



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:26 PM UTC

PDB ID : 7TEO / pdb_00007teo
EMDB ID : EMD-25848
Title : Cryo-EM structure of the 20S Alpha 3 Deletion proteasome core particle in complex with FUB1
Authors : Walsh Jr., R.M.; Rawson, S.; Schnell, H.M.; Hanna, J.
Deposited on : 2022-01-05
Resolution : 2.97 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:

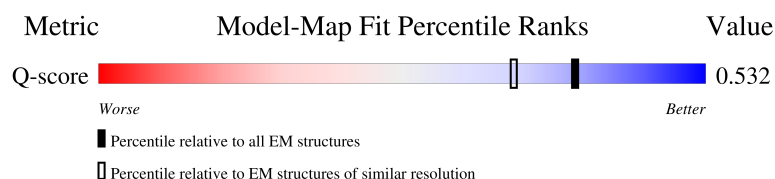
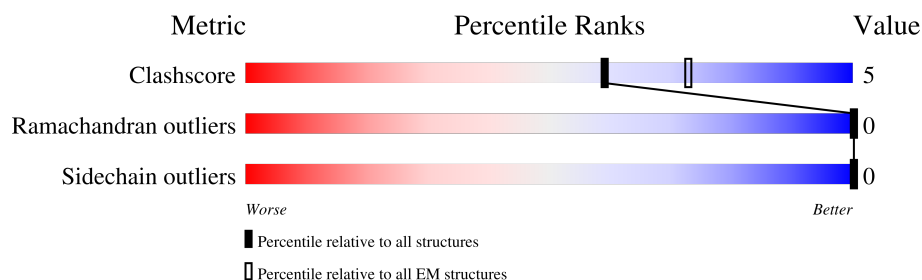
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.97 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	13205 (2.47 - 3.47)

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	 82% 10% 8%
1	M	241	 80% 11% 8%
2	2	266	 78% 8% 14%
2	N	266	 79% 7% 14%

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Mol	Chain	Length	Quality of chain
3	A	252	
3	O	252	
4	B	250	
4	P	250	
5	C	254	
5	D	254	
5	Q	254	
5	R	254	
6	E	260	
6	S	260	
7	F	234	
7	T	234	
8	G	288	
8	U	288	
9	H	215	
9	V	215	
10	I	261	
10	W	261	
11	J	205	
11	X	205	
12	K	198	
12	Y	198	
13	L	287	
13	Z	287	
14	a	250	

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Mol	Chain	Length	Quality of chain
14	b	250	32% 68%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 97522 atoms, of which 48612 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	221	Total	C	H	N	O	S	0	0
			3449	1110	1701	301	333	4		
1	M	221	Total	C	H	N	O	S	0	0
			3449	1110	1701	301	333	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	230	Total	C	H	N	O	S	0	0
			3595	1137	1798	307	346	7		
2	N	230	Total	C	H	N	O	S	0	0
			3595	1137	1798	307	346	7		

- Molecule 3 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	234	Total	C	H	N	O	S	0	0
			3687	1176	1841	308	354	8		
3	O	234	Total	C	H	N	O	S	0	0
			3687	1176	1841	308	354	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	241	Total	C	H	N	O	S	0	0
			3694	1170	1856	303	362	3		
4	P	241	Total	C	H	N	O	S	0	0
			3694	1170	1856	303	362	3		

- Molecule 5 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	222	Total	C	H	N	O	S	0	0
			3521	1098	1771	304	344	4		
5	D	208	Total	C	H	N	O	S	0	0
			3288	1025	1650	284	325	4		
5	Q	222	Total	C	H	N	O	S	0	0
			3521	1098	1771	304	344	4		
5	R	208	Total	C	H	N	O	S	0	0
			3287	1025	1649	284	325	4		

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	207	Total	C	H	N	O	S	0	0
			3176	997	1583	266	324	6		
6	S	207	Total	C	H	N	O	S	0	0
			3176	997	1583	266	324	6		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	231	Total	C	H	N	O	S	0	0
			3551	1114	1778	307	348	4		
7	T	231	Total	C	H	N	O	S	0	0
			3551	1114	1778	307	348	4		

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	243	Total	C	H	N	O	S	0	0
			3776	1203	1884	329	356	4		
8	U	243	Total	C	H	N	O	S	0	0
			3776	1203	1884	329	356	4		

- Molecule 9 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	196	Total	C	H	N	O	S	0	0
			2992	955	1480	250	300	7		
9	V	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	220	Total	C	H	N	O	S	0	0
			3347	1054	1677	291	319	6		
10	W	220	Total	C	H	N	O	S	0	0
			3347	1054	1677	291	319	6		

- Molecule 11 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	203	Total	C	H	N	O	S	0	0
			3142	1007	1567	257	303	8		
11	X	203	Total	C	H	N	O	S	0	0
			3142	1007	1567	257	303	8		

- Molecule 12 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		
12	Y	195	Total	C	H	N	O	S	0	0
			3130	992	1569	264	299	6		

- Molecule 13 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		
13	Z	212	Total	C	H	N	O	S	0	0
			3237	1045	1593	280	312	7		

- Molecule 14 is a protein called Silencing boundary-establishment protein FUB1.

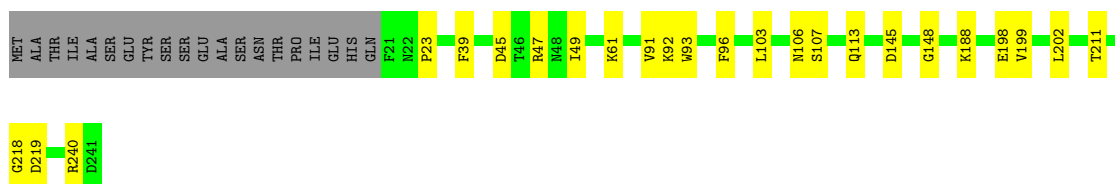
Mol	Chain	Residues	Atoms						AltConf	Trace
14	a	81	Total	C	H	N	O	S	0	0
			1177	393	559	101	121	3		
14	b	81	Total	C	H	N	O	S	0	0
			1177	393	559	101	121	3		

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.

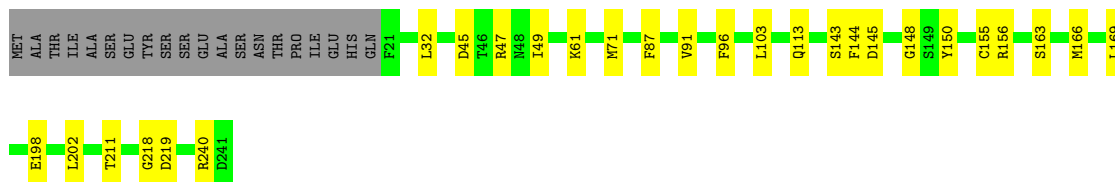
• Molecule 1: Proteasome subunit beta type-6

Chain 1: 



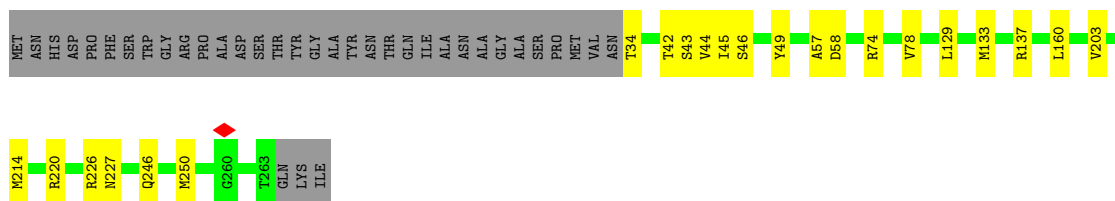
• Molecule 1: Proteasome subunit beta type-6

Chain M: 



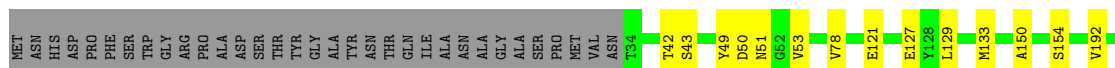
• Molecule 2: Proteasome subunit beta type-7

Chain 2: 



• Molecule 2: Proteasome subunit beta type-7

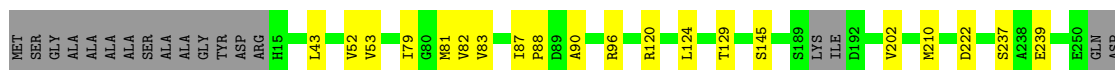
Chain N: 





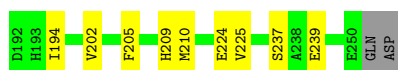
- Molecule 3: Proteasome subunit alpha type-1

Chain A: 85% 8% 7%



- Molecule 3: Proteasome subunit alpha type-1

Chain O: 80% 13% 7%



- Molecule 4: Proteasome subunit alpha type-2

Chain B: 90% 6% 4%



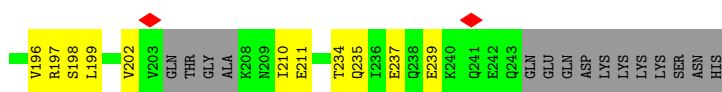
- Molecule 4: Proteasome subunit alpha type-2

Chain P: 89% 7% 4%



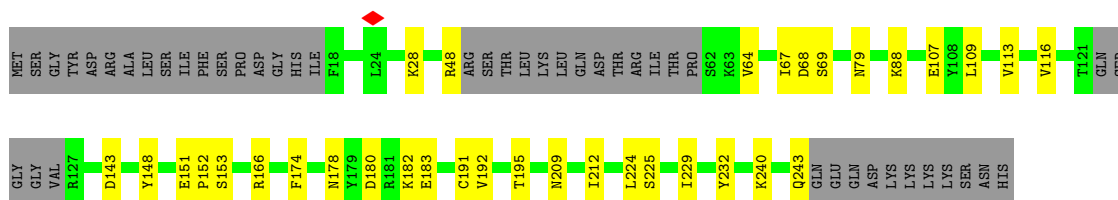
- Molecule 5: Proteasome subunit alpha type-4

Chain C: 76% 12% 13%

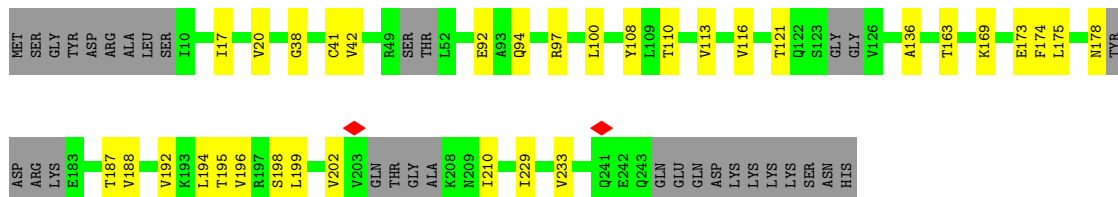
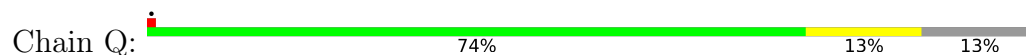


