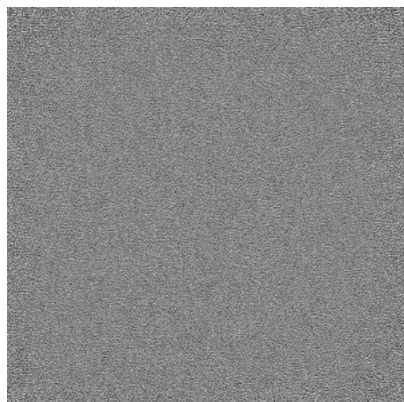


Y Index: 241

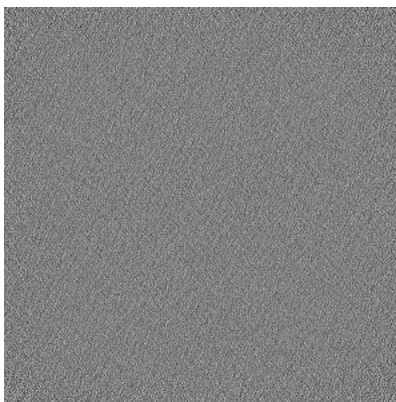


Z Index: 165

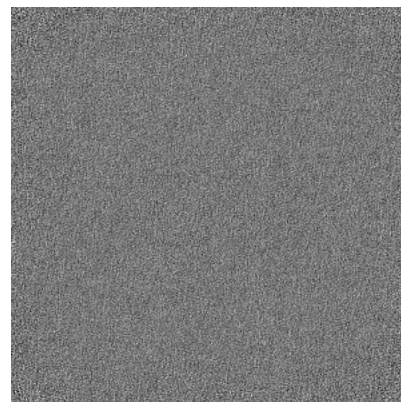
6.3.2 Raw map



X Index: 0



Y Index: 0

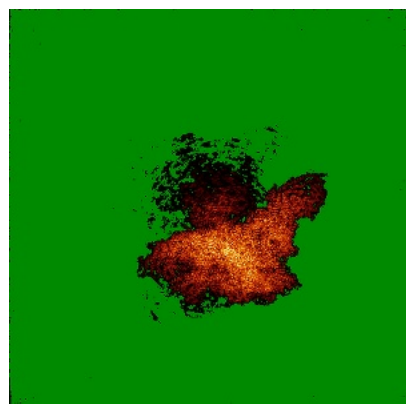


Z Index: 419

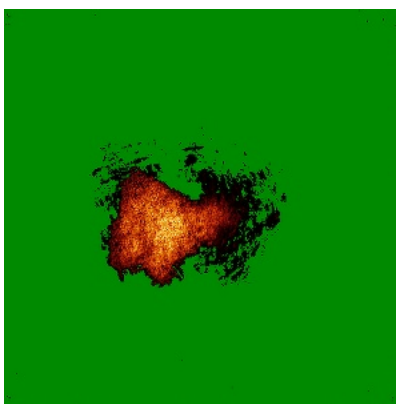
The images above show the largest variance slices of the map in three orthogonal directions.

