



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 02:38 AM EST

PDB ID : 7UT9
EMDB ID : EMD-26763
Title : CryoEM structure of Azotobacter vinelandii nitrogenase complex (1:1 FeP:MoFeP, ADP/ATP-bound) during catalytic N₂ reduction
Authors : Rutledge, H.L.; Cook, B.; Tezcan, F.A.; Herzik, M.A.
Deposited on : 2022-04-26
Resolution : 2.44 Å(reported)
Based on initial model : 4WZA

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

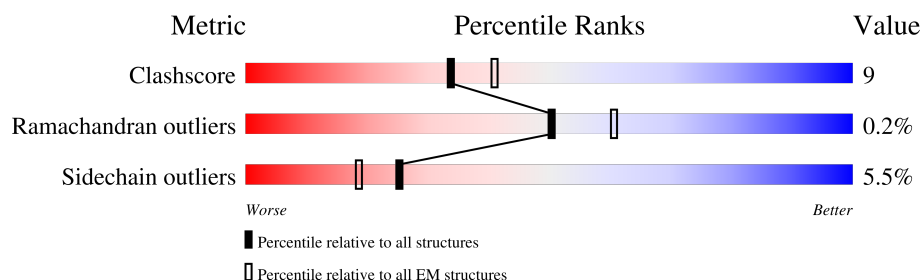
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	492	
1	C	492	
2	B	523	
2	D	523	
3	E	290	
3	F	290	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 20243 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	477	Total	C	N	O	S	0	0
			3790	2410	646	709	25		
1	C	475	Total	C	N	O	S	0	0
			3776	2402	644	706	24		

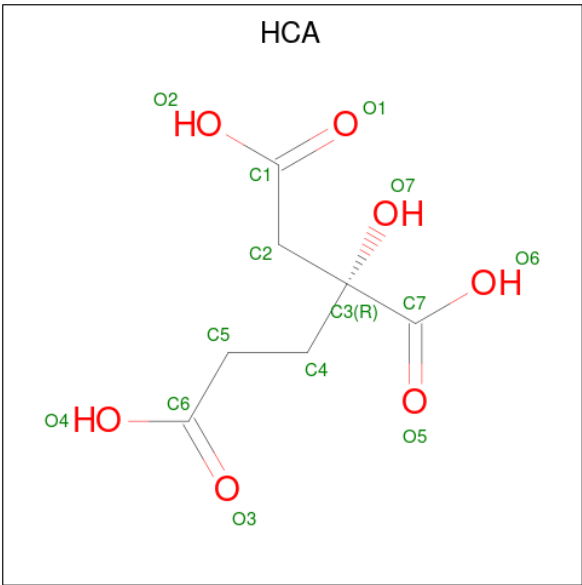
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		
2	D	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		

- Molecule 3 is a protein called Nitrogenase iron protein gamma chain.

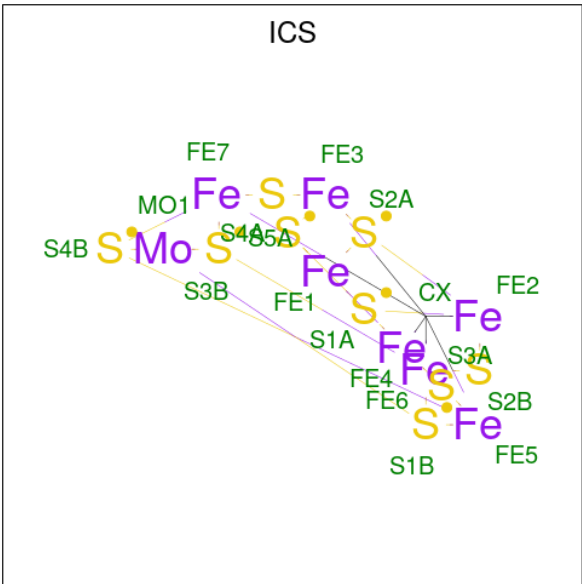
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	271	Total	C	N	O	S	0	0
			2052	1282	350	400	20		
3	F	271	Total	C	N	O	S	0	0
			2053	1283	350	400	20		

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C₇H₁₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			14	7	7	
4	C	1	Total	C	O	0
			14	7	7	

- Molecule 5 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe₇MoS₉) (labeled as "Ligand of Interest" by depositor).



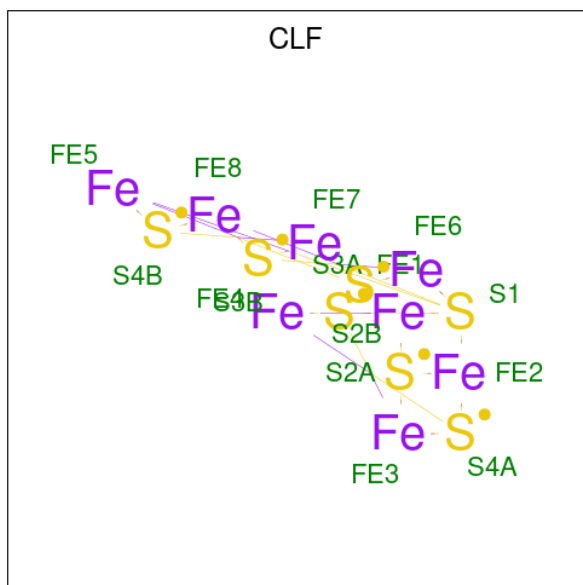
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	

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Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	

- Molecule 6 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	Fe	S	0
			15	8	7	
6	D	1	Total	Fe	S	0
			15	8	7	

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

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Fe	0
			1	1	
7	D	1	Total	Fe	0
			1	1	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

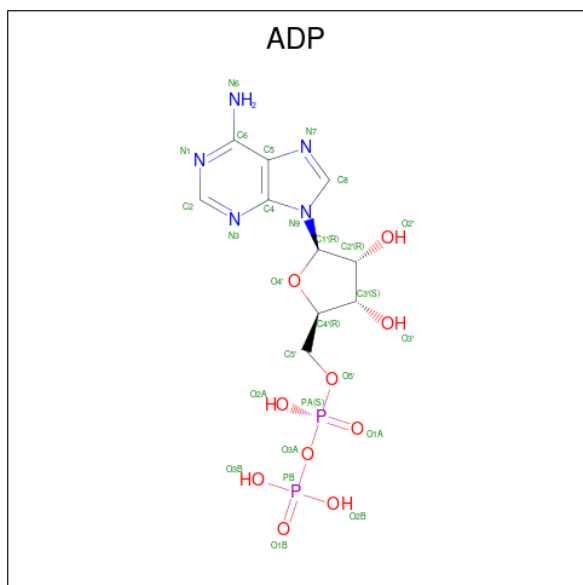
Mol	Chain	Residues	Atoms		AltConf
8	E	1	Total	Mg	0
			1	1	

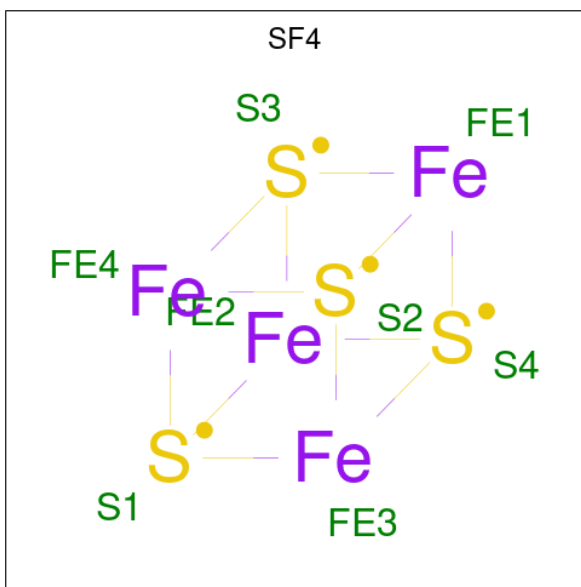
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Mol	Chain	Residues	Atoms		AltConf
8	F	1	Total	Mg	0
			1	1	

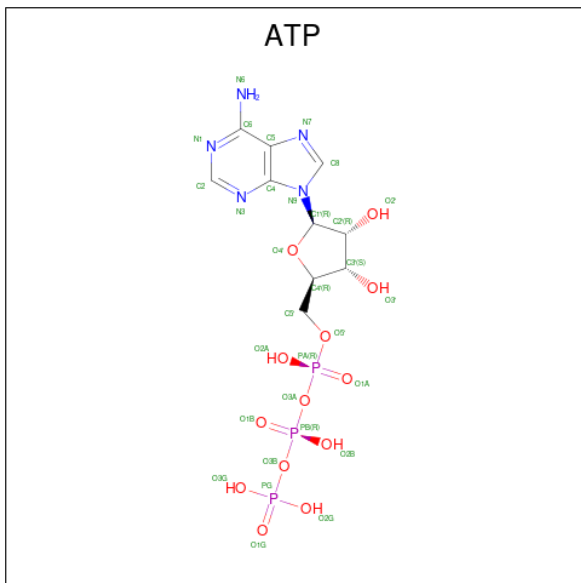
- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf
10	F	1	Total	Fe	S		0
			8	4	4		

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

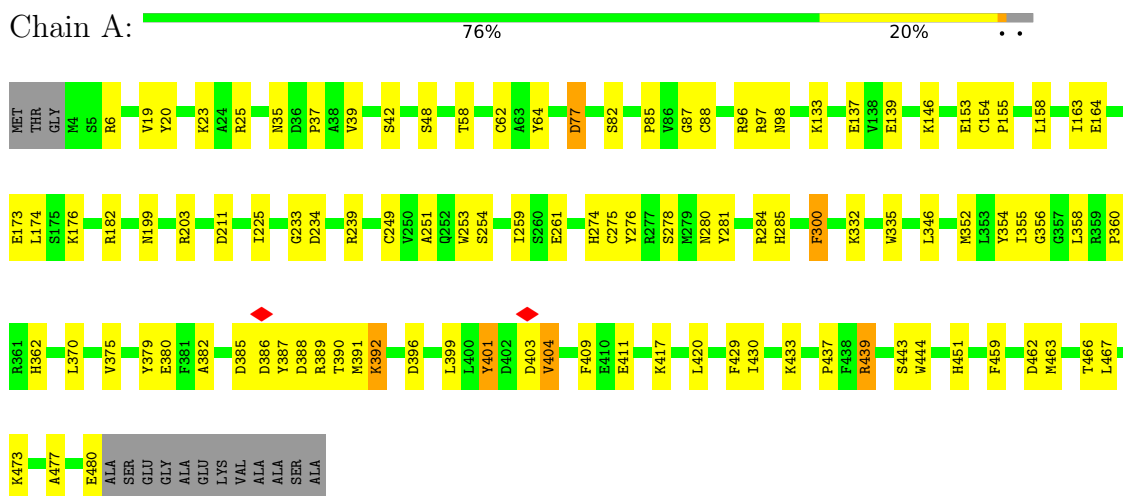
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	13	Total 13	O 13	0
12	B	20	Total 20	O 20	0
12	C	11	Total 11	O 11	0
12	D	8	Total 8	O 8	0
12	E	3	Total 3	O 3	0
12	F	5	Total 5	O 5	0

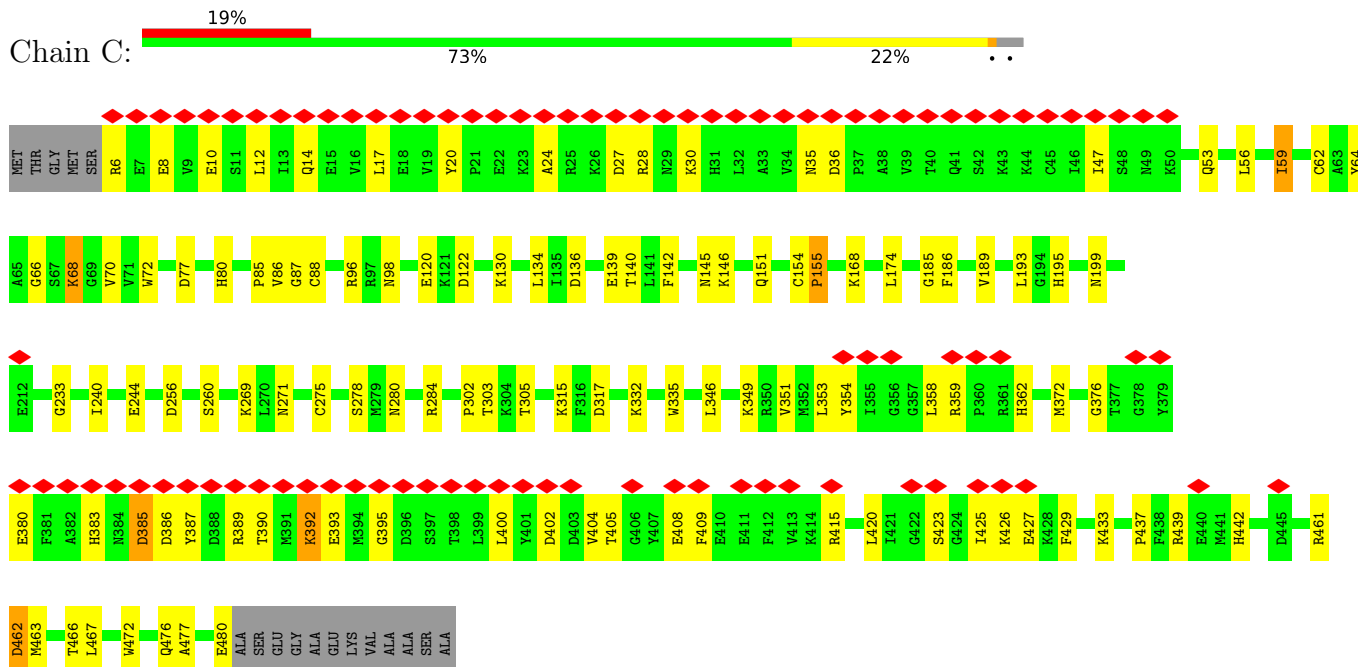
3 Residue-property plots

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


• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

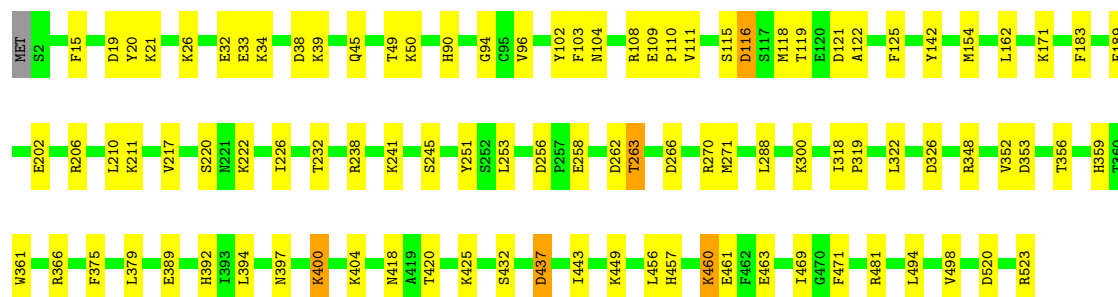


• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain




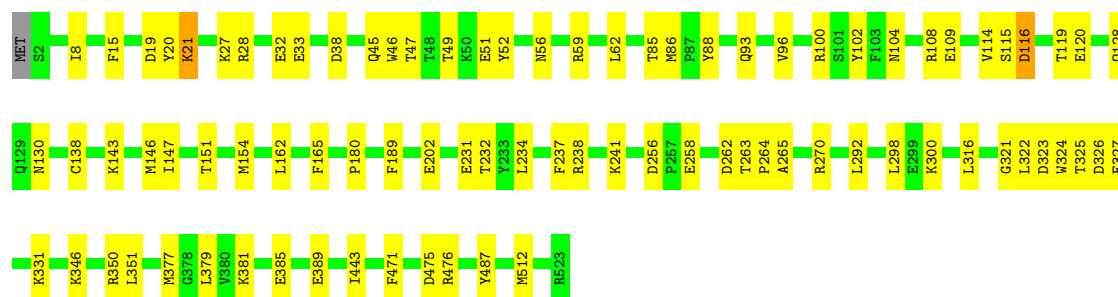
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B:  81% 18%



