



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:18 AM UTC

PDB ID : 8T08 / pdb_00008t08
EMDB ID : EMD-40938
Title : Preholo-Proteasome from Pre1-1 Pre4-1 Double Mutant
Authors : Walsh Jr., R.M.; Rawson, S.; Schnell, H.; Velez, B.; Hanna, J.
Deposited on : 2023-05-31
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

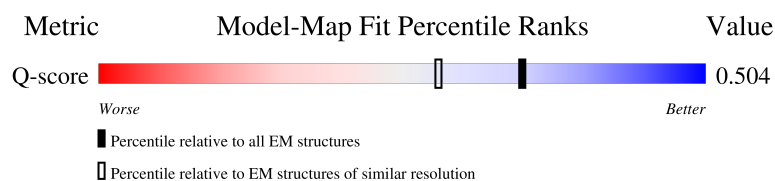
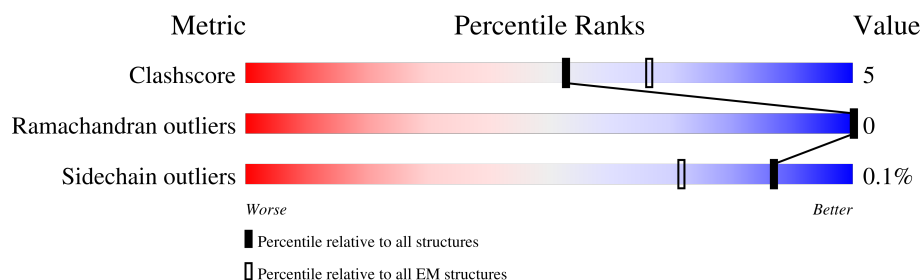
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	A	252	 80% 12% 8%
1	R	252	 80% 12% 8%
2	B	250	 89% 10% .
2	S	250	 89% 10% .

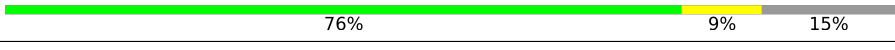
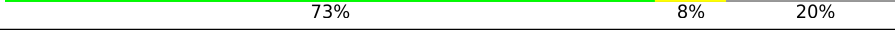
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	258	
3	T	258	
4	D	254	
4	U	254	
5	E	260	
5	V	260	
6	F	234	
6	W	234	
7	G	288	
7	X	288	
8	H	148	
8	Y	148	
9	I	261	
9	Z	261	
10	J	205	
10	a	205	
11	K	198	
11	b	198	
12	L	287	
12	c	287	
13	M	241	
13	d	241	
14	N	215	
14	e	215	
15	O	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	f	276	 76% 9% 14%
16	P	267	 76% 9% 15%
16	g	267	 78% 7% 15%
17	Q	251	 73% 7% 20%
17	h	251	 73% 8% 20%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 55104 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	231	Total	C	N	O	S	0	0
			1823	1162	304	349	8		
1	R	231	Total	C	N	O	S	0	0
			1823	1162	304	349	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	247	Total	C	N	O	S	0	0
			1891	1204	312	372	3		
2	S	247	Total	C	N	O	S	0	0
			1891	1204	312	372	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	233	Total	C	N	O	S	0	0
			1827	1160	303	361	3		
3	T	233	Total	C	N	O	S	0	0
			1827	1160	303	361	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	223	Total	C	N	O	S	0	0
			1752	1101	303	344	4		
4	U	223	Total	C	N	O	S	0	0
			1752	1101	303	344	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	242	Total	C	N	O	S	0	0
			1881	1180	317	376	8		
5	V	242	Total	C	N	O	S	0	0
			1881	1180	317	376	8		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	234	Total	C	N	O	S	0	0
			1803	1134	313	351	5		
6	W	234	Total	C	N	O	S	0	0
			1803	1134	313	351	5		

- Molecule 7 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	234	Total	C	N	O	S	0	0
			1809	1155	314	336	4		
7	X	234	Total	C	N	O	S	0	0
			1809	1155	314	336	4		

- Molecule 8 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	122	Total	C	N	O	S	0	0
			977	603	174	194	6		
8	Y	122	Total	C	N	O	S	0	0
			977	603	174	194	6		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	229	Total	C	N	O	S	0	0
			1738	1098	301	333	6		
9	Z	229	Total	C	N	O	S	0	0
			1738	1098	301	333	6		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1359	879	215	258	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	175	Total	C	N	O	S	0	0
			1359	879	215	258	7		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	181	Total	C	N	O	S	0	0
			1458	931	245	278	4		
11	b	181	Total	C	N	O	S	0	0
			1458	931	245	278	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	conflict	UNP P22141
b	142	PHE	SER	conflict	UNP P22141

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	101	Total	C	N	O	S	0	0
			821	528	139	148	6		
12	c	101	Total	C	N	O	S	0	0
			821	528	139	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	202	Total	C	N	O	S	0	0
			1590	1006	274	306	4		
13	d	202	Total	C	N	O	S	0	0
			1590	1006	274	306	4		

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1550	978	256	309	7		
14	e	202	Total	C	N	O	S	0	0
			1550	978	256	309	7		

- Molecule 15 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	237	Total	C	N	O	S	0	0
			1845	1199	286	347	13		
15	f	237	Total	C	N	O	S	0	0
			1845	1199	286	347	13		

- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	227	Total	C	N	O	S	0	0
			1852	1214	294	337	7		
16	g	227	Total	C	N	O	S	0	0
			1852	1214	294	337	7		

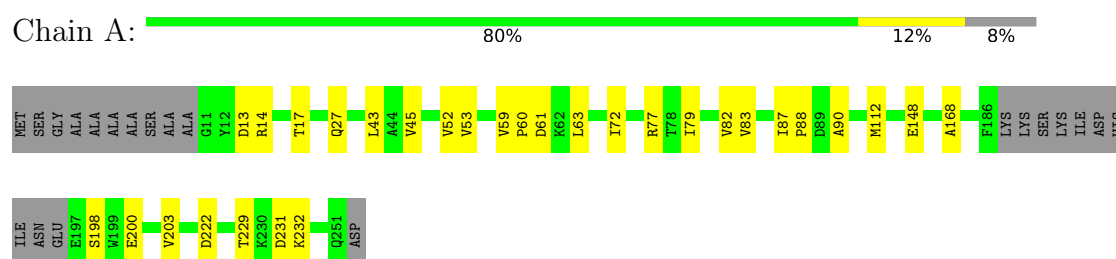
- Molecule 17 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	202	Total	C	N	O	S	0	0
			1576	1000	271	299	6		
17	h	202	Total	C	N	O	S	0	0
			1576	1000	271	299	6		

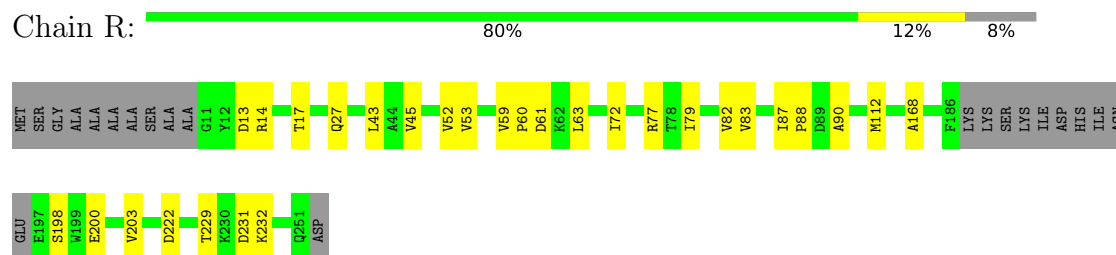
3 Residue-property plots [i](#)

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

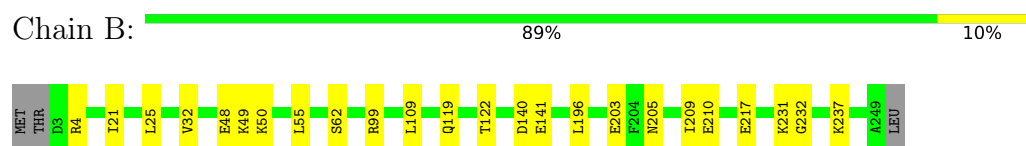
- Molecule 1: Proteasome subunit alpha type-1



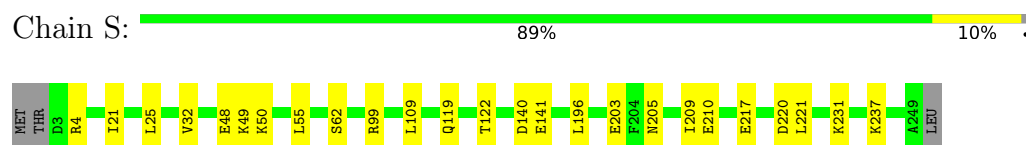
- Molecule 1: Proteasome subunit alpha type-1



- Molecule 2: Proteasome subunit alpha type-2

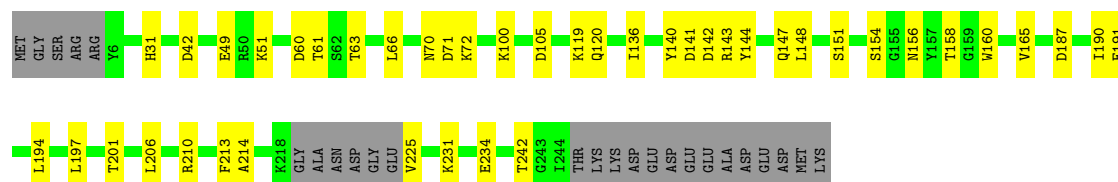


- Molecule 2: Proteasome subunit alpha type-2

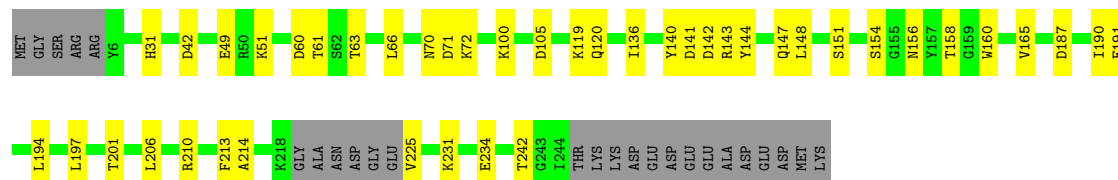


- Molecule 3: Proteasome subunit alpha type-3

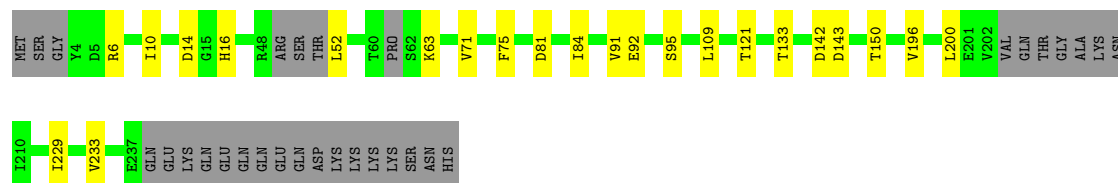
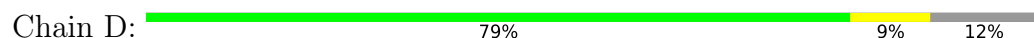




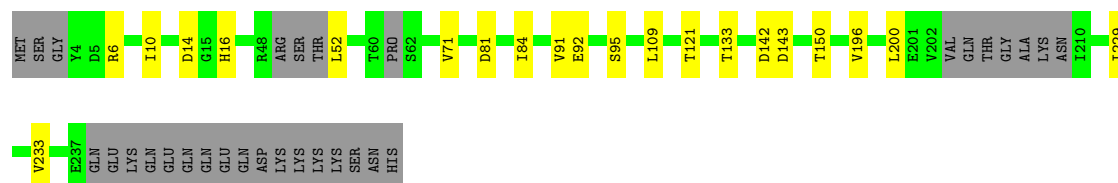
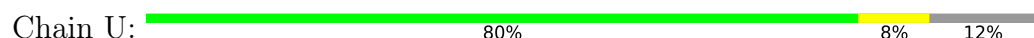
• Molecule 3: Proteasome subunit alpha type-3



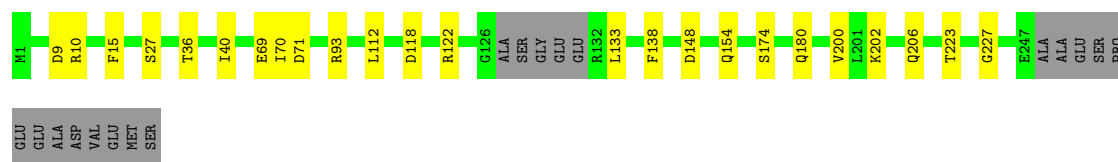
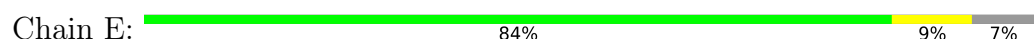
• Molecule 4: Proteasome subunit alpha type-4



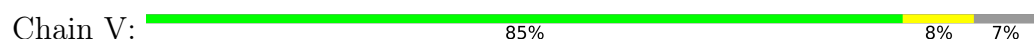
• Molecule 4: Proteasome subunit alpha type-4



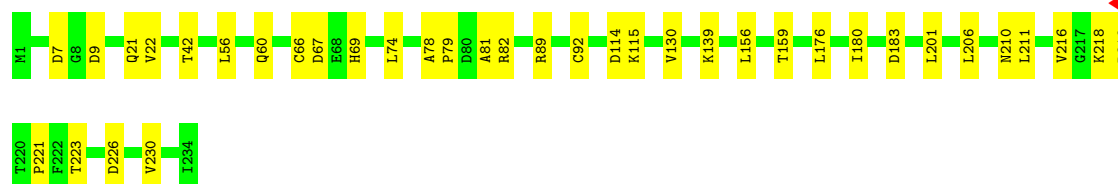
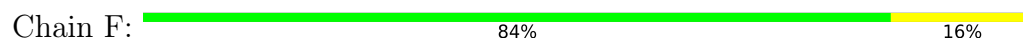
• Molecule 5: Proteasome subunit alpha type-5



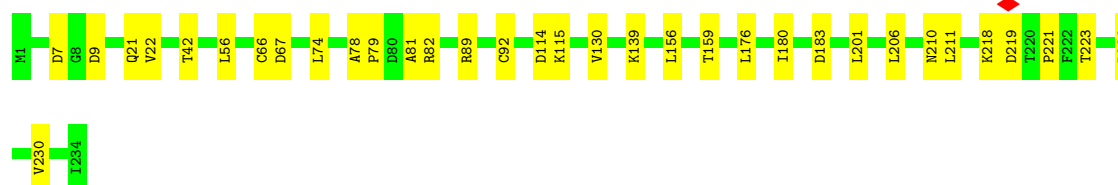
• Molecule 5: Proteasome subunit alpha type-5



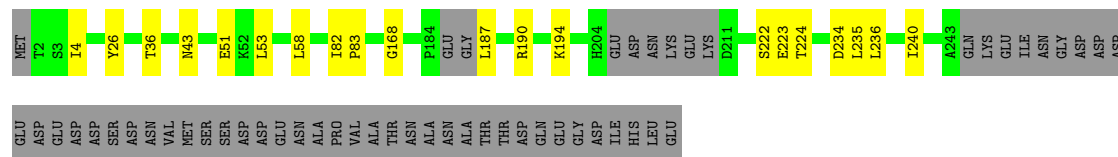
- Molecule 6: Proteasome subunit alpha type-6



