



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:13 PM UTC

PDB ID : 8RVP / pdb_00008rvp
EMDB ID : EMD-19528
Title : Proteasomal late precursor complex from prel-1, state 2
Authors : Mark, E.; Ramos, P.C.; Kayser, F.; Hoeckendorff, J.; Dohmen, R.J.; Wendler, P.
Deposited on : 2024-02-01
Resolution : 2.28 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:

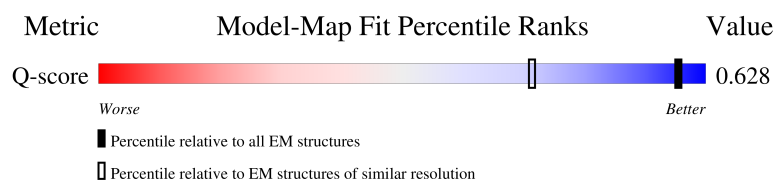
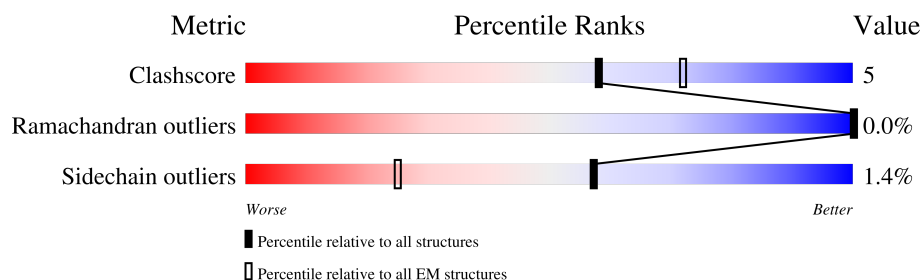
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.28 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.



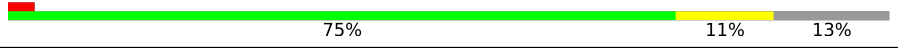
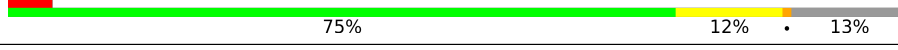
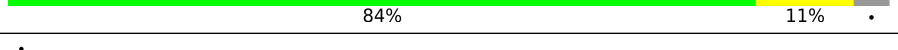
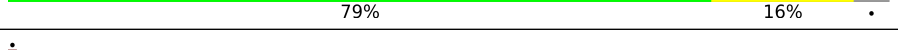
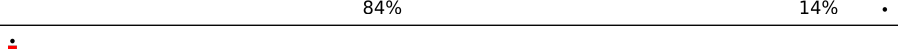
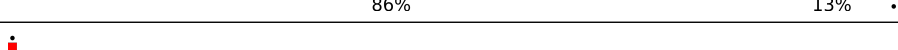
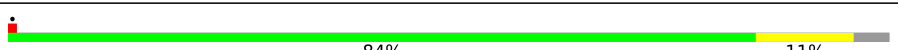
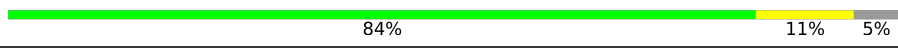
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3643 (1.78 - 2.78)

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	1	241	
1	M	241	
2	2	266	
2	N	266	

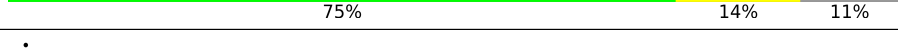
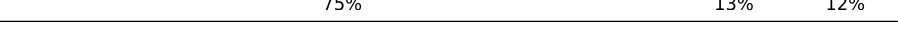
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	3	148	
3	6	148	
4	4	276	
4	7	276	
5	5	267	
5	8	267	
6	A	252	
6	O	252	
7	B	250	
7	P	250	
8	C	258	
8	Q	258	
9	D	254	
9	R	254	
10	E	260	
10	S	260	
11	F	234	
11	T	234	
12	G	288	
12	U	288	
13	H	215	
13	V	215	
14	I	261	
14	W	261	
15	J	205	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	X	205	 9% 82% 10% 8%
16	K	212	 9% 78% 12% 10%
16	Y	212	 6% 81% 8% 10%
17	L	287	 5% 75% 14% 11%
17	Z	287	 75% 13% 12%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 61572 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 beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	210	Total	C	N	O	S	0	0
			1663	1058	286	315	4		
1	M	210	Total	C	N	O	S	0	0
			1663	1058	286	315	4		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	224	Total	C	N	O	S	0	0
			1753	1108	300	338	7		
2	N	223	Total	C	N	O	S	0	0
			1745	1104	299	335	7		

- Molecule 3 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	142	Total	C	N	O	S	0	0
			1133	698	200	228	7		
3	6	143	Total	C	N	O	S	0	0
			1139	701	201	230	7		

- Molecule 4 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	239	Total	C	N	O	S	0	0
			1861	1211	288	349	13		
4	7	241	Total	C	N	O	S	0	0
			1879	1222	292	352	13		

- Molecule 5 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	244	Total	C	N	O	S	0	0
			1980	1285	320	367	8		
5	8	249	Total	C	N	O	S	0	0
			2025	1315	323	380	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	241	Total	C	N	O	S	0	0
			1900	1210	319	363	8		
6	O	241	Total	C	N	O	S	0	0
			1900	1210	319	363	8		

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	249	Total	C	N	O	S	0	0
			1906	1213	314	375	4		
7	P	250	Total	C	N	O	S	0	0
			1914	1219	315	376	4		

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	236	Total	C	N	O	S	0	0
			1856	1176	312	365	3		
8	Q	243	Total	C	N	O	S	0	0
			1900	1199	320	378	3		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	245	Total	C	N	O	S	0	0
			1923	1199	337	383	4		
9	R	242	Total	C	N	O	S	0	0
			1899	1186	333	376	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	250	Total	C	N	O	S	0	0
			1933	1209	325	391	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	249	Total	C	N	O	S	0	0
			1924	1204	324	388	8		

- Molecule 11 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		
11	T	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		

- Molecule 12 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	245	Total	C	N	O	S	0	0
			1900	1208	329	359	4		
12	U	244	Total	C	N	O	S	0	0
			1892	1205	328	355	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	207	LYS	ASN	conflict	UNP P21242
U	208	LYS	ASN	conflict	UNP P21242

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	205	Total	C	N	O	S	0	0
			1575	996	261	311	7		
13	V	205	Total	C	N	O	S	0	0
			1575	996	261	311	7		

- Molecule 14 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	208	Total	C	N	O	S	0	0
			1576	992	274	304	6		
14	W	215	Total	C	N	O	S	0	0
			1629	1024	285	314	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	191	THR	LEU	conflict	UNP P25043
I	192	PRO	THR	conflict	UNP P25043
I	193	THR	-	insertion	UNP P25043
W	191	THR	LEU	conflict	UNP P25043
W	192	PRO	THR	conflict	UNP P25043
W	193	THR	-	insertion	UNP P25043

- Molecule 15 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	186	Total	C	N	O	S	0	0
			1452	937	234	273	8		
15	X	189	Total	C	N	O	S	0	0
			1469	948	237	276	8		

- Molecule 16 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	191	Total	C	N	O	S	0	0
			1532	973	260	294	5		
16	Y	190	Total	C	N	O	S	0	0
			1529	975	259	290	5		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	engineered mutation	UNP P22141
K	199	ASP	-	expression tag	UNP P22141
K	200	TYR	-	expression tag	UNP P22141
K	201	LYS	-	expression tag	UNP P22141
K	202	ASP	-	expression tag	UNP P22141
K	203	ASP	-	expression tag	UNP P22141
K	204	ASP	-	expression tag	UNP P22141
K	205	ASP	-	expression tag	UNP P22141
K	206	LYS	-	expression tag	UNP P22141
K	207	HIS	-	expression tag	UNP P22141
K	208	HIS	-	expression tag	UNP P22141
K	209	HIS	-	expression tag	UNP P22141
K	210	HIS	-	expression tag	UNP P22141
K	211	HIS	-	expression tag	UNP P22141
K	212	HIS	-	expression tag	UNP P22141
Y	142	PHE	SER	engineered mutation	UNP P22141
Y	199	ASP	-	expression tag	UNP P22141

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	200	TYR	-	expression tag	UNP P22141
Y	201	LYS	-	expression tag	UNP P22141
Y	202	ASP	-	expression tag	UNP P22141
Y	203	ASP	-	expression tag	UNP P22141
Y	204	ASP	-	expression tag	UNP P22141
Y	205	ASP	-	expression tag	UNP P22141
Y	206	LYS	-	expression tag	UNP P22141
Y	207	HIS	-	expression tag	UNP P22141
Y	208	HIS	-	expression tag	UNP P22141
Y	209	HIS	-	expression tag	UNP P22141
Y	210	HIS	-	expression tag	UNP P22141
Y	211	HIS	-	expression tag	UNP P22141
Y	212	HIS	-	expression tag	UNP P22141

- Molecule 17 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	254	Total	C	N	O	S	0	0
			1969	1248	338	374	9		
17	Z	252	Total	C	N	O	S	0	0
			1958	1241	337	371	9		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	1	60	Total	O	0
			60	60	
18	2	66	Total	O	0
			66	66	
18	3	35	Total	O	0
			35	35	
18	4	50	Total	O	0
			50	50	
18	5	49	Total	O	0
			49	49	
18	6	50	Total	O	0
			50	50	
18	7	41	Total	O	0
			41	41	
18	8	76	Total	O	0
			76	76	
18	A	64	Total	O	0
			64	64	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	B	67	Total O 67 67	0
18	C	56	Total O 56 56	0
18	D	63	Total O 63 63	0
18	E	72	Total O 72 72	0
18	F	63	Total O 63 63	0
18	G	66	Total O 66 66	0
18	H	62	Total O 62 62	0
18	I	53	Total O 53 53	0
18	J	57	Total O 57 57	0
18	K	56	Total O 56 56	0
18	L	53	Total O 53 53	0
18	M	73	Total O 73 73	0
18	N	60	Total O 60 60	0
18	O	62	Total O 62 62	0
18	P	75	Total O 75 75	0
18	Q	59	Total O 59 59	0
18	R	56	Total O 56 56	0
18	S	76	Total O 76 76	0
18	T	53	Total O 53 53	0
18	U	54	Total O 54 54	0
18	V	69	Total O 69 69	0

Continued on next page...

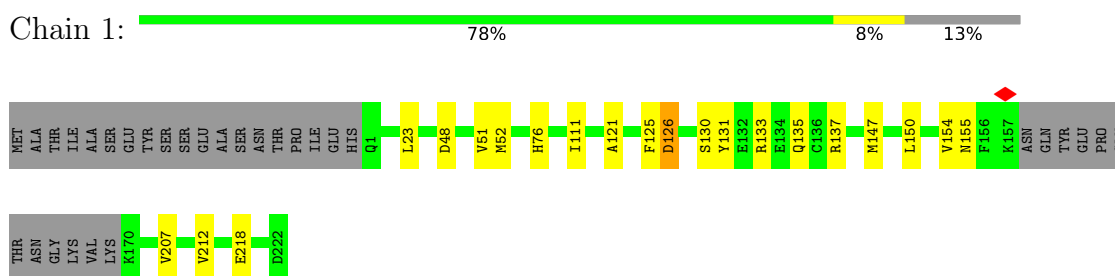
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
18	W	61	Total 61	O 61	0
18	X	64	Total 64	O 64	0
18	Y	44	Total 44	O 44	0
18	Z	51	Total 51	O 51	0

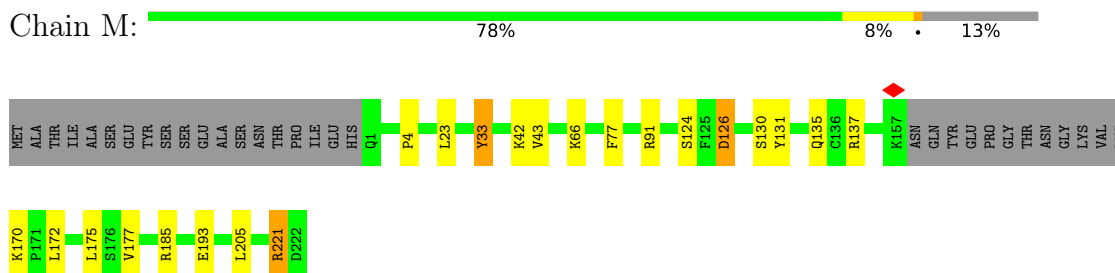
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

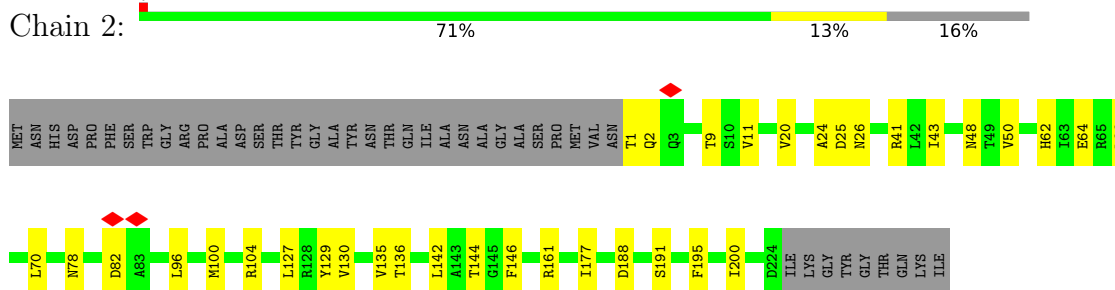
- Molecule 1: Proteasome subunit beta type-6



- Molecule 1: Proteasome subunit beta type-6

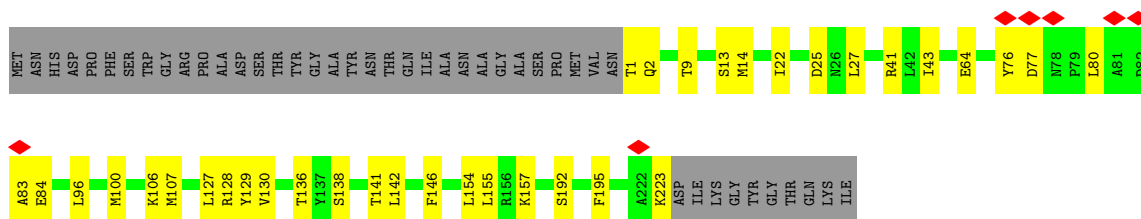


- Molecule 2: Proteasome subunit beta type-7

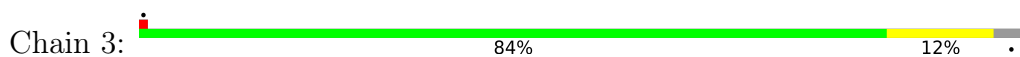


- Molecule 2: Proteasome subunit beta type-7

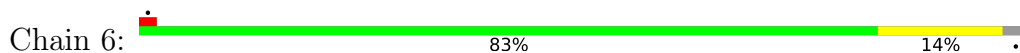




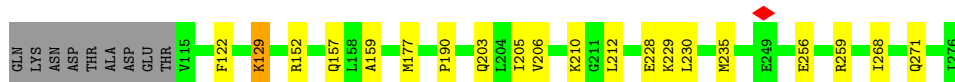
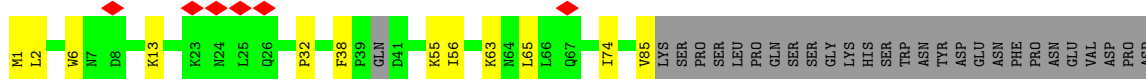
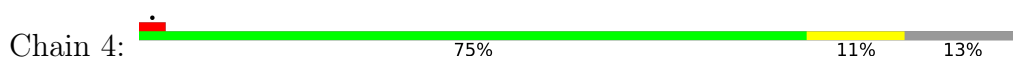
- Molecule 3: Proteasome maturation factor UMP1



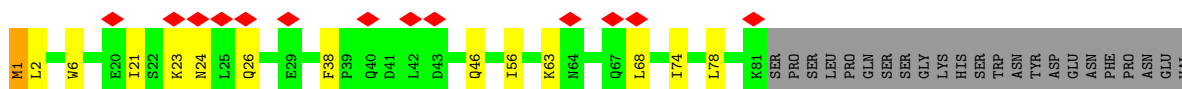
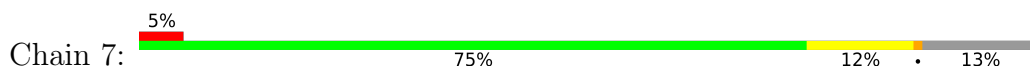
- Molecule 3: Proteasome maturation factor UMP1