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

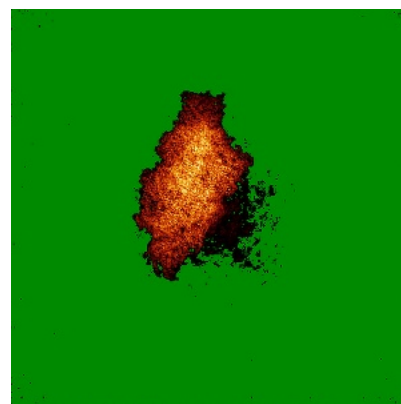
6.4.1 Primary map



X

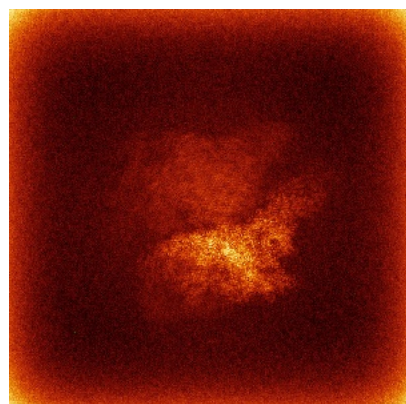


Y

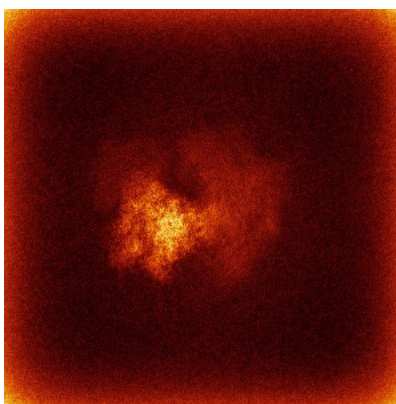


Z

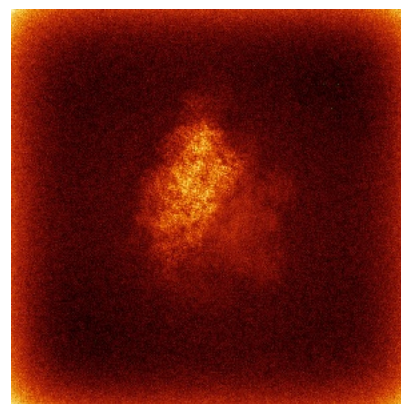
6.4.2 Raw map



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](#)

This section was not generated.

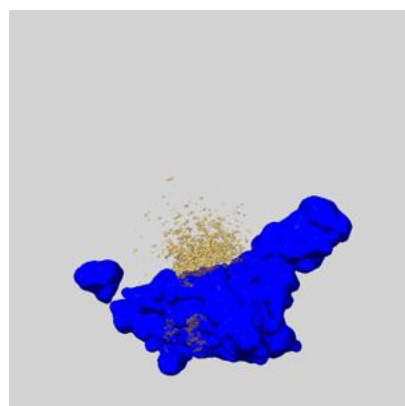
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

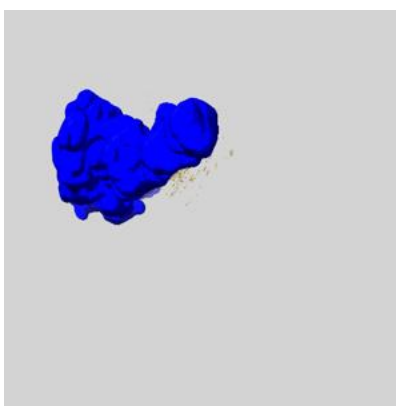
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

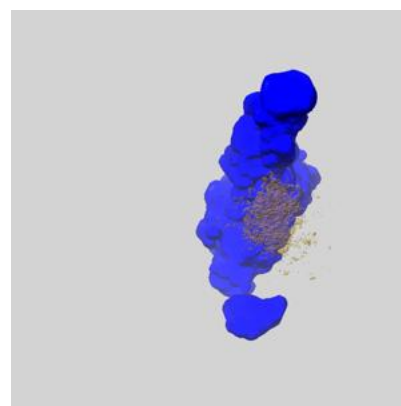
6.6.1 emd_50470_msk_1.map [i](#)



