



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 04:32 pm BST

PDB ID : 7ZC6
EMDB ID : EMD-14622
Title : Na⁺ - translocating ferredoxin: NAD⁺ reductase (Rnf) of *C. tetanomorphum*
Authors : Ermler, U.; Vitt, S.; Buckel, W.
Deposited on : 2022-03-25
Resolution : 4.27 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

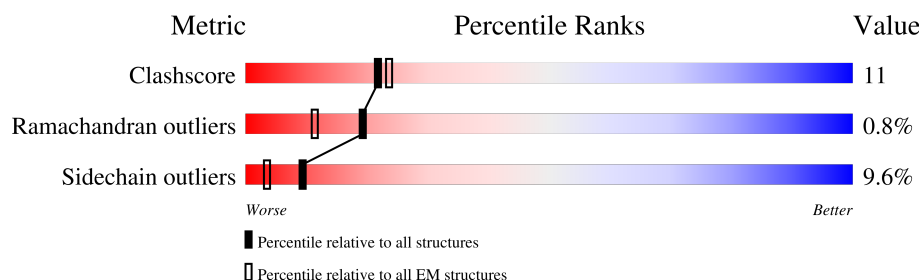
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.27 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	191	<div> <div>12%</div> <div>75%</div> <div>19%</div> <div>5%</div> </div>
2	B	274	<div> <div>10%</div> <div>61%</div> <div>11%</div> <div>26%</div> </div>
3	C	435	<div> <div>11%</div> <div>75%</div> <div>20%</div> <div>.</div> </div>
4	D	310	<div> <div>6%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
5	E	201	<div> <div>12%</div> <div>71%</div> <div>20%</div> <div>5%</div> <div>.</div> </div>
6	G	189	<div> <div>51%</div> <div>95%</div> <div>..</div> </div>

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
10	RBF	D	401	-	-	X	-
8	SF4	B	302	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11428 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 RnfA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	191	Total	C	N	O	S	0	0
			1446	965	221	250	10		

- Molecule 2 is a protein called RnfB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	202	Total	C	N	O	S	0	0
			1451	906	242	278	25		

- Molecule 3 is a protein called RnfC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	435	Total	C	N	O	S	0	0
			3291	2077	562	625	27		

- Molecule 4 is a protein called RnfD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	304	Total	C	N	O	S	0	0
			2282	1518	363	392	9		

- Molecule 5 is a protein called RnfE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	194	Total	C	N	O	S	0	0
			1435	945	231	252	7		

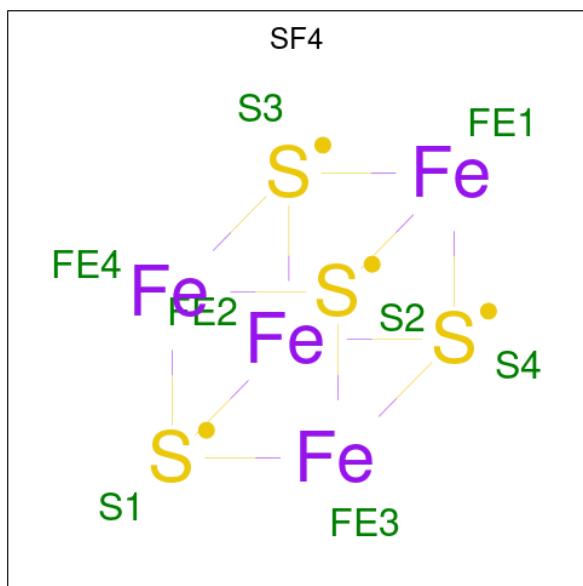
- Molecule 6 is a protein called RnfG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	187	Total	C	N	O	S	0	0
			1348	858	222	264	4		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

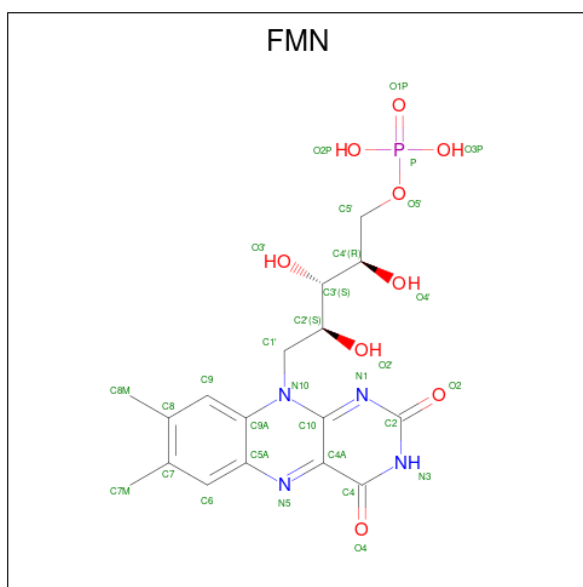
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Fe	0
			1	1	

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



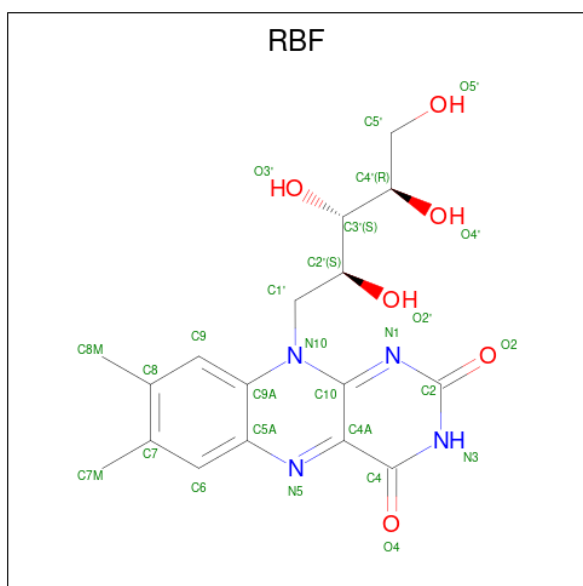
Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	Fe	S	0
			8	4	4	
8	B	1	Total	Fe	S	0
			8	4	4	
8	B	1	Total	Fe	S	0
			8	4	4	
8	B	1	Total	Fe	S	0
			8	4	4	
8	B	1	Total	Fe	S	0
			8	4	4	
8	C	1	Total	Fe	S	0
			8	4	4	
8	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 9 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
9	D	1	Total	C	N	O	P	0
			30	17	4	8	1	
9	G	1	Total	C	N	O	P	0
			30	17	4	8	1	

- Molecule 10 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

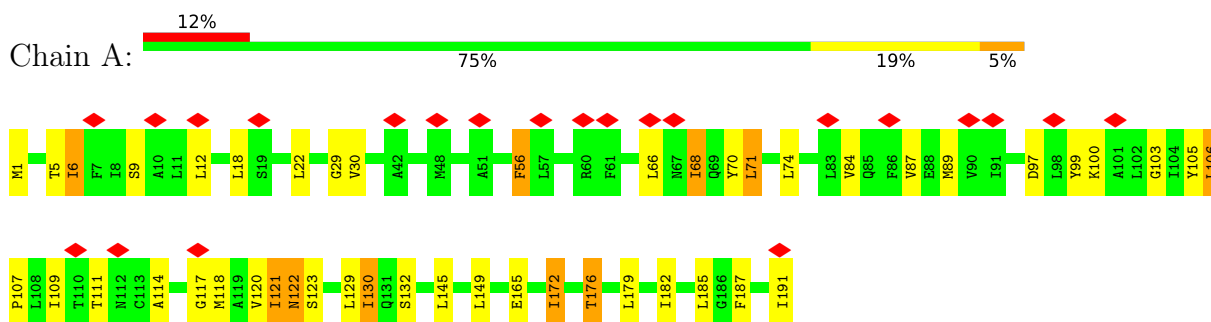


Mol	Chain	Residues	Atoms				AltConf
10	D	1	Total	C	N	O	0
			27	17	4	6	

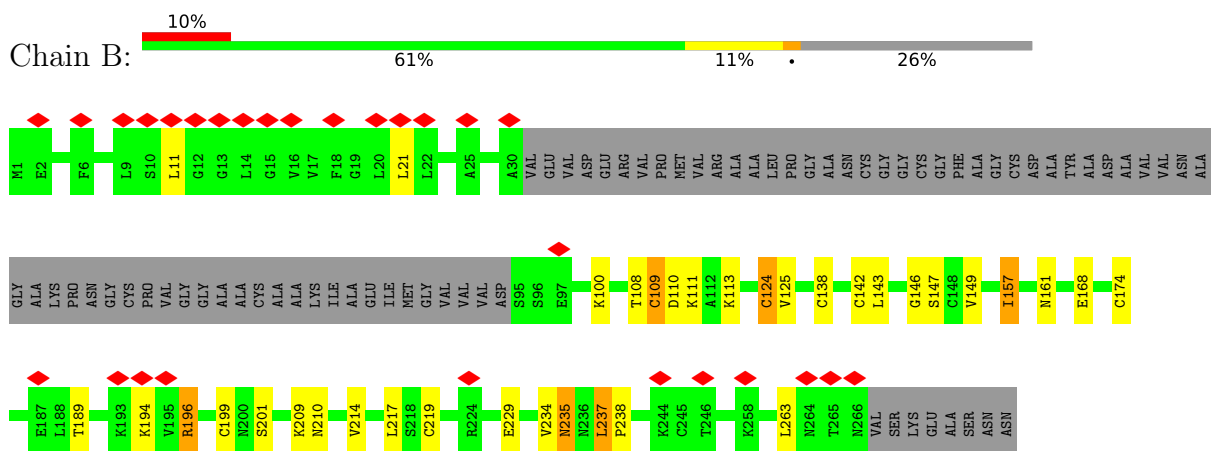
3 Residue-property plots

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.

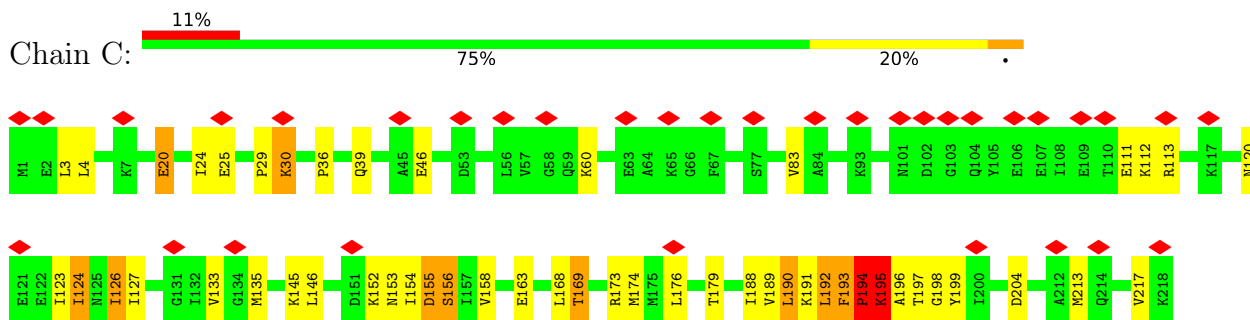
• Molecule 1: RnfA

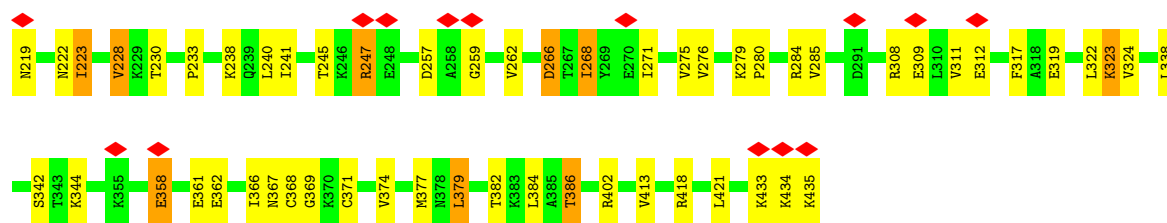


• Molecule 2: RnfB

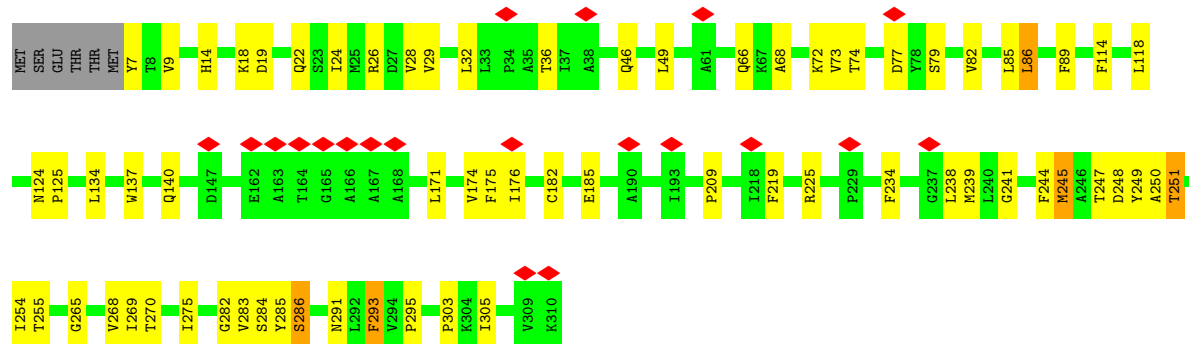
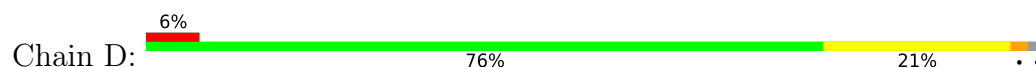


