



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 09:36 PM EST

PDB ID : 7KTR
EMDB ID : EMD-23027
Title : Cryo-EM structure of the human SAGA coactivator complex (TRRAP, core)
Authors : Herbst, D.A.; Esbin, M.N.; Nogales, E.
Deposited on : 2020-11-24
Resolution : 2.93 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:

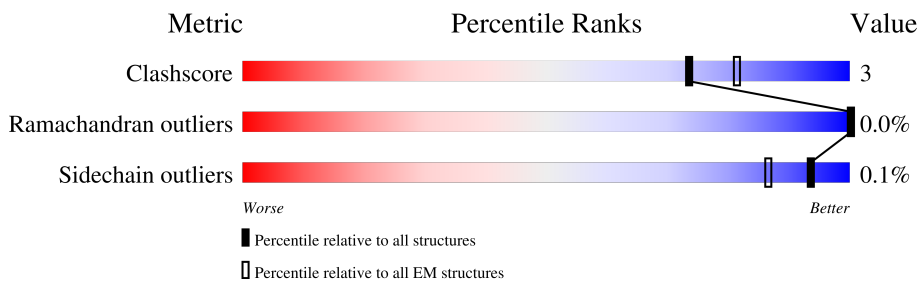
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.93 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.



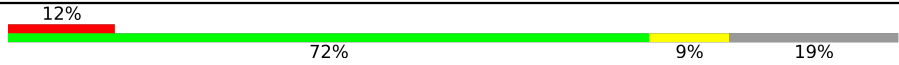
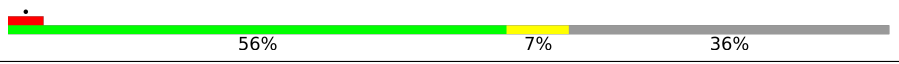
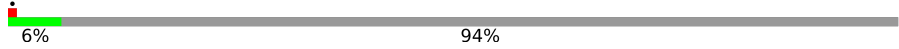
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	3195	
2	B	589	
3	C	811	
4	D	704	
5	E	251	
6	F	622	
7	G	161	
8	H	218	

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Mol	Chain	Length	Quality of chain
9	I	299	
10	J	335	
11	N	892	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 79406 atoms, of which 39069 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 Transformation/transcription domain-associated protein, Transformation/transcription domain-associated protein, Transformation/transcription domain-associated protein, Transformation/transcription domain-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	3042	45850	14890	22456	4097	4249	158	3	0

- Molecule 2 is a protein called TAF5-like RNA polymerase II p300/CBP-associated factor-associated factor 65 kDa subunit 5L.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	534	8338	2657	4113	727	819	22	0	0

- Molecule 3 is a protein called Isoform 3 of Transcription factor SPT20 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	407	6608	2066	3315	580	624	23	1	0

- Molecule 4 is a protein called STAGA complex 65 subunit gamma, DhaA, STAGA complex 65 subunit gamma, STAGA complex 65 subunit gamma, DhaA, STAGA complex 65 subunit gamma, STAGA complex 65 subunit gamma, DhaA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	219	3149	1045	1485	299	312	8	0	0

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 9B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	124	2013	635	1018	175	180	5	0	0

- Molecule 6 is a protein called TAF6-like RNA polymerase II p300/CBP-associated factor-

associated factor 65 kDa subunit 6L.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	130	2069	645	1030	188	200	6	0	0

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	103	1704	527	859	152	161	5	0	0

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	99	1566	501	782	128	151	4	0	0

- Molecule 9 is a protein called Transcription initiation protein SPT3 homolog, Transcription initiation protein SPT3 homolog, Transcription initiation protein SPT3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	243	3823	1207	1911	343	350	12	0	0

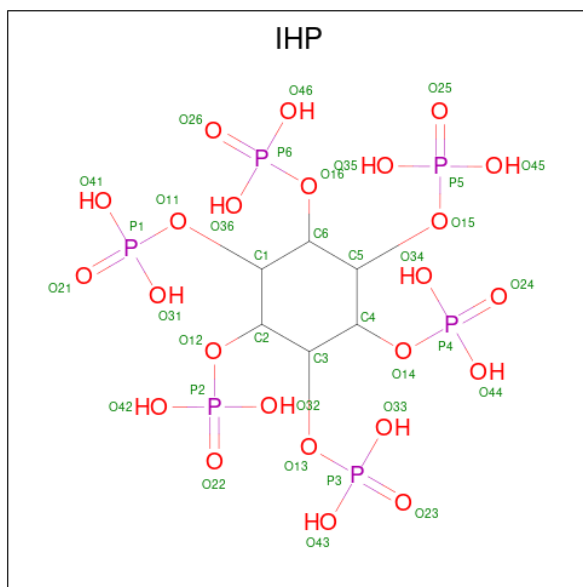
- Molecule 10 is a protein called Transcriptional adapter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	214	3380	1073	1675	305	321	6	0	0

- Molecule 11 is a protein called Ataxin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	N	53	864	280	419	87	74	4	1	0

- Molecule 12 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

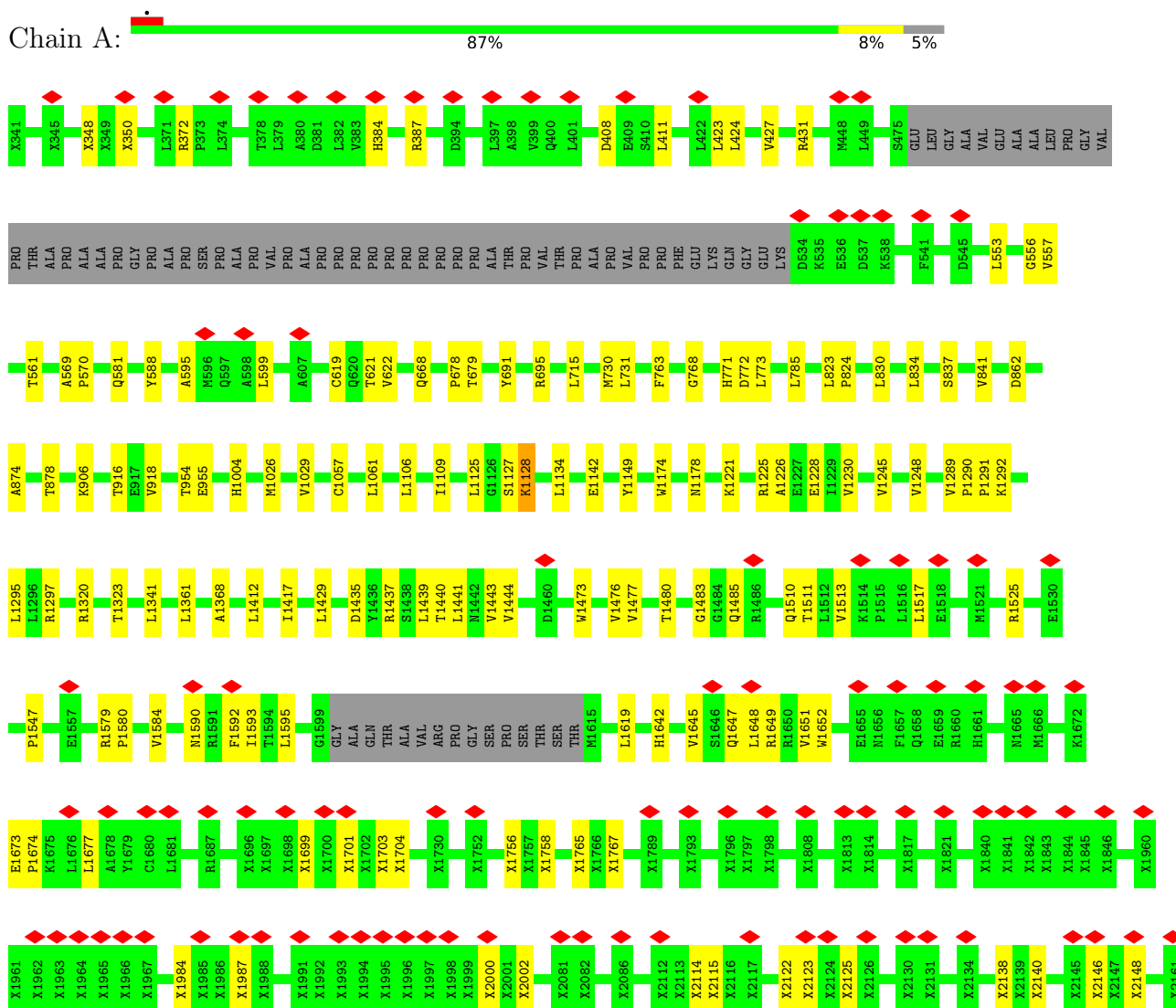


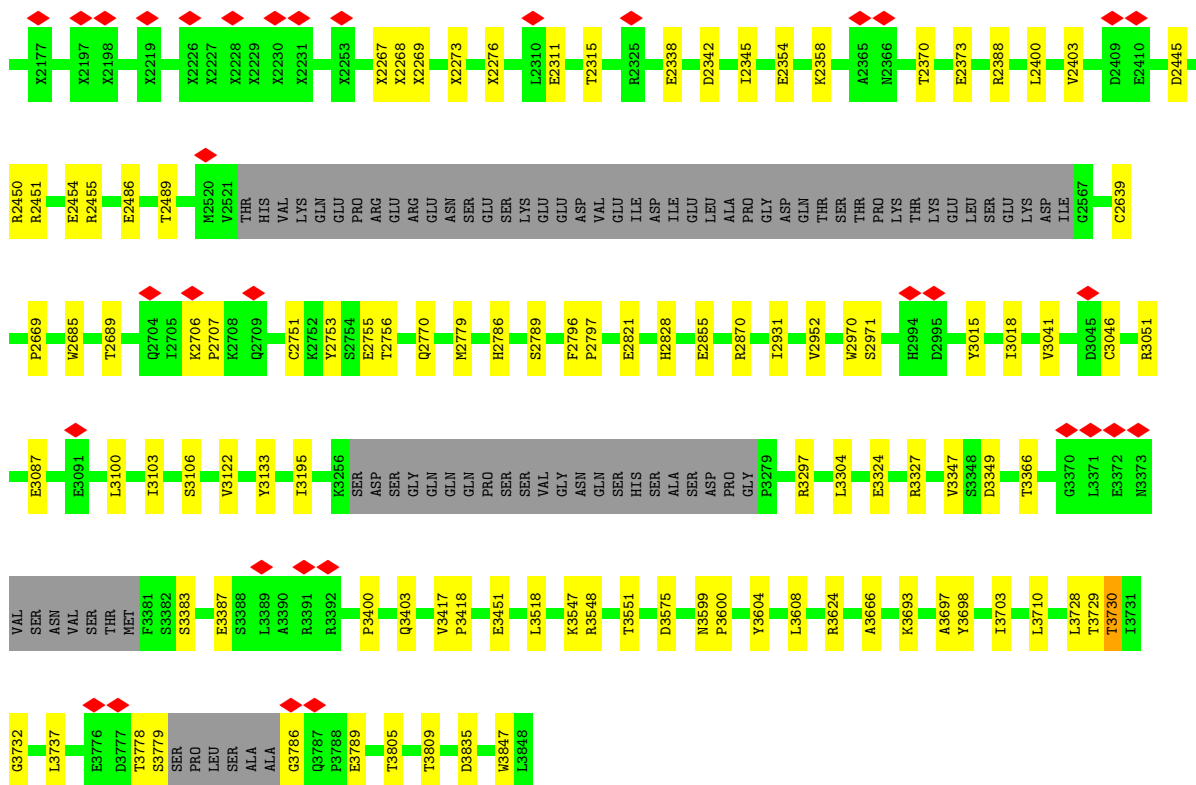
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	O		P
12	A	1	42	6	6	24	6	0