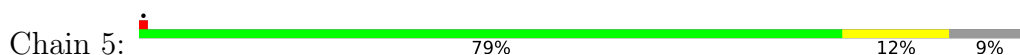
- Molecule 4: Proteasome chaperone 1

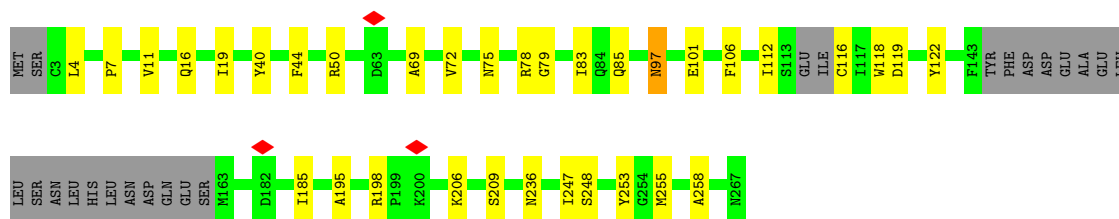


- Molecule 4: Proteasome chaperone 1



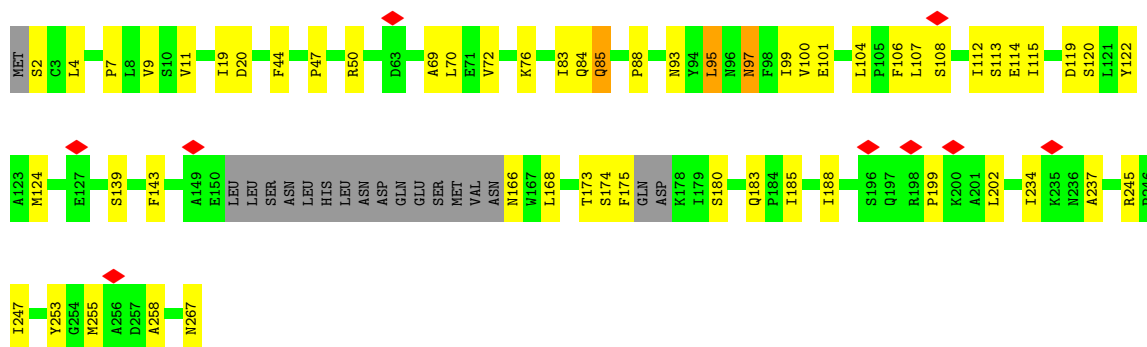
- Molecule 5: Proteasome assembly chaperone 2





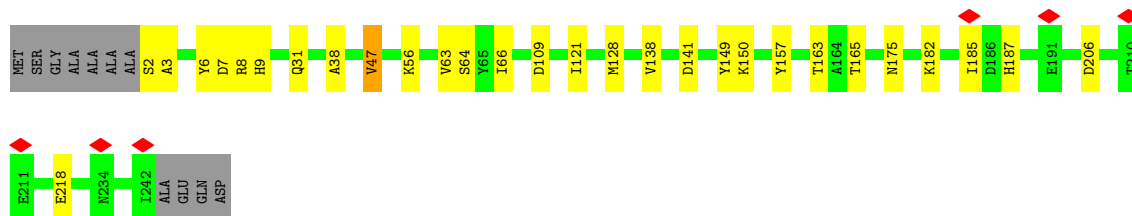
- Molecule 5: Proteasome assembly chaperone 2

Chain 8: 72% 20% 7%



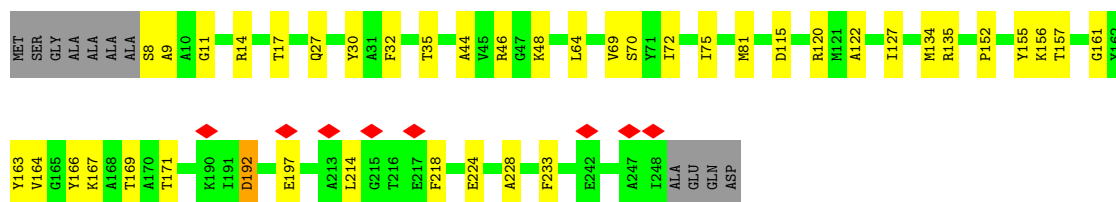
- Molecule 6: Proteasome subunit alpha type-1

Chain A: 84% 11% 5%



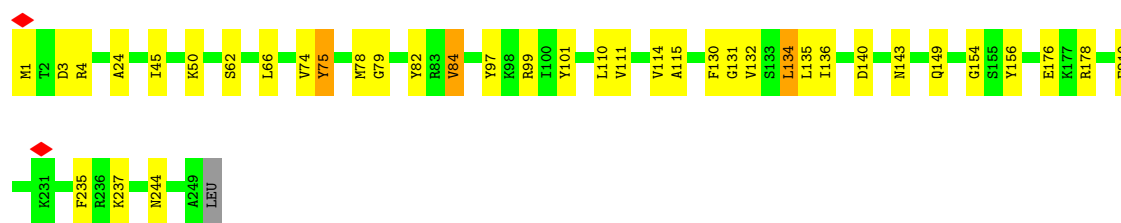
- Molecule 6: Proteasome subunit alpha type-1

Chain O: 79% 16% 5%

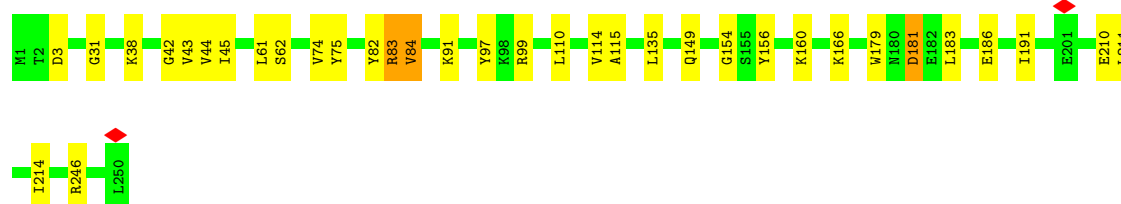
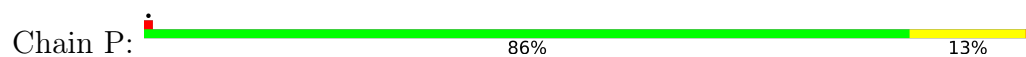


- Molecule 7: Proteasome subunit alpha type-2

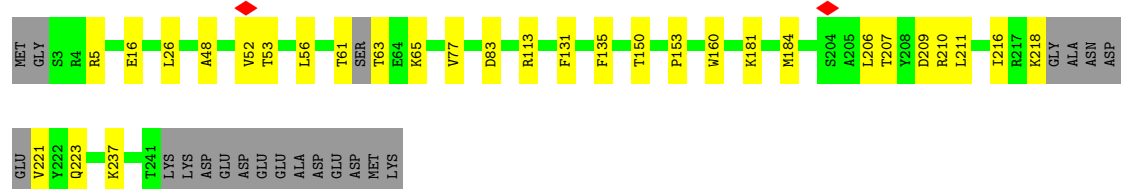
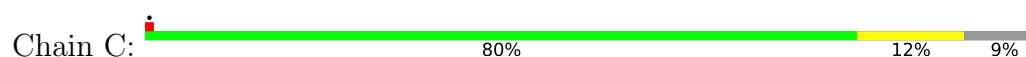
Chain B: 84% 14% 2%



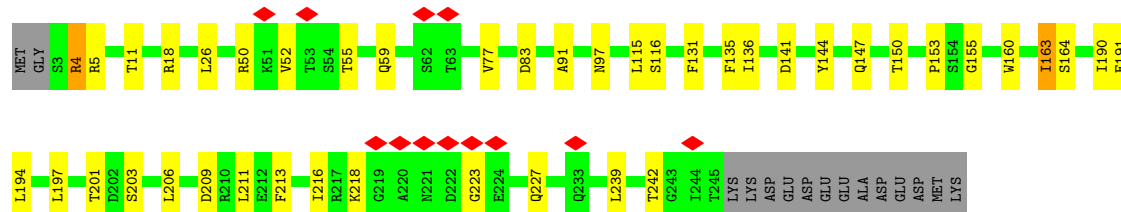
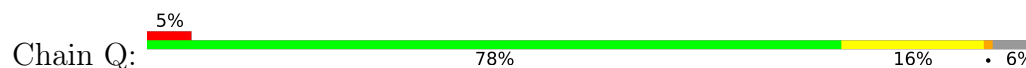
• Molecule 7: Proteasome subunit alpha type-2



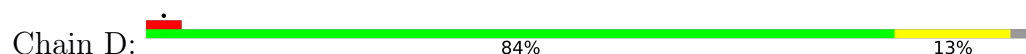
• Molecule 8: Proteasome subunit alpha type-3

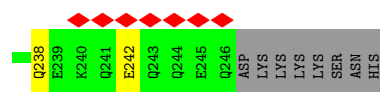


• Molecule 8: Proteasome subunit alpha type-3

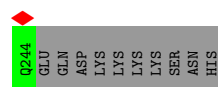
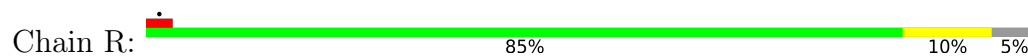


• Molecule 9: Proteasome subunit alpha type-4

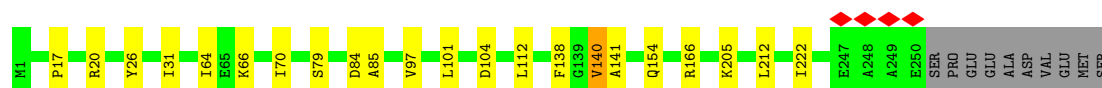
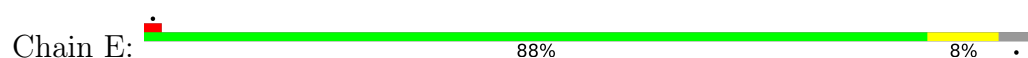




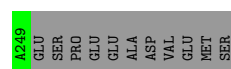
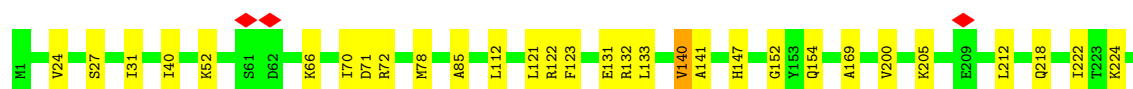
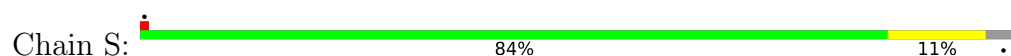
- Molecule 9: Proteasome subunit alpha type-4



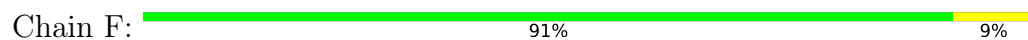
- Molecule 10: Proteasome subunit alpha type-5



- Molecule 10: Proteasome subunit alpha type-5



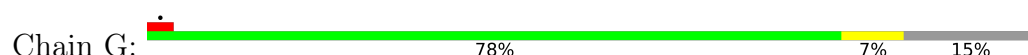
- Molecule 11: Proteasome subunit alpha type-6



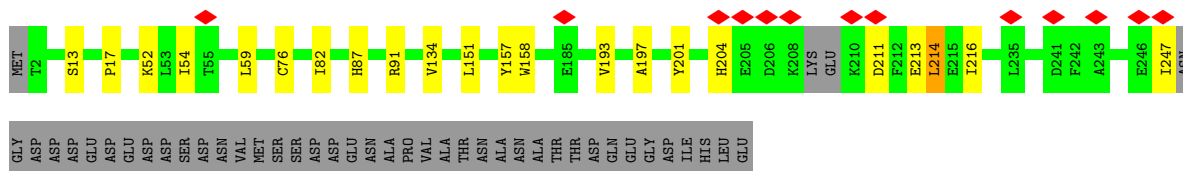
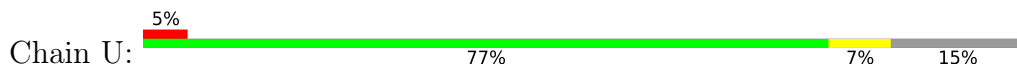
- Molecule 11: Proteasome subunit alpha type-6



- Molecule 12: Probable proteasome subunit alpha type-7



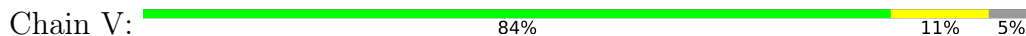
- Molecule 12: Probable proteasome subunit alpha type-7



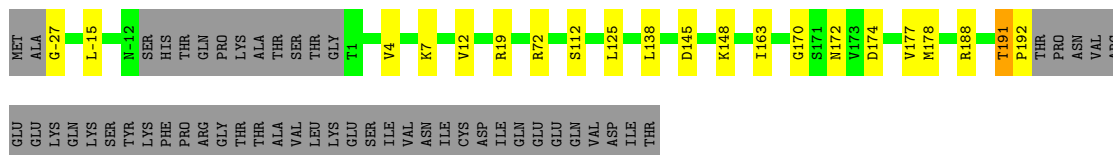
- Molecule 13: Proteasome subunit beta type-1



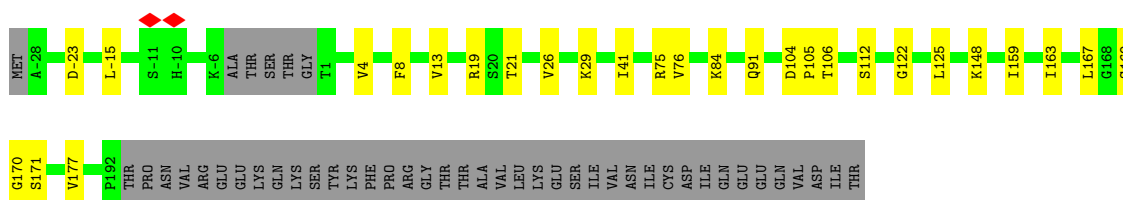
- Molecule 13: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-2

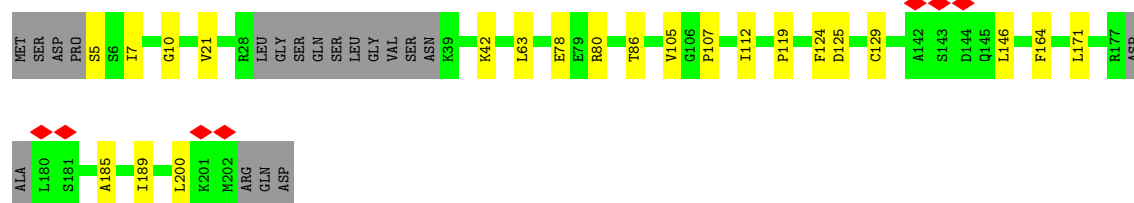


- Molecule 14: Proteasome subunit beta type-2



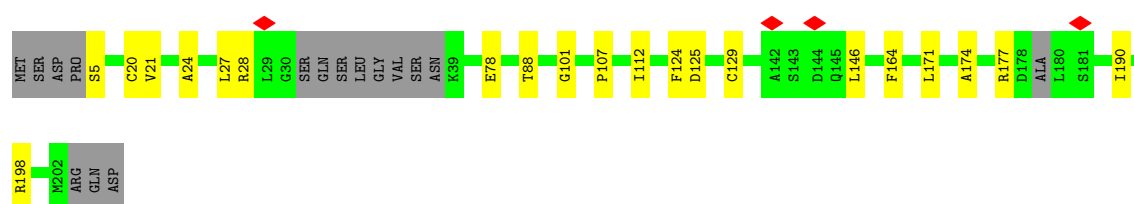
- Molecule 15: Proteasome subunit beta type-3

Chain J: 



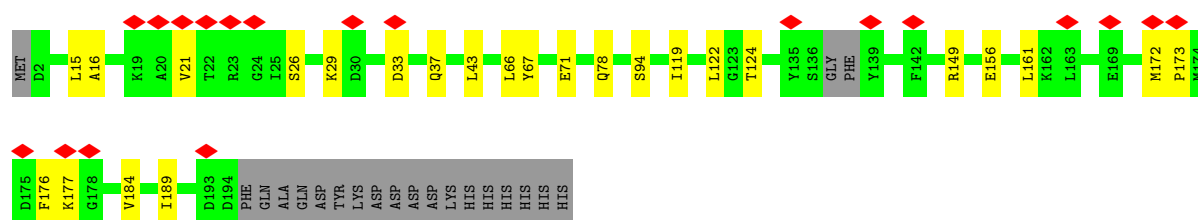
- Molecule 15: Proteasome subunit beta type-3

Chain X: 



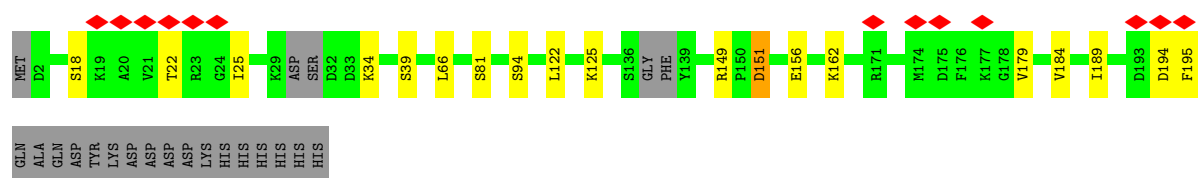
- Molecule 16: Proteasome subunit beta type-4

Chain K: 



