



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 03:51 PM UTC

PDB ID : 8FZ6 / pdb_00008fz6
EMDB ID : EMD-29604
Title : The human PI31 complexed with bovine 20S proteasome
Authors : Hsu, H.-C.; Li, H.
Deposited on : 2023-01-27
Resolution : 2.54 Å(reported)
Based on initial model : 1IRU

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

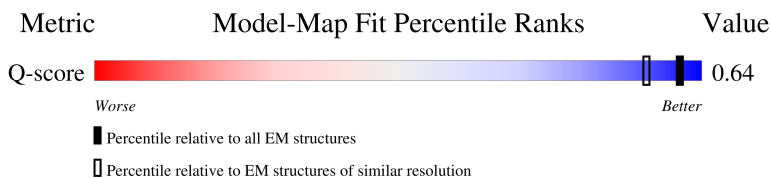
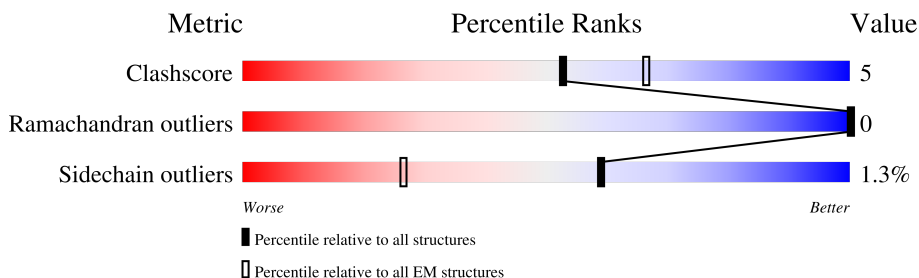
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 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.



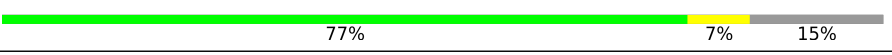
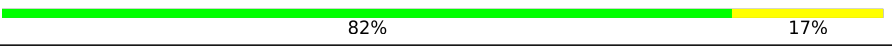
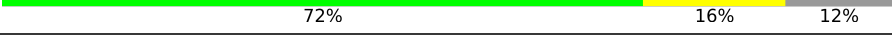
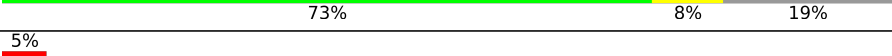
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7403 (2.04 - 3.04)

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	246	5% 88% 11%
1	O	246	6% 87% 12%
2	B	234	• 85% 14%
2	P	234	5% 82% 16% •

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Mol	Chain	Length	Quality of chain
3	C	261	
3	Q	261	
4	D	248	
4	R	248	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	239	
8	V	239	
9	I	277	
9	W	277	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	263	
12	Z	263	
13	M	241	
13	a	241	
14	N	264	
14	b	264	
15	c	271	

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Mol	Chain	Length	Quality of chain
15	d	271	19%5%76%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 49780 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	245	Total	C	N	O	S	0	0
			1911	1211	321	365	14		
1	O	245	Total	C	N	O	S	0	0
			1911	1211	321	365	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	233	Total	C	N	O	S	0	0
			1820	1163	308	342	7		
2	P	233	Total	C	N	O	S	0	0
			1820	1163	308	342	7		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	250	Total	C	N	O	S	0	0
			1971	1245	339	377	10		
3	Q	250	Total	C	N	O	S	0	0
			1971	1245	339	377	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	243	Total	C	N	O	S	0	0
			1922	1208	340	369	5		
4	R	243	Total	C	N	O	S	0	0
			1922	1208	340	369	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1805	1133	297	364	11		
5	S	236	Total	C	N	O	S	0	0
			1805	1133	297	364	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		
6	T	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	241	Total	C	N	O	S	0	0
			1888	1196	322	359	11		
7	U	241	Total	C	N	O	S	0	0
			1888	1196	322	359	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1519	955	258	294	12		
8	V	202	Total	C	N	O	S	0	0
			1519	955	258	294	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1660	1045	283	320	12		
9	W	220	Total	C	N	O	S	0	0
			1660	1045	283	320	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	197	Total	C	N	O	S	0	0
			1584	1017	268	291	8		
11	Y	197	Total	C	N	O	S	0	0
			1584	1017	268	291	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1557	980	272	296	9		
12	Z	201	Total	C	N	O	S	0	0
			1557	980	272	296	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		
13	a	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	214	Total	C	N	O	S	0	0
			1671	1056	287	316	12		
14	b	214	Total	C	N	O	S	0	0
			1671	1056	287	316	12		

- Molecule 15 is a protein called Proteasome inhibitor PI31 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	65	Total	C	N	O	S	0	0
			470	302	84	83	1		
15	d	65	Total	C	N	O	S	0	0
			470	302	84	83	1		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	18	ARG	ALA	conflict	UNP Q3SX30
c	36	PHE	TYR	conflict	UNP Q3SX30
c	40	VAL	ALA	conflict	UNP Q3SX30
c	56	ALA	VAL	conflict	UNP Q3SX30
c	57	GLY	GLU	conflict	UNP Q3SX30
c	60	ASN	SER	conflict	UNP Q3SX30
c	71	TYR	SER	conflict	UNP Q3SX30
c	83	ILE	VAL	conflict	UNP Q3SX30
c	87	SER	ASN	conflict	UNP Q3SX30
c	91	LEU	ILE	conflict	UNP Q3SX30
c	96	TYR	HIS	conflict	UNP Q3SX30
c	102	ALA	SER	conflict	UNP Q3SX30
c	109	ASP	ASN	conflict	UNP Q3SX30
c	114	ALA	SER	conflict	UNP Q3SX30
c	118	GLY	VAL	conflict	UNP Q3SX30
c	123	THR	VAL	conflict	UNP Q3SX30
c	151	VAL	-	insertion	UNP Q3SX30
c	152	SER	LEU	conflict	UNP Q3SX30
c	172	PRO	HIS	conflict	UNP Q3SX30
c	174	HIS	GLN	conflict	UNP Q3SX30
c	183	PRO	THR	conflict	UNP Q3SX30
c	192	VAL	ALA	conflict	UNP Q3SX30
c	203	PRO	CYS	conflict	UNP Q3SX30
c	254	PRO	SER	conflict	UNP Q3SX30
d	18	ARG	ALA	conflict	UNP Q3SX30
d	36	PHE	TYR	conflict	UNP Q3SX30
d	40	VAL	ALA	conflict	UNP Q3SX30
d	56	ALA	VAL	conflict	UNP Q3SX30
d	57	GLY	GLU	conflict	UNP Q3SX30
d	60	ASN	SER	conflict	UNP Q3SX30
d	71	TYR	SER	conflict	UNP Q3SX30
d	83	ILE	VAL	conflict	UNP Q3SX30
d	87	SER	ASN	conflict	UNP Q3SX30
d	91	LEU	ILE	conflict	UNP Q3SX30
d	96	TYR	HIS	conflict	UNP Q3SX30
d	102	ALA	SER	conflict	UNP Q3SX30
d	109	ASP	ASN	conflict	UNP Q3SX30
d	114	ALA	SER	conflict	UNP Q3SX30
d	118	GLY	VAL	conflict	UNP Q3SX30
d	123	THR	VAL	conflict	UNP Q3SX30
d	151	VAL	-	insertion	UNP Q3SX30
d	152	SER	LEU	conflict	UNP Q3SX30

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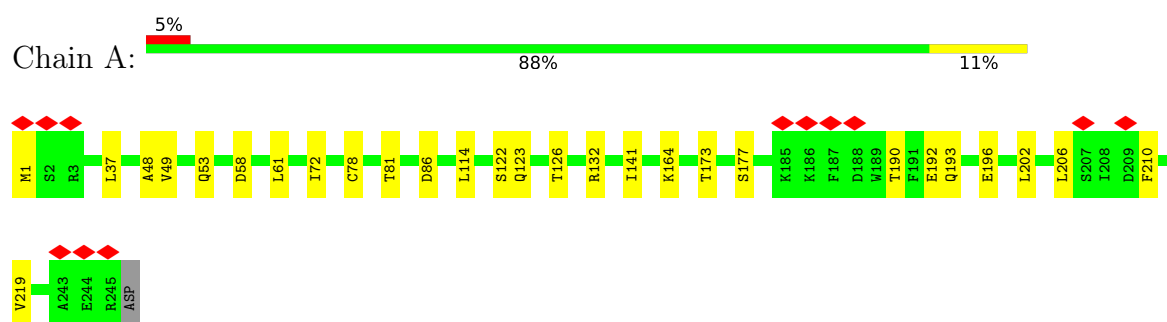
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Chain	Residue	Modelled	Actual	Comment	Reference
d	172	PRO	HIS	conflict	UNP Q3SX30
d	174	HIS	GLN	conflict	UNP Q3SX30
d	183	PRO	THR	conflict	UNP Q3SX30
d	192	VAL	ALA	conflict	UNP Q3SX30
d	203	PRO	CYS	conflict	UNP Q3SX30
d	254	PRO	SER	conflict	UNP Q3SX30

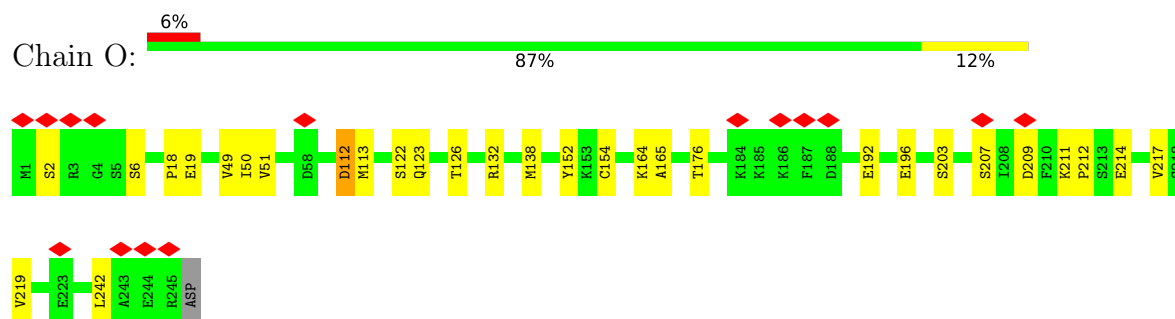
3 Residue-property plots [i](#)

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.

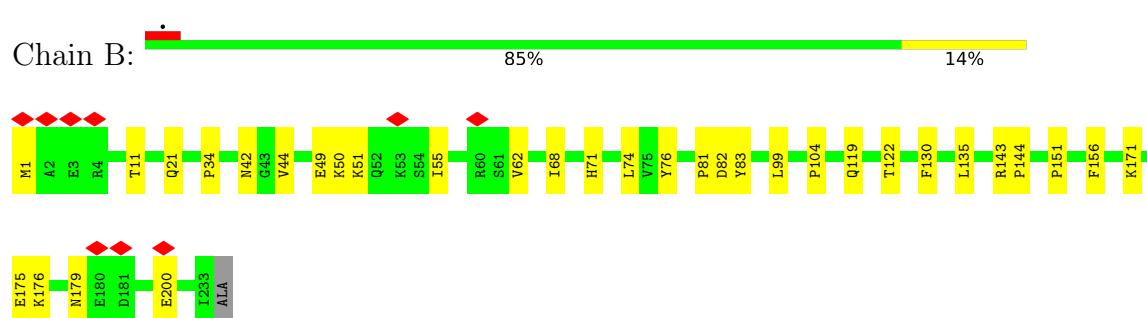
- Molecule 1: Proteasome subunit alpha type-6



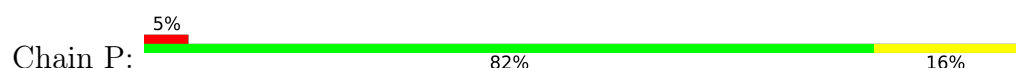
- Molecule 1: Proteasome subunit alpha type-6

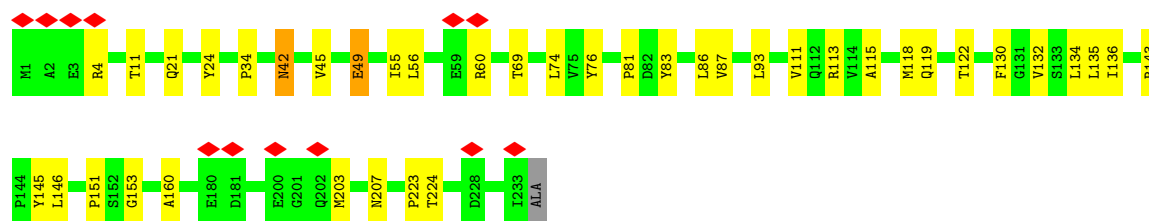


- Molecule 2: Proteasome subunit alpha type-2

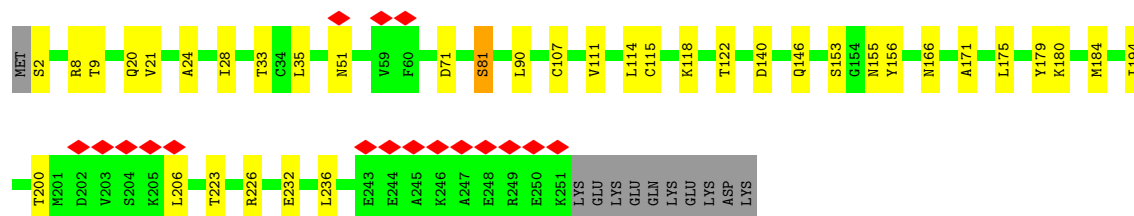
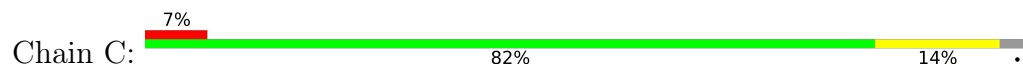


- Molecule 2: Proteasome subunit alpha type-2

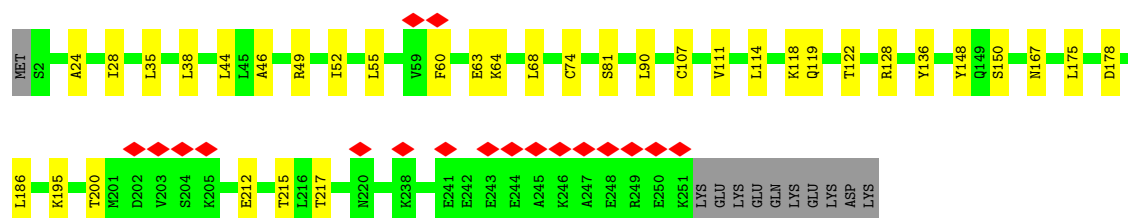
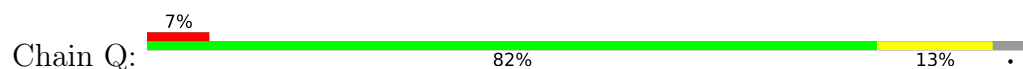




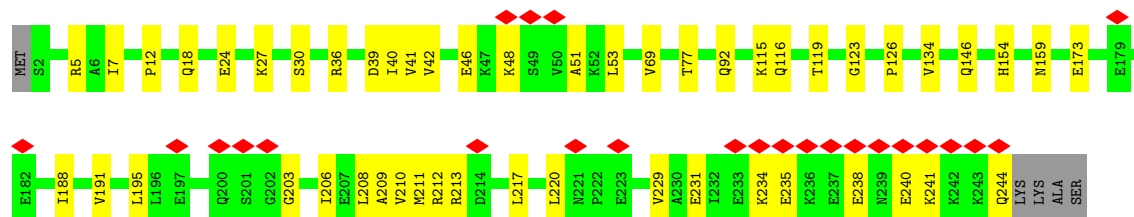
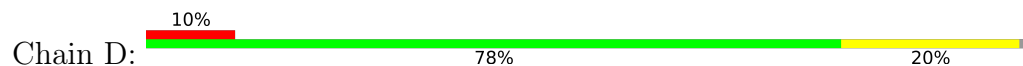
• Molecule 3: Proteasome subunit alpha type-4



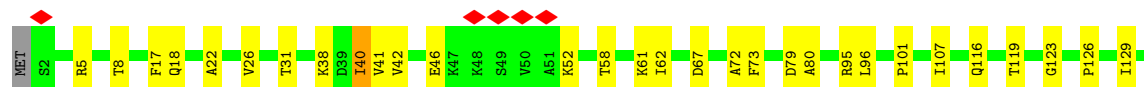
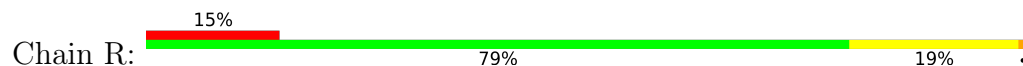
• Molecule 3: Proteasome subunit alpha type-4