3 Residue-property plots

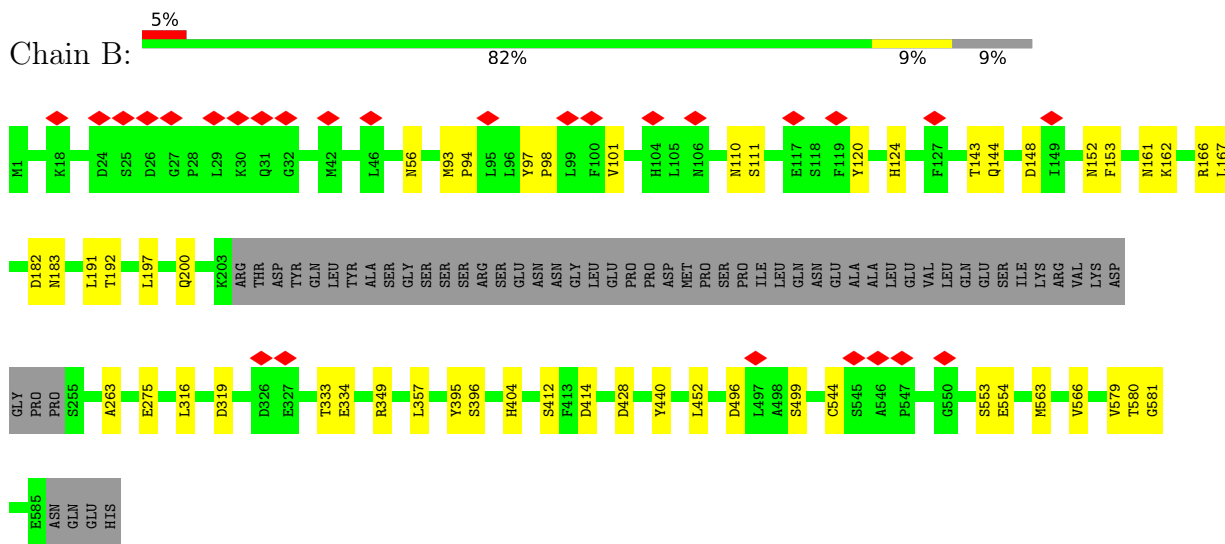
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Transformation/transcription domain-associated protein, Transformation/transcription domain-associated protein, Transformation/transcription domain-associated protein, Transformation/transcription domain-associated protein

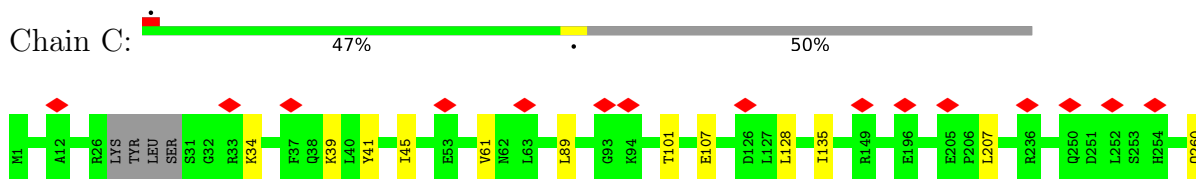


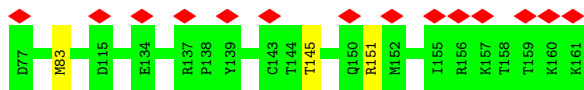


• Molecule 2: TAF5-like RNA polymerase II p300/CBP-associated factor-associated factor 65 kDa subunit 5L



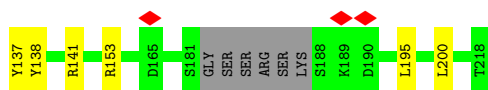
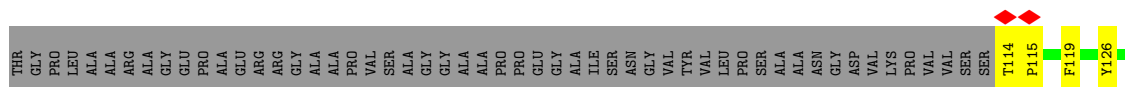
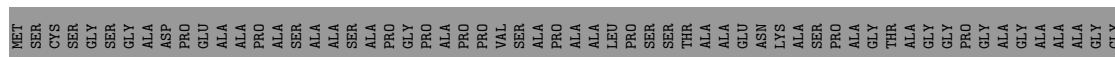
• Molecule 3: Isoform 3 of Transcription factor SPT20 homolog





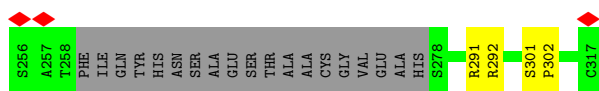
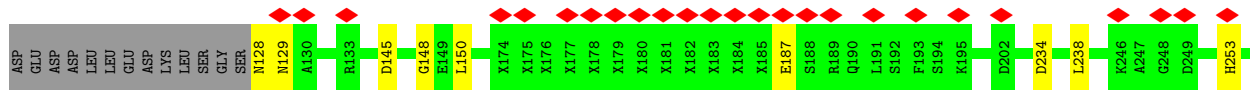
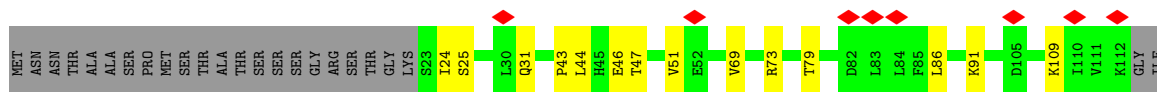
- Molecule 8: Transcription initiation factor TFIID subunit 10

Chain H: 41% 5% 55%



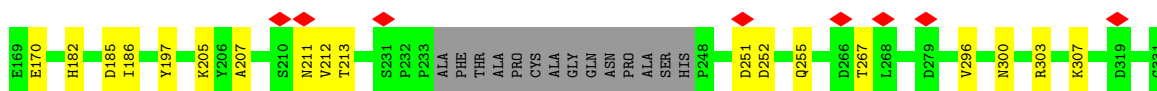
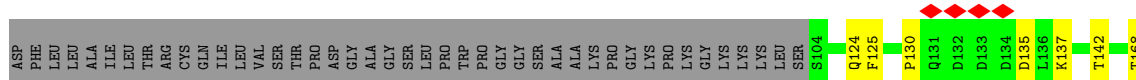
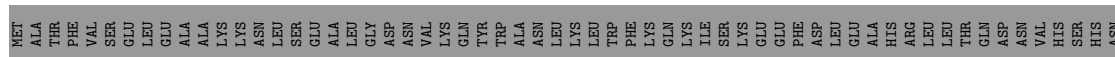
- Molecule 9: Transcription initiation protein SPT3 homolog, Transcription initiation protein SPT3 homolog, Transcription initiation protein SPT3 homolog

Chain I: 12% 72% 9% 19%



- Molecule 10: Transcriptional adapter 1

Chain J: 56% 7% 36%



- Molecule 11: Ataxin-7

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209435	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	25.375	Depositor
Minimum map value	0.000	Depositor
Average map value	0.172	Depositor
Map value standard deviation	0.753	Depositor
Recommended contour level	6.37	Depositor
Map size (\AA)	427.32, 427.32, 427.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.187, 1.187, 1.187	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/22230	0.41	0/30095
2	B	0.28	0/4315	0.43	0/5856
3	C	0.28	0/3355	0.40	0/4527
4	D	0.28	0/1513	0.41	0/2050
5	E	0.29	0/1018	0.40	0/1384
6	F	0.28	0/1055	0.43	0/1424
7	G	0.26	0/857	0.40	0/1150
8	H	0.30	0/800	0.41	0/1082
9	I	0.27	0/1879	0.39	0/2523
10	J	0.28	0/1745	0.40	0/2373
11	N	0.29	0/459	0.39	0/619
All	All	0.28	0/39226	0.41	0/53083

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23394	22456	22469	154	0
2	B	4225	4113	4113	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3293	3315	3313	20	0
4	D	1664	1485	1488	21	0
5	E	995	1018	1018	3	0
6	F	1039	1030	1029	10	0
7	G	845	859	859	2	0
8	H	784	782	781	7	0
9	I	1912	1911	1910	19	0
10	J	1705	1675	1675	18	0
11	N	445	419	418	3	0
12	A	36	6	6	2	0
All	All	40337	39069	39079	261	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 3.