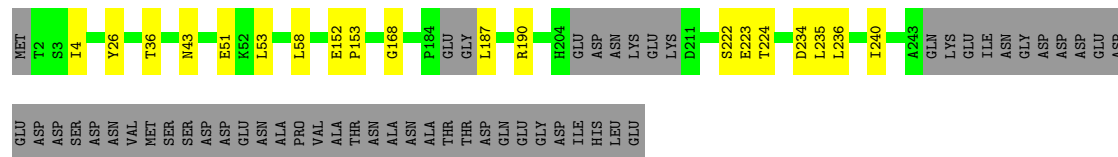
- Molecule 6: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-7

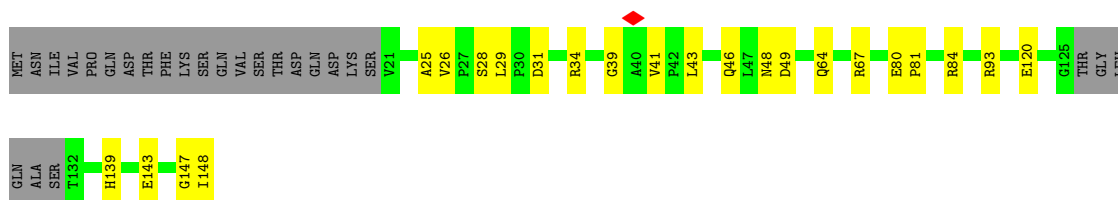


- Molecule 7: Proteasome subunit alpha type-7

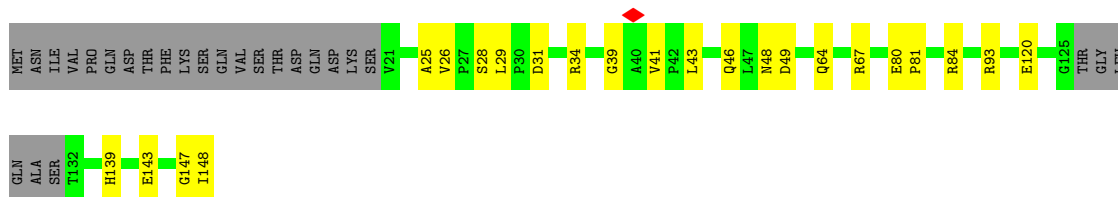


- Molecule 8: Proteasome maturation factor UMP1

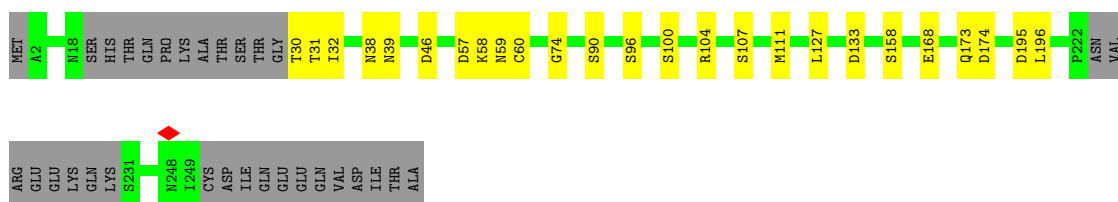
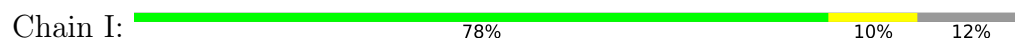




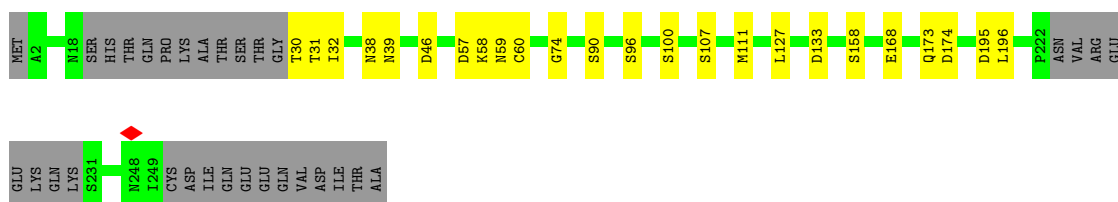
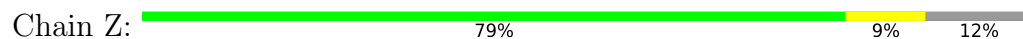
- Molecule 8: Proteasome maturation factor UMP1



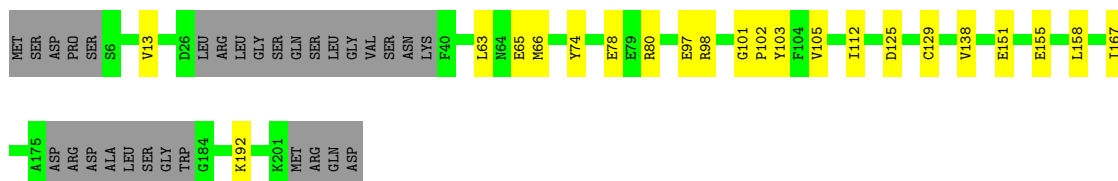
- Molecule 9: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-2

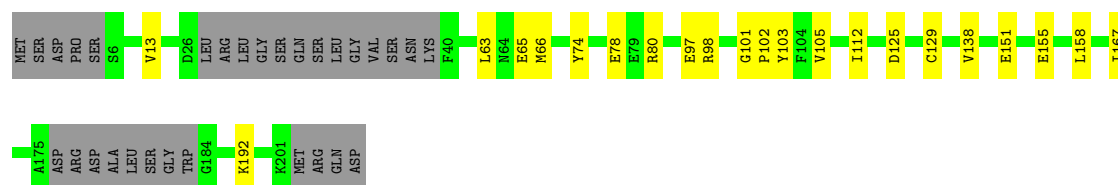


- Molecule 10: Proteasome subunit beta type-3



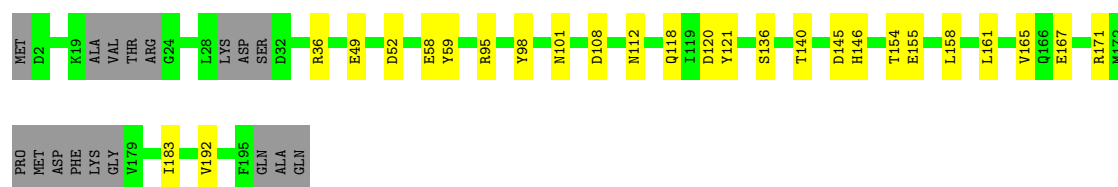
- Molecule 10: Proteasome subunit beta type-3

Chain a: 



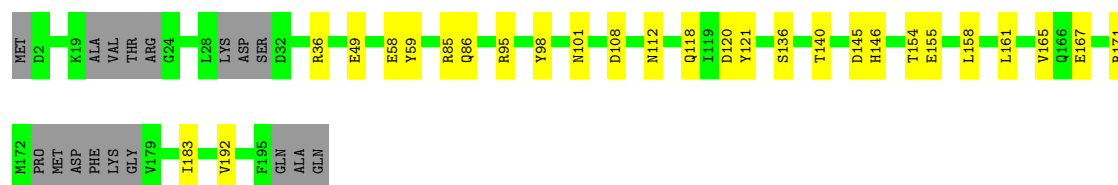
- Molecule 11: Proteasome subunit beta type-4

Chain K: 



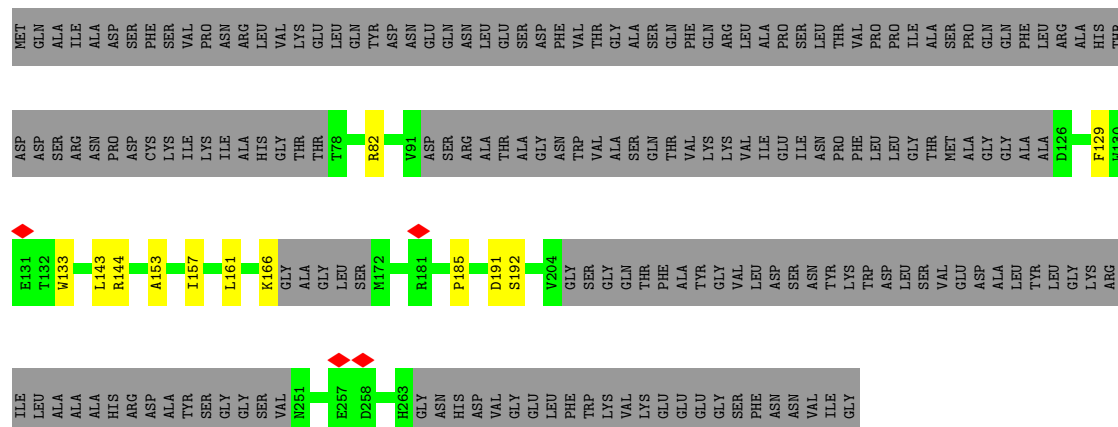
- Molecule 11: Proteasome subunit beta type-4

Chain b: 



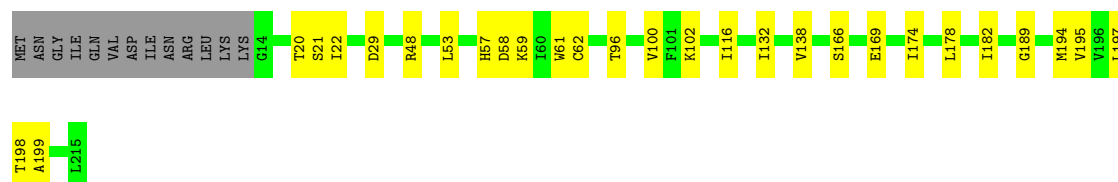
- Molecule 12: Proteasome subunit beta type-5

Chain L: 

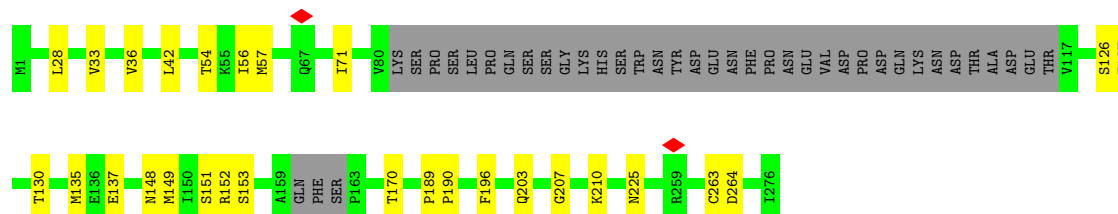
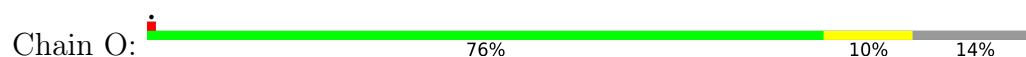


- Molecule 12: Proteasome subunit beta type-5

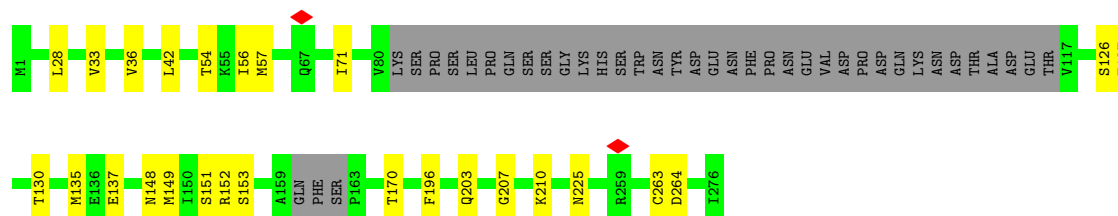
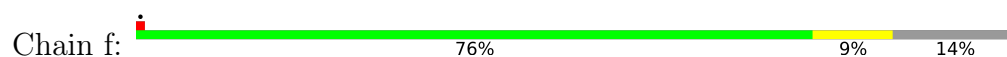
Chain c: 



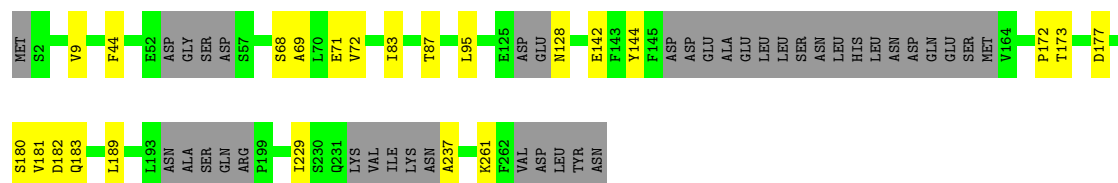
- Molecule 15: Proteasome chaperone 1



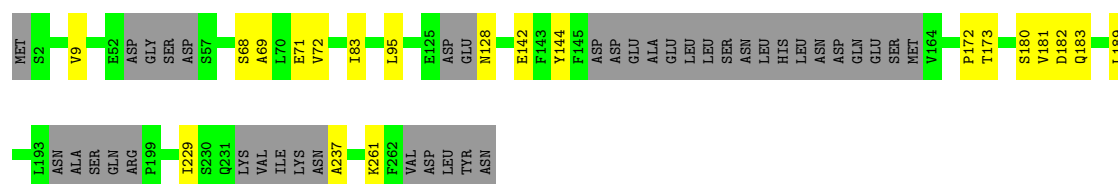
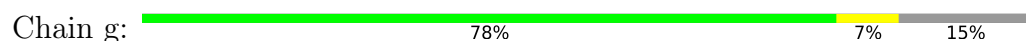
- Molecule 15: Proteasome chaperone 1



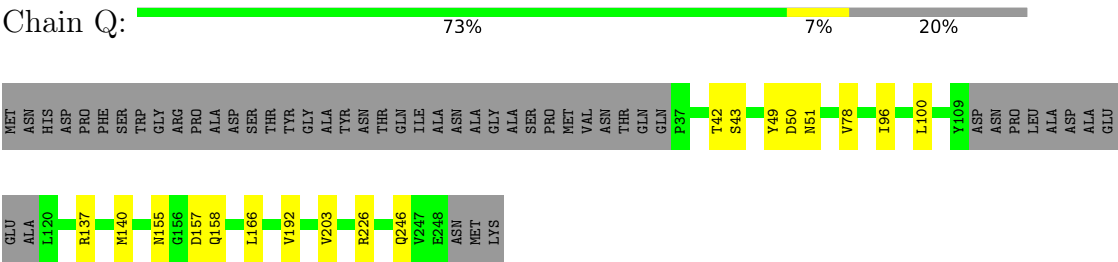
- Molecule 16: Proteasome assembly chaperone 2



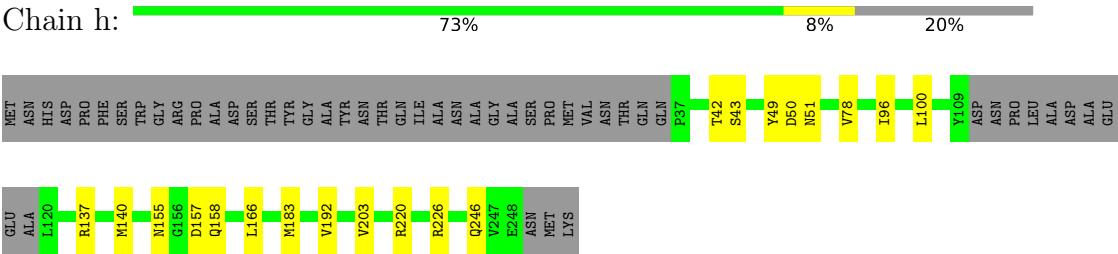
- Molecule 16: Proteasome assembly chaperone 2



