



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:12 PM UTC

PDB ID : 8ADN / pdb_00008adn
EMDB ID : EMD-15365
Title : Vairimorpha necatrix 20S proteasome from spores
Authors : Jespersen, N.; Ehrenbolger, K.; Winiger, R.; Svedberg, D.; Vossbrinck, C.R.;
Barandun, J.
Deposited on : 2022-07-08
Resolution : 2.77 Å(reported)
Based on initial model : 5CZ4

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

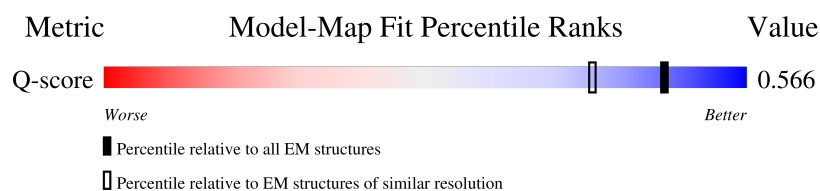
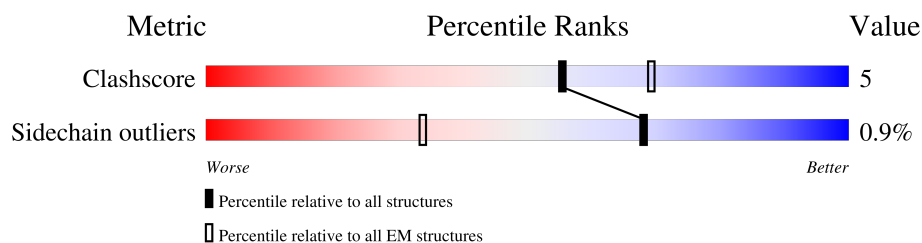
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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.



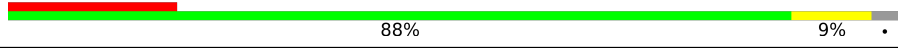
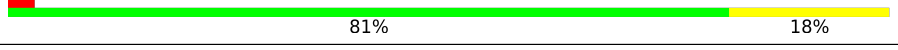
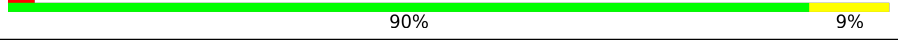
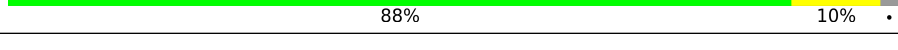
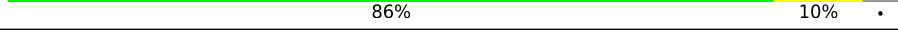
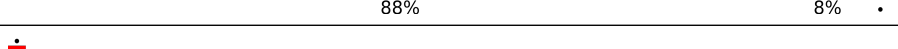
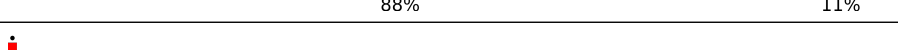
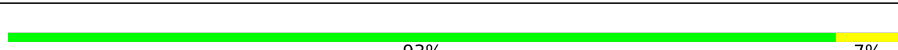
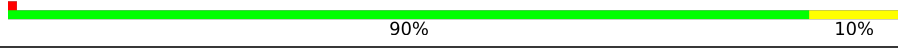
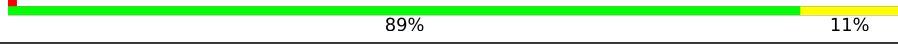
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10695 (2.27 - 3.27)

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	3	147	
1	4	147	
2	A	227	
2	O	227	
3	B	231	

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Mol	Chain	Length	Quality of chain
3	P	231	
4	C	225	
4	Q	225	
5	D	234	
5	R	234	
6	E	230	
6	S	230	
7	F	243	
7	T	243	
8	G	234	
8	U	234	
9	H	227	
9	V	227	
10	I	205	
10	W	205	
11	J	193	
11	X	193	
12	K	228	
12	Y	228	
13	L	297	
13	Z	297	
14	M	212	
14	a	212	
15	N	216	
15	b	216	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 48318 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 Inhibitor 31-Like.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	60	Total	C	N	O	0	0
			478	304	78	96		
1	4	60	Total	C	N	O	0	0
			478	304	78	96		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	225	Total	C	N	O	S	0	0
			1686	1063	284	334	5		
2	O	225	Total	C	N	O	S	0	0
			1686	1063	284	334	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	228	Total	C	N	O	S	0	0
			1858	1187	299	362	10		
3	P	228	Total	C	N	O	S	0	0
			1858	1187	299	362	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	219	Total	C	N	O	S	0	0
			1613	1020	275	311	7		
4	Q	219	Total	C	N	O	S	0	0
			1613	1020	275	311	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	233	Total	C	N	O	S	0	0
			1853	1174	307	365	7		
5	R	233	Total	C	N	O	S	0	0
			1853	1174	307	365	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	225	Total	C	N	O	S	0	0
			1811	1152	308	346	5		
6	S	225	Total	C	N	O	S	0	0
			1811	1152	308	346	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	234	Total	C	N	O	S	0	0
			1879	1188	317	365	9		
7	T	234	Total	C	N	O	S	0	0
			1879	1188	317	365	9		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	233	Total	C	N	O	S	0	0
			1843	1186	290	359	8		
8	U	233	Total	C	N	O	S	0	0
			1843	1186	290	359	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	218	Total	C	N	O	S	0	0
			1659	1037	293	318	11		
9	V	218	Total	C	N	O	S	0	0
			1659	1037	293	318	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	203	Total	C	N	O	S	0	0
			1594	1015	257	308	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	203	Total	C	N	O	S	0	0
			1594	1015	257	308	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	193	Total	C	N	O	S	0	0
			1542	983	250	303	6		
11	X	193	Total	C	N	O	S	0	0
			1542	983	250	303	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	195	Total	C	N	O	S	0	0
			1509	961	254	285	9		
12	Y	195	Total	C	N	O	S	0	0
			1509	961	254	285	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	208	Total	C	N	O	S	0	0
			1690	1074	280	330	6		
13	Z	208	Total	C	N	O	S	0	0
			1690	1074	280	330	6		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	212	Total	C	N	O	S	0	0
			1662	1041	285	323	13		
14	a	212	Total	C	N	O	S	0	0
			1662	1041	285	323	13		

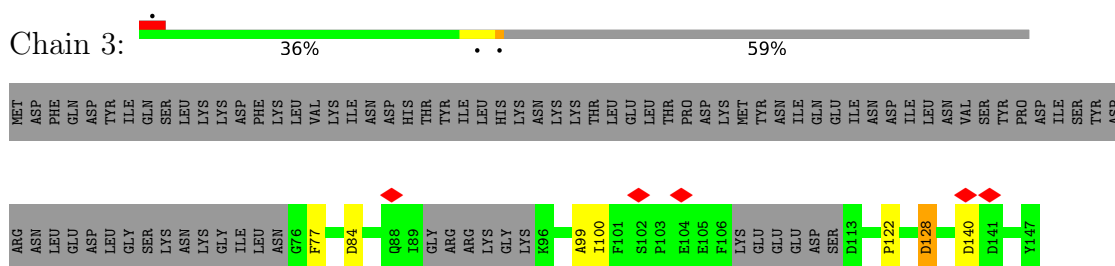
- Molecule 15 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	194	Total	C	N	O	S	0	0
			1482	934	249	286	13		
15	b	194	Total	C	N	O	S	0	0
			1482	934	249	286	13		

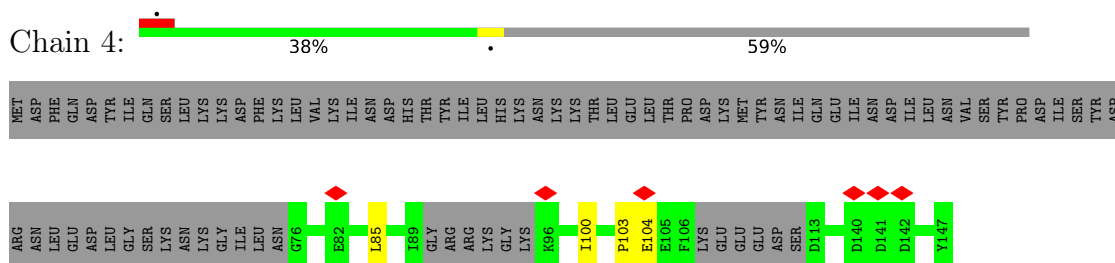
3 Residue-property plots [i](#)

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.

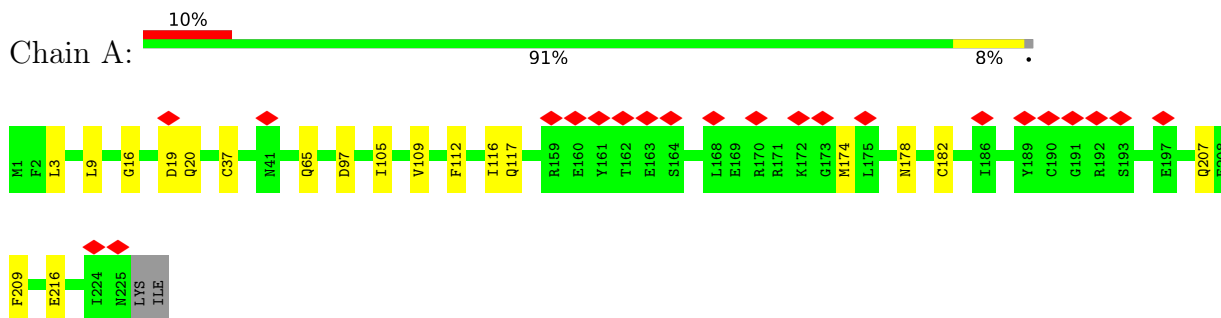
- Molecule 1: Proteasome Inhibitor 31-Like



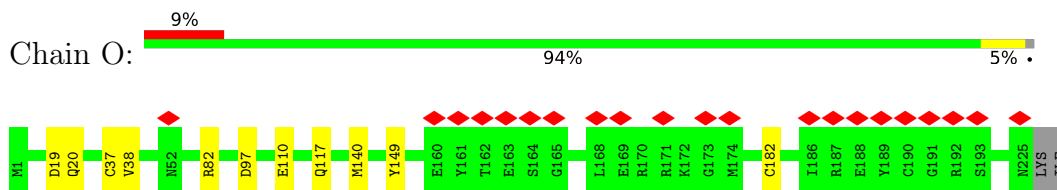
- Molecule 1: Proteasome Inhibitor 31-Like



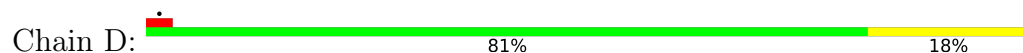
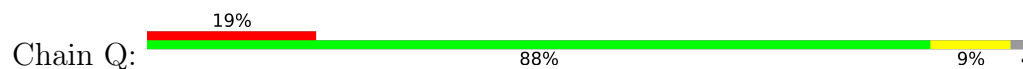
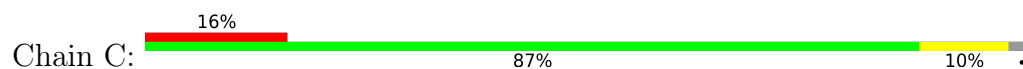
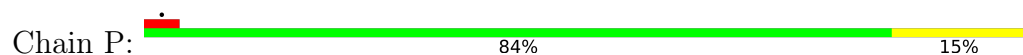
- Molecule 2: Proteasome subunit alpha type-2

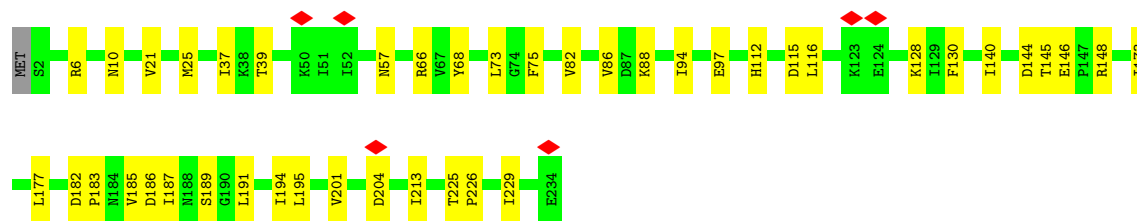


- Molecule 2: Proteasome subunit alpha type-2

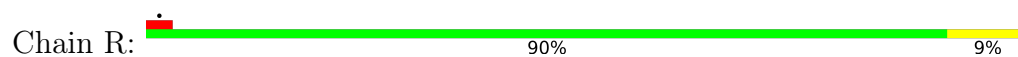


Chain B: 85% 13%

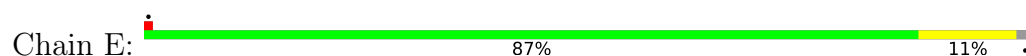




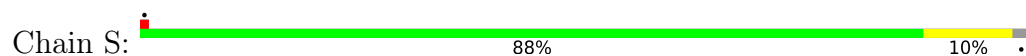
• Molecule 5: Proteasome subunit alpha type-5