All (261) 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)
1:A:2931:ILE:HD11	1:A:2952:VAL:HG11	1.61	0.82
6:F:22:GLU:OE2	7:G:145:THR:OG1	1.99	0.80
2:B:144:GLN:N	2:B:148:ASP:OD2	2.14	0.78
1:A:2639:CYS:O	10:J:255:GLN:NE2	2.16	0.78
10:J:135:ASP:OD2	10:J:137:LYS:NZ	2.17	0.78
1:A:2445:ASP:OD2	1:A:2450:ARG:NH2	2.18	0.77
3:C:332:ASP:OD1	3:C:358:LEU:N	2.19	0.76
1:A:2370:THR:N	1:A:2373:GLU:OE1	2.20	0.74
1:A:1701:UNK:O	1:A:1703:UNK:N	2.20	0.74
1:A:2311:GLU:O	1:A:2315:THR:HG23	1.88	0.73
1:A:2821:GLU:OE1	3:C:270:ARG:NH1	2.22	0.72
10:J:212:VAL:HG13	10:J:213:THR:H	1.55	0.72
3:C:34:LYS:O	3:C:39:LYS:NZ	2.24	0.71
4:D:80:ILE:O	4:D:84:GLN:NE2	2.24	0.71
2:B:544:CYS:N	2:B:553:SER:OG	2.24	0.71
5:E:34:ARG:NE	6:F:87:GLU:O	2.22	0.70
4:D:62:LEU:HD23	4:D:243:HIS:NE2	2.07	0.70
9:I:187:GLU:OE1	9:I:187:GLU:N	2.25	0.69
6:F:111:GLU:N	6:F:111:GLU:OE1	2.24	0.69
1:A:2669:PRO:HB2	10:J:267:THR:HG21	1.73	0.69
1:A:3728:LEU:O	1:A:3729:THR:OG1	2.10	0.69
1:A:2146:UNK:O	1:A:2148:UNK:N	2.26	0.68
1:A:2931:ILE:HD11	1:A:2952:VAL:CG1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:HIS:ND1	1:A:1142:GLU:OE1	2.26	0.68
2:B:200:GLN:N	2:B:200:GLN:OE1	2.27	0.68
1:A:1652:TRP:CD1	1:A:1677:LEU:HD21	2.29	0.67
1:A:3324:GLU:OE2	1:A:3327:ARG:NH2	2.28	0.67
10:J:124:GLN:OE1	10:J:125:PHE:N	2.27	0.67
1:A:1125:LEU:HD11	1:A:1134:LEU:HD11	1.76	0.67
1:A:581:GLN:OE1	1:A:1525:ARG:NH2	2.28	0.67
1:A:2970:TRP:CE3	1:A:3018:ILE:HD13	2.30	0.66
2:B:275:GLU:OE1	2:B:349:ARG:NH1	2.27	0.66
1:A:1510:GLN:O	1:A:1511:THR:OG1	2.10	0.65
2:B:143:THR:HG23	2:B:148:ASP:CB	2.27	0.65
1:A:1595:LEU:HD22	1:A:1619:LEU:HD21	1.78	0.64
10:J:300:ASN:OD1	10:J:303:ARG:NH1	2.31	0.64
2:B:316:LEU:N	2:B:319:ASP:OD2	2.32	0.63
1:A:595:ALA:O	1:A:599:LEU:HD23	1.99	0.63
1:A:2342:ASP:HB2	1:A:2345:ILE:HD12	1.81	0.63
3:C:41:TYR:CE2	3:C:45:ILE:HD11	2.34	0.63
1:A:1361:LEU:O	1:A:1361:LEU:HD23	1.98	0.62
1:A:906:LYS:O	1:A:3693:LYS:NZ	2.25	0.62
9:I:73:ARG:NH2	9:I:79:THR:OG1	2.32	0.62
1:A:3624:ARG:NH1	1:A:3835:ASP:OD1	2.33	0.62
1:A:916:THR:HG22	1:A:918:VAL:H	1.65	0.61
9:I:253:HIS:ND1	10:J:211:ASN:OD1	2.33	0.61
1:A:561:THR:HG22	1:A:588:TYR:OH	2.00	0.61
1:A:3051:ARG:NH2	12:A:4001:IHP:O34	2.33	0.61
1:A:2138:UNK:O	1:A:2140:UNK:N	2.34	0.61
1:A:3547:LYS:NZ	12:A:4001:IHP:O21	2.26	0.61
2:B:152:ASN:OD1	2:B:153:PHE:N	2.34	0.61
1:A:3297:ARG:HA	1:A:3304:LEU:HD12	1.83	0.60
2:B:182:ASP:OD1	2:B:183:ASN:N	2.31	0.58
10:J:296:VAL:O	10:J:300:ASN:ND2	2.37	0.58
1:A:1320:ARG:HE	1:A:1323:THR:HG22	1.68	0.58
9:I:31:GLN:NE2	9:I:43:PRO:O	2.37	0.57
10:J:251:ASP:OD1	10:J:252:ASP:N	2.37	0.57
5:E:34:ARG:NE	6:F:85:SER:OG	2.38	0.57
1:A:3786:GLY:N	1:A:3789:GLU:OE2	2.38	0.57
1:A:768:GLY:O	1:A:771:HIS:NE2	2.37	0.56
1:A:2971:SER:HG	1:A:3015:TYR:HH	1.52	0.56
1:A:837:SER:O	1:A:841:VAL:HG23	2.05	0.56
1:A:408:ASP:CB	1:A:411:LEU:HD12	2.36	0.56
2:B:161:ASN:HA	3:C:61:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3548:ARG:O	1:A:3551:THR:OG1	2.20	0.56
2:B:554:GLU:N	2:B:554:GLU:OE1	2.38	0.56
7:G:83:MET:SD	10:J:307:LYS:NZ	2.62	0.56
10:J:142:THR:HG23	10:J:142:THR:O	2.06	0.55
1:A:1228:GLU:N	1:A:1228:GLU:OE1	2.40	0.55
1:A:619:CYS:SG	1:A:621:THR:HG22	2.47	0.55
1:A:730:MET:SD	1:A:731:LEU:N	2.80	0.55
2:B:143:THR:HG23	2:B:148:ASP:HB3	1.88	0.55
2:B:98:PRO:HA	2:B:101:VAL:HG12	1.89	0.55
3:C:128:LEU:HD13	3:C:135:ILE:HD11	1.88	0.55
6:F:60:ARG:NH2	6:F:67:ASP:OD2	2.37	0.55
1:A:3195:ILE:HG23	3:C:328:TRP:CB	2.37	0.54
1:A:1245:VAL:O	1:A:1248:VAL:HG12	2.08	0.54
1:A:3729:THR:O	1:A:3732:GLY:N	2.41	0.54
1:A:1652:TRP:CG	1:A:1677:LEU:HD21	2.43	0.54
1:A:1127:SER:OG	1:A:1127:SER:O	2.24	0.54
10:J:168:THR:HG23	10:J:170:GLU:H	1.73	0.54
1:A:1648:LEU:O	1:A:1651:VAL:HG22	2.08	0.53
1:A:2970:TRP:CZ3	1:A:3018:ILE:HD13	2.43	0.53
1:A:3087:GLU:N	1:A:3087:GLU:OE1	2.36	0.53
1:A:763:PHE:HZ	1:A:785:LEU:HD21	1.74	0.53
1:A:2486:GLU:OE1	1:A:2489:THR:HG23	2.08	0.53
1:A:1647:GLN:O	1:A:1651:VAL:HG13	2.08	0.53
9:I:73:ARG:HH22	9:I:79:THR:HG1	1.55	0.53
4:D:43:UNK:O	4:D:45:UNK:N	2.42	0.52
9:I:145:ASP:OD2	9:I:148:GLY:N	2.39	0.52
1:A:2855:GLU:OE2	1:A:2870:ARG:NH2	2.43	0.52
1:A:1595:LEU:HD22	1:A:1619:LEU:CD2	2.39	0.52
4:D:198:ARG:NE	4:D:202:ASP:OD2	2.42	0.52
1:A:2273:UNK:O	1:A:2276:UNK:N	2.43	0.51
2:B:56:ASN:O	2:B:192:THR:HG21	2.11	0.51
9:I:47:THR:O	9:I:51:VAL:HG23	2.11	0.51
2:B:404:HIS:ND1	2:B:428:ASP:OD2	2.44	0.51
6:F:89:LEU:HD23	6:F:89:LEU:O	2.11	0.51
9:I:291:ARG:NH1	10:J:185:ASP:OD1	2.40	0.51
1:A:569:ALA:HB1	1:A:570:PRO:HD2	1.93	0.50
1:A:1984:UNK:O	1:A:1987:UNK:N	2.44	0.50
1:A:1439:LEU:HD12	1:A:1443:VAL:HB	1.94	0.50
4:D:245:TYR:CE2	4:D:249:ILE:HD11	2.46	0.50
1:A:2828:HIS:CD2	3:C:262:ARG:HD2	2.46	0.50
2:B:496:ASP:OD2	2:B:499:SER:OG	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:LEU:HD11	1:A:1443:VAL:HG13	1.94	0.50
1:A:3366:THR:HG23	1:A:3366:THR:O	2.11	0.49
3:C:107:GLU:N	3:C:107:GLU:OE1	2.45	0.49
2:B:97:TYR:HB3	2:B:98:PRO:HD3	1.94	0.49
4:D:206:ARG:HH21	4:D:207:LEU:HD21	1.77	0.49
1:A:569:ALA:HB1	1:A:570:PRO:CD	2.43	0.49
1:A:954:THR:HG22	1:A:955:GLU:N	2.28	0.48
2:B:333:THR:HG22	2:B:334:GLU:N	2.28	0.48
4:D:43:UNK:O	4:D:44:UNK:C	2.61	0.48
4:D:243:HIS:O	4:D:247:LEU:HD23	2.13	0.48
1:A:1483:GLY:O	1:A:1485:GLN:NE2	2.46	0.48
1:A:2685:TRP:O	1:A:2689:THR:HG23	2.13	0.48
1:A:3778:THR:O	1:A:3779:SER:HB2	2.14	0.48
4:D:146:VAL:HG12	4:D:147:THR:N	2.28	0.48
9:I:145:ASP:HB2	9:I:150:LEU:HD12	1.94	0.48
1:A:2000:UNK:O	1:A:2002:UNK:N	2.47	0.48
1:A:1226:ALA:O	1:A:1230:VAL:HG23	2.13	0.48
1:A:862:ASP:OD2	3:C:404:ARG:NH2	2.42	0.48
1:A:1547:PRO:HB2	1:A:1584:VAL:HG21	1.96	0.48
3:C:101:THR:HG22	11:N:550:MET:HB2	1.95	0.48
8:H:137:TYR:O	8:H:141:ARG:NH1	2.47	0.48
9:I:292:ARG:HD3	10:J:205:LYS:O	2.14	0.48
4:D:107:UNK:O	4:D:108:UNK:C	2.61	0.48
2:B:162:LYS:H	3:C:61:VAL:HG21	1.78	0.48
1:A:2267:UNK:O	1:A:2268:UNK:C	2.61	0.48
9:I:24:ILE:HG22	9:I:25:SER:N	2.29	0.48
9:I:44:LEU:HD21	9:I:46:GLU:OE2	2.13	0.47
1:A:1435:ASP:OD2	1:A:1437:ARG:NH2	2.47	0.47
3:C:207:LEU:HD12	3:C:207:LEU:N	2.30	0.47
1:A:1174:TRP:O	1:A:1178:ASN:ND2	2.45	0.47
2:B:143:THR:HG23	2:B:148:ASP:HB2	1.96	0.47
4:D:157:LEU:HD11	6:F:119:PRO:HG3	1.96	0.47
5:E:71:VAL:HG11	6:F:36:LEU:HD11	1.97	0.47
1:A:2796:PHE:N	1:A:2797:PRO:CD	2.78	0.47
2:B:349:ARG:O	2:B:357:LEU:HD12	2.15	0.47
1:A:2451:ARG:O	1:A:2455:ARG:HG2	2.15	0.47
9:I:24:ILE:HG22	9:I:25:SER:H	1.79	0.46
1:A:3195:ILE:HG23	3:C:328:TRP:HB3	1.97	0.46
9:I:301:SER:N	9:I:302:PRO:CD	2.78	0.46
1:A:772:ASP:C	1:A:772:ASP:OD1	2.54	0.46
1:A:691:TYR:OH	1:A:695:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1592:PHE:HA	1:A:1595:LEU:HD12	1.98	0.46
1:A:1642:HIS:HA	1:A:1645:VAL:HG12	1.98	0.46
1:A:3122:VAL:HG12	1:A:3122:VAL:O	2.13	0.46
2:B:395:TYR:O	2:B:396:SER:OG	2.28	0.46
9:I:46:GLU:OE1	9:I:46:GLU:N	2.36	0.46
1:A:3106:SER:OG	1:A:3133:TYR:OH	2.25	0.46
3:C:419:CYS:HB2	3:C:420:PRO:CD	2.46	0.46
9:I:234:ASP:O	9:I:238:LEU:HD23	2.16	0.46
4:D:159:TYR:OH	4:D:179:LEU:HD23	2.15	0.45
9:I:69:VAL:HG21	9:I:86:LEU:HD21	1.98	0.45
1:A:668:GLN:HE21	1:A:715:LEU:HD11	1.82	0.45
1:A:3400:PRO:O	1:A:3403:GLN:N	2.50	0.45
1:A:2338:GLU:O	1:A:2388:ARG:NH1	2.49	0.45
3:C:289:CYS:SG	3:C:290:VAL:N	2.90	0.45
10:J:212:VAL:HG13	10:J:213:THR:N	2.27	0.45
1:A:1149:TYR:OH	1:A:3451:GLU:OE2	2.26	0.45
1:A:1221:LYS:O	1:A:1225:ARG:HG3	2.16	0.45
1:A:1289:VAL:HB	1:A:1290:PRO:CD	2.47	0.45
1:A:1579:ARG:N	1:A:1580:PRO:HD2	2.31	0.45
2:B:440:TYR:HB3	2:B:452:LEU:HD11	1.98	0.45
1:A:2755:GLU:OE1	1:A:2755:GLU:N	2.46	0.45
4:D:204:GLU:OE2	4:D:210:THR:OG1	2.35	0.45
1:A:423:LEU:O	1:A:427:VAL:HG23	2.17	0.45
1:A:1295:LEU:O	1:A:1297:ARG:N	2.50	0.45
1:A:1473:TRP:O	1:A:1476:VAL:HG12	2.16	0.44
1:A:678:PRO:O	1:A:679:THR:OG1	2.24	0.44
1:A:3805:THR:O	1:A:3809:THR:HG23	2.17	0.44
2:B:120:TYR:O	2:B:124:HIS:ND1	2.50	0.44
4:D:37:UNK:CB	6:F:128:ARG:NH2	2.80	0.44
6:F:131:VAL:HG12	6:F:132:SER:N	2.31	0.44
1:A:372:ARG:HD2	1:A:411:LEU:HD21	1.99	0.44
1:A:2122:UNK:O	1:A:2123:UNK:C	2.66	0.44
4:D:261:VAL:HG13	4:D:262:ASN:N	2.33	0.44
1:A:2114:UNK:O	1:A:2115:UNK:C	2.65	0.44
1:A:3604:TYR:CE2	1:A:3608:LEU:HD11	2.52	0.44
1:A:2400:LEU:HA	1:A:2403:VAL:HG22	2.00	0.44
1:A:2779:MET:CE	3:C:263:LEU:HD23	2.48	0.44
1:A:3041:VAL:HG23	1:A:3046:CYS:SG	2.57	0.44
1:A:874:ALA:O	1:A:878:THR:HG23	2.18	0.44
1:A:3599:ASN:N	1:A:3600:PRO:CD	2.81	0.44
1:A:1590:ASN:HA	1:A:1593:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2706:LYS:HB3	1:A:2707:PRO:HD3	2.01	0.43
4:D:228:VAL:HG22	8:H:119:PHE:CZ	2.52	0.43
1:A:2451:ARG:HB2	1:A:2454:GLU:OE1	2.18	0.43
1:A:3100:LEU:O	1:A:3103:ILE:O	2.37	0.43
1:A:3697:ALA:HA	1:A:3698:TYR:CG	2.53	0.43
8:H:126:TYR:O	8:H:153:ARG:NH2	2.52	0.43
1:A:1106:LEU:O	1:A:1109:ILE:HG22	2.18	0.43
1:A:2751:CYS:SG	1:A:2753:TYR:O	2.77	0.43
10:J:182:HIS:CE1	10:J:186:ILE:HD11	2.54	0.43
1:A:954:THR:HG22	1:A:955:GLU:H	1.84	0.42
1:A:2370:THR:OG1	1:A:2373:GLU:OE1	2.31	0.42
2:B:191:LEU:HD22	2:B:197:LEU:HD11	2.01	0.42
1:A:2122:UNK:O	1:A:2125:UNK:N	2.52	0.42
4:D:159:TYR:CZ	4:D:179:LEU:HD23	2.54	0.42
4:D:178:VAL:HG13	8:H:200:LEU:HD22	1.99	0.42
1:A:1673:GLU:N	1:A:1674:PRO:CD	2.82	0.42
1:A:3729:THR:O	1:A:3730:THR:C	2.56	0.42
1:A:3383:SER:O	1:A:3387:GLU:OE1	2.38	0.42
1:A:823:LEU:N	1:A:824:PRO:CD	2.82	0.42
1:A:2354:GLU:OE2	1:A:2358:LYS:NZ	2.42	0.42
1:A:1127:SER:O	1:A:1128:LYS:C	2.58	0.42
1:A:1513:VAL:HG12	1:A:1517:LEU:HD12	2.01	0.42
1:A:1703:UNK:O	1:A:1704:UNK:CB	2.67	0.42
1:A:3703:ILE:HD13	1:A:3710:LEU:HD23	2.02	0.42
1:A:1026:MET:O	1:A:1029:VAL:HG22	2.19	0.42
2:B:93:MET:N	2:B:94:PRO:CD	2.82	0.42
4:D:178:VAL:HG11	8:H:195:LEU:CD2	2.49	0.42
1:A:384:HIS:O	1:A:387:ARG:NH1	2.49	0.42
1:A:1440:THR:OG1	1:A:1441:LEU:N	2.53	0.42
1:A:3600:PRO:HB2	1:A:3847:TRP:CZ2	2.55	0.42
2:B:110:ASN:O	2:B:111:SER:OG	2.32	0.42
2:B:563:MET:HE1	2:B:566:VAL:HG13	2.02	0.42
1:A:1756:UNK:C	1:A:1758:UNK:N	2.83	0.42
1:A:2770:GLN:OE1	1:A:2770:GLN:N	2.52	0.42
1:A:3518:LEU:HG	1:A:3575:ASP:OD2	2.20	0.42
1:A:553:LEU:O	1:A:557:VAL:HG23	2.20	0.42
1:A:2267:UNK:O	1:A:2269:UNK:N	2.53	0.41
10:J:197:TYR:HA	10:J:207:ALA:O	2.20	0.41
1:A:772:ASP:OD1	1:A:773:LEU:N	2.53	0.41
1:A:1441:LEU:HA	1:A:1444:VAL:HG22	2.01	0.41
1:A:1699:UNK:C	1:A:1701:UNK:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3347:VAL:HG12	1:A:3349:ASP:HB2	2.02	0.41
1:A:1412:LEU:HD21	1:A:1417:ILE:HD12	2.02	0.41
3:C:89:LEU:HD12	11:N:547:LEU:HD21	2.02	0.41
1:A:1510:GLN:C	1:A:1511:THR:HG23	2.41	0.41
2:B:412:SER:OG	2:B:414:ASP:OD1	2.32	0.41
1:A:1649:ARG:HA	1:A:1652:TRP:CD1	2.56	0.41
4:D:187:HIS:ND1	8:H:138:TYR:OH	2.28	0.41
1:A:1477:VAL:O	1:A:1480:THR:HG22	2.21	0.41
1:A:1510:GLN:O	1:A:1511:THR:CB	2.68	0.41
1:A:3417:VAL:HB	1:A:3418:PRO:HD2	2.02	0.41
2:B:263:ALA:HA	2:B:581:GLY:O	2.21	0.41
8:H:114:THR:N	8:H:115:PRO:CD	2.83	0.41
1:A:622:VAL:HG22	1:A:622:VAL:O	2.21	0.41
1:A:1649:ARG:HA	1:A:1652:TRP:NE1	2.35	0.41
10:J:130:PRO:HG3	11:N:549:LEU:HD22	2.03	0.41
1:A:348:UNK:C	1:A:350:UNK:N	2.84	0.41
1:A:424:LEU:HD12	1:A:556:GLY:HA2	2.03	0.41
2:B:166:ARG:C	2:B:167:LEU:HD12	2.41	0.41
2:B:579:VAL:HG12	2:B:580:THR:N	2.36	0.41
9:I:128:ASN:OD1	9:I:129:ASN:N	2.54	0.41
1:A:1341:LEU:HD23	1:A:1368:ALA:HB2	2.03	0.41
3:C:260:GLN:C	3:C:261:LEU:HD12	2.40	0.40
9:I:91:LYS:HD2	9:I:91:LYS:N	2.36	0.40
1:A:1057:CYS:HA	1:A:1061:LEU:HD21	2.04	0.40
1:A:2000:UNK:C	1:A:2002:UNK:N	2.83	0.40
1:A:2751:CYS:SG	1:A:2756:THR:HB	2.60	0.40
1:A:2786:HIS:HA	1:A:2789:SER:O	2.21	0.40
4:D:200:ALA:CB	4:D:215:VAL:HG13	2.51	0.40
1:A:3666:ALA:HB2	1:A:3737:LEU:HD12	2.03	0.40
3:C:345:THR:HG22	3:C:346:GLN:N	2.36	0.40
1:A:830:LEU:O	1:A:834:LEU:HD23	2.21	0.40
1:A:1291:PRO:O	1:A:1292:LYS:HB3	2.22	0.40
1:A:1765:UNK:O	1:A:1767:UNK:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
						51	80
1	A	2703/3195 (85%)	2570 (95%)	131 (5%)	2 (0%)	51	80
2	B	530/589 (90%)	494 (93%)	36 (7%)	0	100	100
3	C	402/811 (50%)	373 (93%)	29 (7%)	0	100	100
4	D	178/704 (25%)	171 (96%)	7 (4%)	0	100	100
5	E	122/251 (49%)	115 (94%)	7 (6%)	0	100	100
6	F	128/622 (21%)	124 (97%)	4 (3%)	0	100	100
7	G	101/161 (63%)	97 (96%)	4 (4%)	0	100	100
8	H	95/218 (44%)	93 (98%)	2 (2%)	0	100	100
9	I	223/299 (75%)	211 (95%)	12 (5%)	0	100	100
10	J	210/335 (63%)	196 (93%)	14 (7%)	0	100	100
11	N	52/892 (6%)	50 (96%)	2 (4%)	0	100	100
All	All	4744/8077 (59%)	4494 (95%)	248 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3730	THR
1	A	1128	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2409/2532 (95%)	2408 (100%)	1 (0%)	100	100
2	B	472/521 (91%)	472 (100%)	0	100	100
3	C	375/716 (52%)	373 (100%)	2 (0%)	88	96
4	D	164/579 (28%)	164 (100%)	0	100	100
5	E	110/224 (49%)	110 (100%)	0	100	100
6	F	112/505 (22%)	112 (100%)	0	100	100
7	G	94/141 (67%)	93 (99%)	1 (1%)	73	90
8	H	86/154 (56%)	86 (100%)	0	100	100
9	I	202/246 (82%)	201 (100%)	1 (0%)	88	96
10	J	188/287 (66%)	188 (100%)	0	100	100
11	N	47/779 (6%)	47 (100%)	0	100	100
All	All	4259/6684 (64%)	4254 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	ARG
3	C	331[A]	HIS
3	C	331[B]	HIS
7	G	151	ARG
9	I	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	620	GLN
1	A	668	GLN
1	A	865	GLN
1	A	2367	GLN
1	A	2396	ASN
1	A	2655	ASN
1	A	2772	GLN
1	A	2921	GLN
1	A	2979	HIS
1	A	2982	GLN
1	A	3498	HIS
1	A	3617	GLN
2	B	307	HIS