- Molecule 17: Proteasome subunit beta type-7



● Molecule 17: Proteasome subunit beta type-7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	68930	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 ($e^-/\text{\AA}^2$)	54.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.594	Depositor
Minimum map value	-1.707	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.305	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/1859	0.23	0/2519
1	R	0.12	0/1859	0.23	0/2519
2	B	0.12	0/1928	0.23	0/2611
2	S	0.12	0/1928	0.23	0/2611
3	C	0.13	0/1856	0.25	0/2513
3	T	0.13	0/1856	0.25	0/2513
4	D	0.11	0/1777	0.21	0/2403
4	U	0.11	0/1777	0.21	0/2403
5	E	0.10	0/1907	0.23	0/2567
5	V	0.10	0/1907	0.23	0/2567
6	F	0.11	0/1831	0.26	0/2473
6	W	0.11	0/1831	0.26	0/2473
7	G	0.11	0/1847	0.23	0/2495
7	X	0.11	0/1847	0.23	0/2495
8	H	0.13	0/993	0.26	0/1341
8	Y	0.12	0/993	0.26	0/1341
9	I	0.14	0/1770	0.30	0/2400
9	Z	0.14	0/1770	0.30	0/2400
10	J	0.11	0/1384	0.23	0/1867
10	a	0.11	0/1384	0.23	0/1867
11	K	0.10	0/1482	0.25	0/1995
11	b	0.10	0/1482	0.24	0/1995
12	L	0.09	0/838	0.21	0/1128
12	c	0.09	0/838	0.21	0/1128
13	M	0.12	0/1622	0.31	0/2187
13	d	0.12	0/1622	0.31	0/2187
14	N	0.11	0/1579	0.22	0/2138
14	e	0.11	0/1579	0.22	0/2138
15	O	0.12	0/1887	0.31	0/2557
15	f	0.12	0/1887	0.31	0/2557
16	P	0.08	0/1898	0.24	0/2574
16	g	0.08	0/1898	0.24	0/2574
17	Q	0.12	0/1601	0.32	0/2170
17	h	0.12	0/1601	0.32	0/2170

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.11	0/56118	0.26	0/75876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1823	0	1811	22	0
1	R	1823	0	1811	21	0
2	B	1891	0	1899	16	0
2	S	1891	0	1899	16	0
3	C	1827	0	1832	29	0
3	T	1827	0	1832	29	0
4	D	1752	0	1762	16	0
4	U	1752	0	1762	15	0
5	E	1881	0	1866	17	0
5	V	1881	0	1866	16	0
6	F	1803	0	1807	27	0
6	W	1803	0	1807	25	0
7	G	1809	0	1806	15	0
7	X	1809	0	1806	14	0
8	H	977	0	959	21	0
8	Y	977	0	959	21	0
9	I	1738	0	1722	23	0
9	Z	1738	0	1722	20	0
10	J	1359	0	1356	16	0
10	a	1359	0	1356	16	0
11	K	1458	0	1457	20	0
11	b	1458	0	1457	20	0
12	L	821	0	799	12	0
12	c	821	0	799	12	0
13	M	1590	0	1534	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	d	1590	0	1534	27	0
14	N	1550	0	1515	25	0
14	e	1550	0	1515	25	0
15	O	1845	0	1875	20	0
15	f	1845	0	1875	19	0
16	P	1852	0	1832	15	0
16	g	1852	0	1832	13	0
17	Q	1576	0	1596	11	0
17	h	1576	0	1596	12	0
All	All	55104	0	54856	582	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 5.