X



Y

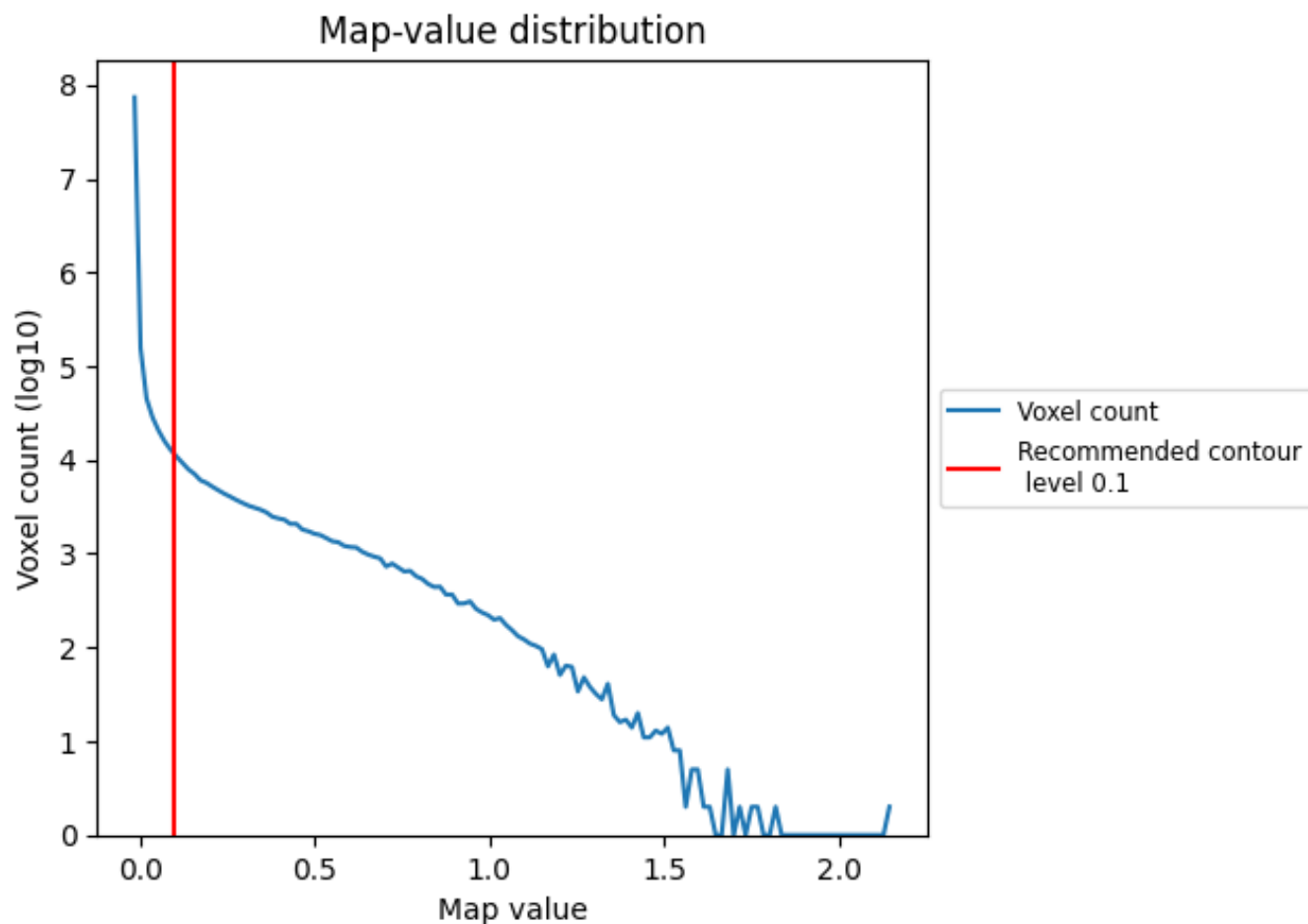


Z

7 Map analysis [i](#)

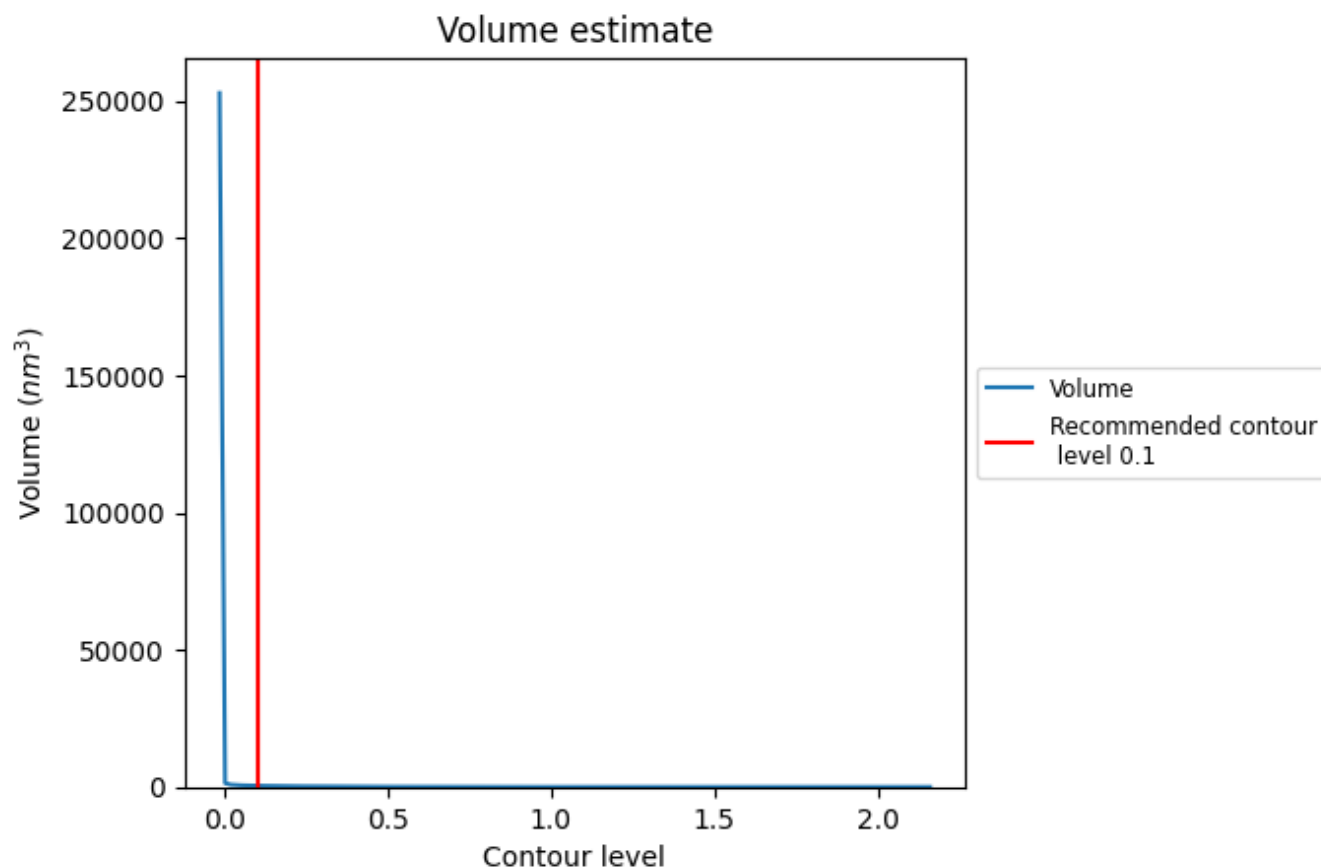
This section contains the results of statistical analysis of the map.