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Mol	Chain	Res	Type
3	C	153	ASN
3	C	171	GLN
3	C	220	ASN
4	D	84	GLN
7	G	86	GLN
8	H	122	GLN
10	J	220	ASN
10	J	285	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	IHP	A	4001	-	36,36,36	1.42	6 (16%)	54,60,60	0.71	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	IHP	A	4001	-	-	6/30/54/54	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	4001	IHP	P3-O13	3.23	1.65	1.59
12	A	4001	IHP	P2-O12	3.06	1.65	1.59
12	A	4001	IHP	P4-O14	2.99	1.65	1.59
12	A	4001	IHP	P6-O16	2.95	1.64	1.59
12	A	4001	IHP	P1-O11	2.93	1.64	1.59
12	A	4001	IHP	P5-O15	2.87	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	4001	IHP	C6-C1-C2	2.41	115.69	110.41
12	A	4001	IHP	C5-C6-C1	2.22	115.27	110.41

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	4001	IHP	C4-O14-P4-O24
12	A	4001	IHP	C5-O15-P5-O45
12	A	4001	IHP	C2-O12-P2-O22
12	A	4001	IHP	C6-O16-P6-O26
12	A	4001	IHP	C1-O11-P1-O31
12	A	4001	IHP	C6-O16-P6-O36

