Full wwPDB EM Validation Report ⓘ

Aug 12, 2023 – 10:38 am BST

PDB ID	:	8OLU
EMDB ID	:	EMD-16963
Title	:	Leishmania tarentolae proteasome 20S subunit in complex with 1-Benzyl-N-(3-(cyclopropylcarbamoyl)phenyl)-6-oxo-1,6-dihydropyridazine-3-carboxamide
Authors	:	Rowland, P.
Deposited on	:	2023-03-30
Resolution	:	2.59 Å(reported)
Based on initial model	:	.

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

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

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

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

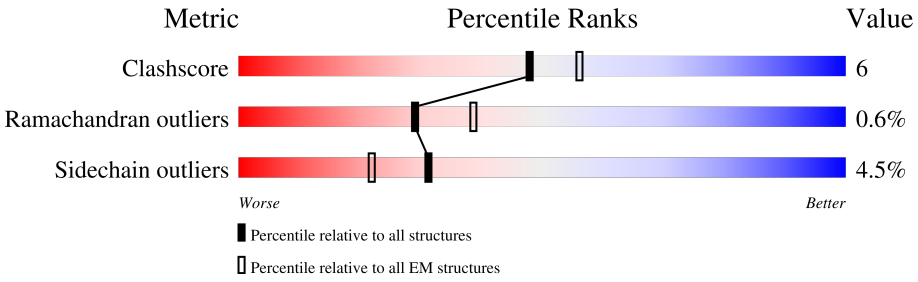
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.59 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	250	14% 78% 19% ••
1	O	250	14% 76% 21% ••
2	B	231	17% 85% 13% ••
2	P	231	17% 84% 13% ••
3	C	285	25% 71% 20% • 5%
3	Q	285	25% 71% 21% • 5%
4	D	248	29% 73% 19% • 6%
4	R	248	29% 72% 19% • 6%

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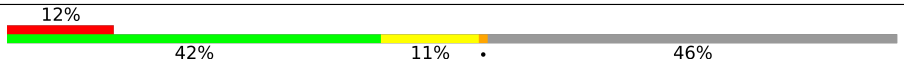
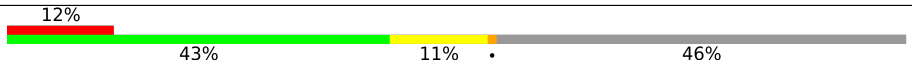
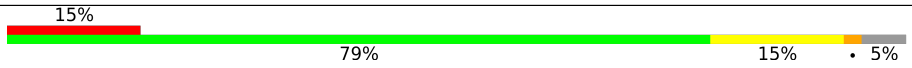
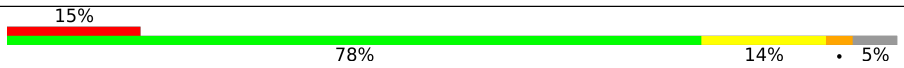
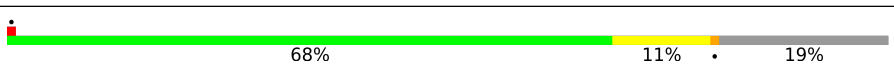
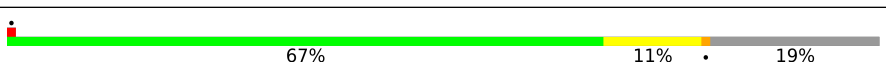
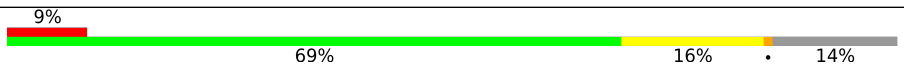
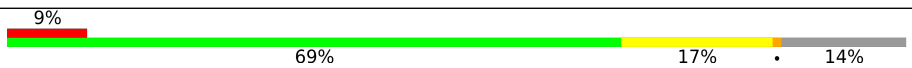
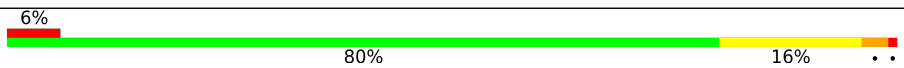
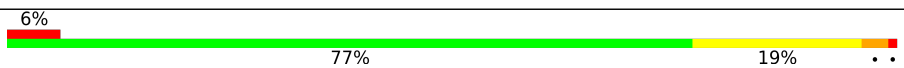
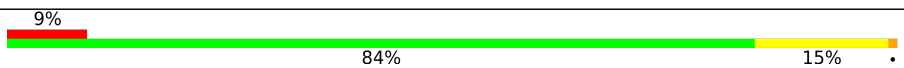
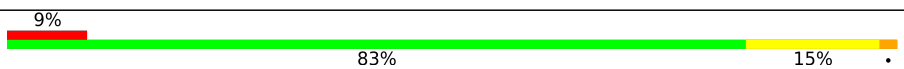
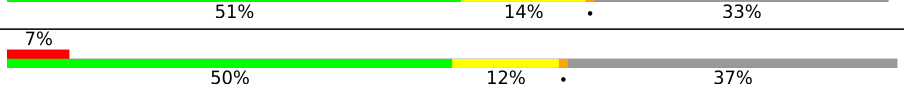
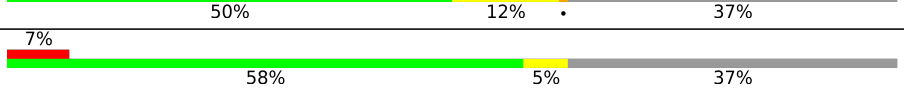
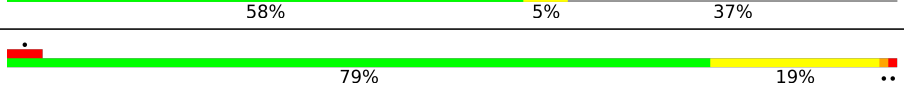
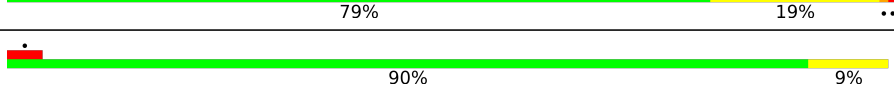
Mol	Chain	Length	Quality of chain
5	E	344	
5	S	344	
6	F	428	
6	T	428	
7	G	238	
7	U	238	
8	H	283	
8	V	283	
9	I	254	
9	W	254	
10	J	205	
10	X	205	
11	K	206	
11	Y	206	
12	L	301	
12	Z	301	
13	M	339	
13	a	339	
14	N	220	
14	b	220	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 48930 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 Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		
1	O	244	Total	C	N	O	S	0	0
			1857	1169	323	353	12		

- Molecule 2 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		
2	P	229	Total	C	N	O	S	0	0
			1754	1112	292	342	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2150	1354	370	414	12		
3	Q	271	Total	C	N	O	S	0	0
			2150	1354	370	414	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	234	Total	C	N	O	S	0	0
			1840	1160	316	356	8		
4	R	234	Total	C	N	O	S	0	0
			1840	1160	316	356	8		

- Molecule 5 is a protein called Proteasome alpha 5 subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		
5	S	229	Total	C	N	O	S	0	0
			1756	1094	302	347	13		

- Molecule 6 is a protein called Proteasome alpha 1 subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	232	Total	C	N	O	S	0	0
			1819	1140	315	353	11		
6	T	232	Total	C	N	O	S	0	0
			1819	1140	315	353	11		

- Molecule 7 is a protein called Proteasome alpha 7 subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	226	Total	C	N	O	S	0	0
			1714	1069	304	331	10		
7	U	226	Total	C	N	O	S	0	0
			1714	1069	304	331	10		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	228	Total	C	N	O	S	0	0
			1705	1060	294	339	12		
8	V	228	Total	C	N	O	S	0	0
			1705	1060	294	339	12		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		
9	W	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		

- 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
			1557	980	259	302	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		
11	Y	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		

- 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
			1579	998	277	297	7		
12	Z	202	Total	C	N	O	S	0	0
			1579	998	277	297	7		

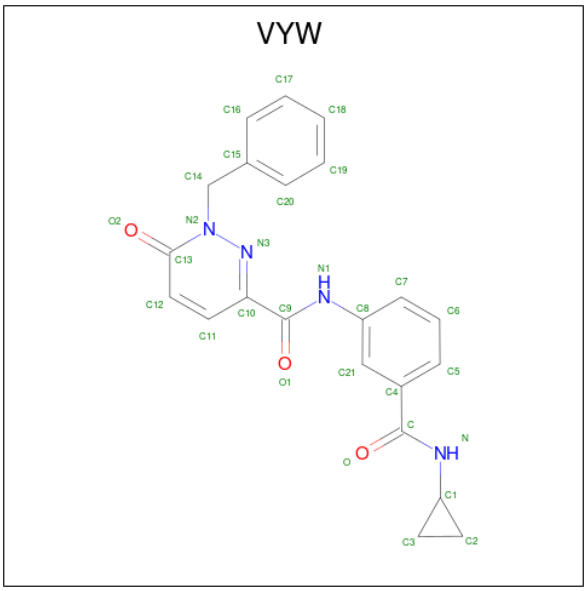
- Molecule 13 is a protein called Proteasome beta 6 subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		
13	a	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	220	Total	C	N	O	S	0	0
			1732	1094	297	326	15		
14	b	220	Total	C	N	O	S	0	0
			1732	1094	297	326	15		

- Molecule 15 is {N}-[3-(cyclopropylcarbamoyl)phenyl]-6-oxidanylidene-1-(phenylmethyl)pyridazine-3-carboxamide (three-letter code: VYW) (formula: $C_{22}H_{20}N_4O_3$).



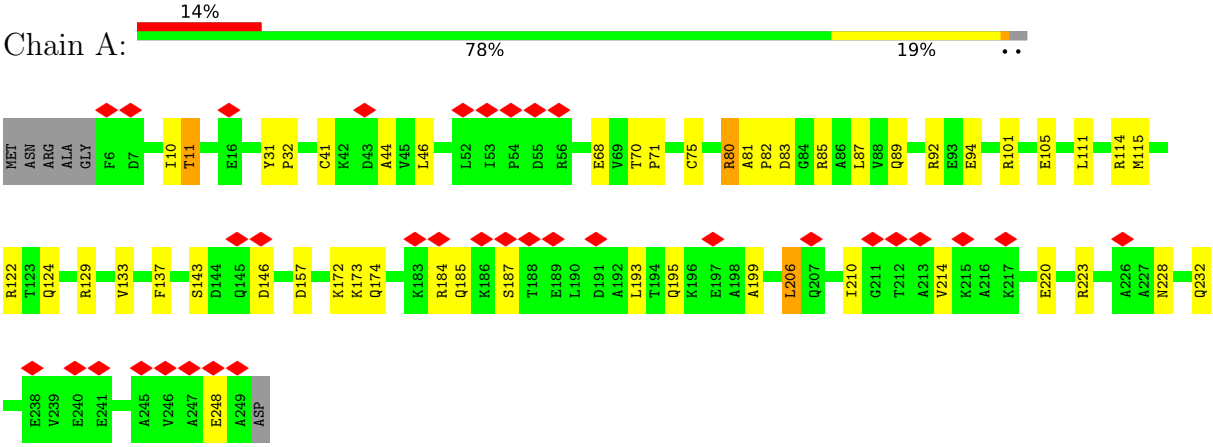
Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	N	O	0
			29	22	4	3	
15	Z	1	Total	C	N	O	0
			29	22	4	3	

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.

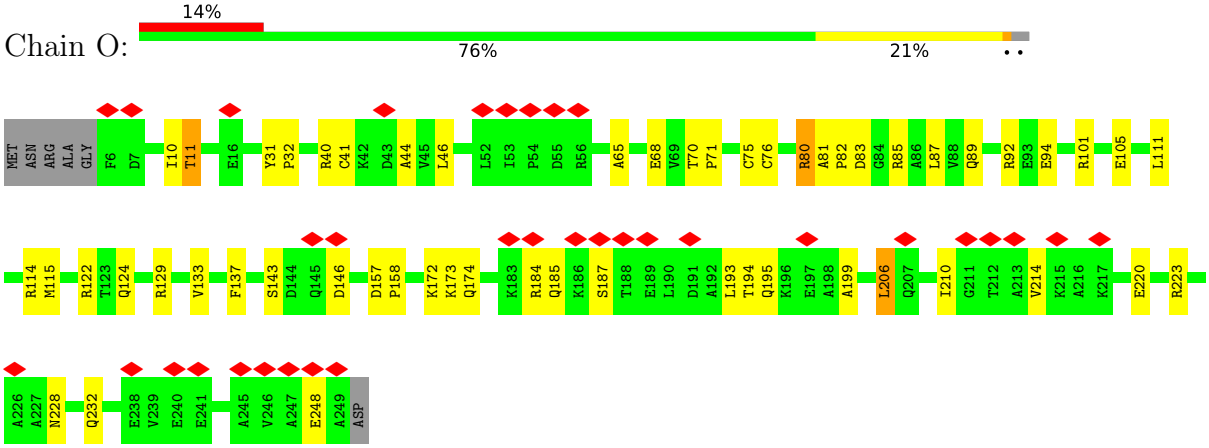
• Molecule 1: Proteasome subunit alpha type

Chain A:



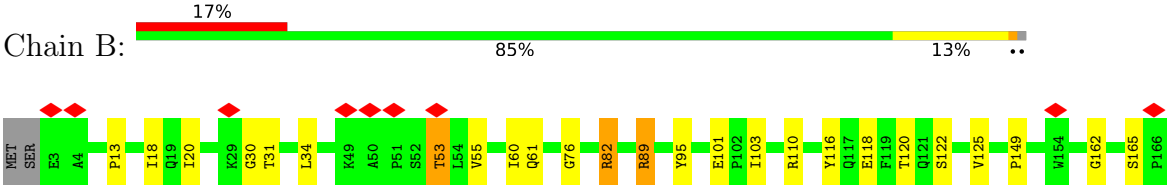
• Molecule 1: Proteasome subunit alpha type

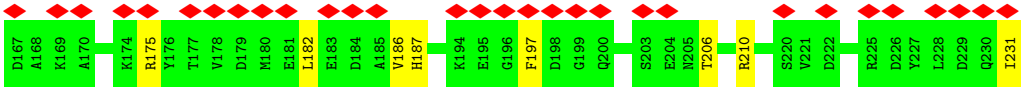
Chain O:



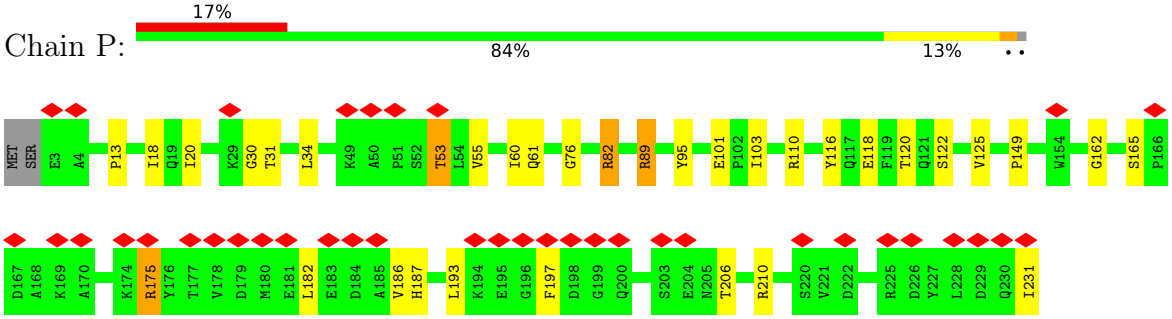
• Molecule 2: Proteasome subunit alpha type

Chain B:

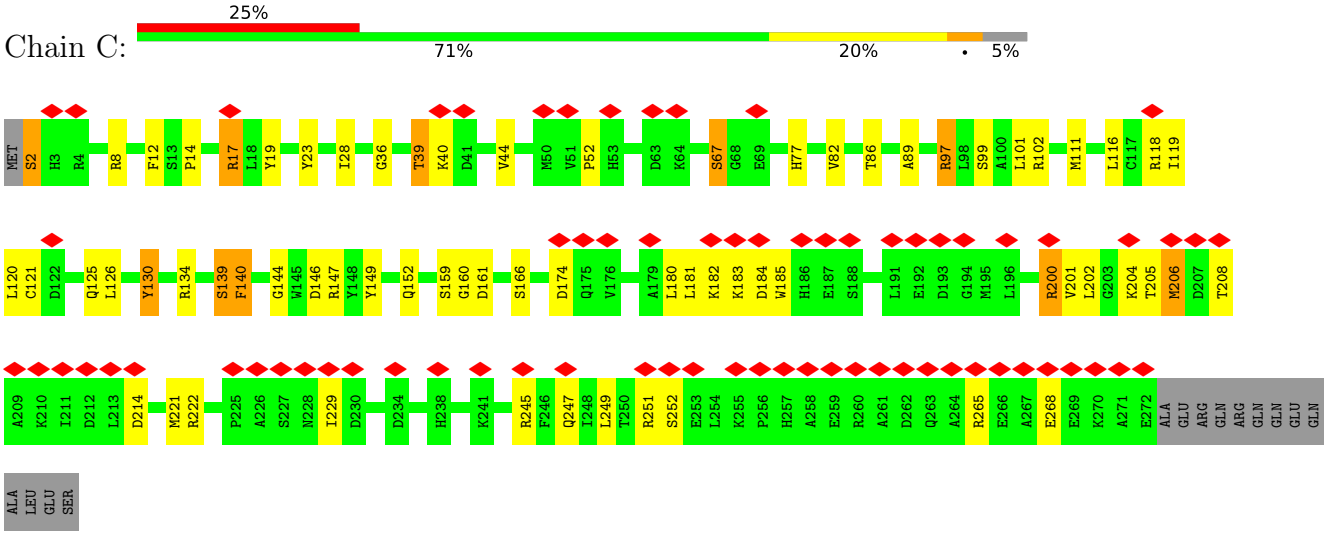




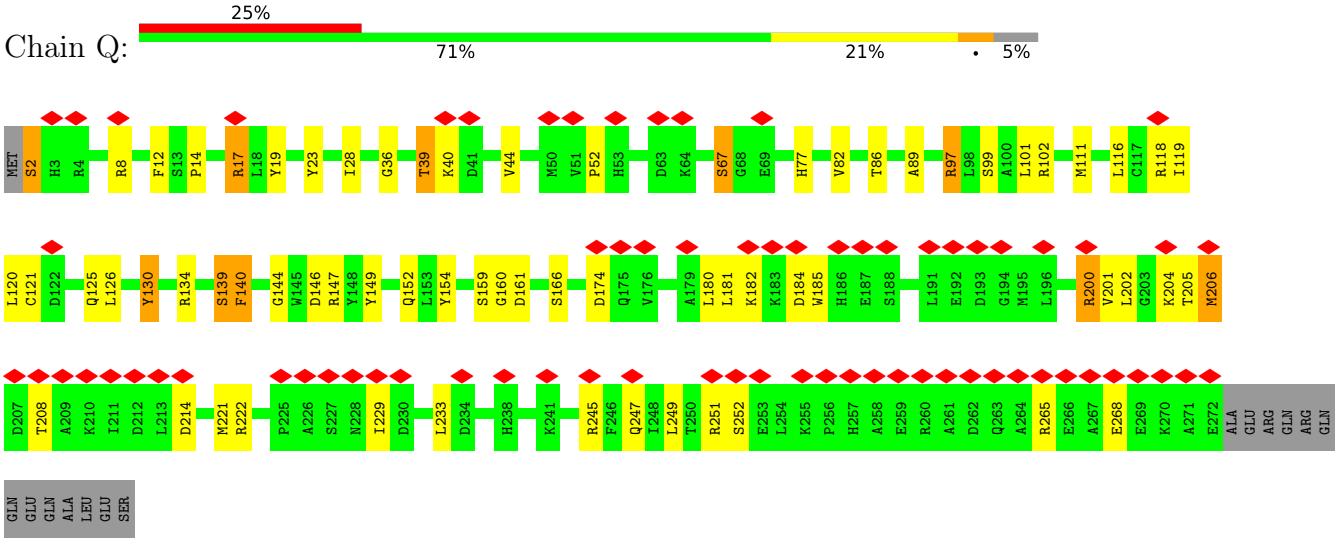
• Molecule 2: Proteasome subunit alpha type



• Molecule 3: Proteasome subunit alpha type

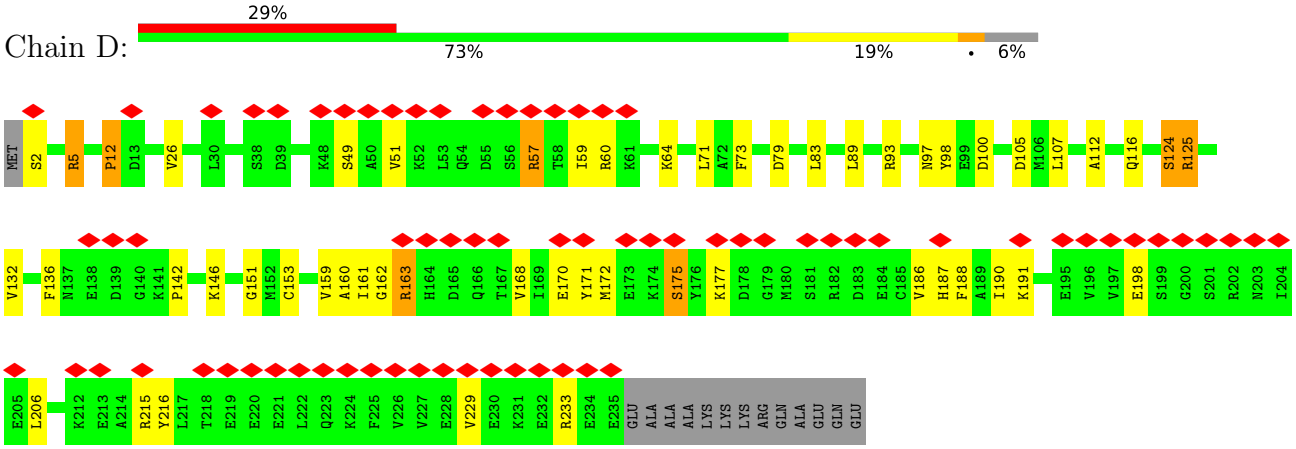


• Molecule 3: Proteasome subunit alpha type



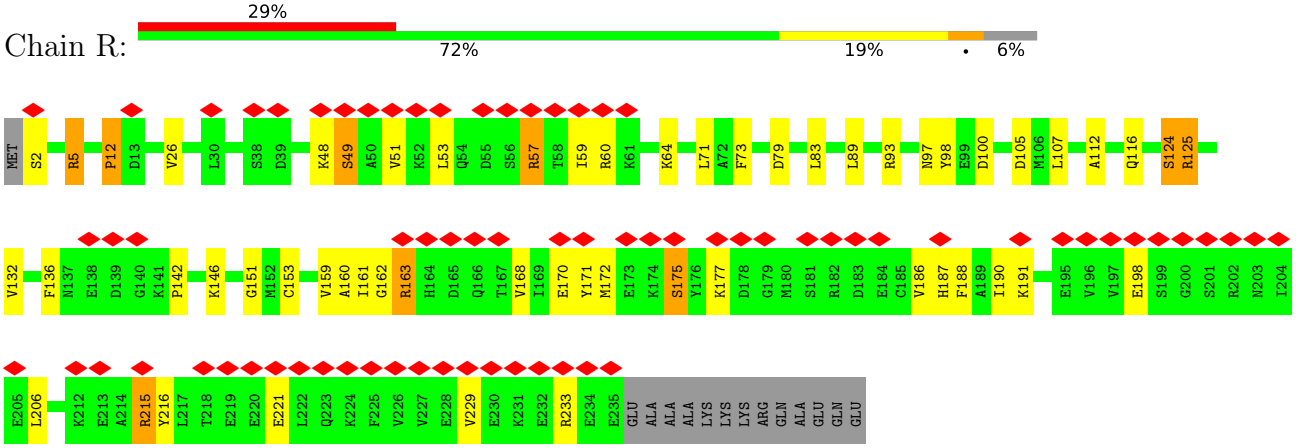
• Molecule 4: Proteasome subunit alpha type