All (582) 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)
14:e:20:THR:CG2	14:e:22:ILE:HG23	1.62	1.28
14:N:20:THR:CG2	14:N:22:ILE:HG23	1.62	1.28
14:N:20:THR:HG22	14:N:22:ILE:HG23	1.26	1.12
14:e:20:THR:HG22	14:e:22:ILE:HG23	1.26	1.11
14:e:20:THR:CG2	14:e:22:ILE:CG2	2.38	1.00
14:N:20:THR:CG2	14:N:22:ILE:CG2	2.38	1.00
14:N:20:THR:HG21	14:N:22:ILE:CG2	1.98	0.94
14:e:20:THR:HG21	14:e:22:ILE:CG2	1.98	0.94
14:N:20:THR:HG21	14:N:22:ILE:HG23	1.50	0.92
14:e:20:THR:HG21	14:e:22:ILE:HG23	1.50	0.92
11:b:101:ASN:OD1	11:b:118:GLN:NE2	2.10	0.84
15:f:152:ARG:NH1	15:f:203:GLN:OE1	2.11	0.84
15:O:152:ARG:NH1	15:O:203:GLN:OE1	2.11	0.83
11:K:101:ASN:OD1	11:K:118:GLN:NE2	2.10	0.83
4:D:133:THR:HG1	4:D:150:THR:HG1	1.20	0.80
14:N:166:SER:OG	14:N:169:GLU:OE1	2.01	0.79
3:T:120:GLN:NE2	4:U:81:ASP:OD1	2.16	0.78
3:C:120:GLN:NE2	4:D:81:ASP:OD1	2.17	0.78
13:d:47:ARG:NH2	13:d:240:ARG:O	2.18	0.77
16:P:172:PRO:O	16:P:173:THR:OG1	2.03	0.77
14:e:166:SER:OG	14:e:169:GLU:OE1	2.01	0.76
7:G:4:ILE:O	7:G:26:TYR:OH	2.04	0.76
13:M:47:ARG:NH2	13:M:240:ARG:O	2.18	0.76
7:X:4:ILE:O	7:X:26:TYR:OH	2.04	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:172:PRO:O	16:g:173:THR:OG1	2.03	0.76
6:F:206:LEU:HD12	6:F:211:LEU:HD22	1.65	0.76
3:T:141:ASP:OD1	3:T:147:GLN:NE2	2.19	0.75
6:W:206:LEU:HD12	6:W:211:LEU:HD22	1.65	0.75
13:M:212:GLU:OE2	9:Z:58:LYS:NZ	2.18	0.74
3:C:141:ASP:OD1	3:C:147:GLN:NE2	2.19	0.74
8:Y:64:GLN:OE1	8:Y:67:ARG:NH1	2.22	0.73
13:d:47:ARG:HD3	13:d:49:ILE:HD11	1.71	0.72
8:H:64:GLN:OE1	8:H:67:ARG:NH1	2.22	0.71
13:M:47:ARG:HD3	13:M:49:ILE:HD11	1.71	0.71
2:S:119:GLN:O	2:S:122:THR:OG1	2.11	0.69
5:E:36:THR:OG1	5:E:174:SER:O	2.11	0.69
9:Z:158:SER:OG	9:Z:195:ASP:OD2	2.07	0.69
2:S:62:SER:OG	2:S:237:LYS:NZ	2.26	0.69
6:W:221:PRO:O	6:W:223:THR:HG23	1.93	0.69
13:d:117:TYR:CZ	13:d:120:ARG:HD3	2.28	0.68
17:Q:50:ASP:OD1	17:Q:51:ASN:N	2.26	0.68
5:V:36:THR:OG1	5:V:174:SER:O	2.11	0.68
8:H:25:ALA:O	12:L:144:ARG:NH2	2.27	0.68
2:B:62:SER:OG	2:B:237:LYS:NZ	2.26	0.68
13:M:117:TYR:CZ	13:M:120:ARG:HD3	2.28	0.68
8:Y:25:ALA:O	12:c:144:ARG:NH2	2.27	0.68
6:F:221:PRO:O	6:F:223:THR:HG23	1.93	0.67
17:h:50:ASP:OD1	17:h:51:ASN:N	2.26	0.67
2:B:119:GLN:O	2:B:122:THR:OG1	2.11	0.67
11:K:136:SER:O	11:K:140:THR:OG1	2.08	0.67
17:h:226:ARG:NH1	17:h:246:GLN:OE1	2.29	0.66
7:X:43:ASN:OD1	7:X:187:LEU:N	2.29	0.66
9:I:58:LYS:NZ	13:d:212:GLU:OE2	2.25	0.66
1:A:77:ARG:NH1	1:A:231:ASP:O	2.29	0.66
1:R:77:ARG:NH1	1:R:231:ASP:O	2.29	0.66
7:G:43:ASN:OD1	7:G:187:LEU:N	2.29	0.65
1:A:231:ASP:OD1	1:A:232:LYS:N	2.29	0.65
1:R:231:ASP:OD1	1:R:232:LYS:N	2.29	0.65
9:Z:38:ASN:OD1	9:Z:39:ASN:N	2.30	0.65
11:K:167:GLU:O	11:K:171:ARG:NE	2.28	0.65
17:Q:226:ARG:NH1	17:Q:246:GLN:OE1	2.29	0.65
3:T:49:GLU:OE1	3:T:201:THR:HG22	1.96	0.65
15:f:148:ASN:O	15:f:151:SER:OG	2.13	0.65
3:T:201:THR:HG21	3:T:206:LEU:HD13	1.79	0.65
3:C:201:THR:HG21	3:C:206:LEU:HD13	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:38:ASN:OD1	9:I:39:ASN:N	2.30	0.64
1:R:61:ASP:OD1	1:R:63:LEU:N	2.30	0.64
3:C:49:GLU:OE1	3:C:201:THR:HG22	1.96	0.64
5:E:202:LYS:O	5:E:206:GLN:NE2	2.30	0.64
5:V:202:LYS:O	5:V:206:GLN:NE2	2.30	0.64
13:M:81:ASP:OD1	13:M:82:ALA:N	2.31	0.64
13:d:81:ASP:OD1	13:d:82:ALA:N	2.31	0.64
7:X:236:LEU:O	7:X:240:ILE:HD12	1.98	0.64
10:a:98:ARG:NH1	10:a:103:TYR:OH	2.31	0.64
16:P:68:SER:N	16:P:71:GLU:OE2	2.32	0.63
16:g:68:SER:N	16:g:71:GLU:OE2	2.32	0.63
1:A:61:ASP:OD1	1:A:63:LEU:N	2.30	0.63
10:J:98:ARG:NH1	10:J:103:TYR:OH	2.31	0.63
7:G:236:LEU:O	7:G:240:ILE:HD12	1.99	0.63
12:L:129:PHE:HD2	13:M:117:TYR:CE2	2.17	0.63
9:I:158:SER:OG	9:I:195:ASP:OD2	2.07	0.62
4:U:95:SER:OG	8:Y:31:ASP:OD1	2.15	0.62
17:Q:49:TYR:CE2	17:Q:203:VAL:HG22	2.34	0.62
10:J:63:LEU:CD1	10:J:105:VAL:HG21	2.29	0.62
12:L:129:PHE:O	12:L:133:TRP:N	2.26	0.62
14:e:20:THR:HG21	14:e:22:ILE:HG21	1.81	0.62
11:b:120:ASP:OD1	11:b:121:TYR:N	2.32	0.62
17:h:49:TYR:CE2	17:h:203:VAL:HG22	2.34	0.62
7:G:224:THR:HG22	7:G:224:THR:O	2.00	0.61
10:J:125:ASP:OD1	10:J:129:CYS:N	2.30	0.61
12:c:129:PHE:HD2	13:d:117:TYR:CE2	2.17	0.61
10:a:125:ASP:OD1	10:a:129:CYS:N	2.30	0.61
15:f:71:ILE:HD11	15:f:126:SER:OG	2.01	0.61
10:J:151:GLU:OE1	13:d:213:ARG:NE	2.19	0.61
2:S:48:GLU:OE2	2:S:50:LYS:NZ	2.27	0.61
10:a:63:LEU:CD1	10:a:105:VAL:HG21	2.30	0.61
17:h:155:ASN:ND2	17:h:157:ASP:OD2	2.34	0.61
3:C:197:LEU:O	3:C:201:THR:HG23	2.01	0.60
11:K:120:ASP:OD1	11:K:121:TYR:N	2.32	0.60
15:O:71:ILE:HD11	15:O:126:SER:OG	2.01	0.60
17:Q:155:ASN:ND2	17:Q:157:ASP:OD2	2.34	0.60
1:R:222:ASP:OD1	1:R:222:ASP:O	2.19	0.60
1:A:222:ASP:OD1	1:A:222:ASP:O	2.19	0.60
15:O:148:ASN:O	15:O:151:SER:OG	2.13	0.60
7:X:224:THR:HG22	7:X:224:THR:O	2.00	0.60
12:c:129:PHE:CE1	12:c:133:TRP:HB2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:145:ASP:OD1	13:M:147:VAL:HG22	2.02	0.60
7:X:222:SER:OG	7:X:223:GLU:OE1	2.19	0.60
11:K:161:LEU:HD12	11:K:165:VAL:HG23	1.84	0.59
11:b:167:GLU:O	11:b:171:ARG:NE	2.29	0.59
12:L:129:PHE:CE1	12:L:133:TRP:HB2	2.37	0.59
4:D:95:SER:OG	8:H:31:ASP:OD1	2.15	0.59
6:W:201:LEU:HD11	6:W:206:LEU:CD2	2.32	0.59
17:h:49:TYR:O	17:h:158:GLN:NE2	2.30	0.59
6:F:211:LEU:HD23	6:F:230:VAL:CG1	2.32	0.59
4:U:133:THR:OG1	4:U:150:THR:OG1	2.06	0.59
8:H:80:GLU:OE2	8:H:84:ARG:NE	2.36	0.59
6:W:211:LEU:HD23	6:W:230:VAL:CG1	2.32	0.59
11:b:161:LEU:HD12	11:b:165:VAL:HG23	1.84	0.59
6:F:201:LEU:HD11	6:F:206:LEU:CD2	2.32	0.59
11:b:155:GLU:OE1	11:b:155:GLU:N	2.36	0.59
13:M:139:GLY:O	13:M:152:ARG:NH2	2.36	0.59
13:d:145:ASP:OD1	13:d:147:VAL:HG22	2.02	0.59
3:T:197:LEU:O	3:T:201:THR:HG23	2.01	0.58
12:c:129:PHE:O	12:c:133:TRP:N	2.26	0.58
12:L:129:PHE:CD2	13:M:117:TYR:CE2	2.92	0.58
13:d:139:GLY:O	13:d:152:ARG:NH2	2.35	0.58
17:Q:49:TYR:O	17:Q:158:GLN:NE2	2.30	0.58
3:C:70:ASN:OD1	3:C:71:ASP:N	2.37	0.58
5:V:148:ASP:OD1	5:V:154:GLN:NE2	2.36	0.58
11:K:155:GLU:N	11:K:155:GLU:OE1	2.36	0.58
5:E:148:ASP:OD1	5:E:154:GLN:NE2	2.36	0.57
8:Y:80:GLU:OE2	8:Y:84:ARG:NE	2.36	0.57
13:d:165:ILE:HG23	13:d:206:SER:OG	2.04	0.57
13:M:165:ILE:HG23	13:M:206:SER:OG	2.04	0.57
16:P:142:GLU:OE1	16:P:144:TYR:OH	2.19	0.57
3:T:70:ASN:OD1	3:T:71:ASP:N	2.37	0.57
3:T:154:SER:OG	3:T:156:ASN:OD1	2.22	0.57
11:b:136:SER:O	11:b:140:THR:OG1	2.08	0.57
5:V:15:PHE:N	6:W:21:GLN:OE1	2.35	0.57
7:G:222:SER:OG	7:G:223:GLU:OE1	2.19	0.57
3:T:142:ASP:OD1	3:T:143:ARG:N	2.38	0.57
12:c:129:PHE:CD2	13:d:117:TYR:CE2	2.92	0.57
6:F:42:THR:OG1	6:F:183:ASP:OD1	2.11	0.57
3:T:158:THR:OG1	3:T:160:TRP:NE1	2.38	0.57
17:h:192:VAL:HG23	17:h:192:VAL:O	2.05	0.56
3:C:142:ASP:OD1	3:C:143:ARG:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:63:LEU:HD11	10:a:105:VAL:HG21	1.87	0.56
14:N:20:THR:HG21	14:N:22:ILE:HG21	1.81	0.56
1:A:53:VAL:HG21	1:A:82:VAL:HG21	1.88	0.56
12:c:191:ASP:OD1	12:c:192:SER:N	2.39	0.56
5:E:15:PHE:N	6:F:21:GLN:OE1	2.33	0.56
12:L:191:ASP:OD1	12:L:192:SER:N	2.39	0.56
3:C:158:THR:OG1	3:C:160:TRP:NE1	2.38	0.56
10:J:63:LEU:HD11	10:J:105:VAL:HG21	1.87	0.56
5:E:122:ARG:HG3	5:E:133:LEU:H	1.72	0.55
17:Q:192:VAL:O	17:Q:192:VAL:HG23	2.05	0.55
14:N:58:ASP:OD1	14:N:59:LYS:N	2.40	0.55
17:Q:137:ARG:HD3	17:Q:166:LEU:HA	1.88	0.55
1:R:53:VAL:HG21	1:R:82:VAL:HG21	1.87	0.55
6:W:42:THR:OG1	6:W:183:ASP:OD1	2.11	0.55
3:C:154:SER:OG	3:C:156:ASN:OD1	2.22	0.55
1:R:87:ILE:N	1:R:88:PRO:HD2	2.22	0.55
16:g:9:VAL:O	16:g:9:VAL:HG13	2.07	0.55
8:H:48:ASN:OD1	8:H:49:ASP:N	2.41	0.54
5:V:122:ARG:HG3	5:V:133:LEU:H	1.71	0.54
14:e:58:ASP:OD1	14:e:59:LYS:N	2.40	0.54
10:a:13:VAL:HG23	10:a:138:VAL:HG12	1.89	0.54
17:h:137:ARG:HD3	17:h:166:LEU:HA	1.88	0.54
1:A:87:ILE:N	1:A:88:PRO:HD2	2.22	0.54
4:D:84:ILE:HD13	8:H:139:HIS:NE2	2.22	0.54
10:J:13:VAL:HG23	10:J:138:VAL:HG12	1.89	0.54
14:N:20:THR:HG22	14:N:21:SER:N	2.22	0.54
8:Y:48:ASN:OD1	8:Y:49:ASP:N	2.40	0.54
2:B:48:GLU:OE2	2:B:50:LYS:NZ	2.27	0.54
3:C:136:ILE:HD11	3:C:165:VAL:HG12	1.90	0.54
6:F:210:ASN:OD1	6:F:211:LEU:N	2.41	0.54
14:e:96:THR:O	14:e:100:VAL:HG23	2.08	0.54
1:R:83:VAL:HG11	1:R:90:ALA:CB	2.39	0.53
15:f:152:ARG:CZ	15:f:203:GLN:OE1	2.56	0.53
4:U:84:ILE:HD13	8:Y:139:HIS:NE2	2.23	0.53
13:d:32:LEU:HD23	13:d:203:VAL:HG23	1.91	0.53
15:O:152:ARG:CZ	15:O:203:GLN:OE1	2.56	0.53
3:T:60:ASP:OD1	3:T:61:THR:N	2.42	0.53
9:Z:30:THR:HG23	9:Z:46:ASP:OD1	2.09	0.53
13:M:32:LEU:HD23	13:M:203:VAL:HG23	1.91	0.53
6:W:210:ASN:OD1	6:W:211:LEU:N	2.41	0.53
13:M:135:GLU:OE1	13:M:135:GLU:CA	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:96:THR:O	14:N:100:VAL:HG23	2.08	0.53
13:d:135:GLU:CA	13:d:135:GLU:OE1	2.57	0.53
14:e:61:TRP:CD1	14:e:197:LEU:HD21	2.44	0.53
5:V:93:ARG:HD3	12:c:143:LEU:HD13	1.91	0.52
1:A:83:VAL:HG11	1:A:90:ALA:CB	2.39	0.52
13:M:239:LYS:NZ	13:M:241:ASP:O	2.42	0.52
14:N:53:LEU:CD1	14:N:195:VAL:HG23	2.39	0.52
13:d:239:LYS:NZ	13:d:241:ASP:O	2.42	0.52
14:e:20:THR:HG22	14:e:21:SER:N	2.22	0.52
14:N:61:TRP:CD1	14:N:197:LEU:HD21	2.44	0.52
5:V:9:ASP:OD1	5:V:10:ARG:NH1	2.43	0.52
9:Z:30:THR:HG22	9:Z:31:THR:N	2.24	0.52
14:e:53:LEU:CD1	14:e:195:VAL:HG23	2.40	0.52
1:A:83:VAL:HG11	1:A:90:ALA:HB2	1.91	0.52
7:G:36:THR:OG1	7:G:168:GLY:O	2.22	0.52
3:T:136:ILE:HD11	3:T:165:VAL:HG12	1.90	0.52
2:S:109:LEU:HD11	10:a:78:GLU:HG2	1.92	0.52
7:X:51:GLU:O	7:X:51:GLU:HG3	2.10	0.52
9:I:30:THR:HG22	9:I:31:THR:N	2.24	0.52
9:I:30:THR:HG23	9:I:46:ASP:OD1	2.09	0.52
16:P:9:VAL:O	16:P:9:VAL:HG13	2.07	0.52
2:B:109:LEU:HD11	10:J:78:GLU:HG2	1.92	0.52
9:I:195:ASP:OD1	9:I:196:LEU:N	2.43	0.52
1:R:83:VAL:HG11	1:R:90:ALA:HB2	1.91	0.52
16:P:229:ILE:HG23	16:P:237:ALA:CB	2.40	0.52
11:b:36:ARG:NE	11:b:58:GLU:OE2	2.36	0.52
5:E:9:ASP:OD1	5:E:10:ARG:NH1	2.43	0.51
7:G:51:GLU:O	7:G:51:GLU:HG3	2.10	0.51
15:O:263:CYS:O	15:O:264:ASP:OD1	2.28	0.51
9:Z:195:ASP:OD1	9:Z:196:LEU:N	2.43	0.51
1:A:59:VAL:HB	1:A:60:PRO:HA	1.92	0.51
16:g:142:GLU:OE1	16:g:144:TYR:OH	2.19	0.51
3:C:194:LEU:HD22	3:C:213:PHE:CZ	2.45	0.51
11:b:108:ASP:O	11:b:112:ASN:N	2.44	0.51
5:E:93:ARG:HD3	12:L:143:LEU:HD13	1.93	0.51
14:e:57:HIS:ND1	14:e:58:ASP:OD1	2.44	0.51
15:f:263:CYS:O	15:f:264:ASP:OD1	2.28	0.51
4:D:121:THR:HG22	4:D:121:THR:O	2.11	0.51
1:R:59:VAL:HB	1:R:60:PRO:HA	1.92	0.51
3:T:194:LEU:HD22	3:T:213:PHE:CZ	2.45	0.51
11:K:108:ASP:O	11:K:112:ASN:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:121:THR:HG22	4:U:121:THR:O	2.11	0.50
3:C:60:ASP:OD1	3:C:61:THR:N	2.42	0.50
9:I:57:ASP:OD1	9:I:58:LYS:O	2.28	0.50
7:X:36:THR:OG1	7:X:168:GLY:O	2.22	0.50
10:a:112:ILE:HG21	10:a:192:LYS:HD2	1.92	0.50
16:g:229:ILE:HG23	16:g:237:ALA:CB	2.40	0.50
10:J:74:TYR:OH	10:J:80:ARG:NH2	2.45	0.50
13:M:200:ILE:HA	13:M:203:VAL:HG12	1.93	0.50
14:N:169:GLU:OE1	14:N:169:GLU:N	2.44	0.50
9:Z:57:ASP:OD1	9:Z:58:LYS:O	2.28	0.50
13:d:239:LYS:NZ	13:d:241:ASP:OD1	2.36	0.50
1:R:198:SER:OG	1:R:200:GLU:OE1	2.27	0.50
10:J:112:ILE:HG21	10:J:192:LYS:HD2	1.92	0.50
5:E:223:THR:O	5:E:227:GLY:N	2.40	0.50
14:N:57:HIS:ND1	14:N:58:ASP:OD1	2.44	0.50
11:b:154:THR:O	11:b:158:LEU:HD12	2.12	0.50
10:a:74:TYR:OH	10:a:80:ARG:NH2	2.45	0.49
4:U:142:ASP:OD1	4:U:143:ASP:N	2.45	0.49
14:e:169:GLU:OE1	14:e:169:GLU:N	2.44	0.49
6:W:230:VAL:HG12	6:W:230:VAL:O	2.11	0.49
11:b:154:THR:HG23	11:b:155:GLU:N	2.28	0.49
5:E:180:GLN:OE1	6:F:56:LEU:HD12	2.12	0.49
11:K:154:THR:HG23	11:K:155:GLU:N	2.28	0.49
5:V:180:GLN:OE1	6:W:56:LEU:HD12	2.12	0.49
13:d:132:GLY:O	13:d:140:ALA:N	2.45	0.49
17:Q:78:VAL:HG12	17:Q:78:VAL:O	2.13	0.49
1:R:229:THR:OG1	1:R:231:ASP:OD1	2.29	0.49
13:d:200:ILE:HA	13:d:203:VAL:HG12	1.93	0.49
4:D:142:ASP:OD1	4:D:143:ASP:N	2.46	0.49
11:K:154:THR:O	11:K:158:LEU:HD12	2.12	0.49
13:M:135:GLU:OE1	13:M:135:GLU:N	2.45	0.49
13:M:212:GLU:HG2	10:a:151:GLU:OE2	2.12	0.49
16:P:128:ASN:OD1	16:P:180:SER:OG	2.31	0.49
13:d:135:GLU:OE1	13:d:135:GLU:N	2.45	0.49
3:C:140:TYR:CD2	3:C:225:VAL:HG21	2.48	0.49
5:V:223:THR:O	5:V:227:GLY:N	2.40	0.49
8:H:28:SER:C	8:H:29:LEU:HD12	2.38	0.49
15:f:135:MET:HE1	15:f:196:PHE:HB2	1.95	0.49
1:R:52:VAL:HG21	1:R:203:VAL:HG22	1.95	0.49
3:T:140:TYR:CD2	3:T:225:VAL:HG21	2.48	0.49
5:V:180:GLN:HG2	15:f:263:CYS:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:230:VAL:O	6:F:230:VAL:HG12	2.11	0.49
17:h:78:VAL:O	17:h:78:VAL:HG12	2.13	0.49
1:A:229:THR:OG1	1:A:231:ASP:OD1	2.29	0.48
13:M:46:THR:CG2	13:M:222:GLU:HG2	2.44	0.48
3:T:136:ILE:CG2	3:T:148:LEU:HD11	2.43	0.48
12:c:82:ARG:HE	12:c:185:PRO:HG2	1.78	0.48
16:g:128:ASN:OD1	16:g:180:SER:OG	2.31	0.48
12:L:82:ARG:HE	12:L:185:PRO:HG2	1.78	0.48
14:N:53:LEU:HD13	14:N:195:VAL:HG23	1.96	0.48
3:T:63:THR:HG23	3:T:63:THR:O	2.13	0.48
8:Y:28:SER:C	8:Y:29:LEU:HD12	2.38	0.48
3:C:136:ILE:CG2	3:C:148:LEU:HD11	2.43	0.48
3:C:187:ASP:O	3:C:191:GLU:OE1	2.30	0.48
13:M:213:ARG:NE	10:a:151:GLU:OE1	2.24	0.48
15:O:263:CYS:SG	15:O:264:ASP:N	2.87	0.48
3:T:187:ASP:O	3:T:191:GLU:OE1	2.30	0.48
15:f:36:VAL:HG11	15:f:153:SER:OG	2.13	0.48
15:f:54:THR:HG23	15:f:56:ILE:HG22	1.95	0.48
3:C:63:THR:HG23	3:C:63:THR:O	2.13	0.48
14:N:29:ASP:O	14:N:198:THR:HG23	2.14	0.48
17:Q:42:THR:HG23	17:Q:43:SER:N	2.28	0.48
4:U:14:ASP:OD2	4:U:16:HIS:NE2	2.47	0.48
9:Z:58:LYS:O	9:Z:59:ASN:OD1	2.32	0.48
15:O:54:THR:HG23	15:O:56:ILE:HG22	1.95	0.48
15:f:137:GLU:OE2	15:f:225:ASN:ND2	2.47	0.48
6:F:74:LEU:HD13	6:F:81:ALA:HB1	1.95	0.48
9:I:58:LYS:O	9:I:59:ASN:OD1	2.32	0.48
15:O:137:GLU:OE2	15:O:225:ASN:ND2	2.47	0.48
4:D:14:ASP:OD2	4:D:16:HIS:NE2	2.47	0.48
17:Q:96:ILE:O	17:Q:100:LEU:HD13	2.13	0.48
3:T:231:LYS:N	3:T:234:GLU:OE2	2.42	0.48
4:U:6:ARG:NH1	4:U:10:ILE:HD12	2.29	0.48
5:V:118:ASP:OD1	6:W:82:ARG:NH2	2.47	0.48
1:A:14:ARG:O	1:A:27:GLN:NE2	2.47	0.48
2:B:196:LEU:HD23	2:B:209:ILE:HD12	1.96	0.48
2:S:196:LEU:HD23	2:S:209:ILE:HD12	1.96	0.48
1:A:52:VAL:HG21	1:A:203:VAL:HG22	1.95	0.48
9:I:58:LYS:O	9:I:60:CYS:N	2.47	0.48
3:T:42:ASP:N	3:T:42:ASP:OD1	2.47	0.48
5:V:70:ILE:HG21	5:V:112:LEU:HD21	1.96	0.48
9:Z:168:GLU:OE2	14:e:48:ARG:NH2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:140:ASP:OD1	2:S:141:GLU:N	2.47	0.47
15:f:127:PHE:O	15:f:130:THR:OG1	2.28	0.47
3:C:42:ASP:N	3:C:42:ASP:OD1	2.47	0.47
7:G:36:THR:HG22	7:G:51:GLU:CD	2.39	0.47
6:W:74:LEU:HD13	6:W:81:ALA:HB1	1.95	0.47
17:h:42:THR:HG23	17:h:43:SER:N	2.28	0.47
17:h:96:ILE:O	17:h:100:LEU:HD13	2.13	0.47
4:D:6:ARG:NH1	4:D:10:ILE:HD12	2.29	0.47
5:E:118:ASP:OD1	6:F:82:ARG:NH2	2.47	0.47
15:O:36:VAL:HG11	15:O:153:SER:OG	2.13	0.47
15:O:135:MET:HE1	15:O:196:PHE:HB2	1.95	0.47
1:R:14:ARG:O	1:R:27:GLN:NE2	2.47	0.47
14:e:29:ASP:O	14:e:198:THR:HG23	2.14	0.47
5:E:180:GLN:HG2	15:O:263:CYS:HB2	1.95	0.47
13:d:46:THR:CG2	13:d:222:GLU:HG2	2.44	0.47
2:B:140:ASP:OD1	2:B:141:GLU:N	2.47	0.47
4:D:196:VAL:O	4:D:200:LEU:HD23	2.15	0.47
3:T:187:ASP:O	3:T:190:ILE:N	2.48	0.47
14:e:53:LEU:HD13	14:e:195:VAL:HG23	1.96	0.47
2:B:217:GLU:HG3	2:B:231:LYS:HD2	1.97	0.47
5:E:27:SER:OG	5:E:138:PHE:O	2.33	0.47
6:W:81:ALA:HB2	6:W:130:VAL:HG21	1.96	0.47
15:f:263:CYS:SG	15:f:264:ASP:N	2.87	0.47
2:B:49:LYS:HG3	2:B:210:GLU:OE1	2.15	0.47
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.96	0.47
13:M:132:GLY:O	13:M:140:ALA:N	2.45	0.47
