



Full wwPDB EM Validation Report ⓘ

Oct 6, 2022 – 10:12 PM EDT

PDB ID : 8E9H
EMDB ID : EMD-27964
Title : Mycobacterial respiratory complex I, fully-inserted quinone
Authors : Liang, Y.; Rubinstein, J.L.
Deposited on : 2022-08-26
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

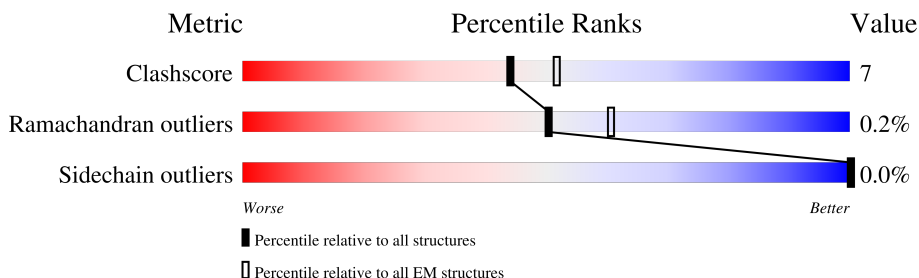
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	O	132	
2	B	184	
3	A	122	
4	C	238	
5	D	442	
6	E	245	
7	G	794	
8	F	443	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	180	
10	H	408	
11	J	252	
12	K	99	
13	L	629	
14	N	521	
15	M	529	

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
16	SF4	I	201	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 36670 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 Two-component system response regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	125	Total	C	N	O	S	0	0
			896	574	162	156	4		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	183	Total	C	N	O	S	0	0
			1338	860	231	233	14		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	122	Total	C	N	O	S	0	0
			951	647	149	150	5		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	220	Total	C	N	O	S	0	0
			1677	1071	304	297	5		

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	407	Total	C	N	O	S	0	0
			3051	1943	549	537	22		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	232	Total	C	N	O	S	0	0
			1614	1019	287	299	9		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	782	Total	C	N	O	S	0	0
			5637	3545	1038	1022	32		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	436	Total	C	N	O	S	0	0
			3170	2040	557	557	16		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	165	Total	C	N	O	S	0	0
			1225	775	212	225	13		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	395	Total	C	N	O	S	0	0
			2936	1967	474	483	12		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	231	Total	C	N	O	S	0	0
			1624	1064	274	280	6		

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	99	Total	C	N	O	S	0	0
			748	484	131	124	9		

- Molecule 13 is a protein called NADH-quinone oxidoreductase, L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	625	Total	C	N	O	S	0	0
			4132	2694	704	713	21		

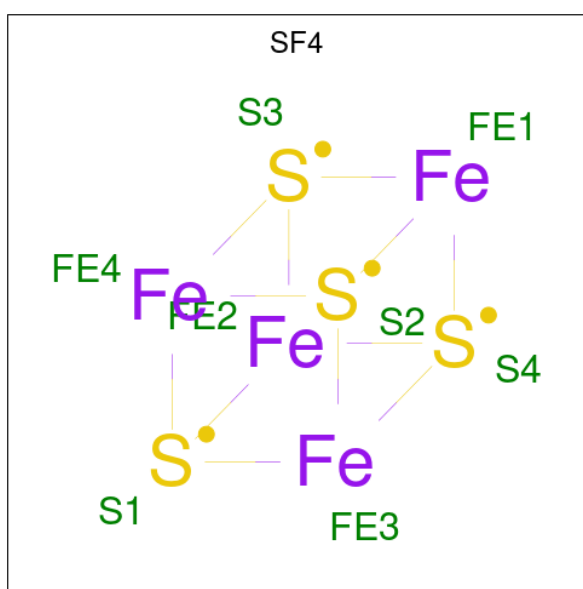
- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	519	Total	C	N	O	S	0	0
			3665	2435	589	627	14		

- Molecule 15 is a protein called NADH-quinone oxidoreductase, M subunit.

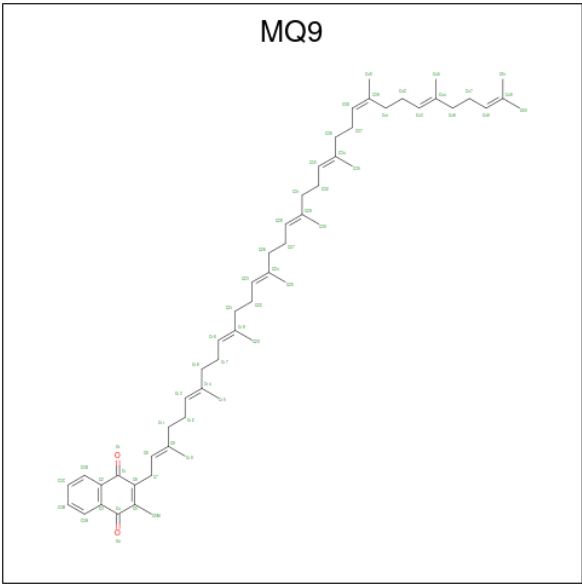
Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	517	Total	C	N	O	S	0	0
			3744	2513	598	617	16		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



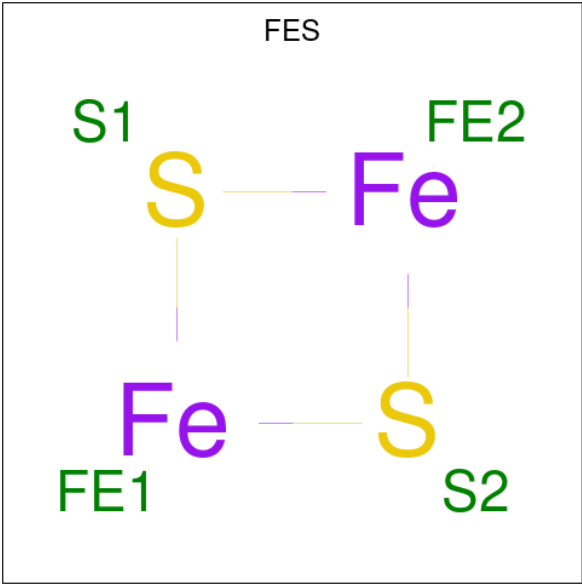
Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	Fe	S	0
			8	4	4	
16	G	1	Total	Fe	S	0
			24	12	12	
16	G	1	Total	Fe	S	0
			24	12	12	
16	G	1	Total	Fe	S	0
			24	12	12	
16	F	1	Total	Fe	S	0
			8	4	4	
16	I	1	Total	Fe	S	0
			16	8	8	
16	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 17 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	D	1	58	56	2	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