Chain D:



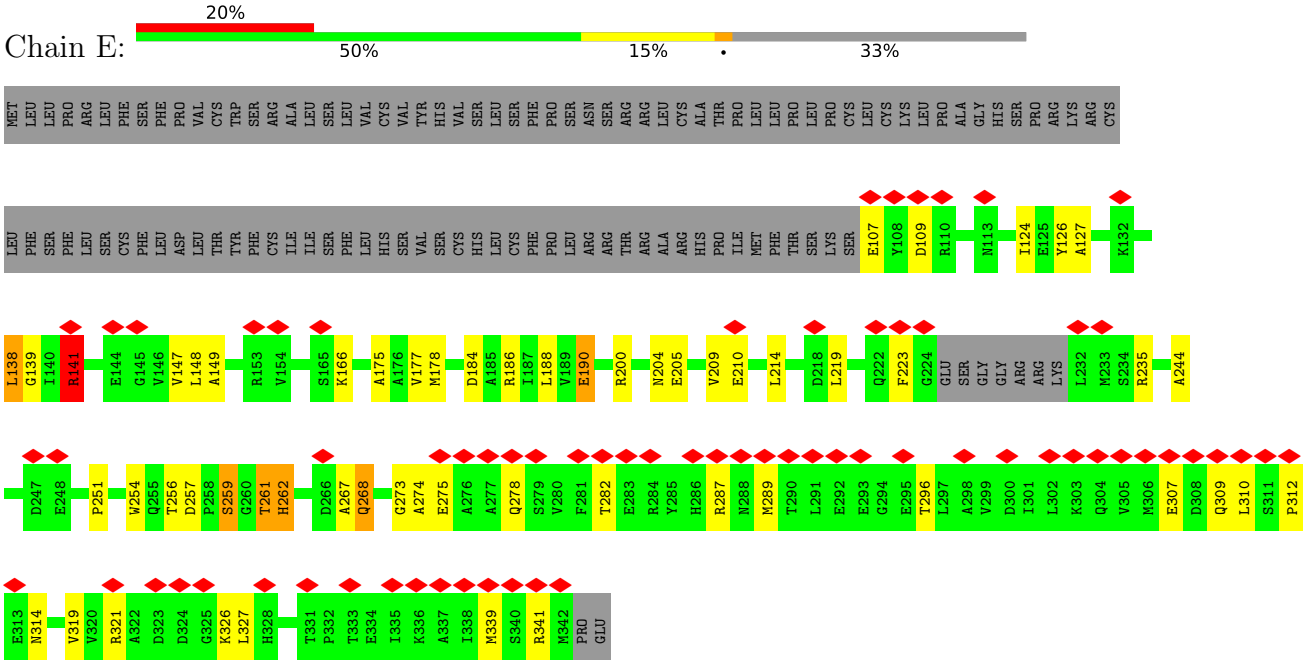
• Molecule 4: Proteasome subunit alpha type

Chain R:

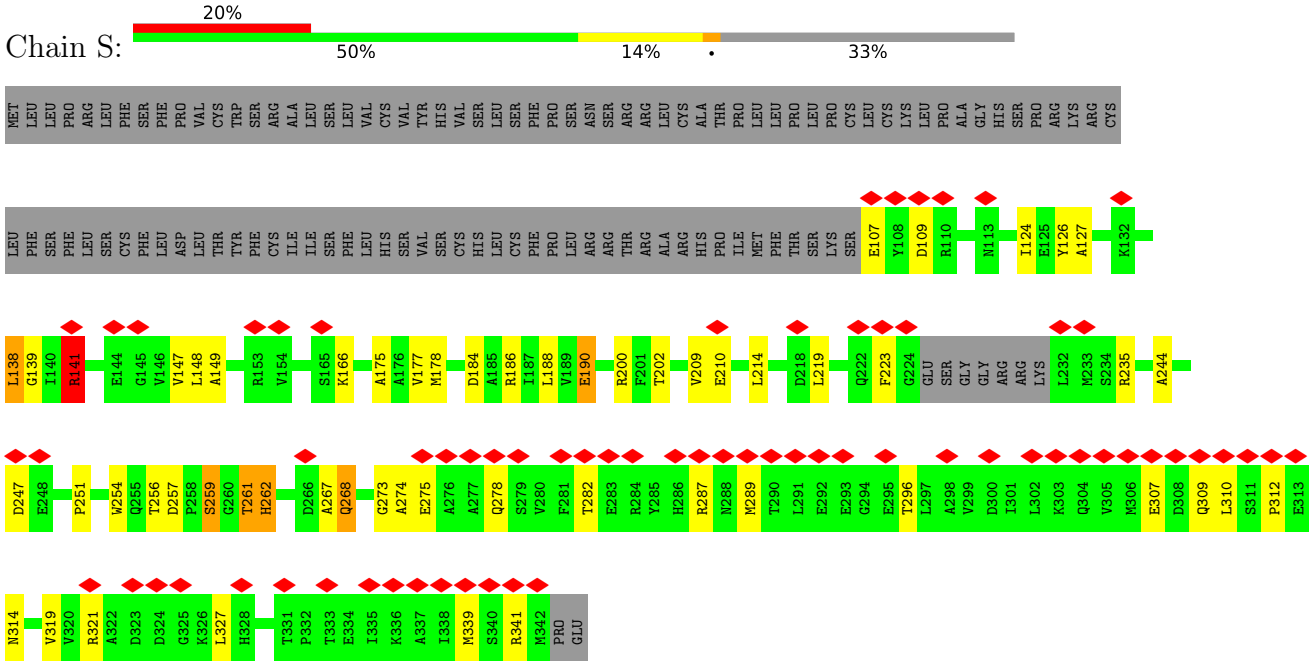


• Molecule 5: Proteasome alpha 5 subunit, putative

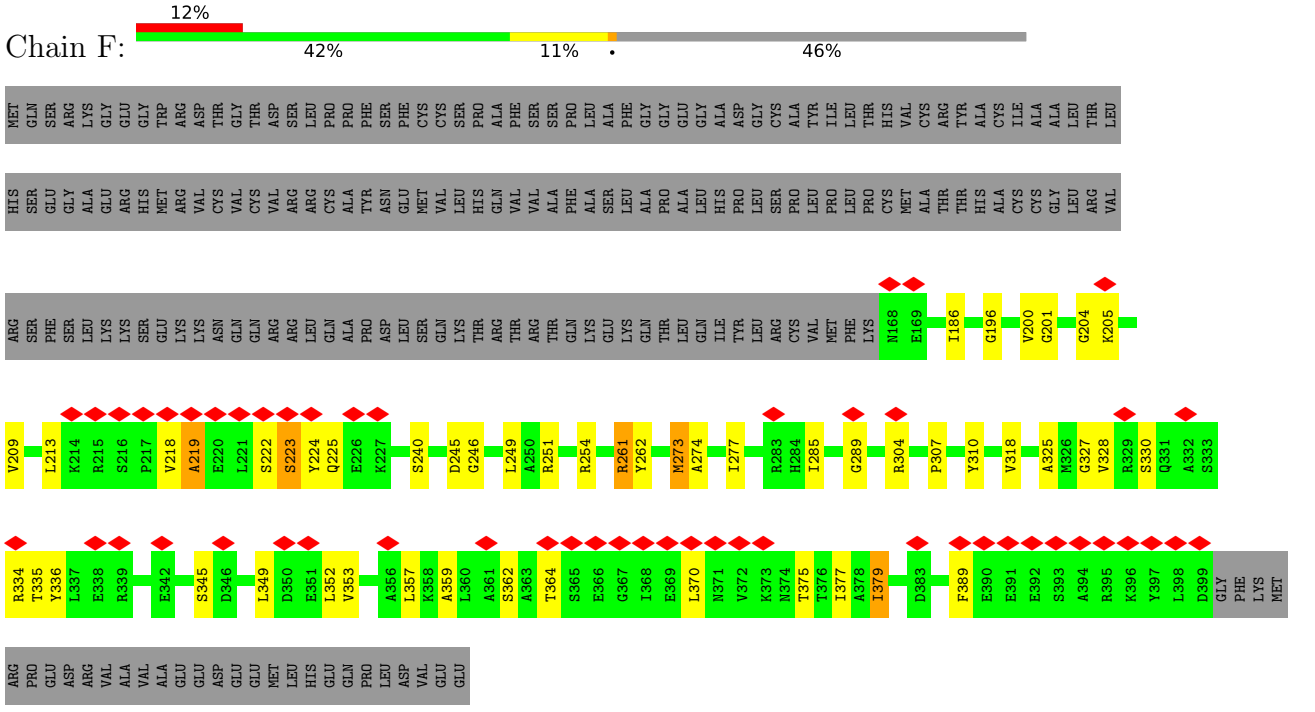
Chain E:



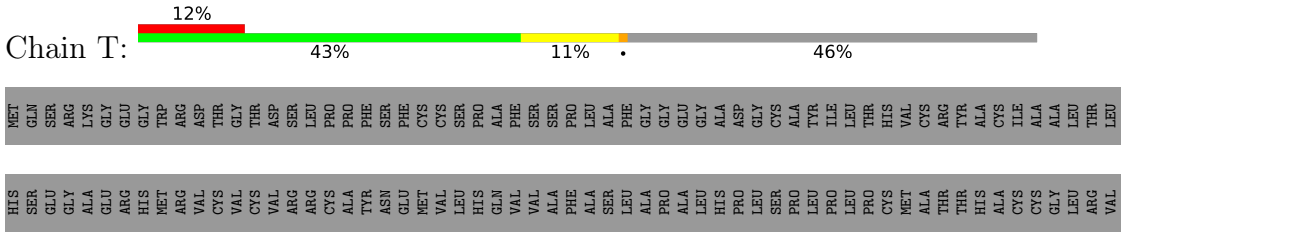
• Molecule 5: Proteasome alpha 5 subunit, putative

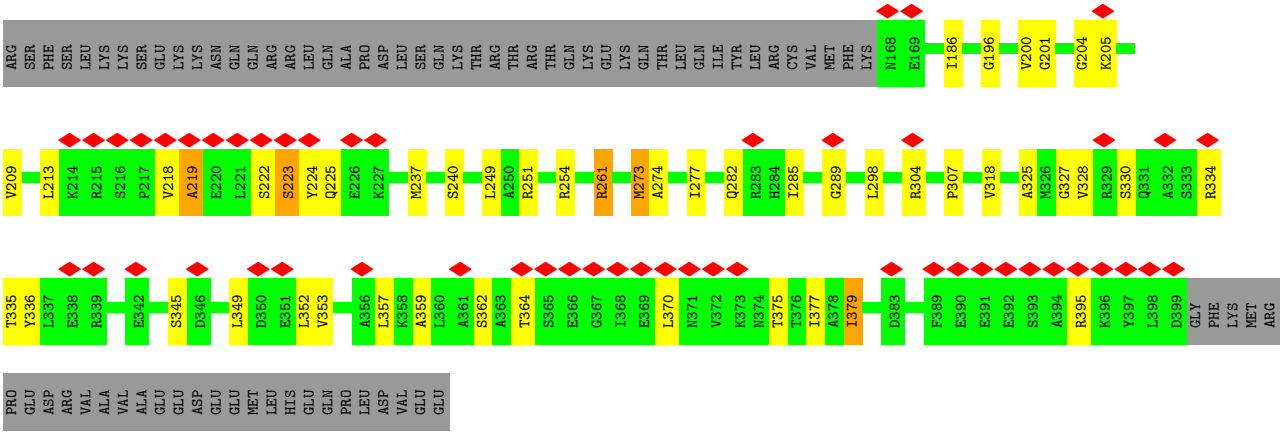


• Molecule 6: Proteasome alpha 1 subunit, putative



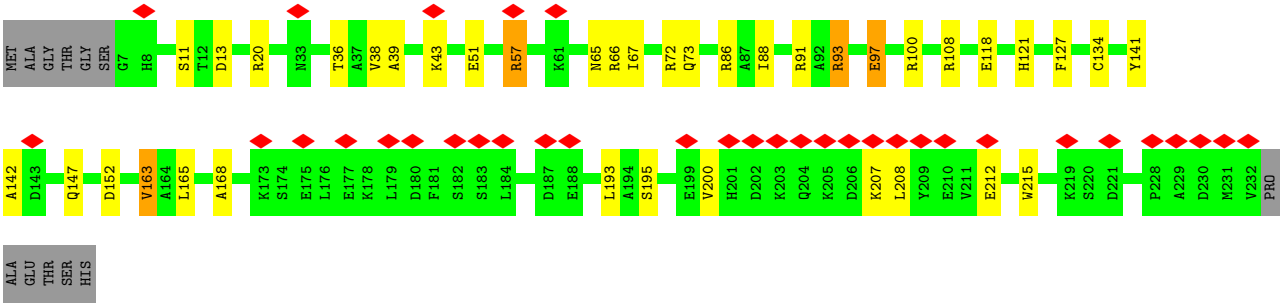
• Molecule 6: Proteasome alpha 1 subunit, putative





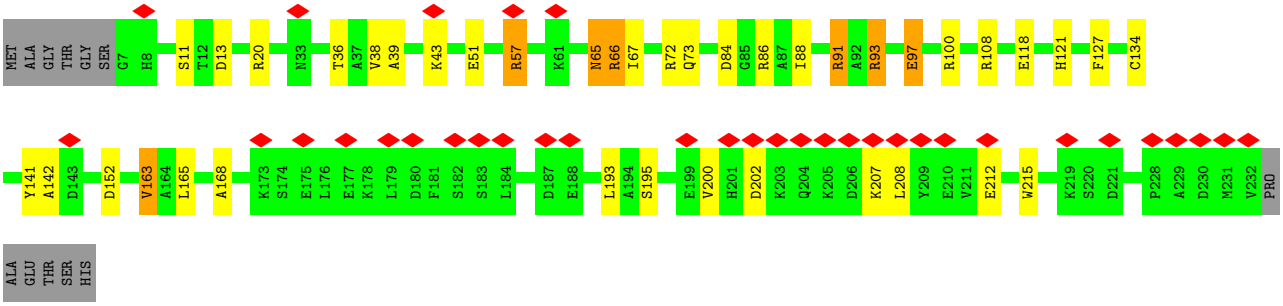
• Molecule 7: Proteasome alpha 7 subunit, putative

Chain G:



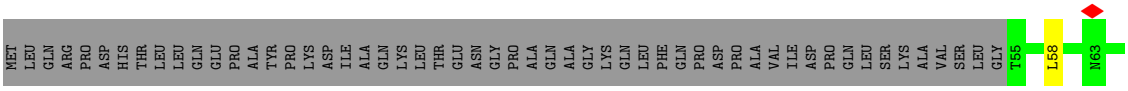
• Molecule 7: Proteasome alpha 7 subunit, putative

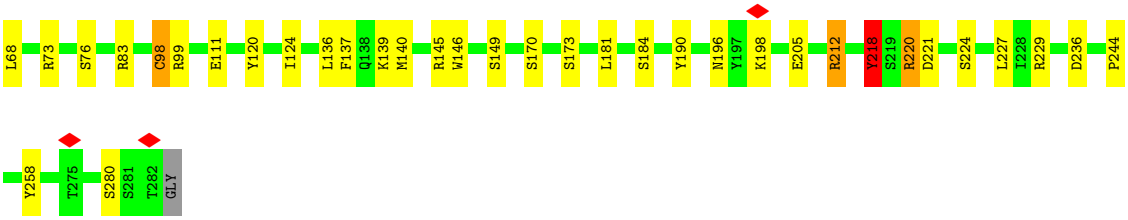
Chain U:



• Molecule 8: Proteasome subunit beta

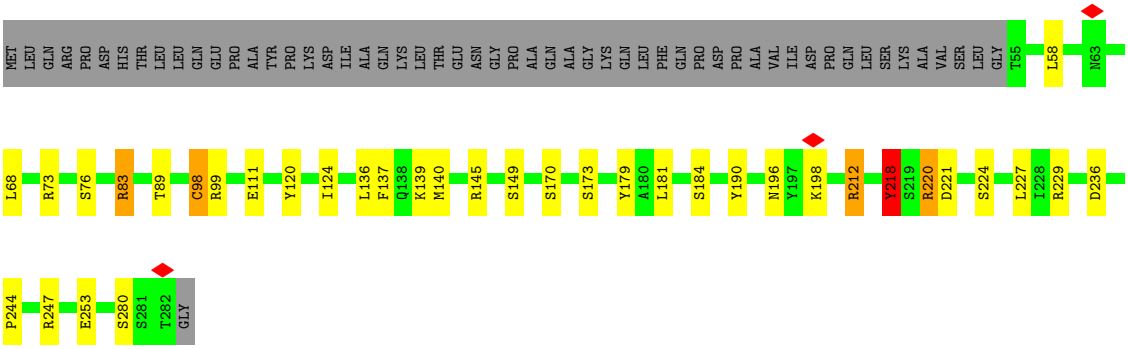
Chain H:





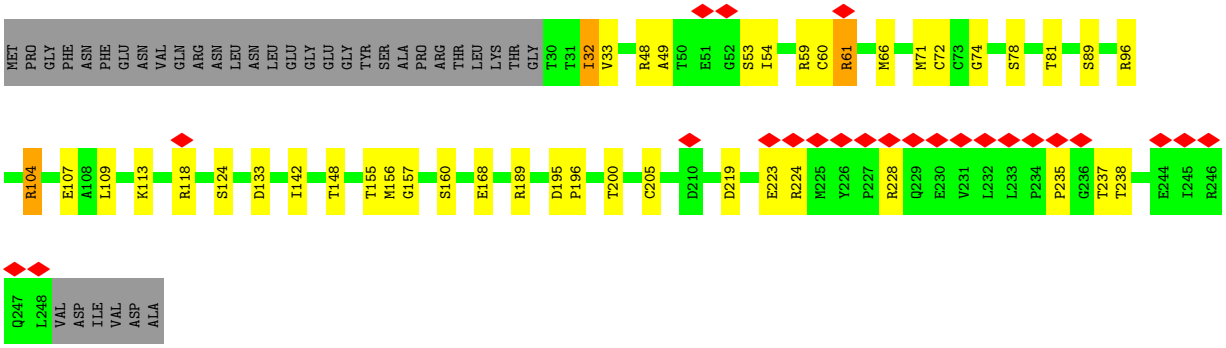
• Molecule 8: Proteasome subunit beta

Chain V:



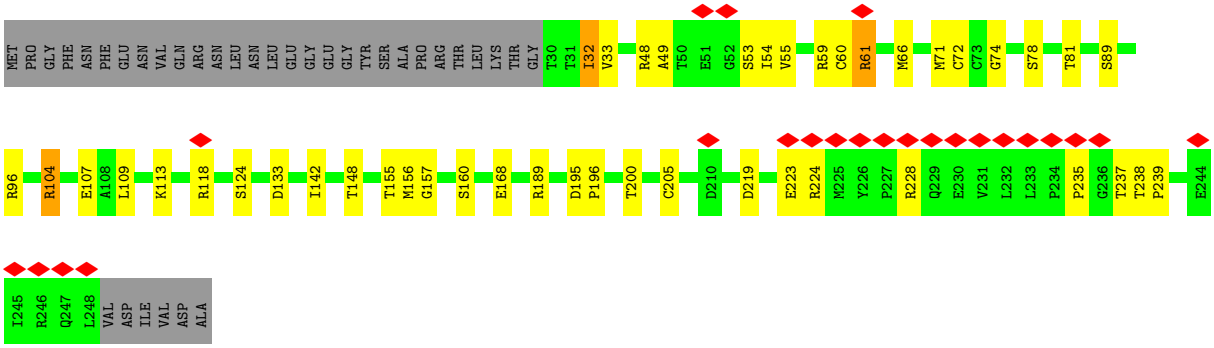
• Molecule 9: Proteasome subunit beta

Chain I:



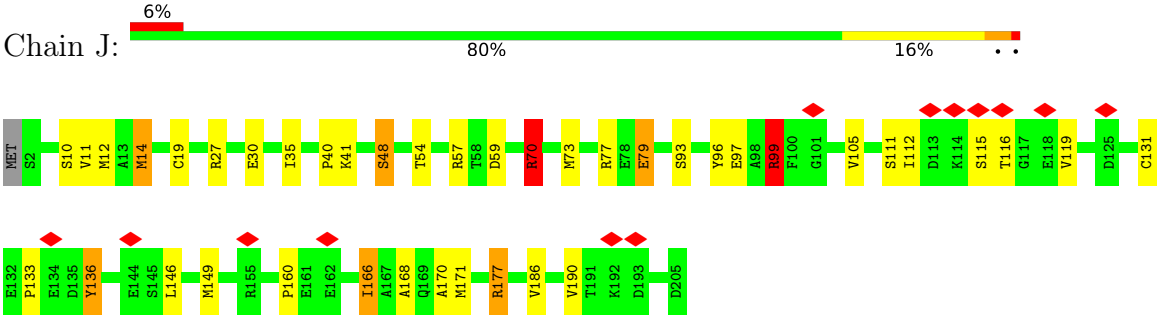
• Molecule 9: Proteasome subunit beta

Chain W:



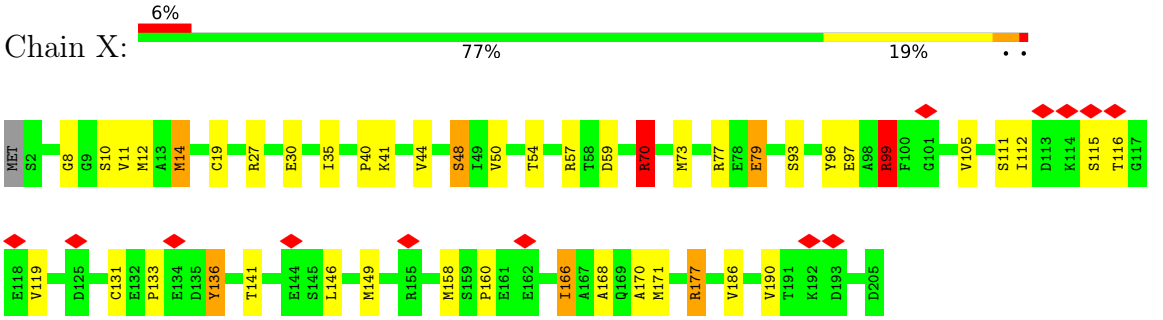
• Molecule 10: Proteasome subunit beta

Chain J:



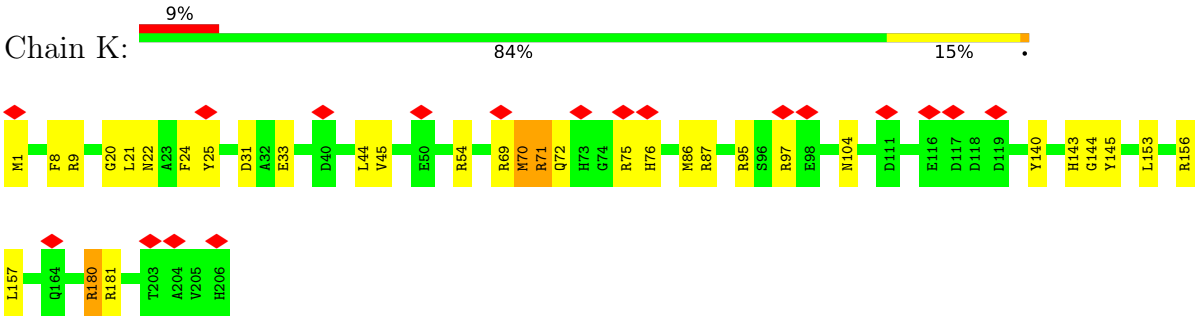
• Molecule 10: Proteasome subunit beta

Chain X:



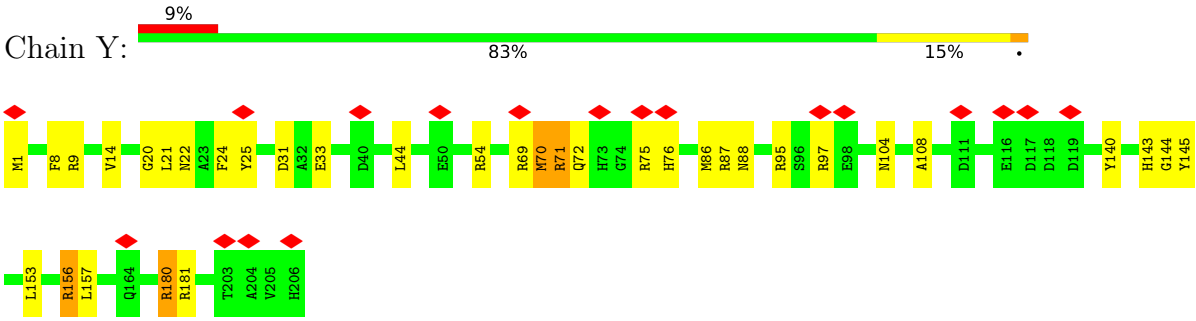
• Molecule 11: Proteasome subunit beta

Chain K:



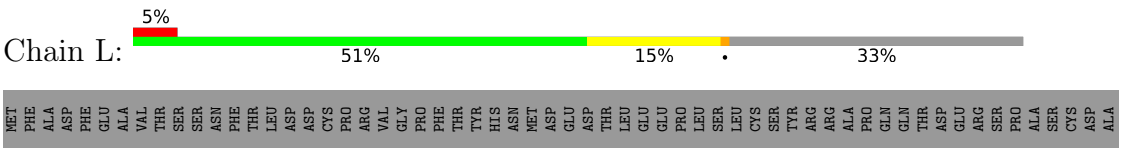
• Molecule 11: Proteasome subunit beta

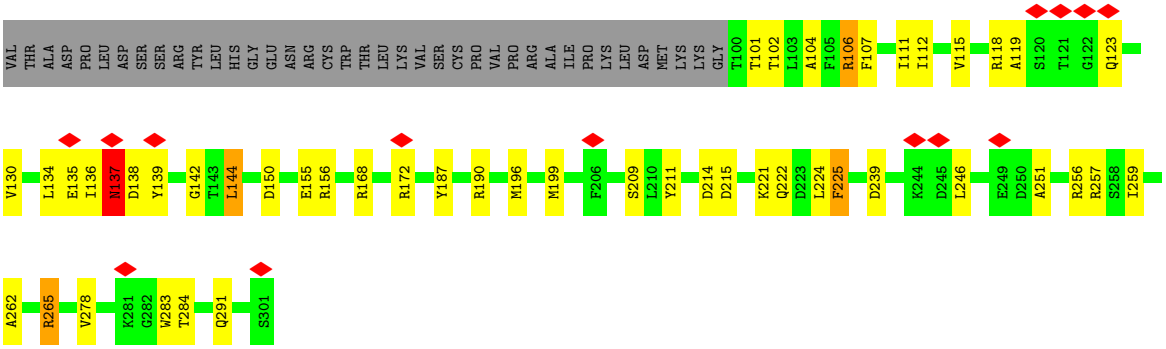
Chain Y:



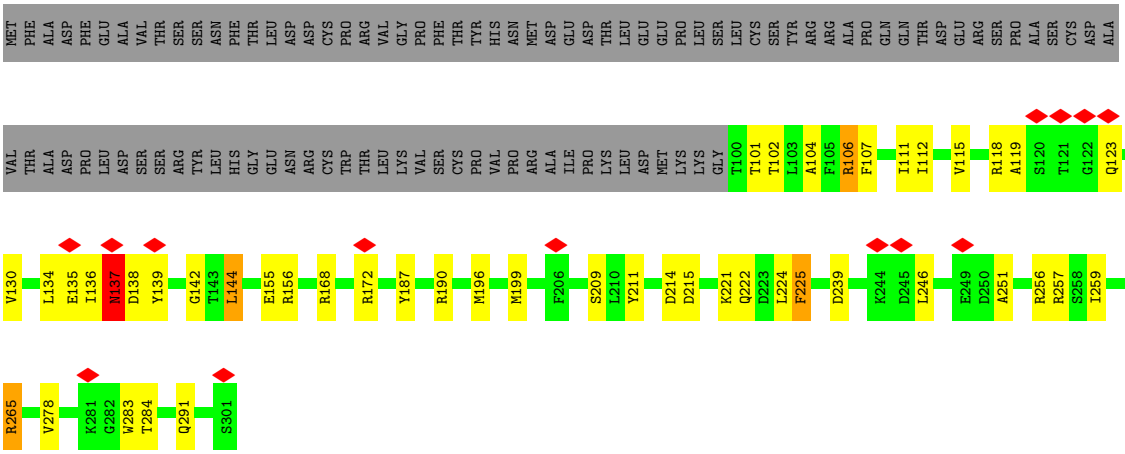
• Molecule 12: Proteasome subunit beta

Chain L:

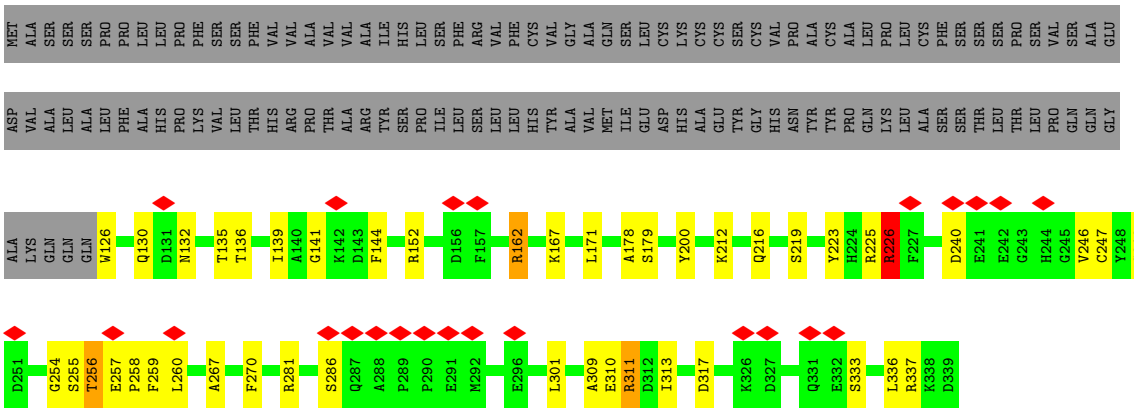




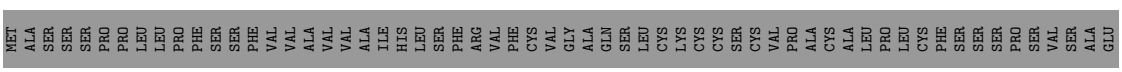
• Molecule 12: Proteasome subunit beta

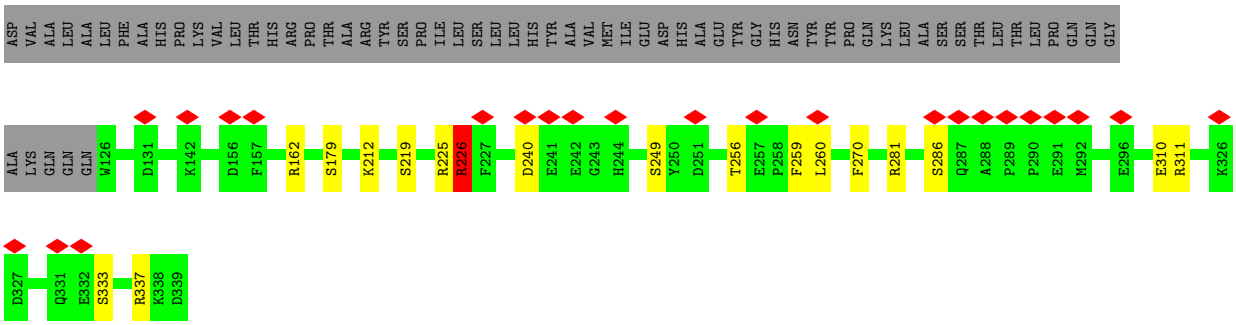


• Molecule 13: Proteasome beta 6 subunit, putative



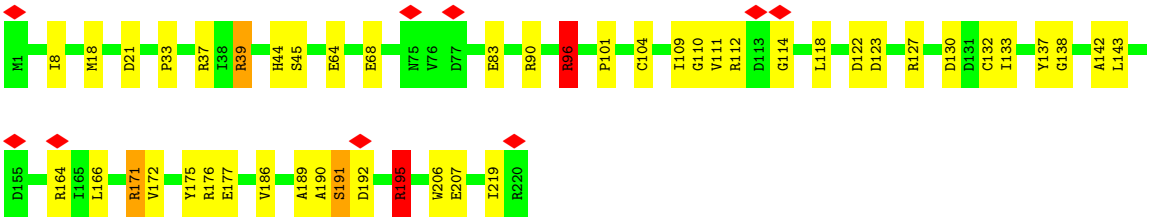
• Molecule 13: Proteasome beta 6 subunit, putative





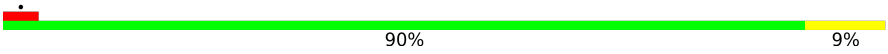
• Molecule 14: Proteasome subunit beta

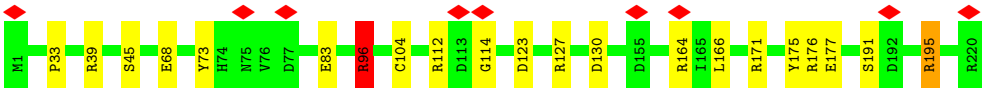
Chain N:



• Molecule 14: Proteasome subunit beta

Chain b:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	94595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.403	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.81	2/1889 (0.1%)	1.06	6/2562 (0.2%)
1	O	0.81	2/1889 (0.1%)	1.06	6/2562 (0.2%)
2	B	0.80	0/1787	1.04	5/2421 (0.2%)
2	P	0.80	0/1787	1.04	5/2421 (0.2%)
3	C	0.73	1/2197 (0.0%)	1.00	3/2975 (0.1%)
3	Q	0.73	1/2197 (0.0%)	1.00	4/2975 (0.1%)
4	D	0.70	0/1869	0.96	1/2518 (0.0%)
4	R	0.70	0/1869	0.96	1/2518 (0.0%)
5	E	0.71	1/1784 (0.1%)	0.98	2/2414 (0.1%)
5	S	0.71	1/1784 (0.1%)	0.98	2/2414 (0.1%)
6	F	0.76	0/1855	1.03	3/2507 (0.1%)
6	T	0.76	0/1855	1.02	2/2507 (0.1%)
7	G	0.89	3/1745 (0.2%)	1.08	5/2359 (0.2%)
7	U	0.89	4/1745 (0.2%)	1.08	4/2359 (0.2%)
8	H	1.04	2/1737 (0.1%)	1.23	13/2354 (0.6%)
8	V	1.03	2/1737 (0.1%)	1.23	13/2354 (0.6%)
9	I	0.93	2/1685 (0.1%)	1.13	5/2284 (0.2%)
9	W	0.93	2/1685 (0.1%)	1.13	5/2284 (0.2%)
10	J	1.03	4/1583 (0.3%)	1.21	10/2135 (0.5%)
10	X	1.03	4/1583 (0.3%)	1.21	10/2135 (0.5%)
11	K	0.87	0/1643	1.13	2/2222 (0.1%)
11	Y	0.87	0/1643	1.13	3/2222 (0.1%)
12	L	0.89	0/1613	1.22	10/2183 (0.5%)
12	Z	0.89	0/1613	1.22	10/2183 (0.5%)
13	M	0.82	1/1743 (0.1%)	1.11	3/2354 (0.1%)
13	a	0.82	1/1743 (0.1%)	1.11	2/2354 (0.1%)
14	N	1.12	4/1768 (0.2%)	1.18	9/2387 (0.4%)
14	b	1.13	4/1768 (0.2%)	1.18	10/2387 (0.4%)
All	All	0.87	41/49796 (0.1%)	1.10	154/67350 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	O	0	3
2	B	0	3
2	P	0	4
3	C	0	12
3	Q	0	12
4	D	0	5
4	R	0	5
5	E	0	4
5	S	0	4
6	F	0	6
6	T	0	7
7	G	0	5
7	U	0	6
8	H	0	2
8	V	0	2
9	I	0	6
9	W	0	6
10	J	0	4
10	X	0	4
11	K	0	6
11	Y	0	6
12	L	0	3
12	Z	0	3
13	M	0	7
13	a	0	7
14	N	0	3
14	b	0	3
All	All	0	140

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	83	GLU	CD-OE2	9.02	1.35	1.25
14	N	83	GLU	CD-OE2	8.69	1.35	1.25
14	b	83	GLU	CD-OE1	8.31	1.34	1.25
14	N	83	GLU	CD-OE1	8.03	1.34	1.25
7	G	118	GLU	CD-OE1	6.69	1.33	1.25
14	b	177	GLU	CD-OE2	6.67	1.32	1.25
5	S	190	GLU	CD-OE1	6.50	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	190	GLU	CD-OE1	6.44	1.32	1.25
7	U	118	GLU	CD-OE1	6.43	1.32	1.25
3	Q	99	SER	CA-CB	-6.31	1.43	1.52
3	C	99	SER	CA-CB	-6.27	1.43	1.52
14	N	177	GLU	CD-OE2	6.27	1.32	1.25
10	X	93	SER	CA-CB	-6.12	1.43	1.52
14	b	68	GLU	CD-OE2	6.08	1.32	1.25
1	O	220	GLU	CD-OE2	6.05	1.32	1.25
10	J	93	SER	CA-CB	-6.03	1.44	1.52
7	G	118	GLU	CD-OE2	5.96	1.32	1.25
7	U	118	GLU	CD-OE2	5.89	1.32	1.25
1	A	220	GLU	CD-OE2	5.87	1.32	1.25
14	N	68	GLU	CD-OE2	5.80	1.32	1.25
9	W	168	GLU	CD-OE1	5.70	1.31	1.25
9	I	168	GLU	CD-OE1	5.62	1.31	1.25
8	H	111	GLU	CD-OE1	5.59	1.31	1.25
8	V	111	GLU	CD-OE1	5.52	1.31	1.25
10	J	30	GLU	CD-OE2	5.31	1.31	1.25
7	G	97	GLU	CD-OE1	5.30	1.31	1.25
8	V	253	GLU	CD-OE2	5.29	1.31	1.25
1	O	94	GLU	CD-OE1	5.28	1.31	1.25
7	U	97	GLU	CD-OE1	5.27	1.31	1.25
13	M	249	SER	CA-CB	-5.21	1.45	1.52
1	A	94	GLU	CD-OE1	5.20	1.31	1.25
7	U	97	GLU	CD-OE2	5.16	1.31	1.25
10	X	10	SER	CA-CB	-5.10	1.45	1.52
10	X	30	GLU	CD-OE2	5.09	1.31	1.25
8	H	205	GLU	CD-OE1	5.08	1.31	1.25
10	X	79	GLU	CD-OE1	5.08	1.31	1.25
13	a	249	SER	CA-CB	-5.08	1.45	1.52
10	J	79	GLU	CD-OE1	5.06	1.31	1.25
9	W	89	SER	CA-CB	-5.06	1.45	1.52
10	J	10	SER	CA-CB	-5.03	1.45	1.52
9	I	89	SER	CA-CB	-5.03	1.45	1.52

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	70	ARG	NE-CZ-NH2	-11.36	114.62	120.30
10	X	70	ARG	NE-CZ-NH2	-11.30	114.65	120.30
6	T	254	ARG	NE-CZ-NH2	-10.96	114.82	120.30
12	Z	265	ARG	NE-CZ-NH2	-10.81	114.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	265	ARG	NE-CZ-NH2	-10.78	114.91	120.30
6	F	254	ARG	NE-CZ-NH2	-10.63	114.99	120.30
8	V	229	ARG	NE-CZ-NH2	-10.61	115.00	120.30
8	H	229	ARG	NE-CZ-NH2	-10.47	115.06	120.30
13	a	270	PHE	CB-CA-C	-10.20	90.00	110.40
13	M	270	PHE	CB-CA-C	-10.13	90.14	110.40
10	J	27	ARG	NE-CZ-NH2	-9.43	115.58	120.30
10	X	27	ARG	NE-CZ-NH2	-9.40	115.60	120.30
12	L	256	ARG	NE-CZ-NH2	-9.18	115.71	120.30
3	Q	97	ARG	NE-CZ-NH2	-9.02	115.79	120.30
12	Z	256	ARG	NE-CZ-NH2	-9.02	115.79	120.30
14	b	176	ARG	NE-CZ-NH2	-8.93	115.84	120.30
12	Z	257	ARG	NE-CZ-NH2	-8.74	115.93	120.30
10	J	27	ARG	NE-CZ-NH1	8.72	124.66	120.30
14	N	176	ARG	NE-CZ-NH2	-8.72	115.94	120.30
12	L	257	ARG	NE-CZ-NH2	-8.62	115.99	120.30
3	C	97	ARG	NE-CZ-NH2	-8.60	116.00	120.30
7	U	100	ARG	NE-CZ-NH2	-8.57	116.02	120.30
14	N	171	ARG	NE-CZ-NH2	-8.53	116.03	120.30
10	X	27	ARG	NE-CZ-NH1	8.53	124.56	120.30
8	H	83	ARG	NE-CZ-NH2	-8.53	116.04	120.30
9	I	96	ARG	NE-CZ-NH2	-8.48	116.06	120.30
8	V	99	ARG	NE-CZ-NH2	-8.47	116.06	120.30
8	V	83	ARG	NE-CZ-NH2	-8.46	116.07	120.30
14	b	171	ARG	NE-CZ-NH2	-8.42	116.09	120.30
7	G	100	ARG	NE-CZ-NH2	-8.41	116.10	120.30
8	H	99	ARG	NE-CZ-NH2	-8.39	116.11	120.30
9	W	48	ARG	NE-CZ-NH2	-8.32	116.14	120.30
9	W	96	ARG	NE-CZ-NH2	-8.21	116.19	120.30
9	I	48	ARG	NE-CZ-NH2	-8.00	116.30	120.30
12	L	137	ASN	CB-CA-C	7.86	126.12	110.40
12	Z	137	ASN	CB-CA-C	7.85	126.11	110.40
8	H	218	TYR	CB-CG-CD1	7.80	125.68	121.00
9	I	96	ARG	NE-CZ-NH1	7.79	124.19	120.30
8	V	218	TYR	CB-CG-CD1	7.76	125.66	121.00
12	Z	265	ARG	NE-CZ-NH1	7.51	124.06	120.30
9	W	96	ARG	NE-CZ-NH1	7.33	123.97	120.30
2	P	101	GLU	CB-CA-C	-7.30	95.80	110.40
2	B	101	GLU	CB-CA-C	-7.29	95.81	110.40
12	L	225	PHE	CB-CA-C	-7.26	95.88	110.40
12	Z	225	PHE	CB-CA-C	-7.22	95.95	110.40
12	L	118	ARG	NE-CZ-NH2	-7.06	116.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	265	ARG	NE-CZ-NH1	7.05	123.83	120.30
12	Z	118	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	80	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	B	82	ARG	NE-CZ-NH2	-6.95	116.83	120.30
10	X	177	ARG	NE-CZ-NH2	-6.94	116.83	120.30
10	J	136	TYR	CB-CG-CD1	-6.88	116.87	121.00
7	U	93	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	114	ARG	NE-CZ-NH2	-6.87	116.86	120.30
5	E	200	ARG	NE-CZ-NH1	-6.86	116.87	120.30
10	X	136	TYR	CB-CG-CD1	-6.85	116.89	121.00
8	H	212	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	P	82	ARG	NE-CZ-NH2	-6.77	116.91	120.30
5	S	200	ARG	NE-CZ-NH1	-6.77	116.92	120.30
10	J	177	ARG	NE-CZ-NH2	-6.76	116.92	120.30
7	G	93	ARG	NE-CZ-NH2	-6.74	116.93	120.30
14	b	104	CYS	CB-CA-C	-6.70	97.00	110.40
14	N	104	CYS	CB-CA-C	-6.69	97.02	110.40
1	O	114	ARG	NE-CZ-NH2	-6.67	116.97	120.30
8	V	212	ARG	NE-CZ-NH2	-6.66	116.97	120.30
8	H	218	TYR	CB-CG-CD2	-6.63	117.02	121.00
12	Z	106	ARG	CB-CA-C	-6.63	97.15	110.40
8	V	218	TYR	CB-CG-CD2	-6.62	117.03	121.00
12	L	106	ARG	CB-CA-C	-6.62	97.15	110.40
1	O	80	ARG	NE-CZ-NH2	-6.59	117.00	120.30
5	S	235	ARG	NE-CZ-NH2	-6.54	117.03	120.30
7	G	66	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	P	89	ARG	NE-CZ-NH1	-6.46	117.07	120.30
10	X	177	ARG	NE-CZ-NH1	6.43	123.52	120.30
5	E	235	ARG	NE-CZ-NH2	-6.43	117.09	120.30
8	H	220	ARG	NE-CZ-NH2	-6.42	117.09	120.30
8	V	220	ARG	NE-CZ-NH2	-6.42	117.09	120.30
8	V	220	ARG	NE-CZ-NH1	6.39	123.50	120.30
7	U	66	ARG	NE-CZ-NH2	-6.26	117.17	120.30
8	H	73	ARG	NE-CZ-NH2	-6.23	117.18	120.30
8	H	220	ARG	NE-CZ-NH1	6.18	123.39	120.30
14	N	127	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	B	89	ARG	NE-CZ-NH1	-6.17	117.22	120.30
9	I	133	ASP	CB-CA-C	6.17	122.74	110.40
10	J	177	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	B	118	GLU	CB-CA-C	-6.16	98.07	110.40
14	N	127	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	P	118	GLU	CB-CA-C	-6.13	98.14	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	125	ARG	NE-CZ-NH2	-6.12	117.24	120.30
9	W	133	ASP	CB-CA-C	6.11	122.63	110.40
14	b	127	ARG	NE-CZ-NH1	6.09	123.34	120.30
10	X	99	ARG	NE-CZ-NH2	-6.03	117.29	120.30
13	M	310	GLU	CB-CA-C	-6.02	98.36	110.40
4	R	125	ARG	NE-CZ-NH2	-6.01	117.29	120.30
8	H	145	ARG	NE-CZ-NH1	5.99	123.30	120.30
11	K	70	MET	CB-CA-C	-5.99	98.43	110.40
10	J	99	ARG	NE-CZ-NH2	-5.98	117.31	120.30
13	a	310	GLU	CB-CA-C	-5.98	98.45	110.40
11	Y	70	MET	CB-CA-C	-5.96	98.49	110.40
14	b	127	ARG	NE-CZ-NH2	-5.87	117.37	120.30
8	V	73	ARG	NE-CZ-NH2	-5.86	117.37	120.30
8	V	139	LYS	CB-CA-C	-5.84	98.71	110.40
1	A	122	ARG	NE-CZ-NH2	-5.84	117.38	120.30
8	H	139	LYS	CB-CA-C	-5.82	98.76	110.40
3	Q	134	ARG	NE-CZ-NH2	-5.76	117.42	120.30
8	V	145	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	O	68	GLU	CB-CA-C	5.74	121.87	110.40
1	A	68	GLU	CB-CA-C	5.73	121.85	110.40
12	L	137	ASN	CA-CB-CG	5.72	125.98	113.40
8	V	170	SER	C-N-CA	-5.72	110.29	122.30
10	J	70	ARG	NE-CZ-NH1	5.71	123.15	120.30
12	Z	137	ASN	CA-CB-CG	5.70	125.93	113.40
1	O	122	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	B	118	GLU	N-CA-CB	5.65	120.78	110.60
2	P	118	GLU	N-CA-CB	5.65	120.77	110.60
10	X	70	ARG	NE-CZ-NH1	5.64	123.12	120.30
8	H	170	SER	C-N-CA	-5.62	110.50	122.30
10	X	57	ARG	NE-CZ-NH2	-5.59	117.50	120.30
6	F	261	ARG	NE-CZ-NH2	-5.58	117.51	120.30
3	C	134	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	129	ARG	NE-CZ-NH2	-5.51	117.55	120.30
14	N	96	ARG	NE-CZ-NH2	-5.51	117.55	120.30
11	Y	87	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	92	ARG	NE-CZ-NH2	-5.50	117.55	120.30
14	N	33	PRO	N-CA-CB	-5.44	96.62	102.60
14	N	112	ARG	NE-CZ-NH2	-5.44	117.58	120.30
14	b	96	ARG	NE-CZ-NH2	-5.43	117.59	120.30
8	V	99	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	O	129	ARG	NE-CZ-NH2	-5.39	117.61	120.30
14	b	33	PRO	N-CA-CB	-5.37	96.69	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	261	ARG	NE-CZ-NH2	-5.33	117.64	120.30
3	C	174	ASP	CB-CA-C	5.31	121.02	110.40
3	Q	174	ASP	CB-CA-C	5.29	120.97	110.40
1	O	92	ARG	NE-CZ-NH2	-5.26	117.67	120.30
12	Z	138	ASP	CB-CA-C	-5.24	99.91	110.40
7	G	91	ARG	NE-CZ-NH2	-5.24	117.68	120.30
11	Y	156	ARG	NE-CZ-NH2	-5.23	117.69	120.30
7	U	91	ARG	NE-CZ-NH2	-5.23	117.69	120.30
12	L	138	ASP	CB-CA-C	-5.22	99.95	110.40
14	b	112	ARG	NE-CZ-NH2	-5.21	117.69	120.30
14	N	175	TYR	CB-CA-C	-5.20	99.99	110.40
9	W	96	ARG	CB-CA-C	-5.18	100.04	110.40
9	I	96	ARG	CB-CA-C	-5.16	100.08	110.40
13	M	152	ARG	NE-CZ-NH1	-5.15	117.72	120.30
14	b	175	TYR	CB-CA-C	-5.15	100.10	110.40
11	K	87	ARG	NE-CZ-NH2	-5.14	117.73	120.30
10	J	57	ARG	NE-CZ-NH2	-5.11	117.75	120.30
8	H	83	ARG	NE-CZ-NH1	5.06	122.83	120.30
7	G	147	GLN	CB-CA-C	-5.06	100.28	110.40
10	X	97	GLU	CB-CA-C	-5.04	100.32	110.40
3	Q	154	TYR	CB-CG-CD2	-5.03	117.98	121.00
6	F	310	TYR	CB-CG-CD2	-5.01	117.99	121.00
10	J	97	GLU	CB-CA-C	-5.01	100.37	110.40
14	b	73	TYR	CB-CA-C	-5.00	100.39	110.40