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.

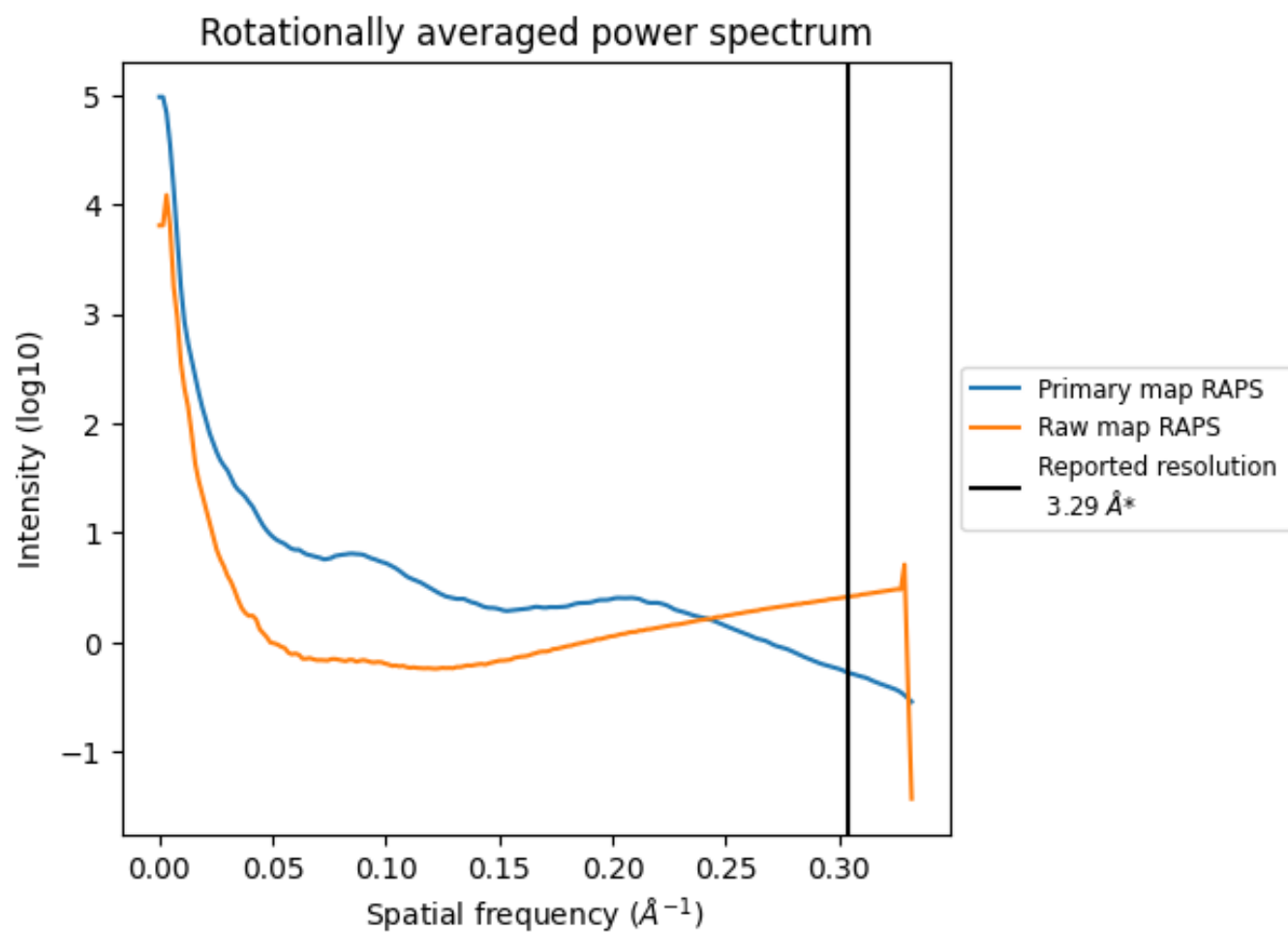
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm^3 ; this corresponds to an approximate mass of 397 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 ⓘ