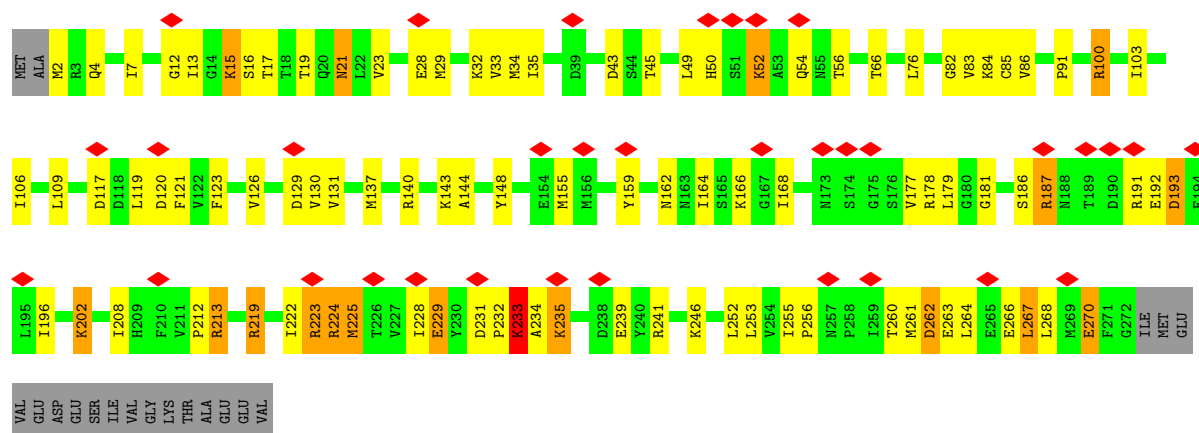
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:  83% 16%



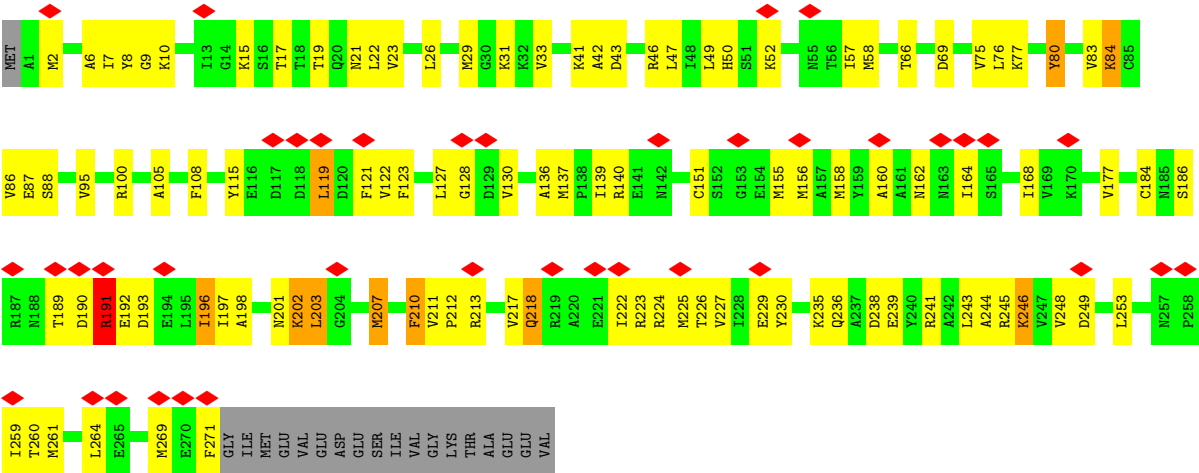
- Molecule 3: Nitrogenase iron protein gamma chain

Chain E:  12% 60% 28% 6% 7%



- Molecule 3: Nitrogenase iron protein gamma chain

Chain F:  13% 56% 33% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	135000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.459	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.075	Depositor
Map size (\AA)	320.63998, 320.63998, 320.63998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HCA, ADP, SF4, CLF, FE, ATP, ICS

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	0.27	0/3878	0.51	0/5229
1	C	0.27	0/3864	0.50	0/5211
2	B	0.26	0/4280	0.48	0/5786
2	D	0.25	0/4280	0.46	0/5786
3	E	0.29	0/2076	0.56	1/2796 (0.0%)
3	F	0.28	0/2077	0.58	0/2798
All	All	0.27	0/20455	0.51	1/27606 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	267	LEU	CA-CB-CG	5.74	128.50	115.30

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	3790	0	3729	64	0
1	C	3776	0	3715	74	0
2	B	4174	0	4088	59	0
2	D	4174	0	4088	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2052	0	2063	69	0
3	F	2053	0	2069	66	0
4	A	14	0	7	1	0
4	C	14	0	7	1	0
5	A	18	0	0	1	0
5	C	18	0	0	2	0
6	B	15	0	0	1	0
6	D	15	0	0	3	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	E	27	0	12	3	0
10	F	8	0	0	0	0
11	F	31	0	12	2	0
12	A	13	0	0	0	0
12	B	20	0	0	0	0
12	C	11	0	0	0	0
12	D	8	0	0	0	0
12	E	3	0	0	1	0
12	F	5	0	0	0	0
All	All	20243	0	19790	361	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 9.