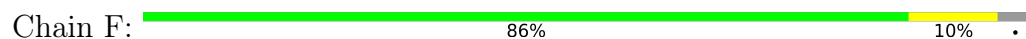
• Molecule 6: Proteasome subunit alpha type-6



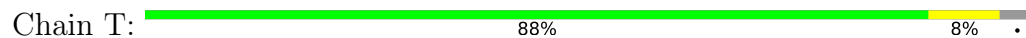
• Molecule 6: Proteasome subunit alpha type-6



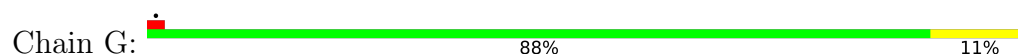
• Molecule 7: Proteasome subunit alpha type-7



• Molecule 7: Proteasome subunit alpha type-7

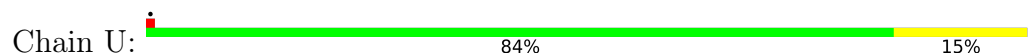


• Molecule 8: Proteasome subunit alpha type-1

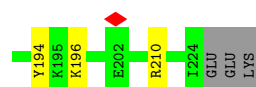
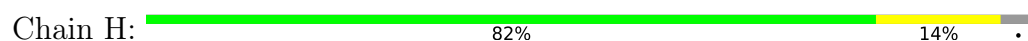




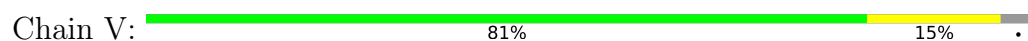
- Molecule 8: Proteasome subunit alpha type-1



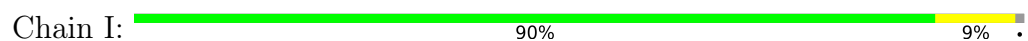
- Molecule 9: Proteasome subunit beta type-2



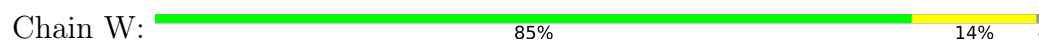
- Molecule 9: Proteasome subunit beta type-2



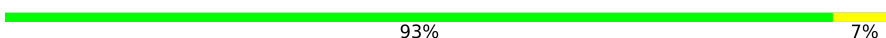
- Molecule 10: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-3



- Molecule 11: Proteasome subunit beta type-4

Chain J:  93% 7%



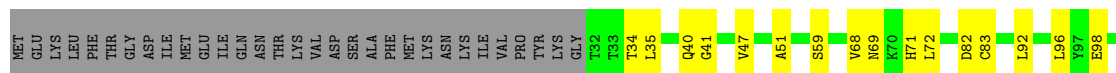
- Molecule 11: Proteasome subunit beta type-4

Chain X:  83% 17%



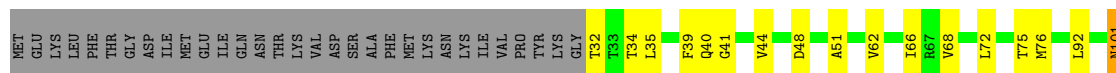
- Molecule 12: Proteasome subunit beta type-5

Chain K:  74% 11% 14%



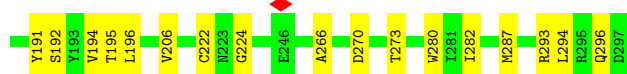
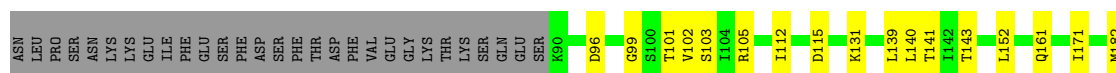
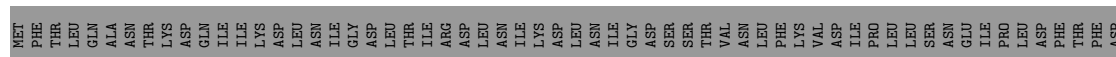
- Molecule 12: Proteasome subunit beta type-5

Chain Y:  74% 11% 14%



- Molecule 13: Proteasome subunit beta type-6

Chain L:  59% 11% 30%

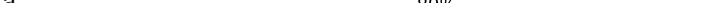


- Molecule 13: Proteasome subunit beta type-6

M182	M191	T195	L196	V206	D210	H214	V218	V221	D257	R280	A286	D270	T273	D274	D275	W280	I281	L282	K289	L294	E295	Q296	D297							
ASN	LEU	PRO	SER	ASN	LYS	GLY	THR	LYS	ASP	PHE	VAL	GLU	GLY	THR	LYS	ASP	ASN	ASN	GLN	GLU	SER	ASN	GLU	ILE	PRO	LEU	ASP	PHE	THR	PHE

- Chain M: 90% 10%

#1	V10	V19	D24	R40	R43	S53	F61	E65 L66	M77	L85 V86	V107	G108	V109	D110	D111	F114	C132	M137	V184	V189	E205	E206	E207	E208	L212
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- Chain a:  89% 11%

M1	S8	G9	V10	I11	S12	K16	N17	D24	R40	R43	S46	N47	T48	L49	S53	L66	V96	V107	C132	N137	M138	R171	S172	S175	I181	W201	N206	E207	E208	L212
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- Chain N:  79% 11% 10%

Diagram illustrating a protein sequence alignment. The top sequence is MET VAL ALA TTR ASP ASN LYS ASN ASN GLU GLY PHE SER PRO ASN ASN LEU PRO GLU MET THR GLY T22 T33 R40 M43 S48 I76 Y79 I80 R86 D91 K99 M102 D106 I107 M114 G117 L118 A121 Y152 E168 M186. The bottom sequence is R199 D210 N214 S215 THR. Red diamonds indicate mismatches between the two sequences: VAL vs D210, ASN vs N214, and ASN vs S215.

- Chain b: 80% 10% 10%

Amino Acid	Frequency (approx.)
MET	25
VAL	24
ALA	23
THR	22
ASP	21
ASN	20
LYS	19
ASN	18
ASN	17
GLU	16
GLY	15
PHE	14
SER	13
PRO	12
ASN	11
LEU	10
PRO	9
GLU	8
MET	7
THR	6
GLY	5
T22	4
I33	3
R40	2
M43	1
Y46	1
S48	1
Y79	1
V84	1
A100	1
A101	1
M102	1
D106	1
I107	1
A121	1
G122	1
Y123	1
M138	1
S148	1
A151	1
N186	1
R199	1
D210	1
V211	1
N214	0.5
S215	0.5
THR	0.5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	52679	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35.01, 36.334	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	4.477	Depositor
Minimum map value	-2.358	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	416.80002, 416.80002, 416.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.042, 1.042, 1.042	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	3	0.13	0/489	0.34	0/653
1	4	0.13	0/489	0.35	0/653
2	A	0.15	0/1711	0.32	0/2316
2	O	0.16	0/1711	0.34	0/2316
3	B	0.14	0/1891	0.32	0/2535
3	P	0.13	0/1891	0.30	0/2535
4	C	0.15	0/1636	0.33	0/2214
4	Q	0.14	0/1636	0.36	0/2214
5	D	0.14	0/1883	0.31	0/2537
5	R	0.14	0/1883	0.35	0/2537
6	E	0.14	0/1841	0.32	0/2478
6	S	0.14	0/1841	0.30	0/2478
7	F	0.15	0/1903	0.33	0/2556
7	T	0.16	0/1903	0.32	0/2556
8	G	0.15	0/1880	0.29	0/2543
8	U	0.15	0/1880	0.31	0/2543
9	H	0.16	0/1687	0.32	0/2280
9	V	0.15	0/1687	0.32	0/2280
10	I	0.17	0/1625	0.34	0/2183
10	W	0.16	0/1625	0.32	0/2183
11	J	0.16	0/1567	0.31	0/2114
11	X	0.17	0/1567	0.33	0/2114
12	K	0.16	0/1542	0.32	0/2078
12	Y	0.15	0/1542	0.30	0/2078
13	L	0.16	0/1727	0.34	0/2332
13	Z	0.16	0/1727	0.34	0/2332
14	M	0.17	0/1684	0.33	0/2279
14	a	0.16	0/1684	0.33	0/2279
15	N	0.16	0/1504	0.32	0/2027
15	b	0.16	0/1504	0.30	0/2027
All	All	0.15	0/49140	0.32	0/66250