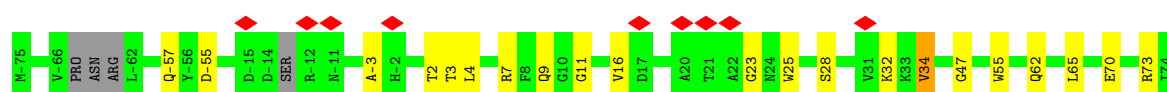
- Molecule 16: Proteasome subunit beta type-4

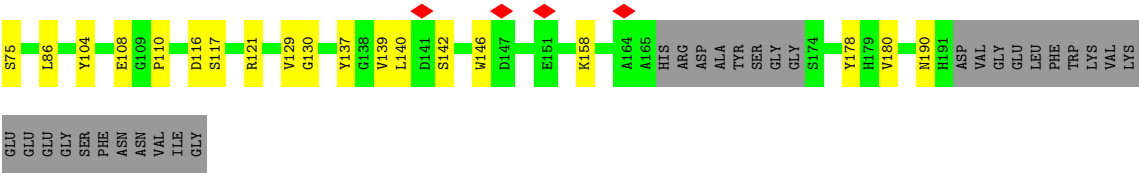
Chain Y: 



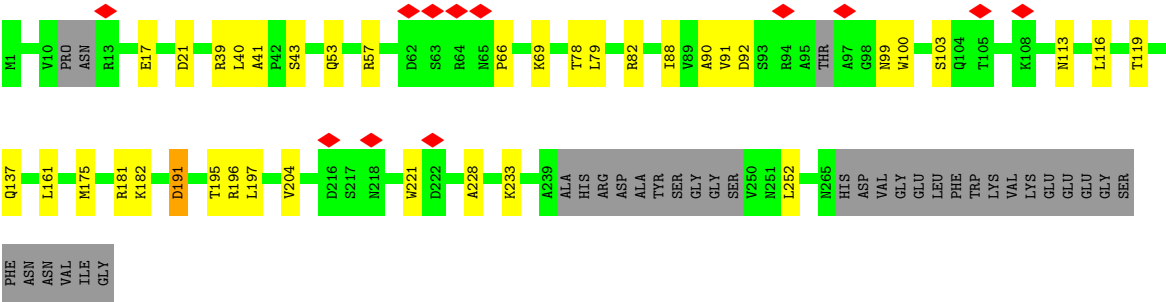
- Molecule 17: Proteasome subunit beta type-5

Chain L: 





● Molecule 17: Proteasome subunit beta type-5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169652	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.702	Depositor
Minimum map value	-0.922	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.205	Depositor
Map size ($\text{\AA}$)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.834, 0.834, 0.834	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	1	0.13	0/1698	0.30	0/2289
1	M	0.12	0/1698	0.32	0/2289
2	2	0.13	0/1783	0.32	0/2420
2	N	0.13	0/1775	0.32	0/2409
3	3	0.11	0/1151	0.25	0/1556
3	6	0.11	0/1157	0.25	0/1564
4	4	0.11	0/1904	0.26	0/2582
4	7	0.11	0/1923	0.27	0/2608
5	5	0.10	0/2028	0.25	0/2754
5	8	0.10	0/2075	0.27	0/2818
6	A	0.13	0/1938	0.31	0/2625
6	O	0.13	0/1938	0.30	0/2625
7	B	0.13	0/1943	0.31	0/2631
7	P	0.13	0/1951	0.30	0/2642
8	C	0.12	0/1884	0.30	0/2548
8	Q	0.13	0/1930	0.31	0/2613
9	D	0.11	0/1952	0.27	0/2642
9	R	0.12	0/1927	0.29	0/2607
10	E	0.11	0/1960	0.26	0/2640
10	S	0.12	0/1951	0.28	0/2628
11	F	0.11	0/1830	0.29	0/2473
11	T	0.12	0/1830	0.29	0/2473
12	G	0.12	0/1939	0.28	0/2618
12	U	0.11	0/1931	0.26	0/2606
13	H	0.13	0/1604	0.31	0/2171
13	V	0.13	0/1604	0.34	0/2171
14	I	0.13	0/1606	0.32	0/2179
14	W	0.13	0/1661	0.33	1/2254 (0.0%)
15	J	0.13	0/1479	0.30	0/1993
15	X	0.12	0/1496	0.31	0/2016
16	K	0.10	0/1558	0.28	0/2100
16	Y	0.10	0/1555	0.27	0/2094
17	L	0.11	0/2009	0.26	0/2720
17	Z	0.11	0/1997	0.26	0/2702

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.12	0/60665	0.29	1/82060 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	W	171	SER	CB-CA-C	-5.38	109.91	117.23