All (361) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:CYS:HB2	1:C:155:PRO:HD3	1.59	0.84
1:A:173:GLU:HG2	1:A:174:LEU:HD12	1.61	0.82
2:B:253:LEU:HD23	2:B:256:ASP:HB3	1.66	0.77
1:C:359:ARG:NH1	5:C:502:ICS:S4B	2.57	0.77
1:C:96:ARG:NH2	5:C:502:ICS:S5A	2.59	0.76
2:D:28:ARG:HA	2:D:32:GLU:HG3	1.66	0.76
3:E:186:SER:HB3	3:E:212:PRO:HA	1.70	0.73
1:A:158:LEU:HD11	2:B:154:MET:HG2	1.70	0.73
2:B:353:ASP:HB2	2:D:265:ALA:HB2	1.70	0.72
1:A:146:LYS:NZ	2:B:33:GLU:O	2.23	0.72
3:E:255:ILE:H	3:E:255:ILE:HD12	1.55	0.71
3:F:137:MET:HA	3:F:140:ARG:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:GLU:OE1	2:B:34:LYS:NZ	2.24	0.70
2:D:104:ASN:ND2	2:D:109:GLU:O	2.26	0.69
1:A:477:ALA:HB3	1:A:480:GLU:HG3	1.74	0.69
2:B:125:PHE:HA	3:E:91:PRO:HB3	1.75	0.69
1:C:386:ASP:OD1	1:C:389:ARG:NH2	2.27	0.68
2:B:162:LEU:HD23	2:B:183:PHE:HB2	1.75	0.67
3:E:84:LYS:HE3	3:E:84:LYS:HA	1.77	0.67
1:C:139:GLU:HG3	1:C:174:LEU:HD13	1.76	0.67
2:B:238:ARG:NH1	2:B:258:GLU:OE2	2.28	0.67
1:C:390:THR:HA	1:C:393:GLU:HB2	1.77	0.67
2:B:226:ILE:HB	2:B:253:LEU:HD12	1.77	0.66
1:A:85:PRO:HB2	6:B:601:CLF:S2B	2.36	0.66
3:E:262:ASP:OD1	3:E:262:ASP:N	2.24	0.66
1:C:142:PHE:O	1:C:145:ASN:ND2	2.25	0.66
1:C:28:ARG:HH22	1:C:404:VAL:HA	1.59	0.66
3:E:33:VAL:HG23	3:E:121:PHE:HB2	1.78	0.66
2:B:19:ASP:OD1	2:B:20:TYR:N	2.30	0.65
3:E:164:ILE:O	3:E:168:ILE:HG12	1.97	0.64
3:E:223:ARG:O	3:E:224:ARG:HG3	1.98	0.64
1:A:154:CYS:HB2	1:A:155:PRO:HD3	1.79	0.64
3:F:29:MET:SD	3:F:31:LYS:NZ	2.70	0.64
1:C:136:ASP:O	1:C:140:THR:HG23	1.98	0.63
1:C:30:LYS:HB3	1:C:47:ILE:HD13	1.80	0.63
3:F:213:ARG:HD2	11:F:303:ATP:C2	2.34	0.63
3:F:225:MET:HG2	3:F:229:GLU:HB3	1.79	0.62
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.80	0.62
3:F:10:LYS:HE2	3:F:160:ALA:HB2	1.80	0.62
3:F:213:ARG:NH1	3:F:218:GLN:OE1	2.32	0.62
1:A:399:LEU:HD22	1:A:401:TYR:HD2	1.64	0.62
3:E:181:GLY:HA3	3:E:208:ILE:HD11	1.81	0.62
1:A:37:PRO:O	1:A:392:LYS:NZ	2.31	0.62
1:C:359:ARG:NH1	1:C:442:HIS:HA	2.15	0.61
1:A:139:GLU:HG3	1:A:174:LEU:HD23	1.83	0.61
3:E:193:ASP:N	3:E:193:ASP:OD1	2.32	0.61
1:A:355:ILE:HG22	1:A:356:GLY:H	1.66	0.60
2:B:103:PHE:HB3	2:B:111:VAL:HG21	1.82	0.60
3:E:32:LYS:NZ	3:E:82:GLY:O	2.34	0.60
3:E:263:GLU:O	3:E:267:LEU:HD22	2.02	0.60
1:A:389:ARG:HG3	1:A:389:ARG:HH11	1.67	0.59
4:A:501:HCA:O1	4:A:501:HCA:O7	2.20	0.59
1:A:433:LYS:NZ	2:B:263:THR:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:57:ILE:HD13	3:F:105:ALA:HB1	1.85	0.59
2:B:104:ASN:ND2	2:B:109:GLU:O	2.36	0.59
2:B:361:TRP:NE1	2:B:523:ARG:O	2.34	0.59
3:E:86:VAL:HG21	3:E:109:LEU:HD11	1.84	0.59
1:C:461:ARG:NH1	2:D:8:ILE:O	2.35	0.58
3:F:46:ARG:HG3	3:F:224:ARG:NH2	2.18	0.58
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.84	0.58
1:C:195:HIS:O	1:C:199:ASN:ND2	2.27	0.58
3:E:23:VAL:HG11	3:E:35:ILE:HD11	1.86	0.58
3:F:223:ARG:HH11	3:F:225:MET:HE2	1.69	0.58
2:D:324:TRP:HH2	2:D:377:MET:HG2	1.69	0.58
3:E:19:THR:O	3:E:23:VAL:HG13	2.04	0.58
3:E:228:ILE:HG13	3:E:229:GLU:N	2.18	0.58
3:F:158:MET:SD	3:F:158:MET:N	2.77	0.58
1:A:275:CYS:HA	1:A:358:LEU:HD13	1.85	0.57
1:C:35:ASN:ND2	1:C:395:GLY:O	2.37	0.57
3:E:106:ILE:HD12	3:E:137:MET:HG2	1.86	0.57
3:F:66:THR:OG1	3:F:69:ASP:OD1	2.21	0.57
1:A:385:ASP:HB2	1:A:389:ARG:HH12	1.69	0.56
2:B:222:LYS:HD3	2:B:288:LEU:HD21	1.87	0.56
3:E:267:LEU:HA	3:E:270:GLU:OE1	2.04	0.56
3:F:43:ASP:OD1	3:F:43:ASP:N	2.38	0.56
1:A:199:ASN:ND2	1:A:278:SER:O	2.38	0.56
1:C:256:ASP:O	2:D:27:LYS:NZ	2.38	0.56
1:A:251:ALA:HA	1:A:261:GLU:HB3	1.86	0.56
1:C:20:TYR:HB3	1:C:24:ALA:HB3	1.85	0.56
1:C:439:ARG:NH2	1:C:462:ASP:OD2	2.39	0.56
1:C:8:GLU:O	1:C:12:LEU:HG	2.05	0.56
3:E:4:GLN:HB2	3:E:144:ALA:HA	1.88	0.56
1:A:387:TYR:O	1:A:391:MET:HG2	2.06	0.56
2:D:38:ASP:OD1	2:D:38:ASP:N	2.39	0.56
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.21	0.56
3:E:52:LYS:NZ	12:E:401:HOH:O	2.27	0.56
1:A:459:PHE:O	1:A:463:MET:HG2	2.06	0.56
3:F:186:SER:HB3	3:F:212:PRO:HA	1.86	0.56
3:F:26:LEU:HD12	3:F:31:LYS:HG2	1.87	0.55
3:F:164:ILE:O	3:F:168:ILE:HG13	2.05	0.55
3:E:219:ARG:HA	3:E:222:ILE:HD12	1.88	0.55
1:A:6:ARG:NH2	1:A:35:ASN:O	2.36	0.55
2:B:241:LYS:NZ	2:B:253:LEU:HD22	2.22	0.55
1:C:240:ILE:O	1:C:244:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:235:LYS:O	3:E:239:GLU:HG3	2.06	0.55
1:A:39:VAL:O	1:A:392:LYS:NZ	2.38	0.55
1:A:42:SER:N	1:A:388:ASP:OD1	2.41	0.54
1:C:56:LEU:HD13	1:C:405:THR:HG21	1.87	0.54
2:B:397:ASN:OD1	2:B:397:ASN:N	2.36	0.54
3:E:50:HIS:HA	3:E:224:ARG:HH22	1.71	0.54
3:F:184:CYS:HB3	3:F:210:PHE:HA	1.89	0.54
3:F:238:ASP:HA	3:F:241:ARG:HD2	1.89	0.54
3:E:208:ILE:HA	3:E:246:LYS:NZ	2.23	0.54
1:C:6:ARG:NH1	1:C:36:ASP:OD1	2.40	0.54
3:E:192:GLU:O	3:E:196:ILE:HG13	2.07	0.54
3:E:28:GLU:OE1	3:E:241:ARG:NH1	2.41	0.54
3:E:260:THR:OG1	3:E:263:GLU:OE1	2.25	0.54
3:F:22:LEU:HD13	3:F:243:LEU:HG	1.90	0.53
2:D:116:ASP:HB2	2:D:130:ASN:HB3	1.89	0.53
1:A:276:TYR:OH	1:A:284:ARG:NH2	2.42	0.53
1:C:275:CYS:HA	1:C:358:LEU:HG	1.91	0.53
1:C:420:LEU:HD22	1:C:467:LEU:HD11	1.90	0.53
3:F:235:LYS:HZ1	3:F:239:GLU:HB2	1.73	0.53
2:D:322:LEU:HD13	2:D:351:LEU:HD23	1.90	0.53
3:E:106:ILE:HD13	3:E:143:LYS:HZ1	1.74	0.52
1:C:68:LYS:HG3	1:C:151:GLN:HG3	1.91	0.52
1:C:439:ARG:HD3	1:C:466:THR:OG1	2.09	0.52
1:C:233:GLY:HA3	2:D:15:PHE:CZ	2.45	0.52
2:D:202:GLU:HG2	2:D:300:LYS:HE2	1.91	0.52
1:C:154:CYS:HB2	1:C:155:PRO:CD	2.34	0.52
1:C:185:GLY:HA3	6:D:602:CLF:S2A	2.49	0.52
1:C:189:VAL:O	2:D:93:GLN:NE2	2.43	0.51
2:D:56:ASN:OD1	2:D:59:ARG:NH2	2.34	0.51
3:F:9:GLY:O	3:F:128:GLY:HA2	2.10	0.51
1:A:20:TYR:O	1:A:25:ARG:NH2	2.43	0.51
2:B:241:LYS:HG2	2:B:251:TYR:CE1	2.46	0.51
2:D:51:GLU:CD	2:D:51:GLU:H	2.14	0.51
3:E:264:LEU:O	3:E:268:LEU:HG	2.11	0.51
3:F:2:MET:HE1	3:F:115:TYR:HB3	1.92	0.51
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.26	0.51
3:E:228:ILE:HG13	3:E:229:GLU:H	1.76	0.51
2:B:38:ASP:OD1	2:B:39:LYS:N	2.43	0.51
3:F:227:VAL:HG11	3:F:236:GLN:HB2	1.92	0.51
2:B:266:ASP:OD2	2:B:270:ARG:NH2	2.44	0.51
2:B:523:ARG:OXT	2:D:108:ARG:NH2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:LEU:HD21	2:D:443:ILE:HG21	1.92	0.50
2:B:26:LYS:NZ	2:B:26:LYS:HB2	2.26	0.50
3:E:52:LYS:HZ3	3:E:224:ARG:HD2	1.76	0.50
3:F:190:ASP:O	3:F:191:ARG:C	2.49	0.50
2:B:375:PHE:HZ	2:B:469:ILE:HG22	1.75	0.50
2:B:322:LEU:HD21	2:B:352:VAL:HG22	1.92	0.50
2:D:119:THR:HG22	2:D:120:GLU:N	2.26	0.50
3:F:50:HIS:NE2	3:F:229:GLU:OE2	2.44	0.50
2:D:119:THR:HG22	2:D:120:GLU:H	1.77	0.50
2:B:394:LEU:HD11	2:B:425:LYS:HB2	1.94	0.50
1:C:280:ASN:O	1:C:284:ARG:HG3	2.12	0.50
3:E:35:ILE:HD12	3:E:123:PHE:HB2	1.93	0.50
3:F:193:ASP:O	3:F:197:ILE:HG23	2.12	0.50
3:E:50:HIS:HA	3:E:224:ARG:NH2	2.26	0.50
2:D:21:LYS:NZ	2:D:21:LYS:HB3	2.27	0.49
2:B:456:LEU:HB2	2:B:463:GLU:HG3	1.93	0.49
1:C:423:SER:OG	1:C:427:GLU:OE2	2.23	0.49
1:C:134:LEU:HD12	2:D:62:LEU:HA	1.95	0.49
1:A:276:TYR:O	1:A:280:ASN:HB3	2.12	0.49
3:F:33:VAL:HG13	3:F:83:VAL:HG22	1.95	0.48
2:B:96:VAL:HG21	2:B:115:SER:HB3	1.96	0.48
3:E:202:LYS:O	3:E:202:LYS:HD3	2.13	0.48
3:F:226:THR:HG23	3:F:229:GLU:H	1.78	0.48
3:F:15:LYS:O	3:F:19:THR:HG22	2.13	0.48
3:E:12:GLY:H	9:E:302:ADP:PB	2.37	0.48
3:F:235:LYS:NZ	3:F:239:GLU:HB2	2.28	0.48
1:C:146:LYS:NZ	2:D:33:GLU:O	2.46	0.48
2:B:392:HIS:CE1	2:B:437:ASP:HB3	2.48	0.48
3:E:268:LEU:HD13	3:F:222:ILE:HG22	1.96	0.48
3:E:17:THR:HG21	9:E:302:ADP:C8	2.49	0.48
1:C:433:LYS:NZ	2:D:263:THR:O	2.47	0.47
2:D:238:ARG:NH2	2:D:262:ASP:OD2	2.47	0.47
1:A:64:TYR:CE2	1:A:88:CYS:HB3	2.50	0.47
1:A:82:SER:HB3	1:A:153:GLU:OE2	2.13	0.47
1:C:402:ASP:O	1:C:404:VAL:HG23	2.13	0.47
3:F:42:ALA:HA	3:F:87:GLU:OE1	2.15	0.47
3:F:162:ASN:HD21	3:F:259:ILE:HD11	1.79	0.47
3:F:198:ALA:HA	3:F:201:ASN:HD21	1.79	0.47
1:A:356:GLY:HA2	1:A:380:GLU:HB2	1.96	0.47
3:F:202:LYS:HE3	3:F:202:LYS:HA	1.96	0.47
2:B:400:LYS:HE2	2:B:400:LYS:HB2	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:LYS:N	3:E:120:ASP:OD2	2.44	0.47
1:C:87:GLY:HA3	6:D:602:CLF:S2B	2.53	0.47
3:E:17:THR:O	3:E:21:ASN:ND2	2.48	0.47
2:B:118:MET:HG2	2:B:122:ALA:HB1	1.97	0.47
2:B:481:ARG:HH22	2:D:350:ARG:HB3	1.80	0.47
1:C:386:ASP:HA	1:C:389:ARG:HE	1.79	0.47
2:D:323:ASP:O	2:D:327:GLU:HG3	2.14	0.47
3:E:13:ILE:HA	3:E:187:ARG:HH22	1.80	0.47
3:F:162:ASN:HD22	3:F:264:LEU:HD11	1.79	0.47
1:A:77:ASP:OD1	1:A:77:ASP:N	2.40	0.47
3:E:261:MET:HG2	3:F:52:LYS:HE3	1.96	0.47
1:C:59:ILE:HG23	1:C:426:LYS:HD2	1.97	0.47
1:C:392:LYS:HB3	1:C:392:LYS:HE2	1.44	0.47
2:B:119:THR:OG1	2:B:121:ASP:OD1	2.24	0.47
2:D:316:LEU:HD11	2:D:331:LYS:HG2	1.97	0.47
3:F:122:VAL:HG12	3:F:122:VAL:O	2.15	0.46
1:A:58:THR:OG1	1:A:403:ASP:OD1	2.34	0.46
2:D:241:LYS:NZ	2:D:256:ASP:OD2	2.49	0.46
3:E:159:TYR:OH	3:F:41:LYS:O	2.29	0.46
3:F:245:ARG:HH11	3:F:249:ASP:HB3	1.79	0.46
1:A:48:SER:OG	1:A:382:ALA:O	2.23	0.46
2:B:238:ARG:NH2	2:B:262:ASP:OD2	2.48	0.46
2:B:241:LYS:HZ2	2:B:253:LEU:HD22	1.80	0.46
1:C:35:ASN:HB2	1:C:400:LEU:HG	1.97	0.46
1:C:85:PRO:HB2	6:D:602:CLF:S2B	2.56	0.46
2:D:86:MET:HG2	2:D:138:CYS:SG	2.55	0.46
1:A:274:HIS:CE1	1:A:451:HIS:CE1	3.04	0.46
1:A:385:ASP:HB2	1:A:389:ARG:NH1	2.30	0.46
3:E:7:ILE:HD12	3:E:148:TYR:HB2	1.97	0.46
1:C:429:PHE:HE2	2:D:104:ASN:HB3	1.81	0.46
3:F:10:LYS:HE3	3:F:156:MET:SD	2.55	0.46
1:A:96:ARG:NH2	5:A:502:ICS:S5A	2.75	0.46
1:A:239:ARG:NH1	1:A:249:CYS:SG	2.88	0.46
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.29	0.46
1:C:359:ARG:HH11	1:C:442:HIS:HA	1.81	0.46
3:E:83:VAL:HG12	3:E:85:CYS:SG	2.56	0.46
1:A:225:ILE:HD12	1:A:249:CYS:SG	2.55	0.46
1:C:12:LEU:HD22	1:C:415:ARG:HG2	1.97	0.46
3:E:235:LYS:HE2	3:E:235:LYS:HB3	1.41	0.46
2:B:375:PHE:CZ	2:B:469:ILE:HG22	2.50	0.45
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HE3	1:A:23:LYS:HB2	1.65	0.45
3:E:264:LEU:HA	3:E:267:LEU:HD23	1.97	0.45
3:F:8:TYR:HE2	3:F:130:VAL:HG21	1.81	0.45
3:F:217:VAL:HG11	11:F:303:ATP:C8	2.52	0.45
1:A:133:LYS:O	1:A:137:GLU:HG3	2.15	0.45
2:B:142:TYR:HD1	2:B:271:MET:HE1	1.81	0.45
3:E:34:MET:C	3:E:35:ILE:HD13	2.37	0.45
3:E:208:ILE:HA	3:E:246:LYS:HZ2	1.82	0.45
1:A:346:LEU:HD13	1:A:370:LEU:HD13	1.97	0.45
2:B:210:LEU:HD23	2:B:211:LYS:HG2	1.97	0.45
3:E:103:ILE:HA	3:E:137:MET:SD	2.56	0.45
3:F:58:MET:HG2	3:F:88:SER:O	2.17	0.45
3:F:244:ALA:O	3:F:248:VAL:HG12	2.15	0.45
1:C:62:CYS:HB2	1:C:185:GLY:HA2	1.99	0.45
2:D:46:TRP:O	2:D:49:THR:OG1	2.23	0.45
3:E:32:LYS:HB3	3:E:119:LEU:HG	1.99	0.45
3:F:76:LEU:HG	3:F:86:VAL:HB	1.98	0.44
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.32	0.44
1:A:439:ARG:HG2	1:A:466:THR:HG21	1.99	0.44
3:F:119:LEU:HD13	3:F:119:LEU:HA	1.83	0.44
2:D:19:ASP:OD1	2:D:20:TYR:N	2.47	0.44
2:D:475:ASP:O	2:D:476:ARG:NH1	2.43	0.44
1:A:259:ILE:HD12	1:A:259:ILE:HA	1.86	0.44
2:B:494:LEU:O	2:B:498:VAL:HG12	2.17	0.44
2:D:146:MET:HB3	2:D:180:PRO:HG2	2.00	0.44
1:A:97:ARG:NH1	1:A:443:SER:O	2.50	0.44
1:A:346:LEU:HD23	1:A:467:LEU:HD22	2.00	0.44
2:B:457:HIS:HB2	2:D:512:MET:HG3	1.98	0.44
1:C:56:LEU:O	1:C:405:THR:HB	2.17	0.44
2:D:292:LEU:HB3	2:D:298:LEU:HD12	2.00	0.44
3:E:177:VAL:O	3:E:178:ARG:NH1	2.49	0.44
2:D:264:PRO:HG2	2:D:270:ARG:HH21	1.82	0.44
2:B:318:ILE:HG13	2:B:319:PRO:HD2	2.00	0.44
3:E:223:ARG:HA	3:E:223:ARG:HD2	1.46	0.44
1:C:477:ALA:HB3	1:C:480:GLU:HG3	2.00	0.43
2:D:143:LYS:HE2	2:D:143:LYS:HB2	1.64	0.43
3:E:34:MET:HA	3:E:84:LYS:O	2.18	0.43
1:A:439:ARG:NH1	1:A:462:ASP:HB3	2.33	0.43
2:B:366:ARG:HA	2:B:389:GLU:O	2.18	0.43
2:D:128:GLN:HG2	2:D:165:PHE:CE2	2.52	0.43
3:F:84:LYS:HB3	3:F:84:LYS:HE2	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:ASP:OD1	2:B:523:ARG:NH1	2.51	0.43
2:D:88:TYR:HB2	2:D:147:ILE:HG23	1.99	0.43
2:D:234:LEU:HB3	2:D:258:GLU:OE2	2.17	0.43
3:E:15:LYS:HE3	3:E:126:VAL:O	2.18	0.43
3:E:263:GLU:HA	3:E:266:GLU:OE1	2.18	0.43
1:C:64:TYR:CE1	1:C:88:CYS:HB3	2.54	0.43
1:A:233:GLY:HA3	2:B:15:PHE:CE2	2.53	0.43
2:B:356:THR:O	2:B:359:HIS:ND1	2.39	0.43
1:C:404:VAL:HG13	1:C:408:GLU:HB2	2.00	0.43
2:D:45:GLN:O	2:D:49:THR:HG23	2.19	0.43
3:F:19:THR:O	3:F:23:VAL:HG12	2.18	0.43
1:A:233:GLY:HA3	2:B:15:PHE:CZ	2.52	0.43
3:F:203:LEU:HD13	3:F:203:LEU:HA	1.91	0.43
2:D:381:LYS:O	2:D:385:GLU:HG3	2.19	0.43
3:E:13:ILE:O	3:E:187:ARG:NH1	2.46	0.43
3:E:213:ARG:HA	9:E:302:ADP:N1	2.33	0.43
3:F:211:VAL:HA	3:F:239:GLU:OE1	2.18	0.43
1:C:186:PHE:HB3	2:D:154:MET:SD	2.59	0.43
3:F:75:VAL:HG21	3:F:108:PHE:HE2	1.83	0.43
3:F:191:ARG:CZ	3:F:271:PHE:HB3	2.48	0.43
3:E:100:ARG:HA	3:E:100:ARG:HD2	1.60	0.43
1:A:352:MET:HG3	1:A:375:VAL:HG23	2.01	0.42
1:A:429:PHE:CZ	2:B:108:ARG:HA	2.54	0.42
2:B:266:ASP:OD1	2:B:266:ASP:N	2.50	0.42
1:C:72:TRP:O	1:C:80:HIS:NE2	2.52	0.42
2:D:96:VAL:O	2:D:100:ARG:HG3	2.19	0.42
3:E:76:LEU:HG	3:E:86:VAL:HG13	2.00	0.42
3:E:179:LEU:HB2	3:E:256:PRO:HD3	2.01	0.42
3:F:186:SER:HB2	3:F:210:PHE:CE1	2.54	0.42
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.55	0.42
1:C:27:ASP:OD2	1:C:53:GLN:NE2	2.44	0.42
3:F:245:ARG:O	3:F:245:ARG:HD3	2.19	0.42
1:A:203:ARG:HG3	1:A:285:HIS:CD2	2.55	0.42
3:F:10:LYS:HE2	3:F:10:LYS:HB2	1.80	0.42
2:B:366:ARG:NH2	2:B:437:ASP:OD2	2.44	0.42
2:B:449:LYS:HB2	2:B:449:LYS:HE3	1.91	0.42
1:C:17:LEU:HD21	1:C:28:ARG:HB2	2.00	0.42
1:C:70:VAL:HA	1:C:96:ARG:NH1	2.33	0.42
1:A:62:CYS:HB3	2:B:94:GLY:HA3	2.01	0.42
1:A:392:LYS:HD3	1:A:392:LYS:HA	1.71	0.42
2:B:217:VAL:O	2:B:220:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ARG:HG3	1:C:463:MET:HE1	2.01	0.42
2:D:321:GLY:O	2:D:325:THR:OG1	2.31	0.42
3:E:129:ASP:HB3	3:E:131:VAL:HG13	2.01	0.42
2:D:326:ASP:OD1	2:D:487:TYR:OH	2.26	0.42
1:A:253:TRP:HA	1:A:254:SER:HA	1.67	0.42
2:B:326:ASP:OD2	2:B:348:ARG:NE	2.44	0.42
1:C:154:CYS:CB	1:C:155:PRO:CD	2.97	0.42
1:C:346:LEU:HB3	1:C:372:MET:SD	2.60	0.42
1:C:437:PRO:HA	1:C:472:TRP:CZ2	2.55	0.42
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.54	0.41
1:A:356:GLY:O	1:A:379:TYR:HD1	2.03	0.41
1:C:404:VAL:HG12	1:C:405:THR:O	2.20	0.41
3:E:223:ARG:HB3	3:E:225:MET:SD	2.60	0.41
1:A:163:ILE:HG12	1:A:182:ARG:NH1	2.35	0.41
3:F:196:ILE:CG2	3:F:207:MET:HG3	2.50	0.41
1:C:351:VAL:HG22	1:C:420:LEU:HD23	2.02	0.41
1:C:385:ASP:N	1:C:385:ASP:OD1	2.53	0.41
2:D:231:GLU:HB3	2:D:237:PHE:CZ	2.55	0.41
3:F:6:ALA:C	3:F:7:ILE:HD13	2.41	0.41
1:A:430:ILE:HG12	2:B:110:PRO:HB3	2.02	0.41
3:E:231:ASP:O	3:E:233:LYS:N	2.53	0.41
3:F:198:ALA:HA	3:F:201:ASN:ND2	2.35	0.41
2:B:45:GLN:O	2:B:49:THR:HG23	2.20	0.41
2:D:346:LYS:HE3	2:D:346:LYS:HB2	1.74	0.41
3:F:46:ARG:HG2	3:F:47:LEU:HD23	2.01	0.41
3:F:76:LEU:HD21	3:F:84:LYS:HB2	2.03	0.41
1:C:332:LYS:HA	1:C:335:TRP:CD1	2.55	0.41
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.55	0.41
1:A:382:ALA:HB1	1:A:386:ASP:HB2	2.02	0.41
1:C:354:TYR:OH	1:C:380:GLU:HB3	2.20	0.41
2:D:47:THR:HG22	2:D:52:TYR:CE2	2.55	0.41
3:E:45:THR:HB	3:E:49:LEU:HD23	2.01	0.41
3:F:80:TYR:CD2	3:F:229:GLU:HG2	2.55	0.41
1:C:387:TYR:HA	1:C:390:THR:HG22	2.03	0.41
3:F:223:ARG:CZ	3:F:223:ARG:O	2.69	0.41
1:C:302:PRO:HA	1:C:305:THR:HG22	2.03	0.41
1:C:425:ILE:HG22	4:C:501:HCA:O3	2.21	0.41
3:E:178:ARG:HA	3:E:178:ARG:HD3	1.76	0.41
3:F:136:ALA:O	3:F:139:ILE:HG12	2.19	0.41
1:A:300:PHE:HZ	1:A:444:TRP:CH2	2.39	0.41
1:A:386:ASP:O	1:A:390:THR:OG1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:PHE:CE2	2:D:104:ASN:HB3	2.57	0.41
3:E:2:MET:HE2	3:E:117:ASP:HA	2.03	0.41
2:B:460:LYS:HD2	2:B:460:LYS:HA	1.79	0.40
1:C:10:GLU:O	1:C:14:GLN:HG2	2.21	0.40
1:C:66:GLY:O	1:C:195:HIS:HD2	2.04	0.40
3:F:100:ARG:HA	3:F:100:ARG:HD2	1.82	0.40
3:F:246:LYS:HA	3:F:249:ASP:OD1	2.20	0.40
3:E:137:MET:HA	3:E:140:ARG:HG3	2.03	0.40
3:E:178:ARG:HB3	3:E:253:LEU:HB3	2.02	0.40
1:A:411:GLU:H	1:A:411:GLU:HG2	1.76	0.40
2:B:379:LEU:HD21	2:B:443:ILE:HG21	2.03	0.40
2:B:461:GLU:H	2:B:461:GLU:CD	2.24	0.40
1:C:275:CYS:SG	1:C:278:SER:OG	2.70	0.40
1:C:353:LEU:N	1:C:376:GLY:O	2.43	0.40
3:F:121:PHE:HB3	3:F:123:PHE:HD1	1.86	0.40
1:C:439:ARG:HA	1:C:439:ARG:HD2	1.75	0.40
2:D:85:THR:HG23	2:D:146:MET:HG3	2.03	0.40
1:A:332:LYS:HA	1:A:335:TRP:CD1	2.57	0.40
1:A:420:LEU:HD12	1:A:437:PRO:HB2	2.04	0.40
1:C:122:ASP:OD1	1:C:130:LYS:HD2	2.22	0.40
3:E:16:SER:O	3:E:17:THR:C	2.59	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	475/492 (96%)	460 (97%)	14 (3%)	1 (0%)	47	57
1	C	473/492 (96%)	453 (96%)	20 (4%)	0	100	100
2	B	520/523 (99%)	511 (98%)	9 (2%)	0	100	100
2	D	520/523 (99%)	511 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	269/290 (93%)	253 (94%)	12 (4%)	4 (2%)	10	9
3	F	269/290 (93%)	249 (93%)	19 (7%)	1 (0%)	34	41
All	All	2526/2610 (97%)	2437 (96%)	83 (3%)	6 (0%)	50	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	GLY
3	E	233	LYS
3	E	234	ALA
3	E	130	VAL
3	F	191	ARG
3	E	232	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	407/415 (98%)	390 (96%)	17 (4%)	30	39
1	C	405/415 (98%)	382 (94%)	23 (6%)	20	26
2	B	454/455 (100%)	436 (96%)	18 (4%)	31	41
2	D	454/455 (100%)	448 (99%)	6 (1%)	69	80
3	E	218/234 (93%)	191 (88%)	27 (12%)	4	3
3	F	218/234 (93%)	191 (88%)	27 (12%)	4	3
All	All	2156/2208 (98%)	2038 (94%)	118 (6%)	25	28