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	3	478	0	444	9	0
1	4	478	0	444	4	0
2	A	1686	0	1583	14	0
2	O	1686	0	1583	9	0
3	B	1858	0	1827	26	0
3	P	1858	0	1827	27	0
4	C	1613	0	1502	16	0
4	Q	1613	0	1502	17	0
5	D	1853	0	1851	31	0
5	R	1853	0	1851	20	0
6	E	1811	0	1827	17	0
6	S	1811	0	1827	15	0
7	F	1879	0	1919	17	0
7	T	1879	0	1919	12	0
8	G	1843	0	1817	19	0
8	U	1843	0	1817	24	0
9	H	1659	0	1663	23	0
9	V	1659	0	1663	22	0
10	I	1594	0	1574	12	0
10	W	1594	0	1574	17	0
11	J	1542	0	1539	8	0
11	X	1542	0	1539	22	0
12	K	1509	0	1467	20	0
12	Y	1509	0	1467	18	0
13	L	1690	0	1630	23	0
13	Z	1690	0	1630	29	0
14	M	1662	0	1669	13	0
14	a	1662	0	1669	13	0
15	N	1482	0	1493	17	0
15	b	1482	0	1493	14	0
All	All	48318	0	47610	478	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 (478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:103:SER:OG	15:N:91:ASP:OD2	1.81	0.98
9:H:186:GLU:OE1	9:H:186:GLU:N	2.09	0.86
13:Z:96:ASP:OD1	13:Z:98:SER:OG	1.94	0.84
2:O:82:ARG:NH2	8:U:150:ALA:O	2.13	0.82
8:U:177:GLU:OE1	8:U:177:GLU:N	2.13	0.81
9:V:7:THR:N	9:V:135:SER:HG	1.76	0.81
5:D:186:ASP:OD1	5:D:187:ILE:N	2.14	0.80
6:E:200:GLU:OE2	6:E:200:GLU:N	2.14	0.80
2:A:216:GLU:N	2:A:216:GLU:OE1	2.15	0.79
1:4:100:ILE:HD11	12:K:51:ALA:HB1	1.67	0.77
9:H:157:MET:HE1	9:H:180:VAL:HG11	1.67	0.76
11:X:38:ILE:HD11	11:X:44:PHE:HD2	1.49	0.75
2:A:117:GLN:NE2	3:B:71:ASP:OD2	2.20	0.75
10:W:114:THR:OG1	10:W:116:ASP:OD2	2.04	0.75
5:D:73:LEU:HD23	5:D:86:VAL:HG22	1.70	0.74
13:L:115:ASP:OD1	13:L:131:LYS:NZ	2.21	0.73
2:O:110:GLU:OE1	2:O:149:TYR:OH	2.04	0.73
2:O:117:GLN:NE2	3:P:71:ASP:OD1	2.21	0.72
12:K:82:ASP:OD1	12:K:83:CYS:N	2.23	0.71
11:X:38:ILE:HD11	11:X:44:PHE:CD2	2.24	0.71
3:P:40:LEU:HD21	3:P:42:ILE:HD11	1.72	0.71
8:U:221:ASP:OD1	8:U:222:LYS:N	2.24	0.70
10:I:166:THR:O	10:I:170:THR:HG23	1.92	0.70
6:S:93:VAL:HG21	13:Z:161:GLN:OE1	1.91	0.69
10:W:166:THR:O	10:W:170:THR:HG23	1.93	0.69
4:C:130:ARG:NE	4:C:146:GLU:OE1	2.25	0.69
13:L:270:ASP:OD2	13:L:273:THR:OG1	2.11	0.69
11:X:1:MET:HE3	11:X:171:VAL:HG21	1.73	0.68
15:N:210:ASP:OD1	15:N:214:ASN:ND2	2.26	0.68
11:X:67:GLU:OE2	11:X:71:ASN:ND2	2.23	0.68
1:3:128:ASP:OD1	9:H:122:HIS:ND1	2.27	0.67
8:G:69:LEU:HD21	8:G:107:LEU:HD22	1.77	0.66
7:T:186:GLU:OE2	7:T:233:LYS:NZ	2.27	0.66
11:J:67:GLU:OE1	11:J:71:ASN:ND2	2.27	0.66
8:G:189:VAL:HG21	8:G:227:LEU:HD21	1.78	0.66
10:I:125:ASP:OD1	10:I:129:ALA:N	2.28	0.65
5:R:17:ARG:H	5:R:17:ARG:HD2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:105:VAL:HG23	9:V:133:LEU:HD12	1.78	0.65
12:Y:35:LEU:HD13	12:Y:170:LEU:HD11	1.77	0.65
12:Y:40:GLN:OE1	12:Y:41:GLY:N	2.29	0.65
4:C:13:ASP:OD2	4:C:15:ARG:NH1	2.30	0.65
7:F:19:ILE:HG21	7:F:149:THR:HG22	1.78	0.65
11:X:39:ASN:OD1	11:X:40:ASN:N	2.31	0.64
5:D:195:LEU:HD21	5:D:213:ILE:HD11	1.79	0.64
12:K:35:LEU:HD13	12:K:170:LEU:HD11	1.80	0.64
12:Y:66:ILE:HD11	12:Y:76:MET:SD	2.39	0.63
5:D:66:ARG:NH2	12:K:98:GLU:OE2	2.31	0.63
4:C:43:LEU:HD12	4:C:45:ILE:HD11	1.80	0.63
3:B:40:LEU:HD21	3:B:42:ILE:HD11	1.81	0.62
5:D:88:LYS:NZ	5:D:128:LYS:O	2.29	0.62
7:F:91:LEU:HD22	7:F:102:VAL:HG11	1.81	0.62
13:L:152:LEU:HD21	13:L:182:MET:HE2	1.81	0.62
3:P:107:LYS:O	3:P:111:THR:HG23	2.00	0.62
6:E:40:ASN:ND2	6:E:178:PHE:O	2.32	0.62
9:H:135:SER:OG	9:H:171:ASP:OD2	2.13	0.62
9:H:157:MET:CE	9:H:180:VAL:HG11	2.30	0.61
12:K:40:GLN:OE1	12:K:41:GLY:N	2.33	0.61
1:3:84:ASP:OD2	1:3:99:ALA:HB2	2.00	0.61
3:B:107:LYS:O	3:B:111:THR:HG23	2.00	0.61
10:W:153:LEU:HD12	10:W:170:THR:HG22	1.82	0.61
10:I:169:GLN:O	10:I:173:ASN:ND2	2.35	0.60
4:Q:49:THR:HG23	4:Q:49:THR:O	2.02	0.60
10:W:169:GLN:O	10:W:173:ASN:ND2	2.33	0.60
1:4:100:ILE:CD1	12:K:51:ALA:HB1	2.30	0.60
13:L:293:ARG:NH1	13:L:294:LEU:O	2.34	0.60
7:T:19:ILE:HG21	7:T:149:THR:HG22	1.84	0.60
8:U:189:VAL:HG21	8:U:227:LEU:HD21	1.84	0.59
7:T:207:GLU:OE2	7:T:221:ARG:NH1	2.35	0.59
2:A:207:GLN:OE1	2:A:207:GLN:N	2.30	0.59
5:D:6:ARG:O	5:D:10:ASN:ND2	2.35	0.59
9:H:24:THR:HG22	9:H:179:ASP:OD1	2.03	0.59
3:B:73:MET:HE2	3:B:73:MET:HA	1.84	0.59
1:3:122:PRO:HB2	14:a:138:MET:HE1	1.84	0.59
10:I:6:GLN:N	10:I:6:GLN:OE1	2.35	0.59
14:a:24:ASP:O	14:a:40:ARG:NH2	2.36	0.59
14:M:110:ASP:O	14:M:110:ASP:OD2	2.21	0.59
14:a:172:SER:HG	14:a:175:SER:HG	1.51	0.58
8:U:69:LEU:HD21	8:U:107:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:152:LEU:HD21	13:Z:182:MET:HE2	1.86	0.58
3:B:4:ASN:ND2	3:B:116:THR:O	2.37	0.58
14:a:172:SER:OG	14:a:175:SER:OG	2.18	0.58
2:A:19:ASP:OD1	2:A:20:GLN:N	2.37	0.58
7:F:87:LEU:HD11	7:F:111:ILE:HD13	1.86	0.58
13:L:266:ALA:O	13:L:270:ASP:N	2.34	0.58
8:U:69:LEU:HD21	8:U:107:LEU:CD2	2.34	0.58
13:L:152:LEU:HD23	13:L:194:VAL:HG21	1.85	0.58
13:Z:152:LEU:HD23	13:Z:194:VAL:HG21	1.85	0.58
6:E:61:LYS:HG3	6:E:61:LYS:O	2.04	0.57
11:J:177:GLU:OE2	11:J:179:LYS:NZ	2.37	0.57
12:K:223:VAL:HG21	10:W:205:ASP:HB3	1.87	0.57
6:E:191:ILE:HD11	6:E:211:ILE:HD11	1.86	0.57
14:M:24:ASP:O	14:M:40:ARG:NH2	2.37	0.57
3:B:128:MET:SD	3:B:206:ASN:ND2	2.78	0.57
13:Z:270:ASP:OD2	13:Z:273:THR:OG1	2.21	0.57
13:Z:296:GLN:OE1	13:Z:296:GLN:N	2.32	0.57
13:L:296:GLN:OE1	13:L:296:GLN:N	2.34	0.57
3:B:8:GLU:OE1	3:B:8:GLU:O	2.23	0.57
4:C:103:SER:OG	4:C:106:GLU:OE1	2.22	0.56
10:I:153:LEU:HD12	10:I:170:THR:HG22	1.87	0.56
9:V:157:MET:HE1	9:V:180:VAL:HG11	1.87	0.56
4:Q:132:ILE:HD11	4:Q:159:VAL:HG21	1.86	0.56
7:T:43:MET:HE3	7:T:134:CYS:SG	2.45	0.56
11:X:140:VAL:HG21	11:X:164:VAL:HG21	1.87	0.56
11:X:80:THR:O	11:X:84:ILE:HG12	2.05	0.56
6:S:191:ILE:HD11	6:S:211:ILE:HD11	1.88	0.56
2:O:19:ASP:OD1	2:O:20:GLN:N	2.37	0.55
11:X:38:ILE:H	11:X:38:ILE:HD12	1.70	0.55
13:L:101:THR:HG23	13:L:143:THR:CG2	2.36	0.55
6:S:98:ARG:N	6:S:98:ARG:HD3	2.21	0.55
13:Z:152:LEU:CD2	13:Z:194:VAL:HG21	2.36	0.55
7:F:47:LYS:NZ	7:F:59:ASN:O	2.31	0.55
3:P:65:VAL:HG22	3:P:123:PHE:CE1	2.41	0.55
7:T:87:LEU:HD11	7:T:111:ILE:HD13	1.87	0.55
3:P:65:VAL:HG22	3:P:123:PHE:HE1	1.72	0.55
3:P:162:GLY:HA3	3:P:184:ILE:HD11	1.87	0.55
8:G:69:LEU:HD21	8:G:107:LEU:CD2	2.36	0.55
9:H:130:TYR:OH	9:H:145:GLU:OE2	2.24	0.54
5:R:144:ASP:OD1	5:R:144:ASP:N	2.39	0.54
8:U:193:LEU:O	8:U:197:GLY:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:157:MET:CE	9:V:180:VAL:HG11	2.38	0.54
2:O:97:ASP:OD1	9:V:63:ARG:NE	2.36	0.54
4:Q:210:VAL:HG12	4:Q:210:VAL:O	2.06	0.54
2:A:174:MET:O	2:A:178:ASN:N	2.39	0.54
5:D:68:TYR:OH	5:D:97:GLU:OE2	2.23	0.54
7:T:15:ASP:OD1	8:U:29:LYS:NZ	2.39	0.54
14:a:132:CYS:O	14:a:137:ASN:ND2	2.40	0.53
6:E:40:ASN:OD1	6:E:41:LYS:N	2.42	0.53
10:W:186:GLU:OE2	10:W:197:ARG:NH1	2.39	0.53
9:H:23:ASP:OD2	9:H:23:ASP:C	2.50	0.53
3:P:124:ILE:HD11	3:P:152:PHE:HD2	1.73	0.53
8:G:189:VAL:HG21	8:G:227:LEU:CD2	2.38	0.53
3:P:55:TYR:CE2	3:P:73:MET:HE1	2.43	0.53
13:Z:133:PHE:O	13:Z:140:LEU:N	2.32	0.53
11:X:10:ASN:O	11:X:11:ASP:OD2	2.27	0.52
5:R:17:ARG:H	5:R:17:ARG:CD	2.21	0.52
10:I:116:ASP:OD2	10:I:116:ASP:O	2.27	0.52
3:B:65:VAL:HG22	3:B:123:PHE:CE1	2.45	0.52
4:C:43:LEU:CD1	4:C:45:ILE:HD11	2.39	0.52
8:G:66:TYR:CD2	8:G:67:PRO:HD2	2.45	0.52
4:Q:83:VAL:HG21	4:Q:129:ILE:HD11	1.90	0.52
13:Z:140:LEU:HD11	13:Z:194:VAL:CG1	2.40	0.52
5:D:146:GLU:OE1	5:D:148:ARG:NH2	2.41	0.52
9:V:23:ASP:OD1	9:V:23:ASP:C	2.52	0.52
9:V:202:GLU:OE1	9:V:203:VAL:N	2.42	0.52
4:Q:171:GLU:HA	5:R:55:LEU:HD21	1.92	0.52
13:L:139:LEU:HD12	13:L:282:ILE:HD11	1.92	0.52
6:S:147:ASP:OD1	6:S:147:ASP:C	2.51	0.52
6:E:93:VAL:HG21	13:L:161:GLN:NE2	2.25	0.52
11:J:140:VAL:HG21	11:J:164:VAL:HG21	1.92	0.52
6:S:26:ASN:O	6:S:29:VAL:HG22	2.10	0.52
13:Z:121:GLU:O	13:Z:122:MET:HG2	2.10	0.52
5:D:10:ASN:ND2	6:E:124:GLY:O	2.43	0.52
13:Z:266:ALA:O	13:Z:270:ASP:N	2.36	0.52
15:b:43:MET:HE3	15:b:48:SER:HB2	1.92	0.51
11:X:17:THR:HG22	11:X:35:PHE:CE1	2.46	0.51