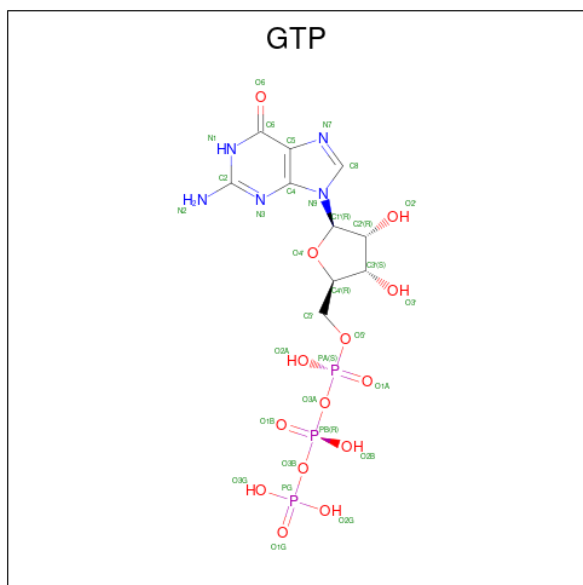
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	E	1	4	2	2	0

Continued on next page...

Continued from previous page...

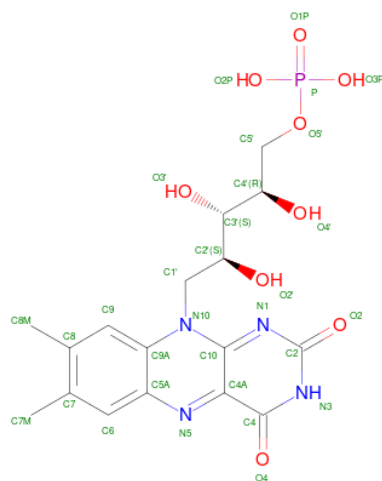
Mol	Chain	Residues	Atoms			AltConf
18	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 19 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

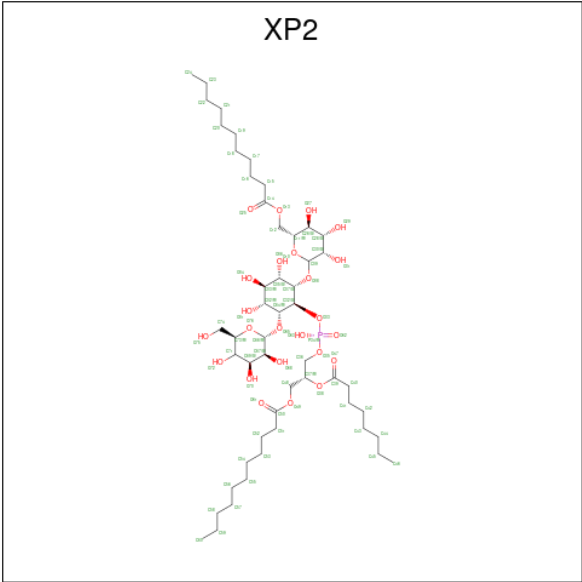


Mol	Chain	Residues	Atoms					AltConf
20	F	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
21	F	1	Total Zn 1 1	0

- Molecule 22 is (2R)-3-[[[(R)-hydroxy({(1S,2R,3R,4R,5S,6S)-3,4,5-trihydroxy-2-(alpha-D-mannopyranosyloxy)-6-[(6-O-undecanoyl-beta-D-mannopyranosyl)oxy]cyclohexyl}oxy)phosphoryl]oxy}-2-(octanoyloxy)propyl undecanoate (three-letter code: XP2) (formula: C₅₁H₉₃O₂₄P) (labeled as "Ligand of Interest" by depositor).




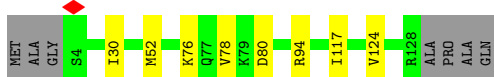
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	L	1	76	51	24	1	0

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.

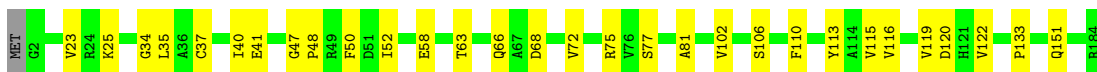
- Molecule 1: Two-component system response regulator

Chain O: 




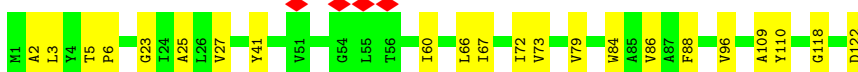
- Molecule 2: NADH-quinone oxidoreductase subunit B

Chain B: 




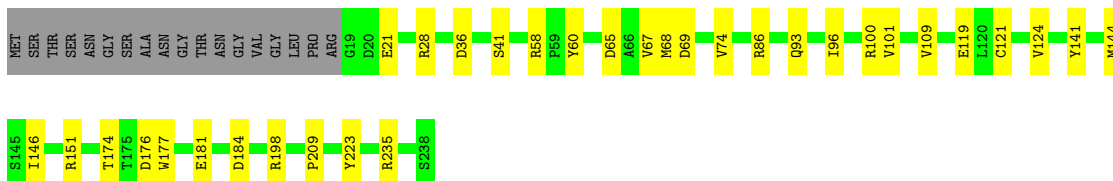
- Molecule 3: NADH-quinone oxidoreductase subunit A

Chain A: 



- Molecule 4: NADH-quinone oxidoreductase subunit C

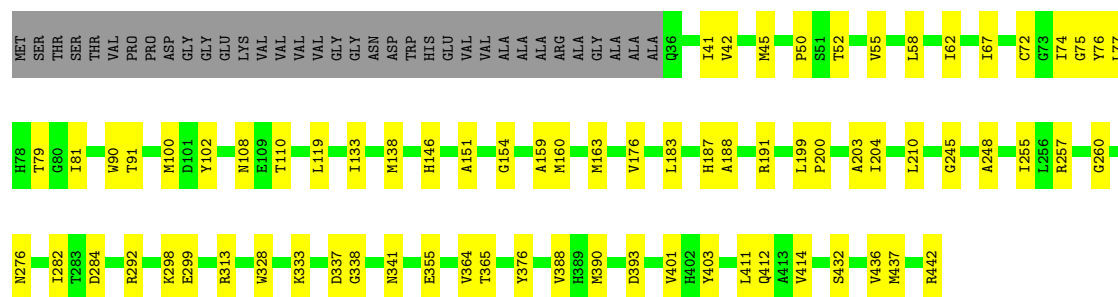
Chain C: 