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

Mol	Chain	Res	Type
1	A	19	VAL
1	A	77	ASP
1	A	98	ASN
1	A	164	GLU

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Mol	Chain	Res	Type
1	A	176	LYS
1	A	211	ASP
1	A	281	TYR
1	A	300	PHE
1	A	362	HIS
1	A	392	LYS
1	A	396	ASP
1	A	401	TYR
1	A	404	VAL
1	A	409	PHE
1	A	417	LYS
1	A	439	ARG
1	A	473	LYS
2	B	21	LYS
2	B	50	LYS
2	B	102	TYR
2	B	116	ASP
2	B	171	LYS
2	B	189	PHE
2	B	202	GLU
2	B	206	ARG
2	B	245	SER
2	B	263	THR
2	B	300	LYS
2	B	400	LYS
2	B	404	LYS
2	B	418	ASN
2	B	420	THR
2	B	432	SER
2	B	437	ASP
2	B	460	LYS
1	C	59	ILE
1	C	68	LYS
1	C	77	ASP
1	C	86	VAL
1	C	98	ASN
1	C	120	GLU
1	C	155	PRO
1	C	168	LYS
1	C	193	LEU
1	C	260	SER
1	C	269	LYS

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Mol	Chain	Res	Type
1	C	271	ASN
1	C	303	THR
1	C	315	LYS
1	C	317	ASP
1	C	349	LYS
1	C	362	HIS
1	C	383	HIS
1	C	385	ASP
1	C	392	LYS
1	C	409	PHE
1	C	462	ASP
1	C	476	GLN
2	D	21	LYS
2	D	102	TYR
2	D	114	VAL
2	D	116	ASP
2	D	189	PHE
2	D	389	GLU
3	E	15	LYS
3	E	21	ASN
3	E	29	MET
3	E	43	ASP
3	E	52	LYS
3	E	54	GLN
3	E	56	THR
3	E	66	THR
3	E	100	ARG
3	E	155	MET
3	E	162	ASN
3	E	166	LYS
3	E	187	ARG
3	E	191	ARG
3	E	193	ASP
3	E	202	LYS
3	E	213	ARG
3	E	219	ARG
3	E	223	ARG
3	E	224	ARG
3	E	225	MET
3	E	229	GLU
3	E	233	LYS
3	E	235	LYS

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Mol	Chain	Res	Type
3	E	252	LEU
3	E	262	ASP
3	E	270	GLU
3	F	17	THR
3	F	21	ASN
3	F	49	LEU
3	F	77	LYS
3	F	80	TYR
3	F	84	LYS
3	F	95	VAL
3	F	119	LEU
3	F	127	LEU
3	F	151	CYS
3	F	155	MET
3	F	177	VAL
3	F	189	THR
3	F	191	ARG
3	F	192	GLU
3	F	196	ILE
3	F	202	LYS
3	F	203	LEU
3	F	207	MET
3	F	210	PHE
3	F	218	GLN
3	F	230	TYR
3	F	246	LYS
3	F	253	LEU
3	F	260	THR
3	F	261	MET
3	F	269	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	HIS
2	B	477	HIS
1	C	451	HIS
2	D	294	GLN
2	D	297	HIS
3	E	21	ASN
3	F	188	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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
11	ATP	F	303	8	26,33,33	0.68	0	31,52,52	0.81	1 (3%)
4	HCA	A	501	-	13,13,13	1.11	1 (7%)	14,18,18	1.39	2 (14%)
6	CLF	B	601	2,1	0,24,24	-	-	-	-	-
9	ADP	E	302	8	24,29,29	0.69	0	29,45,45	0.75	1 (3%)
6	CLF	D	602	2,1	0,24,24	-	-	-	-	-
10	SF4	F	301	3	0,12,12	-	-	-	-	-
5	ICS	A	502	1	18,30,30	2.63	11 (61%)	-	-	-
4	HCA	C	501	-	13,13,13	1.11	1 (7%)	14,18,18	1.43	2 (14%)
5	ICS	C	502	1	18,30,30	2.61	11 (61%)	-	-	-

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
11	ATP	F	303	8	-	1/18/38/38	0/3/3/3
4	HCA	A	501	-	-	5/17/17/17	-
6	CLF	B	601	2,1	-	-	0/12/10/10
9	ADP	E	302	8	-	3/12/32/32	0/3/3/3
6	CLF	D	602	2,1	-	-	0/12/10/10
10	SF4	F	301	3	-	-	0/6/5/5
4	HCA	C	501	-	-	5/17/17/17	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	ICS	S4B-FE7	-4.32	2.21	2.32
5	C	502	ICS	S4B-FE7	-4.26	2.21	2.32
5	A	502	ICS	S3B-FE6	-4.23	2.22	2.32
5	C	502	ICS	S3B-FE6	-4.22	2.22	2.32
5	A	502	ICS	S1B-FE6	-3.73	2.23	2.32
5	C	502	ICS	S1B-FE6	-3.73	2.23	2.32
5	C	502	ICS	S2A-FE2	-3.24	2.24	2.32
5	A	502	ICS	S2A-FE2	-3.19	2.24	2.32
5	C	502	ICS	S3B-FE7	-3.17	2.24	2.32
5	A	502	ICS	S3B-FE7	-3.12	2.24	2.32
5	A	502	ICS	S4B-FE5	-3.06	2.24	2.32
5	C	502	ICS	S4B-FE5	-3.05	2.24	2.32
5	C	502	ICS	S2B-FE6	-3.00	2.17	2.24
5	A	502	ICS	S2B-FE6	-2.96	2.17	2.24
5	A	502	ICS	S4A-FE3	-2.87	2.25	2.32
5	C	502	ICS	S4A-FE3	-2.83	2.25	2.32
5	A	502	ICS	S1A-FE2	-2.56	2.26	2.32
5	C	502	ICS	S1A-FE2	-2.43	2.26	2.32
5	A	502	ICS	S1B-FE5	-2.27	2.26	2.32
5	C	502	ICS	S1B-FE5	-2.25	2.26	2.32
4	A	501	HCA	C3-C7	-2.24	1.51	1.53
4	C	501	HCA	C3-C7	-2.20	1.51	1.53
5	A	502	ICS	S2A-FE3	-2.15	2.27	2.32
5	C	502	ICS	S2A-FE3	-2.03	2.27	2.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HCA	O6-C7-C3	3.16	118.53	113.05
4	A	501	HCA	O6-C7-C3	3.10	118.43	113.05
4	A	501	HCA	O5-C7-C3	-2.65	118.50	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	HCA	O5-C7-C3	-2.65	118.50	122.25
11	F	303	ATP	C5-C6-N6	2.31	123.86	120.35
9	E	302	ADP	C5-C6-N6	2.21	123.72	120.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	501	HCA	C1-C2-C3-C4
4	C	501	HCA	C1-C2-C3-C7
4	C	501	HCA	C1-C2-C3-O7
4	A	501	HCA	C1-C2-C3-C4
4	A	501	HCA	C1-C2-C3-C7
4	A	501	HCA	C1-C2-C3-O7
9	E	302	ADP	PA-O3A-PB-O1B
9	E	302	ADP	PB-O3A-PA-O2A
4	A	501	HCA	C4-C5-C6-O4
4	C	501	HCA	C4-C5-C6-O4
4	A	501	HCA	C4-C5-C6-O3
4	C	501	HCA	C4-C5-C6-O3
9	E	302	ADP	PB-O3A-PA-O1A
11	F	303	ATP	O4'-C4'-C5'-O5'

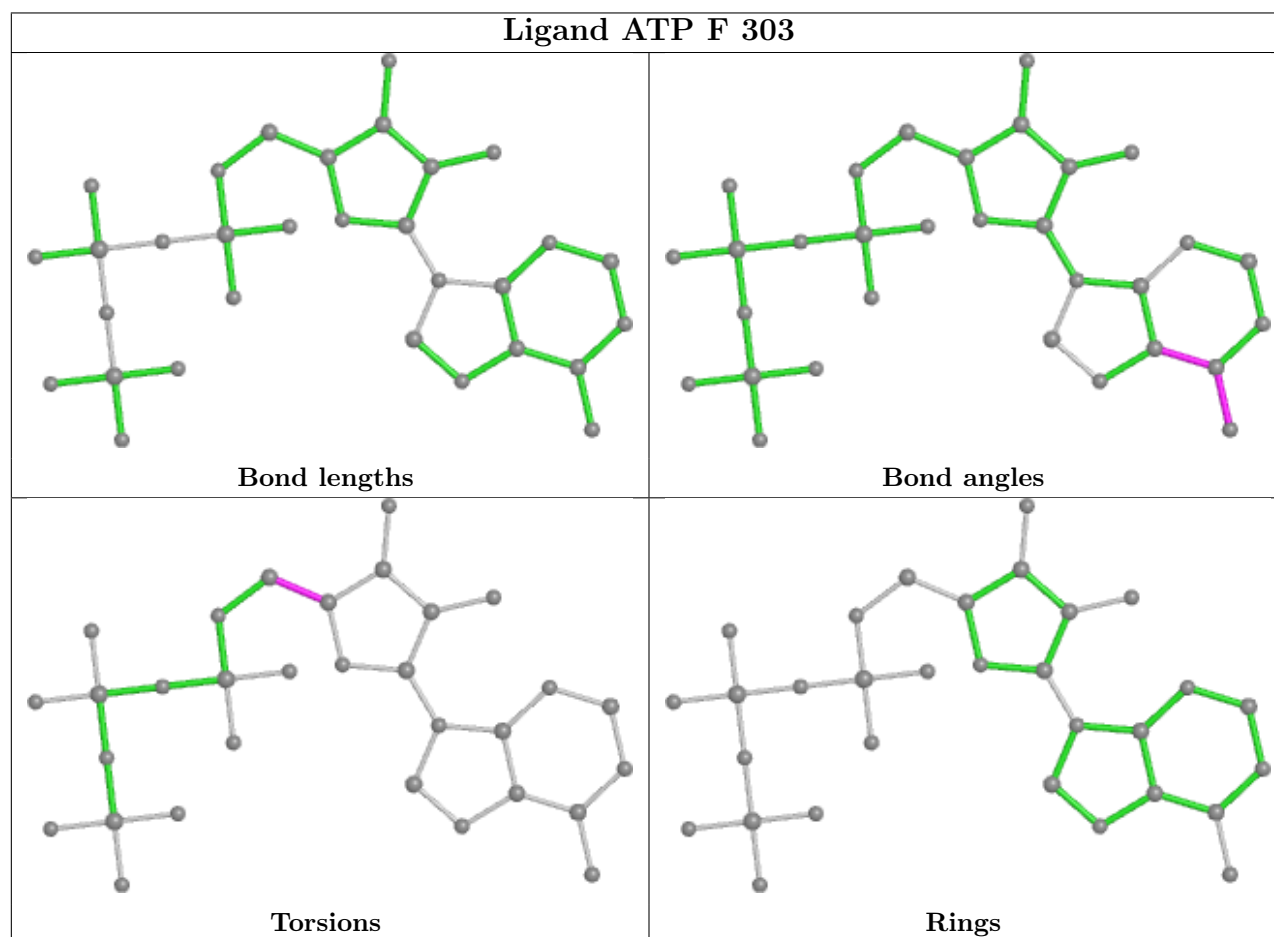
There are no ring outliers.