13:Z:210:ASP:OD2	13:Z:214:HIS:N	2.44	0.51
5:R:68:TYR:OH	5:R:97:GLU:OE1	2.23	0.51
5:D:75:PHE:CD2	5:D:82:VAL:HG21	2.46	0.50
5:D:213:ILE:HD12	5:D:229:ILE:HG12	1.93	0.50
9:H:168:ILE:HG23	9:H:175:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:189:VAL:HG21	8:U:227:LEU:CD2	2.40	0.50
3:B:28:ILE:HD12	3:B:124:ILE:HD12	1.93	0.50
3:B:96:ILE:HD11	3:B:125:TYR:HB2	1.93	0.50
3:P:4:ASN:ND2	3:P:116:THR:O	2.45	0.50
3:B:65:VAL:HG22	3:B:123:PHE:HE1	1.76	0.50
7:F:15:ASP:OD1	8:G:29:LYS:NZ	2.44	0.50
14:a:17:ASN:O	14:a:17:ASN:ND2	2.45	0.50
15:b:199:ARG:NH1	15:b:199:ARG:HB2	2.26	0.50
1:3:140:ASP:O	1:3:140:ASP:OD2	2.30	0.50
1:4:85:LEU:HD12	1:4:85:LEU:O	2.11	0.50
6:S:94:PHE:CD1	6:S:94:PHE:C	2.90	0.50
12:Y:34:THR:HB	12:Y:75:THR:HG21	1.93	0.50
13:Z:121:GLU:C	13:Z:122:MET:HG2	2.37	0.50
4:Q:158:ALA:O	4:Q:163:SER:OG	2.26	0.50
9:V:25:ARG:HD2	9:V:32:VAL:HG13	1.94	0.50
13:Z:257:ASP:OD1	13:Z:260:ARG:NH2	2.45	0.50
6:S:209:VAL:HG21	6:S:229:LEU:HD21	1.94	0.49
11:X:3:SER:OG	11:X:133:SER:OG	2.22	0.49
8:G:159:MET:HE3	8:G:168:TYR:HA	1.94	0.49
14:a:8:SER:OG	14:a:24:ASP:OD1	2.30	0.49
1:3:77:PHE:O	13:Z:186:ARG:NH2	2.42	0.49
2:A:105:ILE:O	2:A:109:VAL:HG23	2.12	0.49
4:Q:64:ASP:OD2	4:Q:92:ARG:NH2	2.45	0.49
8:G:221:ASP:OD2	8:G:222:LYS:N	2.45	0.49
3:B:48:LEU:HD11	3:B:214:PHE:CE2	2.48	0.49
13:L:152:LEU:CD2	13:L:194:VAL:HG21	2.43	0.49
5:R:153:ASP:OD1	5:R:155:SER:N	2.44	0.49
11:X:14:ILE:HD13	11:X:180:ILE:HG23	1.94	0.49
15:b:43:MET:N	15:b:46:TYR:O	2.45	0.49
4:C:41:ILE:HD11	4:C:140:ALA:HB1	1.95	0.49
15:N:168:GLU:CD	15:N:168:GLU:H	2.21	0.49
8:G:89:ASP:OD2	15:N:86:ARG:NH1	2.45	0.48
9:H:8:THR:HG22	9:H:8:THR:O	2.13	0.48
3:P:40:LEU:C	3:P:40:LEU:HD23	2.38	0.48
5:R:112:HIS:NE2	5:R:116:LEU:HD11	2.28	0.48
8:G:23:GLY:HA3	8:G:148:ILE:HD13	1.95	0.48
5:D:94:ILE:HD12	12:K:96:LEU:HD13	1.96	0.48
5:D:185:VAL:HG12	5:D:189:SER:OG	2.13	0.48
12:Y:101:ASN:OD1	12:Y:101:ASN:N	2.46	0.48
5:R:97:GLU:HG2	12:Y:92:LEU:HD21	1.95	0.48
7:T:91:LEU:HD22	7:T:102:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:96:TYR:CD2	9:V:100:ILE:HD12	2.48	0.48
15:b:33:ILE:HG21	15:b:121:ALA:HB1	1.96	0.48
14:M:109:VAL:HG22	14:M:114:PHE:CD2	2.49	0.48
5:R:173:ILE:HD11	5:R:201:VAL:HG11	1.96	0.48
9:V:157:MET:SD	9:V:180:VAL:HG11	2.54	0.48
5:R:21:VAL:O	5:R:25:MET:HE2	2.14	0.48
15:b:22:THR:N	15:b:148:SER:HG	2.11	0.48
15:b:79:TYR:HD2	15:b:107:ILE:HD11	1.78	0.48
8:G:181:ASP:OD1	8:G:182:GLU:N	2.44	0.48
3:P:157:ASP:OD2	3:P:157:ASP:N	2.45	0.48
5:R:37:ILE:CG1	5:R:194:ILE:HD12	2.44	0.48
4:C:86:GLU:HG3	4:C:114:TYR:CZ	2.48	0.47
7:F:91:LEU:HD21	7:F:110:GLN:HG3	1.96	0.47
10:I:13:LEU:HD23	10:I:24:LEU:HD11	1.97	0.47
14:a:12:SER:HB3	14:a:107:VAL:HG11	1.96	0.47
5:D:182:ASP:O	5:D:185:VAL:HG23	2.15	0.47
2:A:97:ASP:OD1	9:H:63:ARG:NE	2.40	0.47
8:G:215:VAL:HG22	8:G:216:LEU:N	2.29	0.47
15:N:33:ILE:HG21	15:N:121:ALA:HB1	1.96	0.47
12:Y:195:THR:HB	12:Y:202:GLY:HA2	1.97	0.47
14:M:77:MET:HE1	14:M:85:LEU:HD22	1.97	0.47
5:R:115:ASP:OD2	5:R:115:ASP:C	2.58	0.47
13:L:140:LEU:HD11	13:L:194:VAL:CG1	2.45	0.47
3:P:124:ILE:HD11	3:P:152:PHE:CD2	2.50	0.47
11:X:98:ASN:OD1	11:X:98:ASN:O	2.32	0.47
13:Z:103:SER:OG	13:Z:195:THR:HG21	2.15	0.47
10:I:123:SER:HB3	10:I:137:VAL:HG21	1.96	0.47
10:W:21:VAL:HG13	10:W:190:ILE:HB	1.96	0.47
13:Z:139:LEU:HD12	13:Z:282:ILE:HD11	1.96	0.47
15:N:117:GLY:C	15:N:118:LEU:HD12	2.40	0.46
13:L:296:GLN:HG2	9:V:169:MET:HE1	1.97	0.46
9:V:112:THR:OG1	9:V:115:HIS:NE2	2.45	0.46
5:D:115:ASP:OD1	5:D:115:ASP:C	2.59	0.46
12:K:68:VAL:HG22	12:K:72:LEU:O	2.16	0.46
12:K:181:GLU:HA	12:K:181:GLU:OE2	2.15	0.46
11:X:152:GLU:OE1	11:X:152:GLU:N	2.45	0.46
12:Y:51:ALA:CB	12:Y:62:VAL:HG21	2.46	0.46
12:Y:216:GLU:OE1	12:Y:218:LEU:HD21	2.15	0.46
3:B:73:MET:HE2	3:B:73:MET:CA	2.45	0.46
7:F:83:ILE:HG22	7:F:87:LEU:HD12	1.96	0.46
7:F:108:ARG:NH1	8:G:57:GLU:OE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:59:GLN:O	8:U:59:GLN:HG3	2.16	0.46
13:Z:275:ASP:O	13:Z:294:LEU:N	2.39	0.46
9:H:79:LEU:HD23	9:H:79:LEU:H	1.81	0.46
3:P:18:ALA:O	3:P:22:VAL:HG23	2.16	0.46
13:Z:142:ILE:CD1	13:Z:194:VAL:HG22	2.45	0.46
5:R:191:LEU:O	5:R:194:ILE:HG22	2.15	0.46
15:b:84:VAL:HG11	15:b:100:ALA:HB2	1.98	0.46
2:O:97:ASP:OD1	9:V:63:ARG:NH2	2.48	0.46
4:Q:13:ASP:OD2	4:Q:13:ASP:C	2.58	0.46
7:F:37:ASN:OD1	7:F:38:LYS:N	2.49	0.46
4:Q:56:ASP:O	4:Q:56:ASP:OD2	2.34	0.46
13:Z:164:GLU:OE1	13:Z:164:GLU:O	2.33	0.46
3:P:96:ILE:HD11	3:P:125:TYR:HB2	1.97	0.46
11:J:79:VAL:O	11:J:83:VAL:HG23	2.16	0.45
7:T:108:ARG:NH1	8:U:57:GLU:OE2	2.48	0.45
4:C:49:THR:HG22	4:C:194:LYS:O	2.16	0.45
5:R:37:ILE:HG12	5:R:194:ILE:HD12	1.98	0.45
5:D:21:VAL:O	5:D:25:MET:HG2	2.17	0.45
5:D:75:PHE:CG	5:D:82:VAL:HG21	2.51	0.45
5:D:191:LEU:HA	5:D:194:ILE:HG22	1.98	0.45
15:N:40:ARG:NH1	15:N:186:ASN:O	2.46	0.45
6:S:11:ILE:O	6:S:12:ILE:HG23	2.16	0.45
14:a:10:VAL:HG23	14:a:53:SER:HB3	1.98	0.45
14:M:10:VAL:HG23	14:M:53:SER:HB3	1.99	0.45
3:P:40:LEU:HD21	3:P:42:ILE:CD1	2.45	0.45
14:a:66:LEU:HD21	14:a:86:VAL:HG22	1.97	0.45
14:M:110:ASP:OD2	14:M:110:ASP:C	2.59	0.45
9:V:178:ILE:O	9:V:194:TYR:N	2.48	0.45
10:W:54:PHE:CE1	10:W:108:VAL:HG13	2.52	0.45
11:X:44:PHE:HB2	11:X:103:VAL:HG22	1.99	0.45
13:Z:142:ILE:HD13	13:Z:194:VAL:HG22	1.99	0.45
15:b:210:ASP:OD1	15:b:211:LYS:N	2.49	0.45
11:J:98:ASN:OD1	11:J:98:ASN:O	2.35	0.45
2:O:38:VAL:HG23	2:O:140:MET:HE3	1.98	0.45
5:D:39:THR:HG23	5:D:183:PRO:O	2.17	0.45
3:P:77:LYS:NZ	10:W:78:ASP:OD1	2.40	0.45
6:S:167:CYS:SG	6:S:197:ALA:HB2	2.57	0.45
7:T:47:LYS:NZ	7:T:59:ASN:O	2.41	0.45
13:Z:140:LEU:HD11	13:Z:194:VAL:HG11	1.98	0.45
5:R:153:ASP:OD1	5:R:153:ASP:C	2.60	0.45
3:B:108:GLN:NE2	4:C:79:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:66:LEU:HD21	14:M:86:VAL:HG22	1.98	0.45
10:W:138:THR:HG21	10:W:146:LEU:HB3	1.99	0.45
12:K:138:ASP:N	12:K:138:ASP:OD1	2.50	0.45
5:D:73:LEU:HD13	5:D:140:ILE:HG13	1.99	0.44
11:J:11:ASP:N	11:J:11:ASP:OD1	2.50	0.44
8:U:181:ASP:OD1	8:U:182:GLU:N	2.47	0.44
5:D:112:HIS:NE2	5:D:116:LEU:HD11	2.32	0.44
5:D:173:ILE:HD11	5:D:201:VAL:HG11	1.98	0.44
10:I:24:LEU:HB3	10:I:187:CYS:HA	1.99	0.44
14:M:132:CYS:O	14:M:137:ASN:ND2	2.48	0.44
2:O:37:CYS:SG	2:O:182:CYS:CB	3.05	0.44
10:W:123:SER:CB	10:W:137:VAL:HG21	2.48	0.44
15:N:199:ARG:NH1	15:N:199:ARG:HB2	2.33	0.44
14:a:46:SER:O	14:a:47:ASN:CG	2.61	0.44
7:F:87:LEU:HD11	7:F:111:ILE:CD1	2.48	0.44
9:H:11:GLY:O	9:H:131:THR:N	2.47	0.44
4:Q:13:ASP:OD2	4:Q:13:ASP:O	2.35	0.44
9:V:181:CYS:SG	9:V:190:MET:HE3	2.57	0.44
11:J:114:TYR:CD1	11:J:122:LEU:HD11	2.53	0.44
10:W:183:MET:SD	10:W:205:ASP:N	2.91	0.44
10:W:191:ASN:HB2	10:W:192:PRO:HD2	1.98	0.44
4:C:43:LEU:HD13	4:C:43:LEU:C	2.42	0.44
7:F:179:MET:HE3	7:F:184:LEU:HD23	1.99	0.44
9:H:27:THR:HG21	9:H:173:TYR:HD1	1.83	0.44
15:b:102:MET:O	15:b:106:ASP:OD1	2.35	0.44
13:L:171:ILE:HD11	13:L:196:LEU:HG	1.99	0.44
10:I:116:ASP:O	10:I:117:LYS:HB2	2.17	0.44
15:N:80:ILE:HD11	15:N:107:ILE:HD12	1.99	0.44
15:N:102:MET:O	15:N:106:ASP:OD1	2.36	0.44
5:D:225:THR:HG22	5:D:226:PRO:HD2	2.00	0.44
3:B:109:LEU:HD13	3:B:109:LEU:C	2.43	0.43
15:b:40:ARG:NH1	15:b:186:ASN:O	2.45	0.43
5:D:37:ILE:HG12	5:D:194:ILE:HD12	2.00	0.43
9:H:82:VAL:HG23	9:H:110:ASP:OD2	2.18	0.43
3:P:225:GLU:OE1	3:P:228:LYS:NZ	2.48	0.43
9:H:96:TYR:CD2	9:H:100:ILE:HD12	2.52	0.43
8:U:23:GLY:HA3	8:U:148:ILE:HD13	1.99	0.43
11:X:122:LEU:C	11:X:122:LEU:HD23	2.43	0.43
2:A:37:CYS:SG	2:A:182:CYS:CB	3.06	0.43
13:L:103:SER:OG	13:L:195:THR:HG21	2.18	0.43
15:N:79:TYR:HD2	15:N:107:ILE:HD11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:160:ASP:N	10:W:160:ASP:OD2	2.51	0.43
3:B:124:ILE:CG2	3:B:135:LEU:HD11	2.49	0.43
6:E:11:ILE:O	6:E:12:ILE:HG23	2.19	0.43
7:F:41:LEU:O	7:F:211:MET:N	2.48	0.43