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	1	1663	0	1620	13	0
1	M	1663	0	1620	19	0
2	2	1753	0	1754	18	0
2	N	1745	0	1750	20	0
3	3	1133	0	1113	12	0
3	6	1139	0	1118	17	0
4	4	1861	0	1888	21	0
4	7	1879	0	1910	22	0
5	5	1980	0	1957	20	0
5	8	2025	0	1986	33	0
6	A	1900	0	1897	19	0
6	O	1900	0	1897	32	0
7	B	1906	0	1918	29	0
7	P	1914	0	1929	22	0
8	C	1856	0	1864	21	0
8	Q	1900	0	1898	27	0
9	D	1923	0	1927	22	0
9	R	1899	0	1907	16	0
10	E	1933	0	1908	14	0
10	S	1924	0	1902	16	0
11	F	1802	0	1809	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	T	1802	0	1809	14	0
12	G	1900	0	1889	17	0
12	U	1892	0	1890	12	0
13	H	1575	0	1555	11	0
13	V	1575	0	1555	15	0
14	I	1576	0	1554	14	0
14	W	1629	0	1606	20	0
15	J	1452	0	1453	13	0
15	X	1469	0	1469	13	0
16	K	1532	0	1539	18	0
16	Y	1529	0	1538	12	0
17	L	1969	0	1932	28	0
17	Z	1958	0	1920	27	0
18	1	60	0	0	1	0
18	2	66	0	0	2	0
18	3	35	0	0	1	0
18	4	50	0	0	0	0
18	5	49	0	0	0	0
18	6	50	0	0	0	0
18	7	41	0	0	1	0
18	8	76	0	0	1	0
18	A	64	0	0	1	0
18	B	67	0	0	2	0
18	C	56	0	0	2	0
18	D	63	0	0	2	0
18	E	72	0	0	0	0
18	F	63	0	0	0	0
18	G	66	0	0	2	0
18	H	62	0	0	1	0
18	I	53	0	0	2	0
18	J	57	0	0	0	0
18	K	56	0	0	2	0
18	L	53	0	0	2	0
18	M	73	0	0	4	0
18	N	60	0	0	1	0
18	O	62	0	0	2	0
18	P	75	0	0	0	0
18	Q	59	0	0	1	0
18	R	56	0	0	0	0
18	S	76	0	0	1	0
18	T	53	0	0	0	0
18	U	54	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	V	69	0	0	1	0
18	W	61	0	0	1	0
18	X	64	0	0	2	0
18	Y	44	0	0	0	0
18	Z	51	0	0	2	0
All	All	61572	0	59281	556	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 (556) 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)
7:B:75:TYR:HE1	7:B:134:LEU:HG	1.37	0.89
8:Q:150:THR:HG21	8:Q:163:ILE:HD12	1.62	0.79
4:4:1:MET:HG3	11:F:124:GLY:HA3	1.65	0.79
5:8:11:VAL:HG21	5:8:122:TYR:HB2	1.66	0.77
13:H:34:LEU:HD13	13:H:176:VAL:HG23	1.69	0.75
9:R:73:LEU:HD11	9:R:133:THR:HB	1.67	0.74
8:Q:141:ASP:OD1	8:Q:147:GLN:NE2	2.22	0.73
4:4:74:ILE:HB	4:4:122:PHE:HB3	1.72	0.72
9:D:73:LEU:HD11	9:D:133:THR:HB	1.70	0.72
17:L:7:ARG:HG3	17:L:110:PRO:HB2	1.74	0.70
9:D:73:LEU:HD13	9:D:135:ILE:HG12	1.73	0.70
8:C:53:THR:HG21	8:C:210:ARG:HG2	1.75	0.69
8:Q:197:LEU:O	8:Q:201:THR:OG1	2.11	0.69
14:I:163:ILE:HG23	14:I:170:GLY:HA2	1.75	0.68
3:3:105:ILE:HG21	7:B:84:VAL:HG13	1.75	0.68
9:R:73:LEU:HD13	9:R:135:ILE:HG12	1.75	0.68
17:L:25:TRP:HB3	1:M:137:ARG:HD3	1.73	0.68
4:7:74:ILE:HB	4:7:122:PHE:HB3	1.76	0.68
9:R:81:ASP:HB3	9:R:129:PHE:HD1	1.59	0.67
4:4:230:LEU:O	4:4:271:GLN:NE2	2.29	0.66
4:4:229:LYS:HZ1	10:E:20:ARG:HD3	1.60	0.66
6:A:175:ASN:ND2	6:A:206:ASP:OD1	2.28	0.66
7:P:181:ASP:N	7:P:181:ASP:OD1	2.29	0.66
10:S:123:PHE:O	10:S:132:ARG:NH1	2.30	0.65
14:W:163:ILE:HG23	14:W:170:GLY:HA2	1.78	0.65
9:R:141:ARG:HD3	17:Z:182:LYS:HB3	1.77	0.65
17:Z:39:ARG:NH1	17:Z:43:SER:OG	2.30	0.65
7:B:75:TYR:CE1	7:B:134:LEU:HG	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:75:TYR:CE2	7:B:132:VAL:HB	2.32	0.65
15:J:107:PRO:HG2	15:J:124:PHE:HB2	1.78	0.65
14:I:7:LYS:HG3	14:I:12:VAL:HG12	1.79	0.64
2:N:25:ASP:OD1	2:N:41:ARG:NH2	2.28	0.64
5:8:267:ASN:HB2	12:U:82:ILE:HD11	1.79	0.64
14:W:104:ASP:OD1	14:W:106:THR:OG1	2.14	0.64
17:Z:66:PRO:HA	17:Z:69:LYS:HE2	1.79	0.64
8:C:48:ALA:HB1	8:C:65:LYS:HD3	1.80	0.64
10:S:154:GLN:NE2	18:S:303:HOH:O	2.30	0.64
13:V:19:ARG:HB2	13:V:170:GLY:HA3	1.80	0.63
13:V:34:LEU:HD13	13:V:176:VAL:HG23	1.78	0.63
10:E:104:ASP:HB2	1:M:91:ARG:HD2	1.81	0.63
3:6:105:ILE:HG21	7:P:84:VAL:HG13	1.81	0.63
10:E:85:ALA:HB2	10:E:140:VAL:HG11	1.80	0.63
15:X:146:LEU:HD13	15:X:174:ALA:HB2	1.80	0.63
7:B:97:TYR:OH	15:J:78:GLU:OE2	2.10	0.62
16:K:149:ARG:NH2	16:K:156:GLU:OE1	2.32	0.62
5:5:11:VAL:HG21	5:5:122:TYR:HB2	1.82	0.62
1:M:221:ARG:NH2	14:W:169:SER:O	2.32	0.62
8:Q:201:THR:HG22	8:Q:203:SER:H	1.65	0.62
15:J:185:ALA:HB3	15:J:200:LEU:HB2	1.81	0.62
2:N:14:MET:HE2	2:N:155:LEU:HD22	1.81	0.62
10:S:31:ILE:HD13	10:S:141:ALA:HB2	1.82	0.62
3:6:114:GLU:OE2	6:O:120:ARG:NH1	2.32	0.61
15:J:10:GLY:HA3	15:J:42:LYS:HE2	1.82	0.61
4:7:21:ILE:HB	5:8:93:ASN:HD21	1.66	0.61
14:W:19:ARG:NH2	14:W:167:LEU:O	2.31	0.61
17:Z:113:ASN:HD21	17:Z:116:LEU:HD12	1.65	0.61
6:A:185:ILE:HG22	6:A:187:HIS:H	1.66	0.61
14:I:15:LEU:HD21	16:K:122:LEU:HD11	1.83	0.61
13:V:53:GLN:OE1	14:W:84:LYS:NZ	2.34	0.61
10:E:17:PRO:HB3	11:F:3:ARG:HH12	1.66	0.61
6:O:122:ALA:HB3	7:P:83:ARG:HH12	1.66	0.61
14:I:172:ASN:HA	14:I:192:PRO:HG2	1.84	0.60
10:E:31:ILE:HD13	10:E:141:ALA:HB2	1.84	0.60
9:D:81:ASP:HB3	9:D:129:PHE:HD1	1.67	0.59
8:C:5:ARG:O	9:D:6:ARG:NH2	2.34	0.59
6:O:214:LEU:HD12	6:O:218:PHE:HZ	1.68	0.59
5:5:195:ALA:HB3	5:5:198:ARG:HB3	1.82	0.59
7:P:97:TYR:OH	15:X:78:GLU:OE2	2.13	0.59
6:O:14:ARG:NH2	18:O:305:HOH:O	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:109:ILE:O	6:O:120:ARG:NH2	2.36	0.59
17:L:7:ARG:NH2	18:L:303:HOH:O	2.33	0.59
11:T:156:LEU:HB3	12:U:59:LEU:HD23	1.83	0.59
5:5:255:MET:HB2	5:5:258:ALA:HB2	1.84	0.59
8:Q:26:LEU:HD23	8:Q:153:PRO:HD2	1.85	0.59
10:S:205:LYS:HB2	10:S:212:LEU:HD22	1.85	0.58
15:X:107:PRO:HG2	15:X:124:PHE:HB2	1.84	0.58
17:L:2:THR:HA	17:L:130:GLY:HA3	1.84	0.58
6:O:46:ARG:NH1	18:O:304:HOH:O	2.35	0.58
14:W:104:ASP:HB2	14:W:105:PRO:HD2	1.85	0.58
8:Q:191:GLU:HG2	8:Q:242:THR:HG22	1.83	0.58
1:M:185:ARG:NH2	18:M:306:HOH:O	2.36	0.58
6:A:141:ASP:OD2	14:I:72:ARG:NH2	2.25	0.58
7:P:62:SER:OG	7:P:210:GLU:OE2	2.21	0.58
1:I:155:ASN:ND2	18:I:305:HOH:O	2.35	0.58
8:Q:216:ILE:HG12	8:Q:227:GLN:HG2	1.84	0.58
9:R:62:SER:OG	9:R:211:GLU:OE2	2.22	0.58
5:5:116:CYS:SG	5:5:118:TRP:NE1	2.75	0.58
17:Z:191:ASP:OD1	17:Z:191:ASP:N	2.37	0.58
6:O:32:PHE:O	6:O:35:THR:OG1	2.19	0.57
3:3:50:ARG:HH22	16:K:94:SER:HB3	1.68	0.57
5:5:7:PRO:HG3	5:5:19:ILE:HG13	1.86	0.57
8:C:113:ARG:NH2	16:K:71:GLU:OE2	2.34	0.57
1:M:172:LEU:HD12	1:M:175:LEU:HD12	1.87	0.57
8:C:206:LEU:HD11	8:C:211:LEU:HD21	1.86	0.57
10:E:70:ILE:HG21	10:E:112:LEU:HD21	1.86	0.57
7:P:149:GLN:O	7:P:156:TYR:HA	2.03	0.57
5:8:255:MET:HB2	5:8:258:ALA:HB2	1.85	0.57
7:B:78:MET:H	7:B:132:VAL:HG12	1.69	0.57
17:L:62:GLN:NE2	18:L:304:HOH:O	2.35	0.57
2:2:127:LEU:HG	2:2:142:LEU:HD12	1.86	0.57
2:N:1:THR:N	18:N:304:HOH:O	2.37	0.57
15:X:28:ARG:NH2	18:X:307:HOH:O	2.38	0.57
9:D:238:GLN:NE2	9:D:242:GLU:OE2	2.37	0.56
17:Z:119:THR:HB	17:Z:175:MET:H	1.69	0.56
14:I:191:THR:HG23	14:I:192:PRO:HD3	1.87	0.56
4:7:68:LEU:HD23	4:7:127:PHE:HB3	1.87	0.56
7:B:62:SER:OG	7:B:210:GLU:OE2	2.21	0.56
5:5:253:TYR:HA	11:F:3:ARG:HB2	1.87	0.56
2:N:80:LEU:HB3	2:N:83:ALA:HB3	1.87	0.56
6:O:70:SER:OG	6:O:224:GLU:OE2	2.22	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:4:LEU:HD11	5:5:83:ILE:HG13	1.88	0.56
3:6:131:SER:HB2	8:Q:97:ASN:HB3	1.86	0.55
9:R:103:PRO:HG2	9:R:140:PRO:HG3	1.88	0.55
3:3:133:MET:HE1	16:K:67:TYR:HB2	1.87	0.55
7:B:111:VAL:HG22	7:B:136:ILE:HD12	1.88	0.55
1:M:193:GLU:OE1	14:W:29:LYS:NZ	2.31	0.55
16:Y:184:VAL:HG22	16:Y:189:ILE:HG12	1.88	0.55
3:6:13:VAL:HG11	3:6:47:LEU:HD11	1.89	0.55
4:7:189:PRO:HA	5:8:47:PRO:HG2	1.89	0.55
5:8:2:SER:HB2	5:8:113:SER:H	1.71	0.55
9:D:62:SER:OG	9:D:211:GLU:OE2	2.24	0.55
16:K:184:VAL:HG22	16:K:189:ILE:HG12	1.88	0.55
17:L:55:TRP:CE3	17:L:86:LEU:HD21	2.42	0.55
10:S:122:ARG:NH1	10:S:131:GLU:O	2.39	0.55
5:8:180:SER:HB3	5:8:183:GLN:HG3	1.88	0.55
1:M:4:PRO:HG3	2:N:107:MET:HE1	1.89	0.55
8:C:218:LYS:HG2	8:C:221:VAL:HG22	1.89	0.54
8:Q:4:ARG:HD3	8:Q:5:ARG:HG3	1.90	0.54
17:L:28:SER:HA	1:M:135:GLN:HG3	1.88	0.54
2:2:43:ILE:HG12	2:2:64:GLU:HG2	1.88	0.54
12:G:12:ASN:O	18:G:301:HOH:O	2.18	0.54
12:U:87:HIS:O	12:U:91:ARG:HG2	2.07	0.54
5:5:40:TYR:OH	5:5:101:GLU:OE1	2.25	0.54
5:8:166:ASN:N	18:8:308:HOH:O	2.39	0.54
11:F:80:ASP:HB2	11:F:130:VAL:HG23	1.89	0.54
11:T:52:ASN:ND2	11:T:54:ASP:O	2.41	0.54
1:1:207:VAL:HG22	1:1:212:VAL:HG22	1.90	0.54
5:5:16:GLN:NE2	5:5:85:GLN:O	2.36	0.54
17:Z:233:LYS:NZ	18:Z:305:HOH:O	2.40	0.54
9:R:34:VAL:HG22	9:R:163:THR:HG22	1.90	0.54
13:V:101:GLY:O	13:V:108:GLY:HA2	2.07	0.54
8:C:26:LEU:HD23	8:C:153:PRO:HD2	1.90	0.54
9:D:58:ARG:HG3	9:D:59:ILE:HG23	1.89	0.54
8:Q:77:VAL:HG22	8:Q:135:PHE:HE1	1.73	0.54
13:V:171:GLY:O	13:V:193:TYR:OH	2.22	0.54
1:1:23:LEU:HD23	1:1:51:VAL:HG12	1.89	0.54
5:8:72:VAL:HG22	5:8:83:ILE:HG12	1.90	0.54
8:C:237:LYS:NZ	18:C:309:HOH:O	2.41	0.54
5:8:70:LEU:HD13	5:8:85:GLN:HG3	1.90	0.53
14:I:-27:GLY:N	18:I:303:HOH:O	2.40	0.53
2:2:129:TYR:O	2:2:136:THR:HA	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:210:ARG:NH2	18:C:308:HOH:O	2.41	0.53
4:4:235:MET:HE1	4:4:268:ILE:HB	1.89	0.53
4:4:256:GLU:OE1	4:4:259:ARG:NH2	2.41	0.53
6:A:31:GLN:NE2	12:G:19:GLY:O	2.42	0.53
12:G:173:LYS:NZ	18:G:308:HOH:O	2.41	0.53
11:T:176:LEU:HA	11:T:179:PHE:CE1	2.43	0.53
12:G:214:LEU:HD21	12:G:216:ILE:HD11	1.89	0.53
13:H:4:MET:HE1	13:H:158:SER:HB2	1.91	0.53
13:V:152:VAL:HG13	13:V:175:MET:HE1	1.91	0.53
4:7:46:GLN:O	4:7:129:LYS:NZ	2.37	0.53
4:7:170:THR:HG21	4:7:230:LEU:HD21	1.91	0.53
7:B:74:VAL:HG22	7:B:75:TYR:H	1.74	0.53
1:M:66:LYS:NZ	18:M:311:HOH:O	2.42	0.53
2:N:128:ARG:HD3	2:N:138:SER:HB2	1.90	0.53
2:2:25:ASP:OD1	2:2:41:ARG:NH2	2.41	0.53
5:8:7:PRO:HG3	5:8:19:ILE:HG13	1.91	0.53
5:8:99:ILE:HD13	5:8:188:ILE:HA	1.91	0.53
6:O:48:LYS:HD2	6:O:197:GLU:HG2	1.90	0.53
9:D:205:THR:OG1	9:D:209:ASN:OD1	2.20	0.53
17:L:-3:ALA:HB3	17:L:47:GLY:H	1.73	0.52
6:O:115:ASP:HB3	6:O:155:TYR:CZ	2.44	0.52
16:Y:149:ARG:NH2	16:Y:156:GLU:OE1	2.42	0.52
7:B:176:GLU:HG2	8:C:56:LEU:HD23	1.91	0.52
17:L:158:LYS:NZ	17:L:190:ASN:O	2.41	0.52
13:V:-8:LYS:NZ	14:W:91:GLN:OE1	2.37	0.52
13:V:107:LYS:NZ	18:V:205:HOH:O	2.42	0.52
16:Y:22:THR:HG21	17:Z:197:LEU:HD22	1.90	0.52
4:7:276:ILE:HD12	11:T:62:LYS:HE3	1.90	0.52
8:Q:206:LEU:HD11	8:Q:211:LEU:HD21	1.92	0.52
14:W:122:GLY:HA3	14:W:125:LEU:HD21	1.90	0.52
6:O:228:ALA:HB2	6:O:233:PHE:HD1	1.75	0.52
8:Q:83:ASP:HB3	8:Q:131:PHE:HD1	1.75	0.52
5:5:72:VAL:HG22	5:5:83:ILE:HG12	1.90	0.52
17:L:73:ARG:NH2	17:L:104:TYR:O	2.41	0.52
10:E:154:GLN:HG2	10:E:166:ARG:HH21	1.75	0.52
17:L:32:LYS:NZ	17:L:178:TYR:OH	2.35	0.52
12:U:54:ILE:HD12	12:U:211:ASP:HB3	1.90	0.52
1:1:218:GLU:OE2	2:2:161:ARG:NH1	2.38	0.52
9:D:172:ARG:NH2	18:D:307:HOH:O	2.43	0.52
6:A:64:SER:OG	6:A:218:GLU:OE2	2.26	0.52
2:N:43:ILE:HG12	2:N:64:GLU:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:74:VAL:HG12	7:B:135:LEU:HB2	1.93	0.51
16:Y:151:ASP:OD1	16:Y:151:ASP:N	2.34	0.51
7:B:75:TYR:CD2	7:B:82:TYR:HB2	2.45	0.51
8:C:216:ILE:HG12	8:C:223:GLN:HG2	1.92	0.51
12:G:87:HIS:O	12:G:91:ARG:HG2	2.11	0.51
2:N:127:LEU:HG	2:N:142:LEU:HD12	1.92	0.51
2:N:154:LEU:O	2:N:157:LYS:HB2	2.10	0.51
8:C:83:ASP:HB3	8:C:131:PHE:HD1	1.76	0.51
2:N:129:TYR:O	2:N:136:THR:HA	2.11	0.51
6:O:46:ARG:NH2	6:O:192:ASP:OD2	2.44	0.51
8:Q:218:LYS:HD2	8:Q:223:GLY:HA2	1.92	0.51
5:8:115:ILE:HG13	5:8:202:LEU:HD11	1.93	0.50
2:2:82:ASP:N	2:2:82:ASP:OD1	2.44	0.50
3:6:34:ARG:HG2	3:6:134:VAL:HG11	1.93	0.50
5:8:20:ASP:OD1	5:8:84:GLN:NE2	2.44	0.50
17:L:3:THR:HG23	17:L:16:VAL:HG12	1.93	0.50
3:3:42:PRO:HG2	3:3:45:THR:HG23	1.92	0.50
9:D:48:ARG:O	9:D:209:ASN:ND2	2.44	0.50
11:F:11:VAL:HA	12:G:130:ARG:HB2	1.94	0.50
11:T:88:LEU:HD11	11:T:108:ALA:HB1	1.94	0.50
14:W:-15:LEU:HD21	16:Y:122:LEU:HD11	1.94	0.50
7:B:1:MET:HB3	7:B:4:ARG:HG3	1.93	0.50
7:B:134:LEU:HD13	7:B:136:ILE:HD11	1.93	0.50
4:4:32:PRO:HG2	4:4:85:VAL:HG22	1.93	0.50
5:5:119:ASP:O	5:5:209:SER:HA	2.11	0.50
5:8:108:SER:HB3	5:8:199:PRO:HB3	1.93	0.50
2:2:66:LEU:HD21	17:Z:17:GLU:HG3	1.92	0.50
3:6:42:PRO:O	3:6:45:THR:OG1	2.30	0.50
4:4:190:PRO:HB3	5:5:248:SER:HB2	1.94	0.50
1:1:126:ASP:OD1	1:1:130:SER:N	2.45	0.49
3:3:60:TRP:O	3:3:64:GLN:HG2	2.12	0.49
4:4:205:ILE:HG22	4:4:206:VAL:HG13	1.93	0.49
5:5:116:CYS:HB3	5:5:206:LYS:HB2	1.93	0.49
11:F:88:LEU:HD11	11:F:108:ALA:HB1	1.93	0.49
9:R:226:SER:O	9:R:227:GLU:N	2.44	0.49
17:Z:40:LEU:HG	17:Z:137:GLN:HE22	1.77	0.49
2:2:78:ASN:ND2	18:2:307:HOH:O	2.40	0.49
12:U:52:LYS:HG3	12:U:213:GLU:HB2	1.94	0.49
2:2:62:HIS:NE2	17:Z:17:GLU:OE2	2.38	0.49
6:O:164:VAL:HG23	7:P:61:LEU:HB2	1.95	0.49
3:6:60:TRP:O	3:6:64:GLN:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:121:THR:HG22	9:R:128:PRO:HB3	1.93	0.49
3:3:34:ARG:NH1	18:3:203:HOH:O	2.36	0.49
3:3:91:VAL:HG23	6:A:128:MET:HE1	1.95	0.49
1:M:170:LYS:N	18:M:313:HOH:O	2.44	0.49
1:1:125:PHE:CD2	1:1:131:TYR:HB3	2.48	0.49
5:8:119:ASP:OD1	5:8:120:SER:N	2.42	0.49
7:P:38:LYS:HG3	7:P:43:VAL:HG22	1.94	0.49
8:Q:11:THR:HA	9:R:127:ARG:HB2	1.94	0.49
6:A:2:SER:N	18:A:307:HOH:O	2.45	0.49
14:I:12:VAL:HG23	14:I:178:MET:HE3	1.94	0.49
7:P:183:LEU:HD21	7:P:191:ILE:HD12	1.95	0.49
13:V:90:LYS:HD3	13:V:116:GLY:O	2.12	0.48
16:Y:25:ILE:HD12	17:Z:204:VAL:HG22	1.95	0.48
9:D:101:GLU:OE1	17:L:121:ARG:NH2	2.39	0.48
12:G:216:ILE:HB	12:G:231:VAL:HG21	1.94	0.48
11:T:74:LEU:HD22	11:T:81:ALA:HB1	1.94	0.48
13:H:-5:GLU:OE2	13:H:48:SER:OG	2.23	0.48
13:H:90:LYS:HD3	13:H:116:GLY:O	2.14	0.48
2:2:1:THR:OG1	2:2:2:GLN:N	2.45	0.48
5:5:75:ASN:O	5:5:79:GLY:N	2.47	0.48
8:C:218:LYS:HA	8:C:221:VAL:HA	1.96	0.48
4:4:13:LYS:NZ	11:F:4:ASN:O	2.46	0.48
4:4:152:ARG:NH1	4:4:203:GLN:OE1	2.46	0.48
3:6:91:VAL:HG23	6:O:134:MET:HE1	1.95	0.48
8:C:77:VAL:HG22	8:C:135:PHE:HE1	1.79	0.48
9:R:67:ILE:HG21	9:R:109:LEU:HD21	1.96	0.48
5:5:78:ARG:HB3	5:5:236:ASN:HB3	1.95	0.48
17:L:116:ASP:OD1	17:L:117:SER:N	2.45	0.48
9:R:81:ASP:N	9:R:81:ASP:OD1	2.45	0.48
17:Z:88:ILE:HG13	17:Z:228:ALA:HB1	1.96	0.48
16:K:177:LYS:NZ	18:K:307:HOH:O	2.46	0.48
17:L:23:GLY:O	15:X:177:ARG:NH1	2.46	0.48
2:N:14:MET:HG3	2:N:141:THR:HG22	1.95	0.48
8:Q:91:ALA:HB2	8:Q:115:LEU:HD11	1.96	0.48
14:I:112:SER:HB3	14:I:125:LEU:HD13	1.96	0.48
2:N:1:THR:OG1	2:N:2:GLN:N	2.47	0.48
5:8:97:ASN:OD1	5:8:97:ASN:N	2.46	0.47
9:D:34:VAL:HG23	9:D:163:THR:HG22	1.96	0.47
5:5:44:PHE:HB3	5:5:69:ALA:HB2	1.95	0.47
8:Q:190:ILE:HG23	8:Q:213:PHE:CZ	2.49	0.47
14:W:75:ARG:NH1	18:W:307:HOH:O	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:21:VAL:HG23	15:X:190:ILE:HB	1.95	0.47
4:4:65:LEU:HD22	4:4:256:GLU:HG3	1.95	0.47
3:6:42:PRO:HG2	3:6:45:THR:HG23	1.96	0.47
4:7:205:ILE:HG22	4:7:206:VAL:HG13	1.96	0.47
10:S:52:LYS:HE3	10:S:218:GLN:HB2	1.96	0.47
4:7:256:GLU:OE2	4:7:259:ARG:NH2	2.48	0.47
8:C:61:THR:O	8:C:63:THR:N	2.47	0.47
13:V:37:VAL:HG12	13:V:63:LEU:HD12	1.97	0.47
12:G:54:ILE:HD13	12:G:211:ASP:HB3	1.96	0.47
10:E:84:ASP:HB3	10:E:138:PHE:CD1	2.49	0.47
13:H:143:ARG:NH1	18:H:208:HOH:O	2.44	0.47
6:O:135:ARG:HD3	12:U:13:SER:HB2	1.96	0.47
1:1:52:MET:HG3	1:1:111:ILE:HG22	1.96	0.47
15:J:63:LEU:HD11	15:J:105:VAL:HG21	1.95	0.47
6:O:8:SER:OG	6:O:9:ALA:N	2.46	0.47
7:P:186:GLU:OE1	7:P:246:ARG:NH1	2.35	0.47
10:S:70:ILE:HG21	10:S:112:LEU:HD21	1.95	0.47
13:V:175:MET:HE2	13:V:188:PHE:HE2	1.80	0.47
16:Y:81:SER:HB3	16:Y:125:LYS:HD2	1.96	0.47
7:B:149:GLN:O	7:B:156:TYR:HA	2.14	0.47
4:7:24:ASN:ND2	18:7:307:HOH:O	2.47	0.47
11:F:63:ILE:HG21	11:F:214:ALA:HB2	1.97	0.47
16:K:172:MET:HG3	16:K:173:PRO:HD2	1.96	0.47
2:N:130:VAL:HB	2:N:136:THR:HG22	1.97	0.47
15:J:5:SER:O	15:J:7:ILE:HG12	2.15	0.47
8:Q:18:ARG:NH1	18:Q:309:HOH:O	2.46	0.47
9:R:101:GLU:OE1	17:Z:196:ARG:NH2	2.38	0.47
17:Z:82:ARG:HH21	17:Z:221:TRP:HH2	1.63	0.47
6:A:38:ALA:HB3	6:A:163:THR:HG22	1.97	0.46
10:E:205:LYS:HB2	10:E:212:LEU:HD22	1.97	0.46
11:F:74:LEU:HD22	11:F:81:ALA:HB1	1.97	0.46
12:G:51:GLU:HB2	12:G:200:ILE:HG23	1.97	0.46
8:Q:50:ARG:HB3	8:Q:52:VAL:HG13	1.97	0.46
17:L:32:LYS:HG3	17:L:34:VAL:H	1.80	0.46
2:N:13:SER:HB3	2:N:22:ILE:HG13	1.97	0.46
14:W:112:SER:HB3	14:W:125:LEU:HD13	1.97	0.46
17:L:11:GLY:HA3	17:L:180:VAL:O	2.16	0.46
7:B:244:ASN:ND2	18:B:310:HOH:O	2.48	0.46
13:V:4:MET:HE3	13:V:4:MET:HB2	1.64	0.46
7:B:62:SER:OG	7:B:237:LYS:NZ	2.43	0.46
14:I:174:ASP:OD2	14:I:188:ARG:NH1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:109:ILE:HB	6:O:127:ILE:HD11	1.98	0.46
12:G:218:TRP:NE1	12:G:231:VAL:HG22	2.30	0.46
10:S:66:LYS:HA	10:S:78:MET:HE2	1.97	0.46
4:4:2:LEU:N	7:B:3:ASP:OD2	2.49	0.46
9:D:204:GLN:HG3	9:D:205:THR:HG23	1.97	0.46
6:O:44:ALA:HB3	6:O:169:THR:HG22	1.98	0.46
5:8:4:LEU:HB2	5:8:112:ILE:HD13	1.98	0.46
11:F:227:GLY:O	11:F:230:VAL:HG22	2.15	0.46
1:M:43:VAL:HG12	1:M:205:LEU:HD12	1.98	0.46
13:V:148:LYS:NZ	13:V:184:GLU:OE1	2.37	0.46
3:3:80:GLU:HB3	3:3:81:PRO:HD3	1.97	0.46
5:8:253:TYR:HA	11:T:3:ARG:HB2	1.97	0.46
14:W:148:LYS:HE3	14:W:177:VAL:HG11	1.97	0.46
5:8:139:SER:HG	5:8:174:SER:HG	1.59	0.45
17:L:75:SER:OG	17:L:108:GLU:OE2	2.34	0.45
4:4:56:ILE:HD12	4:4:228:GLU:HB2	1.98	0.45
1:M:126:ASP:OD1	1:M:130:SER:N	2.43	0.45
12:U:151:LEU:HD13	12:U:157:TYR:HB3	1.98	0.45
15:X:88:THR:HG23	15:X:124:PHE:CZ	2.52	0.45
5:8:100:VAL:HG23	5:8:101:GLU:HG3	1.98	0.45
16:K:37:GLN:HA	16:K:43:LEU:HD12	1.98	0.45
12:U:193:VAL:HG13	12:U:216:ILE:HG21	1.98	0.45
1:1:137:ARG:CZ	17:Z:100:TRP:HB3	2.46	0.45
5:8:143:PHE:HB2	5:8:168:LEU:HD23	1.98	0.45
11:F:80:ASP:HB2	11:F:130:VAL:CG2	2.46	0.45
1:M:33:TYR:HD1	1:M:33:TYR:HA	1.62	0.45
8:Q:77:VAL:HG22	8:Q:135:PHE:CE1	2.51	0.45
2:2:50:VAL:HG23	2:2:200:ILE:HD11	1.98	0.45
5:5:97:ASN:OD1	5:5:97:ASN:N	2.49	0.45
8:Q:59:GLN:HG2	8:Q:209:ASP:HB2	1.98	0.45
4:4:206:VAL:HA	4:4:210:LYS:HE2	1.98	0.45
11:F:164:ARG:HH11	11:F:202:ARG:HD3	1.81	0.45
9:R:79:ASN:O	9:R:82:SER:OG	2.20	0.45
10:S:85:ALA:HB2	10:S:140:VAL:HG11	1.98	0.45
17:Z:79:LEU:HG	17:Z:90:ALA:HB3	1.97	0.45
6:A:109:ASP:HB3	6:A:149:TYR:CZ	2.52	0.45
11:F:45:VAL:HG12	11:F:215:ILE:HG13	1.99	0.45
5:8:234:ILE:HB	5:8:237:ALA:HB2	1.98	0.45
7:B:24:ALA:HB1	7:B:131:GLY:HA2	1.98	0.45
7:P:75:TYR:HB3	7:P:82:TYR:CD1	2.52	0.45
16:Y:18:SER:OG	16:Y:34:LYS:NZ	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:200:ILE:HG21	12:G:214:LEU:HD13	1.99	0.44
13:H:20:THR:HB	13:H:28:ASN:HB3	1.98	0.44
14:I:4:VAL:HG23	14:I:138:LEU:HD11	1.97	0.44
6:O:69:VAL:HA	12:U:158:TRP:CZ3	2.51	0.44
6:O:156:LYS:O	6:O:163:TYR:HA	2.17	0.44
3:3:106:HIS:CD2	6:A:121:ILE:HG12	2.51	0.44
7:B:110:LEU:O	7:B:114:VAL:HG23	2.17	0.44
7:B:176:GLU:HA	8:C:56:LEU:HD21	1.98	0.44
9:D:163:THR:O	9:D:172:ARG:NH2	2.48	0.44
2:N:84:GLU:CD	2:N:84:GLU:H	2.25	0.44
9:R:12:SER:OG	9:R:14:ASP:OD1	2.32	0.44
5:5:4:LEU:HB2	5:5:112:ILE:HD13	1.99	0.44
6:O:115:ASP:OD1	6:O:115:ASP:N	2.44	0.44
4:7:63:LYS:HE3	4:7:63:LYS:HB2	1.87	0.44
11:T:227:GLY:O	11:T:230:VAL:HG22	2.17	0.44
12:U:201:TYR:HB3	12:U:247:ILE:HD11	1.98	0.44
17:Z:233:LYS:HE3	17:Z:252:LEU:HD11	1.99	0.44
4:4:177:MET:HE2	4:4:177:MET:HB3	1.81	0.44
3:6:50:ARG:HH22	16:Y:94:SER:HG	1.63	0.44
4:7:262:ARG:HA	4:7:268:ILE:HD12	2.00	0.44
10:E:101:LEU:O	1:M:91:ARG:HD3	2.17	0.44
16:K:15:LEU:HD12	16:K:43:LEU:HD23	2.00	0.44
8:Q:144:TYR:HB2	8:Q:147:GLN:NE2	2.32	0.44
4:7:177:MET:HG3	4:7:218:VAL:O	2.18	0.44
13:H:152:VAL:HA	13:H:175:MET:HE1	2.00	0.44
3:6:106:HIS:CD2	6:O:127:ILE:HG12	2.53	0.44
5:8:50:ARG:HE	5:8:247:ILE:HD13	1.83	0.44
6:A:9:HIS:HA	12:G:14:VAL:HG22	2.00	0.44
8:C:207:THR:OG1	8:C:209:ASP:OD1	2.29	0.44
12:G:193:VAL:HG21	12:G:218:TRP:CE2	2.52	0.44
2:N:76:TYR:HA	2:N:77:ASP:HA	1.79	0.44
14:W:21:THR:HG22	14:W:26:VAL:HA	2.00	0.44
17:Z:78:THR:HG23	17:Z:91:VAL:HG12	1.99	0.44
4:7:56:ILE:HD12	4:7:228:GLU:HB2	2.00	0.44
2:N:27:LEU:HB2	2:N:192:SER:HB2	2.00	0.44
15:X:164:PHE:CE1	15:X:198:ARG:HD2	2.53	0.44
11:F:80:ASP:OD1	11:F:80:ASP:N	2.50	0.43
10:S:169:ALA:HB3	11:T:56:LEU:HD13	2.00	0.43
15:X:125:ASP:OD1	15:X:129:CYS:N	2.40	0.43
17:Z:181:ARG:NH2	18:Z:306:HOH:O	2.46	0.43
2:2:96:LEU:O	2:2:100:MET:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:28:SER:HB2	17:Z:41:ALA:HB2	2.00	0.43
13:H:39:ASP:OD1	13:H:39:ASP:N	2.51	0.43
14:I:148:LYS:HE3	14:I:177:VAL:HG11	1.99	0.43
1:1:135:GLN:HG3	17:Z:103:SER:HA	2.00	0.43
3:3:79:ALA:HA	3:3:82:MET:HE2	2.00	0.43
5:8:95:LEU:HD22	5:8:99:ILE:HD11	2.01	0.43
7:B:178:ARG:NH1	18:B:313:HOH:O	2.51	0.43
6:O:75:ILE:HD11	6:O:81:MET:HE2	2.00	0.43
7:P:74:VAL:HG12	7:P:135:LEU:HB2	2.00	0.43
4:7:74:ILE:HG13	4:7:124:ILE:HD11	1.99	0.43
5:8:139:SER:HA	5:8:173:THR:HB	2.01	0.43
15:J:112:ILE:HD13	15:J:119:PRO:HA	1.99	0.43
16:K:16:ALA:HB2	16:K:161:LEU:HD21	2.01	0.43
8:Q:160:TRP:CD2	8:Q:163:ILE:HG13	2.53	0.43
11:T:201:LEU:HD11	11:T:206:LEU:HG	2.00	0.43
11:T:63:ILE:HG21	11:T:214:ALA:HB2	1.99	0.43
6:A:66:ILE:HD12	6:A:218:GLU:HG2	2.01	0.43
8:C:150:THR:HG22	8:C:160:TRP:HE1	1.84	0.43
9:D:216:LYS:HB2	9:D:220:ASP:HB2	2.00	0.43
16:K:78:GLN:HE21	16:K:78:GLN:HB3	1.65	0.43
12:U:197:ALA:HA	12:U:214:LEU:HD11	2.01	0.43
7:B:101:TYR:HB3	15:J:86:THR:HG23	1.99	0.43
7:P:42:GLY:HA2	7:P:214:ILE:O	2.18	0.43
2:N:96:LEU:O	2:N:100:MET:HG2	2.19	0.43
4:4:38:PHE:CD2	4:4:157:GLN:HG3	2.54	0.43
4:4:129:LYS:H	4:4:129:LYS:HD3	1.83	0.43
15:J:78:GLU:OE1	15:J:80:ARG:NH1	2.51	0.43
16:K:172:MET:HG2	16:K:176:PHE:CD1	2.53	0.43
6:O:156:LYS:HB3	6:O:166:TYR:HE1	1.83	0.43
12:G:193:VAL:HG13	12:G:216:ILE:HG21	2.01	0.42
15:J:125:ASP:OD1	15:J:129:CYS:N	2.42	0.42
16:K:26:SER:HB3	17:L:137:TYR:CG	2.54	0.42
17:L:4:LEU:HD21	17:L:140:LEU:HD11	2.01	0.42
6:O:46:ARG:HB2	6:O:152:PRO:HB2	2.01	0.42
17:Z:53:GLN:OE1	17:Z:57:ARG:NH2	2.52	0.42
1:1:147:MET:HG2	17:Z:99:ASN:HA	2.01	0.42
3:6:79:ALA:HA	3:6:82:MET:HE2	2.00	0.42
5:8:124:MET:HG3	6:O:11:GLY:HA2	2.01	0.42
6:O:72:ILE:HD12	6:O:224:GLU:HG2	2.00	0.42
2:2:25:ASP:HA	2:2:195:PHE:HA	2.01	0.42
11:T:72:LEU:HA	11:T:133:LEU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:24:ASN:HB2	4:7:26:GLN:HE22	1.84	0.42
13:H:18:SER:HB2	13:H:31:THR:H	1.83	0.42
17:Z:21:ASP:OD1	17:Z:21:ASP:N	2.52	0.42
5:8:44:PHE:HB3	5:8:69:ALA:HB2	2.01	0.42
7:B:130:PHE:HB3	7:B:132:VAL:HG22	2.02	0.42
10:E:97:VAL:HG21	17:L:65:LEU:HD13	2.01	0.42
11:F:72:LEU:HA	11:F:133:LEU:O	2.20	0.42
17:L:9:GLN:HB3	17:L:146:TRP:O	2.20	0.42
4:7:2:LEU:N	7:P:3:ASP:OD2	2.53	0.42
17:L:65:LEU:HD12	17:L:65:LEU:HA	1.85	0.42
17:L:139:VAL:O	17:L:142:SER:OG	2.32	0.42
2:N:25:ASP:HA	2:N:195:PHE:HA	2.00	0.42
7:P:44:VAL:HG13	7:P:211:LEU:HD21	2.01	0.42
15:X:5:SER:N	18:X:314:HOH:O	2.51	0.42
5:8:72:VAL:HG11	5:8:106:PHE:CZ	2.54	0.42
16:K:119:ILE:HA	16:K:124:THR:O	2.20	0.42
17:L:-55:ASP:OD1	17:L:-55:ASP:N	2.53	0.42
15:X:24:ALA:HB1	15:X:171:LEU:HD11	2.01	0.42
3:3:109:ILE:HB	6:A:121:ILE:HD11	2.02	0.42
8:C:77:VAL:HG22	8:C:135:PHE:CE1	2.54	0.42
13:H:4:MET:HE3	13:H:4:MET:HB2	1.65	0.42
7:P:110:LEU:O	7:P:114:VAL:HG23	2.19	0.42
14:W:4:VAL:HG22	14:W:159:ILE:HD11	2.01	0.42
15:X:20:CYS:HA	15:X:112:ILE:HD11	2.02	0.42
16:Y:162:LYS:HE2	16:Y:195:PHE:CE2	2.54	0.42
5:8:99:ILE:HD11	5:8:188:ILE:HG12	2.02	0.42
8:C:16:GLU:HB3	9:D:29:ARG:NH2	2.34	0.42
13:H:1:THR:OG1	13:H:2:SER:N	2.53	0.42
1:M:42:LYS:HE3	1:M:42:LYS:HB2	1.74	0.42
6:O:157:THR:HG22	6:O:163:TYR:HB2	2.01	0.42
14:W:13:VAL:HG22	14:W:177:VAL:HG22	2.01	0.42
17:Z:191:ASP:OD1	17:Z:195:THR:HB	2.20	0.42
5:5:72:VAL:HG11	5:5:106:PHE:CZ	2.54	0.42
8:Q:163:ILE:HD13	8:Q:164:SER:N	2.35	0.42
8:Q:194:LEU:HD13	8:Q:239:LEU:HD23	2.02	0.42
11:T:71:GLY:HA3	11:T:222:PHE:CE1	2.54	0.42
4:4:152:ARG:HG2	4:4:203:GLN:CD	2.45	0.41
6:A:63:VAL:HA	12:G:158:TRP:CZ3	2.55	0.41
6:O:30:TYR:CD1	12:U:17:PRO:HA	2.55	0.41
4:7:78:LEU:HD23	4:7:118:TYR:HD2	1.84	0.41
4:7:177:MET:HE3	4:7:177:MET:HB2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:150:LYS:O	6:A:157:TYR:HA	2.20	0.41
11:F:107:ARG:HA	11:F:107:ARG:HD2	1.89	0.41
10:S:40:ILE:HD12	10:S:200:VAL:HG23	2.01	0.41
3:6:105:ILE:O	3:6:109:ILE:HG13	2.19	0.41
14:I:145:ASP:OD1	14:I:145:ASP:N	2.51	0.41
15:J:164:PHE:CD1	15:J:189:ILE:HD11	2.54	0.41
16:K:177:LYS:NZ	18:K:306:HOH:O	2.45	0.41
1:1:48:ASP:OD2	1:1:76:HIS:NE2	2.53	0.41
2:2:26:ASN:ND2	18:2:306:HOH:O	2.39	0.41
3:3:5:PRO:HG2	3:3:56:THR:HA	2.01	0.41
4:7:1:MET:HG3	7:P:3:ASP:OD1	2.19	0.41
7:B:79:GLY:O	7:B:82:TYR:HB3	2.20	0.41
4:4:159:ALA:HA	4:4:212:LEU:HD11	2.03	0.41
7:P:160:LYS:HD3	7:P:179:TRP:CH2	2.56	0.41
13:V:8:PHE:CE2	13:V:10:ASP:HB2	2.56	0.41
6:A:63:VAL:HA	12:G:158:TRP:HZ3	1.86	0.41
10:S:147:HIS:HA	10:S:152:GLY:O	2.21	0.41
9:D:8:LEU:HD11	9:D:128:PRO:HD3	2.02	0.41
11:F:77:LEU:N	11:F:130:VAL:HG22	2.36	0.41
10:S:71:ASP:OD1	10:S:72:ARG:N	2.51	0.41
10:S:121:LEU:HD22	11:T:79:PRO:HB3	2.02	0.41
16:Y:194:ASP:OD1	16:Y:194:ASP:N	2.54	0.41
4:4:55:LYS:HB3	4:4:55:LYS:HE2	1.81	0.41
5:8:99:ILE:O	5:8:104:LEU:HB2	2.20	0.41
6:A:3:ALA:O	6:A:8:ARG:NH2	2.54	0.41
9:D:12:SER:OG	9:D:14:ASP:OD1	2.30	0.41
10:E:84:ASP:HB3	10:E:138:PHE:HD1	1.86	0.41
15:J:21:VAL:HG13	15:J:119:PRO:HB3	2.03	0.41
15:J:171:LEU:HD23	15:J:171:LEU:HA	1.89	0.41
17:L:25:TRP:HB3	1:M:137:ARG:CD	2.46	0.41
1:M:124:SER:O	1:M:131:TYR:HA	2.21	0.41
8:Q:116:SER:HB3	8:Q:155:GLY:O	2.21	0.41
9:R:94:GLN:HG3	16:Y:66:LEU:HB2	2.03	0.41
1:1:150:LEU:O	1:1:154:VAL:HG22	2.21	0.41
2:2:129:TYR:HE2	2:2:144:THR:HG22	1.86	0.41
2:2:130:VAL:HA	2:2:135:VAL:O	2.21	0.41
5:5:50:ARG:HE	5:5:247:ILE:HD13	1.86	0.41
5:8:9:VAL:HG21	5:8:88:PRO:HA	2.03	0.41
7:B:66:LEU:HD12	7:B:235:PHE:CD1	2.55	0.41
7:B:140:ASP:OD2	7:B:143:ASN:ND2	2.47	0.41
9:D:13:PRO:HA	10:E:26:TYR:CD1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:94:GLN:HG3	16:K:66:LEU:HB2	2.03	0.41
10:E:64:ILE:HG23	10:E:66:LYS:HE2	2.02	0.41
17:L:-57:GLN:NE2	2:N:106:LYS:HD2	2.36	0.41
1:M:91:ARG:NH1	18:M:319:HOH:O	2.54	0.41
7:P:115:ALA:HB1	7:P:154:GLY:O	2.20	0.41
3:6:113:LYS:O	7:P:91:LYS:NZ	2.53	0.41
14:I:19:ARG:NH2	18:I:309:HOH:O	2.54	0.41
1:M:23:LEU:HD23	1:M:43:VAL:HG13	2.02	0.41
14:W:8:PHE:HE1	14:W:13:VAL:HG23	1.86	0.41
5:8:9:VAL:HG11	5:8:88:PRO:HB3	2.03	0.40
7:B:115:ALA:HB1	7:B:154:GLY:O	2.22	0.40
6:O:17:THR:HG22	6:O:27:GLN:HB2	2.03	0.40
6:O:167:LYS:HD2	6:O:192:ASP:HB2	2.03	0.40
8:Q:4:ARG:H	8:Q:4:ARG:HG3	1.55	0.40
14:W:-23:ASP:O	15:X:101:GLY:HA3	2.21	0.40
17:Z:92:ASP:OD1	17:Z:92:ASP:N	2.54	0.40
1:1:121:ALA:HB2	1:1:133:ARG:HH21	1.87	0.40
2:2:11:VAL:HG22	2:2:24:ALA:HB2	2.04	0.40
2:2:188:ASP:HB3	2:2:191:SER:HB3	2.03	0.40
6:A:6:TYR:C	6:A:8:ARG:H	2.29	0.40
14:W:41:ILE:HG12	14:W:76:VAL:HG22	2.02	0.40
6:A:47:VAL:HG13	6:A:138:VAL:HG11	2.04	0.40
7:B:75:TYR:CE2	7:B:82:TYR:HB2	2.55	0.40
8:C:181:LYS:HB2	8:C:184:MET:HG3	2.03	0.40
9:D:6:ARG:NH1	18:D:309:HOH:O	2.44	0.40
16:K:43:LEU:HD13	16:K:189:ILE:HD13	2.02	0.40
7:P:31:GLY:O	7:P:166:LYS:HG3	2.22	0.40
8:Q:136:ILE:HG12	8:Q:150:THR:HG22	2.03	0.40
10:S:24:VAL:O	10:S:27:SER:OG	2.26	0.40
4:7:38:PHE:CG	4:7:157:GLN:HG3	2.57	0.40
9:D:111:ARG:NH2	17:L:70:GLU:OE2	2.55	0.40
10:S:147:HIS:NE2	10:S:224:LYS:HD3	2.36	0.40
13:V:-8:LYS:HZ3	14:W:91:GLN:HB3	1.87	0.40
4:7:169:GLY:HA3	4:7:197:ILE:HG12	2.04	0.40
12:G:183:HIS:HB3	12:G:186:GLY:O	2.21	0.40
6:O:161:GLY:O	7:P:83:ARG:NH2	2.55	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	1	206/241 (86%)	201 (98%)	5 (2%)	0	100	100
1	M	206/241 (86%)	201 (98%)	5 (2%)	0	100	100
2	2	222/266 (84%)	215 (97%)	7 (3%)	0	100	100
2	N	221/266 (83%)	215 (97%)	6 (3%)	0	100	100
3	3	138/148 (93%)	137 (99%)	1 (1%)	0	100	100
3	6	139/148 (94%)	137 (99%)	2 (1%)	0	100	100
4	4	233/276 (84%)	228 (98%)	5 (2%)	0	100	100
4	7	237/276 (86%)	231 (98%)	6 (2%)	0	100	100
5	5	238/267 (89%)	237 (100%)	1 (0%)	0	100	100
5	8	243/267 (91%)	231 (95%)	12 (5%)	0	100	100
6	A	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
6	O	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	B	247/250 (99%)	243 (98%)	4 (2%)	0	100	100
7	P	248/250 (99%)	247 (100%)	1 (0%)	0	100	100
8	C	230/258 (89%)	227 (99%)	3 (1%)	0	100	100
8	Q	241/258 (93%)	233 (97%)	8 (3%)	0	100	100
9	D	243/254 (96%)	236 (97%)	7 (3%)	0	100	100
9	R	238/254 (94%)	231 (97%)	6 (2%)	1 (0%)	30	36
10	E	248/260 (95%)	246 (99%)	2 (1%)	0	100	100
10	S	247/260 (95%)	247 (100%)	0	0	100	100
11	F	232/234 (99%)	227 (98%)	5 (2%)	0	100	100
11	T	232/234 (99%)	226 (97%)	6 (3%)	0	100	100
12	G	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
12	U	240/288 (83%)	234 (98%)	6 (2%)	0	100	100
13	H	203/215 (94%)	201 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	V	203/215 (94%)	197 (97%)	6 (3%)	0	100	100
14	I	204/261 (78%)	201 (98%)	3 (2%)	0	100	100
14	W	211/261 (81%)	209 (99%)	2 (1%)	0	100	100
15	J	180/205 (88%)	166 (92%)	14 (8%)	0	100	100
15	X	183/205 (89%)	176 (96%)	7 (4%)	0	100	100
16	K	187/212 (88%)	178 (95%)	8 (4%)	1 (0%)	24	29
16	Y	184/212 (87%)	177 (96%)	7 (4%)	0	100	100
17	L	246/287 (86%)	236 (96%)	10 (4%)	0	100	100
17	Z	244/287 (85%)	239 (98%)	5 (2%)	0	100	100
All	All	7493/8348 (90%)	7315 (98%)	176 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	R	221	ILE
16	K	21	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	175/201 (87%)	174 (99%)	1 (1%)	78	87
1	M	175/201 (87%)	170 (97%)	5 (3%)	37	52
2	2	192/224 (86%)	185 (96%)	7 (4%)	31	44
2	N	191/224 (85%)	188 (98%)	3 (2%)	55	71
3	3	132/136 (97%)	131 (99%)	1 (1%)	73	84
3	6	133/136 (98%)	132 (99%)	1 (1%)	73	84
4	4	216/251 (86%)	213 (99%)	3 (1%)	59	74
4	7	218/251 (87%)	213 (98%)	5 (2%)	44	60
5	5	222/244 (91%)	220 (99%)	2 (1%)	70	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	8	226/244 (93%)	217 (96%)	9 (4%)	28	40
6	A	205/210 (98%)	200 (98%)	5 (2%)	43	59
6	O	205/210 (98%)	202 (98%)	3 (2%)	57	72
7	B	208/209 (100%)	202 (97%)	6 (3%)	37	52
7	P	209/209 (100%)	204 (98%)	5 (2%)	43	59
8	C	199/216 (92%)	198 (100%)	1 (0%)	81	89
8	Q	203/216 (94%)	200 (98%)	3 (2%)	57	72
9	D	217/226 (96%)	215 (99%)	2 (1%)	70	82
9	R	214/226 (95%)	212 (99%)	2 (1%)	70	82
10	E	206/215 (96%)	203 (98%)	3 (2%)	57	72
10	S	205/215 (95%)	202 (98%)	3 (2%)	57	72
11	F	193/193 (100%)	191 (99%)	2 (1%)	68	81
11	T	193/193 (100%)	190 (98%)	3 (2%)	55	71
12	G	202/239 (84%)	201 (100%)	1 (0%)	81	89
12	U	201/239 (84%)	197 (98%)	4 (2%)	48	65
13	H	169/178 (95%)	169 (100%)	0	100	100
13	V	169/178 (95%)	168 (99%)	1 (1%)	78	87
14	I	167/215 (78%)	166 (99%)	1 (1%)	78	87
14	W	173/215 (80%)	173 (100%)	0	100	100
15	J	157/173 (91%)	156 (99%)	1 (1%)	78	87
15	X	158/173 (91%)	157 (99%)	1 (1%)	78	87
16	K	170/189 (90%)	168 (99%)	2 (1%)	63	77
16	Y	169/189 (89%)	166 (98%)	3 (2%)	51	68
17	L	208/235 (88%)	206 (99%)	2 (1%)	68	81
17	Z	207/235 (88%)	205 (99%)	2 (1%)	68	81
All	All	6487/7108 (91%)	6394 (99%)	93 (1%)	57	74

