



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:30 AM UTC

PDB ID : 9DJW / pdb\_00009djw  
Title : X-ray crystal structure of TNFa-VNAR D1 complex  
Authors : Ubah, O.C.; Shi, K.; Aihara, H.; Barelle, C.J.; LeBeau, A.M.  
Deposited on : 2024-09-06  
Resolution : 3.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

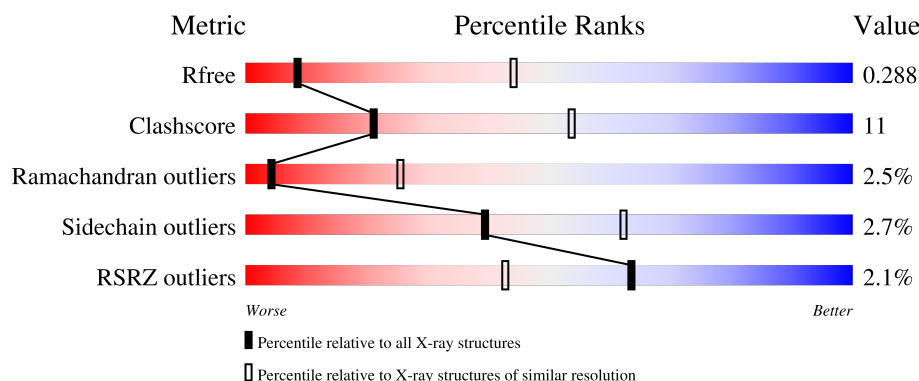
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.43 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.






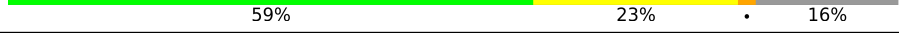


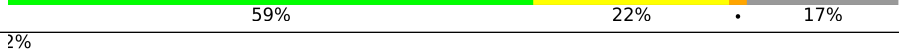




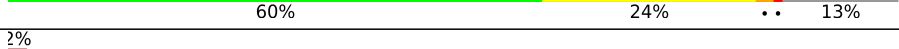
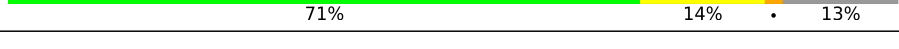












Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	129	
1	1	129	
1	5	129	
1	6	129	
1	7	129	

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Mol	Chain	Length	Quality of chain
1	D	129	% 
1	E	129	
1	F	129	% 
1	J	129	
1	K	129	
1	L	129	3% 
1	P	129	
1	Q	129	2% 
1	R	129	2% 
1	V	129	4% 
1	W	129	
1	X	129	2% 
1	b	129	
1	c	129	
1	d	129	2% 
1	h	129	% 
1	i	129	7% 
1	j	129	3% 
1	n	129	% 
1	o	129	2% 
1	p	129	
1	t	129	2% 
1	u	129	2% 
1	v	129	3% 
1	z	129	

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Mol	Chain	Length	Quality of chain
2	2	156	
2	3	156	
2	4	156	
2	A	156	
2	B	156	
2	C	156	
2	G	156	
2	H	156	
2	I	156	
2	M	156	
2	N	156	
2	O	156	
2	S	156	
2	T	156	
2	U	156	
2	Y	156	
2	Z	156	
2	a	156	
2	e	156	
2	f	156	
2	g	156	
2	k	156	
2	l	156	
2	m	156	
2	q	156	

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Mol	Chain	Length	Quality of chain
2	r	156	<div><div><div>%</div><div><div></div><div>76%</div><div>21%</div><div></div></div><div>• •</div></div></div>
2	s	156	<div><div><div>%</div><div><div></div><div>68%</div><div>29%</div><div></div></div><div>• •</div></div></div>
2	w	156	<div><div><div>%</div><div><div></div><div>76%</div><div>22%</div><div></div></div><div>•</div></div></div>
2	x	156	<div><div><div>3%</div><div><div></div><div>71%</div><div>26%</div><div></div></div><div>• •</div></div></div>
2	y	156	<div><div><div>%</div><div><div></div><div>78%</div><div>19%</div><div></div></div><div>•</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60848 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Antigen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	1	104	Total	C	N	O	S	0	0	0
			797	485	137	171	4			
1	5	108	Total	C	N	O	S	0	0	0
			820	498	142	176	4			
1	6	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	7	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	D	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			
1	E	108	Total	C	N	O	S	0	0	0
			820	498	142	176	4			
1	F	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			
1	J	108	Total	C	N	O	S	0	0	0
			820	498	142	176	4			
1	K	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			
1	L	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	P	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	Q	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	R	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	V	106	Total	C	N	O	S	0	1	0
			821	498	144	175	4			
1	W	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	b	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	c	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	d	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	h	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	i	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	j	105	Total	C	N	O	S	0	0	0
			802	488	138	172	4			
1	n	109	Total	C	N	O	S	0	0	0
			825	501	143	177	4			
1	o	104	Total	C	N	O	S	0	0	0
			797	485	137	171	4			
1	p	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	t	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	u	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	v	105	Total	C	N	O	S	0	0	0
			802	488	138	172	4			
1	z	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			