There are no chirality outliers.

All (140) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	85	ARG	Sidechain
2	B	110	ARG	Sidechain
2	B	210	ARG	Sidechain
2	B	89	ARG	Sidechain
3	C	102	ARG	Sidechain
3	C	118	ARG	Sidechain
3	C	130	TYR	Peptide
3	C	140	PHE	Peptide
3	C	147	ARG	Sidechain
3	C	17	ARG	Sidechain
3	C	200	ARG	Sidechain
3	C	206	MET	Peptide

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Mol	Chain	Res	Type	Group
3	C	222	ARG	Sidechain
3	C	245	ARG	Sidechain
3	C	251	ARG	Sidechain
3	C	97	ARG	Sidechain
4	D	163	ARG	Sidechain
4	D	215	ARG	Sidechain
4	D	233	ARG	Sidechain
4	D	5	ARG	Sidechain
4	D	57	ARG	Sidechain
5	E	141	ARG	Sidechain
5	E	186	ARG	Sidechain
5	E	287	ARG	Sidechain
5	E	321	ARG	Sidechain
6	F	224	TYR	Peptide
6	F	251	ARG	Sidechain
6	F	261	ARG	Sidechain
6	F	289	GLY	Peptide
6	F	304	ARG	Sidechain
6	F	334	ARG	Sidechain
7	G	108	ARG	Sidechain
7	G	20	ARG	Sidechain
7	G	57	ARG	Sidechain
7	G	72	ARG	Sidechain
7	G	86	ARG	Sidechain
8	H	212	ARG	Sidechain
8	H	220	ARG	Sidechain
9	I	104	ARG	Sidechain
9	I	118	ARG	Sidechain
9	I	224	ARG	Sidechain
9	I	228	ARG	Sidechain
9	I	59	ARG	Sidechain
9	I	61	ARG	Sidechain
10	J	177	ARG	Sidechain
10	J	70	ARG	Sidechain
10	J	77	ARG	Sidechain
10	J	99	ARG	Sidechain
11	K	156	ARG	Sidechain
11	K	180	ARG	Sidechain
11	K	181	ARG	Sidechain
11	K	71	ARG	Sidechain
11	K	9	ARG	Sidechain
11	K	97	ARG	Sidechain

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Mol	Chain	Res	Type	Group
12	L	106	ARG	Sidechain
12	L	172	ARG	Sidechain
12	L	265	ARG	Sidechain
13	M	162	ARG	Sidechain
13	M	225	ARG	Sidechain
13	M	226	ARG	Sidechain
13	M	256	THR	Peptide
13	M	281	ARG	Sidechain
13	M	311	ARG	Sidechain
13	M	337	ARG	Sidechain
14	N	195	ARG	Sidechain
14	N	39	ARG	Sidechain
14	N	96	ARG	Sidechain
1	O	101	ARG	Sidechain
1	O	40	ARG	Sidechain
1	O	85	ARG	Sidechain
2	P	110	ARG	Sidechain
2	P	175	ARG	Sidechain
2	P	210	ARG	Sidechain
2	P	89	ARG	Sidechain
3	Q	102	ARG	Sidechain
3	Q	118	ARG	Sidechain
3	Q	130	TYR	Peptide
3	Q	140	PHE	Peptide
3	Q	147	ARG	Sidechain
3	Q	17	ARG	Sidechain
3	Q	200	ARG	Sidechain
3	Q	206	MET	Peptide
3	Q	222	ARG	Sidechain
3	Q	245	ARG	Sidechain
3	Q	251	ARG	Sidechain
3	Q	97	ARG	Sidechain
4	R	163	ARG	Sidechain
4	R	215	ARG	Sidechain
4	R	233	ARG	Sidechain
4	R	5	ARG	Sidechain
4	R	57	ARG	Sidechain
5	S	141	ARG	Sidechain
5	S	186	ARG	Sidechain
5	S	287	ARG	Sidechain
5	S	321	ARG	Sidechain
6	T	224	TYR	Peptide

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Mol	Chain	Res	Type	Group
6	T	251	ARG	Sidechain
6	T	261	ARG	Sidechain
6	T	289	GLY	Peptide
6	T	304	ARG	Sidechain
6	T	334	ARG	Sidechain
6	T	395	ARG	Sidechain
7	U	108	ARG	Sidechain
7	U	20	ARG	Sidechain
7	U	57	ARG	Sidechain
7	U	66	ARG	Sidechain
7	U	72	ARG	Sidechain
7	U	86	ARG	Sidechain
8	V	212	ARG	Sidechain
8	V	220	ARG	Sidechain
9	W	104	ARG	Sidechain
9	W	118	ARG	Sidechain
9	W	224	ARG	Sidechain
9	W	228	ARG	Sidechain
9	W	59	ARG	Sidechain
9	W	61	ARG	Sidechain
10	X	177	ARG	Sidechain
10	X	70	ARG	Sidechain
10	X	77	ARG	Sidechain
10	X	99	ARG	Sidechain
11	Y	156	ARG	Sidechain
11	Y	180	ARG	Sidechain
11	Y	181	ARG	Sidechain
11	Y	71	ARG	Sidechain
11	Y	9	ARG	Sidechain
11	Y	97	ARG	Sidechain
12	Z	106	ARG	Sidechain
12	Z	172	ARG	Sidechain
12	Z	265	ARG	Sidechain
13	a	162	ARG	Sidechain
13	a	225	ARG	Sidechain
13	a	226	ARG	Sidechain
13	a	256	THR	Peptide
13	a	281	ARG	Sidechain
13	a	311	ARG	Sidechain
13	a	337	ARG	Sidechain
14	b	195	ARG	Sidechain
14	b	39	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	b	96	ARG	Sidechain

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	1857	0	1871	28	0
1	O	1857	0	1871	30	0
2	B	1754	0	1741	12	0
2	P	1754	0	1741	13	0
3	C	2150	0	2097	40	0
3	Q	2150	0	2097	39	0
4	D	1840	0	1834	36	0
4	R	1840	0	1834	38	0
5	E	1756	0	1736	33	0
5	S	1756	0	1736	32	0
6	F	1819	0	1769	22	0
6	T	1819	0	1769	23	0
7	G	1714	0	1679	13	0
7	U	1714	0	1679	16	0
8	H	1705	0	1662	13	0
8	V	1705	0	1662	15	0
9	I	1659	0	1684	18	0
9	W	1659	0	1684	21	0
10	J	1557	0	1552	22	0
10	X	1557	0	1552	26	0
11	K	1612	0	1571	25	0
11	Y	1612	0	1571	23	0
12	L	1579	0	1538	27	0
12	Z	1579	0	1538	25	0
13	M	1702	0	1638	23	0
13	a	1702	0	1638	0	0
14	N	1732	0	1693	23	0
14	b	1732	0	1693	0	0
15	L	29	0	0	0	0
15	Z	29	0	0	0	0
All	All	48930	0	48130	570	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 6.