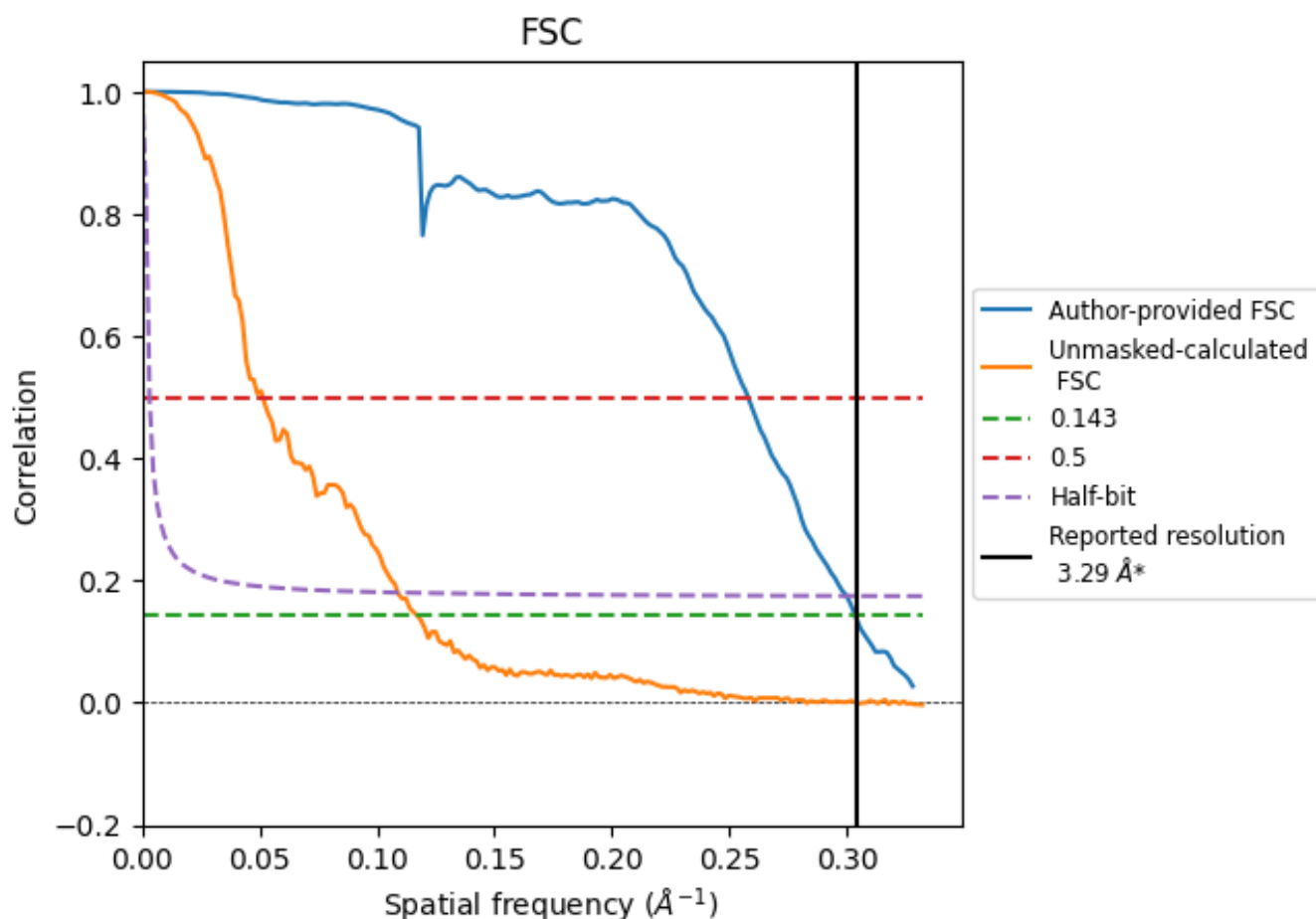


*Reported resolution corresponds to spatial frequency of 0.304 \AA^{-1}

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 0.304 \AA^{-1}

8.2 Resolution estimates [i](#)

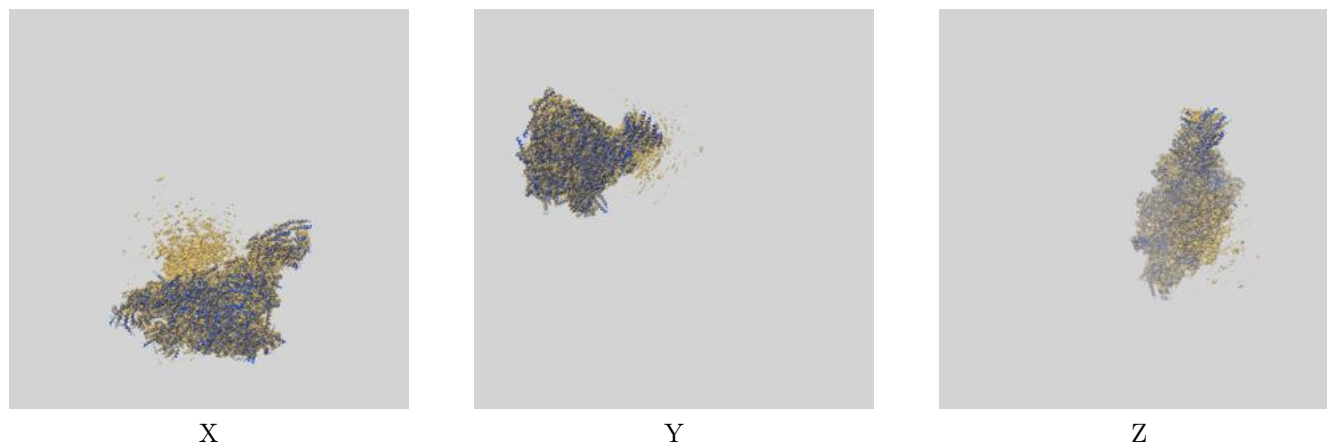
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.29	3.88	3.33