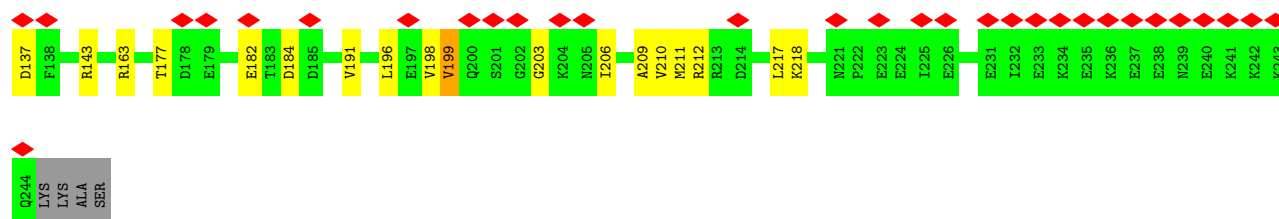


• Molecule 4: Proteasome subunit alpha type-7

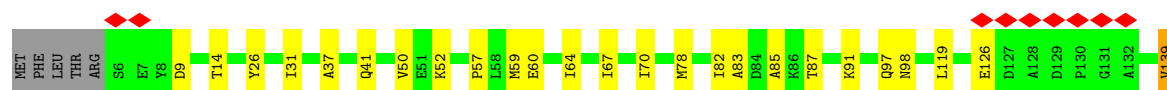
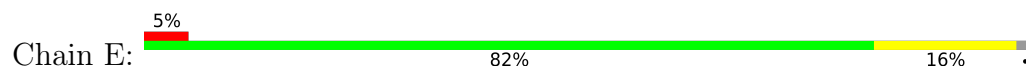


• Molecule 4: Proteasome subunit alpha type-7

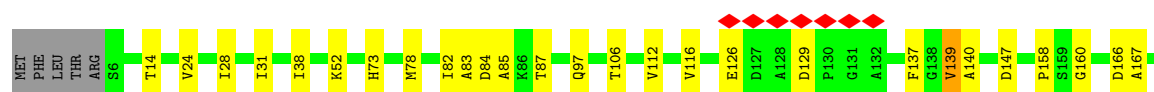
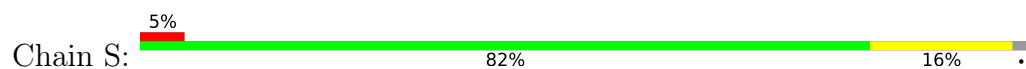




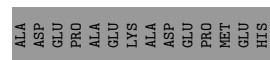
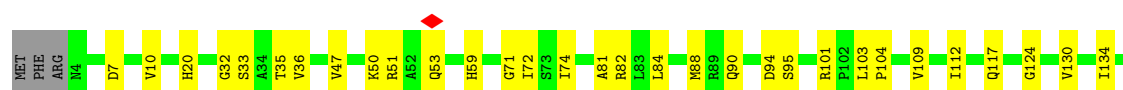
• Molecule 5: Proteasome subunit alpha type-5



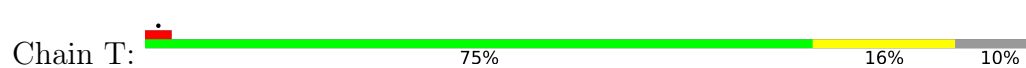
• Molecule 5: Proteasome subunit alpha type-5

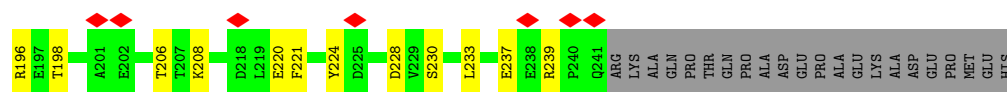


• Molecule 6: Proteasome subunit alpha type-1



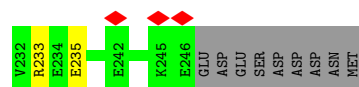
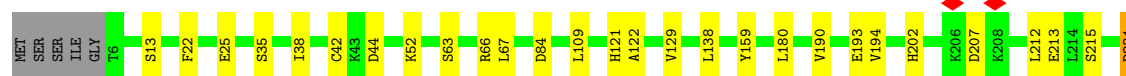
• Molecule 6: Proteasome subunit alpha type-1





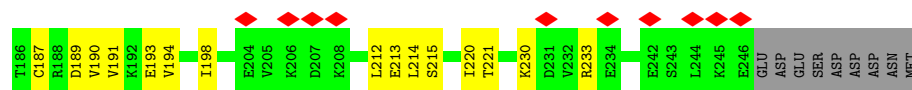
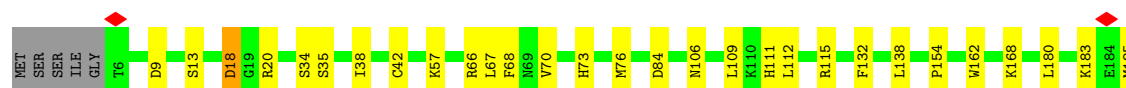
- Molecule 7: Proteasome subunit alpha type-3

Chain G: 83% 11% 5%



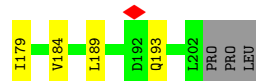
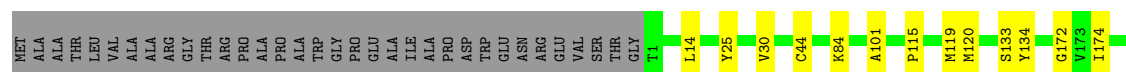
- Molecule 7: Proteasome subunit alpha type-3

Chain U: 5% 77% 17% 5%



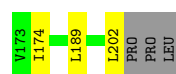
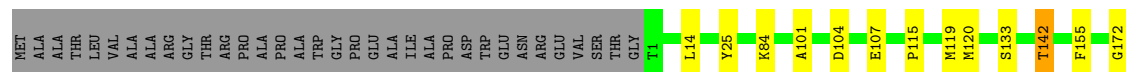
- Molecule 8: Proteasome subunit beta type-6

Chain H: 77% 7% 15%



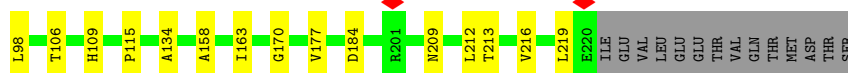
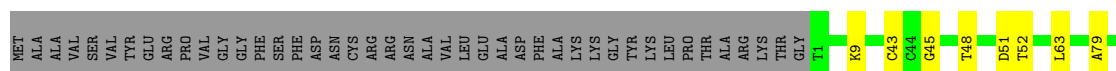
- Molecule 8: Proteasome subunit beta type-6

Chain V: 78% 6% 15%

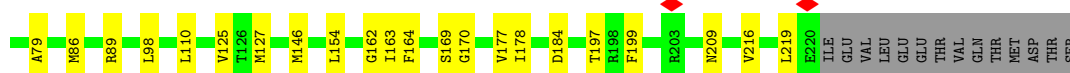
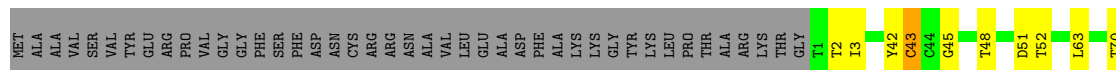


- Molecule 9: Proteasome subunit beta type-7

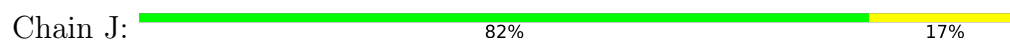
Chain I: 71% 8% 21%



• Molecule 9: Proteasome subunit beta type-7



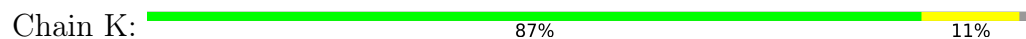
• Molecule 10: Proteasome subunit beta type-3



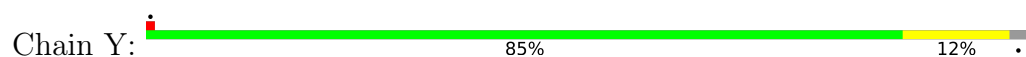
• Molecule 10: Proteasome subunit beta type-3



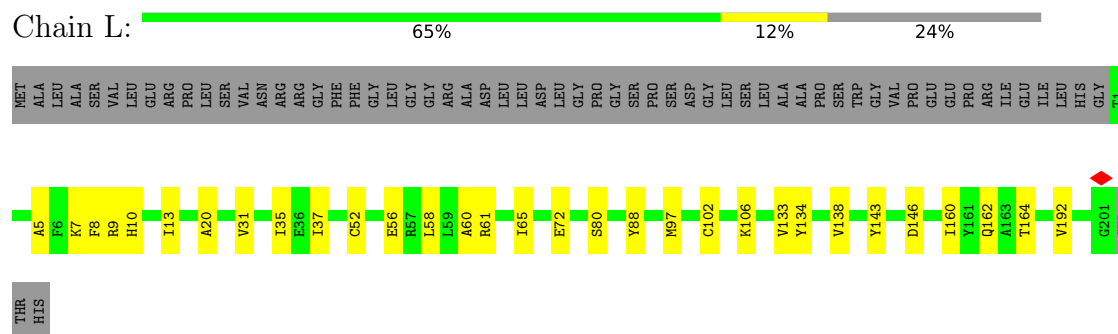
• Molecule 11: Proteasome subunit beta type-2



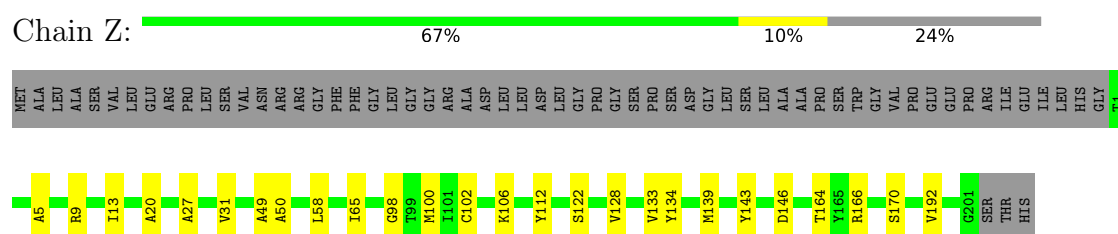
• Molecule 11: Proteasome subunit beta type-2



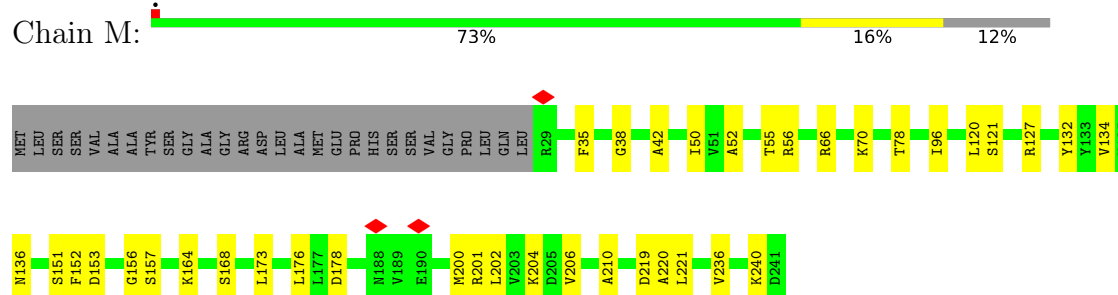
- Molecule 12: Proteasome subunit beta type-5



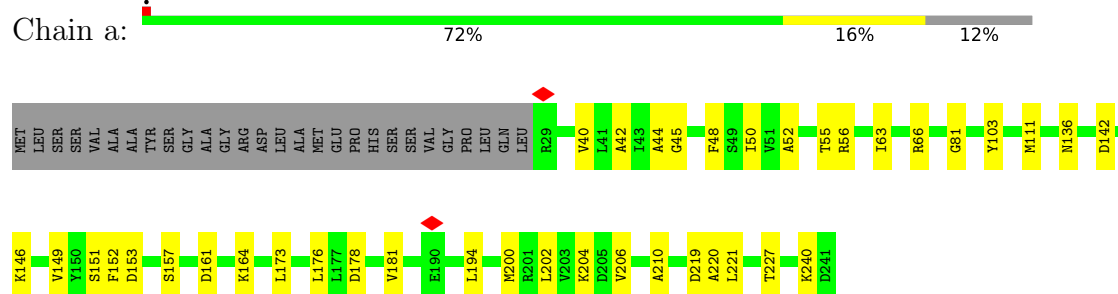
- Molecule 12: Proteasome subunit beta type-5



- Molecule 13: Proteasome subunit beta type-1

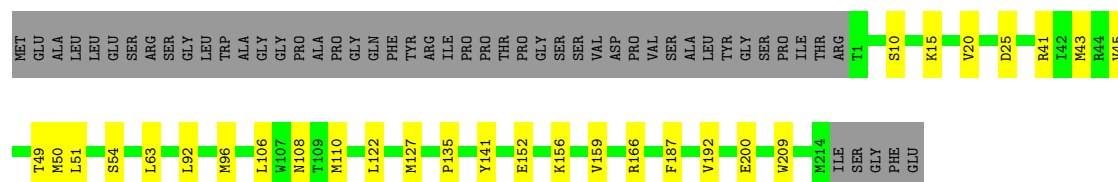


- Molecule 13: Proteasome subunit beta type-1

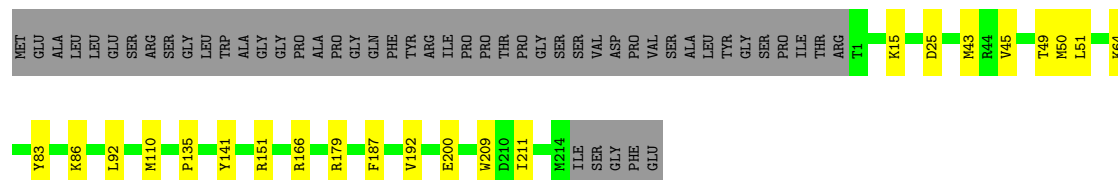


- Molecule 14: Proteasome subunit beta type-4

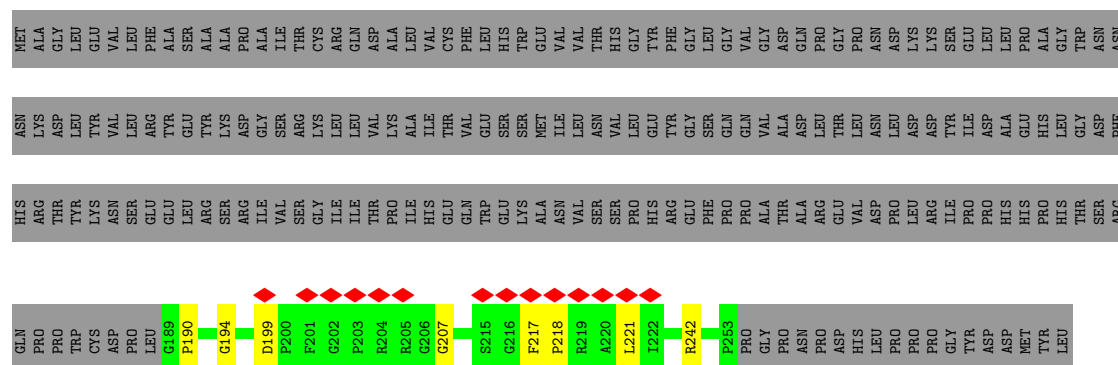




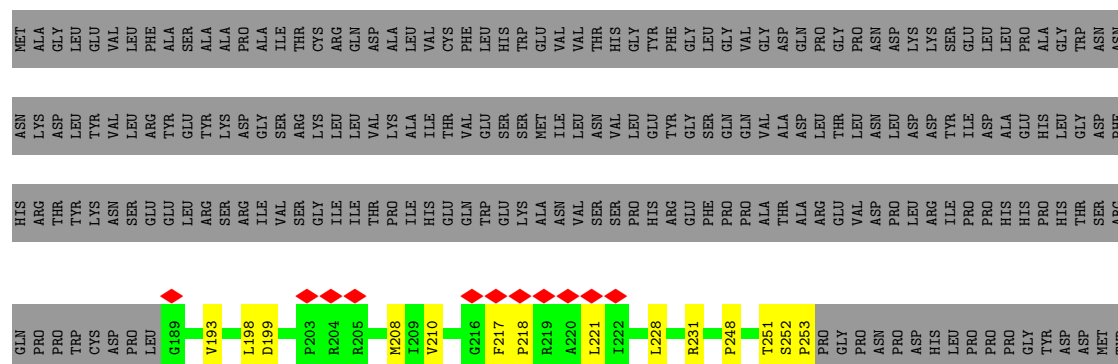
• Molecule 14: Proteasome subunit beta type-4