All (570) 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)
3:C:101:LEU:HD12	10:J:73:MET:HE2	1.51	0.93
1:O:228:ASN:HD21	1:O:232:GLN:HE22	1.17	0.91
1:A:228:ASN:HD21	1:A:232:GLN:HE22	1.17	0.89
1:A:228:ASN:HD21	1:A:232:GLN:NE2	1.69	0.89
3:Q:101:LEU:HD12	10:X:73:MET:HE2	1.55	0.89
5:E:268:GLN:HE21	5:E:268:GLN:HA	1.37	0.88
1:O:228:ASN:HD21	1:O:232:GLN:NE2	1.70	0.88
5:S:268:GLN:HE21	5:S:268:GLN:HA	1.37	0.88
5:E:259:SER:HB2	5:E:261:THR:HG22	1.56	0.88
5:S:259:SER:HB2	5:S:261:THR:HG22	1.57	0.87
13:M:130:GLN:HE21	13:M:132:ASN:HD21	1.20	0.86
3:C:8:ARG:HD2	4:D:5:ARG:HH12	1.40	0.86
3:Q:8:ARG:HD2	4:R:5:ARG:HH12	1.39	0.85
13:M:223:TYR:O	13:M:226:ARG:HB2	1.81	0.81
4:D:132:VAL:HG23	4:D:161:ILE:HD13	1.63	0.80
12:L:134:LEU:HD23	12:L:155:GLU:HB3	1.64	0.79
3:C:101:LEU:HD12	10:J:73:MET:CE	2.13	0.78
3:Q:101:LEU:HD12	10:X:73:MET:CE	2.13	0.78
4:R:132:VAL:HG23	4:R:161:ILE:HD13	1.63	0.78
12:Z:134:LEU:HD23	12:Z:155:GLU:HB3	1.64	0.78
3:Q:8:ARG:HD2	4:R:5:ARG:NH1	2.02	0.74
3:C:8:ARG:HD2	4:D:5:ARG:NH1	2.03	0.74
11:K:1:MET:HB3	11:K:145:TYR:CE1	2.23	0.74
11:Y:1:MET:HB3	11:Y:145:TYR:CE1	2.23	0.73
6:T:357:LEU:HD21	6:T:377:ILE:HD11	1.70	0.72
6:F:204:GLY:HA3	6:F:352:LEU:HD11	1.71	0.72
4:D:116:GLN:NE2	5:E:184:ASP:OD1	2.23	0.71
6:F:357:LEU:HD21	6:F:377:ILE:HD11	1.71	0.71
11:K:44:LEU:HD12	11:K:44:LEU:C	2.11	0.71
6:T:204:GLY:HA3	6:T:352:LEU:HD11	1.71	0.71
11:Y:44:LEU:HD12	11:Y:44:LEU:C	2.11	0.71
1:O:11:THR:HG23	1:O:11:THR:O	1.92	0.69
4:R:116:GLN:NE2	5:S:184:ASP:OD1	2.24	0.68
12:Z:135:GLU:OE2	12:Z:283:TRP:CH2	2.46	0.68
12:L:135:GLU:OE2	12:L:283:TRP:CH2	2.45	0.68
1:A:11:THR:HG23	1:A:11:THR:O	1.92	0.68
12:L:119:ALA:HB2	12:L:130:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:1:MET:HA	11:Y:144:GLY:HA2	1.76	0.67
4:R:71:LEU:HD23	4:R:71:LEU:C	2.15	0.67
4:D:71:LEU:HD23	4:D:71:LEU:C	2.15	0.67
12:L:144:LEU:C	12:L:144:LEU:HD23	2.15	0.67
9:I:157:GLY:O	9:I:160:SER:HB3	1.96	0.66
12:Z:144:LEU:HD23	12:Z:144:LEU:C	2.16	0.66
5:S:138:LEU:HD11	5:S:149:ALA:HB3	1.78	0.66
5:E:147:VAL:HG22	5:E:319:VAL:HG12	1.77	0.66
7:U:88:ILE:HD12	7:U:134:CYS:SG	2.36	0.66
7:G:88:ILE:HD12	7:G:134:CYS:SG	2.36	0.66
5:E:138:LEU:HD11	5:E:149:ALA:HB3	1.78	0.65
12:Z:119:ALA:HB2	12:Z:130:VAL:HG21	1.77	0.65
11:K:1:MET:HA	11:K:144:GLY:HA2	1.77	0.65
5:S:147:VAL:HG22	5:S:319:VAL:HG12	1.77	0.65
8:H:196:ASN:HD21	8:V:196:ASN:HD21	1.44	0.65
5:S:175:ALA:HB2	5:S:327:LEU:HD13	1.79	0.65
9:W:157:GLY:O	9:W:160:SER:HB3	1.96	0.64
1:O:81:ALA:N	1:O:82:PRO:HD2	2.13	0.64
14:N:39:ARG:NH1	14:N:64:GLU:OE1	2.31	0.63
5:E:175:ALA:HB2	5:E:327:LEU:HD13	1.79	0.63
1:A:81:ALA:N	1:A:82:PRO:HD2	2.14	0.63
1:O:195:GLN:OE1	1:O:223:ARG:NH1	2.32	0.62
13:M:136:THR:HG21	13:M:178:ALA:HB1	1.82	0.61
2:B:34:LEU:C	2:B:34:LEU:HD12	2.22	0.60
2:P:187:HIS:CE1	2:P:231:ILE:HG22	2.36	0.60
5:E:214:LEU:HD21	5:E:262:HIS:NE2	2.17	0.60
2:P:34:LEU:C	2:P:34:LEU:HD12	2.22	0.60
2:B:187:HIS:CE1	2:B:231:ILE:HG22	2.36	0.59
4:D:175:SER:HB2	4:D:188:PHE:HE2	1.67	0.59
4:R:132:VAL:HG23	4:R:161:ILE:CD1	2.32	0.59
4:R:136:PHE:CE1	4:R:142:PRO:HB3	2.38	0.59
4:D:136:PHE:CE1	4:D:142:PRO:HB3	2.38	0.59
5:S:214:LEU:HD21	5:S:262:HIS:NE2	2.17	0.59
6:T:249:LEU:HD22	6:T:277:ILE:HD11	1.84	0.59
7:U:38:VAL:HG23	7:U:193:LEU:HD13	1.85	0.59
3:C:166:SER:HB3	3:C:185:TRP:CZ2	2.38	0.59
6:F:249:LEU:HD22	6:F:277:ILE:HD11	1.84	0.59
4:R:98:TYR:O	4:R:100:ASP:N	2.35	0.59
3:Q:166:SER:HB3	3:Q:185:TRP:CZ2	2.38	0.58
4:R:175:SER:HB2	4:R:188:PHE:HE2	1.67	0.58
11:K:70:MET:C	11:K:72:GLN:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:GLY:O	2:B:165:SER:HB3	2.03	0.58
7:G:38:VAL:HG23	7:G:193:LEU:HD13	1.85	0.58
2:P:162:GLY:O	2:P:165:SER:HB3	2.04	0.58
8:H:184:SER:OG	8:H:221:ASP:OD2	2.18	0.58
12:L:246:LEU:HD13	12:L:251:ALA:HA	1.86	0.58
11:Y:1:MET:HB3	11:Y:145:TYR:CD1	2.39	0.58
11:Y:44:LEU:HD12	11:Y:44:LEU:O	2.04	0.58
4:D:98:TYR:O	4:D:100:ASP:N	2.35	0.57
14:N:190:ALA:O	14:N:192:ASP:N	2.37	0.57
4:D:132:VAL:HG23	4:D:161:ILE:CD1	2.32	0.57
11:K:44:LEU:HD12	11:K:44:LEU:O	2.04	0.57
4:D:186:VAL:O	4:D:190:ILE:HG12	2.05	0.57
3:Q:17:ARG:HH11	3:Q:19:TYR:HE1	1.51	0.57
12:Z:246:LEU:HD13	12:Z:251:ALA:HA	1.86	0.57
4:R:186:VAL:O	4:R:190:ILE:HG12	2.04	0.57
14:N:122:ASP:C	14:N:122:ASP:OD1	2.42	0.57
11:K:1:MET:HB3	11:K:145:TYR:CD1	2.39	0.57
3:C:101:LEU:CD1	10:J:73:MET:HE2	2.28	0.57
11:Y:70:MET:C	11:Y:72:GLN:H	2.07	0.57
9:I:142:ILE:N	9:I:142:ILE:HD12	2.20	0.56
11:Y:69:ARG:HD2	11:Y:76:HIS:CE1	2.40	0.56
12:Z:283:TRP:CE3	12:Z:283:TRP:O	2.58	0.56
8:H:68:LEU:N	8:H:68:LEU:HD12	2.20	0.56
12:L:283:TRP:O	12:L:283:TRP:CE3	2.57	0.56
2:B:55:VAL:HG11	2:B:60:ILE:HD11	1.87	0.56
5:S:214:LEU:CD2	5:S:262:HIS:NE2	2.69	0.56
5:S:268:GLN:HE21	5:S:268:GLN:CA	2.16	0.56
8:V:68:LEU:HD12	8:V:68:LEU:N	2.20	0.56
9:W:142:ILE:N	9:W:142:ILE:HD12	2.20	0.56
6:T:274:ALA:HB1	6:T:318:VAL:HG11	1.87	0.56
1:A:195:GLN:OE1	1:A:223:ARG:NH1	2.32	0.56
8:H:181:LEU:HD12	8:H:190:TYR:CE1	2.41	0.56
14:N:118:LEU:HG	14:N:133:ILE:HG13	1.88	0.56
5:E:214:LEU:CD2	5:E:262:HIS:NE2	2.69	0.56
6:F:274:ALA:HB1	6:F:318:VAL:HG11	1.87	0.56
2:P:55:VAL:HG11	2:P:60:ILE:HD11	1.87	0.56
1:A:210:ILE:HD11	1:A:214:VAL:HG12	1.88	0.55
5:E:148:LEU:HD21	5:E:244:ALA:HB2	1.89	0.55
11:K:69:ARG:HD2	11:K:76:HIS:CE1	2.41	0.55
13:M:311:ARG:NH1	9:W:55:VAL:O	2.39	0.55
3:C:204:LYS:CD	3:C:265:ARG:HH22	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:LEU:C	4:D:206:LEU:HD23	2.26	0.55
5:S:148:LEU:HD21	5:S:244:ALA:HB2	1.89	0.55
9:I:189:ARG:HD3	9:I:219:ASP:OD2	2.06	0.55
9:W:189:ARG:HD3	9:W:219:ASP:OD2	2.06	0.55
1:A:195:GLN:OE1	1:A:223:ARG:CD	2.55	0.55
1:O:210:ILE:HD11	1:O:214:VAL:HG12	1.88	0.55
1:O:195:GLN:OE1	1:O:223:ARG:CD	2.55	0.55
3:Q:101:LEU:CD1	10:X:73:MET:HE2	2.32	0.55
12:Z:102:THR:HG22	12:Z:115:VAL:HG12	1.88	0.55
3:C:17:ARG:HH11	3:C:19:TYR:HE1	1.53	0.55
12:L:102:THR:HG22	12:L:115:VAL:HG12	1.88	0.55
3:Q:204:LYS:CD	3:Q:265:ARG:HH22	2.18	0.55
5:S:310:LEU:C	5:S:310:LEU:HD23	2.27	0.55
5:E:310:LEU:C	5:E:310:LEU:HD23	2.26	0.54
4:R:206:LEU:C	4:R:206:LEU:HD23	2.26	0.54
8:V:181:LEU:HD12	8:V:190:TYR:CE1	2.41	0.54
1:A:195:GLN:OE1	1:A:223:ARG:HD2	2.07	0.54
12:L:239:ASP:HB3	11:Y:180:ARG:HH11	1.71	0.54
11:Y:153:LEU:HD11	11:Y:157:LEU:HD12	1.89	0.54
3:C:204:LYS:HD2	3:C:265:ARG:HH22	1.72	0.54
1:O:195:GLN:OE1	1:O:223:ARG:HD2	2.07	0.54
12:L:214:ASP:C	12:L:214:ASP:OD1	2.46	0.54
5:E:268:GLN:HE21	5:E:268:GLN:CA	2.17	0.53
14:N:109:ILE:HG22	14:N:118:LEU:HD13	1.90	0.53
3:Q:204:LYS:HD2	3:Q:265:ARG:HH22	1.72	0.53
12:Z:137:ASN:OD1	12:Z:139:TYR:N	2.40	0.53
12:Z:214:ASP:OD1	12:Z:214:ASP:C	2.46	0.53
9:W:109:LEU:HD12	9:W:142:ILE:HD11	1.91	0.53
5:E:214:LEU:HD23	5:E:262:HIS:CD2	2.44	0.53
5:S:214:LEU:HD23	5:S:262:HIS:CD2	2.44	0.53
1:O:87:LEU:HD12	1:O:133:VAL:CG2	2.39	0.53
11:K:180:ARG:HH11	12:Z:239:ASP:HB3	1.73	0.52
11:K:153:LEU:HD11	11:K:157:LEU:HD12	1.90	0.52
1:A:206:LEU:HD23	1:A:214:VAL:HG11	1.91	0.52
9:W:32:ILE:HD11	9:W:156:MET:HB2	1.92	0.52
12:L:137:ASN:OD1	12:L:139:TYR:N	2.40	0.52
6:F:349:LEU:O	6:F:353:VAL:HG23	2.09	0.52
1:A:87:LEU:HD12	1:A:133:VAL:CG2	2.40	0.52
5:E:124:ILE:HD11	5:E:223:PHE:CZ	2.45	0.52
6:F:327:GLY:O	6:F:330:SER:OG	2.25	0.52
9:I:32:ILE:HD11	9:I:156:MET:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:2:SER:HB2	7:U:127:PHE:CD1	2.45	0.52
7:G:67:ILE:HD12	7:G:212:GLU:HG2	1.92	0.52
3:C:2:SER:HB2	7:G:127:PHE:CD1	2.45	0.51
9:W:71:MET:HG3	9:W:205:CYS:SG	2.50	0.51
3:C:201:VAL:O	3:C:205:THR:HG23	2.11	0.51
3:C:247:GLN:HE21	3:C:249:LEU:HD22	1.75	0.51
13:M:126:TRP:CZ2	14:N:101:PRO:HB3	2.45	0.51
3:Q:52:PRO:HG3	3:Q:214:ASP:HB3	1.93	0.51
10:X:14:MET:SD	10:X:166:ILE:HD11	2.50	0.51
6:T:349:LEU:O	6:T:353:VAL:HG23	2.09	0.51
9:I:66:MET:HE3	9:I:72:CYS:HB2	1.92	0.51
9:I:109:LEU:HD12	9:I:142:ILE:HD11	1.91	0.51
10:J:14:MET:SD	10:J:166:ILE:HD11	2.50	0.51
11:K:20:GLY:O	11:K:21:LEU:C	2.49	0.51
11:K:22:ASN:HD22	11:K:33:GLU:CD	2.14	0.51
1:O:11:THR:O	1:O:11:THR:CG2	2.58	0.51
1:A:11:THR:O	1:A:11:THR:CG2	2.58	0.51
2:B:116:TYR:CD1	2:B:149:PRO:HA	2.46	0.51
5:S:124:ILE:HD11	5:S:223:PHE:CZ	2.45	0.51
3:Q:201:VAL:O	3:Q:205:THR:HG23	2.11	0.51
3:Q:247:GLN:HE21	3:Q:249:LEU:HD22	1.75	0.51
8:V:184:SER:OG	8:V:221:ASP:OD2	2.19	0.51
11:Y:22:ASN:HD22	11:Y:33:GLU:CD	2.15	0.51
11:Y:54:ARG:NH1	11:Y:54:ARG:HG2	2.26	0.51
3:C:202:LEU:O	3:C:206:MET:HG2	2.11	0.51
6:F:370:LEU:HD22	6:F:375:THR:OG1	2.11	0.50
9:I:66:MET:CE	9:I:72:CYS:HB2	2.41	0.50
13:M:256:THR:OG1	13:M:257:GLU:N	2.45	0.50
13:M:309:ALA:HB2	13:M:336:LEU:HD13	1.93	0.50
9:I:71:MET:HG3	9:I:205:CYS:SG	2.50	0.50
2:P:116:TYR:CD1	2:P:149:PRO:HA	2.46	0.50
6:T:370:LEU:HD22	6:T:375:THR:OG1	2.11	0.50
1:O:31:TYR:N	1:O:32:PRO:CD	2.75	0.50
1:O:206:LEU:HD23	1:O:214:VAL:HG11	1.91	0.50
11:K:24:PHE:O	11:K:25:TYR:C	2.49	0.50
9:W:49:ALA:HB2	9:W:60:CYS:SG	2.51	0.50
5:E:309:GLN:O	5:E:314:ASN:ND2	2.45	0.50
10:J:59:ASP:OD2	11:K:95:ARG:NH2	2.44	0.50
7:U:67:ILE:HD12	7:U:212:GLU:HG2	1.93	0.50
11:Y:20:GLY:O	11:Y:21:LEU:C	2.48	0.50
11:Y:44:LEU:C	11:Y:44:LEU:CD1	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:72:GLN:HB3	11:K:75:ARG:CZ	2.41	0.50
3:Q:77:HIS:NE2	3:Q:111:MET:O	2.40	0.50
9:W:66:MET:CE	9:W:72:CYS:HB2	2.41	0.50
13:M:141:GLY:HA3	13:M:144:PHE:CZ	2.46	0.50
11:Y:72:GLN:HB3	11:Y:75:ARG:CZ	2.41	0.50
5:E:205:GLU:OE2	13:M:200:TYR:OH	2.27	0.49
6:F:262:TYR:CZ	14:N:90:ARG:HD2	2.47	0.49
3:C:146:ASP:CG	3:C:152:GLN:HE22	2.15	0.49
1:O:80:ARG:HD3	1:O:83:ASP:CG	2.33	0.49
5:S:210:GLU:HB2	5:S:254:TRP:CZ2	2.47	0.49
11:K:44:LEU:C	11:K:44:LEU:CD1	2.80	0.49
11:K:54:ARG:NH1	11:K:54:ARG:HG2	2.27	0.49
3:Q:202:LEU:O	3:Q:206:MET:HG2	2.12	0.49
4:R:89:LEU:O	4:R:89:LEU:HD12	2.12	0.49
4:D:12:PRO:HA	5:E:126:TYR:CD1	2.47	0.49
6:F:349:LEU:HD21	6:F:379:ILE:HD12	1.94	0.49
12:L:134:LEU:HD23	12:L:155:GLU:CB	2.39	0.49
3:Q:146:ASP:CG	3:Q:152:GLN:HE22	2.15	0.49
9:I:49:ALA:HB2	9:I:60:CYS:SG	2.52	0.49
14:N:207:GLU:OE2	8:V:247:ARG:NH1	2.44	0.49
4:R:12:PRO:HA	5:S:126:TYR:CD1	2.47	0.49
4:R:187:HIS:CE1	4:R:229:VAL:HG22	2.48	0.49
2:B:95:TYR:CD1	2:B:103:ILE:HG13	2.48	0.49
3:C:206:MET:O	3:C:208:THR:HG23	2.13	0.49
3:Q:86:THR:O	3:Q:89:ALA:HB3	2.12	0.49
3:C:52:PRO:HG3	3:C:214:ASP:HB3	1.93	0.49
1:A:31:TYR:N	1:A:32:PRO:CD	2.76	0.49
1:A:80:ARG:HD3	1:A:83:ASP:OD2	2.13	0.49
13:M:257:GLU:HB2	13:M:258:PRO:HD2	1.95	0.49
9:W:238:THR:HG21	10:X:168:ALA:HB1	1.94	0.49
4:D:187:HIS:CE1	4:D:229:VAL:HG22	2.48	0.49
3:Q:121:CYS:HB3	3:Q:160:GLY:O	2.13	0.49
5:S:188:LEU:HD23	5:S:219:LEU:HD23	1.95	0.49
5:E:210:GLU:HB2	5:E:254:TRP:CZ2	2.47	0.48
5:S:309:GLN:O	5:S:314:ASN:ND2	2.45	0.48
11:Y:24:PHE:O	11:Y:25:TYR:C	2.49	0.48
3:C:77:HIS:NE2	3:C:111:MET:O	2.39	0.48
3:C:121:CYS:HB3	3:C:160:GLY:O	2.13	0.48
5:E:141:ARG:HD3	5:E:251:PRO:O	2.13	0.48
13:M:246:VAL:HG22	13:M:247:CYS:N	2.28	0.48
9:W:104:ARG:HB2	9:W:107:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:THR:O	3:C:89:ALA:HB3	2.13	0.48
14:N:21:ASP:O	14:N:37:ARG:HD3	2.13	0.48
7:U:65:ASN:HD22	7:U:65:ASN:HA	1.56	0.48
10:X:11:VAL:HG12	10:X:12:MET:N	2.29	0.48
1:A:70:THR:HB	1:A:71:PRO:CD	2.43	0.48
10:X:136:TYR:CD1	10:X:136:TYR:C	2.87	0.48
3:C:181:LEU:HD23	3:C:201:VAL:HG21	1.96	0.48
3:C:200:ARG:NH1	3:C:268:GLU:OE1	2.47	0.48
4:D:89:LEU:HD12	4:D:89:LEU:O	2.13	0.48
5:E:188:LEU:HD23	5:E:219:LEU:HD23	1.95	0.48
3:Q:36:GLY:HA2	3:Q:44:VAL:O	2.14	0.48
3:Q:181:LEU:HD23	3:Q:201:VAL:HG21	1.96	0.48
5:S:141:ARG:HD3	5:S:251:PRO:O	2.13	0.48
6:T:349:LEU:HD21	6:T:379:ILE:HD12	1.95	0.48
6:F:218:VAL:O	6:F:219:ALA:HB3	2.13	0.48
6:T:218:VAL:O	6:T:219:ALA:HB3	2.13	0.48
3:C:36:GLY:HA2	3:C:44:VAL:O	2.14	0.48
8:H:227:LEU:HD23	8:H:244:PRO:HA	1.95	0.48
10:J:112:ILE:HG23	10:J:112:ILE:O	2.13	0.48
2:P:95:TYR:CD1	2:P:103:ILE:HG13	2.48	0.48
1:A:80:ARG:HD3	1:A:83:ASP:CG	2.33	0.48
1:O:87:LEU:HD12	1:O:133:VAL:HG21	1.96	0.48
3:Q:206:MET:O	3:Q:208:THR:HG23	2.12	0.48
1:A:83:ASP:OD1	7:G:121:HIS:NE2	2.37	0.48
9:I:104:ARG:HB2	9:I:107:GLU:HG3	1.95	0.48
10:J:136:TYR:CD1	10:J:136:TYR:C	2.87	0.48
12:L:156:ARG:NH1	12:L:156:ARG:HG3	2.29	0.48
9:I:238:THR:HG21	10:J:168:ALA:HB1	1.94	0.48
1:O:41:CYS:SG	1:O:44:ALA:HB3	2.54	0.48
3:Q:116:LEU:C	3:Q:116:LEU:HD13	2.35	0.48
8:V:227:LEU:HD23	8:V:244:PRO:HA	1.95	0.48
12:L:222:GLN:HB2	12:L:225:PHE:CZ	2.49	0.47
2:P:13:PRO:HA	3:Q:23:TYR:CD1	2.49	0.47
2:P:20:ILE:HD11	2:P:120:THR:HB	1.96	0.47
1:A:41:CYS:SG	1:A:44:ALA:HB3	2.54	0.47
2:B:13:PRO:HA	3:C:23:TYR:CD1	2.49	0.47
3:Q:200:ARG:NH1	3:Q:268:GLU:OE1	2.47	0.47
10:X:112:ILE:HG23	10:X:112:ILE:O	2.13	0.47
12:Z:222:GLN:HB2	12:Z:225:PHE:CZ	2.49	0.47
1:A:87:LEU:HD12	1:A:133:VAL:HG21	1.96	0.47
1:O:70:THR:HB	1:O:71:PRO:CD	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:66:MET:HE3	9:W:72:CYS:HB2	1.96	0.47
3:C:116:LEU:HD13	3:C:116:LEU:C	2.34	0.47
4:D:107:LEU:HD13	4:D:107:LEU:C	2.35	0.47
2:B:20:ILE:HD11	2:B:120:THR:HB	1.96	0.47
10:X:59:ASP:OD2	11:Y:95:ARG:NH2	2.45	0.47
12:Z:156:ARG:HG3	12:Z:156:ARG:NH1	2.29	0.47
10:J:112:ILE:O	10:J:112:ILE:CG2	2.63	0.47
13:M:139:ILE:HD12	13:M:301:LEU:HG	1.95	0.47
7:U:168:ALA:HB1	7:U:200:VAL:HB	1.96	0.47
9:W:53:SER:C	9:W:54:ILE:HD12	2.35	0.47
12:Z:134:LEU:HD23	12:Z:155:GLU:CB	2.39	0.47
13:M:254:GLY:O	13:M:255:SER:C	2.49	0.47
7:G:168:ALA:HB1	7:G:200:VAL:HB	1.96	0.47
13:M:162:ARG:HD3	13:M:317:ASP:OD1	2.15	0.47
6:T:200:VAL:HG22	6:T:325:ALA:HB2	1.97	0.47
5:E:261:THR:OG1	6:F:225:GLN:NE2	2.48	0.47
9:I:53:SER:C	9:I:54:ILE:HD12	2.35	0.46
12:L:156:ARG:HG3	12:L:156:ARG:HH11	1.80	0.46
7:U:73:GLN:HG3	7:U:142:ALA:HB2	1.98	0.46
4:R:107:LEU:C	4:R:107:LEU:HD13	2.34	0.46
5:E:190:GLU:OE2	12:L:168:ARG:NH1	2.42	0.46
12:L:211:TYR:CE2	12:L:221:LYS:HB2	2.51	0.46
1:O:83:ASP:OD1	7:U:121:HIS:NE2	2.37	0.46
4:D:64:LYS:HG2	11:K:70:MET:SD	2.56	0.46
12:L:144:LEU:C	12:L:144:LEU:CD2	2.84	0.46
1:O:80:ARG:HD3	1:O:83:ASP:OD2	2.14	0.46
1:O:46:LEU:CD1	1:O:199:ALA:HB2	2.46	0.46
10:X:112:ILE:O	10:X:112:ILE:CG2	2.63	0.46
6:T:201:GLY:HA2	6:T:209:VAL:O	2.16	0.46
6:F:201:GLY:HA2	6:F:209:VAL:O	2.16	0.46
10:J:11:VAL:HG12	10:J:12:MET:N	2.29	0.46
4:R:64:LYS:HG2	11:Y:70:MET:SD	2.56	0.46
5:S:139:GLY:O	5:S:267:ALA:HA	2.16	0.46
6:T:327:GLY:O	6:T:330:SER:OG	2.24	0.46
12:Z:224:LEU:C	12:Z:224:LEU:HD23	2.37	0.46
6:F:200:VAL:HG22	6:F:325:ALA:HB2	1.97	0.46
3:C:28:ILE:HD13	3:C:139:SER:HB2	1.98	0.46
5:E:138:LEU:C	5:E:138:LEU:HD12	2.36	0.46
5:E:312:PRO:N	5:E:339:MET:HE1	2.31	0.46
9:I:195:ASP:HA	9:I:196:PRO:HD2	1.80	0.46
10:J:112:ILE:HG13	10:J:119:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:142:ALA:O	14:N:143:LEU:C	2.49	0.46
3:C:144:GLY:HA2	3:C:221:MET:HG2	1.98	0.45
13:M:313:ILE:HD13	9:W:53:SER:HA	1.98	0.45
5:E:139:GLY:O	5:E:267:ALA:HA	2.16	0.45
6:F:273:MET:HE2	6:F:273:MET:HB2	1.85	0.45
12:L:150:ASP:OD1	13:M:223:TYR:OH	2.23	0.45
3:Q:144:GLY:HA2	3:Q:221:MET:HG2	1.98	0.45
7:G:73:GLN:HG3	7:G:142:ALA:HB2	1.98	0.45
3:Q:184:ASP:OD1	3:Q:200:ARG:NH2	2.43	0.45
3:C:149:TYR:CE1	4:D:57:ARG:HD2	2.51	0.45
9:I:33:VAL:HG22	9:I:155:THR:HG22	1.98	0.45
12:Z:211:TYR:CE2	12:Z:221:LYS:HB2	2.51	0.45
14:N:132:CYS:C	14:N:133:ILE:HG12	2.37	0.45
6:T:336:TYR:CD2	6:T:359:ALA:HB2	2.52	0.45
3:C:184:ASP:OD1	3:C:200:ARG:NH2	2.43	0.45
6:T:277:ILE:HD12	6:T:277:ILE:HA	1.88	0.45
12:Z:156:ARG:HG3	12:Z:156:ARG:HH11	1.81	0.45
3:C:182:LYS:HE2	4:D:51:VAL:HG23	1.99	0.45
6:F:186:ILE:HD11	6:F:285:ILE:HB	1.98	0.45
2:P:182:LEU:O	2:P:186:VAL:HG23	2.17	0.45
3:C:82:VAL:HG12	3:C:140:PHE:CD1	2.52	0.45
4:D:168:VAL:O	4:D:172:MET:HG3	2.17	0.45
6:F:336:TYR:CD2	6:F:359:ALA:HB2	2.52	0.45
10:J:54:THR:O	10:J:105:VAL:HA	2.17	0.45
12:L:224:LEU:C	12:L:224:LEU:HD23	2.37	0.45
6:T:196:GLY:O	6:T:328:VAL:HG23	2.17	0.45
8:V:58:LEU:C	8:V:58:LEU:HD12	2.37	0.45
8:H:58:LEU:C	8:H:58:LEU:HD12	2.37	0.45
1:O:81:ALA:N	1:O:82:PRO:CD	2.79	0.45
5:S:138:LEU:CD1	5:S:149:ALA:HB3	2.46	0.45
10:X:112:ILE:HG13	10:X:119:VAL:HG22	1.99	0.45
11:Y:72:GLN:O	11:Y:75:ARG:HD3	2.17	0.45
9:I:113:LYS:CE	9:I:148:THR:HG23	2.47	0.44
11:K:54:ARG:HG2	11:K:54:ARG:HH11	1.82	0.44
3:Q:82:VAL:HG12	3:Q:140:PHE:CE1	2.52	0.44
3:Q:149:TYR:CE1	4:R:57:ARG:HD2	2.52	0.44
1:A:46:LEU:CD1	1:A:199:ALA:HB2	2.46	0.44
3:Q:120:LEU:HD12	3:Q:120:LEU:HA	1.80	0.44
6:T:186:ILE:HD11	6:T:285:ILE:HB	1.97	0.44
5:E:268:GLN:HA	5:E:268:GLN:NE2	2.20	0.44
14:N:137:TYR:O	14:N:138:GLY:C	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:182:LYS:HE2	4:R:51:VAL:HG23	2.00	0.44
4:R:60:ARG:HD2	4:R:216:TYR:CE1	2.53	0.44
5:S:138:LEU:C	5:S:138:LEU:HD12	2.36	0.44
5:S:261:THR:OG1	6:T:225:GLN:NE2	2.49	0.44
9:W:113:LYS:CE	9:W:148:THR:HG23	2.47	0.44
1:A:81:ALA:N	1:A:82:PRO:CD	2.80	0.44
6:F:222:SER:O	6:F:223:SER:CB	2.66	0.44
12:L:111:ILE:HB	12:L:278:VAL:HB	2.00	0.44
5:S:190:GLU:OE2	12:Z:168:ARG:NH1	2.39	0.44
8:V:68:LEU:HD23	8:V:98:CYS:SG	2.58	0.44
1:A:228:ASN:ND2	1:A:232:GLN:NE2	2.51	0.44
6:F:213:LEU:HD23	6:F:213:LEU:HA	1.86	0.44
9:I:74:GLY:HA3	9:I:81:THR:HG21	1.99	0.44
10:X:54:THR:O	10:X:105:VAL:HA	2.17	0.44
2:B:182:LEU:O	2:B:186:VAL:HG23	2.17	0.44
4:D:60:ARG:HD2	4:D:216:TYR:CE1	2.52	0.44
3:Q:28:ILE:HD13	3:Q:139:SER:HB2	1.99	0.44
9:W:195:ASP:HA	9:W:196:PRO:HD2	1.80	0.44
11:K:104:ASN:HB3	11:K:143:HIS:CE1	2.53	0.44
3:Q:130:TYR:CD2	4:R:124:SER:HB2	2.52	0.44
6:T:213:LEU:HD23	6:T:213:LEU:HA	1.86	0.44
11:Y:54:ARG:HG2	11:Y:54:ARG:HH11	1.81	0.44
10:J:146:LEU:HD21	10:J:171:MET:HA	2.00	0.44
12:L:142:GLY:HA2	12:L:199:MET:O	2.18	0.44
1:O:75:CYS:HB3	1:O:137:PHE:CD1	2.53	0.44
7:G:39:ALA:HB3	7:G:163:VAL:HG12	1.99	0.44
8:H:68:LEU:HD23	8:H:98:CYS:SG	2.58	0.44
9:I:61:ARG:HH21	9:I:61:ARG:HG3	1.83	0.44
6:T:222:SER:O	6:T:223:SER:CB	2.65	0.44
9:W:33:VAL:HG22	9:W:155:THR:HG22	1.99	0.44
12:Z:144:LEU:C	12:Z:144:LEU:CD2	2.84	0.44
1:A:75:CYS:HB3	1:A:137:PHE:CD1	2.53	0.43
8:H:218:TYR:CD1	8:H:218:TYR:C	2.92	0.43
3:Q:82:VAL:HG12	3:Q:140:PHE:CD1	2.52	0.43
3:C:130:TYR:CD2	4:D:124:SER:HB2	2.53	0.43
4:D:171:TYR:OH	4:D:191:LYS:HE3	2.18	0.43
11:K:72:GLN:O	11:K:75:ARG:HD3	2.18	0.43
8:V:136:LEU:O	8:V:140:MET:HG3	2.19	0.43
3:C:130:TYR:CE2	4:D:124:SER:HB2	2.54	0.43
8:H:136:LEU:O	8:H:140:MET:HG3	2.18	0.43
10:J:70:ARG:HA	10:J:70:ARG:HD2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:88:ILE:CD1	7:U:134:CYS:SG	3.05	0.43
11:Y:104:ASN:HB3	11:Y:143:HIS:CE1	2.52	0.43
4:D:97:ASN:N	4:D:97:ASN:HD22	2.15	0.43
4:R:171:TYR:OH	4:R:191:LYS:HE3	2.19	0.43
11:Y:86:MET:HB3	11:Y:86:MET:HE2	1.96	0.43
1:A:157:ASP:OD2	1:A:157:ASP:C	2.57	0.43
4:D:190:ILE:HD11	4:D:206:LEU:HD13	2.01	0.43
7:G:11:SER:HB3	7:G:13:ASP:OD2	2.19	0.43
4:R:97:ASN:N	4:R:97:ASN:HD22	2.16	0.43
4:R:168:VAL:O	4:R:172:MET:HG3	2.18	0.43
3:C:120:LEU:HD12	3:C:120:LEU:HA	1.80	0.43
3:C:125:GLN:NE2	4:D:79:ASP:OD1	2.46	0.43
11:K:8:PHE:HB3	11:K:140:TYR:HB3	2.01	0.43
14:N:44:HIS:O	14:N:110:GLY:HA2	2.18	0.43
14:N:195:ARG:NH1	14:N:195:ARG:HG3	2.32	0.43
7:U:93:ARG:O	7:U:97:GLU:HG3	2.17	0.43
5:E:204:ASN:HB2	13:M:216:GLN:HG2	2.01	0.43
7:G:93:ARG:O	7:G:97:GLU:HG3	2.18	0.43
3:Q:130:TYR:CE2	4:R:124:SER:HB2	2.53	0.43
3:Q:125:GLN:NE2	4:R:79:ASP:OD1	2.48	0.43
5:S:166:LYS:O	5:S:177:VAL:HG23	2.18	0.43
5:S:268:GLN:HA	5:S:268:GLN:NE2	2.19	0.43
6:T:282:GLN:NE2	7:U:84:ASP:OD1	2.47	0.43
7:U:39:ALA:HB3	7:U:163:VAL:HG12	1.99	0.43
12:Z:111:ILE:HB	12:Z:278:VAL:HB	2.00	0.43
12:Z:142:GLY:HA2	12:Z:199:MET:O	2.18	0.43
3:C:82:VAL:HG12	3:C:140:PHE:CE1	2.52	0.43
10:J:40:PRO:HB3	10:J:186:VAL:HG21	2.01	0.43
13:M:167:LYS:O	13:M:178:ALA:HA	2.19	0.43
8:V:218:TYR:CD1	8:V:218:TYR:C	2.92	0.43
10:X:48:SER:O	10:X:111:SER:HA	2.18	0.43
3:C:39:THR:OG1	3:C:40:LYS:N	2.52	0.43
5:E:166:LYS:O	5:E:177:VAL:HG23	2.19	0.43
10:J:48:SER:O	10:J:111:SER:HA	2.19	0.43
10:J:131:CYS:O	10:J:133:PRO:HD3	2.19	0.43
1:O:228:ASN:ND2	1:O:232:GLN:NE2	2.53	0.43
10:X:19:CYS:HA	10:X:190:VAL:O	2.19	0.43
7:G:88:ILE:CD1	7:G:134:CYS:SG	3.05	0.42
13:M:226:ARG:HA	13:M:226:ARG:HD2	1.73	0.42
4:R:190:ILE:HD11	4:R:206:LEU:HD13	2.01	0.42
7:U:36:THR:HA	7:U:165:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:107:PHE:CD1	12:Z:107:PHE:N	2.87	0.42
4:D:107:LEU:HD13	4:D:107:LEU:O	2.19	0.42
3:Q:39:THR:OG1	3:Q:40:LYS:N	2.52	0.42
4:R:159:VAL:HG22	4:R:160:ALA:N	2.35	0.42
9:W:74:GLY:HA3	9:W:81:THR:HG21	1.99	0.42
4:D:159:VAL:HG22	4:D:160:ALA:N	2.35	0.42
14:N:171:ARG:HH21	14:N:171:ARG:HD2	1.62	0.42
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.84	0.42
3:C:183:LYS:HB3	3:C:183:LYS:HE2	1.87	0.42
13:M:171:LEU:HD23	13:M:171:LEU:HA	1.93	0.42
5:S:312:PRO:N	5:S:339:MET:HE1	2.33	0.42
4:D:112:ALA:HB1	4:D:151:GLY:O	2.19	0.42
5:E:138:LEU:CD1	5:E:149:ALA:HB3	2.46	0.42
14:N:8:ILE:HD13	14:N:8:ILE:HG21	1.84	0.42
14:N:219:ILE:HD12	8:V:89:THR:CG2	2.50	0.42
1:O:194:THR:O	1:O:195:GLN:C	2.57	0.42
4:R:107:LEU:HD13	4:R:107:LEU:O	2.19	0.42
5:S:209:VAL:O	5:S:209:VAL:HG12	2.19	0.42
8:V:218:TYR:C	8:V:218:TYR:HD1	2.22	0.42
10:X:40:PRO:HB3	10:X:186:VAL:HG21	2.02	0.42
5:E:209:VAL:HG12	5:E:209:VAL:O	2.19	0.42
6:T:205:LYS:HB2	6:T:345:SER:O	2.20	0.42
7:U:11:SER:HB3	7:U:13:ASP:OD2	2.20	0.42
10:J:19:CYS:HA	10:J:190:VAL:O	2.20	0.42
14:N:111:VAL:HG23	14:N:189:ALA:HB1	2.02	0.42
1:O:157:ASP:OD2	1:O:157:ASP:C	2.57	0.42
10:X:146:LEU:HD21	10:X:171:MET:HA	2.00	0.42
1:A:111:LEU:O	1:A:115:MET:HG2	2.20	0.42
5:E:273:GLY:O	5:E:275:GLU:N	2.53	0.42
8:H:218:TYR:C	8:H:218:TYR:HD1	2.22	0.42
3:C:149:TYR:CD1	4:D:57:ARG:HD2	2.55	0.42
4:D:73:PHE:CD2	4:D:73:PHE:C	2.93	0.42
7:G:36:THR:HA	7:G:165:LEU:O	2.19	0.42
10:X:149:MET:HE2	10:X:170:ALA:HA	2.01	0.42
7:G:152:ASP:OD2	7:G:152:ASP:C	2.58	0.42
12:L:107:PHE:CD1	12:L:107:PHE:N	2.87	0.42
1:O:185:GLN:OE1	2:P:53:THR:HB	2.20	0.42
4:R:51:VAL:C	4:R:53:LEU:H	2.24	0.42
10:X:131:CYS:O	10:X:133:PRO:HD3	2.19	0.42
5:E:126:TYR:O	5:E:127:ALA:C	2.57	0.41
5:S:273:GLY:O	5:S:275:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:61:ARG:HH21	9:W:61:ARG:HG3	1.84	0.41
3:C:12:PHE:CE2	4:D:125:ARG:HD2	2.55	0.41
8:H:120:TYR:CE2	8:H:124:ILE:HD13	2.55	0.41
7:U:91:ARG:HH21	7:U:91:ARG:HD2	1.64	0.41
12:Z:101:THR:HG21	12:Z:262:ALA:CB	2.50	0.41
12:L:259:ILE:HD13	12:L:259:ILE:HA	1.84	0.41
13:M:311:ARG:O	9:W:54:ILE:HA	2.20	0.41
1:O:111:LEU:O	1:O:115:MET:HG2	2.20	0.41
4:R:215:ARG:HH12	4:R:221:GLU:CD	2.20	0.41
5:S:247:ASP:OD1	5:S:247:ASP:N	2.53	0.41
7:U:152:ASP:OD2	7:U:152:ASP:C	2.58	0.41
11:Y:8:PHE:HB3	11:Y:140:TYR:HB3	2.01	0.41
10:J:35:ILE:O	10:J:35:ILE:HG22	2.20	0.41
11:K:86:MET:HB3	11:K:86:MET:HE2	1.95	0.41
12:L:101:THR:HG21	12:L:262:ALA:CB	2.50	0.41
14:N:190:ALA:O	14:N:191:SER:C	2.59	0.41
4:R:26:VAL:O	4:R:162:GLY:HA2	2.20	0.41
5:S:296:THR:OG1	5:S:341:ARG:NH1	2.54	0.41
10:X:70:ARG:HA	10:X:70:ARG:HD2	1.85	0.41
11:Y:14:VAL:HG21	11:Y:108:ALA:HB1	2.03	0.41
5:E:326:LYS:HA	5:E:326:LYS:HD3	1.81	0.41
6:F:196:GLY:O	6:F:328:VAL:HG23	2.19	0.41
6:T:273:MET:HE2	6:T:273:MET:HB2	1.86	0.41
10:X:44:VAL:HG22	10:X:50:VAL:HG22	2.03	0.41
4:D:93:ARG:NH1	4:D:97:ASN:OD1	2.54	0.41
12:L:187:TYR:O	12:L:190:ARG:HG2	2.21	0.41
4:R:93:ARG:NH1	4:R:97:ASN:OD1	2.54	0.41
12:Z:187:TYR:O	12:Z:190:ARG:HG2	2.20	0.41
12:Z:259:ILE:HD13	12:Z:259:ILE:HA	1.84	0.41
4:D:83:LEU:HA	4:D:83:LEU:HD12	1.76	0.41
6:F:205:LYS:HB2	6:F:345:SER:O	2.19	0.41
6:F:389:PHE:HD1	6:F:389:PHE:HA	1.78	0.41
14:N:21:ASP:OD1	14:N:37:ARG:NH1	2.54	0.41
14:N:206:TRP:CE3	8:V:83:ARG:NH1	2.88	0.41
3:Q:12:PHE:CE2	4:R:125:ARG:HD2	2.55	0.41
5:S:312:PRO:CD	5:S:339:MET:HE1	2.50	0.41
12:Z:104:ALA:HA	12:Z:112:ILE:O	2.21	0.41
4:D:26:VAL:O	4:D:162:GLY:HA2	2.21	0.41
11:K:1:MET:HB3	11:K:145:TYR:CZ	2.56	0.41
12:L:104:ALA:HA	12:L:112:ILE:O	2.21	0.41
1:O:124:GLN:O	2:P:125:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:83:LEU:HD12	4:R:83:LEU:HA	1.76	0.41
4:R:112:ALA:HB1	4:R:151:GLY:O	2.21	0.41
6:T:237:MET:HA	6:T:298:LEU:O	2.21	0.41
8:V:120:TYR:CE2	8:V:124:ILE:HD13	2.55	0.41
10:X:96:TYR:CE1	10:X:99:ARG:HD3	2.55	0.41
1:A:124:GLN:O	2:B:125:VAL:HA	2.21	0.41
11:K:70:MET:C	11:K:72:GLN:N	2.74	0.41
12:L:278:VAL:HG22	12:L:283:TRP:HB3	2.03	0.41
13:M:135:THR:HG21	13:M:267:ALA:HB3	2.03	0.41
4:R:146:LYS:O	4:R:153:CYS:HA	2.21	0.41
10:X:35:ILE:O	10:X:35:ILE:HG22	2.20	0.41
6:F:245:ASP:O	6:F:246:GLY:C	2.60	0.40
10:J:149:MET:HE2	10:J:170:ALA:HA	2.03	0.40
1:O:157:ASP:HB2	1:O:158:PRO:CD	2.51	0.40
10:J:96:TYR:CE1	10:J:99:ARG:HD3	2.56	0.40
4:R:73:PHE:CD2	4:R:73:PHE:C	2.93	0.40
5:S:126:TYR:O	5:S:127:ALA:C	2.56	0.40
1:A:172:LYS:O	1:A:173:LYS:HB2	2.21	0.40
2:B:30:GLY:HA3	2:B:76:GLY:H	1.87	0.40
5:E:296:THR:OG1	5:E:341:ARG:NH1	2.55	0.40
8:H:146:TRP:CE3	8:H:146:TRP:HA	2.57	0.40
9:I:113:LYS:NZ	9:I:148:THR:HG23	2.36	0.40
13:M:250:TYR:CE2	13:M:256:THR:HB	2.55	0.40
1:O:65:ALA:O	1:O:76:CYS:HA	2.22	0.40
1:O:172:LYS:O	1:O:173:LYS:HB2	2.21	0.40
6:T:249:LEU:HD23	6:T:249:LEU:HA	1.86	0.40
1:A:185:GLN:OE1	2:B:53:THR:HB	2.20	0.40
2:P:193:LEU:HD23	2:P:193:LEU:HA	1.93	0.40
4:R:48:LYS:O	4:R:49:SER:HB2	2.22	0.40
9:W:238:THR:HA	9:W:239:PRO:HD3	1.93	0.40
3:C:67:SER:HB3	10:J:79:GLU:OE1	2.21	0.40
4:D:146:LYS:O	4:D:153:CYS:HA	2.22	0.40
8:H:258:TYR:OH	8:V:179:TYR:OH	2.33	0.40
11:K:45:VAL:O	11:K:45:VAL:HG13	2.22	0.40
14:N:18:MET:O	14:N:186:VAL:HA	2.22	0.40
14:N:172:VAL:O	14:N:172:VAL:HG12	2.21	0.40
2:P:30:GLY:HA3	2:P:76:GLY:H	1.87	0.40
3:Q:67:SER:HB3	10:X:79:GLU:OE1	2.22	0.40
3:Q:101:LEU:HD12	10:X:73:MET:HE3	2.02	0.40
10:X:8:GLY:HA2	10:X:141:THR:HG21	2.04	0.40
10:X:158:MET:HE3	10:X:166:ILE:HG21	2.03	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	242/250 (97%)	235 (97%)	5 (2%)	2 (1%)	19	39
1	O	242/250 (97%)	235 (97%)	5 (2%)	2 (1%)	19	39
2	B	227/231 (98%)	219 (96%)	8 (4%)	0	100	100
2	P	227/231 (98%)	219 (96%)	8 (4%)	0	100	100
3	C	269/285 (94%)	254 (94%)	14 (5%)	1 (0%)	34	57
3	Q	269/285 (94%)	253 (94%)	15 (6%)	1 (0%)	34	57
4	D	232/248 (94%)	213 (92%)	18 (8%)	1 (0%)	34	57
4	R	232/248 (94%)	214 (92%)	17 (7%)	1 (0%)	34	57
5	E	225/344 (65%)	214 (95%)	10 (4%)	1 (0%)	34	57
5	S	225/344 (65%)	214 (95%)	10 (4%)	1 (0%)	34	57
6	F	230/428 (54%)	220 (96%)	8 (4%)	2 (1%)	17	35
6	T	230/428 (54%)	220 (96%)	8 (4%)	2 (1%)	17	35
7	G	224/238 (94%)	216 (96%)	8 (4%)	0	100	100
7	U	224/238 (94%)	216 (96%)	8 (4%)	0	100	100
8	H	226/283 (80%)	217 (96%)	9 (4%)	0	100	100
8	V	226/283 (80%)	217 (96%)	9 (4%)	0	100	100
9	I	217/254 (85%)	205 (94%)	9 (4%)	3 (1%)	11	22
9	W	217/254 (85%)	205 (94%)	9 (4%)	3 (1%)	11	22
10	J	202/205 (98%)	195 (96%)	6 (3%)	1 (0%)	29	52
10	X	202/205 (98%)	194 (96%)	7 (4%)	1 (0%)	29	52
11	K	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	29	52
11	Y	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	200/301 (66%)	191 (96%)	8 (4%)	1 (0%)	29	52
12	Z	200/301 (66%)	190 (95%)	9 (4%)	1 (0%)	29	52
13	M	212/339 (62%)	203 (96%)	6 (3%)	3 (1%)	11	22
13	a	212/339 (62%)	203 (96%)	6 (3%)	3 (1%)	11	22
14	N	218/220 (99%)	210 (96%)	6 (3%)	2 (1%)	17	35
14	b	218/220 (99%)	209 (96%)	7 (3%)	2 (1%)	17	35
All	All	6256/7664 (82%)	5969 (95%)	251 (4%)	36 (1%)	29	47