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	126	ASP
2	2	9	THR
2	2	20	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	48	ASN
2	2	70	LEU
2	2	104	ARG
2	2	146	PHE
2	2	177	ILE
3	3	144	LYS
4	4	6	TRP
4	4	63	LYS
4	4	129	LYS
5	5	97	ASN
5	5	185	ILE
3	6	21	VAL
4	7	1	MET
4	7	6	TRP
4	7	23	LYS
4	7	218	VAL
4	7	268	ILE
5	8	76	LYS
5	8	85	GLN
5	8	95	LEU
5	8	97	ASN
5	8	107	LEU
5	8	114	GLU
5	8	175	PHE
5	8	185	ILE
5	8	245	ARG
6	A	7	ASP
6	A	47	VAL
6	A	56	LYS
6	A	165	THR
6	A	182	LYS
7	B	45	ILE
7	B	50	LYS
7	B	75	TYR
7	B	84	VAL
7	B	99	ARG
7	B	134	LEU
8	C	52	VAL
9	D	42	VAL
9	D	126	VAL
10	E	79	SER
10	E	140	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	E	222	ILE
11	F	74	LEU
11	F	80	ASP
12	G	165	THR
14	I	191	THR
15	J	146	LEU
16	K	29	LYS
16	K	33	ASP
17	L	34	VAL
17	L	129	VAL
1	M	33	TYR
1	M	77	PHE
1	M	126	ASP
1	M	177	VAL
1	M	221	ARG
2	N	9	THR
2	N	146	PHE
2	N	223	LYS
6	O	64	LEU
6	O	171	THR
6	O	192	ASP
7	P	45	ILE
7	P	83	ARG
7	P	84	VAL
7	P	99	ARG
7	P	181	ASP
8	Q	4	ARG
8	Q	55	THR
8	Q	163	ILE
9	R	81	ASP
9	R	126	VAL
10	S	133	LEU
10	S	140	VAL
10	S	222	ILE
11	T	11	VAL
11	T	153	VAL
11	T	156	LEU
12	U	76	CYS
12	U	134	VAL
12	U	204	HIS
12	U	214	LEU
13	V	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	X	27	LEU
16	Y	39	SER
16	Y	151	ASP
16	Y	179	VAL
17	Z	161	LEU
17	Z	191	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	135	GLN
1	1	195	HIS
2	2	26	ASN
3	3	71	GLN
5	5	13	ASN
5	5	213	ASN
5	8	85	GLN
5	8	183	GLN
7	B	41	ASN
7	B	190	HIS
8	C	59	GLN
8	C	229	GLN
9	D	94	GLN
13	H	161	GLN
14	I	91	GLN
14	I	160	GLN
15	J	64	ASN
16	K	86	GLN
16	K	101	ASN
16	K	118	GLN
17	L	-17	HIS
17	L	62	GLN
1	M	135	GLN
2	N	26	ASN
6	O	15	HIS
7	P	123	GLN
8	Q	147	GLN
12	U	237	GLN
14	W	30	ASN
14	W	93	HIS
15	X	64	ASN
16	Y	41	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Y	147	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