There are 990 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	28	HIS	ASN	conflict	UNP Q8JGJ1
0	31	THR	LEU	conflict	UNP Q8JGJ1
0	?	-	ASN	deletion	UNP Q8JGJ1
0	?	-	VAL	deletion	UNP Q8JGJ1
0	84	ALA	TYR	conflict	UNP Q8JGJ1
0	86	GLU	TRP	conflict	UNP Q8JGJ1
0	87	CYS	TYR	conflict	UNP Q8JGJ1
0	88	GLN	GLY	conflict	UNP Q8JGJ1
0	90	GLY	ASP	conflict	UNP Q8JGJ1
0	91	LEU	CYS	conflict	UNP Q8JGJ1
0	94	TYR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
0	107	ALA	-	expression tag	UNP Q8JGJ1
0	108	ALA	-	expression tag	UNP Q8JGJ1
0	109	ALA	-	expression tag	UNP Q8JGJ1
0	110	HIS	-	expression tag	UNP Q8JGJ1
0	111	HIS	-	expression tag	UNP Q8JGJ1
0	112	HIS	-	expression tag	UNP Q8JGJ1
0	113	HIS	-	expression tag	UNP Q8JGJ1
0	114	HIS	-	expression tag	UNP Q8JGJ1
0	115	HIS	-	expression tag	UNP Q8JGJ1
0	116	GLY	-	expression tag	UNP Q8JGJ1
0	117	ALA	-	expression tag	UNP Q8JGJ1
0	118	ALA	-	expression tag	UNP Q8JGJ1
0	119	GLU	-	expression tag	UNP Q8JGJ1
0	120	SER	-	expression tag	UNP Q8JGJ1
0	121	LYS	-	expression tag	UNP Q8JGJ1
0	122	LEU	-	expression tag	UNP Q8JGJ1
0	123	ILE	-	expression tag	UNP Q8JGJ1
0	124	SER	-	expression tag	UNP Q8JGJ1
0	125	GLU	-	expression tag	UNP Q8JGJ1
0	126	GLU	-	expression tag	UNP Q8JGJ1
0	127	ASP	-	expression tag	UNP Q8JGJ1
0	128	LEU	-	expression tag	UNP Q8JGJ1
1	28	HIS	ASN	conflict	UNP Q8JGJ1
1	31	THR	LEU	conflict	UNP Q8JGJ1
1	?	-	ASN	deletion	UNP Q8JGJ1
1	?	-	VAL	deletion	UNP Q8JGJ1
1	84	ALA	TYR	conflict	UNP Q8JGJ1
1	86	GLU	TRP	conflict	UNP Q8JGJ1
1	87	CYS	TYR	conflict	UNP Q8JGJ1
1	88	GLN	GLY	conflict	UNP Q8JGJ1
1	90	GLY	ASP	conflict	UNP Q8JGJ1
1	91	LEU	CYS	conflict	UNP Q8JGJ1
1	94	TYR	LEU	conflict	UNP Q8JGJ1
1	107	ALA	-	expression tag	UNP Q8JGJ1
1	108	ALA	-	expression tag	UNP Q8JGJ1
1	109	ALA	-	expression tag	UNP Q8JGJ1
1	110	HIS	-	expression tag	UNP Q8JGJ1
1	111	HIS	-	expression tag	UNP Q8JGJ1
1	112	HIS	-	expression tag	UNP Q8JGJ1
1	113	HIS	-	expression tag	UNP Q8JGJ1
1	114	HIS	-	expression tag	UNP Q8JGJ1
1	115	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
1	116	GLY	-	expression tag	UNP Q8JGJ1
1	117	ALA	-	expression tag	UNP Q8JGJ1
1	118	ALA	-	expression tag	UNP Q8JGJ1
1	119	GLU	-	expression tag	UNP Q8JGJ1
1	120	SER	-	expression tag	UNP Q8JGJ1
1	121	LYS	-	expression tag	UNP Q8JGJ1
1	122	LEU	-	expression tag	UNP Q8JGJ1
1	123	ILE	-	expression tag	UNP Q8JGJ1
1	124	SER	-	expression tag	UNP Q8JGJ1
1	125	GLU	-	expression tag	UNP Q8JGJ1
1	126	GLU	-	expression tag	UNP Q8JGJ1
1	127	ASP	-	expression tag	UNP Q8JGJ1
1	128	LEU	-	expression tag	UNP Q8JGJ1
5	28	HIS	ASN	conflict	UNP Q8JGJ1
5	31	THR	LEU	conflict	UNP Q8JGJ1
5	?	-	ASN	deletion	UNP Q8JGJ1
5	?	-	VAL	deletion	UNP Q8JGJ1
5	84	ALA	TYR	conflict	UNP Q8JGJ1
5	86	GLU	TRP	conflict	UNP Q8JGJ1
5	87	CYS	TYR	conflict	UNP Q8JGJ1
5	88	GLN	GLY	conflict	UNP Q8JGJ1
5	90	GLY	ASP	conflict	UNP Q8JGJ1
5	91	LEU	CYS	conflict	UNP Q8JGJ1
5	94	TYR	LEU	conflict	UNP Q8JGJ1
5	107	ALA	-	expression tag	UNP Q8JGJ1
5	108	ALA	-	expression tag	UNP Q8JGJ1
5	109	ALA	-	expression tag	UNP Q8JGJ1
5	110	HIS	-	expression tag	UNP Q8JGJ1
5	111	HIS	-	expression tag	UNP Q8JGJ1
5	112	HIS	-	expression tag	UNP Q8JGJ1
5	113	HIS	-	expression tag	UNP Q8JGJ1
5	114	HIS	-	expression tag	UNP Q8JGJ1
5	115	HIS	-	expression tag	UNP Q8JGJ1
5	116	GLY	-	expression tag	UNP Q8JGJ1
5	117	ALA	-	expression tag	UNP Q8JGJ1
5	118	ALA	-	expression tag	UNP Q8JGJ1
5	119	GLU	-	expression tag	UNP Q8JGJ1
5	120	SER	-	expression tag	UNP Q8JGJ1
5	121	LYS	-	expression tag	UNP Q8JGJ1
5	122	LEU	-	expression tag	UNP Q8JGJ1
5	123	ILE	-	expression tag	UNP Q8JGJ1
5	124	SER	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
5	125	GLU	-	expression tag	UNP Q8JGJ1
5	126	GLU	-	expression tag	UNP Q8JGJ1
5	127	ASP	-	expression tag	UNP Q8JGJ1
5	128	LEU	-	expression tag	UNP Q8JGJ1
6	28	HIS	ASN	conflict	UNP Q8JGJ1
6	31	THR	LEU	conflict	UNP Q8JGJ1
6	?	-	ASN	deletion	UNP Q8JGJ1
6	?	-	VAL	deletion	UNP Q8JGJ1
6	84	ALA	TYR	conflict	UNP Q8JGJ1
6	86	GLU	TRP	conflict	UNP Q8JGJ1
6	87	CYS	TYR	conflict	UNP Q8JGJ1
6	88	GLN	GLY	conflict	UNP Q8JGJ1
6	90	GLY	ASP	conflict	UNP Q8JGJ1
6	91	LEU	CYS	conflict	UNP Q8JGJ1
6	94	TYR	LEU	conflict	UNP Q8JGJ1
6	107	ALA	-	expression tag	UNP Q8JGJ1
6	108	ALA	-	expression tag	UNP Q8JGJ1
6	109	ALA	-	expression tag	UNP Q8JGJ1
6	110	HIS	-	expression tag	UNP Q8JGJ1
6	111	HIS	-	expression tag	UNP Q8JGJ1
6	112	HIS	-	expression tag	UNP Q8JGJ1
6	113	HIS	-	expression tag	UNP Q8JGJ1
6	114	HIS	-	expression tag	UNP Q8JGJ1
6	115	HIS	-	expression tag	UNP Q8JGJ1
6	116	GLY	-	expression tag	UNP Q8JGJ1
6	117	ALA	-	expression tag	UNP Q8JGJ1
6	118	ALA	-	expression tag	UNP Q8JGJ1
6	119	GLU	-	expression tag	UNP Q8JGJ1
6	120	SER	-	expression tag	UNP Q8JGJ1
6	121	LYS	-	expression tag	UNP Q8JGJ1
6	122	LEU	-	expression tag	UNP Q8JGJ1
6	123	ILE	-	expression tag	UNP Q8JGJ1
6	124	SER	-	expression tag	UNP Q8JGJ1
6	125	GLU	-	expression tag	UNP Q8JGJ1
6	126	GLU	-	expression tag	UNP Q8JGJ1
6	127	ASP	-	expression tag	UNP Q8JGJ1
6	128	LEU	-	expression tag	UNP Q8JGJ1
7	28	HIS	ASN	conflict	UNP Q8JGJ1
7	31	THR	LEU	conflict	UNP Q8JGJ1
7	?	-	ASN	deletion	UNP Q8JGJ1
7	?	-	VAL	deletion	UNP Q8JGJ1
7	84	ALA	TYR	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
7	86	GLU	TRP	conflict	UNP Q8JGJ1
7	87	CYS	TYR	conflict	UNP Q8JGJ1
7	88	GLN	GLY	conflict	UNP Q8JGJ1
7	90	GLY	ASP	conflict	UNP Q8JGJ1
7	91	LEU	CYS	conflict	UNP Q8JGJ1
7	94	TYR	LEU	conflict	UNP Q8JGJ1
7	107	ALA	-	expression tag	UNP Q8JGJ1
7	108	ALA	-	expression tag	UNP Q8JGJ1
7	109	ALA	-	expression tag	UNP Q8JGJ1
7	110	HIS	-	expression tag	UNP Q8JGJ1
7	111	HIS	-	expression tag	UNP Q8JGJ1
7	112	HIS	-	expression tag	UNP Q8JGJ1
7	113	HIS	-	expression tag	UNP Q8JGJ1
7	114	HIS	-	expression tag	UNP Q8JGJ1
7	115	HIS	-	expression tag	UNP Q8JGJ1
7	116	GLY	-	expression tag	UNP Q8JGJ1
7	117	ALA	-	expression tag	UNP Q8JGJ1
7	118	ALA	-	expression tag	UNP Q8JGJ1
7	119	GLU	-	expression tag	UNP Q8JGJ1
7	120	SER	-	expression tag	UNP Q8JGJ1
7	121	LYS	-	expression tag	UNP Q8JGJ1
7	122	LEU	-	expression tag	UNP Q8JGJ1
7	123	ILE	-	expression tag	UNP Q8JGJ1
7	124	SER	-	expression tag	UNP Q8JGJ1
7	125	GLU	-	expression tag	UNP Q8JGJ1
7	126	GLU	-	expression tag	UNP Q8JGJ1
7	127	ASP	-	expression tag	UNP Q8JGJ1
7	128	LEU	-	expression tag	UNP Q8JGJ1
D	28	HIS	ASN	conflict	UNP Q8JGJ1
D	31	THR	LEU	conflict	UNP Q8JGJ1
D	?	-	ASN	deletion	UNP Q8JGJ1
D	?	-	VAL	deletion	UNP Q8JGJ1
D	84	ALA	TYR	conflict	UNP Q8JGJ1
D	86	GLU	TRP	conflict	UNP Q8JGJ1
D	87	CYS	TYR	conflict	UNP Q8JGJ1
D	88	GLN	GLY	conflict	UNP Q8JGJ1
D	90	GLY	ASP	conflict	UNP Q8JGJ1
D	91	LEU	CYS	conflict	UNP Q8JGJ1
D	94	TYR	LEU	conflict	UNP Q8JGJ1
D	107	ALA	-	expression tag	UNP Q8JGJ1
D	108	ALA	-	expression tag	UNP Q8JGJ1
D	109	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	110	HIS	-	expression tag	UNP Q8JGJ1
D	111	HIS	-	expression tag	UNP Q8JGJ1
D	112	HIS	-	expression tag	UNP Q8JGJ1
D	113	HIS	-	expression tag	UNP Q8JGJ1
D	114	HIS	-	expression tag	UNP Q8JGJ1
D	115	HIS	-	expression tag	UNP Q8JGJ1
D	116	GLY	-	expression tag	UNP Q8JGJ1
D	117	ALA	-	expression tag	UNP Q8JGJ1
D	118	ALA	-	expression tag	UNP Q8JGJ1
D	119	GLU	-	expression tag	UNP Q8JGJ1
D	120	SER	-	expression tag	UNP Q8JGJ1
D	121	LYS	-	expression tag	UNP Q8JGJ1
D	122	LEU	-	expression tag	UNP Q8JGJ1
D	123	ILE	-	expression tag	UNP Q8JGJ1
D	124	SER	-	expression tag	UNP Q8JGJ1
D	125	GLU	-	expression tag	UNP Q8JGJ1
D	126	GLU	-	expression tag	UNP Q8JGJ1
D	127	ASP	-	expression tag	UNP Q8JGJ1
D	128	LEU	-	expression tag	UNP Q8JGJ1
E	28	HIS	ASN	conflict	UNP Q8JGJ1
E	31	THR	LEU	conflict	UNP Q8JGJ1
E	?	-	ASN	deletion	UNP Q8JGJ1
E	?	-	VAL	deletion	UNP Q8JGJ1
E	84	ALA	TYR	conflict	UNP Q8JGJ1
E	86	GLU	TRP	conflict	UNP Q8JGJ1
E	87	CYS	TYR	conflict	UNP Q8JGJ1
E	88	GLN	GLY	conflict	UNP Q8JGJ1
E	90	GLY	ASP	conflict	UNP Q8JGJ1
E	91	LEU	CYS	conflict	UNP Q8JGJ1
E	94	TYR	LEU	conflict	UNP Q8JGJ1
E	107	ALA	-	expression tag	UNP Q8JGJ1
E	108	ALA	-	expression tag	UNP Q8JGJ1
E	109	ALA	-	expression tag	UNP Q8JGJ1
E	110	HIS	-	expression tag	UNP Q8JGJ1
E	111	HIS	-	expression tag	UNP Q8JGJ1
E	112	HIS	-	expression tag	UNP Q8JGJ1
E	113	HIS	-	expression tag	UNP Q8JGJ1
E	114	HIS	-	expression tag	UNP Q8JGJ1
E	115	HIS	-	expression tag	UNP Q8JGJ1
E	116	GLY	-	expression tag	UNP Q8JGJ1
E	117	ALA	-	expression tag	UNP Q8JGJ1
E	118	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	119	GLU	-	expression tag	UNP Q8JGJ1
E	120	SER	-	expression tag	UNP Q8JGJ1
E	121	LYS	-	expression tag	UNP Q8JGJ1
E	122	LEU	-	expression tag	UNP Q8JGJ1
E	123	ILE	-	expression tag	UNP Q8JGJ1
E	124	SER	-	expression tag	UNP Q8JGJ1
E	125	GLU	-	expression tag	UNP Q8JGJ1
E	126	GLU	-	expression tag	UNP Q8JGJ1
E	127	ASP	-	expression tag	UNP Q8JGJ1
E	128	LEU	-	expression tag	UNP Q8JGJ1
F	28	HIS	ASN	conflict	UNP Q8JGJ1
F	31	THR	LEU	conflict	UNP Q8JGJ1
F	?	-	ASN	deletion	UNP Q8JGJ1
F	?	-	VAL	deletion	UNP Q8JGJ1
F	84	ALA	TYR	conflict	UNP Q8JGJ1
F	86	GLU	TRP	conflict	UNP Q8JGJ1
F	87	CYS	TYR	conflict	UNP Q8JGJ1
F	88	GLN	GLY	conflict	UNP Q8JGJ1
F	90	GLY	ASP	conflict	UNP Q8JGJ1
F	91	LEU	CYS	conflict	UNP Q8JGJ1
F	94	TYR	LEU	conflict	UNP Q8JGJ1
F	107	ALA	-	expression tag	UNP Q8JGJ1
F	108	ALA	-	expression tag	UNP Q8JGJ1
F	109	ALA	-	expression tag	UNP Q8JGJ1
F	110	HIS	-	expression tag	UNP Q8JGJ1
F	111	HIS	-	expression tag	UNP Q8JGJ1
F	112	HIS	-	expression tag	UNP Q8JGJ1
F	113	HIS	-	expression tag	UNP Q8JGJ1
F	114	HIS	-	expression tag	UNP Q8JGJ1
F	115	HIS	-	expression tag	UNP Q8JGJ1
F	116	GLY	-	expression tag	UNP Q8JGJ1
F	117	ALA	-	expression tag	UNP Q8JGJ1
F	118	ALA	-	expression tag	UNP Q8JGJ1
F	119	GLU	-	expression tag	UNP Q8JGJ1
F	120	SER	-	expression tag	UNP Q8JGJ1
F	121	LYS	-	expression tag	UNP Q8JGJ1
F	122	LEU	-	expression tag	UNP Q8JGJ1
F	123	ILE	-	expression tag	UNP Q8JGJ1
F	124	SER	-	expression tag	UNP Q8JGJ1
F	125	GLU	-	expression tag	UNP Q8JGJ1
F	126	GLU	-	expression tag	UNP Q8JGJ1
F	127	ASP	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	128	LEU	-	expression tag	UNP Q8JGJ1
J	28	HIS	ASN	conflict	UNP Q8JGJ1
J	31	THR	LEU	conflict	UNP Q8JGJ1
J	?	-	ASN	deletion	UNP Q8JGJ1
J	?	-	VAL	deletion	UNP Q8JGJ1
J	84	ALA	TYR	conflict	UNP Q8JGJ1
J	86	GLU	TRP	conflict	UNP Q8JGJ1
J	87	CYS	TYR	conflict	UNP Q8JGJ1
J	88	GLN	GLY	conflict	UNP Q8JGJ1
J	90	GLY	ASP	conflict	UNP Q8JGJ1
J	91	LEU	CYS	conflict	UNP Q8JGJ1
J	94	TYR	LEU	conflict	UNP Q8JGJ1
J	107	ALA	-	expression tag	UNP Q8JGJ1
J	108	ALA	-	expression tag	UNP Q8JGJ1
J	109	ALA	-	expression tag	UNP Q8JGJ1
J	110	HIS	-	expression tag	UNP Q8JGJ1
J	111	HIS	-	expression tag	UNP Q8JGJ1
J	112	HIS	-	expression tag	UNP Q8JGJ1
J	113	HIS	-	expression tag	UNP Q8JGJ1
J	114	HIS	-	expression tag	UNP Q8JGJ1
J	115	HIS	-	expression tag	UNP Q8JGJ1
J	116	GLY	-	expression tag	UNP Q8JGJ1
J	117	ALA	-	expression tag	UNP Q8JGJ1
J	118	ALA	-	expression tag	UNP Q8JGJ1
J	119	GLU	-	expression tag	UNP Q8JGJ1
J	120	SER	-	expression tag	UNP Q8JGJ1
J	121	LYS	-	expression tag	UNP Q8JGJ1
J	122	LEU	-	expression tag	UNP Q8JGJ1
J	123	ILE	-	expression tag	UNP Q8JGJ1
J	124	SER	-	expression tag	UNP Q8JGJ1
J	125	GLU	-	expression tag	UNP Q8JGJ1
J	126	GLU	-	expression tag	UNP Q8JGJ1
J	127	ASP	-	expression tag	UNP Q8JGJ1
J	128	LEU	-	expression tag	UNP Q8JGJ1
K	28	HIS	ASN	conflict	UNP Q8JGJ1
K	31	THR	LEU	conflict	UNP Q8JGJ1
K	?	-	ASN	deletion	UNP Q8JGJ1
K	?	-	VAL	deletion	UNP Q8JGJ1
K	84	ALA	TYR	conflict	UNP Q8JGJ1
K	86	GLU	TRP	conflict	UNP Q8JGJ1
K	87	CYS	TYR	conflict	UNP Q8JGJ1
K	88	GLN	GLY	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	90	GLY	ASP	conflict	UNP Q8JGJ1
K	91	LEU	CYS	conflict	UNP Q8JGJ1
K	94	TYR	LEU	conflict	UNP Q8JGJ1
K	107	ALA	-	expression tag	UNP Q8JGJ1
K	108	ALA	-	expression tag	UNP Q8JGJ1
K	109	ALA	-	expression tag	UNP Q8JGJ1
K	110	HIS	-	expression tag	UNP Q8JGJ1
K	111	HIS	-	expression tag	UNP Q8JGJ1
K	112	HIS	-	expression tag	UNP Q8JGJ1
K	113	HIS	-	expression tag	UNP Q8JGJ1
K	114	HIS	-	expression tag	UNP Q8JGJ1
K	115	HIS	-	expression tag	UNP Q8JGJ1
K	116	GLY	-	expression tag	UNP Q8JGJ1
K	117	ALA	-	expression tag	UNP Q8JGJ1
K	118	ALA	-	expression tag	UNP Q8JGJ1
K	119	GLU	-	expression tag	UNP Q8JGJ1
K	120	SER	-	expression tag	UNP Q8JGJ1
K	121	LYS	-	expression tag	UNP Q8JGJ1
K	122	LEU	-	expression tag	UNP Q8JGJ1
K	123	ILE	-	expression tag	UNP Q8JGJ1
K	124	SER	-	expression tag	UNP Q8JGJ1
K	125	GLU	-	expression tag	UNP Q8JGJ1
K	126	GLU	-	expression tag	UNP Q8JGJ1
K	127	ASP	-	expression tag	UNP Q8JGJ1
K	128	LEU	-	expression tag	UNP Q8JGJ1
L	28	HIS	ASN	conflict	UNP Q8JGJ1
L	31	THR	LEU	conflict	UNP Q8JGJ1
L	?	-	ASN	deletion	UNP Q8JGJ1
L	?	-	VAL	deletion	UNP Q8JGJ1
L	84	ALA	TYR	conflict	UNP Q8JGJ1
L	86	GLU	TRP	conflict	UNP Q8JGJ1
L	87	CYS	TYR	conflict	UNP Q8JGJ1
L	88	GLN	GLY	conflict	UNP Q8JGJ1
L	90	GLY	ASP	conflict	UNP Q8JGJ1
L	91	LEU	CYS	conflict	UNP Q8JGJ1
L	94	TYR	LEU	conflict	UNP Q8JGJ1
L	107	ALA	-	expression tag	UNP Q8JGJ1
L	108	ALA	-	expression tag	UNP Q8JGJ1
L	109	ALA	-	expression tag	UNP Q8JGJ1
L	110	HIS	-	expression tag	UNP Q8JGJ1
L	111	HIS	-	expression tag	UNP Q8JGJ1
L	112	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	113	HIS	-	expression tag	UNP Q8JGJ1
L	114	HIS	-	expression tag	UNP Q8JGJ1
L	115	HIS	-	expression tag	UNP Q8JGJ1
L	116	GLY	-	expression tag	UNP Q8JGJ1
L	117	ALA	-	expression tag	UNP Q8JGJ1
L	118	ALA	-	expression tag	UNP Q8JGJ1
L	119	GLU	-	expression tag	UNP Q8JGJ1
L	120	SER	-	expression tag	UNP Q8JGJ1
L	121	LYS	-	expression tag	UNP Q8JGJ1
L	122	LEU	-	expression tag	UNP Q8JGJ1
L	123	ILE	-	expression tag	UNP Q8JGJ1
L	124	SER	-	expression tag	UNP Q8JGJ1
L	125	GLU	-	expression tag	UNP Q8JGJ1
L	126	GLU	-	expression tag	UNP Q8JGJ1
L	127	ASP	-	expression tag	UNP Q8JGJ1
L	128	LEU	-	expression tag	UNP Q8JGJ1
P	28	HIS	ASN	conflict	UNP Q8JGJ1
P	31	THR	LEU	conflict	UNP Q8JGJ1
P	?	-	ASN	deletion	UNP Q8JGJ1
P	?	-	VAL	deletion	UNP Q8JGJ1
P	84	ALA	TYR	conflict	UNP Q8JGJ1
P	86	GLU	TRP	conflict	UNP Q8JGJ1
P	87	CYS	TYR	conflict	UNP Q8JGJ1
P	88	GLN	GLY	conflict	UNP Q8JGJ1
P	90	GLY	ASP	conflict	UNP Q8JGJ1
P	91	LEU	CYS	conflict	UNP Q8JGJ1
P	94	TYR	LEU	conflict	UNP Q8JGJ1
P	107	ALA	-	expression tag	UNP Q8JGJ1
P	108	ALA	-	expression tag	UNP Q8JGJ1
P	109	ALA	-	expression tag	UNP Q8JGJ1
P	110	HIS	-	expression tag	UNP Q8JGJ1
P	111	HIS	-	expression tag	UNP Q8JGJ1
P	112	HIS	-	expression tag	UNP Q8JGJ1
P	113	HIS	-	expression tag	UNP Q8JGJ1
P	114	HIS	-	expression tag	UNP Q8JGJ1
P	115	HIS	-	expression tag	UNP Q8JGJ1
P	116	GLY	-	expression tag	UNP Q8JGJ1
P	117	ALA	-	expression tag	UNP Q8JGJ1
P	118	ALA	-	expression tag	UNP Q8JGJ1
P	119	GLU	-	expression tag	UNP Q8JGJ1
P	120	SER	-	expression tag	UNP Q8JGJ1
P	121	LYS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	122	LEU	-	expression tag	UNP Q8JGJ1
P	123	ILE	-	expression tag	UNP Q8JGJ1
P	124	SER	-	expression tag	UNP Q8JGJ1
P	125	GLU	-	expression tag	UNP Q8JGJ1
P	126	GLU	-	expression tag	UNP Q8JGJ1
P	127	ASP	-	expression tag	UNP Q8JGJ1
P	128	LEU	-	expression tag	UNP Q8JGJ1
Q	28	HIS	ASN	conflict	UNP Q8JGJ1
Q	31	THR	LEU	conflict	UNP Q8JGJ1
Q	?	-	ASN	deletion	UNP Q8JGJ1
Q	?	-	VAL	deletion	UNP Q8JGJ1
Q	84	ALA	TYR	conflict	UNP Q8JGJ1
Q	86	GLU	TRP	conflict	UNP Q8JGJ1
Q	87	CYS	TYR	conflict	UNP Q8JGJ1
Q	88	GLN	GLY	conflict	UNP Q8JGJ1
Q	90	GLY	ASP	conflict	UNP Q8JGJ1
Q	91	LEU	CYS	conflict	UNP Q8JGJ1
Q	94	TYR	LEU	conflict	UNP Q8JGJ1
Q	107	ALA	-	expression tag	UNP Q8JGJ1
Q	108	ALA	-	expression tag	UNP Q8JGJ1
Q	109	ALA	-	expression tag	UNP Q8JGJ1
Q	110	HIS	-	expression tag	UNP Q8JGJ1
Q	111	HIS	-	expression tag	UNP Q8JGJ1
Q	112	HIS	-	expression tag	UNP Q8JGJ1
Q	113	HIS	-	expression tag	UNP Q8JGJ1
Q	114	HIS	-	expression tag	UNP Q8JGJ1
Q	115	HIS	-	expression tag	UNP Q8JGJ1
Q	116	GLY	-	expression tag	UNP Q8JGJ1
Q	117	ALA	-	expression tag	UNP Q8JGJ1
Q	118	ALA	-	expression tag	UNP Q8JGJ1
Q	119	GLU	-	expression tag	UNP Q8JGJ1
Q	120	SER	-	expression tag	UNP Q8JGJ1
Q	121	LYS	-	expression tag	UNP Q8JGJ1
Q	122	LEU	-	expression tag	UNP Q8JGJ1
Q	123	ILE	-	expression tag	UNP Q8JGJ1
Q	124	SER	-	expression tag	UNP Q8JGJ1
Q	125	GLU	-	expression tag	UNP Q8JGJ1
Q	126	GLU	-	expression tag	UNP Q8JGJ1
Q	127	ASP	-	expression tag	UNP Q8JGJ1
Q	128	LEU	-	expression tag	UNP Q8JGJ1
R	28	HIS	ASN	conflict	UNP Q8JGJ1
R	31	THR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	ASN	deletion	UNP Q8JGJ1
R	?	-	VAL	deletion	UNP Q8JGJ1
R	84	ALA	TYR	conflict	UNP Q8JGJ1
R	86	GLU	TRP	conflict	UNP Q8JGJ1
R	87	CYS	TYR	conflict	UNP Q8JGJ1
R	88	GLN	GLY	conflict	UNP Q8JGJ1
R	90	GLY	ASP	conflict	UNP Q8JGJ1
R	91	LEU	CYS	conflict	UNP Q8JGJ1
R	94	TYR	LEU	conflict	UNP Q8JGJ1
R	107	ALA	-	expression tag	UNP Q8JGJ1
R	108	ALA	-	expression tag	UNP Q8JGJ1
R	109	ALA	-	expression tag	UNP Q8JGJ1
R	110	HIS	-	expression tag	UNP Q8JGJ1
R	111	HIS	-	expression tag	UNP Q8JGJ1
R	112	HIS	-	expression tag	UNP Q8JGJ1
R	113	HIS	-	expression tag	UNP Q8JGJ1
R	114	HIS	-	expression tag	UNP Q8JGJ1
R	115	HIS	-	expression tag	UNP Q8JGJ1
R	116	GLY	-	expression tag	UNP Q8JGJ1
R	117	ALA	-	expression tag	UNP Q8JGJ1
R	118	ALA	-	expression tag	UNP Q8JGJ1
R	119	GLU	-	expression tag	UNP Q8JGJ1
R	120	SER	-	expression tag	UNP Q8JGJ1
R	121	LYS	-	expression tag	UNP Q8JGJ1
R	122	LEU	-	expression tag	UNP Q8JGJ1
R	123	ILE	-	expression tag	UNP Q8JGJ1
R	124	SER	-	expression tag	UNP Q8JGJ1
R	125	GLU	-	expression tag	UNP Q8JGJ1
R	126	GLU	-	expression tag	UNP Q8JGJ1
R	127	ASP	-	expression tag	UNP Q8JGJ1
R	128	LEU	-	expression tag	UNP Q8JGJ1
V	28	HIS	ASN	conflict	UNP Q8JGJ1
V	31	THR	LEU	conflict	UNP Q8JGJ1
V	?	-	ASN	deletion	UNP Q8JGJ1
V	?	-	VAL	deletion	UNP Q8JGJ1
V	84	ALA	TYR	conflict	UNP Q8JGJ1
V	86	GLU	TRP	conflict	UNP Q8JGJ1
V	87	CYS	TYR	conflict	UNP Q8JGJ1
V	88	GLN	GLY	conflict	UNP Q8JGJ1
V	90	GLY	ASP	conflict	UNP Q8JGJ1
V	91	LEU	CYS	conflict	UNP Q8JGJ1
V	94	TYR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
V	107	ALA	-	expression tag	UNP Q8JGJ1
V	108	ALA	-	expression tag	UNP Q8JGJ1
V	109	ALA	-	expression tag	UNP Q8JGJ1
V	110	HIS	-	expression tag	UNP Q8JGJ1
V	111	HIS	-	expression tag	UNP Q8JGJ1
V	112	HIS	-	expression tag	UNP Q8JGJ1
V	113	HIS	-	expression tag	UNP Q8JGJ1
V	114	HIS	-	expression tag	UNP Q8JGJ1
V	115	HIS	-	expression tag	UNP Q8JGJ1
V	116	GLY	-	expression tag	UNP Q8JGJ1
V	117	ALA	-	expression tag	UNP Q8JGJ1
V	118	ALA	-	expression tag	UNP Q8JGJ1
V	119	GLU	-	expression tag	UNP Q8JGJ1
V	120	SER	-	expression tag	UNP Q8JGJ1
V	121	LYS	-	expression tag	UNP Q8JGJ1
V	122	LEU	-	expression tag	UNP Q8JGJ1
V	123	ILE	-	expression tag	UNP Q8JGJ1
V	124	SER	-	expression tag	UNP Q8JGJ1
V	125	GLU	-	expression tag	UNP Q8JGJ1
V	126	GLU	-	expression tag	UNP Q8JGJ1
V	127	ASP	-	expression tag	UNP Q8JGJ1
V	128	LEU	-	expression tag	UNP Q8JGJ1
W	28	HIS	ASN	conflict	UNP Q8JGJ1
W	31	THR	LEU	conflict	UNP Q8JGJ1
W	?	-	ASN	deletion	UNP Q8JGJ1
W	?	-	VAL	deletion	UNP Q8JGJ1
W	84	ALA	TYR	conflict	UNP Q8JGJ1
W	86	GLU	TRP	conflict	UNP Q8JGJ1
W	87	CYS	TYR	conflict	UNP Q8JGJ1
W	88	GLN	GLY	conflict	UNP Q8JGJ1
W	90	GLY	ASP	conflict	UNP Q8JGJ1
W	91	LEU	CYS	conflict	UNP Q8JGJ1
W	94	TYR	LEU	conflict	UNP Q8JGJ1
W	107	ALA	-	expression tag	UNP Q8JGJ1
W	108	ALA	-	expression tag	UNP Q8JGJ1
W	109	ALA	-	expression tag	UNP Q8JGJ1
W	110	HIS	-	expression tag	UNP Q8JGJ1
W	111	HIS	-	expression tag	UNP Q8JGJ1
W	112	HIS	-	expression tag	UNP Q8JGJ1
W	113	HIS	-	expression tag	UNP Q8JGJ1
W	114	HIS	-	expression tag	UNP Q8JGJ1
W	115	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
W	116	GLY	-	expression tag	UNP Q8JGJ1
W	117	ALA	-	expression tag	UNP Q8JGJ1
W	118	ALA	-	expression tag	UNP Q8JGJ1
W	119	GLU	-	expression tag	UNP Q8JGJ1
W	120	SER	-	expression tag	UNP Q8JGJ1
W	121	LYS	-	expression tag	UNP Q8JGJ1
W	122	LEU	-	expression tag	UNP Q8JGJ1
W	123	ILE	-	expression tag	UNP Q8JGJ1
W	124	SER	-	expression tag	UNP Q8JGJ1
W	125	GLU	-	expression tag	UNP Q8JGJ1
W	126	GLU	-	expression tag	UNP Q8JGJ1
W	127	ASP	-	expression tag	UNP Q8JGJ1
W	128	LEU	-	expression tag	UNP Q8JGJ1
X	28	HIS	ASN	conflict	UNP Q8JGJ1
X	31	THR	LEU	conflict	UNP Q8JGJ1
X	?	-	ASN	deletion	UNP Q8JGJ1
X	?	-	VAL	deletion	UNP Q8JGJ1
X	84	ALA	TYR	conflict	UNP Q8JGJ1
X	86	GLU	TRP	conflict	UNP Q8JGJ1
X	87	CYS	TYR	conflict	UNP Q8JGJ1
X	88	GLN	GLY	conflict	UNP Q8JGJ1
X	90	GLY	ASP	conflict	UNP Q8JGJ1
X	91	LEU	CYS	conflict	UNP Q8JGJ1
X	94	TYR	LEU	conflict	UNP Q8JGJ1
X	107	ALA	-	expression tag	UNP Q8JGJ1
X	108	ALA	-	expression tag	UNP Q8JGJ1
X	109	ALA	-	expression tag	UNP Q8JGJ1
X	110	HIS	-	expression tag	UNP Q8JGJ1
X	111	HIS	-	expression tag	UNP Q8JGJ1
X	112	HIS	-	expression tag	UNP Q8JGJ1
X	113	HIS	-	expression tag	UNP Q8JGJ1
X	114	HIS	-	expression tag	UNP Q8JGJ1
X	115	HIS	-	expression tag	UNP Q8JGJ1
X	116	GLY	-	expression tag	UNP Q8JGJ1
X	117	ALA	-	expression tag	UNP Q8JGJ1
X	118	ALA	-	expression tag	UNP Q8JGJ1
X	119	GLU	-	expression tag	UNP Q8JGJ1
X	120	SER	-	expression tag	UNP Q8JGJ1
X	121	LYS	-	expression tag	UNP Q8JGJ1
X	122	LEU	-	expression tag	UNP Q8JGJ1
X	123	ILE	-	expression tag	UNP Q8JGJ1
X	124	SER	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
X	125	GLU	-	expression tag	UNP Q8JGJ1
X	126	GLU	-	expression tag	UNP Q8JGJ1
X	127	ASP	-	expression tag	UNP Q8JGJ1
X	128	LEU	-	expression tag	UNP Q8JGJ1
b	28	HIS	ASN	conflict	UNP Q8JGJ1
b	31	THR	LEU	conflict	UNP Q8JGJ1
b	?	-	ASN	deletion	UNP Q8JGJ1
b	?	-	VAL	deletion	UNP Q8JGJ1
b	84	ALA	TYR	conflict	UNP Q8JGJ1
b	86	GLU	TRP	conflict	UNP Q8JGJ1
b	87	CYS	TYR	conflict	UNP Q8JGJ1
b	88	GLN	GLY	conflict	UNP Q8JGJ1
b	90	GLY	ASP	conflict	UNP Q8JGJ1
b	91	LEU	CYS	conflict	UNP Q8JGJ1
b	94	TYR	LEU	conflict	UNP Q8JGJ1
b	107	ALA	-	expression tag	UNP Q8JGJ1
b	108	ALA	-	expression tag	UNP Q8JGJ1
b	109	ALA	-	expression tag	UNP Q8JGJ1
b	110	HIS	-	expression tag	UNP Q8JGJ1
b	111	HIS	-	expression tag	UNP Q8JGJ1
b	112	HIS	-	expression tag	UNP Q8JGJ1
b	113	HIS	-	expression tag	UNP Q8JGJ1
b	114	HIS	-	expression tag	UNP Q8JGJ1
b	115	HIS	-	expression tag	UNP Q8JGJ1
b	116	GLY	-	expression tag	UNP Q8JGJ1
b	117	ALA	-	expression tag	UNP Q8JGJ1
b	118	ALA	-	expression tag	UNP Q8JGJ1
b	119	GLU	-	expression tag	UNP Q8JGJ1
b	120	SER	-	expression tag	UNP Q8JGJ1
b	121	LYS	-	expression tag	UNP Q8JGJ1
b	122	LEU	-	expression tag	UNP Q8JGJ1
b	123	ILE	-	expression tag	UNP Q8JGJ1
b	124	SER	-	expression tag	UNP Q8JGJ1
b	125	GLU	-	expression tag	UNP Q8JGJ1
b	126	GLU	-	expression tag	UNP Q8JGJ1
b	127	ASP	-	expression tag	UNP Q8JGJ1
b	128	LEU	-	expression tag	UNP Q8JGJ1
c	28	HIS	ASN	conflict	UNP Q8JGJ1
c	31	THR	LEU	conflict	UNP Q8JGJ1
c	?	-	ASN	deletion	UNP Q8JGJ1
c	?	-	VAL	deletion	UNP Q8JGJ1
c	84	ALA	TYR	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
c	86	GLU	TRP	conflict	UNP Q8JGJ1
c	87	CYS	TYR	conflict	UNP Q8JGJ1
c	88	GLN	GLY	conflict	UNP Q8JGJ1
c	90	GLY	ASP	conflict	UNP Q8JGJ1
c	91	LEU	CYS	conflict	UNP Q8JGJ1
c	94	TYR	LEU	conflict	UNP Q8JGJ1
c	107	ALA	-	expression tag	UNP Q8JGJ1
c	108	ALA	-	expression tag	UNP Q8JGJ1
c	109	ALA	-	expression tag	UNP Q8JGJ1
c	110	HIS	-	expression tag	UNP Q8JGJ1
c	111	HIS	-	expression tag	UNP Q8JGJ1
c	112	HIS	-	expression tag	UNP Q8JGJ1
c	113	HIS	-	expression tag	UNP Q8JGJ1
c	114	HIS	-	expression tag	UNP Q8JGJ1
c	115	HIS	-	expression tag	UNP Q8JGJ1
c	116	GLY	-	expression tag	UNP Q8JGJ1
c	117	ALA	-	expression tag	UNP Q8JGJ1
c	118	ALA	-	expression tag	UNP Q8JGJ1
c	119	GLU	-	expression tag	UNP Q8JGJ1
c	120	SER	-	expression tag	UNP Q8JGJ1
c	121	LYS	-	expression tag	UNP Q8JGJ1
c	122	LEU	-	expression tag	UNP Q8JGJ1
c	123	ILE	-	expression tag	UNP Q8JGJ1
c	124	SER	-	expression tag	UNP Q8JGJ1
c	125	GLU	-	expression tag	UNP Q8JGJ1
c	126	GLU	-	expression tag	UNP Q8JGJ1
c	127	ASP	-	expression tag	UNP Q8JGJ1
c	128	LEU	-	expression tag	UNP Q8JGJ1
d	28	HIS	ASN	conflict	UNP Q8JGJ1
d	31	THR	LEU	conflict	UNP Q8JGJ1
d	?	-	ASN	deletion	UNP Q8JGJ1
d	?	-	VAL	deletion	UNP Q8JGJ1
d	84	ALA	TYR	conflict	UNP Q8JGJ1
d	86	GLU	TRP	conflict	UNP Q8JGJ1
d	87	CYS	TYR	conflict	UNP Q8JGJ1
d	88	GLN	GLY	conflict	UNP Q8JGJ1
d	90	GLY	ASP	conflict	UNP Q8JGJ1
d	91	LEU	CYS	conflict	UNP Q8JGJ1
d	94	TYR	LEU	conflict	UNP Q8JGJ1
d	107	ALA	-	expression tag	UNP Q8JGJ1
d	108	ALA	-	expression tag	UNP Q8JGJ1
d	109	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
d	110	HIS	-	expression tag	UNP Q8JGJ1
d	111	HIS	-	expression tag	UNP Q8JGJ1
d	112	HIS	-	expression tag	UNP Q8JGJ1
d	113	HIS	-	expression tag	UNP Q8JGJ1
d	114	HIS	-	expression tag	UNP Q8JGJ1
d	115	HIS	-	expression tag	UNP Q8JGJ1
d	116	GLY	-	expression tag	UNP Q8JGJ1
d	117	ALA	-	expression tag	UNP Q8JGJ1
d	118	ALA	-	expression tag	UNP Q8JGJ1
d	119	GLU	-	expression tag	UNP Q8JGJ1
d	120	SER	-	expression tag	UNP Q8JGJ1
d	121	LYS	-	expression tag	UNP Q8JGJ1
d	122	LEU	-	expression tag	UNP Q8JGJ1
d	123	ILE	-	expression tag	UNP Q8JGJ1
d	124	SER	-	expression tag	UNP Q8JGJ1
d	125	GLU	-	expression tag	UNP Q8JGJ1
d	126	GLU	-	expression tag	UNP Q8JGJ1
d	127	ASP	-	expression tag	UNP Q8JGJ1
d	128	LEU	-	expression tag	UNP Q8JGJ1
h	28	HIS	ASN	conflict	UNP Q8JGJ1
h	31	THR	LEU	conflict	UNP Q8JGJ1
h	?	-	ASN	deletion	UNP Q8JGJ1
h	?	-	VAL	deletion	UNP Q8JGJ1
h	84	ALA	TYR	conflict	UNP Q8JGJ1
h	86	GLU	TRP	conflict	UNP Q8JGJ1
h	87	CYS	TYR	conflict	UNP Q8JGJ1
h	88	GLN	GLY	conflict	UNP Q8JGJ1
h	90	GLY	ASP	conflict	UNP Q8JGJ1
h	91	LEU	CYS	conflict	UNP Q8JGJ1
h	94	TYR	LEU	conflict	UNP Q8JGJ1
h	107	ALA	-	expression tag	UNP Q8JGJ1
h	108	ALA	-	expression tag	UNP Q8JGJ1
h	109	ALA	-	expression tag	UNP Q8JGJ1
h	110	HIS	-	expression tag	UNP Q8JGJ1
h	111	HIS	-	expression tag	UNP Q8JGJ1
h	112	HIS	-	expression tag	UNP Q8JGJ1
h	113	HIS	-	expression tag	UNP Q8JGJ1
h	114	HIS	-	expression tag	UNP Q8JGJ1
h	115	HIS	-	expression tag	UNP Q8JGJ1
h	116	GLY	-	expression tag	UNP Q8JGJ1
h	117	ALA	-	expression tag	UNP Q8JGJ1
h	118	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
h	119	GLU	-	expression tag	UNP Q8JGJ1
h	120	SER	-	expression tag	UNP Q8JGJ1
h	121	LYS	-	expression tag	UNP Q8JGJ1
h	122	LEU	-	expression tag	UNP Q8JGJ1
h	123	ILE	-	expression tag	UNP Q8JGJ1
h	124	SER	-	expression tag	UNP Q8JGJ1
h	125	GLU	-	expression tag	UNP Q8JGJ1
h	126	GLU	-	expression tag	UNP Q8JGJ1
h	127	ASP	-	expression tag	UNP Q8JGJ1
h	128	LEU	-	expression tag	UNP Q8JGJ1
i	28	HIS	ASN	conflict	UNP Q8JGJ1
i	31	THR	LEU	conflict	UNP Q8JGJ1
i	?	-	ASN	deletion	UNP Q8JGJ1
i	?	-	VAL	deletion	UNP Q8JGJ1
i	84	ALA	TYR	conflict	UNP Q8JGJ1
i	86	GLU	TRP	conflict	UNP Q8JGJ1
i	87	CYS	TYR	conflict	UNP Q8JGJ1
i	88	GLN	GLY	conflict	UNP Q8JGJ1
i	90	GLY	ASP	conflict	UNP Q8JGJ1
i	91	LEU	CYS	conflict	UNP Q8JGJ1
i	94	TYR	LEU	conflict	UNP Q8JGJ1
i	107	ALA	-	expression tag	UNP Q8JGJ1
i	108	ALA	-	expression tag	UNP Q8JGJ1
i	109	ALA	-	expression tag	UNP Q8JGJ1
i	110	HIS	-	expression tag	UNP Q8JGJ1
i	111	HIS	-	expression tag	UNP Q8JGJ1
i	112	HIS	-	expression tag	UNP Q8JGJ1
i	113	HIS	-	expression tag	UNP Q8JGJ1
i	114	HIS	-	expression tag	UNP Q8JGJ1
i	115	HIS	-	expression tag	UNP Q8JGJ1
i	116	GLY	-	expression tag	UNP Q8JGJ1
i	117	ALA	-	expression tag	UNP Q8JGJ1
i	118	ALA	-	expression tag	UNP Q8JGJ1
i	119	GLU	-	expression tag	UNP Q8JGJ1
i	120	SER	-	expression tag	UNP Q8JGJ1
i	121	LYS	-	expression tag	UNP Q8JGJ1
i	122	LEU	-	expression tag	UNP Q8JGJ1
i	123	ILE	-	expression tag	UNP Q8JGJ1
i	124	SER	-	expression tag	UNP Q8JGJ1
i	125	GLU	-	expression tag	UNP Q8JGJ1
i	126	GLU	-	expression tag	UNP Q8JGJ1
i	127	ASP	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
i	128	LEU	-	expression tag	UNP Q8JGJ1
j	28	HIS	ASN	conflict	UNP Q8JGJ1
j	31	THR	LEU	conflict	UNP Q8JGJ1
j	?	-	ASN	deletion	UNP Q8JGJ1
j	?	-	VAL	deletion	UNP Q8JGJ1
j	84	ALA	TYR	conflict	UNP Q8JGJ1
j	86	GLU	TRP	conflict	UNP Q8JGJ1
j	87	CYS	TYR	conflict	UNP Q8JGJ1
j	88	GLN	GLY	conflict	UNP Q8JGJ1
j	90	GLY	ASP	conflict	UNP Q8JGJ1
j	91	LEU	CYS	conflict	UNP Q8JGJ1
j	94	TYR	LEU	conflict	UNP Q8JGJ1
j	107	ALA	-	expression tag	UNP Q8JGJ1
j	108	ALA	-	expression tag	UNP Q8JGJ1
j	109	ALA	-	expression tag	UNP Q8JGJ1
j	110	HIS	-	expression tag	UNP Q8JGJ1
j	111	HIS	-	expression tag	UNP Q8JGJ1
j	112	HIS	-	expression tag	UNP Q8JGJ1
j	113	HIS	-	expression tag	UNP Q8JGJ1
j	114	HIS	-	expression tag	UNP Q8JGJ1
j	115	HIS	-	expression tag	UNP Q8JGJ1
j	116	GLY	-	expression tag	UNP Q8JGJ1
j	117	ALA	-	expression tag	UNP Q8JGJ1
j	118	ALA	-	expression tag	UNP Q8JGJ1
j	119	GLU	-	expression tag	UNP Q8JGJ1
j	120	SER	-	expression tag	UNP Q8JGJ1
j	121	LYS	-	expression tag	UNP Q8JGJ1
j	122	LEU	-	expression tag	UNP Q8JGJ1
j	123	ILE	-	expression tag	UNP Q8JGJ1
j	124	SER	-	expression tag	UNP Q8JGJ1
j	125	GLU	-	expression tag	UNP Q8JGJ1
j	126	GLU	-	expression tag	UNP Q8JGJ1
j	127	ASP	-	expression tag	UNP Q8JGJ1
j	128	LEU	-	expression tag	UNP Q8JGJ1
n	28	HIS	ASN	conflict	UNP Q8JGJ1
n	31	THR	LEU	conflict	UNP Q8JGJ1
n	?	-	ASN	deletion	UNP Q8JGJ1
n	?	-	VAL	deletion	UNP Q8JGJ1
n	84	ALA	TYR	conflict	UNP Q8JGJ1
n	86	GLU	TRP	conflict	UNP Q8JGJ1
n	87	CYS	TYR	conflict	UNP Q8JGJ1
n	88	GLN	GLY	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
n	90	GLY	ASP	conflict	UNP Q8JGJ1
n	91	LEU	CYS	conflict	UNP Q8JGJ1
n	94	TYR	LEU	conflict	UNP Q8JGJ1
n	107	ALA	-	expression tag	UNP Q8JGJ1
n	108	ALA	-	expression tag	UNP Q8JGJ1
n	109	ALA	-	expression tag	UNP Q8JGJ1
n	110	HIS	-	expression tag	UNP Q8JGJ1
n	111	HIS	-	expression tag	UNP Q8JGJ1
n	112	HIS	-	expression tag	UNP Q8JGJ1
n	113	HIS	-	expression tag	UNP Q8JGJ1
n	114	HIS	-	expression tag	UNP Q8JGJ1
n	115	HIS	-	expression tag	UNP Q8JGJ1
n	116	GLY	-	expression tag	UNP Q8JGJ1
n	117	ALA	-	expression tag	UNP Q8JGJ1
n	118	ALA	-	expression tag	UNP Q8JGJ1
n	119	GLU	-	expression tag	UNP Q8JGJ1
n	120	SER	-	expression tag	UNP Q8JGJ1
n	121	LYS	-	expression tag	UNP Q8JGJ1
n	122	LEU	-	expression tag	UNP Q8JGJ1
n	123	ILE	-	expression tag	UNP Q8JGJ1
n	124	SER	-	expression tag	UNP Q8JGJ1
n	125	GLU	-	expression tag	UNP Q8JGJ1
n	126	GLU	-	expression tag	UNP Q8JGJ1
n	127	ASP	-	expression tag	UNP Q8JGJ1
n	128	LEU	-	expression tag	UNP Q8JGJ1
o	28	HIS	ASN	conflict	UNP Q8JGJ1
o	31	THR	LEU	conflict	UNP Q8JGJ1
o	?	-	ASN	deletion	UNP Q8JGJ1
o	?	-	VAL	deletion	UNP Q8JGJ1
o	84	ALA	TYR	conflict	UNP Q8JGJ1
o	86	GLU	TRP	conflict	UNP Q8JGJ1
o	87	CYS	TYR	conflict	UNP Q8JGJ1
o	88	GLN	GLY	conflict	UNP Q8JGJ1
o	90	GLY	ASP	conflict	UNP Q8JGJ1
o	91	LEU	CYS	conflict	UNP Q8JGJ1
o	94	TYR	LEU	conflict	UNP Q8JGJ1
o	107	ALA	-	expression tag	UNP Q8JGJ1
o	108	ALA	-	expression tag	UNP Q8JGJ1
o	109	ALA	-	expression tag	UNP Q8JGJ1
o	110	HIS	-	expression tag	UNP Q8JGJ1
o	111	HIS	-	expression tag	UNP Q8JGJ1
o	112	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
o	113	HIS	-	expression tag	UNP Q8JGJ1
o	114	HIS	-	expression tag	UNP Q8JGJ1
o	115	HIS	-	expression tag	UNP Q8JGJ1
o	116	GLY	-	expression tag	UNP Q8JGJ1
o	117	ALA	-	expression tag	UNP Q8JGJ1
o	118	ALA	-	expression tag	UNP Q8JGJ1
o	119	GLU	-	expression tag	UNP Q8JGJ1
o	120	SER	-	expression tag	UNP Q8JGJ1
o	121	LYS	-	expression tag	UNP Q8JGJ1
o	122	LEU	-	expression tag	UNP Q8JGJ1
o	123	ILE	-	expression tag	UNP Q8JGJ1
o	124	SER	-	expression tag	UNP Q8JGJ1
o	125	GLU	-	expression tag	UNP Q8JGJ1
o	126	GLU	-	expression tag	UNP Q8JGJ1
o	127	ASP	-	expression tag	UNP Q8JGJ1
o	128	LEU	-	expression tag	UNP Q8JGJ1
p	28	HIS	ASN	conflict	UNP Q8JGJ1
p	31	THR	LEU	conflict	UNP Q8JGJ1
p	?	-	ASN	deletion	UNP Q8JGJ1
p	?	-	VAL	deletion	UNP Q8JGJ1
p	84	ALA	TYR	conflict	UNP Q8JGJ1
p	86	GLU	TRP	conflict	UNP Q8JGJ1
p	87	CYS	TYR	conflict	UNP Q8JGJ1
p	88	GLN	GLY	conflict	UNP Q8JGJ1
p	90	GLY	ASP	conflict	UNP Q8JGJ1
p	91	LEU	CYS	conflict	UNP Q8JGJ1
p	94	TYR	LEU	conflict	UNP Q8JGJ1
p	107	ALA	-	expression tag	UNP Q8JGJ1
p	108	ALA	-	expression tag	UNP Q8JGJ1
p	109	ALA	-	expression tag	UNP Q8JGJ1
p	110	HIS	-	expression tag	UNP Q8JGJ1
p	111	HIS	-	expression tag	UNP Q8JGJ1
p	112	HIS	-	expression tag	UNP Q8JGJ1
p	113	HIS	-	expression tag	UNP Q8JGJ1
p	114	HIS	-	expression tag	UNP Q8JGJ1
p	115	HIS	-	expression tag	UNP Q8JGJ1
p	116	GLY	-	expression tag	UNP Q8JGJ1
p	117	ALA	-	expression tag	UNP Q8JGJ1
p	118	ALA	-	expression tag	UNP Q8JGJ1
p	119	GLU	-	expression tag	UNP Q8JGJ1
p	120	SER	-	expression tag	UNP Q8JGJ1
p	121	LYS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
p	122	LEU	-	expression tag	UNP Q8JGJ1
p	123	ILE	-	expression tag	UNP Q8JGJ1
p	124	SER	-	expression tag	UNP Q8JGJ1
p	125	GLU	-	expression tag	UNP Q8JGJ1
p	126	GLU	-	expression tag	UNP Q8JGJ1
p	127	ASP	-	expression tag	UNP Q8JGJ1
p	128	LEU	-	expression tag	UNP Q8JGJ1
t	28	HIS	ASN	conflict	UNP Q8JGJ1
t	31	THR	LEU	conflict	UNP Q8JGJ1
t	?	-	ASN	deletion	UNP Q8JGJ1
t	?	-	VAL	deletion	UNP Q8JGJ1
t	84	ALA	TYR	conflict	UNP Q8JGJ1
t	86	GLU	TRP	conflict	UNP Q8JGJ1
t	87	CYS	TYR	conflict	UNP Q8JGJ1
t	88	GLN	GLY	conflict	UNP Q8JGJ1
t	90	GLY	ASP	conflict	UNP Q8JGJ1
t	91	LEU	CYS	conflict	UNP Q8JGJ1
t	94	TYR	LEU	conflict	UNP Q8JGJ1
t	107	ALA	-	expression tag	UNP Q8JGJ1
t	108	ALA	-	expression tag	UNP Q8JGJ1
t	109	ALA	-	expression tag	UNP Q8JGJ1
t	110	HIS	-	expression tag	UNP Q8JGJ1
t	111	HIS	-	expression tag	UNP Q8JGJ1
t	112	HIS	-	expression tag	UNP Q8JGJ1
t	113	HIS	-	expression tag	UNP Q8JGJ1
t	114	HIS	-	expression tag	UNP Q8JGJ1
t	115	HIS	-	expression tag	UNP Q8JGJ1
t	116	GLY	-	expression tag	UNP Q8JGJ1
t	117	ALA	-	expression tag	UNP Q8JGJ1
t	118	ALA	-	expression tag	UNP Q8JGJ1
t	119	GLU	-	expression tag	UNP Q8JGJ1
t	120	SER	-	expression tag	UNP Q8JGJ1
t	121	LYS	-	expression tag	UNP Q8JGJ1
t	122	LEU	-	expression tag	UNP Q8JGJ1
t	123	ILE	-	expression tag	UNP Q8JGJ1
t	124	SER	-	expression tag	UNP Q8JGJ1
t	125	GLU	-	expression tag	UNP Q8JGJ1
t	126	GLU	-	expression tag	UNP Q8JGJ1
t	127	ASP	-	expression tag	UNP Q8JGJ1
t	128	LEU	-	expression tag	UNP Q8JGJ1
u	28	HIS	ASN	conflict	UNP Q8JGJ1
u	31	THR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
u	?	-	ASN	deletion	UNP Q8JGJ1
u	?	-	VAL	deletion	UNP Q8JGJ1
u	84	ALA	TYR	conflict	UNP Q8JGJ1
u	86	GLU	TRP	conflict	UNP Q8JGJ1
u	87	CYS	TYR	conflict	UNP Q8JGJ1
u	88	GLN	GLY	conflict	UNP Q8JGJ1
u	90	GLY	ASP	conflict	UNP Q8JGJ1
u	91	LEU	CYS	conflict	UNP Q8JGJ1
u	94	TYR	LEU	conflict	UNP Q8JGJ1
u	107	ALA	-	expression tag	UNP Q8JGJ1
u	108	ALA	-	expression tag	UNP Q8JGJ1
u	109	ALA	-	expression tag	UNP Q8JGJ1
u	110	HIS	-	expression tag	UNP Q8JGJ1
u	111	HIS	-	expression tag	UNP Q8JGJ1
u	112	HIS	-	expression tag	UNP Q8JGJ1
u	113	HIS	-	expression tag	UNP Q8JGJ1
u	114	HIS	-	expression tag	UNP Q8JGJ1
u	115	HIS	-	expression tag	UNP Q8JGJ1
u	116	GLY	-	expression tag	UNP Q8JGJ1
u	117	ALA	-	expression tag	UNP Q8JGJ1
u	118	ALA	-	expression tag	UNP Q8JGJ1
u	119	GLU	-	expression tag	UNP Q8JGJ1
u	120	SER	-	expression tag	UNP Q8JGJ1
u	121	LYS	-	expression tag	UNP Q8JGJ1
u	122	LEU	-	expression tag	UNP Q8JGJ1
u	123	ILE	-	expression tag	UNP Q8JGJ1
u	124	SER	-	expression tag	UNP Q8JGJ1
u	125	GLU	-	expression tag	UNP Q8JGJ1
u	126	GLU	-	expression tag	UNP Q8JGJ1
u	127	ASP	-	expression tag	UNP Q8JGJ1
u	128	LEU	-	expression tag	UNP Q8JGJ1
v	28	HIS	ASN	conflict	UNP Q8JGJ1
v	31	THR	LEU	conflict	UNP Q8JGJ1
v	?	-	ASN	deletion	UNP Q8JGJ1
v	?	-	VAL	deletion	UNP Q8JGJ1
v	84	ALA	TYR	conflict	UNP Q8JGJ1
v	86	GLU	TRP	conflict	UNP Q8JGJ1
v	87	CYS	TYR	conflict	UNP Q8JGJ1
v	88	GLN	GLY	conflict	UNP Q8JGJ1
v	90	GLY	ASP	conflict	UNP Q8JGJ1
v	91	LEU	CYS	conflict	UNP Q8JGJ1
v	94	TYR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
v	107	ALA	-	expression tag	UNP Q8JGJ1
v	108	ALA	-	expression tag	UNP Q8JGJ1
v	109	ALA	-	expression tag	UNP Q8JGJ1
v	110	HIS	-	expression tag	UNP Q8JGJ1
v	111	HIS	-	expression tag	UNP Q8JGJ1
v	112	HIS	-	expression tag	UNP Q8JGJ1
v	113	HIS	-	expression tag	UNP Q8JGJ1
v	114	HIS	-	expression tag	UNP Q8JGJ1
v	115	HIS	-	expression tag	UNP Q8JGJ1
v	116	GLY	-	expression tag	UNP Q8JGJ1
v	117	ALA	-	expression tag	UNP Q8JGJ1
v	118	ALA	-	expression tag	UNP Q8JGJ1
v	119	GLU	-	expression tag	UNP Q8JGJ1
v	120	SER	-	expression tag	UNP Q8JGJ1
v	121	LYS	-	expression tag	UNP Q8JGJ1
v	122	LEU	-	expression tag	UNP Q8JGJ1
v	123	ILE	-	expression tag	UNP Q8JGJ1
v	124	SER	-	expression tag	UNP Q8JGJ1
v	125	GLU	-	expression tag	UNP Q8JGJ1
v	126	GLU	-	expression tag	UNP Q8JGJ1
v	127	ASP	-	expression tag	UNP Q8JGJ1
v	128	LEU	-	expression tag	UNP Q8JGJ1
z	28	HIS	ASN	conflict	UNP Q8JGJ1
z	31	THR	LEU	conflict	UNP Q8JGJ1
z	?	-	ASN	deletion	UNP Q8JGJ1
z	?	-	VAL	deletion	UNP Q8JGJ1
z	84	ALA	TYR	conflict	UNP Q8JGJ1
z	86	GLU	TRP	conflict	UNP Q8JGJ1
z	87	CYS	TYR	conflict	UNP Q8JGJ1
z	88	GLN	GLY	conflict	UNP Q8JGJ1
z	90	GLY	ASP	conflict	UNP Q8JGJ1
z	91	LEU	CYS	conflict	UNP Q8JGJ1
z	94	TYR	LEU	conflict	UNP Q8JGJ1
z	107	ALA	-	expression tag	UNP Q8JGJ1
z	108	ALA	-	expression tag	UNP Q8JGJ1
z	109	ALA	-	expression tag	UNP Q8JGJ1
z	110	HIS	-	expression tag	UNP Q8JGJ1
z	111	HIS	-	expression tag	UNP Q8JGJ1
z	112	HIS	-	expression tag	UNP Q8JGJ1
z	113	HIS	-	expression tag	UNP Q8JGJ1
z	114	HIS	-	expression tag	UNP Q8JGJ1
z	115	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
z	116	GLY	-	expression tag	UNP Q8JGJ1
z	117	ALA	-	expression tag	UNP Q8JGJ1
z	118	ALA	-	expression tag	UNP Q8JGJ1
z	119	GLU	-	expression tag	UNP Q8JGJ1
z	120	SER	-	expression tag	UNP Q8JGJ1
z	121	LYS	-	expression tag	UNP Q8JGJ1
z	122	LEU	-	expression tag	UNP Q8JGJ1
z	123	ILE	-	expression tag	UNP Q8JGJ1
z	124	SER	-	expression tag	UNP Q8JGJ1
z	125	GLU	-	expression tag	UNP Q8JGJ1
z	126	GLU	-	expression tag	UNP Q8JGJ1
z	127	ASP	-	expression tag	UNP Q8JGJ1
z	128	LEU	-	expression tag	UNP Q8JGJ1

- Molecule 2 is a protein called Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	154	Total	C	N	O	S	0	0	0
			1202	764	209	227	2			
2	3	151	Total	C	N	O	S	0	0	0
			1183	754	206	221	2			
2	4	155	Total	C	N	O	S	0	0	0
			1208	767	210	229	2			
2	A	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	B	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	C	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	G	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	H	152	Total	C	N	O	S	0	0	0
			1188	757	207	222	2			
2	I	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	M	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	N	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	O	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	S	154	Total	C	N	O	S	0	0	0
			1202	764	209	227	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	U	150	Total	C	N	O	S	0	0	0
			1172	748	202	220	2			
2	Y	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	Z	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	a	154	Total	C	N	O	S	0	0	0
			1202	764	209	227	2			
2	e	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	f	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	g	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	k	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	l	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	m	151	Total	C	N	O	S	0	0	0
			1179	752	203	222	2			
2	q	146	Total	C	N	O	S	0	0	0
			1145	733	198	212	2			
2	r	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	s	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	w	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	x	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	y	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).