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	49	SER
6	F	223	SER
13	M	226	ARG
14	N	191	SER
4	R	49	SER
6	T	223	SER
13	a	226	ARG
14	b	191	SER
1	A	248	GLU
6	F	219	ALA
9	I	223	GLU
1	O	248	GLU
6	T	219	ALA
9	W	223	GLU
1	A	187	SER
5	E	274	ALA
9	I	200	THR
11	K	71	ARG
13	M	286	SER
1	O	187	SER
5	S	274	ALA
9	W	200	THR
11	Y	71	ARG
12	L	136	ILE
12	Z	136	ILE
13	a	286	SER
14	b	114	GLY
10	J	115	SER
14	N	114	GLY

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Mol	Chain	Res	Type
10	X	115	SER
13	a	240	ASP
13	M	240	ASP
3	C	229	ILE
9	I	235	PRO
3	Q	229	ILE
9	W	235	PRO

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	193/197 (98%)	183 (95%)	10 (5%)	23	46
1	O	193/197 (98%)	183 (95%)	10 (5%)	23	46
2	B	188/190 (99%)	179 (95%)	9 (5%)	25	49
2	P	188/190 (99%)	179 (95%)	9 (5%)	25	49
3	C	229/241 (95%)	218 (95%)	11 (5%)	25	49
3	Q	229/241 (95%)	217 (95%)	12 (5%)	23	46
4	D	198/208 (95%)	188 (95%)	10 (5%)	24	46
4	R	198/208 (95%)	188 (95%)	10 (5%)	24	46
5	E	193/301 (64%)	178 (92%)	15 (8%)	12	25
5	S	193/301 (64%)	177 (92%)	16 (8%)	11	22
6	F	195/363 (54%)	188 (96%)	7 (4%)	35	61
6	T	195/363 (54%)	188 (96%)	7 (4%)	35	61
7	G	182/190 (96%)	172 (94%)	10 (6%)	21	43
7	U	182/190 (96%)	171 (94%)	11 (6%)	19	39
8	H	184/229 (80%)	174 (95%)	10 (5%)	22	44
8	V	184/229 (80%)	174 (95%)	10 (5%)	22	44
9	I	180/209 (86%)	176 (98%)	4 (2%)	52	76
9	W	180/209 (86%)	176 (98%)	4 (2%)	52	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	167/168 (99%)	161 (96%)	6 (4%)	35 61
10	X	167/168 (99%)	161 (96%)	6 (4%)	35 61
11	K	172/172 (100%)	171 (99%)	1 (1%)	86 95
11	Y	172/172 (100%)	170 (99%)	2 (1%)	71 87
12	L	163/252 (65%)	155 (95%)	8 (5%)	25 48
12	Z	163/252 (65%)	155 (95%)	8 (5%)	25 48
13	M	181/288 (63%)	174 (96%)	7 (4%)	32 58
13	a	181/288 (63%)	174 (96%)	7 (4%)	32 58
14	N	183/183 (100%)	176 (96%)	7 (4%)	33 59
14	b	183/183 (100%)	176 (96%)	7 (4%)	33 59
All	All	5216/6382 (82%)	4982 (96%)	234 (4%)	31 52

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	THR
1	A	89	GLN
1	A	105	GLU
1	A	143	SER
1	A	146	ASP
1	A	174	GLN
1	A	184	ARG
1	A	193	LEU
1	A	206	LEU
2	B	18	ILE
2	B	31	THR
2	B	53	THR
2	B	61	GLN
2	B	82	ARG
2	B	122	SER
2	B	175	ARG
2	B	197	PHE
2	B	206	THR
3	C	2	SER
3	C	14	PRO
3	C	39	THR
3	C	67	SER

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Mol	Chain	Res	Type
3	C	119	ILE
3	C	126	LEU
3	C	139	SER
3	C	159	SER
3	C	161	ASP
3	C	180	LEU
3	C	252	SER
4	D	2	SER
4	D	12	PRO
4	D	59	ILE
4	D	105	ASP
4	D	124	SER
4	D	163	ARG
4	D	170	GLU
4	D	175	SER
4	D	177	LYS
4	D	198	GLU
5	E	107	GLU
5	E	109	ASP
5	E	138	LEU
5	E	141	ARG
5	E	178	MET
5	E	256	THR
5	E	257	ASP
5	E	259	SER
5	E	261	THR
5	E	262	HIS
5	E	268	GLN
5	E	278	GLN
5	E	282	THR
5	E	289	MET
5	E	307	GLU
6	F	240	SER
6	F	273	MET
6	F	307	PRO
6	F	335	THR
6	F	362	SER
6	F	364	THR
6	F	379	ILE
7	G	43	LYS
7	G	51	GLU
7	G	57	ARG

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Mol	Chain	Res	Type
7	G	65	ASN
7	G	141	TYR
7	G	163	VAL
7	G	195	SER
7	G	207	LYS
7	G	208	LEU
7	G	215	TRP
8	H	76	SER
8	H	98	CYS
8	H	137	PHE
8	H	149	SER
8	H	173	SER
8	H	198	LYS
8	H	218	TYR
8	H	224	SER
8	H	236	ASP
8	H	280	SER
9	I	32	ILE
9	I	78	SER
9	I	124	SER
9	I	237	THR
10	J	14	MET
10	J	41	LYS
10	J	48	SER
10	J	116	THR
10	J	160	PRO
10	J	166	ILE
11	K	31	ASP
12	L	123	GLN
12	L	137	ASN
12	L	144	LEU
12	L	196	MET
12	L	209	SER
12	L	215	ASP
12	L	284	THR
12	L	291	GLN
13	M	179	SER
13	M	212	LYS
13	M	219	SER
13	M	226	ARG
13	M	259	PHE
13	M	260	LEU

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Mol	Chain	Res	Type
13	M	333	SER
14	N	45	SER
14	N	96	ARG
14	N	123	ASP
14	N	130	ASP
14	N	164	ARG
14	N	166	LEU
14	N	195	ARG
1	O	10	ILE
1	O	11	THR
1	O	89	GLN
1	O	105	GLU
1	O	143	SER
1	O	146	ASP
1	O	174	GLN
1	O	184	ARG
1	O	193	LEU
1	O	206	LEU
2	P	18	ILE
2	P	31	THR
2	P	53	THR
2	P	61	GLN
2	P	82	ARG
2	P	122	SER
2	P	175	ARG
2	P	197	PHE
2	P	206	THR
3	Q	2	SER
3	Q	14	PRO
3	Q	39	THR
3	Q	67	SER
3	Q	119	ILE
3	Q	126	LEU
3	Q	139	SER
3	Q	159	SER
3	Q	161	ASP
3	Q	180	LEU
3	Q	233	LEU
3	Q	252	SER
4	R	2	SER
4	R	12	PRO
4	R	59	ILE

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Mol	Chain	Res	Type
4	R	105	ASP
4	R	124	SER
4	R	163	ARG
4	R	170	GLU
4	R	175	SER
4	R	177	LYS
4	R	198	GLU
5	S	107	GLU
5	S	109	ASP
5	S	138	LEU
5	S	141	ARG
5	S	178	MET
5	S	202	THR
5	S	256	THR
5	S	257	ASP
5	S	259	SER
5	S	261	THR
5	S	262	HIS
5	S	268	GLN
5	S	278	GLN
5	S	282	THR
5	S	289	MET
5	S	307	GLU
6	T	240	SER
6	T	273	MET
6	T	307	PRO
6	T	335	THR
6	T	362	SER
6	T	364	THR
6	T	379	ILE
7	U	43	LYS
7	U	51	GLU
7	U	57	ARG
7	U	65	ASN
7	U	141	TYR
7	U	163	VAL
7	U	195	SER
7	U	202	ASP
7	U	207	LYS
7	U	208	LEU
7	U	215	TRP
8	V	76	SER

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Mol	Chain	Res	Type
8	V	98	CYS
8	V	137	PHE
8	V	149	SER
8	V	173	SER
8	V	198	LYS
8	V	218	TYR
8	V	224	SER
8	V	236	ASP
8	V	280	SER
9	W	32	ILE
9	W	78	SER
9	W	124	SER
9	W	237	THR
10	X	14	MET
10	X	41	LYS
10	X	48	SER
10	X	116	THR
10	X	160	PRO
10	X	166	ILE
11	Y	31	ASP
11	Y	88	ASN
12	Z	123	GLN
12	Z	137	ASN
12	Z	144	LEU
12	Z	196	MET
12	Z	209	SER
12	Z	215	ASP
12	Z	284	THR
12	Z	291	GLN
13	a	179	SER
13	a	212	LYS
13	a	219	SER
13	a	226	ARG
13	a	259	PHE
13	a	260	LEU
13	a	333	SER
14	b	45	SER
14	b	96	ARG
14	b	123	ASP
14	b	130	ASP
14	b	164	ARG
14	b	166	LEU

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Mol	Chain	Res	Type
14	b	195	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
2	B	107	GLN
2	B	187	HIS
2	B	200	GLN
3	C	29	GLN
3	C	152	GLN
4	D	23	GLN
4	D	97	ASN
5	E	191	HIS
5	E	252	GLN
5	E	255	GLN
5	E	268	GLN
5	E	288	ASN
6	F	225	GLN
6	F	272	GLN
6	F	331	GLN
7	G	65	ASN
8	H	196	ASN
8	H	211	GLN
8	H	241	GLN
9	I	115	HIS
9	I	201	GLN
10	J	65	ASN
11	K	22	ASN
11	K	102	GLN
11	K	186	ASN
11	K	197	ASN
13	M	130	GLN
14	N	70	GLN
1	O	232	GLN
2	P	107	GLN
2	P	187	HIS
2	P	200	GLN
3	Q	29	GLN
3	Q	152	GLN
4	R	23	GLN
4	R	97	ASN

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Mol	Chain	Res	Type
5	S	191	HIS
5	S	222	GLN
5	S	252	GLN
5	S	255	GLN
5	S	268	GLN
5	S	288	ASN
6	T	225	GLN
6	T	272	GLN
6	T	331	GLN
7	U	65	ASN
8	V	211	GLN
8	V	241	GLN
9	W	115	HIS
9	W	201	GLN
10	X	65	ASN
10	X	68	GLN
11	Y	22	ASN
11	Y	102	GLN
11	Y	186	ASN
11	Y	197	ASN
13	a	130	GLN
14	b	70	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	VYW	Z	4000	-	32,32,32	0.58	1 (3%)	39,44,44	0.45	0
15	VYW	L	4000	-	32,32,32	0.59	1 (3%)	39,44,44	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	VYW	Z	4000	-	-	1/20/22/22	0/4/4/4
15	VYW	L	4000	-	-	1/20/22/22	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	4000	VYW	C12-C13	-2.42	1.37	1.43
15	Z	4000	VYW	C12-C13	-2.38	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	4000	VYW	C2-C1-N-C
15	Z	4000	VYW	C2-C1-N-C

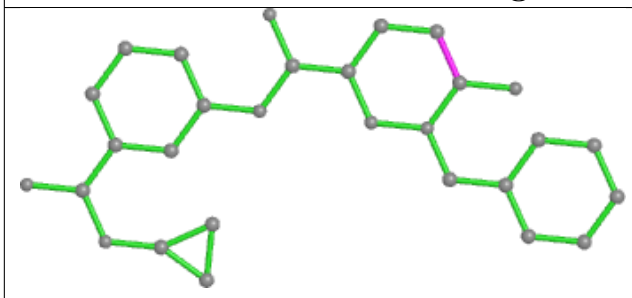
There are no ring outliers.

