Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:40 AM UTC

PDB ID	:	8P0T / pdb_00008p0t
EMDB ID	:	EMD-17337
Title	:	CryoEM structure of 20S Trichomonas vaginalis proteasome in complex with proteasome inhibitor CP-17
Authors	:	Silhan, J.; Boura, E.; Fajtova, P.
Deposited on	:	2023-05-10
Resolution	:	2.65 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

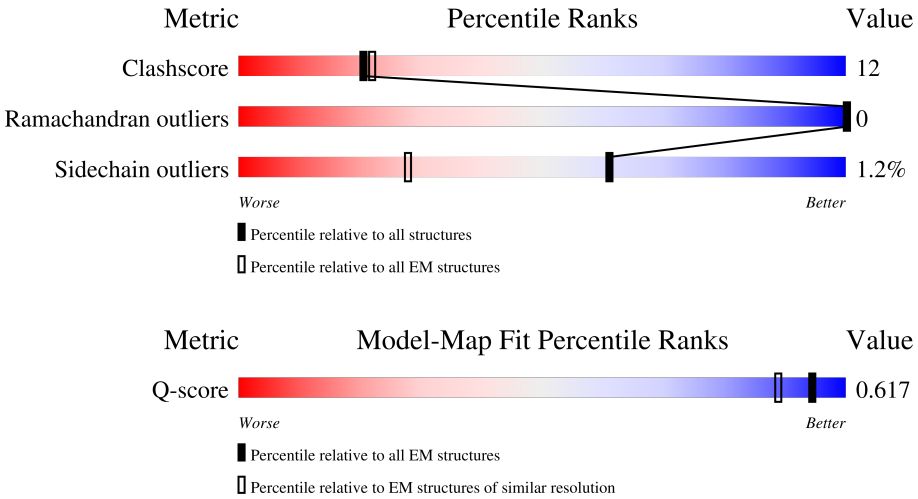
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9050 (2.15 - 3.15)

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

Mol	Chain	Length	Quality of chain
1	A	241	5% 77% 22%
1	O	241	5% 76% 23%
2	B	232	66% 31%
2	P	232	69% 28%

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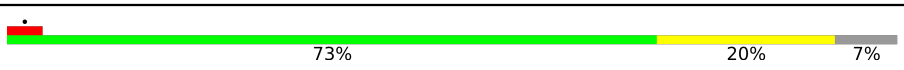
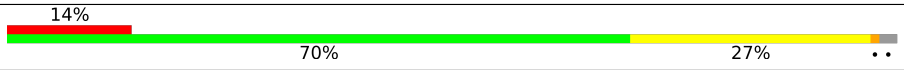
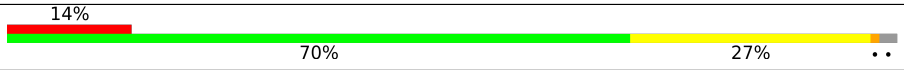
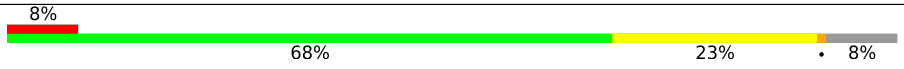
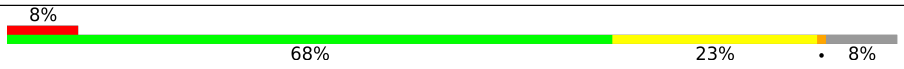
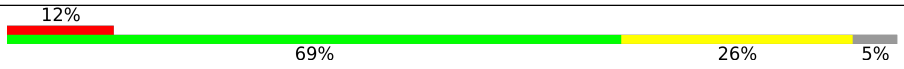
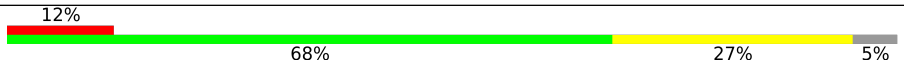
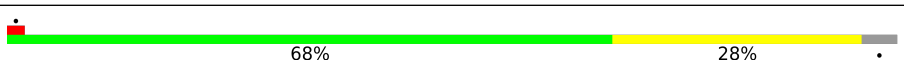
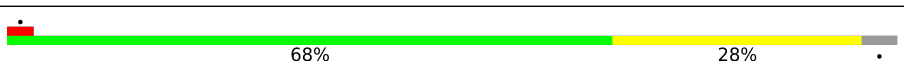
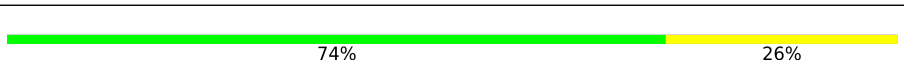
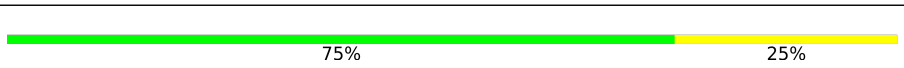
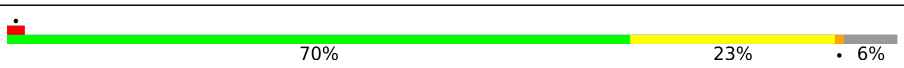
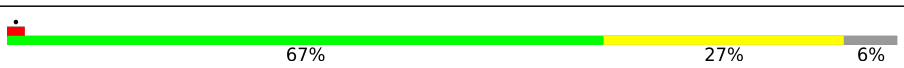
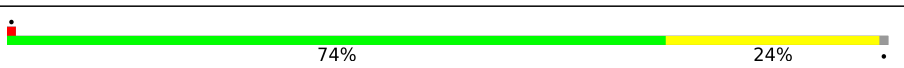
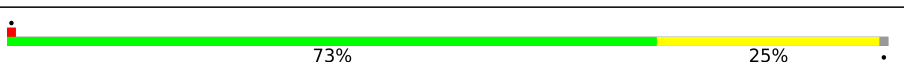
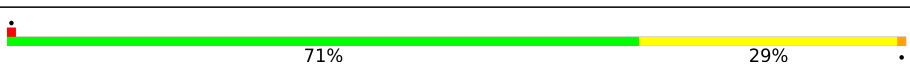
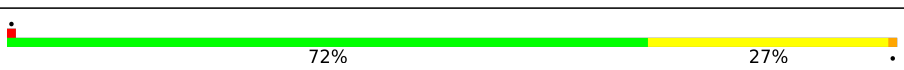
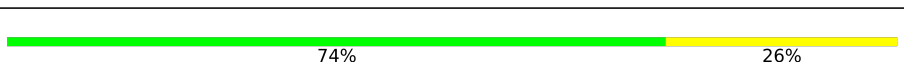
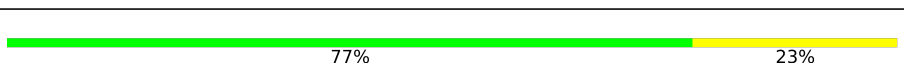
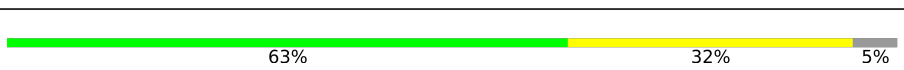
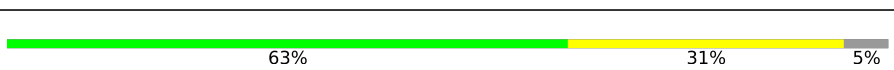
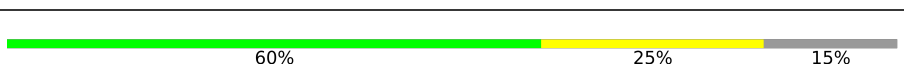
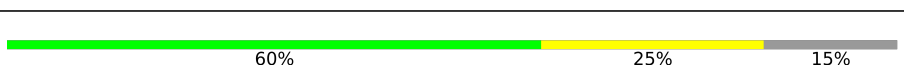
Mol	Chain	Length	Quality of chain
3	C	251	
3	Q	251	
4	D	235	
4	R	235	
5	E	251	
5	S	251	
6	F	233	
6	T	233	
7	G	240	
7	U	240	
8	H	204	
8	V	204	
9	I	243	
9	W	243	
10	J	206	
10	X	206	
11	K	191	
11	Y	191	
12	L	202	
12	Z	202	
13	M	224	
13	a	224	
14	N	244	
14	b	244	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 47778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1843	1171	304	359	9		
1	O	239	Total	C	N	O	S	0	0
			1843	1171	304	359	9		

- Molecule 2 is a protein called Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1770	1121	305	340	4		
2	P	229	Total	C	N	O	S	0	0
			1770	1121	305	340	4		

- Molecule 3 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	233	Total	C	N	O	S	0	0
			1819	1148	307	354	10		
3	Q	233	Total	C	N	O	S	0	0
			1819	1148	307	354	10		

- Molecule 4 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	231	Total	C	N	O	S	0	0
			1806	1123	320	351	12		
4	R	231	Total	C	N	O	S	0	0
			1806	1123	320	351	12		

- Molecule 5 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	231	Total	C	N	O	S	0	0
			1754	1093	309	342	10		
5	S	231	Total	C	N	O	S	0	0
			1754	1093	309	342	10		

- Molecule 6 is a protein called Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	222	Total	C	N	O	S	0	0
			1709	1074	304	322	9		
6	T	222	Total	C	N	O	S	0	0
			1709	1074	304	322	9		

- Molecule 7 is a protein called Family T1, proteasome alpha subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1836	1176	310	343	7		
7	U	230	Total	C	N	O	S	0	0
			1836	1176	310	343	7		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	204	Total	C	N	O	S	0	0
			1536	955	273	301	7		
8	V	204	Total	C	N	O	S	0	0
			1536	955	273	301	7		

- Molecule 9 is a protein called proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	229	Total	C	N	O	S	0	0
			1773	1116	311	336	10		
9	W	229	Total	C	N	O	S	0	0
			1773	1116	311	336	10		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1599	1021	266	301	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1599	1021	266	301	11		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	191	Total	C	N	O	S	0	0
			1502	959	249	283	11		
11	Y	191	Total	C	N	O	S	0	0
			1502	959	249	283	11		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	202	Total	C	N	O	S	0	0
			1578	998	277	293	10		
12	Z	202	Total	C	N	O	S	0	0
			1578	998	277	293	10		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1656	1043	283	320	10		
13	a	212	Total	C	N	O	S	0	0
			1656	1043	283	320	10		

- Molecule 14 is a protein called Family T1, proteasome beta subunit, threonine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	208	Total	C	N	O	S	0	0
			1594	1012	270	304	8		
14	b	208	Total	C	N	O	S	0	0
			1594	1012	270	304	8		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	215	SER	-	expression tag	UNP A2F3X4
N	216	ALA	-	expression tag	UNP A2F3X4
N	217	TRP	-	expression tag	UNP A2F3X4
N	218	SER	-	expression tag	UNP A2F3X4

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Chain	Residue	Modelled	Actual	Comment	Reference
N	219	HIS	-	expression tag	UNP A2F3X4
N	220	PRO	-	expression tag	UNP A2F3X4
N	221	GLN	-	expression tag	UNP A2F3X4
N	222	PHE	-	expression tag	UNP A2F3X4
N	223	GLU	-	expression tag	UNP A2F3X4
N	224	LYS	-	expression tag	UNP A2F3X4
N	225	GLY	-	expression tag	UNP A2F3X4
N	226	GLY	-	expression tag	UNP A2F3X4
N	227	GLY	-	expression tag	UNP A2F3X4
N	228	SER	-	expression tag	UNP A2F3X4
N	229	GLY	-	expression tag	UNP A2F3X4
N	230	GLY	-	expression tag	UNP A2F3X4
N	231	GLY	-	expression tag	UNP A2F3X4
N	232	SER	-	expression tag	UNP A2F3X4
N	233	GLY	-	expression tag	UNP A2F3X4
N	234	GLY	-	expression tag	UNP A2F3X4
N	235	SER	-	expression tag	UNP A2F3X4
N	236	ALA	-	expression tag	UNP A2F3X4
N	237	TRP	-	expression tag	UNP A2F3X4
N	238	SER	-	expression tag	UNP A2F3X4
N	239	HIS	-	expression tag	UNP A2F3X4
N	240	PRO	-	expression tag	UNP A2F3X4
N	241	GLN	-	expression tag	UNP A2F3X4
N	242	PHE	-	expression tag	UNP A2F3X4
N	243	GLU	-	expression tag	UNP A2F3X4
N	244	LYS	-	expression tag	UNP A2F3X4
b	215	SER	-	expression tag	UNP A2F3X4
b	216	ALA	-	expression tag	UNP A2F3X4
b	217	TRP	-	expression tag	UNP A2F3X4
b	218	SER	-	expression tag	UNP A2F3X4
b	219	HIS	-	expression tag	UNP A2F3X4
b	220	PRO	-	expression tag	UNP A2F3X4
b	221	GLN	-	expression tag	UNP A2F3X4
b	222	PHE	-	expression tag	UNP A2F3X4
b	223	GLU	-	expression tag	UNP A2F3X4
b	224	LYS	-	expression tag	UNP A2F3X4
b	225	GLY	-	expression tag	UNP A2F3X4
b	226	GLY	-	expression tag	UNP A2F3X4
b	227	GLY	-	expression tag	UNP A2F3X4
b	228	SER	-	expression tag	UNP A2F3X4
b	229	GLY	-	expression tag	UNP A2F3X4
b	230	GLY	-	expression tag	UNP A2F3X4

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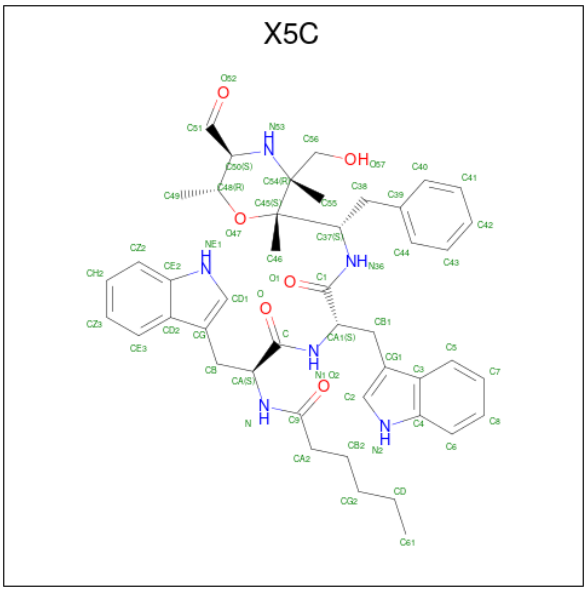
Chain	Residue	Modelled	Actual	Comment	Reference
b	231	GLY	-	expression tag	UNP A2F3X4
b	232	SER	-	expression tag	UNP A2F3X4
b	233	GLY	-	expression tag	UNP A2F3X4
b	234	GLY	-	expression tag	UNP A2F3X4
b	235	SER	-	expression tag	UNP A2F3X4
b	236	ALA	-	expression tag	UNP A2F3X4
b	237	TRP	-	expression tag	UNP A2F3X4
b	238	SER	-	expression tag	UNP A2F3X4
b	239	HIS	-	expression tag	UNP A2F3X4
b	240	PRO	-	expression tag	UNP A2F3X4
b	241	GLN	-	expression tag	UNP A2F3X4
b	242	PHE	-	expression tag	UNP A2F3X4
b	243	GLU	-	expression tag	UNP A2F3X4
b	244	LYS	-	expression tag	UNP A2F3X4

- Molecule 15 is N-[(2S)-1-[[(2S)-1-[[(1S)-1-[(2S,3R,5S,6R)-3-(hydroxymethyl)-5-methanoyl-2,3,6-trimethyl-morpholin-2-yl]-2-phenyl-ethyl]amino]-3-(1H-indol-3-yl)-1-oxidanylidene-propan-2-yl]amino]-3-(1H-indol-3-yl)-1-oxidanylidene-propan-2-yl]hexanamide (CCD ID: X5C) (formula: $C_{45}H_{56}N_6O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	I	1	Total	C	N	O	0
			57	45	6	6	
15	L	1	Total	C	N	O	0
			57	45	6	6	
15	W	1	Total	C	N	O	0
			57	45	6	6	

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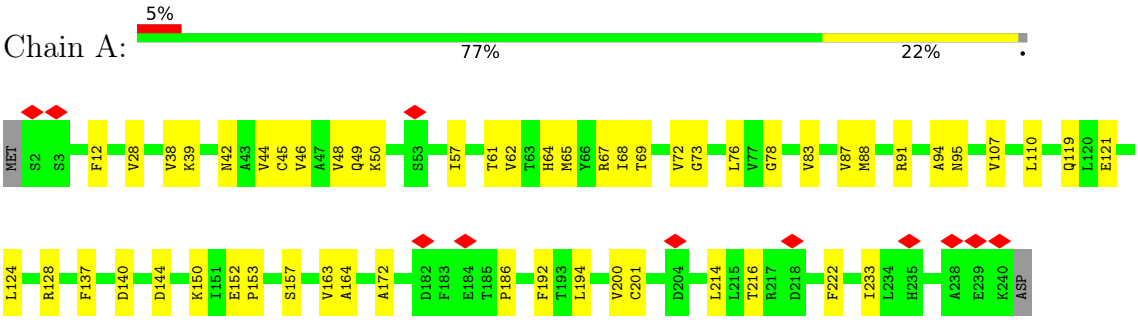
Mol	Chain	Residues	Atoms				AltConf
15	Z	1	Total	C	N	O	0
			57	45	6	6	

3 Residue-property plots (i)

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

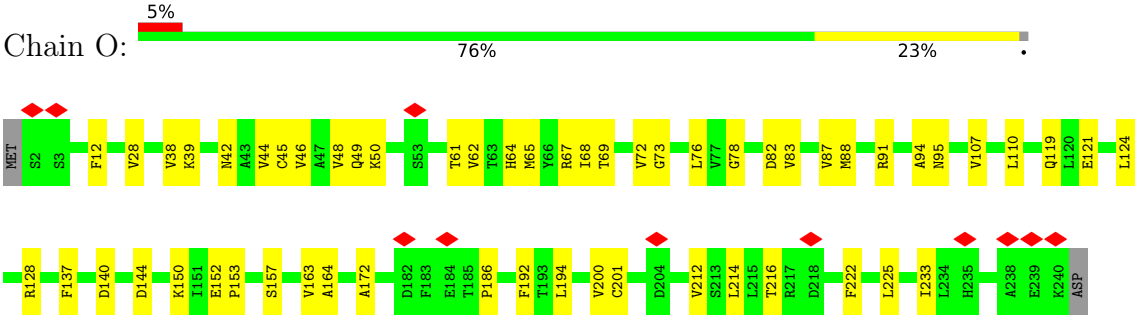
• Molecule 1: Family T1, proteasome alpha subunit, threonine peptidase

Chain A:



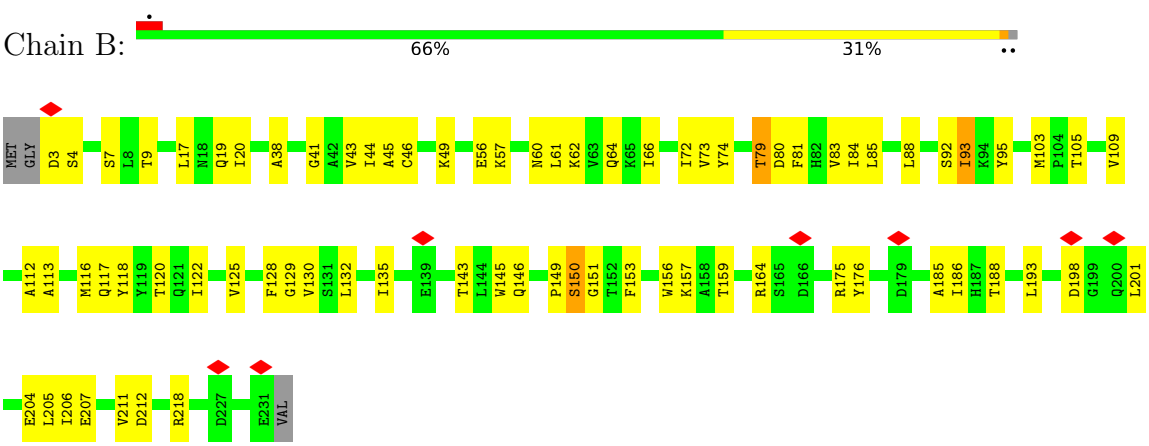
• Molecule 1: Family T1, proteasome alpha subunit, threonine peptidase

Chain O:



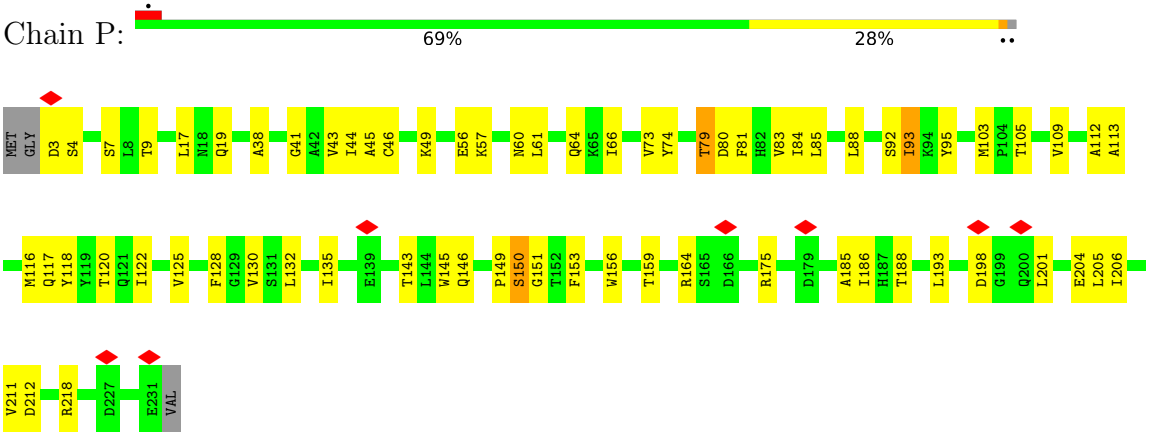
• Molecule 2: Family T1, proteasome alpha subunit, threonine peptidase

Chain B:



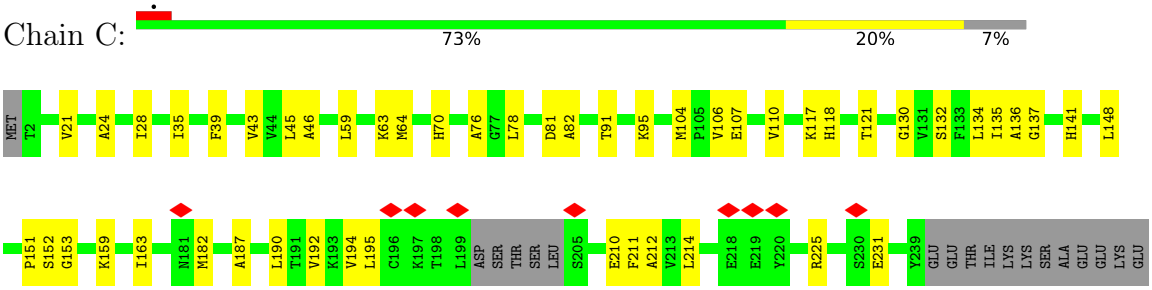
• Molecule 2: Family T1, proteasome alpha subunit, threonine peptidase

Chain P:



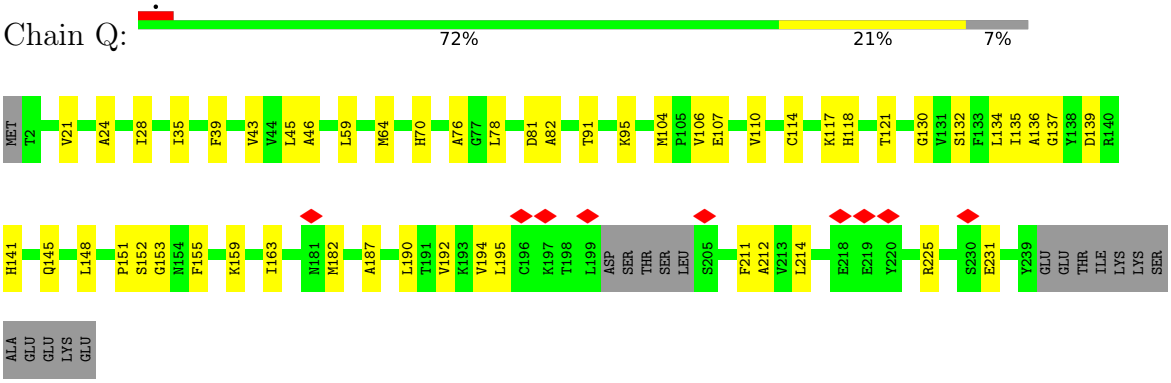
• Molecule 3: Proteasome subunit alpha type

Chain C:



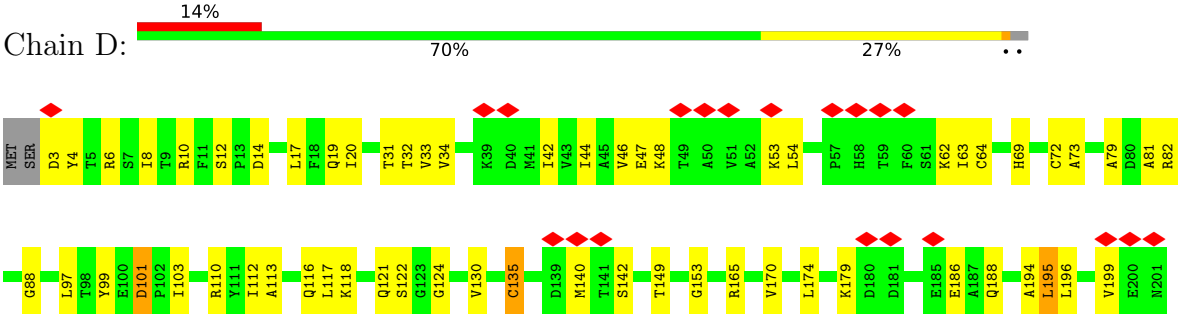
• Molecule 3: Proteasome subunit alpha type

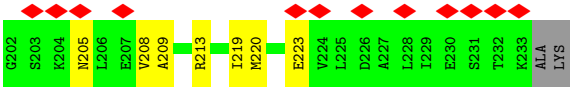
Chain Q:



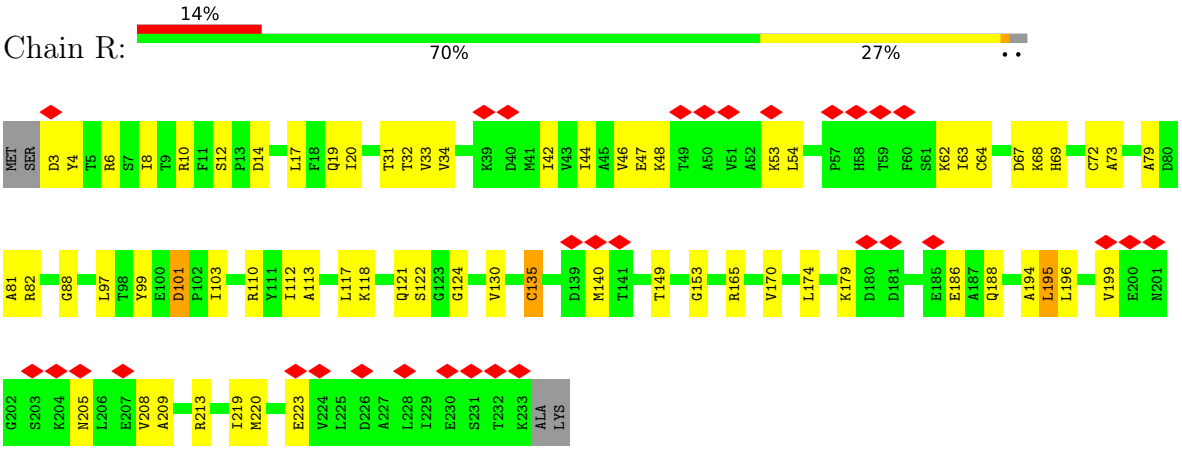
• Molecule 4: Proteasome subunit alpha type