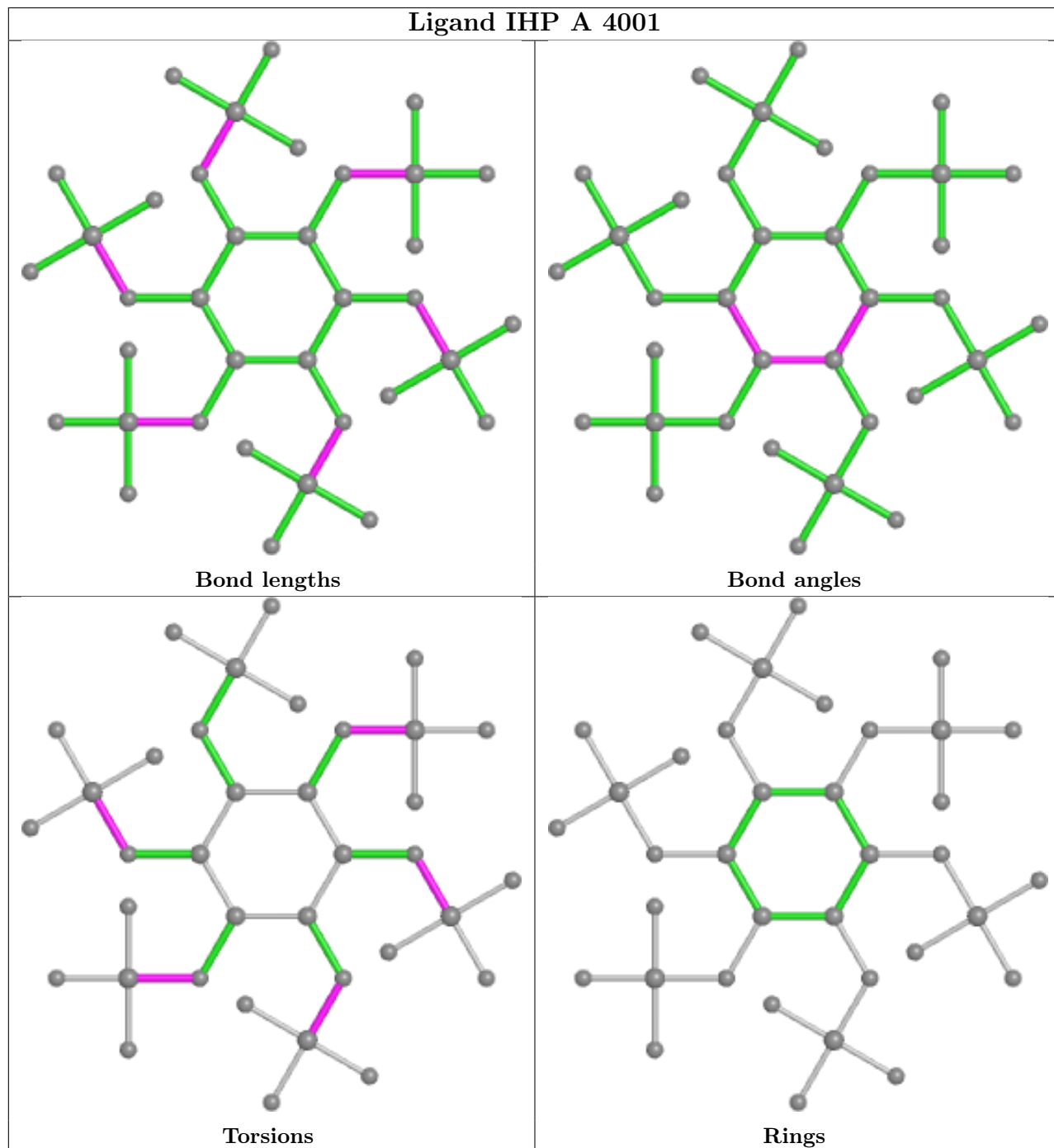
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	4001	IHP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	16
4	D	3
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1848:UNK	C	1960:UNK	N	31.46
1	A	1768:UNK	C	1787:UNK	N	19.99
1	A	2002:UNK	C	2077:UNK	N	18.56
1	A	1822:UNK	C	1838:UNK	N	16.12
1	A	360:UNK	C	369:GLU	N	14.95
1	D	87:ASN	C	96:UNK	N	14.89
1	A	1799:UNK	C	1806:UNK	N	13.57
1	A	2290:UNK	C	2300:ALA	N	13.41
1	I	156:ASP	C	174:UNK	N	13.21
1	A	2238:UNK	C	2249:UNK	N	13.11
1	A	1721:UNK	C	1729:UNK	N	11.31
1	A	2180:UNK	C	2193:UNK	N	10.68
1	A	2208:UNK	C	2218:UNK	N	10.31
1	A	1688:ASN	C	1693:UNK	N	10.13
1	A	2088:UNK	C	2102:UNK	N	8.89
1	A	2148:UNK	C	2153:UNK	N	7.97
1	D	47:UNK	C	52:MET	N	7.56
1	D	117:UNK	C	119:ASP	N	6.99
1	A	350:UNK	C	354:UNK	N	5.27
1	I	185:UNK	C	187:GLU	N	5.10
1	A	1973:UNK	C	1984:UNK	N	4.89

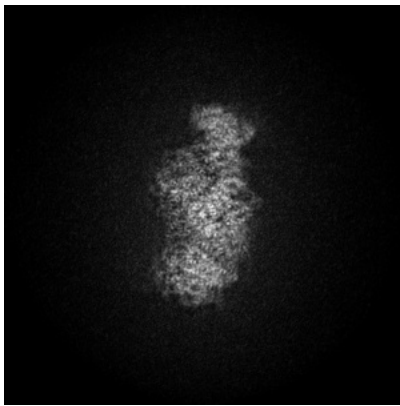
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23027. These allow visual inspection of the internal detail of the map and identification of artifacts.

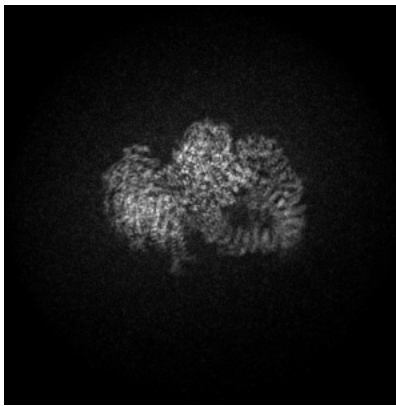
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

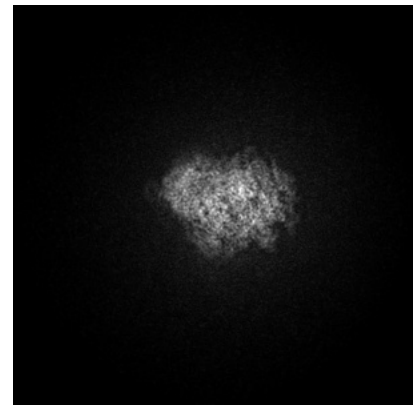
6.1.1 Primary map



X

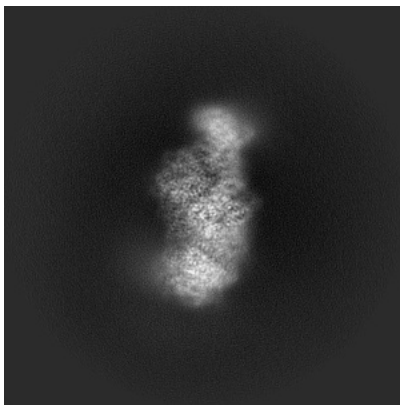


Y

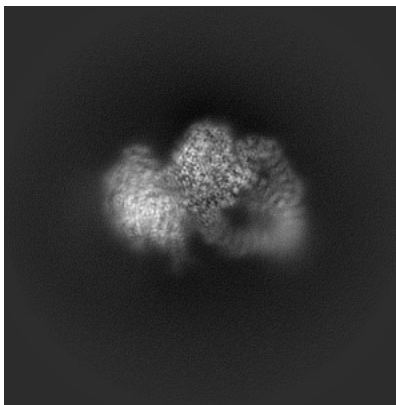


Z

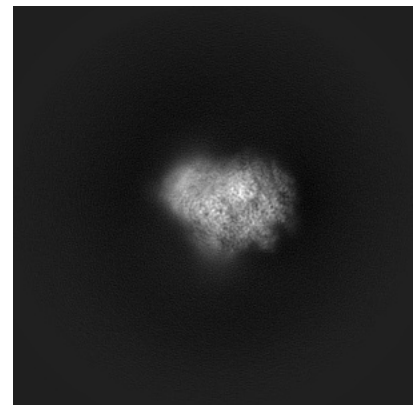
6.1.2 Raw map



X



Y

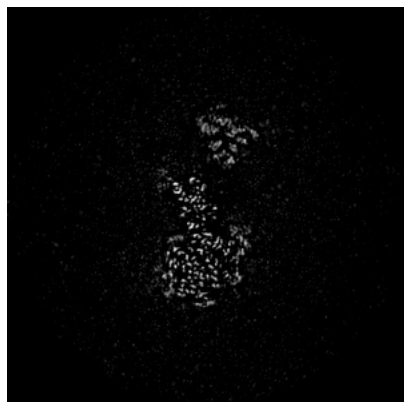


Z

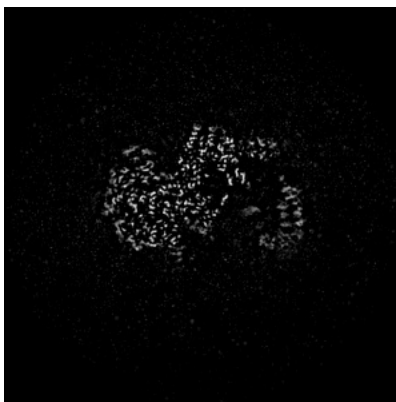
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