- Molecule 5: Proteasome subunit alpha type-4

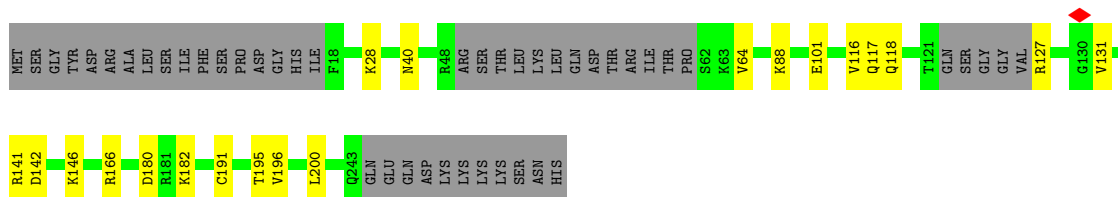
Chain D: 69% 13% 18%



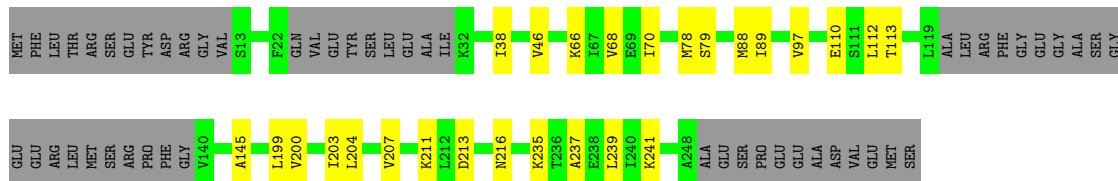
• Molecule 5: Proteasome subunit alpha type-4



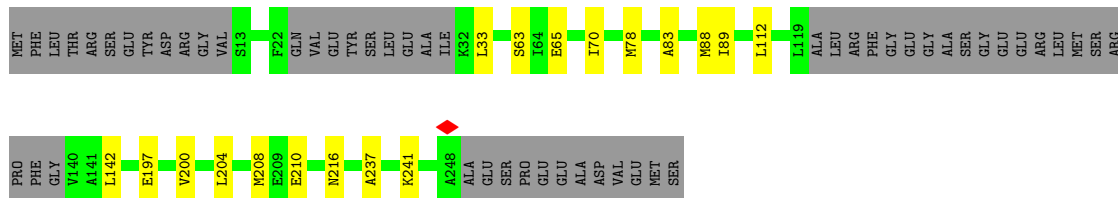
• Molecule 5: Proteasome subunit alpha type-4



• Molecule 6: Proteasome subunit alpha type-5



• Molecule 6: Proteasome subunit alpha type-5



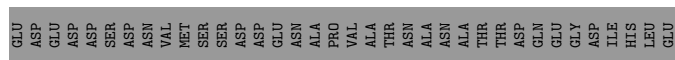
• Molecule 7: Proteasome subunit alpha type-6

MET
PHE
ARG
N4
D9
T10
V11
V45
I64
K65
C66
L74
A78
F79
D90
A81
R82
L88
N93
L97
N100
A108
V130
L156
T159
N185
E188
L189
V194
I197
I213
V230
I234

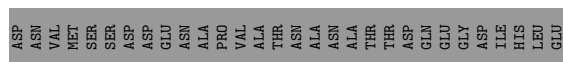
MET	PHE	ARG	N4	A25	A28	G32	V45	K50	G66	D67	E68	H69	S73	L74	A81	N86	Y87	L88	R89	N93	L97	K102	V105	A108	Q117	L145	L156	T159	A163	D183	L189	E204	T207	V208	R208
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NET					T5		E31	M32	G33		C41	G44	K56	L57	L58	O61	R90	K103	M149	L150	E151	K166	G167	H168	E190	Q194	I199	L213	V217	T223	V230	L235	Q236	T239	D240	Q243	J247	GLY	ASP	ASP	SEN
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MET	THR	SER	ILE	GLY	T5	V13	R19	N20	E24	V30	K56	Q61	D83	R90	K103	S134	E190	Q194	I198	I199	L213	W217	T223	V230	L235	Q236	I239	D240	N247	GLY	ASP	ASP	ASP	GLU	ASP	ASP	GLU	ASP	ASP	ASP	SER
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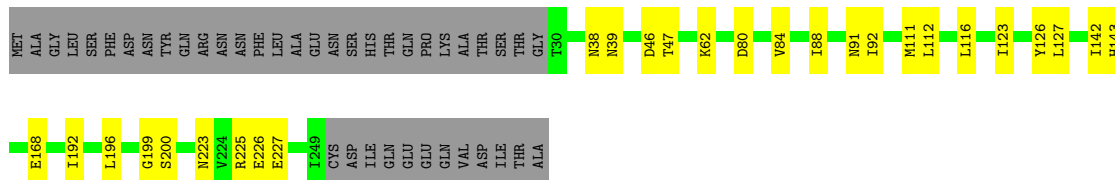
MET	ASN	GLY	ILE	GLN	VAL	ASP	ILE	ASN	ARG	LEU	LYS	LYS	GLY	GLU	VAL	SER	LEU	GLY	T20	T22	S37	R36	T39	T40	T41	T50	L53	C63	I74	A96	K102	E103	L112	D122	K126	Y130	T131	I132	S137	V138	H139	K140	A146	T152
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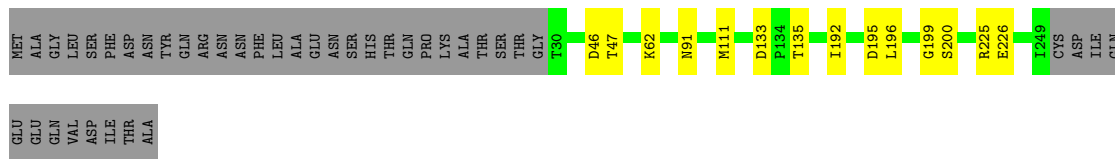
• Molecule 10: Proteasome subunit beta type-2

Chain I: 74% 10% 16%



• Molecule 10: Proteasome subunit beta type-2

Chain W: 79% 5% 16%



• Molecule 11: Proteasome subunit beta type-3

Chain J: 89% 10% .



• Molecule 11: Proteasome subunit beta type-3

Chain X: 89% 10% .



• Molecule 12: Proteasome subunit beta type-4

Chain K: 91% 8% .



• Molecule 12: Proteasome subunit beta type-4

Chain Y: 82% 16% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	56059	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 ($e^-/\text{\AA}^2$)	53.85	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.742	Depositor
Minimum map value	-1.746	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.306	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.14	0/1786	0.35	0/2408
1	M	0.14	0/1786	0.32	0/2408
2	2	0.13	0/1828	0.31	0/2480
2	N	0.13	0/1828	0.31	0/2480
3	A	0.13	0/1882	0.29	0/2549
3	O	0.13	0/1882	0.31	0/2549
4	B	0.14	0/1873	0.30	0/2536
4	P	0.14	0/1873	0.31	0/2536
5	C	0.14	0/1773	0.33	0/2396
5	D	0.14	0/1660	0.33	0/2244
5	Q	0.15	0/1773	0.35	0/2396
5	R	0.15	0/1660	0.34	0/2244
6	E	0.12	0/1612	0.29	0/2171
6	S	0.12	0/1612	0.29	0/2171
7	F	0.13	0/1800	0.32	0/2433
7	T	0.13	0/1800	0.30	0/2433
8	G	0.13	0/1932	0.31	0/2609
8	U	0.14	0/1932	0.33	0/2609
9	H	0.14	0/1541	0.31	0/2087
9	V	0.14	0/1541	0.30	0/2087
10	I	0.14	0/1701	0.32	0/2307
10	W	0.14	0/1701	0.32	0/2307
11	J	0.15	0/1605	0.32	0/2166
11	X	0.15	0/1605	0.31	0/2166
12	K	0.13	0/1589	0.30	0/2142
12	Y	0.15	0/1589	0.33	0/2142
13	L	0.15	0/1681	0.34	0/2274
13	Z	0.16	0/1681	0.32	0/2274
14	a	0.16	0/641	0.32	0/873
14	b	0.10	0/641	0.30	0/873
All	All	0.14	0/49808	0.32	0/67350