8:G:25:GLU:OE2	8:G:25:GLU:HA	2.19	0.43
15:N:76:ILE:HG13	15:N:114:MET:HE1	1.99	0.43
6:S:210:ASP:OD1	6:S:222:GLN:NE2	2.51	0.43
7:T:42:ILE:HG22	7:T:210:ILE:HG22	2.00	0.43
14:a:43:ARG:HA	14:a:49:LEU:HD23	2.00	0.43
4:C:210:VAL:HG12	4:C:211:GLU:N	2.33	0.43
9:H:86:VAL:HG21	9:H:117:TYR:CG	2.53	0.43
10:I:79:ASN:O	10:I:80:ASN:HB2	2.19	0.43
8:U:9:ASN:H	8:U:122:THR:HG22	1.84	0.43
8:U:66:TYR:O	8:U:67:PRO:C	2.62	0.43
3:B:58:ASN:OD1	3:B:58:ASN:C	2.61	0.43
6:S:212:TRP:NE1	6:S:222:GLN:OE1	2.52	0.43
8:G:9:ASN:H	8:G:122:THR:HG22	1.84	0.43
13:L:141:THR:HG22	13:L:195:THR:HB	2.01	0.43
15:N:199:ARG:HB2	15:N:199:ARG:HH11	1.84	0.43
2:O:82:ARG:NH1	8:U:113:ASP:OD1	2.52	0.43
9:H:196:LYS:HG3	9:H:196:LYS:O	2.19	0.43
3:P:214:PHE:C	3:P:214:PHE:CD1	2.97	0.43
6:S:93:VAL:HG21	13:Z:161:GLN:CD	2.44	0.43
11:X:54:PHE:CD1	11:X:54:PHE:C	2.96	0.43
13:Z:145:PHE:N	13:Z:191:TYR:O	2.47	0.43
2:A:9:LEU:HD13	8:G:10:ILE:CG2	2.49	0.43
8:U:215:VAL:HG22	8:U:216:LEU:N	2.34	0.43
13:Z:171:ILE:HD11	13:Z:196:LEU:HG	2.00	0.43
3:B:157:ASP:OD1	3:B:157:ASP:N	2.51	0.42
11:J:23:ASN:OD1	11:J:26:LEU:N	2.46	0.42
5:R:16:GLY:O	5:R:17:ARG:C	2.62	0.42
7:T:103:SER:O	7:T:107:VAL:HG23	2.19	0.42
9:V:168:ILE:HG23	9:V:175:GLY:O	2.19	0.42
15:b:123:TYR:OH	15:b:199:ARG:NH1	2.51	0.42
2:A:16:GLY:O	3:B:21:ASN:ND2	2.52	0.42
15:N:43:MET:HE3	15:N:48:SER:HB3	2.01	0.42
5:R:108:ARG:NH2	13:Z:167:ASN:OD1	2.52	0.42
9:V:154:GLU:HA	9:V:154:GLU:OE1	2.19	0.42
11:X:61:ASN:O	11:X:65:VAL:HG23	2.19	0.42
13:L:112:ILE:HG23	13:L:280:TRP:HB2	2.00	0.42
13:L:143:THR:O	13:L:192:SER:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:156:CYS:SG	5:R:55:LEU:HD22	2.59	0.42
12:Y:68:VAL:HG22	12:Y:72:LEU:O	2.20	0.42
14:M:19:VAL:HG11	14:M:107:VAL:HB	2.02	0.42
3:P:38:ILE:HD11	3:P:174:MET:HG3	2.02	0.42
15:b:79:TYR:CD2	15:b:107:ILE:HD11	2.54	0.42
12:K:107:VAL:HG23	12:K:136:ASP:OD1	2.19	0.42
3:P:112:GLN:NE2	4:Q:125:ARG:O	2.52	0.42
12:K:223:VAL:HG23	12:K:224:ASP:OD1	2.19	0.42
13:L:105:ARG:HB3	13:L:206:VAL:HG23	2.02	0.42
14:M:43:ARG:HG3	14:M:189:VAL:HG11	2.02	0.42
8:U:225:GLU:OE1	8:U:225:GLU:C	2.61	0.42
10:W:63:MET:HE2	10:W:66:LYS:HE3	2.01	0.42
12:Y:39:PHE:CE1	12:Y:44:VAL:HG23	2.54	0.42
15:N:91:ASP:OD1	15:N:99:LYS:NZ	2.53	0.42
4:C:132:ILE:HD11	4:C:159:VAL:HG21	2.01	0.42
13:L:102:VAL:HG23	13:L:222:CYS:SG	2.59	0.42
14:M:110:ASP:O	14:M:111:ASP:C	2.62	0.42
11:X:26:LEU:HD21	12:Y:167:TYR:CE2	2.54	0.42
6:E:167:CYS:SG	6:E:197:ALA:HB2	2.60	0.42
8:U:38:ASN:OD1	8:U:41:MET:N	2.46	0.42
1:3:100:ILE:CD1	12:Y:51:ALA:HB1	2.50	0.42
1:3:100:ILE:HD11	12:Y:51:ALA:HB1	2.02	0.42
4:C:120:LEU:HD22	5:D:130:PHE:CD1	2.55	0.42
12:K:51:ALA:HB3	12:K:59:SER:HB3	2.01	0.42
12:K:69:ASN:OD1	12:K:71:HIS:N	2.43	0.42
13:L:96:ASP:OD2	13:L:191:TYR:OH	2.23	0.42
3:P:124:ILE:CG2	3:P:135:LEU:HD11	2.50	0.42
5:R:153:ASP:HB2	5:R:154:PRO:HD2	2.01	0.41
5:D:97:GLU:HG2	12:K:92:LEU:HD21	2.02	0.41
6:E:17:GLY:O	7:F:25:ALA:HB2	2.20	0.41
6:E:183:LYS:HG2	6:E:184:GLU:N	2.35	0.41
9:H:8:THR:O	9:H:164:ILE:HD13	2.20	0.41
12:K:181:GLU:OE2	12:K:181:GLU:CA	2.68	0.41
15:N:48:SER:O	14:a:171:ARG:NH1	2.52	0.41
3:P:16:GLU:OE1	3:P:16:GLU:HA	2.20	0.41
12:K:34:THR:HG22	12:K:47:VAL:HG12	2.01	0.41
13:L:139:LEU:HD21	13:L:287:MET:HE1	2.01	0.41
3:P:28:ILE:HD12	3:P:124:ILE:HD12	2.03	0.41
6:S:183:LYS:HG2	6:S:184:GLU:N	2.35	0.41
10:W:123:SER:HB2	10:W:137:VAL:HG21	2.02	0.41
2:A:3:LEU:HD21	8:G:7:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:82:ASP:OD2	12:K:126:LEU:HD12	2.20	0.41
15:N:152:TYR:HA	15:b:151:ALA:O	2.20	0.41
3:P:42:ILE:HD12	3:P:199:TYR:CE1	2.56	0.41
3:P:63:VAL:HA	3:P:124:ILE:O	2.20	0.41
8:U:149:SER:O	8:U:150:ALA:HB3	2.21	0.41
3:B:63:VAL:HG12	3:B:125:TYR:CD1	2.55	0.41
9:H:178:ILE:O	9:H:194:TYR:N	2.54	0.41
4:Q:72:THR:HG23	4:Q:132:ILE:HB	2.03	0.41
11:X:117:ASP:OD1	11:X:117:ASP:C	2.64	0.41
13:Z:218:VAL:HG21	13:Z:221:VAL:HB	2.02	0.41
6:E:43:PHE:HA	6:E:141:ILE:HG13	2.02	0.41
4:Q:153:GLU:OE1	4:Q:154:TYR:N	2.54	0.41
11:X:69:ILE:HG23	11:X:70:GLN:N	2.35	0.41
4:C:32:VAL:HG22	4:C:45:ILE:HG23	2.02	0.41
14:M:61:PHE:O	14:M:65:GLU:HG2	2.19	0.41
9:V:82:VAL:HG23	9:V:110:ASP:OD2	2.21	0.41
15:b:102:MET:HE2	15:b:138:MET:CE	2.51	0.41
5:D:37:ILE:HD11	5:D:177:LEU:HD21	2.02	0.41
6:E:222:GLN:OE1	6:E:223:ILE:N	2.54	0.41
7:F:108:ARG:O	7:F:112:VAL:HG23	2.21	0.41
4:Q:43:LEU:CD1	4:Q:45:ILE:HD11	2.50	0.41
4:Q:56:ASP:OD2	4:Q:56:ASP:C	2.64	0.41
5:R:75:PHE:CD2	5:R:82:VAL:HG21	2.55	0.41
8:U:159:MET:HE3	8:U:168:TYR:HA	2.03	0.41
12:Y:128:LEU:C	12:Y:128:LEU:HD23	2.46	0.41
7:F:4:LEU:HD22	8:G:7:ILE:HD11	2.02	0.41
7:F:42:ILE:HG22	7:F:210:ILE:HG22	2.02	0.41
8:G:73:PHE:HB2	8:G:80:VAL:HG13	2.03	0.41
9:H:210:ARG:HA	10:I:165:THR:HG21	2.01	0.41
3:P:40:LEU:HD23	3:P:41:GLY:N	2.36	0.41
3:P:197:LYS:HG3	3:P:214:PHE:CD2	2.56	0.41
7:T:87:LEU:HD11	7:T:111:ILE:CD1	2.51	0.41
9:V:43:ILE:HD13	9:V:85:CYS:SG	2.61	0.41
12:Y:107:VAL:HG23	12:Y:136:ASP:OD1	2.21	0.41
6:E:166:SER:O	6:E:169:THR:HG22	2.20	0.41
6:S:183:LYS:O	6:S:187:VAL:HG23	2.21	0.41
9:V:151:MET:HE3	9:V:151:MET:HB2	1.99	0.41
11:X:2:GLU:OE2	11:X:34:LYS:NZ	2.40	0.41
3:B:40:LEU:C	3:B:40:LEU:HD23	2.46	0.40
5:D:82:VAL:O	5:D:86:VAL:HG23	2.21	0.40
5:D:144:ASP:C	5:D:145:THR:HG23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:15:ARG:HB3	4:Q:15:ARG:NH1	2.36	0.40
8:U:31:LEU:C	8:U:31:LEU:HD12	2.46	0.40
1:3:84:ASP:OD1	1:3:84:ASP:O	2.39	0.40
1:3:84:ASP:OD1	12:Y:32:THR:N	2.55	0.40
2:A:112:PHE:O	2:A:116:ILE:HG12	2.21	0.40
2:A:65:GLN:NE2	2:A:209:PHE:O	2.54	0.40
3:B:63:VAL:HA	3:B:124:ILE:O	2.21	0.40
3:B:112:GLN:NE2	4:C:125:ARG:O	2.54	0.40
6:E:43:PHE:CE1	6:E:186:LEU:HD12	2.57	0.40
6:E:183:LYS:O	6:E:187:VAL:HG23	2.20	0.40
13:L:99:GLY:HA3	13:L:224:GLY:HA3	2.04	0.40
14:M:184:VAL:HG23	14:M:189:VAL:HG22	2.03	0.40
6:S:116:ALA:O	6:S:120:THR:HG23	2.21	0.40
9:V:27:THR:HG21	9:V:173:TYR:HD1	1.86	0.40
13:Z:280:TRP:CZ2	13:Z:289:LYS:HE2	2.57	0.40
1:4:103:PRO:O	1:4:104:GLU:HG2	2.22	0.40
2:A:97:ASP:OD2	9:H:67:LYS:CE	2.69	0.40
3:B:7:THR:HG21	3:B:13:LEU:HD23	2.03	0.40
3:B:8:GLU:O	4:C:24:GLN:OE1	2.40	0.40
3:B:167:PHE:CE1	3:B:172:MET:HE3	2.56	0.40
5:D:57:ASN:O	5:D:57:ASN:OD1	2.39	0.40
5:D:204:ASP:OD1	5:D:204:ASP:N	2.54	0.40
6:E:68:SER:O	6:E:69:LYS:HG2	2.22	0.40
8:U:177:GLU:N	8:U:177:GLU:CD	2.79	0.40
10:W:12:LEU:HB2	10:W:109:ILE:HD12	2.02	0.40
9:H:23:ASP:OD2	9:H:23:ASP:O	2.39	0.40
12:K:205:VAL:N	12:K:221:PHE:O	2.51	0.40
8:U:36:LEU:HD23	8:U:157:GLY:HA3	2.03	0.40
9:V:128:VAL:HG21	9:V:131:THR:HG21	2.04	0.40
12:Y:51:ALA:HB2	12:Y:62:VAL:HG21	2.03	0.40
13:Z:105:ARG:HB3	13:Z:206:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	3	52/135 (38%)	51 (98%)	1 (2%)	50	78
1	4	1/135 (1%)	1 (100%)	0	100	100
6	S	102/209 (49%)	101 (99%)	1 (1%)	68	86
7	T	215/223 (96%)	215 (100%)	0	100	100
8	U	200/201 (100%)	195 (98%)	5 (2%)	42	73
9	V	182/190 (96%)	180 (99%)	2 (1%)	65	85
10	I	23/181 (13%)	23 (100%)	0	100	100
10	W	179/181 (99%)	178 (99%)	1 (1%)	78	91
11	X	177/177 (100%)	177 (100%)	0	100	100
12	Y	157/187 (84%)	155 (99%)	2 (1%)	61	83
13	Z	186/271 (69%)	185 (100%)	1 (0%)	81	92
14	a	195/195 (100%)	192 (98%)	3 (2%)	57	81
15	b	159/178 (89%)	159 (100%)	0	100	100
All	All	1828/2463 (74%)	1812 (99%)	16 (1%)	68	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	128	ASP
6	S	218	GLN
8	U	30	SER
8	U	58	VAL
8	U	66	TYR
8	U	92	HIS
8	U	137	ASP
9	V	77	ASN
9	V	125	SER
10	W	80	ASN
12	Y	48	ASP
12	Y	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	Z	275	ASP
14	a	16	LYS
14	a	181	ILE
14	a	201	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
6	S	131	GLN
7	T	98	ASN
7	T	178	ASN
7	T	226	GLN
10	W	7	HIS
11	X	190	ASN
12	Y	204	ASN
12	Y	217	HIS
13	Z	231	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