• Molecule 15: Proteasome inhibitor PI31 subunit



• Molecule 15: Proteasome inhibitor PI31 subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	350283	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.080	Depositor
Minimum map value	-1.526	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.44	Depositor
Map size (Å)	291.456, 291.456, 291.456	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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	0.11	0/1945	0.24	0/2627
1	O	0.10	0/1945	0.25	0/2627
2	B	0.11	0/1859	0.24	0/2517
2	P	0.10	0/1859	0.24	0/2517
3	C	0.10	0/2001	0.23	0/2694
3	Q	0.10	0/2001	0.23	0/2694
4	D	0.09	0/1949	0.23	0/2627
4	R	0.09	0/1949	0.23	0/2627
5	E	0.10	0/1833	0.23	0/2475
5	S	0.09	0/1833	0.23	0/2475
6	F	0.10	0/1908	0.26	0/2579
6	T	0.10	0/1908	0.25	0/2579
7	G	0.10	0/1923	0.23	0/2590
7	U	0.09	0/1923	0.23	0/2590
8	H	0.11	0/1547	0.25	0/2097
8	V	0.11	0/1547	0.24	0/2097
9	I	0.11	0/1687	0.27	0/2280
9	W	0.10	0/1687	0.25	0/2280
10	J	0.12	0/1623	0.27	0/2188
10	X	0.11	0/1623	0.26	0/2188
11	K	0.11	0/1618	0.24	0/2190
11	Y	0.11	0/1618	0.26	0/2190
12	L	0.11	0/1588	0.24	0/2144
12	Z	0.10	0/1588	0.25	0/2144
13	M	0.11	0/1676	0.28	0/2258
13	a	0.11	0/1676	0.27	0/2258
14	N	0.11	0/1704	0.26	0/2305
14	b	0.11	0/1704	0.26	0/2305
15	c	0.11	0/488	0.29	0/668
15	d	0.10	0/488	0.28	0/668
All	All	0.10	0/50698	0.25	0/68478