- Molecule 5: NADH-quinone oxidoreductase subunit D

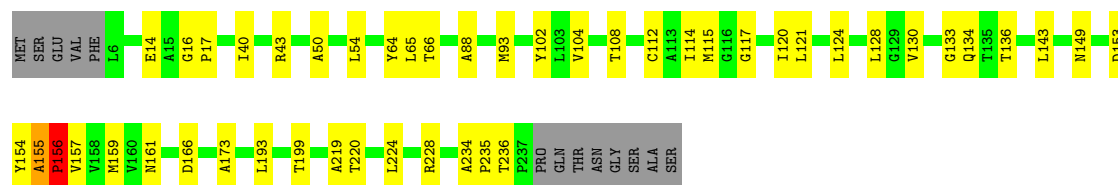
Chain D: 





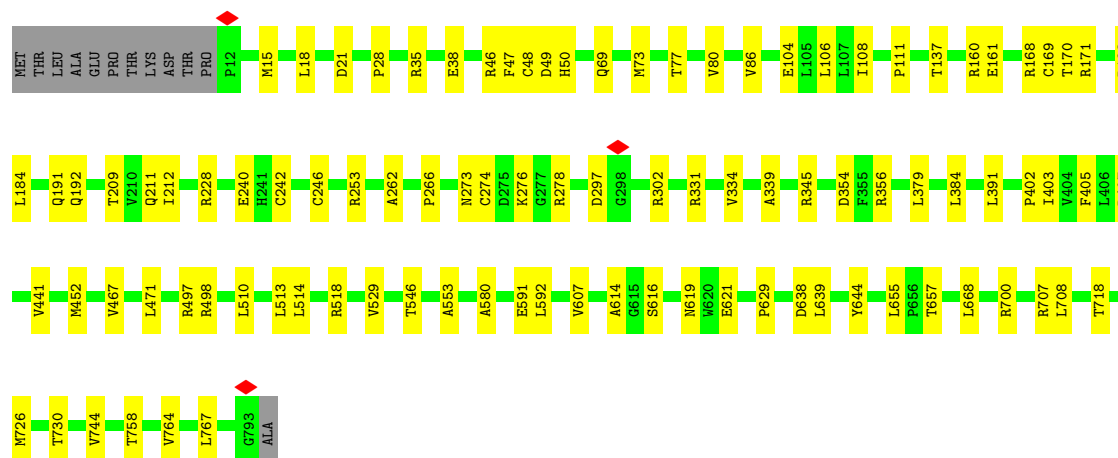
• Molecule 6: NADH-quinone oxidoreductase subunit E

Chain E: 76% 18% 5%



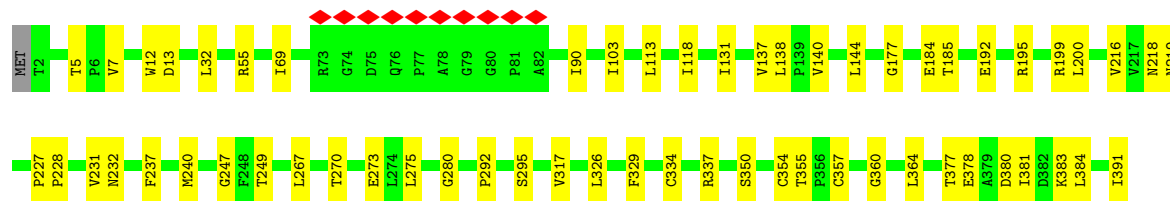
• Molecule 7: NADH-quinone oxidoreductase subunit G

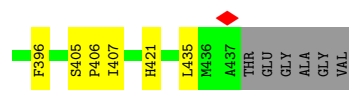
Chain G: 86% 12% 2%



• Molecule 8: NADH-quinone oxidoreductase subunit F

Chain F: 84% 15% 1%





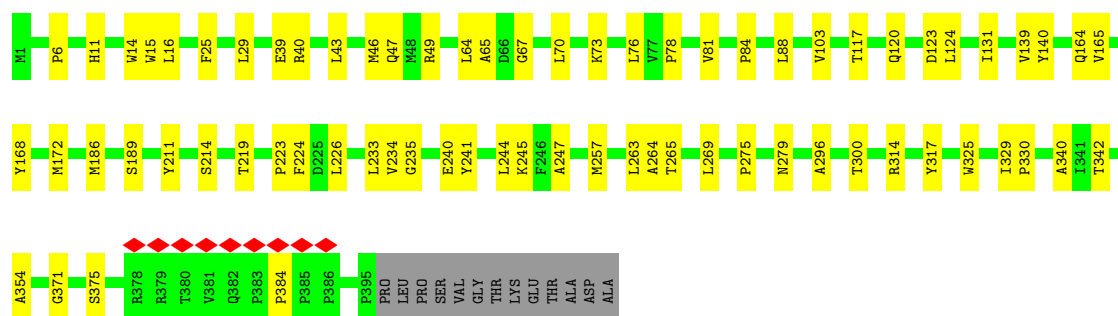
• Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I: 80% 12% 8%



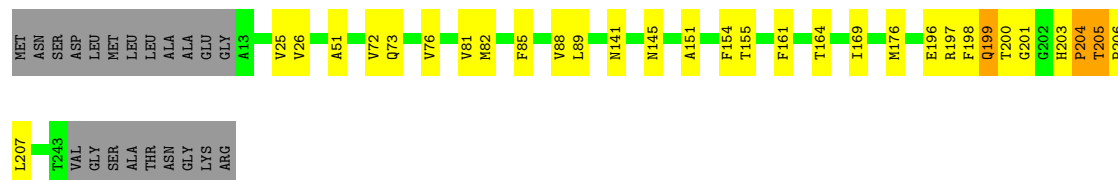
• Molecule 10: NADH-quinone oxidoreductase subunit H

Chain H: 79% 17% .