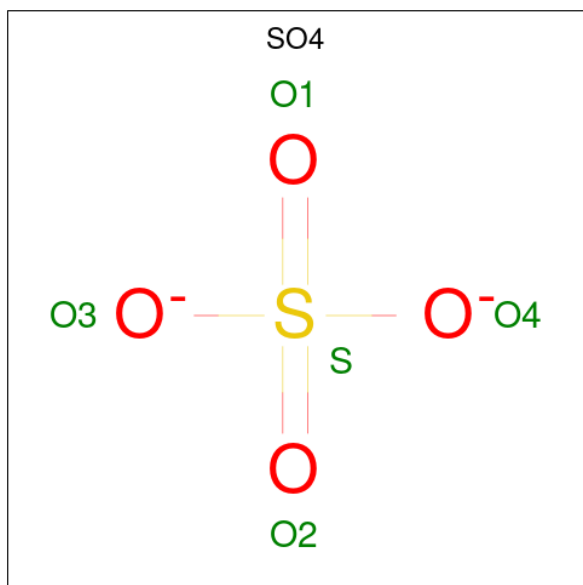
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	0	1	Total	C	O	0	0
			6	3	3		
3	1	1	Total	C	O	0	0
			6	3	3		
3	5	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		
3	W	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		
3	c	1	Total	C	O	0	0
			6	3	3		
3	h	1	Total	C	O	0	0
			6	3	3		
3	n	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	t	1	Total	C	O	0	0
			6	3	3		
3	t	1	Total	C	O	0	0
			6	3	3		
3	z	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	O	S	0	0
			5	4	1		
4	h	1	Total	O	S	0	0
			5	4	1		
4	t	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	S	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

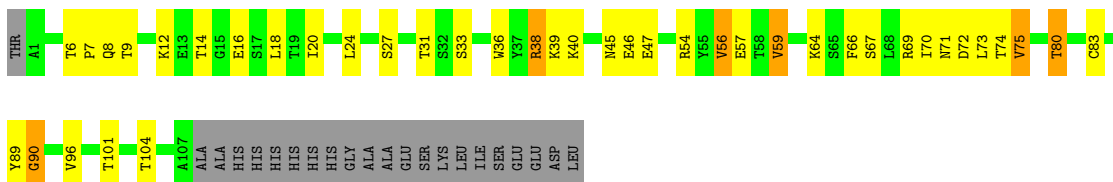
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total 2	O 2	0	0
6	I	1	Total 1	O 1	0	0
6	J	1	Total 1	O 1	0	0
6	P	1	Total 1	O 1	0	0
6	S	1	Total 1	O 1	0	0
6	V	2	Total 2	O 2	0	0
6	X	1	Total 1	O 1	0	0

### 3 Residue-property plots

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

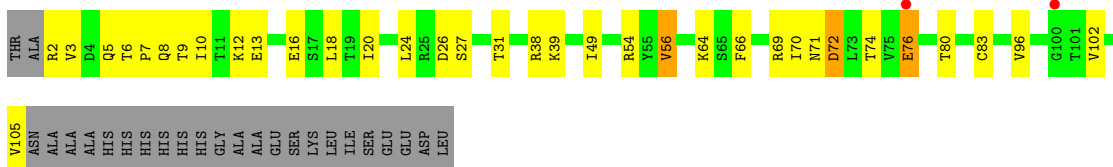
- Molecule 1: Antigen receptor

Chain 0: 



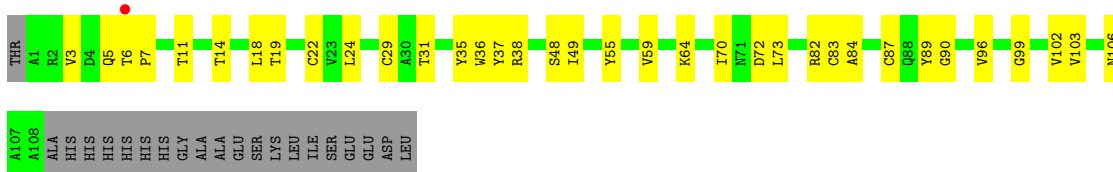
- Molecule 1: Antigen receptor

Chain 1: 



- Molecule 1: Antigen receptor

Chain 5: 



- Molecule 1: Antigen receptor

Chain 6: 

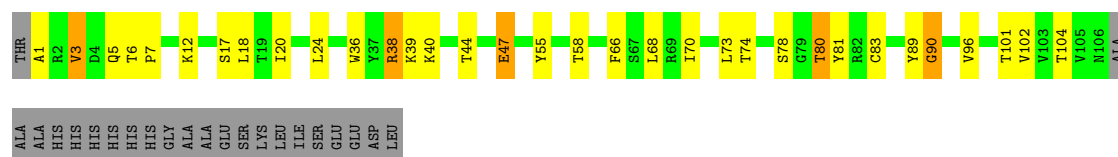


Chain J:  59% 23% • 16%



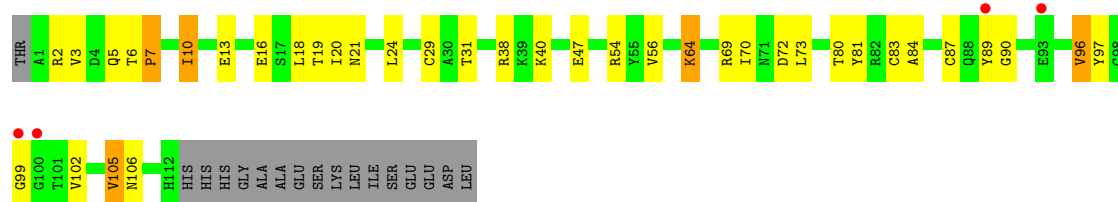
• Molecule 1: Antigen receptor

Chain K: 57% 22% 18%



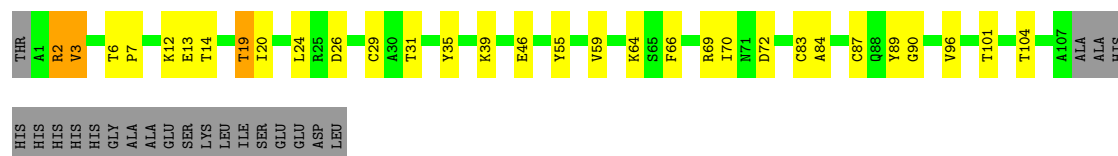
• Molecule 1: Antigen receptor

Chain L: 3% 57% 26% 13%



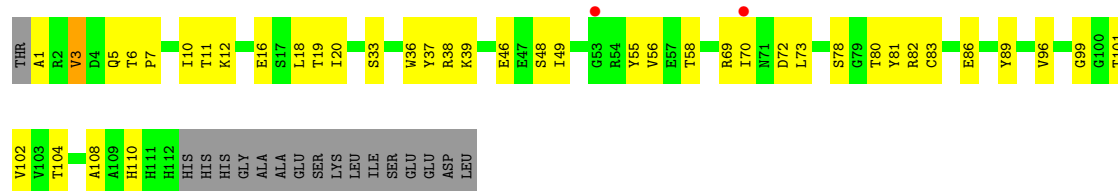
• Molecule 1: Antigen receptor

Chain P: 59% 22% 17%



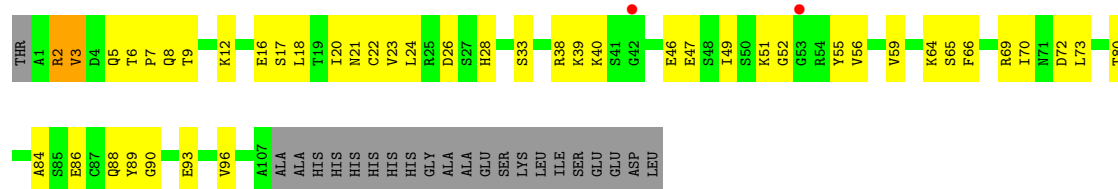
• Molecule 1: Antigen receptor

Chain Q: 2% 55% 31% 13%

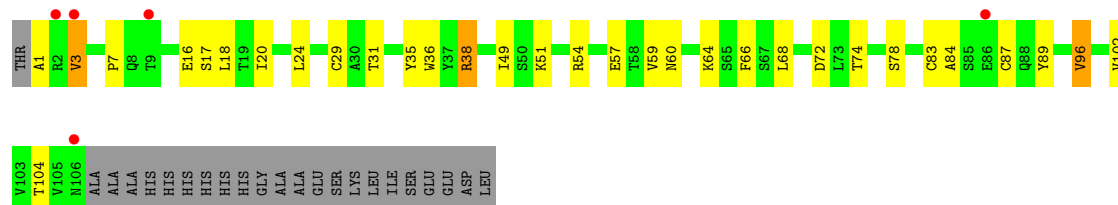


• Molecule 1: Antigen receptor

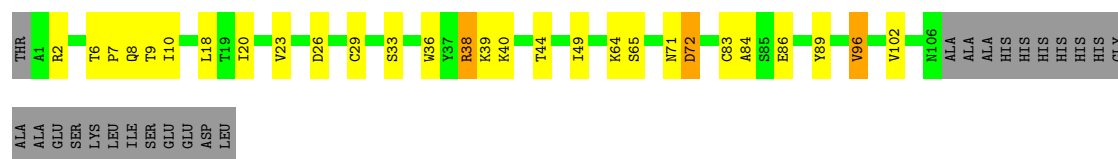
Chain R: 2% 48% 33% 17%



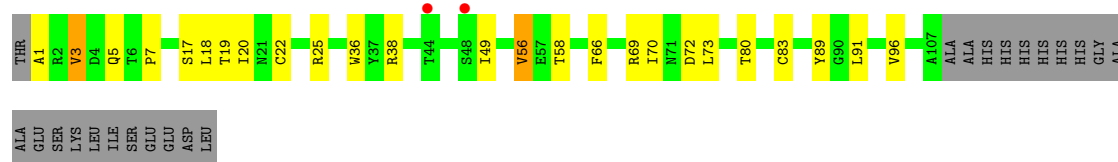
• Molecule 1: Antigen receptor



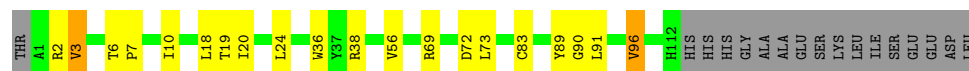
• Molecule 1: Antigen receptor



• Molecule 1: Antigen receptor



• Molecule 1: Antigen receptor



• Molecule 1: Antigen receptor



ALA  
GLU  
SER  
LYS  
LEU  
ILE  
SER  
GLU  
ASP  
LEU

• Molecule 1: Antigen receptor



THR A1 R2 V3 T6 P7 T11 L18 T19 I20 L24 S33 T34 Y35 W36 Y37 R38 K39 T44 M45 I49 V56 F66 S67 L68 R69 D72 L73 T74 V75 E76 C83 A84 S85 E86 E93 G99 T104 H112 HIS HIS HIS GLY ALA ALA

GLU  
SER  
LYS  
LEU  
ILE  
SER  
GLU  
ASP  
LEU

• Molecule 1: Antigen receptor



THR A1 R2 V3 T6 P7 T10 L18 T19 I20 R25 C29 A30 T31 Y37 E46 T58 K64 R69 D72 L73 A84 C87 D88 Y89 G90 L91 V96 G99 A109 H112 HIS HIS HIS GLY ALA ALA GLU SER LYS LEU ILE SER

GLU  
GLU  
ASP  
LEU

• Molecule 1: Antigen receptor



THR A1 R2 V3 D4 Q5 T6 P7 T10 E13 T11 T14 G15 E16 S17 L18 N21 C22 V23 L24 C29 Y37 R38 K39 T44 M45 E46 E47 S48 I49 R54 Y55 S63 K64 S65 F66 I70 D71 D72 G79 T80 Y81 H82 C83 A84 C87 Q88 R89 G90 L91

V96 G100 T101 V102 N106 H111 H112 HIS HIS HIS GLY ALA ALA SER LYS LEU ILE SER SER GLU ASP LEU

• Molecule 1: Antigen receptor



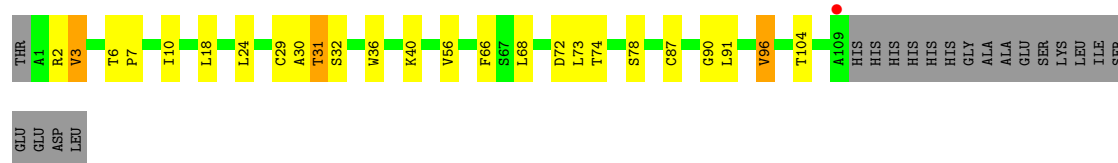
THR A1 R2 V3 T6 P7 Q8 T9 T10 T11 K12 E13 T14 G15 S17 L18 T19 I20 L24 S27 H28 W36 K40 S41 I49 Y55 V56 E57 T58 V59 K64 S65 F66 S67 L68 R69 I70 N71 D72 L73 T74 S78 G79 T80 Y81 L91 Y94 D95

V96 G100 T101 V103 T104 V105 ASN ALA ALA ALA HIS HIS HIS HIS HIS HIS GLY ALA ALA GLU SER LYS LEU ILE SER SER GLU ASP LEU

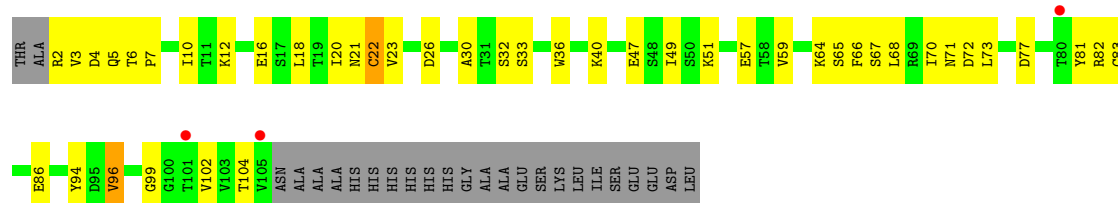
• Molecule 1: Antigen receptor



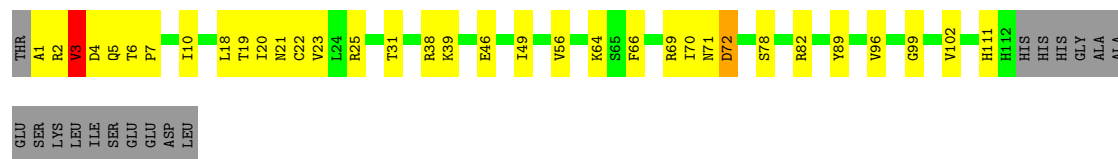




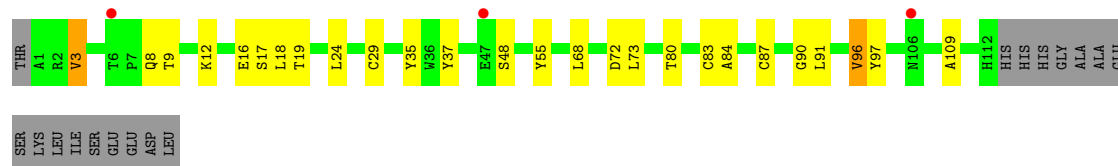
- Molecule 1: Antigen receptor



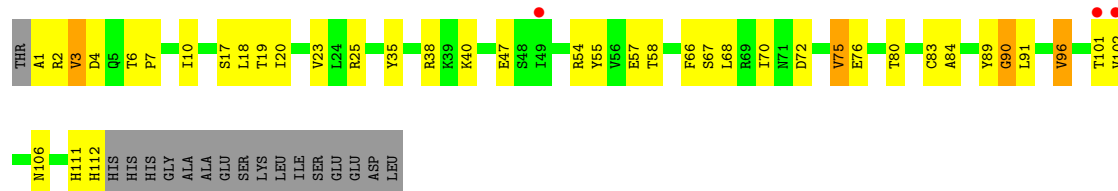
- Molecule 1: Antigen receptor



- Molecule 1: Antigen receptor



- Molecule 1: Antigen receptor

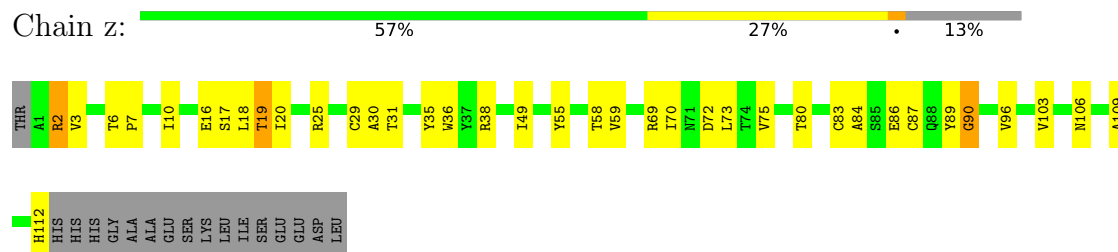


- Molecule 1: Antigen receptor

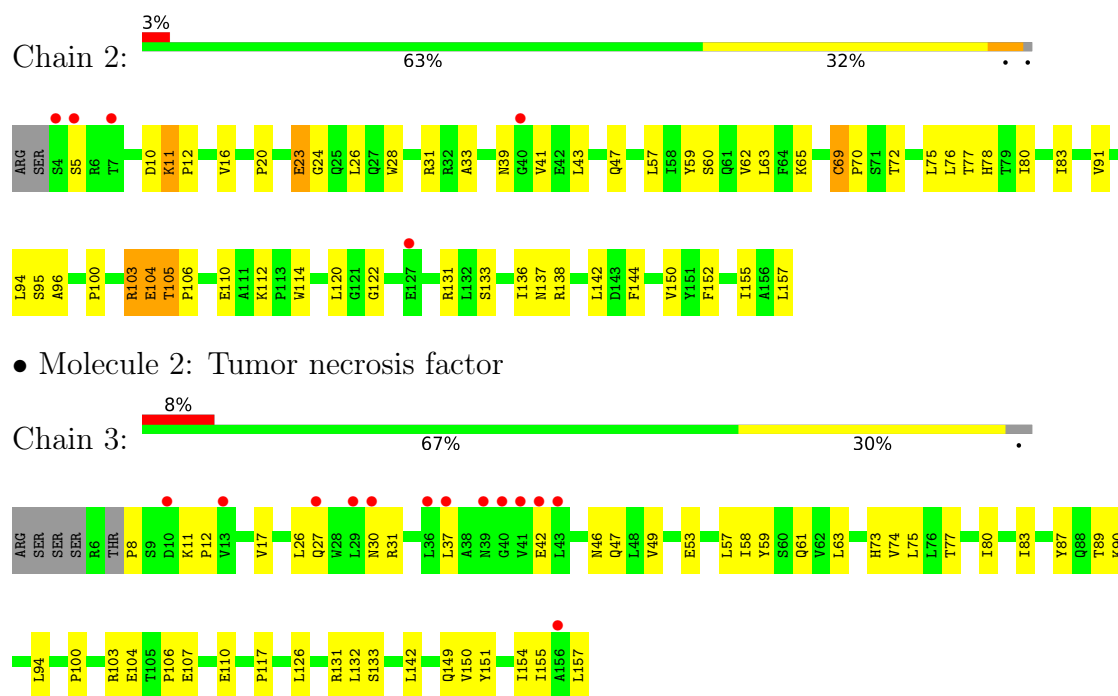




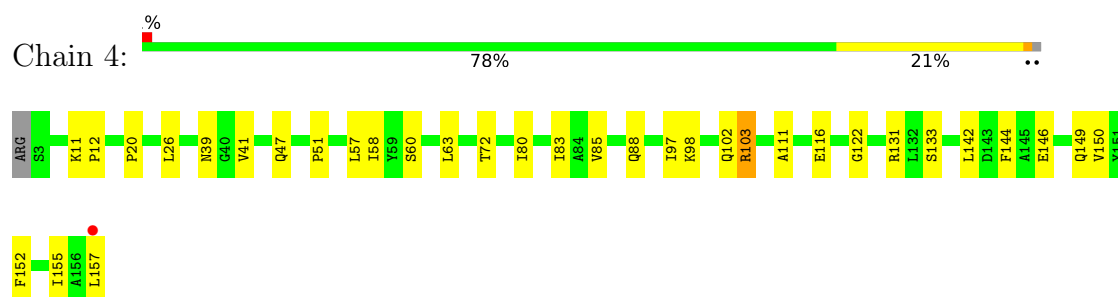
### • Molecule 1: Antigen receptor



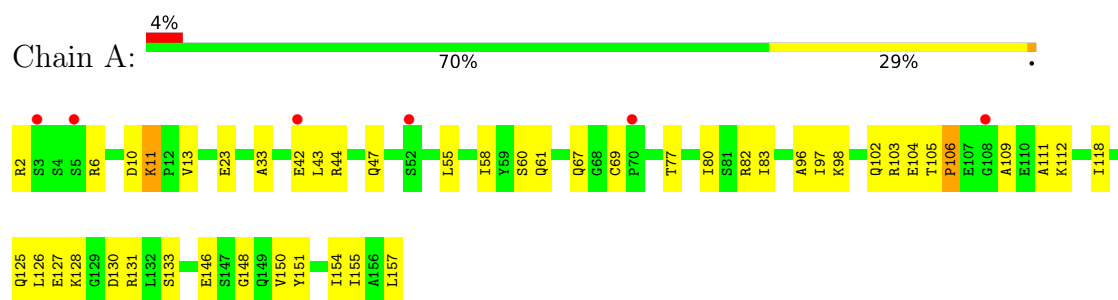
### • Molecule 2: Tumor necrosis factor



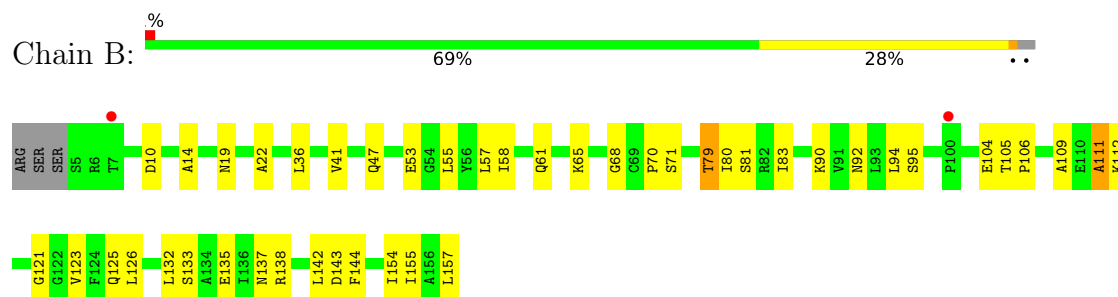
### • Molecule 2: Tumor necrosis factor



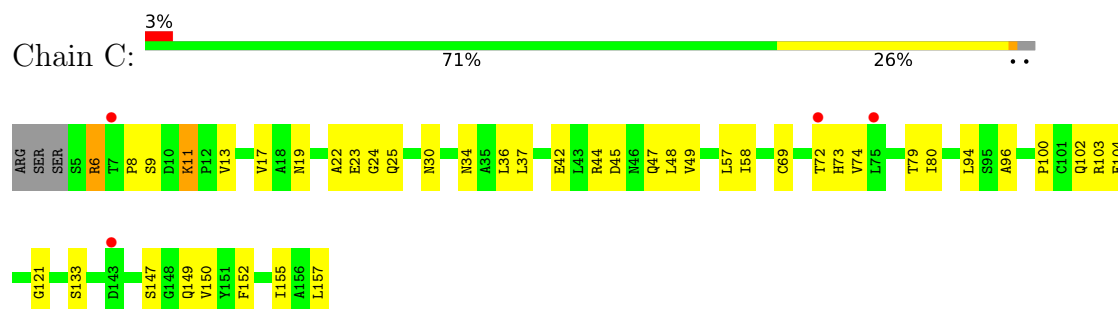
### • Molecule 2: Tumor necrosis factor



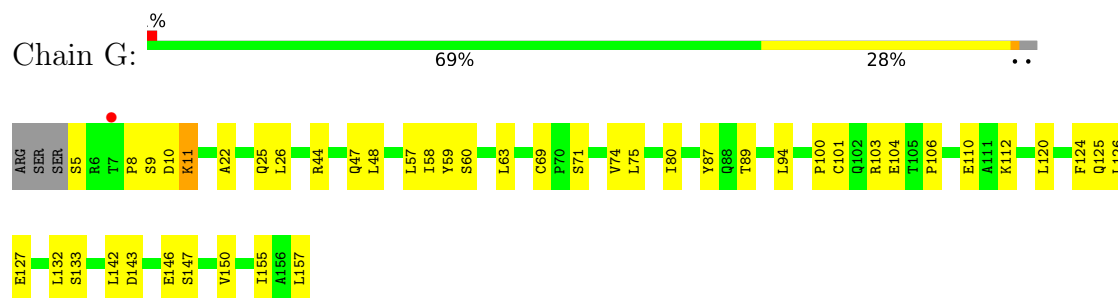
• Molecule 2: Tumor necrosis factor



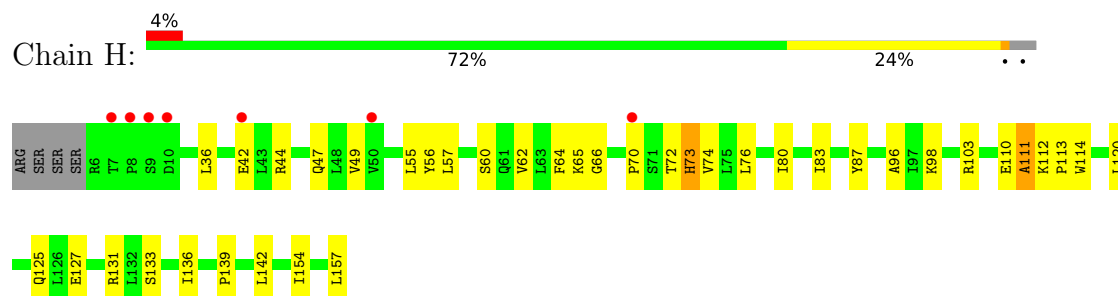
• Molecule 2: Tumor necrosis factor



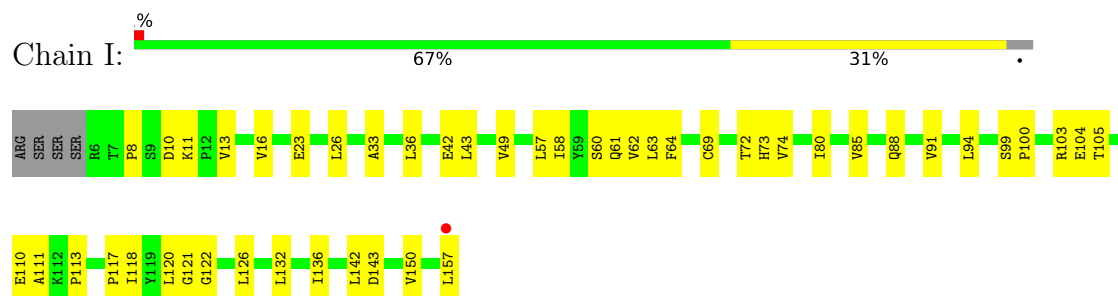
• Molecule 2: Tumor necrosis factor



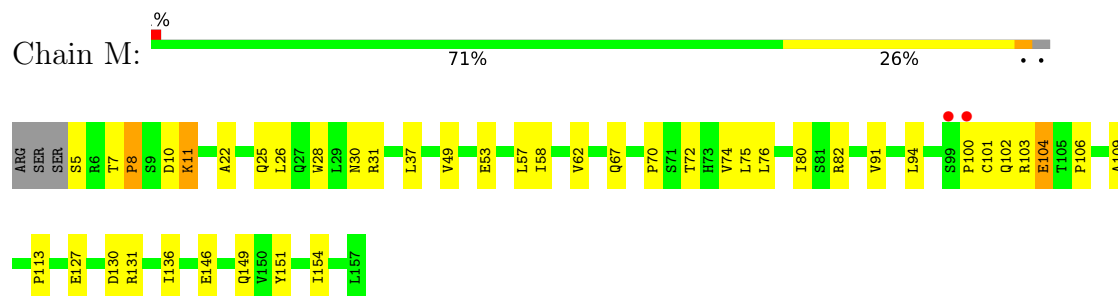
• Molecule 2: Tumor necrosis factor



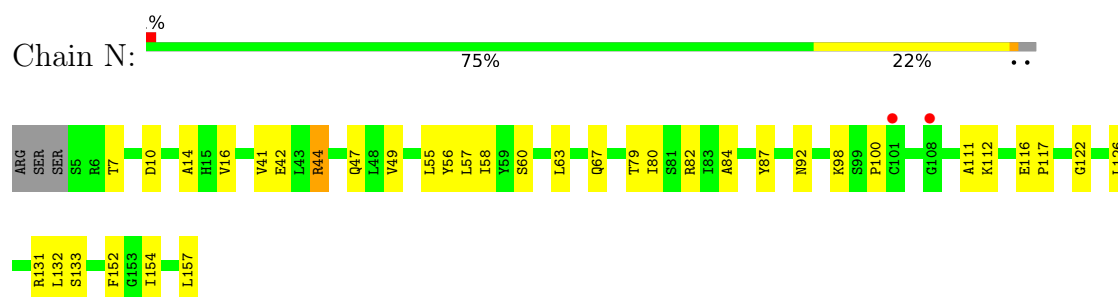
- Molecule 2: Tumor necrosis factor



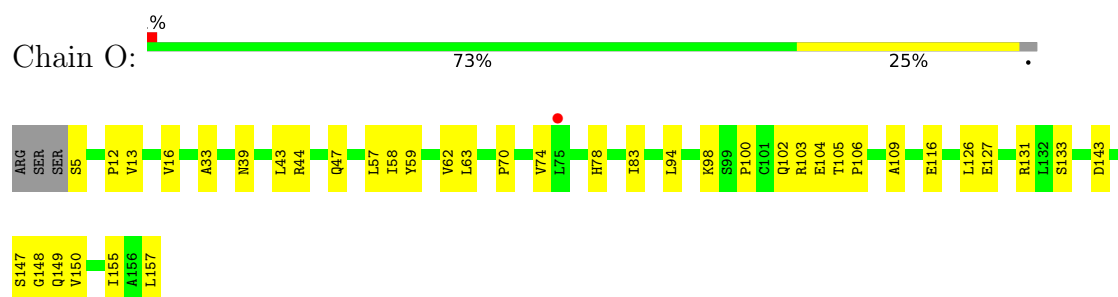
- Molecule 2: Tumor necrosis factor



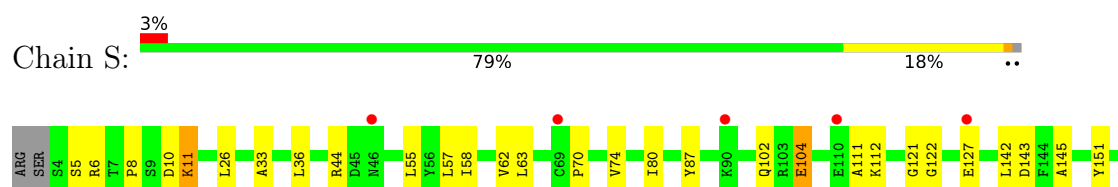
- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor

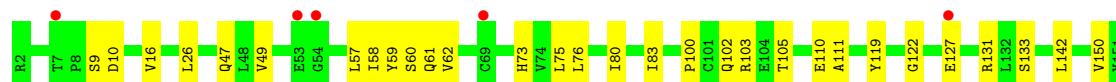
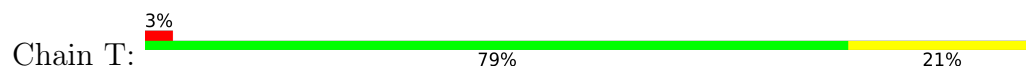


- Molecule 2: Tumor necrosis factor



L157

- Molecule 2: Tumor necrosis factor



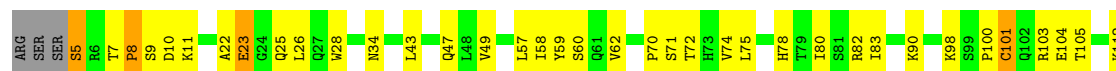
F152 I155 A156 L157

- Molecule 2: Tumor necrosis factor



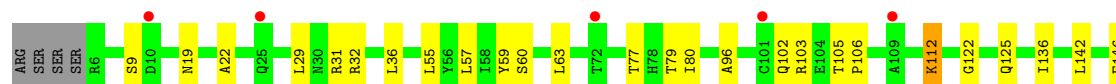
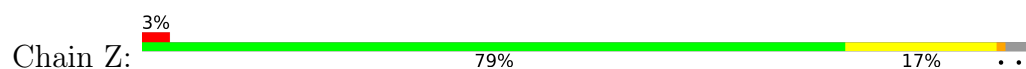
R103 E104 T105 E116 L120 F124 Q125 L126 L132 S133 A134 I136 Y141 L142 D143 V150 Y151 F152 I155 A156 L157

- Molecule 2: Tumor necrosis factor



E116 G121 G122 V123 F124 Q125 L126 D130 R131 L132 S133 R138 L142 D143 F144 A145 E146 L157

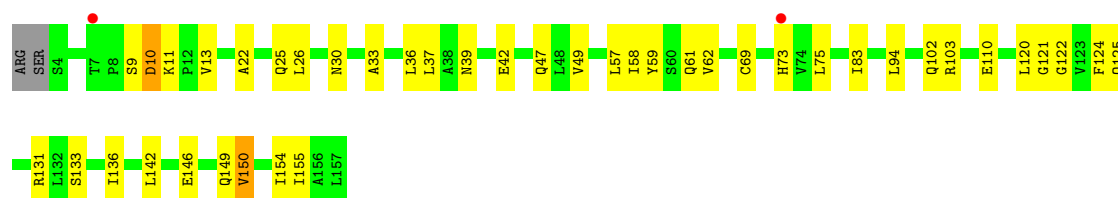
- Molecule 2: Tumor necrosis factor



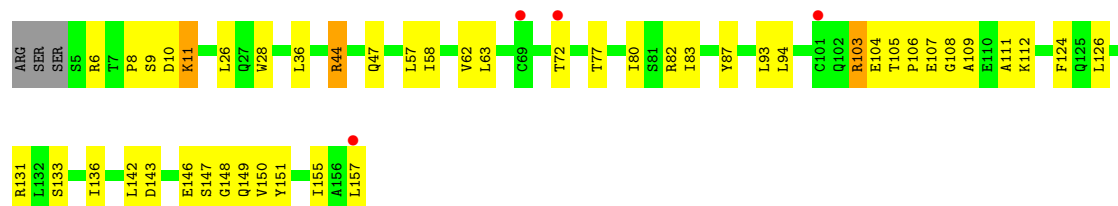
Q149 V150 L157

- Molecule 2: Tumor necrosis factor

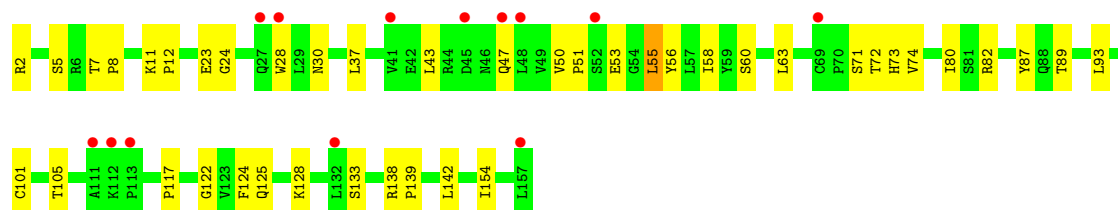




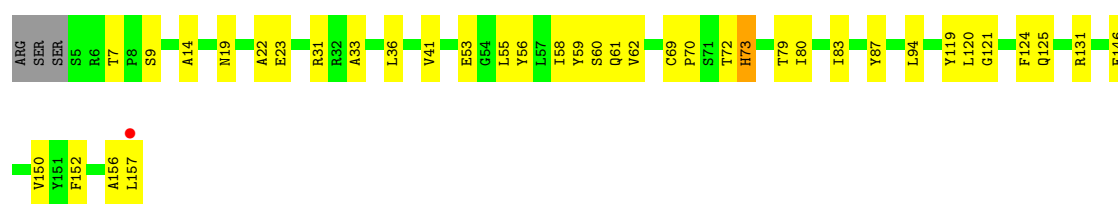
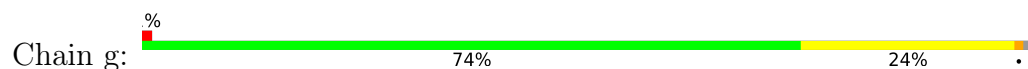
- Molecule 2: Tumor necrosis factor



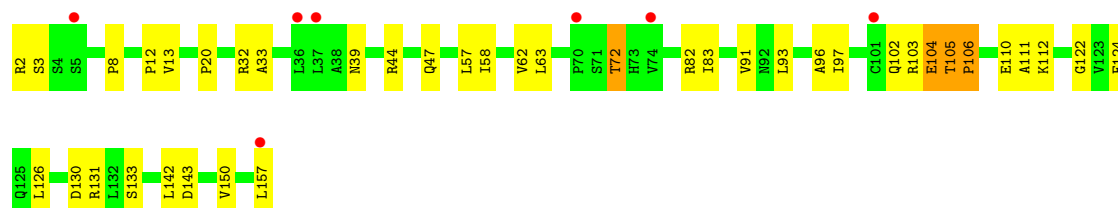
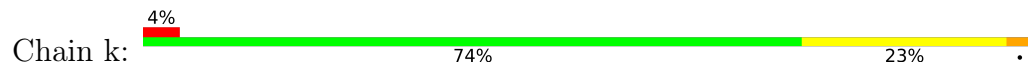
- Molecule 2: Tumor necrosis factor



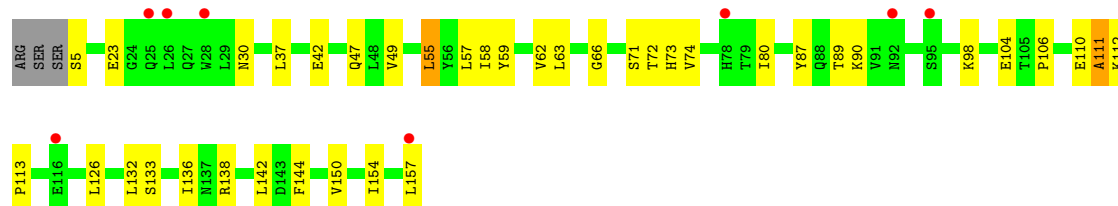
- Molecule 2: Tumor necrosis factor



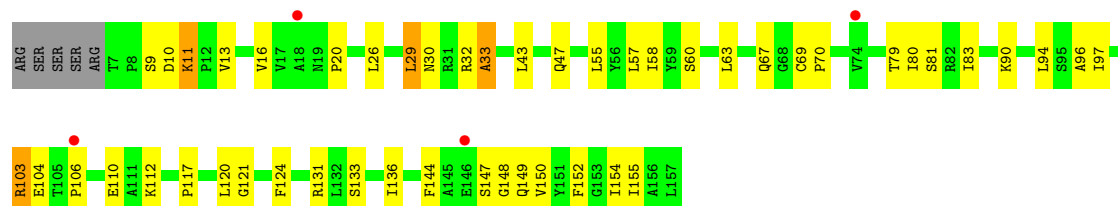
- Molecule 2: Tumor necrosis factor



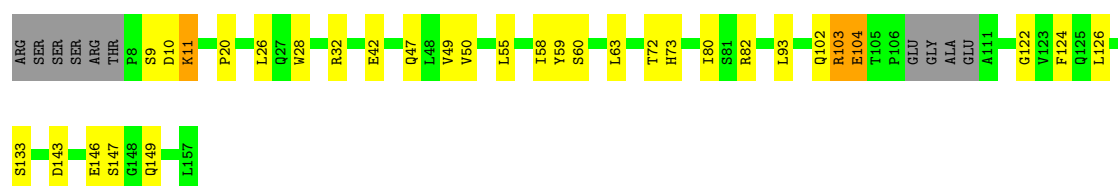
- Molecule 2: Tumor necrosis factor



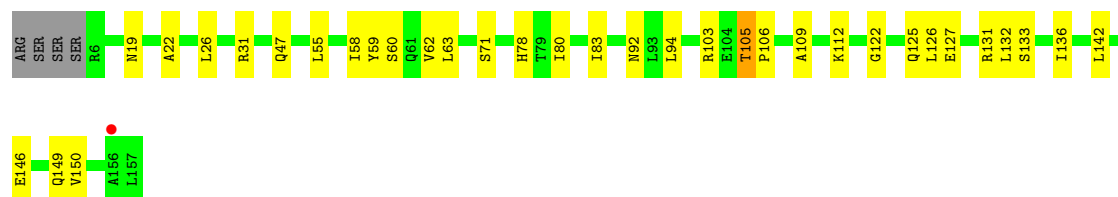
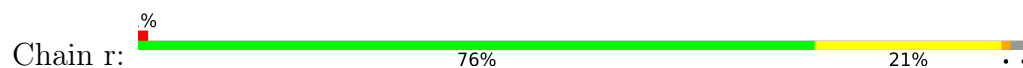
- Molecule 2: Tumor necrosis factor



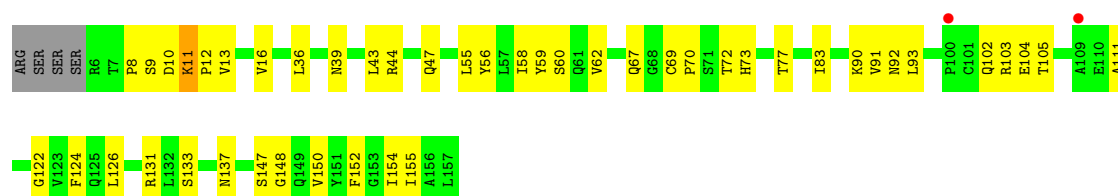
- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor

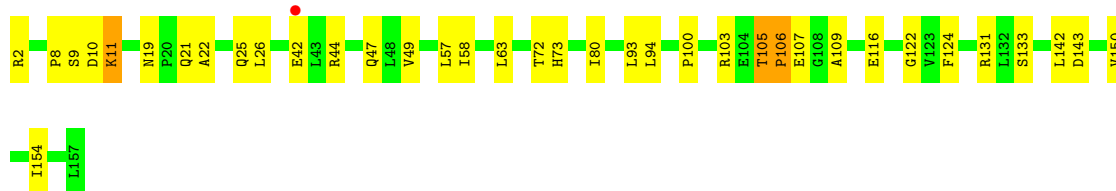
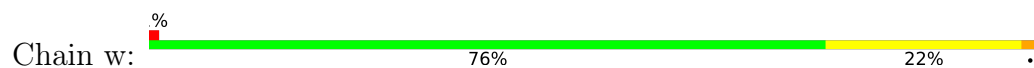


- Molecule 2: Tumor necrosis factor





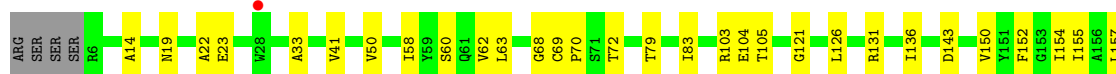
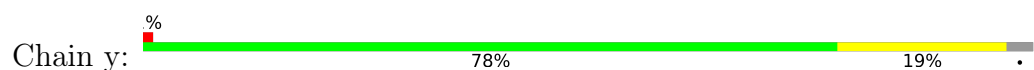
- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.32Å 218.13Å 236.49Å 90.00° 96.28° 90.00°	Depositor
Resolution (Å)	109.06 – 3.43 109.06 – 3.43	Depositor EDS
% Data completeness (in resolution range)	99.4 (109.06-3.43) 99.5 (109.06-3.43)	Depositor EDS
$R_{merge}$	0.58	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.230 , 0.288 0.230 , 0.288	Depositor DCC
$R_{free}$ test set	7793 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.5	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 83.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	60848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, GOL

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	0	0.23	0/826	0.55	0/1118
1	1	0.20	0/808	0.53	0/1093
1	5	0.25	0/831	0.52	0/1125
1	6	0.22	0/826	0.55	0/1118
1	7	0.22	0/826	0.64	0/1118
1	D	0.26	0/821	0.62	0/1111
1	E	0.24	0/831	0.56	0/1125
1	F	0.24	0/821	0.65	0/1111
1	J	0.24	0/831	0.52	0/1125
1	K	0.19	0/821	0.51	0/1111
1	L	0.23	0/869	0.54	0/1177
1	P	0.22	0/826	0.55	0/1118
1	Q	0.23	0/869	0.52	0/1177
1	R	0.18	0/826	0.48	0/1118
1	V	0.22	0/832	0.54	0/1125
1	W	0.18	0/821	0.44	0/1111
1	X	0.21	0/826	0.52	0/1118
1	b	0.19	0/869	0.53	0/1177
1	c	0.23	0/869	0.55	0/1177
1	d	0.20	0/869	0.49	0/1177
1	h	0.20	0/869	0.57	0/1177
1	i	0.22	0/869	0.54	0/1177
1	j	0.22	0/813	0.60	0/1100
1	n	0.24	0/836	0.56	0/1132
1	o	0.25	0/808	0.60	0/1093
1	p	0.16	0/869	0.46	0/1177
1	t	0.22	0/869	0.54	0/1177
1	u	0.20	0/869	0.47	0/1177
1	v	0.19	0/813	0.54	0/1100
1	z	0.23	0/869	0.56	0/1177
2	2	0.20	0/1229	0.57	0/1672
2	3	0.20	0/1209	0.52	0/1642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	4	0.21	0/1235	0.53	0/1680
2	A	0.23	0/1246	0.52	0/1694
2	B	0.20	0/1223	0.53	0/1664
2	C	0.21	0/1223	0.56	0/1664
2	G	0.20	0/1223	0.53	0/1664
2	H	0.22	0/1215	0.52	0/1653
2	I	0.19	0/1217	0.53	0/1656
2	M	0.20	0/1223	0.51	0/1664
2	N	0.18	0/1223	0.52	2/1664 (0.1%)
2	O	0.20	0/1223	0.54	0/1664
2	S	0.21	0/1229	0.55	0/1672
2	T	0.19	0/1246	0.52	0/1694
2	U	0.24	0/1199	0.57	0/1631
2	Y	0.20	0/1223	0.57	0/1664
2	Z	0.22	0/1217	0.50	0/1656
2	a	0.19	0/1229	0.53	2/1672 (0.1%)
2	e	0.20	0/1223	0.56	0/1664
2	f	0.17	0/1246	0.48	0/1694
2	g	0.20	0/1223	0.51	0/1664
2	k	0.18	0/1246	0.51	0/1694
2	l	0.19	0/1223	0.48	0/1664
2	m	0.20	0/1206	0.52	0/1642
2	q	0.19	0/1171	0.57	0/1592
2	r	0.18	0/1217	0.49	0/1656
2	s	0.19	0/1217	0.54	0/1656
2	w	0.20	0/1246	0.58	0/1694
2	x	0.22	0/1223	0.53	0/1664
2	y	0.21	0/1217	0.51	0/1656
All	All	0.21	0/61892	0.54	4/84027 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	10	ASP	CA-C-N	5.57	135.38	121.80
2	a	10	ASP	C-N-CA	5.57	135.38	121.80
2	N	10	ASP	CA-C-N	-5.13	110.23	122.74
2	N	10	ASP	C-N-CA	-5.13	110.23	122.74

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	815	0	775	26	0
1	1	797	0	756	23	0
1	5	820	0	780	22	0
1	6	815	0	775	15	0
1	7	815	0	775	31	0
1	D	810	0	770	22	0
1	E	820	0	780	24	0
1	F	810	0	772	25	0
1	J	820	0	780	21	0
1	K	810	0	770	23	0
1	L	855	0	806	23	0
1	P	815	0	775	16	0
1	Q	855	0	806	21	0
1	R	815	0	775	29	0
1	V	821	0	782	22	0
1	W	810	0	770	19	0
1	X	815	0	775	14	0
1	b	855	0	806	12	0
1	c	855	0	806	22	0
1	d	855	0	806	15	0
1	h	855	0	806	17	0
1	i	855	0	806	28	0
1	j	802	0	764	32	0
1	n	825	0	785	17	0
1	o	797	0	756	40	0
1	p	855	0	806	24	0
1	t	855	0	806	13	0
1	u	855	0	806	27	0
1	v	802	0	764	15	0
1	z	855	0	806	20	0
2	2	1202	0	1195	45	0
2	3	1183	0	1178	33	0
2	4	1208	0	1200	22	0
2	A	1219	0	1213	37	0
2	B	1196	0	1190	36	0
2	C	1196	0	1190	28	0
2	G	1196	0	1190	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1188	0	1180	28	0
2	I	1190	0	1185	27	0
2	M	1196	0	1190	26	0
2	N	1196	0	1190	24	0
2	O	1196	0	1190	21	0
2	S	1202	0	1195	21	0
2	T	1219	0	1213	24	0
2	U	1172	0	1166	36	0
2	Y	1196	0	1190	32	0
2	Z	1190	0	1185	21	0
2	a	1202	0	1195	30	0
2	e	1196	0	1190	34	0
2	f	1219	0	1213	25	0
2	g	1196	0	1190	29	0
2	k	1219	0	1213	30	0
2	l	1196	0	1190	33	0
2	m	1179	0	1172	33	0
2	q	1145	0	1145	23	0
2	r	1190	0	1185	25	0
2	s	1190	0	1185	26	0
2	w	1219	0	1213	22	0
2	x	1196	0	1190	23	0
2	y	1190	0	1185	20	0
3	0	6	0	8	0	0
3	1	6	0	8	2	0
3	5	6	0	8	0	0
3	D	6	0	8	1	0
3	J	6	0	8	2	0
3	P	6	0	8	0	0
3	V	6	0	8	1	0
3	W	6	0	8	1	0
3	b	18	0	24	0	0
3	c	6	0	8	1	0
3	h	6	0	8	1	0
3	n	6	0	8	0	0
3	t	12	0	16	1	0
3	z	6	0	8	1	0
4	P	5	0	0	0	0
4	h	5	0	0	0	0
4	t	5	0	0	0	0
5	S	1	0	0	0	0
6	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	P	1	0	0	0	0
6	S	1	0	0	0	0
6	V	2	0	0	0	0
6	X	1	0	0	0	0
All	All	60848	0	59387	1325	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 11.