Unmasked-calculated*	8.55	19.46	9.18

*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 8.55 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

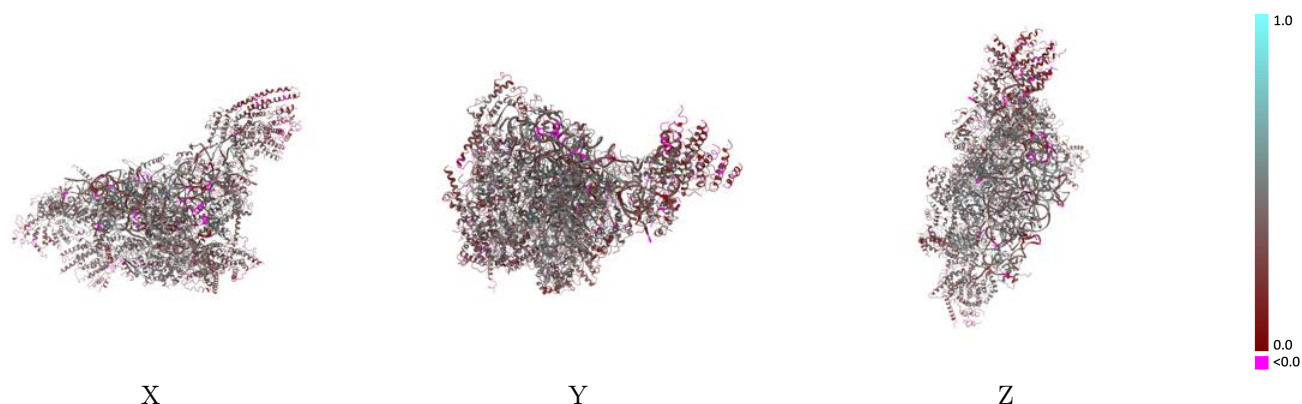
This section contains information regarding the fit between EMDB map EMD-50470 and PDB model 9FIA. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