Chain D:

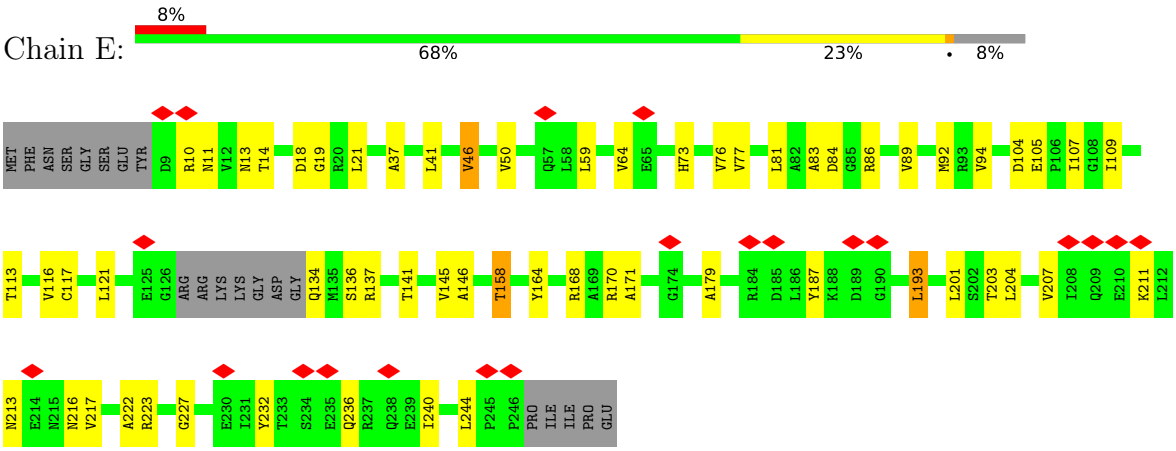




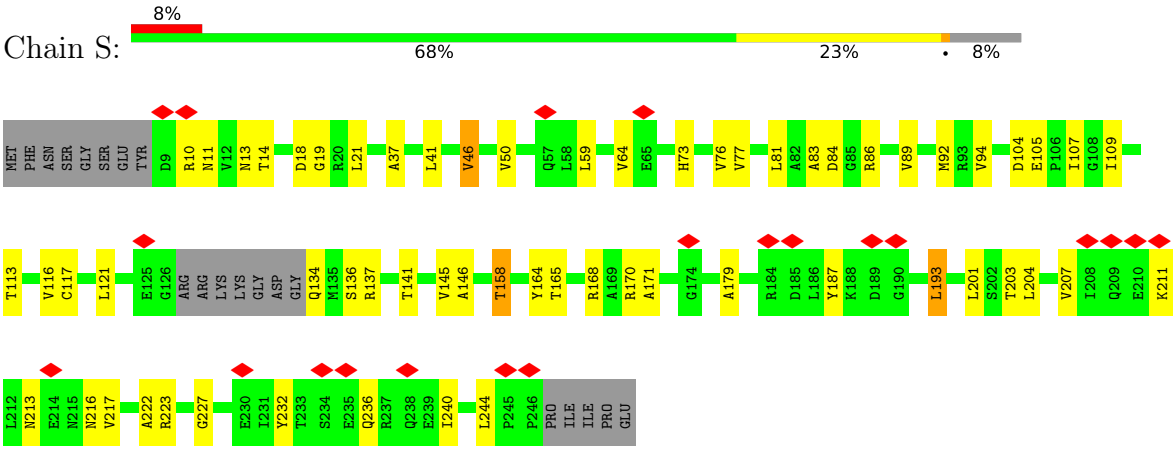
• Molecule 4: Proteasome subunit alpha type



• Molecule 5: Proteasome subunit alpha type

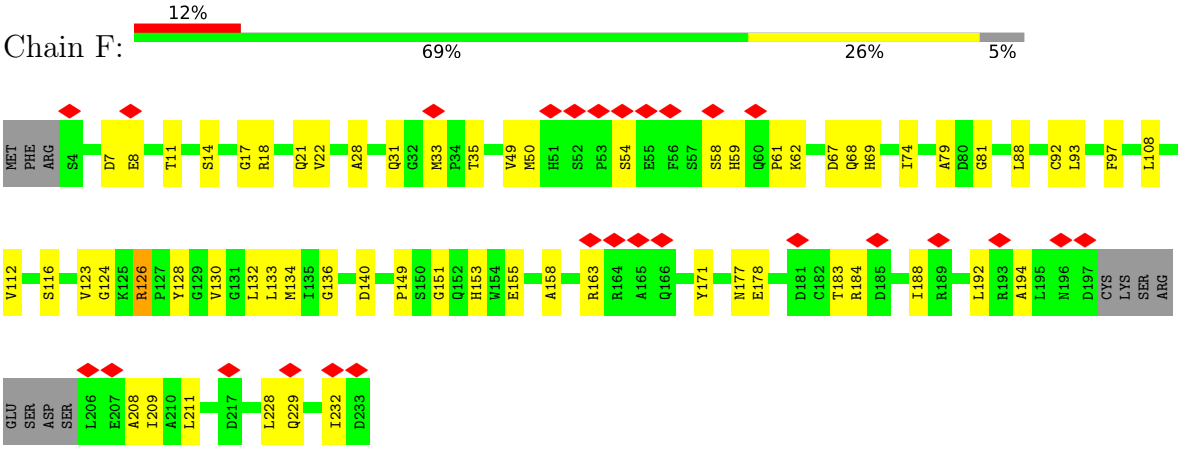


• Molecule 5: Proteasome subunit alpha type



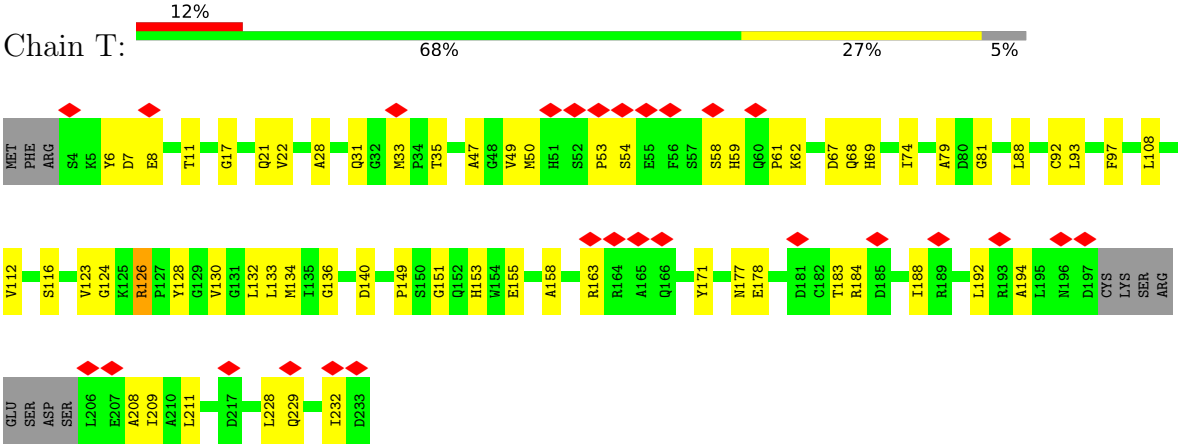
• Molecule 6: Family T1, proteasome alpha subunit, threonine peptidase

Chain F:



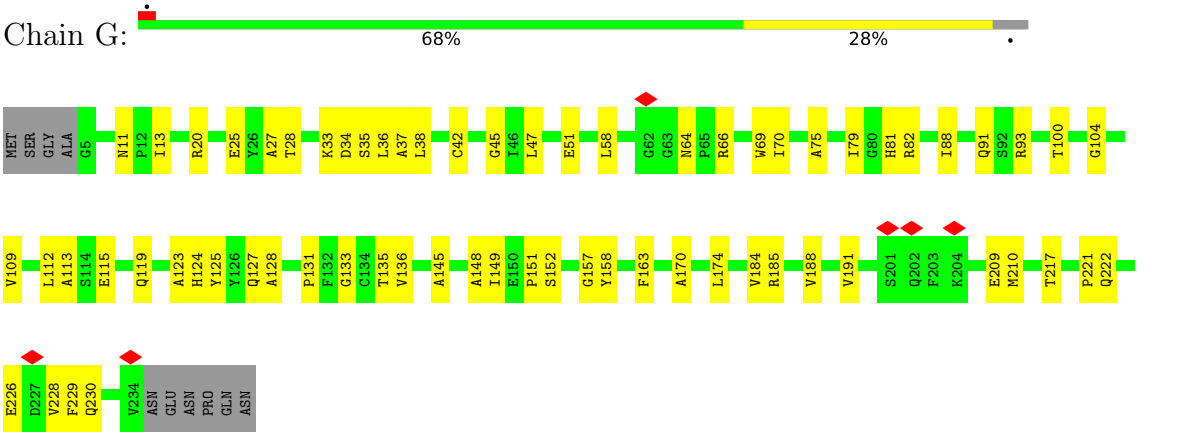
• Molecule 6: Family T1, proteasome alpha subunit, threonine peptidase

Chain T:



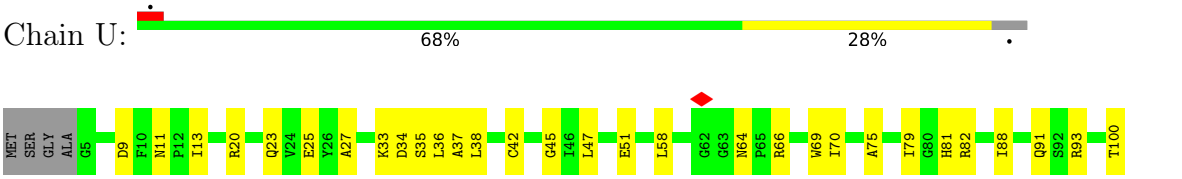
• Molecule 7: Family T1, proteasome alpha subunit, threonine peptidase

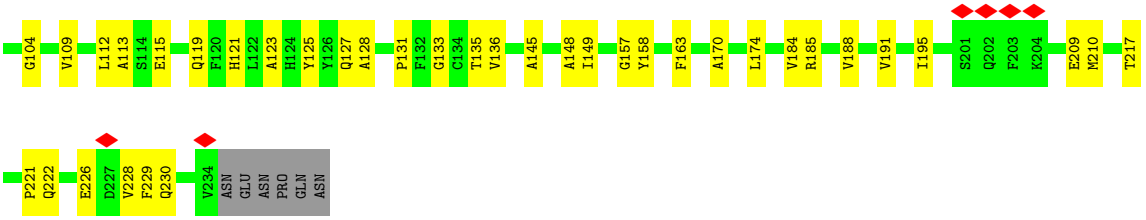
Chain G:



• Molecule 7: Family T1, proteasome alpha subunit, threonine peptidase

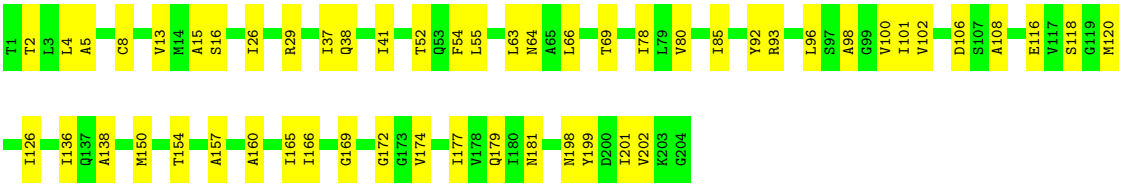
Chain U:





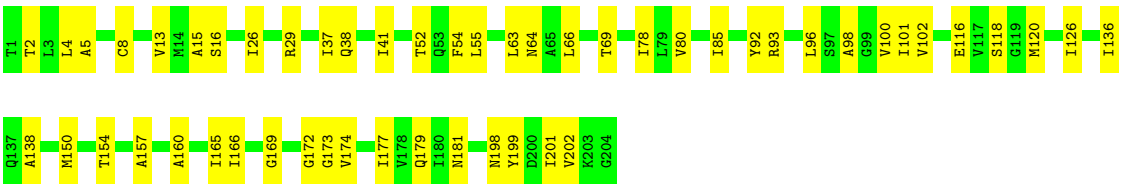
• Molecule 8: Proteasome subunit beta

Chain H:



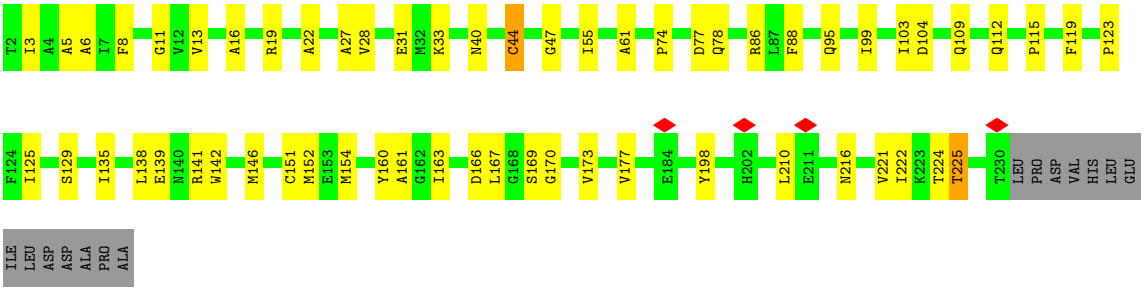
• Molecule 8: Proteasome subunit beta

Chain V:



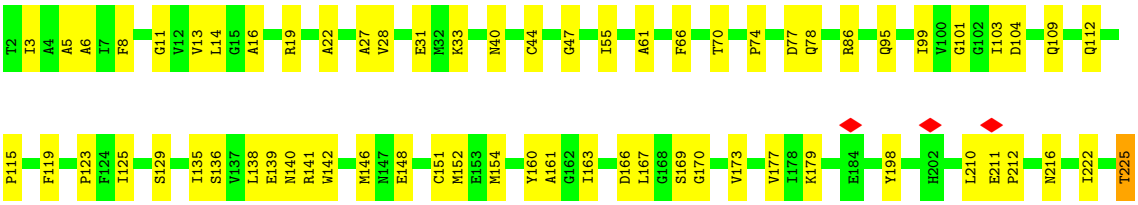
• Molecule 9: proteasome endopeptidase complex

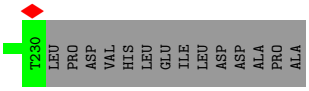
Chain I:



• Molecule 9: proteasome endopeptidase complex

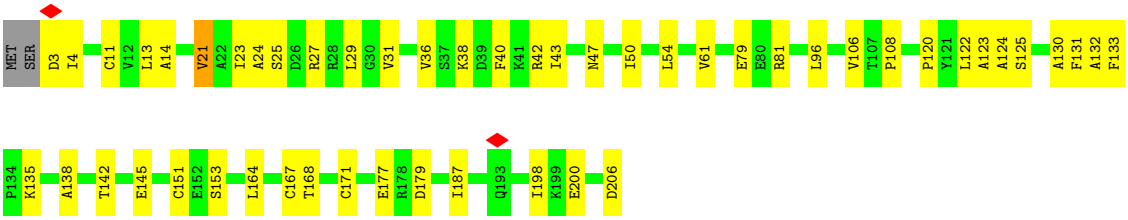
Chain W:





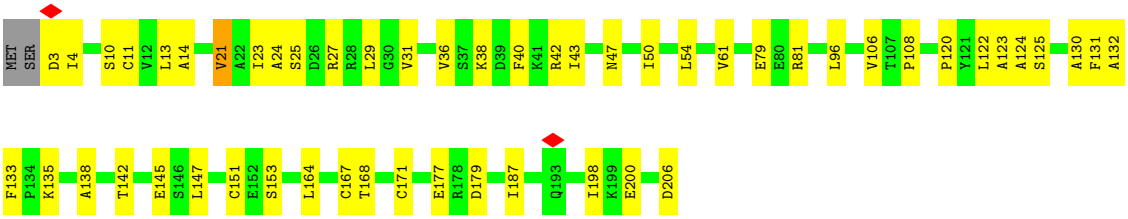
• Molecule 10: Proteasome subunit beta

Chain J:



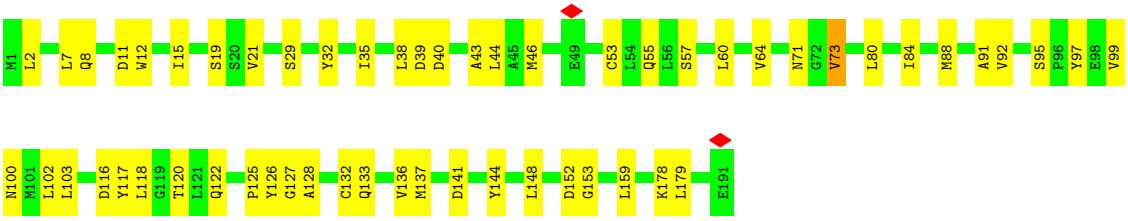
• Molecule 10: Proteasome subunit beta

Chain X:



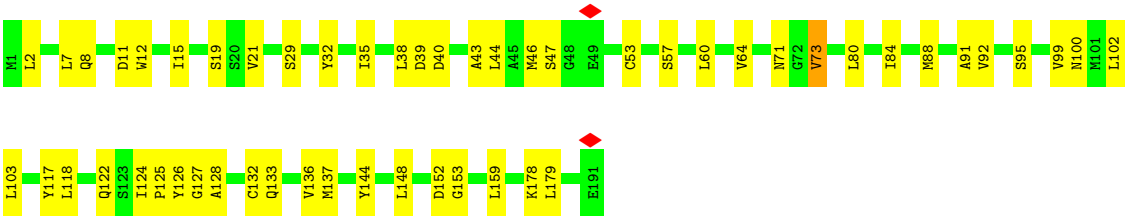
• Molecule 11: Proteasome subunit beta

Chain K:



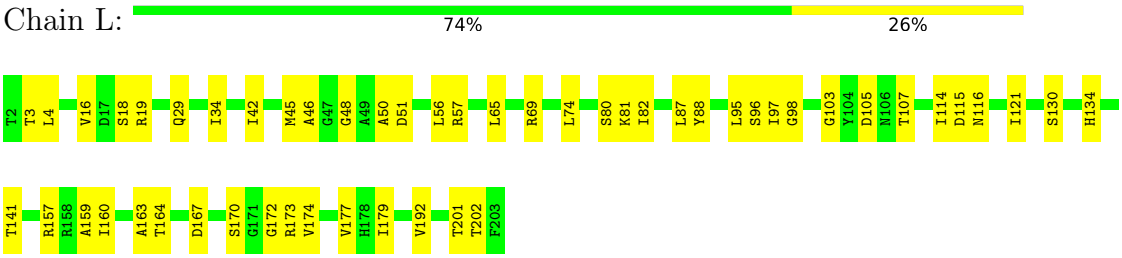
• Molecule 11: Proteasome subunit beta

Chain Y:



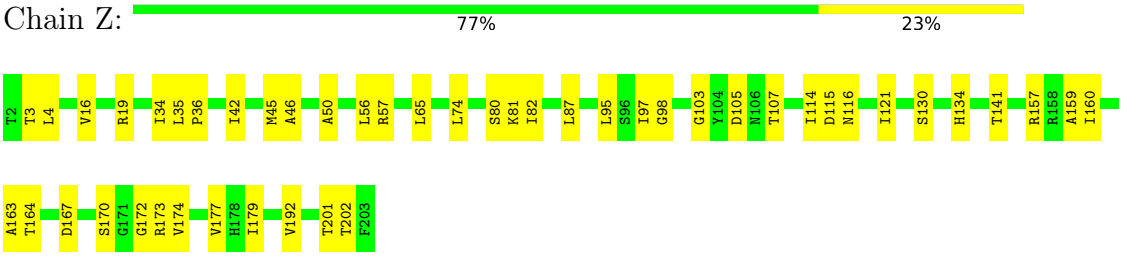
• Molecule 12: Proteasome subunit beta

Chain L:



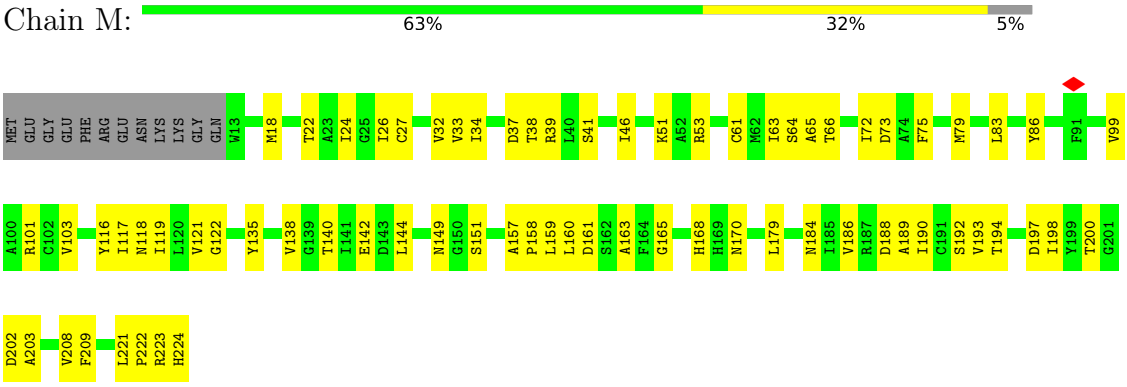
• Molecule 12: Proteasome subunit beta

Chain Z:



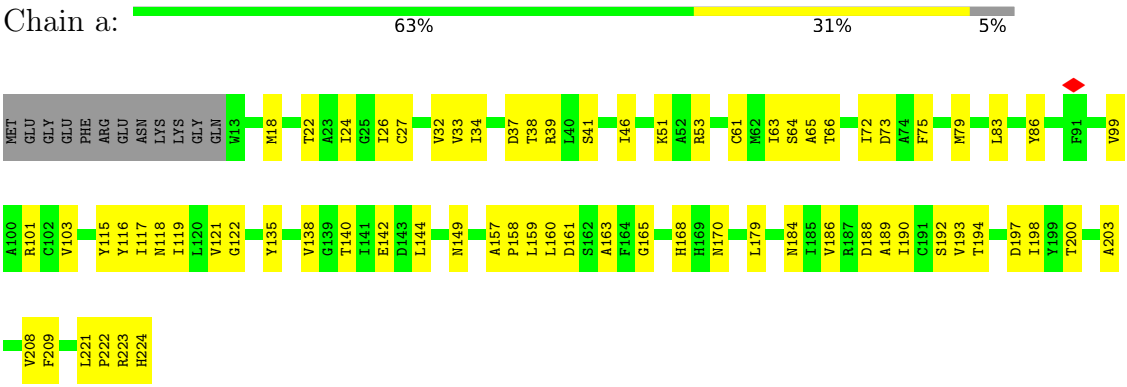
• Molecule 13: Proteasome subunit beta

Chain M:



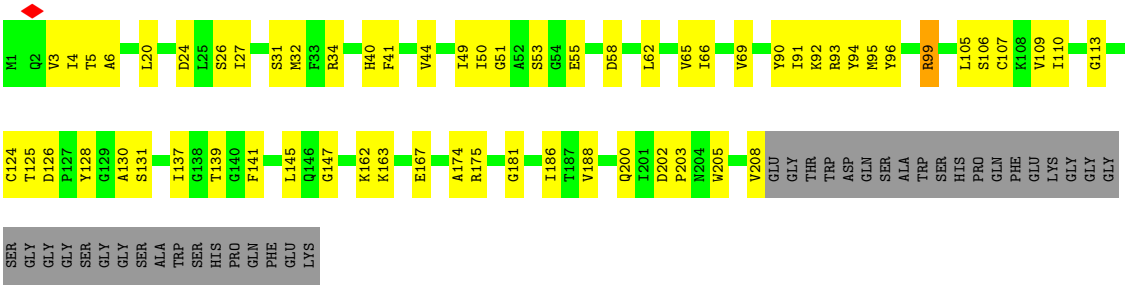
• Molecule 13: Proteasome subunit beta

Chain a:



• Molecule 14: Family T1, proteasome beta subunit, threonine peptidase

Chain N:



• Molecule 14: Family T1, proteasome beta subunit, threonine peptidase

Chain b:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.677	Depositor
Minimum map value	-1.154	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.195	Depositor
Map size (Å)	313.6, 313.6, 313.6	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7, 0.7, 0.7	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: X5C

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.19	0/1875	0.30	0/2538
1	O	0.19	0/1875	0.29	0/2538
2	B	0.18	0/1801	0.32	0/2434
2	P	0.18	0/1801	0.32	0/2434
3	C	0.17	0/1848	0.28	0/2497
3	Q	0.17	0/1848	0.28	0/2497
4	D	0.16	0/1836	0.29	0/2480
4	R	0.16	0/1836	0.29	0/2480
5	E	0.15	0/1778	0.27	0/2402
5	S	0.15	0/1778	0.27	0/2402
6	F	0.15	0/1741	0.28	0/2350
6	T	0.15	0/1741	0.28	0/2350
7	G	0.18	0/1884	0.29	0/2553
7	U	0.18	0/1884	0.29	0/2553
8	H	0.22	0/1555	0.33	0/2106
8	V	0.22	0/1555	0.33	0/2106
9	I	0.23	0/1807	0.33	0/2452
9	W	0.23	0/1807	0.33	0/2452
10	J	0.26	0/1629	0.37	0/2204
10	X	0.26	0/1629	0.37	0/2204
11	K	0.21	0/1532	0.31	0/2065
11	Y	0.21	0/1532	0.31	0/2065
12	L	0.21	0/1613	0.33	0/2180
12	Z	0.21	0/1613	0.33	0/2180
13	M	0.22	0/1695	0.34	0/2295
13	a	0.22	0/1695	0.34	0/2295
14	N	0.22	0/1627	0.31	0/2209
14	b	0.22	0/1627	0.31	0/2209
All	All	0.20	0/48442	0.31	0/65530

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1843	0	1843	41	0
1	O	1843	0	1843	42	0
2	B	1770	0	1789	58	0
2	P	1770	0	1789	54	0
3	C	1819	0	1813	34	0
3	Q	1819	0	1813	35	0
4	D	1806	0	1781	63	0
4	R	1806	0	1781	60	0
5	E	1754	0	1743	50	0
5	S	1754	0	1743	51	0
6	F	1709	0	1703	46	0
6	T	1709	0	1703	48	0
7	G	1836	0	1782	45	0
7	U	1836	0	1782	47	0
8	H	1536	0	1551	46	0
8	V	1536	0	1551	43	0
9	I	1773	0	1747	53	0
9	W	1773	0	1747	55	0
10	J	1599	0	1604	38	0
10	X	1599	0	1604	39	0
11	K	1502	0	1495	43	0
11	Y	1502	0	1495	41	0
12	L	1578	0	1541	45	0
12	Z	1578	0	1541	40	0
13	M	1656	0	1582	60	0
13	a	1656	0	1582	58	0
14	N	1594	0	1566	49	0
14	b	1594	0	1566	48	0
15	I	57	0	0	6	0
15	L	57	0	0	3	0
15	W	57	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Z	57	0	0	3	0
All	All	47778	0	47080	1145	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 12.