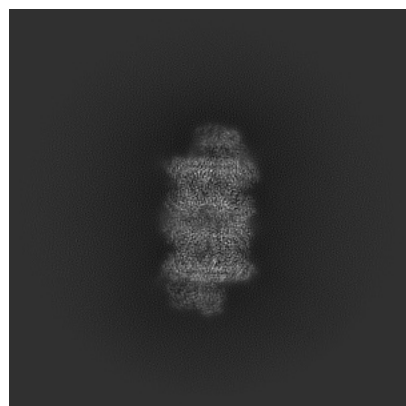
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19528. These allow visual inspection of the internal detail of the map and identification of artifacts.

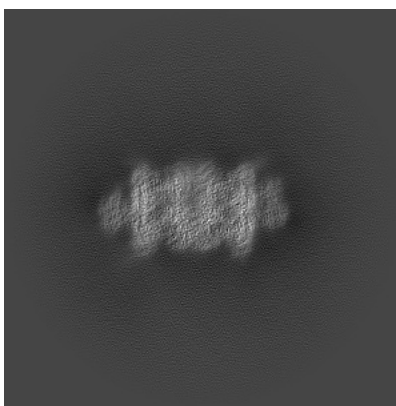
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

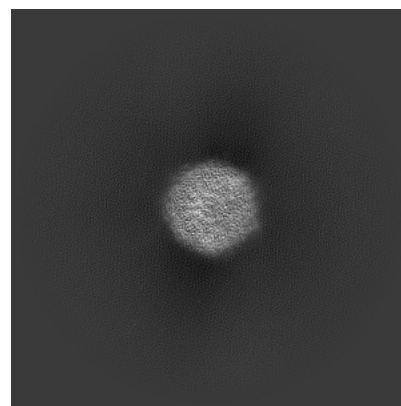
6.1.1 Primary map



X

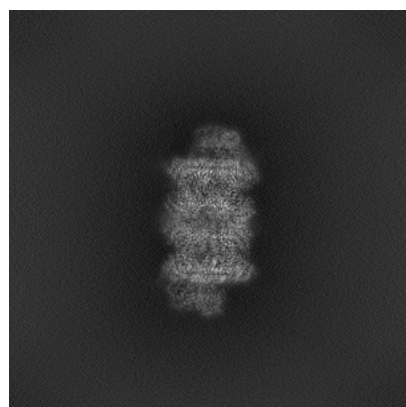


Y

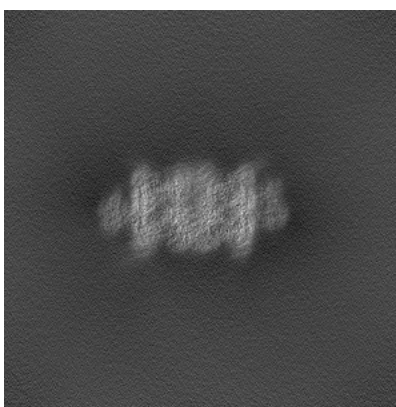


Z

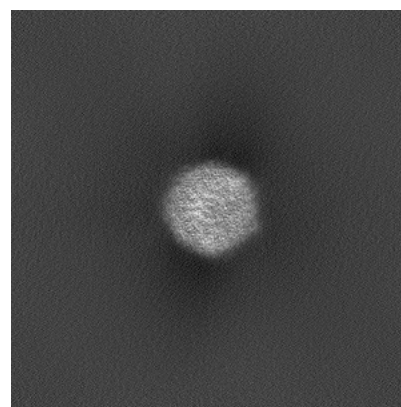
6.1.2 Raw map



X



Y

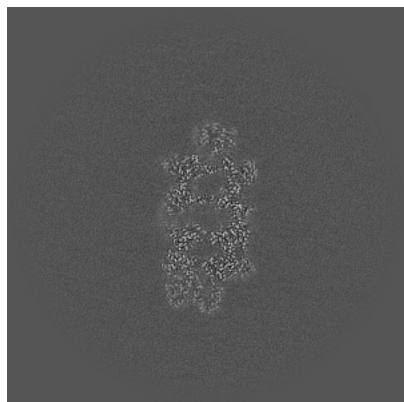


Z

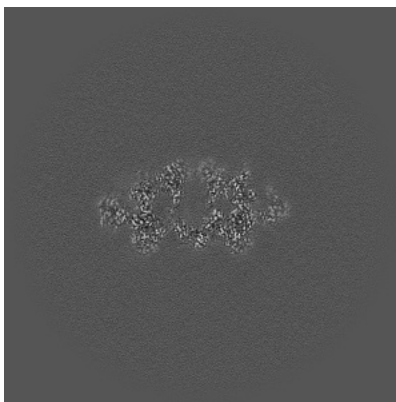
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