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	1	1748	1701	1700	18	0
1	M	1748	1701	1700	18	0
2	2	1797	1798	1797	17	0
2	N	1797	1798	1797	12	0
3	A	1846	1841	1839	13	0
3	O	1846	1841	1839	22	0
4	B	1838	1856	1854	11	0
4	P	1838	1856	1854	14	0
5	C	1750	1771	1766	21	0
5	D	1638	1650	1646	21	0
5	Q	1750	1771	1766	21	0
5	R	1638	1649	1646	13	0
6	E	1593	1583	1579	18	0
6	S	1593	1583	1579	13	0
7	F	1773	1778	1775	16	0
7	T	1773	1778	1775	23	0
8	G	1892	1884	1883	19	0
8	U	1892	1884	1883	16	0
9	H	1512	1480	1478	22	0
9	V	1512	1479	1478	19	0
10	I	1670	1677	1676	21	0
10	W	1670	1677	1676	9	0
11	J	1575	1567	1566	12	0
11	X	1575	1567	1566	13	0
12	K	1561	1569	1569	12	0
12	Y	1561	1569	1569	21	0
13	L	1644	1593	1592	19	0
13	Z	1644	1593	1592	23	0
14	a	618	559	556	2	0
14	b	618	559	556	1	0
All	All	48910	48612	48552	445	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 (445) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:74:ILE:HD11	9:H:112:LEU:HD23	1.50	0.91
4:B:224:TYR:OH	4:B:230:ASP:OD2	1.88	0.91
12:K:25:ILE:O	12:Y:139:TYR:OH	1.90	0.90
1:M:47:ARG:NE	1:M:219:ASP:OD2	2.04	0.89
9:V:74:ILE:HD11	9:V:112:LEU:HD23	1.54	0.87
4:P:224:TYR:OH	4:P:230:ASP:OD2	1.93	0.86
1:1:47:ARG:NE	1:1:219:ASP:OD2	2.08	0.85
1:1:188:LYS:NZ	13:Z:270:GLU:OE2	2.09	0.85
5:D:151:GLU:OE1	5:D:153:SER:OG	1.94	0.85
5:D:240:LYS:O	5:D:243:GLN:NE2	2.09	0.84
12:K:96:ARG:NH2	13:L:166:LYS:O	2.11	0.83
8:G:31:GLU:OE1	8:G:168:ARG:NH2	2.12	0.82
10:W:46:ASP:OD1	10:W:62:LYS:NZ	2.14	0.79
2:N:121:GLU:OE2	2:N:154:SER:OG	2.00	0.79
10:I:116:LEU:HG	10:I:123:ILE:HD11	1.66	0.78
12:Y:107:TYR:OH	12:Y:112:ASN:OD1	2.02	0.77
12:Y:193:ASP:OD1	12:Y:194:ASP:N	2.19	0.76
5:R:142:ASP:OD2	5:R:146:LYS:NZ	2.19	0.76
9:V:190:GLY:O	9:V:212:TYR:OH	2.04	0.75
13:L:92:ASP:OD2	13:L:108:LYS:NZ	2.18	0.75
7:F:78:ALA:HB1	7:F:82:ARG:NH1	2.02	0.74
8:U:217:TRP:CZ3	8:U:223:THR:HG23	2.21	0.74
1:M:218:GLY:O	1:M:240:ARG:N	2.23	0.71
6:S:208:MET:HE1	6:S:216:ASN:HB2	1.72	0.71
8:G:217:TRP:CZ3	8:G:223:THR:HG23	2.25	0.71
1:1:218:GLY:O	1:1:240:ARG:N	2.25	0.70
13:Z:92:ASP:OD1	13:Z:108:LYS:NZ	2.22	0.70
6:S:210:GLU:OE1	6:S:216:ASN:ND2	2.25	0.69
1:M:145:ASP:OD1	1:M:148:GLY:N	2.26	0.69
5:Q:42:VAL:HG11	5:Q:136:ALA:HB1	1.73	0.69
9:V:37:SER:O	9:V:50:THR:HG22	1.93	0.69
9:H:74:ILE:HD11	9:H:112:LEU:CD2	2.23	0.68
5:R:180:ASP:OD2	5:R:182:LYS:N	2.26	0.68
9:H:190:GLY:O	9:H:212:TYR:OH	2.08	0.68
9:V:39:THR:OG1	9:V:50:THR:HG21	1.94	0.68
10:W:225:ARG:NH1	10:W:226:GLU:O	2.28	0.67
10:W:47:THR:OG1	10:W:200:SER:OG	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:1:MET:HE1	12:Y:174:MET:HB2	1.75	0.67
10:I:225:ARG:NH1	10:I:226:GLU:O	2.26	0.67
1:M:211:THR:HG23	1:M:218:GLY:HA3	1.77	0.67
5:C:196:VAL:HG23	5:C:210:ILE:CD1	2.26	0.66
9:V:74:ILE:HD11	9:V:112:LEU:CD2	2.24	0.66
3:A:43:LEU:HD22	3:A:210:MET:HE3	1.76	0.66
3:O:43:LEU:HD22	3:O:210:MET:HE3	1.77	0.66
8:G:103:LYS:NZ	9:H:103:GLU:OE1	2.29	0.66
12:K:23:ARG:NH1	13:L:191:ASP:OD2	2.29	0.66
6:E:199:LEU:O	6:E:203:ILE:HD12	1.95	0.65
13:Z:95:ALA:HB2	13:Z:106:VAL:HG21	1.79	0.65
3:A:81:MET:HE3	3:A:83:VAL:CG2	2.27	0.64
8:U:103:LYS:NZ	9:V:103:GLU:OE2	2.26	0.64
8:U:190:GLU:OE2	8:U:194:GLN:NE2	2.30	0.64
9:H:39:THR:OG1	9:H:50:THR:HG21	1.98	0.64
5:C:235:GLN:NE2	5:C:239:GLU:OE2	2.30	0.64
5:R:196:VAL:O	5:R:200:LEU:HD13	1.98	0.63
1:I:145:ASP:OD1	1:I:148:GLY:N	2.31	0.63
2:2:227:ASN:OD1	2:2:246:GLN:NE2	2.31	0.63
7:T:74:LEU:HD22	7:T:81:ALA:HB1	1.81	0.63
6:E:66:LYS:NZ	6:E:79:SER:O	2.31	0.62
7:T:213:ILE:HD12	7:T:230:VAL:HG23	1.81	0.62
6:S:78:MET:HE1	6:S:89:ILE:CG1	2.30	0.62
6:S:70:ILE:HG21	6:S:112:LEU:HD21	1.81	0.62
11:J:135:ASP:OD1	11:J:136:PHE:N	2.31	0.62
7:F:74:LEU:HD22	7:F:81:ALA:HB1	1.82	0.62
13:Z:245:TYR:OH	14:a:195:GLN:OE1	2.18	0.62
8:G:41:CYS:SG	8:G:44:GLY:N	2.73	0.61
9:H:41:THR:O	9:H:41:THR:HG23	1.98	0.61
2:N:78:VAL:HG12	2:N:78:VAL:O	1.99	0.61
5:D:180:ASP:OD2	5:D:182:LYS:N	2.33	0.61
1:I:106:ASN:OD1	1:I:107:SER:N	2.33	0.61
12:Y:115:GLU:OE1	12:Y:117:TYR:OH	2.15	0.61
6:E:70:ILE:HG21	6:E:112:LEU:HD21	1.82	0.61
4:B:196:LEU:HD23	4:B:209:ILE:HD11	1.83	0.61
9:H:122:ASP:O	9:H:126:LYS:N	2.35	0.60
3:O:237:SER:OG	3:O:239:GLU:OE2	2.18	0.60
3:O:81:MET:HE3	3:O:83:VAL:CG2	2.31	0.60
2:N:42:THR:HG23	2:N:43:SER:N	2.16	0.60
13:L:138:CYS:O	13:L:142:GLU:OE1	2.20	0.60
1:I:23:PRO:O	2:2:137:ARG:NH2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:78:VAL:HG12	2:2:78:VAL:O	2.00	0.60
13:Z:138:CYS:O	13:Z:142:GLU:OE1	2.20	0.60
7:F:100:ASN:ND2	2:N:127:GLU:OE1	2.34	0.59
7:T:117:GLN:NE2	8:U:83:ASP:OD1	2.34	0.59
5:Q:196:VAL:HG23	5:Q:210:ILE:CD1	2.33	0.59
5:D:48:ARG:N	5:D:209:ASN:O	2.31	0.58
10:W:199:GLY:O	10:W:200:SER:OG	2.19	0.58
6:E:78:MET:HE1	6:E:89:ILE:CG1	2.34	0.58
7:F:9:ASP:OD2	7:F:11:VAL:HG22	2.02	0.58
5:D:180:ASP:OD2	5:D:183:GLU:N	2.37	0.57
2:2:226:ARG:HH12	2:2:250:MET:HE2	1.68	0.57
13:L:78:THR:HG22	13:L:91:VAL:HG12	1.85	0.57
10:I:46:ASP:OD1	10:I:62:LYS:NZ	2.32	0.57
4:P:21:ILE:HD11	4:P:122:THR:HG23	1.86	0.57
1:1:49:ILE:HD12	10:I:196:LEU:HD11	1.87	0.56
2:2:220:ARG:NH1	10:I:168:GLU:OE2	2.38	0.56
13:Z:256:THR:N	13:Z:259:GLY:O	2.32	0.56
1:M:49:ILE:HD12	10:W:196:LEU:HD11	1.88	0.56
11:J:149:MET:HE3	11:J:153:LEU:HD11	1.87	0.56
4:P:118:MET:CE	4:P:150:VAL:HG12	2.35	0.56
5:D:225:SER:O	5:D:229:ILE:HD12	2.06	0.56
12:Y:50:ALA:HB1	13:Z:195:THR:OG1	2.06	0.55
1:1:198:GLU:O	1:1:202:LEU:HD23	2.06	0.55
9:H:102:LYS:HD3	9:H:138:VAL:HG23	1.88	0.55
4:P:84:VAL:O	4:P:87:ASP:OD2	2.23	0.55
5:Q:198:SER:O	5:Q:202:VAL:HG12	2.06	0.55
8:G:199:ILE:HG21	8:G:213:LEU:HD13	1.88	0.55
8:G:217:TRP:CH2	8:G:223:THR:HG23	2.41	0.55
1:1:211:THR:HG23	1:1:218:GLY:HA3	1.89	0.55
13:L:128:GLN:OE1	1:M:113:GLN:NE2	2.40	0.55
3:A:53:VAL:HG11	3:A:82:VAL:HG21	1.89	0.55
2:N:226:ARG:HH12	2:N:250:MET:HE2	1.72	0.55
2:2:42:THR:HG23	2:2:43:SER:N	2.22	0.54
13:L:95:ALA:HB2	13:L:106:VAL:HG21	1.89	0.54
1:M:47:ARG:HD3	1:M:49:ILE:HD11	1.88	0.54
3:O:205:PHE:CE1	3:O:209:HIS:CD2	2.95	0.54
8:G:236:GLN:O	8:G:240:ASP:OD1	2.26	0.54
10:I:192:ILE:HG23	10:I:199:GLY:HA2	1.88	0.54
4:B:196:LEU:HD23	4:B:209:ILE:CD1	2.38	0.54
5:Q:42:VAL:HG11	5:Q:136:ALA:CB	2.37	0.54
5:D:192:VAL:HG21	5:D:232:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:172:MET:HE2	12:K:174:MET:HB2	1.89	0.54
2:N:227:ASN:OD1	2:N:246:GLN:NE2	2.33	0.54
10:I:116:LEU:CG	10:I:123:ILE:HD11	2.38	0.54
3:O:53:VAL:HG11	3:O:82:VAL:HG21	1.89	0.54
6:E:200:VAL:O	6:E:204:LEU:HD23	2.08	0.53
4:B:21:ILE:O	4:B:25:LEU:HD23	2.08	0.53
9:V:122:ASP:O	9:V:126:LYS:N	2.41	0.53
7:F:185:ASN:ND2	7:F:188:GLU:OE1	2.37	0.53
10:I:199:GLY:O	10:I:200:SER:OG	2.19	0.53
10:I:47:THR:OG1	10:I:200:SER:OG	2.21	0.53
13:Z:270:GLU:N	13:Z:270:GLU:OE1	2.42	0.53
8:U:236:GLN:O	8:U:240:ASP:OD1	2.27	0.53
5:Q:121:THR:O	5:R:127:ARG:NH1	2.42	0.53
12:K:139:TYR:OH	12:Y:25:ILE:O	2.20	0.53
9:H:130:TYR:HE1	9:H:140:LYS:HG3	1.74	0.52
7:T:67:ASP:OD1	7:T:69:HIS:CD2	2.63	0.52
5:C:197:ARG:NH2	5:C:239:GLU:OE1	2.41	0.52
4:P:35:LEU:HD23	4:P:163:ALA:HB2	1.90	0.52
2:2:49:TYR:CE2	2:2:203:VAL:HG22	2.45	0.52
7:F:81:ALA:HB2	7:F:130:VAL:HG21	1.90	0.52
3:O:28:VAL:HG21	3:O:129:THR:HG23	1.91	0.52
12:K:1:MET:HE1	12:K:172:MET:HE3	1.92	0.51
5:D:64:VAL:HG13	5:D:64:VAL:O	2.08	0.51
5:R:118:GLN:OE1	6:S:83:ALA:HB1	2.10	0.51
13:Z:110:ILE:HD11	13:Z:120:MET:SD	2.51	0.51
13:Z:130:TRP:CE3	13:Z:161:LEU:HD21	2.46	0.51
1:I:96:PHE:CE1	7:T:66:CYS:O	2.64	0.51
1:M:198:GLU:O	1:M:202:LEU:HD23	2.11	0.51
8:U:199:ILE:HG21	8:U:213:LEU:HD13	1.91	0.51
9:V:130:TYR:HE1	9:V:140:LYS:HG3	1.75	0.51
5:C:17:ILE:HD12	5:C:20:VAL:HG21	1.93	0.51
3:A:83:VAL:HG11	3:A:90:ALA:CB	2.41	0.51
9:H:22:ILE:HG21	9:H:63:CYS:SG	2.51	0.51
8:U:19:ARG:NH2	8:U:24:GLU:OE1	2.44	0.51
5:C:174:PHE:O	5:C:178:ASN:N	2.41	0.51
7:F:194:VAL:HA	7:F:197:ILE:HG22	1.93	0.51
3:O:87:ILE:N	3:O:88:PRO:HD2	2.26	0.50
6:E:235:LYS:O	6:E:239:LEU:HD23	2.11	0.50
7:F:93:ASN:O	7:F:97:LEU:HD13	2.11	0.50
4:B:21:ILE:HD11	4:B:122:THR:HG23	1.93	0.50
13:Z:111:GLU:OE1	13:Z:260:TRP:CH2	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:95:ALA:CB	13:Z:106:VAL:HG21	2.42	0.50