16:P:68:SER:OG	16:P:69:ALA:N	2.48	0.47
5:V:27:SER:OG	5:V:138:PHE:O	2.33	0.47
7:X:36:THR:HG22	7:X:51:GLU:CD	2.39	0.47
3:C:31:HIS:O	3:C:51:LYS:NZ	2.45	0.47
8:H:120:GLU:OE2	8:H:120:GLU:N	2.48	0.47
9:I:168:GLU:OE2	14:N:48:ARG:NH2	2.48	0.47
3:T:160:TRP:HH2	4:U:52:LEU:HD12	1.79	0.47
1:A:198:SER:OG	1:A:200:GLU:OE1	2.27	0.46
10:J:151:GLU:OE2	13:d:212:GLU:HG2	2.16	0.46
11:K:36:ARG:NE	11:K:58:GLU:OE2	2.36	0.46
10:a:13:VAL:HG13	10:a:167:ILE:HD11	1.97	0.46
6:F:211:LEU:HD23	6:F:230:VAL:HG11	1.97	0.46
16:P:95:LEU:HD22	16:P:183:GLN:OE1	2.16	0.46
4:U:196:VAL:O	4:U:200:LEU:HD23	2.15	0.46
9:Z:58:LYS:O	9:Z:60:CYS:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:161:LEU:CD1	11:b:165:VAL:HG23	2.45	0.46
3:C:160:TRP:HH2	4:D:52:LEU:HD12	1.80	0.46
6:F:66:CYS:SG	6:F:89:ARG:HA	2.56	0.46
2:S:99:ARG:NH1	9:Z:90:SER:OG	2.49	0.46
2:S:217:GLU:HG3	2:S:231:LYS:HD2	1.97	0.46
15:f:33:VAL:CG1	15:f:149:MET:HE3	2.45	0.46
8:H:26:VAL:HG13	8:H:26:VAL:O	2.16	0.46
10:J:13:VAL:HG13	10:J:167:ILE:HD11	1.97	0.46
2:S:49:LYS:HG3	2:S:210:GLU:OE1	2.15	0.46
9:Z:74:GLY:HA3	9:Z:127:LEU:HD23	1.98	0.46
16:g:68:SER:OG	16:g:69:ALA:N	2.49	0.46
5:E:70:ILE:HG21	5:E:112:LEU:HD21	1.96	0.46
6:W:66:CYS:SG	6:W:89:ARG:HA	2.56	0.46
8:Y:26:VAL:HG13	8:Y:26:VAL:O	2.16	0.46
15:O:33:VAL:CG1	15:O:149:MET:HE3	2.45	0.46
15:O:42:LEU:HD13	15:O:71:ILE:HG21	1.98	0.46
15:O:57:MET:HE2	15:O:170:THR:HG23	1.98	0.46
6:W:22:VAL:HG13	16:g:261:LYS:HE2	1.98	0.46
6:W:211:LEU:HD23	6:W:230:VAL:HG11	1.98	0.46
14:e:198:THR:HG22	14:e:199:ALA:N	2.30	0.46
3:C:119:LYS:NZ	3:C:151:SER:OG	2.48	0.46
11:b:154:THR:HG23	11:b:155:GLU:H	1.81	0.46
14:N:198:THR:HG22	14:N:199:ALA:N	2.30	0.46
2:B:4:ARG:HD2	8:H:93:ARG:HH22	1.81	0.45
15:f:42:LEU:HD13	15:f:71:ILE:HG21	1.98	0.45
13:M:104:SER:HB2	13:M:135:GLU:OE2	2.17	0.45
2:S:4:ARG:HD2	8:Y:93:ARG:HH22	1.81	0.45
6:W:7:ASP:O	6:W:21:GLN:NE2	2.50	0.45
11:K:154:THR:HG23	11:K:155:GLU:H	1.81	0.45
3:T:119:LYS:NZ	3:T:151:SER:OG	2.48	0.45
11:K:161:LEU:CD1	11:K:165:VAL:HG23	2.45	0.45
14:N:132:ILE:HG12	14:N:138:VAL:HG22	1.99	0.45
8:Y:120:GLU:OE2	8:Y:120:GLU:N	2.48	0.45
13:d:104:SER:HB2	13:d:135:GLU:OE2	2.17	0.45
17:h:140:MET:O	17:h:140:MET:HG3	2.16	0.45
2:B:32:VAL:HG23	2:B:50:LYS:NZ	2.32	0.45
15:f:57:MET:HE2	15:f:170:THR:HG23	1.98	0.45
3:C:187:ASP:O	3:C:190:ILE:N	2.48	0.45
6:F:7:ASP:O	6:F:21:GLN:NE2	2.49	0.45
6:F:9:ASP:OD1	6:F:9:ASP:N	2.50	0.45
16:P:72:VAL:HG22	16:P:83:ILE:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:140:MET:HG3	17:Q:140:MET:O	2.16	0.45
13:d:169:LEU:O	13:d:173:VAL:HG22	2.16	0.45
1:A:79:ILE:HD11	1:A:112:MET:O	2.17	0.45
1:R:79:ILE:HD11	1:R:112:MET:O	2.17	0.45
2:S:32:VAL:HG23	2:S:50:LYS:NZ	2.32	0.45
6:F:22:VAL:HG13	16:P:261:LYS:HE2	1.98	0.45
7:G:190:ARG:NH1	7:G:235:LEU:HD13	2.32	0.44
9:I:74:GLY:HA3	9:I:127:LEU:HD23	1.98	0.44
4:U:84:ILE:HD13	8:Y:139:HIS:HE2	1.81	0.44
1:A:17:THR:HG23	1:A:17:THR:O	2.17	0.44
5:E:180:GLN:CG	15:O:263:CYS:HB2	2.48	0.44
7:G:190:ARG:HH12	7:G:235:LEU:HD13	1.83	0.44
11:K:49:GLU:OE1	11:K:98:TYR:HB2	2.17	0.44
13:M:169:LEU:O	13:M:173:VAL:HG22	2.16	0.44
14:N:102:LYS:HD2	14:N:138:VAL:HG23	1.99	0.44
1:A:72:ILE:HG12	1:A:82:VAL:HG22	1.99	0.44
3:C:143:ARG:NH2	3:C:144:TYR:OH	2.51	0.44
10:J:97:GLU:O	10:J:98:ARG:HB2	2.18	0.44
1:R:72:ILE:HG12	1:R:82:VAL:HG22	1.99	0.44
3:T:31:HIS:O	3:T:51:LYS:NZ	2.45	0.44
14:e:174:ILE:HG21	14:e:194:MET:HE3	1.99	0.44
16:g:95:LEU:HD22	16:g:183:GLN:OE1	2.16	0.44
2:B:49:LYS:HD2	2:B:210:GLU:OE1	2.18	0.44
4:D:84:ILE:HD13	8:H:139:HIS:HE2	1.81	0.44
10:J:63:LEU:HD23	10:J:66:MET:HE3	2.00	0.44
4:U:91:VAL:HG11	8:Y:34:ARG:HG2	1.99	0.44
15:f:207:GLY:O	15:f:210:LYS:NZ	2.46	0.44
16:g:72:VAL:HG22	16:g:83:ILE:HG12	1.99	0.44
4:D:91:VAL:HG11	8:H:34:ARG:HG2	1.99	0.44
1:R:53:VAL:CG2	1:R:82:VAL:HG21	2.47	0.44
3:T:143:ARG:NH2	3:T:144:TYR:OH	2.51	0.44
1:R:13:ASP:OD1	1:R:14:ARG:N	2.51	0.44
14:e:132:ILE:HG12	14:e:138:VAL:HG22	1.98	0.44
15:O:127:PHE:O	15:O:130:THR:OG1	2.28	0.44
3:T:190:ILE:O	3:T:194:LEU:HD23	2.18	0.44
8:Y:41:VAL:O	11:b:95:ARG:NH1	2.51	0.44
2:B:99:ARG:NH1	9:I:90:SER:OG	2.49	0.44
3:C:190:ILE:O	3:C:194:LEU:HD23	2.18	0.44
8:H:41:VAL:O	11:K:95:ARG:NH1	2.51	0.44
14:N:174:ILE:HG21	14:N:194:MET:HE3	1.99	0.44
13:d:196:VAL:HG22	13:d:196:VAL:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ASP:OD1	1:A:14:ARG:N	2.51	0.44
8:H:29:LEU:HD11	12:L:161:LEU:HD21	2.00	0.44
8:H:80:GLU:HB3	8:H:81:PRO:HD3	1.99	0.44
13:M:196:VAL:O	13:M:196:VAL:HG22	2.18	0.44
6:W:176:LEU:HD12	7:X:58:LEU:HD23	2.00	0.44
7:X:190:ARG:NH1	7:X:235:LEU:HD13	2.32	0.44
9:Z:107:SER:O	9:Z:111:MET:HG2	2.18	0.44
10:a:97:GLU:O	10:a:98:ARG:HB2	2.18	0.44
14:e:102:LYS:HD2	14:e:138:VAL:HG23	1.99	0.44
3:C:242:THR:O	3:C:242:THR:HG22	2.18	0.43
13:d:35:ALA:N	13:d:154:GLN:O	2.43	0.43
1:A:53:VAL:CG2	1:A:82:VAL:HG21	2.48	0.43
6:F:226:ASP:N	6:F:226:ASP:OD1	2.51	0.43
6:W:218:LYS:HD2	6:W:219:ASP:N	2.33	0.43
11:b:49:GLU:OE1	11:b:98:TYR:HB2	2.17	0.43
14:e:20:THR:CG2	14:e:21:SER:N	2.81	0.43
14:N:20:THR:CG2	14:N:21:SER:N	2.81	0.43
8:Y:29:LEU:HD11	12:c:161:LEU:HD21	2.00	0.43
3:C:72:LYS:NZ	3:C:105:ASP:OD2	2.41	0.43
6:F:176:LEU:HD12	7:G:58:LEU:HD23	2.00	0.43
1:R:17:THR:HG23	1:R:17:THR:O	2.17	0.43
5:V:69:GLU:OE2	5:V:71:ASP:C	2.61	0.43
5:E:69:GLU:OE2	5:E:71:ASP:C	2.61	0.43
7:G:234:ASP:OD1	7:G:235:LEU:N	2.51	0.43
8:H:143:GLU:HA	8:H:148:ILE:HG22	2.00	0.43
8:Y:80:GLU:HB3	8:Y:81:PRO:HD3	1.99	0.43
14:e:62:CYS:SG	14:e:116:ILE:HG23	2.59	0.43
3:C:100:LYS:HG3	10:J:65:GLU:HB3	2.01	0.43
1:R:168:ALA:O	2:S:55:LEU:HD13	2.19	0.43
1:A:168:ALA:O	2:B:55:LEU:HD13	2.19	0.43
3:T:242:THR:O	3:T:242:THR:HG22	2.18	0.43
1:A:43:LEU:HD21	1:A:45:VAL:HG13	2.01	0.43
4:D:63:LYS:NZ	4:D:75:PHE:O	2.42	0.43
6:F:218:LYS:HD2	6:F:219:ASP:N	2.33	0.43
10:J:101:GLY:N	10:J:102:PRO:HD3	2.34	0.43
3:T:100:LYS:HG3	10:a:65:GLU:HB3	2.01	0.43
7:X:190:ARG:HH12	7:X:235:LEU:HD13	1.83	0.43
6:F:78:ALA:N	6:F:79:PRO:HD2	2.34	0.43
9:I:173:GLN:O	9:I:174:ASP:OD1	2.37	0.43
1:A:43:LEU:C	1:A:43:LEU:HD23	2.44	0.43
7:G:190:ARG:O	7:G:194:LYS:NZ	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:39:GLY:HA2	11:K:59:TYR:CG	2.54	0.43
14:N:62:CYS:SG	14:N:116:ILE:HG23	2.59	0.43
3:T:72:LYS:NZ	3:T:105:ASP:OD2	2.41	0.43
9:Z:173:GLN:O	9:Z:174:ASP:OD1	2.37	0.43
10:a:63:LEU:HD23	10:a:66:MET:HE3	2.00	0.43
11:b:183:ILE:CD1	11:b:192:VAL:HG21	2.49	0.43
2:S:49:LYS:HD2	2:S:210:GLU:OE1	2.18	0.42
6:W:226:ASP:N	6:W:226:ASP:OD1	2.51	0.42
8:Y:39:GLY:HA2	11:b:59:TYR:CG	2.54	0.42
9:I:107:SER:O	9:I:111:MET:HG2	2.18	0.42
9:Z:96:SER:O	9:Z:100:SER:N	2.52	0.42
15:f:71:ILE:O	15:f:71:ILE:HG22	2.19	0.42
13:M:135:GLU:OE1	13:M:135:GLU:HA	2.19	0.42
5:V:180:GLN:CG	15:f:263:CYS:HB2	2.48	0.42
6:W:78:ALA:N	6:W:79:PRO:HD2	2.34	0.42
15:f:28:LEU:HD12	16:g:189:LEU:HD23	2.01	0.42
16:g:182:ASP:OD1	16:g:182:ASP:N	2.52	0.42
11:K:183:ILE:CD1	11:K:192:VAL:HG21	2.49	0.42
7:X:234:ASP:OD1	7:X:235:LEU:N	2.51	0.42
11:b:85:ARG:NH2	11:b:86:GLN:OE1	2.50	0.42
6:F:114:ASP:OD1	6:F:115:LYS:N	2.53	0.42
8:H:43:LEU:HD12	8:H:46:GLN:H	1.83	0.42
9:I:96:SER:O	9:I:100:SER:N	2.52	0.42
10:J:155:GLU:HB2	10:J:158:LEU:HD11	2.02	0.42
8:Y:43:LEU:HD12	8:Y:46:GLN:H	1.83	0.42
8:Y:143:GLU:HA	8:Y:148:ILE:HG22	2.00	0.42
5:E:69:GLU:OE1	12:L:143:LEU:CD2	2.68	0.42
6:F:67:ASP:OD2	6:F:92:CYS:HB3	2.19	0.42
4:U:229:ILE:O	4:U:233:VAL:HG23	2.20	0.42
6:W:9:ASP:OD1	6:W:9:ASP:N	2.50	0.42
6:W:114:ASP:OD1	6:W:115:LYS:N	2.53	0.42
8:H:41:VAL:HG11	11:K:98:TYR:CE1	2.55	0.42
9:I:30:THR:HG22	9:I:32:ILE:CD1	2.50	0.42
13:M:30:THR:HG21	13:M:165:ILE:HD12	2.02	0.42
9:I:30:THR:CG2	9:I:31:THR:N	2.83	0.42
14:e:174:ILE:HG23	14:e:178:LEU:HD13	2.02	0.42
14:e:182:ILE:HG23	14:e:189:GLY:HA2	2.01	0.42
11:K:145:ASP:OD1	11:K:146:HIS:N	2.53	0.42
14:N:174:ILE:HG23	14:N:178:LEU:HD13	2.02	0.42
14:N:182:ILE:HG23	14:N:189:GLY:HA2	2.01	0.42
16:P:182:ASP:OD1	16:P:182:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:69:GLU:OE1	12:c:143:LEU:CD2	2.67	0.42
9:Z:195:ASP:OD1	9:Z:195:ASP:C	2.62	0.42
4:D:71:VAL:HG11	4:D:109:LEU:HD22	2.02	0.41
9:Z:30:THR:CG2	9:Z:31:THR:N	2.82	0.41
2:B:21:ILE:O	2:B:25:LEU:HD23	2.21	0.41
16:P:181:VAL:O	16:P:181:VAL:HG22	2.21	0.41
1:R:43:LEU:HD21	1:R:45:VAL:HG13	2.01	0.41
9:Z:30:THR:HG22	9:Z:32:ILE:CD1	2.50	0.41
11:b:183:ILE:HD13	11:b:192:VAL:HG21	2.01	0.41
3:C:231:LYS:N	3:C:234:GLU:OE2	2.42	0.41
1:R:43:LEU:C	1:R:43:LEU:HD23	2.44	0.41
10:a:101:GLY:N	10:a:102:PRO:HD3	2.34	0.41
13:d:30:THR:HG21	13:d:165:ILE:HD12	2.02	0.41
7:G:51:GLU:O	7:G:53:LEU:HD22	2.21	0.41
8:H:143:GLU:O	8:H:147:GLY:N	2.53	0.41
15:O:71:ILE:O	15:O:71:ILE:HG22	2.20	0.41
2:S:21:ILE:O	2:S:25:LEU:HD23	2.21	0.41
3:T:210:ARG:O	3:T:210:ARG:HG2	2.21	0.41
8:Y:41:VAL:HG11	11:b:98:TYR:CE1	2.55	0.41
8:Y:143:GLU:O	8:Y:147:GLY:N	2.53	0.41
9:Z:133:ASP:C	9:Z:133:ASP:OD1	2.64	0.41
11:K:52:ASP:OD2	12:L:166:LYS:NZ	2.53	0.41
15:O:28:LEU:HD12	16:P:189:LEU:HD23	2.02	0.41
10:a:155:GLU:HB2	10:a:158:LEU:HD11	2.02	0.41
11:b:145:ASP:OD1	11:b:146:HIS:N	2.53	0.41
12:c:180:THR:HG22	12:c:181:ARG:N	2.36	0.41
3:C:210:ARG:O	3:C:210:ARG:HG2	2.20	0.41
4:D:229:ILE:O	4:D:233:VAL:HG23	2.20	0.41
12:L:153:ALA:O	12:L:157:ILE:HG12	2.21	0.41
15:O:207:GLY:O	15:O:210:LYS:NZ	2.46	0.41
9:I:133:ASP:OD1	9:I:133:ASP:C	2.64	0.41
2:S:203:GLU:OE2	2:S:205:ASN:ND2	2.54	0.41
4:U:92:GLU:HB2	8:Y:34:ARG:HH21	1.86	0.41
6:W:67:ASP:OD2	6:W:92:CYS:HB3	2.19	0.41
7:X:152:GLU:HB3	7:X:153:PRO:HD2	2.03	0.41
9:Z:30:THR:CG2	9:Z:32:ILE:HD11	2.51	0.41
6:F:156:LEU:HD13	6:F:159:THR:HB	2.02	0.41
9:I:30:THR:CG2	9:I:32:ILE:HD11	2.51	0.41
9:I:195:ASP:OD1	9:I:195:ASP:C	2.62	0.41
9:I:196:LEU:HD12	13:d:52:TYR:HA	2.03	0.41
11:K:183:ILE:HD13	11:K:192:VAL:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:44:PHE:HB2	16:P:87:THR:HG21	2.03	0.41
4:U:71:VAL:HG11	4:U:109:LEU:HD22	2.02	0.41
6:W:156:LEU:HD13	6:W:159:THR:HB	2.02	0.41
12:c:153:ALA:O	12:c:157:ILE:HG12	2.21	0.41
6:F:69:HIS:O	6:F:216:VAL:HG21	2.21	0.41
15:O:189:PRO:N	15:O:190:PRO:CD	2.84	0.40
13:M:239:LYS:NZ	13:M:241:ASP:OD1	2.36	0.40
7:X:51:GLU:O	7:X:53:LEU:HD22	2.21	0.40
13:d:135:GLU:OE1	13:d:135:GLU:HA	2.19	0.40
1:A:148:GLU:OE2	9:I:104:ARG:NH2	2.49	0.40
4:D:92:GLU:HB2	8:H:34:ARG:HH21	1.86	0.40
6:F:176:LEU:CD2	6:F:180:ILE:HD12	2.52	0.40
3:T:66:LEU:HD23	3:T:214:ALA:CB	2.51	0.40
6:W:176:LEU:CD2	6:W:180:ILE:HD12	2.52	0.40
2:B:203:GLU:OE2	2:B:205:ASN:ND2	2.54	0.40
6:F:60:GLN:OE1	6:F:60:GLN:HA	2.21	0.40
7:G:82:ILE:N	7:G:83:PRO:HD2	2.36	0.40
9:I:57:ASP:OD1	9:I:57:ASP:C	2.64	0.40
17:h:183:MET:HE1	17:h:220:ARG:HG3	2.03	0.40
2:B:217:GLU:OE1	2:B:232:GLY:O	2.40	0.40
3:C:66:LEU:HD23	3:C:214:ALA:CB	2.51	0.40
5:E:40:ILE:HD12	5:E:200:VAL:HG23	2.04	0.40
16:P:177:ASP:OD1	16:P:177:ASP:N	2.54	0.40
2:S:220:ASP:OD1	2:S:221:LEU:N	2.55	0.40
16:g:181:VAL:O	16:g:181:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	227/252 (90%)	225 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	227/252 (90%)	225 (99%)	2 (1%)	0	100	100
2	B	245/250 (98%)	242 (99%)	3 (1%)	0	100	100
2	S	245/250 (98%)	242 (99%)	3 (1%)	0	100	100
3	C	229/258 (89%)	225 (98%)	4 (2%)	0	100	100
3	T	229/258 (89%)	225 (98%)	4 (2%)	0	100	100
4	D	215/254 (85%)	214 (100%)	1 (0%)	0	100	100
4	U	215/254 (85%)	214 (100%)	1 (0%)	0	100	100
5	E	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
5	V	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
6	F	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
6	W	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
7	G	228/288 (79%)	225 (99%)	3 (1%)	0	100	100
7	X	228/288 (79%)	225 (99%)	3 (1%)	0	100	100
8	H	118/148 (80%)	114 (97%)	4 (3%)	0	100	100
8	Y	118/148 (80%)	114 (97%)	4 (3%)	0	100	100
9	I	223/261 (85%)	218 (98%)	5 (2%)	0	100	100
9	Z	223/261 (85%)	218 (98%)	5 (2%)	0	100	100
10	J	169/205 (82%)	165 (98%)	4 (2%)	0	100	100
10	a	169/205 (82%)	165 (98%)	4 (2%)	0	100	100
11	K	173/198 (87%)	169 (98%)	4 (2%)	0	100	100
11	b	173/198 (87%)	169 (98%)	4 (2%)	0	100	100
12	L	93/287 (32%)	93 (100%)	0	0	100	100
12	c	93/287 (32%)	93 (100%)	0	0	100	100
13	M	198/241 (82%)	195 (98%)	3 (2%)	0	100	100
13	d	198/241 (82%)	195 (98%)	3 (2%)	0	100	100
14	N	200/215 (93%)	195 (98%)	5 (2%)	0	100	100
14	e	200/215 (93%)	195 (98%)	5 (2%)	0	100	100
15	O	231/276 (84%)	229 (99%)	2 (1%)	0	100	100
15	f	231/276 (84%)	229 (99%)	2 (1%)	0	100	100
16	P	215/267 (80%)	211 (98%)	4 (2%)	0	100	100
16	g	215/267 (80%)	211 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	198/251 (79%)	190 (96%)	8 (4%)	0	100	100
17	h	198/251 (79%)	190 (96%)	8 (4%)	0	100	100
All	All	6864/8290 (83%)	6742 (98%)	122 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/210 (93%)	196 (100%)	0	100	100
1	R	196/210 (93%)	196 (100%)	0	100	100
2	B	206/209 (99%)	206 (100%)	0	100	100
2	S	206/209 (99%)	206 (100%)	0	100	100
3	C	196/216 (91%)	196 (100%)	0	100	100
3	T	196/216 (91%)	196 (100%)	0	100	100
4	D	198/226 (88%)	198 (100%)	0	100	100
4	U	198/226 (88%)	198 (100%)	0	100	100
5	E	202/215 (94%)	202 (100%)	0	100	100
5	V	202/215 (94%)	202 (100%)	0	100	100
6	F	193/193 (100%)	192 (100%)	1 (0%)	81	89
6	W	193/193 (100%)	192 (100%)	1 (0%)	81	89
7	G	192/239 (80%)	192 (100%)	0	100	100
7	X	192/239 (80%)	192 (100%)	0	100	100
8	H	112/136 (82%)	112 (100%)	0	100	100
8	Y	112/136 (82%)	112 (100%)	0	100	100
9	I	185/214 (86%)	185 (100%)	0	100	100
9	Z	185/214 (86%)	185 (100%)	0	100	100
10	J	147/173 (85%)	147 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	a	147/173 (85%)	147 (100%)	0	100	100
11	K	161/175 (92%)	161 (100%)	0	100	100
11	b	161/175 (92%)	161 (100%)	0	100	100
12	L	87/235 (37%)	87 (100%)	0	100	100
12	c	87/235 (37%)	87 (100%)	0	100	100
13	M	167/201 (83%)	166 (99%)	1 (1%)	78	88
13	d	167/201 (83%)	166 (99%)	1 (1%)	78	88
14	N	166/178 (93%)	166 (100%)	0	100	100
14	e	166/178 (93%)	166 (100%)	0	100	100
15	O	214/251 (85%)	214 (100%)	0	100	100
15	f	214/251 (85%)	214 (100%)	0	100	100
16	P	207/244 (85%)	207 (100%)	0	100	100
16	g	207/244 (85%)	207 (100%)	0	100	100
17	Q	174/212 (82%)	174 (100%)	0	100	100
17	h	174/212 (82%)	174 (100%)	0	100	100
All	All	6006/7054 (85%)	6002 (100%)	4 (0%)	87	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	139	LYS
13	M	135	GLU
6	W	139	LYS
13	d	135	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	209	HIS
2	B	241	GLN
5	E	114	GLN
5	E	147	HIS
5	E	185	ASN
7	G	183	HIS
7	G	204	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	237	GLN
8	H	102	ASN
9	I	8	ASN
9	I	86	GLN
10	J	64	ASN
10	J	113	ASN
11	K	101	ASN
11	K	118	GLN
11	K	133	HIS
11	K	146	HIS
12	L	164	GLN
13	M	214	HIS
16	P	13	ASN
16	P	16	GLN
16	P	169	HIS
16	P	217	ASN
17	Q	212	ASN
17	Q	227	ASN
1	R	37	GLN
2	S	241	GLN
5	V	114	GLN
5	V	147	HIS
5	V	185	ASN
7	X	183	HIS
7	X	204	HIS
7	X	237	GLN
8	Y	35	GLN
8	Y	102	ASN
9	Z	8	ASN
10	a	64	ASN
10	a	113	ASN
11	b	101	ASN
11	b	118	GLN
11	b	133	HIS
11	b	146	HIS
12	c	164	GLN
13	d	214	HIS
16	g	217	ASN
17	h	95	HIS
17	h	212	ASN
17	h	227	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