• Molecule 11: NADH-quinone oxidoreductase subunit J

Chain J: 79% 11% . 8%



• Molecule 12: NADH-quinone oxidoreductase subunit K

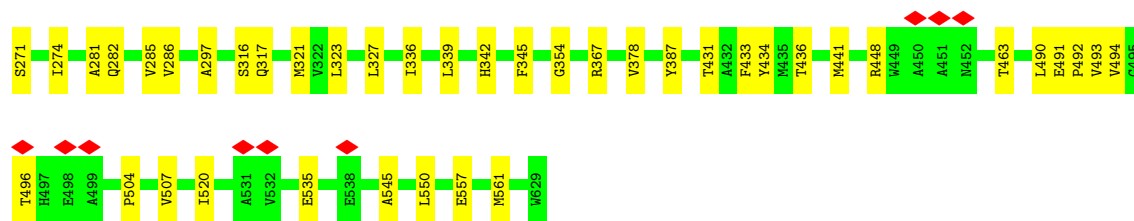
Chain K: 87% 13%



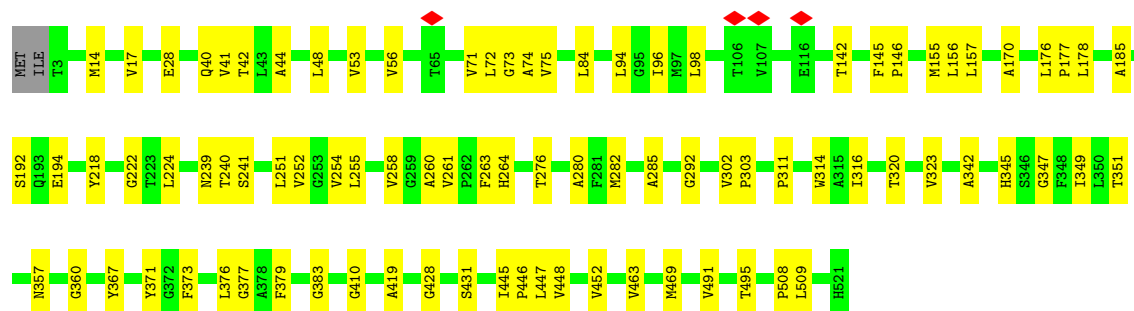
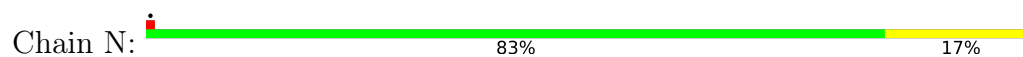
• Molecule 13: NADH-quinone oxidoreductase, L subunit

Chain L: 88% 11% .

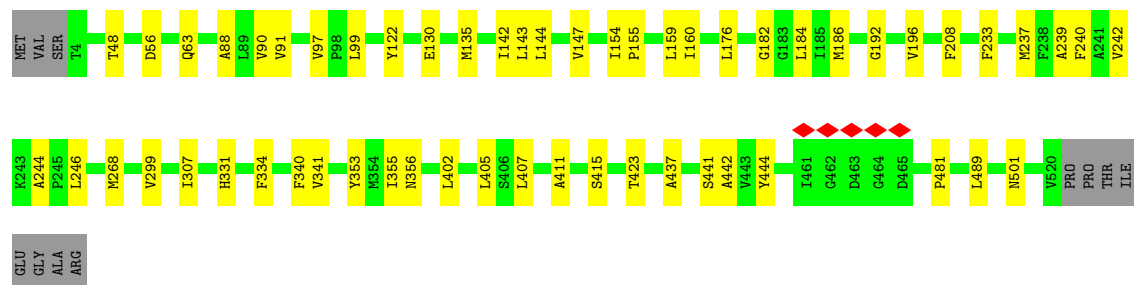




• Molecule 14: NADH-quinone oxidoreductase subunit N



• Molecule 15: NADH-quinone oxidoreductase, M subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45342	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.828	Depositor
Minimum map value	-0.535	Depositor
Average map value	0.036	Depositor
Map value standard deviation	0.184	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	453.19986, 453.19986, 453.19986	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.180208, 1.180208, 1.180208	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MQ9, GTP, SF4, XP2, FMN, FES

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	O	0.32	0/915	0.52	0/1255
2	B	0.33	0/1367	0.51	0/1863
3	A	0.34	0/979	0.46	0/1338
4	C	0.34	0/1728	0.53	0/2367
5	D	0.34	0/3114	0.53	0/4229
6	E	0.30	0/1653	0.53	1/2277 (0.0%)
7	G	0.31	0/5755	0.53	0/7870
8	F	0.31	0/3257	0.48	0/4450
9	I	0.35	0/1258	0.50	0/1718
10	H	0.31	0/3025	0.46	0/4152
11	J	0.30	0/1656	0.48	0/2271
12	K	0.30	0/759	0.47	0/1026
13	L	0.27	0/4223	0.44	0/5798
14	N	0.31	0/3747	0.47	0/5138
15	M	0.30	0/3841	0.45	0/5278
All	All	0.31	0/37277	0.49	1/51030 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	156	PRO	N-CA-CB	-6.91	95.00	102.60

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	O	896	0	898	7	0
2	B	1338	0	1340	28	0
3	A	951	0	983	21	0
4	C	1677	0	1588	24	0
5	D	3051	0	3038	63	0
6	E	1614	0	1543	39	0
7	G	5637	0	5601	66	0
8	F	3170	0	3048	51	0
9	I	1225	0	1141	23	0
10	H	2936	0	2922	51	0
11	J	1624	0	1650	31	0
12	K	748	0	776	14	0
13	L	4132	0	3859	43	0
14	N	3665	0	3764	76	0
15	M	3744	0	3815	37	0
16	B	8	0	0	0	0
16	F	8	0	0	1	0
16	G	24	0	0	0	0
16	I	16	0	0	2	0
17	D	58	0	80	9	0
18	E	4	0	0	0	0
18	G	4	0	0	0	0
19	G	32	0	12	5	0
20	F	31	0	19	3	0
21	F	1	0	0	0	0
22	L	76	0	0	1	0
All	All	36670	0	36077	503	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 7.