5:Q:195:THR:O	5:Q:199:LEU:HD23	2.11	0.50
4:B:118:MET:CE	4:B:150:VAL:HG12	2.41	0.49
1:M:45:ASP:OD2	1:M:61:LYS:NZ	2.45	0.49
5:C:48:ARG:NH2	5:C:211:GLU:OE1	2.45	0.49
5:Q:229:ILE:O	5:Q:233:VAL:HG23	2.13	0.49
9:V:194:MET:HE3	9:V:207:PHE:CD2	2.47	0.49
11:J:11:ILE:HD12	11:J:142:ALA:HB3	1.93	0.49
9:H:39:THR:HG21	14:a:133:TYR:CZ	2.48	0.49
12:K:49:GLU:OE2	12:K:49:GLU:HA	2.13	0.49
13:L:243:ASP:OD2	13:L:246:SER:OG	2.27	0.49
7:T:227:GLY:O	7:T:230:VAL:HG12	2.12	0.49
9:V:130:TYR:CE1	9:V:140:LYS:HG3	2.48	0.49
6:S:200:VAL:O	6:S:204:LEU:HD23	2.13	0.49
11:X:56:LEU:HG	11:X:58:THR:HG22	1.94	0.49
14:b:209:ARG:NH2	14:b:211:GLU:OE1	2.42	0.49
3:A:120:ARG:O	3:A:124:LEU:HD13	2.13	0.48
5:Q:196:VAL:HG23	5:Q:210:ILE:HD11	1.95	0.48
13:L:105:THR:O	13:L:105:THR:HG22	2.13	0.48
7:T:45:VAL:HG23	7:T:189:LEU:HD23	1.95	0.48
8:U:61:GLN:O	8:U:61:GLN:HG2	2.13	0.48
11:X:149:MET:HE3	11:X:153:LEU:HD11	1.94	0.48
12:Y:155:GLU:OE2	12:Y:155:GLU:HA	2.13	0.48
2:2:45:ILE:CD1	2:2:214:MET:HE3	2.43	0.48
3:A:87:ILE:N	3:A:88:PRO:HD2	2.27	0.48
11:X:11:ILE:HD12	11:X:142:ALA:HB3	1.94	0.48
12:Y:49:GLU:O	12:Y:53:THR:HG23	2.14	0.48
12:Y:9:VAL:HG12	12:Y:10:GLN:N	2.28	0.48
2:2:34:THR:OG1	9:V:109:LYS:HD2	2.13	0.48
6:E:78:MET:HE1	6:E:89:ILE:HG13	1.96	0.48
3:O:83:VAL:HG11	3:O:90:ALA:CB	2.44	0.48
11:X:56:LEU:HD23	11:X:59:ASP:OD2	2.14	0.48
5:C:192:VAL:O	5:C:196:VAL:HG12	2.14	0.48
12:Y:108:ASP:O	12:Y:112:ASN:N	2.47	0.48
13:L:130:TRP:CE3	13:L:161:LEU:HD21	2.48	0.48
4:P:196:LEU:HD23	4:P:209:ILE:CD1	2.43	0.48
13:Z:276:LYS:NZ	13:Z:285:VAL:O	2.39	0.48
4:P:196:LEU:HD23	4:P:209:ILE:HD11	1.96	0.48
7:T:25:ALA:O	7:T:28:ALA:HB3	2.13	0.48
2:N:50:ASP:OD1	2:N:51:ASN:N	2.47	0.47
3:O:116:VAL:HG12	3:O:120:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:182:ILE:HG23	9:V:189:GLY:HA2	1.95	0.47
6:S:33:LEU:HD23	6:S:33:LEU:H	1.79	0.47
8:U:194:GLN:O	8:U:198:ILE:HG12	2.14	0.47
1:1:39:PHE:CZ	1:1:199:VAL:HG21	2.49	0.47
5:Q:187:THR:HG22	5:Q:188:VAL:N	2.30	0.47
9:H:37:SER:O	9:H:50:THR:HG22	2.15	0.47
12:K:184:VAL:HG22	12:K:189:ILE:HG12	1.97	0.47
6:S:88:MET:HE2	6:S:142:LEU:CD1	2.45	0.47
5:C:17:ILE:HD12	5:C:20:VAL:CG2	2.43	0.47
10:I:116:LEU:HD23	10:I:143:HIS:O	2.14	0.47
2:N:49:TYR:CE2	2:N:203:VAL:HG22	2.49	0.47
3:A:237:SER:OG	3:A:239:GLU:OE2	2.24	0.47
9:H:182:ILE:HG23	9:H:189:GLY:HA2	1.97	0.47
11:J:54:THR:HG21	11:J:140:GLY:HA2	1.96	0.47
6:S:78:MET:HE1	6:S:89:ILE:HG13	1.97	0.47
7:T:86:ASN:OD1	7:T:87:TYR:N	2.48	0.47
8:U:90:ARG:HD2	8:U:90:ARG:O	2.15	0.47
12:Y:72:ASP:O	12:Y:72:ASP:OD2	2.32	0.47
5:D:67:ILE:HG21	5:D:109:LEU:HD21	1.97	0.47
6:E:46:VAL:HG11	6:E:145:ALA:HB1	1.97	0.47
8:G:190:GLU:OE2	8:G:194:GLN:NE2	2.48	0.47
3:O:194:ILE:HD12	3:O:205:PHE:HE2	1.80	0.47
2:2:45:ILE:HD11	2:2:214:MET:HE3	1.97	0.47
5:Q:174:PHE:O	5:Q:178:ASN:N	2.37	0.47
1:1:96:PHE:CD1	7:T:89:ARG:HD3	2.49	0.47
3:O:126:GLN:NE2	4:P:81:ASP:OD1	2.43	0.47
12:Y:11:ASP:OD1	12:Y:11:ASP:O	2.33	0.47
5:D:28:LYS:O	5:D:166:ARG:HA	2.15	0.46
5:Q:38:GLY:N	5:Q:41:CYS:O	2.44	0.46
5:C:47:GLU:HB2	5:C:199:LEU:HD12	1.97	0.46
5:C:196:VAL:HG23	5:C:210:ILE:HD13	1.97	0.46
7:F:45:VAL:HG23	7:F:189:LEU:HD23	1.97	0.46
10:I:112:LEU:O	10:I:116:LEU:HD13	2.15	0.46
2:N:129:LEU:O	2:N:133:MET:HG2	2.15	0.46
9:V:58:ASP:OD1	9:V:59:LYS:N	2.48	0.46
13:Z:110:ILE:HD13	13:Z:131:GLU:OE2	2.16	0.46
2:N:192:VAL:HG23	2:N:192:VAL:O	2.15	0.46
7:T:207:THR:OG1	7:T:209:ASP:OD1	2.16	0.46
3:A:53:VAL:HG11	3:A:82:VAL:CG2	2.45	0.46
5:C:234:THR:HA	5:C:237:GLU:HG2	1.97	0.46
6:E:211:LYS:O	6:E:216:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:133:ASP:OD1	10:W:135:THR:OG1	2.30	0.46
2:2:58:ASP:OD1	2:2:74:ARG:NH2	2.36	0.46
10:I:126:TYR:C	10:I:127:LEU:HD12	2.41	0.46
7:T:88:LEU:HD11	7:T:108:ALA:HB1	1.98	0.46
8:U:235:LEU:O	8:U:239:ILE:HG12	2.16	0.46
1:1:93:TRP:HA	1:1:96:PHE:HD2	1.79	0.46
7:T:156:LEU:HD13	7:T:159:THR:HB	1.97	0.46
10:I:116:LEU:HD22	10:I:142:ILE:HG22	1.98	0.46
5:Q:17:ILE:HG23	5:Q:20:VAL:HB	1.97	0.46
5:C:198:SER:O	5:C:202:VAL:HG12	2.16	0.46
10:I:91:ASN:HB3	10:I:111:MET:HE1	1.97	0.46
10:I:227:GLU:OE2	10:I:227:GLU:HA	2.15	0.46
7:T:93:ASN:O	7:T:97:LEU:HD13	2.16	0.46
13:Z:203:CYS:SG	13:Z:215:LEU:HD12	2.56	0.46
3:A:52:VAL:HG21	3:A:202:VAL:HG13	1.96	0.46
7:T:204:GLU:OE2	7:T:210:ASN:ND2	2.45	0.46
7:T:230:VAL:O	7:T:230:VAL:HG22	2.16	0.46
11:X:11:ILE:CG2	11:X:146:LEU:HD11	2.46	0.46
6:E:68:VAL:HG21	6:E:89:ILE:HD13	1.98	0.45
8:G:61:GLN:O	8:G:61:GLN:HG2	2.16	0.45
10:I:88:ILE:HG22	10:I:92:ILE:HD12	1.97	0.45
6:S:197:GLU:O	6:S:200:VAL:HG12	2.16	0.45
2:2:129:LEU:O	2:2:133:MET:HG2	2.15	0.45
13:L:113:ASN:OD1	13:L:113:ASN:C	2.60	0.45
3:O:70:SER:HA	3:O:224:GLU:OE2	2.17	0.45
3:O:129:THR:HG22	3:O:129:THR:O	2.16	0.45
8:U:56:LYS:HD3	8:U:56:LYS:N	2.32	0.45
11:J:11:ILE:CD1	11:J:142:ALA:HB3	2.45	0.45
11:J:56:LEU:HG	11:J:58:THR:HG22	1.98	0.45
12:Y:2:ASP:HB2	12:Y:47:ALA:HB1	1.97	0.45
1:1:113:GLN:NE2	13:Z:128:GLN:OE1	2.49	0.45
1:M:71:MET:HE1	1:M:87:PHE:CD2	2.52	0.45
5:R:28:LYS:O	5:R:166:ARG:HA	2.16	0.45
4:B:123:GLN:O	4:B:123:GLN:CD	2.60	0.45
8:G:33:GLY:O	8:G:166:LYS:N	2.47	0.45
5:D:68:ASP:OD2	5:D:69:SER:N	2.41	0.45
13:L:82:ARG:NH1	13:L:200:ASP:OD1	2.49	0.45
5:R:64:VAL:HG13	5:R:64:VAL:O	2.15	0.45
11:X:98:ARG:HD2	11:X:103:TYR:CE2	2.52	0.45
9:H:53:LEU:HD22	9:H:195:VAL:HG23	1.97	0.45
12:Y:96:ARG:NH2	13:Z:166:LYS:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:LYS:O	1:1:96:PHE:CD2	2.69	0.45
8:G:235:LEU:O	8:G:239:ILE:HG12	2.17	0.45
3:O:52:VAL:HG21	3:O:202:VAL:HG13	1.97	0.45
12:Y:185:ASP:OD2	12:Y:190:ARG:NH1	2.41	0.45
2:2:226:ARG:NH1	2:2:250:MET:HE2	2.32	0.45
3:A:222:ASP:OD1	3:A:222:ASP:O	2.34	0.45
6:E:110:GLU:O	6:E:113:THR:HG22	2.17	0.45
8:G:56:LYS:HD3	8:G:56:LYS:N	2.31	0.45
1:M:144:PHE:CE1	1:M:150:TYR:HB3	2.52	0.45
13:L:256:THR:N	13:L:259:GLY:O	2.44	0.45
9:V:24:ALA:HB2	9:V:33:LEU:HD12	1.99	0.45
6:E:78:MET:HE2	6:E:88:MET:HE1	1.99	0.44
5:Q:92:GLU:OE2	5:Q:108:TYR:HE1	2.00	0.44
5:Q:192:VAL:O	5:Q:196:VAL:HG12	2.16	0.44
9:H:41:THR:O	9:H:41:THR:CG2	2.65	0.44
7:T:50:LYS:NZ	7:T:226:ASP:OD2	2.47	0.44
10:W:192:ILE:HG23	10:W:199:GLY:HA2	1.98	0.44
5:C:34:VAL:HG21	5:C:199:LEU:HD21	2.00	0.44
7:F:156:LEU:CD2	8:G:58:LEU:HD23	2.48	0.44
2:N:42:THR:HG23	2:N:43:SER:H	1.80	0.44
4:P:123:GLN:CD	4:P:123:GLN:O	2.61	0.44
5:R:117:GLN:NE2	5:R:131:VAL:O	2.50	0.44
1:M:32:LEU:HD11	1:M:169:LEU:CD1	2.48	0.44
3:O:43:LEU:CD2	3:O:210:MET:HE3	2.46	0.44
8:U:230:VAL:HG12	8:U:235:LEU:HB2	2.00	0.44
5:D:229:ILE:HD12	5:D:229:ILE:H	1.82	0.44
7:F:88:LEU:HD11	7:F:108:ALA:HB1	1.98	0.44
3:O:32:PHE:HZ	3:O:160:ALA:HB2	1.82	0.44
5:Q:110:THR:HA	5:Q:113:VAL:HG22	2.00	0.44
5:Q:178:ASN:HB3	5:Q:194:LEU:HD11	1.99	0.44
5:R:101:GLU:OE1	13:Z:196:ARG:NH2	2.48	0.44
9:V:23:MET:HE2	9:V:25:VAL:CG2	2.48	0.44
12:Y:153:THR:HG22	12:Y:156:GLU:OE2	2.18	0.44
2:2:44:VAL:HG22	2:2:57:ALA:HB2	2.00	0.44
10:I:116:LEU:CD1	10:I:123:ILE:HD11	2.47	0.44
3:O:53:VAL:HG11	3:O:82:VAL:CG2	2.47	0.44
5:R:141:ARG:NH1	13:Z:182:LYS:O	2.48	0.44
7:T:105:VAL:HG12	7:T:145:LEU:HD11	2.00	0.44
3:A:96:ARG:CZ	3:A:124:LEU:HD21	2.48	0.44
1:M:143:SER:CB	1:M:156:ARG:HG2	2.47	0.44
8:G:239:ILE:HG22	8:G:243:GLN:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:118:MET:HE1	4:B:150:VAL:HG12	2.00	0.43
5:C:118:GLN:O	5:C:121:THR:OG1	2.32	0.43
4:P:216:ASP:OD1	4:P:216:ASP:N	2.50	0.43
5:C:110:THR:HA	5:C:113:VAL:HG22	2.01	0.43
9:H:130:TYR:CE1	9:H:140:LYS:HG3	2.52	0.43
4:B:46:ALA:HB2	4:B:211:LEU:CD2	2.49	0.43
9:H:22:ILE:CG2	9:H:63:CYS:SG	3.06	0.43
2:2:42:THR:HG23	2:2:43:SER:H	1.81	0.43
7:F:66:CYS:O	1:M:96:PHE:CE2	2.72	0.43
4:P:204:PHE:CE1	4:P:209:ILE:HD12	2.53	0.43
5:R:40:ASN:OD1	5:R:40:ASN:O	2.37	0.43
10:W:91:ASN:HB3	10:W:111:MET:HE1	1.99	0.43
13:Z:78:THR:HG22	13:Z:91:VAL:HG12	1.99	0.43
6:E:237:ALA:O	6:E:241:LYS:HD3	2.18	0.43
7:F:64:ILE:HD12	7:F:74:LEU:HD21	2.01	0.43
9:H:22:ILE:HD11	9:H:146:ALA:HB3	1.99	0.43
13:L:127:CYS:HA	13:L:172:MET:HE3	2.00	0.43
4:P:122:THR:O	4:P:122:THR:HG22	2.18	0.43
9:V:185:ASP:OD2	9:V:187:SER:OG	2.35	0.43