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	1911	0	1923	18	0
1	O	1911	0	1923	18	0
2	B	1820	0	1818	24	0
2	P	1820	0	1818	28	0
3	C	1971	0	1992	20	0
3	Q	1971	0	1992	23	0
4	D	1922	0	1954	30	0
4	R	1922	0	1954	29	0
5	E	1805	0	1784	27	0
5	S	1805	0	1784	25	0
6	F	1873	0	1860	32	0
6	T	1873	0	1860	25	0
7	G	1888	0	1870	20	0
7	U	1888	0	1870	28	0
8	H	1519	0	1495	12	0
8	V	1519	0	1495	10	0
9	I	1660	0	1680	16	0
9	W	1660	0	1680	22	0
10	J	1594	0	1613	26	0
10	X	1594	0	1613	22	0
11	K	1584	0	1584	14	0
11	Y	1584	0	1584	16	0
12	L	1557	0	1518	17	0
12	Z	1557	0	1518	17	0
13	M	1645	0	1644	22	0
13	a	1645	0	1644	22	0
14	N	1671	0	1652	15	0
14	b	1671	0	1652	16	0
15	c	470	0	463	6	0
15	d	470	0	463	10	0
All	All	49780	0	49700	524	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 (524) 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)
10:J:205:ASP:HB3	12:Z:192:VAL:HG11	1.68	0.75
5:S:85:ALA:HB2	5:S:139:VAL:HG21	1.69	0.73
13:a:151:SER:HB3	13:a:164:LYS:HG2	1.70	0.73
6:T:206:THR:HG23	6:T:208:LYS:H	1.55	0.71
13:M:151:SER:HB3	13:M:164:LYS:HG2	1.72	0.69
5:E:98:ASN:OD1	12:L:61:ARG:NH1	2.25	0.69
9:W:209:ASN:OD1	10:X:169:GLN:NE2	2.27	0.68
5:E:85:ALA:HB2	5:E:139:VAL:HG11	1.75	0.67
4:R:209:ALA:HB1	4:R:217:LEU:HD11	1.74	0.67
5:E:41:GLN:OE1	5:E:164:GLN:NE2	2.29	0.66
1:A:123:GLN:HG3	2:B:81:PRO:HB2	1.77	0.65
4:R:203:GLY:HA2	4:R:206:ILE:HD12	1.77	0.65
6:T:196:ARG:HD3	6:T:239:ARG:HG2	1.78	0.64
9:I:213:THR:HG1	10:J:199:THR:HG1	1.45	0.64
1:O:49:VAL:HG22	1:O:219:VAL:HG12	1.80	0.64
4:D:119:THR:HG22	4:D:126:PRO:HB3	1.80	0.64
7:U:42:CYS:HB3	7:U:190:VAL:HG21	1.81	0.63
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.79	0.63
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.81	0.62
10:X:129:CYS:O	15:c:242:ARG:NH1	2.33	0.62
14:N:15:LYS:HE2	14:N:135:PRO:HA	1.82	0.62
9:I:106:THR:HB	9:I:109:HIS:HE2	1.64	0.62
1:O:132:ARG:HB2	7:U:13:SER:HA	1.81	0.62
2:P:11:THR:HG23	2:P:21:GLN:HB2	1.82	0.62
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.82	0.62
9:W:63:LEU:HD11	9:W:79:ALA:HB2	1.82	0.62
13:M:178:ASP:OD2	10:X:177:ARG:NH1	2.32	0.62
2:B:119:GLN:HG3	3:C:81:SER:HB2	1.82	0.61
3:Q:49:ARG:NH1	3:Q:212:GLU:OE1	2.33	0.61
1:A:123:GLN:NE2	2:B:82:ASP:OD1	2.33	0.61
5:S:209:LYS:O	5:S:214:ASN:ND2	2.33	0.61
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.82	0.61
9:W:216:VAL:HG22	10:X:196:THR:HG23	1.81	0.61
15:d:218:PRO:HB2	15:d:221:LEU:HD22	1.83	0.61
7:G:212:LEU:O	7:G:233:ARG:NH1	2.33	0.61
5:E:91:LYS:HD3	5:E:119:LEU:HD11	1.82	0.60
1:O:123:GLN:HG3	2:P:81:PRO:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:GLN:NE2	7:G:84:ASP:OD1	2.34	0.60
13:a:66:ARG:NH2	13:a:240:LYS:O	2.34	0.60
4:D:24:GLU:HA	4:D:27:LYS:HE3	1.84	0.60
5:E:160:GLY:O	6:F:82:ARG:NH2	2.28	0.60
5:E:236:GLU:HA	5:E:239:LYS:HE2	1.83	0.60
2:P:119:GLN:HG3	3:Q:81:SER:HB2	1.83	0.59
12:L:134:TYR:HB3	11:Y:141:SER:HB3	1.84	0.59
14:N:43:MET:HG2	14:N:51:LEU:HB3	1.85	0.59
4:R:8:THR:HG23	4:R:18:GLN:HB2	1.83	0.59
4:D:39:ASP:OD1	4:D:213:ARG:NH1	2.30	0.59
1:A:132:ARG:HB2	7:G:13:SER:HA	1.85	0.59
6:T:157:ARG:NH1	7:U:57:LYS:O	2.36	0.59
5:E:9:ASP:OD1	5:E:9:ASP:N	2.36	0.58
1:O:164:LYS:NZ	2:P:55:ILE:O	2.36	0.58
13:a:63:ILE:O	14:b:151:ARG:NH2	2.29	0.57
6:F:95:SER:OG	6:F:101:ARG:NH1	2.37	0.57
10:X:15:LYS:HD2	10:X:121:ILE:HG12	1.86	0.57
5:E:59:MET:HE2	5:E:64:ILE:HD11	1.85	0.57
6:T:72:ILE:HG21	6:T:88:MET:HE1	1.87	0.57
4:R:96:LEU:HB2	11:Y:62:LYS:HG3	1.87	0.57
14:N:50:MET:HE2	14:N:192:VAL:HG12	1.87	0.57
11:Y:43:LEU:HB2	11:Y:183:ILE:HD11	1.86	0.57
3:C:90:LEU:HG	3:C:114:LEU:HD13	1.85	0.57
5:E:52:LYS:HE3	5:E:216:GLU:HG3	1.87	0.57
2:B:68:ILE:HD11	2:B:74:LEU:HD12	1.86	0.56
4:R:119:THR:HG22	4:R:126:PRO:HB3	1.86	0.56
2:P:42:ASN:OD1	2:P:42:ASN:N	2.38	0.56
12:L:192:VAL:HG11	10:X:205:ASP:HB3	1.86	0.56
13:M:176:LEU:HD23	13:M:206:VAL:HG12	1.88	0.56
7:G:67:LEU:HD13	7:G:215:SER:HB3	1.88	0.56
13:a:176:LEU:HD12	13:a:206:VAL:HG12	1.87	0.56
5:E:240:ASP:OD1	5:E:240:ASP:N	2.39	0.56
6:F:224:TYR:HD2	6:F:228:ASP:HB3	1.71	0.56
7:U:220:ILE:HG23	7:U:221:THR:HG23	1.87	0.55
5:E:168:ARG:NH1	6:F:53:GLN:OE1	2.29	0.55
3:C:171:ALA:HB2	3:C:200:THR:HG21	1.87	0.55
11:K:46:CYS:HB2	11:K:53:THR:HG23	1.89	0.55
2:P:60:ARG:HH12	2:P:223:PRO:HG3	1.72	0.55
7:G:109:LEU:HD11	7:G:138:LEU:HB3	1.88	0.55
13:a:56:ARG:NE	13:a:219:ASP:OD2	2.37	0.55
7:U:68:PHE:HB2	7:U:76:MET:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:209:ASN:HD21	10:X:165:GLU:HA	1.72	0.55
6:F:199:LEU:HD13	6:F:203:GLN:HG3	1.89	0.54
3:C:194:ILE:HG13	3:C:236:LEU:HB3	1.89	0.54
6:F:196:ARG:HD3	6:F:239:ARG:HG2	1.90	0.54
11:K:59:TYR:O	11:K:63:ASN:ND2	2.38	0.54
6:T:100:ASP:OD2	14:b:86:LYS:NZ	2.41	0.54
7:G:180:LEU:HD21	7:G:193:GLU:HB3	1.89	0.54
4:D:36:ARG:NH1	5:E:60:GLU:OE2	2.41	0.54
6:F:200:PRO:O	6:F:239:ARG:NH1	2.40	0.54
10:J:177:ARG:NH1	13:a:178:ASP:OD2	2.38	0.54
13:M:202:LEU:O	13:M:206:VAL:HG13	2.08	0.54
10:X:205:ASP:OD1	10:X:205:ASP:N	2.39	0.54
9:I:63:LEU:HD11	9:I:79:ALA:HB2	1.90	0.54
11:Y:184:ASP:OD1	11:Y:189:HIS:NE2	2.40	0.54
4:D:240:GLU:OE2	4:D:244:GLN:NE2	2.41	0.54
6:T:117:GLN:NE2	7:U:84:ASP:OD1	2.39	0.54
6:T:224:TYR:HD2	6:T:228:ASP:HB3	1.73	0.54
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.90	0.54
3:Q:178:ASP:OD2	3:Q:195:LYS:NZ	2.39	0.53
13:M:56:ARG:O	13:M:70:LYS:NZ	2.42	0.53
2:P:74:LEU:HD23	2:P:87:VAL:HG22	1.90	0.53
14:N:25:ASP:OD1	14:N:41:ARG:NH2	2.33	0.53
4:D:209:ALA:HB1	4:D:217:LEU:HD11	1.89	0.53
8:H:174:ILE:HB	8:H:189:LEU:HB2	1.89	0.53
4:D:173:GLU:HG2	5:E:57:PRO:HG2	1.91	0.53
5:S:52:LYS:HE3	5:S:216:GLU:HG3	1.89	0.53
14:N:96:MET:HE3	14:N:127:MET:HA	1.91	0.53
2:P:111:VAL:HG22	2:P:136:ILE:HD12	1.89	0.53
4:R:196:LEU:HA	4:R:199:VAL:HG12	1.91	0.53
13:a:153:ASP:OD1	13:a:157:SER:N	2.39	0.53
2:B:51:LYS:NZ	2:B:200:GLU:O	2.42	0.53
3:Q:119:GLN:NE2	4:R:79:ASP:OD1	2.38	0.53
5:S:190:THR:OG1	5:S:193:GLU:OE1	2.24	0.53
3:C:118:LYS:O	3:C:122:THR:HG23	2.09	0.52
10:X:125:ASP:OD1	10:X:129:CYS:N	2.35	0.52
6:F:72:ILE:HG21	6:F:88:MET:HE1	1.92	0.52
9:W:146:MET:HE1	9:W:154:LEU:HD22	1.92	0.52
1:O:122:SER:O	1:O:126:THR:HG23	2.08	0.52
3:C:140:ASP:OD2	3:C:146:GLN:NE2	2.30	0.52
14:b:43:MET:HG2	14:b:51:LEU:HB3	1.92	0.52
4:D:30:SER:HB3	4:D:48:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:LYS:HG3	8:H:120:MET:HB2	1.91	0.52
11:K:1:MET:HG2	11:K:134:TYR:H	1.73	0.52
13:M:173:LEU:HD21	13:M:210:ALA:HB2	1.92	0.52
1:A:48:ALA:HB1	1:A:141:ILE:HD12	1.92	0.52
12:L:52:CYS:HA	12:L:97:MET:HE3	1.92	0.52
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.91	0.52
11:Y:118:MET:HE2	11:Y:124:LEU:HD13	1.92	0.52
15:d:193:VAL:HB	15:d:210:VAL:HG22	1.92	0.52
1:A:86:ASP:OD1	7:G:121:HIS:NE2	2.33	0.52
5:E:147:ASP:N	5:E:147:ASP:OD1	2.40	0.52
10:J:15:LYS:HD2	10:J:121:ILE:HG12	1.92	0.52
9:W:177:VAL:HB	9:W:184:ASP:HB2	1.92	0.52
15:c:218:PRO:HB2	15:c:221:LEU:HB2	1.90	0.52
4:D:203:GLY:HA3	4:D:229:VAL:HG21	1.91	0.52
8:V:84:LYS:HG3	8:V:120:MET:HB2	1.92	0.52
9:W:209:ASN:ND2	10:X:165:GLU:HA	2.25	0.52
14:N:166:ARG:NH2	14:N:200:GLU:OE1	2.43	0.51
4:R:31:THR:OG1	4:R:163:ARG:O	2.24	0.51
4:R:46:GLU:HG3	4:R:199:VAL:HG23	1.91	0.51
9:I:45:GLY:HA3	9:I:52:THR:HG21	1.91	0.51
3:Q:52:ILE:O	3:Q:52:ILE:HD12	2.10	0.51
5:E:209:LYS:O	5:E:214:ASN:ND2	2.43	0.51
10:J:15:LYS:HG2	10:J:119:PRO:HB2	1.91	0.51
1:O:113:MET:HE2	9:W:70:THR:HG22	1.92	0.51
6:T:196:ARG:NH2	6:T:237:GLU:O	2.43	0.51
11:Y:104:LEU:HB3	11:Y:116:TYR:HB2	1.93	0.51
3:C:35:LEU:HD11	3:C:175:LEU:HD11	1.93	0.51
12:L:7:LYS:O	12:L:143:TYR:OH	2.20	0.51
1:O:51:VAL:HG22	1:O:217:VAL:HG22	1.92	0.51
2:B:76:TYR:HB3	2:B:83:TYR:CD1	2.46	0.51
7:U:214:LEU:H	7:U:233:ARG:HH12	1.59	0.51
14:b:43:MET:SD	14:b:64:LYS:HG2	2.50	0.51
7:G:44:ASP:OD1	7:G:44:ASP:N	2.43	0.51
2:B:42:ASN:OD1	2:B:42:ASN:N	2.43	0.51
2:B:156:PHE:HD2	3:C:51:ASN:HD21	1.58	0.51
7:U:187:CYS:O	7:U:191:VAL:HG23	2.11	0.51
7:G:35:SER:HB3	7:G:66:ARG:HH12	1.75	0.51
2:P:86:LEU:HD13	2:P:134:LEU:HD11	1.92	0.51
10:X:28:PHE:HB2	10:X:39:PHE:HB2	1.93	0.51
11:Y:2:GLU:HG3	11:Y:47:VAL:HB	1.92	0.51
5:S:38:ILE:HG23	5:S:181:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:216:VAL:HG22	10:J:196:THR:HG23	1.92	0.50
10:J:14:MET:HB3	10:J:163:LEU:HD11	1.94	0.50
15:d:248:PRO:O	15:d:251:THR:OG1	2.28	0.50
5:S:129:ASP:OD1	5:S:129:ASP:N	2.36	0.50
1:A:1:MET:SD	1:A:1:MET:N	2.80	0.50
3:C:33:THR:OG1	3:C:166:ASN:O	2.28	0.50
4:D:40:ILE:HG13	4:D:212:ARG:HG3	1.94	0.50
10:J:28:PHE:HB2	10:J:39:PHE:HB2	1.93	0.50
11:K:96:THR:O	11:K:96:THR:OG1	2.25	0.50
2:P:76:TYR:HB3	2:P:83:TYR:CD1	2.47	0.50
9:W:219:LEU:HD11	10:X:195:ILE:HG13	1.92	0.50
1:A:37:LEU:HD22	1:A:53:GLN:HG3	1.94	0.50
13:a:181:VAL:HG13	13:a:194:LEU:HD22	1.93	0.50
15:c:217:PHE:CD1	15:c:218:PRO:HD2	2.47	0.50
1:A:58:ASP:OD1	1:A:58:ASP:N	2.44	0.50
4:D:238:GLU:O	4:D:241:LYS:HG2	2.12	0.50
11:K:141:SER:HB3	12:Z:134:TYR:HB3	1.93	0.50
13:M:35:PHE:HZ	13:M:168:SER:HB3	1.77	0.50
3:Q:118:LYS:NZ	3:Q:150:SER:OG	2.42	0.50
6:F:109:VAL:HA	6:F:112:ILE:HD12	1.94	0.50
14:b:15:LYS:HE2	14:b:135:PRO:HA	1.94	0.50
6:F:72:ILE:HG22	6:F:134:ILE:HG12	1.93	0.50
13:M:153:ASP:OD1	13:M:157:SER:N	2.40	0.50
9:I:115:PRO:HG2	15:d:228:LEU:HD21	1.94	0.50
2:P:122:THR:HG22	3:Q:128:ARG:HH21	1.77	0.50
5:S:160:GLY:O	6:T:82:ARG:NH2	2.45	0.50
4:D:41:VAL:HG23	4:D:211:MET:HB3	1.92	0.49
4:D:146:GLN:OE1	4:D:159:ASN:ND2	2.45	0.49
13:a:202:LEU:O	13:a:206:VAL:HG13	2.11	0.49
10:J:51:ILE:HD11	10:J:107:PRO:HB3	1.92	0.49
6:F:226:ASP:OD1	6:F:226:ASP:N	2.45	0.49
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.94	0.49
4:R:116:GLN:NE2	5:S:84:ASP:OD1	2.45	0.49
12:Z:9:ARG:NH2	12:Z:146:ASP:OD1	2.45	0.49
14:b:50:MET:HE2	14:b:192:VAL:HG12	1.93	0.49
2:B:50:LYS:NZ	2:B:62:VAL:O	2.45	0.49
2:B:143:ARG:NH1	2:B:144:PRO:O	2.44	0.49
2:P:74:LEU:HD11	2:P:134:LEU:HB3	1.94	0.49
4:R:137:ASP:OD2	4:R:143:ARG:NH1	2.45	0.49
2:P:135:LEU:HD22	2:P:146:LEU:HD11	1.94	0.49
8:H:25:TYR:HB2	14:b:141:TYR:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:35:MET:HG2	11:K:45:LEU:HG	1.94	0.49
4:R:41:VAL:HG23	4:R:211:MET:HB3	1.94	0.49
2:B:1:MET:HB2	7:G:122:ALA:HB1	1.94	0.49
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.94	0.49
3:C:9:THR:HB	3:C:20:GLN:HG3	1.93	0.49
8:H:30:VAL:HG11	14:b:211:ILE:HG13	1.95	0.49
4:D:5:ARG:O	4:D:123:GLY:N	2.41	0.49
8:H:189:LEU:HD22	8:H:193:GLN:HB3	1.95	0.49
13:a:40:VAL:HG11	13:a:81:GLY:HA3	1.94	0.49
7:U:34:SER:O	7:U:168:LYS:N	2.46	0.48
7:U:109:LEU:HD11	7:U:138:LEU:HB3	1.95	0.48
11:K:4:LEU:HD22	11:K:45:LEU:HB3	1.95	0.48
14:N:141:TYR:HE2	8:V:25:TYR:HB2	1.78	0.48
1:O:196:GLU:OE1	1:O:242:LEU:HB2	2.13	0.48
3:Q:90:LEU:HG	3:Q:114:LEU:HD13	1.95	0.48
2:P:74:LEU:HD13	2:P:136:ILE:HG12	1.93	0.48
7:G:42:CYS:HB3	7:G:190:VAL:HG21	1.95	0.48
2:P:93:LEU:HD13	2:P:113:ARG:HB3	1.94	0.48
3:Q:118:LYS:O	3:Q:122:THR:HG23	2.13	0.48
6:T:88:MET:HE3	6:T:112:ILE:HD11	1.96	0.48
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.95	0.48
5:E:67:ILE:HD12	5:E:216:GLU:HB3	1.96	0.48
6:F:33:SER:HB3	6:F:51:ARG:HG3	1.94	0.48
6:F:71:GLY:HA3	6:F:221:PHE:CZ	2.49	0.48
6:T:32:GLY:O	6:T:163:ALA:N	2.47	0.48
9:W:48:THR:HB	9:W:51:ASP:HB2	1.93	0.48
1:O:211:LYS:HB2	1:O:214:GLU:HG3	1.96	0.48
5:E:78:MET:HG3	5:E:82:ILE:HD12	1.96	0.48
11:Y:35:MET:HG2	11:Y:45:LEU:HG	1.96	0.48
13:a:136:ASN:HB2	13:a:152:PHE:HB2	1.95	0.47
2:B:71:HIS:CE1	2:B:104:PRO:HB2	2.48	0.47
6:F:7:ASP:HA	6:F:20:HIS:HB2	1.96	0.47
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.96	0.47
7:U:230:LYS:HA	7:U:230:LYS:HD3	1.77	0.47
10:X:20:VAL:HG23	10:X:190:ILE:HB	1.97	0.47
6:F:206:THR:HG23	6:F:208:LYS:H	1.79	0.47
10:J:20:VAL:HG23	10:J:190:ILE:HB	1.96	0.47
12:L:72:GLU:OE2	12:L:106:LYS:NZ	2.47	0.47
6:T:36:VAL:HB	6:T:47:VAL:HG23	1.95	0.47
7:U:180:LEU:HD21	7:U:193:GLU:HB3	1.96	0.47
8:V:84:LYS:HE3	8:V:84:LYS:HB3	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:103:TYR:CD1	13:a:111:MET:HG2	2.49	0.47
8:H:172:GLY:HA2	14:b:209:TRP:CH2	2.49	0.47
10:X:14:MET:HB2	10:X:167:ILE:HD12	1.95	0.47
2:B:1:MET:H2	7:G:129:VAL:HG11	1.79	0.47
6:T:192:LEU:HD13	6:T:233:LEU:HD23	1.96	0.47
12:Z:164:THR:HG22	12:Z:170:SER:HB3	1.95	0.47
13:a:52:ALA:HB1	13:a:221:LEU:HD11	1.96	0.47
9:I:48:THR:HB	9:I:51:ASP:HB2	1.97	0.47
3:Q:136:TYR:HE1	3:Q:150:SER:HB3	1.79	0.47
7:U:18:ASP:OD1	7:U:20:ARG:HD3	2.15	0.47
7:U:67:LEU:HD12	7:U:213:GLU:HG2	1.96	0.47
11:K:118:MET:HE2	11:K:124:LEU:HD13	1.96	0.47
2:P:74:LEU:HG	2:P:83:TYR:HE1	1.80	0.47
4:R:199:VAL:HG11	4:R:206:ILE:HD11	1.97	0.47
6:T:71:GLY:HA3	6:T:221:PHE:CZ	2.50	0.47
9:W:209:ASN:ND2	10:X:168:SER:HB2	2.30	0.47
7:G:52:LYS:NZ	7:G:63:SER:O	2.42	0.47
10:J:193:ASP:OD1	10:J:193:ASP:N	2.48	0.47
11:K:62:LYS:HA	11:K:62:LYS:HD3	1.64	0.47
3:Q:167:ASN:HB2	3:Q:200:THR:HG23	1.96	0.47
5:S:78:MET:HG3	5:S:82:ILE:HD12	1.96	0.47
7:U:189:ASP:O	7:U:193:GLU:HG2	2.15	0.47
14:b:45:VAL:HB	14:b:49:THR:HB	1.97	0.47
4:D:188:ILE:HG23	4:D:208:LEU:HD21	1.97	0.46
2:P:4:ARG:HH21	6:T:122:ARG:HH21	1.63	0.46
4:R:40:ILE:HG13	4:R:212:ARG:HG3	1.96	0.46
11:Y:119:ASP:OD1	11:Y:119:ASP:N	2.43	0.46
13:M:52:ALA:HB1	13:M:221:LEU:HD11	1.97	0.46
2:P:160:ALA:HB3	3:Q:55:LEU:HD22	1.98	0.46
1:A:122:SER:O	1:A:126:THR:HG23	2.15	0.46
2:B:130:PHE:O	2:B:151:PRO:HB3	2.15	0.46
3:C:226:ARG:NH2	3:C:232:GLU:OE1	2.37	0.46
4:R:116:GLN:HG3	5:S:83:ALA:HB1	1.98	0.46
6:T:176:MET:HE2	6:T:176:MET:HB3	1.80	0.46
2:B:34:PRO:HD2	2:B:49:GLU:HG2	1.97	0.46
3:C:21:VAL:HG11	3:C:153:SER:HB3	1.96	0.46
6:F:88:MET:HE3	6:F:112:ILE:HD11	1.97	0.46
1:O:203:SER:O	1:O:207:SER:N	2.49	0.46
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.83	0.46
1:O:112:ASP:HB3	1:O:152:TYR:CZ	2.51	0.46
6:T:109:VAL:HA	6:T:112:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:174:ILE:HB	8:V:189:LEU:HB2	1.97	0.46