• Molecule 3: RnfC

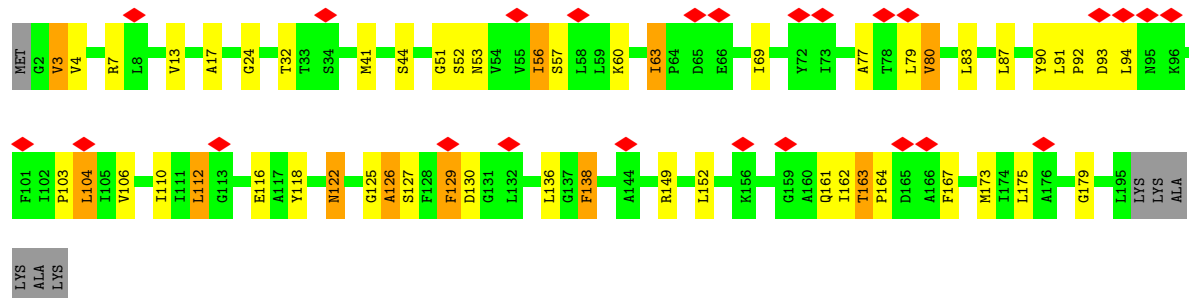




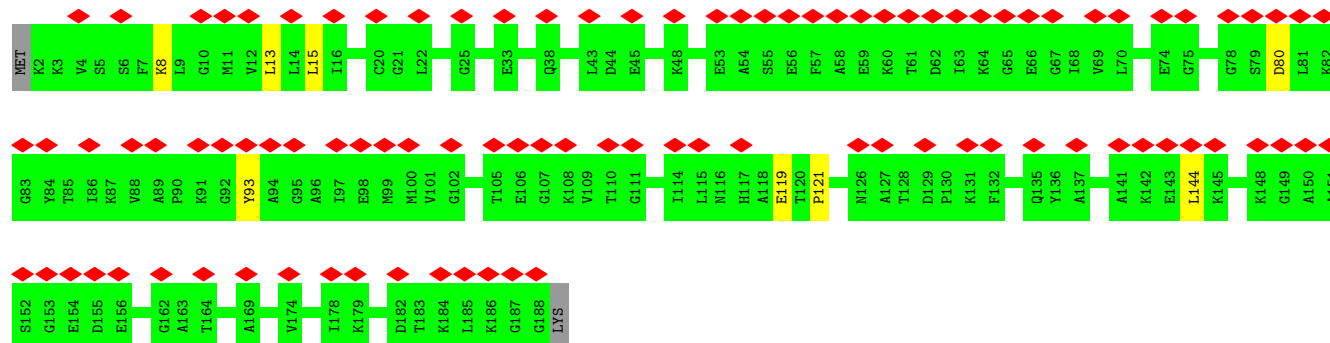
• Molecule 4: RnfD



• Molecule 5: RnfE



• Molecule 6: RnfG



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88423	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	200.88, 200.88, 200.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: FE, FMN, RBF, SF4

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	0.59	0/1469	1.00	2/1994 (0.1%)
2	B	0.58	0/1470	0.97	5/1983 (0.3%)
3	C	0.62	2/3344 (0.1%)	0.90	1/4515 (0.0%)
4	D	0.58	0/2341	0.96	3/3196 (0.1%)
5	E	0.62	0/1457	1.03	1/1981 (0.1%)
6	G	0.60	0/1362	0.98	2/1834 (0.1%)
All	All	0.60	2/11443 (0.0%)	0.96	14/15503 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	194	PRO	N-CA	14.04	1.71	1.47
3	C	193	PHE	C-N	6.04	1.45	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194	PRO	CA-N-CD	-7.74	100.66	111.50
2	B	174	CYS	CA-CB-SG	7.20	126.96	114.00
4	D	49	LEU	CB-CG-CD2	-6.62	99.74	111.00
4	D	295	PRO	CA-N-CD	-6.26	102.74	111.50
2	B	237	LEU	CB-CG-CD2	-5.99	100.83	111.00
2	B	11	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	A	71	LEU	CB-CG-CD1	-5.56	101.54	111.00
2	B	21	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	18	LEU	CB-CG-CD1	5.39	120.17	111.00
6	G	144	LEU	CA-CB-CG	5.30	127.48	115.30
4	D	209	PRO	CA-N-CD	-5.25	104.15	111.50
2	B	199	CYS	CA-CB-SG	5.19	123.34	114.00
6	G	93	TYR	CB-CG-CD1	-5.12	117.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	103	PRO	CA-N-CD	-5.02	104.47	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1446	0	1565	37	0
2	B	1451	0	1453	22	0
3	C	3291	0	3388	70	0
4	D	2282	0	2378	75	0
5	E	1435	0	1539	34	0
6	G	1348	0	1423	0	0
7	A	1	0	0	0	0
8	B	40	0	0	3	0
8	C	16	0	0	1	0
9	C	31	0	19	1	0
9	D	30	0	19	4	0
9	G	30	0	19	2	0
10	D	27	0	20	11	0
All	All	11428	0	11823	234	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 11.