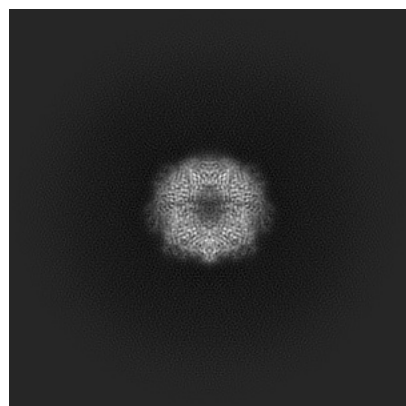
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15365. These allow visual inspection of the internal detail of the map and identification of artifacts.

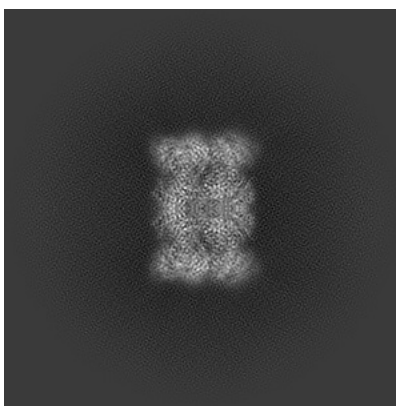
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

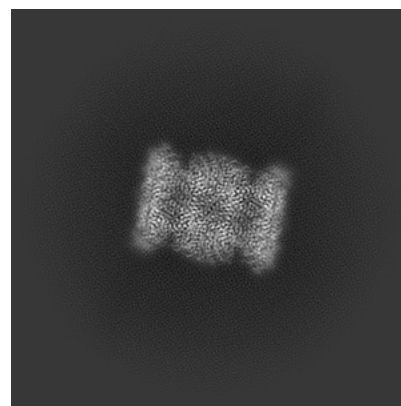
6.1.1 Primary map



X

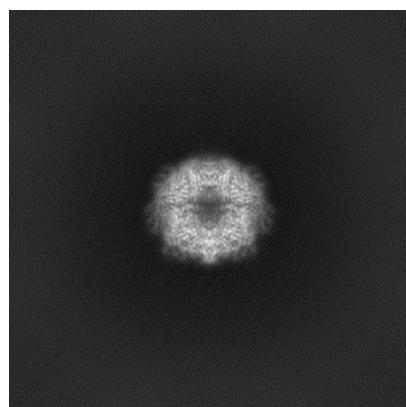


Y

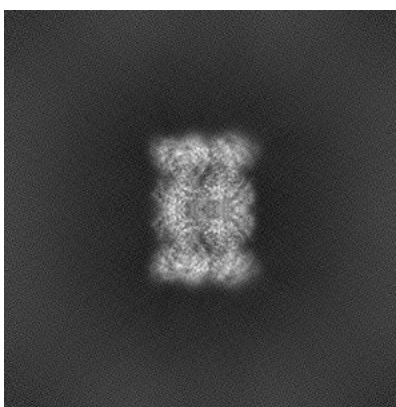


Z

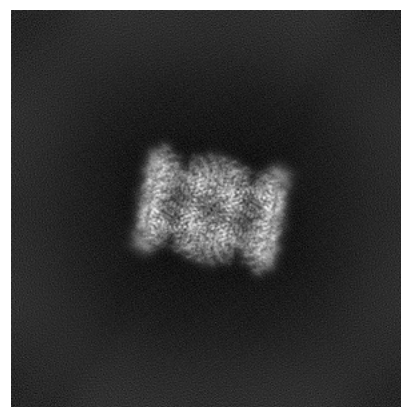
6.1.2 Raw map



X



Y

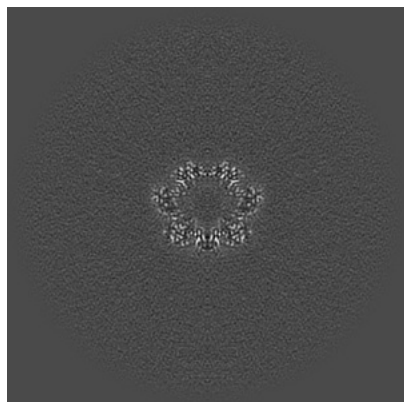


Z

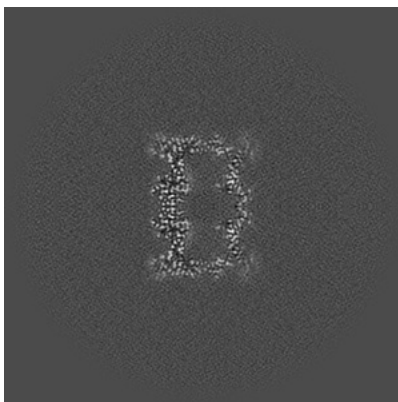
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

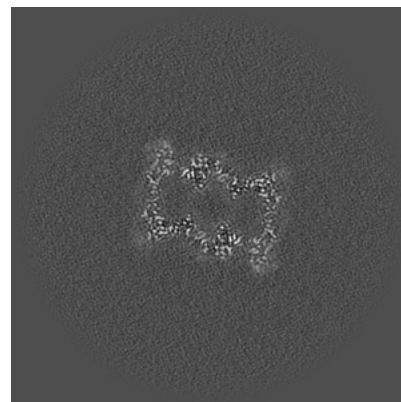
6.2.1 Primary map



X Index: 200

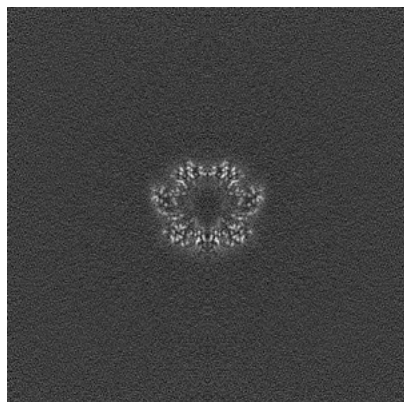


Y Index: 200

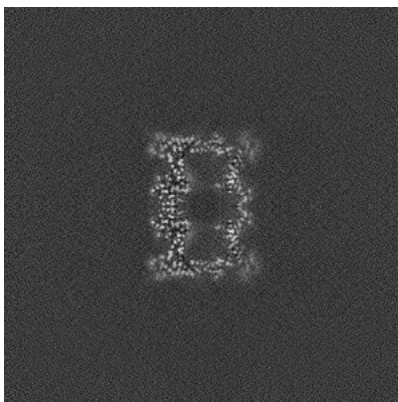


Z Index: 200

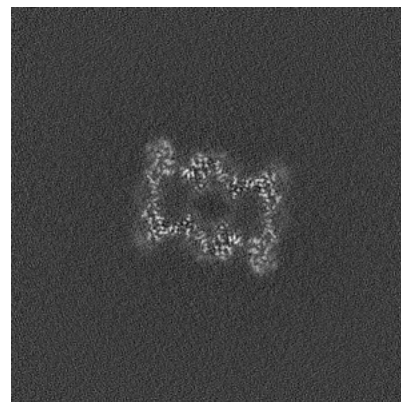
6.2.2 Raw map



X Index: 200



Y Index: 200

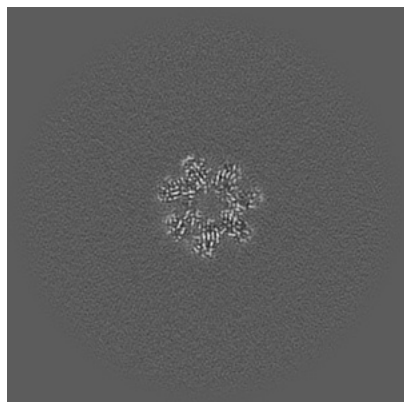


Z Index: 200

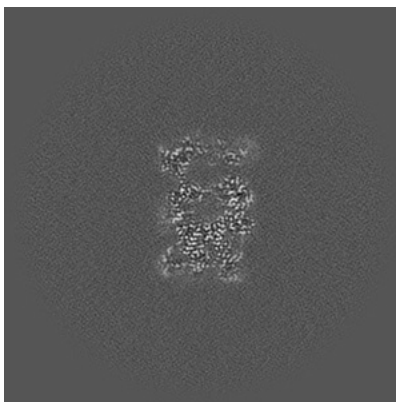
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