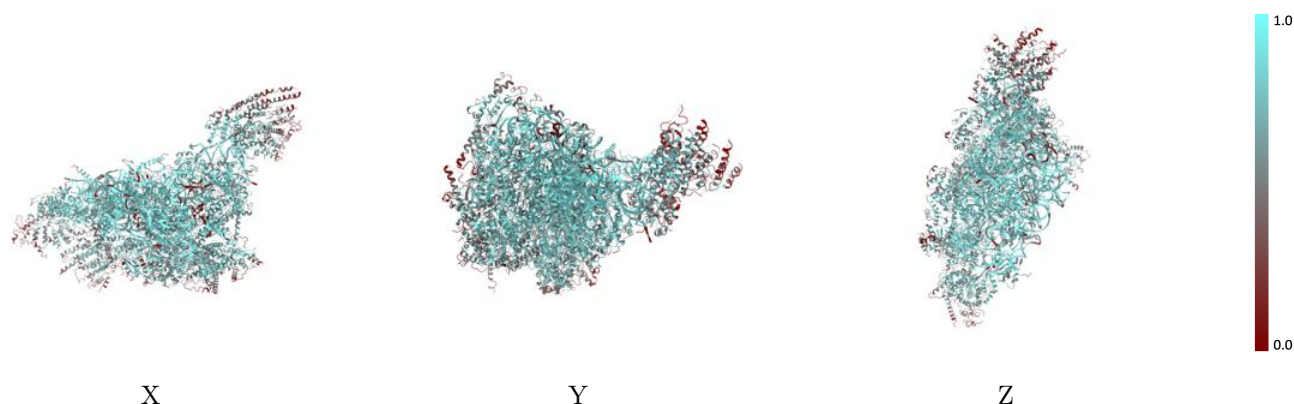
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