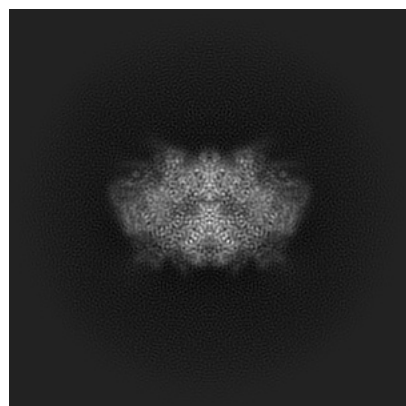
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40938. These allow visual inspection of the internal detail of the map and identification of artifacts.

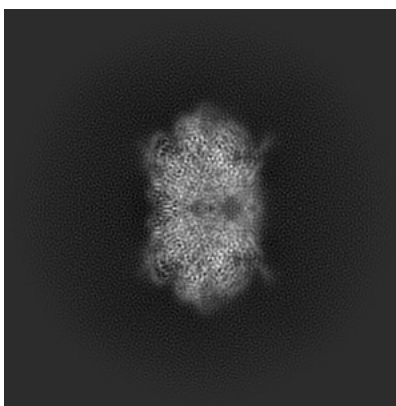
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

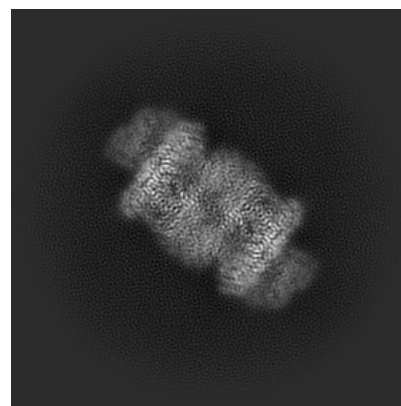
6.1.1 Primary map



X

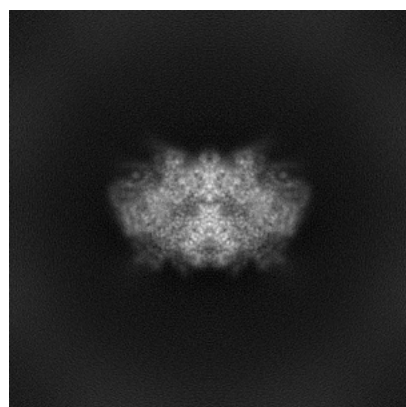


Y

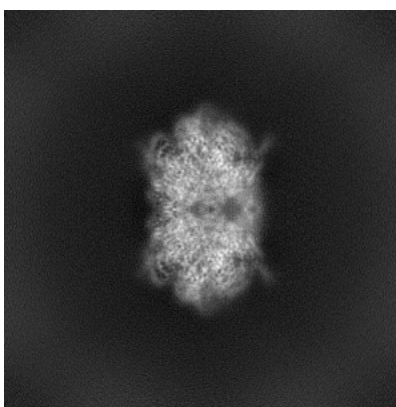


Z

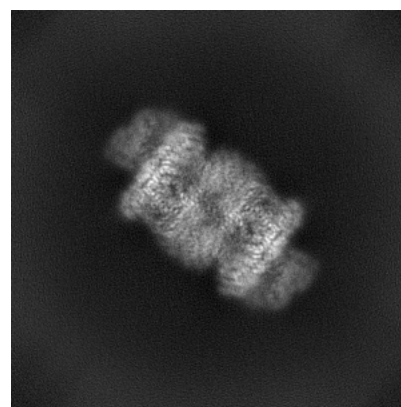
6.1.2 Raw map



X



Y

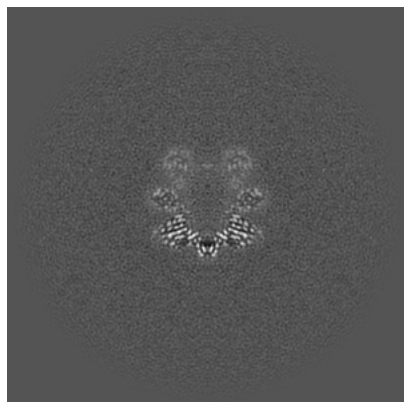


Z

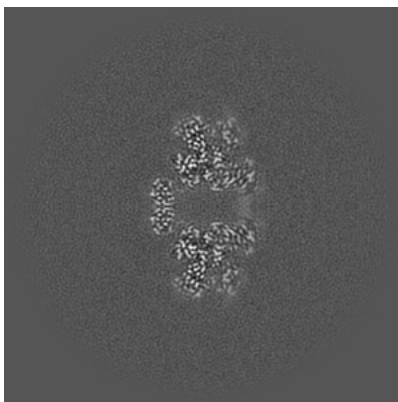
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