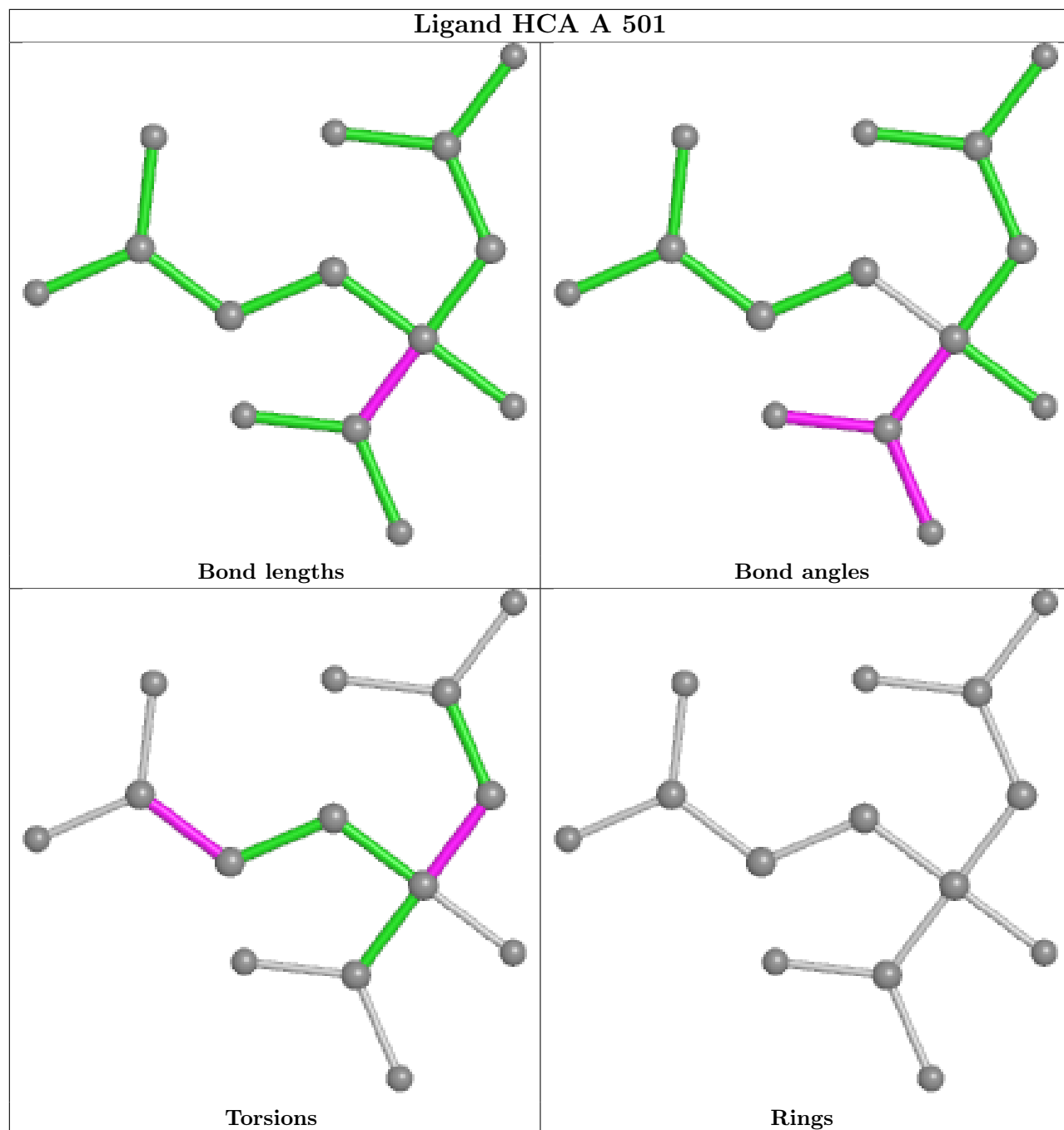
8 monomers are involved in 14 short contacts:

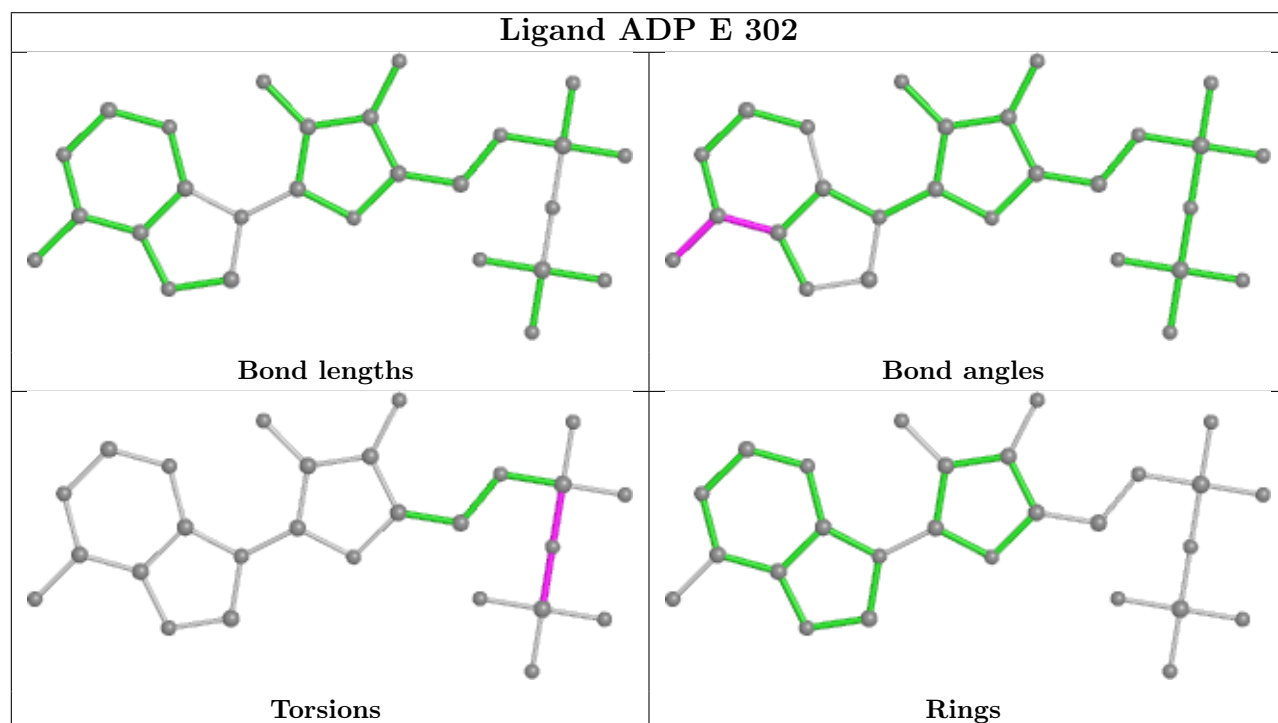
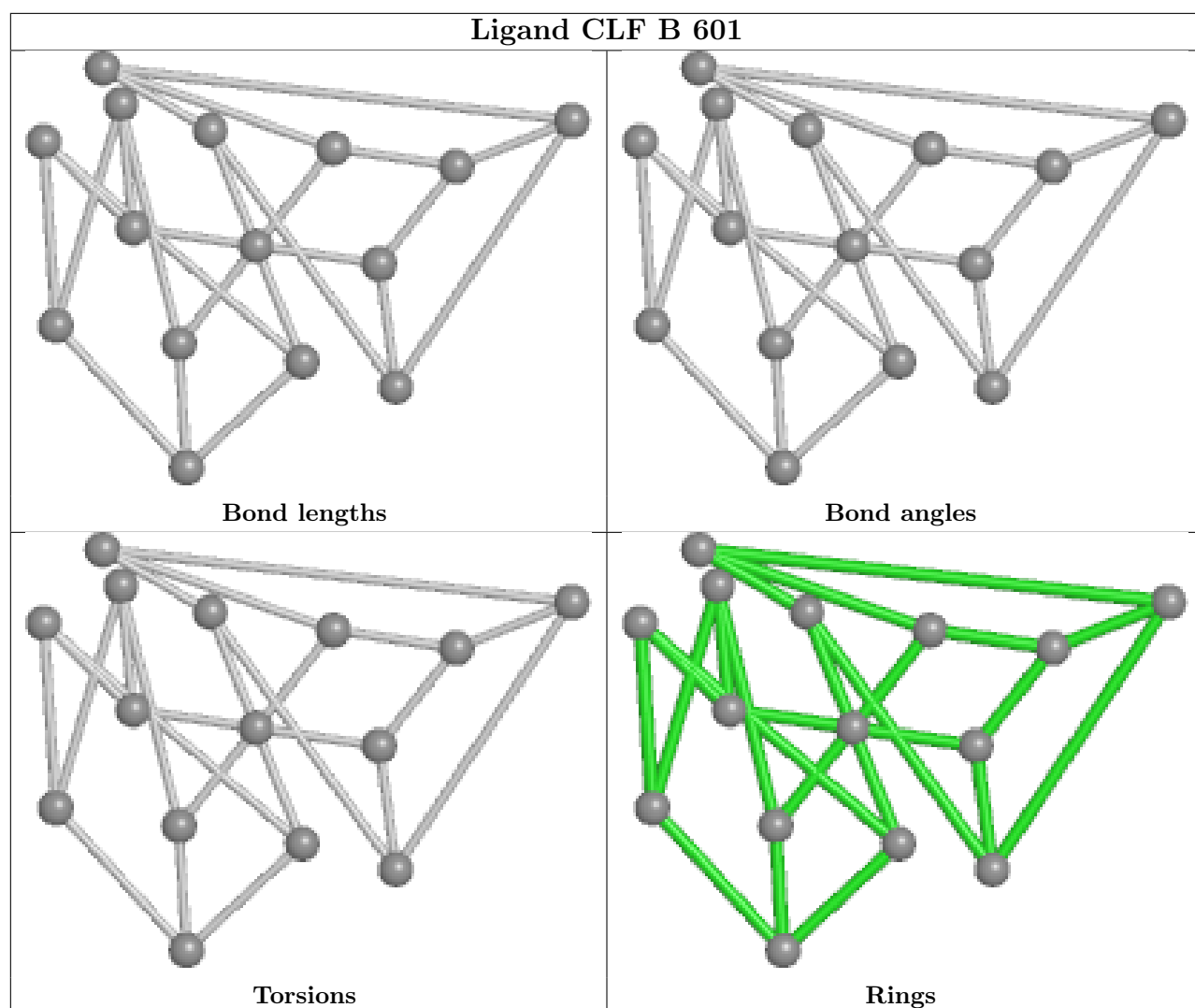
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	303	ATP	2	0
4	A	501	HCA	1	0
6	B	601	CLF	1	0
9	E	302	ADP	3	0
6	D	602	CLF	3	0
5	A	502	ICS	1	0
4	C	501	HCA	1	0
5	C	502	ICS	2	0

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

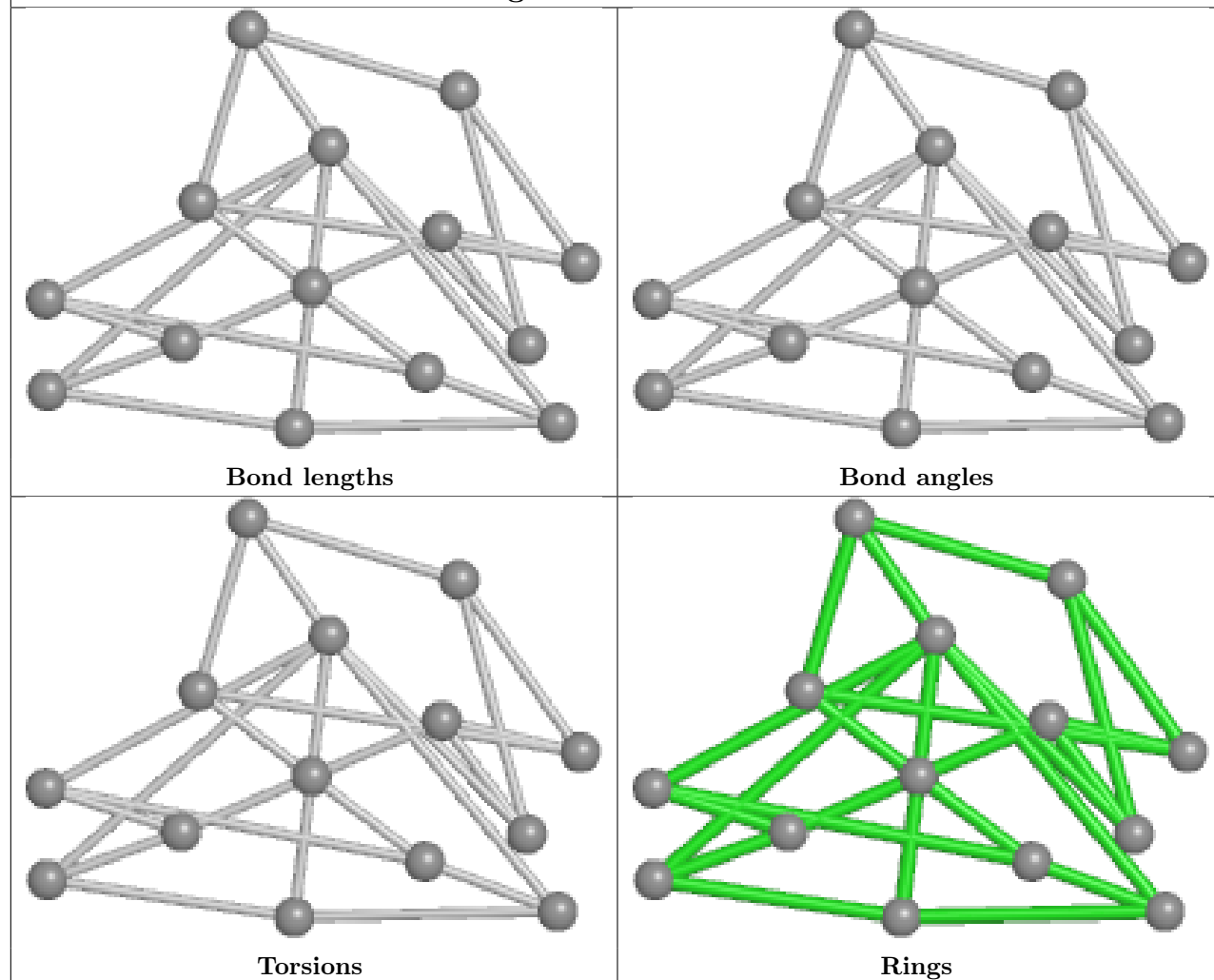
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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