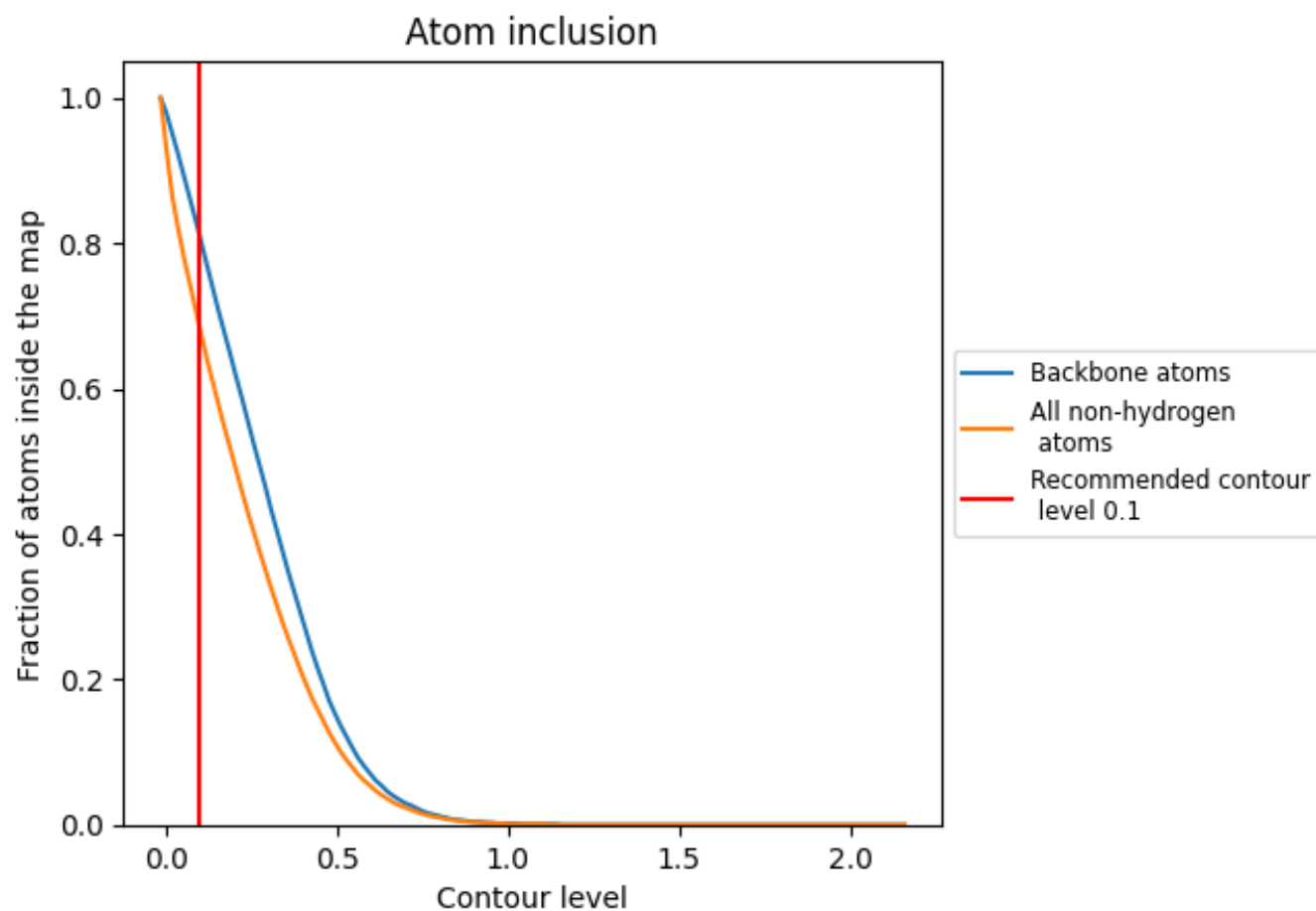
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.3530
B0	 0.5680	 0.3020
B1	 0.7500	 0.4160
B2	 0.6760	 0.3560
B3	 0.7200	 0.3910
B4	 0.7010	 0.4030
B5	 0.7510	 0.3930
B6	 0.8290	 0.4550
B7	 0.2500	 0.2890
B8	 0.6550	 0.4170
B9	 0.7440	 0.3960
BA	 0.6590	 0.3660
BB	 0.5020	 0.2630
BC	 0.6700	 0.3640
BD	 0.5540	 0.2860
BE	 0.5270	 0.3000
BF	 0.6900	 0.3860
BG	 0.6830	 0.3790
BH	 0.8530	 0.4580
BI	 0.8460	 0.4210
BJ	 0.6250	 0.4180
BK	 0.8060	 0.4230
BL	 0.8630	 0.4570
BN	 0.6150	 0.3530
BO	 0.8030	 0.4380
BP	 0.8080	 0.4020
BQ	 0.7070	 0.3770
BS	 0.5640	 0.3120
BT	 0.7310	 0.3420
BU	 0.5890	 0.3880
BV	 0.6830	 0.3720
BW	 0.6510	 0.3050
BX	 0.7880	 0.5010
BY	 0.2270	 0.1740
Ba	 0.4000	 0.3490



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Chain	Atom inclusion	Q-score
Bb	 0.5940	 0.3650
Bc	 0.6780	 0.3710
Bd	 0.7880	 0.3780
Be	 0.7920	 0.4840
Bg	 0.7550	 0.3820
Bh	 0.7780	 0.4300
Bi	 0.7450	 0.4040
Bj	 0.9290	 0.5160
Bk	 0.6500	 0.3530
Bl	 0.6760	 0.3490
HJ	 0.6470	 0.3320
HS	 0.5180	 0.2740
b1	 0.8500	 0.3990
b2	 0.7780	 0.3900
b3	 0.5000	 0.2460
b4	 0.7280	 0.3060
bA	 0.7850	 0.3670
bD	 0.7970	 0.3800
bE	 0.7840	 0.3460
bG	 0.1630	 -0.1460
bH	 0.6500	 0.1360
bI	 0.1330	 -0.1050
bJ	 0.6640	 0.2890
bK	 0.6900	 0.3040
bL	 0.8390	 0.3670
bN	 0.7830	 0.3630
bO	 0.8280	 0.3940
bP	 0.7730	 0.3660
bQ	 0.7040	 0.3080
bR	 0.8140	 0.3820
bS	 0.7660	 0.3670
bT	 0.8130	 0.3740
bU	 0.7760	 0.3190
bV	 0.8830	 0.4030
bY	 0.7680	 0.3110