All (1145) 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)
9:W:19:ARG:O	15:W:301:X5C:O57	1.84	0.94
9:I:19:ARG:O	15:I:301:X5C:O57	1.84	0.93
12:Z:19:ARG:O	15:Z:301:X5C:O57	1.88	0.92
12:L:19:ARG:O	15:L:301:X5C:O57	1.88	0.91
13:a:18:MET:HE2	13:a:18:MET:HA	1.52	0.90
13:M:18:MET:HE2	13:M:18:MET:HA	1.52	0.90
4:R:32:THR:OG1	4:R:165:ARG:O	1.94	0.86
13:a:18:MET:HE1	13:a:116:TYR:HB3	1.58	0.85
4:D:32:THR:OG1	4:D:165:ARG:O	1.94	0.84
13:M:18:MET:HE1	13:M:116:TYR:HB3	1.58	0.84
13:M:159:LEU:HD21	10:X:153:SER:HB2	1.60	0.83
10:J:153:SER:HB2	13:a:159:LEU:HD21	1.60	0.83
2:P:116:MET:O	2:P:120:THR:HG23	1.79	0.83
2:B:116:MET:O	2:B:120:THR:HG23	1.79	0.82
6:T:153:HIS:O	7:U:82:ARG:NH2	2.13	0.81
6:F:31:GLN:O	6:F:163:ARG:NH1	2.13	0.81
6:F:153:HIS:O	7:G:82:ARG:NH2	2.13	0.81
6:T:31:GLN:O	6:T:163:ARG:NH1	2.13	0.81
6:F:33:MET:SD	6:F:163:ARG:NH2	2.56	0.79
6:T:33:MET:SD	6:T:163:ARG:NH2	2.55	0.79
8:H:166:ILE:HG21	8:H:201:ILE:HD11	1.65	0.79
10:J:124:ALA:HB2	10:J:138:ALA:HB1	1.65	0.78
2:B:212:ASP:OD2	2:B:218:ARG:NH1	2.17	0.78
10:X:124:ALA:HB2	10:X:138:ALA:HB1	1.65	0.77
2:P:212:ASP:OD2	2:P:218:ARG:NH1	2.17	0.77
8:V:166:ILE:HG21	8:V:201:ILE:HD11	1.65	0.77
4:R:48:LYS:N	4:R:205:ASN:O	2.18	0.76
14:b:95:MET:HE1	14:b:107:CYS:O	1.86	0.76
4:D:48:LYS:N	4:D:205:ASN:O	2.18	0.76
14:N:95:MET:HE1	14:N:107:CYS:O	1.86	0.75
2:B:95:TYR:OH	10:J:79:GLU:OE2	2.04	0.75
2:B:156:TRP:CG	2:B:159:THR:HG1	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:156:TRP:CG	2:P:159:THR:HG1	2.06	0.73
1:A:48:VAL:HG12	1:A:65:MET:HE2	1.70	0.73
2:P:95:TYR:OH	10:X:79:GLU:OE2	2.04	0.73
9:I:104:ASP:OD1	9:I:109:GLN:NE2	2.22	0.73
1:O:48:VAL:HG12	1:O:65:MET:HE2	1.70	0.73
1:O:172:ALA:HA	1:O:200:VAL:HG11	1.71	0.73
2:P:175:ARG:NH1	2:P:188:THR:OG1	2.22	0.73
1:A:39:LYS:NZ	2:B:56:GLU:OE2	2.15	0.73
11:Y:91:ALA:O	11:Y:95:SER:N	2.22	0.72
1:A:88:MET:SD	8:H:69:THR:HG22	2.30	0.72
2:B:175:ARG:NH1	2:B:188:THR:OG1	2.22	0.72
1:A:172:ALA:HA	1:A:200:VAL:HG11	1.71	0.72
9:W:104:ASP:OD1	9:W:109:GLN:NE2	2.22	0.71
9:W:112:GLN:HB3	9:W:125:ILE:HD13	1.72	0.71
11:K:91:ALA:O	11:K:95:SER:N	2.22	0.71
5:E:105:GLU:OE2	13:M:86:TYR:OH	2.08	0.70
9:I:112:GLN:HB3	9:I:125:ILE:HD13	1.72	0.70
1:O:88:MET:SD	8:V:69:THR:HG22	2.30	0.70
4:D:31:THR:HG21	4:D:47:GLU:O	1.92	0.70
4:R:31:THR:HG21	4:R:47:GLU:O	1.92	0.70
5:S:104:ASP:OD1	13:a:101:ARG:NH2	2.25	0.70
4:D:34:VAL:HG23	4:D:174:LEU:HD11	1.74	0.70
9:I:3:ILE:HG23	15:I:301:X5C:C49	2.22	0.70
11:K:39:ASP:OD1	11:K:40:ASP:N	2.25	0.69
9:W:3:ILE:HG23	15:W:301:X5C:C49	2.22	0.69
5:E:104:ASP:OD1	13:M:101:ARG:NH2	2.25	0.69
4:R:34:VAL:HG23	4:R:174:LEU:HD11	1.74	0.69
5:E:81:LEU:O	5:E:141:THR:OG1	2.10	0.69
14:N:50:ILE:HD13	14:N:66:ILE:HD13	1.74	0.69
12:Z:80:SER:HB2	12:Z:114:ILE:HD11	1.73	0.69
4:D:223:GLU:OE1	4:D:223:GLU:N	2.25	0.69
12:L:80:SER:HB2	12:L:114:ILE:HD11	1.73	0.69
4:R:223:GLU:OE1	4:R:223:GLU:N	2.25	0.69
12:Z:46:ALA:O	12:Z:98:GLY:N	2.24	0.69
9:I:5:ALA:HB3	9:I:99:ILE:HG21	1.75	0.69
5:S:81:LEU:O	5:S:141:THR:OG1	2.10	0.68
11:K:71:ASN:OD1	11:K:73:VAL:HG22	1.94	0.68
11:Y:39:ASP:OD1	11:Y:40:ASP:N	2.25	0.68
13:a:22:THR:N	13:a:37:ASP:OD1	2.27	0.68
14:b:50:ILE:HD13	14:b:66:ILE:HD13	1.75	0.68
13:M:159:LEU:HD21	10:X:153:SER:CB	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:5:ALA:HB3	9:W:99:ILE:HG21	1.75	0.68
11:Y:71:ASN:OD1	11:Y:73:VAL:HG22	1.94	0.68
4:D:12:SER:OG	4:D:14:ASP:OD1	2.06	0.68
13:M:22:THR:N	13:M:37:ASP:OD1	2.27	0.67
14:b:62:LEU:HD22	14:b:109:VAL:HG21	1.76	0.67
4:R:12:SER:OG	4:R:14:ASP:OD1	2.06	0.67
14:N:62:LEU:HD22	14:N:109:VAL:HG21	1.76	0.67
2:B:17:LEU:HD21	3:C:78:LEU:HD11	1.77	0.67
8:V:52:THR:HG22	8:V:98:ALA:HB1	1.77	0.67
6:F:8:GLU:N	6:F:8:GLU:OE1	2.28	0.67
10:J:153:SER:CB	13:a:159:LEU:HD21	2.24	0.67
5:E:170:ARG:NH1	6:F:54:SER:OG	2.28	0.67
13:M:163:ALA:O	9:W:216:ASN:ND2	2.28	0.67
1:O:39:LYS:NZ	2:P:56:GLU:OE2	2.15	0.66
2:P:17:LEU:HD21	3:Q:78:LEU:HD11	1.77	0.66
8:H:136:ILE:HG21	8:H:160:ALA:O	1.94	0.66
5:S:170:ARG:NH1	6:T:54:SER:OG	2.28	0.66
9:I:216:ASN:ND2	13:a:163:ALA:O	2.28	0.66
5:S:18:ASP:O	6:T:31:GLN:NE2	2.28	0.66
8:V:136:ILE:HG21	8:V:160:ALA:O	1.94	0.66
8:H:52:THR:HG22	8:H:98:ALA:HB1	1.76	0.66
9:I:28:VAL:HG22	10:J:132:ALA:HB2	1.78	0.66
12:L:46:ALA:O	12:L:98:GLY:N	2.24	0.65
4:D:97:LEU:O	12:L:81:LYS:NZ	2.29	0.65
5:E:18:ASP:O	6:F:31:GLN:NE2	2.28	0.65
2:P:120:THR:HG21	2:P:150:SER:HA	1.78	0.65
9:W:112:GLN:HB3	9:W:125:ILE:HG21	1.77	0.65
6:T:8:GLU:N	6:T:8:GLU:OE1	2.28	0.65
2:B:120:THR:HG21	2:B:150:SER:HA	1.78	0.65
12:L:87:LEU:HD22	12:L:97:ILE:HD13	1.79	0.65
1:O:121:GLU:OE2	7:U:125:TYR:OH	2.14	0.65
8:V:13:VAL:HG11	8:V:154:THR:HA	1.78	0.65
9:W:28:VAL:HG22	10:X:132:ALA:HB2	1.78	0.65
5:E:134:GLN:OE1	5:E:134:GLN:N	2.30	0.64
9:I:112:GLN:HB3	9:I:125:ILE:HG21	1.77	0.64
13:a:73:ASP:OD1	14:b:93:ARG:NH1	2.29	0.64
12:L:170:SER:OG	15:L:301:X5C:O52	2.15	0.64
4:R:97:LEU:O	12:Z:81:LYS:NZ	2.29	0.64
10:J:38:LYS:NZ	12:Z:201:THR:O	2.27	0.64
2:P:44:ILE:HG23	2:P:135:ILE:HG23	1.80	0.64
5:S:134:GLN:N	5:S:134:GLN:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:170:SER:OG	15:Z:301:X5C:O52	2.15	0.64
13:M:73:ASP:OD1	14:N:93:ARG:NH1	2.29	0.64
8:H:13:VAL:HG11	8:H:154:THR:HA	1.78	0.64
8:H:165:ILE:HG23	8:H:172:GLY:HA2	1.80	0.64
12:Z:3:THR:HG23	15:Z:301:X5C:C49	2.28	0.64
12:L:201:THR:O	10:X:38:LYS:NZ	2.27	0.63
4:R:6:ARG:O	4:R:124:GLY:N	2.30	0.63
2:B:44:ILE:HG23	2:B:135:ILE:HG23	1.80	0.63
1:O:76:LEU:HD12	1:O:87:VAL:HG23	1.80	0.63
8:V:165:ILE:HG23	8:V:172:GLY:HA2	1.80	0.63
10:J:142:THR:OG1	10:J:179:ASP:OD2	2.11	0.63
12:Z:87:LEU:HD22	12:Z:97:ILE:HD13	1.79	0.63
1:A:68:ILE:HG21	1:A:110:LEU:HD21	1.80	0.63
12:L:3:THR:HG23	15:L:301:X5C:C49	2.28	0.63
5:S:41:LEU:O	5:S:187:TYR:OH	2.12	0.63
14:b:53:SER:OG	14:b:139:THR:OG1	2.17	0.63
10:X:133:PHE:O	10:X:135:LYS:NZ	2.32	0.63
11:Y:19:SER:O	11:Y:32:TYR:N	2.32	0.63
3:Q:64:MET:HE2	3:Q:212:ALA:HB3	1.81	0.63
4:D:6:ARG:O	4:D:124:GLY:N	2.30	0.62
3:Q:70:HIS:NE2	3:Q:104:MET:O	2.31	0.62
10:X:142:THR:OG1	10:X:179:ASP:OD2	2.11	0.62
1:O:68:ILE:HG21	1:O:110:LEU:HD21	1.80	0.62
1:A:76:LEU:HD12	1:A:87:VAL:HG23	1.80	0.62
13:a:24:ILE:HG23	13:a:160:LEU:HD11	1.81	0.62
13:M:24:ILE:HG23	13:M:160:LEU:HD11	1.81	0.62
3:C:64:MET:HE2	3:C:212:ALA:HB3	1.81	0.62
10:J:133:PHE:O	10:J:135:LYS:NZ	2.32	0.62
11:Y:35:ILE:HG22	11:Y:43:ALA:HB1	1.82	0.62
13:a:161:ASP:O	13:a:165:GLY:N	2.28	0.62
13:M:161:ASP:O	13:M:165:GLY:N	2.28	0.61
2:P:46:CYS:HB3	2:P:73:VAL:HG21	1.82	0.61
14:N:53:SER:OG	14:N:139:THR:OG1	2.17	0.61
5:S:19:GLY:O	6:T:28:ALA:HB2	2.01	0.61
2:B:46:CYS:HB3	2:B:73:VAL:HG21	1.82	0.61
6:F:88:LEU:HD21	6:F:112:VAL:HG23	1.82	0.61
6:F:50:MET:N	6:F:208:ALA:O	2.34	0.61
11:K:35:ILE:HG22	11:K:43:ALA:HB1	1.82	0.61
5:E:19:GLY:O	6:F:28:ALA:HB2	2.01	0.60
11:K:19:SER:O	11:K:32:TYR:N	2.32	0.60
9:W:19:ARG:O	9:W:33:LYS:NZ	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:192:SER:OG	10:X:153:SER:OG	2.15	0.60
11:Y:21:VAL:HG11	12:Z:121:ILE:HG12	1.83	0.60
13:M:34:ILE:HG21	13:M:64:SER:CB	2.32	0.60
5:S:94:VAL:HA	12:Z:65:LEU:HD21	1.83	0.60
13:M:39:ARG:NH1	13:M:198:ILE:O	2.35	0.60
13:M:188:ASP:OD1	10:X:153:SER:OG	2.19	0.60
14:N:69:VAL:HG21	14:N:90:TYR:CZ	2.36	0.60
1:A:121:GLU:OE2	7:G:125:TYR:OH	2.14	0.60
13:M:63:ILE:HG23	13:M:119:ILE:HG23	1.84	0.60
13:a:34:ILE:HG21	13:a:64:SER:CB	2.32	0.60
14:b:69:VAL:HG21	14:b:90:TYR:CZ	2.36	0.60
4:D:32:THR:HG21	4:D:170:VAL:HG21	1.84	0.60
4:R:32:THR:HG21	4:R:170:VAL:HG21	1.84	0.59
2:B:3:ASP:OD1	2:B:4:SER:N	2.35	0.59
10:J:177:GLU:OE2	13:a:168:HIS:ND1	2.34	0.59
4:R:34:VAL:CG1	4:R:195:LEU:HD23	2.32	0.59
7:U:11:ASN:ND2	7:U:127:GLN:OE1	2.35	0.59
1:A:119:GLN:NE2	2:B:83:VAL:HG21	2.18	0.59
6:T:88:LEU:HD21	6:T:112:VAL:HG23	1.82	0.59
13:a:63:ILE:HG23	13:a:119:ILE:HG23	1.84	0.59
11:K:21:VAL:HG11	12:L:121:ILE:HG12	1.83	0.59
5:E:94:VAL:HA	12:L:65:LEU:HD21	1.83	0.59
7:G:34:ASP:OD1	7:G:35:SER:N	2.35	0.59
2:P:3:ASP:OD1	2:P:4:SER:N	2.35	0.59
4:R:34:VAL:HG12	4:R:195:LEU:HD23	1.85	0.59
7:U:34:ASP:OD1	7:U:35:SER:N	2.35	0.59
8:V:5:ALA:HB3	8:V:101:ILE:HG21	1.84	0.59
2:B:113:ALA:HB1	2:B:151:GLY:O	2.03	0.59
13:a:39:ARG:NH1	13:a:198:ILE:O	2.35	0.59
8:H:5:ALA:HB3	8:H:101:ILE:HG21	1.84	0.59
4:R:170:VAL:HG13	4:R:194:ALA:HB1	1.84	0.59
4:D:31:THR:HG23	4:D:165:ARG:NH2	2.18	0.59
4:D:170:VAL:HG13	4:D:194:ALA:HB1	1.84	0.59
13:M:168:HIS:ND1	10:X:177:GLU:OE2	2.34	0.59
5:E:46:VAL:HG13	5:E:222:ALA:HB3	1.85	0.59
7:G:11:ASN:ND2	7:G:127:GLN:OE1	2.35	0.59
1:O:119:GLN:NE2	2:P:83:VAL:HG21	2.18	0.59
5:S:46:VAL:HG13	5:S:222:ALA:HB3	1.85	0.59
14:N:208:VAL:HG21	8:V:174:VAL:HG11	1.85	0.58
2:P:113:ALA:HB1	2:P:151:GLY:O	2.03	0.58
9:I:210:LEU:HD13	13:a:184:ASN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:31:THR:HG23	4:R:165:ARG:NH2	2.18	0.58
6:F:178:GLU:N	6:F:178:GLU:OE1	2.37	0.58
6:T:178:GLU:OE1	6:T:178:GLU:N	2.37	0.58
4:D:34:VAL:CG1	4:D:195:LEU:HD23	2.32	0.58
3:C:159:LYS:NZ	4:D:53:LYS:O	2.30	0.58
4:R:118:LYS:O	4:R:122:SER:N	2.36	0.58
11:Y:92:VAL:HG21	11:Y:118:LEU:HD23	1.85	0.58
12:Z:105:ASP:OD1	12:Z:107:THR:OG1	2.22	0.58
7:U:113:ALA:HA	7:U:149:ILE:HD11	1.86	0.58
3:C:70:HIS:NE2	3:C:104:MET:O	2.31	0.58
12:L:105:ASP:OD1	12:L:107:THR:OG1	2.22	0.58
5:S:21:LEU:HD21	6:T:126:ARG:CD	2.33	0.58
6:T:50:MET:N	6:T:208:ALA:O	2.34	0.58
4:D:34:VAL:HG12	4:D:195:LEU:HD23	1.85	0.57
5:E:21:LEU:HD21	6:F:126:ARG:CD	2.33	0.57
13:M:184:ASN:HB3	9:W:210:LEU:HD13	1.85	0.57
7:G:113:ALA:HA	7:G:149:ILE:HD11	1.86	0.57
4:R:64:CYS:N	4:R:72:CYS:O	2.33	0.57
6:T:155:GLU:N	7:U:64:ASN:OD1	2.35	0.57
5:E:76:VAL:HG12	5:E:145:VAL:HG22	1.86	0.57
5:E:201:LEU:HD22	5:E:240:ILE:HG22	1.87	0.57
6:F:155:GLU:N	7:G:64:ASN:OD1	2.35	0.57
8:H:174:VAL:HG11	14:b:208:VAL:HG21	1.85	0.57
8:V:154:THR:OG1	8:V:179:GLN:NE2	2.35	0.57
4:D:118:LYS:O	4:D:122:SER:N	2.36	0.57
8:V:85:ILE:HG21	8:V:100:VAL:HB	1.87	0.57
12:Z:157:ARG:HA	12:Z:174:VAL:HG11	1.85	0.57
8:H:201:ILE:HD12	8:H:202:VAL:N	2.20	0.57
8:H:85:ILE:HG21	8:H:100:VAL:HB	1.87	0.57
12:L:202:THR:HG21	11:Y:144:TYR:CE1	2.40	0.57
5:S:76:VAL:HG12	5:S:145:VAL:HG22	1.86	0.57
5:S:201:LEU:HD22	5:S:240:ILE:HG22	1.87	0.57
11:K:144:TYR:CE1	12:Z:202:THR:HG21	2.40	0.57
10:J:153:SER:OG	13:a:192:SER:OG	2.15	0.56
12:L:157:ARG:HA	12:L:174:VAL:HG11	1.85	0.56
8:V:201:ILE:HD12	8:V:202:VAL:N	2.20	0.56
1:A:194:LEU:HD12	1:A:233:ILE:CG2	2.36	0.56
4:D:17:LEU:HD12	4:D:20:ILE:HD12	1.88	0.56
5:E:211:LYS:O	5:E:216:ASN:ND2	2.39	0.56
3:Q:39:PHE:HB3	3:Q:187:ALA:HB2	1.87	0.56
11:K:92:VAL:HG21	11:K:118:LEU:HD23	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:194:LEU:HD12	1:O:233:ILE:CG2	2.35	0.56
5:S:211:LYS:O	5:S:216:ASN:ND2	2.39	0.56
9:W:55:ILE:HD12	9:W:86:ARG:HD3	1.87	0.56
2:B:45:ALA:HB1	2:B:193:LEU:HD11	1.87	0.56
8:H:4:LEU:HD11	8:H:126:ILE:HD11	1.88	0.56
2:P:45:ALA:HB1	2:P:193:LEU:HD11	1.87	0.56
12:Z:3:THR:HG22	12:Z:16:VAL:HG12	1.88	0.56
7:U:38:LEU:HD11	7:U:191:VAL:HG13	1.88	0.56
2:B:201:LEU:HD21	2:B:206:ILE:CG2	2.36	0.56
9:I:55:ILE:HD12	9:I:86:ARG:HD3	1.87	0.56
9:I:129:SER:N	15:I:301:X5C:O52	2.39	0.56
5:E:168:ARG:NH1	6:F:58:SER:OG	2.39	0.56
12:L:3:THR:HG22	12:L:16:VAL:HG12	1.88	0.56
3:C:39:PHE:HB3	3:C:187:ALA:HB2	1.87	0.55
8:V:4:LEU:HD11	8:V:126:ILE:HD11	1.88	0.55
9:W:129:SER:N	15:W:301:X5C:O52	2.39	0.55
1:A:150:LYS:NZ	1:A:152:GLU:OE2	2.33	0.55
5:E:203:THR:O	5:E:207:VAL:HG22	2.05	0.55
7:G:38:LEU:HD11	7:G:191:VAL:HG13	1.88	0.55
2:P:44:ILE:HG23	2:P:135:ILE:CG2	2.36	0.55
5:E:84:ASP:OD2	5:E:137:ARG:NH1	2.39	0.55
2:P:88:LEU:HD11	2:P:112:ALA:HB2	1.88	0.55
2:B:44:ILE:HG23	2:B:135:ILE:CG2	2.36	0.55
9:I:19:ARG:NH1	9:I:167:LEU:O	2.38	0.55
9:W:129:SER:OG	9:W:166:ASP:OD2	2.20	0.55
4:D:64:CYS:N	4:D:72:CYS:O	2.33	0.55
13:M:34:ILE:HG21	13:M:64:SER:HB2	1.89	0.55
2:P:57:LYS:NZ	2:P:204:GLU:O	2.40	0.55
4:R:17:LEU:HD12	4:R:20:ILE:HD12	1.88	0.55
5:S:84:ASP:OD2	5:S:137:ARG:NH1	2.39	0.55
5:S:168:ARG:NH1	6:T:58:SER:OG	2.39	0.55
8:H:154:THR:OG1	8:H:179:GLN:NE2	2.35	0.55
3:Q:159:LYS:NZ	4:R:53:LYS:O	2.30	0.55
5:S:203:THR:O	5:S:207:VAL:HG22	2.05	0.55
11:Y:84:ILE:HD12	11:Y:103:LEU:HD22	1.89	0.55
9:I:129:SER:OG	9:I:166:ASP:OD2	2.21	0.55
10:X:79:GLU:OE1	10:X:81:ARG:NH1	2.40	0.55
10:J:79:GLU:OE1	10:J:81:ARG:NH1	2.40	0.55
11:K:84:ILE:HD12	11:K:103:LEU:HD22	1.89	0.55
14:b:50:ILE:CD1	14:b:66:ILE:HD13	2.37	0.55
2:B:88:LEU:HD11	2:B:112:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:118:TYR:CZ	2:P:122:ILE:HG21	2.43	0.54
3:C:110:VAL:HG22	3:C:135:ILE:HD12	1.90	0.54
3:C:141:HIS:CE1	11:K:73:VAL:HG21	2.42	0.54
10:J:145:GLU:OE1	10:J:145:GLU:N	2.38	0.54
1:O:124:LEU:HD23	2:P:125:VAL:HG12	1.90	0.54
2:P:201:LEU:HD21	2:P:206:ILE:CG2	2.36	0.54
1:A:61:THR:HG21	7:G:157:GLY:HA3	1.90	0.54
3:C:182:MET:HE1	3:C:190:LEU:HD22	1.89	0.54
1:O:61:THR:HG21	7:U:157:GLY:HA3	1.90	0.54
3:Q:110:VAL:HG22	3:Q:135:ILE:HD12	1.90	0.54
2:B:57:LYS:NZ	2:B:204:GLU:O	2.40	0.54
8:H:93:ARG:NH1	14:N:58:ASP:OD1	2.37	0.54
13:a:61:CYS:SG	13:a:99:VAL:HG11	2.48	0.54
7:G:184:VAL:O	7:G:188:VAL:HG23	2.08	0.54
13:M:18:MET:HE2	13:M:18:MET:CA	2.32	0.54
10:J:153:SER:OG	13:a:188:ASP:OD1	2.19	0.54
13:M:61:CYS:SG	13:M:99:VAL:HG11	2.48	0.54
11:Y:53:CYS:SG	11:Y:99:VAL:HG13	2.48	0.54
9:I:19:ARG:O	9:I:33:LYS:NZ	2.34	0.54
11:K:100:ASN:OD1	11:K:117:TYR:N	2.41	0.54
2:P:109:VAL:HG21	2:P:145:TRP:CG	2.43	0.54
3:Q:141:HIS:CE1	11:Y:73:VAL:HG21	2.42	0.54
7:U:69:TRP:O	7:U:93:ARG:NE	2.37	0.54
13:a:34:ILE:HG21	13:a:64:SER:HB2	1.89	0.54
3:C:153:GLY:O	4:D:82:ARG:NH2	2.40	0.54
12:L:74:LEU:HD21	12:L:82:ILE:HD11	1.90	0.54
2:B:118:TYR:CZ	2:B:122:ILE:HG21	2.42	0.54
3:Q:182:MET:HE1	3:Q:190:LEU:HD22	1.89	0.54
9:I:3:ILE:HG22	9:I:16:ALA:CB	2.39	0.53
13:a:159:LEU:HD13	13:a:189:ALA:HA	1.91	0.53
7:U:184:VAL:O	7:U:188:VAL:HG23	2.08	0.53
1:A:124:LEU:HD23	2:B:125:VAL:HG12	1.90	0.53
1:O:150:LYS:NZ	1:O:152:GLU:OE2	2.33	0.53
3:Q:91:THR:HG22	3:Q:95:LYS:HD3	1.91	0.53
7:U:115:GLU:HG2	8:V:69:THR:HG21	1.90	0.53
11:K:21:VAL:HG12	11:K:29:SER:HB3	1.89	0.53
3:Q:153:GLY:O	4:R:82:ARG:NH2	2.40	0.53
7:U:35:SER:O	7:U:66:ARG:NH2	2.41	0.53
5:E:213:ASN:O	5:E:217:VAL:HG12	2.08	0.53
13:M:159:LEU:HD13	13:M:189:ALA:HA	1.91	0.53
2:B:109:VAL:HG21	2:B:145:TRP:CG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:GLU:HG2	8:H:69:THR:HG21	1.90	0.53
11:K:102:LEU:HD11	11:K:128:ALA:HA	1.91	0.53
6:T:97:PHE:O	14:b:93:ARG:NE	2.41	0.53
9:W:77:ASP:OD1	9:W:78:GLN:N	2.42	0.53
11:Y:21:VAL:HG12	11:Y:29:SER:HB3	1.89	0.53
7:G:88:ILE:CG2	7:G:136:VAL:HG11	2.39	0.53
11:K:53:CYS:SG	11:K:99:VAL:HG13	2.48	0.53
5:S:213:ASN:O	5:S:217:VAL:HG12	2.08	0.53
9:W:19:ARG:NH1	9:W:167:LEU:O	2.38	0.53
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.89	0.53
12:Z:130:SER:OG	12:Z:167:ASP:OD2	2.26	0.53
9:I:77:ASP:OD1	9:I:78:GLN:N	2.42	0.53
14:N:50:ILE:CD1	14:N:66:ILE:HD13	2.37	0.53
2:P:201:LEU:HD11	2:P:206:ILE:HD13	1.91	0.53
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.89	0.52
12:L:130:SER:OG	12:L:167:ASP:OD2	2.26	0.52
9:W:3:ILE:HG22	9:W:16:ALA:CB	2.39	0.52
14:b:69:VAL:HG21	14:b:90:TYR:CE1	2.44	0.52
4:D:208:VAL:HG11	4:D:220:MET:HE3	1.89	0.52
12:L:3:THR:HG22	12:L:16:VAL:CG1	2.40	0.52
11:Y:128:ALA:HB3	11:Y:133:GLN:HA	1.92	0.52
11:K:128:ALA:HB3	11:K:133:GLN:HA	1.92	0.52
7:U:88:ILE:CG2	7:U:136:VAL:HG11	2.39	0.52
12:Z:74:LEU:HD21	12:Z:82:ILE:HD11	1.90	0.52
14:N:69:VAL:HG21	14:N:90:TYR:CE1	2.44	0.52
13:a:18:MET:HE2	13:a:18:MET:CA	2.32	0.52
14:b:126:ASP:OD1	14:b:130:ALA:N	2.43	0.52
3:C:91:THR:HG22	3:C:95:LYS:HD3	1.91	0.52
6:F:97:PHE:O	14:N:93:ARG:NE	2.41	0.52
5:E:41:LEU:O	5:E:187:TYR:OH	2.12	0.52
7:U:91:GLN:OE1	7:U:119:GLN:NE2	2.37	0.52
2:B:201:LEU:HD11	2:B:206:ILE:HD13	1.91	0.52
3:C:117:LYS:O	3:C:121:THR:HG23	2.10	0.52
3:C:159:LYS:N	4:D:54:LEU:O	2.43	0.52
8:V:93:ARG:NH1	14:b:58:ASP:OD1	2.37	0.52
4:R:208:VAL:HG11	4:R:220:MET:HE3	1.89	0.52
12:Z:3:THR:HG22	12:Z:16:VAL:CG1	2.40	0.52
6:F:81:GLY:HA2	6:F:130:VAL:HG11	1.92	0.52
7:G:51:GLU:O	7:G:66:ARG:NH1	2.43	0.52
2:P:66:ILE:HD13	2:P:88:LEU:HD13	1.91	0.52
14:b:200:GLN:NE2	14:b:202:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ASP:OD1	2:B:130:VAL:HG13	2.10	0.52
9:I:161:ALA:HB1	14:b:147:GLY:HA2	1.92	0.52
14:N:126:ASP:OD1	14:N:130:ALA:N	2.43	0.52
6:T:81:GLY:HA2	6:T:130:VAL:HG11	1.92	0.52
8:H:66:LEU:HD22	8:H:80:VAL:HG11	1.92	0.51
11:K:7:LEU:HD11	11:K:144:TYR:HD2	1.76	0.51
12:L:134:HIS:HB2	12:L:163:ALA:HA	1.92	0.51
8:V:66:LEU:HD22	8:V:80:VAL:HG11	1.92	0.51
11:Y:102:LEU:HD11	11:Y:128:ALA:HA	1.91	0.51
2:B:117:GLN:O	2:B:120:THR:OG1	2.19	0.51
3:Q:43:VAL:HB	3:Q:136:ALA:HB1	1.93	0.51
2:P:117:GLN:O	2:P:120:THR:OG1	2.19	0.51
2:B:66:ILE:HD13	2:B:88:LEU:HD13	1.91	0.51
14:N:62:LEU:CD2	14:N:66:ILE:HD11	2.41	0.51
10:X:145:GLU:OE1	10:X:145:GLU:N	2.38	0.51
14:b:62:LEU:CD2	14:b:66:ILE:HD11	2.41	0.51
4:D:3:ASP:OD1	4:D:4:TYR:N	2.44	0.51
4:D:188:GLN:NE2	4:D:220:MET:HE2	2.26	0.51
6:F:92:CYS:SG	6:F:108:LEU:HD11	2.51	0.51
14:N:147:GLY:HA2	9:W:161:ALA:HB1	1.92	0.51
3:Q:117:LYS:O	3:Q:121:THR:HG23	2.10	0.51
11:Y:100:ASN:OD1	11:Y:117:TYR:N	2.41	0.51
7:U:188:VAL:HG13	7:U:210:MET:SD	2.51	0.51
11:Y:15:ILE:HG23	11:Y:15:ILE:O	2.10	0.51
1:A:46:VAL:HG12	1:A:65:MET:HE1	1.93	0.51
7:G:115:GLU:CG	8:H:69:THR:HG21	2.41	0.51
7:G:188:VAL:HG13	7:G:210:MET:SD	2.51	0.51
7:U:115:GLU:CG	8:V:69:THR:HG21	2.41	0.51
10:X:24:ALA:C	10:X:43:ILE:HD11	2.36	0.51
1:A:48:VAL:HG11	1:A:64:HIS:HB2	1.93	0.51
2:B:143:THR:HG22	3:C:59:LEU:HD13	1.93	0.51
6:F:88:LEU:HD21	6:F:112:VAL:CG2	2.41	0.51
1:O:46:VAL:HG12	1:O:65:MET:HE1	1.93	0.51
4:R:64:CYS:O	4:R:72:CYS:N	2.30	0.51
9:I:222:ILE:N	10:J:200:GLU:O	2.45	0.51
13:M:26:ILE:HD12	13:M:186:VAL:HG23	1.93	0.51
2:P:143:THR:HG22	3:Q:59:LEU:HD13	1.93	0.51
4:R:3:ASP:OD1	4:R:4:TYR:N	2.44	0.51
7:U:51:GLU:O	7:U:66:ARG:NH1	2.43	0.51
11:Y:46:MET:HE2	11:Y:99:VAL:HG11	1.93	0.51
12:Z:34:ILE:HG23	12:Z:42:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:44:VAL:HG11	14:b:50:ILE:HD12	1.93	0.51
6:F:177:ASN:OD1	6:F:177:ASN:N	2.44	0.50
4:R:117:LEU:HD13	5:S:83:ALA:CB	2.41	0.50
6:T:92:CYS:SG	6:T:108:LEU:HD11	2.51	0.50
13:a:75:PHE:HZ	13:a:103:VAL:HG13	1.76	0.50
3:C:24:ALA:HB1	3:C:130:GLY:HA2	1.93	0.50
4:D:117:LEU:HD13	5:E:83:ALA:CB	2.41	0.50
2:P:80:ASP:OD1	2:P:130:VAL:HG13	2.10	0.50
4:R:153:GLY:O	5:S:86:ARG:NH1	2.43	0.50
7:U:70:ILE:HG21	7:U:112:LEU:HD21	1.93	0.50
14:b:96:TYR:O	14:b:99:ARG:HG3	2.12	0.50
7:G:91:GLN:OE1	7:G:119:GLN:NE2	2.37	0.50
5:S:105:GLU:OE2	13:a:86:TYR:OH	2.08	0.50
4:D:99:TYR:CD2	12:L:82:ILE:HD11	2.47	0.50
7:G:35:SER:O	7:G:66:ARG:NH2	2.41	0.50
7:U:66:ARG:N	7:U:209:GLU:OE1	2.35	0.50
12:Z:134:HIS:HB2	12:Z:163:ALA:HA	1.92	0.50
1:A:12:PHE:O	2:B:19:GLN:NE2	2.45	0.50
3:C:43:VAL:HB	3:C:136:ALA:HB1	1.93	0.50
14:N:96:TYR:O	14:N:99:ARG:HG3	2.12	0.50
6:T:88:LEU:HD21	6:T:112:VAL:CG2	2.41	0.50
13:a:33:VAL:HG22	13:a:208:VAL:HG22	1.93	0.50
1:A:50:LYS:NZ	1:A:62:VAL:O	2.37	0.50
4:D:69:HIS:NE2	4:D:103:ILE:O	2.39	0.50
5:E:113:THR:O	5:E:116:VAL:HG12	2.11	0.50
11:K:15:ILE:HG23	11:K:15:ILE:O	2.10	0.50
1:O:48:VAL:HG11	1:O:64:HIS:HB2	1.93	0.50
2:P:81:PHE:HB2	2:P:130:VAL:HG11	1.93	0.50
5:S:113:THR:O	5:S:116:VAL:HG12	2.11	0.50
2:B:81:PHE:HB2	2:B:130:VAL:HG11	1.93	0.50
11:K:137:MET:HE2	11:K:137:MET:HA	1.94	0.50
14:N:200:GLN:NE2	14:N:202:ASP:OD1	2.43	0.50
4:R:188:GLN:NE2	4:R:220:MET:HE2	2.26	0.50
6:F:50:MET:HE3	6:F:61:PRO:HA	1.94	0.50
7:G:188:VAL:HG11	7:G:229:PHE:HB2	1.93	0.50
10:J:24:ALA:C	10:J:43:ILE:HD11	2.36	0.50
13:M:203:ALA:O	13:M:221:LEU:HD12	2.12	0.50
7:U:42:CYS:N	7:U:45:GLY:O	2.43	0.50
11:Y:2:LEU:O	11:Y:47:SER:OG	2.21	0.50
11:Y:137:MET:HA	11:Y:137:MET:HE2	1.94	0.50
11:K:35:ILE:O	11:K:178:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:24:ALA:HB1	3:Q:130:GLY:HA2	1.93	0.50
10:X:31:VAL:HG23	10:X:36:VAL:HG21	1.94	0.50
13:a:193:VAL:O	13:a:197:ASP:N	2.31	0.50
14:N:44:VAL:HG11	14:N:50:ILE:HD12	1.93	0.49
4:R:99:TYR:CD2	12:Z:82:ILE:HD11	2.47	0.49
4:D:33:VAL:HG22	4:D:46:VAL:HG13	1.94	0.49
7:G:70:ILE:HG21	7:G:112:LEU:HD21	1.93	0.49
11:K:46:MET:HE2	11:K:99:VAL:HG11	1.93	0.49
12:L:34:ILE:HG23	12:L:42:ILE:HD13	1.93	0.49
3:Q:159:LYS:N	4:R:54:LEU:O	2.44	0.49
5:S:11:ASN:OD1	5:S:14:THR:OG1	2.30	0.49
7:G:27:ALA:HB1	7:G:133:GLY:HA2	1.95	0.49
6:T:50:MET:HE3	6:T:61:PRO:HA	1.94	0.49
7:U:188:VAL:HG11	7:U:229:PHE:HB2	1.93	0.49
9:W:3:ILE:HG22	9:W:16:ALA:HB2	1.94	0.49
14:b:124:CYS:HB2	14:b:137:ILE:HD13	1.95	0.49
11:Y:7:LEU:HD11	11:Y:144:TYR:HD2	1.76	0.49
13:a:203:ALA:O	13:a:221:LEU:HD12	2.12	0.49
12:L:45:MET:HG2	12:L:56:LEU:HD12	1.95	0.49
13:M:33:VAL:HG22	13:M:208:VAL:HG22	1.93	0.49
8:V:55:LEU:HD21	8:V:96:LEU:HD23	1.95	0.49
13:a:26:ILE:HD12	13:a:186:VAL:HG23	1.93	0.49
4:D:113:ALA:HB1	4:D:153:GLY:O	2.13	0.49
8:H:55:LEU:HD21	8:H:96:LEU:HD23	1.95	0.49
4:R:33:VAL:HG22	4:R:46:VAL:HG13	1.94	0.49
7:U:27:ALA:HB1	7:U:133:GLY:HA2	1.95	0.49
11:Y:12:TRP:CH2	11:Y:153:GLY:HA3	2.47	0.49
13:M:75:PHE:HZ	13:M:103:VAL:HG13	1.76	0.49
4:D:196:LEU:HA	4:D:199:VAL:HG22	1.94	0.49
4:R:46:VAL:HG11	4:R:62:LYS:CG	2.43	0.49
1:O:45:CYS:HB2	1:O:214:LEU:HD13	1.95	0.49
3:Q:148:LEU:HD11	3:Q:163:ILE:HG21	1.95	0.49
1:O:12:PHE:O	2:P:19:GLN:NE2	2.45	0.49
2:P:73:VAL:HG22	2:P:74:TYR:H	1.77	0.49
6:F:108:LEU:HB3	6:F:134:MET:HE1	1.95	0.48
6:T:192:LEU:HD21	6:T:228:LEU:HD21	1.95	0.48
2:B:73:VAL:HG22	2:B:74:TYR:H	1.78	0.48
4:D:46:VAL:HG11	4:D:62:LYS:CG	2.43	0.48
11:K:12:TRP:CH2	11:K:153:GLY:HA3	2.47	0.48
13:M:118:ASN:HB2	13:M:149:ASN:HB3	1.95	0.48
9:W:222:ILE:N	10:X:200:GLU:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:51:LYS:NZ	14:b:131:SER:O	2.38	0.48
12:Z:45:MET:HG2	12:Z:56:LEU:HD12	1.95	0.48
7:G:69:TRP:O	7:G:93:ARG:NE	2.37	0.48
1:O:50:LYS:NZ	1:O:62:VAL:O	2.37	0.48
6:T:49:VAL:HG22	6:T:209:ILE:HG12	1.96	0.48
6:T:108:LEU:HB3	6:T:134:MET:HE1	1.95	0.48
4:D:63:ILE:HG21	4:D:209:ALA:HB3	1.96	0.48
6:F:192:LEU:HD21	6:F:228:LEU:HD21	1.94	0.48
4:R:196:LEU:HA	4:R:199:VAL:HG22	1.94	0.48
9:W:5:ALA:HB3	9:W:99:ILE:CG2	2.43	0.48
14:b:163:LYS:O	14:b:167:GLU:HG3	2.14	0.48
10:J:31:VAL:HG23	10:J:36:VAL:HG21	1.94	0.48
4:R:113:ALA:HB1	4:R:153:GLY:O	2.13	0.48
5:E:223:ARG:O	5:E:227:GLY:N	2.47	0.48
4:D:110:ARG:NH2	12:L:69:ARG:O	2.34	0.48
9:I:3:ILE:HG22	9:I:16:ALA:HB2	1.95	0.48
1:O:67:ARG:O	1:O:91:ARG:NE	2.44	0.48
4:R:33:VAL:HG13	4:R:46:VAL:HG22	1.96	0.48
5:S:223:ARG:O	5:S:227:GLY:N	2.47	0.48
3:C:46:ALA:HB1	3:C:195:LEU:HD11	1.96	0.48
7:G:42:CYS:N	7:G:45:GLY:O	2.44	0.48
14:N:124:CYS:HB2	14:N:137:ILE:HD13	1.95	0.48
14:N:163:LYS:O	14:N:167:GLU:HG3	2.13	0.48
4:R:140:MET:O	4:R:213:ARG:NH1	2.41	0.48
11:Y:8:GLN:N	11:Y:125:PRO:O	2.42	0.48
4:D:195:LEU:O	4:D:199:VAL:HG13	2.14	0.48
5:E:50:VAL:HB	5:E:77:VAL:HG21	1.96	0.48
6:F:49:VAL:HG22	6:F:209:ILE:HG12	1.96	0.48
4:R:195:LEU:O	4:R:199:VAL:HG13	2.14	0.48
5:S:50:VAL:HB	5:S:77:VAL:HG21	1.96	0.48
4:D:33:VAL:HG13	4:D:46:VAL:HG22	1.96	0.47
4:D:140:MET:O	4:D:213:ARG:NH1	2.41	0.47
5:E:13:ASN:ND2	6:F:124:GLY:O	2.47	0.47
13:a:135:TYR:HA	13:a:140:THR:O	2.14	0.47
14:b:110:ILE:HD13	14:b:124:CYS:HB2	1.95	0.47
3:C:28:ILE:HD13	3:C:132:SER:HB2	1.96	0.47
13:a:118:ASN:HB2	13:a:149:ASN:HB3	1.95	0.47
13:a:194:THR:HG21	13:a:222:PRO:HD2	1.97	0.47
14:b:3:VAL:HG12	14:b:6:ALA:HB2	1.97	0.47
9:I:5:ALA:HB3	9:I:99:ILE:CG2	2.43	0.47
12:L:74:LEU:HD21	12:L:82:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:74:LEU:HD21	12:Z:82:ILE:CD1	2.45	0.47
1:A:157:SER:O	2:B:60:ASN:ND2	2.45	0.47
3:C:148:LEU:HD11	3:C:163:ILE:HG21	1.95	0.47
5:E:21:LEU:HD21	6:F:126:ARG:HD2	1.97	0.47
9:I:11:GLY:HA2	9:I:103:ILE:HD11	1.96	0.47
12:L:141:THR:CG2	11:Y:159:LEU:HD21	2.45	0.47
13:M:135:TYR:HA	13:M:140:THR:O	2.14	0.47
6:F:140:ASP:OD1	6:F:140:ASP:N	2.48	0.47
3:Q:46:ALA:HB1	3:Q:195:LEU:HD11	1.96	0.47
5:S:13:ASN:ND2	6:T:124:GLY:O	2.47	0.47
1:A:45:CYS:HB2	1:A:214:LEU:HD13	1.95	0.47
3:C:225:ARG:NH2	3:C:231:GLU:OE1	2.47	0.47
4:D:64:CYS:O	4:D:72:CYS:N	2.30	0.47
8:H:26:ILE:HB	14:b:175:ARG:HA	1.97	0.47
12:L:18:SER:OG	12:L:29:GLN:O	2.23	0.47
14:N:110:ILE:HD13	14:N:124:CYS:HB2	1.95	0.47
2:P:105:THR:O	2:P:109:VAL:HG23	2.15	0.47
3:Q:225:ARG:NH2	3:Q:231:GLU:OE1	2.47	0.47
5:S:21:LEU:HD21	6:T:126:ARG:HD2	1.97	0.47
5:S:76:VAL:HG11	5:S:92:MET:SD	2.55	0.47
6:T:50:MET:HE2	6:T:59:HIS:O	2.15	0.47
11:Y:127:GLY:HA2	11:Y:137:MET:HE1	1.97	0.47
5:E:76:VAL:HG11	5:E:92:MET:SD	2.55	0.47
6:F:50:MET:HE2	6:F:59:HIS:O	2.15	0.47
10:J:14:ALA:HB1	10:J:122:LEU:HD22	1.97	0.47
13:M:194:THR:HG21	13:M:222:PRO:HD2	1.96	0.47
3:Q:106:VAL:O	3:Q:110:VAL:HG23	2.15	0.47
4:R:10:ARG:NH1	5:S:10:ARG:O	2.48	0.47
5:S:46:VAL:CG1	5:S:222:ALA:HB3	2.45	0.47
1:A:67:ARG:O	1:A:91:ARG:NE	2.44	0.47
4:D:31:THR:HG22	4:D:32:THR:N	2.30	0.47
5:E:11:ASN:OD1	5:E:14:THR:OG1	2.30	0.47
3:Q:28:ILE:HD11	3:Q:151:PRO:HG3	1.97	0.47
6:T:116:SER:HB2	6:T:151:GLY:HA2	1.97	0.47
1:A:194:LEU:HD12	1:A:233:ILE:HG21	1.97	0.47
2:B:93:ILE:HG23	9:I:61:ALA:HB1	1.96	0.47
11:K:159:LEU:HD21	12:Z:141:THR:CG2	2.44	0.47
14:N:181:GLY:HA2	8:V:199:TYR:CG	2.50	0.47
4:R:63:ILE:HG21	4:R:209:ALA:HB3	1.96	0.47
13:a:37:ASP:O	13:a:53:ARG:NH2	2.48	0.47
6:F:183:THR:HG22	6:F:184:ARG:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:93:ILE:HG23	9:W:61:ALA:HB1	1.97	0.46
5:E:46:VAL:CG1	5:E:222:ALA:HB3	2.45	0.46
8:H:199:TYR:CG	14:b:181:GLY:HA2	2.50	0.46
9:I:141:ARG:HB2	9:I:154:MET:HG3	1.98	0.46
6:T:7:ASP:OD1	6:T:21:GLN:NE2	2.41	0.46
14:N:175:ARG:HA	8:V:26:ILE:HB	1.97	0.46
2:P:64:GLN:HG3	2:P:85:LEU:HD22	1.97	0.46
4:R:42:ILE:HG21	4:R:135:CYS:HB3	1.98	0.46
12:Z:172:GLY:O	12:Z:192:VAL:HG22	2.16	0.46
8:H:198:ASN:O	8:H:201:ILE:HG13	2.15	0.46
9:I:47:GLY:O	15:I:301:X5C:N36	2.48	0.46
10:J:29:LEU:HB2	10:J:40:PHE:HB2	1.97	0.46
11:K:8:GLN:N	11:K:125:PRO:O	2.42	0.46
1:O:194:LEU:HD12	1:O:233:ILE:HG21	1.97	0.46
3:Q:28:ILE:HD13	3:Q:132:SER:HB2	1.96	0.46
11:Y:35:ILE:O	11:Y:178:LYS:NZ	2.45	0.46
14:b:50:ILE:HD13	14:b:91:ILE:HD11	1.97	0.46
1:A:76:LEU:HB2	1:A:83:VAL:HG13	1.98	0.46
7:G:66:ARG:N	7:G:209:GLU:OE1	2.35	0.46
9:W:225:THR:HG23	10:X:198:ILE:HB	1.98	0.46
1:A:119:GLN:HB2	2:B:79:THR:HG22	1.97	0.46
2:B:105:THR:O	2:B:109:VAL:HG23	2.15	0.46
3:C:28:ILE:HD11	3:C:151:PRO:HG3	1.97	0.46
6:F:116:SER:HB2	6:F:151:GLY:HA2	1.97	0.46
1:O:157:SER:O	2:P:60:ASN:ND2	2.45	0.46
9:W:11:GLY:HA2	9:W:103:ILE:HD11	1.96	0.46
14:N:31:SER:O	8:V:169:GLY:N	2.48	0.46
1:O:28:VAL:HG21	1:O:153:PRO:HG3	1.98	0.46
1:O:119:GLN:HB2	2:P:79:THR:HG22	1.97	0.46
3:Q:190:LEU:O	3:Q:194:VAL:HG23	2.16	0.46
9:W:47:GLY:O	15:W:301:X5C:N36	2.48	0.46
13:a:75:PHE:CZ	13:a:103:VAL:HG13	2.50	0.46
3:C:190:LEU:O	3:C:194:VAL:HG23	2.16	0.46
12:L:97:ILE:O	12:L:115:ASP:HA	2.16	0.46
14:N:50:ILE:HD13	14:N:91:ILE:HD11	1.97	0.46
14:N:113:GLY:HA2	14:N:188:VAL:HG11	1.98	0.46
4:R:31:THR:HG22	4:R:32:THR:N	2.30	0.46
4:R:69:HIS:NE2	4:R:103:ILE:O	2.39	0.46