All (503) 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)
6:E:155:ALA:HB1	6:E:156:PRO:HD2	1.31	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:110:TYR:OH	10:H:325:TRP:O	1.73	1.06
7:G:744:VAL:HG21	7:G:767:LEU:HD11	1.50	0.93
7:G:498:ARG:NH1	19:G:802:GTP:O1G	2.05	0.90
8:F:131:ILE:HG21	8:F:144:LEU:HD21	1.54	0.89
2:B:58:GLU:OE2	10:H:40:ARG:NE	2.07	0.88
10:H:47:GLN:OE1	10:H:49:ARG:NH1	2.10	0.84
8:F:270:THR:OG1	8:F:273:GLU:OE1	1.95	0.83
7:G:38:GLU:OE2	7:G:46:ARG:NH1	2.11	0.82
7:G:707:ARG:N	19:G:802:GTP:O2B	2.13	0.82
15:M:88:ALA:HB1	15:M:355:ILE:HD11	1.62	0.81
5:D:72:CYS:SG	5:D:414:VAL:HG21	2.21	0.81
13:L:262:THR:HG23	13:L:339:LEU:HD21	1.64	0.79
4:C:176:ASP:O	5:D:412:GLN:NE2	2.16	0.79
2:B:75:ARG:NE	5:D:79:THR:OG1	2.17	0.78
5:D:100:MET:O	5:D:108:ASN:ND2	2.17	0.78
7:G:700:ARG:NH1	19:G:802:GTP:O1G	2.17	0.78
2:B:63:THR:OG1	2:B:66:GLN:OE1	2.01	0.77
5:D:183:LEU:O	5:D:187:HIS:HE1	1.68	0.75
6:E:149:ASN:ND2	6:E:159:MET:SD	2.60	0.75
11:J:196:GLU:O	11:J:199:GLN:N	2.21	0.74
5:D:183:LEU:O	5:D:187:HIS:CE1	2.41	0.73
14:N:261:VAL:HG23	14:N:320:THR:HA	1.69	0.72
2:B:48:PRO:O	9:I:24:THR:HG22	1.89	0.71
5:D:257:ARG:NH1	5:D:299:GLU:OE2	2.22	0.71
8:F:103:ILE:HG23	8:F:140:VAL:HG21	1.72	0.69
17:D:501:MQ9:H503	10:H:244:LEU:HD22	1.73	0.69
8:F:377:THR:N	8:F:380:ASP:OD2	2.26	0.69
6:E:235:PRO:O	6:E:236:THR:OG1	2.08	0.69
14:N:239:ASN:O	14:N:240:THR:OG1	2.09	0.69
2:B:120:ASP:OD2	9:I:127:ARG:NH2	2.26	0.68
8:F:334:CYS:SG	8:F:421:HIS:CE1	2.87	0.68
2:B:25:LYS:NZ	2:B:151:GLN:OE1	2.28	0.67
17:D:501:MQ9:H402	17:D:501:MQ9:H353	1.75	0.67
2:B:102:VAL:HG11	9:I:99:CYS:O	1.94	0.67
10:H:139:VAL:HG11	10:H:165:VAL:CG2	2.24	0.67
14:N:367:TYR:CD1	14:N:431:SER:OG	2.48	0.66
7:G:211:GLN:OE1	7:G:278:ARG:NH2	2.29	0.66
6:E:102:TYR:CE1	6:E:193:LEU:HD21	2.30	0.66
10:H:84:PRO:O	10:H:88:LEU:HD23	1.95	0.66
11:J:161:PHE:O	11:J:164:THR:OG1	2.14	0.66
4:C:184:ASP:OD1	4:C:198:ARG:NH1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:76:LEU:O	10:H:245:LYS:NZ	2.29	0.66
7:G:266:PRO:O	7:G:407:ARG:NH2	2.29	0.66
9:I:42:HIS:CD2	9:I:105:CYS:SG	2.88	0.65
15:M:135:MET:HE1	15:M:144:LEU:HD21	1.78	0.65
3:A:73:VAL:HG13	12:K:73:VAL:HG21	1.78	0.65
5:D:328:TRP:NE1	9:I:107:GLU:OE1	2.28	0.65
5:D:411:LEU:O	5:D:414:VAL:HG22	1.98	0.64
6:E:155:ALA:HB1	6:E:156:PRO:CD	2.16	0.64
9:I:147:ALA:O	9:I:150:HIS:ND1	2.28	0.64
13:L:22:LEU:HB3	13:L:123:ALA:HB2	1.79	0.64
7:G:354:ASP:OD2	7:G:546:THR:N	2.29	0.64
4:C:28:ARG:NH2	5:D:393:ASP:O	2.32	0.63
7:G:591:GLU:OE2	7:G:592:LEU:N	2.30	0.63
14:N:345:HIS:ND1	14:N:367:TYR:OH	2.31	0.63
15:M:182:GLY:HA3	15:M:242:VAL:HG21	1.80	0.63
5:D:146:HIS:NE2	5:D:299:GLU:OE1	2.31	0.63
14:N:72:LEU:O	14:N:72:LEU:HD23	1.99	0.62
6:E:154:TYR:CZ	6:E:219:ALA:HB3	2.34	0.62
13:L:367:ARG:NH2	13:L:535:GLU:O	2.33	0.62
8:F:90:ILE:HG21	8:F:113:LEU:HD11	1.81	0.62
4:C:41:SER:O	7:G:168:ARG:NH2	2.32	0.62
13:L:557:GLU:HG2	22:L:701:XP2:C11	2.29	0.61
7:G:246:CYS:SG	7:G:403:ILE:HG13	2.41	0.61
7:G:619:ASN:ND2	7:G:621:GLU:OE1	2.33	0.61
11:J:198:PHE:CE2	11:J:201:GLY:HA3	2.36	0.61
11:J:200:THR:HG22	11:J:205:THR:O	2.01	0.60
14:N:280:ALA:HB1	14:N:376:LEU:HD12	1.83	0.60
3:A:66:LEU:HD21	11:J:176:MET:SD	2.41	0.60
10:H:342:THR:HG23	10:H:354:ALA:HB1	1.83	0.60
7:G:607:VAL:HG11	7:G:638:ASP:OD1	2.02	0.60
7:G:758:THR:HG22	7:G:758:THR:O	2.00	0.60
8:F:184:GLU:O	8:F:185:THR:OG1	2.09	0.60
13:L:387:TYR:OH	13:L:436:THR:HG22	2.01	0.59
14:N:261:VAL:HG21	14:N:323:VAL:HB	1.83	0.59
4:C:36:ASP:OD2	4:C:235:ARG:NH1	2.34	0.59
8:F:131:ILE:CG2	8:F:144:LEU:HD21	2.28	0.59
8:F:192:GLU:OE2	8:F:199:ARG:NH2	2.34	0.59
8:F:5:THR:HG21	8:F:240:MET:SD	2.43	0.59