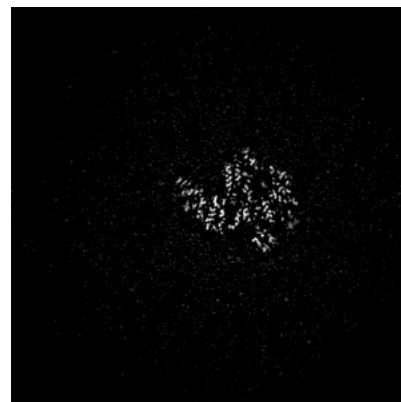
6.2.1 Primary map



X Index: 180

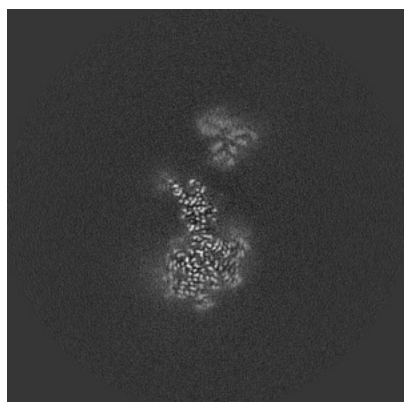


Y Index: 180

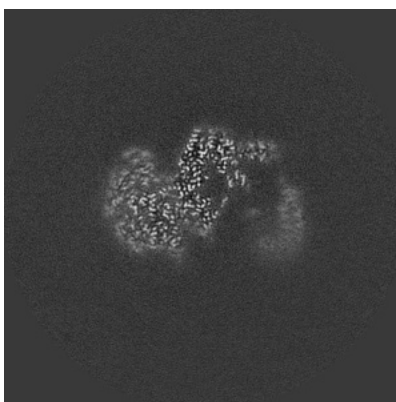


Z Index: 180

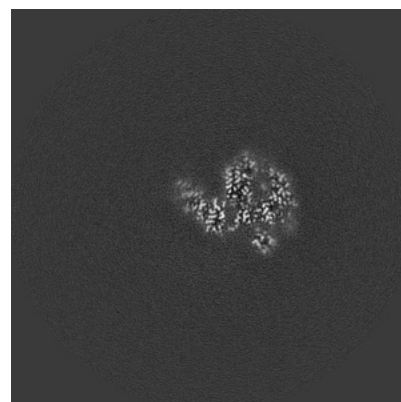
6.2.2 Raw map



X Index: 180



Y Index: 180

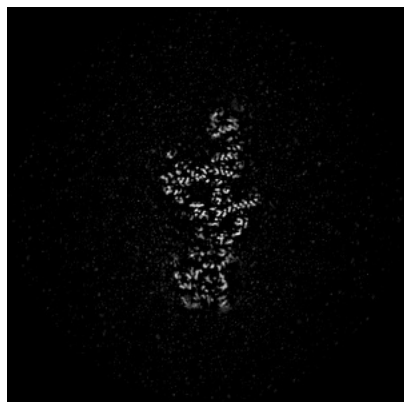


Z Index: 180

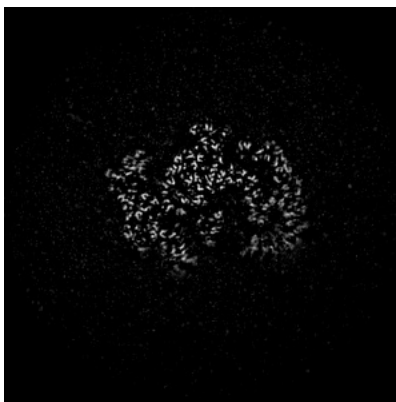
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

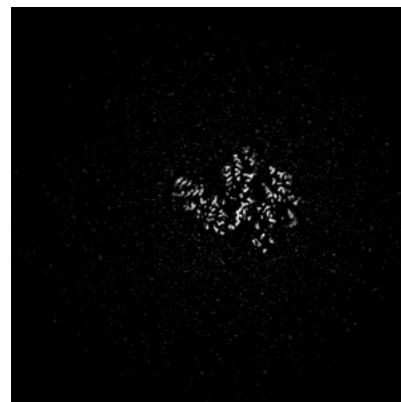
6.3.1 Primary map



X Index: 204

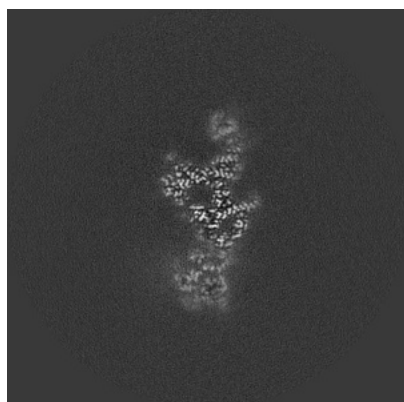


Y Index: 189

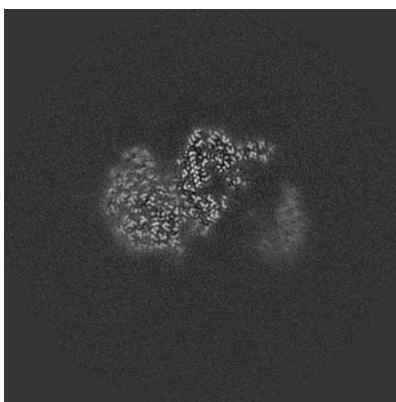


Z Index: 181

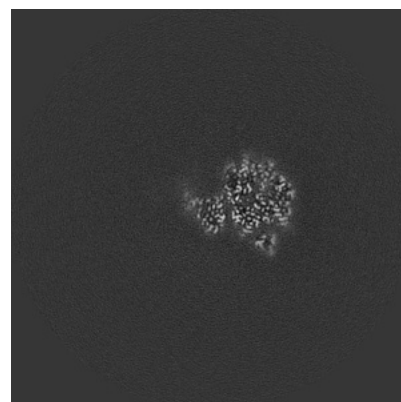
6.3.2 Raw map



X Index: 204



Y Index: 178

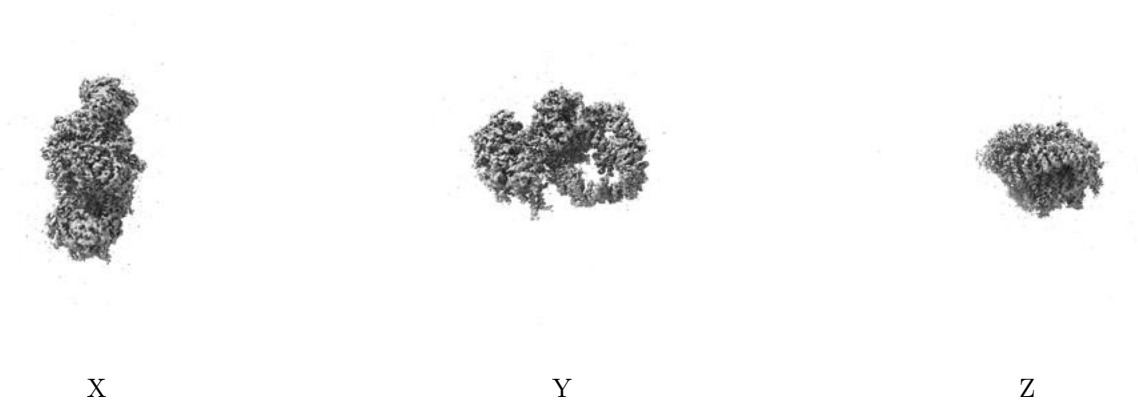


Z Index: 176

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

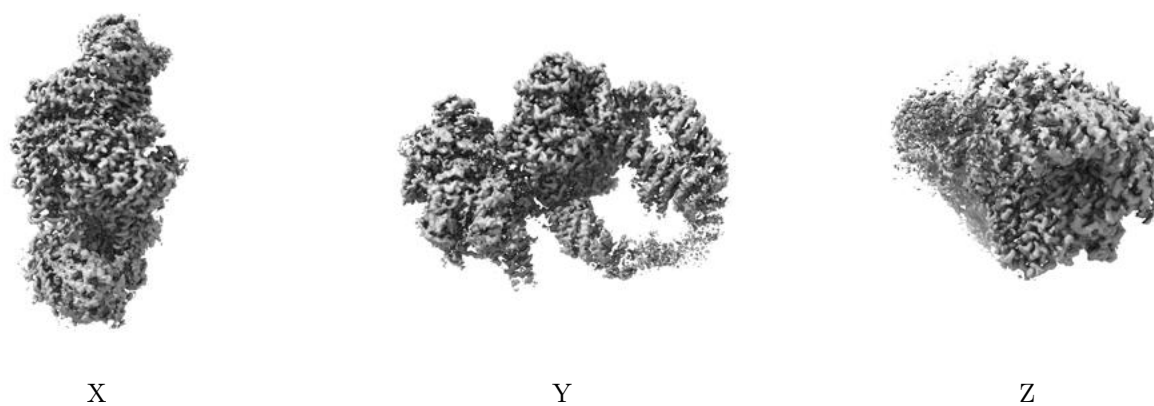
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.37. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

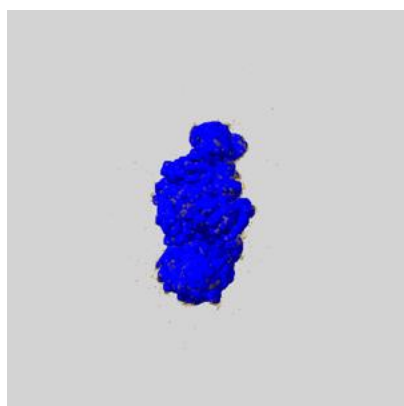
6.5 Mask visualisation [i](#)

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

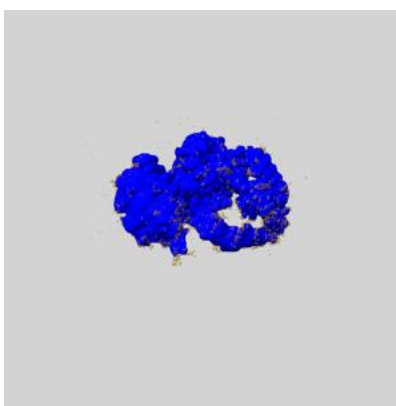
A mask typically either:

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

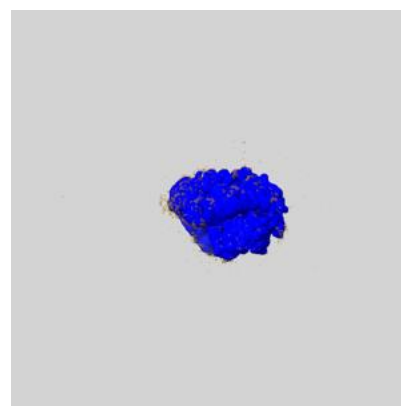
6.5.1 emd_23027_msk_1.map [i](#)