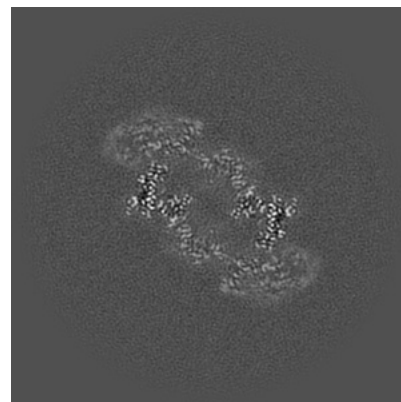
6.2.1 Primary map



X Index: 180

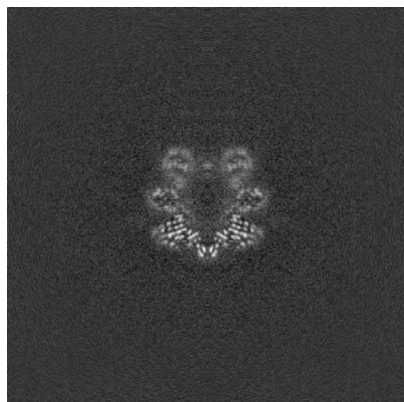


Y Index: 180

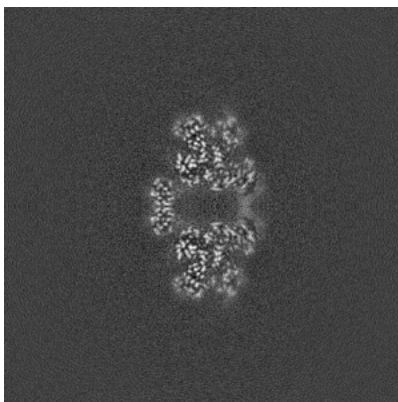


Z Index: 180

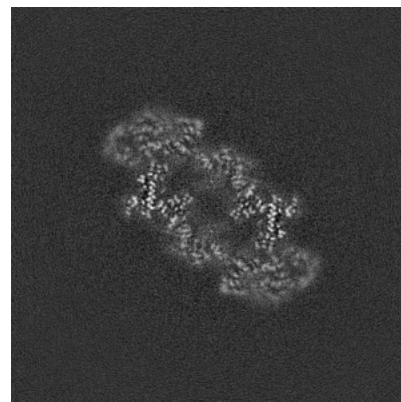
6.2.2 Raw map



X Index: 180



Y Index: 180

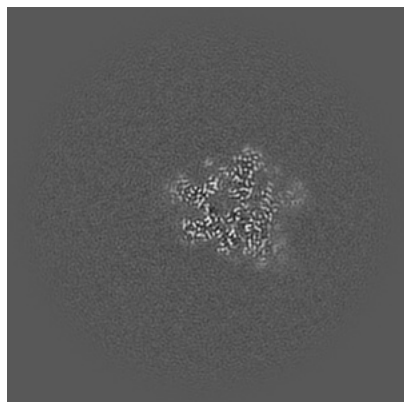


Z Index: 180

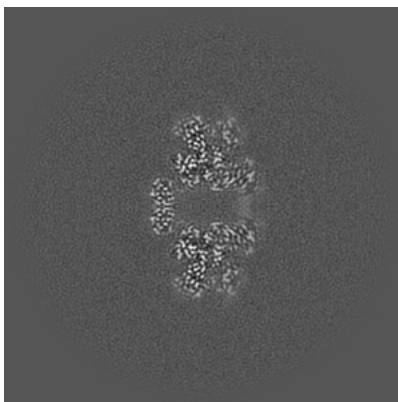
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

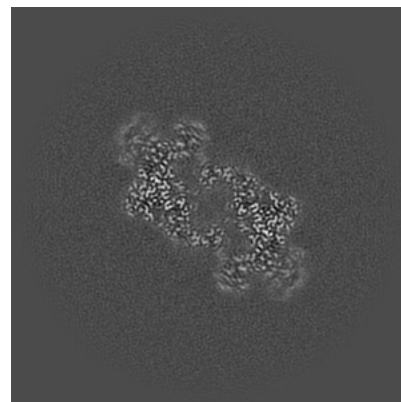
6.3.1 Primary map



X Index: 139

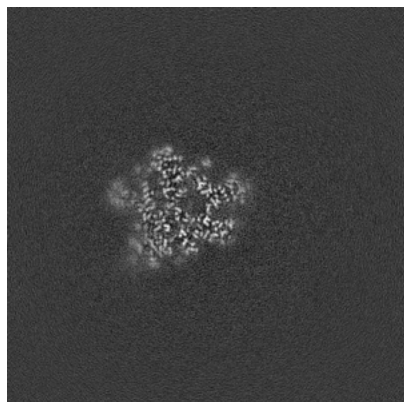


Y Index: 180

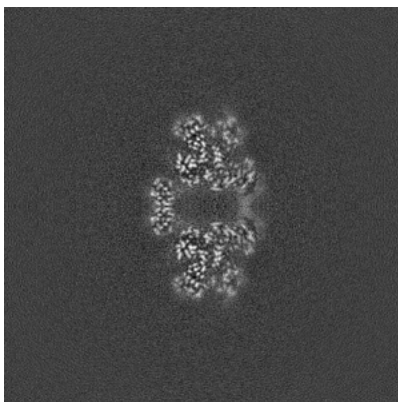


Z Index: 168

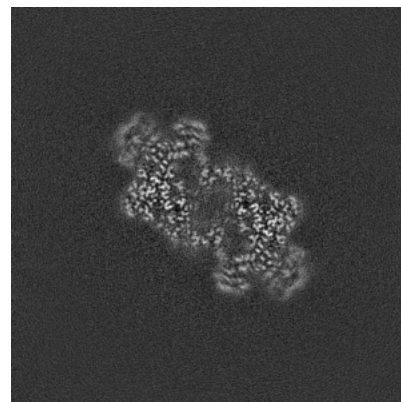
6.3.2 Raw map



X Index: 221



Y Index: 180

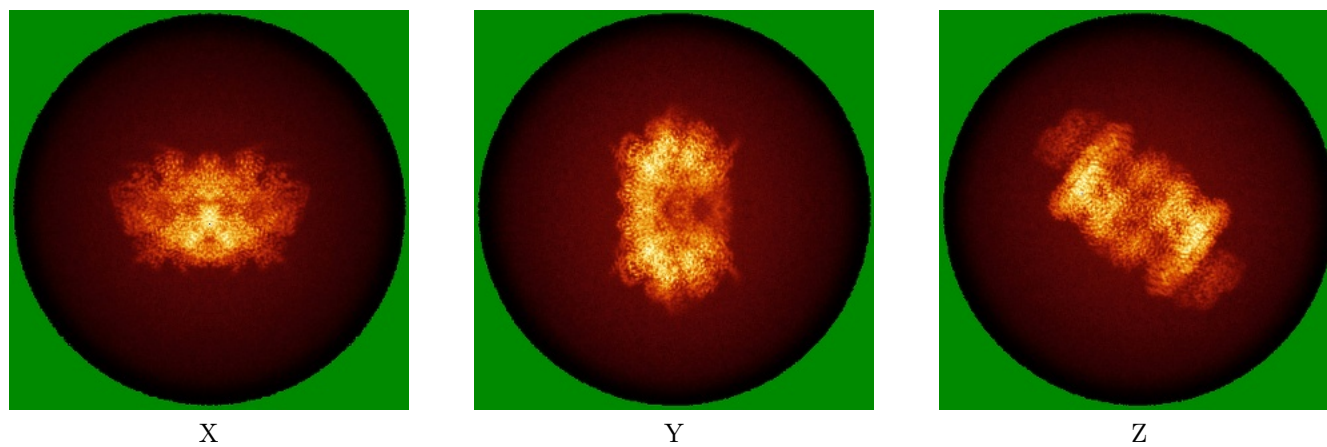


Z Index: 168

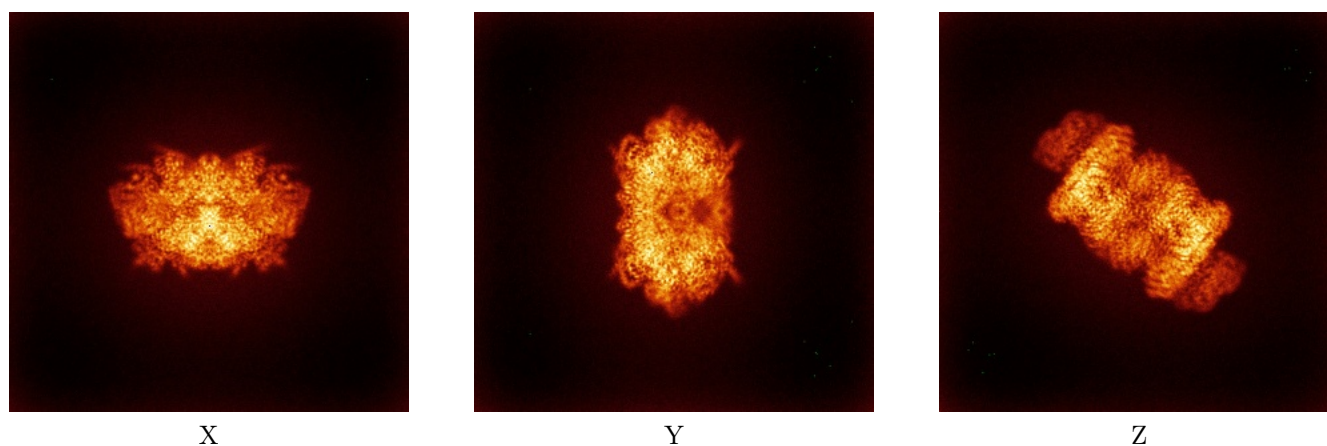
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

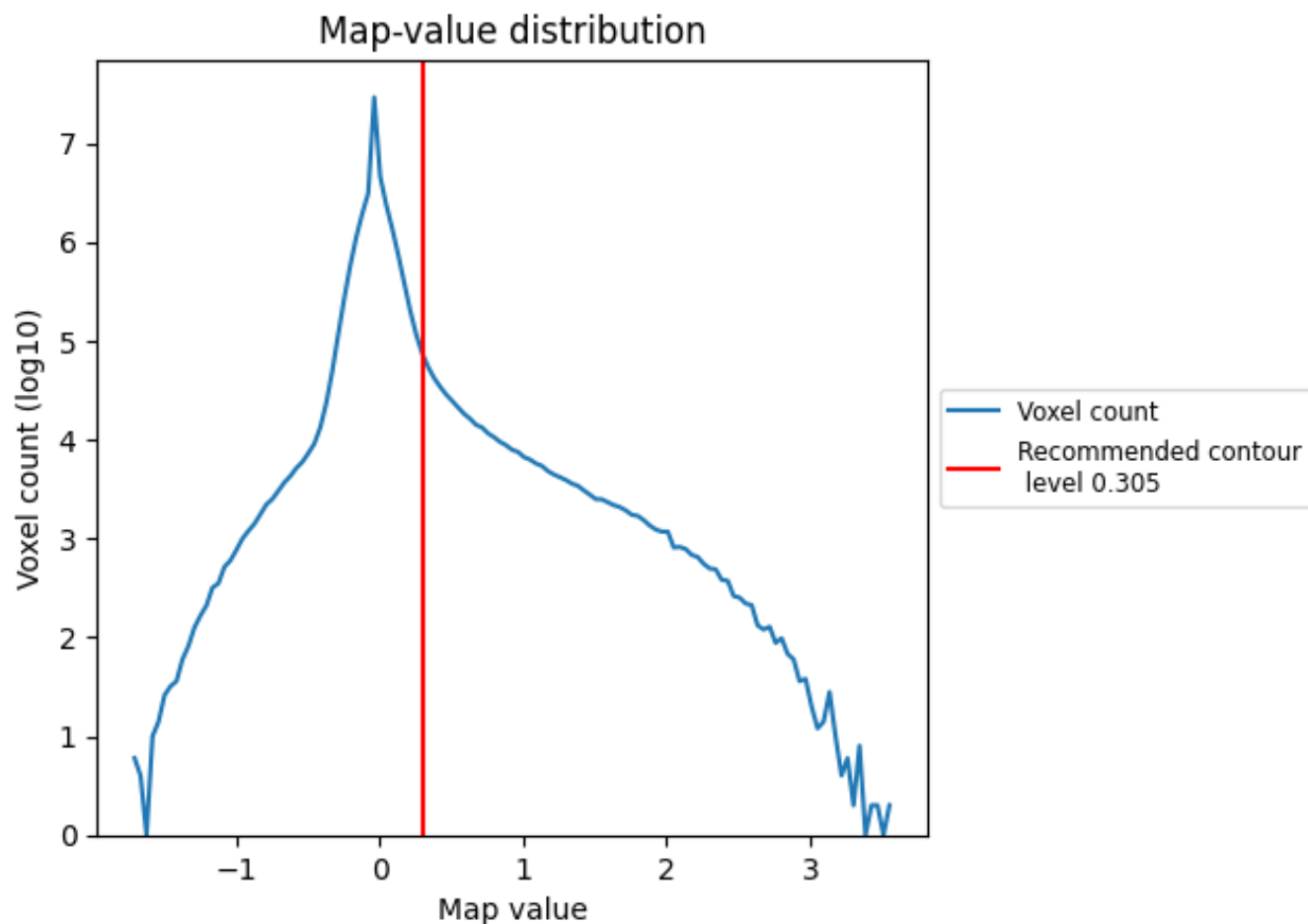
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

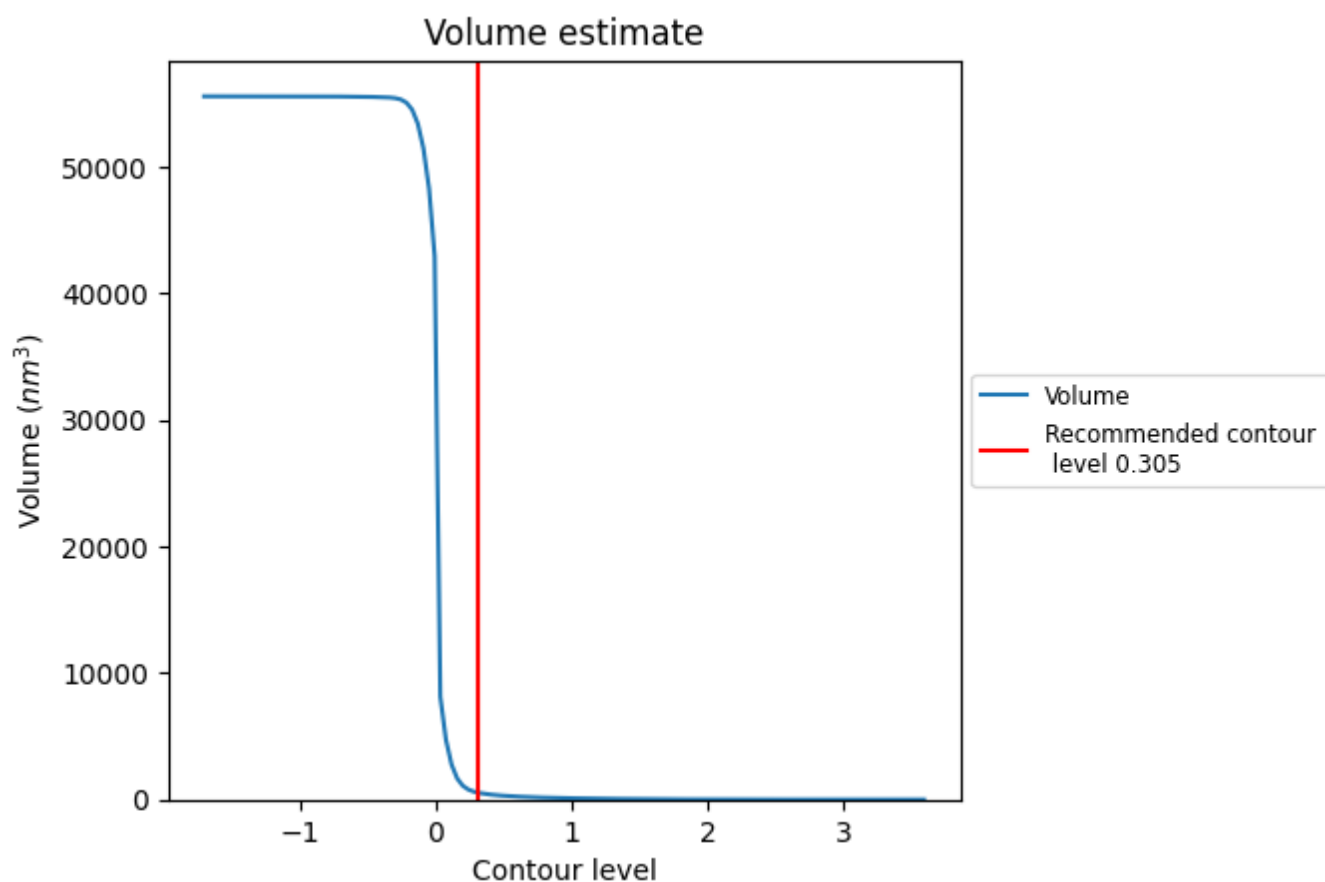
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

