



Full wwPDB EM Validation Report ⓘ

Jul 6, 2024 – 03:32 PM EDT

PDB ID : 8UGP
EMDB ID : EMD-42231
Title : In-situ structure of typeA supercomplex in respiratory chain (local refined map focused on CI iron-sulfur cluster regions)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.00 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.dev92
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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

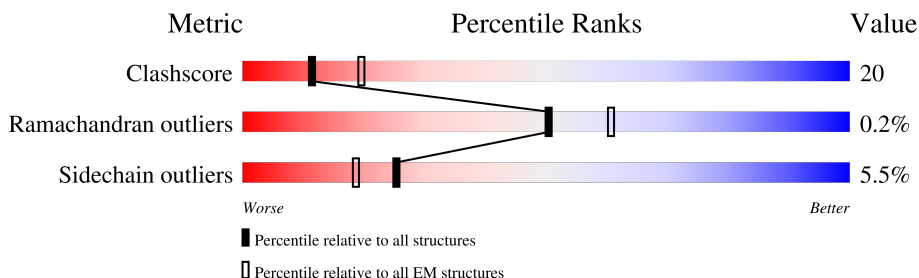
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.00 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.





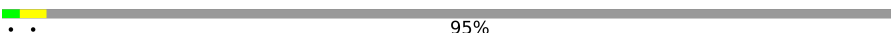

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1A	115	95%
2	1B	258	28% 19% 52%
3	1C	264	16% 8% 76%
4	1D	476	37% 15% 48%
5	1G	727	96%
6	1H	318	98%
7	1I	239	33% 19% 46%
8	1P	377	95%

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Mol	Chain	Length	Quality of chain
9	1Q	175	 7% 89%
10	1R	123	 22% 7% 71%
11	1W	128	 95%
12	1q	145	 28% 70%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	SF4	1B	301	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 5152 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	6	Total	C	N	O	S	0	1
			34	23	5	5	1		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	125	Total	C	N	O	S	0	5
			911	581	157	159	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	63	Total	C	N	O	S	0	8
			433	283	70	79	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	246	Total	C	N	O	S	0	17
			1756	1141	302	300	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	-13	GLY	GLU	conflict	UNP A0A8D0QM68

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1G	30	Total	C	N	O	S	0	4
			196	118	36	38	4		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1H	7	Total	C	N	O	0	2
			34	18	6	10		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1I	128	Total	C	N	O	S	0	1
			997	625	175	188	9		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1P	17	Total	C	N	O	S	0	2
			95	56	21	17	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1Q	20	Total	C	N	O	S	0	0
			150	93	27	29	1		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1R	36	Total	C	N	O	S	0	6
			202	124	42	35	1		

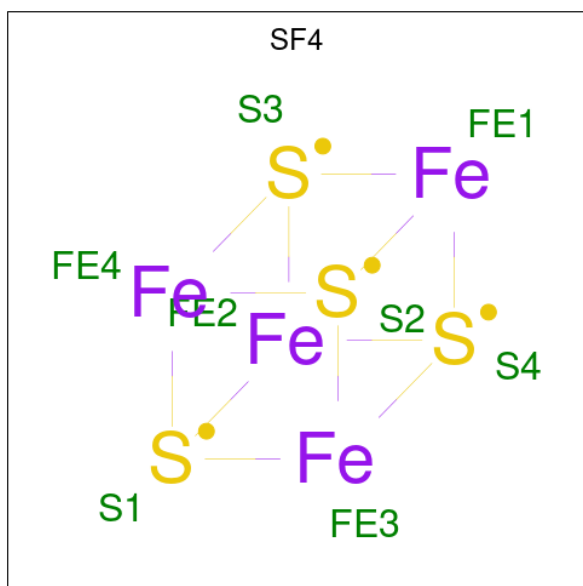
- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	1W	7	Total	C	N	O	0	3
			33	19	9	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1q	44	Total	C	N	O	S	0	5
			286	181	54	49	2		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	1B	1	Total	Fe	S	0
			8	4	4	
13	1I	1	Total	Fe	S	0
			8	4	4	
13	1I	1	Total	Fe	S	0
			8	4	4	

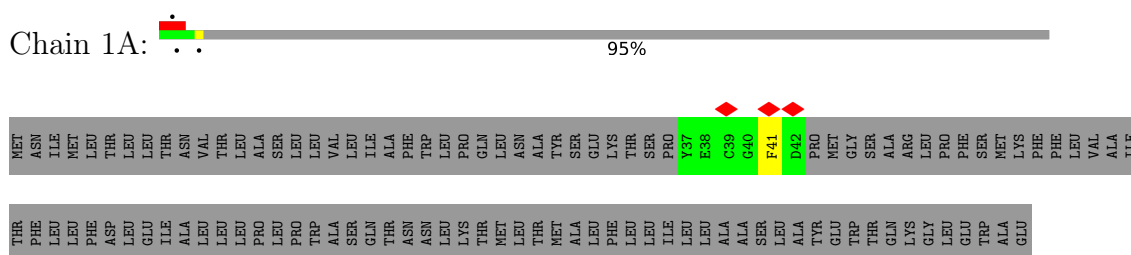
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	1R	1	Total	Zn	0
			1	1	

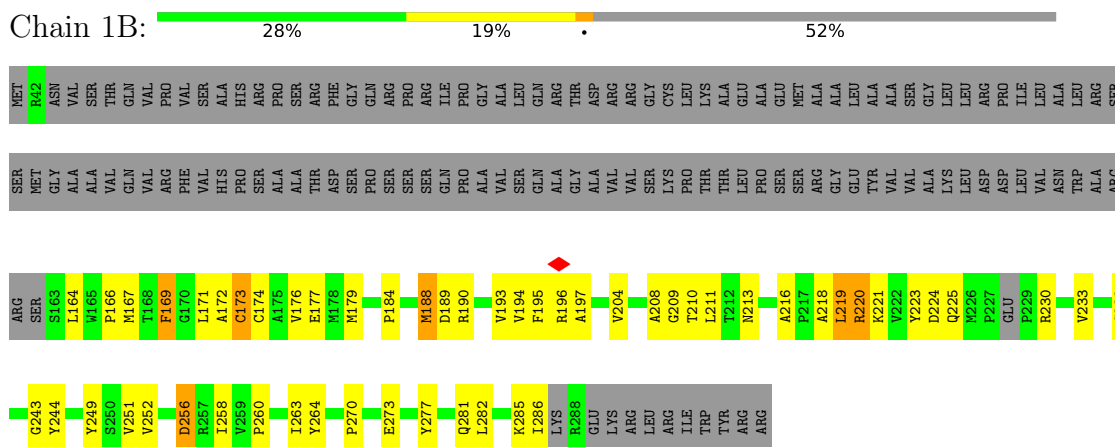
3 Residue-property plots

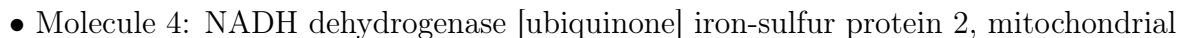
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: NADH-ubiquinone oxidoreductase chain 3



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



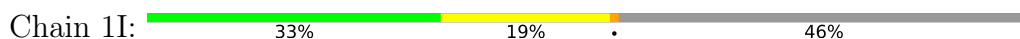


[illegible]

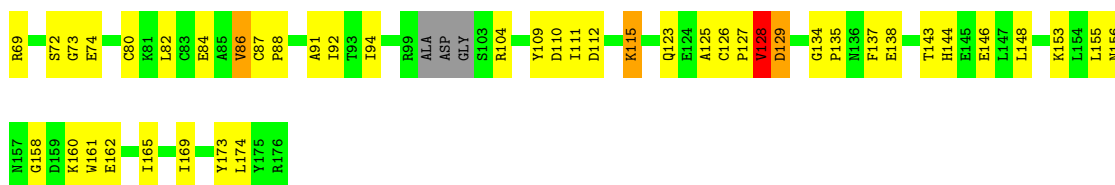
- Molecule 6: NADH-ubiquinone oxidoreductase chain 1

[illegible]

- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

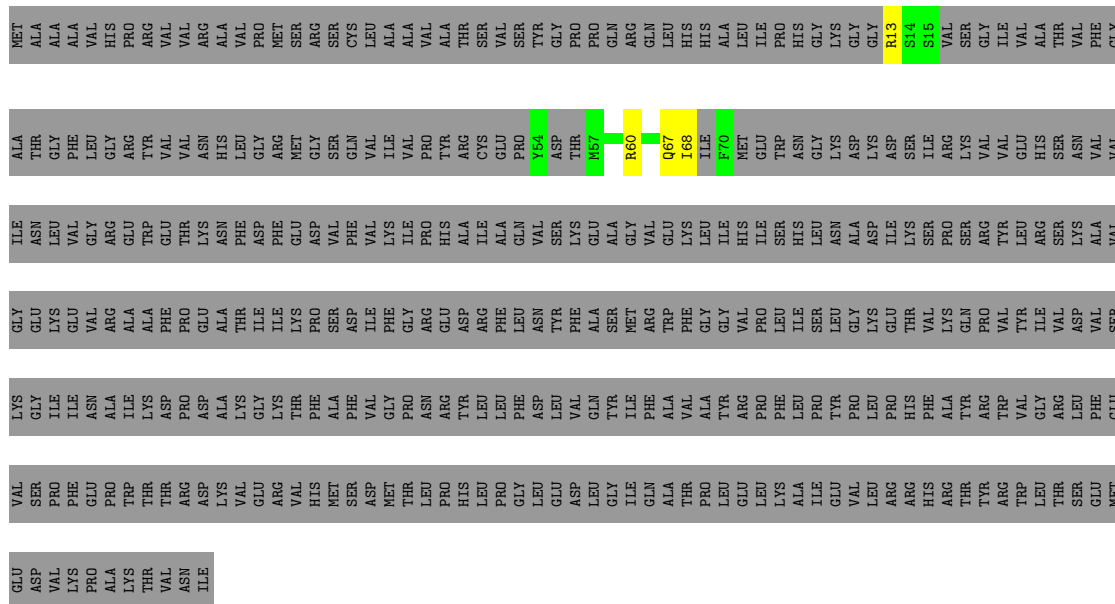


MET	GLU	ALA	ALA	SER	GLN	GLU	CYS	ARG	LEU	VAL	ASP	ARG	PRO	PRO	HIS	GLY	LYS	GLU	ARG	GLN	ARG	PHE	LYS	MET	ARG	CYS	LEU	LEU	SER	THR	PRO	MET	LEU	LEU	ALA	ALA	GLN	ALA	ALA	HIS	ALA	ALA	GLY	HIS	PRO	SER	SER	SER	ALA							
VAL	ALA	ALA	ALA	THR	TYR	LYS	PHE	VAL	VAL	ASN	MET	ARG	ARG	GLU	GLU	PRO	SER	LYS	LYS	SER	VAL	VAL	THR	THR	ASP	ASP	LYS	ARG	ALA	ALA	GLN	THR	THR	GLY	LEU	LEU	GLY	GLY	GLU	THR	SER	THR	LEU	PHE	ARG	GLU	PRO	A46	Y50	P51	K64	E64	H65	A66	L67	F68