X



Y

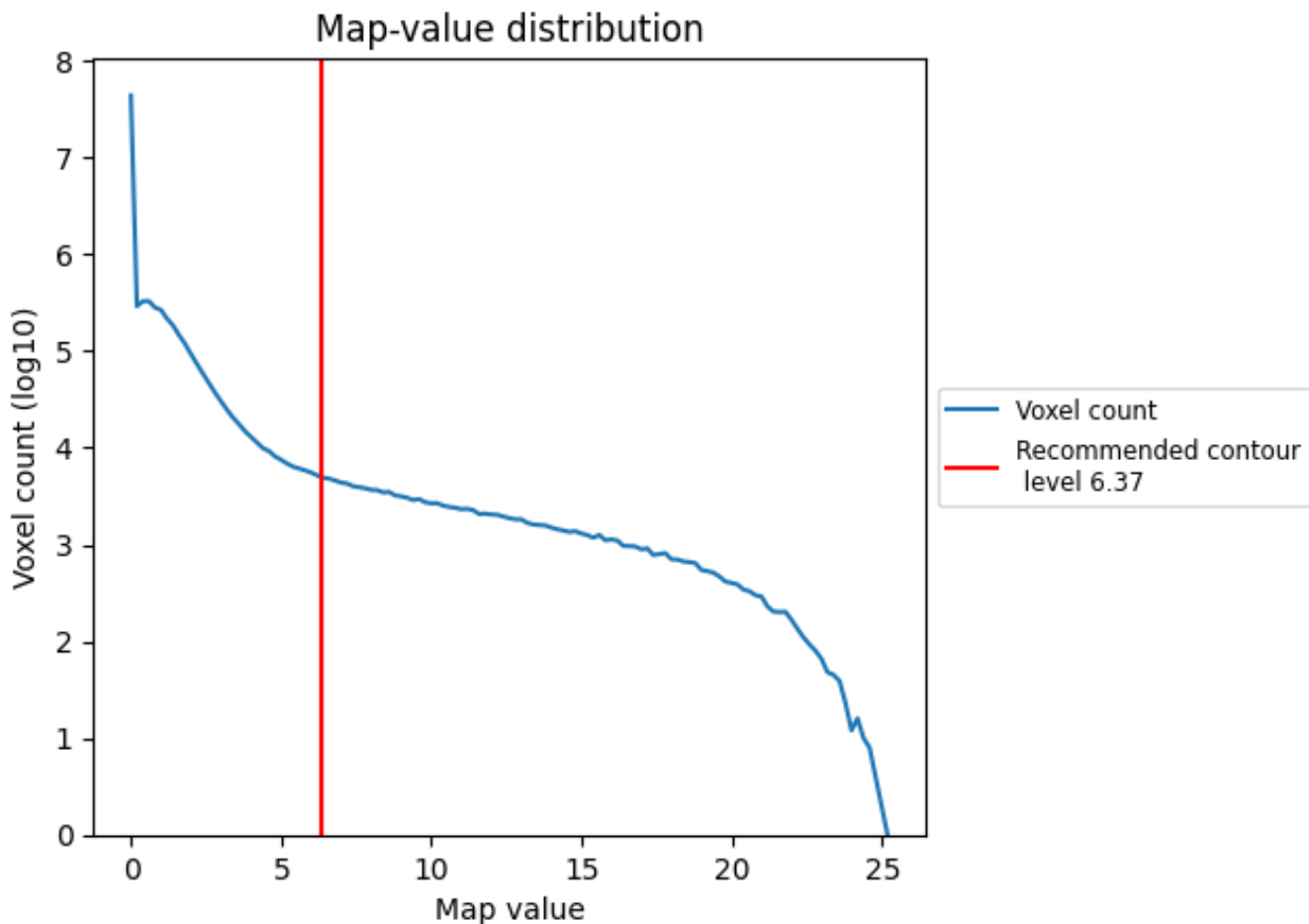


Z

7 Map analysis [i](#)

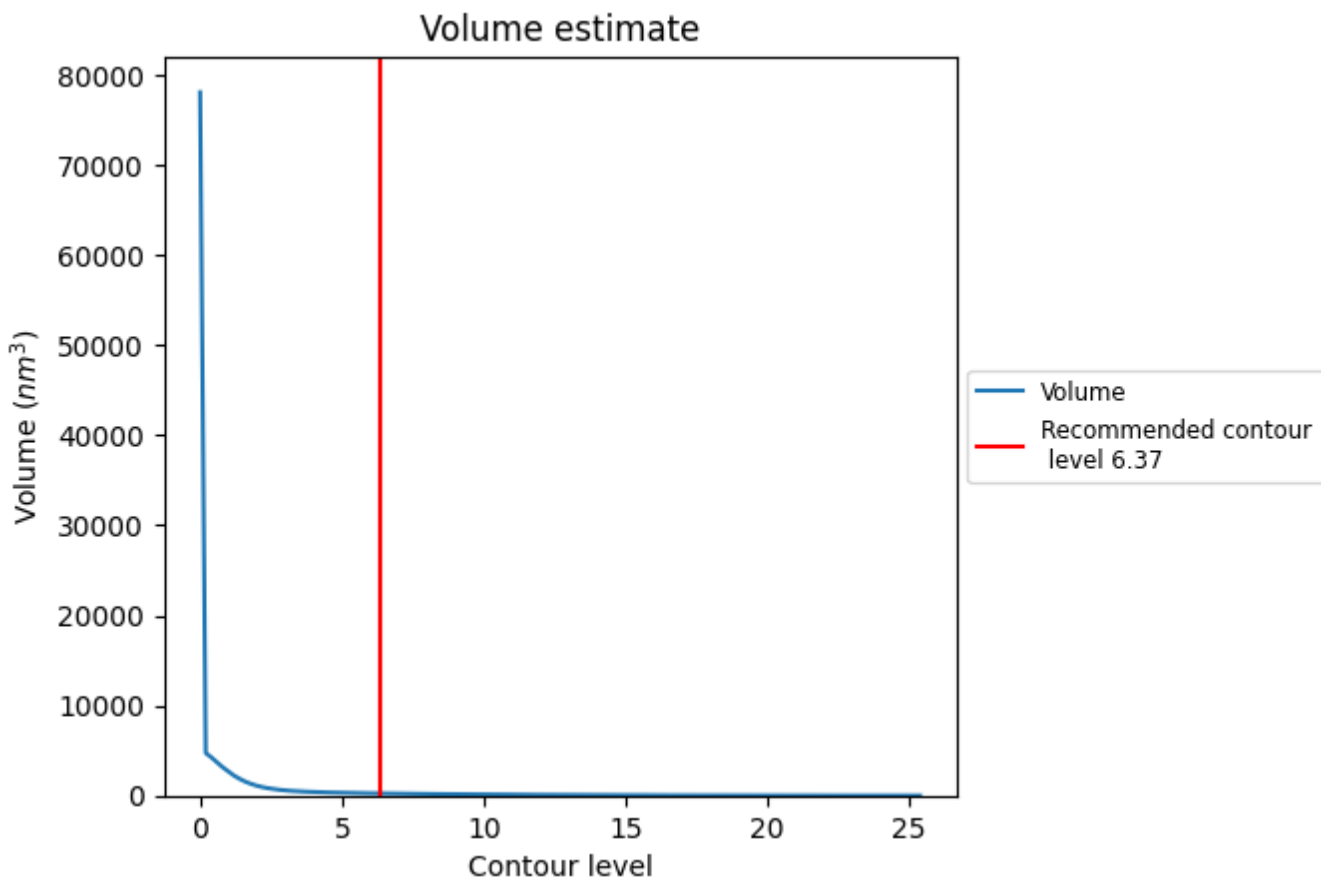
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

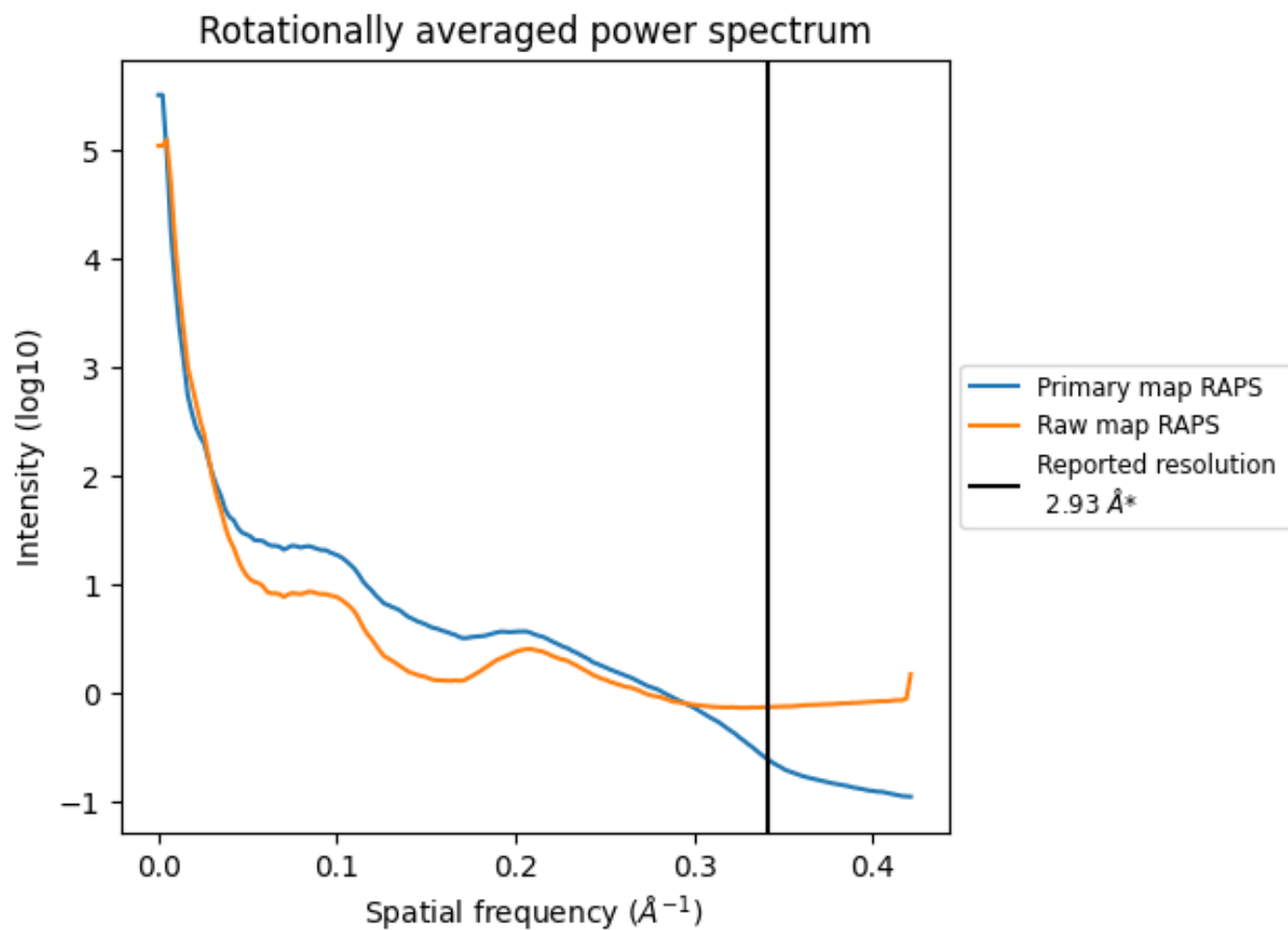
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 237 nm³; this corresponds to an approximate mass of 214 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 i

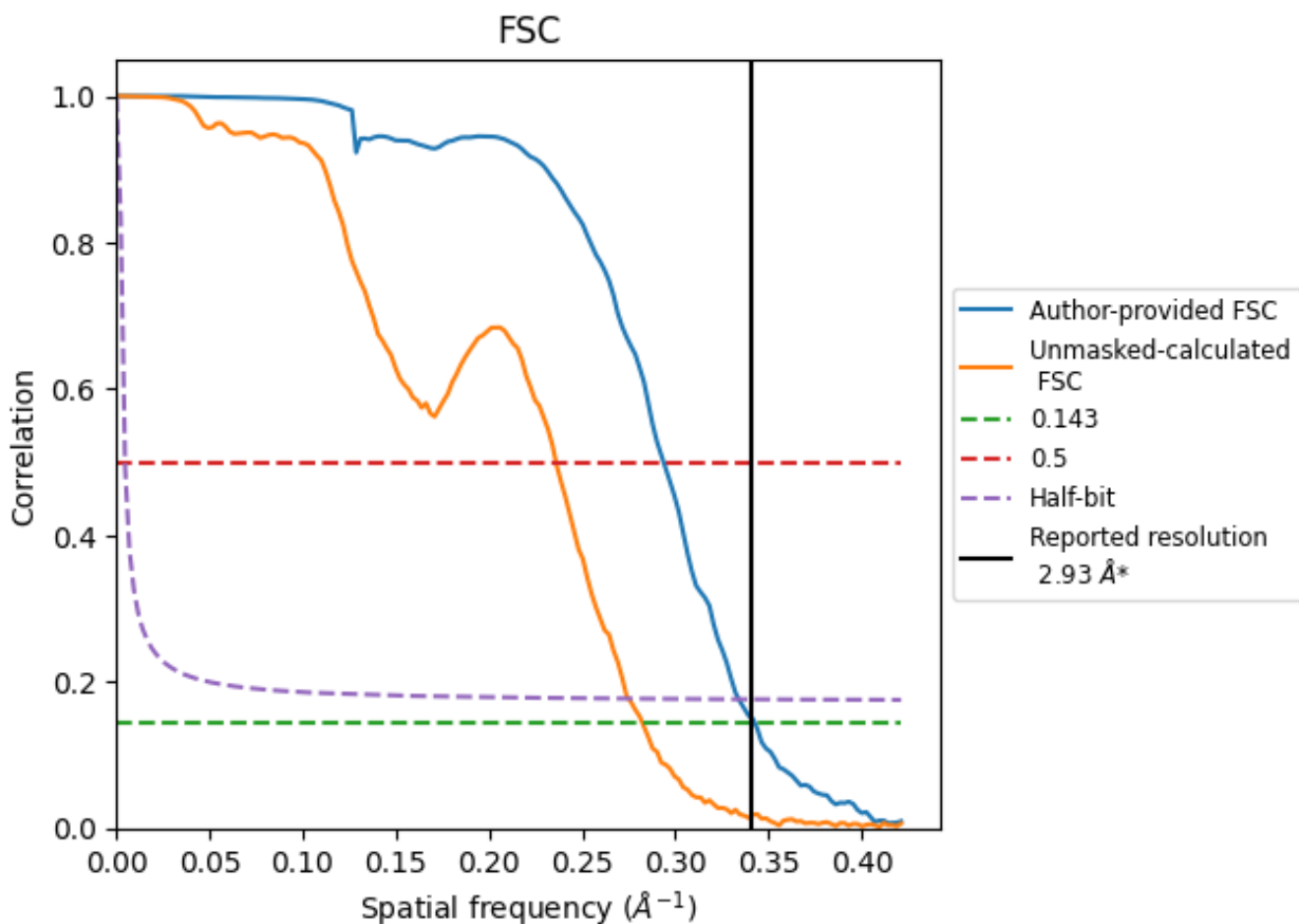


*Reported resolution corresponds to spatial frequency of 0.341 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