All (234) 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)
3:C:194:PRO:CA	3:C:194:PRO:N	1.71	1.47
2:B:234:VAL:HG23	2:B:235:ASN:OD1	1.15	1.25
4:D:32:LEU:HD11	4:D:85:LEU:HD21	1.33	1.09
4:D:79:SER:HB3	4:D:118:LEU:HD12	1.38	1.06
2:B:234:VAL:CG2	2:B:235:ASN:OD1	2.10	1.00
4:D:32:LEU:HD23	4:D:244:PHE:HE2	1.29	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:THR:HG21	5:E:149:ARG:HD3	1.52	0.90
1:A:66:LEU:HB3	1:A:68:ILE:CG1	2.03	0.89
4:D:32:LEU:HD21	4:D:85:LEU:HD23	1.56	0.88
1:A:122:ASN:OD1	1:A:132:SER:HB2	1.74	0.85
3:C:198:GLY:O	3:C:199:TYR:HD1	1.58	0.85
4:D:32:LEU:HD11	4:D:85:LEU:CD2	2.07	0.85
4:D:251:THR:HB	4:D:291:ASN:HD21	1.41	0.85
3:C:120:ASN:OD1	3:C:192:LEU:HD23	1.77	0.85
1:A:97:ASP:HA	1:A:100:LYS:HB2	1.58	0.84
1:A:106:LEU:O	1:A:109:ILE:HG22	1.77	0.83
4:D:268:VAL:HG12	4:D:269:ILE:HD13	1.59	0.82
4:D:79:SER:HB3	4:D:118:LEU:CD1	2.10	0.81
4:D:79:SER:CB	4:D:118:LEU:HD12	2.10	0.81
2:B:194:LYS:O	2:B:196:ARG:HD3	1.82	0.79
4:D:251:THR:HB	4:D:291:ASN:ND2	1.98	0.79
3:C:198:GLY:O	3:C:199:TYR:CD1	2.36	0.79
4:D:32:LEU:HB3	4:D:244:PHE:CZ	2.18	0.78
10:D:401:RBF:HC4'	10:D:401:RBF:N1	1.98	0.78
4:D:32:LEU:HD23	4:D:244:PHE:CE2	2.18	0.77
3:C:154:ILE:HG12	3:C:196:ALA:HB2	1.67	0.76
3:C:153:ASN:OD1	3:C:195:LYS:HE3	1.85	0.75
4:D:86:LEU:HD12	4:D:245:MET:SD	2.26	0.75
2:B:234:VAL:HG23	2:B:235:ASN:CG	2.06	0.74
5:E:32:THR:CG2	5:E:149:ARG:HD3	2.18	0.74
4:D:124:ASN:ND2	4:D:251:THR:HG21	2.04	0.73
1:A:66:LEU:HB3	1:A:68:ILE:HD11	1.69	0.73
3:C:174:MET:HE3	3:C:285:VAL:HG21	1.70	0.73
3:C:135:MET:HG3	3:C:266:ASP:HB3	1.71	0.73
5:E:80:VAL:HG21	5:E:106:VAL:HG13	1.68	0.73
4:D:270:THR:HG23	4:D:282:GLY:C	2.09	0.73
3:C:156:SER:CA	3:C:196:ALA:HB1	2.20	0.72
1:A:12:LEU:HD22	1:A:187:PHE:CE2	2.25	0.71
3:C:156:SER:HA	3:C:196:ALA:HB1	1.71	0.71
4:D:32:LEU:CD2	4:D:244:PHE:HE2	2.00	0.71
3:C:155:ASP:O	3:C:196:ALA:HA	1.88	0.71
4:D:270:THR:HG23	4:D:282:GLY:O	1.90	0.71
5:E:118:TYR:O	5:E:122:ASN:HB2	1.90	0.70
1:A:66:LEU:HB3	1:A:68:ILE:CD1	2.20	0.70
4:D:283:VAL:HG12	9:D:400:FMN:HM72	1.73	0.70
3:C:124:ILE:O	3:C:127:ILE:HG22	1.92	0.69
3:C:158:VAL:HG12	3:C:199:TYR:HD2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:LEU:O	4:D:118:LEU:HD23	1.93	0.68
4:D:24:ILE:HG21	4:D:249:TYR:HE2	1.59	0.67
4:D:269:ILE:HB	4:D:286:SER:OG	1.93	0.67
4:D:282:GLY:O	4:D:286:SER:HB2	1.94	0.67
3:C:158:VAL:HG12	3:C:199:TYR:CD2	2.30	0.67
1:A:111:THR:HG21	5:E:112:LEU:HD13	1.77	0.67
1:A:66:LEU:HD23	1:A:68:ILE:HD11	1.76	0.66
5:E:92:PRO:C	5:E:94:LEU:H	2.00	0.65
3:C:111:GLU:HA	3:C:111:GLU:OE1	1.96	0.64
3:C:358:GLU:O	3:C:358:GLU:HG3	1.98	0.64
4:D:137:TRP:HB3	4:D:140:GLN:HG3	1.79	0.63
4:D:268:VAL:HG12	4:D:269:ILE:CD1	2.28	0.63
5:E:138:PHE:HD1	5:E:138:PHE:O	1.82	0.63
4:D:171:LEU:O	4:D:174:VAL:HG12	1.99	0.62
10:D:401:RBF:N1	10:D:401:RBF:HC2'	2.14	0.62
5:E:149:ARG:NH1	5:E:179:GLY:HA3	2.15	0.61
4:D:32:LEU:CD2	4:D:85:LEU:HD23	2.29	0.61
2:B:146:GLY:O	2:B:149:VAL:HG22	2.00	0.61
1:A:106:LEU:N	1:A:107:PRO:HD2	2.14	0.60
1:A:66:LEU:HB3	1:A:68:ILE:HG12	1.80	0.60
3:C:190:LEU:HD22	3:C:193:PHE:O	2.01	0.60
3:C:367:ASN:OD1	4:D:254:ILE:HD11	2.01	0.60
3:C:379:LEU:HD23	3:C:384:LEU:HD11	1.83	0.60
2:B:111:LYS:HE2	2:B:214:VAL:CG1	2.32	0.60
1:A:29:GLY:HA3	1:A:105:TYR:CE2	2.37	0.59
3:C:198:GLY:C	3:C:199:TYR:CD1	2.76	0.59
5:E:80:VAL:HG21	5:E:106:VAL:CG1	2.33	0.58
2:B:108:THR:HG23	2:B:161:ASN:HB3	1.86	0.58
5:E:17:ALA:HB1	5:E:110:ILE:CD1	2.34	0.58
1:A:68:ILE:HD12	1:A:70:TYR:HE1	1.68	0.58
5:E:161:GLN:HE21	5:E:163:THR:H	1.52	0.57
4:D:118:LEU:HD23	4:D:118:LEU:C	2.25	0.57
4:D:251:THR:HG21	4:D:291:ASN:OD1	2.04	0.57
9:G:300:FMN:O4'	9:G:300:FMN:O2'	2.16	0.57
3:C:4:LEU:CD1	3:C:228:VAL:HG12	2.34	0.57
3:C:268:ILE:N	3:C:268:ILE:HD13	2.19	0.57
3:C:158:VAL:CG1	3:C:199:TYR:HD2	2.17	0.57
4:D:241:GLY:HA2	4:D:245:MET:HB2	1.86	0.57
3:C:20:GLU:HA	3:C:169:THR:HG21	1.87	0.56
4:D:28:VAL:HG21	10:D:401:RBF:C7M	2.35	0.56
5:E:17:ALA:HB1	5:E:110:ILE:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD23	1:A:74:LEU:O	2.06	0.56
5:E:51:GLY:O	5:E:79:LEU:HD11	2.05	0.56
1:A:66:LEU:HD23	1:A:68:ILE:CD1	2.36	0.56
5:E:53:ASN:HA	5:E:56:ILE:HG22	1.86	0.56
5:E:118:TYR:O	5:E:122:ASN:N	2.38	0.56
3:C:275:VAL:HG23	3:C:276:VAL:HG23	1.87	0.56
1:A:66:LEU:C	1:A:68:ILE:HG12	2.27	0.55
3:C:374:VAL:HG11	3:C:413:VAL:HG11	1.88	0.55
3:C:4:LEU:HD12	3:C:228:VAL:HG12	1.88	0.55
3:C:24:ILE:HD11	3:C:173:ARG:HG3	1.90	0.54
4:D:32:LEU:HB3	4:D:244:PHE:HZ	1.72	0.54
1:A:6:ILE:O	1:A:9:SER:HB2	2.08	0.54
4:D:22:GLN:HG2	4:D:77:ASP:HA	1.90	0.54
3:C:36:PRO:O	3:C:39:GLN:HG3	2.07	0.54
5:E:3:VAL:O	5:E:3:VAL:HG13	2.08	0.53
4:D:284:SER:HB2	9:D:400:FMN:H6	1.91	0.53
5:E:4:VAL:HG22	5:E:129:PHE:HB3	1.90	0.53
3:C:324:VAL:HG21	3:C:338:LEU:HD21	1.91	0.53
4:D:137:TRP:HB3	4:D:140:GLN:CG	2.39	0.53
1:A:5:THR:HG23	1:A:191:ILE:HD12	1.91	0.53
4:D:32:LEU:CD2	4:D:244:PHE:CE2	2.87	0.53
4:D:32:LEU:HD21	4:D:85:LEU:CD2	2.35	0.52
1:A:172:ILE:HD11	4:D:114:PHE:O	2.08	0.52
3:C:245:THR:HG23	3:C:247:ARG:HG2	1.92	0.52
5:E:125:GLY:C	5:E:127:SER:H	2.11	0.52
2:B:201:SER:O	2:B:237:LEU:HD13	2.10	0.52
4:D:283:VAL:HG12	4:D:283:VAL:O	2.10	0.52
3:C:190:LEU:HD21	3:C:196:ALA:O	2.10	0.51
10:D:401:RBF:N1	10:D:401:RBF:C2'	2.73	0.51
2:B:149:VAL:HG12	2:B:157:ILE:HG22	1.93	0.51
3:C:197:THR:HG22	3:C:222:ASN:O	2.11	0.51
3:C:311:VAL:HG11	3:C:317:PHE:CE1	2.45	0.51
5:E:44:SER:HB2	5:E:83:LEU:HD21	1.92	0.51
3:C:361:GLU:OE1	3:C:361:GLU:HA	2.11	0.51
5:E:163:THR:HG22	5:E:164:PRO:HD2	1.93	0.51
3:C:379:LEU:HD23	3:C:384:LEU:CD1	2.41	0.51
1:A:149:LEU:HD21	4:D:293:PHE:HD1	1.76	0.50
3:C:3:LEU:HD11	3:C:204:ASP:HB3	1.93	0.50
4:D:251:THR:CG2	4:D:291:ASN:CG	2.80	0.50
2:B:237:LEU:HD12	2:B:238:PRO:HD2	1.93	0.50
10:D:401:RBF:N1	10:D:401:RBF:C4'	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:435:LYS:HG2	3:C:435:LYS:OXT	2.11	0.50
4:D:238:LEU:HA	4:D:283:VAL:HG21	1.93	0.49
4:D:137:TRP:CB	4:D:140:GLN:HG3	2.43	0.49
4:D:32:LEU:CD1	4:D:85:LEU:HD21	2.24	0.49
4:D:251:THR:HG22	4:D:291:ASN:CG	2.33	0.49
4:D:125:PRO:HD2	10:D:401:RBF:O2	2.14	0.48
2:B:142:CYS:SG	2:B:143:LEU:N	2.86	0.48
3:C:158:VAL:CG1	3:C:199:TYR:CD2	2.95	0.48
1:A:30:VAL:HG11	1:A:99:TYR:HE1	1.78	0.48
3:C:29:PRO:O	3:C:30:LYS:HD2	2.13	0.48
3:C:284:ARG:NH2	3:C:344:LYS:O	2.45	0.48
3:C:145:LYS:HZ1	9:C:503:FMN:P	2.37	0.47
3:C:371:CYS:HB3	8:C:502:SF4:S3	2.54	0.47
4:D:22:GLN:O	4:D:26:ARG:HB3	2.14	0.47
3:C:217:VAL:HA	3:C:223:ILE:HD11	1.97	0.47
4:D:66:GLN:HE21	4:D:73:VAL:HA	1.80	0.47
3:C:145:LYS:NZ	3:C:262:VAL:O	2.42	0.47
2:B:111:LYS:HE2	2:B:214:VAL:HG12	1.96	0.47
3:C:156:SER:HA	3:C:196:ALA:CB	2.44	0.47
1:A:74:LEU:HD23	1:A:74:LEU:C	2.36	0.46
4:D:32:LEU:HB3	4:D:244:PHE:CE2	2.51	0.46
5:E:51:GLY:C	5:E:79:LEU:HD11	2.35	0.46
1:A:68:ILE:HB	1:A:70:TYR:HD1	1.80	0.46
4:D:238:LEU:CA	4:D:283:VAL:HG21	2.46	0.46
5:E:126:ALA:HA	5:E:129:PHE:CE2	2.50	0.46
4:D:248:ASP:OD1	10:D:401:RBF:HC12	2.16	0.46
4:D:265:GLY:O	4:D:269:ILE:HG12	2.16	0.46
3:C:146:LEU:O	3:C:193:PHE:HZ	1.99	0.46
3:C:154:ILE:HG12	3:C:196:ALA:CB	2.43	0.46
5:E:17:ALA:CB	5:E:110:ILE:CD1	2.94	0.46
1:A:66:LEU:HB3	1:A:68:ILE:HG13	1.94	0.45
4:D:175:PHE:HE1	4:D:234:PHE:CG	2.34	0.45
10:D:401:RBF:HC4'	10:D:401:RBF:C2	2.46	0.45
1:A:117:GLY:O	1:A:121:ILE:HB	2.16	0.45
4:D:29:VAL:HG23	4:D:82:VAL:HG23	1.98	0.45
3:C:155:ASP:OD1	3:C:259:GLY:HA3	2.17	0.45
3:C:124:ILE:HA	3:C:127:ILE:HG22	1.99	0.45
5:E:136:LEU:HD12	5:E:136:LEU:HA	1.73	0.45
2:B:113:LYS:HE3	2:B:210:ASN:O	2.17	0.45
4:D:32:LEU:CD1	4:D:85:LEU:CD2	2.90	0.45
3:C:188:ILE:O	3:C:191:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:GLU:CD	3:C:113:ARG:HG2	2.37	0.44
2:B:100:LYS:NZ	2:B:168:GLU:O	2.34	0.44
2:B:189:THR:HG21	2:B:196:ARG:HH22	1.82	0.44
3:C:369:GLY:HA2	4:D:254:ILE:HG23	1.99	0.44
5:E:138:PHE:CD1	5:E:138:PHE:C	2.90	0.44
1:A:106:LEU:N	1:A:107:PRO:CD	2.80	0.44
3:C:366:ILE:HG22	4:D:118:LEU:CD2	2.47	0.44
4:D:284:SER:O	4:D:286:SER:N	2.50	0.44
9:D:400:FMN:H9	9:D:400:FMN:H1'1	1.86	0.44
3:C:382:THR:O	3:C:386:THR:HB	2.17	0.44
4:D:250:ALA:HB3	10:D:401:RBF:O5'	2.18	0.44
2:B:138:CYS:CB	8:B:302:SF4:S3	3.06	0.44
1:A:66:LEU:CB	1:A:68:ILE:HD11	2.42	0.43
3:C:311:VAL:HG11	3:C:317:PHE:CZ	2.53	0.43
1:A:176:THR:O	1:A:179:LEU:N	2.51	0.43
2:B:189:THR:HG21	2:B:196:ARG:NH2	2.32	0.43
4:D:36:THR:HG1	4:D:89:PHE:HZ	1.65	0.43
4:D:134:LEU:HD11	9:G:300:FMN:HM83	2.00	0.43
4:D:284:SER:C	4:D:286:SER:H	2.21	0.43
5:E:63:ILE:HD13	5:E:63:ILE:HA	1.81	0.43
1:A:149:LEU:HD21	4:D:293:PHE:CD1	2.52	0.43
3:C:112:LYS:NZ	3:C:126:ILE:HG13	2.33	0.43
1:A:56:PHE:CD2	1:A:129:LEU:HD13	2.54	0.43
4:D:74:THR:HG22	4:D:74:THR:O	2.19	0.43
3:C:189:VAL:HA	3:C:192:LEU:HD12	2.00	0.43
2:B:124:CYS:SG	2:B:125:VAL:N	2.92	0.43
5:E:92:PRO:C	5:E:94:LEU:N	2.70	0.43
1:A:179:LEU:O	1:A:182:ILE:HB	2.19	0.43
1:A:121:ILE:HD12	1:A:121:ILE:HA	1.58	0.42
3:C:322:LEU:HG	4:D:9:VAL:CG2	2.48	0.42
4:D:251:THR:CG2	4:D:291:ASN:OD1	2.66	0.42
1:A:103:GLY:O	1:A:106:LEU:HB2	2.19	0.42
3:C:123:ILE:CG2	3:C:192:LEU:HD21	2.49	0.42
1:A:74:LEU:HA	5:E:77:ALA:HB1	2.00	0.42
5:E:24:GLY:HA3	5:E:110:ILE:HG13	2.00	0.42
5:E:79:LEU:HD23	5:E:79:LEU:HA	1.79	0.42
1:A:84:VAL:HA	1:A:87:VAL:HG22	2.01	0.42
3:C:163:GLU:OE1	3:C:168:LEU:HD23	2.19	0.42
3:C:268:ILE:O	3:C:271:ILE:HG22	2.19	0.42
4:D:255:THR:HG23	4:D:303:PRO:HD3	2.01	0.42
2:B:111:LYS:HE2	2:B:214:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:THR:HG23	2:B:161:ASN:CB	2.48	0.41
2:B:138:CYS:HB3	8:B:302:SF4:S3	2.60	0.41
3:C:36:PRO:HG2	3:C:39:GLN:HG2	2.01	0.41
3:C:317:PHE:HB3	3:C:319:GLU:O	2.21	0.41
5:E:138:PHE:HD1	5:E:138:PHE:C	2.23	0.41
1:A:130:ILE:HD12	1:A:130:ILE:HA	1.74	0.41
1:A:22:LEU:HB3	1:A:114:ALA:HA	2.02	0.41
3:C:238:LYS:HD2	3:C:377:MET:HE1	2.03	0.41
4:D:251:THR:CB	4:D:291:ASN:ND2	2.76	0.41
5:E:87:LEU:HD23	5:E:87:LEU:HA	1.78	0.41
2:B:142:CYS:HB2	8:B:301:SF4:S2	2.60	0.41
5:E:122:ASN:HD22	5:E:122:ASN:HA	1.50	0.41
3:C:268:ILE:HA	3:C:271:ILE:HG22	2.02	0.41
3:C:323:LYS:HG2	4:D:9:VAL:O	2.20	0.41
4:D:284:SER:C	4:D:286:SER:N	2.74	0.41
3:C:323:LYS:NZ	4:D:14:HIS:HA	2.37	0.40
3:C:362:GLU:HG3	3:C:418:ARG:HD2	2.03	0.40
4:D:248:ASP:OD1	10:D:401:RBF:N10	2.55	0.40
4:D:284:SER:HB2	9:D:400:FMN:C6	2.51	0.40
3:C:368:CYS:SG	3:C:369:GLY:N	2.94	0.40
5:E:104:LEU:HD22	5:E:104:LEU:O	2.22	0.40
4:D:28:VAL:CG1	10:D:401:RBF:HC72	2.51	0.40
4:D:225:ARG:HD2	4:D:275:ILE:HD12	2.02	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	A	189/191 (99%)	170 (90%)	19 (10%)	0	100	100
2	B	198/274 (72%)	186 (94%)	11 (6%)	1 (0%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	433/435 (100%)	403 (93%)	25 (6%)	5 (1%)	11	43
4	D	302/310 (97%)	283 (94%)	16 (5%)	3 (1%)	13	48
5	E	192/201 (96%)	174 (91%)	16 (8%)	2 (1%)	13	48
6	G	185/189 (98%)	179 (97%)	5 (3%)	1 (0%)	25	63
All	All	1499/1600 (94%)	1395 (93%)	92 (6%)	12 (1%)	19	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	194	PRO
2	B	109	CYS
3	C	195	LYS
4	D	68	ALA
5	E	93	ASP
4	D	285	TYR
6	G	121	PRO
5	E	126	ALA
3	C	280	PRO
4	D	18	LYS
3	C	83	VAL
3	C	233	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/158 (100%)	140 (89%)	18 (11%)	4	18
2	B	164/211 (78%)	152 (93%)	12 (7%)	11	32
3	C	365/365 (100%)	324 (89%)	41 (11%)	5	19
4	D	240/246 (98%)	224 (93%)	16 (7%)	13	35
5	E	155/160 (97%)	129 (83%)	26 (17%)	1	10
6	G	141/143 (99%)	136 (96%)	5 (4%)	31	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1223/1283 (95%)	1105 (90%)	118 (10%)	9 23

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ILE
1	A	56	PHE
1	A	68	ILE
1	A	71	LEU
1	A	89	MET
1	A	106	LEU
1	A	118	MET
1	A	120	VAL
1	A	121	ILE
1	A	122	ASN
1	A	123	SER
1	A	130	ILE
1	A	145	LEU
1	A	165	GLU
1	A	172	ILE
1	A	176	THR
1	A	185	LEU
2	B	109	CYS
2	B	110	ASP
2	B	124	CYS
2	B	147	SER
2	B	157	ILE
2	B	196	ARG
2	B	209	LYS
2	B	217	LEU
2	B	219	CYS
2	B	229	GLU
2	B	235	ASN
2	B	263	LEU
3	C	20	GLU
3	C	25	GLU
3	C	30	LYS
3	C	46	GLU
3	C	60	LYS
3	C	124	ILE
3	C	126	ILE

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Mol	Chain	Res	Type
3	C	133	VAL
3	C	152	LYS
3	C	155	ASP
3	C	156	SER
3	C	169	THR
3	C	176	LEU
3	C	179	THR
3	C	190	LEU
3	C	192	LEU
3	C	195	LYS
3	C	213	MET
3	C	219	ASN
3	C	223	ILE
3	C	228	VAL
3	C	230	THR
3	C	240	LEU
3	C	241	ILE
3	C	247	ARG
3	C	257	ASP
3	C	266	ASP
3	C	268	ILE
3	C	279	LYS
3	C	308	ARG
3	C	309	GLU
3	C	312	GLU
3	C	323	LYS
3	C	342	SER
3	C	358	GLU
3	C	379	LEU
3	C	386	THR
3	C	402	ARG
3	C	421	LEU
3	C	433	LYS
3	C	434	LYS
4	D	7	TYR
4	D	19	ASP
4	D	46	GLN
4	D	72	LYS
4	D	86	LEU
4	D	176	ILE
4	D	182	CYS
4	D	185	GLU