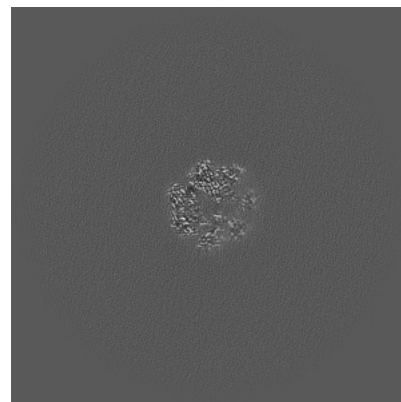
6.2.1 Primary map



X Index: 300

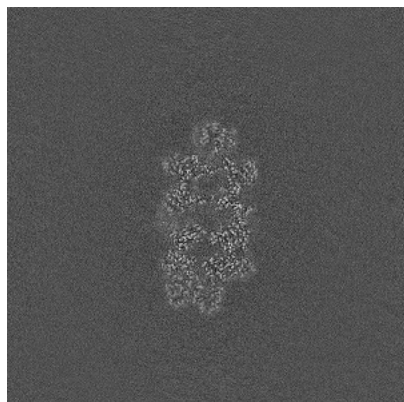


Y Index: 300

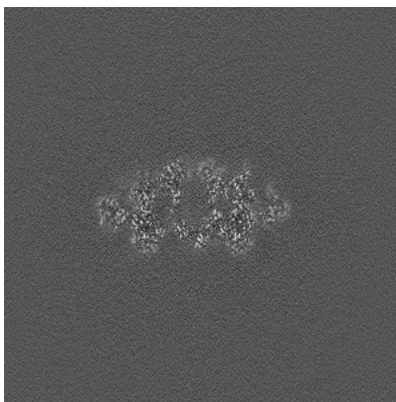


Z Index: 300

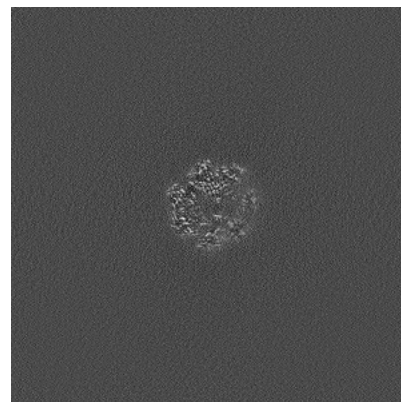
6.2.2 Raw map



X Index: 300



Y Index: 300

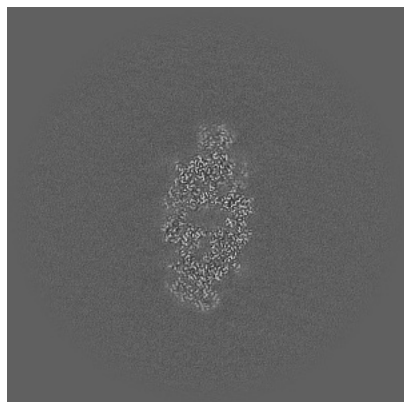


Z Index: 300

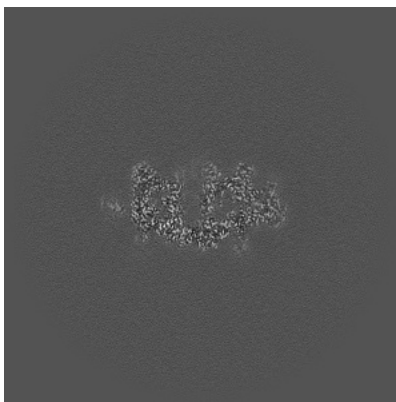
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

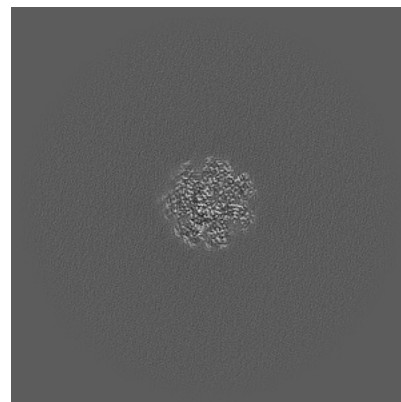
6.3.1 Primary map



X Index: 283

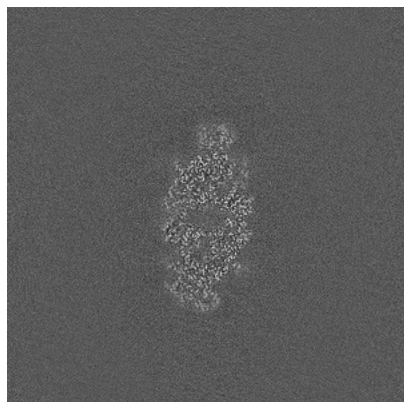


Y Index: 319

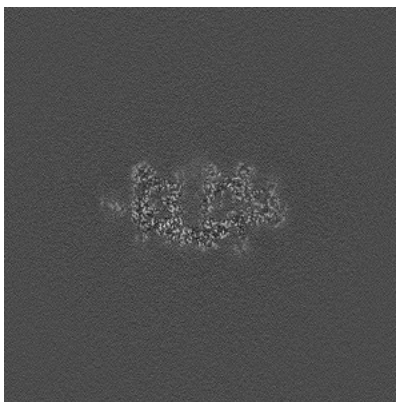


Z Index: 356

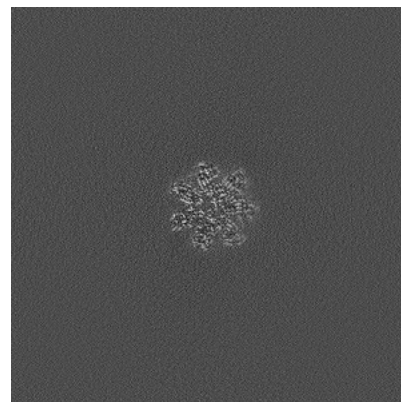
6.3.2 Raw map



X Index: 283



Y Index: 319

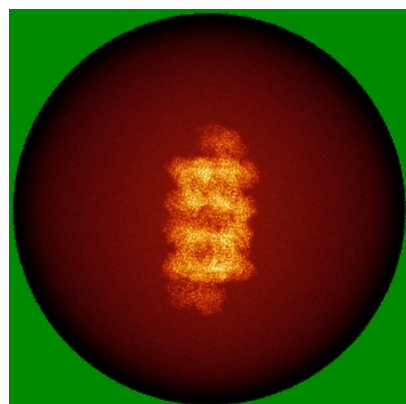


Z Index: 259

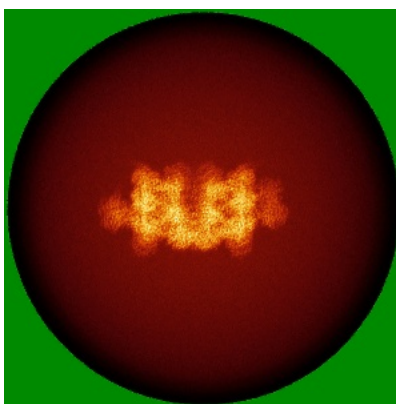
The images above show the largest variance slices of the map in three orthogonal directions.

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

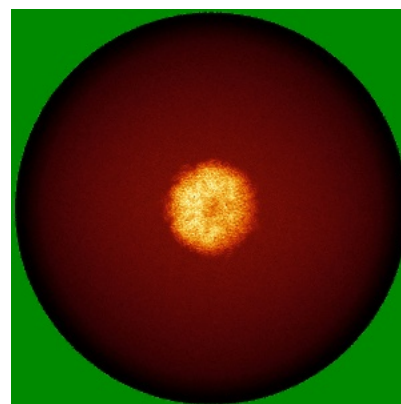
6.4.1 Primary map



X

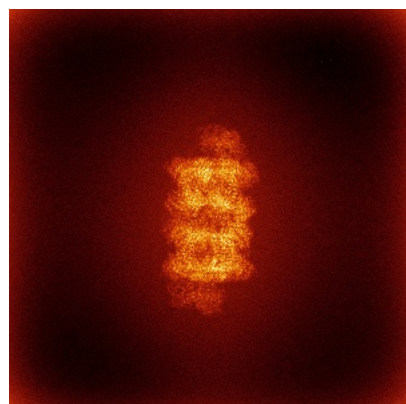


Y

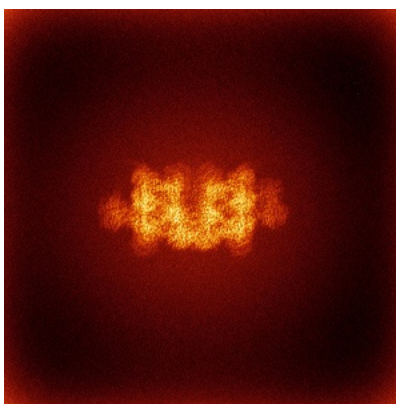


Z

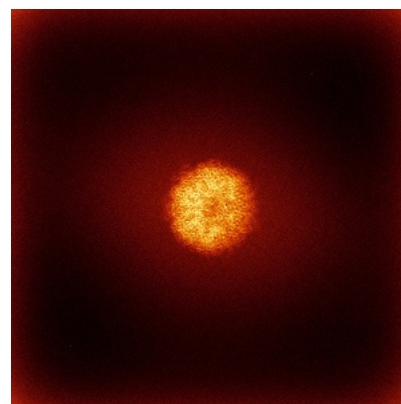
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

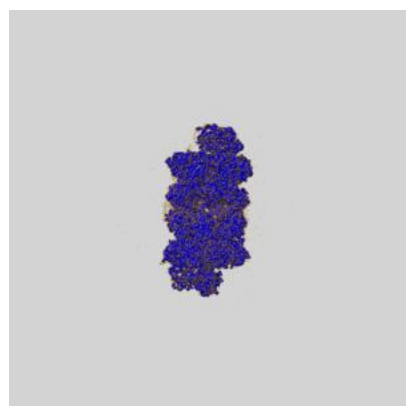
6.6 Mask visualisation [i](#)

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

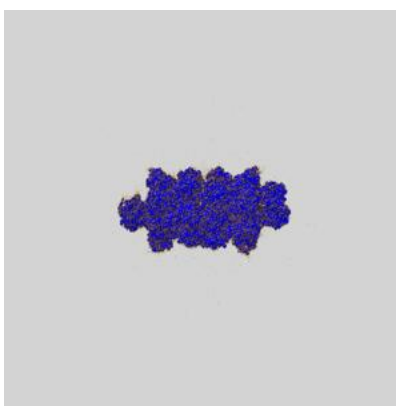
A mask typically either:

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

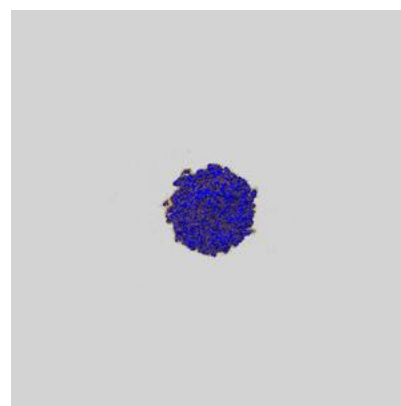
6.6.1 emd_19528_msk_1.map [i](#)



X



Y

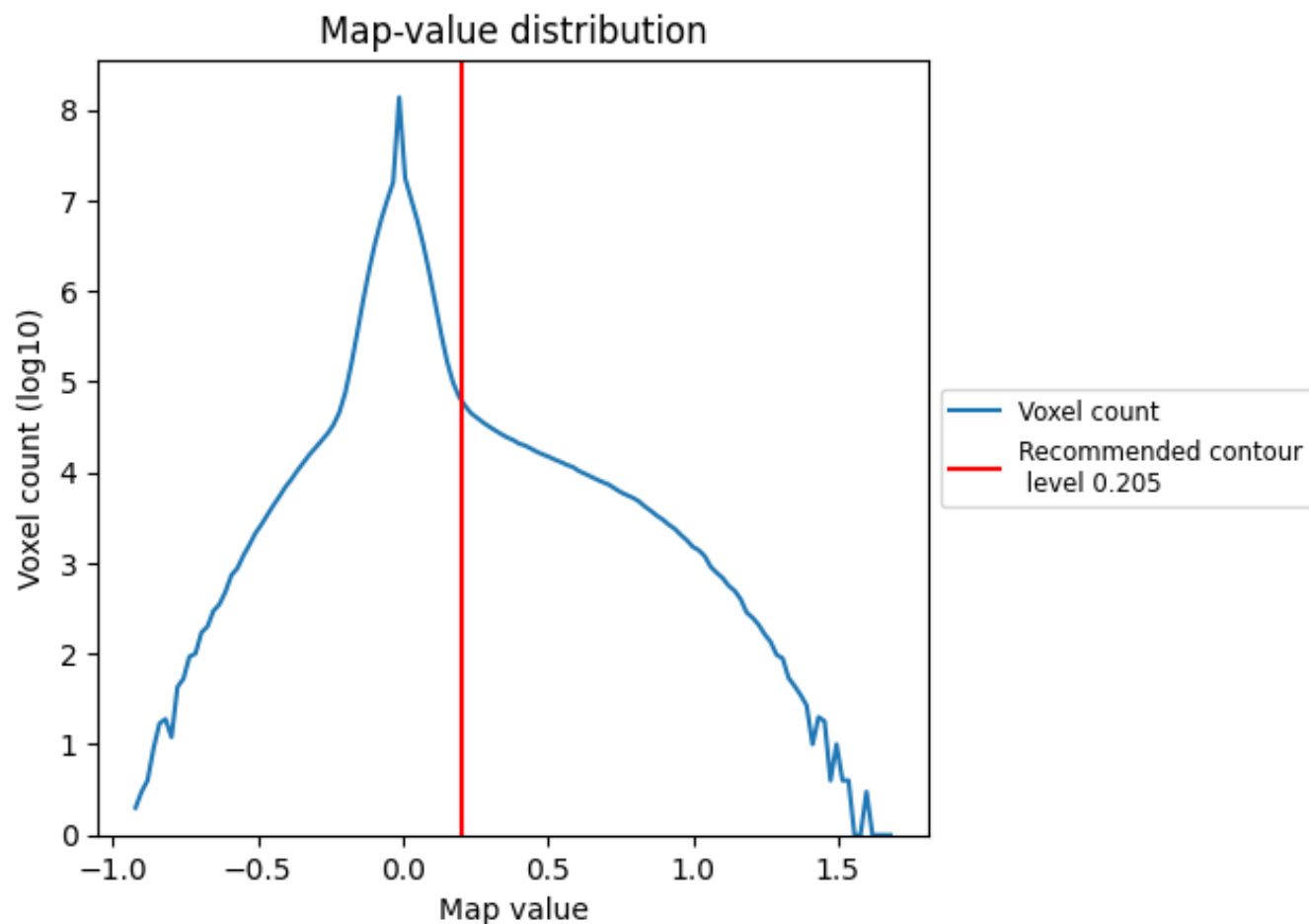


Z

7 Map analysis [i](#)

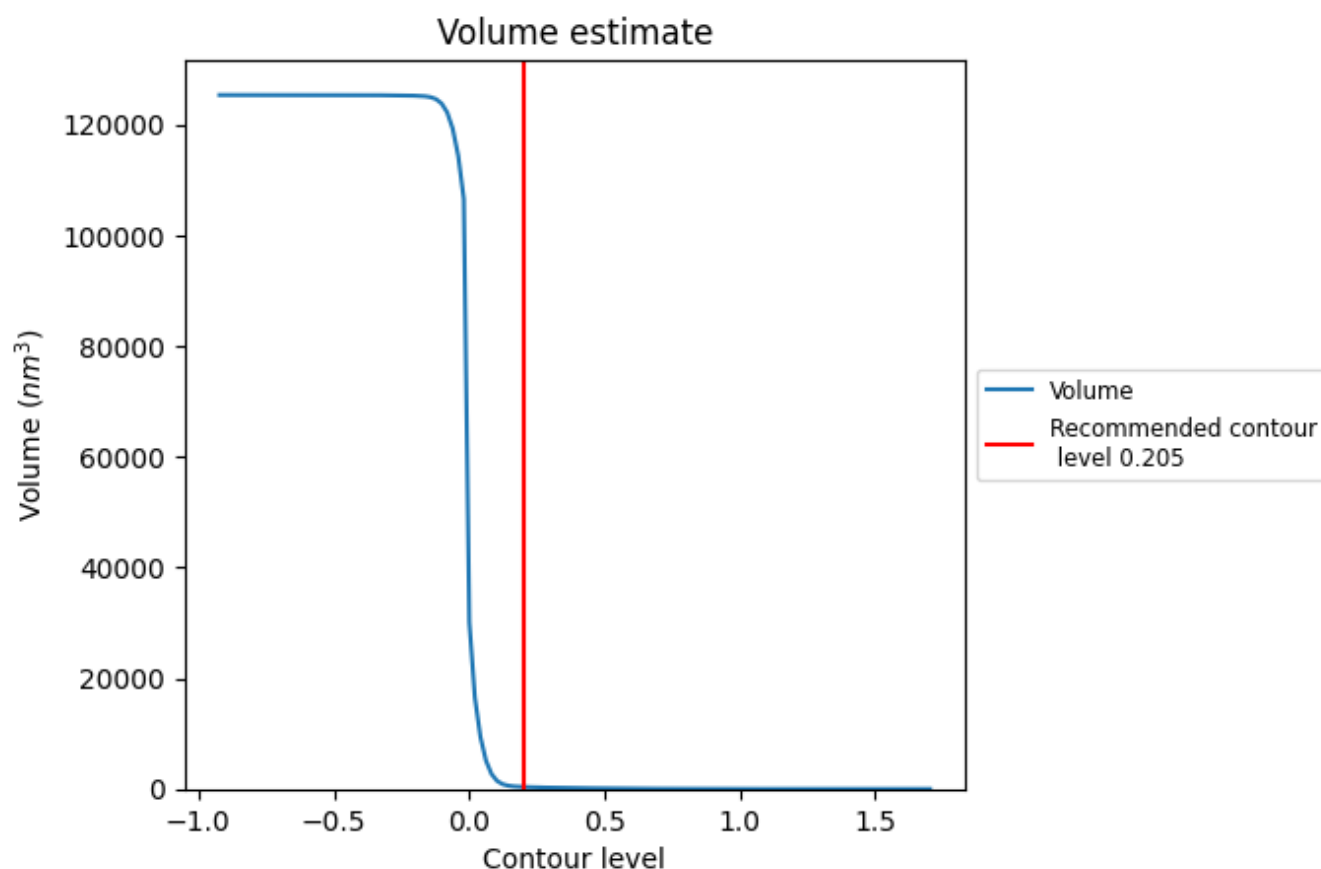
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