7:T:68:GLU:OE2	7:T:102:LYS:NZ	2.52	0.43
10:W:195:ASP:OD1	10:W:196:LEU:N	2.52	0.43
12:Y:149:ARG:O	12:Y:152:MET:HG3	2.18	0.43
8:G:239:ILE:O	8:G:243:GLN:OE1	2.36	0.43
13:L:110:ILE:HD13	13:L:131:GLU:OE1	2.18	0.43
5:D:174:PHE:O	5:D:178:ASN:ND2	2.51	0.43
11:J:102:PRO:HB3	11:J:127:ILE:HG22	2.00	0.43
5:Q:163:THR:OG1	5:Q:175:LEU:CD1	2.67	0.43
5:R:88:LYS:HD3	5:R:116:VAL:HG21	2.00	0.43
7:T:5:ASN:OD1	7:T:5:ASN:N	2.52	0.43
7:F:156:LEU:HD13	7:F:159:THR:HB	2.00	0.42
9:H:194:MET:HE3	9:H:207:PHE:CE2	2.54	0.42
1:M:91:VAL:HG23	1:M:103:LEU:HD22	2.00	0.42
1:I:45:ASP:OD1	1:I:61:LYS:NZ	2.51	0.42
8:G:217:TRP:CD1	8:G:230:VAL:HG22	2.54	0.42
10:I:200:SER:O	10:I:223:ASN:ND2	2.44	0.42
8:G:230:VAL:HG12	8:G:235:LEU:HB2	2.01	0.42
12:K:50:ALA:HB1	13:L:195:THR:OG1	2.19	0.42
5:C:47:GLU:OE1	5:C:49:ARG:NH1	2.52	0.42
6:E:97:VAL:HG21	13:L:140:LEU:HD23	2.01	0.42
1:M:163:SER:HB2	11:X:145:GLN:OE1	2.19	0.42
6:E:203:ILE:O	6:E:207:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:213:ASP:OD1	6:E:213:ASP:C	2.62	0.42
7:T:73:SER:C	7:T:74:LEU:HD23	2.44	0.42
5:D:88:LYS:HD3	5:D:116:VAL:HG21	2.00	0.42
5:D:212:ILE:HG21	5:D:224:LEU:HD12	2.00	0.42
6:E:38:ILE:HD13	6:E:204:LEU:HD22	2.00	0.42
10:I:80:ASP:O	10:I:84:VAL:HG12	2.19	0.42
3:O:53:VAL:O	3:O:225:VAL:HA	2.20	0.42
9:V:33:LEU:HD11	9:V:63:CYS:SG	2.60	0.42
11:X:107:PRO:HD2	11:X:124:PHE:HB2	2.02	0.42
5:C:187:THR:HG22	5:C:188:VAL:N	2.35	0.42
5:D:113:VAL:O	5:D:116:VAL:HG12	2.20	0.42
9:H:98:ALA:CB	9:H:130:TYR:HD2	2.33	0.42
11:J:178:ASP:OD2	11:J:181:SER:OG	2.29	0.42
3:O:53:VAL:CG1	3:O:82:VAL:HG21	2.49	0.42
13:Z:112:ILE:HG21	13:Z:116:LEU:HD23	2.01	0.42
9:H:197:LEU:CD2	9:H:202:VAL:HG12	2.50	0.42
13:Z:92:ASP:OD1	13:Z:92:ASP:C	2.63	0.42
1:1:91:VAL:HG23	1:1:103:LEU:HD22	2.02	0.41
4:B:216:ASP:OD1	4:B:216:ASP:N	2.53	0.41
5:D:143:ASP:OD1	5:D:143:ASP:N	2.49	0.41
7:F:78:ALA:N	7:F:79:PRO:HD2	2.35	0.41
11:X:102:PRO:HB3	11:X:127:ILE:HG22	2.01	0.41
4:B:75:TYR:HB3	4:B:82:TYR:CD1	2.55	0.41
9:H:132:ILE:HA	9:H:137:SER:O	2.21	0.41
5:R:191:CYS:O	5:R:195:THR:HG23	2.19	0.41
5:C:17:ILE:O	5:C:17:ILE:HG13	2.20	0.41
8:G:149:MET:HE3	8:G:151:GLU:OE2	2.20	0.41
10:I:112:LEU:HD21	10:I:127:LEU:HD22	2.02	0.41
3:O:115:ASP:HB3	3:O:155:TYR:CZ	2.56	0.41
5:Q:113:VAL:HA	5:Q:116:VAL:HG12	2.01	0.41
5:Q:169:LYS:O	5:Q:173:GLU:OE1	2.38	0.41
1:M:144:PHE:HE1	1:M:150:TYR:HB2	1.86	0.41
5:Q:97:ARG:HA	5:Q:100:LEU:O	2.20	0.41
8:U:13:VAL:O	8:U:20:ASN:ND2	2.53	0.41
12:Y:1:MET:SD	12:Y:172:MET:HE2	2.61	0.41
13:Z:80:ALA:HA	13:Z:88:ILE:O	2.20	0.41
12:K:49:GLU:HG2	12:K:99:GLN:HB2	2.02	0.41
2:N:53:VAL:HG21	2:N:150:ALA:HB1	2.03	0.41
11:X:159:GLU:H	11:X:159:GLU:CD	2.28	0.41
3:A:79:ILE:HA	3:A:145:SER:OG	2.20	0.41
3:A:129:THR:O	3:A:129:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:151:GLU:HG2	5:D:152:PRO:HD2	2.03	0.41
13:L:95:ALA:CB	13:L:106:VAL:HG21	2.51	0.41
12:Y:101:ASN:OD1	12:Y:121:TYR:N	2.51	0.41
8:G:90:ARG:O	8:G:90:ARG:HD2	2.21	0.41
10:I:38:ASN:OD1	10:I:39:ASN:N	2.54	0.41
11:J:46:TYR:HB3	11:J:71:THR:HG21	2.03	0.41
6:S:63:SER:O	6:S:65:GLU:OE1	2.39	0.41
1:1:211:THR:HG23	1:1:218:GLY:CA	2.50	0.41
11:J:11:ILE:CG2	11:J:146:LEU:HD11	2.50	0.41
3:O:77:ARG:NH1	3:O:111:ASP:OD2	2.51	0.41
4:P:74:VAL:HG22	4:P:75:TYR:H	1.86	0.41
7:T:183:ASP:N	7:T:183:ASP:OD1	2.52	0.41
9:V:98:ALA:CB	9:V:130:TYR:HD2	2.33	0.41
11:X:7:ILE:HG23	11:X:8:ASN:N	2.36	0.41
2:2:46:SER:OG	2:2:160:LEU:HD11	2.21	0.41
5:D:191:CYS:O	5:D:195:THR:HG23	2.21	0.40
11:J:172:LEU:HD22	11:J:202:MET:HB3	2.03	0.40
8:U:30:VAL:HG11	8:U:134:SER:HB3	2.02	0.40
8:U:217:TRP:CD1	8:U:230:VAL:HG22	2.56	0.40
11:X:178:ASP:OD1	11:X:181:SER:OG	2.24	0.40
2:2:45:ILE:HG12	2:2:214:MET:HE3	2.03	0.40
5:D:107:GLU:OE1	5:D:148:TYR:CE2	2.75	0.40
12:K:11:ASP:OD1	12:K:11:ASP:O	2.38	0.40
1:M:155:CYS:SG	1:M:166:MET:HE1	2.61	0.40
6:S:237:ALA:O	6:S:241:LYS:HD3	2.21	0.40
7:T:32:GLY:O	7:T:163:ALA:N	2.44	0.40
9:V:96:THR:O	9:V:100:VAL:HG23	2.22	0.40
12:Y:180:ILE:O	12:Y:180:ILE:HG23	2.20	0.40
13:L:112:ILE:HG21	13:L:116:LEU:HD23	2.02	0.40
4:P:118:MET:HE1	4:P:150:VAL:HG12	2.02	0.40
6:S:78:MET:HE1	6:S:89:ILE:HG12	2.04	0.40
5:C:94:GLN:HB3	11:J:69:TYR:CD2	2.55	0.40
5:C:155:ILE:HG22	5:D:79:ASN:OD1	2.22	0.40
5:C:163:THR:HG21	5:C:171:VAL:CG1	2.51	0.40
12:K:165:VAL:O	12:K:169:GLU:HG3	2.22	0.40
5:Q:94:GLN:HB3	11:X:69:TYR:CD2	2.57	0.40
6:E:199:LEU:HD23	6:E:203:ILE:HD13	2.03	0.40
7:F:213:ILE:HD12	7:F:230:VAL:HG23	2.04	0.40
3:O:79:ILE:HA	3:O:145:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	219/241 (91%)	214 (98%)	5 (2%)	0	100	100
1	M	219/241 (91%)	215 (98%)	4 (2%)	0	100	100
2	2	228/266 (86%)	223 (98%)	5 (2%)	0	100	100
2	N	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
3	A	230/252 (91%)	228 (99%)	2 (1%)	0	100	100
3	O	230/252 (91%)	227 (99%)	3 (1%)	0	100	100
4	B	239/250 (96%)	239 (100%)	0	0	100	100
4	P	239/250 (96%)	239 (100%)	0	0	100	100
5	C	212/254 (84%)	209 (99%)	3 (1%)	0	100	100
5	D	202/254 (80%)	198 (98%)	4 (2%)	0	100	100
5	Q	212/254 (84%)	207 (98%)	5 (2%)	0	100	100
5	R	202/254 (80%)	201 (100%)	1 (0%)	0	100	100
6	E	201/260 (77%)	197 (98%)	4 (2%)	0	100	100
6	S	201/260 (77%)	200 (100%)	1 (0%)	0	100	100
7	F	229/234 (98%)	228 (100%)	1 (0%)	0	100	100
7	T	229/234 (98%)	226 (99%)	3 (1%)	0	100	100
8	G	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
8	U	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
9	H	194/215 (90%)	191 (98%)	3 (2%)	0	100	100
9	V	194/215 (90%)	190 (98%)	4 (2%)	0	100	100
10	I	218/261 (84%)	216 (99%)	2 (1%)	0	100	100
10	W	218/261 (84%)	214 (98%)	4 (2%)	0	100	100
11	J	201/205 (98%)	194 (96%)	7 (4%)	0	100	100
11	X	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
12	K	193/198 (98%)	189 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Y	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
13	L	210/287 (73%)	207 (99%)	3 (1%)	0	100	100
13	Z	210/287 (73%)	207 (99%)	3 (1%)	0	100	100
14	a	73/250 (29%)	72 (99%)	1 (1%)	0	100	100
14	b	73/250 (29%)	73 (100%)	0	0	100	100
All	All	6180/7430 (83%)	6084 (98%)	96 (2%)	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	1	184/201 (92%)	184 (100%)	0	100	100
1	M	184/201 (92%)	184 (100%)	0	100	100
2	2	196/224 (88%)	196 (100%)	0	100	100
2	N	196/224 (88%)	196 (100%)	0	100	100
3	A	200/210 (95%)	200 (100%)	0	100	100
3	O	200/210 (95%)	200 (100%)	0	100	100
4	B	200/209 (96%)	200 (100%)	0	100	100
4	P	200/209 (96%)	200 (100%)	0	100	100
5	C	200/226 (88%)	200 (100%)	0	100	100
5	D	185/226 (82%)	185 (100%)	0	100	100
5	Q	200/226 (88%)	200 (100%)	0	100	100
5	R	185/226 (82%)	185 (100%)	0	100	100
6	E	172/215 (80%)	172 (100%)	0	100	100
6	S	172/215 (80%)	172 (100%)	0	100	100
7	F	190/193 (98%)	190 (100%)	0	100	100
7	T	190/193 (98%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	201/239 (84%)	201 (100%)	0	100	100
8	U	201/239 (84%)	201 (100%)	0	100	100
9	H	162/178 (91%)	162 (100%)	0	100	100
9	V	162/178 (91%)	162 (100%)	0	100	100
10	I	179/214 (84%)	179 (100%)	0	100	100
10	W	179/214 (84%)	179 (100%)	0	100	100
11	J	171/173 (99%)	171 (100%)	0	100	100
11	X	171/173 (99%)	171 (100%)	0	100	100
12	K	173/175 (99%)	173 (100%)	0	100	100
12	Y	173/175 (99%)	173 (100%)	0	100	100
13	L	169/235 (72%)	169 (100%)	0	100	100
13	Z	169/235 (72%)	169 (100%)	0	100	100
14	a	64/207 (31%)	64 (100%)	0	100	100
14	b	64/207 (31%)	64 (100%)	0	100	100
All	All	5292/6250 (85%)	5292 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	111	ASN
1	1	114	HIS
1	1	177	ASN
3	A	176	GLN
5	C	19	GLN
5	C	79	ASN
6	E	147	HIS
6	E	154	GLN
7	F	69	HIS
7	F	93	ASN
7	F	100	ASN
8	G	20	ASN
11	J	64	ASN
11	J	173	ASN
12	K	118	GLN
1	M	113	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	M	177	ASN
2	N	236	ASN
3	O	176	GLN
3	O	193	HIS
3	O	221	ASN
5	Q	19	GLN
5	Q	79	ASN
5	Q	230	ASN
7	T	69	HIS
7	T	93	ASN
10	W	120	GLN
10	W	145	HIS
10	W	223	ASN
11	X	32	GLN
11	X	64	ASN
11	X	157	ASN
11	X	169	GLN
11	X	173	ASN
12	Y	99	GLN
12	Y	118	GLN
13	Z	283	ASN
14	b	134	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