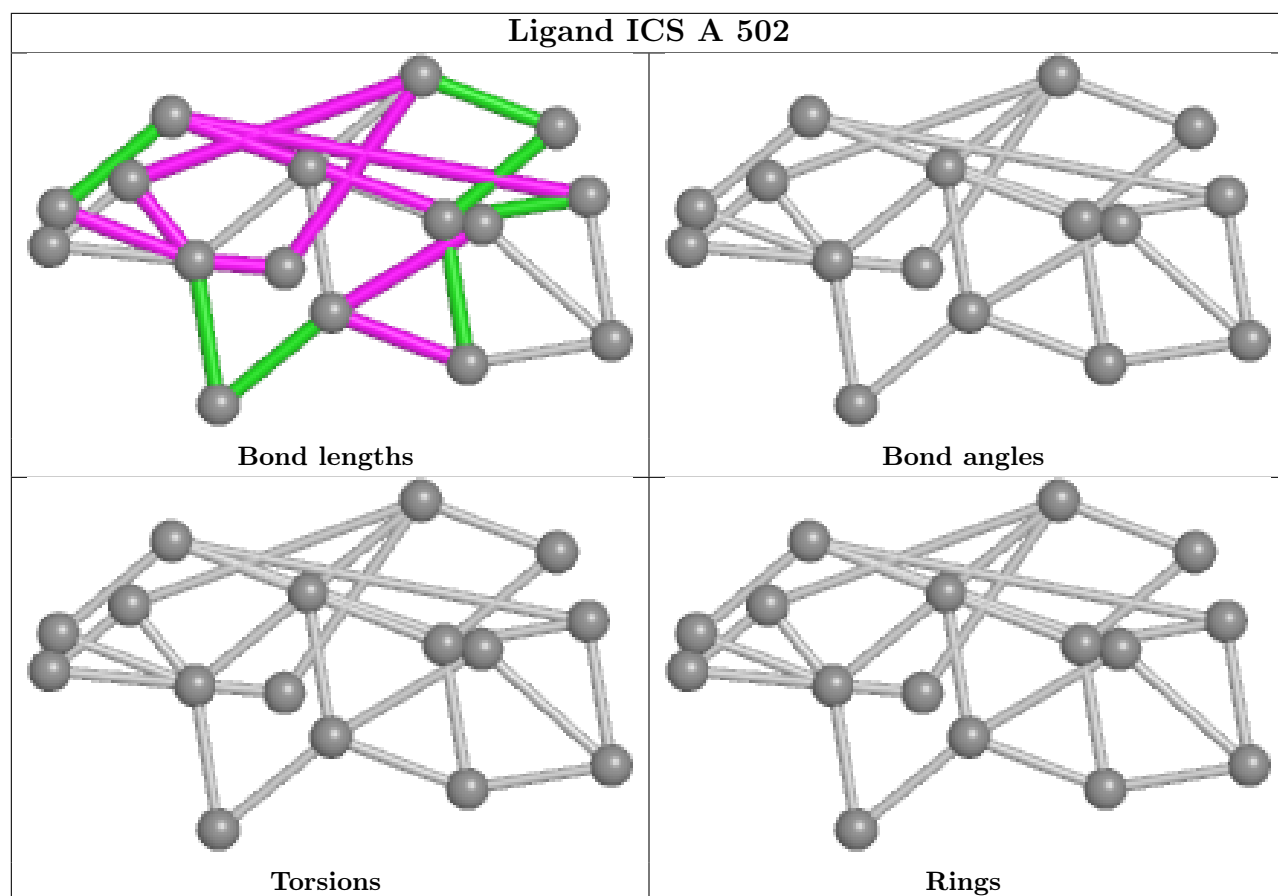
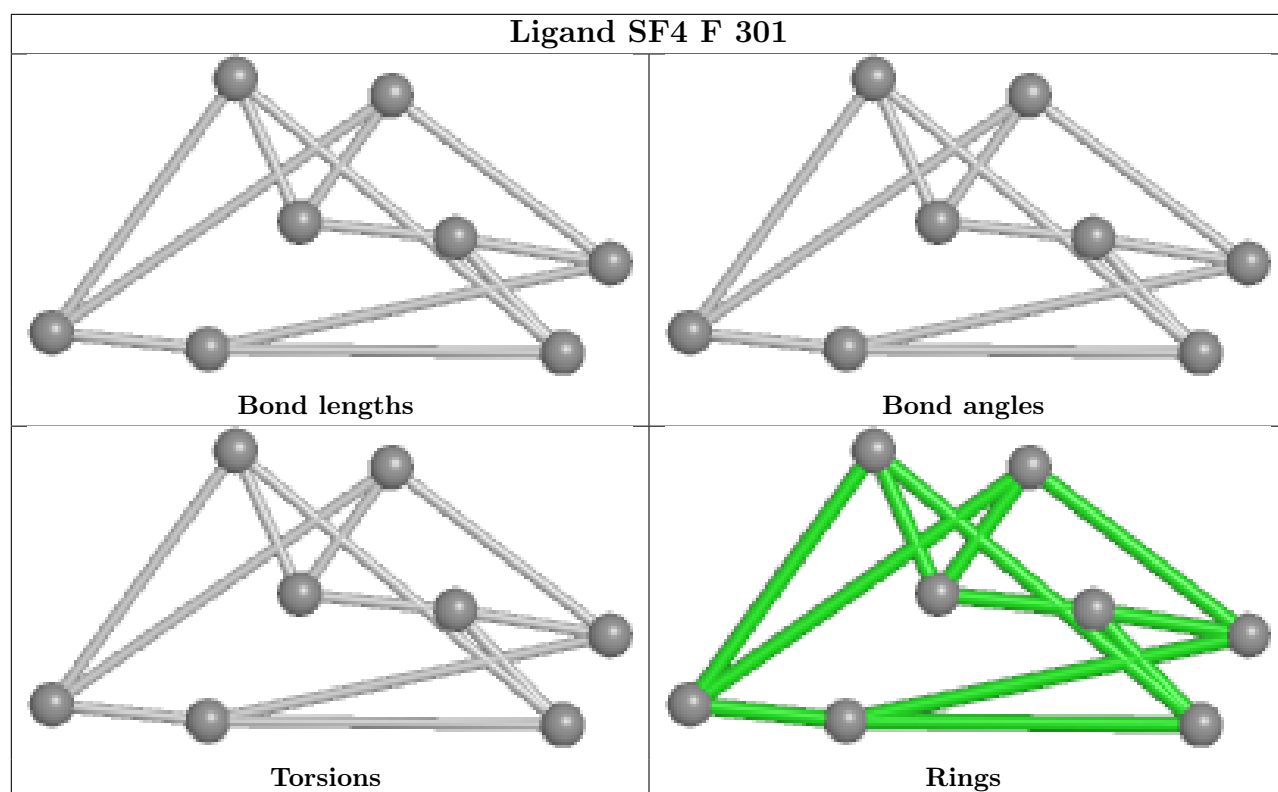


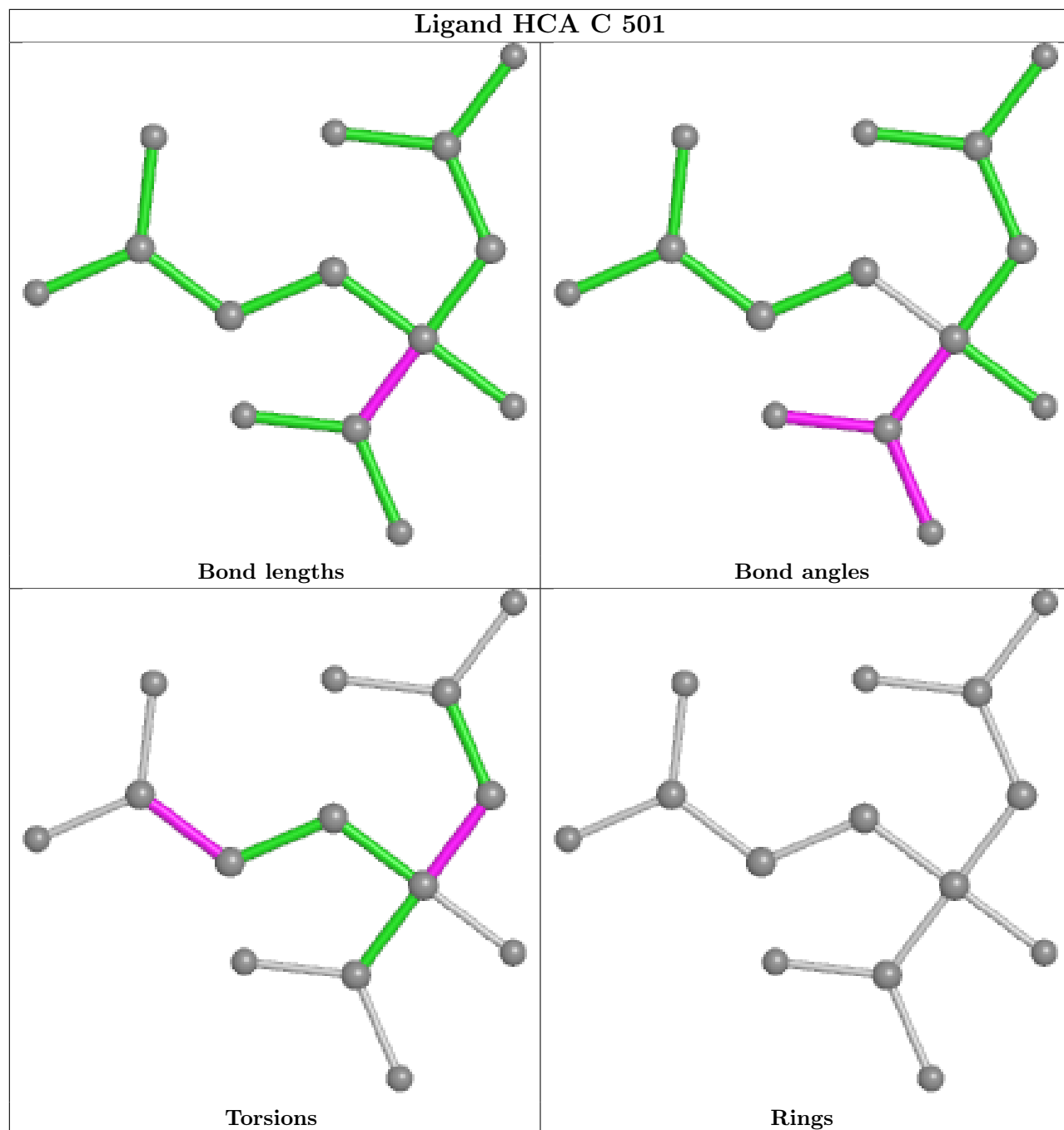


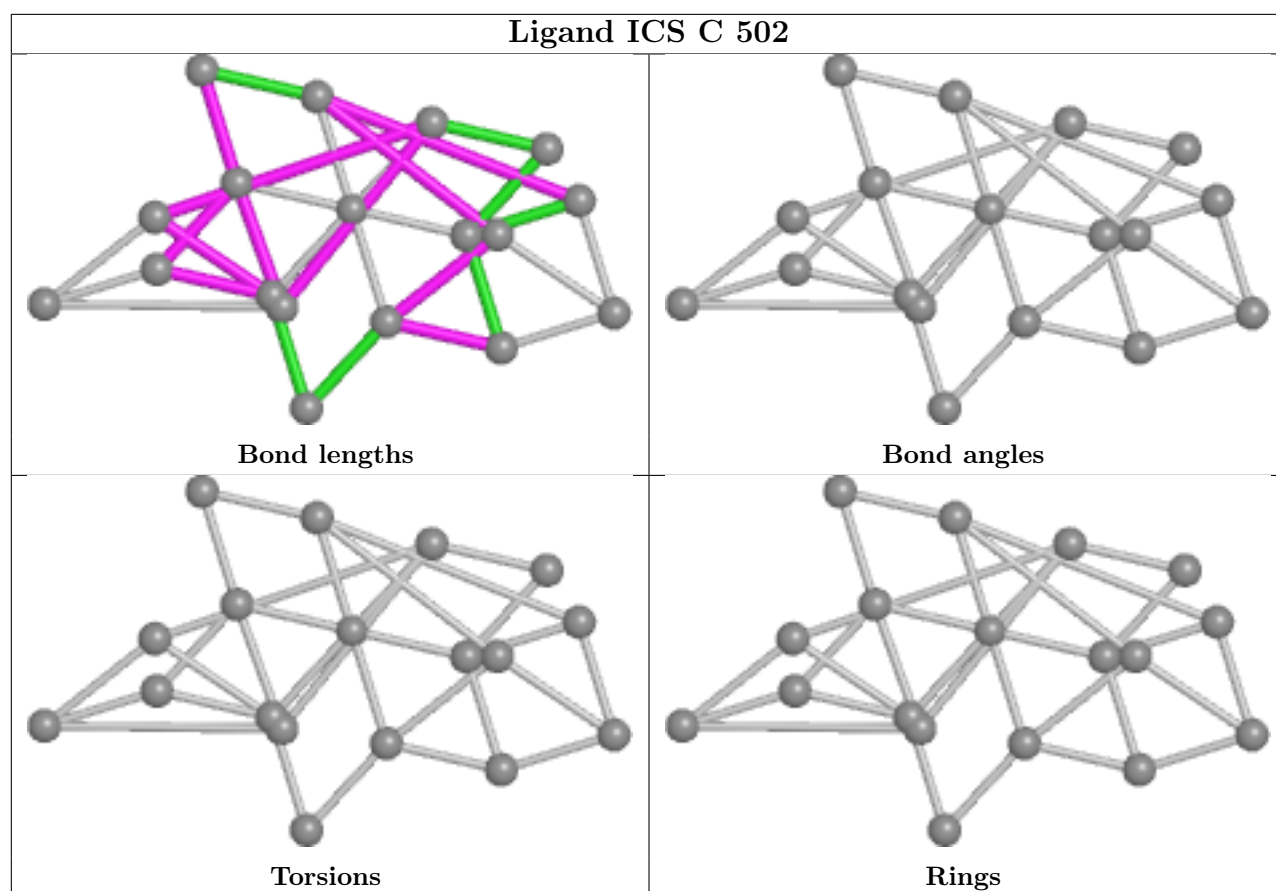


Ligand CLF D 602









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.

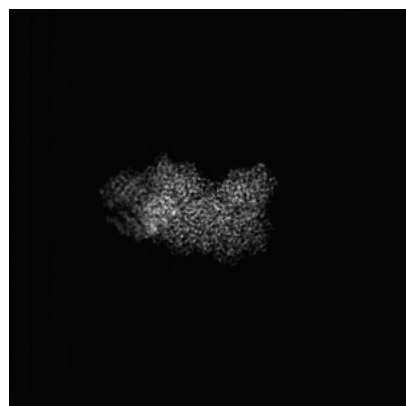
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26763. These allow visual inspection of the internal detail of the map and identification of artifacts.

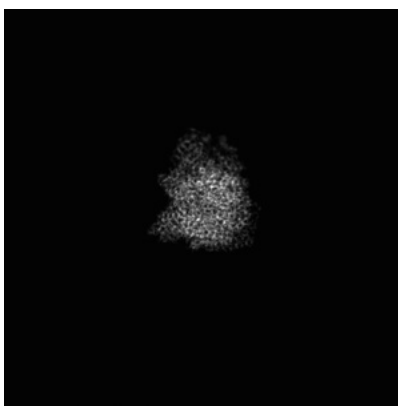
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