4:R:88:GLY:CA	4:R:112:ILE:HD11	2.46	0.46
8:V:15:ALA:HB2	8:V:177:ILE:HD13	1.98	0.46
9:W:142:TRP:HD1	9:W:154:MET:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:SER:OG	2:B:9:THR:O	2.34	0.46
4:D:209:ALA:HB2	4:D:219:ILE:HD13	1.97	0.46
9:I:47:GLY:H	15:I:301:X5C:C46	2.29	0.46
11:K:127:GLY:HA2	11:K:137:MET:HE1	1.97	0.46
13:M:75:PHE:CZ	13:M:103:VAL:HG13	2.50	0.46
14:N:3:VAL:HG12	14:N:6:ALA:HB2	1.97	0.46
3:Q:45:LEU:CB	3:Q:64:MET:HE1	2.46	0.46
4:R:99:TYR:HD2	12:Z:82:ILE:HD11	1.81	0.46
4:D:10:ARG:NH1	5:E:10:ARG:O	2.48	0.46
13:M:37:ASP:O	13:M:53:ARG:NH2	2.48	0.46
4:R:117:LEU:HD13	5:S:83:ALA:HB1	1.98	0.46
8:V:198:ASN:O	8:V:201:ILE:HG13	2.15	0.46
1:A:28:VAL:HG21	1:A:153:PRO:HG3	1.98	0.45
2:B:49:LYS:HD3	2:B:205:LEU:HD22	1.98	0.45
5:E:13:ASN:HB3	6:F:126:ARG:HB2	1.98	0.45
11:K:64:VAL:HG22	11:K:80:LEU:HD13	1.98	0.45
2:P:49:LYS:HD3	2:P:205:LEU:HD22	1.98	0.45
11:Y:64:VAL:HG22	11:Y:80:LEU:HD13	1.98	0.45
12:Z:97:ILE:O	12:Z:115:ASP:HA	2.16	0.45
14:b:113:GLY:HA2	14:b:188:VAL:HG11	1.98	0.45
2:B:64:GLN:HG3	2:B:85:LEU:HD22	1.97	0.45
2:B:156:TRP:CD1	2:B:159:THR:HG1	2.34	0.45
3:C:106:VAL:O	3:C:110:VAL:HG23	2.15	0.45
9:I:22:ALA:HB2	9:I:27:ALA:HB2	1.98	0.45
10:J:206:ASP:OXT	12:Z:19:ARG:NH1	2.50	0.45
13:M:79:MET:O	13:M:83:LEU:HD13	2.17	0.45
9:W:141:ARG:HB2	9:W:154:MET:HG3	1.98	0.45
1:O:128:ARG:HB2	7:U:13:ILE:HB	1.98	0.45
4:R:209:ALA:HB2	4:R:219:ILE:HD13	1.97	0.45
6:T:140:ASP:OD1	6:T:140:ASP:N	2.48	0.45
9:W:22:ALA:HB2	9:W:27:ALA:HB2	1.98	0.45
9:W:47:GLY:H	15:W:301:X5C:C46	2.29	0.45
1:A:95:ASN:CG	8:H:64:ASN:HB3	2.42	0.45
8:H:15:ALA:HB2	8:H:177:ILE:HD13	1.98	0.45
13:M:197:ASP:OD2	13:M:200:THR:OG1	2.34	0.45
2:P:156:TRP:CD1	2:P:159:THR:HG1	2.34	0.45
4:D:42:ILE:HG21	4:D:135:CYS:HB3	1.98	0.45
4:D:88:GLY:CA	4:D:112:ILE:HD11	2.46	0.45
4:D:117:LEU:HD11	4:D:121:GLN:NE2	2.32	0.45
8:H:4:LEU:HD23	8:H:157:ALA:HA	1.98	0.45
8:H:92:TYR:O	8:H:96:LEU:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:ALA:HA	10:J:187:ILE:O	2.17	0.45
2:P:164:ARG:NH1	2:P:198:ASP:OD2	2.49	0.45
5:S:13:ASN:HB3	6:T:126:ARG:HB2	1.99	0.45
6:T:183:THR:HG22	6:T:184:ARG:N	2.30	0.45
10:X:14:ALA:HB1	10:X:122:LEU:HD22	1.97	0.45
10:X:29:LEU:HB2	10:X:40:PHE:HB2	1.97	0.45
13:a:79:MET:O	13:a:83:LEU:HD13	2.17	0.45
4:D:99:TYR:HD2	12:L:82:ILE:HD11	1.81	0.45
4:D:153:GLY:O	5:E:86:ARG:NH1	2.43	0.45
12:L:172:GLY:O	12:L:192:VAL:HG22	2.16	0.45
5:S:117:CYS:SG	5:S:158:THR:HB	2.57	0.45
11:Y:7:LEU:HD11	11:Y:144:TYR:CD2	2.51	0.45
4:D:117:LEU:HD13	5:E:83:ALA:HB1	1.98	0.45
12:L:19:ARG:NH1	10:X:206:ASP:OXT	2.50	0.45
2:P:61:LEU:O	2:P:64:GLN:NE2	2.50	0.45
9:W:28:VAL:CG2	10:X:132:ALA:HB2	2.45	0.45
2:B:164:ARG:NH1	2:B:198:ASP:OD2	2.49	0.45
6:F:123:VAL:HG22	7:G:128:ALA:HB1	1.98	0.45
9:I:142:TRP:HD1	9:I:154:MET:HE1	1.80	0.45
6:T:123:VAL:HG22	7:U:128:ALA:HB1	1.98	0.45
12:Z:50:ALA:N	13:a:140:THR:OG1	2.50	0.45
1:A:128:ARG:HB2	7:G:13:ILE:HB	1.98	0.45
8:H:138:ALA:CB	8:V:136:ILE:HG22	2.47	0.45
9:I:6:ALA:HB3	9:I:151:CYS:SG	2.57	0.45
11:K:38:LEU:HD11	11:K:44:LEU:HD22	1.98	0.45
12:L:50:ALA:N	13:M:140:THR:OG1	2.50	0.45
1:O:95:ASN:CG	8:V:64:ASN:HB3	2.42	0.45
8:H:136:ILE:HG22	8:V:138:ALA:CB	2.47	0.45
8:H:150:MET:HE1	8:H:181:ASN:HB3	1.99	0.45
9:I:225:THR:HG23	10:J:198:ILE:HB	1.98	0.45
11:K:7:LEU:HD11	11:K:144:TYR:CD2	2.51	0.45
1:O:46:VAL:HG21	1:O:137:PHE:CD1	2.52	0.45
7:U:20:ARG:NH2	7:U:25:GLU:OE2	2.49	0.45
8:V:150:MET:HE1	8:V:181:ASN:HB3	1.99	0.45
10:X:24:ALA:HA	10:X:187:ILE:O	2.17	0.45
1:A:38:VAL:HG21	1:A:192:PHE:CD2	2.53	0.44
1:A:186:PRO:HB3	1:A:216:THR:HG22	2.00	0.44
3:C:45:LEU:CB	3:C:64:MET:HE1	2.46	0.44
5:E:76:VAL:HG21	5:E:89:VAL:HG22	1.99	0.44
6:F:74:ILE:HG22	6:F:132:LEU:HD22	1.99	0.44
6:F:158:ALA:O	7:G:58:LEU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:76:LEU:HB2	1:O:83:VAL:HG13	1.98	0.44
6:T:177:ASN:OD1	6:T:177:ASN:N	2.44	0.44
8:V:4:LEU:HD23	8:V:157:ALA:HA	1.98	0.44
9:W:6:ALA:HB3	9:W:151:CYS:SG	2.57	0.44
5:E:59:LEU:HD21	5:E:64:VAL:HG21	1.99	0.44
9:I:8:PHE:HB3	9:I:151:CYS:HB2	2.00	0.44
4:R:117:LEU:HD11	4:R:121:GLN:NE2	2.32	0.44
6:T:17:GLY:O	7:U:33:LYS:NZ	2.50	0.44
6:T:158:ALA:O	7:U:58:LEU:HB3	2.18	0.44
8:V:92:TYR:O	8:V:96:LEU:N	2.46	0.44
12:L:42:ILE:HG12	12:L:179:ILE:HD11	1.99	0.44
13:M:51:LYS:NZ	14:N:131:SER:O	2.38	0.44
13:M:193:VAL:O	13:M:197:ASP:N	2.31	0.44
1:O:69:THR:CG2	1:O:94:ALA:HB1	2.47	0.44
11:Y:46:MET:SD	11:Y:57:SER:HB3	2.57	0.44
5:E:21:LEU:HD21	6:F:126:ARG:HD3	1.98	0.44
1:O:140:ASP:O	1:O:144:ASP:N	2.50	0.44
2:P:38:ALA:HB2	2:P:185:ALA:HB2	1.99	0.44
3:Q:134:LEU:HG	3:Q:163:ILE:HD11	2.00	0.44
12:Z:42:ILE:HG12	12:Z:179:ILE:HD11	1.99	0.44
12:Z:103:GLY:HA2	12:Z:179:ILE:HG21	2.00	0.44
13:a:32:VAL:HG11	13:a:122:GLY:HA3	1.99	0.44
1:A:69:THR:CG2	1:A:94:ALA:HB1	2.47	0.44
6:F:17:GLY:O	7:G:33:LYS:NZ	2.50	0.44
8:H:5:ALA:CB	8:H:101:ILE:HG21	2.47	0.44
11:K:46:MET:SD	11:K:57:SER:HB3	2.57	0.44
14:N:65:VAL:O	14:N:69:VAL:HG23	2.18	0.44
6:T:171:TYR:CD2	6:T:194:ALA:HB2	2.52	0.44
4:D:97:LEU:HD13	4:D:97:LEU:C	2.43	0.44
6:F:171:TYR:CD2	6:F:194:ALA:HB2	2.52	0.44
2:P:84:ILE:HG21	2:P:132:LEU:HD11	2.00	0.44
6:T:192:LEU:HD13	6:T:232:ILE:HA	2.00	0.44
2:B:61:LEU:O	2:B:64:GLN:NE2	2.50	0.44
3:C:76:ALA:HB3	3:C:163:ILE:HD12	2.00	0.44
3:C:134:LEU:HG	3:C:163:ILE:HD11	2.00	0.44
5:E:117:CYS:SG	5:E:158:THR:HB	2.57	0.44
5:E:193:LEU:HD13	5:E:193:LEU:O	2.17	0.44
6:F:192:LEU:HD13	6:F:232:ILE:HA	2.00	0.44
9:I:160:TYR:OH	13:a:223:ARG:NH2	2.51	0.44
5:S:21:LEU:HD21	6:T:126:ARG:HD3	1.98	0.44
9:W:8:PHE:HB3	9:W:151:CYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:66:PHE:O	9:W:70:THR:OG1	2.22	0.44
9:W:123:PRO:HB2	9:W:142:TRP:CZ2	2.53	0.44
11:Y:38:LEU:HD11	11:Y:44:LEU:HD22	1.98	0.44
14:b:65:VAL:O	14:b:69:VAL:HG23	2.18	0.44
3:C:46:ALA:HB1	3:C:195:LEU:CD1	2.48	0.44
8:H:102:VAL:O	8:H:102:VAL:HG13	2.18	0.44
8:H:169:GLY:N	14:b:31:SER:O	2.48	0.44
1:O:44:VAL:HG13	1:O:44:VAL:O	2.18	0.44
2:P:43:VAL:HG21	2:P:186:ILE:HG13	2.00	0.44
5:S:59:LEU:HD21	5:S:64:VAL:HG21	1.99	0.44
12:Z:4:LEU:C	12:Z:4:LEU:HD12	2.43	0.44
13:M:63:ILE:HG12	13:M:121:VAL:HG22	2.00	0.44
13:M:103:VAL:HG11	13:M:119:ILE:HG21	2.00	0.44
5:S:76:VAL:HG21	5:S:89:VAL:HG22	1.99	0.44
13:a:197:ASP:OD2	13:a:200:THR:OG1	2.34	0.44
14:b:49:ILE:CD1	14:b:186:ILE:HD13	2.48	0.44
1:A:46:VAL:HG21	1:A:137:PHE:CD1	2.52	0.43
2:B:38:ALA:HB2	2:B:185:ALA:HB2	1.99	0.43
7:G:75:ALA:HB2	7:G:221:PRO:HB3	2.00	0.43
13:M:151:SER:OG	13:M:197:ASP:OD2	2.33	0.43
5:S:193:LEU:HD13	5:S:193:LEU:O	2.17	0.43
8:V:102:VAL:HG13	8:V:102:VAL:O	2.18	0.43
1:A:140:ASP:O	1:A:144:ASP:N	2.50	0.43
3:C:81:ASP:OD1	3:C:82:ALA:N	2.51	0.43
7:G:20:ARG:NH2	7:G:25:GLU:OE2	2.49	0.43
8:H:116:GLU:HG3	14:N:5:THR:HG21	2.00	0.43
9:I:28:VAL:CG2	10:J:132:ALA:HB2	2.45	0.43
14:N:94:TYR:HE2	14:N:105:LEU:HD11	1.83	0.43
1:O:38:VAL:HG21	1:O:192:PHE:CD2	2.52	0.43
2:P:7:SER:OG	2:P:9:THR:O	2.34	0.43
12:Z:42:ILE:CG1	12:Z:179:ILE:HD11	2.48	0.43
2:B:73:VAL:HG22	2:B:74:TYR:N	2.33	0.43
12:L:4:LEU:HD12	12:L:4:LEU:C	2.43	0.43
14:N:40:HIS:O	14:N:51:GLY:HA2	2.18	0.43
1:O:28:VAL:HA	1:O:78:GLY:HA2	2.01	0.43
2:P:118:TYR:O	2:P:122:ILE:HG12	2.19	0.43
7:U:75:ALA:HB2	7:U:221:PRO:HB3	2.00	0.43
8:V:92:TYR:HB2	8:V:96:LEU:HD22	2.00	0.43
8:V:116:GLU:HG3	14:b:5:THR:HG21	2.00	0.43
13:a:63:ILE:HG12	13:a:121:VAL:HG22	2.00	0.43
1:A:44:VAL:HG13	1:A:44:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:37:ALA:HB2	5:E:50:VAL:HG23	2.01	0.43
5:E:240:ILE:O	5:E:244:LEU:HD23	2.18	0.43
9:I:13:VAL:HG11	9:I:152:MET:HA	2.01	0.43
10:J:42:ARG:NH1	10:J:61:VAL:HG21	2.33	0.43
12:L:103:GLY:HA2	12:L:179:ILE:HG21	2.00	0.43
12:L:173:ARG:NH1	13:M:170:ASN:O	2.52	0.43
13:M:18:MET:HA	13:M:18:MET:CE	2.37	0.43
9:W:173:VAL:O	9:W:198:TYR:N	2.52	0.43
10:X:42:ARG:NH1	10:X:61:VAL:HG21	2.33	0.43
10:X:54:LEU:HB3	10:X:106:VAL:HG21	2.00	0.43
14:b:124:CYS:CB	14:b:137:ILE:HD13	2.49	0.43
7:G:135:THR:HG21	7:G:163:PHE:CD1	2.54	0.43
8:H:166:ILE:HG23	8:H:199:TYR:HA	2.00	0.43
13:M:41:SER:HB2	9:W:167:LEU:HD11	2.00	0.43
14:N:41:PHE:CD2	14:N:186:ILE:HD12	2.54	0.43
5:S:240:ILE:O	5:S:244:LEU:HD23	2.17	0.43
6:T:74:ILE:HG22	6:T:132:LEU:HD22	1.99	0.43
8:V:5:ALA:CB	8:V:101:ILE:HG21	2.47	0.43
1:A:72:VAL:HG13	1:A:107:VAL:HG22	2.00	0.43
6:F:188:ILE:HG23	6:F:211:LEU:HD13	2.00	0.43
7:G:148:ALA:HB3	7:G:158:TYR:CE1	2.54	0.43
8:H:118:SER:HB3	14:N:4:ILE:HB	2.01	0.43
12:L:42:ILE:CG1	12:L:179:ILE:HD11	2.48	0.43
13:M:223:ARG:NH2	9:W:160:TYR:OH	2.51	0.43
14:N:49:ILE:CD1	14:N:186:ILE:HD13	2.48	0.43
3:Q:64:MET:HE2	3:Q:212:ALA:CB	2.47	0.43
12:Z:160:ILE:O	12:Z:164:THR:HG23	2.18	0.43
13:a:103:VAL:HG11	13:a:119:ILE:HG21	2.00	0.43
14:b:40:HIS:O	14:b:51:GLY:HA2	2.18	0.43
2:B:43:VAL:HG21	2:B:186:ILE:HG13	2.00	0.43
9:I:8:PHE:HB2	9:I:146:MET:O	2.19	0.43
9:I:123:PRO:HB2	9:I:142:TRP:CZ2	2.53	0.43
14:N:124:CYS:CB	14:N:137:ILE:HD13	2.49	0.43
1:O:186:PRO:HB3	1:O:216:THR:HG22	2.00	0.43
4:R:97:LEU:C	4:R:97:LEU:HD13	2.43	0.43
6:T:188:ILE:HG23	6:T:211:LEU:HD13	2.00	0.43
7:U:135:THR:HG21	7:U:163:PHE:CD1	2.54	0.43
3:Q:192:VAL:HG22	3:Q:211:PHE:CZ	2.54	0.43
8:V:166:ILE:HG23	8:V:199:TYR:HA	2.00	0.43
10:X:3:ASP:OD1	10:X:4:ILE:N	2.52	0.43
3:C:70:HIS:O	3:C:137:GLY:HA2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:VAL:HG22	3:C:211:PHE:CZ	2.54	0.43
6:F:7:ASP:OD1	6:F:21:GLN:NE2	2.40	0.43
10:J:29:LEU:HD22	11:K:122:GLN:HB2	2.01	0.43
12:L:160:ILE:O	12:L:164:THR:HG23	2.18	0.43
13:M:32:VAL:HG11	13:M:122:GLY:HA3	1.99	0.43
2:P:73:VAL:HG22	2:P:74:TYR:N	2.33	0.43
8:V:2:THR:O	8:V:16:SER:HA	2.19	0.43
11:Y:127:GLY:CA	11:Y:137:MET:HE1	2.49	0.43
14:b:41:PHE:CD2	14:b:186:ILE:HD12	2.54	0.43
14:b:94:TYR:HE2	14:b:105:LEU:HD11	1.84	0.43
2:B:84:ILE:HG21	2:B:132:LEU:HD11	2.00	0.43
3:C:63:LYS:N	3:C:210:GLU:OE2	2.41	0.43
4:D:179:LYS:NZ	4:D:186:GLU:OE2	2.52	0.43
7:G:226:GLU:O	7:G:230:GLN:NE2	2.52	0.43
3:Q:46:ALA:HB1	3:Q:195:LEU:CD1	2.48	0.43
3:Q:76:ALA:HB3	3:Q:163:ILE:HD12	2.00	0.43
3:Q:81:ASP:OD1	3:Q:82:ALA:N	2.51	0.43
5:S:46:VAL:HG11	5:S:146:ALA:HB1	2.01	0.43
7:U:100:THR:O	7:U:104:GLY:N	2.48	0.43
2:B:156:TRP:CG	2:B:159:THR:OG1	2.70	0.42
4:D:44:ILE:HG21	4:D:73:ALA:HB2	2.01	0.42
9:I:167:LEU:HD11	13:a:41:SER:HB2	2.00	0.42
11:K:127:GLY:CA	11:K:137:MET:HE1	2.49	0.42
1:O:68:ILE:HG21	1:O:110:LEU:CD2	2.47	0.42
2:P:92:SER:HA	2:P:103:MET:HB2	2.01	0.42
5:S:11:ASN:OD1	5:S:11:ASN:N	2.52	0.42
3:C:64:MET:HE2	3:C:212:ALA:CB	2.47	0.42
5:E:117:CYS:SG	5:E:164:TYR:HB3	2.59	0.42
9:I:31:GLU:HG2	15:I:301:X5C:C41	2.50	0.42
12:L:80:SER:CB	12:L:114:ILE:HD11	2.46	0.42
14:N:175:ARG:NE	9:W:139:GLU:OE2	2.40	0.42
3:Q:118:HIS:HB2	4:R:79:ALA:HB1	2.01	0.42
4:R:17:LEU:CD1	4:R:20:ILE:HD12	2.49	0.42
7:U:9:ASP:O	7:U:23:GLN:NE2	2.51	0.42
9:W:13:VAL:HG11	9:W:152:MET:HA	2.01	0.42
10:X:29:LEU:HD22	11:Y:122:GLN:HB2	2.01	0.42
1:A:83:VAL:O	1:A:87:VAL:HG23	2.19	0.42
2:B:118:TYR:O	2:B:122:ILE:HG12	2.18	0.42
6:F:229:GLN:O	6:F:232:ILE:HG22	2.19	0.42
8:H:2:THR:O	8:H:16:SER:HA	2.19	0.42
10:J:3:ASP:OD1	10:J:4:ILE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:146:GLN:O	2:P:153:PHE:HA	2.20	0.42
7:U:148:ALA:HB3	7:U:158:TYR:CE1	2.54	0.42
7:U:226:GLU:O	7:U:230:GLN:NE2	2.52	0.42
1:O:72:VAL:HG13	1:O:107:VAL:HG22	2.00	0.42
1:O:83:VAL:O	1:O:87:VAL:HG23	2.19	0.42
6:T:229:GLN:O	6:T:232:ILE:HG22	2.19	0.42
10:X:164:LEU:O	10:X:168:THR:OG1	2.32	0.42
12:Z:4:LEU:CD2	12:Z:159:ALA:HB3	2.49	0.42
14:b:24:ASP:OD2	14:b:26:SER:OG	2.33	0.42
3:C:118:HIS:HB2	4:D:79:ALA:HB1	2.01	0.42
6:F:128:TYR:O	6:F:149:PRO:HB3	2.20	0.42
7:G:100:THR:O	7:G:104:GLY:N	2.48	0.42
9:I:167:LEU:HD21	13:a:46:ILE:CG1	2.50	0.42
9:I:173:VAL:O	9:I:198:TYR:N	2.52	0.42
3:Q:70:HIS:O	3:Q:137:GLY:HA2	2.19	0.42
8:V:118:SER:HB3	14:b:4:ILE:HB	2.01	0.42
1:A:73:GLY:HA3	1:A:222:PHE:CD1	2.54	0.42
2:B:146:GLN:O	2:B:153:PHE:HA	2.20	0.42
4:D:101:ASP:OD1	4:D:101:ASP:N	2.53	0.42
4:D:121:GLN:O	5:E:136:SER:N	2.42	0.42
4:D:142:SER:O	4:D:213:ARG:NH1	2.43	0.42
9:W:148:GLU:OE1	9:W:179:LYS:NZ	2.47	0.42
13:a:65:ALA:HB3	13:a:72:ILE:HG23	2.01	0.42
1:A:68:ILE:HG21	1:A:110:LEU:CD2	2.47	0.42
8:H:54:PHE:CD2	8:H:96:LEU:HD21	2.55	0.42
8:H:92:TYR:HB2	8:H:96:LEU:HD22	2.00	0.42
4:R:81:ALA:N	4:R:130:VAL:HG21	2.34	0.42
5:S:117:CYS:SG	5:S:164:TYR:HB3	2.59	0.42
6:T:128:TYR:O	6:T:149:PRO:HB3	2.20	0.42
9:W:135:ILE:HD12	9:W:138:LEU:HD12	2.02	0.42
11:Y:7:LEU:HD12	11:Y:126:TYR:HB3	2.02	0.42
11:Y:128:ALA:HB3	11:Y:133:GLN:CA	2.50	0.42
12:Z:80:SER:CB	12:Z:114:ILE:HD11	2.46	0.42
13:a:115:TYR:O	13:a:117:ILE:N	2.51	0.42
1:A:28:VAL:HA	1:A:78:GLY:HA2	2.00	0.42
4:D:17:LEU:CD1	4:D:20:ILE:HD12	2.49	0.42
4:D:88:GLY:HA3	4:D:112:ILE:HD11	2.01	0.42
6:F:69:HIS:O	6:F:136:GLY:HA2	2.19	0.42
8:H:106:ASP:OD1	8:H:108:ALA:N	2.47	0.42
10:J:123:ALA:HB1	10:J:131:PHE:CD1	2.55	0.42
10:J:164:LEU:O	10:J:168:THR:OG1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:132:CYS:O	11:K:136:VAL:HG22	2.20	0.42
14:N:110:ILE:HD11	14:N:139:THR:CG2	2.50	0.42
5:S:204:LEU:CD2	5:S:217:VAL:HG23	2.50	0.42
7:U:36:LEU:C	7:U:36:LEU:HD12	2.45	0.42
8:V:120:MET:SD	14:b:27:ILE:HG21	2.60	0.42
9:W:13:VAL:HG22	9:W:177:VAL:HG22	2.02	0.42
10:X:123:ALA:HB1	10:X:131:PHE:CD1	2.55	0.42
8:H:120:MET:SD	14:N:27:ILE:HG21	2.60	0.42
10:J:54:LEU:HB3	10:J:106:VAL:HG21	2.00	0.42
12:L:4:LEU:CD2	12:L:159:ALA:HB3	2.49	0.42
2:P:38:ALA:N	2:P:41:GLY:O	2.53	0.42
2:P:156:TRP:CG	2:P:159:THR:OG1	2.70	0.42
4:R:8:ILE:HG22	4:R:19:GLN:HG3	2.02	0.42
9:W:95:GLN:HA	9:W:115:PRO:HB3	2.01	0.42
12:Z:173:ARG:NH1	13:a:170:ASN:O	2.52	0.42
5:E:109:ILE:HD13	5:E:109:ILE:N	2.35	0.42
10:J:167:CYS:O	10:J:171:CYS:SG	2.78	0.42
11:K:148:LEU:HD22	11:K:152:ASP:HB3	2.01	0.42
12:L:50:ALA:CB	13:M:138:VAL:HG23	2.50	0.42
13:M:65:ALA:HB1	13:M:72:ILE:HG12	2.01	0.42
4:R:31:THR:HG22	4:R:32:THR:H	1.84	0.42
8:V:54:PHE:CD2	8:V:96:LEU:HD21	2.55	0.42
9:W:8:PHE:HB2	9:W:146:MET:O	2.19	0.42
10:X:27:ARG:HD3	10:X:187:ILE:HB	2.02	0.42
10:X:167:CYS:O	10:X:171:CYS:SG	2.78	0.42
12:Z:95:LEU:O	12:Z:116:ASN:ND2	2.53	0.42
13:a:79:MET:HE2	13:a:103:VAL:HG23	2.02	0.42
14:b:174:ALA:HB2	14:b:203:PRO:HB3	2.01	0.42
2:B:211:VAL:O	2:B:211:VAL:HG23	2.20	0.41
7:G:217:THR:HG21	7:G:222:GLN:HB3	2.02	0.41
9:I:95:GLN:HA	9:I:115:PRO:HB3	2.01	0.41
12:L:95:LEU:O	12:L:116:ASN:ND2	2.53	0.41
7:U:170:ALA:O	7:U:174:LEU:HG	2.20	0.41
11:Y:148:LEU:HD22	11:Y:152:ASP:HB3	2.01	0.41
13:a:189:ALA:O	13:a:193:VAL:HG23	2.20	0.41
14:b:32:MET:HE2	14:b:34:ARG:HA	2.02	0.41
2:B:201:LEU:HD13	2:B:201:LEU:C	2.45	0.41
5:E:46:VAL:HG11	5:E:146:ALA:HB1	2.01	0.41
7:G:88:ILE:HG21	7:G:136:VAL:HG11	2.02	0.41
8:H:138:ALA:HB3	8:V:136:ILE:HA	2.02	0.41
11:K:126:TYR:OH	11:K:141:ASP:OD1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:65:ALA:HB3	13:M:72:ILE:HG23	2.01	0.41
1:O:164:ALA:CB	1:O:172:ALA:HB3	2.51	0.41
1:O:212:VAL:O	1:O:225:LEU:N	2.36	0.41
2:P:66:ILE:CD1	2:P:88:LEU:HD13	2.50	0.41
4:R:88:GLY:HA3	4:R:112:ILE:HD11	2.01	0.41
5:S:37:ALA:HB2	5:S:50:VAL:HG23	2.01	0.41
5:S:73:HIS:NE2	5:S:107:ILE:O	2.40	0.41
6:T:6:TYR:OH	7:U:9:ASP:OD2	2.33	0.41
6:T:69:HIS:O	6:T:136:GLY:HA2	2.19	0.41
9:W:40:ASN:HB2	9:W:103:ILE:O	2.20	0.41
10:X:11:CYS:O	10:X:25:SER:HA	2.20	0.41
11:Y:132:CYS:O	11:Y:136:VAL:HG22	2.20	0.41
12:Z:50:ALA:CB	13:a:138:VAL:HG23	2.50	0.41
1:A:163:VAL:HG22	1:A:164:ALA:N	2.35	0.41
2:B:92:SER:HA	2:B:103:MET:HB2	2.01	0.41
3:C:21:VAL:HG11	3:C:152:SER:HB3	2.02	0.41
4:D:31:THR:HG22	4:D:32:THR:H	1.84	0.41
4:D:81:ALA:N	4:D:130:VAL:HG21	2.34	0.41
7:G:170:ALA:O	7:G:174:LEU:HG	2.20	0.41
9:I:135:ILE:HD12	9:I:138:LEU:HD12	2.02	0.41
10:J:27:ARG:HD3	10:J:187:ILE:HB	2.01	0.41
10:J:47:ASN:HD21	10:J:50:ILE:HD12	1.85	0.41
11:K:7:LEU:HD12	11:K:126:TYR:HB3	2.02	0.41
13:M:189:ALA:O	13:M:193:VAL:HG23	2.20	0.41
2:P:128:PHE:O	2:P:149:PRO:HB3	2.20	0.41
2:P:211:VAL:HG23	2:P:211:VAL:O	2.20	0.41
4:R:113:ALA:HB2	4:R:149:THR:HB	2.03	0.41
6:T:93:LEU:C	6:T:93:LEU:HD23	2.45	0.41
7:U:47:LEU:HD11	7:U:210:MET:HG2	2.02	0.41
7:U:88:ILE:HG21	7:U:136:VAL:HG11	2.01	0.41
9:W:31:GLU:HG2	15:W:301:X5C:C41	2.50	0.41
10:X:96:LEU:HD11	10:X:108:PRO:HG3	2.02	0.41
11:Y:12:TRP:HB2	11:Y:179:LEU:HD11	2.02	0.41
4:D:8:ILE:HG22	4:D:19:GLN:HG3	2.02	0.41
5:E:204:LEU:CD2	5:E:217:VAL:HG23	2.50	0.41
6:F:14:SER:N	6:F:18:ARG:O	2.45	0.41
7:G:36:LEU:C	7:G:36:LEU:HD12	2.45	0.41
7:G:81:HIS:N	7:G:133:GLY:O	2.40	0.41
7:G:109:VAL:HB	7:G:145:ALA:HB3	2.02	0.41
9:I:40:ASN:HB2	9:I:103:ILE:O	2.20	0.41
9:I:139:GLU:OE2	14:b:175:ARG:NE	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:13:LEU:HD11	10:J:151:CYS:SG	2.60	0.41
11:K:84:ILE:O	11:K:88:MET:HG2	2.20	0.41
13:M:46:ILE:CG1	9:W:167:LEU:HD21	2.50	0.41
4:R:121:GLN:O	5:S:136:SER:N	2.42	0.41
4:R:179:LYS:NZ	4:R:186:GLU:OE2	2.52	0.41
5:S:121:LEU:CD1	6:T:79:ALA:HB3	2.51	0.41
7:U:217:THR:HG21	7:U:222:GLN:HB3	2.02	0.41
9:W:6:ALA:HB1	9:W:142:TRP:CD1	2.55	0.41
9:W:136:SER:O	9:W:140:ASN:ND2	2.54	0.41
10:X:47:ASN:HD21	10:X:50:ILE:HD12	1.85	0.41
14:b:3:VAL:CG1	14:b:6:ALA:HB2	2.50	0.41
8:H:38:GLN:HB2	8:H:41:ILE:HG12	2.03	0.41
9:I:221:VAL:HG11	9:I:224:THR:OG1	2.21	0.41
13:M:79:MET:HE2	13:M:103:VAL:HG23	2.02	0.41
14:N:32:MET:HE2	14:N:34:ARG:HA	2.02	0.41
5:S:232:TYR:CE2	5:S:240:ILE:HD11	2.55	0.41
10:X:13:LEU:HD11	10:X:151:CYS:SG	2.60	0.41
2:B:72:ILE:HD11	2:B:132:LEU:HD13	2.02	0.41
2:B:74:TYR:HB3	2:B:81:PHE:CD1	2.56	0.41
4:D:110:ARG:HD3	5:E:86:ARG:HD2	2.03	0.41
6:F:93:LEU:C	6:F:93:LEU:HD23	2.45	0.41
7:G:124:HIS:NE2	7:G:152:SER:O	2.37	0.41
8:H:136:ILE:HA	8:V:138:ALA:HB3	2.02	0.41
10:J:21:VAL:HG13	10:J:120:PRO:HB3	2.03	0.41
10:J:23:ILE:HG23	10:J:23:ILE:O	2.20	0.41
11:K:128:ALA:HB3	11:K:133:GLN:CA	2.50	0.41
12:L:46:ALA:HB3	12:L:98:GLY:O	2.21	0.41
14:N:3:VAL:CG1	14:N:6:ALA:HB2	2.50	0.41
1:O:163:VAL:HG22	1:O:164:ALA:N	2.35	0.41
2:P:80:ASP:HB2	2:P:128:PHE:HD1	1.86	0.41
4:R:101:ASP:OD1	4:R:101:ASP:N	2.53	0.41
6:T:67:ASP:OD1	6:T:68:GLN:N	2.54	0.41
7:U:81:HIS:N	7:U:133:GLY:O	2.40	0.41
13:a:38:THR:OG1	13:a:203:ALA:HB3	2.21	0.41
14:b:110:ILE:HD11	14:b:139:THR:CG2	2.50	0.41
14:b:146:GLN:O	14:b:149:GLN:OE1	2.39	0.41
2:B:128:PHE:O	2:B:149:PRO:HB3	2.20	0.41
5:E:232:TYR:CE2	5:E:240:ILE:HD11	2.56	0.41
8:H:37:ILE:CG2	8:H:63:LEU:HD12	2.51	0.41
9:I:112:GLN:O	9:I:119:PHE:HA	2.20	0.41
10:J:96:LEU:HD11	10:J:108:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:32:VAL:HG11	13:M:122:GLY:CA	2.50	0.41
1:O:73:GLY:HA3	1:O:222:PHE:CD1	2.54	0.41
7:U:135:THR:HG21	7:U:163:PHE:CG	2.55	0.41
13:a:32:VAL:HG11	13:a:122:GLY:CA	2.50	0.41
13:a:157:ALA:HB3	13:a:158:PRO:HD3	2.03	0.41
2:B:66:ILE:CD1	2:B:88:LEU:HD13	2.50	0.41
6:F:35:THR:HG22	6:F:133:LEU:HD12	2.02	0.41
6:F:67:ASP:OD1	6:F:68:GLN:N	2.54	0.41
9:I:6:ALA:HB1	9:I:142:TRP:CD1	2.55	0.41
11:K:116:ASP:OD1	11:K:120:THR:N	2.36	0.41
14:N:124:CYS:HB2	14:N:137:ILE:HG21	2.03	0.41
2:P:74:TYR:HB3	2:P:81:PHE:CD1	2.55	0.41
4:R:44:ILE:HG21	4:R:73:ALA:HB2	2.01	0.41
5:S:236:GLN:O	5:S:240:ILE:HG13	2.21	0.41
7:U:123:ALA:HB1	7:U:131:PRO:HA	2.03	0.41
10:X:13:LEU:HD22	10:X:147:LEU:HD22	2.03	0.41
14:b:55:GLU:HG3	14:b:58:ASP:H	1.85	0.41
14:b:124:CYS:HB2	14:b:137:ILE:HG21	2.02	0.41
14:b:141:PHE:HB3	14:b:145:LEU:HD12	2.03	0.41
1:A:164:ALA:CB	1:A:172:ALA:HB3	2.51	0.41
2:B:17:LEU:HB3	2:B:20:ILE:HG12	2.03	0.41
3:C:35:ILE:HD12	3:C:35:ILE:N	2.36	0.41
4:D:34:VAL:CG2	4:D:174:LEU:HD11	2.49	0.41
4:D:116:GLN:NE2	4:D:130:VAL:O	2.54	0.41
5:E:11:ASN:OD1	5:E:11:ASN:N	2.52	0.41
5:E:171:ALA:CB	5:E:179:ALA:HB3	2.51	0.41
7:G:47:LEU:HD11	7:G:210:MET:HG2	2.02	0.41
7:G:135:THR:HG21	7:G:163:PHE:CG	2.55	0.41
11:K:97:TYR:O	11:K:117:TYR:HB2	2.21	0.41
12:L:57:ARG:HD2	13:M:101:ARG:NH1	2.36	0.41
13:M:157:ALA:HB3	13:M:158:PRO:HD3	2.03	0.41
13:M:190:ILE:CG2	13:M:221:LEU:HD11	2.51	0.41
14:N:20:LEU:HD21	14:N:162:LYS:CD	2.51	0.41
14:N:24:ASP:OD2	14:N:26:SER:OG	2.33	0.41
14:N:55:GLU:HG3	14:N:58:ASP:H	1.85	0.41
14:N:99:ARG:HG2	14:N:128:TYR:O	2.21	0.41
14:N:174:ALA:HB2	14:N:203:PRO:HB3	2.01	0.41
14:N:205:TRP:CH2	8:V:173:GLY:HA2	2.56	0.41
4:R:34:VAL:O	4:R:34:VAL:HG13	2.20	0.41
4:R:63:ILE:HD13	4:R:209:ALA:HB3	2.03	0.41
4:R:110:ARG:HD3	5:S:86:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:109:ILE:N	5:S:109:ILE:HD13	2.35	0.41
8:V:37:ILE:CG2	8:V:63:LEU:HD12	2.51	0.41
8:V:38:GLN:HB2	8:V:41:ILE:HG12	2.03	0.41
10:X:21:VAL:HG13	10:X:120:PRO:HB3	2.03	0.41
10:X:125:SER:HA	10:X:130:ALA:O	2.21	0.41
11:Y:2:LEU:HD22	11:Y:2:LEU:N	2.36	0.41
11:Y:60:LEU:O	11:Y:64:VAL:HG23	2.21	0.41
11:Y:124:ILE:HD12	11:Y:127:GLY:HA3	2.03	0.41
13:a:18:MET:HA	13:a:18:MET:CE	2.37	0.41
13:a:65:ALA:HB1	13:a:72:ILE:HG12	2.01	0.41
13:a:66:THR:O	13:a:117:ILE:HA	2.21	0.41
13:a:190:ILE:CG2	13:a:221:LEU:HD11	2.51	0.41
14:b:20:LEU:HD21	14:b:162:LYS:CD	2.51	0.41
14:b:92:LYS:HA	14:b:125:THR:HG21	2.03	0.41
1:A:57:ILE:HG21	1:A:62:VAL:CG2	2.51	0.41
2:B:157:LYS:HB3	2:B:176:TYR:CE2	2.56	0.41
4:D:42:ILE:HG21	4:D:135:CYS:CB	2.51	0.41
4:D:113:ALA:HB2	4:D:149:THR:HB	2.03	0.41
8:H:96:LEU:HD11	9:I:88:PHE:HZ	1.86	0.41
9:I:11:GLY:CA	9:I:103:ILE:HD11	2.51	0.41
9:I:40:ASN:ND2	9:I:74:PRO:O	2.36	0.41
11:K:2:LEU:N	11:K:2:LEU:HD22	2.36	0.41
13:M:38:THR:OG1	13:M:203:ALA:HB3	2.21	0.41
13:M:179:LEU:HD11	13:M:208:VAL:CG1	2.51	0.41
13:M:179:LEU:HD11	13:M:208:VAL:HG11	2.03	0.41
3:Q:21:VAL:HG11	3:Q:152:SER:HB3	2.02	0.41
3:Q:35:ILE:HD12	3:Q:35:ILE:N	2.36	0.41
4:R:33:VAL:HG22	4:R:46:VAL:HG22	2.03	0.41
9:W:11:GLY:CA	9:W:103:ILE:HD11	2.51	0.41
9:W:112:GLN:O	9:W:119:PHE:HA	2.20	0.41
13:a:179:LEU:HD11	13:a:208:VAL:CG1	2.51	0.41
1:A:12:PHE:CZ	2:B:129:GLY:HA3	2.56	0.40
5:E:73:HIS:NE2	5:E:107:ILE:O	2.40	0.40
7:G:28:THR:HA	7:G:151:PRO:HG2	2.03	0.40
7:G:37:ALA:HB3	7:G:79:ILE:HG13	2.03	0.40
7:G:123:ALA:HB1	7:G:131:PRO:HA	2.03	0.40
8:H:126:ILE:HG23	8:H:126:ILE:O	2.21	0.40
10:J:125:SER:HA	10:J:130:ALA:O	2.21	0.40
10:J:153:SER:OG	13:a:159:LEU:HD11	2.22	0.40
11:K:60:LEU:HD22	11:K:84:ILE:HG12	2.03	0.40
12:L:48:GLY:N	12:L:96:SER:O	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:66:THR:O	13:M:117:ILE:HA	2.21	0.40
1:O:49:GLN:NE2	1:O:201:CYS:SG	2.95	0.40
5:S:171:ALA:CB	5:S:179:ALA:HB3	2.51	0.40
6:T:35:THR:HG22	6:T:133:LEU:HD12	2.02	0.40
7:U:185:ARG:HH12	7:U:228:VAL:HG22	1.86	0.40
12:Z:57:ARG:HD2	13:a:101:ARG:NH1	2.36	0.40
8:H:166:ILE:HG21	8:H:201:ILE:CD1	2.45	0.40
10:J:11:CYS:O	10:J:25:SER:HA	2.20	0.40
11:K:12:TRP:HB2	11:K:179:LEU:HD11	2.02	0.40
1:O:150:LYS:CB	1:O:163:VAL:HG21	2.52	0.40
7:U:36:LEU:HD11	7:U:195:ILE:HG12	2.03	0.40
12:Z:35:LEU:HD22	12:Z:36:PRO:HD2	2.04	0.40
4:D:33:VAL:HG22	4:D:46:VAL:HG22	2.03	0.40
5:E:236:GLN:O	5:E:240:ILE:HG13	2.21	0.40
9:I:13:VAL:HG22	9:I:177:VAL:HG22	2.02	0.40
11:K:55:GLN:HG3	12:L:88:TYR:CG	2.57	0.40
13:M:34:ILE:HG21	13:M:64:SER:HB3	2.03	0.40
13:M:202:ASP:O	13:M:203:ALA:HB2	2.21	0.40
14:N:92:LYS:HA	14:N:125:THR:HG21	2.03	0.40
1:O:82:ASP:OD1	7:U:121:HIS:NE2	2.54	0.40
2:P:201:LEU:HD13	2:P:201:LEU:C	2.45	0.40
6:T:47:ALA:HB2	6:T:211:LEU:HD12	2.04	0.40
9:W:14:LEU:HD21	9:W:101:GLY:H	1.86	0.40
11:Y:84:ILE:O	11:Y:88:MET:HG2	2.20	0.40
1:A:49:GLN:NE2	1:A:201:CYS:SG	2.95	0.40
4:D:34:VAL:O	4:D:34:VAL:HG13	2.21	0.40
5:E:121:LEU:CD1	6:F:79:ALA:HB3	2.51	0.40
8:H:29:ARG:NH1	9:I:139:GLU:OE1	2.54	0.40
11:K:11:ASP:OD1	11:K:11:ASP:N	2.54	0.40
14:N:141:PHE:HB3	14:N:145:LEU:HD12	2.03	0.40
3:Q:114:CYS:SG	3:Q:155:PHE:HB3	2.62	0.40
3:Q:139:ASP:OD2	3:Q:145:GLN:NE2	2.46	0.40
8:V:29:ARG:NH1	9:W:139:GLU:OE1	2.54	0.40
9:W:40:ASN:ND2	9:W:74:PRO:O	2.36	0.40
2:B:38:ALA:N	2:B:41:GLY:O	2.53	0.40
2:B:62:LYS:N	2:B:207:GLU:OE1	2.55	0.40
7:G:185:ARG:HH12	7:G:228:VAL:HG22	1.86	0.40
9:I:44:CYS:SG	9:I:99:ILE:HB	2.61	0.40
12:L:51:ASP:HB3	12:L:97:ILE:HD11	2.04	0.40
4:R:67:ASP:OD1	4:R:68:LYS:N	2.48	0.40
5:S:165:THR:HG21	6:T:53:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:37:ALA:HB3	7:U:79:ILE:HG13	2.03	0.40
7:U:109:VAL:HB	7:U:145:ALA:HB3	2.02	0.40
9:W:211:GLU:HB3	9:W:212:PRO:HD3	2.04	0.40
10:X:10:SER:HB3	10:X:42:ARG:CZ	2.51	0.40
10:X:23:ILE:O	10:X:23:ILE:HG23	2.20	0.40
11:Y:11:ASP:OD1	11:Y:11:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/241 (98%)	233 (98%)	4 (2%)	0	100	100
1	O	237/241 (98%)	233 (98%)	4 (2%)	0	100	100
2	B	227/232 (98%)	223 (98%)	4 (2%)	0	100	100
2	P	227/232 (98%)	223 (98%)	4 (2%)	0	100	100
3	C	229/251 (91%)	228 (100%)	1 (0%)	0	100	100
3	Q	229/251 (91%)	228 (100%)	1 (0%)	0	100	100
4	D	229/235 (97%)	222 (97%)	7 (3%)	0	100	100
4	R	229/235 (97%)	222 (97%)	7 (3%)	0	100	100
5	E	227/251 (90%)	226 (100%)	1 (0%)	0	100	100
5	S	227/251 (90%)	226 (100%)	1 (0%)	0	100	100
6	F	218/233 (94%)	216 (99%)	2 (1%)	0	100	100
6	T	218/233 (94%)	216 (99%)	2 (1%)	0	100	100
7	G	228/240 (95%)	221 (97%)	7 (3%)	0	100	100
7	U	228/240 (95%)	221 (97%)	7 (3%)	0	100	100
8	H	202/204 (99%)	199 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	202/204 (99%)	199 (98%)	3 (2%)	0	100	100
9	I	227/243 (93%)	220 (97%)	7 (3%)	0	100	100
9	W	227/243 (93%)	220 (97%)	7 (3%)	0	100	100
10	J	202/206 (98%)	197 (98%)	5 (2%)	0	100	100
10	X	202/206 (98%)	197 (98%)	5 (2%)	0	100	100
11	K	189/191 (99%)	180 (95%)	9 (5%)	0	100	100
11	Y	189/191 (99%)	180 (95%)	9 (5%)	0	100	100
12	L	200/202 (99%)	195 (98%)	5 (2%)	0	100	100
12	Z	200/202 (99%)	195 (98%)	5 (2%)	0	100	100
13	M	210/224 (94%)	205 (98%)	5 (2%)	0	100	100
13	a	210/224 (94%)	205 (98%)	5 (2%)	0	100	100
14	N	206/244 (84%)	203 (98%)	3 (2%)	0	100	100
14	b	206/244 (84%)	203 (98%)	3 (2%)	0	100	100
All	All	6062/6394 (95%)	5936 (98%)	126 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/207 (99%)	204 (100%)	1 (0%)	81	91
1	O	205/207 (99%)	204 (100%)	1 (0%)	81	91
2	B	194/196 (99%)	191 (98%)	3 (2%)	57	75
2	P	194/196 (99%)	191 (98%)	3 (2%)	57	75
3	C	195/212 (92%)	193 (99%)	2 (1%)	68	81
3	Q	195/212 (92%)	193 (99%)	2 (1%)	68	81
4	D	194/198 (98%)	191 (98%)	3 (2%)	57	75
4	R	194/198 (98%)	191 (98%)	3 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	187/204 (92%)	184 (98%)	3 (2%)	55	74
5	S	187/204 (92%)	184 (98%)	3 (2%)	55	74
6	F	182/193 (94%)	178 (98%)	4 (2%)	45	67
6	T	182/193 (94%)	178 (98%)	4 (2%)	45	67
7	G	196/204 (96%)	196 (100%)	0	100	100
7	U	196/204 (96%)	196 (100%)	0	100	100
8	H	164/164 (100%)	162 (99%)	2 (1%)	63	79
8	V	164/164 (100%)	162 (99%)	2 (1%)	63	79
9	I	190/202 (94%)	187 (98%)	3 (2%)	55	74
9	W	190/202 (94%)	187 (98%)	3 (2%)	55	74
10	J	175/177 (99%)	174 (99%)	1 (1%)	78	88
10	X	175/177 (99%)	174 (99%)	1 (1%)	78	88
11	K	163/163 (100%)	162 (99%)	1 (1%)	78	88
11	Y	163/163 (100%)	162 (99%)	1 (1%)	78	88
12	L	167/167 (100%)	166 (99%)	1 (1%)	78	88
12	Z	167/167 (100%)	166 (99%)	1 (1%)	78	88
13	M	180/190 (95%)	175 (97%)	5 (3%)	38	60
13	a	180/190 (95%)	175 (97%)	5 (3%)	38	60
14	N	172/198 (87%)	170 (99%)	2 (1%)	63	79
14	b	172/198 (87%)	170 (99%)	2 (1%)	63	79
All	All	5128/5350 (96%)	5066 (99%)	62 (1%)	61	79