10:H:296:ALA:O	10:H:300:THR:HG23	2.02	0.58
13:L:504:PRO:O	13:L:507:VAL:HG22	2.03	0.58
6:E:234:ALA:HA	8:F:5:THR:HG23	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:436:VAL:HG13	5:D:436:VAL:O	2.04	0.58
7:G:35:ARG:NH2	7:G:49:ASP:OD2	2.37	0.58
11:J:203:HIS:O	11:J:205:THR:N	2.36	0.58
5:D:260:GLY:N	5:D:284:ASP:O	2.37	0.57
2:B:106:SER:OG	9:I:97:LEU:O	2.22	0.57
6:E:155:ALA:O	6:E:156:PRO:C	2.42	0.57
9:I:106:ILE:HG21	9:I:116:MET:HG3	1.85	0.57
11:J:204:PRO:HB2	11:J:207:LEU:HD23	1.85	0.57
6:E:102:TYR:HE1	6:E:193:LEU:HD21	1.67	0.57
6:E:161:ASN:HB3	6:E:199:THR:HG21	1.86	0.57
8:F:350:SER:OG	8:F:357:CYS:SG	2.48	0.57
14:N:48:LEU:HD11	14:N:96:ILE:HD12	1.86	0.57
7:G:339:ALA:HB2	7:G:639:LEU:HD12	1.87	0.56
11:J:205:THR:HB	11:J:206:PRO:CD	2.36	0.56
4:C:93:GLN:NE2	5:D:376:TYR:O	2.38	0.56
5:D:337:ASP:OD1	5:D:338:GLY:N	2.38	0.56
7:G:21:ASP:N	7:G:86:VAL:O	2.39	0.56
14:N:48:LEU:CD1	14:N:96:ILE:HD12	2.36	0.56
14:N:71:VAL:HG12	14:N:71:VAL:O	2.05	0.56
8:F:90:ILE:HD13	8:F:131:ILE:CD1	2.36	0.56
14:N:53:VAL:O	14:N:56:VAL:HG22	2.05	0.56
13:L:228:ALA:O	13:L:232:SER:N	2.34	0.56
15:M:244:ALA:O	15:M:246:LEU:N	2.39	0.56
6:E:124:LEU:HD11	6:E:173:ALA:HB1	1.88	0.56
15:M:135:MET:CE	15:M:144:LEU:HD21	2.35	0.56
14:N:261:VAL:HA	14:N:264:HIS:HD1	1.69	0.55
1:O:117:ILE:HG21	7:G:644:TYR:CZ	2.41	0.55
9:I:97:LEU:HD21	9:I:130:LEU:HD13	1.88	0.55
1:O:117:ILE:HG21	7:G:644:TYR:CE1	2.42	0.55
7:G:441:VAL:HG23	7:G:764:VAL:HG22	1.89	0.55
11:J:196:GLU:O	11:J:198:PHE:N	2.40	0.55
10:H:6:PRO:O	10:H:11:HIS:NE2	2.39	0.55
6:E:155:ALA:CB	6:E:156:PRO:HD2	2.19	0.55
8:F:360:GLY:HA3	8:F:391:ILE:HD11	1.88	0.55
3:A:79:VAL:HG23	12:K:62:PHE:HZ	1.71	0.54
14:N:452:VAL:HG13	15:M:184:LEU:HB3	1.88	0.54
8:F:90:ILE:HD13	8:F:131:ILE:HD13	1.88	0.54
4:C:121:CYS:O	4:C:174:THR:HG21	2.08	0.54
8:F:32:LEU:HD11	8:F:118:ILE:HG21	1.88	0.54
10:H:16:LEU:HD21	10:H:117:THR:HG21	1.88	0.54
13:L:436:THR:HG21	13:L:520:ILE:HA	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:157:LEU:CD2	14:N:170:ALA:HB2	2.38	0.54
13:L:433:PHE:O	13:L:436:THR:OG1	2.23	0.54
7:G:518:ARG:NH2	7:G:668:LEU:O	2.40	0.53
13:L:238:GLN:OE1	13:L:238:GLN:N	2.37	0.53
5:D:133:ILE:HD12	5:D:199:LEU:HD11	1.90	0.53
6:E:108:THR:HG21	6:E:121:LEU:HD22	1.90	0.53
5:D:333:LYS:O	9:I:112:ARG:NH2	2.42	0.53
14:N:377:GLY:CA	14:N:495:THR:HG21	2.39	0.53
7:G:497:ARG:NH2	19:G:802:GTP:O2G	2.40	0.53
6:E:130:VAL:HG13	6:E:134:GLN:HB2	1.90	0.53
7:G:240:GLU:O	7:G:331:ARG:NH2	2.42	0.53
14:N:367:TYR:HA	14:N:431:SER:OG	2.09	0.53
6:E:104:VAL:O	6:E:104:VAL:HG23	2.09	0.52
11:J:198:PHE:O	11:J:199:GLN:C	2.47	0.52
4:C:223:TYR:OH	9:I:67:ASP:O	2.24	0.52
12:K:45:PHE:CZ	12:K:60:VAL:HG11	2.44	0.52
7:G:639:LEU:HD11	7:G:655:LEU:HB3	1.90	0.52
7:G:708:LEU:N	19:G:802:GTP:O2B	2.34	0.52
11:J:200:THR:O	11:J:203:HIS:N	2.42	0.52
15:M:160:ILE:HD11	15:M:268:MET:CE	2.40	0.52
14:N:349:ILE:HG12	14:N:367:TYR:CD2	2.44	0.52
5:D:90:TRP:O	5:D:91:THR:OG1	2.17	0.52
14:N:260:ALA:O	14:N:264:HIS:N	2.43	0.52
7:G:354:ASP:OD1	7:G:356:ARG:NE	2.32	0.52
10:H:371:GLY:O	10:H:375:SER:N	2.41	0.52
13:L:74:PRO:O	15:M:501:ASN:ND2	2.43	0.52
14:N:377:GLY:HA3	14:N:495:THR:HG21	1.92	0.52
3:A:60:ILE:CD1	5:D:41:ILE:HD11	2.40	0.51
7:G:510:LEU:HD12	7:G:513:LEU:HD12	1.91	0.51
5:D:45:MET:HG3	5:D:52:THR:CG2	2.41	0.51
6:E:65:LEU:CD1	6:E:88:ALA:HB1	2.40	0.51
4:C:68:MET:HE3	4:C:96:ILE:HD11	1.91	0.51
6:E:155:ALA:O	6:E:157:VAL:N	2.43	0.51
7:G:297:ASP:OD2	7:G:302:ARG:NE	2.32	0.51
13:L:10:LEU:O	13:L:14:LEU:N	2.43	0.51
5:D:151:ALA:HB1	5:D:163:MET:HA	1.91	0.51
5:D:74:ILE:HG22	5:D:75:GLY:N	2.25	0.51
7:G:191:GLN:OE1	8:F:195:ARG:NH2	2.43	0.51