2:B:176:LYS:HE2	2:B:176:LYS:HB2	1.81	0.46
8:H:115:PRO:HD2	8:H:119:MET:HG3	1.98	0.46
6:F:90:GLN:NE2	6:F:94:ASP:OD1	2.49	0.46
10:J:87:LEU:O	10:J:91:VAL:HG23	2.16	0.46
1:O:211:LYS:HE3	1:O:212:PRO:HD2	1.97	0.46
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.97	0.46
6:F:50:LYS:HB3	6:F:59:HIS:HB3	1.97	0.45
13:M:219:ASP:HA	13:M:240:LYS:HD3	1.98	0.45
11:Y:46:CYS:HB2	11:Y:53:THR:HG23	1.97	0.45
12:Z:49:ALA:HB2	15:d:208:MET:HG2	1.98	0.45
1:A:206:LEU:HD12	1:A:210:PHE:HZ	1.81	0.45
8:H:179:ILE:HG23	8:H:184:VAL:HG22	1.98	0.45
5:S:137:PHE:O	5:S:158:PRO:HB3	2.15	0.45
5:E:37:ALA:HB2	5:E:50:VAL:HG13	1.97	0.45
6:F:47:VAL:HG12	6:F:212:ILE:HG12	1.99	0.45
7:U:35:SER:HB3	7:U:66:ARG:HH12	1.81	0.45
9:W:45:GLY:HA3	9:W:52:THR:HG21	1.98	0.45
11:Y:183:ILE:HG12	11:Y:188:ILE:HG12	1.97	0.45
15:d:217:PHE:CD1	15:d:218:PRO:HD2	2.51	0.45
14:N:20:VAL:HG11	14:N:122:LEU:HD13	1.99	0.45
13:M:66:ARG:NH2	9:W:164:PHE:O	2.49	0.45
1:A:164:LYS:NZ	2:B:55:ILE:O	2.49	0.45
4:D:115:LYS:O	4:D:119:THR:HG23	2.15	0.45
5:E:126:GLU:HB2	6:F:124:GLY:HA3	1.97	0.45
10:J:84:PRO:HB2	10:J:120:PHE:CD1	2.52	0.45
13:M:201:ARG:HG3	9:W:199:PHE:HB3	1.98	0.45
14:N:63:LEU:HD11	14:N:106:LEU:HD13	1.98	0.45
10:X:193:ASP:OD1	10:X:193:ASP:N	2.47	0.45
15:c:190:PRO:HG3	15:c:217:PHE:HD1	1.80	0.45
4:D:42:VAL:HB	4:D:191:VAL:HG21	1.99	0.45
4:D:154:HIS:CG	5:E:59:MET:HE3	2.52	0.45
9:I:177:VAL:HB	9:I:184:ASP:HB2	1.99	0.45
10:J:77:LYS:HB3	10:J:77:LYS:HE3	1.62	0.45
6:T:68:ASN:HB3	6:T:220:GLU:HG2	1.98	0.45
3:C:24:ALA:O	3:C:28:ILE:HG12	2.17	0.45
9:W:86:MET:HA	9:W:89:ARG:HE	1.82	0.45
12:Z:112:TYR:CE2	12:Z:122:SER:HB2	2.52	0.45
13:a:44:ALA:HB2	13:a:149:VAL:HG23	1.98	0.45
3:Q:35:LEU:HD11	3:Q:175:LEU:HD11	1.99	0.44
11:Y:37:LYS:HE2	11:Y:188:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:106:LYS:HB2	12:Z:106:LYS:HE2	1.75	0.44
10:J:35:VAL:HG12	10:J:36:THR:HG23	2.00	0.44
1:O:123:GLN:CG	2:P:81:PRO:HB2	2.47	0.44
4:R:42:VAL:HB	4:R:191:VAL:HG21	1.99	0.44
9:I:219:LEU:HD11	10:J:195:ILE:HG13	1.99	0.44
7:U:70:VAL:HG11	7:U:112:LEU:HD21	1.99	0.44
7:U:162:TRP:CE2	7:U:183:LYS:HE2	2.52	0.44
13:a:55:THR:OG1	13:a:220:ALA:HB3	2.17	0.44
13:a:151:SER:OG	13:a:161:ASP:OD2	2.28	0.44
7:G:202:HIS:CE1	7:G:207:ASP:HB2	2.53	0.44
13:M:221:LEU:N	13:M:236:VAL:O	2.48	0.44
12:Z:139:MET:O	12:Z:143:TYR:N	2.51	0.44
1:A:49:VAL:HG22	1:A:219:VAL:HG12	1.99	0.44
2:B:171:LYS:O	2:B:175:GLU:HG3	2.17	0.44
6:F:36:VAL:HB	6:F:47:VAL:HG23	1.98	0.44
10:J:177:ARG:NH2	12:Z:27:ALA:O	2.51	0.44
11:K:52:ASP:OD1	12:L:88:TYR:OH	2.23	0.44
7:U:35:SER:HB3	7:U:66:ARG:NH1	2.33	0.44
14:b:179:ARG:HA	14:b:179:ARG:HD3	1.87	0.44
11:K:43:LEU:HB2	11:K:183:ILE:HD11	1.98	0.44
14:N:54:SER:O	14:N:108:ASN:ND2	2.49	0.44
5:S:147:ASP:OD1	5:S:147:ASP:N	2.51	0.44
4:D:208:LEU:HD23	4:D:220:LEU:HD12	2.00	0.44
6:T:7:ASP:HA	6:T:20:HIS:HB2	1.99	0.44
7:G:38:ILE:HD11	7:G:194:VAL:HG13	1.99	0.44
3:Q:24:ALA:O	3:Q:28:ILE:HG12	2.17	0.44
5:S:233:GLU:O	5:S:237:VAL:HG23	2.17	0.44
11:Y:160:LEU:O	11:Y:164:LEU:HG	2.18	0.44
4:R:38:LYS:NZ	4:R:182:GLU:OE1	2.51	0.44
1:A:61:LEU:HD11	7:G:159:TYR:HB3	2.00	0.43
3:C:107:CYS:O	3:C:111:VAL:HG23	2.18	0.43
13:M:121:SER:OG	13:M:156:GLY:O	2.31	0.43
7:U:214:LEU:N	7:U:233:ARG:HH12	2.15	0.43
9:W:43:CYS:SG	9:W:98:LEU:HB3	2.58	0.43
2:B:179:ASN:N	2:B:179:ASN:OD1	2.50	0.43
7:G:67:LEU:HD12	7:G:213:GLU:HG2	2.00	0.43
9:I:115:PRO:HD2	15:d:228:LEU:HD11	2.00	0.43
9:I:134:ALA:HB1	9:I:158:ALA:HB1	2.00	0.43
11:K:101:ASN:HB3	11:K:132:HIS:CE1	2.53	0.43
1:O:165:ALA:HB3	2:P:56:LEU:HD22	2.00	0.43
5:S:73:HIS:CE1	5:S:106:THR:HB	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:199:ASP:N	15:c:199:ASP:OD1	2.49	0.43
4:D:203:GLY:HA2	4:D:206:ILE:HD12	1.99	0.43
14:N:92:LEU:HD21	14:N:110:MET:SD	2.58	0.43
5:S:31:ILE:HD11	5:S:158:PRO:CD	2.49	0.43
7:U:111:HIS:O	7:U:115:ARG:HG2	2.18	0.43
8:V:115:PRO:HD2	8:V:119:MET:HG3	2.01	0.43
4:D:116:GLN:HG3	5:E:83:ALA:HB1	2.00	0.43
4:D:231:GLU:O	4:D:235:GLU:HG2	2.17	0.43
10:J:34:MET:O	12:Z:166:ARG:NH1	2.51	0.43
10:J:113:ASP:O	10:J:117:PHE:N	2.44	0.43
5:S:24:VAL:O	5:S:28:ILE:HG12	2.18	0.43
9:W:110:LEU:HD21	9:W:125:VAL:HG22	2.00	0.43
6:F:158:ALA:HB1	6:F:172:LEU:HD22	2.01	0.43
12:L:9:ARG:NH2	12:L:146:ASP:OD1	2.52	0.43
13:M:96:ILE:HD11	13:M:120:LEU:HD13	2.01	0.43
14:N:45:VAL:HB	14:N:49:THR:HB	1.99	0.43
14:N:209:TRP:CH2	8:V:172:GLY:HA2	2.54	0.43
2:P:34:PRO:HD2	2:P:49:GLU:HG2	2.00	0.43
3:Q:44:LEU:HB3	3:Q:215:THR:HG22	2.01	0.43
6:T:103:LEU:HD12	6:T:104:PRO:HD2	2.01	0.43
12:Z:50:ALA:HB2	13:a:157:SER:HB2	1.99	0.43
1:A:123:GLN:CG	2:B:81:PRO:HB2	2.47	0.43
6:F:74:ILE:HG21	6:F:81:ALA:HB1	2.00	0.43
6:F:165:SER:HB2	6:F:169:ARG:HH21	1.84	0.43
4:R:62:ILE:HG12	4:R:72:ALA:HB2	2.01	0.43
6:T:74:ILE:HG21	6:T:81:ALA:HB1	2.01	0.43
6:F:138:ASP:OD1	6:F:143:HIS:NE2	2.45	0.43
4:R:212:ARG:HH12	4:R:218:LYS:NZ	2.16	0.43
8:V:104:ASP:HB3	8:V:107:GLU:H	1.83	0.43
11:K:27:GLN:NE2	11:Y:171:PHE:O	2.51	0.43
12:L:8:PHE:CZ	12:L:10:HIS:HB2	2.53	0.43
13:M:55:THR:OG1	13:M:220:ALA:HB3	2.19	0.43
1:O:138:MET:HB3	1:O:154:CYS:SG	2.59	0.43
9:W:42:TYR:HB2	9:W:178:ILE:HD11	1.99	0.43
10:X:11:VAL:HG11	10:X:52:GLY:HA3	1.99	0.43
10:X:84:PRO:HB2	10:X:120:PHE:CD2	2.54	0.43
13:a:42:ALA:HA	13:a:50:ILE:O	2.19	0.43
6:F:32:GLY:O	6:F:163:ALA:N	2.49	0.43
7:G:231:ASP:O	7:G:235:GLU:HG3	2.19	0.43
13:M:38:GLY:HA3	13:M:70:LYS:HE2	2.00	0.43
3:Q:63:GLU:HG2	3:Q:64:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:148:TYR:HE1	4:R:58:THR:HG21	1.84	0.43
4:D:7:ILE:HG22	4:D:18:GLN:HG3	1.99	0.43
5:E:97:GLN:HG3	12:L:65:ILE:HG13	2.01	0.43
13:M:132:TYR:HB3	13:M:134:VAL:HG23	2.01	0.43
13:M:136:ASN:HB2	13:M:152:PHE:HB2	1.99	0.43
3:Q:60:PHE:HE2	10:X:79:GLY:HA3	1.83	0.43
1:A:72:ILE:HG21	1:A:114:LEU:HD21	2.00	0.42
6:T:101:ARG:HH21	14:b:83:TYR:HE1	1.67	0.42
14:b:166:ARG:NH2	14:b:200:GLU:OE1	2.51	0.42
5:S:97:GLN:HG3	12:Z:65:ILE:HG13	2.01	0.42
7:U:73:HIS:CE1	7:U:106:ASN:HB3	2.53	0.42
10:X:87:LEU:O	10:X:91:VAL:HG23	2.19	0.42
3:Q:35:LEU:HB3	3:Q:46:ALA:HB3	2.01	0.42
3:Q:35:LEU:N	3:Q:46:ALA:O	2.44	0.42
3:Q:68:LEU:HD11	3:Q:74:CYS:HB3	2.01	0.42
15:d:231:ARG:HD2	15:d:253:PRO:HG2	2.02	0.42
3:C:180:LYS:O	3:C:184:MET:HG2	2.20	0.42
12:L:138:VAL:HG21	12:L:162:GLN:HG3	2.00	0.42
4:R:40:ILE:HD12	4:R:184:ASP:HB3	2.01	0.42
4:R:52:LYS:HE3	4:R:52:LYS:HB3	1.77	0.42
12:Z:100:MET:HE2	12:Z:128:VAL:HG23	2.01	0.42
5:S:112:VAL:O	5:S:116:VAL:HG23	2.20	0.42
7:U:67:LEU:HD13	7:U:215:SER:HB3	2.01	0.42
10:X:56:LEU:HD23	10:X:56:LEU:HA	1.92	0.42
4:D:92:GLN:HG3	11:K:66:LEU:HB2	2.00	0.42
4:D:195:LEU:HD23	4:D:195:LEU:HA	1.90	0.42
12:L:58:LEU:HD23	12:L:58:LEU:HA	1.91	0.42
9:W:3:ILE:HG13	9:W:127:MET:HB3	2.01	0.42
12:Z:58:LEU:HD23	12:Z:58:LEU:HA	1.90	0.42
5:E:206:MET:HE1	5:E:214:ASN:HB3	2.02	0.42
12:Z:5:ALA:HA	12:Z:13:ILE:O	2.19	0.42
12:Z:98:GLY:HA3	15:d:198:LEU:HD11	2.00	0.42
9:I:209:ASN:OD1	10:J:200:LEU:HD22	2.20	0.42
8:V:142:THR:HB	8:V:155:PHE:CE1	2.55	0.42
13:a:173:LEU:HD21	13:a:210:ALA:HB2	2.01	0.42
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.87	0.42
13:M:200:MET:HE3	13:M:204:LYS:HE3	2.01	0.42
7:U:38:ILE:HD11	7:U:194:VAL:HG13	2.01	0.42
7:U:198:ILE:HG21	7:U:212:LEU:HD13	2.02	0.42
8:H:84:LYS:HE3	8:H:84:LYS:HB3	1.83	0.41
8:H:134:TYR:HA	8:V:133:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:5:ALA:HA	12:L:13:ILE:O	2.20	0.41
3:Q:186:LEU:HD11	3:Q:217:THR:HG22	2.01	0.41
4:R:107:ILE:HD12	4:R:107:ILE:HA	1.87	0.41
4:D:234:LYS:O	4:D:238:GLU:HG2	2.20	0.41
7:G:22:PHE:HA	7:G:25:GLU:HG3	2.02	0.41
4:R:95:ARG:NH2	4:R:101:PRO:HB3	2.34	0.41
1:O:209:ASP:OD1	1:O:209:ASP:N	2.42	0.41
2:P:49:GLU:O	2:P:49:GLU:HG3	2.20	0.41
7:U:9:ASP:OD1	7:U:9:ASP:N	2.53	0.41
9:W:163:ILE:HA	9:W:169:SER:HB2	2.02	0.41
12:L:160:ILE:O	12:L:164:THR:HG23	2.21	0.41
14:N:152:GLU:HG2	14:N:156:LYS:NZ	2.35	0.41
4:R:5:ARG:O	4:R:123:GLY:N	2.44	0.41
11:Y:9:GLY:HA3	11:Y:12:TYR:CE1	2.55	0.41
2:P:143:ARG:HD2	2:P:145:TYR:CZ	2.55	0.41
5:S:166:ASP:HB3	5:S:185:TYR:CZ	2.55	0.41
5:S:187:LYS:HE2	5:S:187:LYS:HB2	1.85	0.41
14:b:25:ASP:HA	14:b:187:PHE:HA	2.02	0.41
3:C:115:CYS:SG	3:C:156:TYR:HB3	2.60	0.41
6:F:84:LEU:HD23	6:F:84:LEU:HA	1.89	0.41
1:O:18:PRO:HA	2:P:24:TYR:CD1	2.56	0.41
7:U:132:PHE:O	7:U:154:PRO:HB3	2.21	0.41
10:X:113:ASP:O	10:X:117:PHE:N	2.44	0.41
1:A:190:THR:OG1	1:A:193:GLN:HG3	2.21	0.41
1:A:192:GLU:O	1:A:196:GLU:HG2	2.21	0.41
6:F:189:LYS:NZ	6:F:234:GLU:O	2.47	0.41
7:G:35:SER:HB3	7:G:66:ARG:NH1	2.36	0.41
9:I:212:LEU:HD21	10:J:201:LYS:HG3	2.03	0.41
10:J:14:MET:HB2	10:J:167:ILE:HD12	2.03	0.41
12:L:37:ILE:HG23	12:L:60:ALA:HB2	2.02	0.41
13:M:42:ALA:HA	13:M:50:ILE:O	2.21	0.41
5:S:240:ASP:OD1	5:S:240:ASP:N	2.45	0.41
15:d:199:ASP:OD1	15:d:199:ASP:N	2.54	0.41
3:C:71:ASP:HA	3:C:223:THR:HG21	2.03	0.41
8:H:14:LEU:HD23	8:H:44:CYS:SG	2.61	0.41
10:J:34:MET:HE3	10:J:34:MET:HB3	1.96	0.41
13:M:127:ARG:HG3	13:M:132:TYR:CE2	2.56	0.41
2:P:130:PHE:O	2:P:151:PRO:HB3	2.20	0.41
2:B:99:LEU:HD23	2:B:99:LEU:HA	1.94	0.40
3:C:179:TYR:CE1	3:C:184:MET:HG3	2.56	0.40
8:H:14:LEU:HD21	8:H:101:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:68:LYS:HA	10:J:68:LYS:HD2	1.84	0.40
1:O:192:GLU:O	1:O:196:GLU:HG2	2.21	0.40
2:P:118:MET:HE2	2:P:151:PRO:HA	2.02	0.40
7:U:180:LEU:HG	7:U:185:MET:HE1	2.03	0.40
14:b:51:LEU:HD21	14:b:110:MET:HE3	2.02	0.40
14:b:92:LEU:HD12	14:b:92:LEU:HA	1.92	0.40
4:D:12:PRO:HA	5:E:26:TYR:CD1	2.56	0.40
5:E:70:ILE:HG13	5:E:143:PHE:HE1	1.86	0.40
9:I:43:CYS:SG	9:I:98:LEU:HB3	2.61	0.40
10:J:56:LEU:HD23	10:J:56:LEU:HA	1.85	0.40
14:N:25:ASP:HA	14:N:187:PHE:HA	2.03	0.40
4:R:22:ALA:O	4:R:26:VAL:HG23	2.20	0.40
13:a:45:GLY:HA3	13:a:48:PHE:CE2	2.56	0.40
3:C:8:ARG:HH21	4:D:5:ARG:HD2	1.85	0.40
3:C:155:ASN:ND2	4:D:77:THR:HB	2.36	0.40
4:D:51:ALA:C	4:D:53:LEU:H	2.29	0.40
5:E:31:ILE:HD11	5:E:158:PRO:CD	2.51	0.40
2:P:203:MET:HA	2:P:207:ASN:HD22	1.86	0.40
4:R:61:LYS:HD3	4:R:73:PHE:CZ	2.56	0.40
9:W:2:THR:HG21	9:W:162:GLY:HA3	2.03	0.40
13:a:142:ASP:OD1	13:a:146:LYS:N	2.54	0.40
2:B:143:ARG:HG2	2:B:144:PRO:HD2	2.03	0.40
6:F:103:LEU:HD12	6:F:104:PRO:HD2	2.04	0.40
9:I:9:LYS:HE3	9:I:9:LYS:HB2	1.80	0.40
12:L:35:ILE:HD12	12:L:56:GLU:CD	2.46	0.40
2:P:115:ALA:HB1	2:P:153:GLY:O	2.22	0.40
3:Q:107:CYS:O	3:Q:111:VAL:HG23	2.22	0.40
5:S:126:GLU:HB2	6:T:124:GLY:HA3	2.04	0.40
5:S:234:LEU:HD23	5:S:234:LEU:HA	1.93	0.40
15:c:194:GLY:N	15:c:207:GLY:O	2.51	0.40
2:B:11:THR:HG23	2:B:21:GLN:HB2	2.04	0.40
6:F:134:ILE:HB	6:F:145:PHE:HB2	2.04	0.40
10:J:153:LEU:HB3	10:J:166:THR:HG23	2.02	0.40
4:R:17:PHE:HD1	4:R:17:PHE:HA	1.78	0.40
11:Y:101:ASN:HB3	11:Y:132:HIS:CD2	2.56	0.40
13:a:200:MET:HE3	13:a:204:LYS:HE3	2.02	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	243/246 (99%)	241 (99%)	2 (1%)	0	100	100
1	O	243/246 (99%)	240 (99%)	3 (1%)	0	100	100
2	B	231/234 (99%)	229 (99%)	2 (1%)	0	100	100
2	P	231/234 (99%)	230 (100%)	1 (0%)	0	100	100
3	C	248/261 (95%)	244 (98%)	4 (2%)	0	100	100
3	Q	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
4	D	241/248 (97%)	239 (99%)	2 (1%)	0	100	100
4	R	241/248 (97%)	238 (99%)	3 (1%)	0	100	100
5	E	234/241 (97%)	231 (99%)	3 (1%)	0	100	100
5	S	234/241 (97%)	230 (98%)	4 (2%)	0	100	100
6	F	236/263 (90%)	232 (98%)	4 (2%)	0	100	100
6	T	236/263 (90%)	233 (99%)	3 (1%)	0	100	100
7	G	239/255 (94%)	239 (100%)	0	0	100	100
7	U	239/255 (94%)	238 (100%)	1 (0%)	0	100	100
8	H	200/239 (84%)	199 (100%)	1 (0%)	0	100	100
8	V	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
9	I	218/277 (79%)	216 (99%)	2 (1%)	0	100	100
9	W	218/277 (79%)	216 (99%)	2 (1%)	0	100	100
10	J	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	X	202/205 (98%)	198 (98%)	4 (2%)	0	100	100
11	K	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
11	Y	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
12	L	199/263 (76%)	197 (99%)	2 (1%)	0	100	100
12	Z	199/263 (76%)	196 (98%)	3 (2%)	0	100	100
13	M	211/241 (88%)	207 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
14	N	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
14	b	212/264 (80%)	206 (97%)	6 (3%)	0	100	100
15	c	63/271 (23%)	62 (98%)	1 (2%)	0	100	100
15	d	63/271 (23%)	61 (97%)	2 (3%)	0	100	100
All	All	6344/7418 (86%)	6254 (99%)	90 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	209/210 (100%)	205 (98%)	4 (2%)	50	69
1	O	209/210 (100%)	203 (97%)	6 (3%)	37	55
2	B	191/191 (100%)	189 (99%)	2 (1%)	68	80
2	P	191/191 (100%)	185 (97%)	6 (3%)	35	53
3	C	210/221 (95%)	207 (99%)	3 (1%)	59	75
3	Q	210/221 (95%)	209 (100%)	1 (0%)	81	88
4	D	207/211 (98%)	203 (98%)	4 (2%)	50	69
4	R	207/211 (98%)	201 (97%)	6 (3%)	37	55
5	E	198/203 (98%)	195 (98%)	3 (2%)	57	74
5	S	198/203 (98%)	195 (98%)	3 (2%)	57	74
6	F	204/225 (91%)	201 (98%)	3 (2%)	57	74
6	T	204/225 (91%)	200 (98%)	4 (2%)	48	67
7	G	199/212 (94%)	198 (100%)	1 (0%)	81	88
7	U	199/212 (94%)	198 (100%)	1 (0%)	81	88
8	H	158/184 (86%)	157 (99%)	1 (1%)	78	87
8	V	158/184 (86%)	156 (99%)	2 (1%)	61	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	181/228 (79%)	181 (100%)	0	100	100
9	W	181/228 (79%)	179 (99%)	2 (1%)	65	79
10	J	174/175 (99%)	172 (99%)	2 (1%)	65	79
10	X	174/175 (99%)	174 (100%)	0	100	100
11	K	168/171 (98%)	166 (99%)	2 (1%)	63	78
11	Y	168/171 (98%)	167 (99%)	1 (1%)	78	87
12	L	157/205 (77%)	154 (98%)	3 (2%)	50	69
12	Z	157/205 (77%)	155 (99%)	2 (1%)	61	76
13	M	177/198 (89%)	176 (99%)	1 (1%)	78	87
13	a	177/198 (89%)	176 (99%)	1 (1%)	78	87
14	N	176/215 (82%)	174 (99%)	2 (1%)	65	79
14	b	176/215 (82%)	176 (100%)	0	100	100
15	c	50/230 (22%)	50 (100%)	0	100	100
15	d	50/230 (22%)	49 (98%)	1 (2%)	48	67
All	All	5318/6158 (86%)	5251 (99%)	67 (1%)	59	76