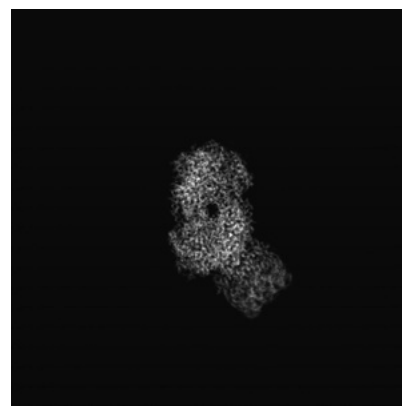
6.1.1 Primary map



X

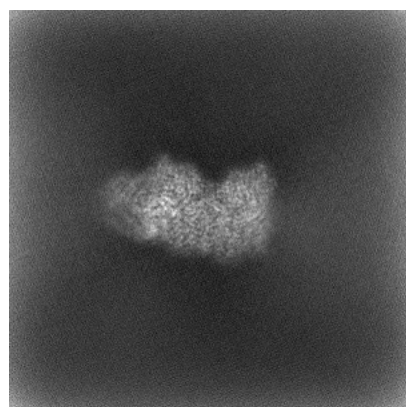


Y

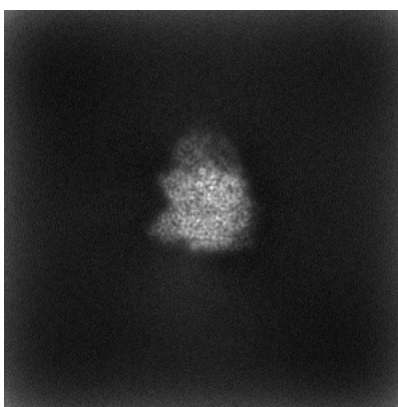


Z

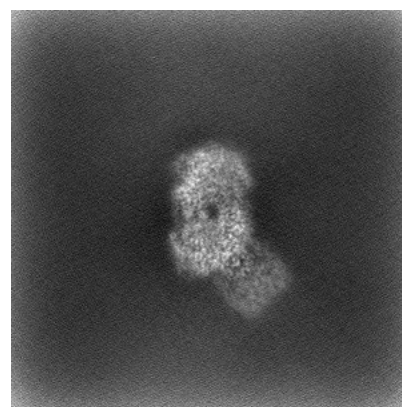
6.1.2 Raw map



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: 192

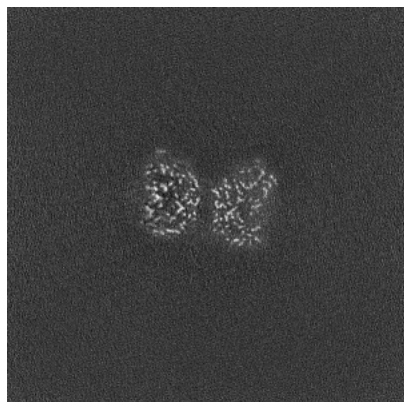


Y Index: 192

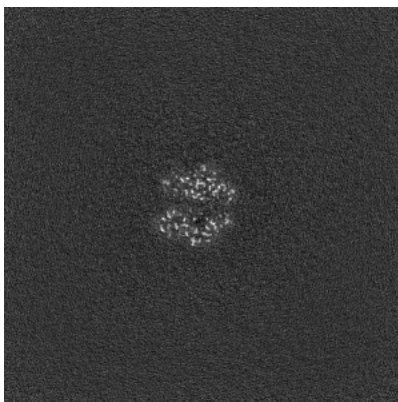


Z Index: 192

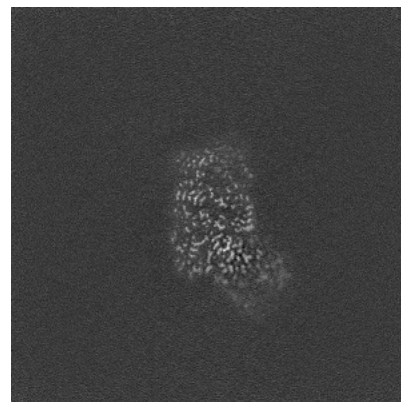
6.2.2 Raw map



X Index: 192



Y Index: 192

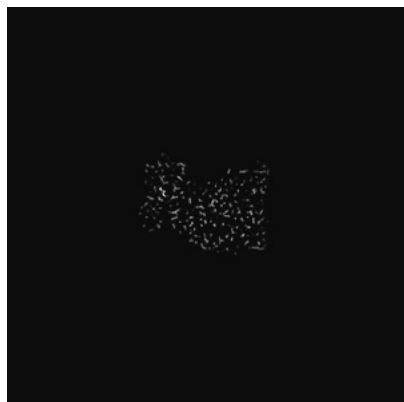


Z Index: 192

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 182

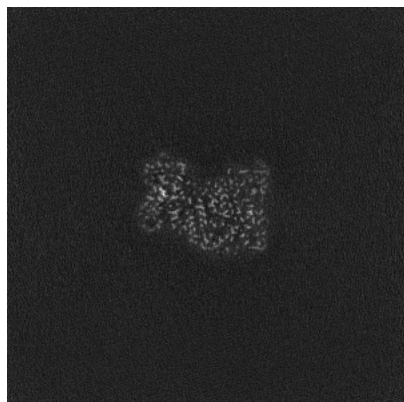


Y Index: 150

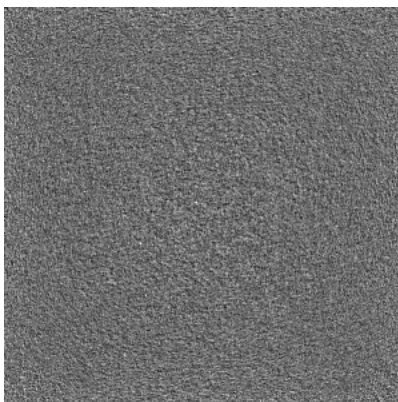


Z Index: 188

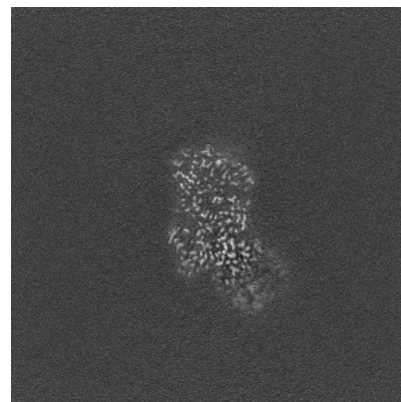
6.3.2 Raw map



X Index: 182



Y Index: 0

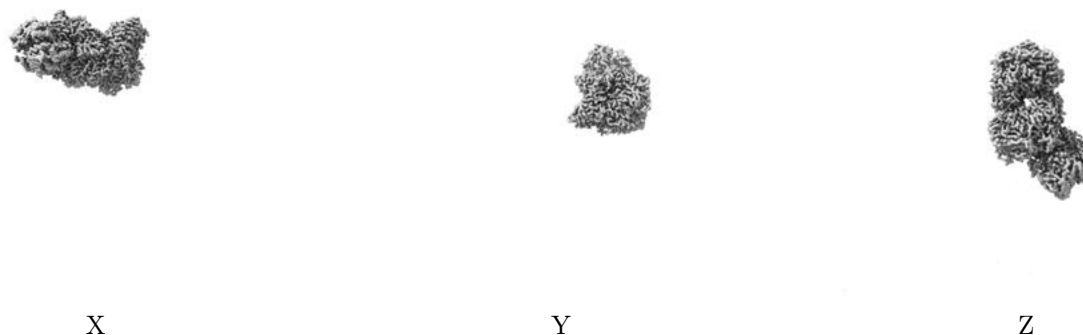


Z Index: 199

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

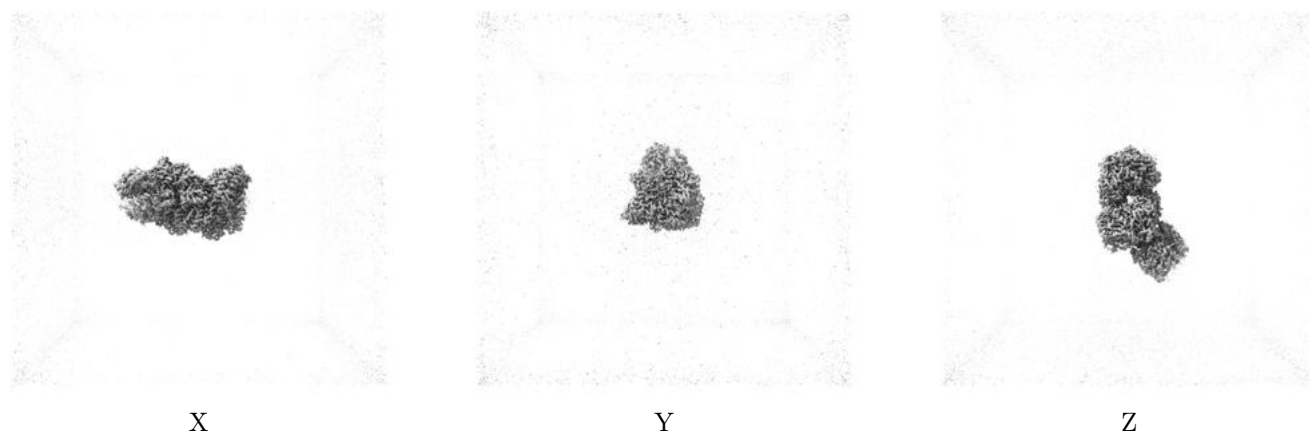
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

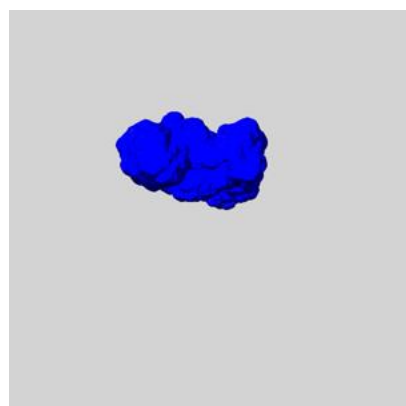
6.5 Mask visualisation [i](#)

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

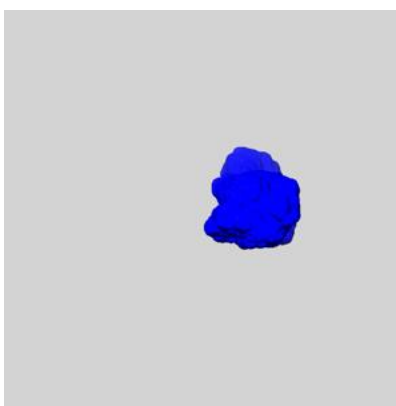
A mask typically either:

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

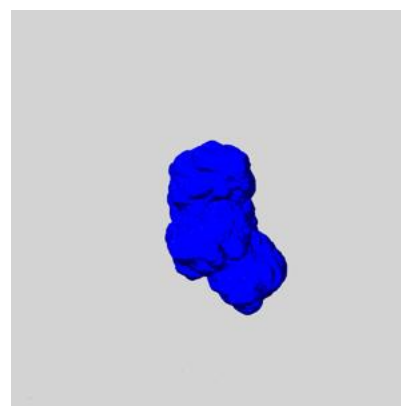
6.5.1 emd_26763_msk_1.map [i](#)



X



Y

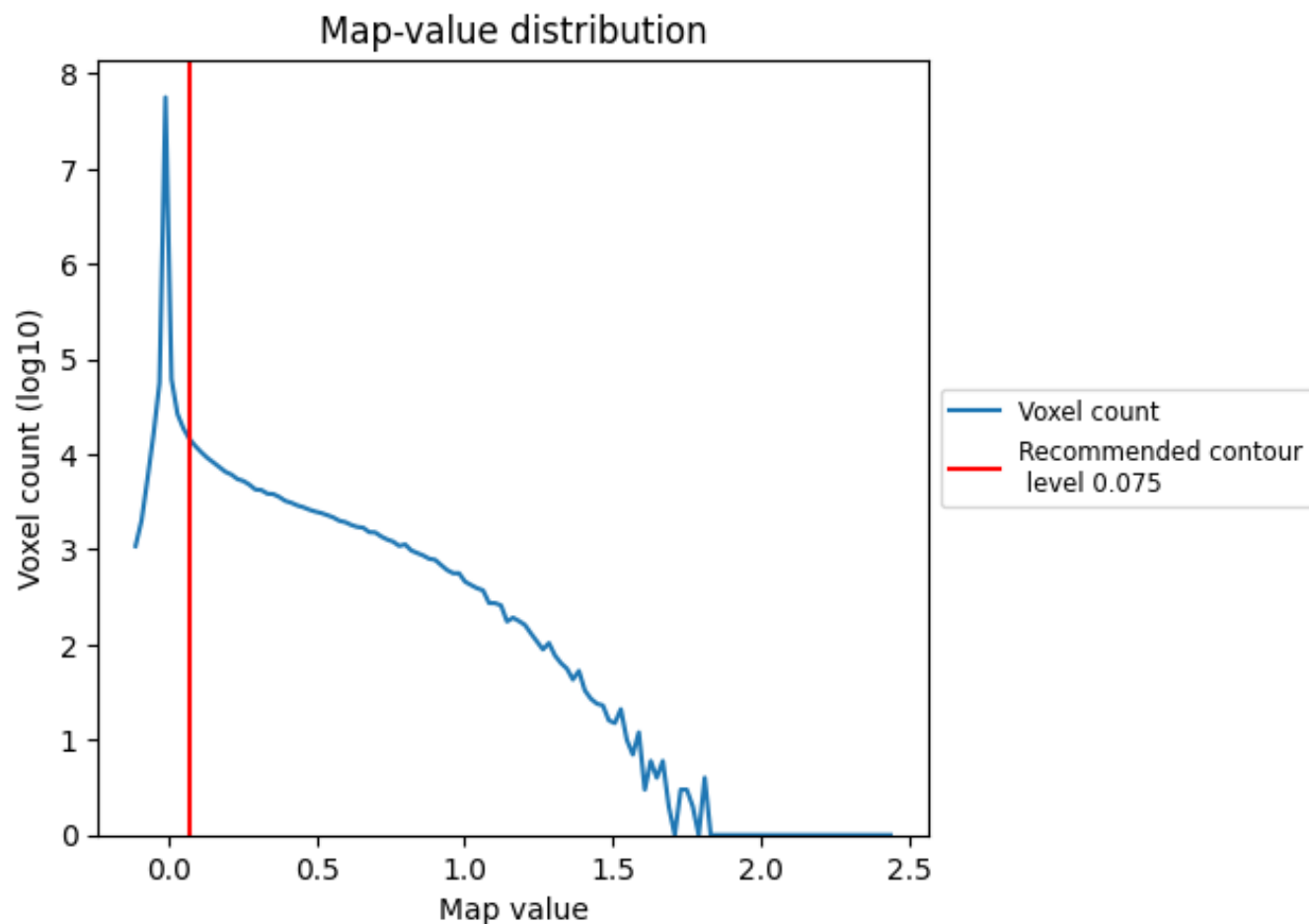


Z

7 Map analysis [i](#)

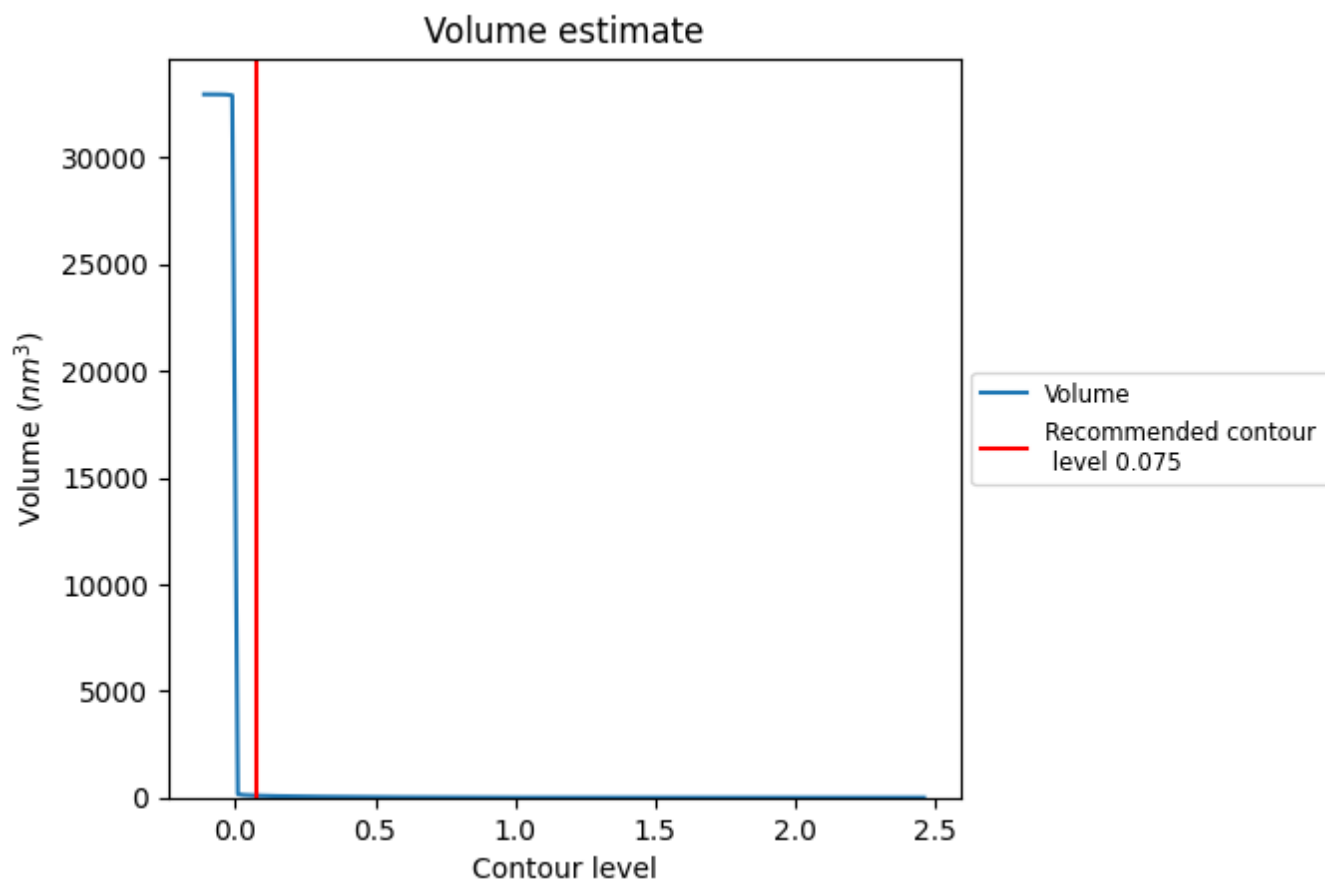
This section contains the results of statistical analysis of the map.

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.