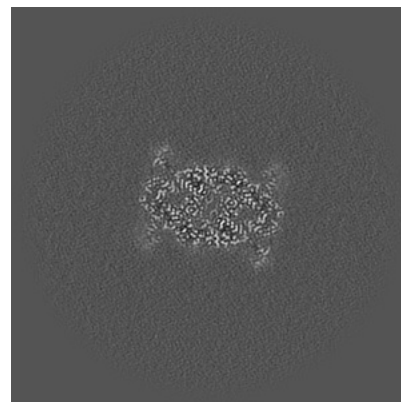
6.3.1 Primary map



X Index: 182

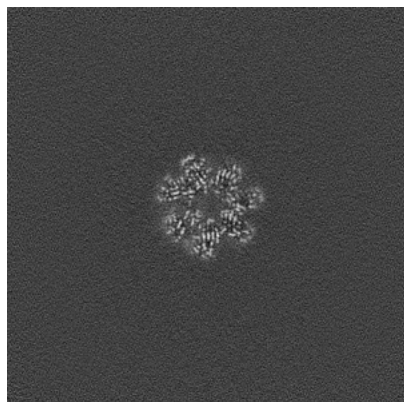


Y Index: 182

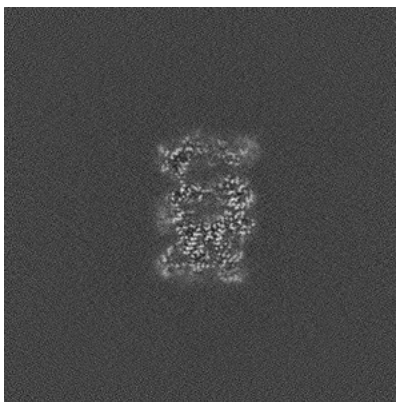


Z Index: 179

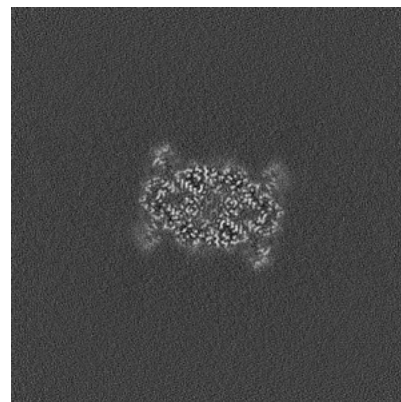
6.3.2 Raw map



X Index: 182



Y Index: 182

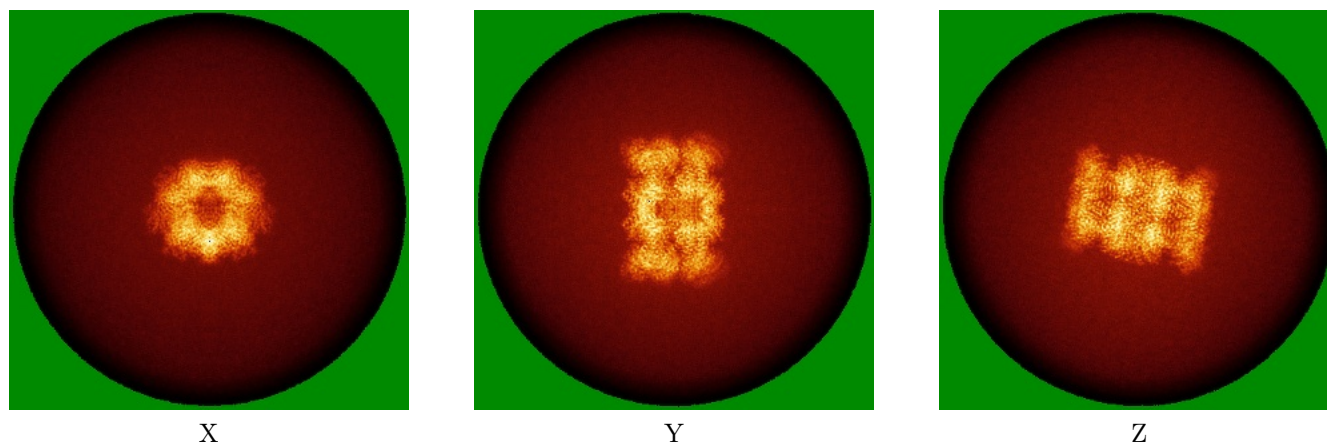


Z Index: 179

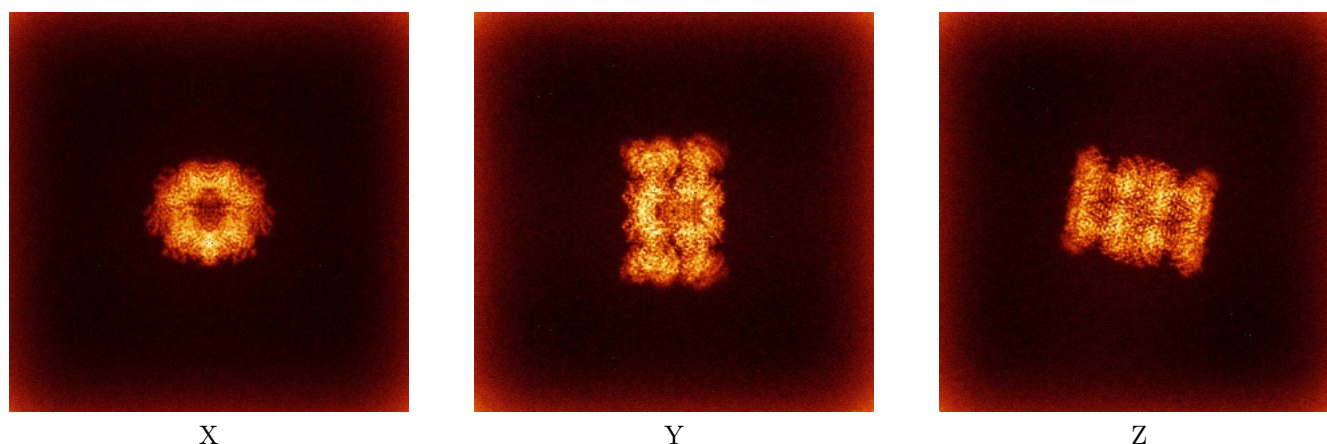
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

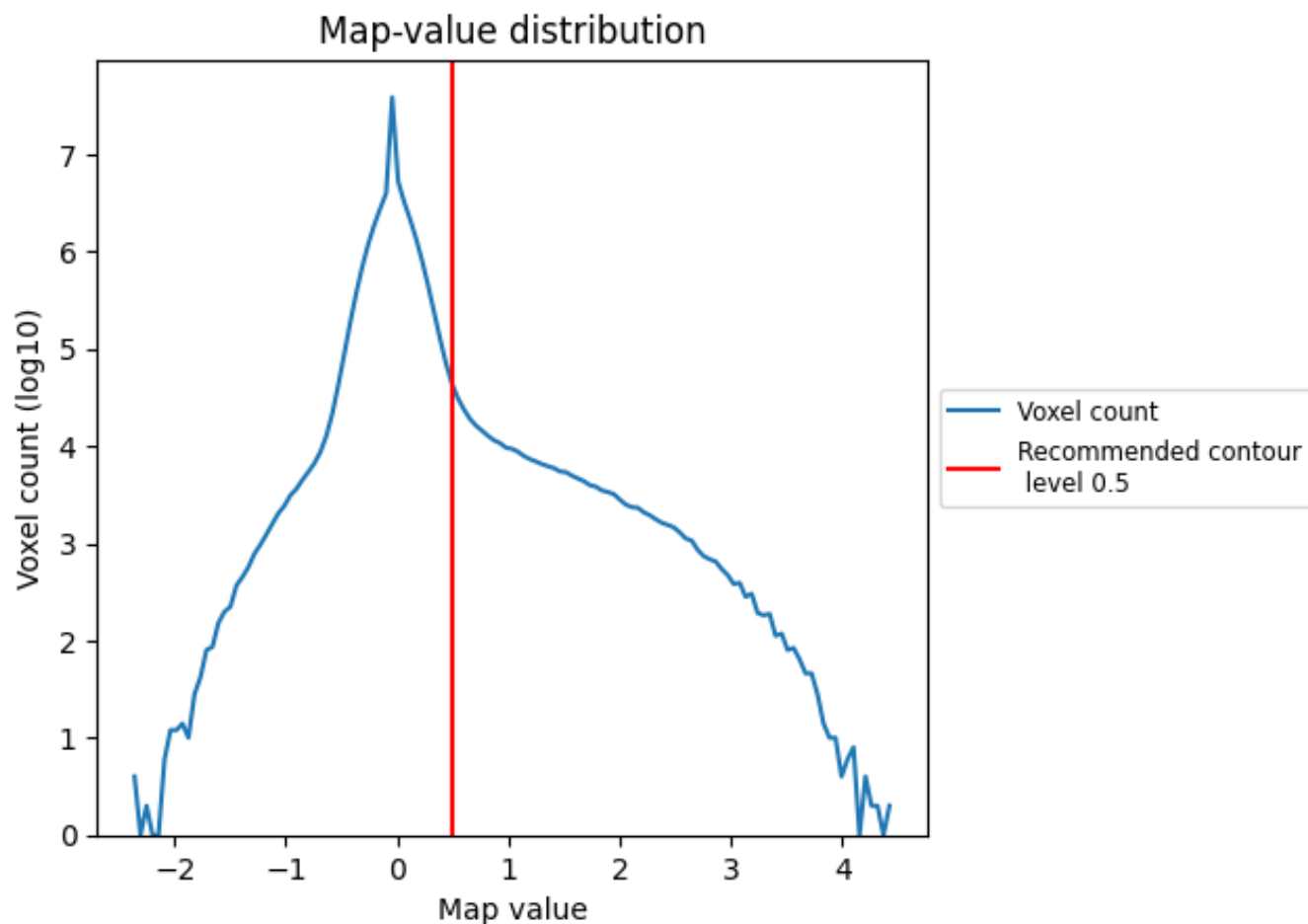
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

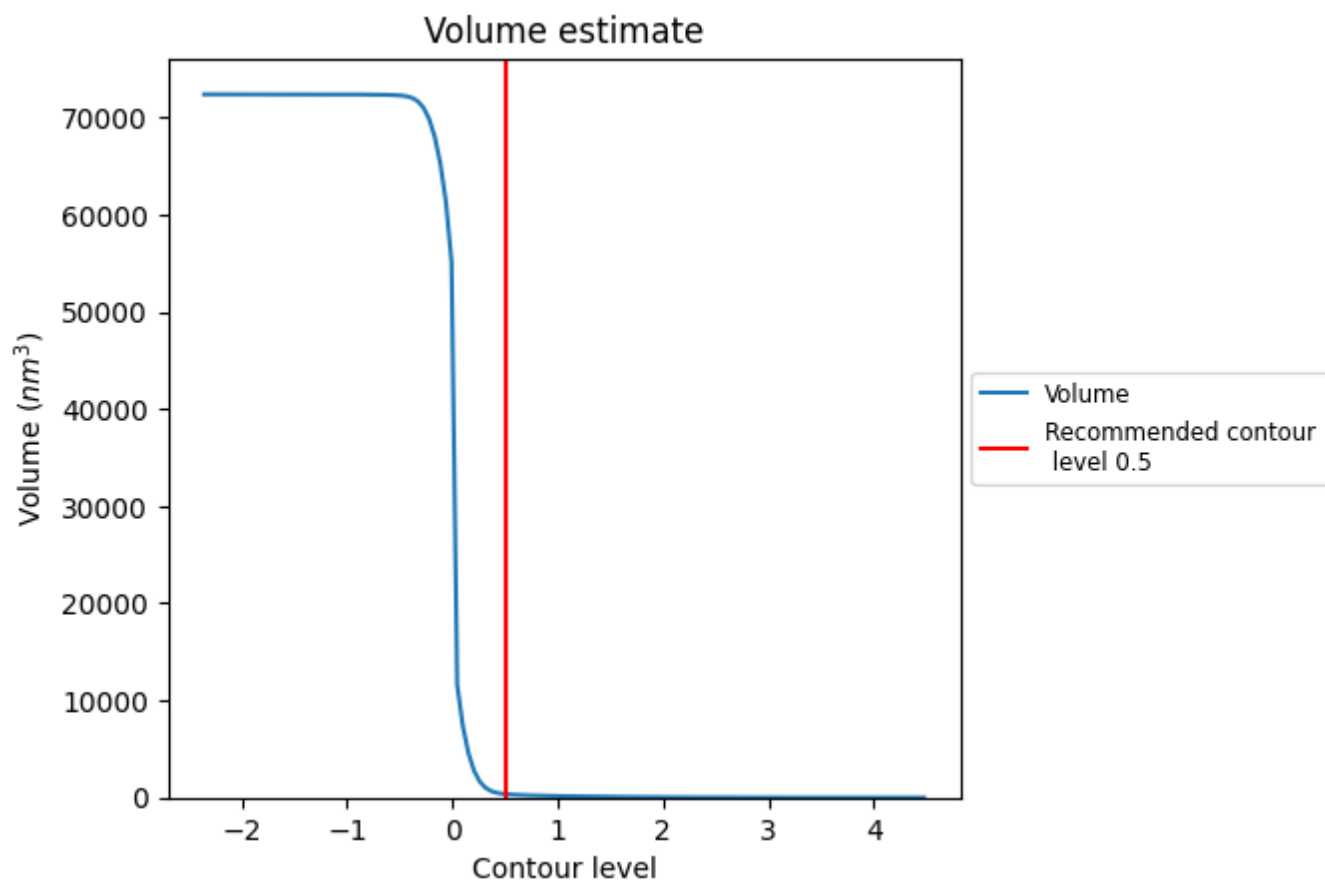
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