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Mol	Chain	Res	Type
4	D	219	PHE
4	D	239	MET
4	D	245	MET
4	D	247	THR
4	D	251	THR
4	D	286	SER
4	D	293	PHE
4	D	305	ILE
5	E	3	VAL
5	E	7	ARG
5	E	13	VAL
5	E	41	MET
5	E	52	SER
5	E	56	ILE
5	E	57	SER
5	E	60	LYS
5	E	63	ILE
5	E	69	ILE
5	E	80	VAL
5	E	90	TYR
5	E	91	LEU
5	E	104	LEU
5	E	112	LEU
5	E	116	GLU
5	E	122	ASN
5	E	129	PHE
5	E	130	ASP
5	E	138	PHE
5	E	152	LEU
5	E	162	ILE
5	E	163	THR
5	E	167	PHE
5	E	173	MET
5	E	175	LEU
6	G	8	LYS
6	G	13	LEU
6	G	15	LEU
6	G	80	ASP
6	G	119	GLU

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

Mol	Chain	Res	Type
1	A	122	ASN
3	C	39	GLN
3	C	208	ASN
4	D	66	GLN
4	D	124	ASN
4	D	161	ASN
4	D	291	ASN
5	E	122	ASN
5	E	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
8	SF4	B	301	2	0,12,12	-	-	-		
10	RBF	D	401	-	29,29,29	0.57	0	41,43,43	0.65	1 (2%)
9	FMN	G	300	6	29,32,33	2.74	8 (27%)	40,47,50	1.53	8 (20%)
8	SF4	C	501	3	0,12,12	-	-	-		
8	SF4	B	302	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SF4	B	300	2	0,12,12	-	-	-		
9	FMN	C	503	-	33,33,33	2.56	7 (21%)	48,50,50	1.77	11 (22%)
8	SF4	B	304	2	0,12,12	-	-	-		
8	SF4	B	303	2	0,12,12	-	-	-		
9	FMN	D	400	4	29,32,33	2.76	8 (27%)	40,47,50	1.76	11 (27%)
8	SF4	C	502	3	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
8	SF4	B	301	2	-	-	0/6/5/5
10	RBF	D	401	-	-	13/14/14/14	0/3/3/3
9	FMN	G	300	6	-	10/15/17/18	0/3/3/3
8	SF4	C	501	3	-	-	0/6/5/5
8	SF4	B	302	2	-	-	0/6/5/5
8	SF4	B	300	2	-	-	0/6/5/5
8	SF4	B	304	2	-	-	0/6/5/5
8	SF4	B	303	2	-	-	0/6/5/5
9	FMN	D	400	4	-	7/15/17/18	0/3/3/3
9	FMN	C	503	-	-	6/18/18/18	0/3/3/3
8	SF4	C	502	3	-	-	0/6/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	300	FMN	O4-C4	8.97	1.40	1.23
9	D	400	FMN	O2-C2	8.61	1.40	1.24
9	G	300	FMN	O2-C2	8.42	1.39	1.24
9	C	503	FMN	O4-C4	8.41	1.39	1.23
9	C	503	FMN	O2-C2	8.33	1.39	1.24
9	D	400	FMN	O4-C4	8.25	1.39	1.23
9	D	400	FMN	C4-N3	-4.09	1.31	1.38
9	C	503	FMN	C4-N3	-3.86	1.31	1.38
9	D	400	FMN	C5A-N5	-3.14	1.33	1.39
9	G	300	FMN	C4-N3	-3.11	1.33	1.38
9	C	503	FMN	C2-N3	-2.89	1.32	1.39
9	G	300	FMN	C5A-N5	-2.87	1.33	1.39
9	C	503	FMN	C5A-N5	-2.76	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	400	FMN	C2-N3	-2.75	1.32	1.39
9	D	400	FMN	C6-C7	-2.68	1.35	1.39
9	G	300	FMN	C2-N3	-2.65	1.32	1.39
9	D	400	FMN	C9A-N10	-2.56	1.36	1.41
9	G	300	FMN	C9A-N10	-2.49	1.36	1.41
9	G	300	FMN	C4A-C10	-2.30	1.37	1.44
9	D	400	FMN	C4A-C10	-2.29	1.37	1.44
9	C	503	FMN	C4A-C10	-2.27	1.37	1.44
9	G	300	FMN	O5'-C5'	-2.25	1.39	1.44
9	C	503	FMN	C9A-N10	-2.18	1.37	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	503	FMN	C4'-C3'-C2'	-5.64	101.64	113.36
9	D	400	FMN	C4A-C10-N1	-3.48	116.65	124.73
9	G	300	FMN	C1'-C2'-C3'	3.39	119.26	109.79
9	C	503	FMN	C4-N3-C2	-3.35	119.44	125.64
9	D	400	FMN	C4-N3-C2	-3.33	119.48	125.64
9	C	503	FMN	C4A-C10-N1	-3.30	117.07	124.73
9	D	400	FMN	C1'-C2'-C3'	3.27	118.91	109.79
9	D	400	FMN	C4A-C4-N3	3.21	121.35	113.19
9	G	300	FMN	O4-C4-C4A	-3.15	118.24	126.60
9	C	503	FMN	C4A-C4-N3	3.15	121.19	113.19
9	C	503	FMN	O4-C4-C4A	-3.13	118.28	126.60
9	D	400	FMN	C10-N1-C2	3.12	123.13	116.90
9	C	503	FMN	C1'-C2'-C3'	3.11	118.47	109.79
9	G	300	FMN	C9A-C5A-N5	-2.85	119.33	122.43
9	G	300	FMN	C4-N3-C2	-2.83	120.42	125.64
9	C	503	FMN	C10-N1-C2	2.81	122.53	116.90
9	G	300	FMN	C4A-C4-N3	2.75	120.18	113.19
9	D	400	FMN	C8M-C8-C7	-2.70	115.21	120.74
9	G	300	FMN	C4A-C10-N1	-2.68	118.52	124.73
9	D	400	FMN	C6-C5A-C9A	2.67	122.72	118.94
9	D	400	FMN	O4-C4-C4A	-2.65	119.56	126.60
9	G	300	FMN	C10-N1-C2	2.56	122.02	116.90
9	C	503	FMN	O3P-P-O2P	2.47	117.06	107.64
9	D	400	FMN	C7M-C7-C8	2.45	125.76	120.74
9	C	503	FMN	O4'-C4'-C3'	-2.43	103.18	109.10
9	G	300	FMN	C6-C5A-C9A	2.20	122.06	118.94
9	D	400	FMN	C4A-C10-N10	2.20	119.69	116.48
9	D	400	FMN	C7M-C7-C6	-2.07	115.67	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	503	FMN	C6-C5A-C9A	2.03	121.81	118.94
10	D	401	RBF	C4-N3-C2	-2.03	121.90	125.64
9	C	503	FMN	O3'-C3'-C4'	2.02	113.69	108.81

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	503	FMN	N10-C1'-C2'-O2'
9	C	503	FMN	N10-C1'-C2'-C3'
9	C	503	FMN	C3'-C4'-C5'-O5'
9	C	503	FMN	C5'-O5'-P-O2P
9	C	503	FMN	C5'-O5'-P-O3P
9	D	400	FMN	N10-C1'-C2'-O2'
9	D	400	FMN	N10-C1'-C2'-C3'
9	D	400	FMN	C2'-C3'-C4'-O4'
9	D	400	FMN	O3'-C3'-C4'-O4'
9	D	400	FMN	O3'-C3'-C4'-C5'
9	G	300	FMN	C1'-C2'-C3'-O3'
9	G	300	FMN	C1'-C2'-C3'-C4'
9	G	300	FMN	O2'-C2'-C3'-O3'
9	G	300	FMN	O2'-C2'-C3'-C4'
9	G	300	FMN	C3'-C4'-C5'-O5'
10	D	401	RBF	C2'-C1'-N10-C10
10	D	401	RBF	N10-C1'-C2'-O2'
10	D	401	RBF	N10-C1'-C2'-C3'
10	D	401	RBF	C1'-C2'-C3'-C4'
10	D	401	RBF	C2'-C3'-C4'-C5'
10	D	401	RBF	O3'-C3'-C4'-C5'
10	D	401	RBF	O4'-C4'-C5'-O5'
10	D	401	RBF	C3'-C4'-C5'-O5'
10	D	401	RBF	O3'-C3'-C4'-O4'
10	D	401	RBF	C2'-C3'-C4'-O4'
9	D	400	FMN	C2'-C3'-C4'-C5'
10	D	401	RBF	O2'-C2'-C3'-C4'
10	D	401	RBF	O2'-C2'-C3'-O3'
9	G	300	FMN	O4'-C4'-C5'-O5'
9	G	300	FMN	C2'-C3'-C4'-O4'
9	G	300	FMN	O3'-C3'-C4'-C5'
9	G	300	FMN	O3'-C3'-C4'-O4'
9	D	400	FMN	O4'-C4'-C5'-O5'
9	C	503	FMN	C5'-O5'-P-O1P

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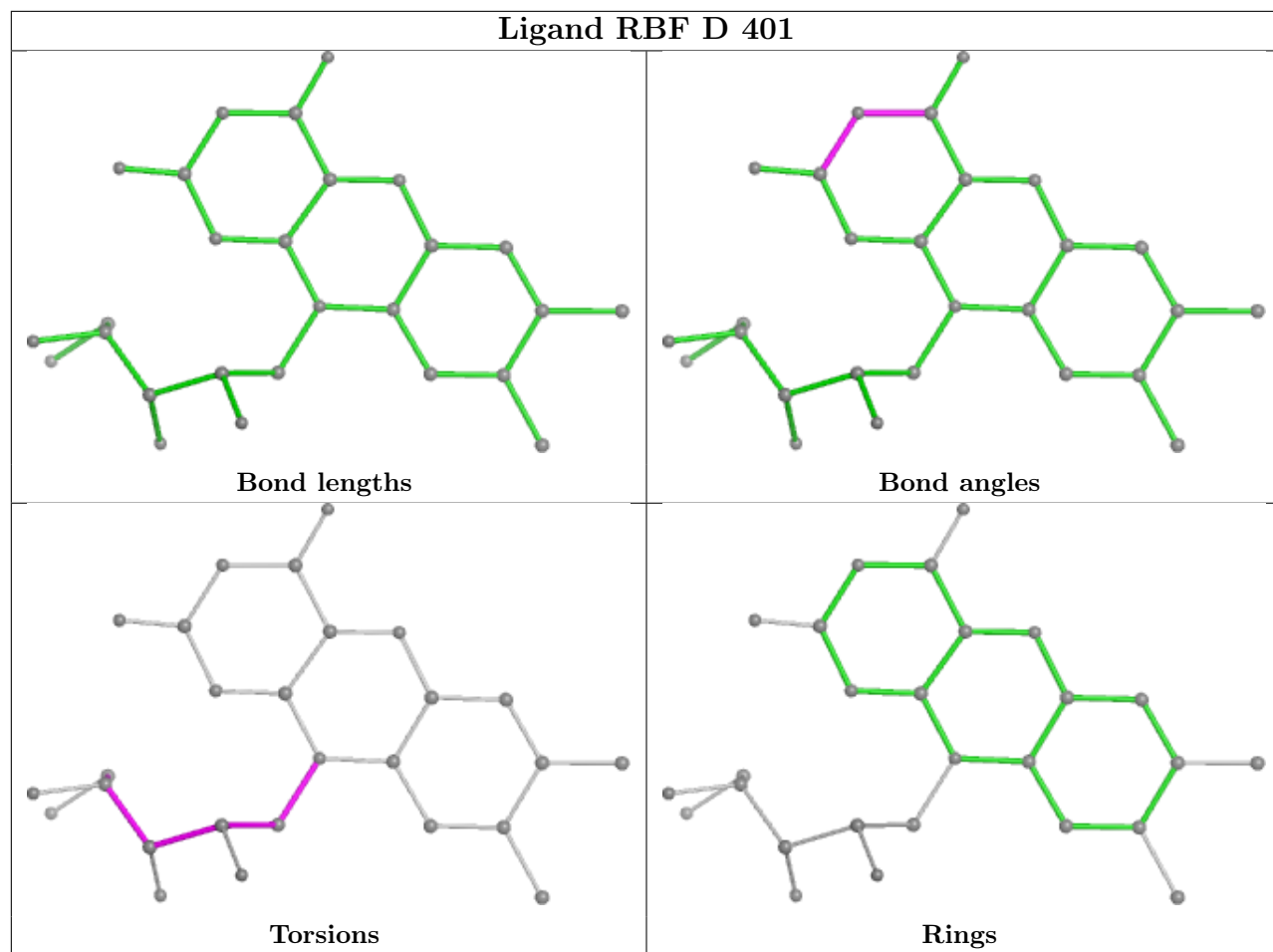
Mol	Chain	Res	Type	Atoms
10	D	401	RBF	C1'-C2'-C3'-O3'
9	G	300	FMN	N10-C1'-C2'-C3'