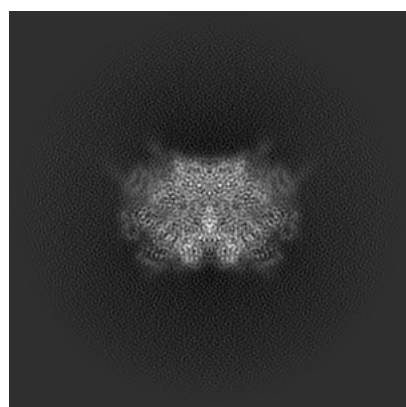
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25848. These allow visual inspection of the internal detail of the map and identification of artifacts.

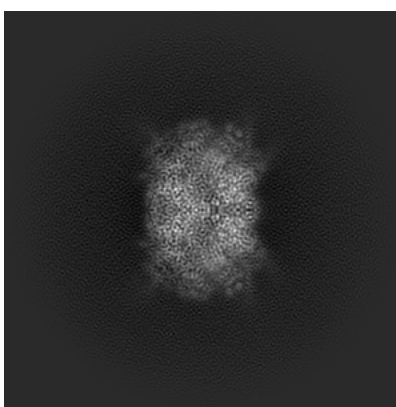
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

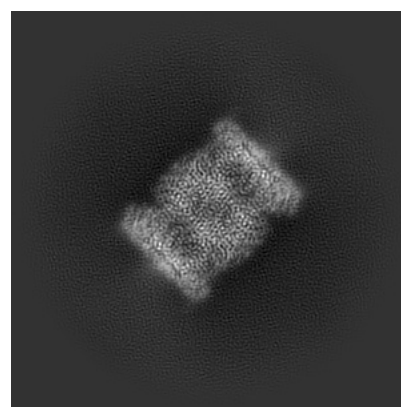
6.1.1 Primary map



X



Y

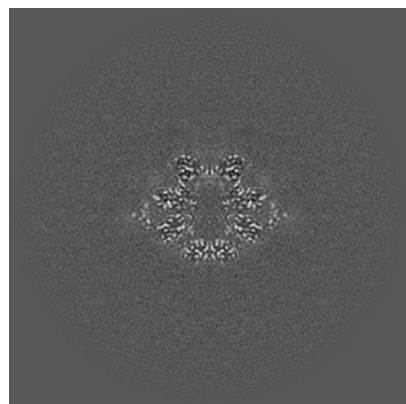


Z

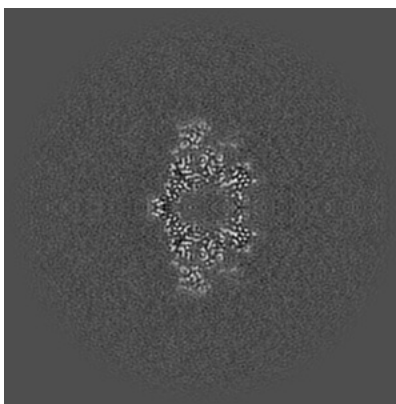
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

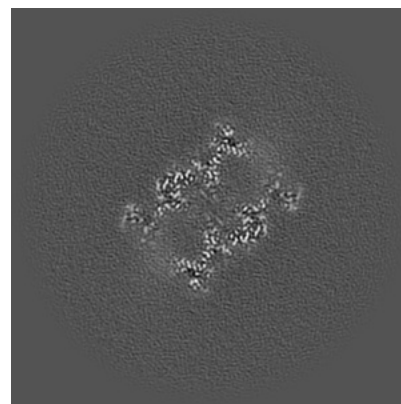
6.2.1 Primary map



X Index: 180



Y Index: 180

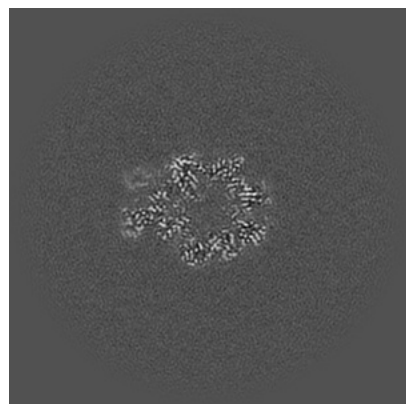


Z Index: 180

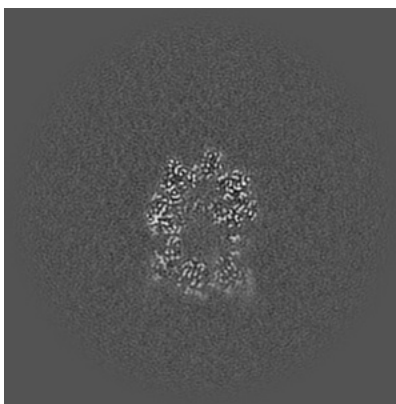
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

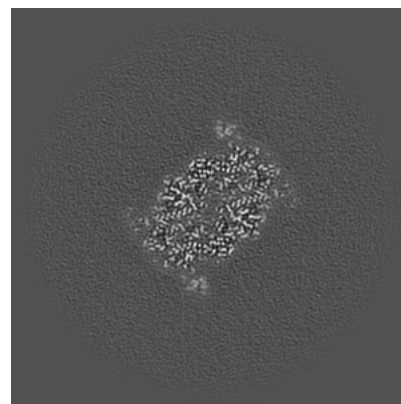
6.3.1 Primary map



X Index: 173



Y Index: 164

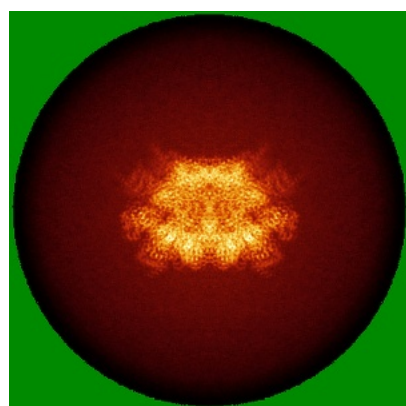


Z Index: 155

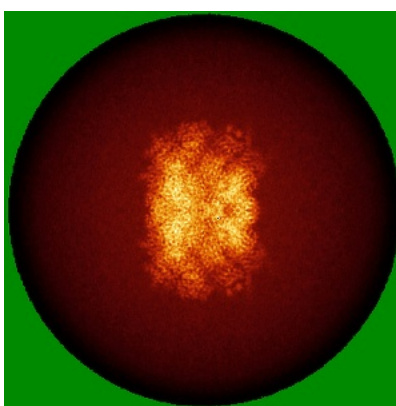
The images above show the largest variance slices of the map in three orthogonal directions.