All (1325) 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)
1:7:7:PRO:HG2	1:7:20:ILE:HA	1.49	0.93
1:E:39:LYS:HG2	1:E:46:GLU:HG2	1.51	0.92
1:F:10:ILE:HD12	1:F:18:LEU:HD11	1.53	0.90
2:a:125:GLN:HE22	1:b:90:GLY:HA3	1.36	0.90
2:M:102:GLN:HE22	2:O:102:GLN:HB2	1.39	0.88
1:1:38:ARG:HD3	1:1:49:ILE:HD11	1.57	0.85
1:1:56:VAL:HG23	1:1:69:ARG:HB3	1.58	0.85
2:m:63:LEU:H	2:m:150:VAL:HG12	1.42	0.85
1:6:18:LEU:HD21	1:6:102:VAL:HG11	1.60	0.84
2:2:47:GLN:HG2	2:2:133:SER:HB3	1.59	0.84
1:j:55:TYR:HB3	1:j:68:LEU:HD11	1.59	0.84
1:h:6:THR:HG23	1:h:7:PRO:HD3	1.60	0.84
1:L:40:LYS:HG3	1:L:47:GLU:OE2	1.78	0.81
1:6:7:PRO:HG2	1:6:20:ILE:HA	1.60	0.81
1:X:56:VAL:HG23	1:X:69:ARG:HB3	1.62	0.81
2:l:136:ILE:HD11	2:l:142:LEU:HD11	1.60	0.81
2:r:136:ILE:HD11	2:r:142:LEU:HD11	1.61	0.81
1:Q:7:PRO:HG2	1:Q:20:ILE:HA	1.63	0.80
1:i:54:ARG:HD2	1:i:72:ASP:HB2	1.62	0.80
1:F:54:ARG:HE	1:F:71:ASN:HB2	1.47	0.78
2:a:62:VAL:HA	2:a:150:VAL:HG12	1.65	0.77
2:s:62:VAL:HA	2:s:150:VAL:HG12	1.64	0.77
1:D:35:TYR:HB2	1:D:84:ALA:HB3	1.67	0.77
1:j:7:PRO:HG2	1:j:20:ILE:HA	1.66	0.77
2:q:58:ILE:HD12	2:q:124:PHE:HD2	1.49	0.77
2:3:103:ARG:HG2	2:3:104:GLU:H	1.49	0.76
1:L:6:THR:HB	1:L:21:ASN:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:36:TRP:HD1	1:o:51:LYS:HE2	1.50	0.75
2:w:80:ILE:HD12	2:w:94:LEU:HD12	1.68	0.75
2:3:8:PRO:HA	2:U:72:THR:HG21	1.68	0.75
2:l:71:SER:HB2	2:l:104:GLU:HG3	1.68	0.75
1:5:35:TYR:HB2	1:5:84:ALA:HB3	1.67	0.75
2:f:125:GLN:HB2	2:g:36:LEU:HD21	1.68	0.74
1:6:38:ARG:HB3	1:6:49:ILE:HD11	1.68	0.74
2:e:82:ARG:HH12	2:e:126:LEU:HA	1.52	0.74
2:A:112:LYS:HG3	2:C:103:ARG:HG3	1.70	0.74
1:t:16:GLU:HG3	1:t:17:SER:H	1.51	0.74
1:j:8:GLN:HG2	1:j:9:THR:H	1.52	0.74
1:X:18:LEU:HD23	1:X:73:LEU:HD21	1.69	0.73
1:F:7:PRO:HG2	1:F:20:ILE:HA	1.70	0.73
1:K:38:ARG:HD2	1:K:40:LYS:HD3	1.69	0.73
1:c:16:GLU:HG3	1:c:17:SER:H	1.53	0.73
2:3:74:VAL:HG23	2:3:100:PRO:HD2	1.70	0.73
2:l:57:LEU:HB2	2:l:157:LEU:HD11	1.70	0.73
1:z:7:PRO:HB2	1:z:10:ILE:HD11	1.71	0.73
2:U:47:GLN:HG2	2:U:133:SER:HB3	1.71	0.73
2:U:103:ARG:HD2	2:U:104:GLU:H	1.51	0.73
1:i:13:GLU:HB3	1:i:16:GLU:HG3	1.72	0.72
1:z:18:LEU:HD23	1:z:73:LEU:HD21	1.71	0.72
2:Z:136:ILE:HD11	2:Z:142:LEU:HD11	1.71	0.72
1:d:38:ARG:HB3	1:d:49:ILE:HD11	1.70	0.72
2:3:49:VAL:HG22	2:3:131:ARG:HG2	1.72	0.72
1:K:7:PRO:HG2	1:K:20:ILE:HA	1.72	0.72
1:E:7:PRO:HG2	1:E:20:ILE:HA	1.70	0.72
2:S:87:TYR:HE1	1:X:1:ALA:HB3	1.55	0.72
1:j:27:SER:HA	1:j:64:LYS:HE2	1.72	0.72
2:y:62:VAL:HA	2:y:150:VAL:HG12	1.70	0.72
1:K:39:LYS:HD2	1:K:44:THR:HA	1.71	0.71
2:T:73:HIS:HB3	1:c:6:THR:HG21	1.73	0.71
2:f:139:PRO:HA	2:f:142:LEU:HD13	1.71	0.71
2:f:2:ARG:HB3	1:i:64:LYS:HE3	1.72	0.70
1:o:36:TRP:CD1	1:o:51:LYS:HE2	2.26	0.70
2:a:22:ALA:HB1	2:a:25:GLN:HG3	1.73	0.70
2:M:72:THR:HG22	2:M:103:ARG:HA	1.74	0.70
2:2:57:LEU:HB2	2:2:157:LEU:HD11	1.73	0.70
2:O:57:LEU:HB2	2:O:157:LEU:HD11	1.71	0.70
1:z:75:VAL:HG21	1:z:106:ASN:HD22	1.57	0.70
1:n:18:LEU:HD23	1:n:73:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:39:LYS:HB2	1:P:46:GLU:HG2	1.73	0.69
1:X:17:SER:HB2	1:X:69:ARG:HE	1.55	0.69
1:o:4:ASP:HB2	1:o:23:VAL:HB	1.73	0.69
1:o:21:ASN:HB3	1:o:65:SER:HB2	1.73	0.69
2:U:103:ARG:CD	2:U:104:GLU:H	2.06	0.69
1:1:10:ILE:HD12	1:1:102:VAL:HG22	1.75	0.69
2:q:47:GLN:HG2	2:q:133:SER:HB3	1.75	0.69
1:F:38:ARG:HD3	1:F:81:TYR:CZ	2.27	0.68
2:H:55:LEU:HD13	2:I:13:VAL:HG11	1.74	0.68
2:s:58:ILE:HD11	2:s:126:LEU:HD11	1.75	0.68
1:0:56:VAL:HG13	1:0:69:ARG:HB3	1.74	0.68
1:6:25:ARG:NH1	1:R:52:GLY:HA3	2.08	0.68
1:V:35:TYR:HB2	1:V:84:ALA:HB3	1.76	0.68
1:J:7:PRO:HG2	1:J:20:ILE:HA	1.76	0.68
1:o:82:ARG:HD3	1:o:99:GLY:HA2	1.76	0.68
1:5:24:LEU:HB2	1:5:64:LYS:HB3	1.75	0.68
1:E:14:THR:HG23	1:E:73:LEU:O	1.94	0.67
2:f:47:GLN:HG2	2:f:133:SER:HB3	1.76	0.67
2:k:3:SER:HB2	1:n:30:ALA:HB2	1.76	0.67
1:X:7:PRO:HG2	1:X:20:ILE:HA	1.76	0.67
2:Z:136:ILE:CD1	2:Z:142:LEU:HD11	2.22	0.67
1:V:7:PRO:HG2	1:V:20:ILE:HA	1.75	0.67
2:m:47:GLN:HG2	2:m:133:SER:HB3	1.77	0.67
2:A:103:ARG:HD2	2:B:112:LYS:HZ2	1.60	0.67
1:L:13:GLU:H	1:L:16:GLU:HG3	1.60	0.67
2:Z:57:LEU:HB2	2:Z:157:LEU:HD11	1.76	0.67
2:w:122:GLY:HA2	2:x:59:TYR:CE2	2.29	0.67
2:Y:82:ARG:HH12	2:Y:126:LEU:HA	1.59	0.67
1:W:2:ARG:HD2	3:W:201:GOL:H32	1.75	0.67
1:j:57:GLU:OE2	1:j:66:PHE:HB2	1.95	0.67
1:7:6:THR:HB	1:7:7:PRO:HD3	1.75	0.67
1:1:27:SER:HA	1:1:64:LYS:HE2	1.76	0.67
2:3:58:ILE:HD11	2:3:126:LEU:HD11	1.76	0.67
2:e:26:LEU:HD21	2:e:28:TRP:CE2	2.30	0.67
1:v:82:ARG:HG3	1:v:99:GLY:HA2	1.76	0.67
2:r:103:ARG:HG2	2:r:106:PRO:HG3	1.75	0.66
2:s:103:ARG:HG2	2:s:104:GLU:H	1.61	0.66
1:R:39:LYS:HB2	1:R:46:GLU:HG2	1.76	0.66
1:c:7:PRO:HG2	1:c:20:ILE:HA	1.76	0.66
2:w:58:ILE:HD12	2:w:124:PHE:HD2	1.59	0.66
2:A:61:GLN:HE22	2:C:96:ALA:HB2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:58:ILE:HD12	2:e:124:PHE:HD2	1.60	0.66
2:4:146:GLU:HB2	2:4:149:GLN:HE22	1.60	0.66
1:L:56:VAL:HG13	1:L:69:ARG:HB3	1.77	0.66
2:M:53:GLU:OE2	1:R:89:TYR:HE1	1.77	0.66
2:B:57:LEU:HB2	2:B:157:LEU:HD11	1.78	0.66
1:Q:5:GLN:HG3	1:Q:99:GLY:H	1.60	0.66
1:1:13:GLU:HA	1:1:105:VAL:HG22	1.76	0.66
1:J:35:TYR:HB2	1:J:84:ALA:HB3	1.78	0.65
1:c:56:VAL:HG23	1:c:69:ARG:HB2	1.77	0.65
2:C:47:GLN:HG2	2:C:133:SER:HB3	1.78	0.65
2:M:80:ILE:HD12	2:M:94:LEU:HD12	1.79	0.65
2:g:9:SER:HB3	1:j:91:LEU:HD11	1.78	0.65
2:g:14:ALA:HB2	2:g:41:VAL:HG11	1.76	0.65
2:k:47:GLN:HG2	2:k:133:SER:HB3	1.78	0.65
1:K:3:VAL:HG22	1:K:24:LEU:HD23	1.77	0.65
2:Z:31:ARG:HE	1:d:93:GLU:HG2	1.59	0.65
1:j:6:THR:HB	1:j:7:PRO:HD3	1.79	0.65
2:A:2:ARG:HA	1:D:30:ALA:HB1	1.77	0.65
1:J:61:SER:HB2	3:J:201:GOL:H11	1.77	0.65
2:H:47:GLN:HG2	2:H:133:SER:HB3	1.78	0.65
1:0:7:PRO:HG2	1:0:20:ILE:HA	1.79	0.65
2:Y:57:LEU:HB2	2:Y:157:LEU:HD11	1.78	0.65
1:R:40:LYS:HE2	1:R:47:GLU:OE2	1.95	0.65
1:j:59:VAL:HA	1:j:66:PHE:HA	1.78	0.64
1:K:38:ARG:O	1:K:47:GLU:HG2	1.96	0.64
1:0:8:GLN:HG3	1:0:9:THR:H	1.61	0.64
1:j:68:LEU:HD23	1:j:81:TYR:HE1	1.62	0.64
1:K:55:TYR:HB3	1:K:68:LEU:HD11	1.79	0.64
2:4:63:LEU:HD22	2:4:149:GLN:HG2	1.79	0.64
2:N:42:GLU:HG3	2:N:49:VAL:HB	1.80	0.64
2:2:76:LEU:HD22	2:2:100:PRO:HB3	1.79	0.64
1:R:88:GLN:HB3	1:R:93:GLU:OE1	1.98	0.64
2:T:57:LEU:HB2	2:T:157:LEU:HD11	1.79	0.64
2:Y:58:ILE:HD12	2:Y:124:PHE:HD2	1.63	0.64
1:V:54:ARG:HH21	3:V:201:GOL:H11	1.63	0.64
1:n:6:THR:HB	1:n:7:PRO:HD3	1.80	0.64
1:6:5:GLN:HE21	1:6:20:ILE:HG21	1.63	0.63
2:G:112:LYS:HE3	2:I:103:ARG:HE	1.63	0.63
2:H:42:GLU:HG3	2:H:49:VAL:HB	1.78	0.63
2:H:72:THR:HG23	2:H:74:VAL:HG13	1.80	0.63
2:e:63:LEU:HD22	2:e:143:ASP:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:VAL:HG22	2:H:131:ARG:HG2	1.80	0.63
2:H:139:PRO:HA	2:H:142:LEU:HD13	1.80	0.63
2:e:57:LEU:HB2	2:e:157:LEU:HD11	1.80	0.63
2:x:80:ILE:HD12	2:x:94:LEU:HD12	1.81	0.63
1:D:24:LEU:HB2	1:D:64:LYS:HB3	1.78	0.63
2:l:98:LYS:HE2	2:m:117:PRO:HD2	1.81	0.63
2:3:31:ARG:HH22	1:7:86:GLU:HG3	1.64	0.63
1:c:12:LYS:HD2	1:c:16:GLU:HG2	1.81	0.63
2:m:69:CYS:HB2	2:m:106:PRO:HD3	1.81	0.63
2:q:82:ARG:HH12	2:q:126:LEU:HA	1.64	0.63
1:1:54:ARG:HG3	1:1:71:ASN:HB2	1.80	0.63
1:h:7:PRO:HB2	1:h:10:ILE:HD11	1.79	0.63
1:j:12:LYS:HG3	1:j:18:LEU:HB3	1.81	0.62
2:B:47:GLN:HG2	2:B:133:SER:HB3	1.81	0.62
2:N:57:LEU:HB2	2:N:157:LEU:HD11	1.80	0.62
1:b:6:THR:OG1	1:b:7:PRO:HD3	2.00	0.62
2:q:103:ARG:HH22	2:r:109:ALA:HB3	1.64	0.62
1:Q:6:THR:OG1	1:Q:7:PRO:HD3	1.98	0.62
1:h:1:ALA:HB1	1:h:25:ARG:HG3	1.82	0.62
2:S:122:GLY:HA2	2:T:59:TYR:CE2	2.35	0.62
2:Y:22:ALA:HB1	2:Y:25:GLN:HG3	1.82	0.61
1:6:18:LEU:HB3	1:6:70:ILE:HB	1.82	0.61
1:t:18:LEU:HD23	1:t:73:LEU:HD21	1.81	0.61
1:1:2:ARG:HH11	3:1:201:GOL:H32	1.64	0.61
1:L:6:THR:HG21	1:L:20:ILE:HA	1.81	0.61
2:U:50:VAL:HG21	2:U:126:LEU:HD13	1.82	0.61
2:G:57:LEU:HB2	2:G:157:LEU:HD11	1.82	0.61
1:j:41:SER:HB2	1:j:78:SER:HB3	1.82	0.61
1:u:18:LEU:HD22	1:u:102:VAL:HG11	1.83	0.61
2:O:98:LYS:HE2	2:O:116:GLU:OE2	1.99	0.61
1:R:7:PRO:HG2	1:R:20:ILE:HA	1.83	0.61
2:f:30:ASN:HD22	2:f:37:LEU:HB3	1.65	0.61
2:g:62:VAL:HA	2:g:150:VAL:HG12	1.81	0.61
2:x:72:THR:HG23	2:x:74:VAL:HG13	1.82	0.61
2:T:60:SER:HB3	2:T:80:ILE:HD11	1.83	0.61
1:o:20:ILE:O	1:o:67:SER:HA	2.00	0.61
1:v:10:ILE:HG13	1:v:102:VAL:HG23	1.83	0.61
2:2:137:ASN:ND2	2:2:138:ARG:HG3	2.16	0.60
1:K:44:THR:HG23	1:z:112:HIS:NE2	2.16	0.60
1:h:37:TYR:HB3	1:h:46:GLU:HG2	1.83	0.60
1:z:38:ARG:HB3	1:z:49:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:19:THR:HG23	1:h:69:ARG:HB2	1.82	0.60
1:j:3:VAL:HG21	1:j:96:VAL:HB	1.82	0.60
2:y:62:VAL:HG11	2:y:136:ILE:HG21	1.83	0.60
2:T:47:GLN:HG2	2:T:133:SER:HB3	1.82	0.60
2:e:44:ARG:HH11	2:e:131:ARG:HH22	1.49	0.60
2:e:112:LYS:HZ1	2:g:72:THR:HA	1.66	0.60
1:u:54:ARG:HD3	1:u:72:ASP:OD2	2.01	0.60
2:y:58:ILE:HD11	2:y:126:LEU:HD11	1.83	0.60
1:5:18:LEU:HD11	1:5:70:ILE:HD12	1.83	0.60
2:r:126:LEU:HD13	2:r:132:LEU:HD11	1.84	0.60
2:y:83:ILE:HG22	2:y:131:ARG:HB2	1.84	0.60
2:G:103:ARG:HB2	2:H:112:LYS:HD2	1.82	0.60
2:f:122:GLY:HA2	2:g:59:TYR:CE2	2.37	0.60
1:R:24:LEU:HB2	1:R:64:LYS:HB3	1.84	0.60
2:x:47:GLN:HG2	2:x:133:SER:HB3	1.84	0.59
2:2:103:ARG:HG3	2:3:103:ARG:HE	1.66	0.59
1:c:2:ARG:HD2	3:c:201:GOL:H11	1.84	0.59
2:N:157:LEU:HD13	2:O:155:ILE:HD13	1.84	0.59
2:U:63:LEU:HD22	2:U:143:ASP:HB3	1.84	0.59
2:H:98:LYS:HE2	2:I:117:PRO:HD2	1.85	0.59
1:6:82:ARG:HD2	1:6:97:TYR:HB3	1.85	0.59
2:A:47:GLN:HG2	2:A:133:SER:HB3	1.83	0.59
2:H:127:GLU:HG2	1:K:89:TYR:HE2	1.68	0.59
1:Q:78:SER:OG	1:Q:104:THR:HG22	2.03	0.59
1:V:24:LEU:HB2	1:V:64:LYS:HB3	1.84	0.59
1:E:14:THR:H	1:E:106:ASN:HB2	1.67	0.59
1:L:105:VAL:HG12	1:L:106:ASN:H	1.68	0.59
1:o:36:TRP:HD1	1:o:51:LYS:CE	2.16	0.59
2:2:23:GLU:HG3	2:2:24:GLY:H	1.66	0.59
2:f:55:LEU:H	2:f:55:LEU:HD12	1.67	0.59
1:p:1:ALA:H2	1:p:25:ARG:HG3	1.68	0.59
2:U:42:GLU:HG3	2:U:49:VAL:HB	1.85	0.59
1:o:10:ILE:HG13	1:o:18:LEU:HD11	1.85	0.59
1:p:7:PRO:HG2	1:p:20:ILE:HA	1.83	0.59
2:w:2:ARG:HG2	1:z:30:ALA:HA	1.85	0.59
2:H:60:SER:HB3	2:H:80:ILE:HD11	1.84	0.58
2:M:102:GLN:HG2	2:M:102:GLN:O	2.03	0.58
1:W:7:PRO:HG2	1:W:20:ILE:HA	1.84	0.58
1:o:57:GLU:HB3	1:o:67:SER:O	2.03	0.58
2:B:80:ILE:HD12	2:B:94:LEU:HD12	1.84	0.58
1:b:18:LEU:HD23	1:b:73:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:VAL:HG12	1:L:24:LEU:HD23	1.85	0.58
1:1:8:GLN:HG2	1:1:9:THR:N	2.19	0.58
2:r:83:ILE:HD13	2:r:131:ARG:HH21	1.68	0.58
2:y:103:ARG:HG2	2:y:104:GLU:H	1.68	0.58
2:3:57:LEU:HB3	2:3:155:ILE:HG23	1.84	0.58
1:E:6:THR:OG1	1:E:7:PRO:HD3	2.03	0.58
2:m:60:SER:HB3	2:m:80:ILE:HD11	1.85	0.58
2:x:57:LEU:HB2	2:x:157:LEU:HD11	1.84	0.58
2:B:55:LEU:HD13	2:C:13:VAL:HG11	1.84	0.58
1:P:2:ARG:HG2	1:P:26:ASP:HB2	1.86	0.58
2:e:62:VAL:HG11	2:e:136:ILE:HG21	1.85	0.58
2:S:36:LEU:HD21	2:U:125:GLN:HB2	1.84	0.58
2:U:98:LYS:HE2	2:U:116:GLU:OE2	2.04	0.58
2:Y:10:ASP:CG	2:Y:11:LYS:H	2.12	0.58
2:m:58:ILE:HD12	2:m:124:PHE:HD2	1.68	0.58
2:N:58:ILE:HD11	2:N:126:LEU:HD11	1.86	0.58
1:h:2:ARG:HD2	3:h:202:GOL:H2	1.86	0.58
1:p:6:THR:OG1	1:p:7:PRO:HD3	2.04	0.58
1:K:12:LYS:O	1:K:104:THR:HA	2.03	0.57
1:6:6:THR:OG1	1:6:7:PRO:HD3	2.03	0.57
2:O:147:SER:O	2:O:149:GLN:HG3	2.04	0.57
2:S:63:LEU:HD22	2:S:143:ASP:HB3	1.87	0.57
1:z:7:PRO:HG2	1:z:20:ILE:HA	1.85	0.57
2:w:47:GLN:HG2	2:w:133:SER:HB3	1.85	0.57
2:4:83:ILE:HG23	2:4:131:ARG:HB2	1.85	0.57
1:D:18:LEU:HD23	1:D:73:LEU:HD11	1.86	0.57
1:D:54:ARG:HH21	3:D:201:GOL:H12	1.68	0.57
2:H:73:HIS:CE1	2:I:113:PRO:HG2	2.39	0.57
1:K:18:LEU:HD23	1:K:73:LEU:HD21	1.87	0.57
2:I:103:ARG:HG2	2:I:104:GLU:H	1.70	0.57
1:u:7:PRO:HG2	1:u:20:ILE:HA	1.85	0.57
2:O:74:VAL:HG23	2:O:100:PRO:HD2	1.87	0.57
2:S:102:GLN:HB3	2:T:103:ARG:HD2	1.86	0.57
1:0:40:LYS:HG2	1:0:47:GLU:OE2	2.05	0.57
1:v:73:LEU:H	1:v:73:LEU:HD23	1.69	0.57
2:O:58:ILE:HD11	2:O:126:LEU:HD11	1.87	0.57
1:R:38:ARG:HB3	1:R:49:ILE:HD11	1.85	0.57
2:e:26:LEU:HD21	2:e:28:TRP:CZ2	2.39	0.57
2:q:122:GLY:HA2	2:r:59:TYR:CE2	2.39	0.57
2:s:69:CYS:HB3	2:s:105:THR:HG22	1.86	0.57
2:T:127:GLU:HG2	1:W:89:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:80:THR:HG22	1:7:100:GLY:H	1.70	0.57
1:F:10:ILE:HB	1:F:102:VAL:HA	1.87	0.57
2:S:57:LEU:HB2	2:S:157:LEU:HD11	1.87	0.57
1:W:38:ARG:HB3	1:W:49:ILE:HD11	1.87	0.57
2:Y:112:LYS:HE2	2:a:103:ARG:HG3	1.86	0.57
1:c:54:ARG:HD2	1:c:72:ASP:OD1	2.04	0.57
2:A:103:ARG:HH12	2:B:109:ALA:H	1.53	0.56
2:s:13:VAL:HG12	2:s:155:ILE:HG13	1.86	0.56
1:0:14:THR:HG23	1:0:74:THR:HA	1.86	0.56
2:G:47:GLN:HG2	2:G:133:SER:HB3	1.86	0.56
1:i:38:ARG:HD3	1:i:49:ILE:HD11	1.87	0.56
2:m:16:VAL:HG11	2:m:43:LEU:HD12	1.86	0.56
1:E:45:ASN:HB2	1:E:47:GLU:OE2	2.05	0.56
1:V:51:LYS:HE2	1:V:57:GLU:OE2	2.04	0.56
2:k:82:ARG:HH12	2:k:126:LEU:HA	1.70	0.56
1:W:38:ARG:NH1	1:W:40:LYS:HE2	2.20	0.56
1:h:29:CYS:HA	1:h:87:CYS:HA	1.88	0.56
2:w:10:ASP:CG	2:w:11:LYS:H	2.14	0.56
2:l:30:ASN:HD22	2:l:37:LEU:HB3	1.70	0.56
2:y:63:LEU:H	2:y:150:VAL:HG12	1.70	0.56
2:A:112:LYS:HB3	2:C:73:HIS:CE1	2.41	0.56
1:c:17:SER:HA	1:c:70:ILE:O	2.05	0.56
1:E:38:ARG:HB2	1:E:49:ILE:HG12	1.87	0.56
2:Y:5:SER:HA	1:b:89:TYR:O	2.05	0.56
2:q:63:LEU:HD22	2:q:143:ASP:HB3	1.88	0.56
2:B:83:ILE:HD11	2:B:90:LYS:HE3	1.87	0.56
1:h:18:LEU:HD23	1:h:73:LEU:HD21	1.88	0.56
1:R:5:GLN:HG3	1:R:22:CYS:SG	2.46	0.56
2:Y:9:SER:HB2	1:b:91:LEU:HD11	1.87	0.56
2:Z:157:LEU:HD13	2:a:155:ILE:HD13	1.87	0.56
1:J:24:LEU:HD11	1:J:66:PHE:HE1	1.71	0.56
1:t:12:LYS:HD2	1:t:16:GLU:HG2	1.88	0.56
2:2:95:SER:HB2	2:3:149:GLN:HG2	1.87	0.55
2:A:2:ARG:N	1:D:31:THR:HG1	2.05	0.55
2:G:58:ILE:HD12	2:G:124:PHE:CD2	2.40	0.55
2:r:122:GLY:HA2	2:s:59:TYR:CE2	2.40	0.55
2:4:12:PRO:HA	2:4:39:ASN:HB2	1.89	0.55
2:A:6:ARG:HB2	1:D:89:TYR:HE1	1.70	0.55
2:f:53:GLU:HG2	2:f:128:LYS:N	2.21	0.55
1:1:7:PRO:HG2	1:1:20:ILE:HA	1.88	0.55
1:i:24:LEU:HB2	1:i:64:LYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:7:PRO:HB2	1:n:10:ILE:HD11	1.89	0.55
1:o:2:ARG:HG2	1:o:26:ASP:HB2	1.87	0.55
1:5:5:GLN:HG3	1:5:99:GLY:H	1.71	0.55
1:5:29:CYS:HA	1:5:87:CYS:HA	1.89	0.55
2:B:125:GLN:HB2	2:C:36:LEU:HD21	1.89	0.55
1:j:8:GLN:HG2	1:j:9:THR:N	2.18	0.55
1:o:73:LEU:HG	1:o:77:ASP:HB3	1.88	0.55
2:B:71:SER:HB3	2:B:104:GLU:HA	1.89	0.55
1:D:45:ASN:HB3	2:U:88:GLN:OE1	2.06	0.55
1:d:74:THR:OG1	1:d:76:GLU:HG3	2.07	0.55
2:w:93:LEU:HB3	2:w:124:PHE:CE2	2.41	0.55
1:z:29:CYS:HA	1:z:87:CYS:HA	1.89	0.55
2:I:63:LEU:HD22	2:I:143:ASP:HB3	1.88	0.55
1:p:7:PRO:HB2	1:p:10:ILE:HD11	1.89	0.55
2:2:112:LYS:HZ2	2:4:102:GLN:HG2	1.71	0.55
1:7:27:SER:HA	1:7:64:LYS:HE2	1.87	0.55
2:G:71:SER:O	2:G:74:VAL:HG13	2.07	0.55
2:2:10:ASP:CG	2:2:11:LYS:H	2.15	0.55
2:I:73:HIS:NE2	2:I:99:SER:HB2	2.21	0.55
2:I:110:GLU:HG2	2:I:111:ALA:H	1.72	0.55
2:r:62:VAL:HG11	2:r:136:ILE:HD13	1.89	0.55
2:s:55:LEU:HD11	1:t:91:LEU:HD12	1.89	0.55
1:0:89:TYR:HE2	2:x:127:GLU:HG2	1.70	0.55
1:o:22:CYS:O	1:o:65:SER:HA	2.07	0.55
1:p:31:THR:HG21	1:p:64:LYS:HA	1.88	0.55
1:d:24:LEU:HD11	1:d:66:PHE:HE1	1.73	0.54
1:i:6:THR:HG23	1:i:7:PRO:HD3	1.89	0.54
1:j:8:GLN:O	1:j:100:GLY:HA2	2.07	0.54
1:7:19:THR:HG22	1:7:69:ARG:HB2	1.88	0.54
1:L:6:THR:OG1	1:L:7:PRO:HD2	2.07	0.54
1:L:29:CYS:HA	1:L:87:CYS:HA	1.89	0.54
1:E:18:LEU:O	1:E:69:ARG:HA	2.07	0.54
2:G:9:SER:HB2	1:J:91:LEU:HD11	1.88	0.54
1:n:2:ARG:HB3	1:n:96:VAL:HG11	1.89	0.54
1:n:29:CYS:HA	1:n:87:CYS:HA	1.89	0.54
1:0:24:LEU:HB2	1:0:64:LYS:HD3	1.90	0.54
2:B:81:SER:HB2	2:B:90:LYS:HE2	1.88	0.54
1:E:13:GLU:HG2	1:E:105:VAL:O	2.07	0.54
2:m:63:LEU:N	2:m:150:VAL:HG12	2.18	0.54
2:I:10:ASP:CG	2:I:11:LYS:H	2.15	0.54
2:O:16:VAL:HG11	2:O:43:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:10:ASP:CG	2:e:11:LYS:H	2.16	0.54
2:f:71:SER:HB3	2:f:105:THR:HB	1.88	0.54
1:E:14:THR:HA	1:E:73:LEU:HB2	1.89	0.54
1:W:8:GLN:HG3	1:W:9:THR:H	1.72	0.54
1:h:7:PRO:HG2	1:h:20:ILE:HA	1.90	0.54
2:l:55:LEU:HD11	2:m:9:SER:HB3	1.89	0.54
2:a:26:LEU:HD13	2:a:142:LEU:HD11	1.90	0.54
2:e:80:ILE:HD12	2:e:94:LEU:HD12	1.89	0.54
1:i:5:GLN:HA	1:i:21:ASN:O	2.07	0.54
1:j:40:LYS:HA	1:j:79:GLY:HA2	1.90	0.54
1:5:6:THR:HB	1:5:7:PRO:HD3	1.89	0.54
2:G:103:ARG:HE	2:G:104:GLU:H	1.56	0.54
2:T:122:GLY:HA2	2:U:59:TYR:CE2	2.43	0.54
2:k:2:ARG:HB3	1:n:31:THR:H	1.72	0.54
2:2:28:TRP:HB2	2:2:43:LEU:HD11	1.90	0.54
1:i:2:ARG:HB3	1:i:96:VAL:HG11	1.90	0.54
2:A:103:ARG:NH1	2:B:109:ALA:H	2.06	0.53
2:B:81:SER:HB3	2:B:90:LYS:HG2	1.89	0.53
2:Z:60:SER:HB3	2:Z:80:ILE:HD11	1.88	0.53
2:l:62:VAL:HG12	2:l:150:VAL:HG13	1.88	0.53
1:o:12:LYS:HD3	1:o:16:GLU:HB2	1.90	0.53
1:o:36:TRP:HB2	1:o:49:ILE:HG21	1.90	0.53
2:O:12:PRO:HA	2:O:39:ASN:HB2	1.89	0.53
2:S:10:ASP:CG	2:S:11:LYS:H	2.16	0.53
1:7:56:VAL:O	1:7:68:LEU:HA	2.08	0.53
2:e:155:ILE:HD13	2:g:157:LEU:HD11	1.90	0.53
1:o:73:LEU:HB3	1:o:104:THR:HG21	1.91	0.53
2:C:23:GLU:O	2:C:25:GLN:HG2	2.09	0.53
1:W:64:LYS:HD2	2:a:110:GLU:OE2	2.08	0.53
2:f:58:ILE:HG21	2:f:80:ILE:HG21	1.89	0.53
1:X:38:ARG:HB2	1:X:49:ILE:HD11	1.90	0.53
2:I:60:SER:HB3	2:I:80:ILE:HD11	1.90	0.53
1:1:2:ARG:NH1	3:1:201:GOL:H32	2.23	0.53
2:G:127:GLU:HG2	1:L:89:TYR:HE2	1.74	0.53
2:N:122:GLY:HA2	2:O:59:TYR:CE2	2.44	0.53
1:p:18:LEU:HD11	1:p:70:ILE:HD12	1.89	0.53
2:C:30:ASN:HD22	2:C:37:LEU:HD23	1.72	0.53
1:K:70:ILE:HD11	1:K:81:TYR:HE2	1.74	0.53
1:K:78:SER:HA	1:K:102:VAL:HG23	1.91	0.53
1:P:7:PRO:HG2	1:P:20:ILE:HA	1.90	0.53
1:X:18:LEU:HD11	1:X:70:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:2:ARG:HB2	3:z:201:GOL:H11	1.90	0.53
1:0:6:THR:OG1	1:0:7:PRO:HD3	2.09	0.53
1:W:18:LEU:HD22	1:W:102:VAL:HG11	1.91	0.53
1:c:22:CYS:HB2	1:c:66:PHE:CE1	2.44	0.53
1:o:21:ASN:HA	1:o:66:PHE:O	2.09	0.53
1:P:12:LYS:O	1:P:104:THR:HA	2.09	0.53
1:W:38:ARG:HG3	1:W:39:LYS:N	2.24	0.53
1:c:1:ALA:H2	1:c:25:ARG:HD3	1.73	0.53
1:t:55:TYR:HB3	1:t:68:LEU:HD11	1.91	0.53
2:B:19:ASN:HD22	2:B:22:ALA:HB2	1.74	0.52
2:y:14:ALA:HB2	2:y:41:VAL:HG11	1.91	0.52
1:7:24:LEU:HB2	1:7:64:LYS:HG2	1.90	0.52
1:E:49:ILE:HG22	1:E:50:SER:H	1.74	0.52
1:K:5:GLN:HE21	1:K:20:ILE:HG21	1.75	0.52
1:7:49:ILE:HG23	1:7:55:TYR:CD2	2.43	0.52
2:g:19:ASN:HB3	2:g:22:ALA:HB2	1.90	0.52
2:l:42:GLU:HB2	2:l:49:VAL:HB	1.92	0.52
1:1:74:THR:OG1	1:1:76:GLU:HG2	2.09	0.52
2:3:42:GLU:HB2	2:3:49:VAL:HB	1.90	0.52
2:C:42:GLU:HG3	2:C:49:VAL:HB	1.92	0.52
2:N:87:TYR:OH	1:Q:1:ALA:HA	2.10	0.52
2:a:47:GLN:HG2	2:a:133:SER:HB3	1.90	0.52
2:e:26:LEU:HD12	2:e:142:LEU:HD11	1.91	0.52
2:e:44:ARG:NH1	2:e:131:ARG:HH22	2.07	0.52
1:7:37:TYR:HD1	1:7:48:SER:HA	1.74	0.52
1:t:55:TYR:HE1	3:t:202:GOL:H32	1.75	0.52
1:6:25:ARG:HH12	1:R:52:GLY:HA3	1.73	0.52
2:G:80:ILE:HD12	2:G:94:LEU:HD12	1.90	0.52
1:j:55:TYR:CE1	1:j:70:ILE:HG12	2.45	0.52
2:r:47:GLN:HG2	2:r:133:SER:HB3	1.90	0.52
2:y:60:SER:HB2	2:y:152:PHE:HD1	1.75	0.52
1:5:18:LEU:HD22	1:5:102:VAL:HG11	1.91	0.52
1:D:55:TYR:HD1	1:D:70:ILE:HG12	1.75	0.52
1:E:39:LYS:HE2	1:E:82:ARG:NE	2.25	0.52
1:R:18:LEU:HD23	1:R:73:LEU:HD21	1.90	0.52
1:X:1:ALA:HB1	1:X:25:ARG:HG3	1.91	0.52
2:s:9:SER:HB2	1:u:91:LEU:HD11	1.90	0.52
1:0:24:LEU:HB2	1:0:64:LYS:HB3	1.92	0.52
2:N:7:THR:HG21	1:R:90:GLY:HA3	1.92	0.52
2:O:83:ILE:CG2	2:O:131:ARG:HB2	2.40	0.52
1:R:6:THR:HB	1:R:7:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:39:LYS:O	1:i:79:GLY:HA3	2.09	0.52
2:l:111:ALA:O	2:l:112:LYS:HD2	2.10	0.52
2:r:78:HIS:HA	2:r:136:ILE:HG22	1.92	0.52
2:w:103:ARG:HG2	2:w:105:THR:H	1.74	0.52
2:x:62:VAL:HG12	2:x:150:VAL:HG13	1.91	0.52
2:4:98:LYS:HE2	2:4:116:GLU:OE1	2.10	0.52
1:5:18:LEU:HD23	1:5:73:LEU:HD21	1.92	0.52
2:N:63:LEU:HD13	2:N:117:PRO:HB3	1.92	0.52
1:d:33:SER:HB2	1:d:86:GLU:HB2	1.90	0.52
2:g:83:ILE:CG2	2:g:131:ARG:HB2	2.40	0.52
2:3:47:GLN:HG2	2:3:133:SER:HB3	1.92	0.52
2:A:55:LEU:HD11	1:F:91:LEU:HD12	1.91	0.52
1:D:6:THR:OG1	1:D:7:PRO:HD3	2.10	0.52
2:Z:29:LEU:HD13	2:Z:32:ARG:NH1	2.25	0.52
2:a:13:VAL:HG12	2:a:155:ILE:HG13	1.92	0.52
2:f:138:ARG:HH21	2:l:138:ARG:HH22	1.58	0.52
2:m:81:SER:HB2	2:m:90:LYS:HG2	1.92	0.52
2:M:53:GLU:OE2	1:R:89:TYR:CE1	2.61	0.51
1:P:29:CYS:HA	1:P:87:CYS:HA	1.91	0.51
1:p:56:VAL:HG23	1:p:69:ARG:HB3	1.92	0.51
2:w:106:PRO:HA	2:y:103:ARG:HE	1.75	0.51
2:N:44:ARG:HD3	2:N:49:VAL:HG21	1.92	0.51
1:Q:55:TYR:HD1	1:Q:70:ILE:HG12	1.75	0.51
2:U:11:LYS:HD2	2:U:156:ALA:O	2.10	0.51
1:u:66:PHE:CE2	1:u:83:CYS:HB2	2.46	0.51
1:5:55:TYR:CD1	1:5:70:ILE:HG12	2.45	0.51
1:L:31:THR:HG21	1:L:64:LYS:HA	1.91	0.51
2:M:106:PRO:HB3	2:M:109:ALA:HB3	1.92	0.51
2:T:102:GLN:HE22	2:U:101:CYS:HA	1.74	0.51
2:U:61:GLN:HB3	2:U:151:TYR:CZ	2.45	0.51
1:o:2:ARG:HD3	1:o:96:VAL:HG11	1.92	0.51
1:o:23:VAL:HA	1:o:64:LYS:O	2.10	0.51
1:E:82:ARG:HG2	1:E:99:GLY:HA2	1.92	0.51
1:P:55:TYR:HD1	1:P:70:ILE:HG12	1.75	0.51
2:e:47:GLN:HG2	2:e:133:SER:HB3	1.91	0.51
2:s:83:ILE:HG13	2:s:90:LYS:HA	1.92	0.51
1:0:14:THR:OG1	1:0:75:VAL:HG22	2.11	0.51
2:C:22:ALA:HB1	2:C:25:GLN:HG3	1.93	0.51
1:d:18:LEU:HD23	1:d:73:LEU:HD21	1.93	0.51
2:k:82:ARG:NH1	2:k:130:ASP:OD2	2.43	0.51
2:l:106:PRO:O	2:l:110:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:1:ALA:N	1:p:25:ARG:HG3	2.25	0.51
1:p:5:GLN:HG2	1:p:22:CYS:SG	2.51	0.51
2:4:60:SER:HB2	2:4:152:PHE:HD1	1.76	0.51
1:5:5:GLN:HG2	1:5:22:CYS:SG	2.51	0.51
2:T:83:ILE:HD13	2:T:131:ARG:NH2	2.26	0.51
2:2:103:ARG:HG3	2:2:104:GLU:H	1.76	0.51
1:R:8:GLN:HG3	1:R:9:THR:H	1.74	0.51
1:R:16:GLU:HG3	1:R:17:SER:H	1.74	0.51
2:A:10:ASP:CG	2:A:11:LYS:H	2.19	0.51
2:C:44:ARG:HD3	2:C:49:VAL:HG21	1.92	0.51
1:j:13:GLU:HB3	1:j:16:GLU:HG3	1.93	0.51
2:G:74:VAL:HG23	2:G:100:PRO:HD2	1.93	0.51
2:q:55:LEU:HD11	1:v:91:LEU:HD12	1.92	0.51
2:4:57:LEU:HB3	2:4:155:ILE:HG23	1.93	0.51
2:M:74:VAL:HG23	2:M:100:PRO:HD2	1.93	0.51
2:l:23:GLU:HA	2:l:144:PHE:HZ	1.76	0.51
1:R:55:TYR:HD1	1:R:70:ILE:HG12	1.75	0.50
1:V:74:THR:O	1:V:104:THR:HG21	2.11	0.50
1:n:24:LEU:HD11	1:n:66:PHE:HE1	1.75	0.50
2:y:63:LEU:HD22	2:y:143:ASP:HB3	1.92	0.50
1:5:55:TYR:HD1	1:5:70:ILE:HG12	1.76	0.50
2:A:98:LYS:HB2	2:A:118:ILE:HD11	1.93	0.50
1:0:54:ARG:HD2	1:0:72:ASP:HB2	1.92	0.50
2:2:103:ARG:CG	2:2:104:GLU:H	2.25	0.50
2:A:96:ALA:HB2	2:B:61:GLN:HE22	1.77	0.50
1:Q:12:LYS:HE2	1:Q:16:GLU:OE1	2.10	0.50
2:U:26:LEU:HD13	2:U:142:LEU:HD11	1.92	0.50
1:u:6:THR:OG1	1:u:7:PRO:HD3	2.11	0.50
2:4:83:ILE:CG2	2:4:131:ARG:HB2	2.42	0.50
1:7:31:THR:HG21	1:7:61:SER:HA	1.93	0.50
1:F:6:THR:HB	1:F:7:PRO:HD3	1.94	0.50
1:F:58:THR:O	1:F:66:PHE:HA	2.11	0.50
1:v:36:TRP:HE1	1:v:57:GLU:CD	2.19	0.50
2:G:26:LEU:HD13	2:G:142:LEU:HD11	1.92	0.50
2:I:57:LEU:HB2	2:I:157:LEU:HD11	1.93	0.50
2:a:10:ASP:CG	2:a:11:LYS:H	2.19	0.50
2:A:82:ARG:NH1	2:A:130:ASP:OD2	2.45	0.50
2:B:70:PRO:HA	2:B:105:THR:HG22	1.92	0.50
2:B:95:SER:HB3	2:C:149:GLN:HG2	1.94	0.50
1:c:1:ALA:N	1:c:25:ARG:HD3	2.26	0.50
2:k:63:LEU:HD11	2:m:97:ILE:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:31:THR:HG22	1:0:59:VAL:HG23	1.93	0.50
2:A:103:ARG:HD2	2:B:112:LYS:NZ	2.26	0.50
1:j:36:TRP:HB3	1:j:49:ILE:HD12	1.94	0.50
1:1:16:GLU:O	1:1:72:ASP:HA	2.12	0.50
2:U:87:TYR:OH	1:V:1:ALA:HA	2.12	0.50
2:Y:98:LYS:HE2	2:Y:116:GLU:OE2	2.12	0.50
1:d:35:TYR:HB2	1:d:84:ALA:HB3	1.94	0.50
1:i:5:GLN:OE1	1:i:100:GLY:HA3	2.11	0.50
2:m:57:LEU:O	2:m:154:ILE:HA	2.12	0.50
1:t:84:ALA:HA	1:t:96:VAL:O	2.11	0.50
2:2:59:TYR:CE2	2:4:122:GLY:HA2	2.47	0.50
1:J:38:ARG:HB2	1:J:49:ILE:HD11	1.94	0.50
2:N:60:SER:HB3	2:N:80:ILE:HD11	1.94	0.50
2:f:28:TRP:HB2	2:f:43:LEU:HD21	1.94	0.50
1:h:1:ALA:C	1:h:3:VAL:H	2.20	0.50
1:D:7:PRO:HG2	1:D:20:ILE:HA	1.93	0.49
2:I:42:GLU:HB2	2:I:49:VAL:HB	1.94	0.49
2:I:62:VAL:HG11	2:I:136:ILE:HG21	1.94	0.49
2:g:83:ILE:HG23	2:g:131:ARG:HB2	1.94	0.49
2:2:23:GLU:HG3	2:2:24:GLY:N	2.26	0.49
1:7:14:THR:OG1	1:7:75:VAL:HG22	2.11	0.49
2:G:60:SER:HB3	2:G:80:ILE:HD11	1.93	0.49
2:U:16:VAL:HG11	2:U:43:LEU:HD12	1.93	0.49
1:d:56:VAL:HG23	1:d:69:ARG:HB3	1.94	0.49
1:Q:39:LYS:HB2	1:Q:46:GLU:HG2	1.93	0.49
1:V:66:PHE:HE2	1:V:83:CYS:HB2	1.77	0.49
1:W:23:VAL:HG22	1:W:65:SER:HB3	1.95	0.49
2:Z:103:ARG:HG2	2:Z:106:PRO:HG3	1.94	0.49
2:l:72:THR:HG23	2:l:74:VAL:HG13	1.93	0.49
1:o:10:ILE:HB	1:o:102:VAL:HA	1.95	0.49
2:y:19:ASN:HB3	2:y:22:ALA:HB2	1.94	0.49
1:K:55:TYR:HD1	1:K:70:ILE:HG12	1.77	0.49
1:K:66:PHE:HE1	1:K:83:CYS:HB2	1.77	0.49
2:O:62:VAL:HG23	2:O:78:HIS:CE1	2.47	0.49
2:U:62:VAL:HG11	2:U:136:ILE:HD13	1.94	0.49
2:Z:19:ASN:HB3	2:Z:22:ALA:HB2	1.93	0.49
1:i:23:VAL:HG22	1:i:65:SER:HB3	1.95	0.49
1:6:71:ASN:O	1:6:72:ASP:C	2.54	0.49
1:K:6:THR:OG1	1:K:7:PRO:HD3	2.12	0.49
2:S:151:TYR:CZ	2:U:94:LEU:HD22	2.48	0.49
2:Z:63:LEU:H	2:Z:150:VAL:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:47:GLN:HG2	2:l:133:SER:HB3	1.95	0.49
2:q:26:LEU:HD11	2:q:28:TRP:CZ2	2.46	0.49
2:e:112:LYS:HG3	2:g:73:HIS:NE2	2.27	0.49
1:h:6:THR:CG2	1:h:7:PRO:HD3	2.38	0.49
1:i:14:THR:OG1	1:i:106:ASN:HA	2.13	0.49
1:j:2:ARG:HD3	1:j:96:VAL:HG12	1.93	0.49
2:k:13:VAL:HG11	2:m:55:LEU:HD21	1.94	0.49
2:k:63:LEU:HD22	2:k:143:ASP:HB3	1.94	0.49
1:o:7:PRO:HG2	1:o:20:ILE:HG23	1.95	0.49
2:4:57:LEU:HB2	2:4:157:LEU:HD11	1.94	0.49
2:G:125:GLN:HB2	2:H:36:LEU:HD21	1.95	0.49
2:H:125:GLN:HB2	2:I:36:LEU:HD21	1.95	0.49
1:R:12:LYS:HE2	1:R:16:GLU:HG2	1.95	0.49
2:a:42:GLU:HB2	2:a:49:VAL:HB	1.94	0.49
2:a:94:LEU:HB2	2:a:120:LEU:HD23	1.94	0.49
2:s:12:PRO:HA	2:s:39:ASN:HB2	1.95	0.49
1:v:6:THR:OG1	1:v:7:PRO:HD3	2.12	0.49
1:1:7:PRO:HG2	1:1:20:ILE:HG12	1.94	0.49
2:2:5:SER:HB3	1:5:89:TYR:O	2.11	0.49
2:H:57:LEU:HB2	2:H:157:LEU:HD11	1.94	0.49
1:Q:36:TRP:CZ3	1:Q:83:CYS:HB3	2.47	0.49
1:W:6:THR:OG1	1:W:7:PRO:HD3	2.13	0.49
2:l:73:HIS:NE2	2:m:112:LYS:HE3	2.27	0.49
1:p:39:LYS:HB2	1:p:46:GLU:HG2	1.93	0.49
1:0:66:PHE:HE2	1:0:83:CYS:HB2	1.78	0.49
1:7:58:THR:O	1:7:66:PHE:HA	2.13	0.49
2:M:62:VAL:HG21	2:M:136:ILE:HG21	1.93	0.49
2:M:101:CYS:SG	2:M:104:GLU:HB2	2.53	0.49
2:k:82:ARG:HD3	2:k:93:LEU:HD21	1.95	0.49
2:k:93:LEU:HB3	2:k:124:PHE:CZ	2.47	0.49
2:s:60:SER:HB3	2:s:152:PHE:HD1	1.76	0.49
2:2:104:GLU:HB2	2:4:103:ARG:HH22	1.78	0.48
2:A:157:LEU:HD13	2:B:155:ILE:HG12	1.95	0.48
2:B:123:VAL:HG21	2:C:155:ILE:HG21	1.93	0.48
2:H:103:ARG:HH21	2:H:112:LYS:HZ1	1.61	0.48
1:P:35:TYR:HB2	1:P:84:ALA:HB3	1.95	0.48
2:r:125:GLN:HB2	2:s:36:LEU:HD21	1.95	0.48
1:0:80:THR:HG23	1:0:101:THR:OG1	2.14	0.48
2:3:103:ARG:CG	2:3:104:GLU:H	2.23	0.48
2:I:64:PHE:HE2	2:I:118:ILE:HD12	1.78	0.48
1:i:13:GLU:HB3	1:i:16:GLU:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:CYS:HA	1:D:87:CYS:HA	1.95	0.48
1:L:5:GLN:HG2	1:L:6:THR:O	2.13	0.48
2:O:47:GLN:HG2	2:O:133:SER:HB3	1.95	0.48
1:W:39:LYS:HZ3	1:W:44:THR:HA	1.78	0.48
2:k:2:ARG:HB2	1:n:31:THR:HG22	1.96	0.48
2:m:103:ARG:HG2	2:m:104:GLU:H	1.78	0.48
2:q:58:ILE:HD12	2:q:124:PHE:CD2	2.37	0.48
2:2:26:LEU:HG	2:2:142:LEU:HD11	1.95	0.48
2:B:65:LYS:HB3	2:B:143:ASP:HB2	1.95	0.48
2:H:64:PHE:CE1	2:H:76:LEU:HD12	2.49	0.48
1:K:80:THR:HG23	1:K:101:THR:OG1	2.13	0.48
2:O:5:SER:HB3	1:Q:89:TYR:CE1	2.48	0.48
2:e:106:PRO:HB3	2:e:109:ALA:HB3	1.95	0.48
1:i:3:VAL:HG22	1:i:24:LEU:HD23	1.95	0.48
1:j:55:TYR:HA	1:j:69:ARG:O	2.13	0.48
1:t:35:TYR:HB2	1:t:84:ALA:HB3	1.95	0.48
1:u:1:ALA:N	1:u:25:ARG:HD2	2.29	0.48
2:x:44:ARG:HD2	2:x:49:VAL:HG21	1.95	0.48
2:2:69:CYS:O	2:2:106:PRO:HD2	2.13	0.48
2:I:94:LEU:HB2	2:I:120:LEU:HD23	1.95	0.48
1:p:5:GLN:NE2	1:p:82:ARG:HA	2.29	0.48
1:l:5:GLN:HG2	1:l:83:CYS:SG	2.53	0.48
1:7:105:VAL:HG12	1:7:106:ASN:H	1.79	0.48
2:G:112:LYS:HE3	2:I:103:ARG:NE	2.28	0.48
2:M:151:TYR:CZ	2:O:94:LEU:HD22	2.47	0.48
2:Y:49:VAL:HG22	2:Y:131:ARG:HD3	1.95	0.48
1:o:40:LYS:HD3	1:o:47:GLU:OE2	2.14	0.48
1:t:83:CYS:O	1:t:97:TYR:HA	2.14	0.48
1:v:18:LEU:HD22	1:v:102:VAL:HG21	1.94	0.48
2:A:109:ALA:HB3	2:C:103:ARG:HD2	1.96	0.48
1:c:39:LYS:HD2	1:c:44:THR:HA	1.96	0.48
2:y:69:CYS:HB3	2:y:105:THR:HG22	1.95	0.48
1:7:19:THR:HA	1:7:69:ARG:HA	1.96	0.48
2:B:57:LEU:O	2:B:154:ILE:HA	2.13	0.48
1:R:3:VAL:HG22	1:R:24:LEU:HD23	1.96	0.48
2:Y:82:ARG:NH1	2:Y:130:ASP:OD2	2.46	0.48
2:A:55:LEU:HD13	2:B:10:ASP:OD2	2.14	0.48
2:M:82:ARG:NH1	2:M:130:ASP:OD2	2.47	0.48
2:M:146:GLU:HB2	2:M:149:GLN:CD	2.38	0.48
2:e:147:SER:O	2:e:149:GLN:N	2.47	0.48
2:f:53:GLU:HG2	2:f:128:LYS:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:12:LYS:O	1:o:104:THR:HA	2.13	0.48
2:A:60:SER:HB3	2:A:80:ILE:HD11	1.96	0.48
2:G:110:GLU:HB3	2:G:112:LYS:HZ2	1.78	0.48
2:S:102:GLN:O	2:S:104:GLU:HG2	2.14	0.48
1:V:24:LEU:HD11	1:V:66:PHE:HE1	1.78	0.48
2:m:26:LEU:HD22	2:m:136:ILE:HG12	1.95	0.48
2:w:49:VAL:HG22	2:w:131:ARG:HG2	1.96	0.48
2:B:53:GLU:OE2	2:C:6:ARG:HB3	2.13	0.47
1:E:36:TRP:CE2	1:E:68:LEU:HB2	2.49	0.47
1:F:3:VAL:HG12	1:F:96:VAL:HG12	1.96	0.47
1:J:18:LEU:HD23	1:J:73:LEU:HD21	1.96	0.47
1:L:10:ILE:HB	1:L:102:VAL:HG12	1.96	0.47
1:V:18:LEU:HD22	1:V:102:VAL:HG11	1.96	0.47
1:W:38:ARG:HH11	1:W:40:LYS:HG2	1.79	0.47
1:X:5:GLN:HG2	1:X:22:CYS:SG	2.54	0.47
1:7:56:VAL:O	1:7:68:LEU:HD12	2.13	0.47
1:W:33:SER:HB2	1:W:86:GLU:HB2	1.96	0.47
2:e:82:ARG:HB2	2:e:93:LEU:HD11	1.96	0.47
2:k:110:GLU:H	2:k:112:LYS:HE2	1.78	0.47
1:o:49:ILE:HG23	1:o:51:LYS:NZ	2.29	0.47