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
2	B	79	THR
2	B	93	ILE
2	B	150	SER
3	C	107	GLU
3	C	214	LEU
4	D	101	ASP
4	D	135	CYS
4	D	195	LEU
5	E	46	VAL

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Mol	Chain	Res	Type
5	E	158	THR
5	E	193	LEU
6	F	11	THR
6	F	22	VAL
6	F	62	LYS
6	F	126	ARG
8	H	8	CYS
8	H	78	ILE
9	I	44	CYS
9	I	169	SER
9	I	225	THR
10	J	21	VAL
11	K	73	VAL
12	L	177	VAL
13	M	27	CYS
13	M	142	GLU
13	M	144	LEU
13	M	209	PHE
13	M	224	HIS
14	N	99	ARG
14	N	106	SER
1	O	42	ASN
2	P	79	THR
2	P	93	ILE
2	P	150	SER
3	Q	107	GLU
3	Q	214	LEU
4	R	101	ASP
4	R	135	CYS
4	R	195	LEU
5	S	46	VAL
5	S	158	THR
5	S	193	LEU
6	T	11	THR
6	T	22	VAL
6	T	62	LYS
6	T	126	ARG
8	V	8	CYS
8	V	78	ILE
9	W	44	CYS
9	W	169	SER
9	W	225	THR