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

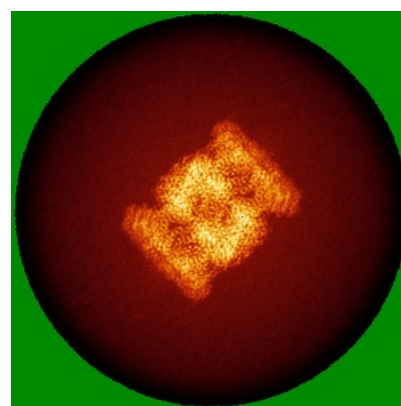
6.4.1 Primary map



X



Y

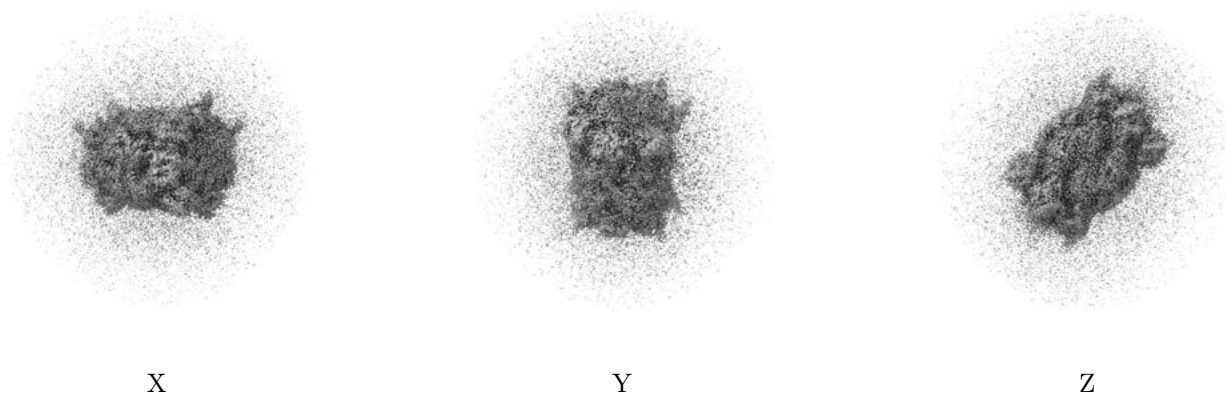


Z

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 0.306. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

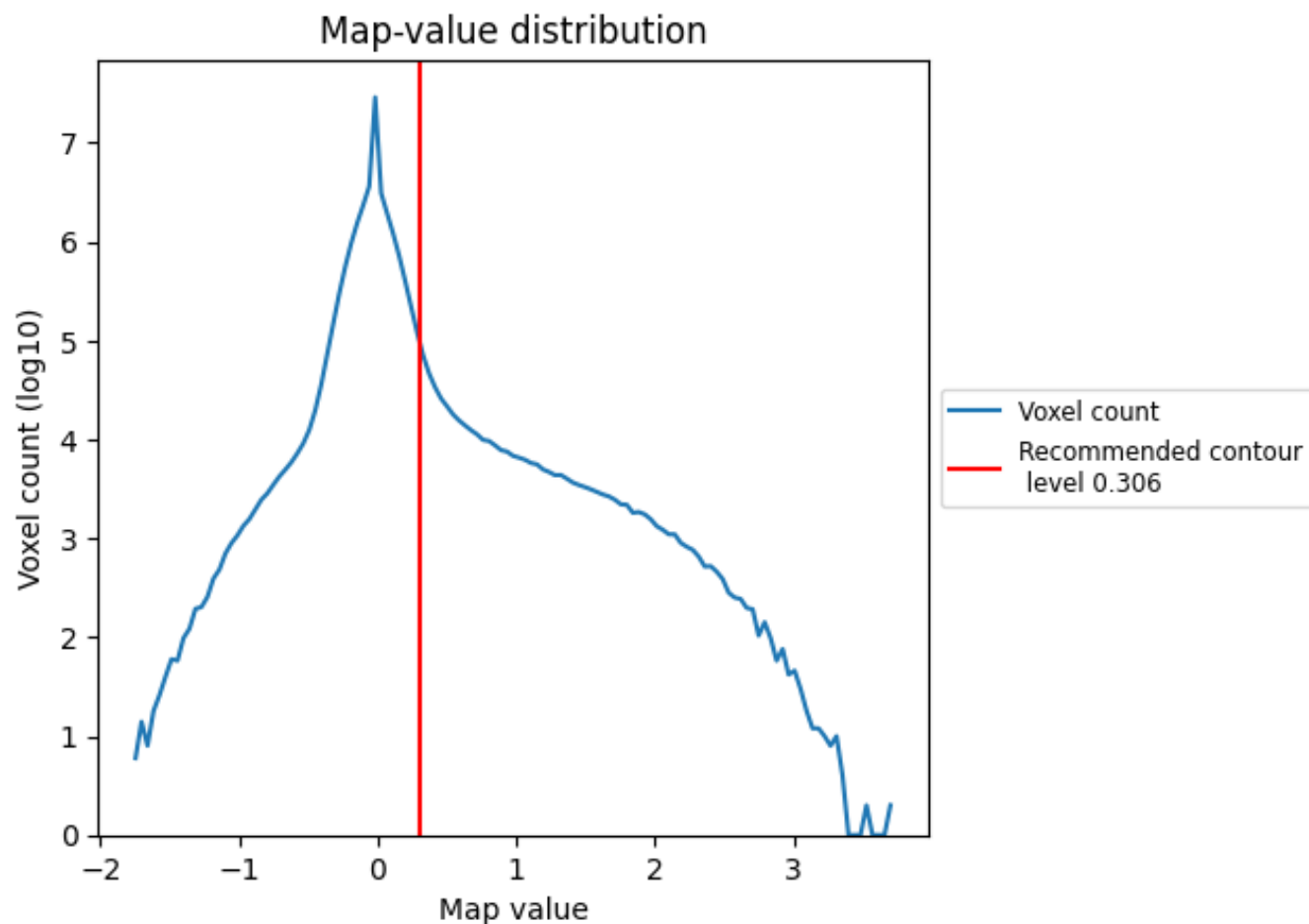
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

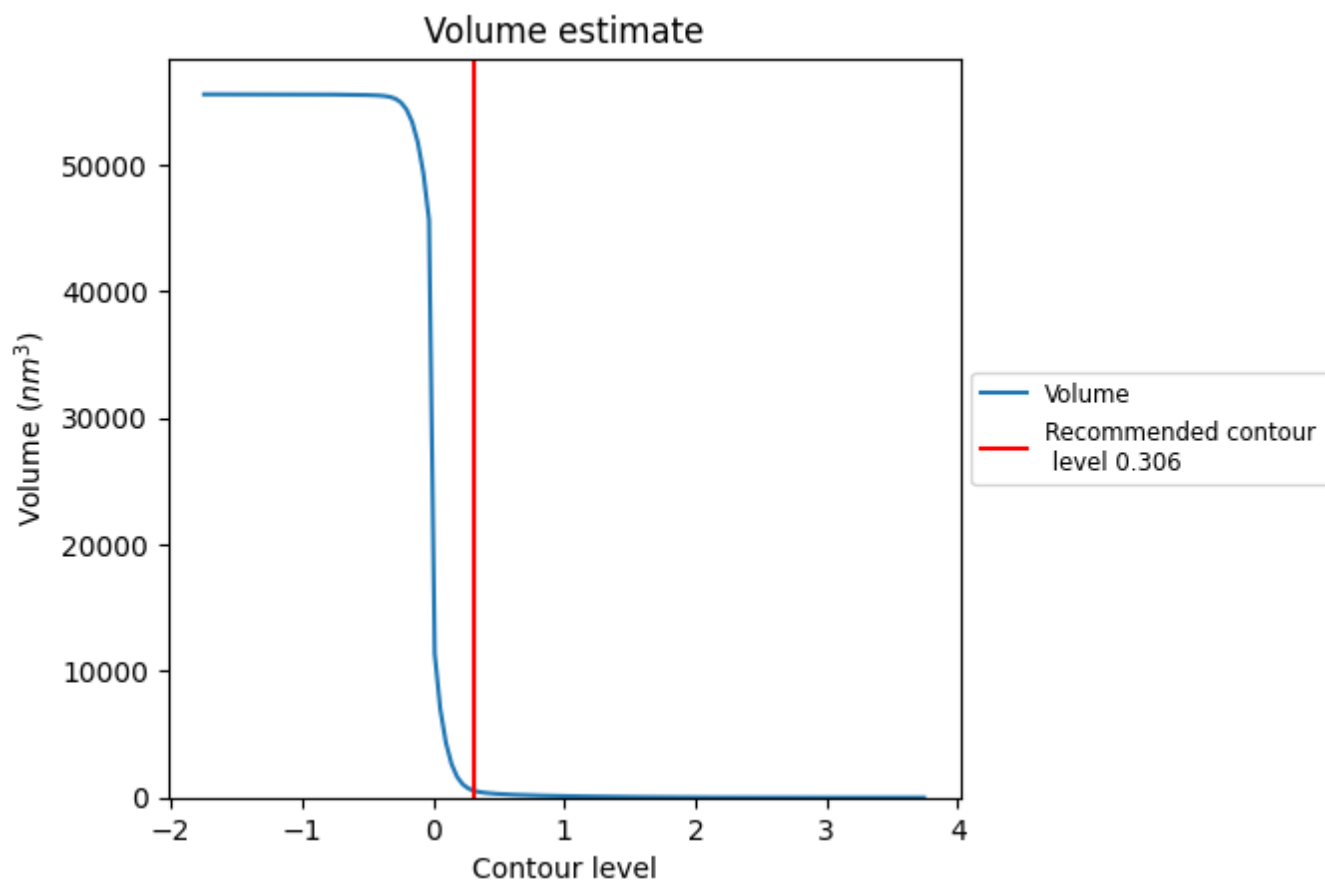
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

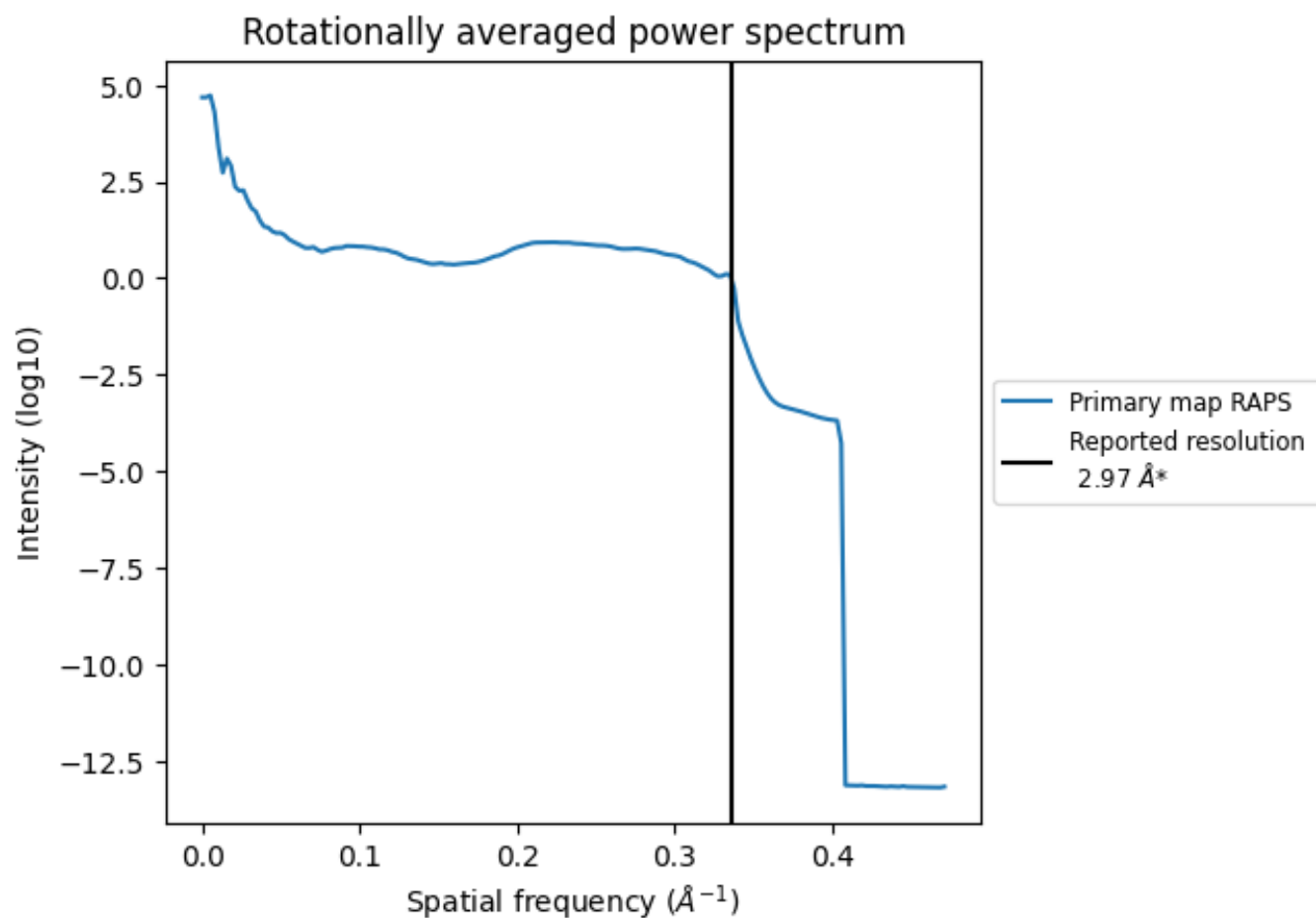
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 563 nm^3 ; this corresponds to an approximate mass of 508 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 0.337 Å⁻¹