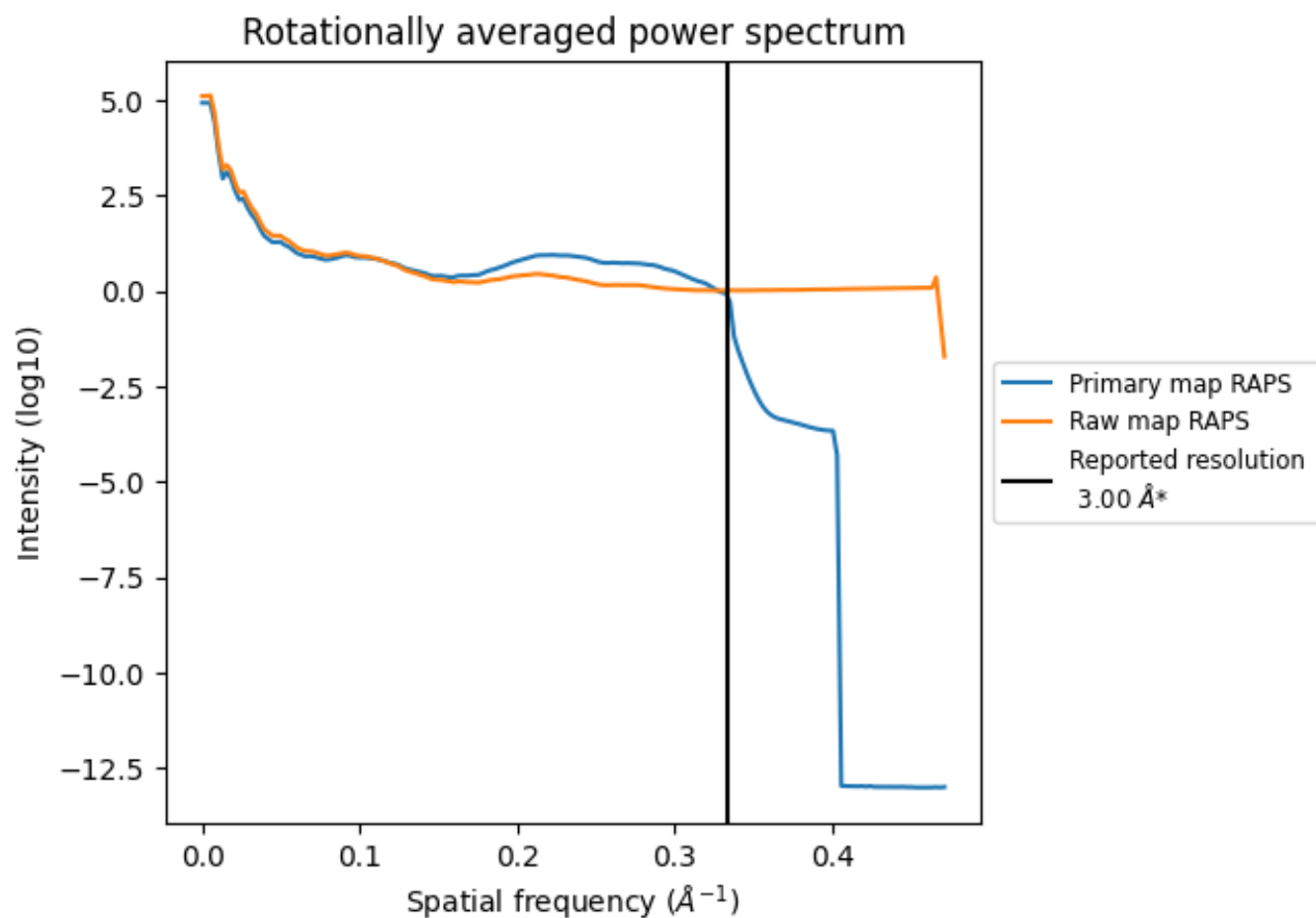
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 561 nm³; this corresponds to an approximate mass of 507 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

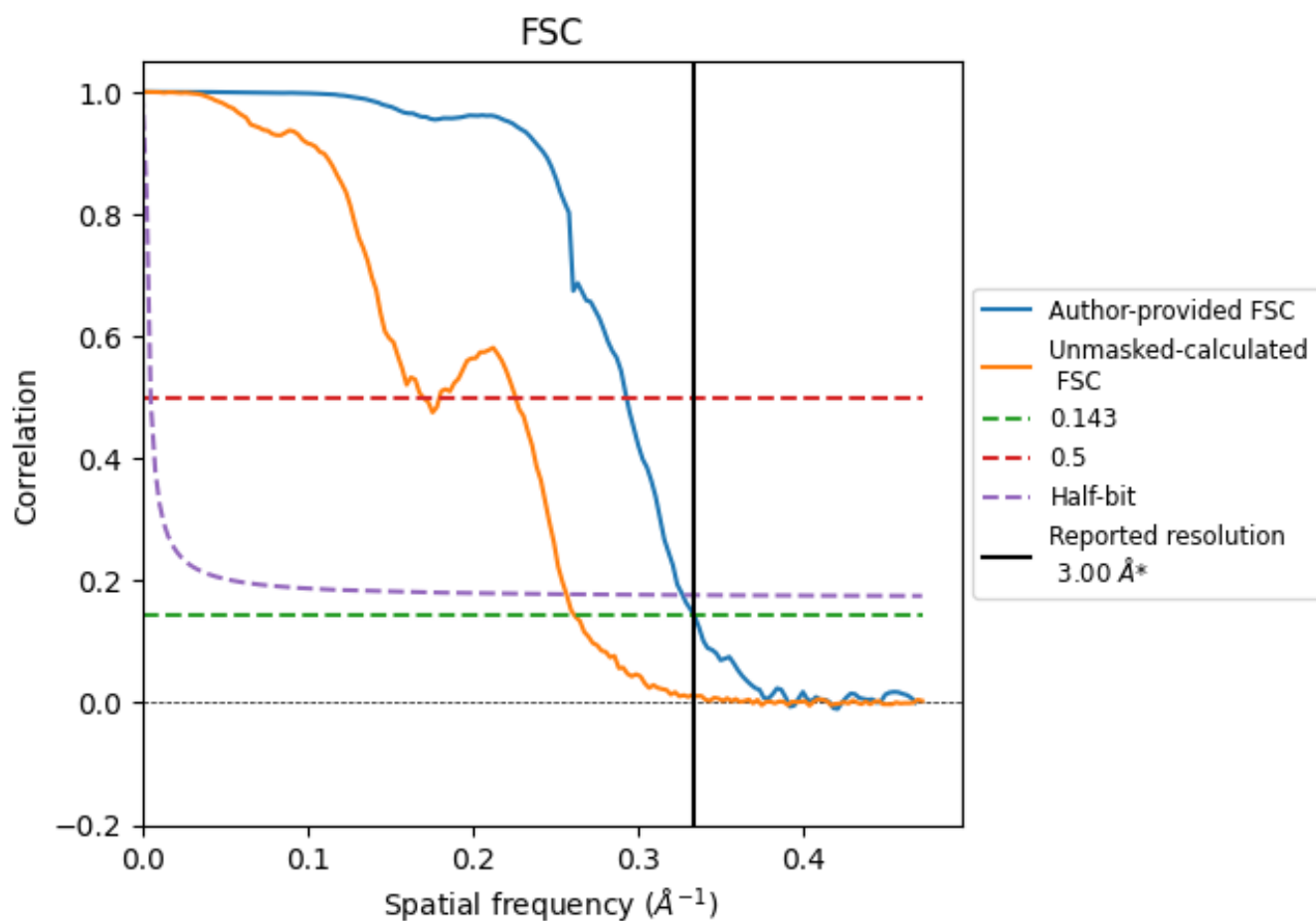


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.42	3.06
Unmasked-calculated*	3.83	5.89	3.90

*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 3.83 differs from the reported value 3.0 by more than 10 %

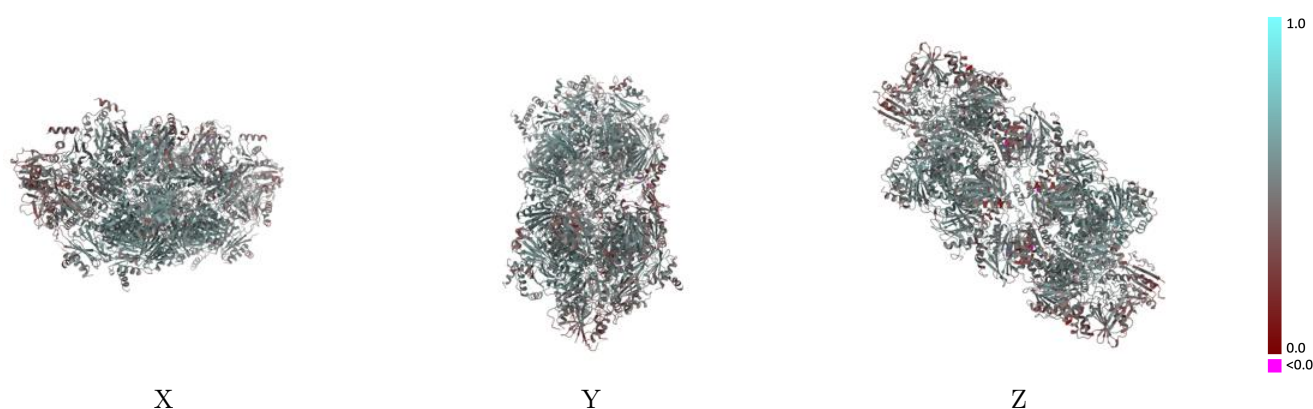
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40938 and PDB model 8T08. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

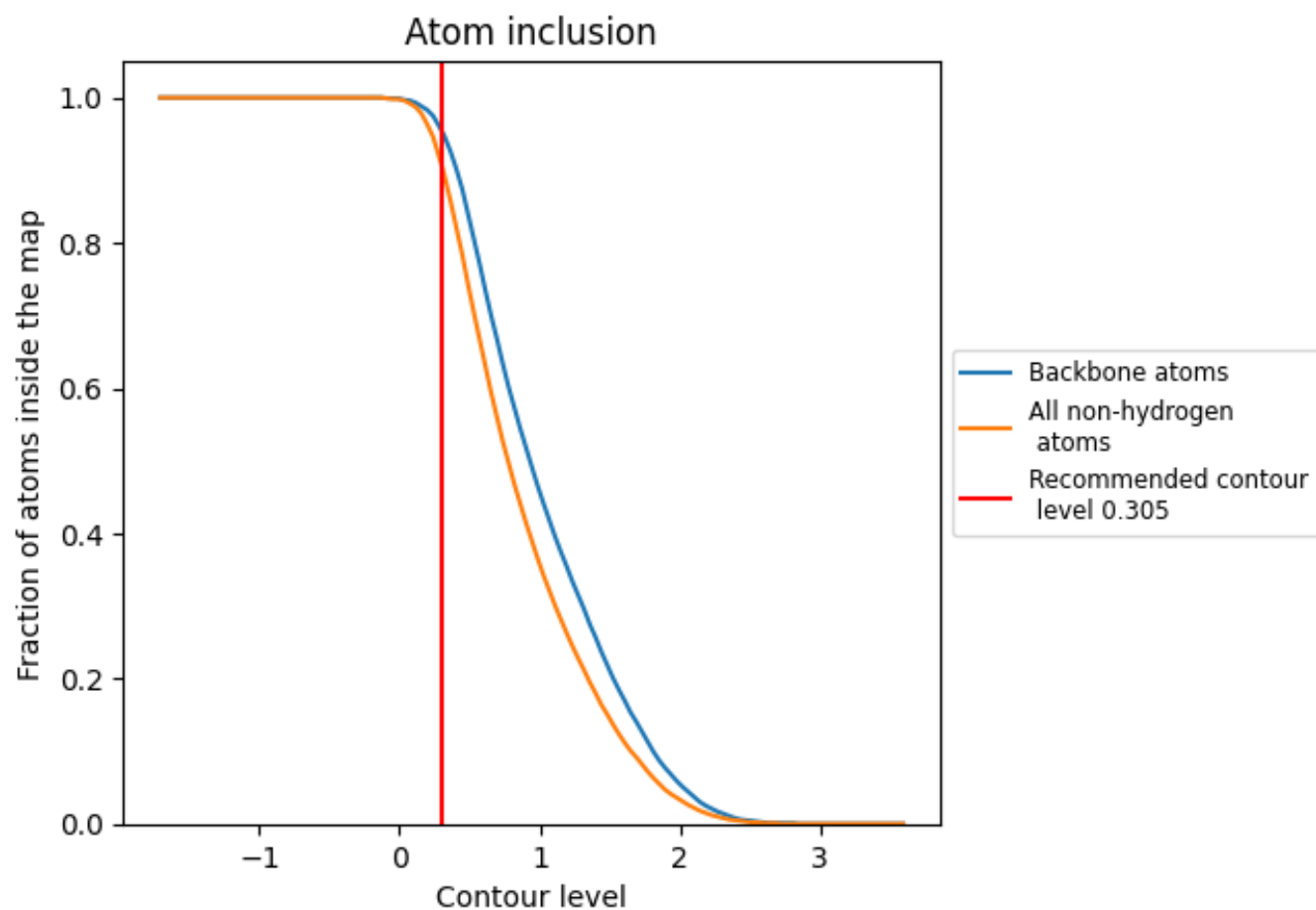


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.5040
A	 0.9340	 0.5420
B	 0.9300	 0.5460
C	 0.9330	 0.5360
D	 0.9190	 0.5190
E	 0.8860	 0.4900
F	 0.9000	 0.4800
G	 0.9300	 0.5230
H	 0.8640	 0.5230
I	 0.9250	 0.5430
J	 0.9180	 0.5280
K	 0.9000	 0.4750
L	 0.8440	 0.4060
M	 0.8960	 0.4970
N	 0.9320	 0.5470
O	 0.8180	 0.4220
P	 0.8650	 0.4260
Q	 0.9410	 0.5400
R	 0.9330	 0.5440
S	 0.9310	 0.5440
T	 0.9330	 0.5350
U	 0.9190	 0.5180
V	 0.8840	 0.4930
W	 0.8980	 0.4790
X	 0.9310	 0.5220
Y	 0.8630	 0.5220
Z	 0.9250	 0.5430
a	 0.9180	 0.5280
b	 0.9010	 0.4780
c	 0.8440	 0.4050
d	 0.8910	 0.4950
e	 0.9320	 0.5470
f	 0.8160	 0.4260
g	 0.8640	 0.4240
h	 0.9400	 0.5400