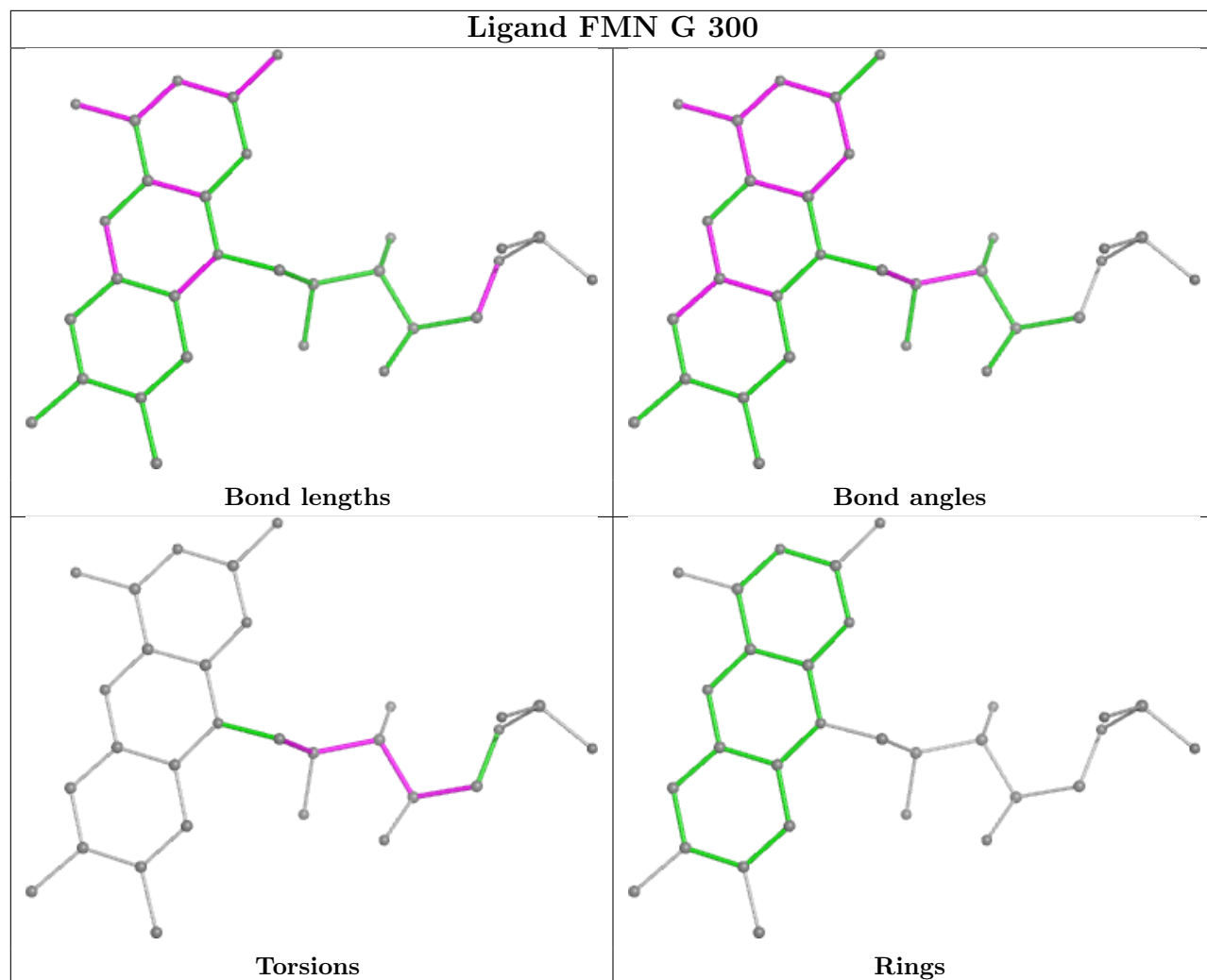
There are no ring outliers.

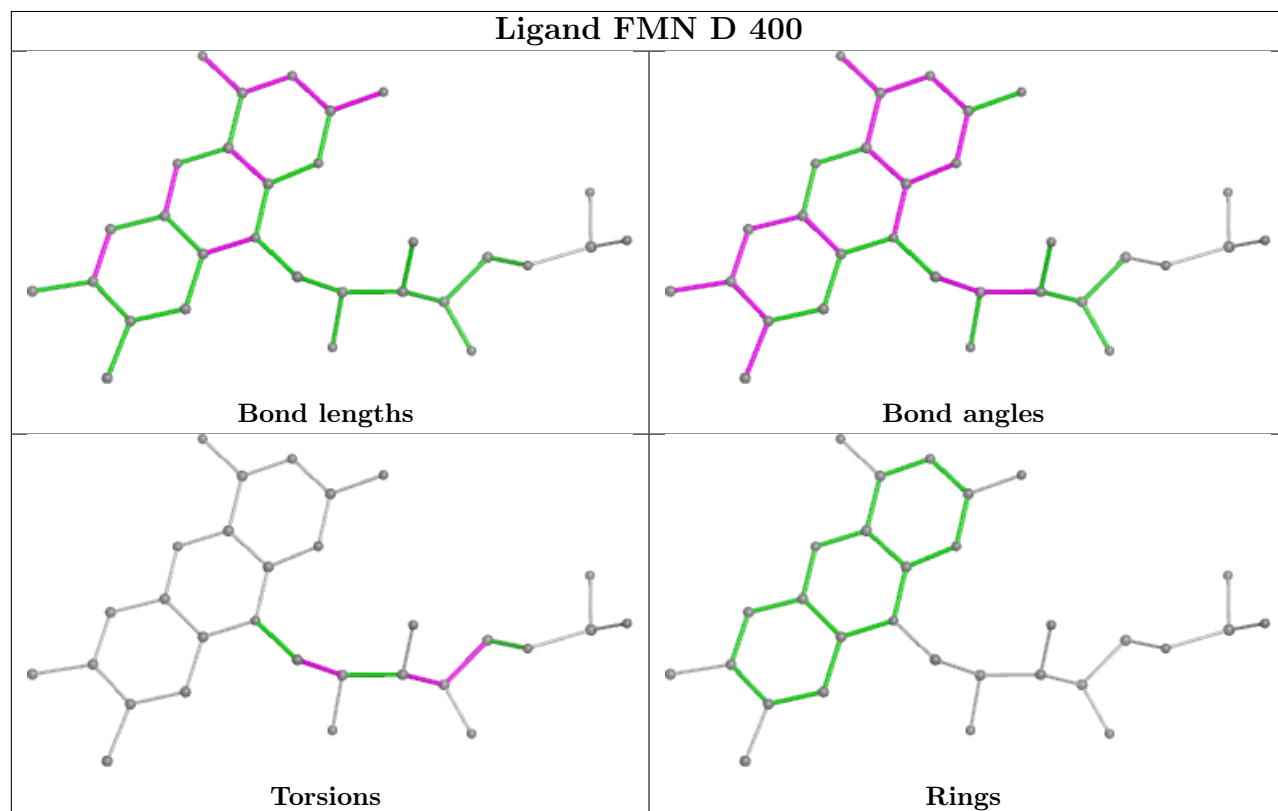
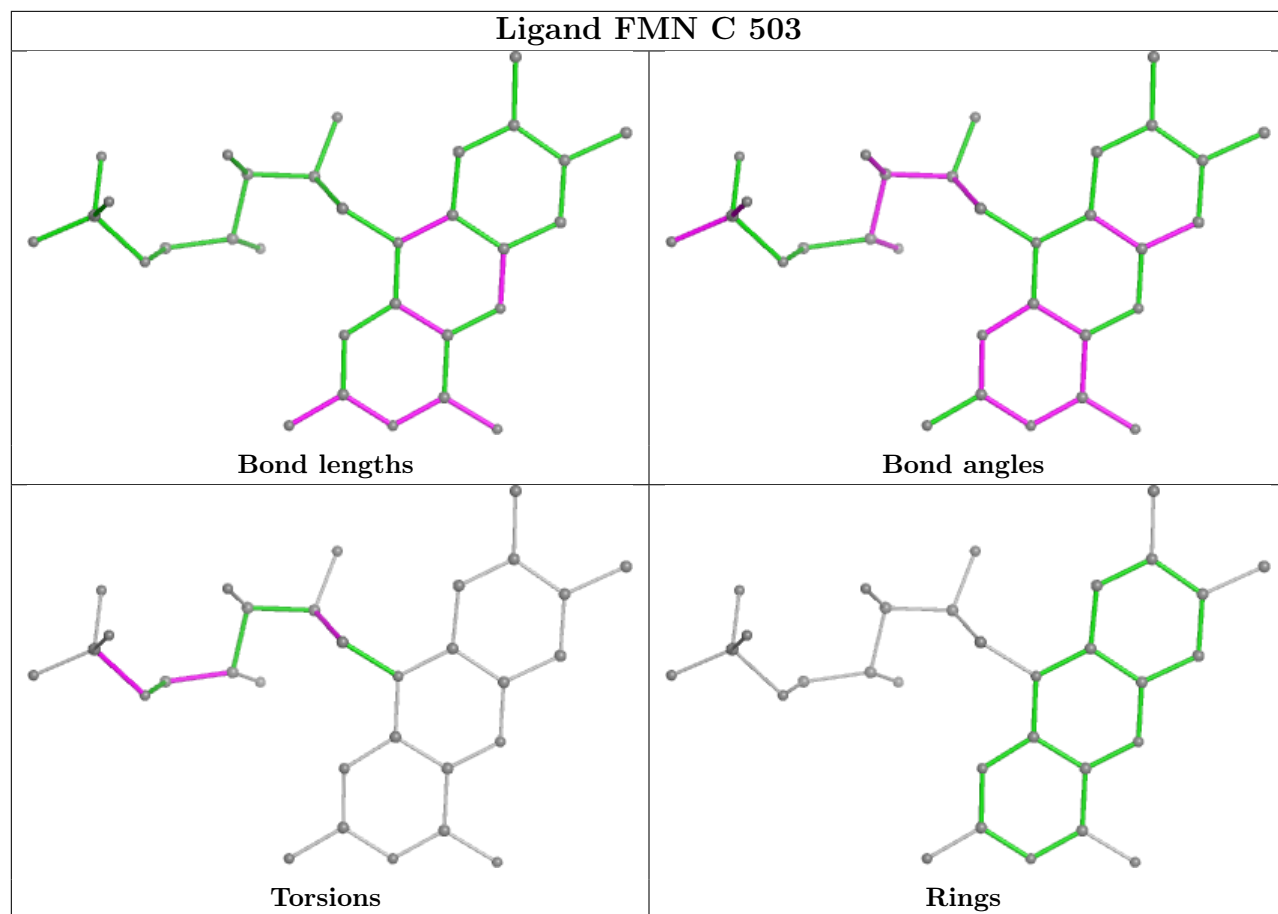
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	301	SF4	1	0
10	D	401	RBF	11	0
9	G	300	FMN	2	0
8	B	302	SF4	2	0
9	C	503	FMN	1	0
9	D	400	FMN	4	0
8	C	502	SF4	1	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.

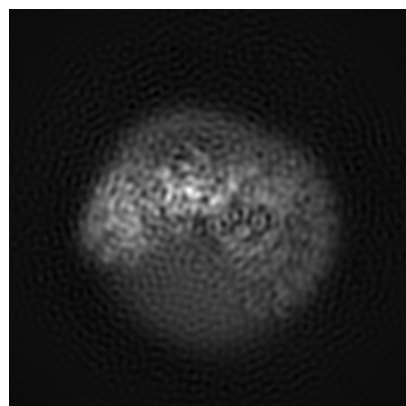
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14622. These allow visual inspection of the internal detail of the map and identification of artifacts.

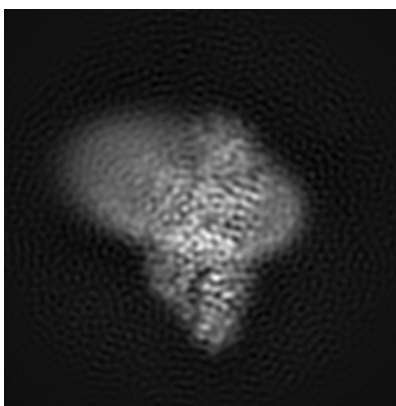
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

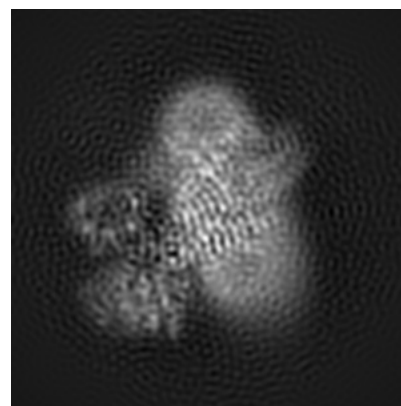
6.1.1 Primary map



X

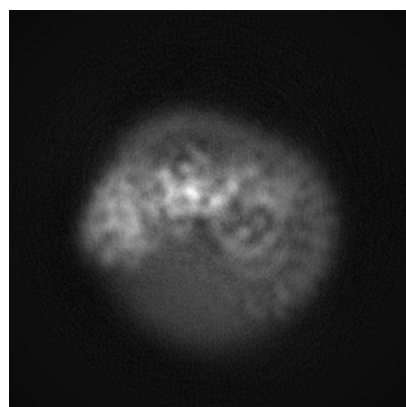


Y

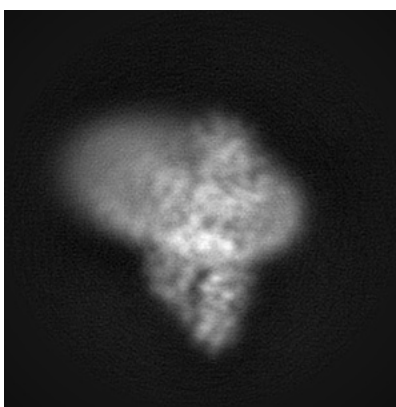


Z

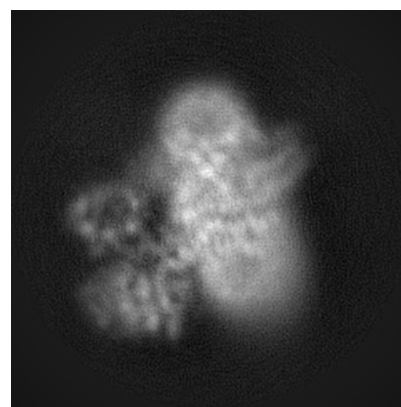
6.1.2 Raw map



X



Y

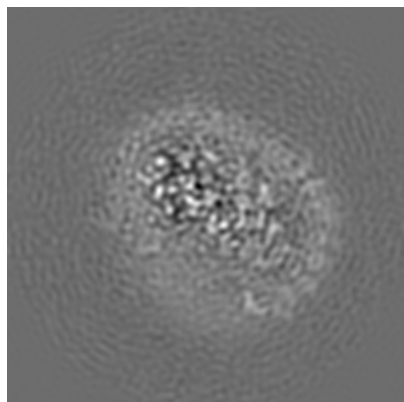


Z

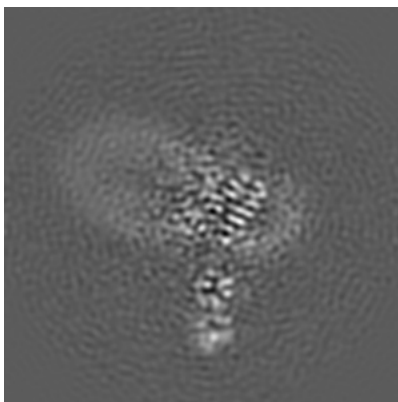
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