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Mol	Chain	Res	Type
10	X	21	VAL
11	Y	73	VAL
12	Z	177	VAL
13	a	27	CYS
13	a	142	GLU
13	a	144	LEU
13	a	209	PHE
13	a	224	HIS
14	b	99	ARG
14	b	106	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	235	HIS
2	B	18	ASN
2	B	69	ASN
4	D	119	ASN
4	D	143	GLN
5	E	99	HIS
5	E	114	GLN
5	E	134	GLN
8	H	28	ASN
8	H	61	ASN
8	H	137	GLN
8	H	143	ASN
8	H	194	GLN
10	J	32	ASN
11	K	55	GLN
11	K	63	ASN
11	K	86	HIS
11	K	173	HIS
12	L	85	ASN
12	L	181	GLN
12	L	196	HIS
13	M	169	HIS
14	N	37	ASN
14	N	180	ASN
14	N	204	ASN
1	O	227	ASN
2	P	18	ASN

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Mol	Chain	Res	Type
2	P	69	ASN
2	P	187	HIS
4	R	119	ASN
5	S	99	HIS
5	S	114	GLN
5	S	134	GLN
8	V	28	ASN
8	V	61	ASN
8	V	137	GLN
8	V	143	ASN
8	V	194	GLN
9	W	149	HIS
9	W	187	GLN
10	X	32	ASN
11	Y	86	HIS
11	Y	173	HIS
12	Z	181	GLN
12	Z	196	HIS
13	a	169	HIS
14	b	180	ASN
14	b	191	GLN
14	b	195	HIS
14	b	204	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
15	X5C	W	301	9	56,62,62	0.50	2 (3%)	70,88,88	0.55	2 (2%)
15	X5C	I	301	9	56,62,62	0.50	2 (3%)	70,88,88	0.55	2 (2%)
15	X5C	L	301	12	56,62,62	0.47	1 (1%)	70,88,88	0.58	2 (2%)
15	X5C	Z	301	12	56,62,62	0.47	1 (1%)	70,88,88	0.58	2 (2%)

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
15	X5C	W	301	9	-	9/43/71/71	0/6/6/6
15	X5C	I	301	9	-	9/43/71/71	0/6/6/6
15	X5C	L	301	12	-	7/43/71/71	0/6/6/6
15	X5C	Z	301	12	-	7/43/71/71	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	X5C	C46-C45	-2.82	1.47	1.51
15	W	301	X5C	C46-C45	-2.79	1.47	1.51
15	L	301	X5C	C46-C45	-2.63	1.47	1.51
15	Z	301	X5C	C46-C45	-2.63	1.47	1.51
15	I	301	X5C	O47-C45	-2.13	1.37	1.44
15	W	301	X5C	O47-C45	-2.12	1.37	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	301	X5C	O47-C45-C46	2.66	115.04	109.62
15	Z	301	X5C	O47-C45-C46	2.66	115.04	109.62
15	W	301	X5C	O47-C45-C46	2.63	114.97	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	301	X5C	O47-C45-C46	2.61	114.93	109.62
15	Z	301	X5C	C55-C54-C45	-2.60	108.76	111.66
15	L	301	X5C	C55-C54-C45	-2.60	108.76	111.66
15	I	301	X5C	C55-C54-C45	-2.50	108.87	111.66
15	W	301	X5C	C55-C54-C45	-2.50	108.87	111.66

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	I	301	X5C	N53-C54-C56-O57
15	L	301	X5C	CA-CB-CG-CD2
15	L	301	X5C	C45-C37-C38-C39
15	L	301	X5C	N53-C54-C56-O57
15	W	301	X5C	N53-C54-C56-O57
15	Z	301	X5C	CA-CB-CG-CD2
15	Z	301	X5C	C45-C37-C38-C39
15	Z	301	X5C	N53-C54-C56-O57
15	L	301	X5C	CA-CB-CG-CD1
15	Z	301	X5C	CA-CB-CG-CD1
15	I	301	X5C	C37-C38-C39-C40
15	W	301	X5C	C37-C38-C39-C40
15	I	301	X5C	C37-C38-C39-C44
15	W	301	X5C	C37-C38-C39-C44
15	L	301	X5C	C37-C38-C39-C40
15	Z	301	X5C	C37-C38-C39-C40
15	L	301	X5C	C37-C38-C39-C44
15	Z	301	X5C	C37-C38-C39-C44
15	I	301	X5C	C1-CA1-CB1-CG1
15	W	301	X5C	C1-CA1-CB1-CG1
15	I	301	X5C	O1-C1-CA1-N1
15	W	301	X5C	O1-C1-CA1-N1
15	I	301	X5C	N36-C1-CA1-N1
15	W	301	X5C	N36-C1-CA1-N1
15	L	301	X5C	C48-C50-C51-O52
15	Z	301	X5C	C48-C50-C51-O52
15	I	301	X5C	C45-C37-C38-C39
15	W	301	X5C	C45-C37-C38-C39
15	I	301	X5C	O1-C1-CA1-CB1
15	W	301	X5C	O1-C1-CA1-CB1
15	I	301	X5C	N36-C1-CA1-CB1
15	W	301	X5C	N36-C1-CA1-CB1

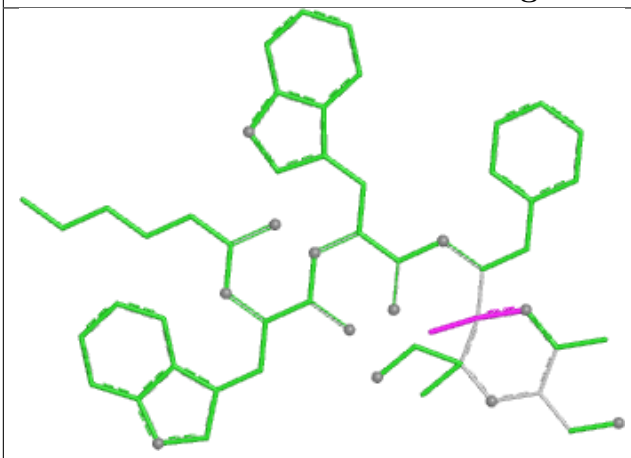
There are no ring outliers.