2:q:72:THR:HG23	2:q:73:HIS:ND1	2.28	0.47
2:w:103:ARG:HG2	2:w:105:THR:N	2.27	0.47
2:2:23:GLU:CG	2:2:24:GLY:H	2.24	0.47
1:F:22:CYS:HB2	1:F:66:PHE:CE2	2.49	0.47
2:e:62:VAL:HG13	2:e:142:LEU:HD21	1.96	0.47
2:g:94:LEU:HB2	2:g:120:LEU:HD23	1.95	0.47
2:C:11:LYS:O	2:C:13:VAL:HG13	2.14	0.47
2:C:74:VAL:O	2:C:100:PRO:HD2	2.14	0.47
1:F:75:VAL:HA	1:F:104:THR:HB	1.95	0.47
1:J:21:ASN:ND2	1:J:67:SER:HB3	2.28	0.47
1:c:3:VAL:HA	1:c:23:VAL:O	2.14	0.47
2:m:10:ASP:CG	2:m:11:LYS:H	2.22	0.47
2:q:10:ASP:CG	2:q:11:LYS:H	2.23	0.47
2:r:127:GLU:HG2	1:u:89:TYR:HE2	1.80	0.47
2:2:104:GLU:O	2:2:105:THR:C	2.57	0.47
1:D:31:THR:HB	1:D:59:VAL:HG21	1.97	0.47
1:E:41:SER:OG	1:E:79:GLY:HA2	2.15	0.47
1:n:74:THR:O	1:n:104:THR:HG21	2.14	0.47
2:4:41:VAL:HG22	2:4:51:PRO:HD3	1.96	0.47
1:F:54:ARG:HB3	1:F:70:ILE:HD12	1.96	0.47
1:L:54:ARG:O	1:L:70:ILE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:94:LEU:HB2	2:m:120:LEU:HD23	1.96	0.47
2:q:147:SER:HB3	2:s:92:ASN:HB2	1.96	0.47
2:r:60:SER:HB3	2:r:80:ILE:HD11	1.96	0.47
1:0:66:PHE:CE2	1:0:83:CYS:HB2	2.49	0.47
2:3:90:LYS:HE2	2:3:90:LYS:HB3	1.68	0.47
2:C:57:LEU:HB2	2:C:157:LEU:HD11	1.95	0.47
1:E:14:THR:HB	1:E:106:ASN:CG	2.40	0.47
1:L:5:GLN:HG3	1:L:99:GLY:O	2.15	0.47
1:Q:38:ARG:HG3	1:Q:81:TYR:CZ	2.50	0.47
2:S:6:ARG:HB2	1:V:89:TYR:CE1	2.50	0.47
2:T:110:GLU:HB3	2:T:111:ALA:H	1.53	0.47
2:U:58:ILE:HD13	2:U:132:LEU:HD11	1.97	0.47
2:Y:112:LYS:HD3	2:a:73:HIS:NE2	2.30	0.47
1:b:7:PRO:HB2	1:b:10:ILE:HD11	1.96	0.47
1:d:6:THR:OG1	1:d:7:PRO:HD3	2.15	0.47
2:f:82:ARG:HD2	2:f:93:LEU:HD11	1.95	0.47
2:s:67:GLN:HG3	2:s:111:ALA:HB1	1.96	0.47
2:x:146:GLU:HB2	2:x:149:GLN:NE2	2.30	0.47
1:z:6:THR:OG1	1:z:7:PRO:HD3	2.14	0.47
1:D:12:LYS:O	1:D:104:THR:HA	2.15	0.47
1:P:6:THR:OG1	1:P:7:PRO:HD3	2.14	0.47
2:Y:7:THR:HG23	2:Y:8:PRO:HD2	1.97	0.47
2:f:93:LEU:HB3	2:f:124:PHE:CZ	2.49	0.47
2:2:76:LEU:CD2	2:2:100:PRO:HB3	2.44	0.47
2:A:127:GLU:HG2	2:A:128:LYS:H	1.80	0.47
2:C:48:LEU:HD13	2:C:152:PHE:CE2	2.49	0.47
2:M:7:THR:HG23	2:M:8:PRO:HD2	1.96	0.47
2:M:10:ASP:CG	2:M:11:LYS:H	2.23	0.47
2:M:49:VAL:HG22	2:M:131:ARG:HG2	1.96	0.47
2:O:106:PRO:HB2	2:O:109:ALA:HB3	1.95	0.47
2:Z:96:ALA:HB2	2:a:61:GLN:HE22	1.79	0.47
2:Z:146:GLU:HB2	2:Z:149:GLN:NE2	2.29	0.47
2:e:103:ARG:O	2:e:104:GLU:HB3	2.14	0.47
1:j:18:LEU:HG	1:j:70:ILE:HD12	1.96	0.47
1:W:84:ALA:HA	1:W:96:VAL:O	2.15	0.47
2:e:72:THR:HG23	2:e:103:ARG:HA	1.97	0.47
2:x:70:PRO:HB2	2:x:72:THR:HG22	1.97	0.47
1:6:39:LYS:HD2	1:6:46:GLU:HG2	1.97	0.46
2:H:96:ALA:HB2	2:H:120:LEU:HD21	1.96	0.46
1:1:24:LEU:HB3	1:1:64:LYS:HG2	1.97	0.46
1:F:56:VAL:O	1:F:68:LEU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:96:ALA:HB2	2:3:61:GLN:HE22	1.79	0.46
2:3:11:LYS:HB2	2:3:12:PRO:HD2	1.97	0.46
2:B:71:SER:H	2:B:105:THR:HG23	1.80	0.46
2:S:127:GLU:HG2	1:X:89:TYR:HE2	1.79	0.46
1:p:2:ARG:O	1:p:3:VAL:HB	2.14	0.46
2:x:62:VAL:HA	2:x:150:VAL:HG22	1.98	0.46
2:A:58:ILE:HD11	2:A:126:LEU:HD11	1.96	0.46
2:I:73:HIS:CE1	2:I:99:SER:HB2	2.50	0.46
1:j:15:GLY:H	1:j:73:LEU:HB3	1.80	0.46
1:o:49:ILE:HG23	1:o:51:LYS:HZ1	1.81	0.46
1:p:5:GLN:HG3	1:p:99:GLY:H	1.80	0.46
2:q:104:GLU:OE2	2:s:102:GLN:O	2.33	0.46
2:q:146:GLU:O	2:q:149:GLN:HG3	2.16	0.46
2:I:85:VAL:HA	2:I:88:GLN:NE2	2.30	0.46
2:S:55:LEU:HD13	2:T:10:ASP:OD2	2.16	0.46
1:j:70:ILE:HG22	1:j:71:ASN:N	2.31	0.46
2:l:106:PRO:HG2	2:l:112:LYS:HG2	1.98	0.46
2:m:60:SER:HB2	2:m:152:PHE:HD1	1.80	0.46
1:Q:37:TYR:HD1	1:Q:48:SER:HA	1.81	0.46
2:U:62:VAL:HG11	2:U:136:ILE:HG21	1.97	0.46
2:f:5:SER:HA	1:i:89:TYR:CD1	2.50	0.46
2:f:63:LEU:HD13	2:f:117:PRO:HB3	1.97	0.46
2:x:26:LEU:HD13	2:x:142:LEU:HD11	1.97	0.46
2:y:63:LEU:H	2:y:150:VAL:CG1	2.28	0.46
1:7:40:LYS:HD3	1:7:47:GLU:OE2	2.15	0.46
1:D:9:THR:HG22	1:D:101:THR:HG22	1.98	0.46
2:G:22:ALA:HB1	2:G:25:GLN:HG3	1.98	0.46
2:Y:70:PRO:HA	2:Y:105:THR:HG23	1.98	0.46
2:g:55:LEU:HD11	1:h:91:LEU:HD12	1.98	0.46
1:j:58:THR:HB	1:j:67:SER:HB3	1.97	0.46
1:7:9:THR:HA	1:7:101:THR:HB	1.98	0.46
1:J:37:TYR:HE2	1:J:97:TYR:HE1	1.64	0.46
2:T:49:VAL:HG22	2:T:131:ARG:HG2	1.97	0.46
2:Y:23:GLU:HA	2:Y:144:PHE:HZ	1.81	0.46
1:d:39:LYS:HE3	1:d:44:THR:HA	1.97	0.46
1:j:68:LEU:HD23	1:j:81:TYR:CE1	2.46	0.46
1:o:4:ASP:O	1:o:22:CYS:HA	2.16	0.46
2:2:60:SER:HB2	2:2:152:PHE:HD1	1.81	0.46
2:B:14:ALA:HB2	2:B:41:VAL:HG11	1.98	0.46
2:U:12:PRO:HA	2:U:39:ASN:HB2	1.97	0.46
2:x:57:LEU:HB3	2:x:155:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:31:THR:HB	1:z:59:VAL:CG2	2.46	0.46
2:H:83:ILE:HD13	2:H:131:ARG:NH2	2.31	0.46
2:Y:74:VAL:HG21	2:Y:101:CYS:HB2	1.98	0.46
1:u:57:GLU:HG3	1:u:67:SER:O	2.16	0.46
2:A:151:TYR:CZ	2:C:94:LEU:HD22	2.51	0.45
1:F:73:LEU:HD22	1:F:77:ASP:CG	2.41	0.45
1:J:24:LEU:HD23	1:J:29:CYS:HB2	1.98	0.45
2:T:9:SER:HA	1:X:91:LEU:HD11	1.98	0.45
1:V:29:CYS:HA	1:V:87:CYS:HA	1.99	0.45
2:Z:122:GLY:HA2	2:a:59:TYR:CE2	2.51	0.45
2:g:33:ALA:HA	1:j:94:TYR:CD2	2.52	0.45
2:m:58:ILE:HD12	2:m:124:PHE:CD2	2.49	0.45
1:u:10:ILE:HD11	1:u:102:VAL:HG22	1.98	0.45
1:v:16:GLU:O	1:v:71:ASN:HA	2.16	0.45
1:v:22:CYS:HB2	1:v:66:PHE:CE1	2.51	0.45
2:w:100:PRO:HB3	2:w:116:GLU:HG3	1.98	0.45
2:2:104:GLU:HB2	2:4:103:ARG:NH2	2.31	0.45
2:3:83:ILE:HD11	2:3:131:ARG:CZ	2.46	0.45
1:7:38:ARG:HB2	1:7:81:TYR:CD1	2.50	0.45
2:a:62:VAL:HG11	2:a:136:ILE:HG21	1.98	0.45
2:l:55:LEU:HD12	2:l:55:LEU:H	1.82	0.45
1:n:36:TRP:CE2	1:n:68:LEU:HB2	2.51	0.45
1:o:68:LEU:HD23	1:o:70:ILE:HD11	1.96	0.45
2:r:55:LEU:HD23	2:s:13:VAL:HG11	1.98	0.45
2:w:105:THR:O	2:w:107:GLU:HB2	2.16	0.45
1:z:55:TYR:HD1	1:z:70:ILE:HG12	1.80	0.45
2:3:30:ASN:HD22	2:3:37:LEU:HD23	1.82	0.45
1:5:14:THR:OG1	1:5:106:ASN:HA	2.16	0.45
2:N:92:ASN:HB2	2:O:147:SER:OG	2.16	0.45
2:O:63:LEU:HD22	2:O:143:ASP:HB3	1.98	0.45
1:o:5:GLN:HG2	1:o:7:PRO:HD2	1.98	0.45
1:u:47:GLU:H	1:u:47:GLU:HG2	1.64	0.45
2:w:22:ALA:HB1	2:w:25:GLN:HG3	1.97	0.45
1:0:38:ARG:HD3	1:0:40:LYS:HD3	1.98	0.45
1:5:36:TRP:CZ3	1:5:83:CYS:HB3	2.51	0.45
2:Z:102:GLN:HG2	2:a:102:GLN:HE21	1.82	0.45
1:d:7:PRO:HG2	1:d:20:ILE:HG12	1.99	0.45
2:e:83:ILE:CG2	2:e:131:ARG:HB2	2.46	0.45
2:k:62:VAL:HG13	2:k:142:LEU:HD21	1.97	0.45
2:l:126:LEU:HD13	2:l:132:LEU:HD11	1.97	0.45
1:o:6:THR:OG1	1:o:7:PRO:HD3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:35:TYR:HB2	1:u:84:ALA:HB3	1.99	0.45
1:5:5:GLN:HE21	1:5:5:GLN:HB3	1.54	0.45
1:6:18:LEU:HD23	1:6:70:ILE:HD12	1.99	0.45
2:C:44:ARG:HB3	2:C:45:ASP:H	1.67	0.45
1:E:36:TRP:CZ3	1:E:83:CYS:HB3	2.51	0.45
2:G:58:ILE:HD12	2:G:124:PHE:HD2	1.81	0.45
2:H:65:LYS:HA	2:H:114:TRP:O	2.16	0.45
1:c:71:ASN:O	1:c:72:ASP:C	2.60	0.45
1:d:7:PRO:HG2	1:d:20:ILE:HA	1.99	0.45
2:k:58:ILE:HD12	2:k:124:PHE:HD2	1.81	0.45
2:3:53:GLU:HA	2:3:126:LEU:O	2.17	0.45
1:P:59:VAL:HG12	1:P:66:PHE:HB3	1.97	0.45
2:s:60:SER:HB3	2:s:152:PHE:CD1	2.52	0.45
1:u:1:ALA:H1	1:u:25:ARG:HD2	1.82	0.45
2:2:103:ARG:HE	2:2:104:GLU:N	2.15	0.45
2:f:56:TYR:CD2	2:f:154:ILE:HD12	2.52	0.45
2:g:23:GLU:O	2:g:23:GLU:HG2	2.17	0.45
1:u:20:ILE:O	1:u:67:SER:HA	2.17	0.45
1:1:18:LEU:HD11	1:1:70:ILE:HD12	1.98	0.45
2:B:58:ILE:HG21	2:B:80:ILE:HG21	1.99	0.45
2:M:57:LEU:O	2:M:154:ILE:HA	2.17	0.45
2:N:98:LYS:HE2	2:N:116:GLU:OE2	2.16	0.45
1:P:26:ASP:HB3	1:P:29:CYS:SG	2.57	0.45
2:S:58:ILE:O	2:S:121:GLY:HA2	2.17	0.45
2:T:58:ILE:HG21	2:T:80:ILE:HG21	1.98	0.45
1:V:38:ARG:HB3	1:V:49:ILE:HD11	1.97	0.45
2:Y:122:GLY:HA2	2:Z:59:TYR:CE2	2.51	0.45
1:i:18:LEU:HD22	1:i:102:VAL:HG11	1.98	0.45
2:m:58:ILE:O	2:m:121:GLY:HA2	2.16	0.45
1:F:38:ARG:HH12	1:F:40:LYS:NZ	2.15	0.45
1:F:80:THR:HG22	1:F:101:THR:HG22	1.99	0.45
2:G:69:CYS:HB2	2:G:106:PRO:HD3	1.98	0.45
2:O:103:ARG:HE	2:O:104:GLU:H	1.65	0.45
2:a:58:ILE:O	2:a:121:GLY:HA2	2.17	0.45
1:b:7:PRO:HG2	1:b:20:ILE:HA	1.99	0.45
2:l:5:SER:HA	1:p:89:TYR:HE1	1.81	0.45
2:q:82:ARG:HD3	2:q:93:LEU:HD21	1.99	0.45
1:v:16:GLU:H	1:v:73:LEU:HD21	1.82	0.45
1:0:39:LYS:HB2	1:0:46:GLU:HG2	1.99	0.45
2:2:62:VAL:HG11	2:2:136:ILE:HG21	1.99	0.45
2:2:80:ILE:HD12	2:2:94:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:ARG:NE	1:F:71:ASN:HB2	2.23	0.45
2:N:55:LEU:HD13	2:O:13:VAL:HG11	1.98	0.45
1:Q:108:ALA:HA	1:Q:110:HIS:CE1	2.52	0.45
2:a:30:ASN:HD22	2:a:37:LEU:HD23	1.82	0.45
1:b:2:ARG:O	1:b:3:VAL:HB	2.16	0.45
2:e:87:TYR:HE1	1:i:1:ALA:H2	1.65	0.45
1:j:56:VAL:O	1:j:68:LEU:HA	2.16	0.45
2:q:102:GLN:O	2:q:103:ARG:HB3	2.17	0.45
2:3:126:LEU:HD13	2:3:132:LEU:HD11	1.99	0.44
1:K:5:GLN:NE2	1:K:20:ILE:HG21	2.31	0.44
2:N:82:ARG:NE	2:N:84:ALA:HB2	2.32	0.44
2:Y:60:SER:HB3	2:Y:80:ILE:HD11	1.99	0.44
1:b:2:ARG:HG2	1:b:96:VAL:HG11	2.00	0.44
2:m:20:PRO:HA	2:m:144:PHE:CD1	2.53	0.44
1:p:6:THR:OG1	1:p:21:ASN:HB2	2.17	0.44
1:z:19:THR:HG23	1:z:69:ARG:HB2	1.98	0.44
1:E:57:GLU:HG3	1:E:67:SER:O	2.17	0.44
2:G:22:ALA:O	2:G:25:GLN:HG2	2.17	0.44
2:H:56:TYR:CD2	2:H:154:ILE:HD12	2.53	0.44
2:H:70:PRO:HB2	2:H:72:THR:HG22	1.98	0.44
1:J:30:ALA:HA	3:J:201:GOL:H2	1.99	0.44
2:N:56:TYR:CD2	2:N:154:ILE:HD12	2.52	0.44
1:Q:10:ILE:HD11	1:Q:102:VAL:HG22	1.98	0.44
1:Q:18:LEU:HD23	1:Q:73:LEU:HD21	1.99	0.44
2:T:61:GLN:HB2	2:T:119:TYR:HD1	1.82	0.44
1:c:2:ARG:O	1:c:3:VAL:HG22	2.16	0.44
2:g:87:TYR:HE1	1:h:1:ALA:HB3	1.83	0.44
2:k:110:GLU:HG2	2:k:111:ALA:H	1.82	0.44
2:2:76:LEU:HD13	2:2:100:PRO:HG3	1.99	0.44
1:J:38:ARG:HG3	1:J:81:TYR:CZ	2.52	0.44
1:R:56:VAL:HG23	1:R:69:ARG:HB3	1.97	0.44
2:m:147:SER:O	2:m:149:GLN:HG3	2.16	0.44
1:o:18:LEU:HD22	1:o:20:ILE:HG12	2.00	0.44
2:x:123:VAL:HG21	2:y:155:ILE:HG21	2.00	0.44
2:2:31:ARG:CZ	1:D:23:VAL:HG21	2.47	0.44
2:3:27:GLN:HA	2:3:46:ASN:HD21	1.81	0.44
2:3:63:LEU:HD13	2:3:117:PRO:HB3	1.98	0.44
1:7:5:GLN:HG2	1:7:22:CYS:SG	2.57	0.44
1:7:19:THR:HB	1:7:67:SER:OG	2.16	0.44
1:7:37:TYR:CD1	1:7:48:SER:HA	2.52	0.44
2:A:105:THR:O	2:A:106:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:HD23	2:B:144:PHE:HD2	1.81	0.44
1:Q:38:ARG:HB2	1:Q:49:ILE:HD11	2.00	0.44
1:X:36:TRP:CZ3	1:X:83:CYS:HB3	2.52	0.44
2:e:151:TYR:CZ	2:g:94:LEU:HD22	2.52	0.44
1:5:31:THR:HG21	1:5:64:LYS:HA	1.98	0.44
1:7:58:THR:HB	1:7:67:SER:HB3	1.99	0.44
1:J:6:THR:OG1	1:J:7:PRO:HD3	2.17	0.44
2:N:44:ARG:NH1	2:N:131:ARG:HD3	2.33	0.44
1:W:26:ASP:HB3	1:W:29:CYS:SG	2.58	0.44
1:d:74:THR:O	1:d:104:THR:HG21	2.17	0.44
2:f:60:SER:HB3	2:f:80:ILE:HD11	2.00	0.44
2:l:87:TYR:CE2	2:l:89:THR:HB	2.53	0.44
1:o:33:SER:OG	1:o:86:GLU:HG3	2.18	0.44
2:s:10:ASP:CG	2:s:11:LYS:H	2.25	0.44
1:v:54:ARG:HD3	1:v:72:ASP:H	1.82	0.44
1:z:16:GLU:HG2	1:z:17:SER:H	1.82	0.44
1:0:36:TRP:CZ3	1:0:83:CYS:HB3	2.52	0.44
2:2:41:VAL:O	1:D:58:THR:HG23	2.18	0.44
2:G:94:LEU:HB2	2:G:120:LEU:HD23	1.98	0.44
1:L:18:LEU:HD21	1:L:73:LEU:HD13	1.99	0.44
1:R:33:SER:HB2	1:R:86:GLU:HB2	2.00	0.44
1:u:111:HIS:HB2	1:u:112:HIS:H	1.68	0.44
1:5:24:LEU:HD12	1:5:31:THR:HG22	2.00	0.44
2:I:58:ILE:O	2:I:121:GLY:HA2	2.17	0.44
1:P:13:GLU:HG2	1:P:14:THR:N	2.33	0.44
2:U:94:LEU:HB2	2:U:120:LEU:HD23	2.00	0.44
2:Y:59:TYR:CE2	2:a:122:GLY:HA2	2.53	0.44
2:a:58:ILE:HD12	2:a:124:PHE:CD2	2.52	0.44
1:b:3:VAL:HG22	1:b:24:LEU:HD23	1.99	0.44
2:l:58:ILE:HG12	2:l:154:ILE:HG22	1.99	0.44
1:o:20:ILE:HD12	1:o:68:LEU:HD23	1.99	0.44
1:o:36:TRP:CZ3	1:o:83:CYS:HB2	2.53	0.44
1:o:71:ASN:O	1:o:73:LEU:HD12	2.18	0.44
2:w:63:LEU:HD22	2:w:143:ASP:HB3	1.99	0.44
2:y:157:LEU:OXT	2:y:157:LEU:HD12	2.17	0.44
2:N:126:LEU:HD13	2:N:132:LEU:HD11	2.00	0.44
1:R:2:ARG:HG2	1:R:26:ASP:HB2	1.99	0.44
2:U:75:LEU:HD23	2:U:75:LEU:HA	1.87	0.44
1:b:36:TRP:CZ3	1:b:83:CYS:HB3	2.52	0.44
2:f:87:TYR:CZ	2:f:89:THR:HB	2.53	0.44
1:u:18:LEU:HD11	1:u:70:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:84:ALA:HA	1:u:96:VAL:O	2.18	0.44
2:w:57:LEU:O	2:w:154:ILE:HA	2.18	0.44
2:2:94:LEU:HD22	2:3:151:TYR:CZ	2.53	0.44
2:2:103:ARG:CG	2:3:103:ARG:HE	2.28	0.44
2:3:17:VAL:HG23	2:3:150:VAL:O	2.17	0.44
2:A:43:LEU:HB3	1:V:60:ASN:HD22	1.83	0.44
2:A:77:THR:HG22	2:A:97:ILE:HG12	1.99	0.44
1:V:84:ALA:HA	1:V:96:VAL:O	2.17	0.44
2:a:83:ILE:CG2	2:a:131:ARG:HB2	2.48	0.44
2:e:6:ARG:HH11	1:h:89:TYR:HE1	1.64	0.44
1:h:31:THR:HG21	1:h:64:LYS:HA	2.00	0.44
1:i:38:ARG:HG2	1:i:47:GLU:HG3	2.00	0.44
1:i:84:ALA:HA	1:i:96:VAL:O	2.17	0.44
2:k:72:THR:HG21	2:k:103:ARG:HD2	2.00	0.44
2:m:103:ARG:CG	2:m:104:GLU:H	2.30	0.44
1:V:31:THR:HG23	1:V:64:LYS:HD3	2.00	0.43
2:a:9:SER:HB2	1:c:91:LEU:HD11	1.99	0.43
1:0:27:SER:HA	1:0:64:LYS:NZ	2.33	0.43
2:2:16:VAL:HG23	2:2:28:TRP:CE3	2.54	0.43
1:5:5:GLN:OE1	1:5:82:ARG:HA	2.18	0.43
2:A:6:ARG:HB2	1:D:89:TYR:CE1	2.52	0.43
1:J:84:ALA:HA	1:J:96:VAL:O	2.18	0.43
1:R:51:LYS:O	1:R:51:LYS:HG3	2.17	0.43
2:Z:55:LEU:CD2	2:a:13:VAL:HG11	2.48	0.43
1:c:40:LYS:HE3	1:c:76:GLU:OE2	2.18	0.43
2:f:50:VAL:HG13	2:f:56:TYR:CZ	2.53	0.43
1:j:3:VAL:HG22	1:j:24:LEU:HD23	1.99	0.43
1:o:59:VAL:HA	1:o:66:PHE:HA	2.00	0.43
2:r:58:ILE:HG21	2:r:80:ILE:HG21	2.00	0.43
1:0:16:GLU:H	1:0:73:LEU:HB3	1.82	0.43
1:1:7:PRO:CG	1:1:20:ILE:HA	2.48	0.43
2:2:83:ILE:CG2	2:2:131:ARG:HB2	2.47	0.43
1:J:6:THR:HG1	1:J:7:PRO:HD3	1.83	0.43
2:O:127:GLU:HG2	1:P:89:TYR:HE2	1.83	0.43
1:P:19:THR:HG23	1:P:69:ARG:HB2	1.99	0.43
1:R:59:VAL:HG12	1:R:66:PHE:HB3	1.99	0.43
2:Z:125:GLN:HB2	2:a:36:LEU:HD21	2.00	0.43
2:f:11:LYS:HB2	2:f:12:PRO:HD2	2.00	0.43
2:g:58:ILE:HD12	2:g:124:PHE:CD2	2.52	0.43
1:i:29:CYS:HA	1:i:87:CYS:HA	2.00	0.43
2:k:122:GLY:HA2	2:l:59:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:10:ILE:HD12	1:p:102:VAL:HG12	1.99	0.43
2:y:58:ILE:O	2:y:121:GLY:HA2	2.17	0.43
2:2:75:LEU:O	2:2:137:ASN:ND2	2.51	0.43
1:5:3:VAL:HG22	1:5:24:LEU:HD23	2.00	0.43
2:C:13:VAL:HG12	2:C:155:ILE:HG13	2.01	0.43
1:E:12:LYS:HE3	1:E:17:SER:C	2.43	0.43
2:I:26:LEU:HB2	2:I:142:LEU:HD11	2.01	0.43
1:L:18:LEU:HD22	1:L:73:LEU:HD22	2.00	0.43
1:P:24:LEU:HB2	1:P:64:LYS:HB3	2.00	0.43
2:S:142:LEU:HD23	2:S:142:LEU:HA	1.82	0.43
2:Y:28:TRP:HB2	2:Y:43:LEU:HD21	2.00	0.43
2:Y:74:VAL:HG23	2:Y:100:PRO:HD2	2.00	0.43
2:g:31:ARG:HG3	1:j:94:TYR:HA	2.01	0.43
2:k:44:ARG:O	2:k:47:GLN:HB2	2.18	0.43
2:k:82:ARG:NH1	2:k:126:LEU:HA	2.33	0.43
2:l:58:ILE:HG21	2:l:80:ILE:HG21	2.00	0.43
2:s:11:LYS:O	2:s:13:VAL:HG13	2.19	0.43
1:t:24:LEU:HD22	1:t:29:CYS:HB2	2.00	0.43
1:z:36:TRP:CZ3	1:z:83:CYS:HB3	2.53	0.43
1:0:18:LEU:HD11	1:0:70:ILE:HD12	2.00	0.43
2:A:102:GLN:O	2:A:104:GLU:HG2	2.18	0.43
2:G:57:LEU:HB3	2:G:155:ILE:HG23	2.00	0.43
2:M:26:LEU:HD21	2:M:28:TRP:CZ2	2.53	0.43
1:Q:80:THR:HG22	1:Q:101:THR:OG1	2.17	0.43
1:i:6:THR:CG2	1:i:7:PRO:HD3	2.48	0.43
1:i:22:CYS:HB2	1:i:66:PHE:CE1	2.53	0.43
1:i:55:TYR:HD1	1:i:70:ILE:HG12	1.83	0.43
1:o:7:PRO:HG3	1:o:18:LEU:HD21	2.01	0.43
2:q:26:LEU:HD11	2:q:28:TRP:CE2	2.53	0.43
2:r:125:GLN:HE22	1:u:90:GLY:H	1.66	0.43
1:5:11:THR:HG22	1:5:103:VAL:HG22	2.01	0.43
2:A:83:ILE:HG23	2:A:131:ARG:HB2	2.01	0.43
1:J:6:THR:HB	1:z:86:GLU:HG2	2.01	0.43
2:N:100:PRO:HB3	2:N:116:GLU:HG3	2.00	0.43
1:R:84:ALA:HA	1:R:96:VAL:O	2.17	0.43
2:U:79:THR:HG23	2:U:135:GLU:HG3	2.01	0.43
2:a:57:LEU:O	2:a:154:ILE:HA	2.19	0.43
2:f:138:ARG:NH2	2:l:138:ARG:HH22	2.15	0.43
1:n:40:LYS:HB2	1:n:40:LYS:HE3	1.63	0.43
1:u:75:VAL:HG21	1:u:106:ASN:ND2	2.34	0.43
1:1:6:THR:HB	1:1:7:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ILE:O	2:B:121:GLY:HA2	2.18	0.43
1:F:20:ILE:O	1:F:67:SER:HA	2.19	0.43
2:H:44:ARG:HH22	2:H:131:ARG:HD3	1.83	0.43
1:X:19:THR:HG22	1:X:69:ARG:HD3	2.00	0.43
2:e:26:LEU:HD23	2:e:26:LEU:C	2.43	0.43
1:o:30:ALA:C	1:o:32:SER:H	2.26	0.43
1:p:78:SER:HA	1:p:102:VAL:HG23	2.00	0.43
1:z:35:TYR:HB2	1:z:84:ALA:HB3	2.00	0.43
2:2:78:HIS:ND1	2:2:120:LEU:HD13	2.34	0.43
2:4:58:ILE:HG21	2:4:80:ILE:HG21	2.01	0.43
1:7:54:ARG:HH21	1:7:74:THR:HG23	1.83	0.43
2:B:79:THR:HG23	2:B:135:GLU:HG3	1.99	0.43
2:G:10:ASP:CG	2:G:11:LYS:H	2.27	0.43
2:I:74:VAL:O	2:I:100:PRO:HD2	2.18	0.43
2:N:16:VAL:HG22	2:N:152:PHE:O	2.18	0.43
1:c:12:LYS:O	1:c:104:THR:HA	2.19	0.43
2:s:16:VAL:HG11	2:s:43:LEU:HD12	2.01	0.43
1:1:2:ARG:HG2	1:1:26:ASP:HB2	2.00	0.43
1:7:36:TRP:CE3	1:7:68:LEU:HD22	2.54	0.43
1:F:79:GLY:H	1:F:102:VAL:HG13	1.84	0.43
2:S:5:SER:HA	1:V:89:TYR:O	2.19	0.43
2:S:58:ILE:HG21	2:S:80:ILE:HG21	2.01	0.43
1:d:7:PRO:HD2	1:d:20:ILE:HG23	2.01	0.43
2:f:55:LEU:HD11	2:g:9:SER:OG	2.18	0.43
2:g:53:GLU:OE2	1:h:89:TYR:CE2	2.71	0.43
2:g:157:LEU:H	2:g:157:LEU:HD23	1.84	0.43
2:k:20:PRO:HG3	2:k:32:ARG:NH2	2.34	0.43
2:k:105:THR:O	2:k:106:PRO:C	2.61	0.43
2:l:5:SER:HA	1:p:89:TYR:CE1	2.53	0.43
2:2:60:SER:HB2	2:2:152:PHE:CD1	2.54	0.43
2:A:125:GLN:HB2	2:B:36:LEU:HD21	2.00	0.43
2:B:112:LYS:HE3	2:B:112:LYS:HB2	1.71	0.43
2:Y:26:LEU:HD21	2:Y:28:TRP:CZ2	2.54	0.43
2:a:39:ASN:H	1:p:111:HIS:HB2	1.84	0.43
2:g:58:ILE:O	2:g:121:GLY:HA2	2.19	0.43
2:m:55:LEU:HD11	1:n:91:LEU:HD12	2.00	0.43
2:s:77:THR:HG22	2:s:137:ASN:HB3	2.01	0.43
1:t:37:TYR:HD1	1:t:48:SER:HA	1.83	0.43
1:7:54:ARG:NH2	1:7:72:ASP:HB3	2.34	0.42
2:B:92:ASN:HB2	2:C:147:SER:CB	2.49	0.42
2:C:19:ASN:HB3	2:C:22:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:PHE:HE2	1:D:83:CYS:HB2	1.84	0.42
2:I:16:VAL:HG11	2:I:43:LEU:HD12	2.01	0.42
1:L:83:CYS:O	1:L:97:TYR:HA	2.19	0.42
2:M:30:ASN:OD1	2:M:31:ARG:HG2	2.19	0.42
2:N:14:ALA:HB2	2:N:41:VAL:HG11	2.01	0.42
2:T:76:LEU:HD13	2:T:100:PRO:HG3	2.00	0.42
2:T:157:LEU:HD13	2:U:155:ILE:HD13	2.01	0.42
1:V:36:TRP:CE2	1:V:68:LEU:HB2	2.54	0.42
2:s:93:LEU:HB3	2:s:124:PHE:CZ	2.54	0.42
1:u:3:VAL:HA	1:u:23:VAL:O	2.19	0.42
1:v:38:ARG:HH22	1:v:79:GLY:H	1.66	0.42
2:x:63:LEU:HD13	2:x:117:PRO:HB3	2.01	0.42
2:x:71:SER:OG	2:x:105:THR:HG22	2.19	0.42
1:6:55:TYR:HD1	1:6:70:ILE:HG12	1.84	0.42
2:C:58:ILE:O	2:C:121:GLY:HA2	2.19	0.42
1:J:59:VAL:HG22	2:w:42:GLU:HG2	2.02	0.42
2:S:58:ILE:HG22	2:S:80:ILE:HD13	2.00	0.42
2:Y:58:ILE:O	2:Y:121:GLY:HA2	2.19	0.42
2:a:22:ALA:HB1	2:a:25:GLN:CG	2.47	0.42
1:o:40:LYS:HB2	1:o:47:GLU:OE2	2.19	0.42
1:0:12:LYS:O	1:0:104:THR:HG23	2.19	0.42
2:2:57:LEU:HB3	2:2:155:ILE:HG23	2.00	0.42
2:2:63:LEU:HD11	2:4:97:ILE:H	1.84	0.42
1:E:12:LYS:O	1:E:104:THR:HA	2.18	0.42
1:J:55:TYR:HD1	1:J:70:ILE:HG12	1.85	0.42
1:Q:5:GLN:HE22	1:Q:82:ARG:HA	1.83	0.42
1:Q:16:GLU:O	1:Q:73:LEU:HD13	2.19	0.42
2:Y:142:LEU:HD23	2:Y:142:LEU:HA	1.73	0.42
2:q:42:GLU:HB2	2:q:49:VAL:HB	2.00	0.42
2:r:146:GLU:HB2	2:r:149:GLN:CD	2.44	0.42
2:A:42:GLU:HG2	1:V:59:VAL:H	1.83	0.42
2:A:44:ARG:HH11	2:A:131:ARG:NH2	2.17	0.42
2:G:69:CYS:O	2:G:106:PRO:HD2	2.19	0.42
2:I:126:LEU:HD13	2:I:132:LEU:HD11	2.00	0.42
2:k:142:LEU:HD23	2:k:142:LEU:HA	1.85	0.42
1:p:7:PRO:HG2	1:p:20:ILE:HG12	2.00	0.42
2:r:63:LEU:H	2:r:150:VAL:HG22	1.85	0.42
2:r:80:ILE:HD12	2:r:94:LEU:HD12	2.00	0.42
2:y:50:VAL:HG21	2:y:126:LEU:HD13	2.01	0.42
2:2:31:ARG:NH1	1:D:23:VAL:HG21	2.34	0.42
2:B:137:ASN:ND2	2:B:138:ARG:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:103:ARG:HE	2:G:104:GLU:N	2.17	0.42
2:Y:71:SER:O	2:Y:74:VAL:HG13	2.19	0.42
1:i:6:THR:HG22	1:i:21:ASN:HB2	2.02	0.42
2:l:57:LEU:CB	2:l:157:LEU:HD11	2.44	0.42
2:m:29:LEU:HD22	2:m:32:ARG:HG2	2.01	0.42
1:o:12:LYS:HG3	1:o:104:THR:HG22	2.01	0.42
2:r:26:LEU:HD13	2:r:142:LEU:HD21	2.02	0.42
2:y:23:GLU:O	2:y:23:GLU:HG2	2.19	0.42
1:l:31:THR:HG22	1:l:66:PHE:HD2	1.84	0.42
2:2:12:PRO:HA	2:2:39:ASN:HB2	2.02	0.42
1:6:55:TYR:CD1	1:6:70:ILE:HG12	2.55	0.42
2:G:63:LEU:HD22	2:G:143:ASP:HB3	2.01	0.42
1:J:14:THR:HG23	1:J:105:VAL:O	2.20	0.42
1:L:38:ARG:HG3	1:L:81:TYR:CZ	2.55	0.42
2:S:62:VAL:HG13	2:S:142:LEU:HD21	2.02	0.42
1:b:56:VAL:HG23	1:b:69:ARG:HB3	2.01	0.42
2:k:57:LEU:HB2	2:k:157:LEU:HD11	2.01	0.42
2:m:83:ILE:HG22	2:m:131:ARG:HB2	2.01	0.42
2:q:20:PRO:HG3	2:q:32:ARG:HH22	1.85	0.42
1:0:8:GLN:HG3	1:0:9:THR:N	2.31	0.42
1:0:71:ASN:O	1:0:72:ASP:C	2.62	0.42
2:3:26:LEU:HD13	2:3:142:LEU:HD21	2.01	0.42
2:3:57:LEU:O	2:3:154:ILE:HA	2.19	0.42
1:F:35:TYR:HB2	1:F:84:ALA:HB3	2.00	0.42
2:H:110:GLU:O	2:H:111:ALA:C	2.62	0.42
1:L:84:ALA:HA	1:L:96:VAL:O	2.20	0.42
2:N:47:GLN:HG2	2:N:133:SER:HB3	2.01	0.42
1:R:7:PRO:HD3	1:R:21:ASN:OD1	2.20	0.42
1:i:3:VAL:HA	1:i:23:VAL:O	2.19	0.42
1:i:24:LEU:HD22	1:i:29:CYS:HB2	2.02	0.42
1:F:37:TYR:HA	1:F:47:GLU:O	2.20	0.42
1:R:6:THR:HB	1:R:21:ASN:OD1	2.19	0.42
2:Y:47:GLN:HG3	2:Y:133:SER:HB3	2.01	0.42
2:Y:125:GLN:HB2	2:Z:36:LEU:HD21	2.02	0.42
1:c:13:GLU:CD	1:c:13:GLU:H	2.27	0.42
1:t:29:CYS:HA	1:t:87:CYS:HA	2.02	0.42
1:u:17:SER:HA	1:u:70:ILE:O	2.20	0.42
2:x:16:VAL:HG11	2:x:43:LEU:HD12	2.02	0.42
2:A:58:ILE:HG23	2:A:154:ILE:HG22	2.02	0.42
1:D:56:VAL:HG23	1:D:69:ARG:HB3	2.01	0.42
1:F:55:TYR:HD2	1:F:68:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:146:GLU:HB2	2:Z:149:GLN:HE21	1.84	0.42
1:c:55:TYR:CD1	1:c:70:ILE:HG12	2.55	0.42
2:e:93:LEU:HB3	2:e:124:PHE:CE2	2.54	0.42
2:r:71:SER:HB3	2:r:105:THR:HG21	2.01	0.42
2:2:112:LYS:NZ	2:4:102:GLN:HG2	2.34	0.42
1:7:71:ASN:O	1:7:72:ASP:C	2.63	0.42
2:A:13:VAL:HB	2:A:155:ILE:HD13	2.01	0.42
2:G:126:LEU:HD13	2:G:132:LEU:HD11	2.02	0.42
1:L:2:ARG:HD2	1:L:96:VAL:HG11	2.02	0.42
2:M:22:ALA:HB1	2:M:25:GLN:HG2	2.02	0.42
2:g:61:GLN:HB2	2:g:119:TYR:HD1	1.84	0.42
2:m:29:LEU:HD23	2:m:30:ASN:H	1.85	0.42
1:p:82:ARG:HG2	1:p:99:GLY:HA2	2.01	0.42
1:1:10:ILE:HG22	1:1:12:LYS:HG2	2.02	0.41
1:7:70:ILE:CG2	1:7:73:LEU:HD13	2.49	0.41
1:K:36:TRP:CZ3	1:K:83:CYS:HB3	2.55	0.41
2:N:57:LEU:O	2:N:154:ILE:HA	2.19	0.41
1:i:3:VAL:CG2	1:i:24:LEU:HD23	2.50	0.41
2:x:20:PRO:HA	2:x:144:PHE:CD1	2.55	0.41
1:z:49:ILE:HG23	1:z:55:TYR:CD2	2.55	0.41
1:E:26:ASP:OD2	1:E:28:HIS:HB2	2.20	0.41
1:F:12:LYS:HG3	1:F:18:LEU:HD12	2.02	0.41
2:I:23:GLU:H	2:I:23:GLU:CD	2.28	0.41
2:M:30:ASN:HD22	2:M:37:LEU:HB3	1.85	0.41
2:T:62:VAL:HG12	2:T:150:VAL:HG13	2.02	0.41
2:U:70:PRO:HB2	2:U:71:SER:H	1.71	0.41
1:W:36:TRP:CZ3	1:W:83:CYS:HB3	2.55	0.41
2:g:56:TYR:CE2	2:g:156:ALA:HB2	2.54	0.41
1:h:84:ALA:HA	1:h:96:VAL:O	2.20	0.41
1:j:73:LEU:HD12	1:j:73:LEU:HA	1.94	0.41
2:m:13:VAL:HG12	2:m:155:ILE:HG13	2.03	0.41
2:m:33:ALA:HA	1:o:94:TYR:CD1	2.55	0.41
2:3:87:TYR:CE2	2:3:89:THR:HB	2.54	0.41
2:4:47:GLN:HG2	2:4:133:SER:HB3	2.01	0.41
1:E:4:ASP:HB2	1:E:23:VAL:HB	2.03	0.41
1:E:5:GLN:HG2	1:E:99:GLY:O	2.20	0.41
1:Q:33:SER:HB2	1:Q:86:GLU:HB2	2.03	0.41
2:Y:58:ILE:HD12	2:Y:124:PHE:CD2	2.49	0.41
2:a:75:LEU:HD23	2:a:75:LEU:HA	1.89	0.41
1:c:10:ILE:HD11	1:c:102:VAL:HG22	2.02	0.41
2:k:12:PRO:HA	2:k:39:ASN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:63:LEU:HD12	2:m:96:ALA:HA	2.01	0.41
2:k:83:ILE:CG1	2:k:131:ARG:HB2	2.51	0.41
1:p:38:ARG:HB3	1:p:49:ILE:HD11	2.03	0.41
2:q:58:ILE:HG21	2:q:80:ILE:HG21	2.01	0.41
2:r:19:ASN:HB3	2:r:22:ALA:HB2	2.02	0.41
2:w:103:ARG:H	2:w:103:ARG:HD3	1.84	0.41
2:x:56:TYR:CD2	2:x:154:ILE:HD12	2.55	0.41
1:z:89:TYR:CG	1:z:90:GLY:N	2.89	0.41
2:3:80:ILE:HD12	2:3:94:LEU:HD12	2.02	0.41
2:4:20:PRO:HA	2:4:144:PHE:CD1	2.55	0.41
2:B:126:LEU:CD1	2:B:132:LEU:HD11	2.50	0.41
2:C:102:GLN:O	2:C:103:ARG:C	2.63	0.41
2:H:87:TYR:OH	1:K:1:ALA:HA	2.21	0.41
2:N:112:LYS:HA	2:N:112:LYS:HD3	1.77	0.41
2:e:26:LEU:HD23	2:e:26:LEU:O	2.20	0.41
1:n:78:SER:OG	1:n:104:THR:HG22	2.21	0.41
2:r:31:ARG:HA	1:v:94:TYR:HA	2.02	0.41
1:F:11:THR:HA	1:F:103:VAL:O	2.20	0.41
2:H:125:GLN:OE1	1:K:90:GLY:HA3	2.21	0.41
2:U:60:SER:HB2	2:U:152:PHE:HD1	1.86	0.41
2:Y:75:LEU:HD12	2:Y:75:LEU:HA	1.86	0.41
2:Y:138:ARG:HA	2:Y:138:ARG:HD2	1.92	0.41
2:l:136:ILE:CD1	2:l:142:LEU:HD11	2.41	0.41
1:u:40:LYS:HD3	1:u:76:GLU:O	2.20	0.41
2:G:59:TYR:CE2	2:I:122:GLY:HA2	2.55	0.41
2:H:66:GLY:O	2:H:113:PRO:HA	2.21	0.41
1:J:24:LEU:HB2	1:J:64:LYS:HB3	2.03	0.41
1:P:31:THR:HG21	1:P:64:LYS:HA	2.03	0.41
1:d:36:TRP:CH2	1:d:83:CYS:HB3	2.56	0.41
2:l:90:LYS:HE2	2:l:90:LYS:HB3	1.83	0.41
2:2:20:PRO:HA	2:2:144:PHE:CD1	2.56	0.41
2:4:85:VAL:HA	2:4:88:GLN:NE2	2.36	0.41
1:7:5:GLN:CD	1:7:99:GLY:H	2.28	0.41
2:G:87:TYR:CE2	2:G:89:THR:HB	2.55	0.41
2:M:76:LEU:HD13	2:M:76:LEU:HA	1.93	0.41
2:M:127:GLU:OE2	1:R:28:HIS:NE2	2.48	0.41
2:S:36:LEU:HD22	2:U:55:LEU:HD21	2.03	0.41
1:V:16:GLU:HB3	1:V:17:SER:H	1.77	0.41
1:V:66:PHE:CE2	1:V:83:CYS:HB2	2.55	0.41
2:a:146:GLU:HB2	2:a:149:GLN:CD	2.46	0.41
2:e:142:LEU:HD23	2:e:142:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:24:LEU:HD23	1:n:29:CYS:HB2	2.01	0.41
1:o:81:TYR:O	1:o:82:ARG:C	2.63	0.41
1:u:55:TYR:HB3	1:u:68:LEU:HD11	2.02	0.41
2:w:58:ILE:HG22	2:w:80:ILE:HD13	2.02	0.41
2:w:72:THR:OG1	2:x:112:LYS:HE2	2.19	0.41
1:1:39:LYS:HG2	1:1:80:THR:HB	2.03	0.41
2:2:122:GLY:HA2	2:3:59:TYR:CE2	2.55	0.41
2:3:75:LEU:HD23	2:3:75:LEU:HA	1.91	0.41
1:D:3:VAL:HA	1:D:23:VAL:O	2.21	0.41
1:K:74:THR:O	1:K:104:THR:HG21	2.21	0.41
2:M:58:ILE:HG22	2:M:80:ILE:HD13	2.03	0.41
2:T:16:VAL:HG22	2:T:152:PHE:O	2.21	0.41
2:T:57:LEU:HB3	2:T:155:ILE:HG23	2.02	0.41
2:U:93:LEU:HB3	2:U:124:PHE:CZ	2.55	0.41
2:e:58:ILE:HG21	2:e:80:ILE:HG21	2.03	0.41
2:k:2:ARG:N	1:n:32:SER:HG	2.18	0.41
2:w:26:LEU:HG	2:w:142:LEU:HD11	2.03	0.41
2:3:106:PRO:HB2	2:3:110:GLU:HA	2.03	0.41
1:5:38:ARG:HB2	1:5:49:ILE:HD11	2.02	0.41
1:E:56:VAL:O	1:E:68:LEU:HD12	2.21	0.41
2:G:142:LEU:HD23	2:G:142:LEU:HA	1.92	0.41
1:K:17:SER:HA	1:K:73:LEU:HD13	2.03	0.41
2:M:67:GLN:HG2	2:M:113:PRO:HB3	2.03	0.41
2:S:112:LYS:HD2	2:U:73:HIS:NE2	2.35	0.41
2:T:157:LEU:CD1	2:U:155:ILE:HD13	2.51	0.41
1:c:51:LYS:HE3	1:c:57:GLU:HB3	2.02	0.41
2:g:60:SER:HB3	2:g:80:ILE:HD11	2.03	0.41
2:q:50:VAL:HG21	2:q:126:LEU:HD13	2.03	0.41
2:q:60:SER:HB3	2:q:80:ILE:HD11	2.03	0.41
1:u:38:ARG:O	1:u:47:GLU:HG2	2.21	0.41
2:x:103:ARG:HB3	2:x:106:PRO:HG3	2.02	0.41
2:y:68:GLY:O	2:y:70:PRO:HD3	2.21	0.41
1:L:18:LEU:HD23	1:L:18:LEU:H	1.84	0.41
1:Q:56:VAL:HG23	1:Q:69:ARG:HB3	2.02	0.41
2:e:107:GLU:HG3	2:e:108:GLY:N	2.36	0.41
2:e:147:SER:O	2:e:149:GLN:HG3	2.21	0.41
1:i:7:PRO:HB2	1:i:10:ILE:HD11	2.03	0.41
2:k:96:ALA:HA	2:l:63:LEU:HD12	2.02	0.41
2:k:97:ILE:H	2:l:63:LEU:HD11	1.85	0.41
2:q:59:TYR:CE2	2:s:122:GLY:HA2	2.55	0.41
1:t:8:GLN:HG2	1:t:9:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:90:GLY:HA3	2:x:125:GLN:HE22	1.85	0.40
2:G:5:SER:HA	1:J:89:TYR:O	2.21	0.40
1:P:66:PHE:CE2	1:P:83:CYS:HB2	2.57	0.40
2:T:75:LEU:HD23	2:T:75:LEU:HA	1.87	0.40
2:U:41:VAL:HG22	2:U:51:PRO:HD3	2.03	0.40
1:V:78:SER:OG	1:V:104:THR:HG22	2.22	0.40
2:g:60:SER:HB2	2:g:152:PHE:HD1	1.86	0.40
2:l:66:GLY:O	2:l:113:PRO:HA	2.21	0.40
2:r:92:ASN:HB2	2:s:147:SER:OG	2.21	0.40
2:r:112:LYS:HE3	2:r:112:LYS:HB2	1.75	0.40
2:w:19:ASN:OD1	2:w:21:GLN:HG2	2.21	0.40
2:x:65:LYS:HB3	2:x:143:ASP:HB2	2.03	0.40
2:y:58:ILE:HG12	2:y:154:ILE:HG22	2.04	0.40
2:2:65:LYS:HA	2:2:114:TRP:O	2.21	0.40
2:3:103:ARG:HG2	2:3:104:GLU:N	2.25	0.40
1:6:12:LYS:HA	1:6:12:LYS:HD2	1.88	0.40
1:7:39:LYS:HB2	1:7:79:GLY:HA3	2.02	0.40
2:B:68:GLY:HA2	2:B:111:ALA:O	2.22	0.40
2:G:48:LEU:HD23	2:G:48:LEU:HA	1.94	0.40
1:L:13:GLU:OE1	1:L:105:VAL:HB	2.21	0.40
2:T:26:LEU:HD13	2:T:142:LEU:HD11	2.03	0.40
2:g:23:GLU:CD	2:g:23:GLU:H	2.28	0.40
2:k:102:GLN:O	2:k:104:GLU:HG2	2.20	0.40
1:p:4:ASP:HB2	1:p:23:VAL:HG23	2.04	0.40
1:p:71:ASN:O	1:p:72:ASP:C	2.64	0.40
2:s:47:GLN:HG2	2:s:133:SER:HB3	2.01	0.40
2:s:56:TYR:CD2	2:s:154:ILE:HD12	2.56	0.40
1:v:78:SER:OG	1:v:103:VAL:HA	2.21	0.40
1:1:8:GLN:HG2	1:1:9:THR:HG23	2.03	0.40
1:5:37:TYR:HD1	1:5:48:SER:HA	1.86	0.40
1:7:38:ARG:HD3	1:7:49:ILE:HD11	2.03	0.40
2:A:106:PRO:HA	2:C:103:ARG:NH1	2.37	0.40
1:F:73:LEU:HD12	1:F:73:LEU:O	2.20	0.40
2:H:62:VAL:HG21	2:H:136:ILE:HG21	2.02	0.40
2:M:75:LEU:HD12	2:M:75:LEU:HA	1.87	0.40
1:R:23:VAL:HG22	1:R:65:SER:HB3	2.03	0.40
2:S:87:TYR:CE1	1:X:1:ALA:HB3	2.45	0.40
2:U:74:VAL:HG11	2:U:141:TYR:HE2	1.86	0.40
1:W:10:ILE:HD11	1:W:102:VAL:HG22	2.04	0.40
1:W:71:ASN:O	1:W:72:ASP:C	2.64	0.40
2:Y:62:VAL:HG23	2:Y:78:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:71:ASN:O	1:j:72:ASP:C	2.64	0.40
1:j:74:THR:O	1:j:104:THR:HG21	2.21	0.40
2:l:157:LEU:HD22	2:m:155:ILE:HD13	2.02	0.40
1:n:36:TRP:CZ2	1:n:68:LEU:HB2	2.56	0.40
1:u:4:ASP:HB2	1:u:23:VAL:HG13	2.02	0.40
1:u:7:PRO:CG	1:u:20:ILE:HA	2.51	0.40
1:0:57:GLU:HG3	1:0:67:SER:O	2.22	0.40
2:3:157:LEU:HD13	2:4:155:ILE:HG12	2.02	0.40
2:4:26:LEU:HD13	2:4:142:LEU:HD11	2.03	0.40
2:U:74:VAL:O	2:U:100:PRO:HD2	2.21	0.40
2:Z:103:ARG:HG2	2:Z:106:PRO:HD3	2.04	0.40
2:l:62:VAL:HA	2:l:150:VAL:HG22	2.03	0.40
2:m:110:GLU:CD	2:m:110:GLU:H	2.29	0.40
2:A:67:GLN:O	2:A:111:ALA:HB1	2.22	0.40
2:A:103:ARG:HD3	2:B:106:PRO:HB3	2.04	0.40
2:C:80:ILE:HD12	2:C:94:LEU:HD12	2.03	0.40
2:G:75:LEU:HD12	2:G:75:LEU:HA	1.96	0.40
2:H:96:ALA:HB2	2:I:61:GLN:HE22	1.87	0.40
2:N:67:GLN:OE1	2:N:111:ALA:HA	2.20	0.40
2:U:80:ILE:HD12	2:U:94:LEU:HD12	2.02	0.40
2:Y:83:ILE:HD11	2:Y:90:LYS:HE2	2.04	0.40
2:Z:112:LYS:HE3	2:Z:112:LYS:HB2	1.73	0.40
2:e:36:LEU:HD21	2:g:125:GLN:HB2	2.03	0.40
2:f:51:PRO:HD2	2:f:56:TYR:OH	2.20	0.40
1:u:80:THR:HG22	1:u:101:THR:OG1	2.20	0.40
1:v:5:GLN:HG3	1:v:99:GLY:O	2.21	0.40
1:z:2:ARG:H	1:z:25:ARG:HB2	1.87	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 X-ray entries followed by that with respect to entries of similar resolution.