10:H:244:LEU:HA	10:H:247:ALA:HB3	1.92	0.51
4:C:41:SER:OG	7:G:50:HIS:NE2	2.42	0.51
14:N:94:LEU:CB	14:N:376:LEU:HD21	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:431:THR:HA	13:L:434:TYR:CE2	2.46	0.51
13:L:496:THR:O	13:L:496:THR:HG23	2.11	0.51
15:M:233:PHE:CZ	15:M:237:MET:HE2	2.46	0.51
6:E:112:CYS:O	6:E:117:GLY:N	2.41	0.51
15:M:356:ASN:ND2	15:M:411:ALA:HB1	2.27	0.50
3:A:86:VAL:HG11	10:H:186:MET:HG3	1.93	0.50
6:E:154:TYR:HB3	6:E:166:ASP:HB3	1.92	0.50
14:N:14:MET:HE1	14:N:157:LEU:HD13	1.92	0.50
7:G:48:CYS:O	7:G:171:ARG:NH1	2.40	0.50
10:H:16:LEU:CD2	10:H:117:THR:HG21	2.41	0.50
7:G:614:ALA:HB2	7:G:629:PRO:HD3	1.94	0.50
5:D:50:PRO:O	17:D:501:MQ9:H5M1	2.12	0.50
5:D:154:GLY:O	5:D:159:ALA:N	2.43	0.50
8:F:354:CYS:SG	8:F:396:PHE:N	2.69	0.50
15:M:48:THR:HG23	15:M:90:VAL:HG12	1.94	0.50
15:M:299:VAL:HG11	15:M:340:PHE:CE2	2.46	0.50
10:H:70:LEU:HD13	10:H:247:ALA:HB2	1.93	0.50
13:L:193:MET:HE1	13:L:205:VAL:HG21	1.93	0.50
14:N:218:TYR:O	14:N:222:GLY:N	2.43	0.50
11:J:141:ASN:OD1	11:J:145:ASN:ND2	2.41	0.50
4:C:58:ARG:O	4:C:60:TYR:N	2.44	0.50
14:N:157:LEU:HD23	14:N:170:ALA:HB2	1.94	0.50
10:H:223:PRO:O	10:H:314:ARG:HA	2.12	0.50
2:B:72:VAL:HG11	2:B:119:VAL:HG21	1.94	0.49
4:C:176:ASP:O	4:C:177:TRP:HB2	2.12	0.49
3:A:79:VAL:HG23	12:K:62:PHE:CZ	2.47	0.49
9:I:97:LEU:HD21	9:I:130:LEU:CD1	2.42	0.49
13:L:101:GLY:O	13:L:105:HIS:ND1	2.39	0.49
13:L:269:VAL:HG21	13:L:336:ILE:HD11	1.94	0.49
14:N:178:LEU:HD22	14:N:282:MET:HE2	1.94	0.49
6:E:133:GLY:N	6:E:143:LEU:O	2.39	0.49
15:M:97:VAL:HG11	15:M:130:GLU:OE1	2.10	0.49
1:O:76:LYS:NZ	1:O:80:ASP:OD2	2.42	0.49
7:G:18:LEU:HD13	7:G:80:VAL:HG13	1.94	0.49
2:B:40:ILE:HD11	17:D:501:MQ9:C3C	2.42	0.49
12:K:45:PHE:CE1	12:K:60:VAL:HG11	2.47	0.49
15:M:405:LEU:HD13	15:M:442:ALA:HA	1.95	0.49
6:E:154:TYR:OH	6:E:220:THR:HG23	2.12	0.49
10:H:25:PHE:O	10:H:29:LEU:HD23	2.12	0.49
4:C:181:GLU:OE2	5:D:442:ARG:NH2	2.37	0.49
14:N:40:GLN:O	14:N:44:ALA:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:255:LEU:HA	14:N:258:VAL:HG22	1.95	0.49
14:N:74:ALA:O	14:N:75:VAL:HG23	2.12	0.49
14:N:185:ALA:HB3	14:N:192:SER:HB2	1.95	0.49
3:A:67:ILE:HD12	3:A:122:ASP:O	2.12	0.48
4:C:119:GLU:OE2	4:C:146:ILE:N	2.45	0.48
7:G:183:ASP:OD1	7:G:184:LEU:N	2.42	0.48
4:C:21:GLU:O	4:C:86:ARG:NH2	2.46	0.48
5:D:119:LEU:HD12	5:D:390:MET:HE2	1.96	0.48
17:D:501:MQ9:H371	10:H:67:GLY:CA	2.43	0.48
14:N:448:VAL:O	14:N:452:VAL:HG23	2.13	0.48
5:D:81:ILE:HG21	5:D:100:MET:CE	2.44	0.48
8:F:292:PRO:HA	8:F:326:LEU:HD23	1.95	0.48
13:L:490:LEU:O	13:L:494:VAL:N	2.43	0.48
14:N:261:VAL:O	14:N:264:HIS:ND1	2.44	0.48
7:G:47:PHE:O	7:G:168:ARG:HD2	2.13	0.48
14:N:311:PRO:O	14:N:314:TRP:HB2	2.14	0.48
8:F:364:LEU:HD13	8:F:407:ILE:CD1	2.44	0.48
5:D:245:GLY:HA2	11:J:198:PHE:CE1	2.49	0.48
13:L:189:ALA:O	13:L:193:MET:HG3	2.14	0.48
11:J:151:ALA:O	11:J:155:THR:OG1	2.14	0.47
15:M:441:SER:HA	15:M:444:TYR:CE1	2.49	0.47
2:B:81:ALA:HB1	2:B:122:VAL:HG11	1.96	0.47
10:H:224:PHE:O	10:H:226:LEU:N	2.46	0.47
10:H:275:PRO:O	10:H:279:ASN:N	2.44	0.47
14:N:98:LEU:HD21	14:N:491:VAL:HG11	1.96	0.47
5:D:79:THR:O	5:D:79:THR:HG22	2.15	0.47
5:D:341:ASN:ND2	9:I:109:CYS:O	2.42	0.47
10:H:120:GLN:NE2	10:H:189:SER:OG	2.44	0.47
13:L:153:LEU:HD22	15:M:407:LEU:CD1	2.43	0.47
15:M:142:ILE:HD12	15:M:208:PHE:O	2.14	0.47
4:C:58:ARG:NH2	4:C:69:ASP:OD1	2.47	0.47
5:D:176:VAL:HG21	5:D:210:LEU:CD1	2.44	0.47
7:G:467:VAL:HG13	7:G:471:LEU:HD22	1.96	0.47
5:D:45:MET:HG3	5:D:52:THR:HG21	1.95	0.47
13:L:281:ALA:O	13:L:285:VAL:HG23	2.14	0.47
7:G:467:VAL:HG13	7:G:471:LEU:CD2	2.44	0.47
2:B:66:GLN:NE2	10:H:241:TYR:O	2.48	0.47