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	A	81	THR
1	A	173	THR
1	A	177	SER
2	B	44	VAL
2	B	122	THR
3	C	2	SER
3	C	81	SER
3	C	206	LEU
4	D	46	GLU
4	D	69	VAL
4	D	134	VAL
4	D	210	VAL
5	E	14	THR
5	E	87	THR
5	E	139	VAL
6	F	10	VAL
6	F	35	THR

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Mol	Chain	Res	Type
6	F	230	SER
7	G	231	ASP
8	H	133	SER
10	J	20	VAL
10	J	108	VAL
11	K	23	SER
11	K	39	SER
12	L	80	SER
12	L	102	CYS
12	L	133	VAL
13	M	78	THR
14	N	10	SER
14	N	159	VAL
1	O	2	SER
1	O	6	SER
1	O	19	GLU
1	O	50	ILE
1	O	112	ASP
1	O	176	THR
2	P	42	ASN
2	P	45	VAL
2	P	49	GLU
2	P	69	THR
2	P	132	VAL
2	P	224	THR
3	Q	38	LEU
4	R	40	ILE
4	R	67	ASP
4	R	177	THR
4	R	198	VAL
4	R	199	VAL
4	R	210	VAL
5	S	14	THR
5	S	87	THR
5	S	139	VAL
6	T	35	THR
6	T	78	THR
6	T	198	THR
6	T	230	SER
7	U	18	ASP
8	V	142	THR
8	V	202	LEU

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Mol	Chain	Res	Type
9	W	43	CYS
9	W	197	THR
11	Y	2	GLU
12	Z	102	CYS
12	Z	133	VAL
13	a	227	THR
15	d	252	SER

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

Mol	Chain	Res	Type
1	A	75	ASN
1	A	90	GLN
2	B	95	GLN
2	B	102	GLN
2	B	109	GLN
3	C	142	HIS
3	C	167	ASN
4	D	92	GLN
4	D	122	ASN
4	D	175	ASN
4	D	215	GLN
5	E	152	GLN
6	F	31	GLN
6	F	59	HIS
8	H	123	GLN
9	I	91	GLN
10	J	93	ASN
11	K	132	HIS
13	M	180	GLN
1	O	147	GLN
1	O	150	GLN
3	Q	198	ASN
4	R	92	GLN
4	R	122	ASN
4	R	175	ASN
4	R	215	GLN
6	T	68	ASN
7	U	144	ASN
8	V	154	GLN
9	W	193	ASN
10	X	188	HIS

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Mol	Chain	Res	Type
13	a	136	ASN
14	b	208	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.

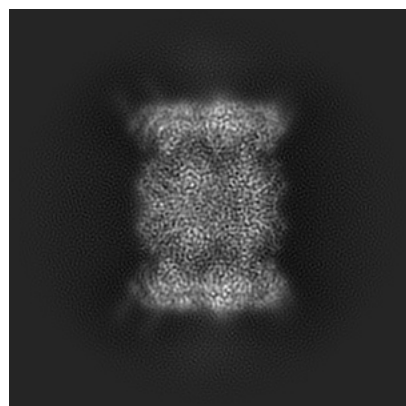
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29604. These allow visual inspection of the internal detail of the map and identification of artifacts.

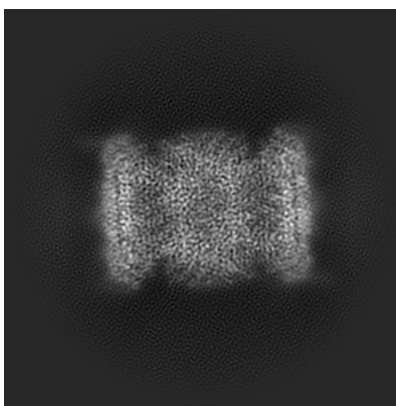
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

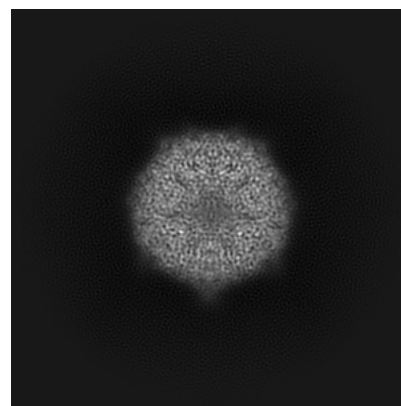
6.1.1 Primary map



X

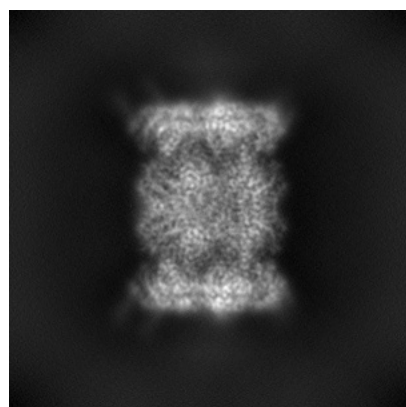


Y

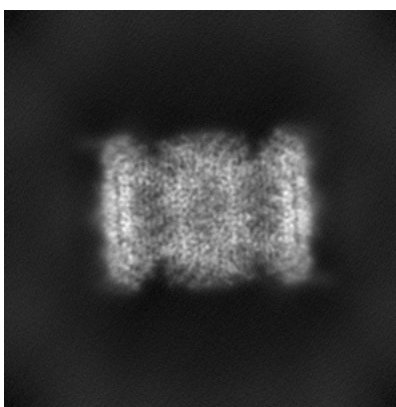


Z

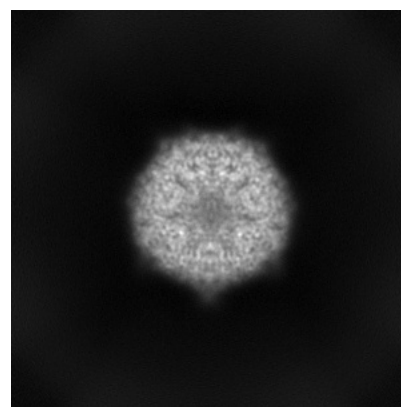
6.1.2 Raw map



X



Y

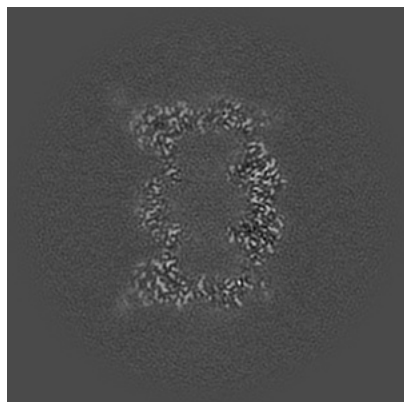


Z

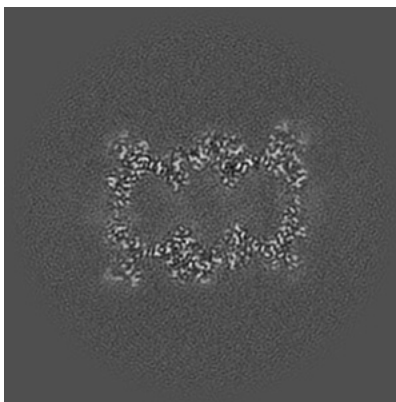
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

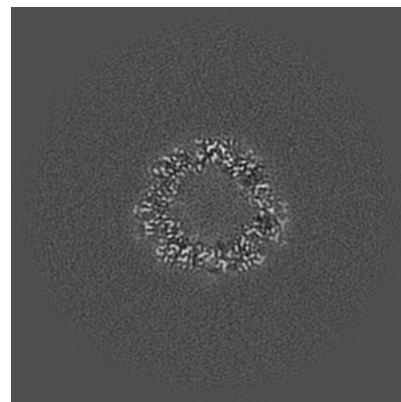
6.2.1 Primary map



X Index: 176

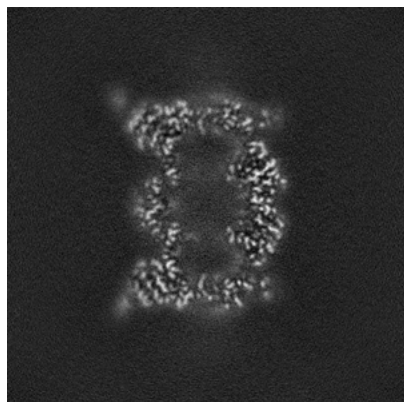


Y Index: 176

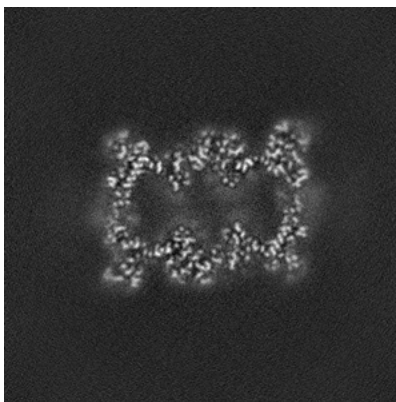


Z Index: 176

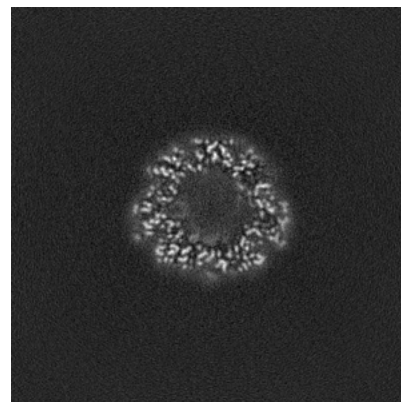
6.2.2 Raw map



X Index: 176



Y Index: 176

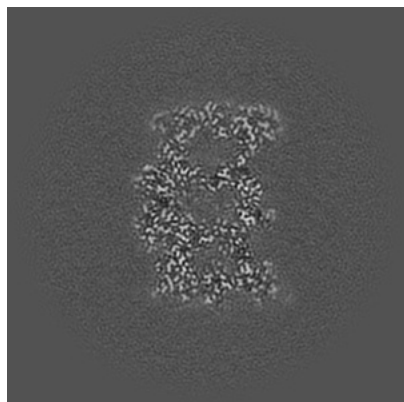


Z Index: 176

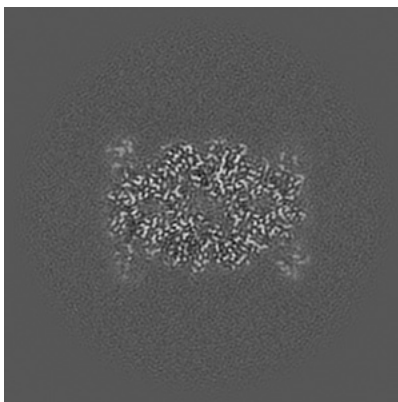
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

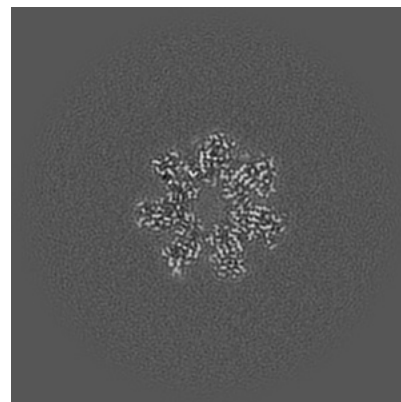
6.3.1 Primary map



X Index: 201

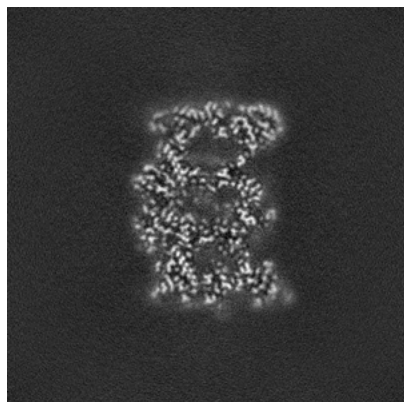


Y Index: 207

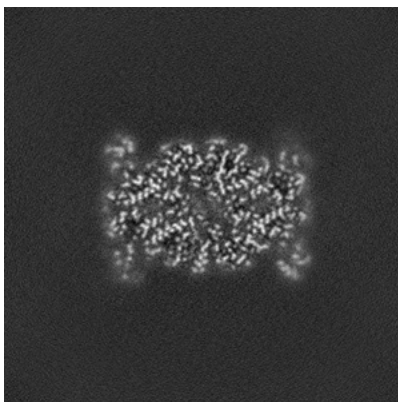


Z Index: 154

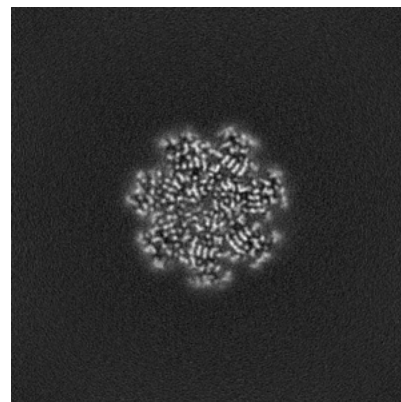
6.3.2 Raw map



X Index: 201



Y Index: 207

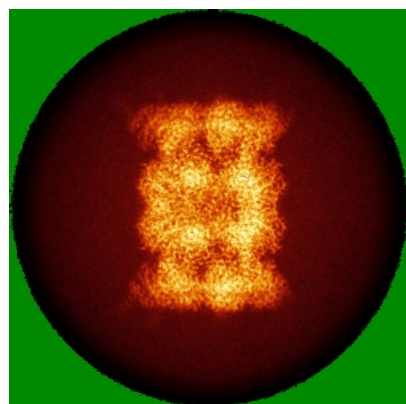


Z Index: 108

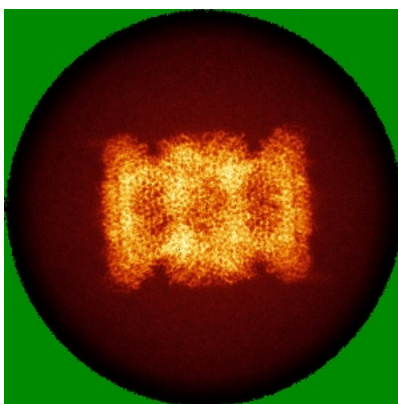
The images above show the largest variance slices of the map in three orthogonal directions.