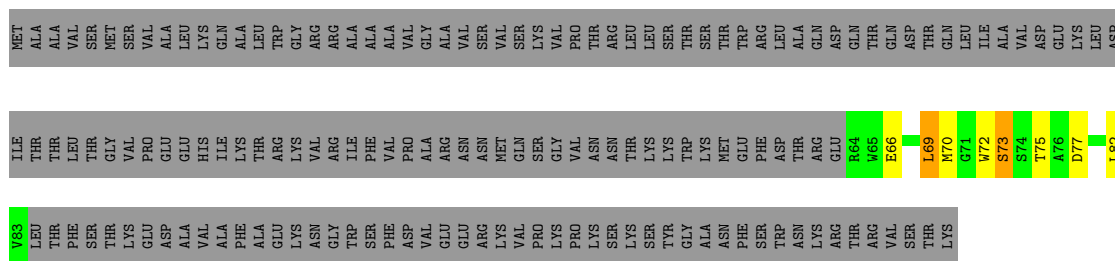
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain 1P: 95%



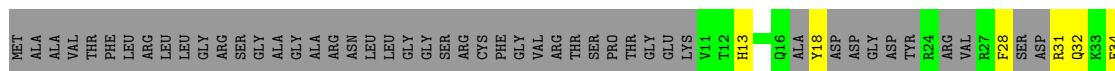
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

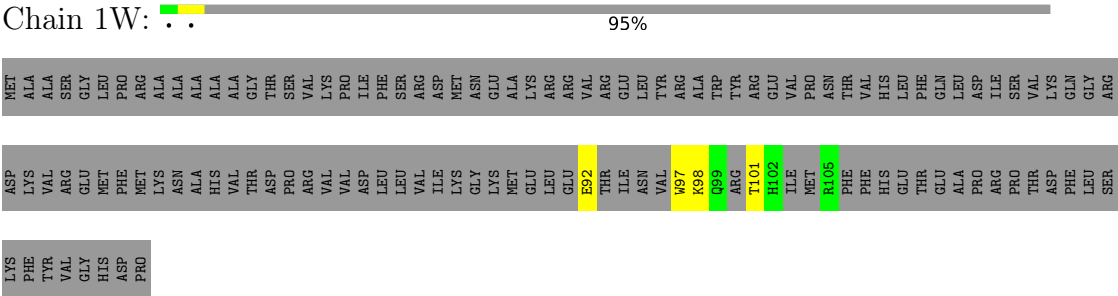
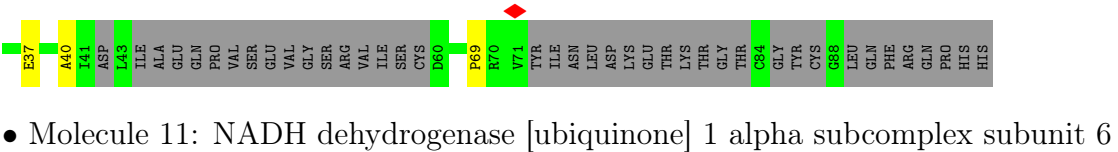
Chain 1Q:  7% 2% 89%



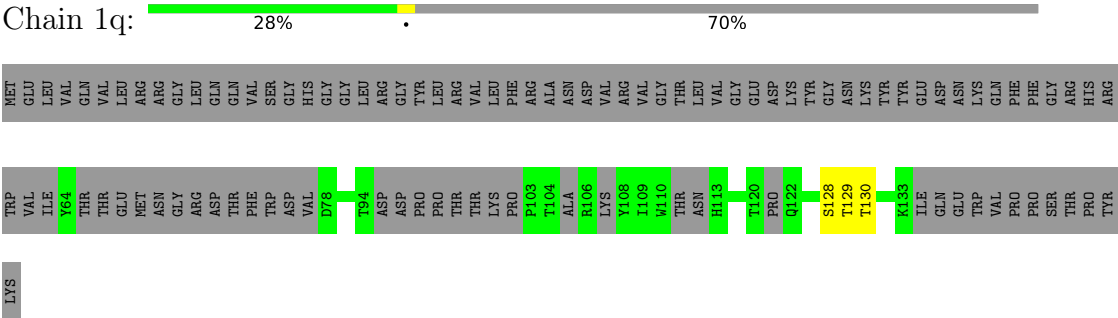
- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:





- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	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)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.369	Depositor
Minimum map value	-1.193	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	108.16, 108.16, 108.16	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.416, 0.416, 0.416	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: SF4, ZN

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	1A	0.30	0/34	0.50	0/43
2	1B	0.45	0/926	0.67	1/1246 (0.1%)
3	1C	0.31	0/425	0.49	0/553
4	1D	0.35	0/1756	0.52	0/2313
5	1G	0.27	0/186	0.62	0/228
6	1H	0.26	0/27	0.68	0/31
7	1I	0.46	0/1014	0.68	1/1363 (0.1%)
8	1P	0.28	0/89	0.61	0/111
9	1Q	0.26	0/153	0.55	0/204
10	1R	0.27	0/190	0.53	0/236
11	1W	0.20	0/29	0.67	0/32
12	1q	0.29	0/284	0.44	0/372
All	All	0.38	0/5113	0.59	2/6732 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1I	123	GLN	C-N-CA	-5.20	108.70	121.70
2	1B	188	MET	CG-SD-CE	-5.14	91.97	100.20