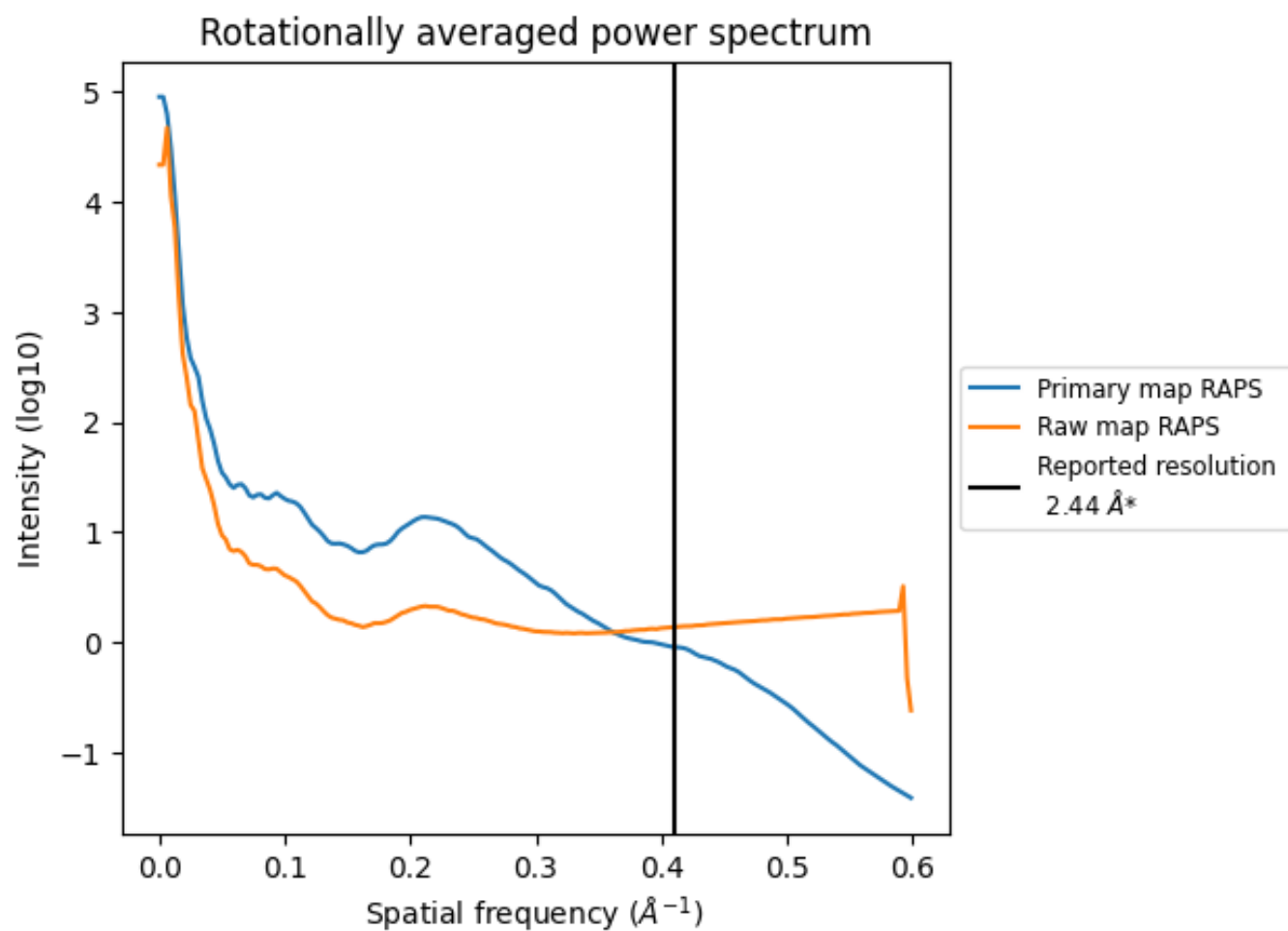
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

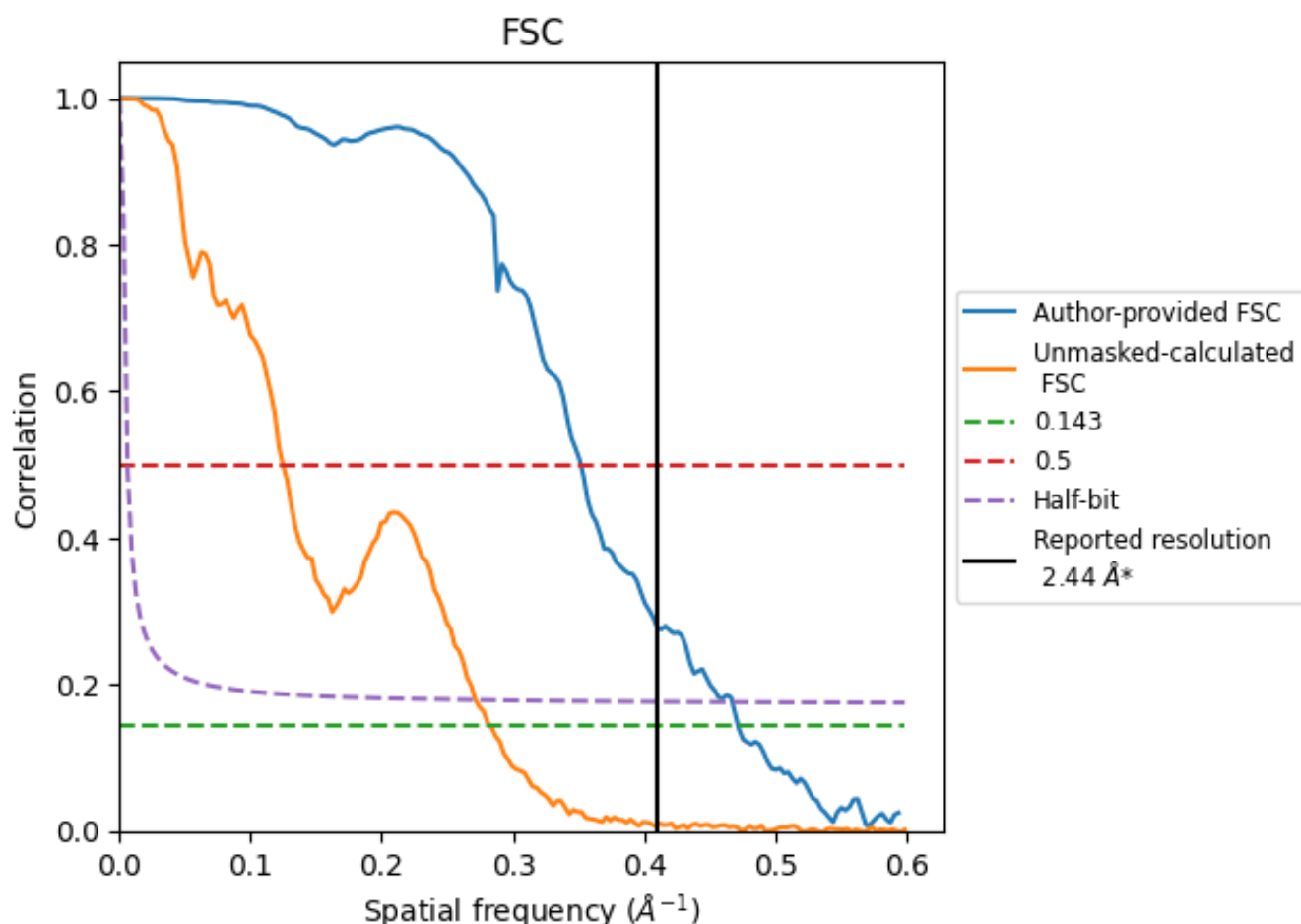


*Reported resolution corresponds to spatial frequency of 0.410 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.410 Å⁻¹

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.12	2.84	2.14
Unmasked-calculated*	3.54	8.03	3.68

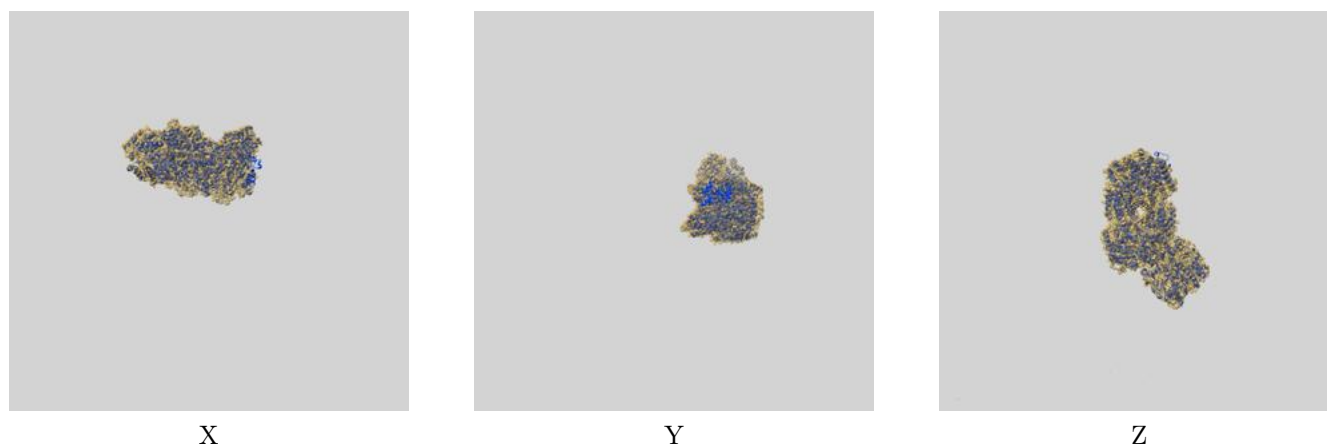
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.12 differs from the reported value 2.44 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 2.44 by more than 10 %

9 Map-model fit [i](#)

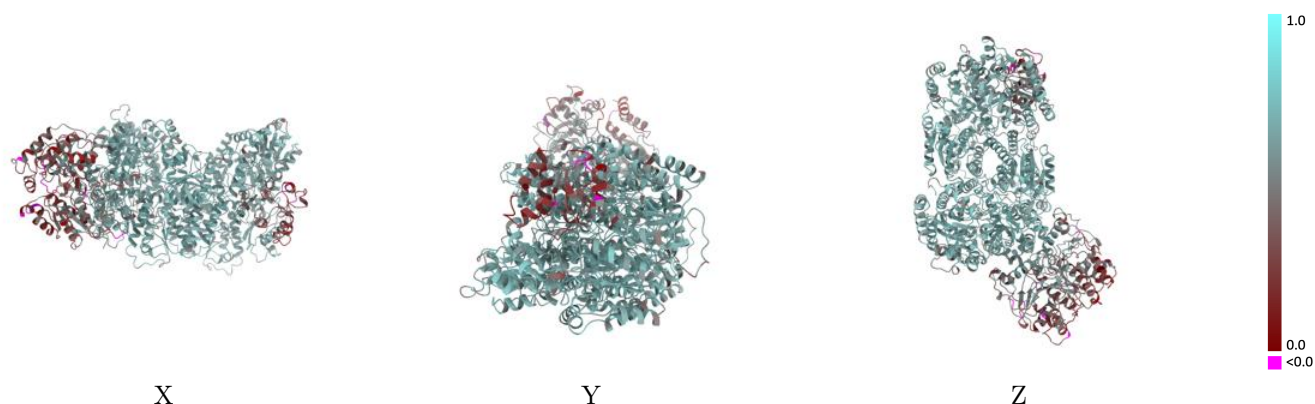
This section contains information regarding the fit between EMDB map EMD-26763 and PDB model 7UT9. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



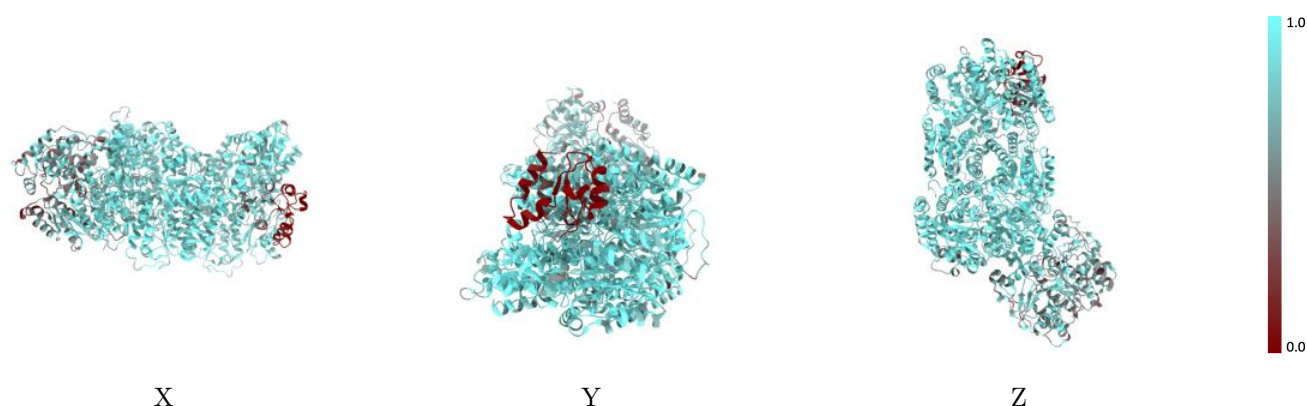
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



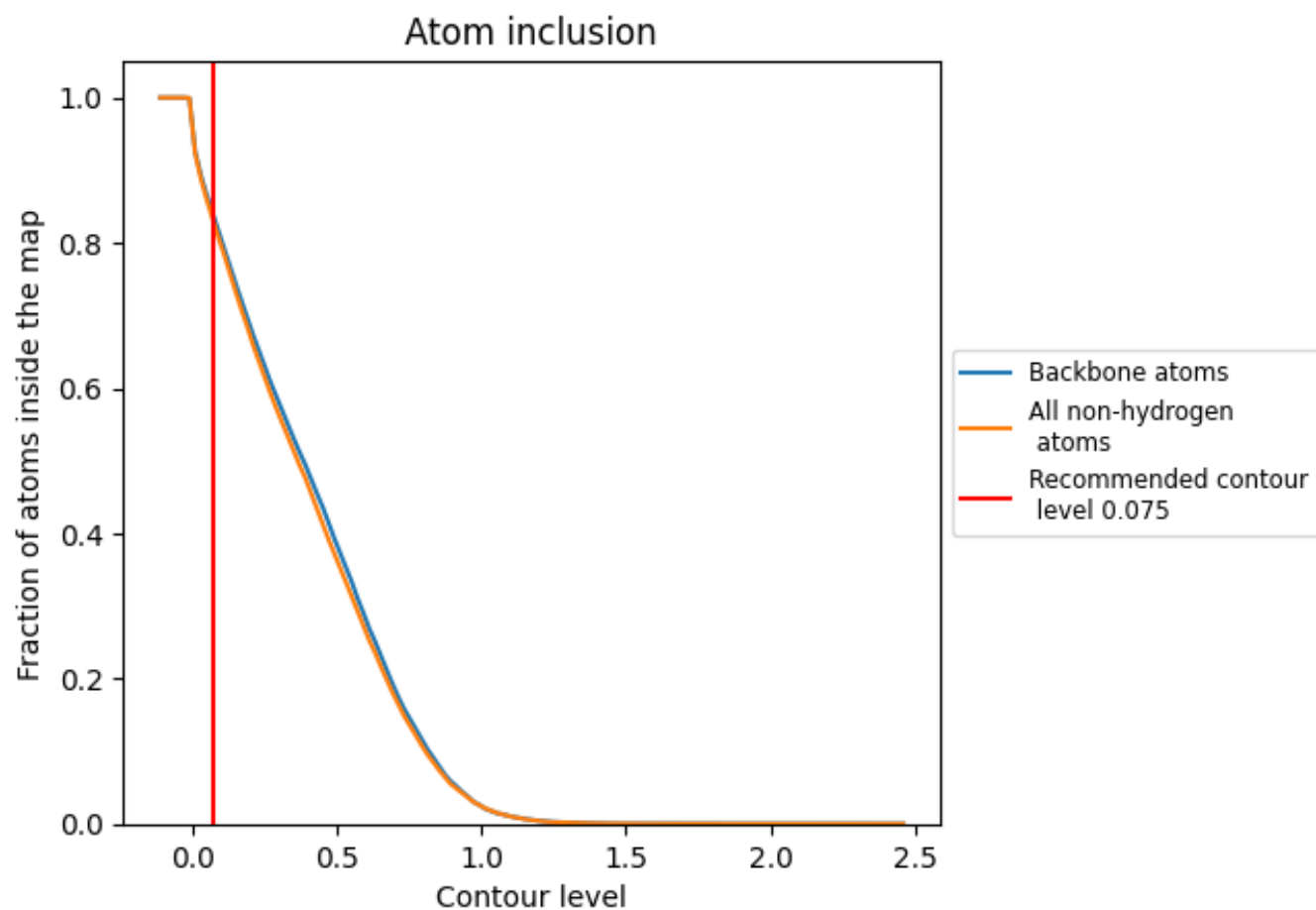
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8271	<div><div></div></div> 0.5700
A	<div><div></div></div> 0.9043	<div><div></div></div> 0.6390
B	<div><div></div></div> 0.9396	<div><div></div></div> 0.6590
C	<div><div></div></div> 0.7084	<div><div></div></div> 0.5240
D	<div><div></div></div> 0.9231	<div><div></div></div> 0.6460
E	<div><div></div></div> 0.6729	<div><div></div></div> 0.3820
F	<div><div></div></div> 0.6676	<div><div></div></div> 0.3850

1.0

0.0

<0.0