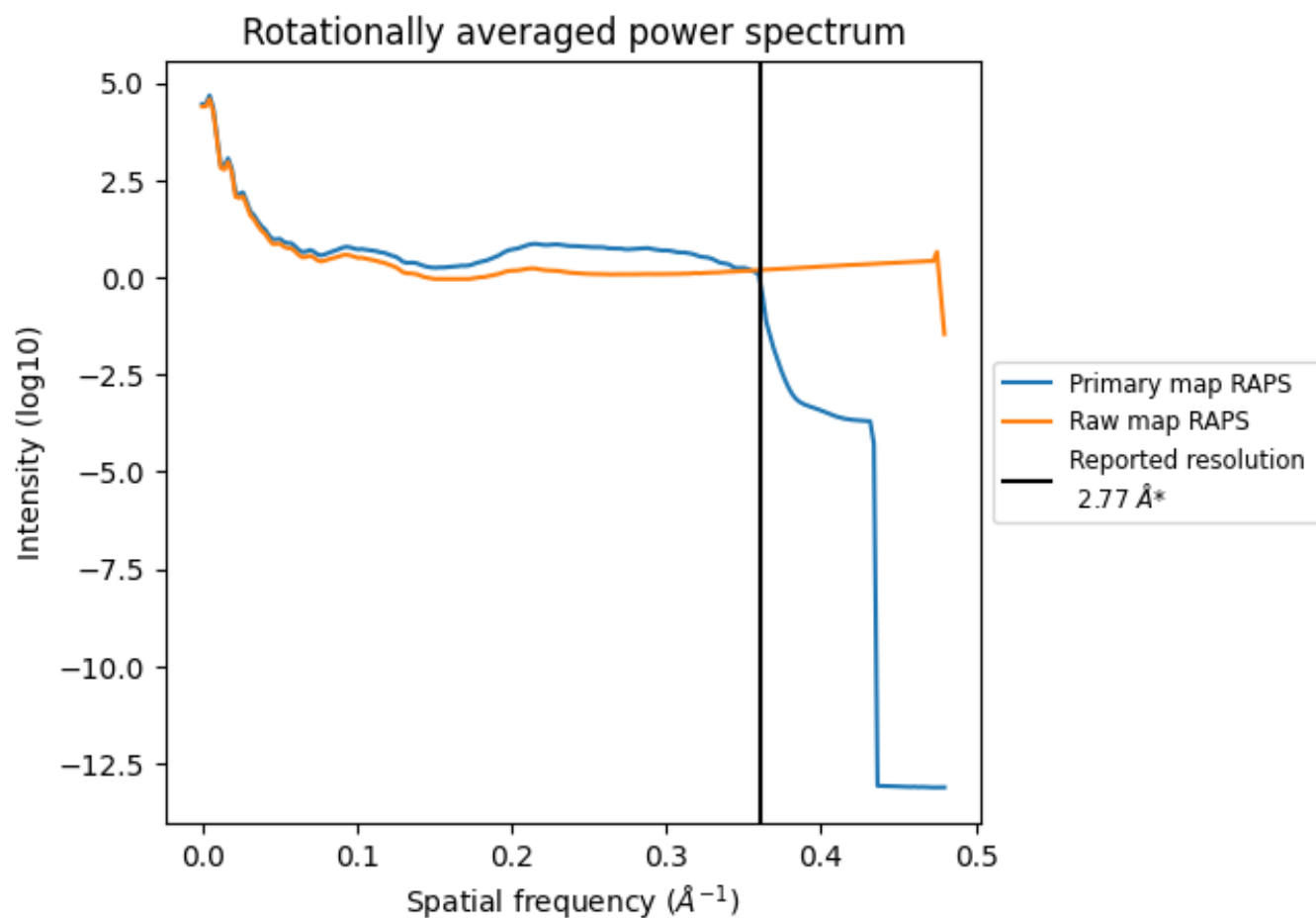
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 364 nm³; this corresponds to an approximate mass of 329 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 ⓘ

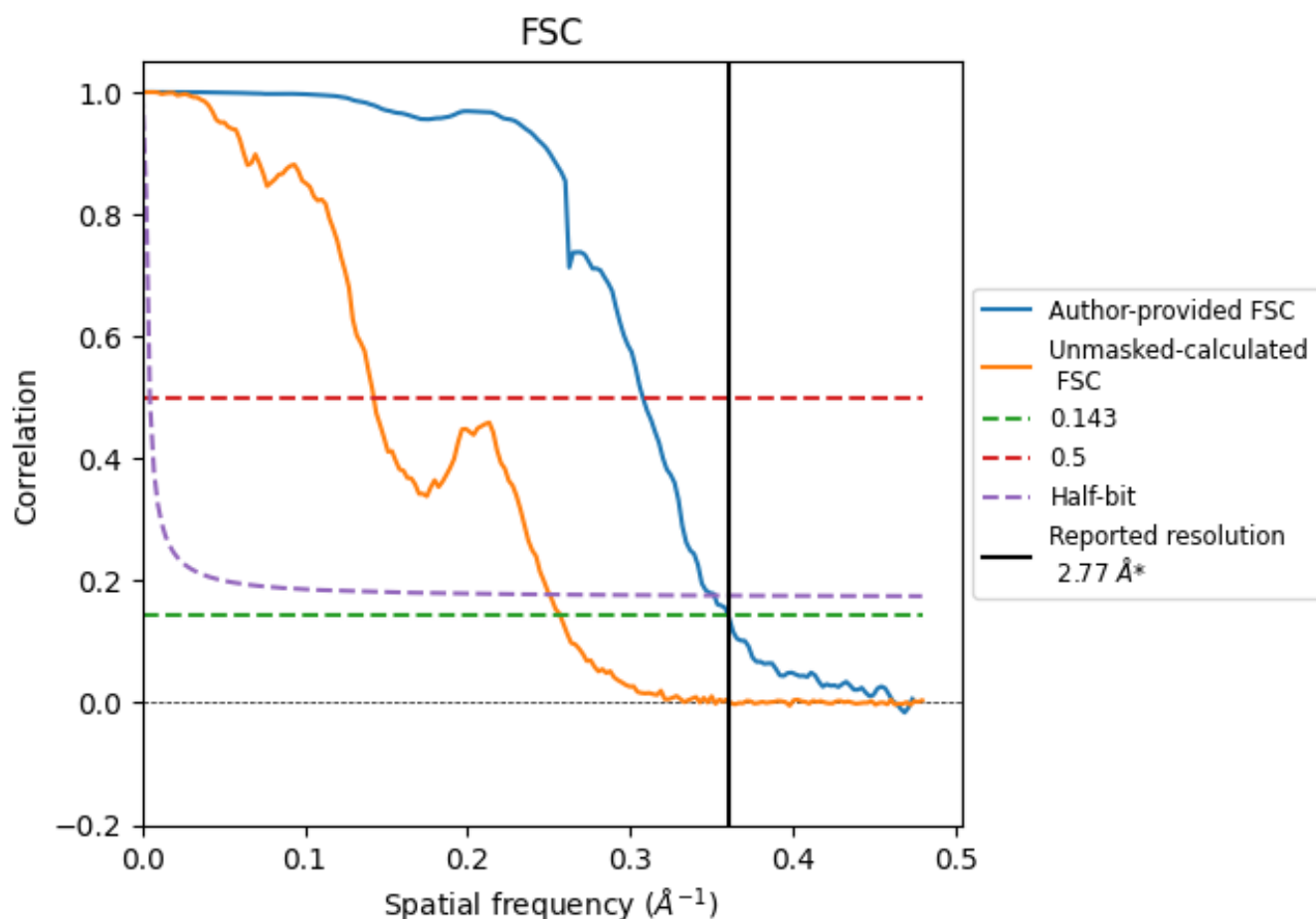


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.361 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.25	2.84
Unmasked-calculated*	3.89	7.03	3.99

*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 3.89 differs from the reported value 2.77 by more than 10 %

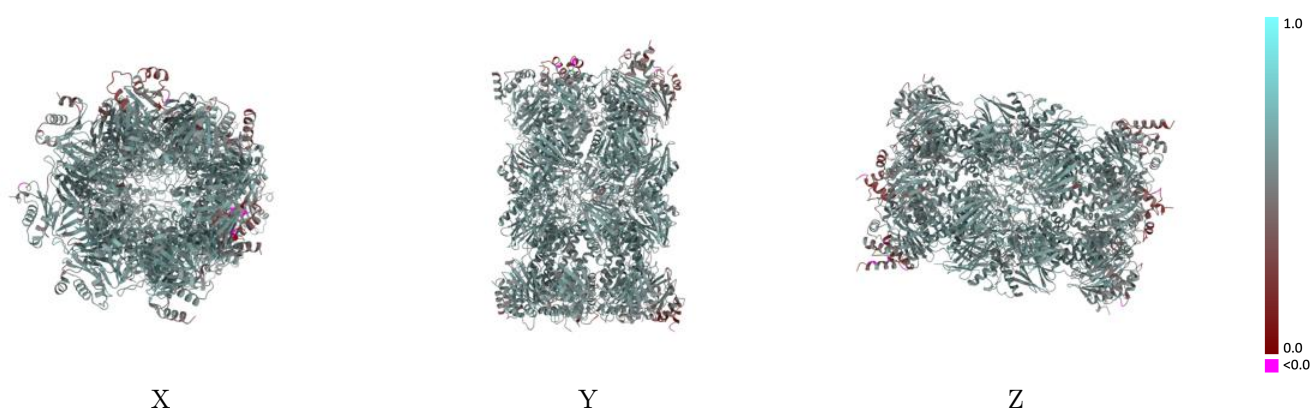
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-15365 and PDB model 8ADN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)

This section was not generated.

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

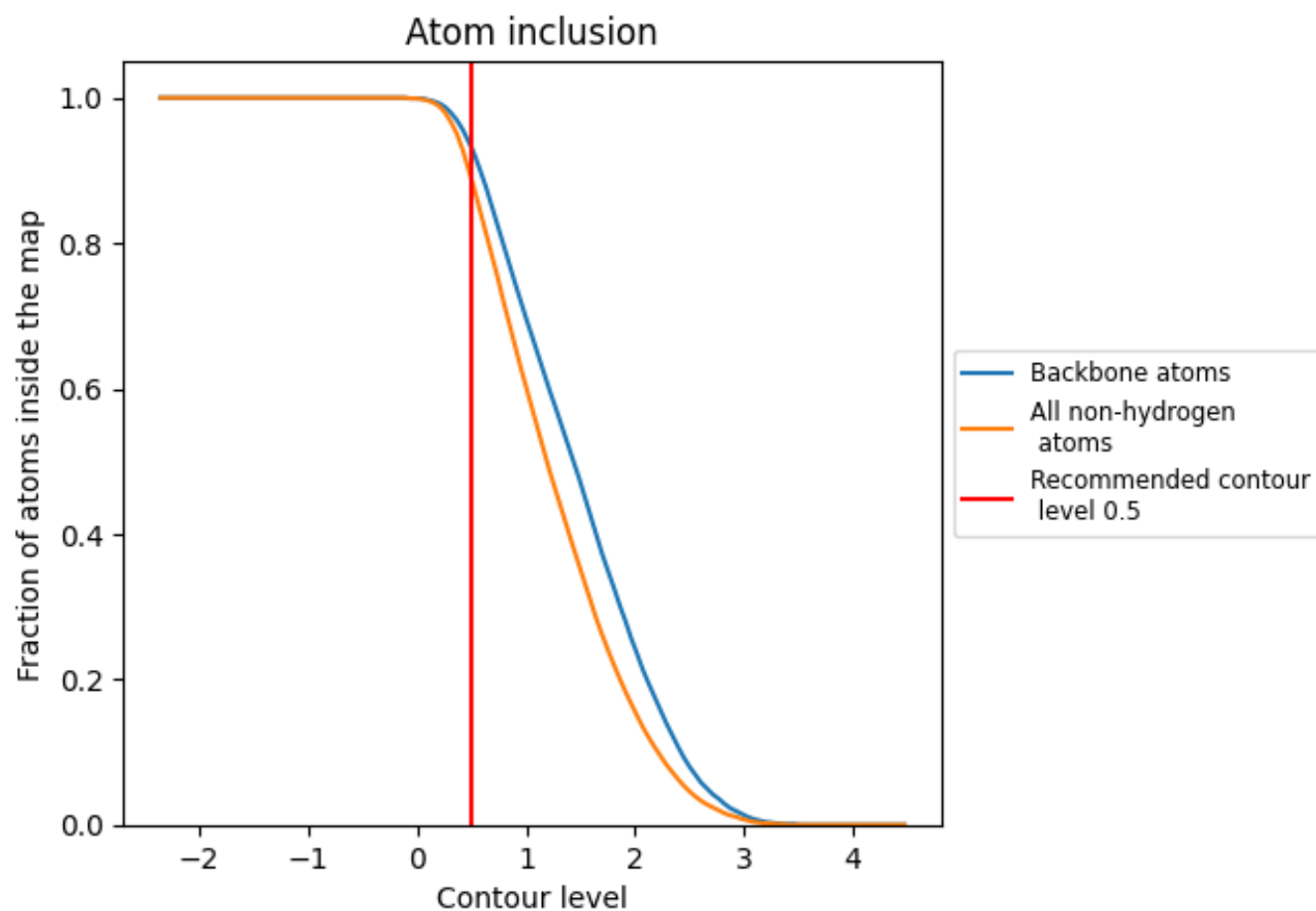


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.5660
3	 0.7120	 0.5340
4	 0.7160	 0.5310
A	 0.8370	 0.5280
B	 0.8560	 0.5340
C	 0.7940	 0.5180
D	 0.8390	 0.5430
E	 0.8830	 0.5510
F	 0.9030	 0.5700
G	 0.8870	 0.5670
H	 0.9190	 0.5890
I	 0.9430	 0.5970
J	 0.9310	 0.5950
K	 0.9360	 0.5910
L	 0.9110	 0.5820
M	 0.9240	 0.5880
N	 0.9300	 0.5920
O	 0.8440	 0.5320
P	 0.8480	 0.5350
Q	 0.7930	 0.5130
R	 0.8390	 0.5350
S	 0.8820	 0.5560
T	 0.8960	 0.5700
U	 0.8950	 0.5690
V	 0.9170	 0.5900
W	 0.9440	 0.5980
X	 0.9310	 0.5910
Y	 0.9360	 0.5930
Z	 0.9090	 0.5830
a	 0.9210	 0.5860
b	 0.9380	 0.5960