4 monomers are involved in 18 short contacts:

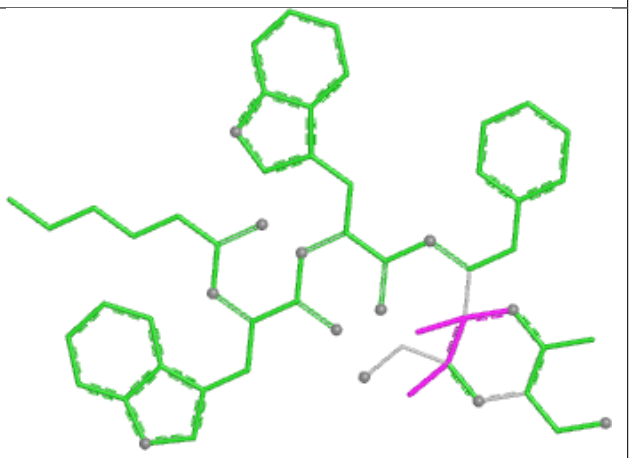
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	W	301	X5C	6	0
15	I	301	X5C	6	0
15	L	301	X5C	3	0
15	Z	301	X5C	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

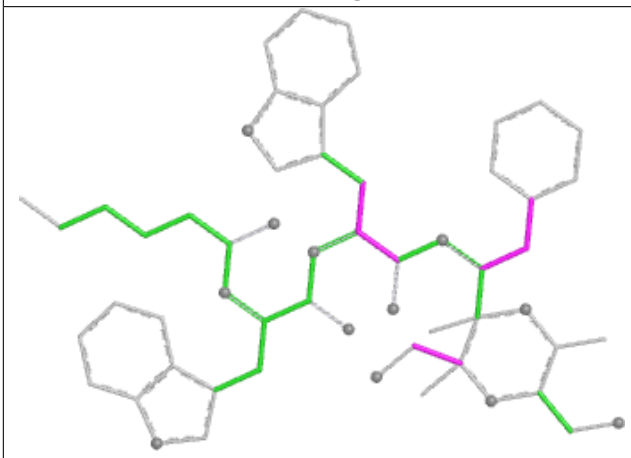
Ligand X5C W 301



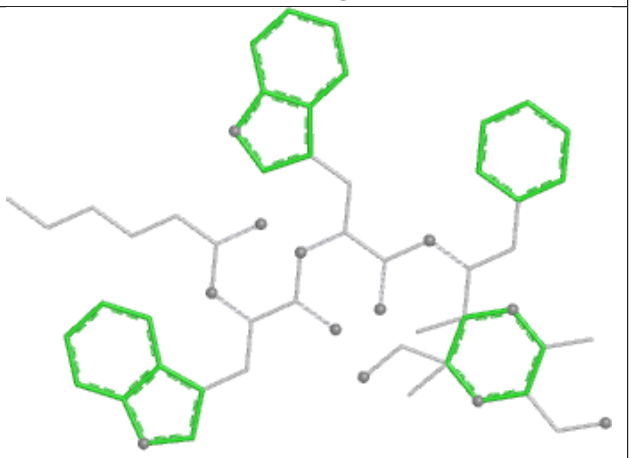
Bond lengths



Bond angles

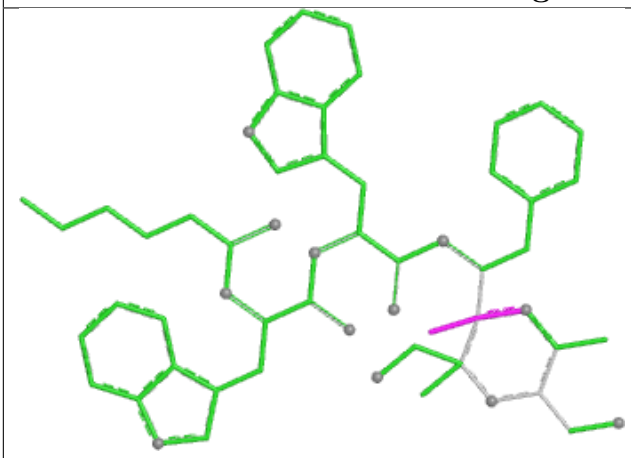


Torsions

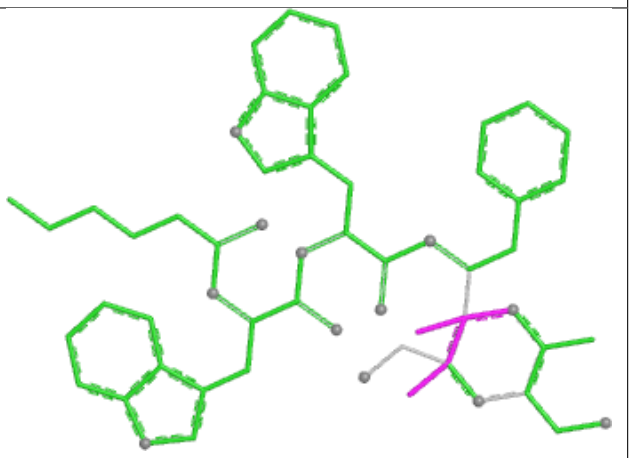


Rings

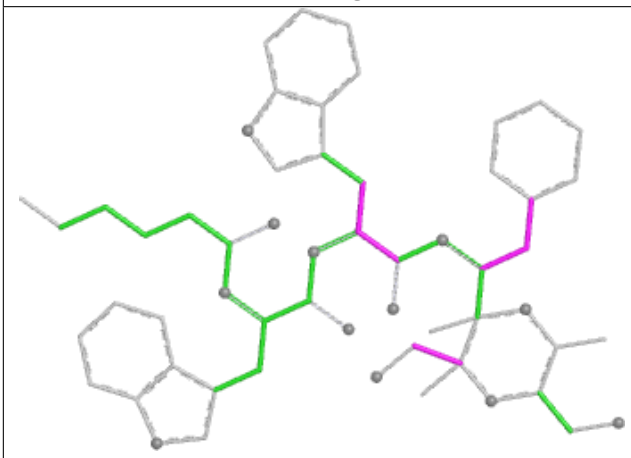
Ligand X5C I 301



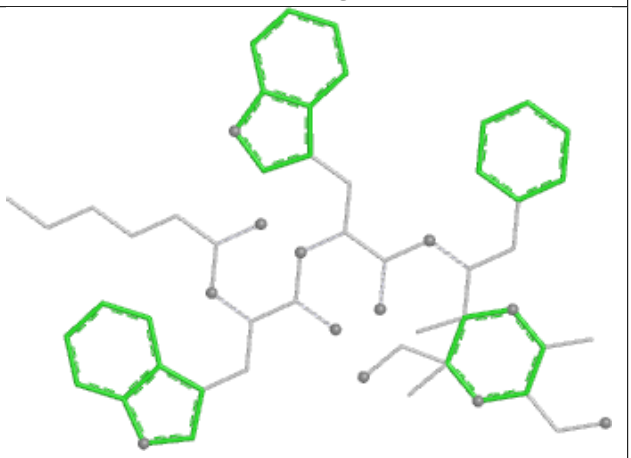
Bond lengths



Bond angles

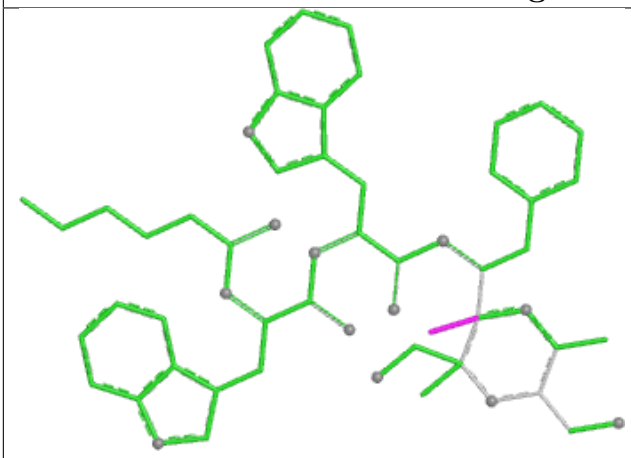


Torsions

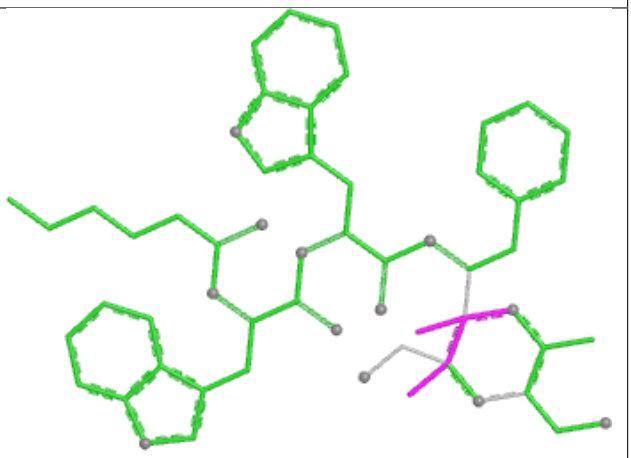


Rings

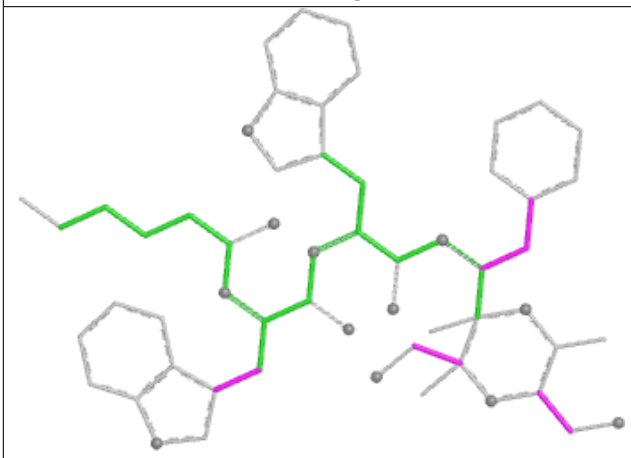
Ligand X5C L 301



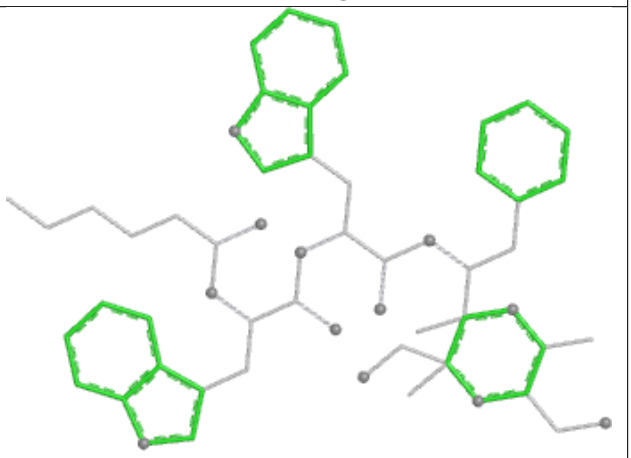
Bond lengths



Bond angles

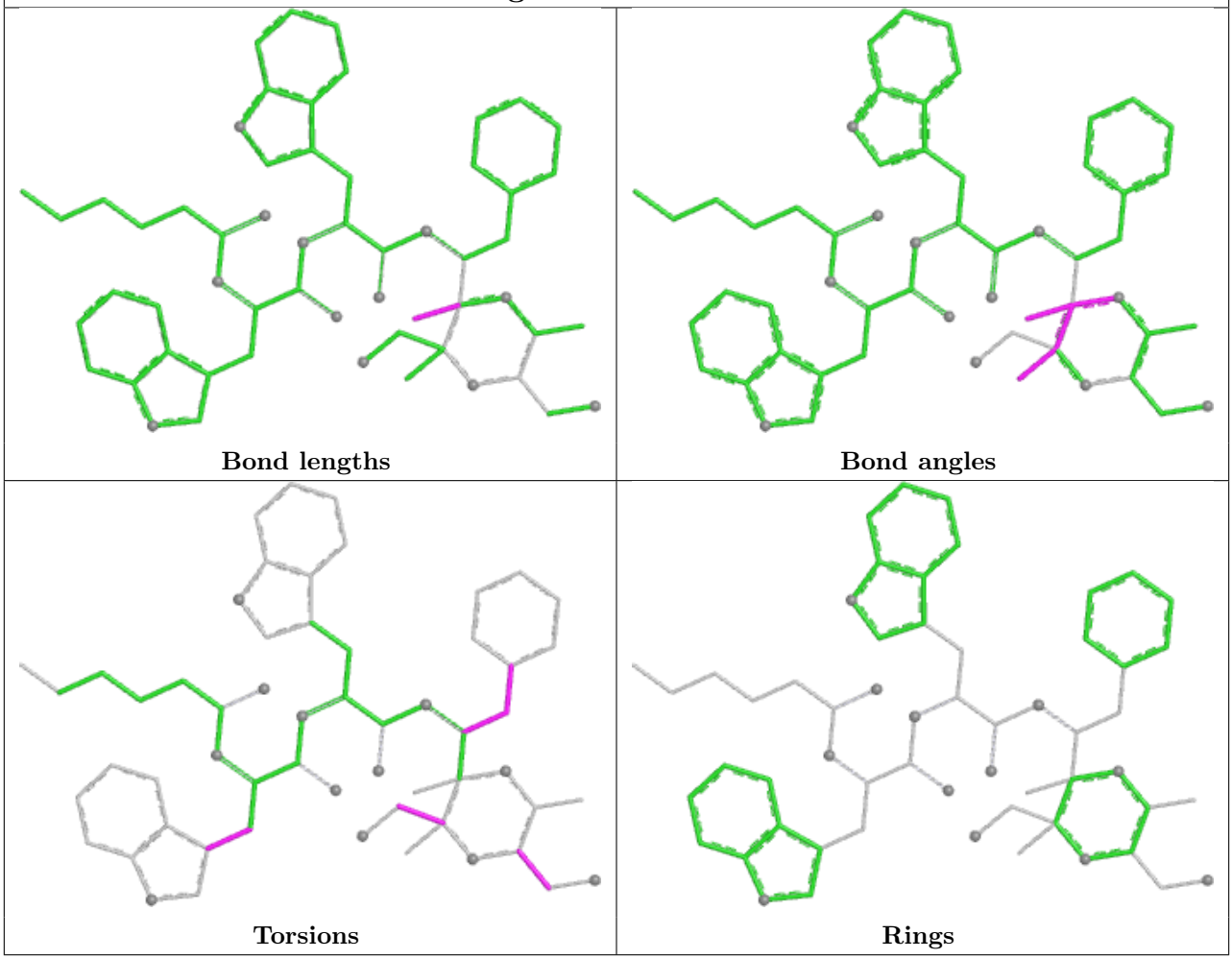


Torsions



Rings

Ligand X5C Z 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

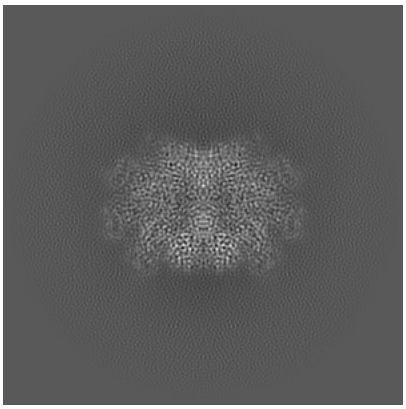
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17337. These allow visual inspection of the internal detail of the map and identification of artifacts.

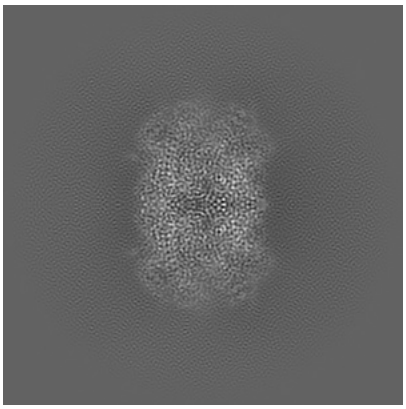
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

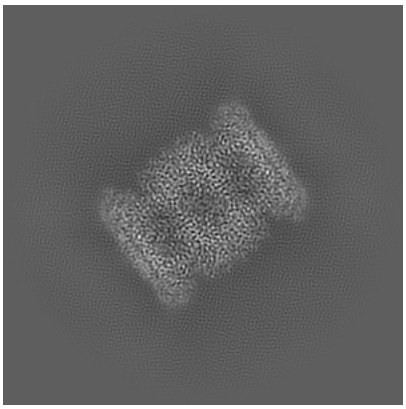
6.1.1 Primary map



X

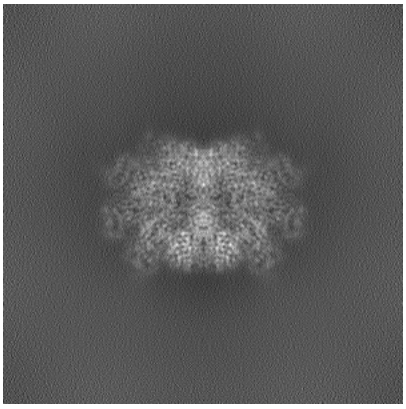


Y

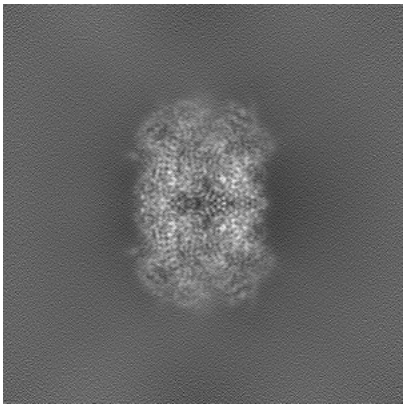


Z

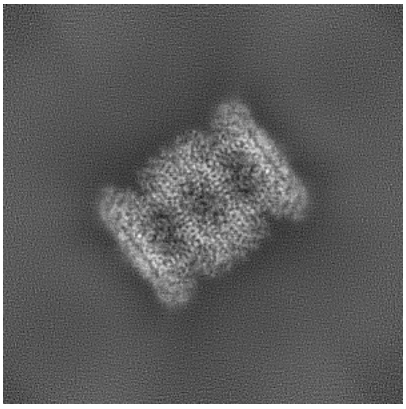
6.1.2 Raw map



X



Y

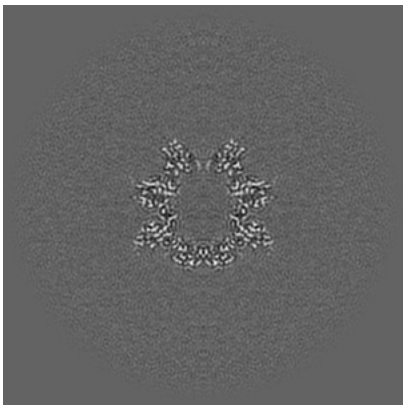


Z

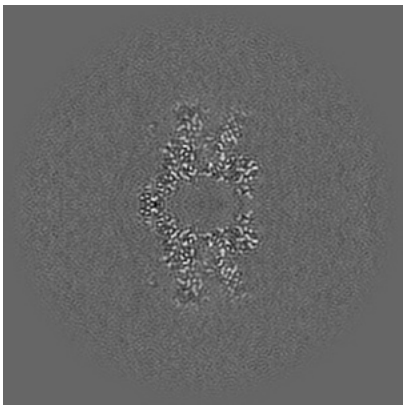
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

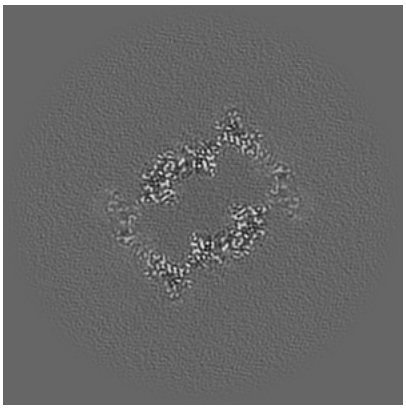
6.2.1 Primary map



X Index: 224

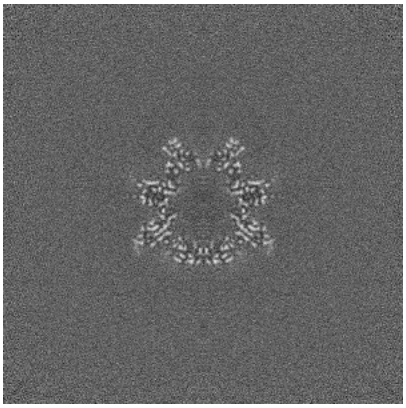


Y Index: 224

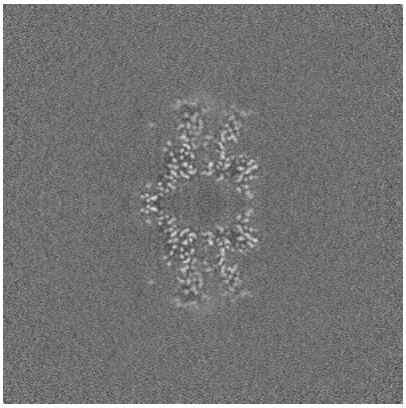


Z Index: 224

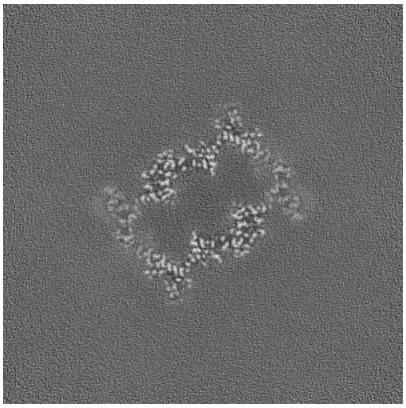
6.2.2 Raw map



X Index: 224



Y Index: 224

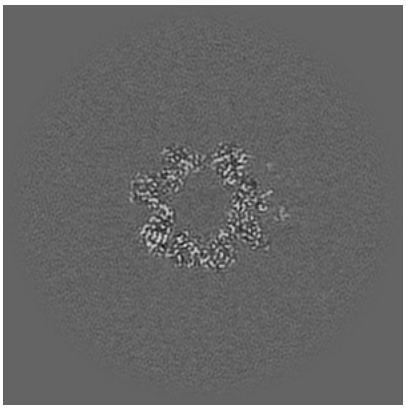


Z Index: 224

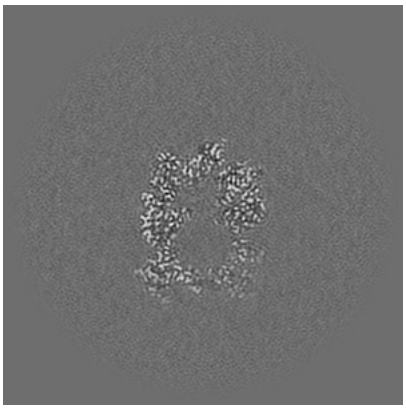
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

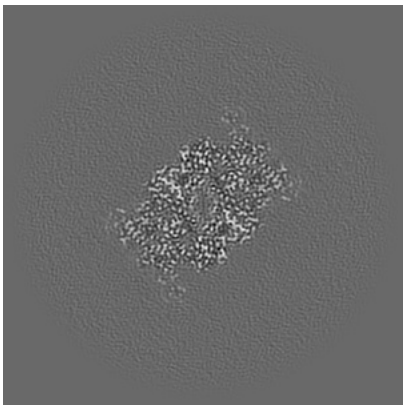
6.3.1 Primary map



X Index: 233

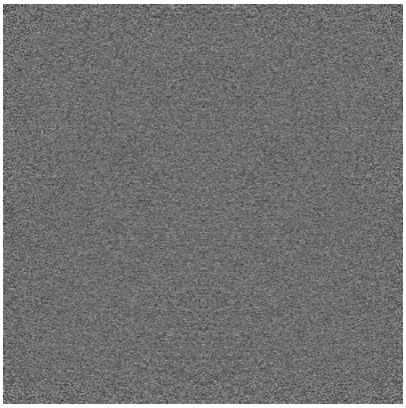


Y Index: 197

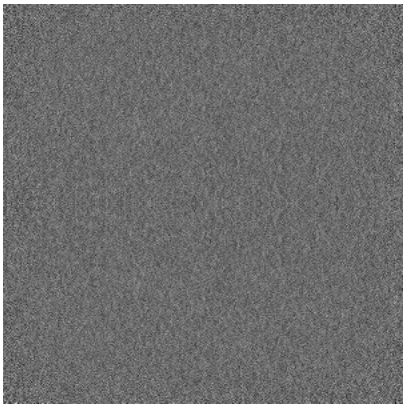


Z Index: 185

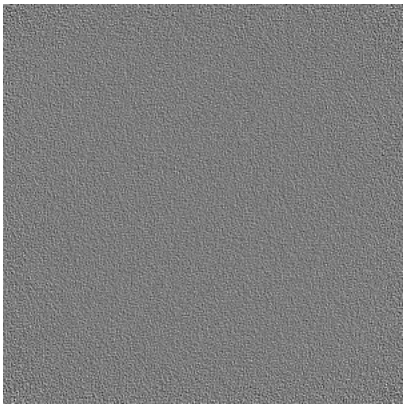
6.3.2 Raw map



X Index: 0



Y Index: 0

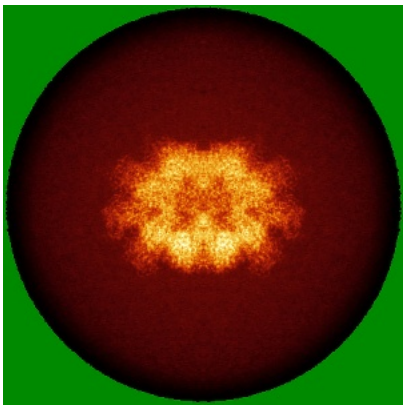


Z Index: 0

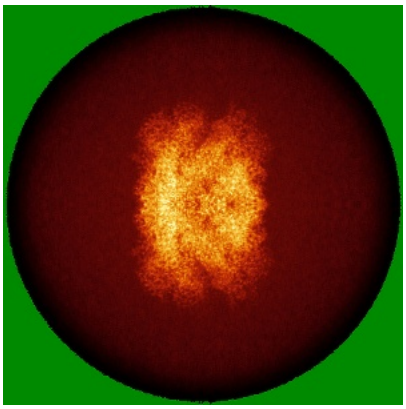
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

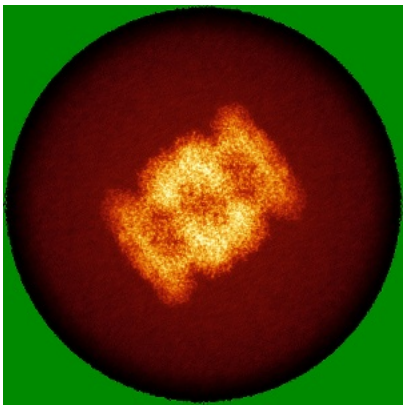
6.4.1 Primary map



X

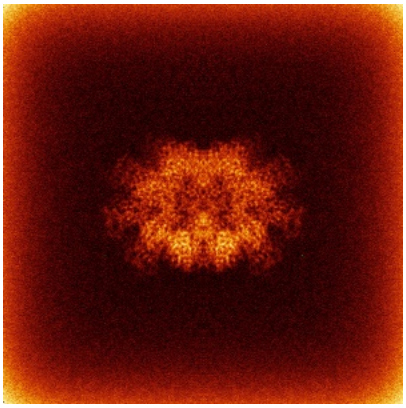


Y

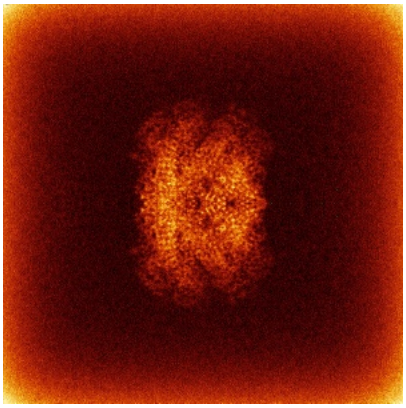


Z

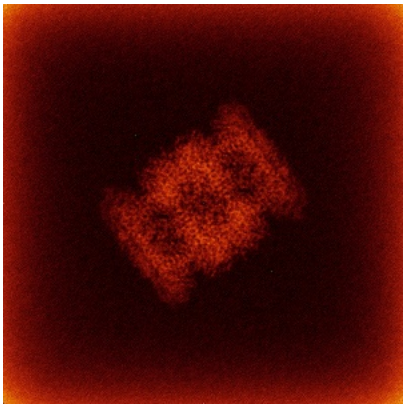
6.4.2 Raw map



X



Y

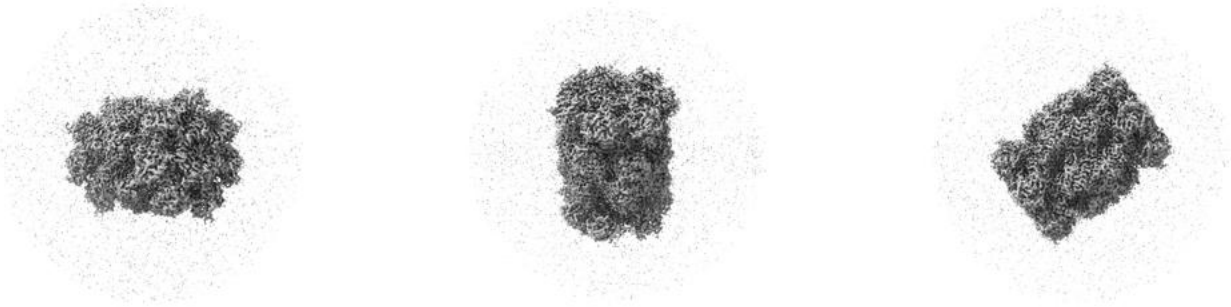


Z

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

6.5 Orthogonal surface views (i)

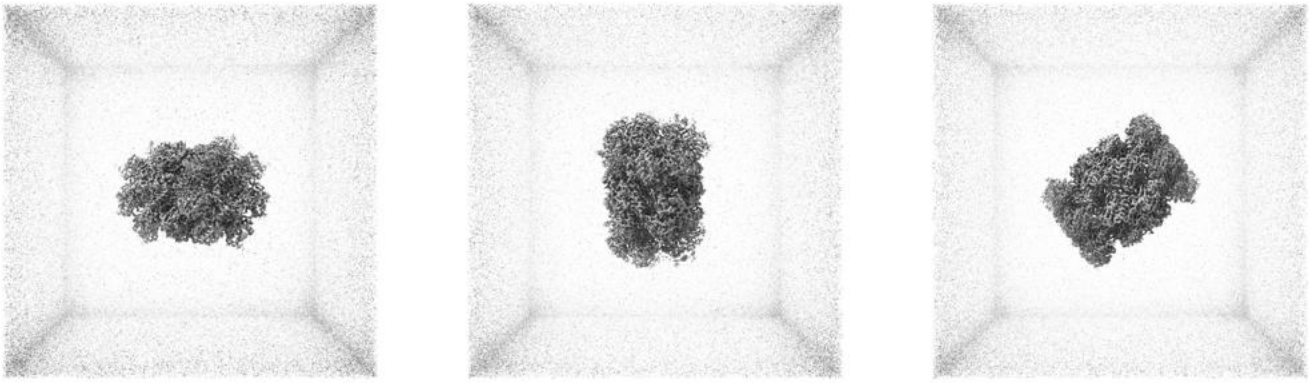
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.195. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