No monomer is involved in short contacts.

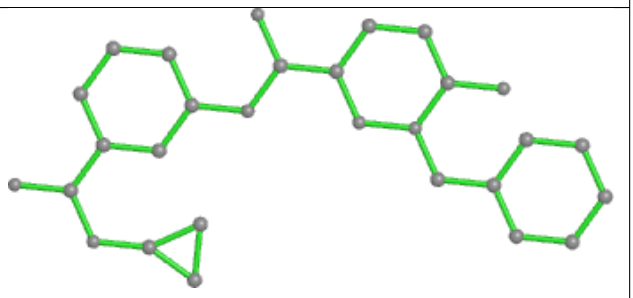
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

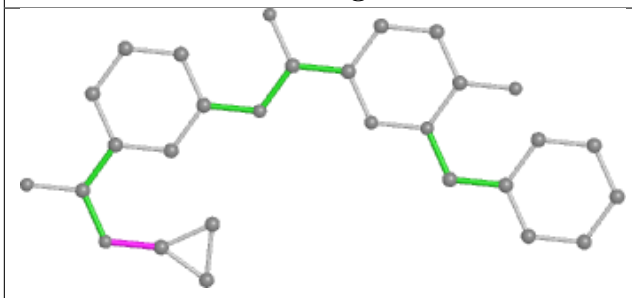
Ligand VYW Z 4000



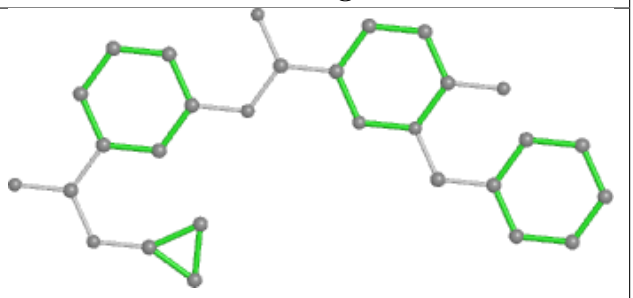
Bond lengths



Bond angles

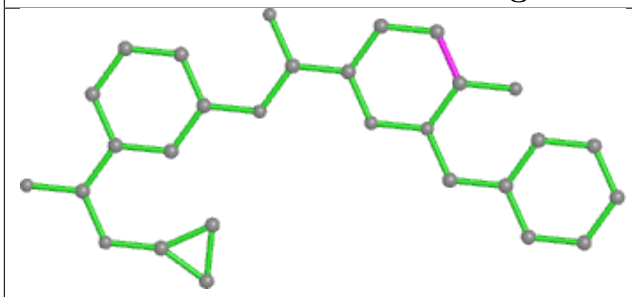


Torsions

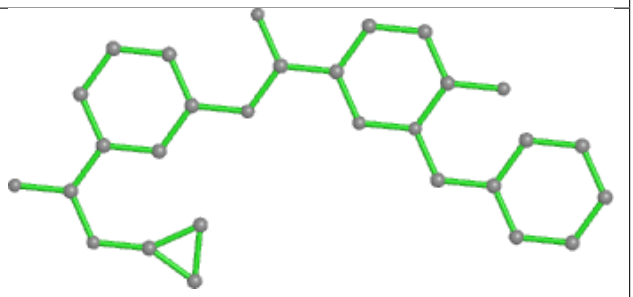


Rings

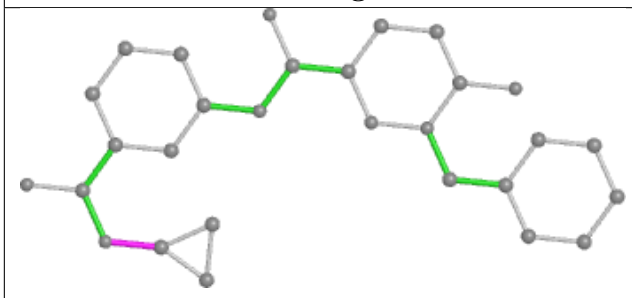
Ligand VYW L 4000



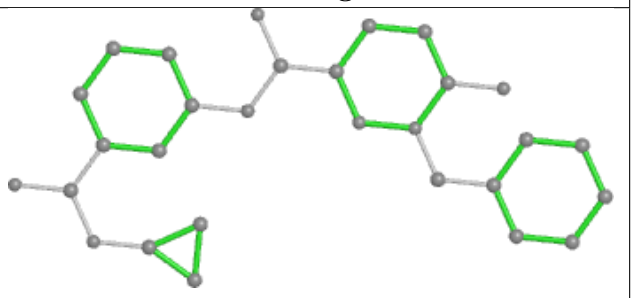
Bond lengths



Bond angles



Torsions



Rings

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.

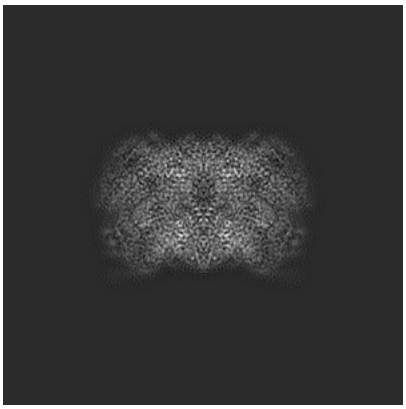
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16963. These allow visual inspection of the internal detail of the map and identification of artifacts.

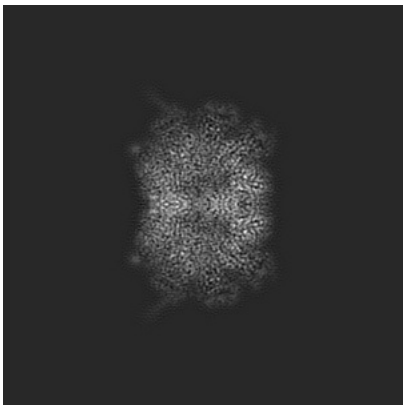
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

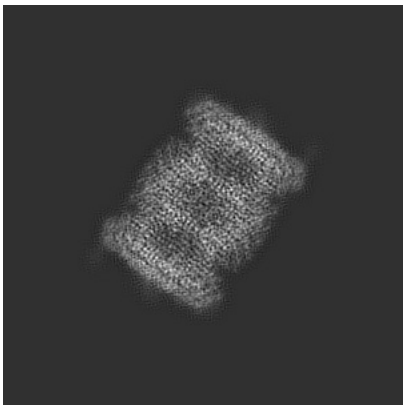
6.1.1 Primary map



X

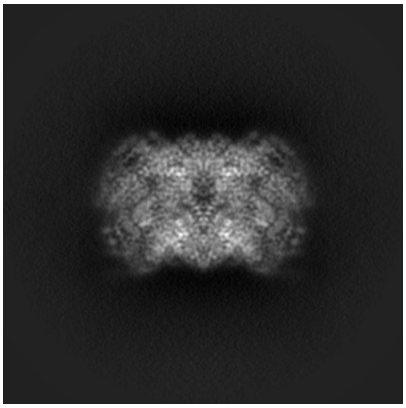


Y

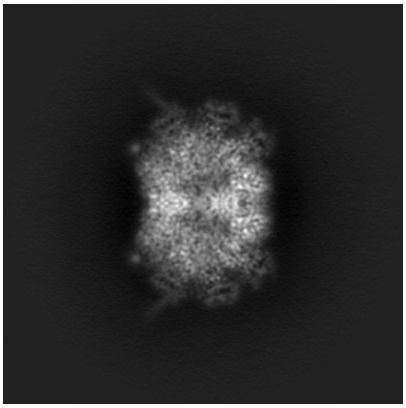


Z

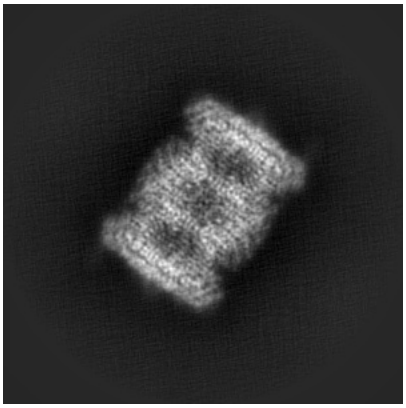
6.1.2 Raw map



X



Y

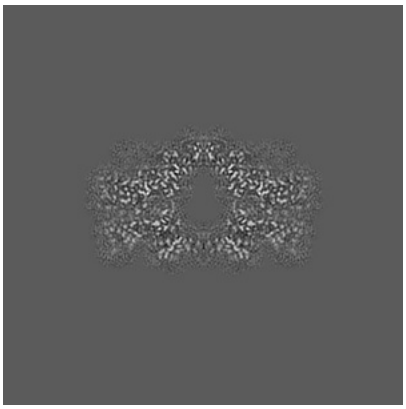


Z

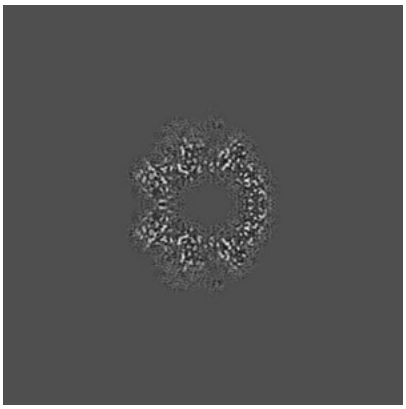
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

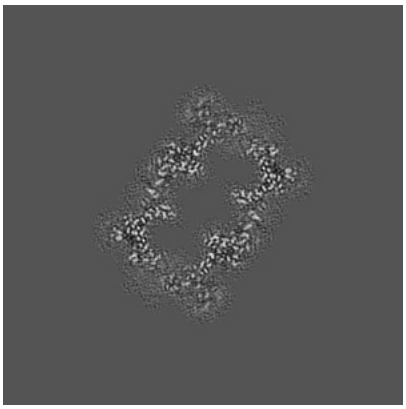
6.2.1 Primary map



X Index: 150

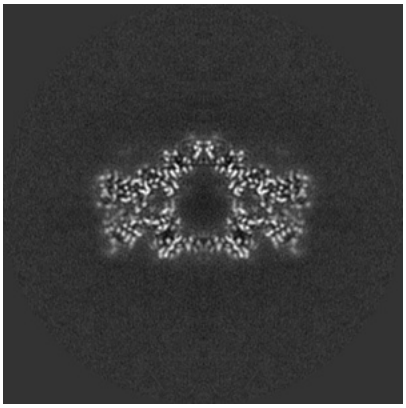


Y Index: 150

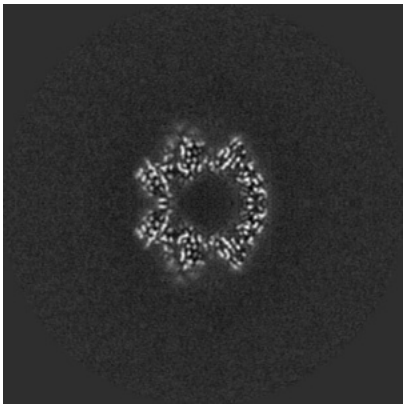


Z Index: 150

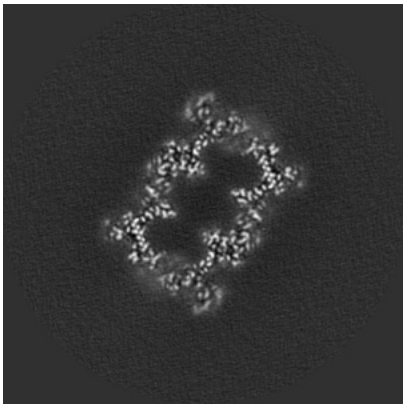
6.2.2 Raw map



X Index: 150



Y Index: 150

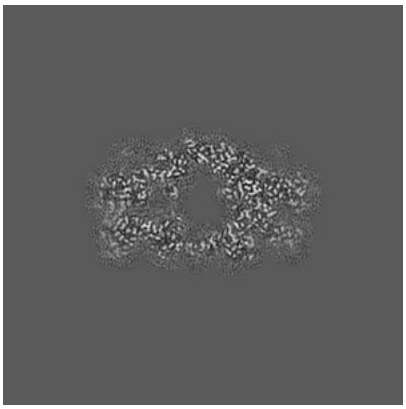


Z Index: 150

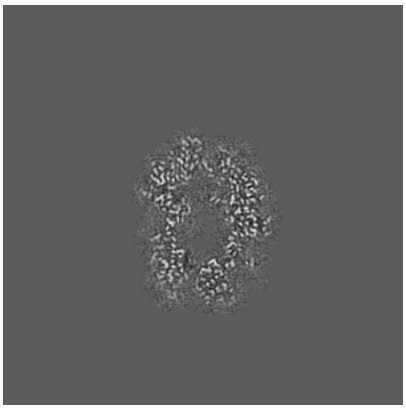
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

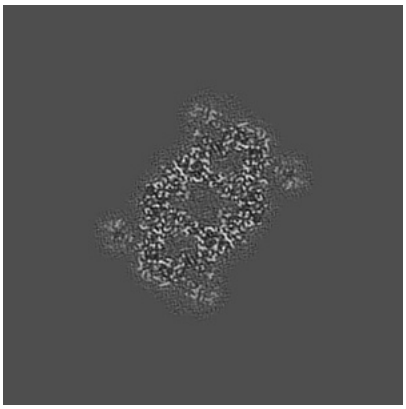
6.3.1 Primary map



X Index: 147

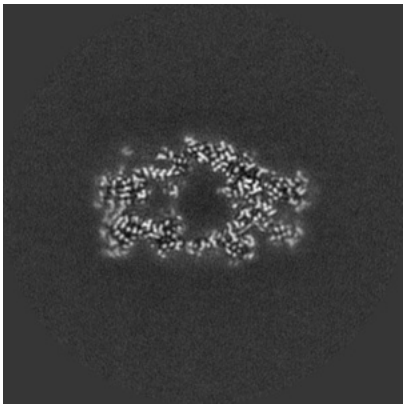


Y Index: 132

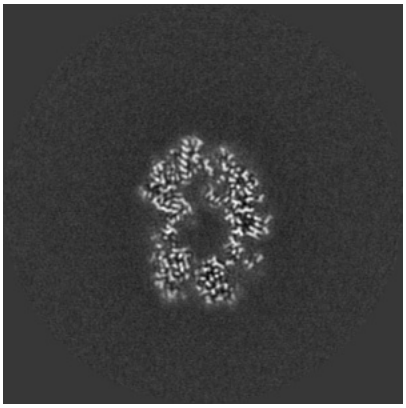


Z Index: 172

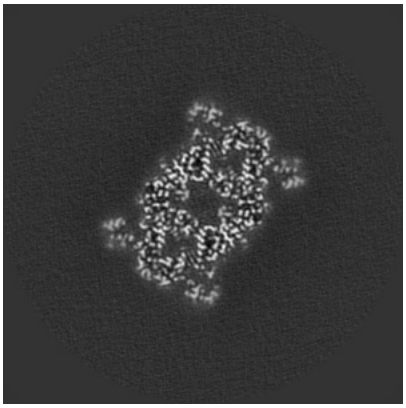
6.3.2 Raw map



X Index: 147



Y Index: 131

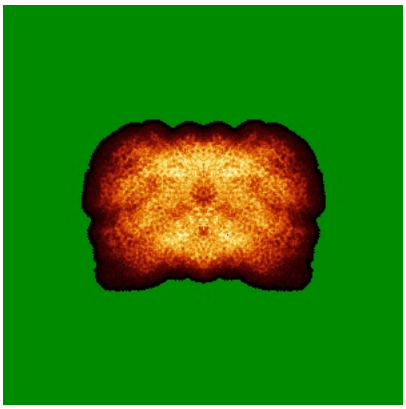


Z Index: 172

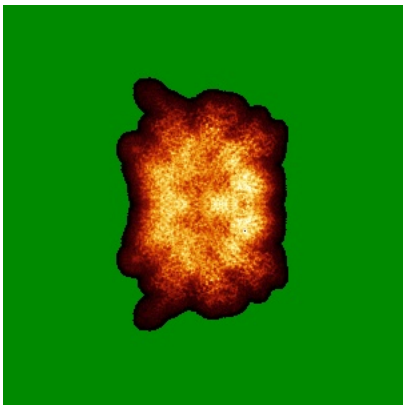
The images above show the largest variance slices of the map in three orthogonal directions.

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

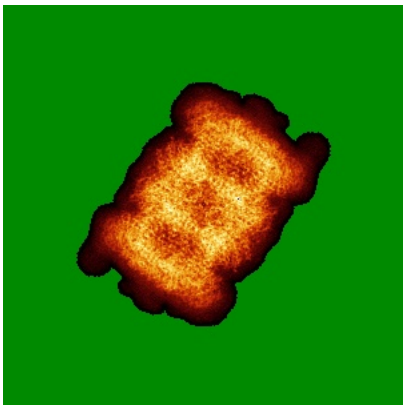
6.4.1 Primary map



X

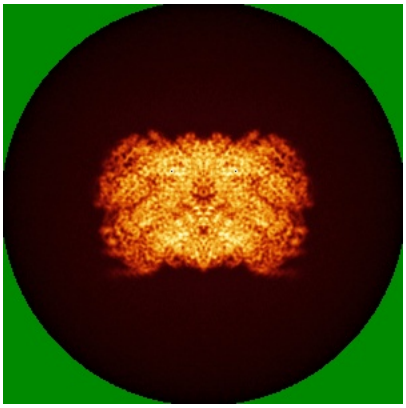


Y

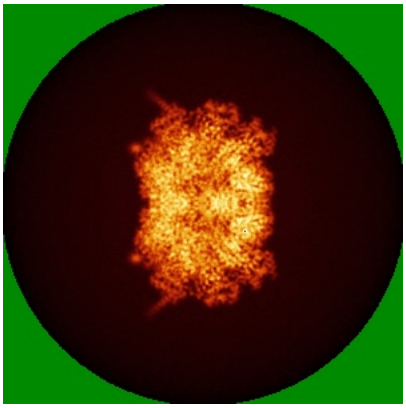


Z

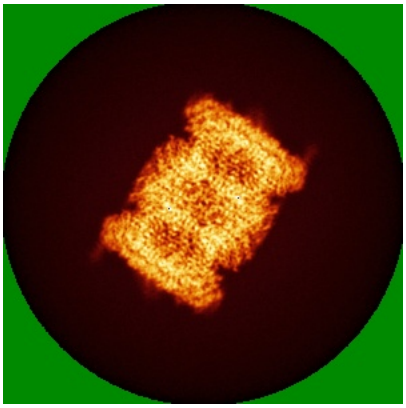
6.4.2 Raw map



X



Y

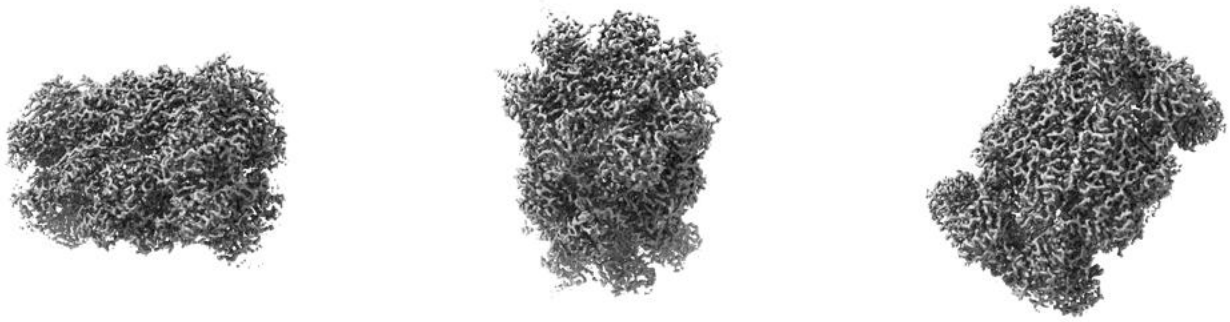


Z

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)

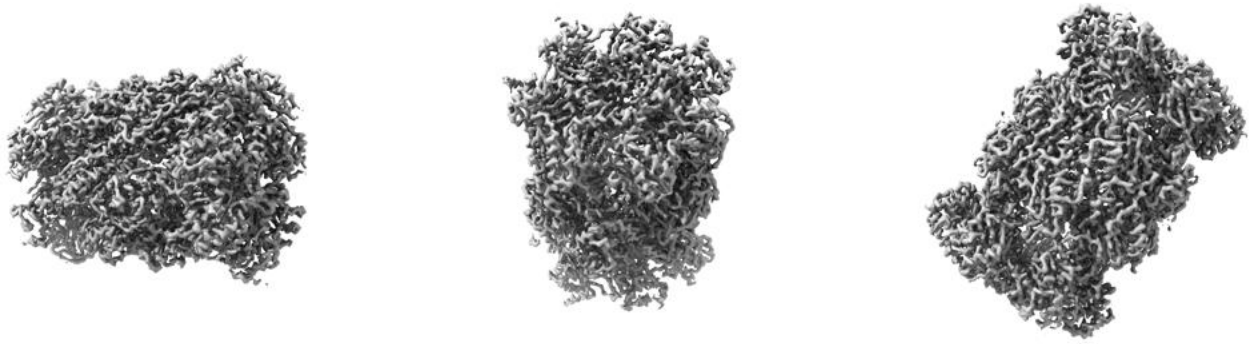
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