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

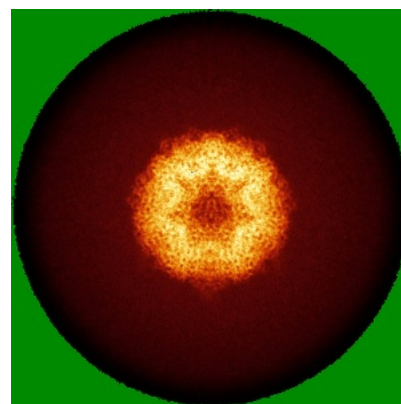
6.4.1 Primary map



X

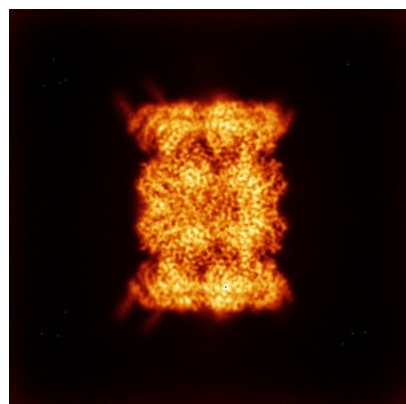


Y

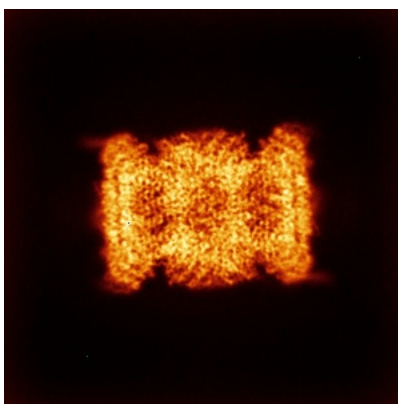


Z

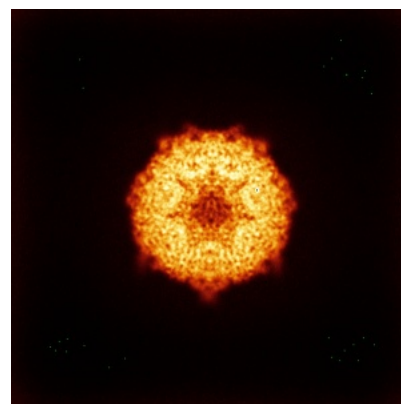
6.4.2 Raw map



X



Y

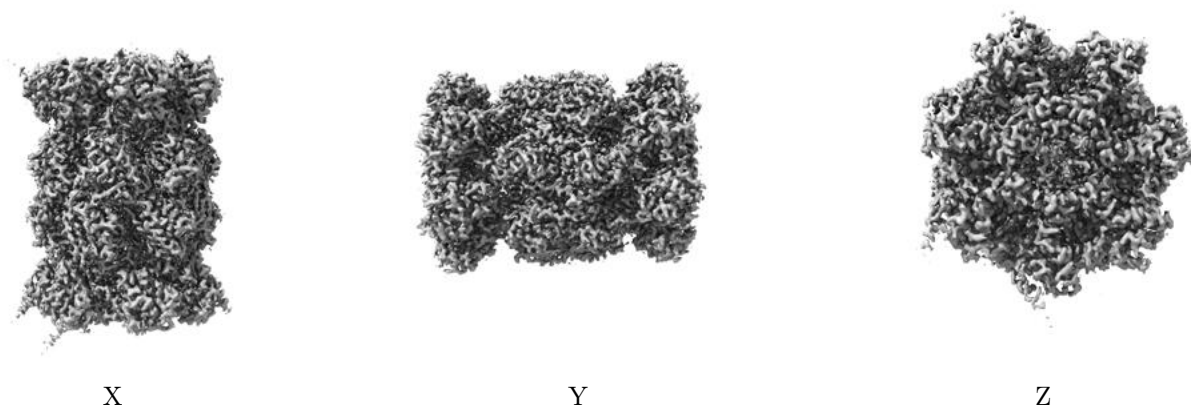


Z

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

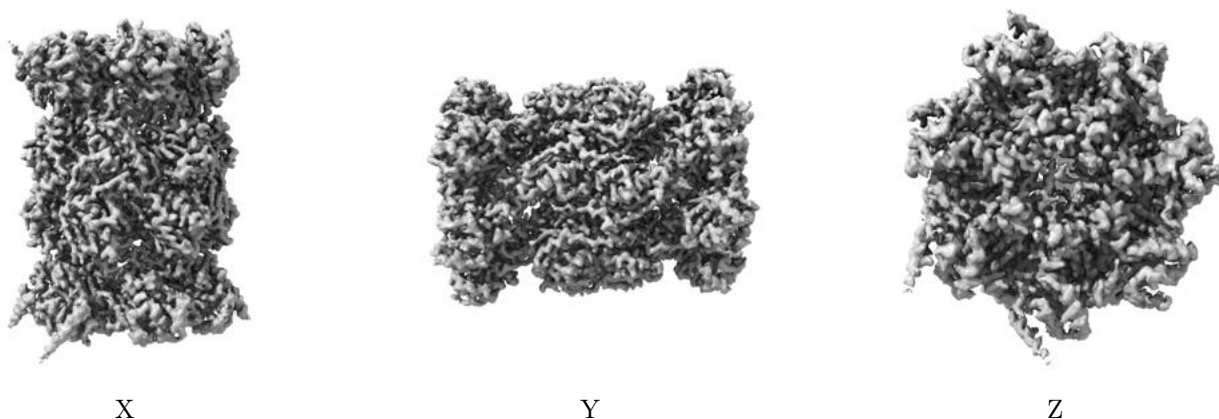
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

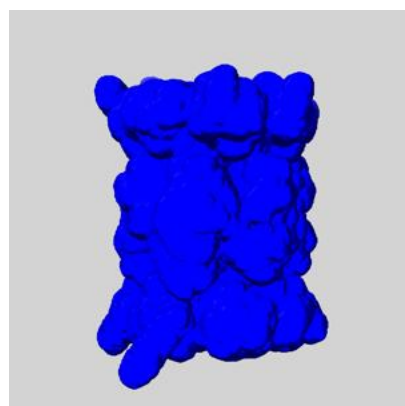
6.6 Mask visualisation [i](#)

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

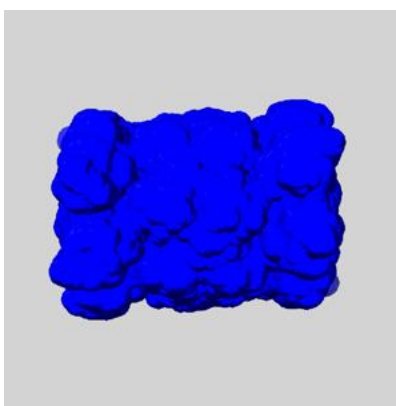
A mask typically either:

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

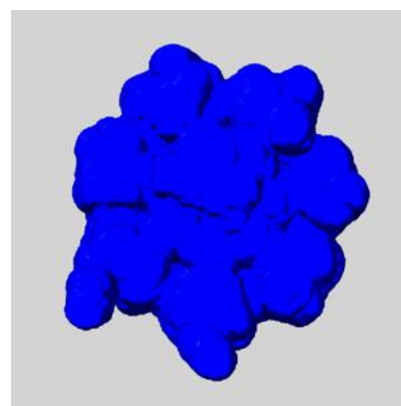
6.6.1 emd_29604_msk_1.map [i](#)



X



Y

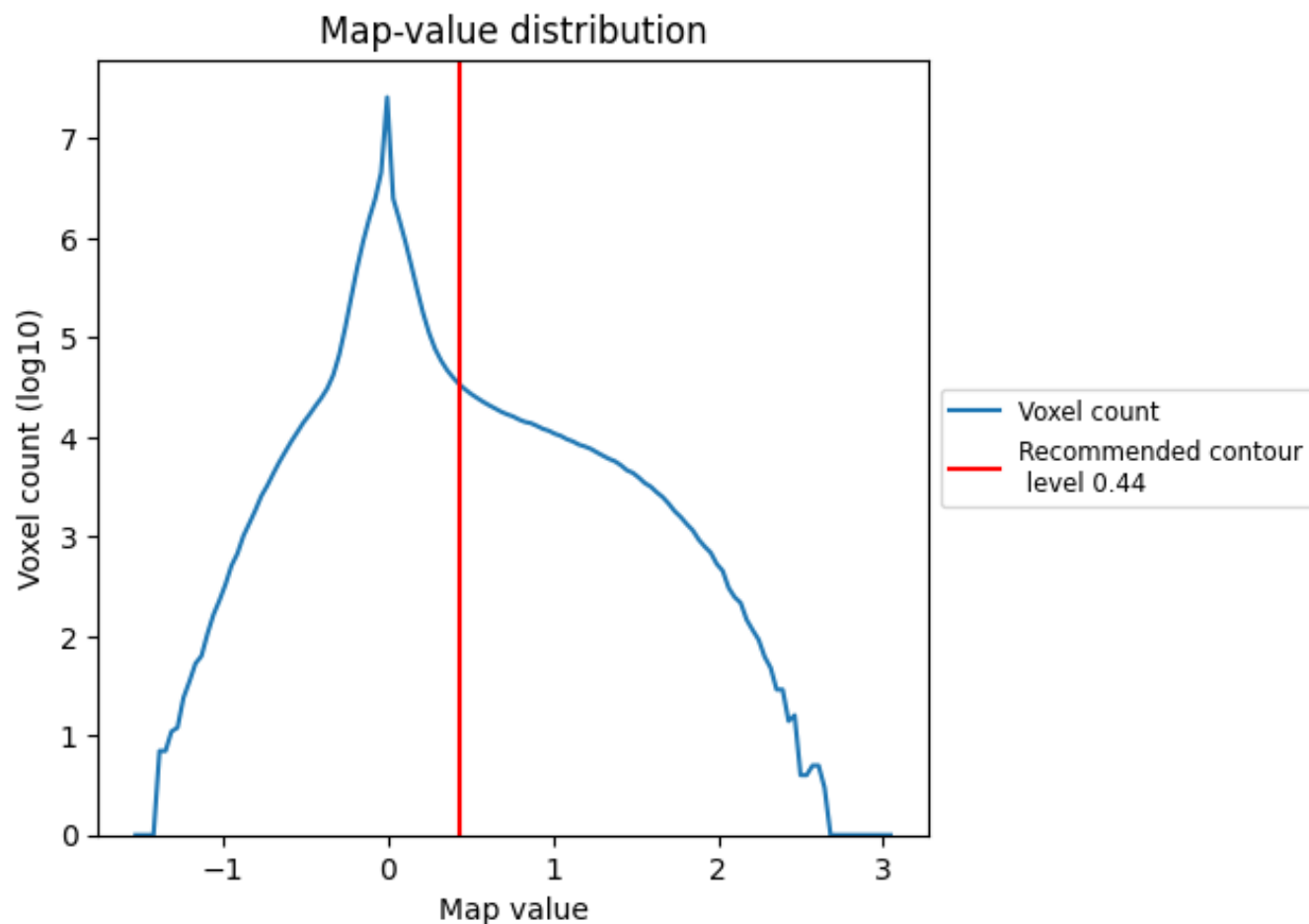


Z

7 Map analysis [i](#)

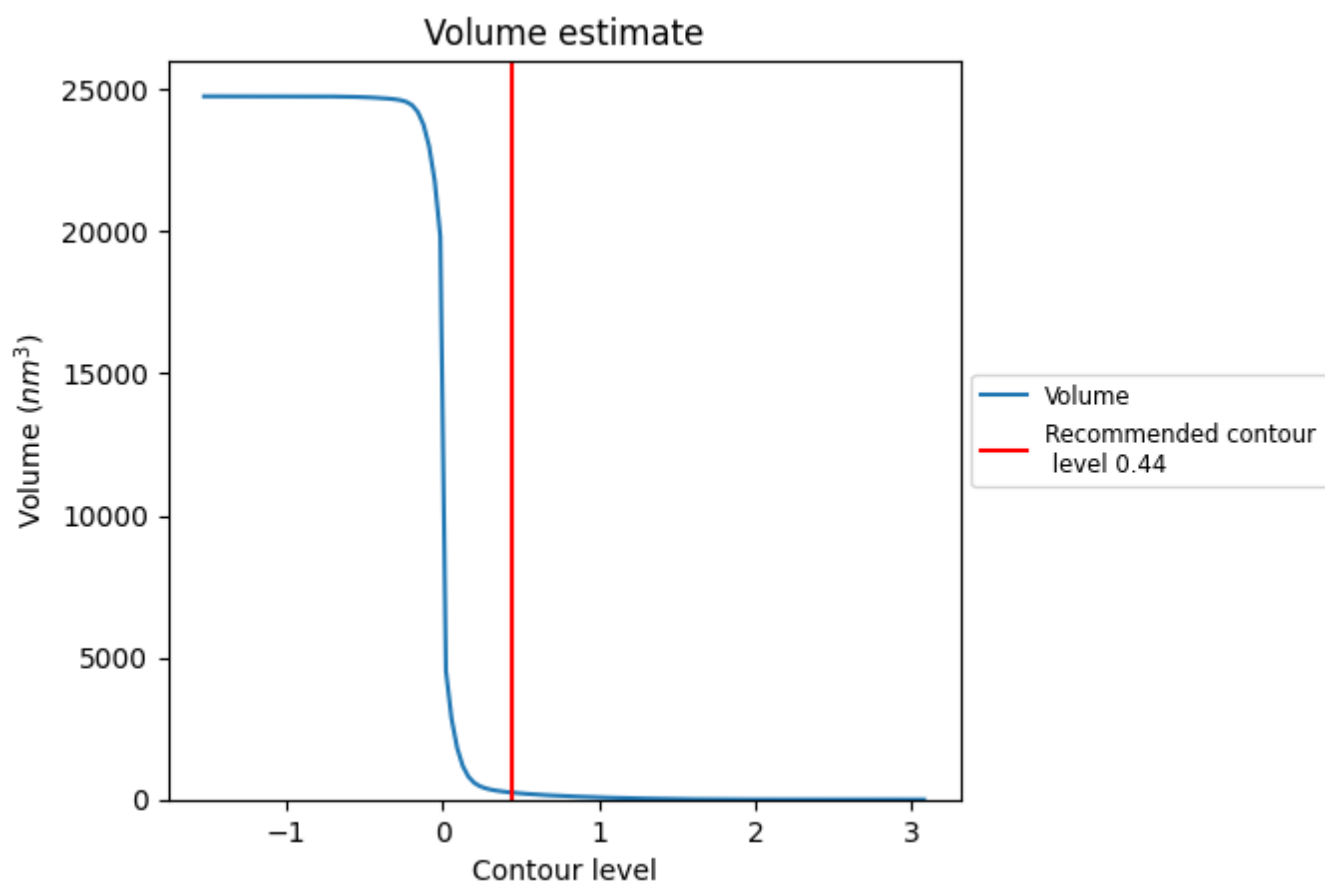
This section contains the results of statistical analysis of the map.

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.