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	1A	34	0	23	1	0
2	1B	911	0	894	64	0
3	1C	433	0	370	19	0
4	1D	1756	0	1678	56	0
5	1G	196	0	162	10	0
6	1H	34	0	27	4	0
7	1I	997	0	942	40	0
8	1P	95	0	76	2	0
9	1Q	150	0	124	11	0
10	1R	202	0	164	9	0
11	1W	33	0	26	2	0
12	1q	286	0	238	0	0
13	1B	8	0	0	3	0
13	1I	16	0	0	0	0
14	1R	1	0	0	0	0
All	All	5152	0	4724	187	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 20.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1R:18:TYR:CD2	10:1R:18:TYR:CD1	2.38	1.05
10:1R:28:PHE:CG	10:1R:28:PHE:CE2	2.39	0.99
4:1D:364:TYR:CE2	4:1D:364:TYR:CG	2.40	0.96
2:1B:238:CYS:HG	13:1B:301:SF4:FE1	0.71	0.96
4:1D:364:TYR:CG	4:1D:364:TYR:CA	2.53	0.92
4:1D:342:MET:CA	4:1D:342:MET:CG	2.52	0.88
4:1D:416:ALA:C	4:1D:417:ILE:CA	2.43	0.86
11:1W:97:TRP:C	11:1W:98:LYS:CA	2.43	0.86
5:1G:213:TYR:C	5:1G:214:ALA:CA	2.43	0.86
3:1C:164:LYS:CA	3:1C:164:LYS:CG	2.54	0.86
3:1C:78:LEU:C	3:1C:79:THR:CA	2.44	0.85
5:1G:224:LYS:CA	5:1G:224:LYS:CG	2.54	0.85
9:1Q:69:LEU:HD23	9:1Q:70:MET:HG2	1.59	0.84
3:1C:79:THR:CA	3:1C:80:ALA:N	2.41	0.83
4:1D:257:GLY:CA	4:1D:258:VAL:N	2.41	0.83
8:1P:67:GLN:CA	8:1P:68:ILE:N	2.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:381:ASP:CA	4:1D:382:GLY:N	2.45	0.80
2:1B:256:ASP:OD1	2:1B:264:TYR:OH	1.98	0.80
2:1B:238:CYS:SG	13:1B:301:SF4:FE1	1.75	0.79
4:1D:258:VAL:N	4:1D:258:VAL:CB	2.46	0.79
2:1B:286:ILE:CB	2:1B:286:ILE:N	2.46	0.78
4:1D:328:ALA:HB3	5:1G:126:ASP:HB2	1.64	0.78
10:1R:31:ARG:NE	10:1R:31:ARG:CG	2.46	0.78
9:1Q:77:ASP:CA	9:1Q:77:ASP:CG	2.53	0.77
8:1P:68:ILE:N	8:1P:68:ILE:CB	2.49	0.75
3:1C:158:GLU:N	3:1C:158:GLU:C	2.42	0.73
7:1I:72:SER:C	7:1I:72:SER:N	2.43	0.72
6:1H:32:GLN:OE1	6:1H:34:ARG:NH1	2.22	0.72
3:1C:130:TYR:CA	3:1C:130:TYR:O	2.38	0.72
3:1C:173:GLU:HG3	3:1C:188:VAL:HA	1.70	0.72
4:1D:210:ASP:CB	4:1D:210:ASP:OD2	2.38	0.71
6:1H:206:GLU:O	6:1H:206:GLU:CA	2.39	0.71
10:1R:37:GLU:OE2	10:1R:37:GLU:CG	2.38	0.70
2:1B:196:ARG:HG3	2:1B:197:ALA:H	1.56	0.69
4:1D:300:ARG:O	4:1D:300:ARG:CA	2.41	0.69
3:1C:134:ILE:CA	3:1C:134:ILE:O	2.41	0.69
5:1G:243:ARG:HG2	5:1G:244:THR:HG23	1.74	0.69
2:1B:209:GLY:HA2	13:1B:301:SF4:S2	2.34	0.68
4:1D:416:ALA:C	4:1D:416:ALA:N	2.46	0.68
4:1D:62:LEU:HB2	4:1D:425:PHE:CZ	2.30	0.67
2:1B:211:LEU:O	2:1B:252:VAL:HG12	1.94	0.67
2:1B:263:ILE:HD12	2:1B:281:GLN:HG2	1.77	0.67
3:1C:151:ILE:HG23	3:1C:152:LEU:HG	1.79	0.65
2:1B:211:LEU:HD11	2:1B:216:ALA:HA	1.78	0.64
2:1B:196:ARG:HH11	2:1B:197:ALA:H	1.43	0.63
2:1B:188:MET:CE	2:1B:195:PHE:HD1	2.10	0.63
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.30	0.62
2:1B:166:PRO:HD2	2:1B:194:VAL:O	1.99	0.62
2:1B:196:ARG:HG3	2:1B:196:ARG:HH11	1.63	0.62
4:1D:143:GLU:OE1	4:1D:278:TYR:OH	2.16	0.62
7:1I:135:PRO:HD3	7:1I:165:ILE:HG22	1.81	0.62
2:1B:179:MET:HA	2:1B:195:PHE:HZ	1.65	0.62
2:1B:223:TYR:O	2:1B:230:ARG:NH1	2.33	0.61
7:1I:156:ASN:ND2	10:1R:34:GLU:OE1	2.34	0.60
2:1B:177:GLU:HG2	2:1B:270:PRO:O	2.02	0.59
4:1D:145:THR:HG1	4:1D:181:TYR:HH	1.46	0.59
9:1Q:77:ASP:OD1	9:1Q:77:ASP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1I:112:ASP:OD2	7:1I:115:LYS:HD3	2.04	0.57
4:1D:100:LEU:HD22	4:1D:195:ARG:HD3	1.85	0.57
9:1Q:75:THR:OG1	9:1Q:77:ASP:OD1	2.22	0.57
2:1B:184:PRO:HA	6:1H:34:ARG:HG2	1.86	0.56
4:1D:94:LYS:HD2	4:1D:102:TYR:HE2	1.70	0.56
2:1B:188:MET:HB2	2:1B:193:VAL:HB	1.88	0.56
2:1B:188:MET:CE	2:1B:195:PHE:CD1	2.88	0.56
1:1A:41:PHE:CZ	2:1B:218:ALA:HB2	2.41	0.55
4:1D:427:GLU:O	4:1D:430:ARG:HG3	2.07	0.55
7:1I:64:GLU:O	7:1I:134:GLY:N	2.33	0.55
4:1D:348:HIS:HE1	7:1I:125:ALA:O	1.89	0.55
5:1G:218:ARG:HD2	5:1G:220:TRP:CH2	2.41	0.55
7:1I:69:ARG:NH1	7:1I:73:GLY:O	2.39	0.55
2:1B:188:MET:HE2	2:1B:195:PHE:HD1	1.70	0.54
2:1B:188:MET:HE2	2:1B:195:PHE:CD1	2.42	0.54
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.88	0.54
2:1B:251:VAL:CG2	4:1D:85:ARG:HG2	2.38	0.54
4:1D:144:ILE:HG23	4:1D:177:MET:HG2	1.90	0.53
5:1G:224:LYS:CG	5:1G:224:LYS:N	2.72	0.53
5:1G:215:PHE:HB3	7:1I:104:ARG:HG3	1.90	0.52
7:1I:91:ALA:O	7:1I:111:ILE:HA	2.09	0.52
4:1D:363:THR:O	4:1D:377:TYR:HA	2.09	0.52
4:1D:428:VAL:O	4:1D:430:ARG:NH1	2.43	0.52
2:1B:213:ASN:HB3	3:1C:174:LEU:HD22	1.92	0.51
4:1D:183:ARG:NH1	4:1D:210:ASP:OD2	2.31	0.51
4:1D:121:ALA:HA	4:1D:365:THR:HG21	1.91	0.51
2:1B:251:VAL:HG21	4:1D:85:ARG:HG2	1.92	0.51
2:1B:169:PHE:CD2	2:1B:219:LEU:HD12	2.45	0.51
2:1B:169:PHE:HD2	2:1B:219:LEU:HD12	1.76	0.51
4:1D:88:GLU:OE2	4:1D:390:LYS:HD2	2.11	0.51
4:1D:151:ILE:HD11	4:1D:218:PHE:CZ	2.46	0.51
3:1C:155:TYR:HD1	11:1W:92:GLU:OE1	1.94	0.51
4:1D:354:GLU:OE2	4:1D:357:GLN:NE2	2.44	0.50
9:1Q:70:MET:HE2	9:1Q:72:TRP:CH2	2.47	0.50
7:1I:80:CYS:SG	7:1I:82:LEU:HG	2.52	0.49
10:1R:13:HIS:HD1	10:1R:13:HIS:H	1.59	0.49
2:1B:220:ARG:HG2	3:1C:176:TYR:CD2	2.46	0.49
7:1I:72:SER:N	7:1I:73:GLY:N	2.60	0.49
2:1B:196:ARG:CG	2:1B:197:ALA:H	2.24	0.49
2:1B:211:LEU:HD23	2:1B:252:VAL:HG11	1.93	0.49
2:1B:188:MET:HE1	2:1B:195:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:134:ILE:O	3:1C:138:PHE:N	2.45	0.49
2:1B:256:ASP:OD2	7:1I:144:HIS:HD2	1.96	0.49
2:1B:184:PRO:HD3	4:1D:168:PHE:HB3	1.95	0.49
7:1I:66:ALA:HB1	7:1I:158:GLY:CA	2.43	0.48
4:1D:373:GLU:OE1	4:1D:392:LYS:NZ	2.46	0.48
7:1I:126:CYS:SG	7:1I:128:VAL:HG23	2.52	0.48
2:1B:263:ILE:HG13	2:1B:282:LEU:HB2	1.95	0.48
4:1D:62:LEU:HD22	4:1D:425:PHE:HZ	1.78	0.48
7:1I:148:LEU:HD23	9:1Q:70:MET:HG3	1.95	0.48
2:1B:273:GLU:HG2	7:1I:137:PHE:HE2	1.77	0.48
4:1D:62:LEU:HD11	4:1D:78:PRO:HB3	1.95	0.47
7:1I:160:LYS:HD2	7:1I:161:TRP:NE1	2.29	0.47
4:1D:371:LYS:HZ2	4:1D:422:ASP:HB2	1.79	0.47
7:1I:84:GLU:HB2	7:1I:94:ILE:HD12	1.96	0.47
2:1B:171:LEU:HB2	2:1B:209:GLY:HA3	1.97	0.47
2:1B:243:GLY:HA2	7:1I:115:LYS:HA	1.97	0.47
2:1B:233:VAL:HG22	2:1B:263:ILE:HB	1.96	0.47
4:1D:349:PHE:CE2	7:1I:82:LEU:HD21	2.49	0.47
3:1C:173:GLU:O	3:1C:174:LEU:HD12	2.15	0.47
7:1I:67:LEU:HD11	7:1I:109:TYR:CD1	2.49	0.47
4:1D:100:LEU:HD13	4:1D:196:PRO:HD3	1.96	0.47
7:1I:50:TYR:CD1	7:1I:51:PRO:HA	2.50	0.46
2:1B:164:LEU:O	2:1B:166:PRO:HD3	2.15	0.46
4:1D:171:PHE:HA	4:1D:174:ARG:HB2	1.97	0.46
4:1D:342:MET:CG	4:1D:342:MET:C	2.84	0.46
7:1I:67:LEU:O	7:1I:158:GLY:HA3	2.14	0.46
3:1C:192:GLN:HB2	9:1Q:72:TRP:CD1	2.50	0.46
2:1B:172:ALA:HB2	4:1D:83:LEU:HD21	1.97	0.46
2:1B:221:LYS:O	2:1B:225:GLN:HG3	2.16	0.46
4:1D:148:LEU:HD23	4:1D:174:ARG:HG2	1.98	0.46
7:1I:153:LYS:HA	7:1I:153:LYS:HD2	1.72	0.46
4:1D:414:VAL:C	4:1D:414:VAL:CG1	2.85	0.46
4:1D:258:VAL:N	4:1D:258:VAL:CG2	2.79	0.45
4:1D:424:VAL:O	4:1D:427:GLU:HG2	2.16	0.45
2:1B:174:CYS:HB3	2:1B:208:ALA:HB1	1.97	0.45
3:1C:199:LEU:HD12	4:1D:385:ARG:HH11	1.80	0.45
7:1I:143:THR:OG1	7:1I:146:GLU:HG3	2.17	0.45
3:1C:184:VAL:HG23	3:1C:186:GLU:OE1	2.16	0.45
7:1I:169:ILE:O	7:1I:173:TYR:N	2.47	0.45
2:1B:164:LEU:HD23	2:1B:164:LEU:HA	1.84	0.45
7:1I:74:GLU:HA	10:1R:40:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:189:ASP:OD1	2:1B:194:VAL:HG12	2.17	0.45
7:1I:92:ILE:HA	7:1I:110:ASP:O	2.17	0.45
2:1B:277:TYR:CE2	7:1I:138:GLU:HB3	2.53	0.44
2:1B:196:ARG:HD2	2:1B:196:ARG:HA	1.75	0.44
2:1B:223:TYR:CZ	2:1B:260:PRO:HD2	2.53	0.44
4:1D:147:LEU:HD22	4:1D:218:PHE:HE2	1.83	0.44
2:1B:173:CYS:HB3	4:1D:108:TYR:HB2	2.00	0.44
2:1B:196:ARG:HH11	2:1B:197:ALA:N	2.13	0.44
5:1G:213:TYR:HE1	5:1G:248:MET:HB3	1.82	0.44
7:1I:129:ASP:N	7:1I:129:ASP:OD1	2.51	0.43
4:1D:78:PRO:HG3	4:1D:402:LEU:HD23	2.00	0.43
2:1B:285:LYS:HB3	2:1B:285:LYS:HE2	1.65	0.43
2:1B:176:VAL:HA	2:1B:179:MET:HG2	2.00	0.43
2:1B:179:MET:HG3	4:1D:171:PHE:HE2	1.83	0.43
4:1D:151:ILE:HD11	4:1D:218:PHE:HZ	1.84	0.43
2:1B:184:PRO:HB3	6:1H:33:LEU:O	2.19	0.43
7:1I:162:GLU:HA	7:1I:165:ILE:HG12	1.99	0.42
2:1B:164:LEU:O	2:1B:193:VAL:HG13	2.20	0.42
7:1I:174:LEU:HD23	7:1I:174:LEU:HA	1.76	0.42
2:1B:220:ARG:NH1	2:1B:224:ASP:OD1	2.52	0.42
2:1B:273:GLU:OE1	7:1I:54:LYS:HB3	2.19	0.42
7:1I:86:VAL:O	7:1I:87:CYS:C	2.56	0.42
2:1B:211:LEU:HD11	2:1B:216:ALA:CA	2.49	0.42
4:1D:121:ALA:HB2	4:1D:365:THR:OG1	2.19	0.42
7:1I:66:ALA:HB1	7:1I:158:GLY:HA2	2.02	0.42
9:1Q:82:LEU:HD23	9:1Q:82:LEU:HA	1.79	0.42
2:1B:188:MET:HE1	2:1B:195:PHE:CD1	2.53	0.42
4:1D:64:LEU:HD22	4:1D:76:CYS:SG	2.60	0.41
5:1G:218:ARG:O	5:1G:221:GLU:HG2	2.20	0.41
2:1B:249:TYR:CZ	3:1C:161:PRO:HB3	2.55	0.41
2:1B:196:ARG:HG3	2:1B:196:ARG:NH1	2.30	0.41
2:1B:196:ARG:NH1	2:1B:197:ALA:HB3	2.35	0.41
3:1C:195:ARG:NH2	7:1I:92:ILE:O	2.54	0.41
2:1B:216:ALA:HB1	2:1B:258:ILE:HD12	2.03	0.41
4:1D:64:LEU:HD11	4:1D:418:ILE:HD11	2.02	0.41
4:1D:328:ALA:HA	4:1D:331:SER:O	2.20	0.41
5:1G:244:THR:HB	9:1Q:73:SER:HB2	2.03	0.41
9:1Q:66:GLU:HA	9:1Q:72:TRP:O	2.20	0.41
10:1R:31:ARG:CB	10:1R:32:GLN:N	2.83	0.41
2:1B:179:MET:HA	2:1B:195:PHE:CZ	2.50	0.41
3:1C:193:GLU:HG2	9:1Q:73:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:119:SER:HA	4:1D:196:PRO:HG3	2.02	0.41
7:1I:84:GLU:HG3	7:1I:92:ILE:O	2.20	0.41
2:1B:167:MET:O	2:1B:167:MET:HG3	2.20	0.40
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.39	0.40
7:1I:127:PRO:O	10:1R:69:PRO:HD3	2.21	0.40
7:1I:87:CYS:HA	7:1I:88:PRO:HD3	1.98	0.40
7:1I:155:LEU:HD23	7:1I:155:LEU:HA	1.88	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	
1	1A	3/115 (3%)	2 (67%)	1 (33%)	0	100	100
2	1B	117/258 (45%)	104 (89%)	13 (11%)	0	100	100
3	1C	42/264 (16%)	41 (98%)	1 (2%)	0	100	100
4	1D	200/476 (42%)	189 (94%)	11 (6%)	0	100	100
5	1G	14/727 (2%)	14 (100%)	0	0	100	100
6	1H	1/318 (0%)	1 (100%)	0	0	100	100
7	1I	121/239 (51%)	115 (95%)	5 (4%)	1 (1%)	19	13
8	1P	10/377 (3%)	7 (70%)	3 (30%)	0	100	100
9	1Q	18/175 (10%)	17 (94%)	1 (6%)	0	100	100
10	1R	21/123 (17%)	20 (95%)	1 (5%)	0	100	100
12	1q	31/145 (21%)	30 (97%)	1 (3%)	0	100	100
All	All	578/3217 (18%)	540 (93%)	37 (6%)	1 (0%)	50	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1I	128	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	2/100 (2%)	2 (100%)	0	100	100
2	1B	96/212 (45%)	87 (91%)	9 (9%)	8	5
3	1C	37/227 (16%)	37 (100%)	0	100	100
4	1D	169/405 (42%)	164 (97%)	5 (3%)	41	41
5	1G	16/610 (3%)	15 (94%)	1 (6%)	18	13
6	1H	2/275 (1%)	2 (100%)	0	100	100
7	1I	103/201 (51%)	99 (96%)	4 (4%)	32	30
8	1P	8/323 (2%)	6 (75%)	2 (25%)	0	0
9	1Q	15/152 (10%)	13 (87%)	2 (13%)	4	2
10	1R	14/97 (14%)	14 (100%)	0	100	100
11	1W	3/112 (3%)	2 (67%)	1 (33%)	0	0
12	1q	25/131 (19%)	22 (88%)	3 (12%)	5	2
All	All	490/2845 (17%)	463 (94%)	27 (6%)	25	17