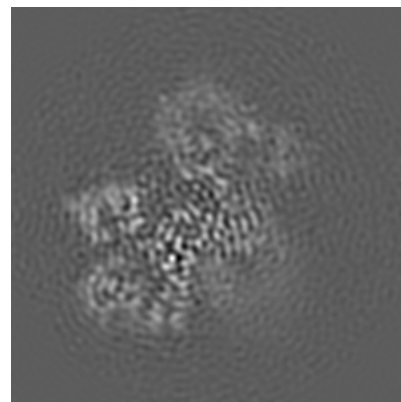
6.2.1 Primary map



X Index: 120

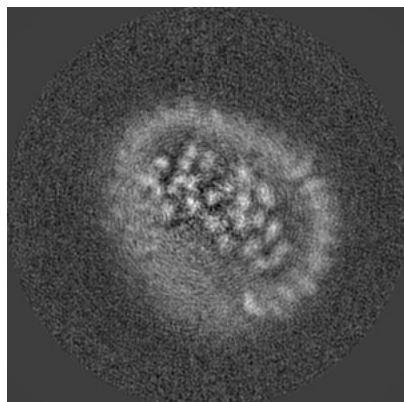


Y Index: 120

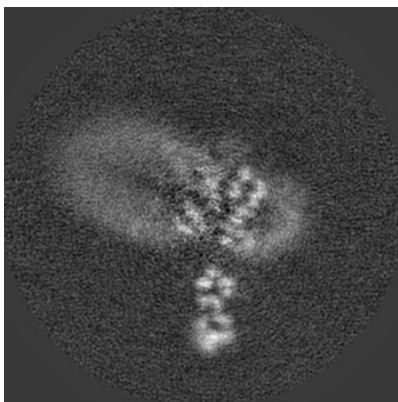


Z Index: 120

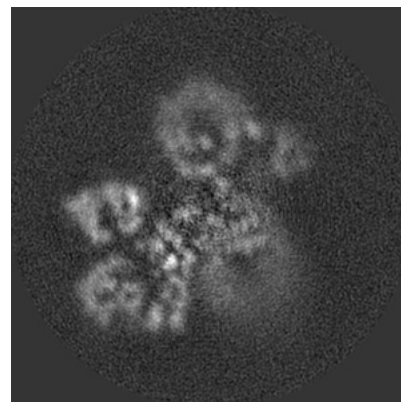
6.2.2 Raw map



X Index: 120



Y Index: 120

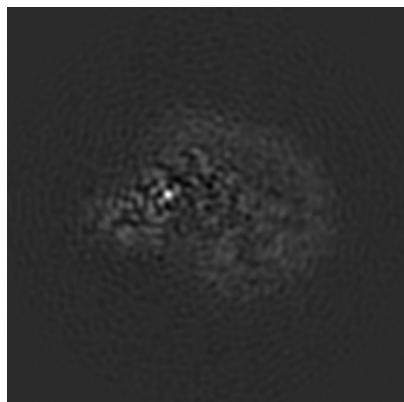


Z Index: 120

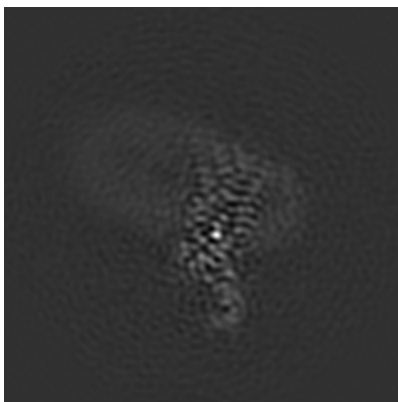
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

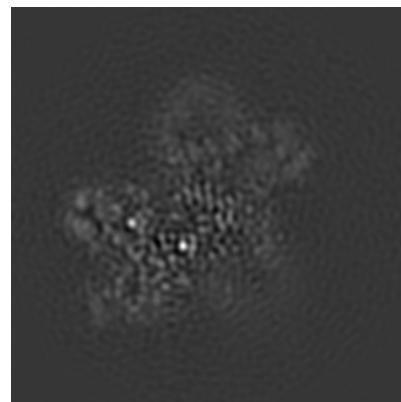
6.3.1 Primary map



X Index: 103

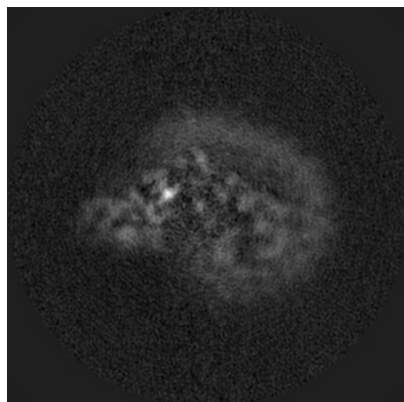


Y Index: 96

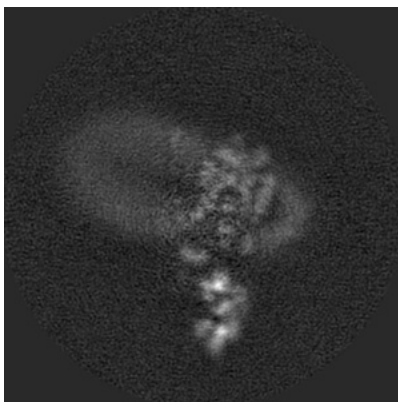


Z Index: 127

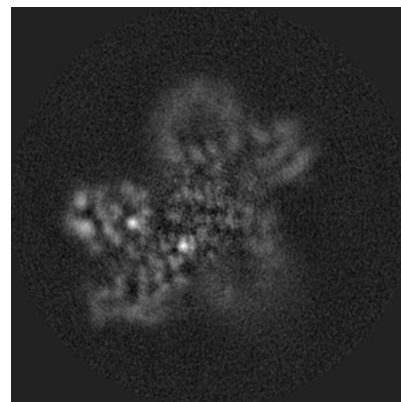
6.3.2 Raw map



X Index: 103



Y Index: 109

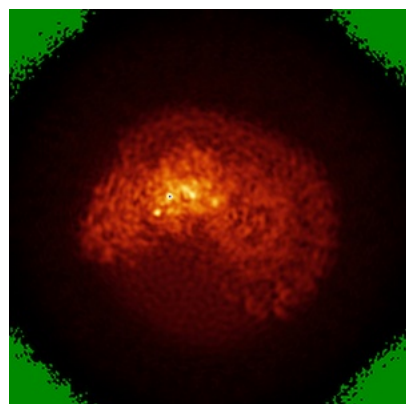


Z Index: 128

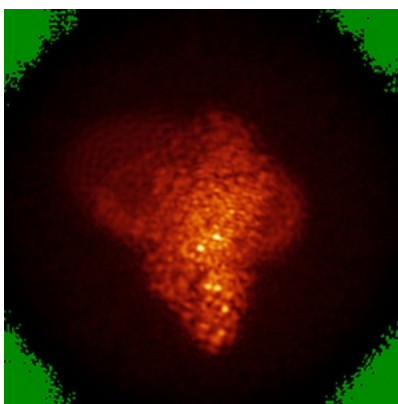
The images above show the largest variance slices of the map in three orthogonal directions.

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

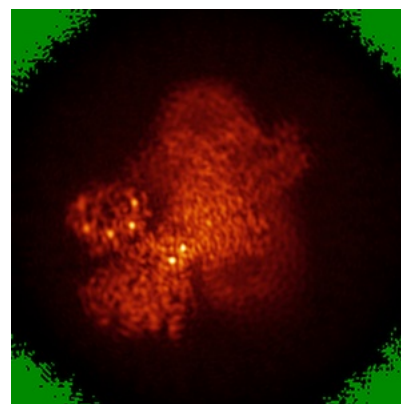
6.4.1 Primary map



X

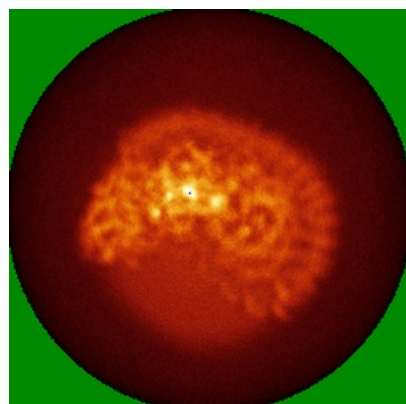


Y

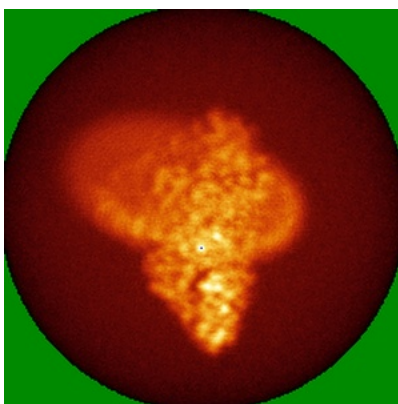


Z

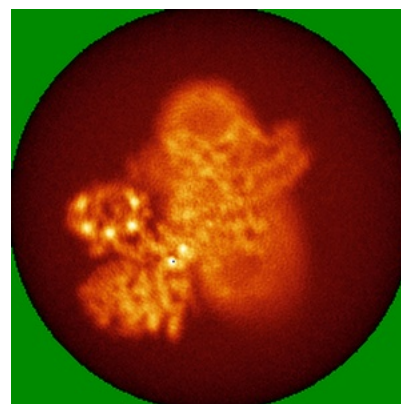
6.4.2 Raw map



X



Y

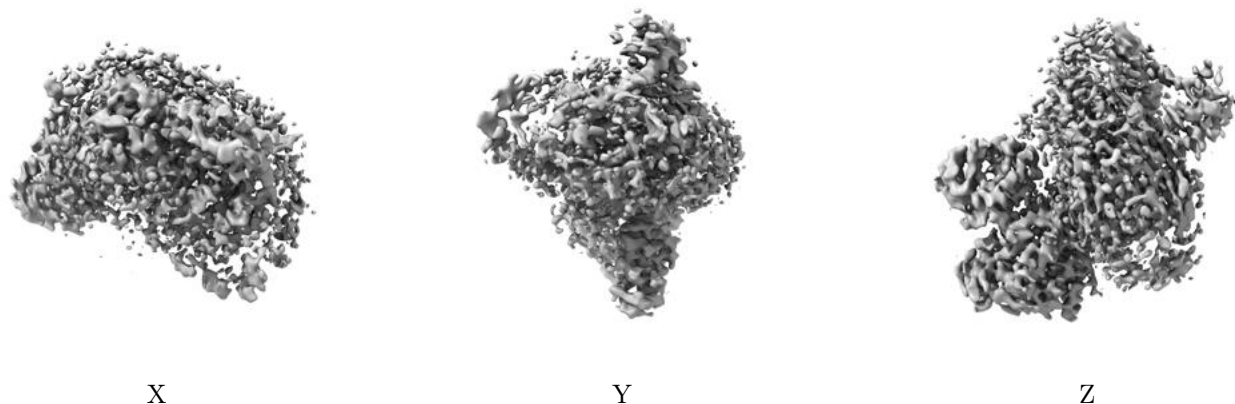


Z

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

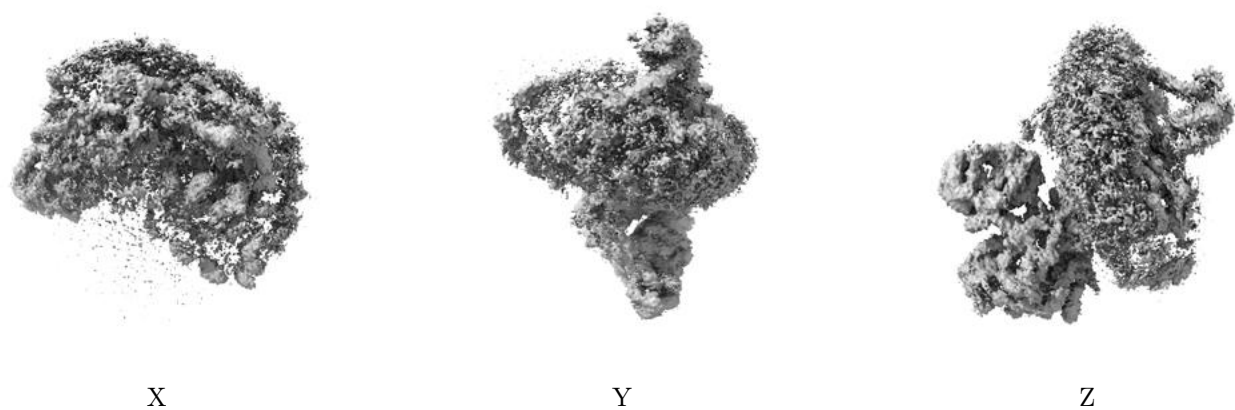
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