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	0	105/129 (81%)	91 (87%)	13 (12%)	1 (1%)	12	42
1	1	102/129 (79%)	89 (87%)	12 (12%)	1 (1%)	12	42
1	5	106/129 (82%)	93 (88%)	11 (10%)	2 (2%)	6	30
1	6	105/129 (81%)	91 (87%)	10 (10%)	4 (4%)	2	18
1	7	105/129 (81%)	88 (84%)	16 (15%)	1 (1%)	12	42
1	D	104/129 (81%)	93 (89%)	7 (7%)	4 (4%)	2	18
1	E	106/129 (82%)	89 (84%)	14 (13%)	3 (3%)	4	24
1	F	104/129 (81%)	83 (80%)	16 (15%)	5 (5%)	2	14
1	J	106/129 (82%)	95 (90%)	9 (8%)	2 (2%)	6	30
1	K	104/129 (81%)	89 (86%)	13 (12%)	2 (2%)	6	30
1	L	110/129 (85%)	93 (84%)	14 (13%)	3 (3%)	4	24
1	P	105/129 (81%)	90 (86%)	11 (10%)	4 (4%)	2	18
1	Q	110/129 (85%)	91 (83%)	17 (16%)	2 (2%)	6	31
1	R	105/129 (81%)	92 (88%)	10 (10%)	3 (3%)	3	23
1	V	105/129 (81%)	93 (89%)	10 (10%)	2 (2%)	6	30
1	W	104/129 (81%)	94 (90%)	9 (9%)	1 (1%)	12	42
1	X	105/129 (81%)	90 (86%)	13 (12%)	2 (2%)	6	30
1	b	110/129 (85%)	95 (86%)	13 (12%)	2 (2%)	6	31
1	c	110/129 (85%)	92 (84%)	14 (13%)	4 (4%)	2	19
1	d	110/129 (85%)	92 (84%)	16 (14%)	2 (2%)	6	31
1	h	110/129 (85%)	97 (88%)	11 (10%)	2 (2%)	6	31
1	i	110/129 (85%)	93 (84%)	15 (14%)	2 (2%)	6	31
1	j	103/129 (80%)	88 (85%)	13 (13%)	2 (2%)	6	30
1	n	107/129 (83%)	93 (87%)	11 (10%)	3 (3%)	4	24
1	o	102/129 (79%)	73 (72%)	27 (26%)	2 (2%)	6	29
1	p	110/129 (85%)	95 (86%)	13 (12%)	2 (2%)	6	31
1	t	110/129 (85%)	95 (86%)	11 (10%)	4 (4%)	2	19
1	u	110/129 (85%)	93 (84%)	14 (13%)	3 (3%)	4	24
1	v	103/129 (80%)	92 (89%)	11 (11%)	0	100	100
1	z	110/129 (85%)	94 (86%)	11 (10%)	5 (4%)	2	15
2	2	152/156 (97%)	123 (81%)	21 (14%)	8 (5%)	1	12
2	3	148/156 (95%)	126 (85%)	21 (14%)	1 (1%)	18	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4	153/156 (98%)	131 (86%)	19 (12%)	3 (2%)	6	29
2	A	154/156 (99%)	132 (86%)	16 (10%)	6 (4%)	2	18
2	B	151/156 (97%)	127 (84%)	23 (15%)	1 (1%)	18	50
2	C	151/156 (97%)	120 (80%)	24 (16%)	7 (5%)	2	15
2	G	151/156 (97%)	129 (85%)	17 (11%)	5 (3%)	3	21
2	H	150/156 (96%)	125 (83%)	23 (15%)	2 (1%)	9	37
2	I	150/156 (96%)	127 (85%)	20 (13%)	3 (2%)	6	29
2	M	151/156 (97%)	126 (83%)	21 (14%)	4 (3%)	4	25
2	N	151/156 (97%)	135 (89%)	15 (10%)	1 (1%)	18	50
2	O	151/156 (97%)	134 (89%)	12 (8%)	5 (3%)	3	21
2	S	152/156 (97%)	122 (80%)	22 (14%)	8 (5%)	1	12
2	T	154/156 (99%)	135 (88%)	18 (12%)	1 (1%)	21	52
2	U	148/156 (95%)	131 (88%)	14 (10%)	3 (2%)	6	29
2	Y	151/156 (97%)	126 (83%)	20 (13%)	5 (3%)	3	21
2	Z	150/156 (96%)	128 (85%)	19 (13%)	3 (2%)	6	29
2	a	152/156 (97%)	133 (88%)	18 (12%)	1 (1%)	18	50
2	e	151/156 (97%)	127 (84%)	15 (10%)	9 (6%)	1	10
2	f	154/156 (99%)	126 (82%)	23 (15%)	5 (3%)	3	22
2	g	151/156 (97%)	126 (83%)	22 (15%)	3 (2%)	6	29
2	k	154/156 (99%)	129 (84%)	20 (13%)	5 (3%)	3	22
2	l	151/156 (97%)	134 (89%)	16 (11%)	1 (1%)	18	50
2	m	149/156 (96%)	131 (88%)	13 (9%)	5 (3%)	3	21
2	q	142/156 (91%)	125 (88%)	13 (9%)	4 (3%)	4	24
2	r	150/156 (96%)	130 (87%)	19 (13%)	1 (1%)	18	50
2	s	150/156 (96%)	125 (83%)	18 (12%)	7 (5%)	2	15
2	w	154/156 (99%)	128 (83%)	18 (12%)	8 (5%)	1	13
2	x	151/156 (97%)	132 (87%)	15 (10%)	4 (3%)	4	25
2	y	150/156 (96%)	132 (88%)	17 (11%)	1 (1%)	18	50
All	All	7723/8550 (90%)	6591 (85%)	937 (12%)	195 (2%)	4	25