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1B	169	PHE
2	1B	173	CYS
2	1B	190	ARG
2	1B	204	VAL
2	1B	210	THR
2	1B	219	LEU
2	1B	220	ARG
2	1B	244	TYR
2	1B	256	ASP
4	1D	61	VAL

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Mol	Chain	Res	Type
4	1D	79	HIS
4	1D	109	VAL
4	1D	140	LEU
4	1D	184	VAL
5	1G	242	THR
7	1I	86	VAL
7	1I	115	LYS
7	1I	128	VAL
7	1I	129	ASP
8	1P	13	ARG
8	1P	60	ARG
9	1Q	69	LEU
9	1Q	73	SER
11	1W	101	THR
12	1q	128	SER
12	1q	129	THR
12	1q	130	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	1D	79	HIS
4	1D	190	HIS
4	1D	348	HIS
4	1D	421	GLN
7	1I	144	HIS

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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
13	SF4	1I	202	7	0,12,12	-	-	-		
13	SF4	1I	201	7	0,12,12	-	-	-		
13	SF4	1B	301	2	0,12,12	-	-	-		

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
13	SF4	1I	202	7	-	-	0/6/5/5
13	SF4	1I	201	7	-	-	0/6/5/5
13	SF4	1B	301	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

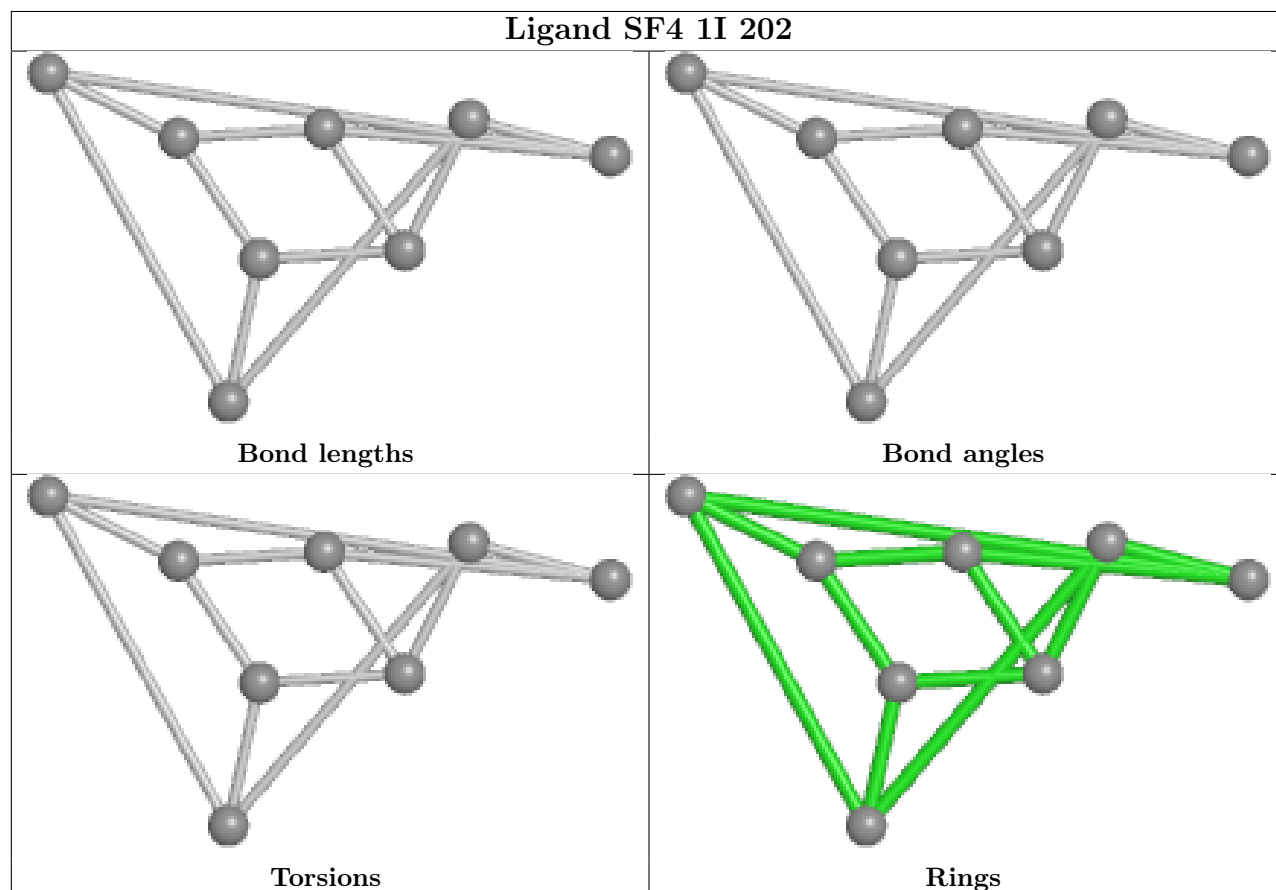
There are no ring outliers.

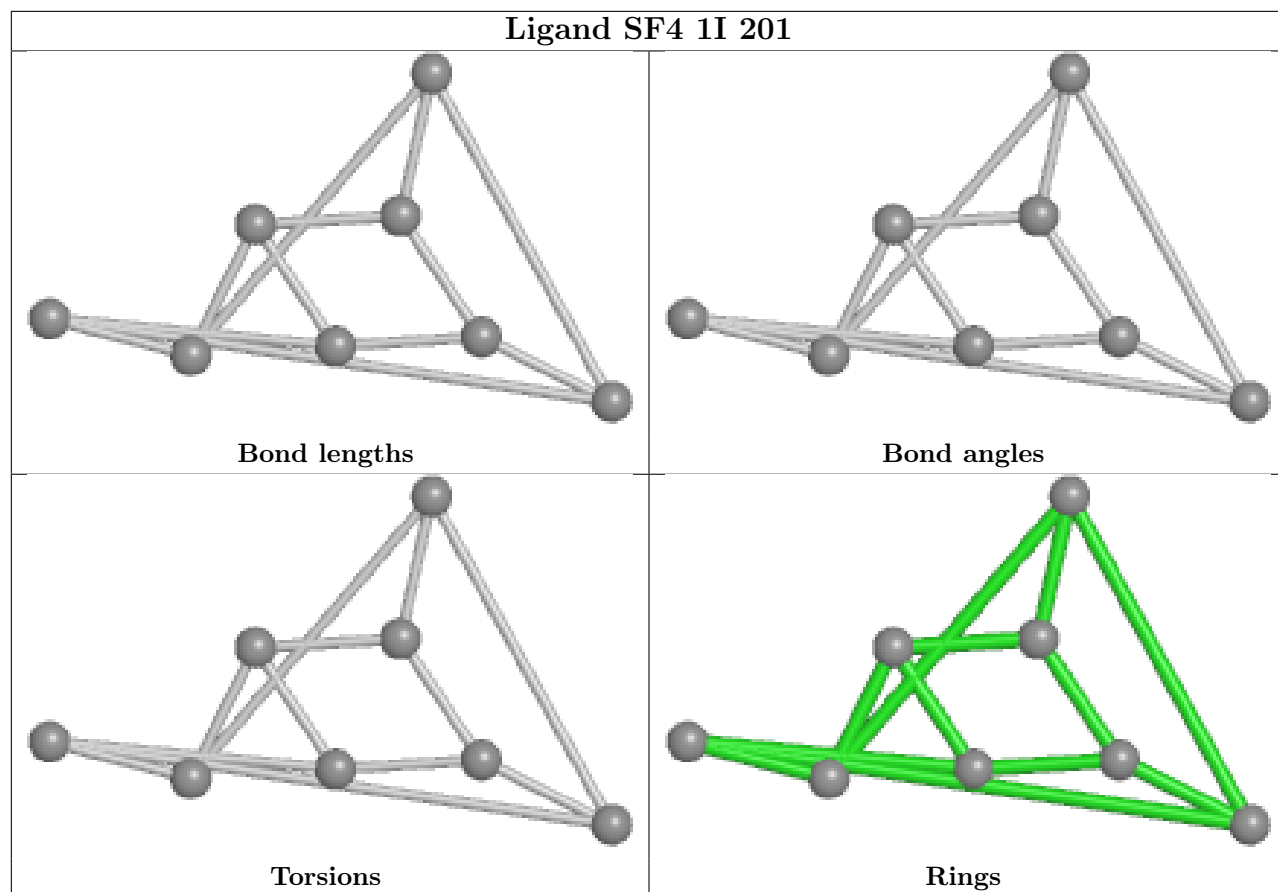
1 monomer is involved in 3 short contacts:

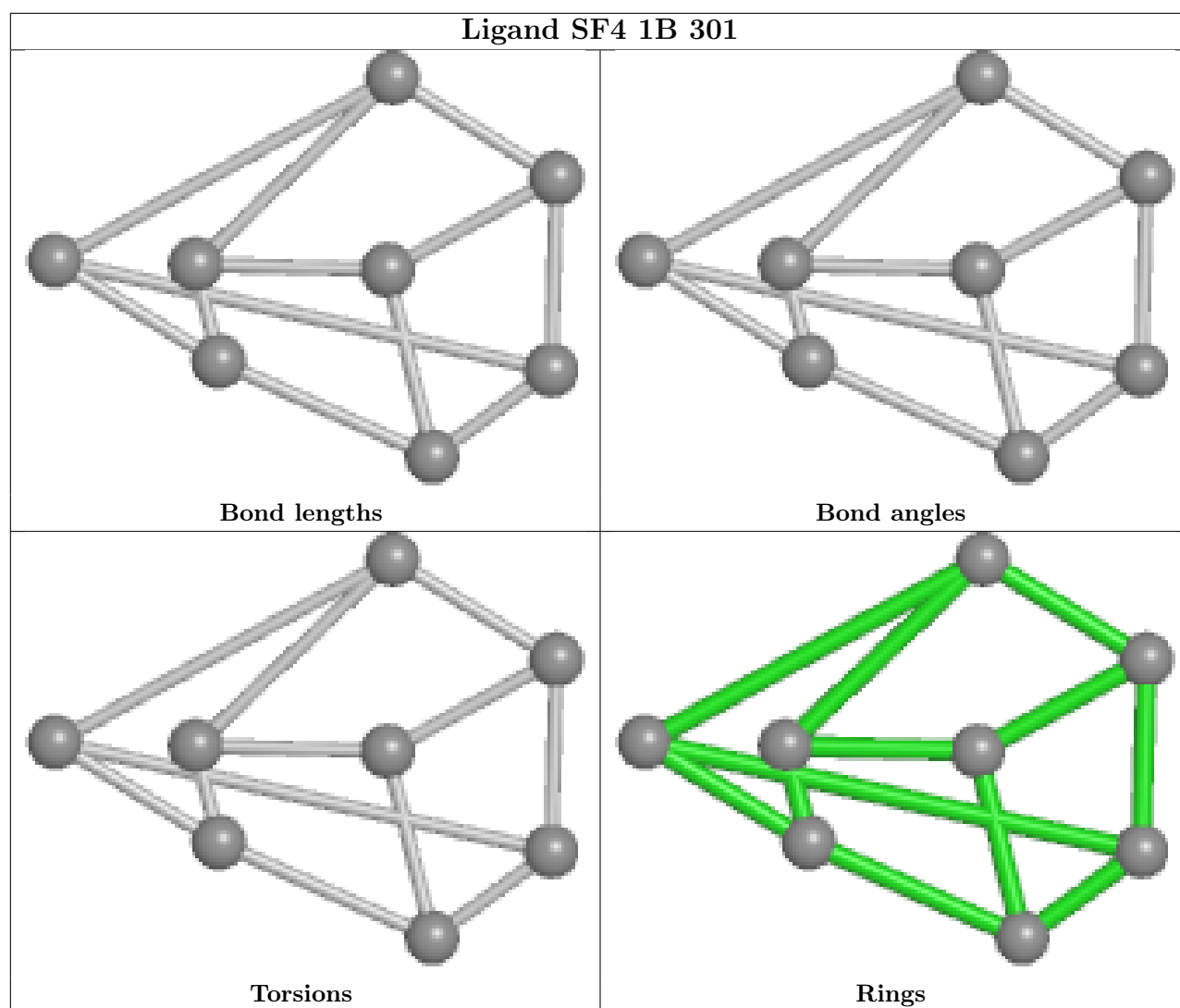
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1B	301	SF4	3	0

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](#)

There are no chain breaks in this entry.

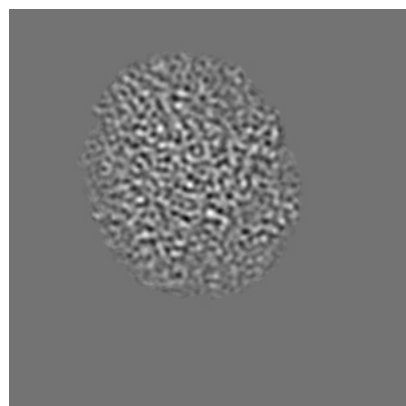
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42231. These allow visual inspection of the internal detail of the map and identification of artifacts.

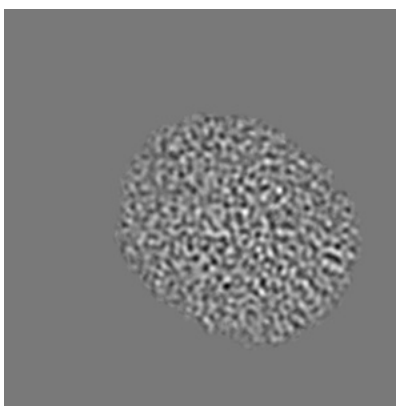
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

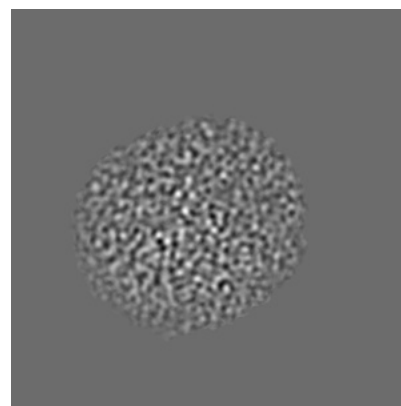
6.1.1 Primary map



X

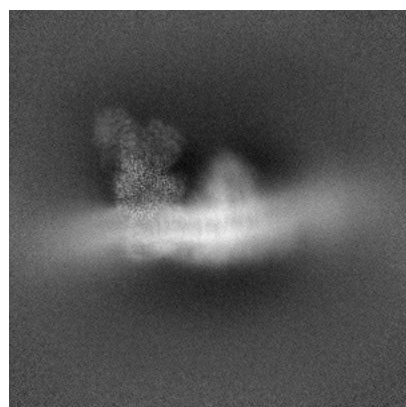


Y

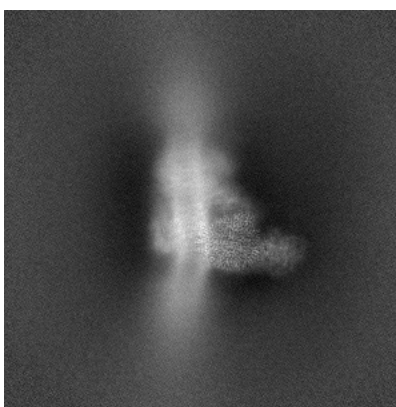


Z

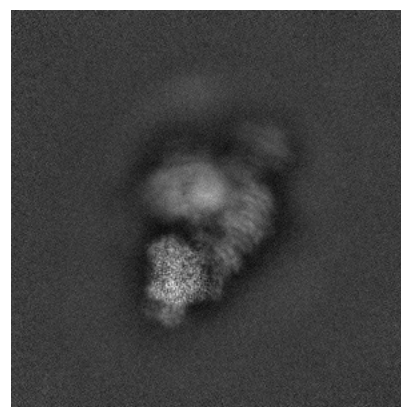
6.1.2 Raw map



X



Y

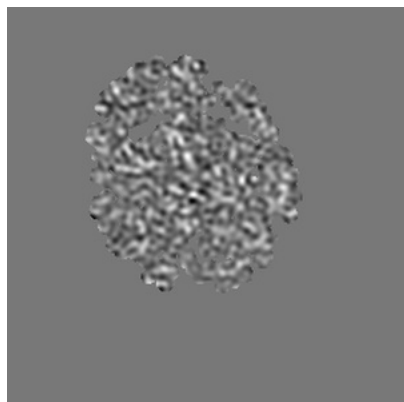


Z

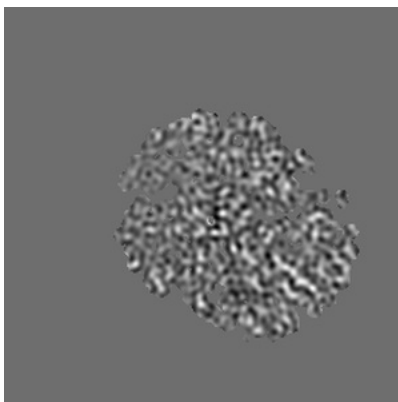
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

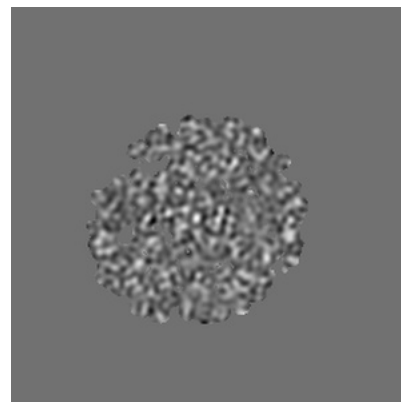
6.2.1 Primary map



X Index: 130



Y Index: 130

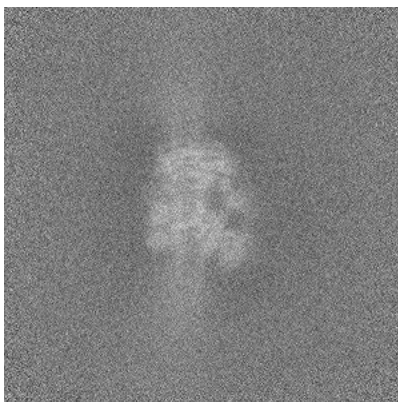


Z Index: 130

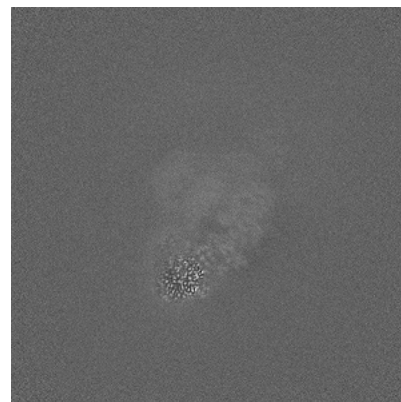
6.2.2 Raw map



X Index: 320



Y Index: 320

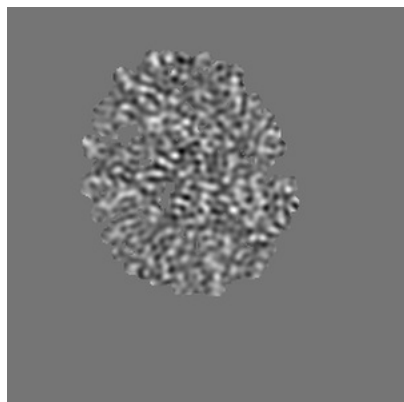


Z Index: 320

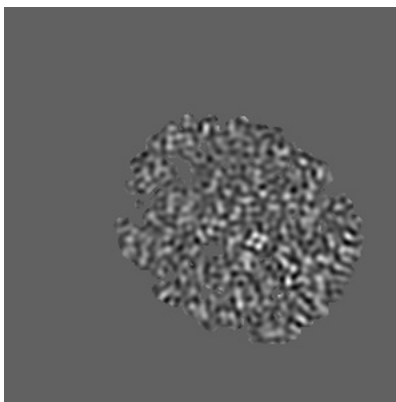
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