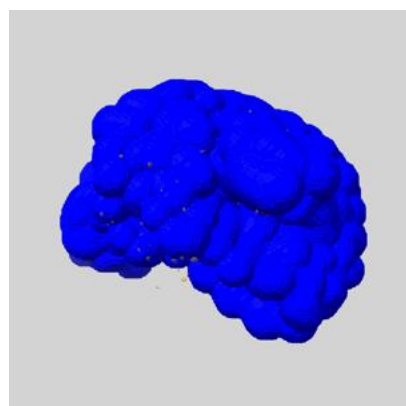
6.6 Mask visualisation [i](#)

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

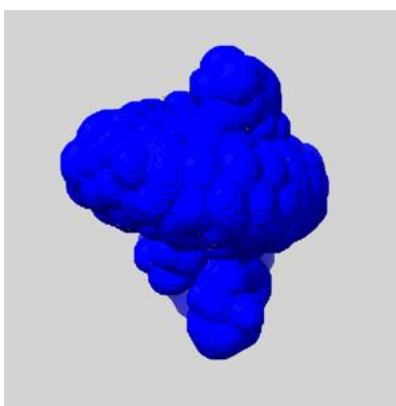
A mask typically either:

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

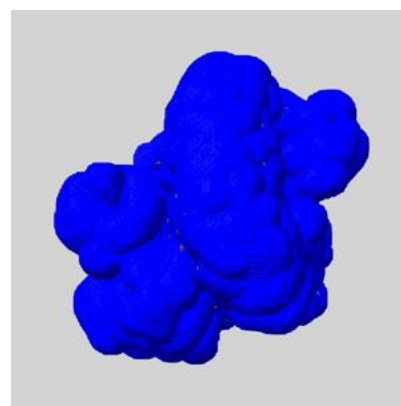
6.6.1 emd_14622_msk_1.map [i](#)



X



Y

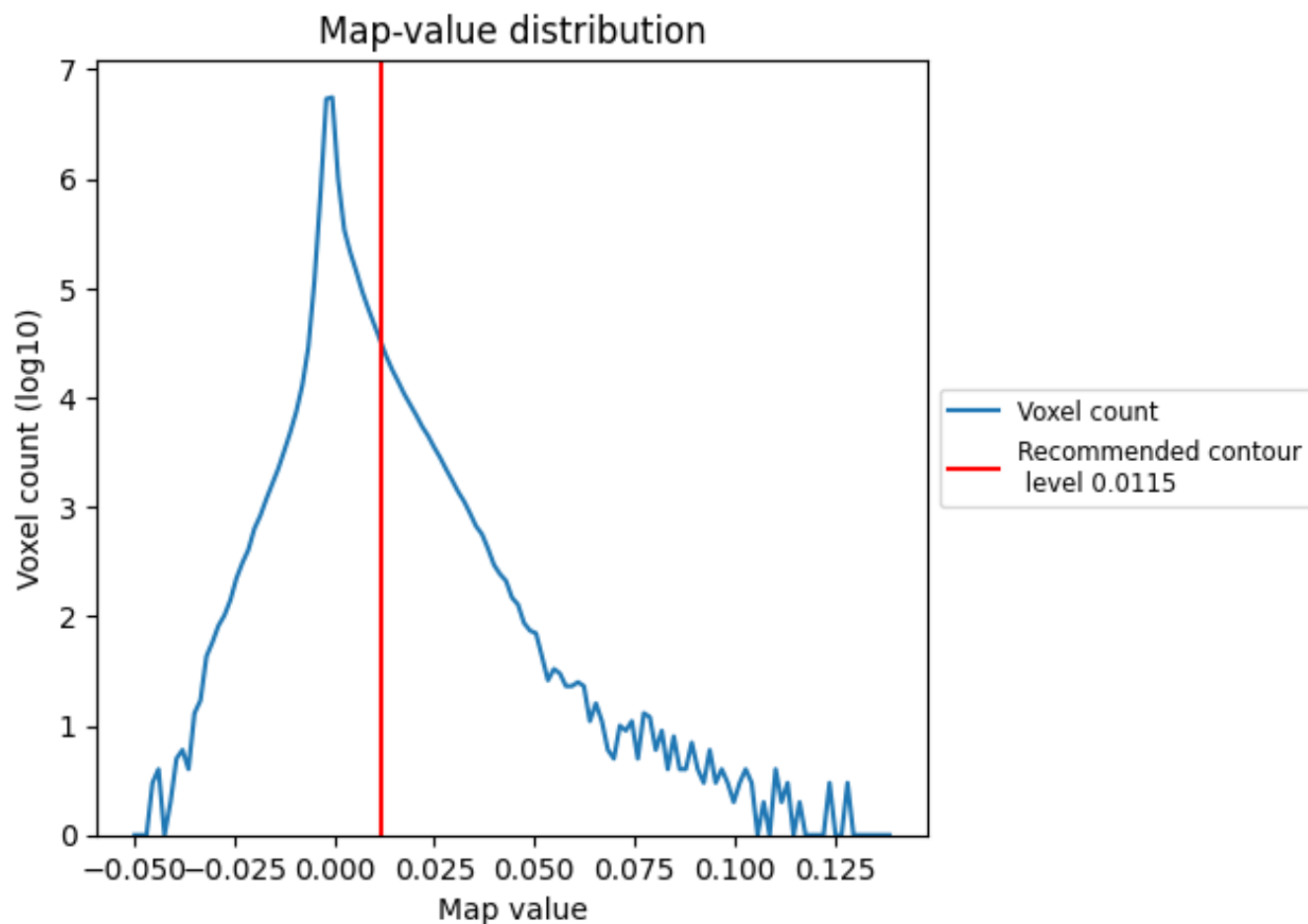


Z

7 Map analysis [i](#)

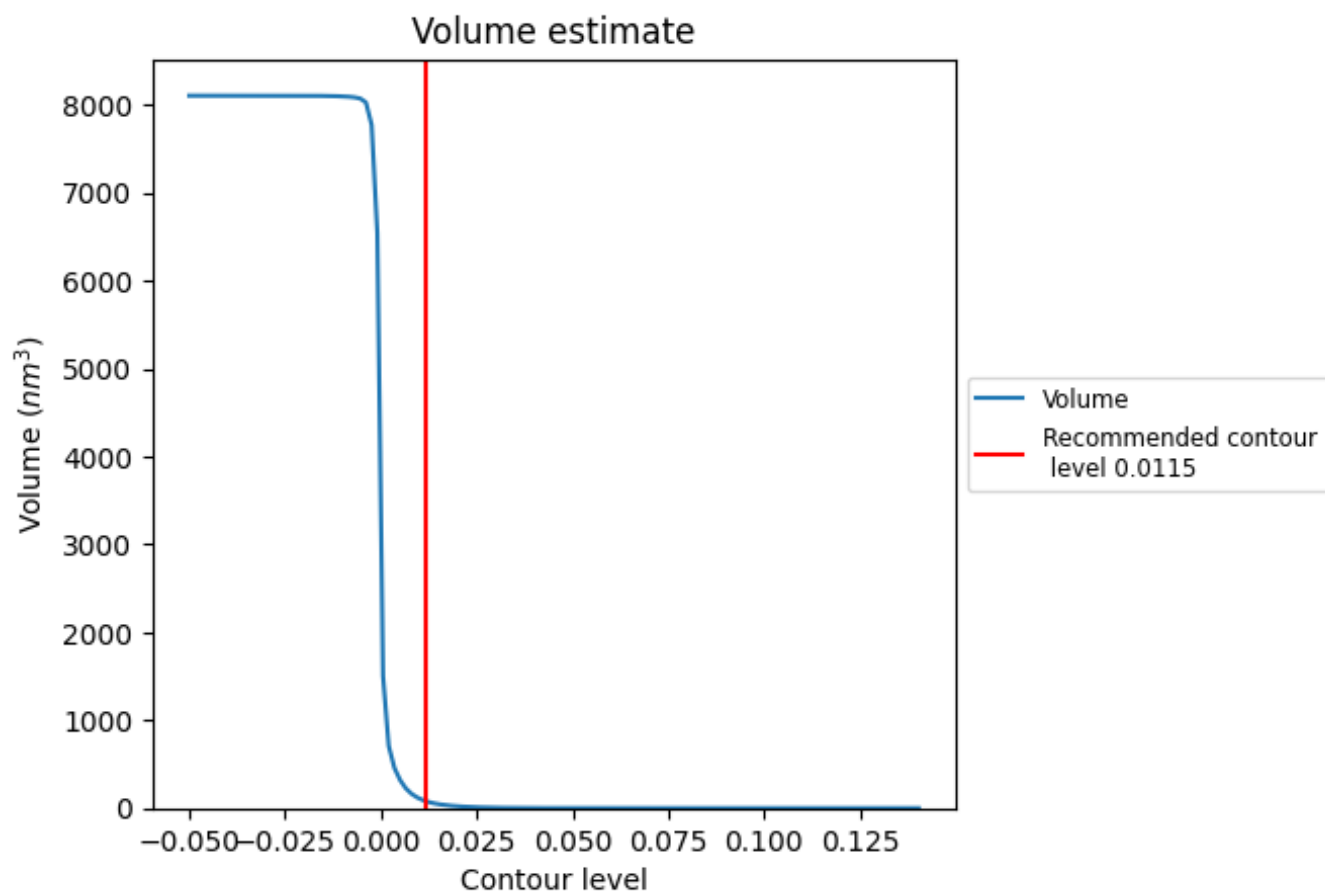
This section contains the results of statistical analysis of the map.

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.

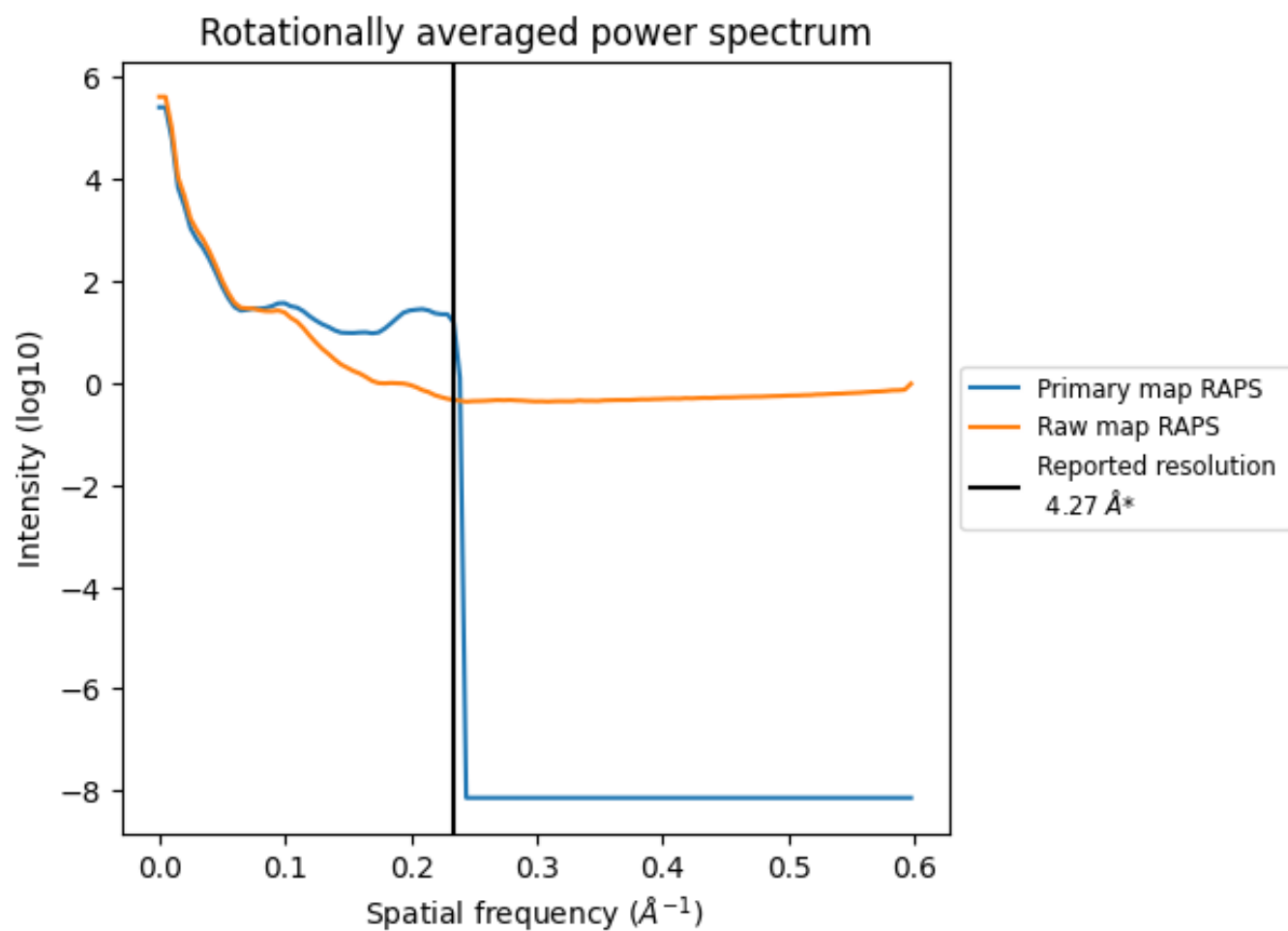
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm^3 ; this corresponds to an approximate mass of 76 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 ⓘ