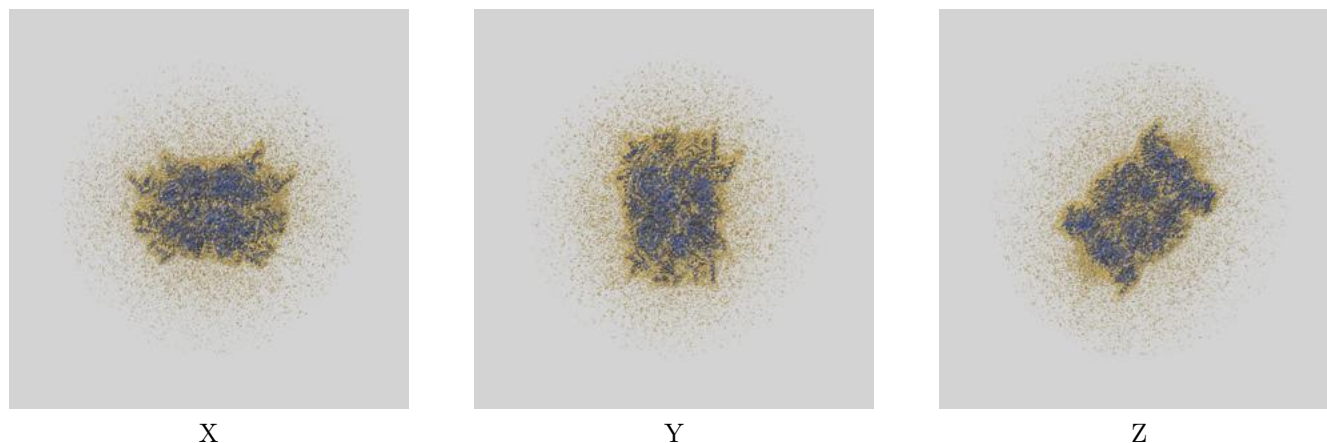
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

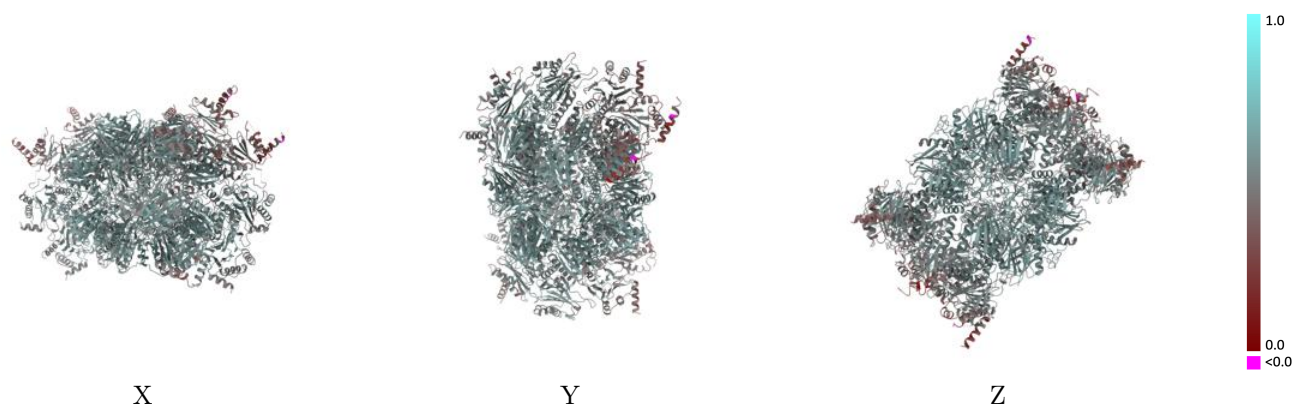
This section contains information regarding the fit between EMDB map EMD-25848 and PDB model 7TEO. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



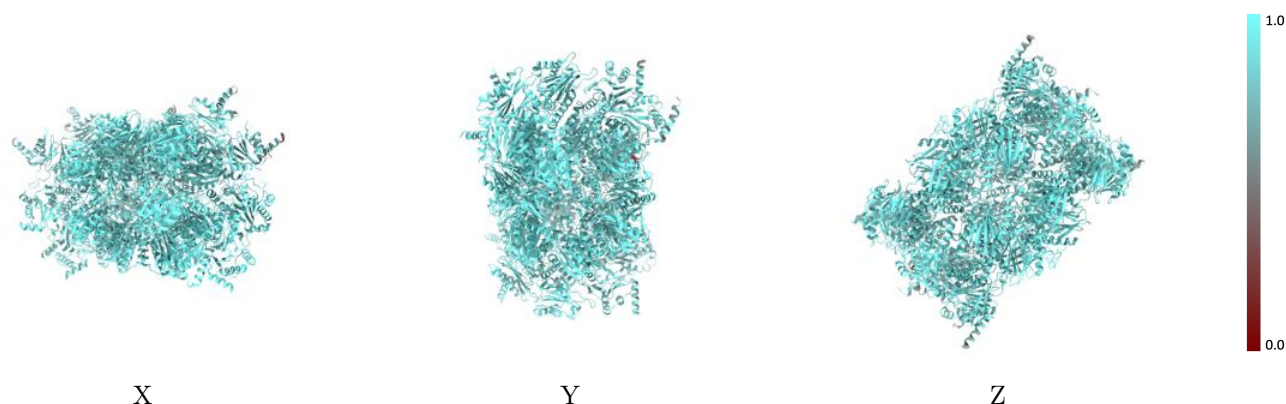
The images above show the 3D surface view of the map at the recommended contour level 0.306 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



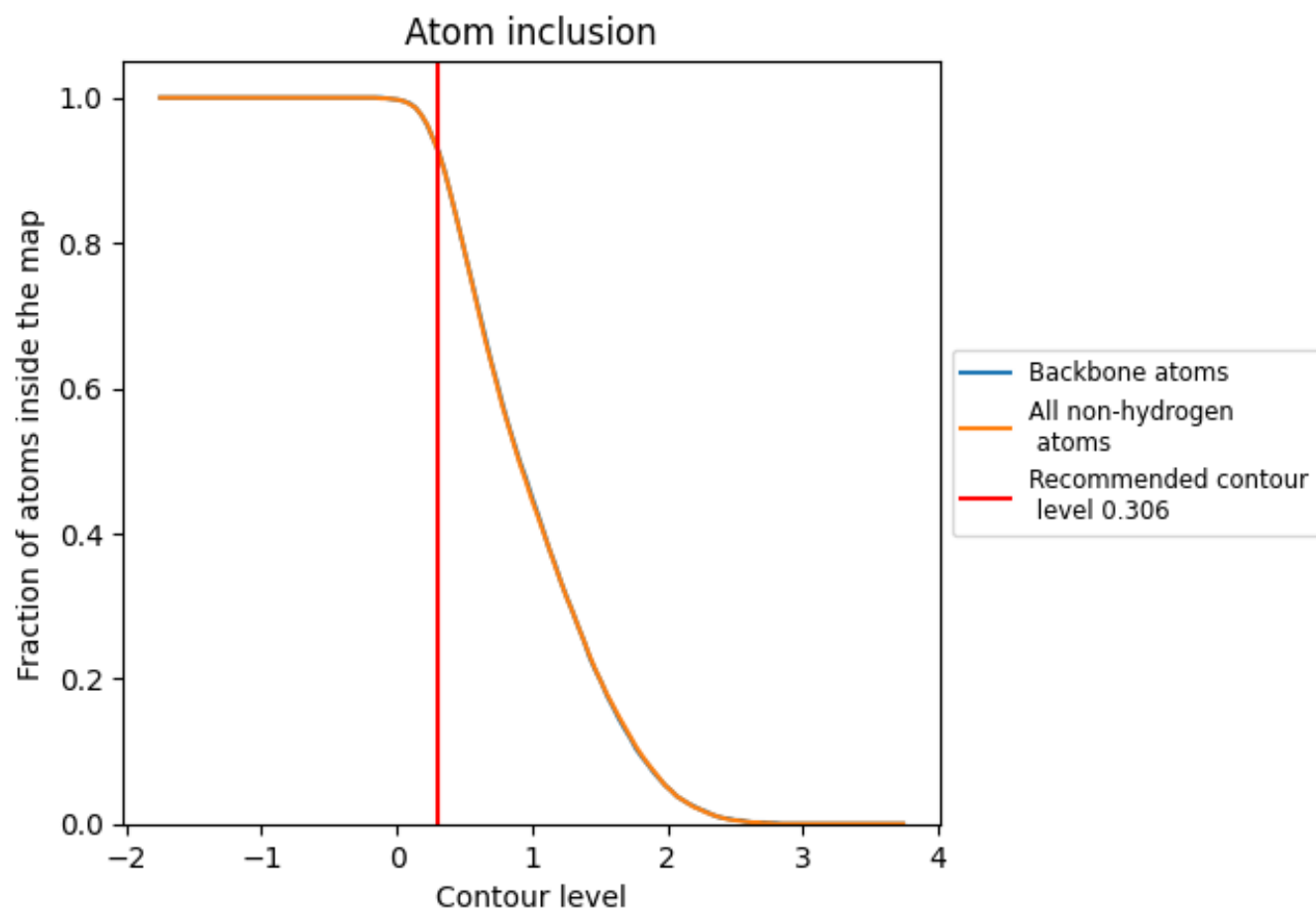
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.306).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.306) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9270	 0.5320
1	 0.9480	 0.5560
2	 0.9490	 0.5690
A	 0.9500	 0.5350
B	 0.9270	 0.5380
C	 0.8490	 0.4300
D	 0.8740	 0.4460
E	 0.8820	 0.4610
F	 0.9370	 0.5320
G	 0.9390	 0.5350
H	 0.9540	 0.5640
I	 0.9630	 0.5750
J	 0.9630	 0.5790
K	 0.9590	 0.5680
L	 0.9570	 0.5740
M	 0.9520	 0.5620
N	 0.9530	 0.5700
O	 0.9530	 0.5340
P	 0.9290	 0.5380
Q	 0.8430	 0.4280
R	 0.8670	 0.4400
S	 0.8820	 0.4640
T	 0.9290	 0.5300
U	 0.9440	 0.5330
V	 0.9580	 0.5630
W	 0.9650	 0.5790
X	 0.9600	 0.5760
Y	 0.9560	 0.5670
Z	 0.9630	 0.5700
a	 0.8430	 0.5100
b	 0.8650	 0.5210