8.2 Resolution estimates [i](#)

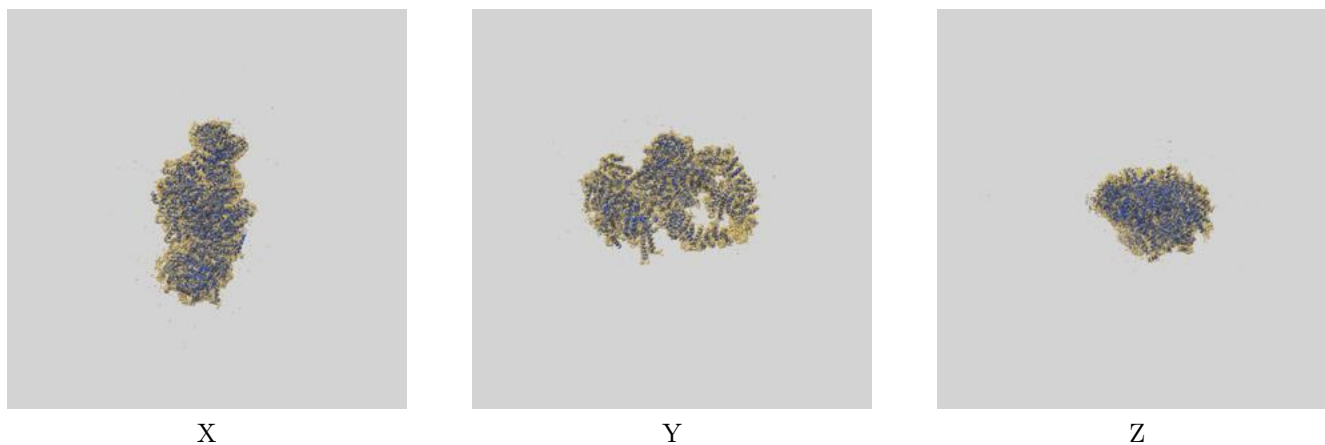
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.92	3.40	2.99
Unmasked-calculated*	3.54	4.24	3.64

*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 3.54 differs from the reported value 2.93 by more than 10 %

9 Map-model fit [i](#)

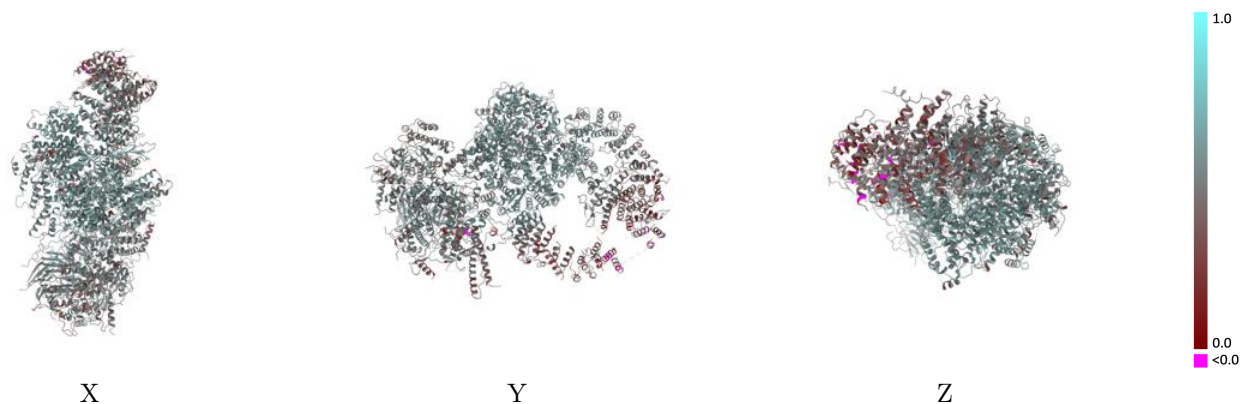
This section contains information regarding the fit between EMDB map EMD-23027 and PDB model 7KTR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



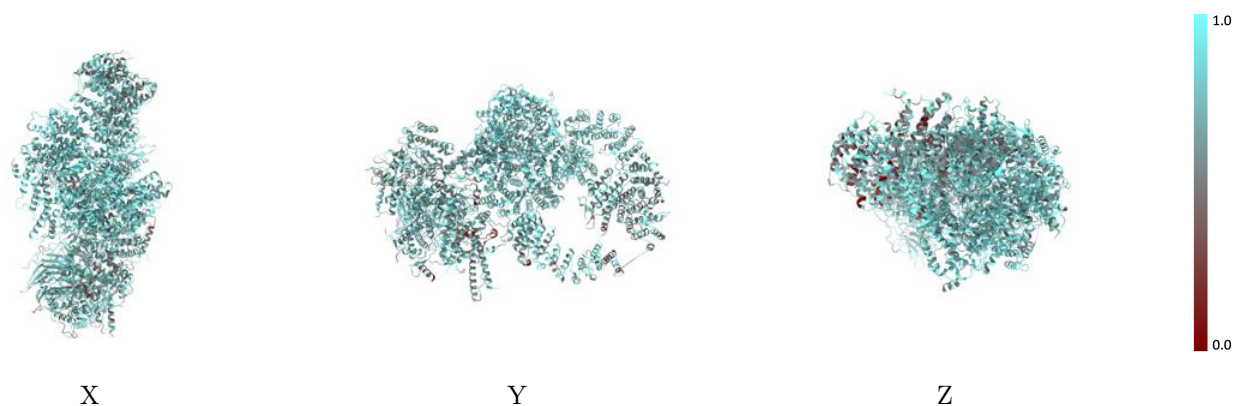
The images above show the 3D surface view of the map at the recommended contour level 6.37 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



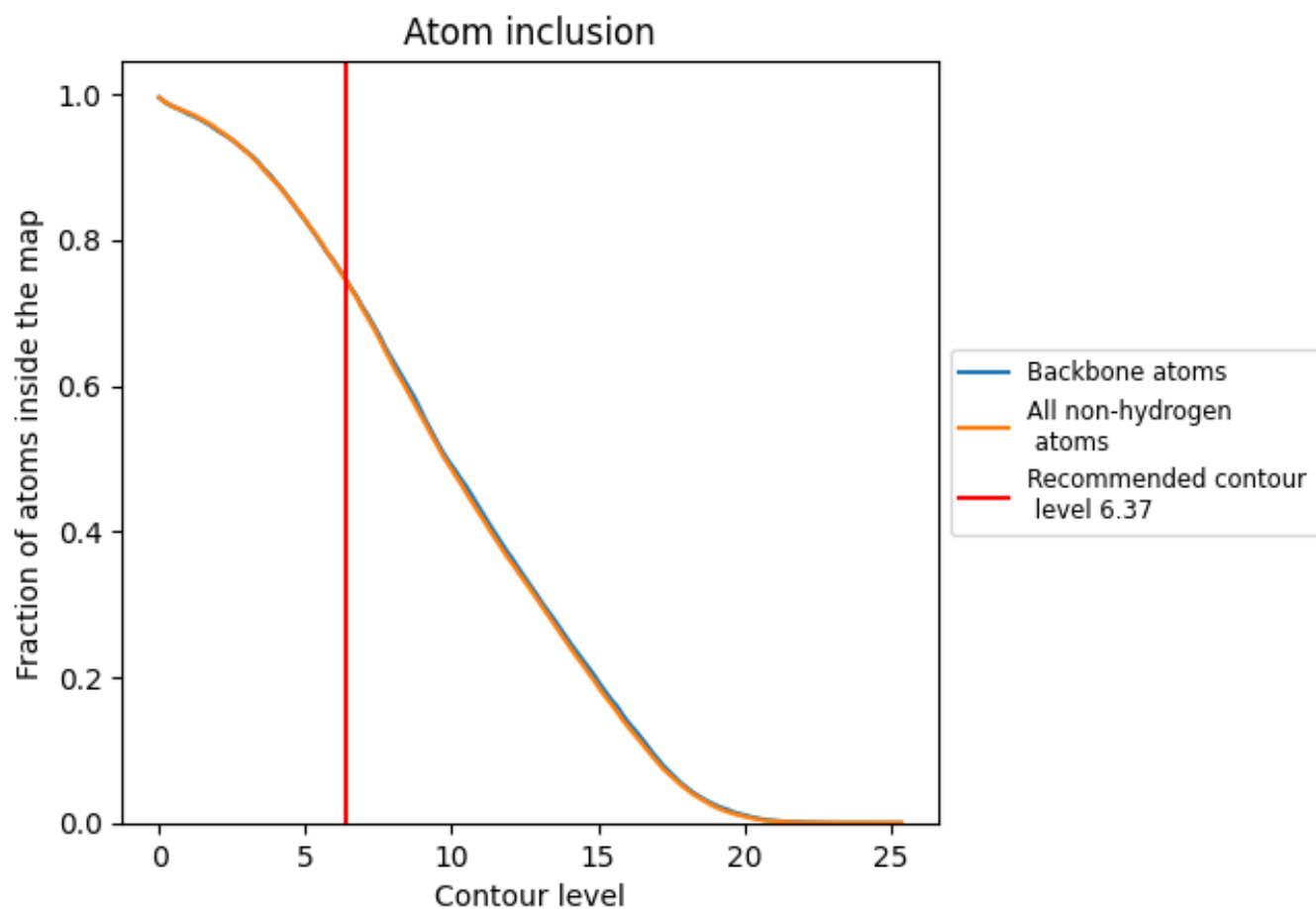
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.37).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (6.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7453	 0.5130
A	 0.7650	 0.5210
B	 0.7439	 0.5090
C	 0.7165	 0.4910
D	 0.7375	 0.5040
E	 0.7585	 0.5320
F	 0.7465	 0.5040
G	 0.6461	 0.4800
H	 0.7623	 0.5480
I	 0.6456	 0.4500
J	 0.7542	 0.5250
N	 0.6936	 0.4910