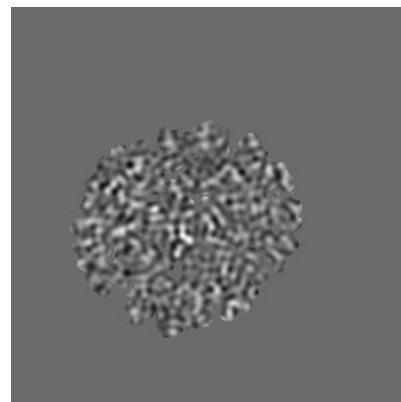
6.3.1 Primary map



X Index: 114

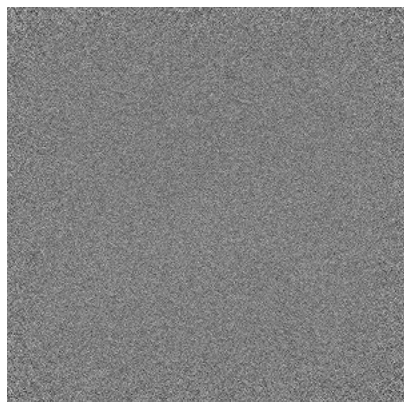


Y Index: 111

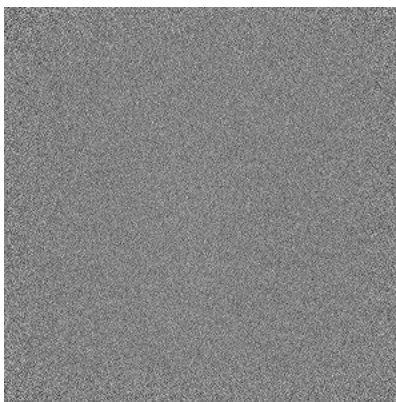


Z Index: 163

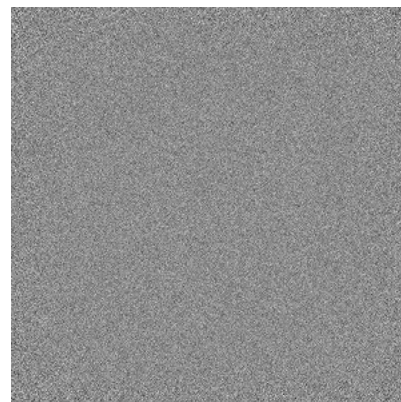
6.3.2 Raw map



X Index: 0



Y Index: 0

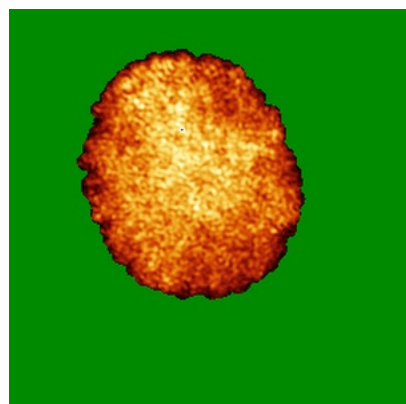


Z Index: 0

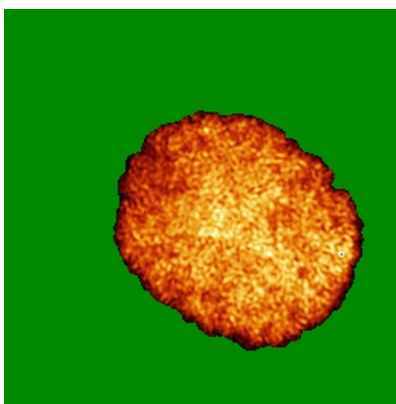
The images above show the largest variance slices of the map in three orthogonal directions.

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

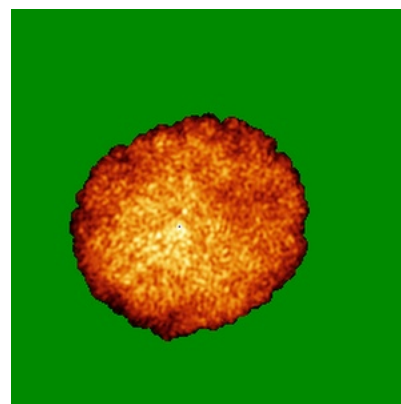
6.4.1 Primary map



X

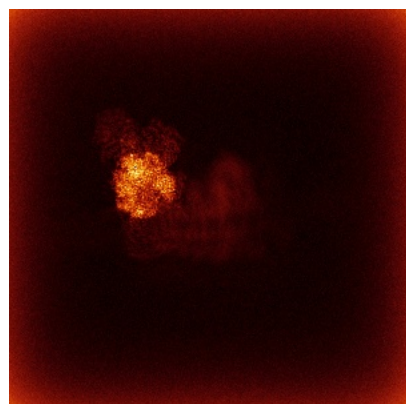


Y

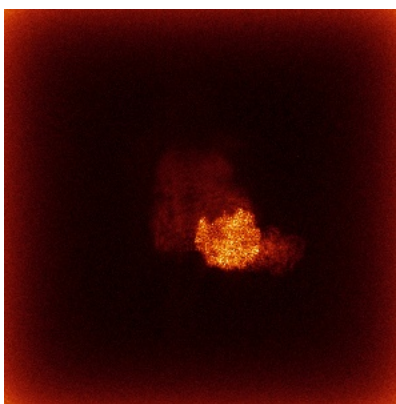


Z

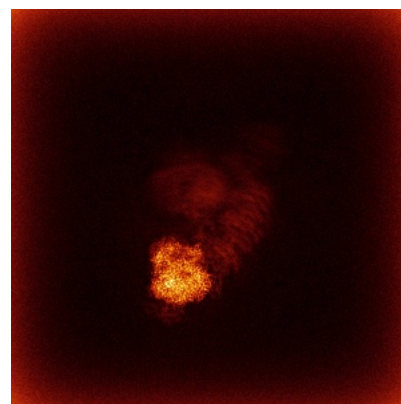
6.4.2 Raw map



X



Y



Z

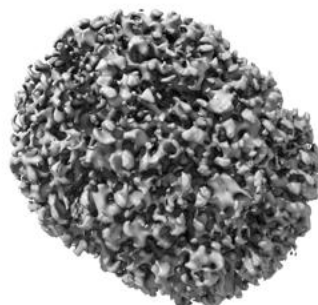
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

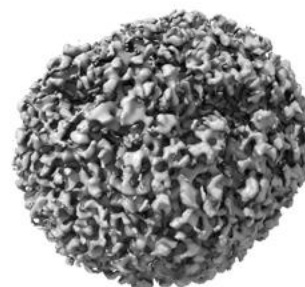
6.5.1 Primary map



X



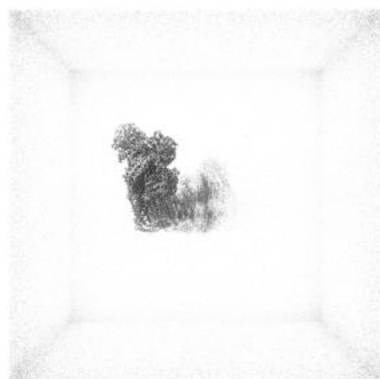
Y



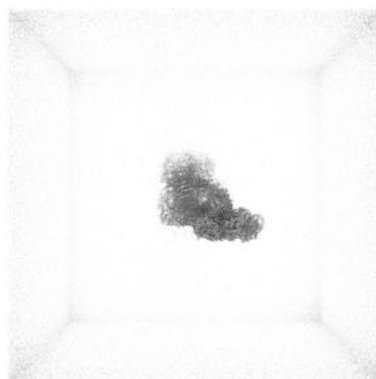
Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

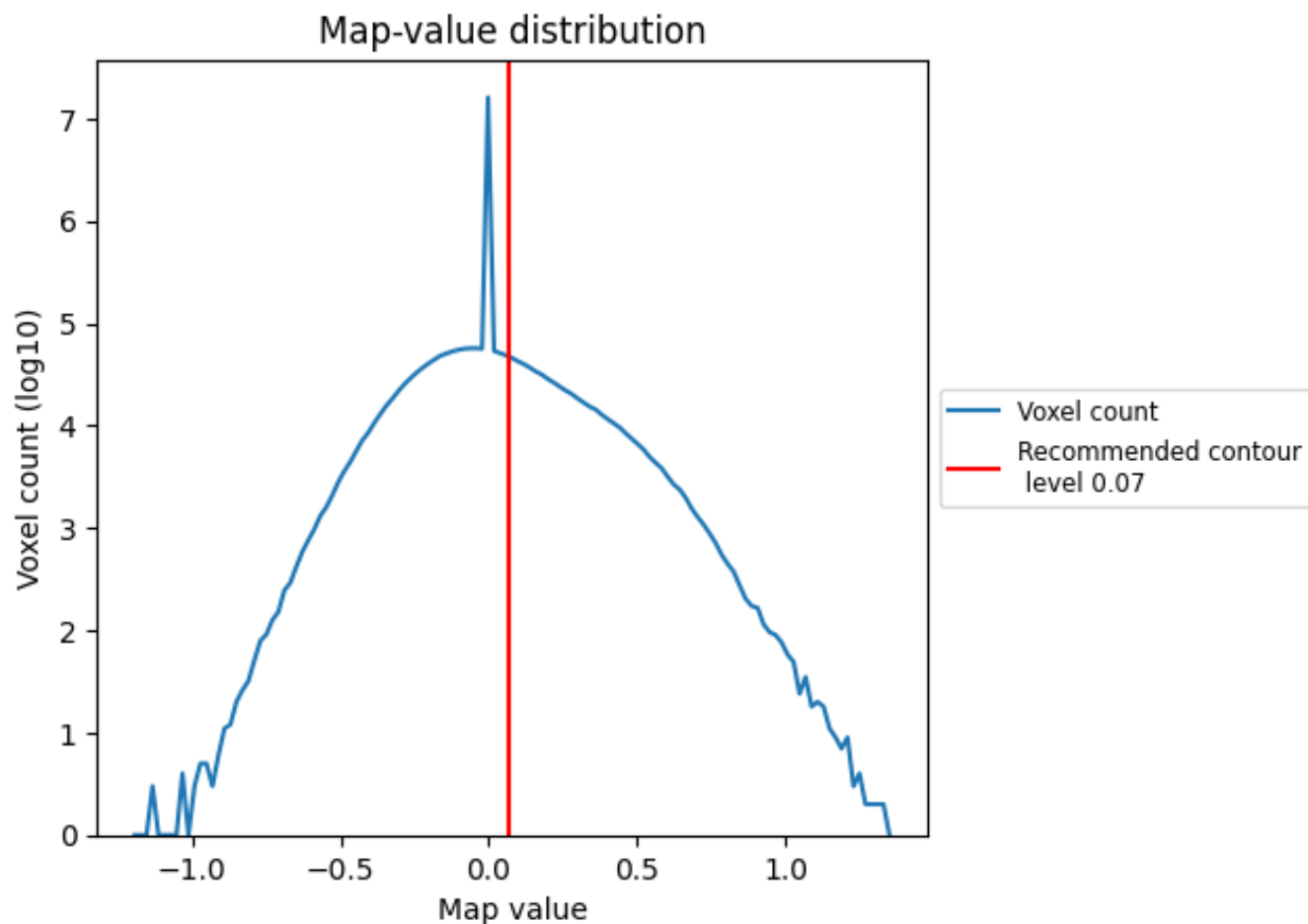
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