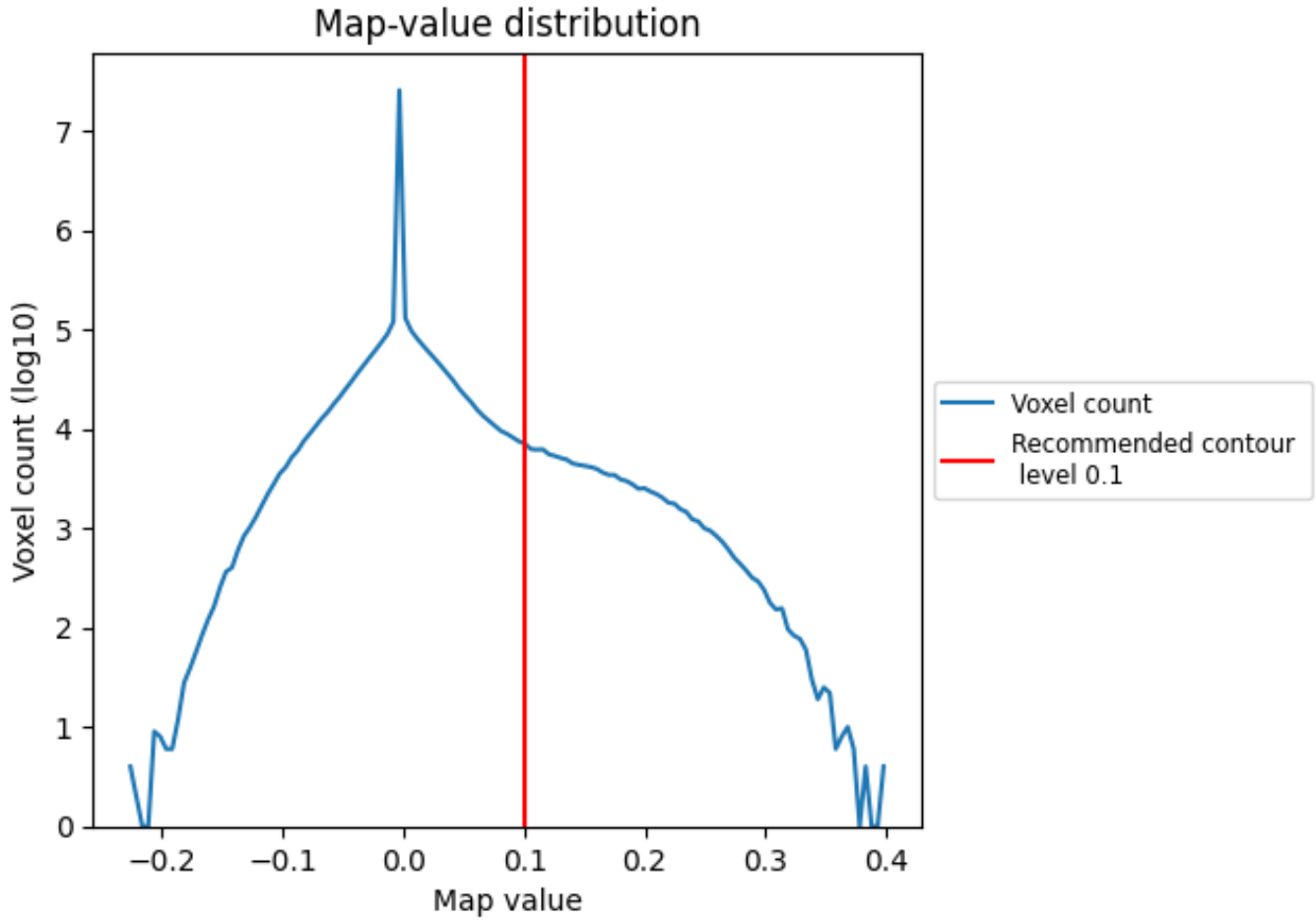
6.6 Mask visualisation (i)

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

7 Map analysis

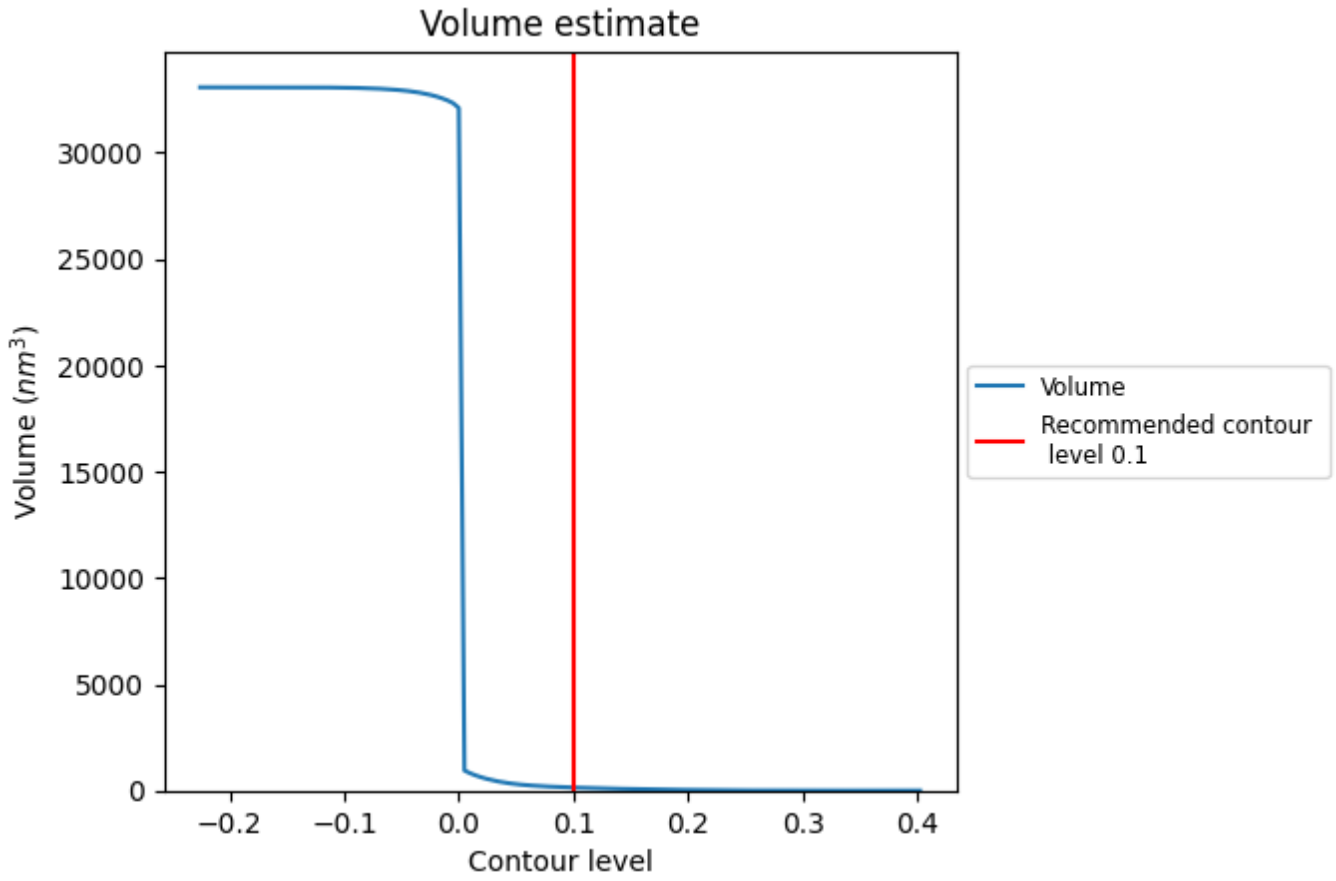
This section contains the results of statistical analysis of the map.

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.

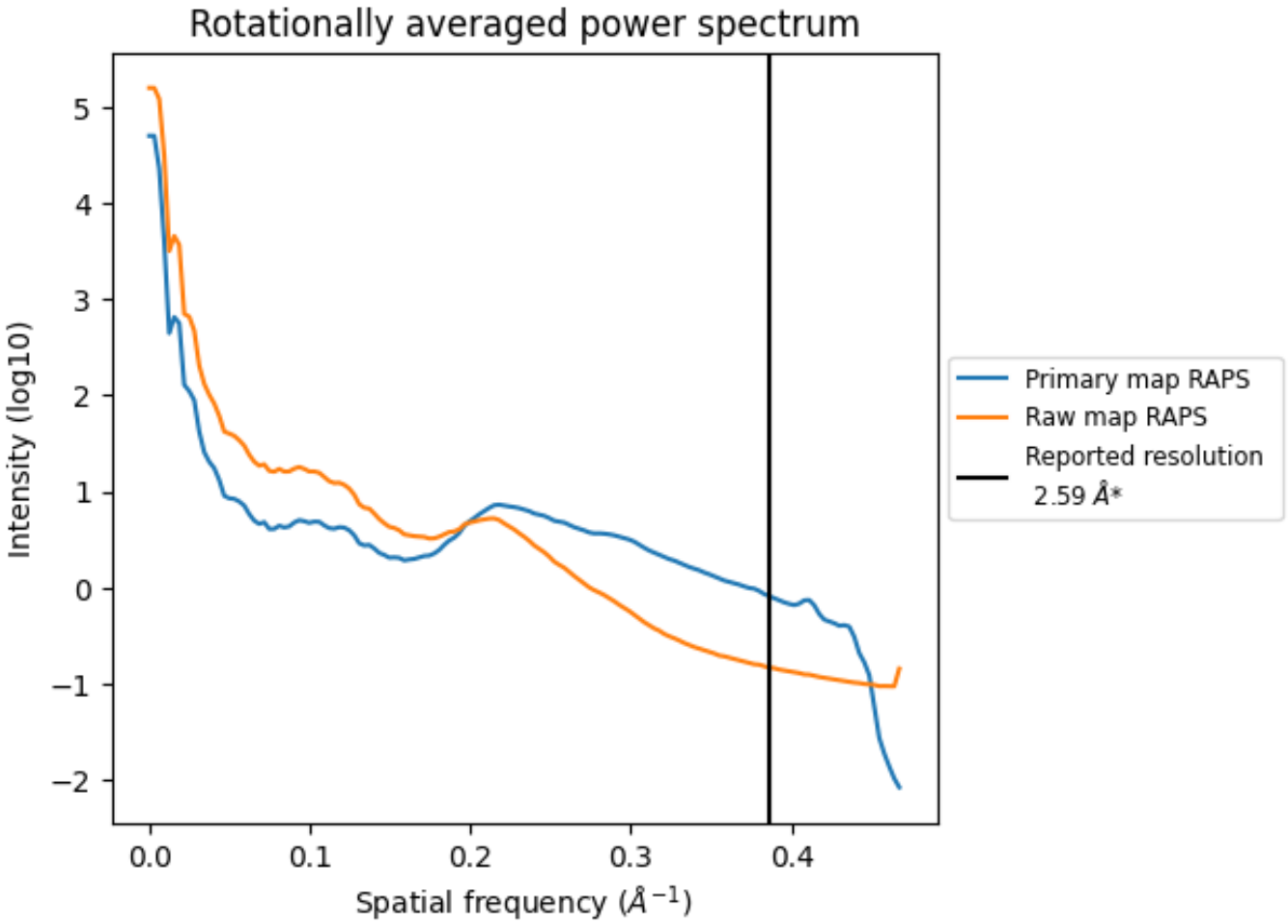
7.2 Volume estimate (i)



The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 128 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)

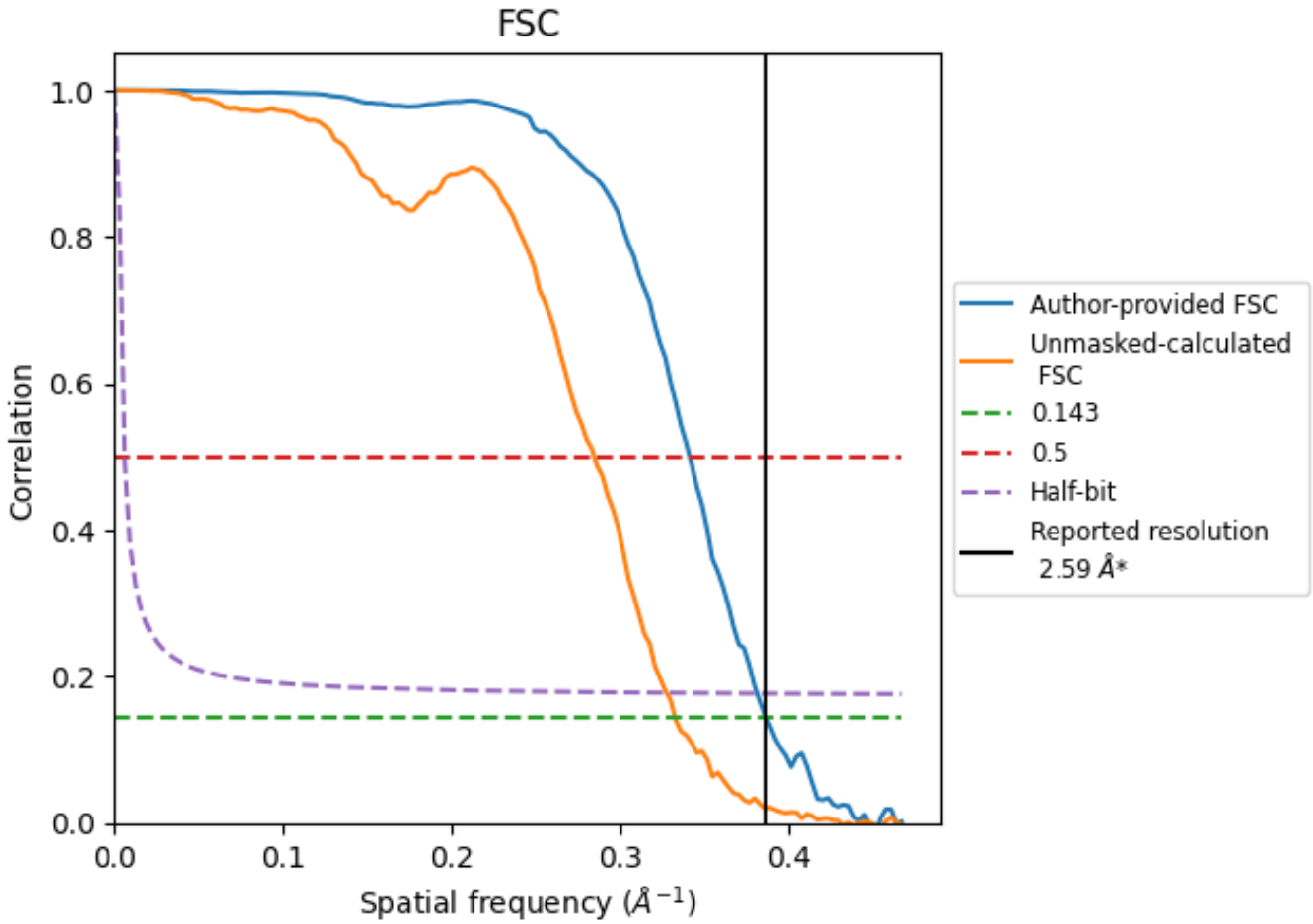


*Reported resolution corresponds to spatial frequency of 0.386 $Å^{-1}$

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 0.386 Å^{-1}

8.2 Resolution estimates (i)

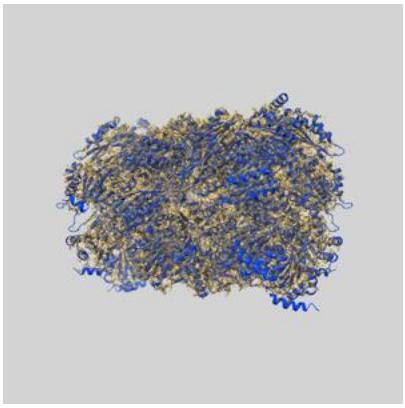
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.58	2.93	2.62
Unmasked-calculated*	3.00	3.51	3.05

*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 3.00 differs from the reported value 2.59 by more than 10 %

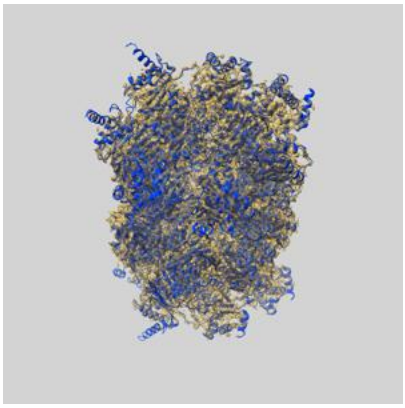
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16963 and PDB model 8OLU. Per-residue inclusion information can be found in section 3 on page 8.

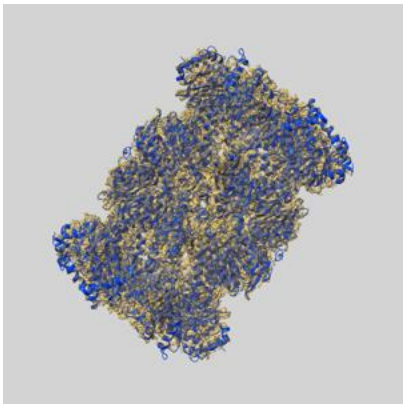
9.1 Map-model overlay



X



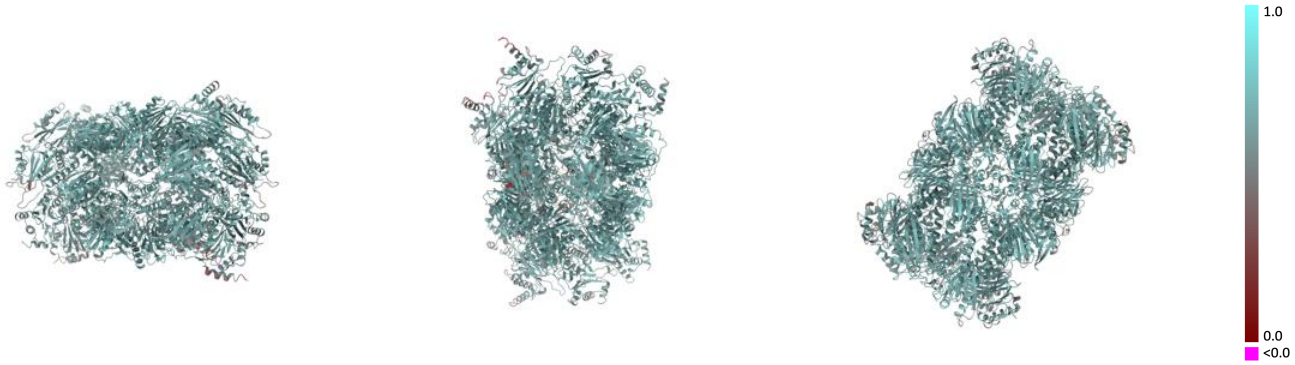
Y



Z

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

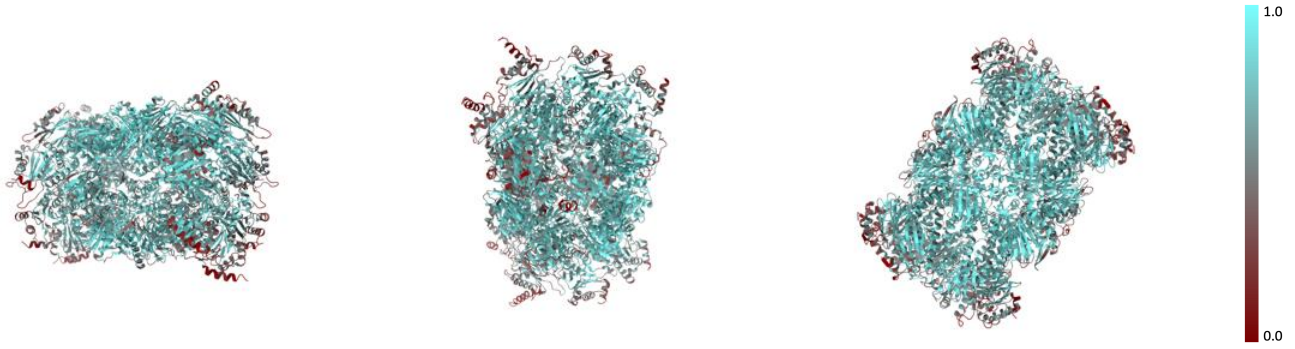
9.2 Q-score mapped to coordinate model (i)



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.

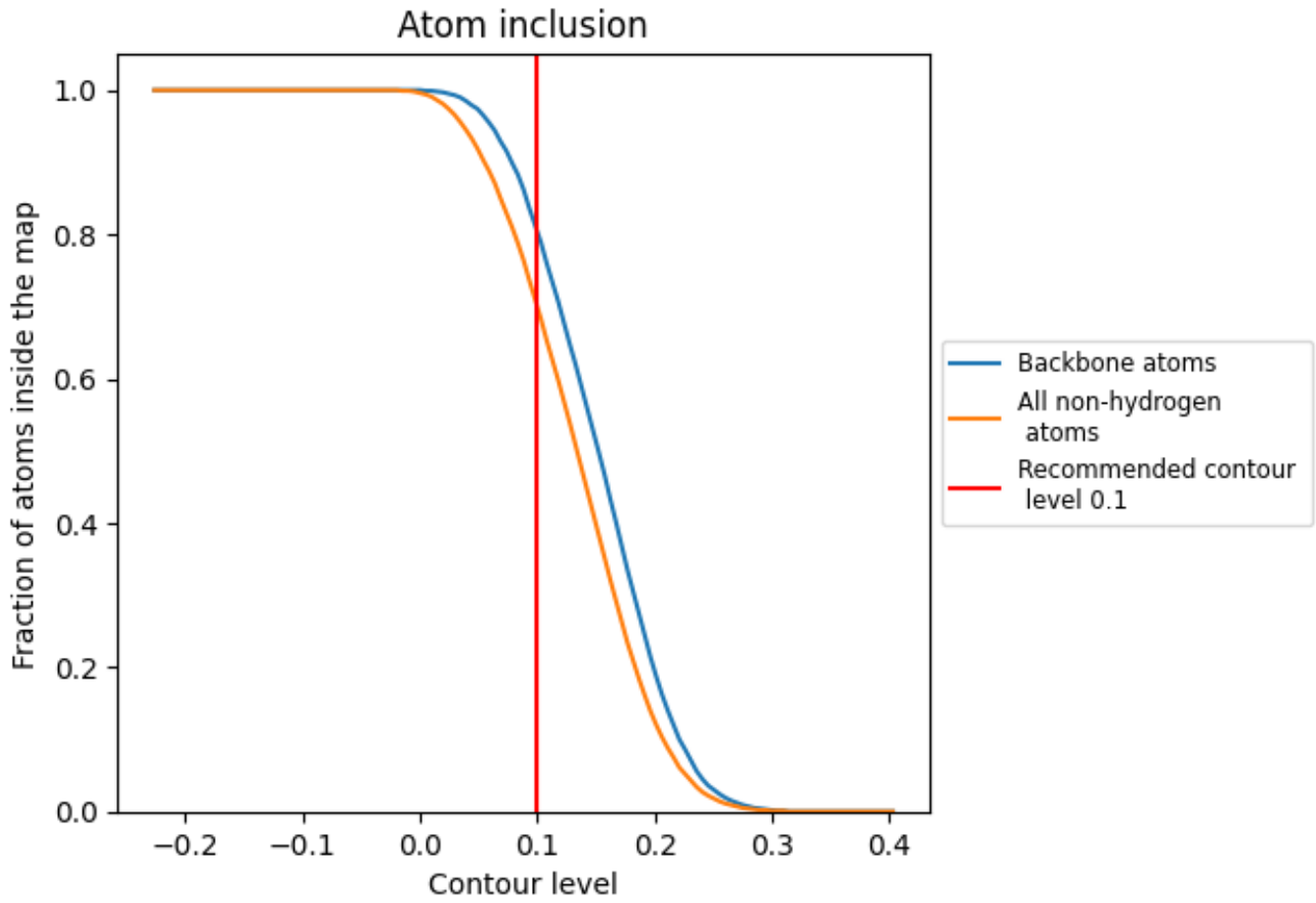
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7000	0.6490
A	0.6890	0.6470
B	0.6800	0.6450
C	0.5930	0.6230
D	0.5650	0.6060
E	0.5520	0.6110
F	0.6150	0.6320
G	0.6970	0.6520
H	0.8490	0.6940
I	0.7430	0.6540
J	0.7940	0.6720
K	0.7600	0.6640
L	0.7880	0.6710
M	0.7210	0.6560
N	0.8210	0.6760
O	0.6880	0.6480
P	0.6780	0.6440
Q	0.5920	0.6220
R	0.5660	0.6080
S	0.5510	0.6130
T	0.6150	0.6320
U	0.6980	0.6530
V	0.8510	0.6930
W	0.7440	0.6580
X	0.7950	0.6700
Y	0.7590	0.6630
Z	0.7880	0.6700
a	0.7210	0.6560
b	0.8190	0.6760