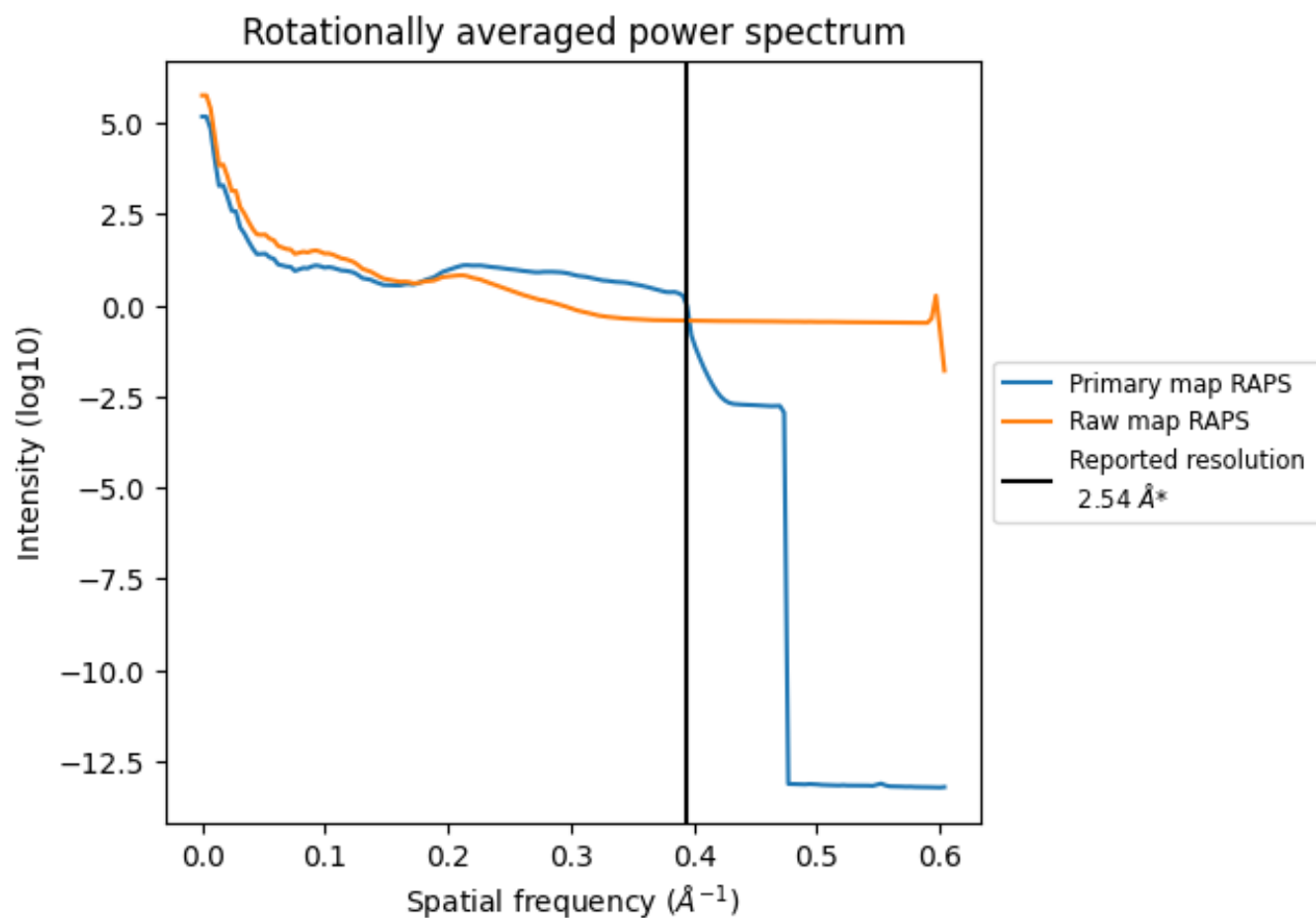
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm³; this corresponds to an approximate mass of 223 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 ⓘ

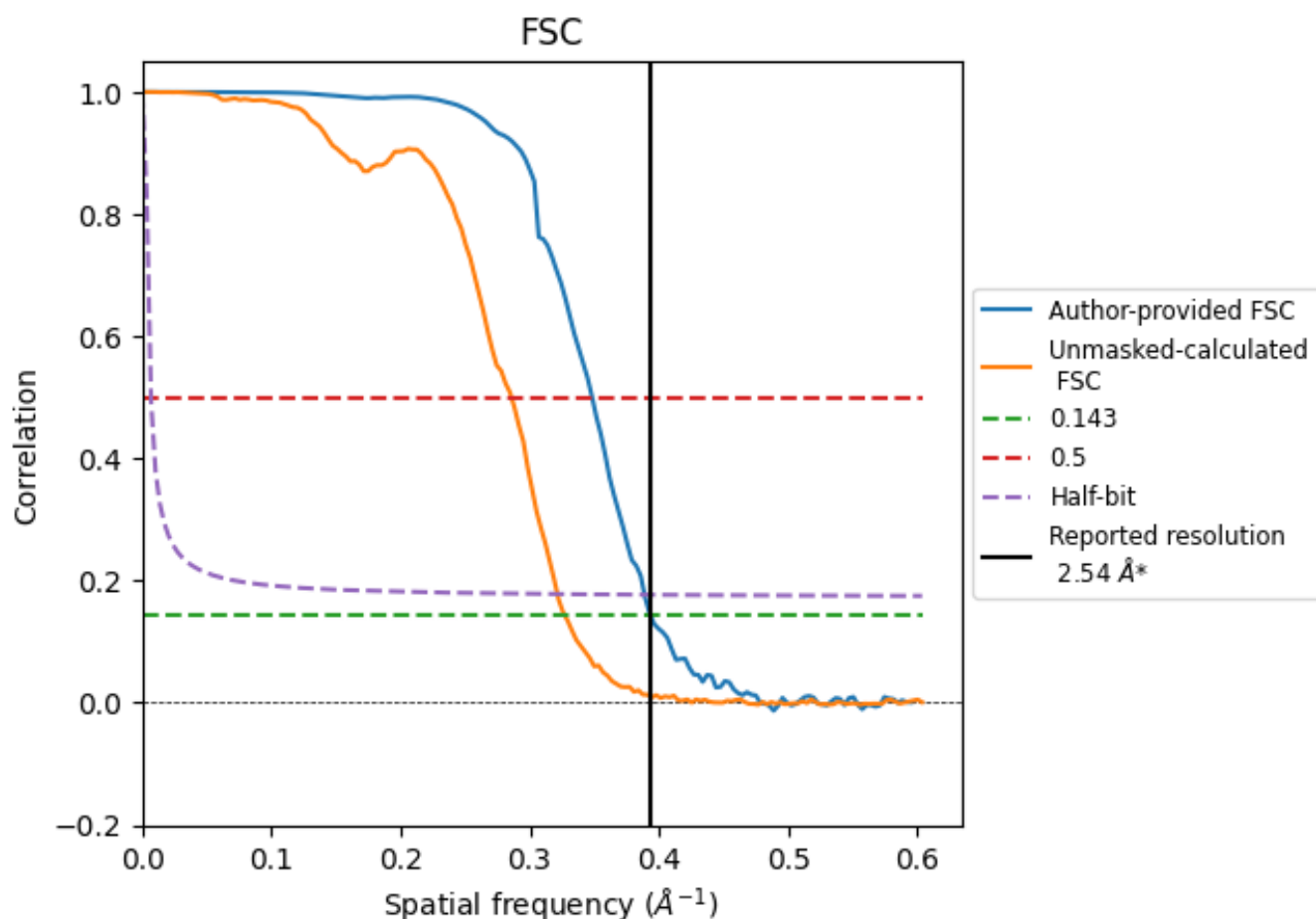


*Reported resolution corresponds to spatial frequency of 0.394 $\text{\AA}^{-1}$

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 0.394 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

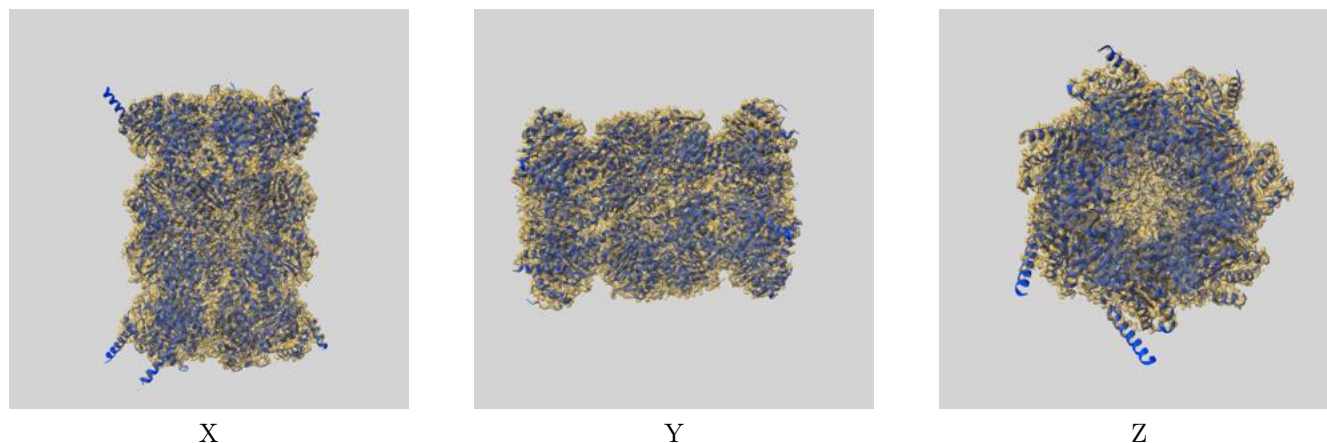
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.87	2.57
Unmasked-calculated*	3.06	3.50	3.11

*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 3.06 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

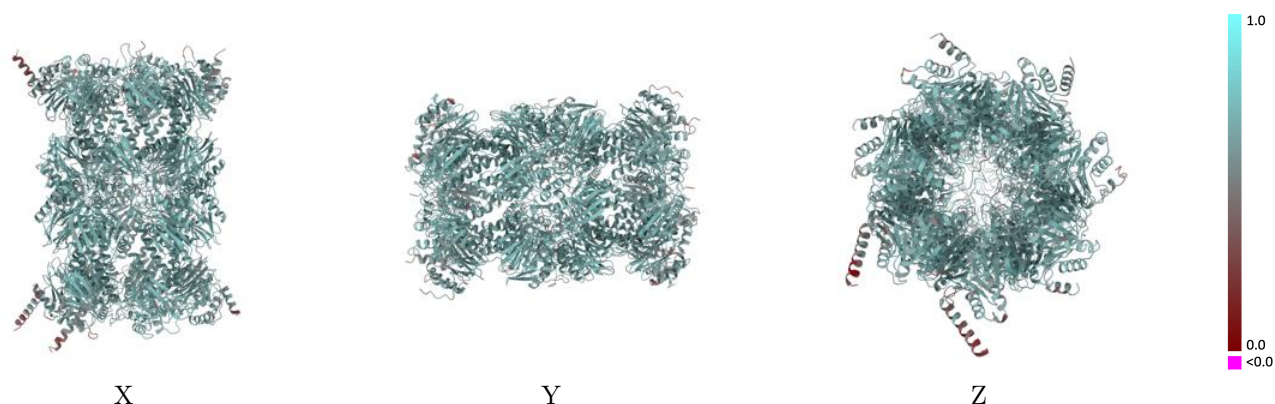
This section contains information regarding the fit between EMDB map EMD-29604 and PDB model 8FZ6. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



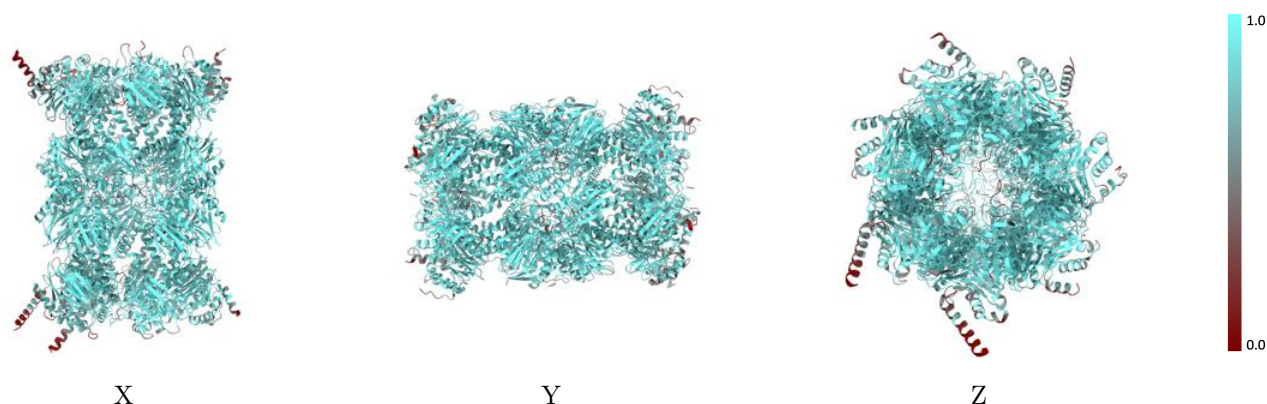
The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



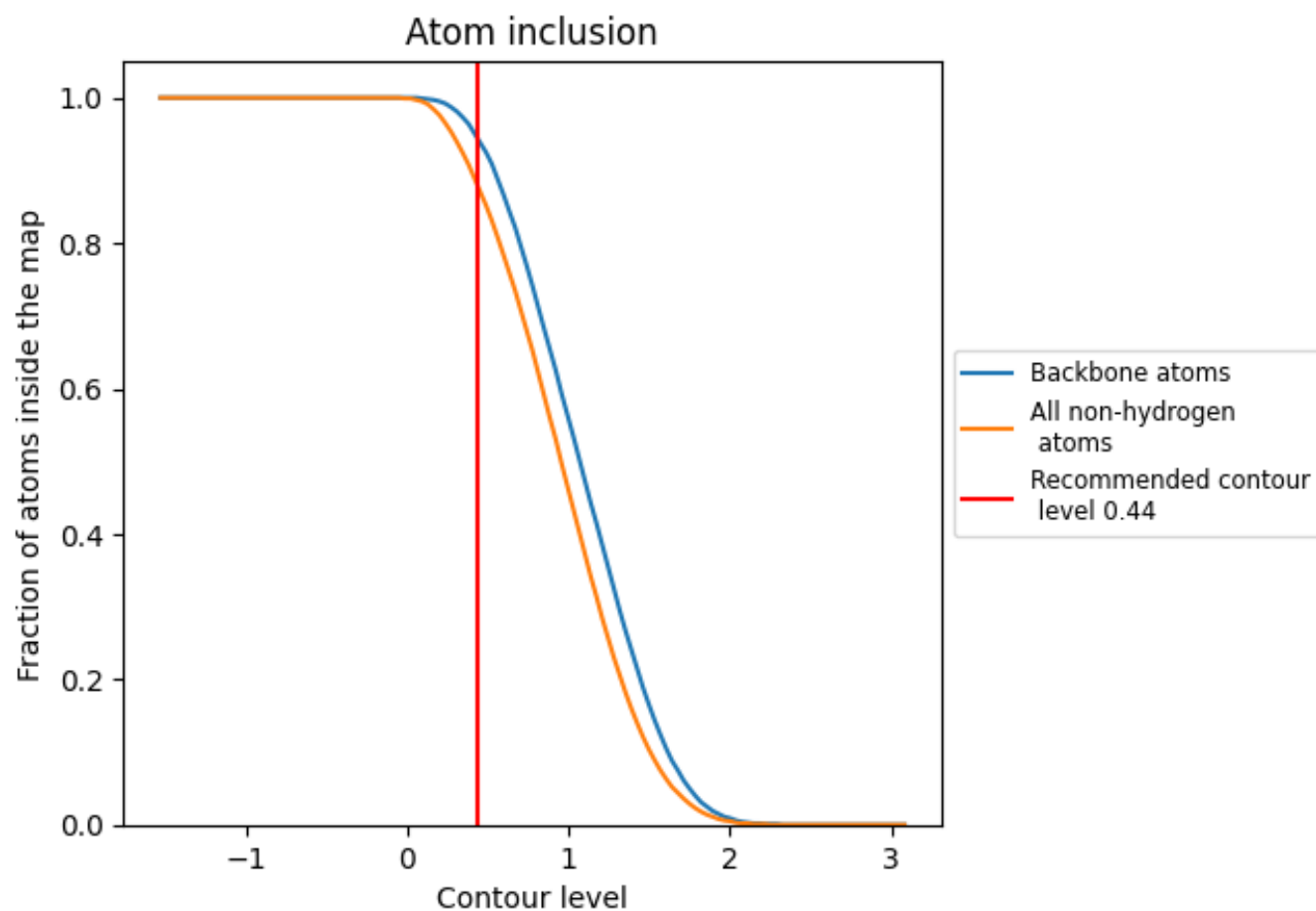
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.44).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.6400
A	 0.8580	 0.6340
B	 0.8820	 0.6350
C	 0.8220	 0.6140
D	 0.7820	 0.6030
E	 0.8380	 0.6200
F	 0.8750	 0.6360
G	 0.8690	 0.6350
H	 0.9500	 0.6730
I	 0.9360	 0.6630
J	 0.9460	 0.6690
K	 0.9400	 0.6650
L	 0.9450	 0.6660
M	 0.9200	 0.6560
N	 0.9430	 0.6690
O	 0.8320	 0.6250
P	 0.8590	 0.6290
Q	 0.7950	 0.6010
R	 0.7480	 0.5860
S	 0.8150	 0.6210
T	 0.8630	 0.6280
U	 0.8470	 0.6250
V	 0.9400	 0.6730
W	 0.9220	 0.6620
X	 0.9380	 0.6660
Y	 0.9380	 0.6640
Z	 0.9400	 0.6640
a	 0.9170	 0.6570
b	 0.9440	 0.6680
c	 0.6810	 0.5920
d	 0.6720	 0.5900