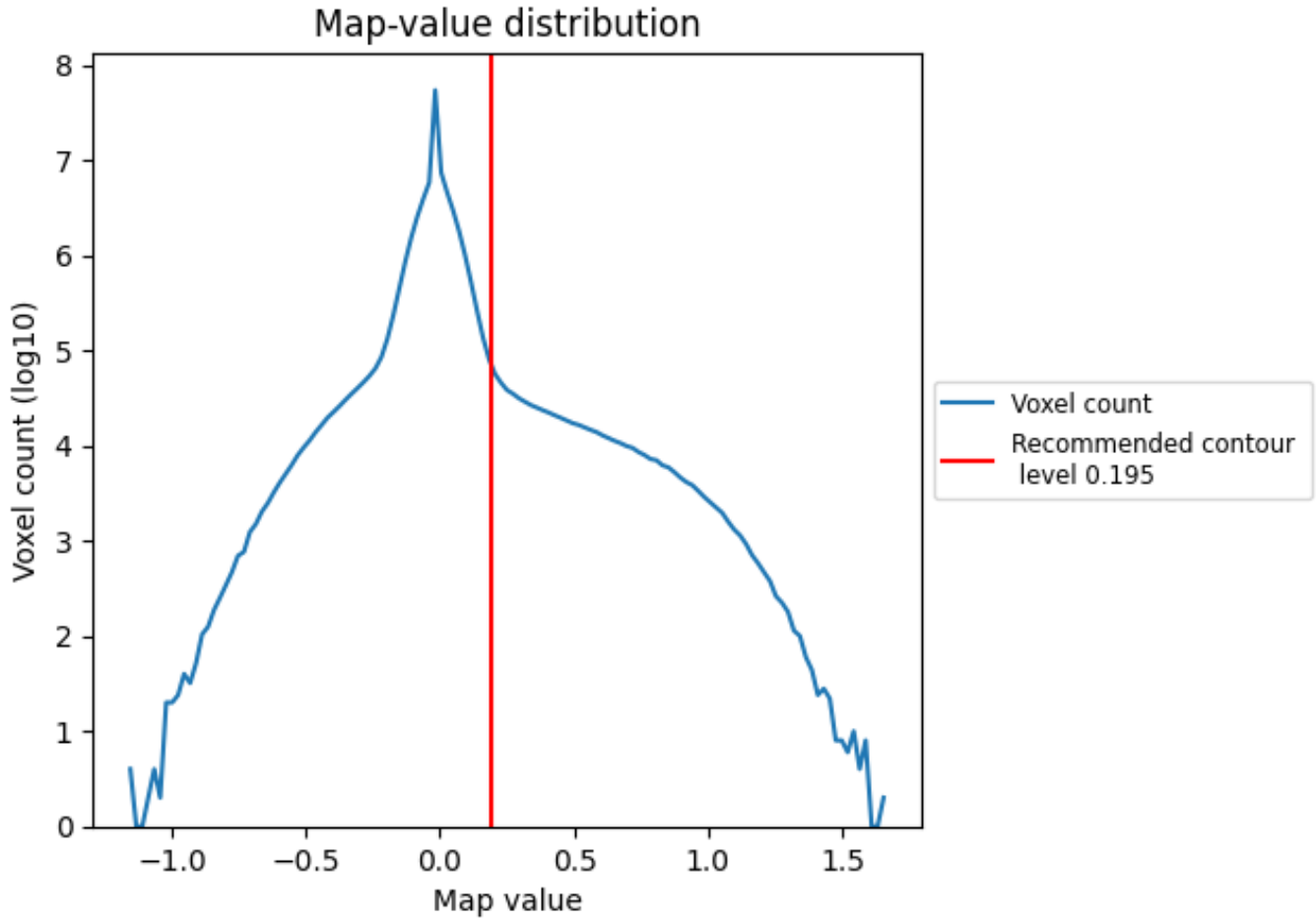
6.6 Mask visualisation (i)

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

7 Map analysis

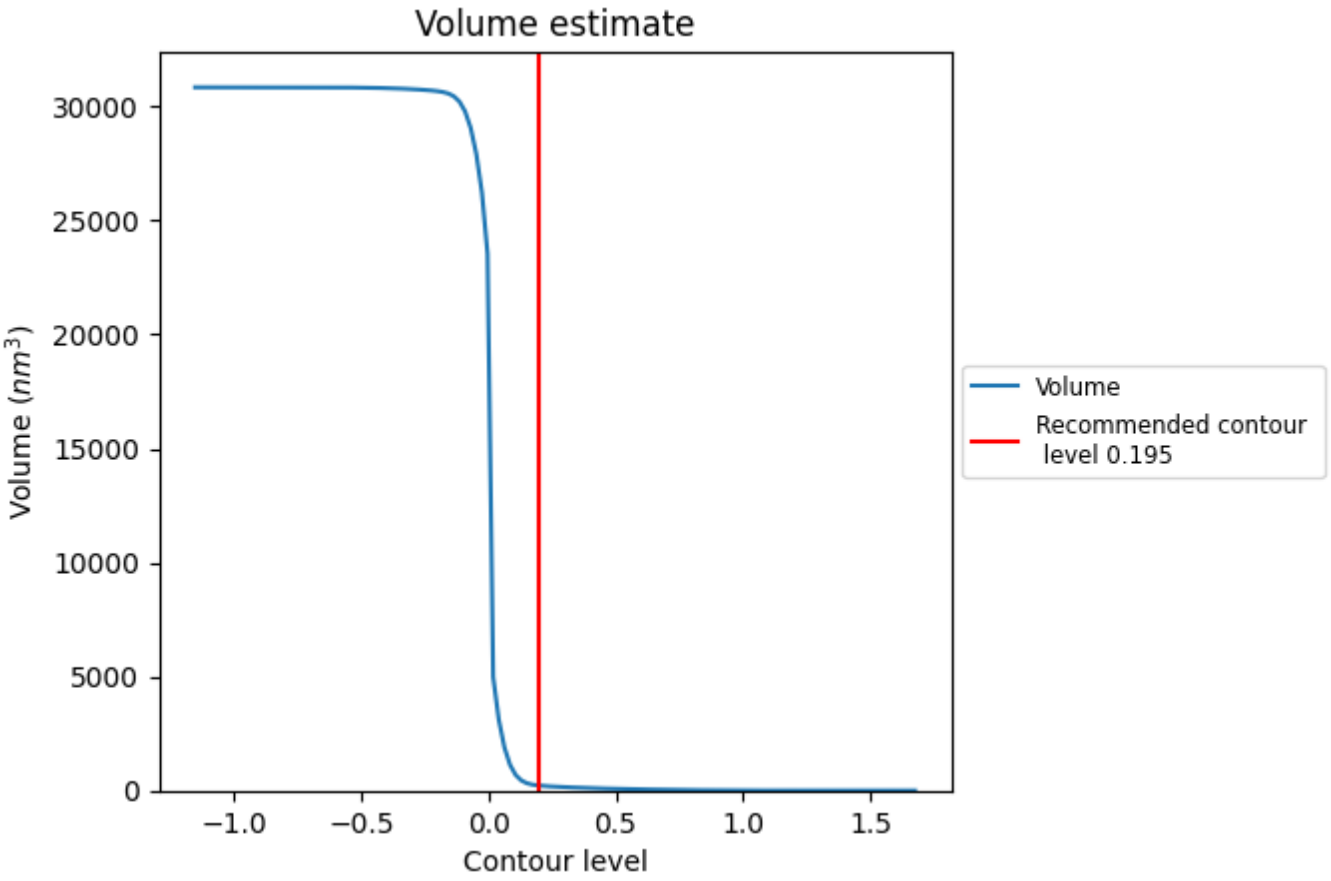
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

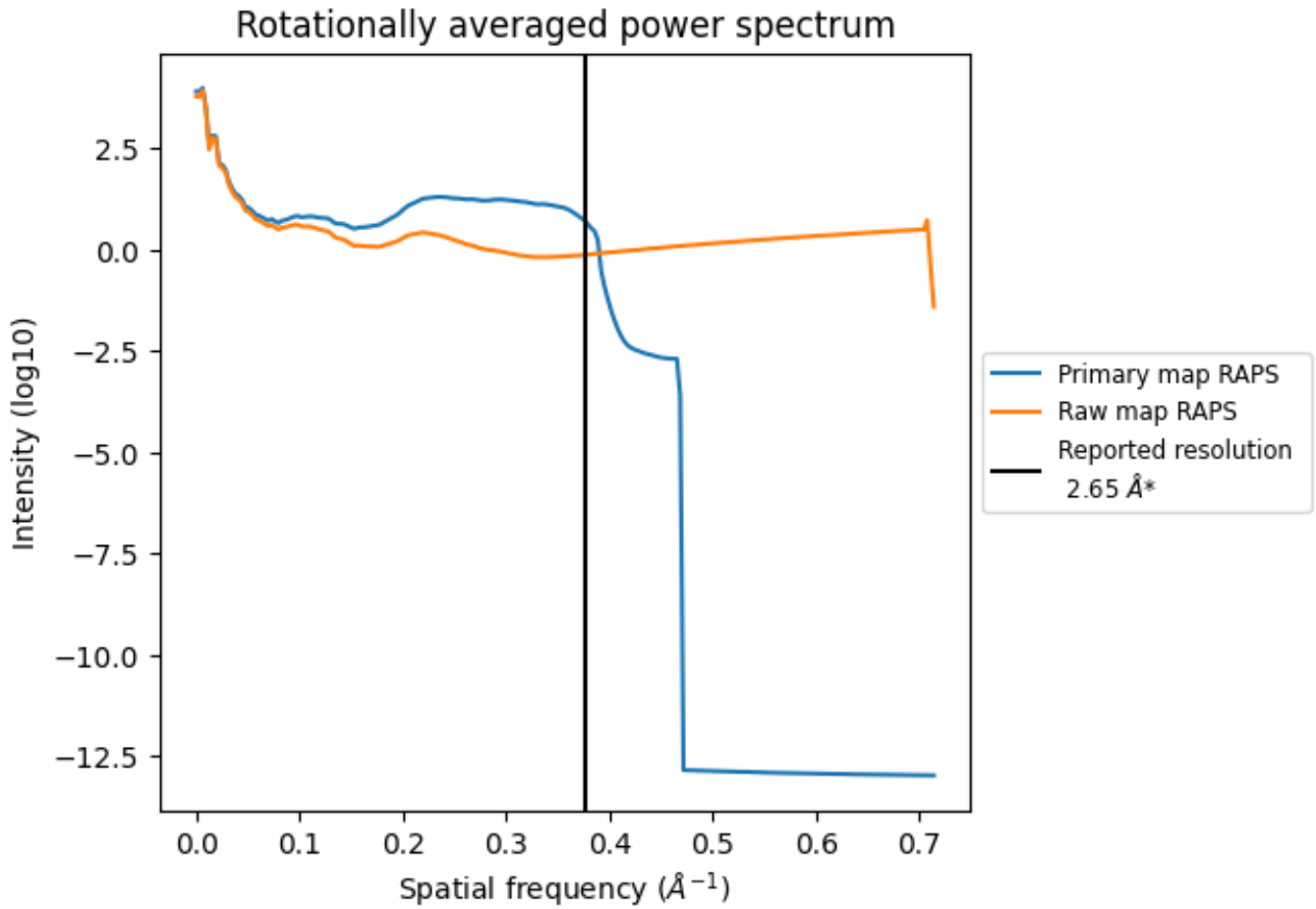
7.2 Volume estimate



The volume at the recommended contour level is 225 nm^3; this corresponds to an approximate mass of 203 kDa.

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

7.3 Rotationally averaged power spectrum (i)

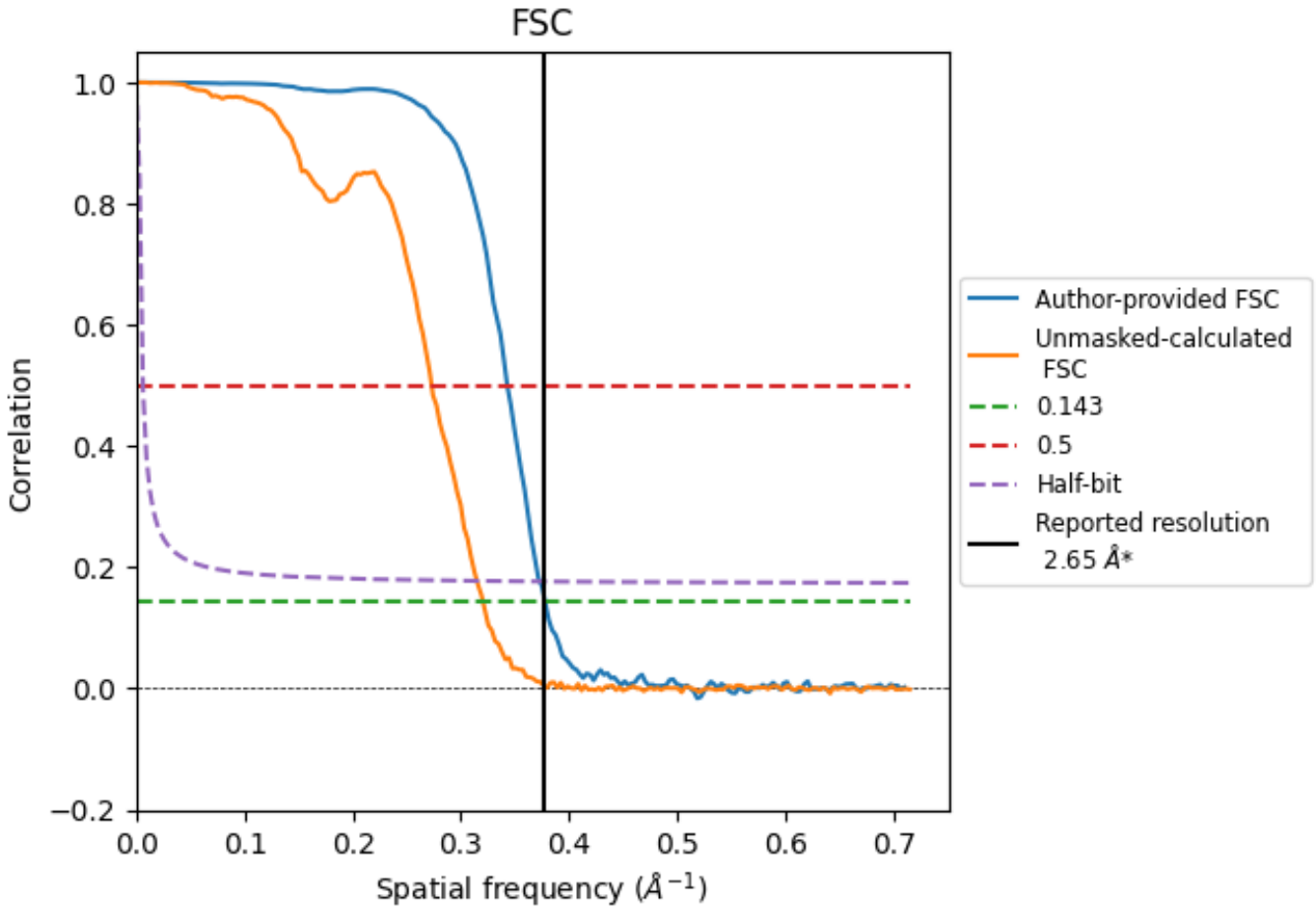


*Reported resolution corresponds to spatial frequency of 0.377 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.377 $Å^{-1}$

8.2 Resolution estimates (i)

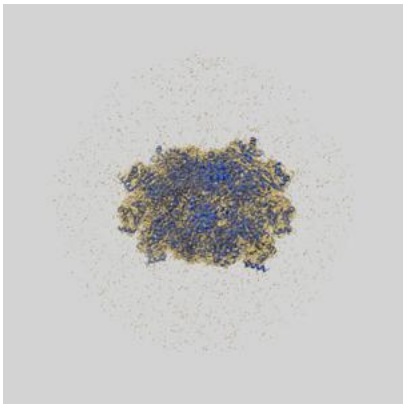
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	2.92	2.68
Unmasked-calculated*	3.12	3.66	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.65 by more than 10 %

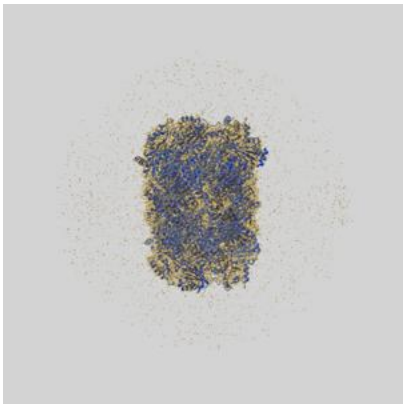
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17337 and PDB model 8P0T. Per-residue inclusion information can be found in section 3 on page 10.

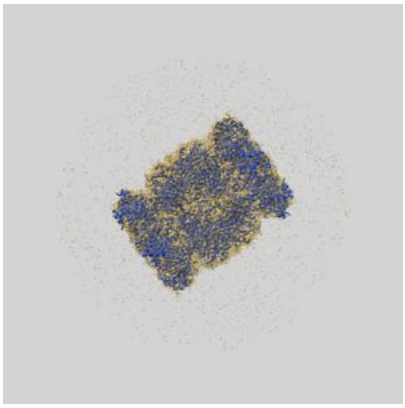
9.1 Map-model overlay



X



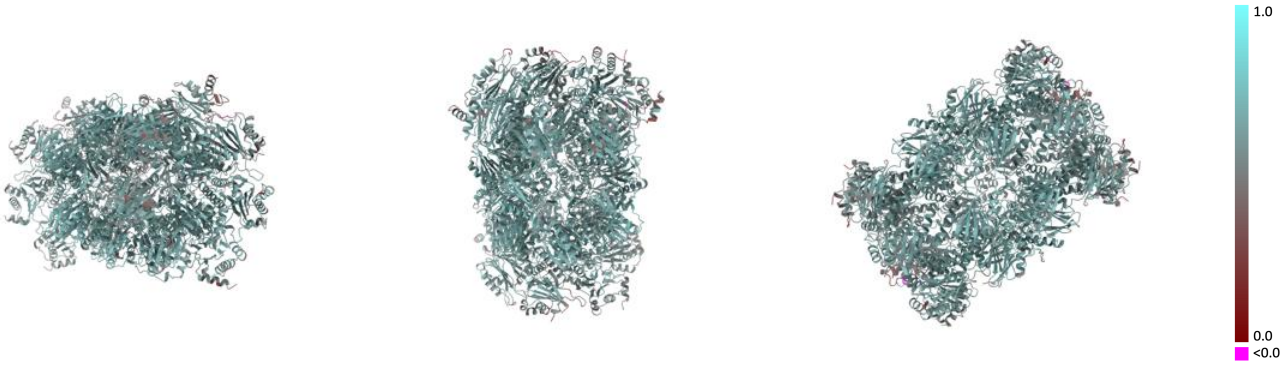
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.195 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

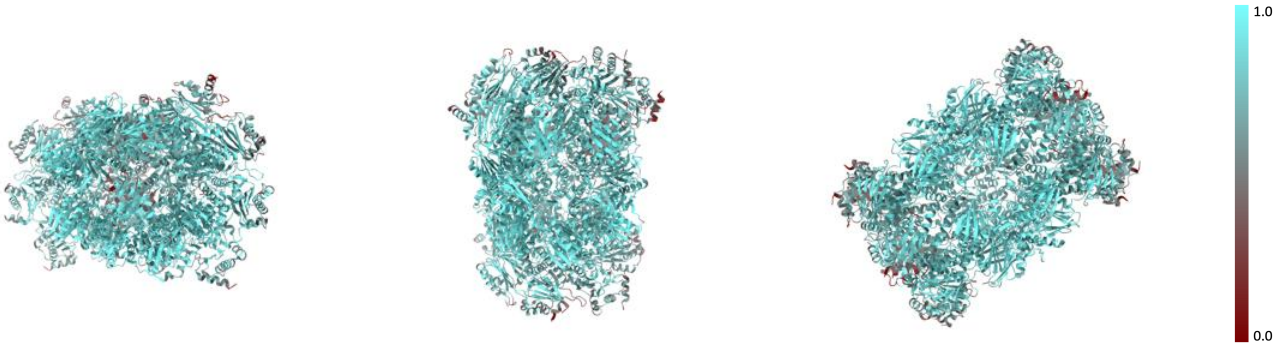
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

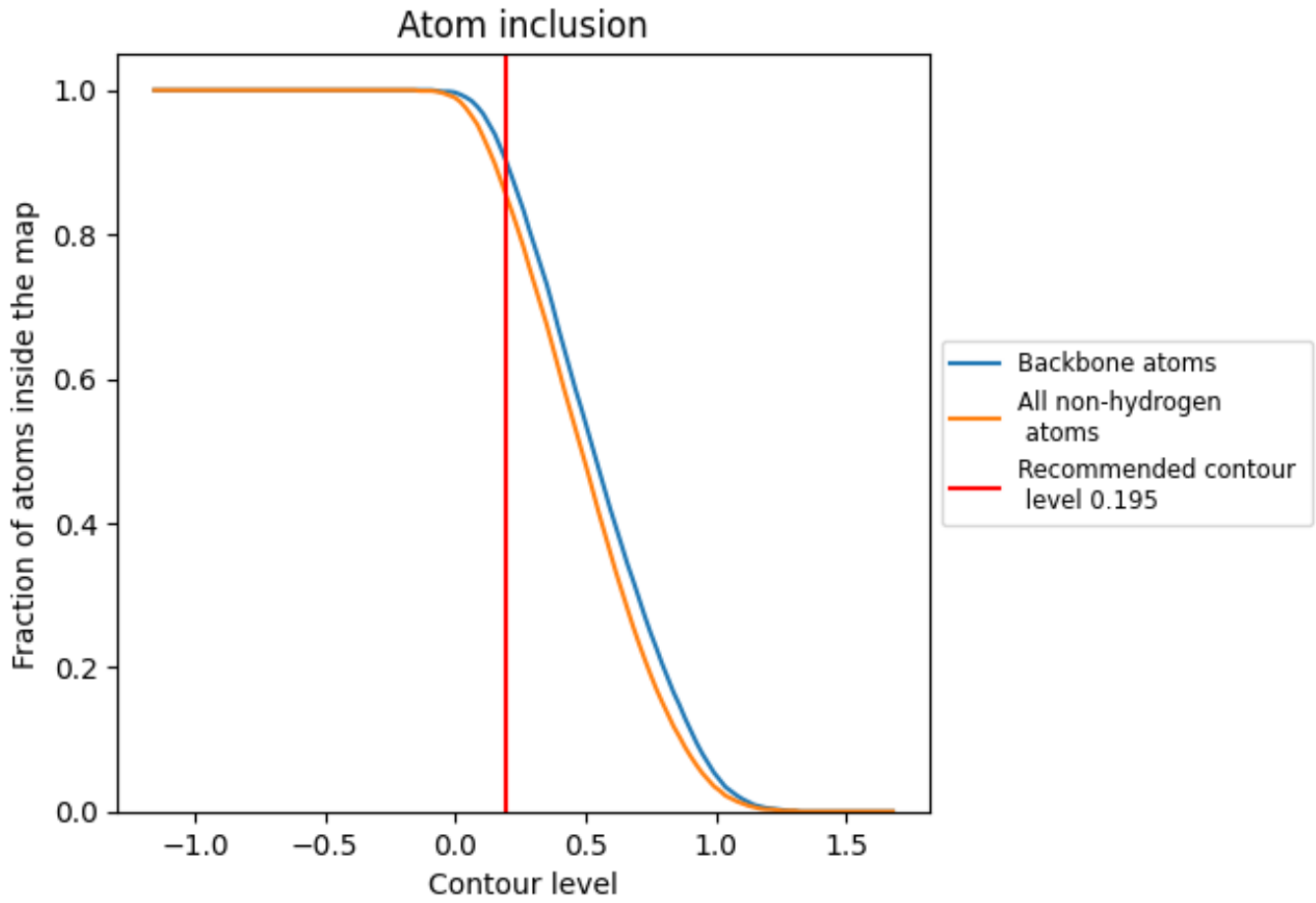
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.195).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.195) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8540	0.6170
A	0.8290	0.6080
B	0.8420	0.6120
C	0.8160	0.6030
D	0.7200	0.5700
E	0.7440	0.5760
F	0.7160	0.5580
G	0.8560	0.6200
H	0.9450	0.6530
I	0.9290	0.6480
J	0.9180	0.6440
K	0.8930	0.6270
L	0.9180	0.6420
M	0.9300	0.6440
N	0.9440	0.6500
O	0.8290	0.6080
P	0.8420	0.6120
Q	0.8160	0.6040
R	0.7200	0.5690
S	0.7440	0.5780
T	0.7170	0.5580
U	0.8550	0.6170
V	0.9450	0.6520
W	0.9290	0.6480
X	0.9180	0.6430
Y	0.8930	0.6250
Z	0.9180	0.6390
a	0.9300	0.6460
b	0.9440	0.6500