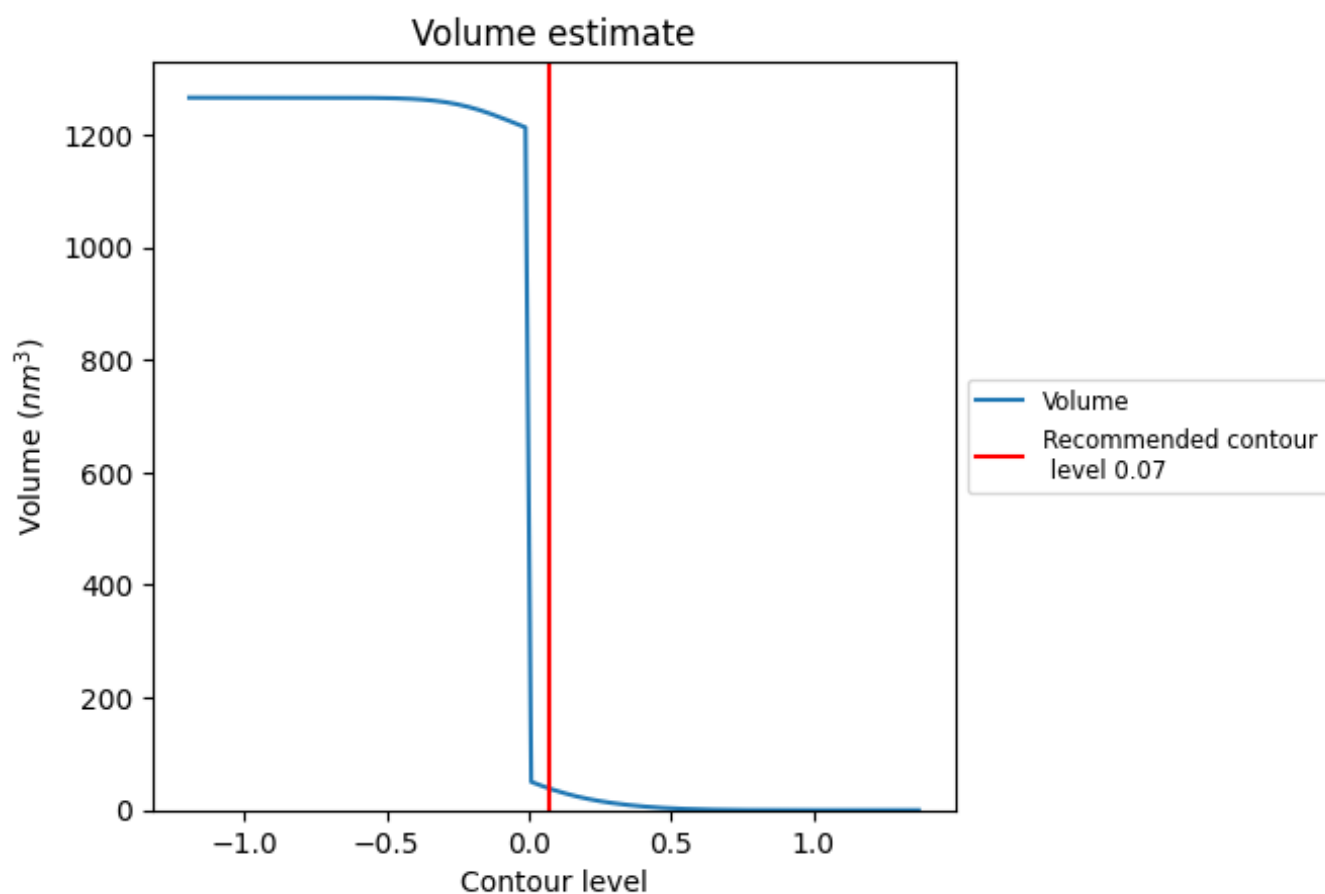
This section contains the results of statistical analysis of the map.

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.

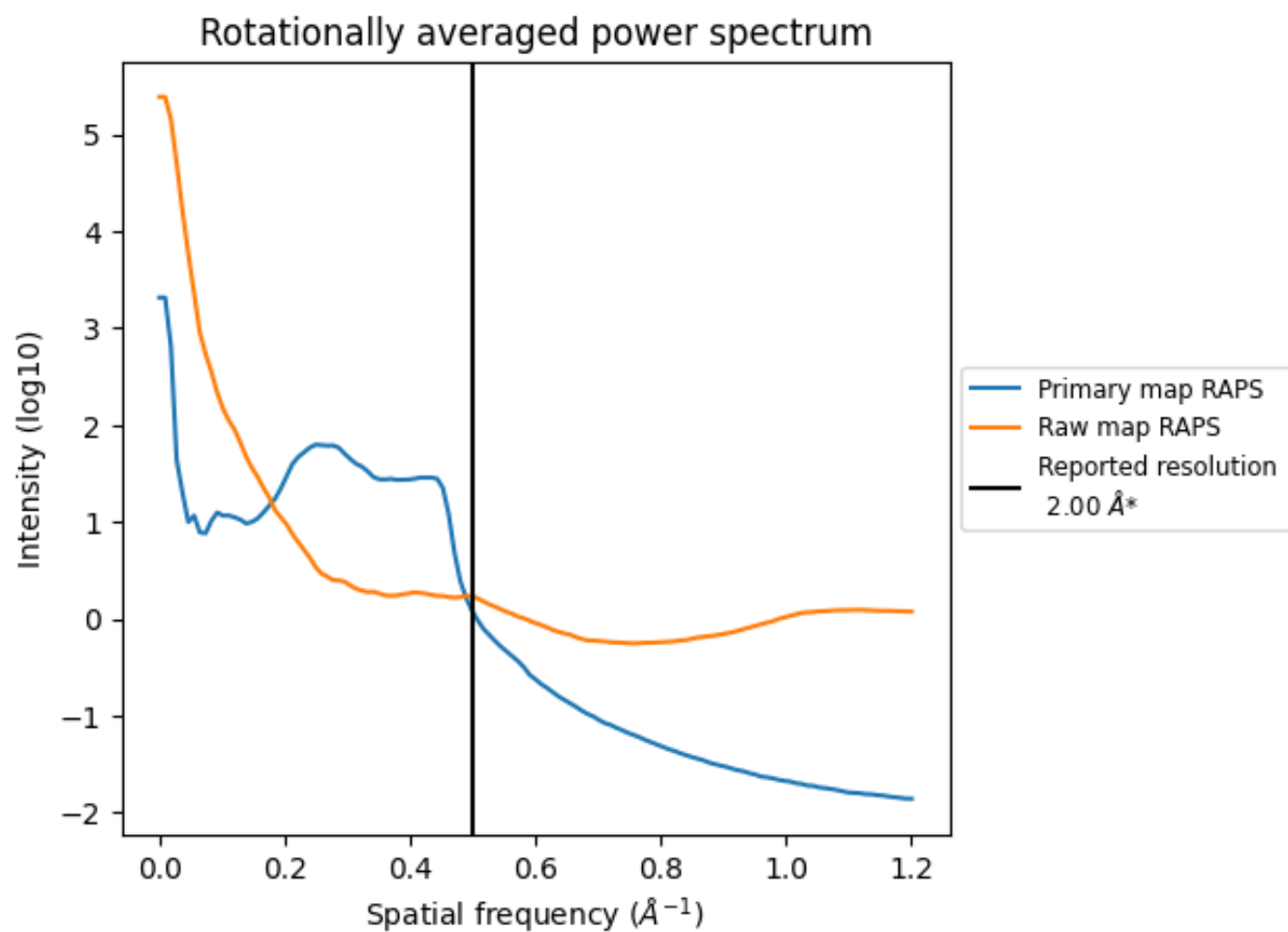
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm^3 ; this corresponds to an approximate mass of 35 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 ⓘ