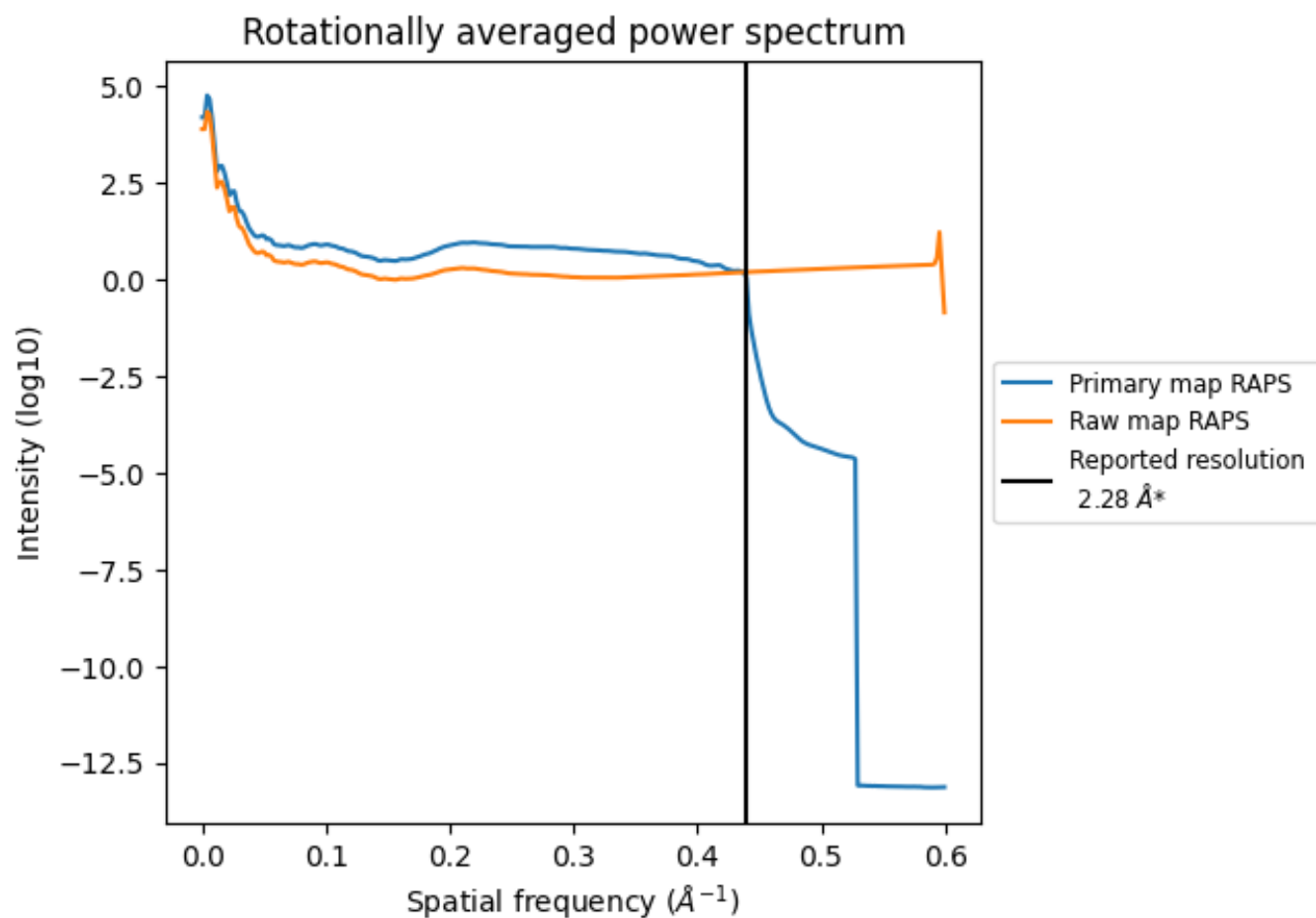
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm³; this corresponds to an approximate mass of 318 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 ⓘ

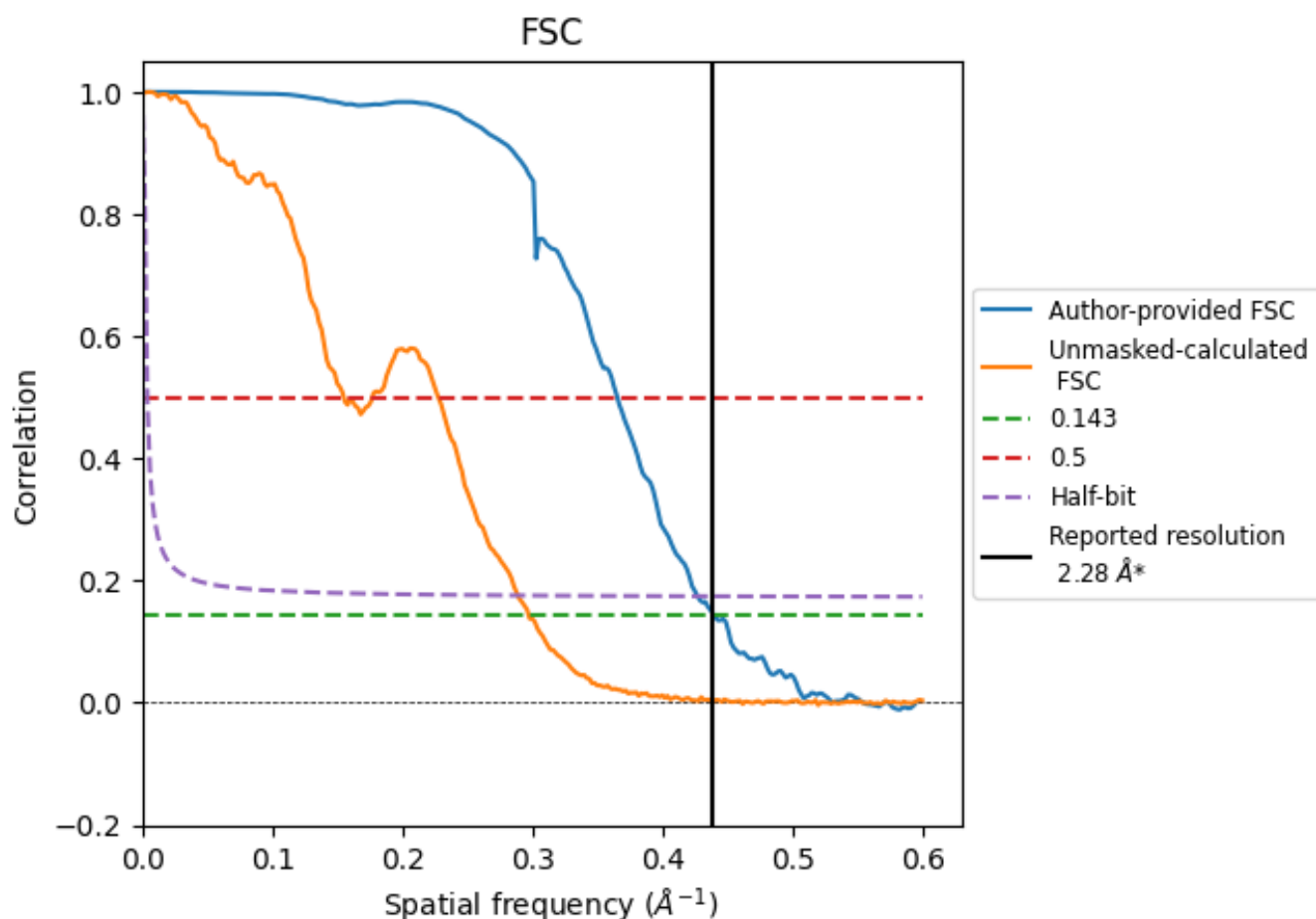


*Reported resolution corresponds to spatial frequency of 0.439 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.439 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

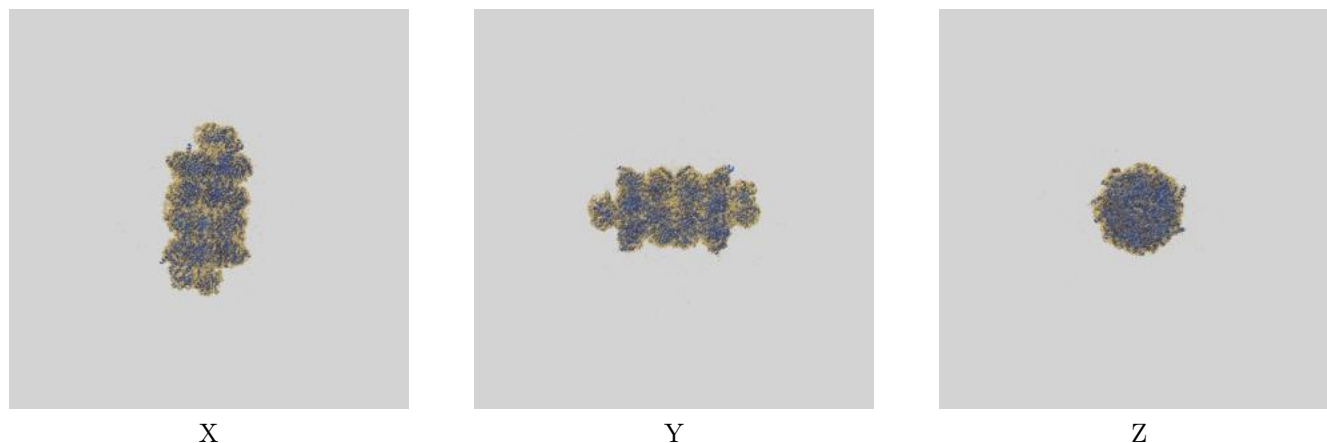
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.28	-	-
Author-provided FSC curve	2.28	2.74	2.34
Unmasked-calculated*	3.37	6.46	3.46

*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 3.37 differs from the reported value 2.28 by more than 10 %

9 Map-model fit [i](#)

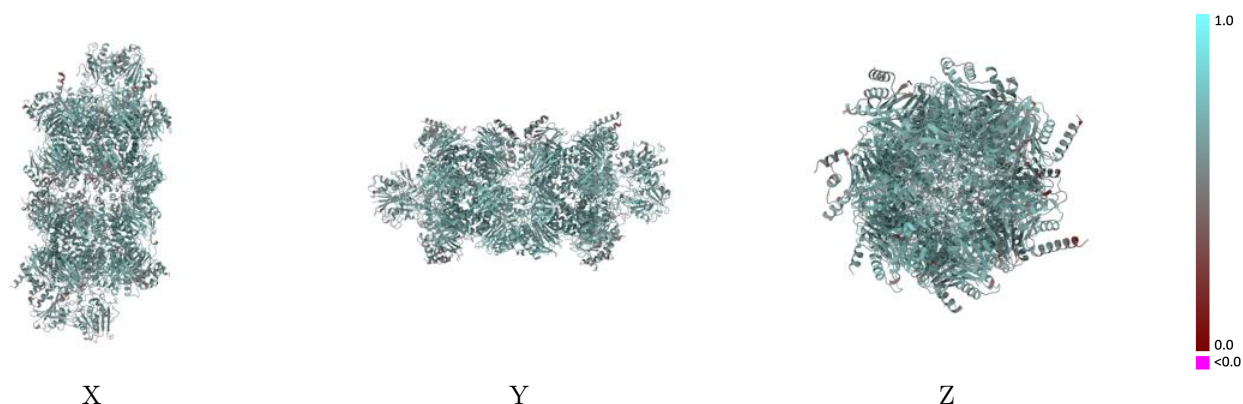
This section contains information regarding the fit between EMDB map EMD-19528 and PDB model 8RVP. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.205 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

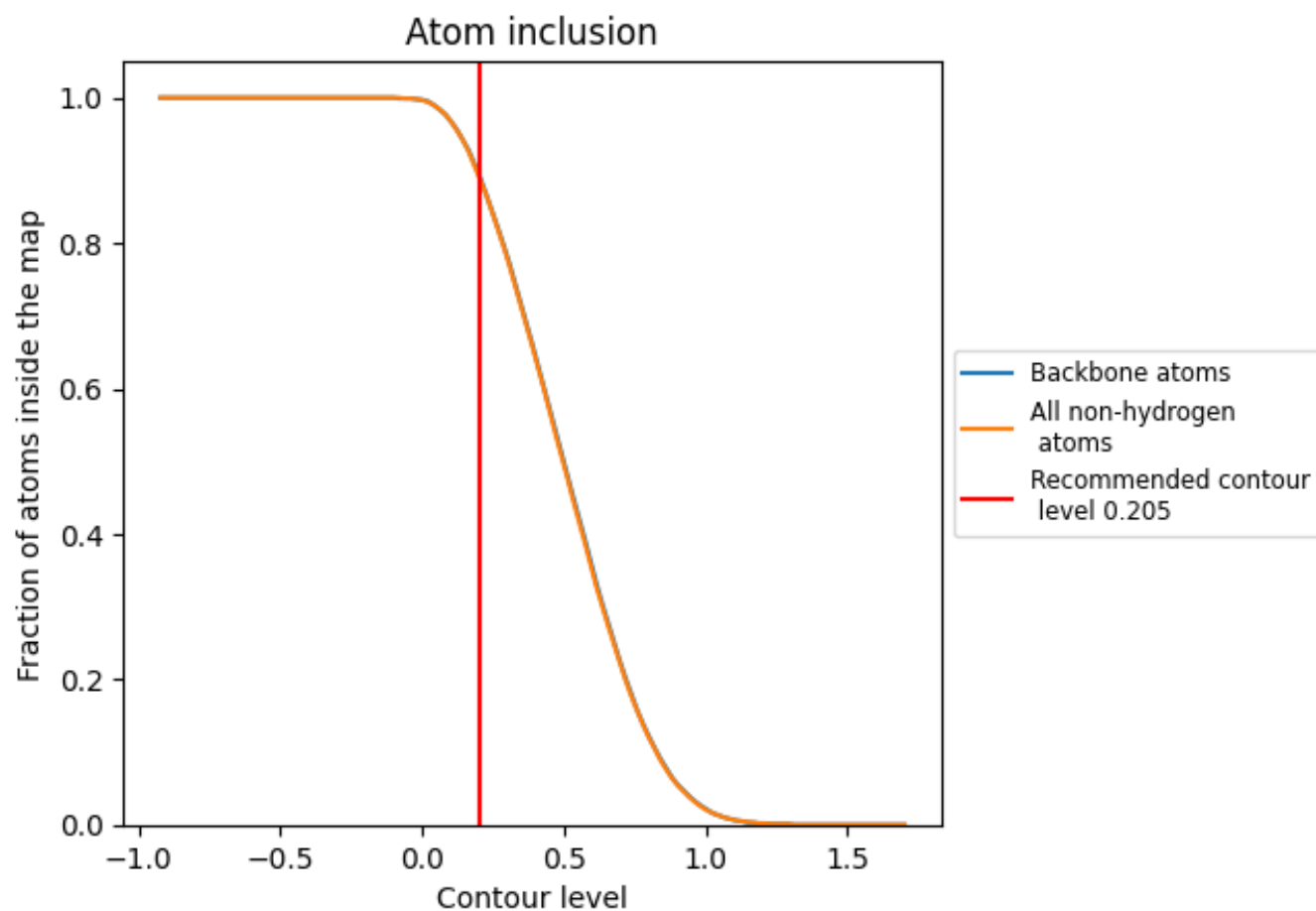


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.6280
1	 0.9410	 0.6510
2	 0.9340	 0.6520
3	 0.9370	 0.6660
4	 0.8320	 0.5910
5	 0.8770	 0.6030
6	 0.9200	 0.6600
7	 0.7950	 0.5730
8	 0.8400	 0.5780
A	 0.8780	 0.6210
B	 0.9130	 0.6390
C	 0.9000	 0.6320
D	 0.8710	 0.6220
E	 0.9090	 0.6420
F	 0.9340	 0.6510
G	 0.8680	 0.6160
H	 0.9610	 0.6740
I	 0.9680	 0.6720
J	 0.8920	 0.6260
K	 0.8120	 0.5910
L	 0.8310	 0.5940
M	 0.9430	 0.6540
N	 0.9330	 0.6640
O	 0.8780	 0.6250
P	 0.9140	 0.6410
Q	 0.8630	 0.6170
R	 0.8670	 0.6110
S	 0.9010	 0.6310
T	 0.9240	 0.6390
U	 0.8480	 0.6090
V	 0.9630	 0.6740
W	 0.9550	 0.6750
X	 0.8990	 0.6340
Y	 0.8230	 0.5920
Z	 0.8460	 0.5980