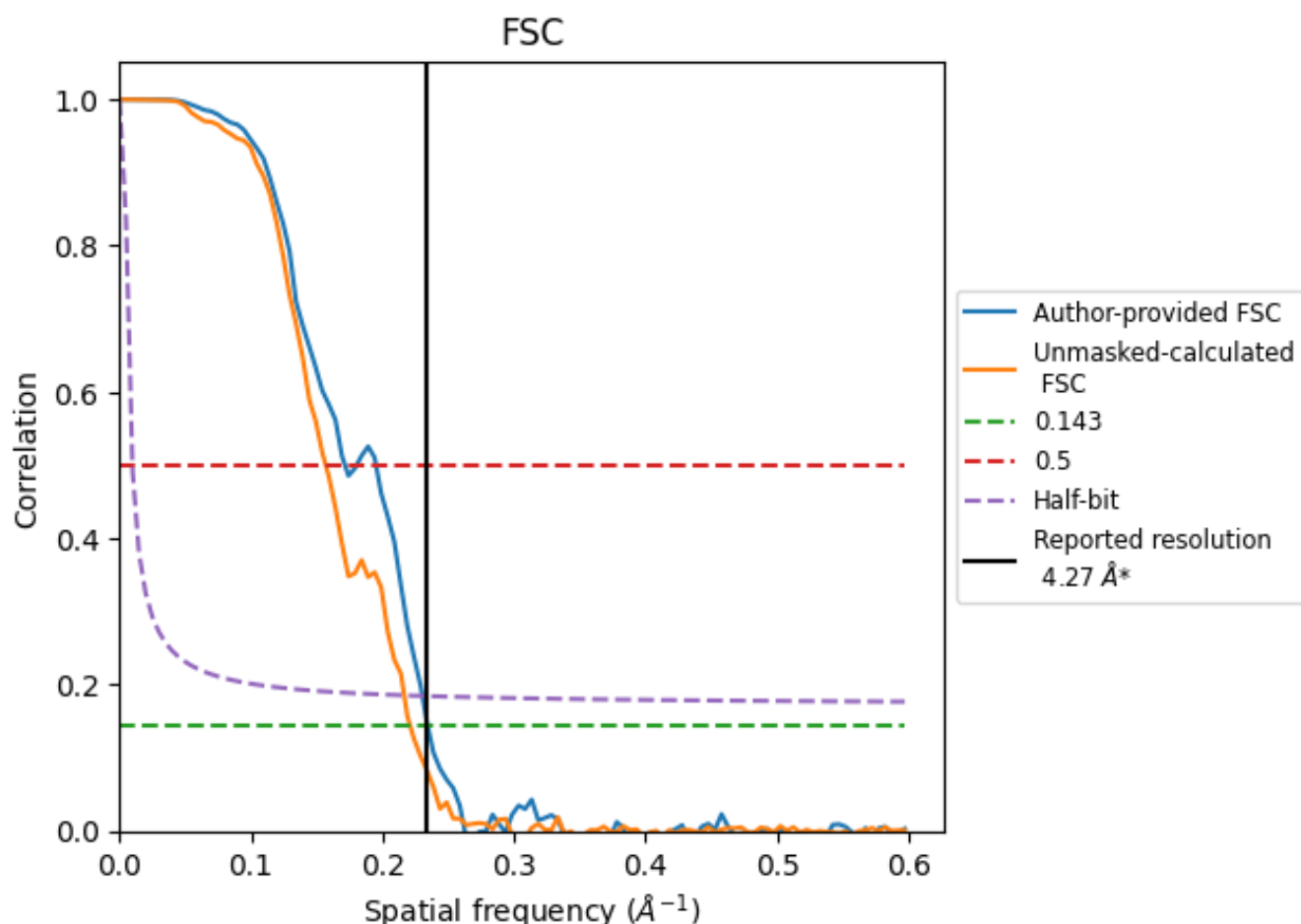


*Reported resolution corresponds to spatial frequency of 0.234 Å⁻¹

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 0.234 Å⁻¹

8.2 Resolution estimates [i](#)

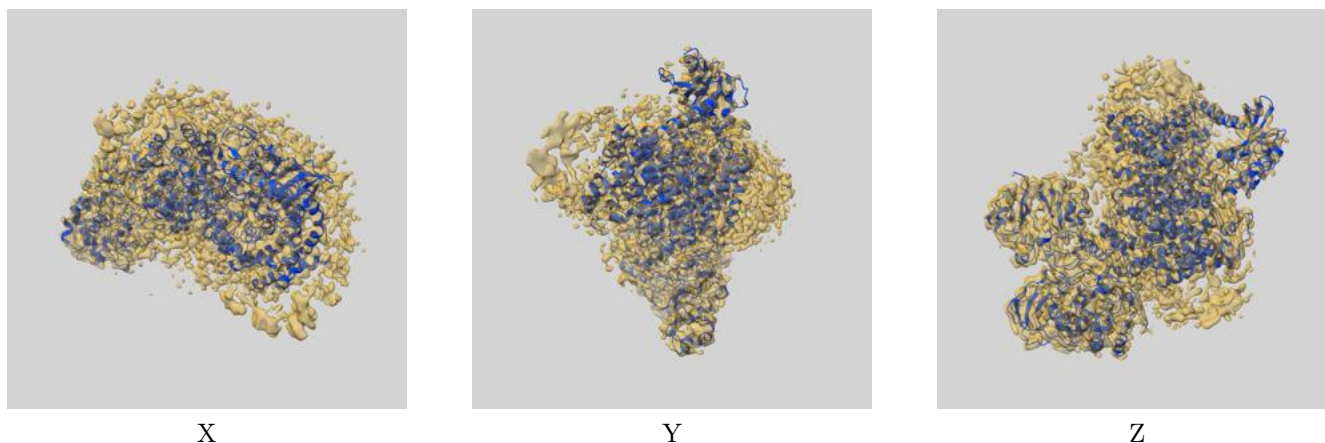
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.27	-	-
Author-provided FSC curve	4.26	5.83	4.34
Unmasked-calculated*	4.52	6.37	4.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

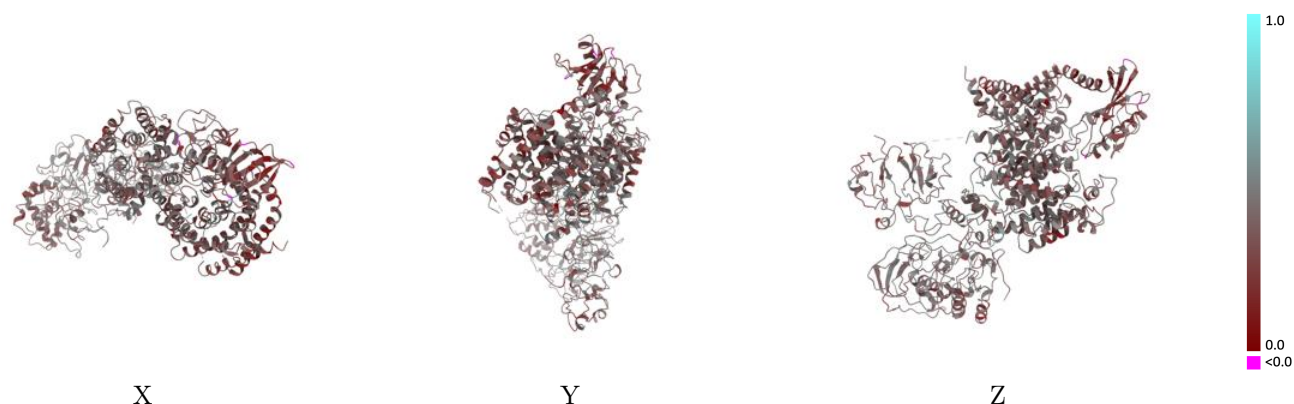
This section contains information regarding the fit between EMDB map EMD-14622 and PDB model 7ZC6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



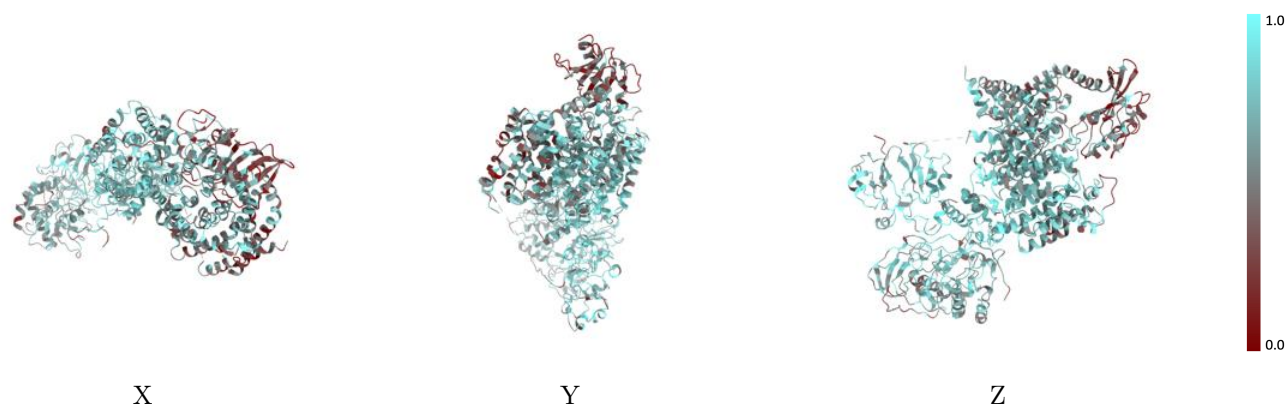
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



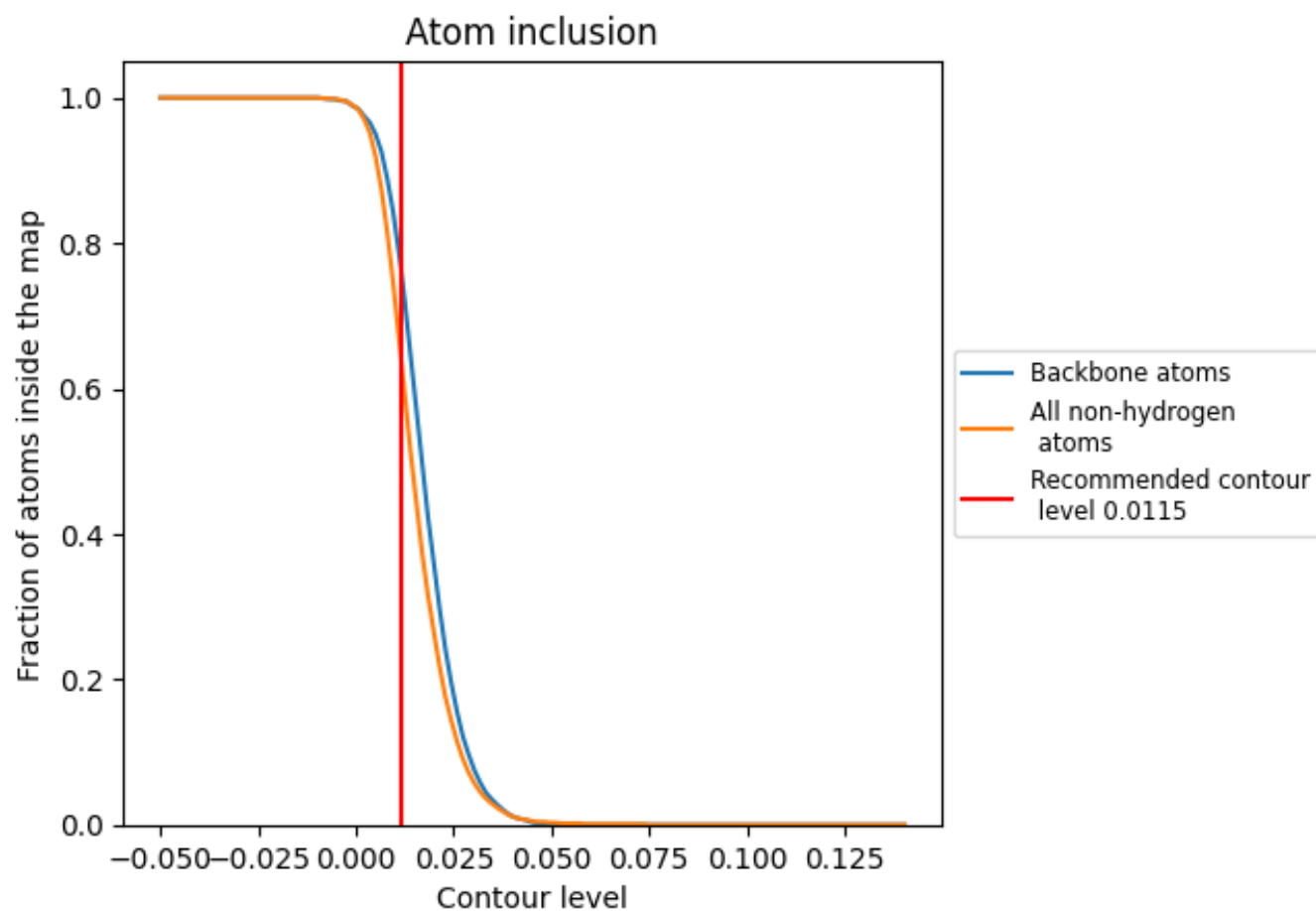
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0115).

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6440</div>	<div><div></div>0.3800</div>
A	<div><div></div>0.6430</div>	<div><div></div>0.3840</div>
B	<div><div></div>0.6860</div>	<div><div></div>0.3780</div>
C	<div><div></div>0.6680</div>	<div><div></div>0.4010</div>
D	<div><div></div>0.7250</div>	<div><div></div>0.3960</div>
E	<div><div></div>0.6530</div>	<div><div></div>0.3750</div>
G	<div><div></div>0.3940</div>	<div><div></div>0.3060</div>

1.0

0.0

<0.0