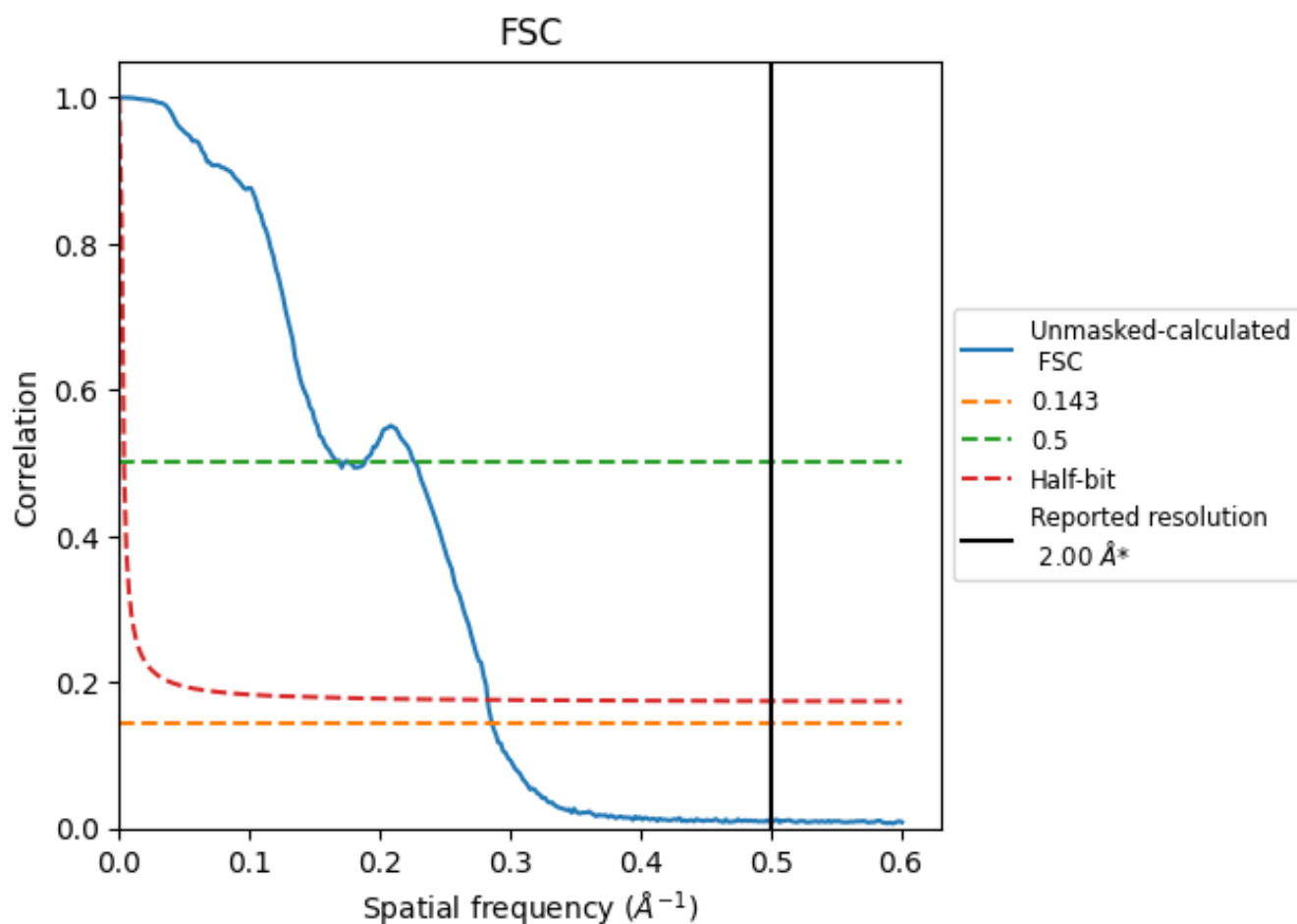


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

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 0.500 Å⁻¹

8.2 Resolution estimates [i](#)

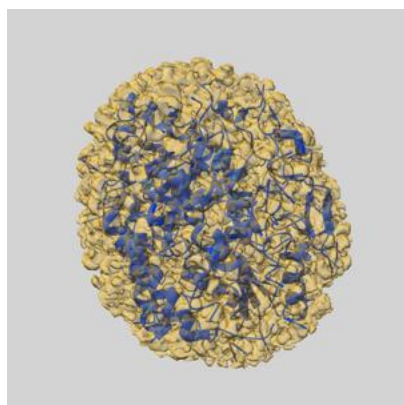
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	5.90	3.53

*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 3.49 differs from the reported value 2.0 by more than 10 %

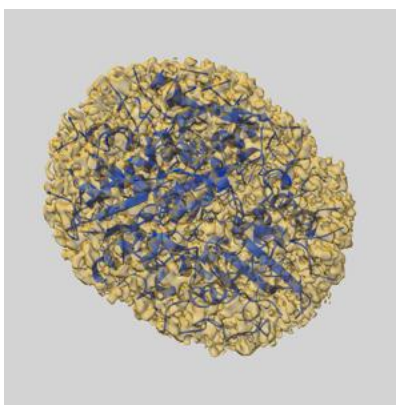
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42231 and PDB model 8UGP. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

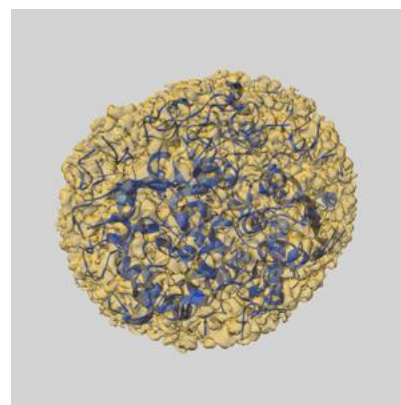
9.1 Map-model overlay [i](#)



X



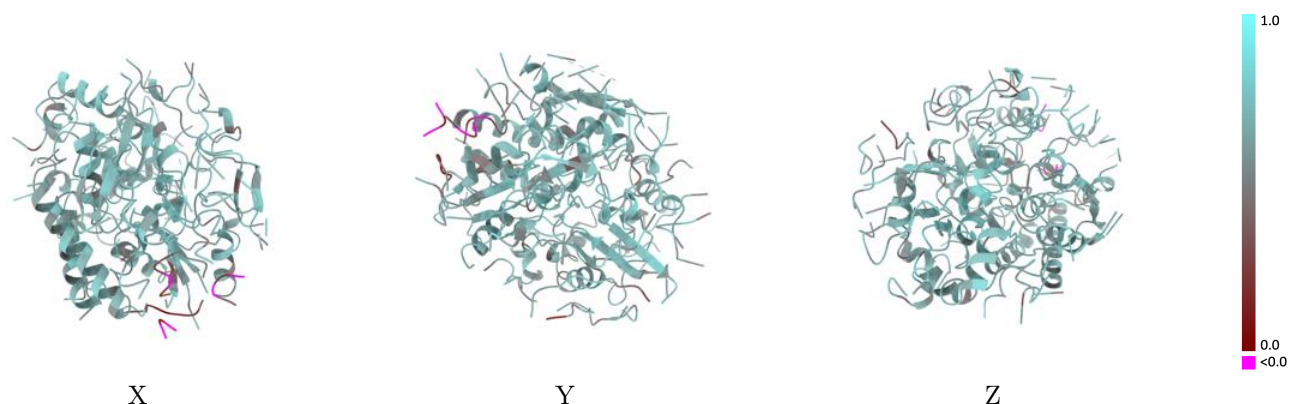
Y



Z

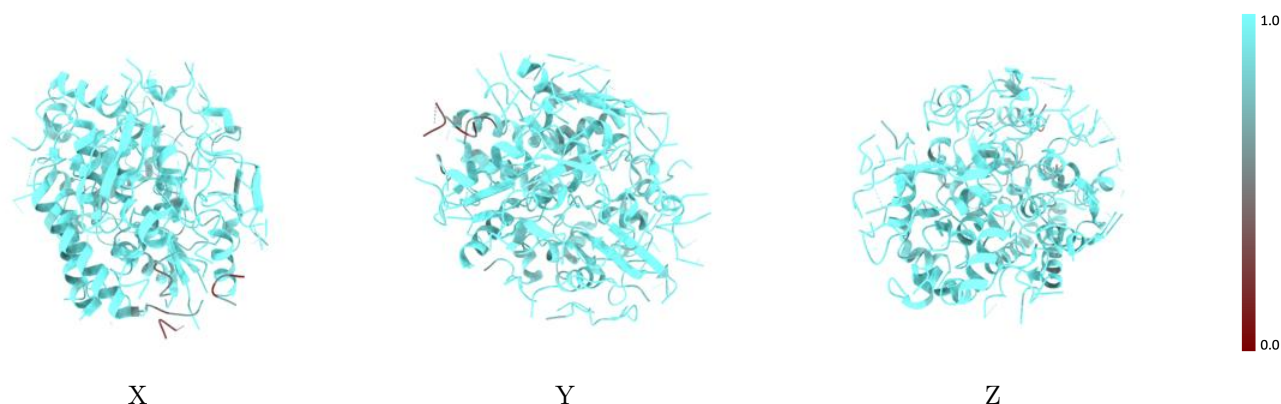
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



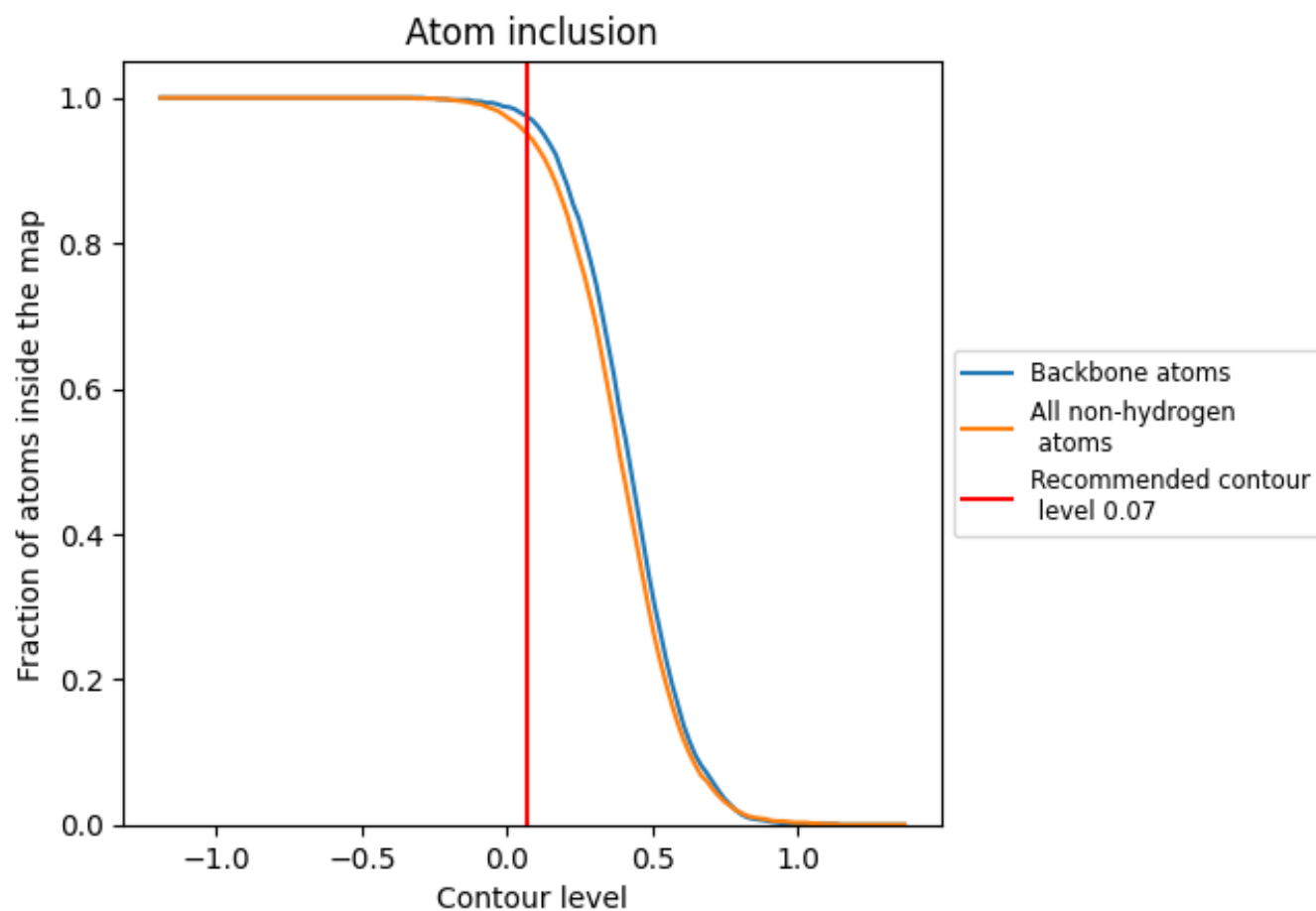
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.6100
1A	 0.3640	 0.0350
1B	 0.9590	 0.6230
1C	 0.9600	 0.6140
1D	 0.9550	 0.6170
1G	 0.9570	 0.5870
1H	 0.4690	 0.1210
1I	 0.9720	 0.6480
1P	 0.9120	 0.5620
1Q	 0.9380	 0.5860
1R	 0.9500	 0.5660
1W	 0.9680	 0.6040
1q	 0.9460	 0.5840