All (195) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	33	ALA
2	2	104	GLU
2	A	106	PRO
2	A	146	GLU
2	C	72	THR
1	F	49	ILE
2	G	8	PRO
2	G	11	LYS
2	H	111	ALA
2	I	33	ALA
2	O	148	GLY
2	T	105	THR
2	U	11	LYS
2	Y	34	ASN
2	Y	104	GLU
2	Y	146	GLU
2	Z	9	SER
2	a	33	ALA
1	c	3	VAL
2	e	111	ALA
2	e	146	GLU
2	e	148	GLY
2	k	106	PRO
2	l	111	ALA
2	m	148	GLY
1	0	90	GLY
1	1	72	ASP
2	2	23	GLU
1	5	90	GLY
1	6	14	THR
1	6	90	GLY
2	A	33	ALA
2	C	24	GLY
2	C	34	ASN
2	C	104	GLU
1	D	90	GLY
1	E	3	VAL
1	E	49	ILE
1	F	77	ASP
1	J	3	VAL
1	K	90	GLY
1	L	90	GLY
2	M	11	LYS

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Mol	Chain	Res	Type
2	M	104	GLU
1	P	2	ARG
1	R	3	VAL
2	S	104	GLU
2	U	70	PRO
1	V	3	VAL
1	X	3	VAL
2	Y	23	GLU
1	c	2	ARG
1	c	90	GLY
1	d	3	VAL
2	e	8	PRO
2	f	8	PRO
1	i	14	THR
1	n	3	VAL
1	n	90	GLY
1	o	3	VAL
1	p	3	VAL
2	s	11	LYS
2	s	148	GLY
1	t	3	VAL
1	t	90	GLY
1	u	3	VAL
1	u	90	GLY
2	x	146	GLU
1	z	3	VAL
1	z	90	GLY
1	z	109	ALA
2	2	105	THR
2	3	107	GLU
2	4	103	ARG
2	4	111	ALA
1	5	72	ASP
1	6	16	GLU
1	6	72	ASP
2	C	11	LYS
1	D	2	ARG
1	D	3	VAL
1	E	72	ASP
1	F	14	THR
1	F	80	THR
2	G	146	GLU

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Mol	Chain	Res	Type
2	G	147	SER
1	J	72	ASP
2	O	33	ALA
2	O	70	PRO
1	P	3	VAL
1	P	72	ASP
1	R	72	ASP
2	S	33	ALA
2	S	111	ALA
1	V	72	ASP
1	X	72	ASP
2	Z	105	THR
1	b	3	VAL
1	b	72	ASP
1	c	72	ASP
1	d	72	ASP
2	g	70	PRO
1	h	72	ASP
1	i	3	VAL
2	k	8	PRO
2	k	33	ALA
2	m	33	ALA
2	m	70	PRO
1	n	72	ASP
1	o	72	ASP
1	p	72	ASP
2	q	103	ARG
2	q	104	GLU
2	s	72	THR
2	s	73	HIS
1	t	72	ASP
2	w	73	HIS
2	w	105	THR
2	x	72	THR
1	z	72	ASP
2	2	11	LYS
2	2	110	GLU
2	4	11	LYS
2	A	11	LYS
2	A	23	GLU
2	A	148	GLY
2	H	73	HIS

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Mol	Chain	Res	Type
1	L	7	PRO
1	L	72	ASP
2	M	8	PRO
1	Q	3	VAL
1	Q	72	ASP
2	S	70	PRO
2	U	33	ALA
1	W	72	ASP
2	Y	8	PRO
2	e	105	THR
2	f	23	GLU
2	f	24	GLY
2	f	72	THR
2	f	73	HIS
2	g	146	GLU
1	j	72	ASP
2	k	104	GLU
2	m	103	ARG
2	q	9	SER
2	r	105	THR
2	s	70	PRO
1	t	109	ALA
1	u	2	ARG
2	w	8	PRO
2	y	33	ALA
1	z	2	ARG
2	2	70	PRO
2	2	103	ARG
2	C	8	PRO
2	C	9	SER
1	D	16	GLU
2	G	44	ARG
2	I	8	PRO
2	I	105	THR
1	K	3	VAL
2	M	70	PRO
2	N	44	ARG
1	R	2	ARG
2	S	44	ARG
2	S	145	ALA
2	e	11	LYS
2	e	103	ARG

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Mol	Chain	Res	Type
2	g	73	HIS
1	h	109	ALA
1	j	3	VAL
2	k	105	THR
2	s	44	ARG
2	w	9	SER
2	w	44	ARG
2	w	109	ALA
2	x	111	ALA
2	x	148	GLY
1	7	72	ASP
2	B	111	ALA
2	O	44	ARG
2	O	105	THR
2	S	8	PRO
2	e	9	SER
2	e	44	ARG
2	q	11	LYS
2	s	8	PRO
2	w	11	LYS
1	P	90	GLY
1	F	79	GLY
2	S	11	LYS
2	w	106	PRO
2	Z	112	LYS
2	m	11	LYS

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	0	92/109 (84%)	84 (91%)	8 (9%)	9	33
1	1	91/109 (84%)	87 (96%)	4 (4%)	25	52
1	5	92/109 (84%)	89 (97%)	3 (3%)	33	59
1	6	92/109 (84%)	88 (96%)	4 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	92/109 (84%)	88 (96%)	4 (4%)	26	52
1	D	92/109 (84%)	88 (96%)	4 (4%)	26	52
1	E	92/109 (84%)	88 (96%)	4 (4%)	26	52
1	F	92/109 (84%)	91 (99%)	1 (1%)	65	74
1	J	92/109 (84%)	88 (96%)	4 (4%)	26	52
1	K	92/109 (84%)	87 (95%)	5 (5%)	20	47
1	L	95/109 (87%)	89 (94%)	6 (6%)	16	43
1	P	92/109 (84%)	88 (96%)	4 (4%)	26	52
1	Q	95/109 (87%)	90 (95%)	5 (5%)	20	48
1	R	92/109 (84%)	91 (99%)	1 (1%)	65	74
1	V	93/109 (85%)	90 (97%)	3 (3%)	34	59
1	W	92/109 (84%)	90 (98%)	2 (2%)	45	65
1	X	92/109 (84%)	86 (94%)	6 (6%)	15	43
1	b	95/109 (87%)	92 (97%)	3 (3%)	34	59
1	c	95/109 (87%)	92 (97%)	3 (3%)	34	59
1	d	95/109 (87%)	92 (97%)	3 (3%)	34	59
1	h	95/109 (87%)	90 (95%)	5 (5%)	20	48
1	i	95/109 (87%)	92 (97%)	3 (3%)	34	59
1	j	91/109 (84%)	88 (97%)	3 (3%)	33	59
1	n	92/109 (84%)	88 (96%)	4 (4%)	26	52
1	o	91/109 (84%)	89 (98%)	2 (2%)	45	65
1	p	95/109 (87%)	91 (96%)	4 (4%)	26	53
1	t	95/109 (87%)	91 (96%)	4 (4%)	26	53
1	u	95/109 (87%)	91 (96%)	4 (4%)	26	53
1	v	91/109 (84%)	87 (96%)	4 (4%)	25	52
1	z	95/109 (87%)	90 (95%)	5 (5%)	20	48
2	2	130/132 (98%)	125 (96%)	5 (4%)	29	56
2	3	127/132 (96%)	125 (98%)	2 (2%)	55	70
2	4	131/132 (99%)	129 (98%)	2 (2%)	57	71
2	A	132/132 (100%)	130 (98%)	2 (2%)	57	71
2	B	129/132 (98%)	128 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	129/132 (98%)	124 (96%)	5 (4%)	28	55
2	G	129/132 (98%)	127 (98%)	2 (2%)	55	70
2	H	127/132 (96%)	127 (100%)	0	100	100
2	I	128/132 (97%)	124 (97%)	4 (3%)	35	60
2	M	129/132 (98%)	127 (98%)	2 (2%)	55	70
2	N	129/132 (98%)	128 (99%)	1 (1%)	73	77
2	O	129/132 (98%)	128 (99%)	1 (1%)	73	77
2	S	130/132 (98%)	128 (98%)	2 (2%)	57	71
2	T	132/132 (100%)	132 (100%)	0	100	100
2	U	126/132 (96%)	123 (98%)	3 (2%)	43	64
2	Y	129/132 (98%)	125 (97%)	4 (3%)	35	60
2	Z	128/132 (97%)	125 (98%)	3 (2%)	44	64
2	a	130/132 (98%)	128 (98%)	2 (2%)	57	71
2	e	129/132 (98%)	127 (98%)	2 (2%)	55	70
2	f	132/132 (100%)	128 (97%)	4 (3%)	36	60
2	g	129/132 (98%)	126 (98%)	3 (2%)	44	64
2	k	132/132 (100%)	129 (98%)	3 (2%)	44	64
2	l	129/132 (98%)	128 (99%)	1 (1%)	73	77
2	m	127/132 (96%)	124 (98%)	3 (2%)	43	64
2	q	124/132 (94%)	124 (100%)	0	100	100
2	r	128/132 (97%)	128 (100%)	0	100	100
2	s	128/132 (97%)	126 (98%)	2 (2%)	55	70
2	w	132/132 (100%)	131 (99%)	1 (1%)	73	77
2	x	129/132 (98%)	126 (98%)	3 (2%)	44	64
2	y	128/132 (97%)	126 (98%)	2 (2%)	55	70
All	All	6661/7230 (92%)	6481 (97%)	180 (3%)	39	62

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	33	SER
1	0	38	ARG
1	0	45	ASN

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Mol	Chain	Res	Type
1	0	56	VAL
1	0	59	VAL
1	0	75	VAL
1	0	80	THR
1	0	96	VAL
1	1	3	VAL
1	1	56	VAL
1	1	76	GLU
1	1	96	VAL
2	2	69	CYS
2	2	72	THR
2	2	77	THR
2	2	91	VAL
2	2	150	VAL
2	3	73	HIS
2	3	77	THR
2	4	72	THR
2	4	150	VAL
1	5	19	THR
1	5	59	VAL
1	5	96	VAL
1	6	3	VAL
1	6	19	THR
1	6	54	ARG
1	6	96	VAL
1	7	3	VAL
1	7	75	VAL
1	7	80	THR
1	7	96	VAL
2	A	69	CYS
2	A	150	VAL
2	B	79	THR
2	C	6	ARG
2	C	17	VAL
2	C	69	CYS
2	C	79	THR
2	C	150	VAL
1	D	19	THR
1	D	38	ARG
1	D	80	THR
1	D	96	VAL
1	E	3	VAL

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Mol	Chain	Res	Type
1	E	59	VAL
1	E	80	THR
1	E	96	VAL
1	F	20	ILE
2	G	101	CYS
2	G	150	VAL
2	I	69	CYS
2	I	72	THR
2	I	91	VAL
2	I	150	VAL
1	J	3	VAL
1	J	19	THR
1	J	87	CYS
1	J	96	VAL
1	K	38	ARG
1	K	47	GLU
1	K	58	THR
1	K	80	THR
1	K	96	VAL
1	L	10	ILE
1	L	19	THR
1	L	64	LYS
1	L	80	THR
1	L	96	VAL
1	L	105	VAL
2	M	5	SER
2	M	91	VAL
2	N	79	THR
2	O	150	VAL
1	P	3	VAL
1	P	19	THR
1	P	96	VAL
1	P	101	THR
1	Q	3	VAL
1	Q	11	THR
1	Q	19	THR
1	Q	58	THR
1	Q	96	VAL
1	R	80	THR
2	S	26	LEU
2	S	74	VAL
2	U	105	THR

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Mol	Chain	Res	Type
2	U	132	LEU
2	U	150	VAL
1	V	3	VAL
1	V	38	ARG
1	V	96	VAL
1	W	38	ARG
1	W	96	VAL
1	X	3	VAL
1	X	56	VAL
1	X	58	THR
1	X	66	PHE
1	X	80	THR
1	X	96	VAL
2	Y	5	SER
2	Y	72	THR
2	Y	101	CYS
2	Y	103	ARG
2	Z	77	THR
2	Z	79	THR
2	Z	157	LEU
2	a	69	CYS
2	a	150	VAL
1	b	19	THR
1	b	38	ARG
1	b	96	VAL
1	c	3	VAL
1	c	38	ARG
1	c	96	VAL
1	d	3	VAL
1	d	11	THR
1	d	19	THR
2	e	77	THR
2	e	150	VAL
2	f	7	THR
2	f	55	LEU
2	f	74	VAL
2	f	101	CYS
2	g	7	THR
2	g	69	CYS
2	g	79	THR
1	h	3	VAL
1	h	6	THR

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Mol	Chain	Res	Type
1	h	19	THR
1	h	58	THR
1	h	96	VAL
1	i	80	THR
1	i	96	VAL
1	i	111	HIS
1	j	28	HIS
1	j	58	THR
1	j	96	VAL
2	k	72	THR
2	k	91	VAL
2	k	150	VAL
2	l	55	LEU
2	m	29	LEU
2	m	67	GLN
2	m	79	THR
1	n	3	VAL
1	n	31	THR
1	n	56	VAL
1	n	96	VAL
1	o	22	CYS
1	o	96	VAL
1	p	3	VAL
1	p	19	THR
1	p	66	PHE
1	p	96	VAL
2	s	91	VAL
2	s	131	ARG
1	t	3	VAL
1	t	19	THR
1	t	80	THR
1	t	96	VAL
1	u	19	THR
1	u	58	THR
1	u	75	VAL
1	u	96	VAL
1	v	54	ARG
1	v	56	VAL
1	v	80	THR
1	v	96	VAL
2	w	150	VAL
2	x	55	LEU

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Mol	Chain	Res	Type
2	x	69	CYS
2	x	79	THR
2	y	72	THR
2	y	79	THR
1	z	19	THR
1	z	58	THR
1	z	80	THR
1	z	96	VAL
1	z	103	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	47	GLN
2	3	61	GLN
2	4	73	HIS
1	5	21	ASN
1	6	21	ASN
1	7	45	ASN
2	A	61	GLN
2	B	102	GLN
2	G	39	ASN
2	G	47	GLN
2	G	149	GLN
2	I	34	ASN
1	J	21	ASN
2	M	34	ASN
2	M	61	GLN
2	M	102	GLN
2	N	34	ASN
2	N	61	GLN
2	N	102	GLN
2	O	30	ASN
2	O	149	GLN
1	Q	45	ASN
1	Q	60	ASN
1	R	71	ASN
2	S	15	HIS
2	S	149	GLN
2	T	39	ASN
2	T	73	HIS
1	V	60	ASN

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Mol	Chain	Res	Type
1	V	88	GLN
1	W	71	ASN
1	X	71	ASN
2	Y	73	HIS
2	Z	34	ASN
2	a	102	GLN
1	c	21	ASN
1	c	71	ASN
2	e	46	ASN
2	f	47	GLN
2	k	47	GLN
2	k	61	GLN
2	l	34	ASN
2	l	125	GLN
1	o	5	GLN
1	p	60	ASN
2	q	47	GLN
2	r	61	GLN
2	r	149	GLN
2	s	46	ASN
1	u	71	ASN
2	x	61	GLN
1	z	111	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	P	201	-	4,4,4	0.67	0	6,6,6	0.06	0
3	GOL	J	201	-	5,5,5	0.32	0	5,5,5	0.45	0
3	GOL	b	202	-	5,5,5	0.35	0	5,5,5	0.48	0
3	GOL	W	201	-	5,5,5	0.38	0	5,5,5	0.52	0
4	SO4	h	201	-	4,4,4	0.66	0	6,6,6	0.10	0
3	GOL	b	203	-	5,5,5	0.34	0	5,5,5	0.38	0
3	GOL	n	201	-	5,5,5	0.35	0	5,5,5	0.39	0
3	GOL	D	201	-	5,5,5	0.37	0	5,5,5	0.46	0
4	SO4	t	201	-	4,4,4	0.66	0	6,6,6	0.15	0
3	GOL	5	201	-	5,5,5	0.34	0	5,5,5	0.47	0
3	GOL	h	202	-	5,5,5	0.38	0	5,5,5	0.47	0
3	GOL	b	201	-	5,5,5	0.37	0	5,5,5	0.68	0
3	GOL	V	201	-	5,5,5	0.35	0	5,5,5	0.46	0
3	GOL	c	201	-	5,5,5	0.35	0	5,5,5	0.40	0
3	GOL	t	203	-	5,5,5	0.33	0	5,5,5	0.53	0
3	GOL	l	201	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	t	202	-	5,5,5	0.35	0	5,5,5	0.48	0
3	GOL	P	202	-	5,5,5	0.34	0	5,5,5	0.45	0
3	GOL	z	201	-	5,5,5	0.36	0	5,5,5	0.44	0
3	GOL	0	201	-	5,5,5	0.36	0	5,5,5	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	t	203	-	-	2/4/4/4	-
3	GOL	b	202	-	-	0/4/4/4	-
3	GOL	b	203	-	-	4/4/4/4	-
3	GOL	h	202	-	-	0/4/4/4	-
3	GOL	n	201	-	-	0/4/4/4	-
3	GOL	D	201	-	-	0/4/4/4	-
3	GOL	l	201	-	-	0/4/4/4	-
3	GOL	b	201	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	t	202	-	-	4/4/4/4	-
3	GOL	J	201	-	-	2/4/4/4	-
3	GOL	W	201	-	-	0/4/4/4	-
3	GOL	V	201	-	-	1/4/4/4	-
3	GOL	0	201	-	-	2/4/4/4	-
3	GOL	P	202	-	-	2/4/4/4	-
3	GOL	c	201	-	-	0/4/4/4	-
3	GOL	z	201	-	-	2/4/4/4	-
3	GOL	5	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	5	201	GOL	O1-C1-C2-C3
3	J	201	GOL	O1-C1-C2-C3
3	t	202	GOL	O1-C1-C2-O2
3	t	202	GOL	O1-C1-C2-C3
3	t	202	GOL	C1-C2-C3-O3
3	t	203	GOL	O1-C1-C2-C3
3	J	201	GOL	O1-C1-C2-O2
3	t	203	GOL	O1-C1-C2-O2
3	0	201	GOL	O1-C1-C2-C3
3	P	202	GOL	O1-C1-C2-C3
3	z	201	GOL	O1-C1-C2-C3
3	0	201	GOL	O1-C1-C2-O2
3	t	202	GOL	O2-C2-C3-O3
3	z	201	GOL	O1-C1-C2-O2
3	V	201	GOL	O1-C1-C2-O2
3	5	201	GOL	O1-C1-C2-O2
3	P	202	GOL	O1-C1-C2-O2
3	b	203	GOL	O2-C2-C3-O3
3	b	203	GOL	O1-C1-C2-C3
3	b	203	GOL	C1-C2-C3-O3
3	b	201	GOL	O2-C2-C3-O3
3	b	203	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	201	GOL	2	0
3	W	201	GOL	1	0
3	D	201	GOL	1	0
3	h	202	GOL	1	0
3	V	201	GOL	1	0
3	c	201	GOL	1	0
3	1	201	GOL	2	0
3	t	202	GOL	1	0
3	z	201	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	107/129 (82%)	0.23	0 100 100	58, 119, 171, 224	0
1	1	104/129 (80%)	0.24	2 (1%) 66 45	52, 127, 182, 224	0
1	5	108/129 (83%)	-0.06	1 (0%) 81 62	39, 62, 100, 157	0
1	6	107/129 (82%)	0.16	0 100 100	95, 122, 157, 179	0
1	7	107/129 (82%)	0.59	6 (5%) 30 20	97, 169, 222, 243	0
1	D	106/129 (82%)	0.04	1 (0%) 81 62	44, 67, 112, 144	0
1	E	108/129 (83%)	0.14	0 100 100	74, 130, 187, 213	0
1	F	106/129 (82%)	0.13	1 (0%) 81 62	78, 154, 207, 222	0
1	J	108/129 (83%)	-0.09	0 100 100	38, 60, 97, 155	0
1	K	106/129 (82%)	0.10	0 100 100	69, 110, 166, 182	0
1	L	112/129 (86%)	0.48	4 (3%) 46 30	62, 134, 188, 256	0
1	P	107/129 (82%)	-0.11	0 100 100	43, 65, 91, 111	0
1	Q	112/129 (86%)	0.30	2 (1%) 67 47	84, 124, 175, 210	0
1	R	107/129 (82%)	0.17	2 (1%) 66 45	64, 131, 179, 210	0
1	V	106/129 (82%)	0.11	5 (4%) 36 23	42, 62, 95, 117	1 (0%)
1	W	106/129 (82%)	0.17	0 100 100	59, 107, 149, 195	0
1	X	107/129 (82%)	0.31	2 (1%) 66 45	69, 104, 149, 175	0
1	b	112/129 (86%)	0.09	0 100 100	50, 73, 151, 270	0
1	c	112/129 (86%)	0.11	0 100 100	58, 98, 177, 221	0
1	d	112/129 (86%)	0.45	3 (2%) 56 37	60, 131, 176, 222	0
1	h	112/129 (86%)	-0.02	1 (0%) 81 62	40, 69, 160, 273	0
1	i	112/129 (86%)	0.72	9 (8%) 18 14	95, 151, 206, 233	0
1	j	105/129 (81%)	0.46	4 (3%) 44 28	121, 168, 202, 253	0
1	n	109/129 (84%)	-0.01	1 (0%) 81 62	41, 66, 117, 191	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	o	104/129 (80%)	0.50	3 (2%) 53 35	109, 190, 244, 284	0
1	p	112/129 (86%)	0.21	0 100 100	89, 131, 173, 195	0
1	t	112/129 (86%)	0.17	3 (2%) 56 37	43, 74, 242, 333	0
1	u	112/129 (86%)	0.31	3 (2%) 56 37	68, 128, 193, 210	0
1	v	105/129 (81%)	0.48	4 (3%) 44 28	73, 181, 241, 295	0
1	z	112/129 (86%)	-0.11	0 100 100	44, 61, 109, 222	0
2	2	154/156 (98%)	0.17	5 (3%) 50 33	45, 85, 204, 322	0
2	3	151/156 (96%)	0.42	13 (8%) 16 13	59, 106, 210, 265	0
2	4	155/156 (99%)	-0.07	1 (0%) 85 69	42, 82, 200, 242	0
2	A	156/156 (100%)	0.11	6 (3%) 44 28	38, 76, 195, 231	0
2	B	153/156 (98%)	0.15	2 (1%) 75 55	54, 89, 212, 262	0
2	C	153/156 (98%)	0.09	4 (2%) 57 38	42, 76, 186, 259	0
2	G	153/156 (98%)	-0.01	1 (0%) 84 67	35, 64, 162, 227	0
2	H	152/156 (97%)	0.35	7 (4%) 37 24	39, 69, 188, 254	0
2	I	152/156 (97%)	-0.04	1 (0%) 84 67	37, 63, 161, 249	0
2	M	153/156 (98%)	-0.03	2 (1%) 75 55	37, 73, 265, 305	0
2	N	153/156 (98%)	0.08	2 (1%) 75 55	55, 90, 197, 238	0
2	O	153/156 (98%)	0.13	1 (0%) 84 67	44, 80, 222, 282	0
2	S	154/156 (98%)	0.18	5 (3%) 50 33	30, 65, 164, 205	0
2	T	156/156 (100%)	0.21	5 (3%) 50 33	34, 66, 172, 217	0
2	U	150/156 (96%)	-0.10	1 (0%) 84 67	34, 61, 139, 194	0
2	Y	153/156 (98%)	0.03	1 (0%) 84 67	32, 59, 136, 188	0
2	Z	152/156 (97%)	0.13	5 (3%) 49 32	27, 65, 157, 203	0
2	a	154/156 (98%)	-0.12	2 (1%) 75 55	34, 62, 143, 182	0
2	e	153/156 (98%)	0.28	4 (2%) 57 38	52, 93, 171, 237	0
2	f	156/156 (100%)	0.70	13 (8%) 17 14	81, 130, 213, 266	0
2	g	153/156 (98%)	0.19	1 (0%) 84 67	59, 106, 181, 205	0
2	k	156/156 (100%)	0.43	7 (4%) 38 24	52, 91, 193, 285	0
2	l	153/156 (98%)	0.51	8 (5%) 33 21	79, 119, 199, 290	0
2	m	151/156 (96%)	0.26	4 (2%) 57 38	58, 99, 177, 218	0
2	q	146/156 (93%)	-0.20	0 100 100	37, 71, 157, 275	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
2	r	152/156 (97%)	-0.00	1 (0%)	84 67	48, 80, 184, 220	0
2	s	152/156 (97%)	0.04	2 (1%)	75 55	40, 75, 205, 242	0
2	w	156/156 (100%)	-0.03	1 (0%)	85 69	36, 67, 172, 238	0
2	x	153/156 (98%)	0.17	4 (2%)	57 38	34, 74, 191, 225	0
2	y	152/156 (97%)	-0.04	1 (0%)	84 67	32, 64, 160, 223	0
All	All	7845/8550 (91%)	0.17	167 (2%)	63 43	27, 90, 193, 333	1 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	7	91	LEU	5.8
2	H	42	GLU	5.6
2	3	41	VAL	5.3
2	3	42	GLU	5.1
1	V	2[A]	ARG	4.6
2	3	43	LEU	4.5
1	7	93	GLU	4.0
1	Q	53	GLY	3.8
1	i	49	ILE	3.6
2	f	28	TRP	3.5
2	l	157	LEU	3.4
2	3	13	VAL	3.4
2	3	27	GLN	3.4
2	f	112	LYS	3.4
1	v	81	TYR	3.4
2	3	10	ASP	3.4
1	1	76	GLU	3.4
2	H	7	THR	3.4
2	H	70	PRO	3.4
1	L	100	GLY	3.3
1	j	1	ALA	3.3
2	M	99	SER	3.2
1	j	10	ILE	3.2
1	d	68	LEU	3.2
2	3	29	LEU	3.2
1	7	90	GLY	3.2
2	H	9	SER	3.2
2	3	39	ASN	3.0
2	T	54	GLY	3.0
2	l	25	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	42	GLU	3.0
1	d	99	GLY	3.0
2	2	4	SER	3.0
2	x	9	SER	3.0
2	Z	10	ASP	2.9
1	L	89	TYR	2.9
2	x	7	THR	2.9
2	H	8	PRO	2.9
2	f	69	CYS	2.9
2	e	157	LEU	2.9
1	i	48	SER	2.8
1	i	44	THR	2.8
2	T	127	GLU	2.8
2	w	42	GLU	2.8
1	V	106	ASN	2.8
2	f	52	SER	2.8
2	x	8	PRO	2.8
2	T	53	GLU	2.8
1	t	47	GLU	2.8
2	2	7	THR	2.8
2	Z	72	THR	2.8
2	f	113	PRO	2.8
2	3	30	ASN	2.7
2	k	36	LEU	2.7
2	Z	109	ALA	2.7
1	L	99	GLY	2.7
2	Y	157	LEU	2.7
2	S	127	GLU	2.6
2	T	7	THR	2.6
2	a	7	THR	2.6
2	k	5	SER	2.6
1	j	9	THR	2.6
2	4	157	LEU	2.6
2	f	47	GLN	2.6
2	3	37	LEU	2.6
2	A	70	PRO	2.5
1	i	37	TYR	2.5
2	Z	101	CYS	2.5
1	v	48	SER	2.5
2	f	157	LEU	2.5
1	7	95	ASP	2.5
1	X	44	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	u	101	THR	2.5
2	C	7	THR	2.5
1	F	53	GLY	2.5
2	k	101	CYS	2.5
2	G	7	THR	2.5
1	7	35	TYR	2.5
2	S	69	CYS	2.5
2	x	72	THR	2.5
2	f	41	VAL	2.5
2	f	27	GLN	2.5
2	Z	25	GLN	2.4
1	5	6	THR	2.4
2	y	28	TRP	2.4
2	M	100	PRO	2.4
1	i	112	HIS	2.4
1	i	82	ARG	2.4
2	A	3	SER	2.4
2	l	95	SER	2.4
1	i	91	LEU	2.4
2	H	10	ASP	2.4
1	l	100	GLY	2.4
1	o	101	THR	2.4
2	B	7	THR	2.4
2	S	46	ASN	2.4
1	u	49	ILE	2.4
2	f	48	LEU	2.4
1	t	6	THR	2.3
2	A	108	GLY	2.3
1	L	93	GLU	2.3
2	2	127	GLU	2.3
2	S	110	GLU	2.3
1	R	42	GLY	2.3
2	S	90	LYS	2.3
2	m	18	ALA	2.3
2	l	26	LEU	2.3
1	Q	70	ILE	2.3
2	2	40	GLY	2.3
2	e	69	CYS	2.3
1	V	86	GLU	2.3
2	r	156	ALA	2.3
2	A	5	SER	2.3
2	A	52	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	o	105	VAL	2.3
1	n	109	ALA	2.3
2	f	111	ALA	2.3
2	I	157	LEU	2.3
2	m	146	GLU	2.2
2	f	132	LEU	2.2
2	e	72	THR	2.2
2	2	5	SER	2.2
1	7	88	GLN	2.2
2	N	101	CYS	2.2
1	o	80	THR	2.2
2	s	109	ALA	2.2
2	k	74	VAL	2.2
1	V	9	THR	2.2
1	v	49	ILE	2.2
2	U	9	SER	2.2
2	g	157	LEU	2.2
1	h	99	GLY	2.2
2	k	70	PRO	2.2
2	C	75	LEU	2.1
2	m	106	PRO	2.1
2	C	143	ASP	2.1
2	a	73	HIS	2.1
2	3	36	LEU	2.1
1	j	102	VAL	2.1
2	k	157	LEU	2.1
2	B	100	PRO	2.1
2	l	116	GLU	2.1
1	i	63	SER	2.1
1	V	3	VAL	2.1
2	T	69	CYS	2.1
2	l	78	HIS	2.1
1	v	100	GLY	2.1
2	H	50	VAL	2.1
2	O	75	LEU	2.1
2	k	37	LEU	2.1
2	C	72	THR	2.1
2	e	101	CYS	2.1
2	3	156	ALA	2.1
1	D	98	GLY	2.1
2	N	108	GLY	2.1
1	t	106	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	X	48	SER	2.0
1	d	45	ASN	2.0
2	l	92	ASN	2.0
2	l	28	TRP	2.0
2	f	45	ASP	2.0
1	R	53	GLY	2.0
2	3	40	GLY	2.0
2	s	100	PRO	2.0
1	i	46	GLU	2.0
1	u	102	VAL	2.0
2	m	74	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	b	202	6/6	0.75	0.09	74,81,88,89	0
3	GOL	0	201	6/6	0.80	0.11	54,63,65,73	0
3	GOL	b	203	6/6	0.80	0.11	66,67,70,76	0
3	GOL	l	201	6/6	0.81	0.11	63,69,73,74	0
3	GOL	t	203	6/6	0.82	0.11	49,76,82,86	0
3	GOL	c	201	6/6	0.83	0.14	57,65,71,75	0
3	GOL	P	202	6/6	0.83	0.09	59,62,74,81	0
3	GOL	D	201	6/6	0.84	0.09	54,61,69,73	0
3	GOL	z	201	6/6	0.84	0.09	53,58,65,70	0
3	GOL	b	201	6/6	0.85	0.11	42,56,61,67	0
4	SO4	h	201	5/5	0.87	0.11	68,85,106,117	0
3	GOL	n	201	6/6	0.88	0.08	67,74,75,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	W	201	6/6	0.88	0.08	64,67,79,80	0
3	GOL	t	202	6/6	0.90	0.08	58,71,81,89	0
3	GOL	5	201	6/6	0.90	0.10	53,62,65,70	0
3	GOL	h	202	6/6	0.90	0.08	50,56,58,58	0
3	GOL	V	201	6/6	0.90	0.11	61,65,66,67	0
3	GOL	J	201	6/6	0.92	0.09	38,41,51,59	0
4	SO4	P	201	5/5	0.93	0.10	66,71,83,84	0
4	SO4	t	201	5/5	0.93	0.12	68,74,81,104	0
5	CL	S	201	1/1	0.95	0.04	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.