2:B:72:VAL:HG11	2:B:119:VAL:CG2	2.45	0.47
3:A:88:PHE:CE2	3:A:96:VAL:HG22	2.50	0.47
8:F:357:CYS:HB2	16:F:503:SF4:S4	2.54	0.47
10:H:123:ASP:OD1	10:H:124:LEU:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:140:TYR:OH	11:J:82:MET:N	2.48	0.47
13:L:491:GLU:N	13:L:492:PRO:HD2	2.30	0.47
2:B:34:GLY:O	2:B:35:LEU:HD12	2.15	0.47
7:G:209:THR:HA	7:G:212:ILE:HG22	1.96	0.47
7:G:228:ARG:NH1	9:I:57:CYS:O	2.48	0.47
10:H:172:MET:HG3	10:H:214:SER:OG	2.14	0.47
14:N:94:LEU:HB2	14:N:376:LEU:HD21	1.96	0.47
14:N:314:TRP:CD2	14:N:447:LEU:HD11	2.50	0.47
7:G:345:ARG:NH2	7:G:510:LEU:O	2.40	0.47
8:F:5:THR:HG22	8:F:7:VAL:HG23	1.96	0.47
14:N:157:LEU:HG	14:N:170:ALA:HB2	1.97	0.47
6:E:114:ILE:HD11	8:F:329:PHE:CD1	2.50	0.47
15:M:160:ILE:HD11	15:M:268:MET:HE1	1.97	0.47
1:O:52:MET:SD	1:O:78:VAL:HG11	2.54	0.46
5:D:204:ILE:HD12	5:D:204:ILE:H	1.80	0.46
6:E:120:ILE:O	6:E:124:LEU:HD13	2.14	0.46
10:H:131:ILE:HG21	10:H:263:LEU:HD22	1.97	0.46
11:J:72:VAL:O	11:J:76:VAL:HG22	2.15	0.46
5:D:248:ALA:HB3	11:J:198:PHE:CE2	2.50	0.46
8:F:227:PRO:HG2	8:F:228:PRO:HD3	1.96	0.46
14:N:463:VAL:HG21	15:M:176:LEU:HD23	1.97	0.46
13:L:245:MET:HE2	13:L:245:MET:HA	1.97	0.46
14:N:261:VAL:HA	14:N:264:HIS:ND1	2.30	0.46
2:B:23:VAL:HG13	10:H:65:ALA:O	2.16	0.46
7:G:253:ARG:NH2	9:I:71:VAL:O	2.46	0.46
11:J:73:GLN:HA	12:K:65:MET:HE1	1.97	0.46
14:N:302:VAL:O	14:N:302:VAL:HG13	2.16	0.46
8:F:275:LEU:O	8:F:280:GLY:N	2.40	0.46
9:I:105:CYS:N	16:I:201:SF4:S1	2.89	0.46
13:L:184:MET:O	13:L:188:ILE:HG12	2.15	0.46
13:L:271:SER:O	13:L:274:ILE:N	2.46	0.46
14:N:251:LEU:HA	14:N:254:VAL:HG22	1.98	0.46
5:D:364:VAL:HG11	9:I:108:ALA:HA	1.98	0.46
6:E:16:GLY:O	6:E:17:PRO:C	2.54	0.46
14:N:508:PRO:O	14:N:509:LEU:HB3	2.16	0.46
3:A:2:ALA:O	3:A:3:LEU:HB2	2.16	0.46
7:G:77:THR:CG2	8:F:200:LEU:HD11	2.46	0.46
1:O:30:ILE:HG21	1:O:124:VAL:HG23	1.97	0.46
13:L:80:VAL:HG11	13:L:142:LEU:HD23	1.97	0.46
5:D:188:ALA:O	5:D:191:ARG:NE	2.46	0.46
6:E:64:TYR:CE2	6:E:66:THR:HG22	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:128:LEU:HD12	6:E:136:THR:CG2	2.46	0.46
15:M:411:ALA:HB2	15:M:489:LEU:HB2	1.98	0.46
2:B:110:PHE:CE1	5:D:81:ILE:HG12	2.51	0.45
2:B:116:VAL:HG12	2:B:116:VAL:O	2.17	0.45
13:L:297:ALA:N	13:L:316:SER:OG	2.49	0.45
14:N:276:THR:HG21	14:N:383:GLY:CA	2.46	0.45
8:F:219:ASN:ND2	20:F:501:FMN:O2	2.49	0.45
14:N:280:ALA:HB2	14:N:379:PHE:CB	2.45	0.45
14:N:445:ILE:N	14:N:446:PRO:CD	2.79	0.45
8:F:69:ILE:HD11	8:F:216:VAL:HG23	1.98	0.45
3:A:5:THR:N	3:A:6:PRO:CD	2.79	0.45
11:J:204:PRO:O	11:J:205:THR:C	2.54	0.45
13:L:493:VAL:HG23	13:L:494:VAL:N	2.31	0.45
6:E:154:TYR:CE2	6:E:219:ALA:HB3	2.52	0.45
10:H:39:GLU:O	10:H:40:ARG:C	2.54	0.45
5:D:292:ARG:NE	5:D:432:SER:OG	2.43	0.45
7:G:379:LEU:HD21	7:G:384:LEU:HD21	1.98	0.45
8:F:381:ILE:HD12	8:F:381:ILE:H	1.82	0.45
11:J:51:ALA:HB2	11:J:81:VAL:HG11	1.99	0.45
14:N:357:ASN:OD1	14:N:360:GLY:N	2.45	0.45
11:J:25:VAL:HG23	11:J:26:VAL:N	2.32	0.45
6:E:154:TYR:CE2	6:E:220:THR:HG23	2.52	0.45
11:J:88:VAL:HG23	12:K:28:ILE:HG21	1.99	0.45
13:L:282:GLN:O	13:L:286:VAL:HG23	2.17	0.45
3:A:25:ALA:HB2	10:H:244:LEU:HB2	1.99	0.45
5:D:119:LEU:HD12	5:D:390:MET:CE	2.47	0.45
5:D:282:ILE:HG21	5:D:298:LYS:HB2	1.99	0.45
6:E:50:ALA:O	6:E:54:LEU:HD13	2.16	0.45
7:G:553:ALA:HB3	7:G:580:ALA:HB1	1.99	0.45
10:H:139:VAL:HG11	10:H:165:VAL:HG21	1.98	0.45
12:K:96:LEU:N	14:N:194:GLU:OE1	2.48	0.45
14:N:302:VAL:O	14:N:302:VAL:HG22	2.17	0.45
2:B:77:SER:OG	5:D:76:TYR:O	2.29	0.45
7:G:106:LEU:HD13	8:F:355:THR:HG21	1.98	0.45
13:L:323:LEU:O	13:L:327:LEU:HG	2.17	0.45
14:N:252:VAL:HG13	14:N:263:PHE:CE1	2.52	0.45
2:B:47:GLY:O	2:B:50:PHE:O	2.34	0.44
10:H:164:GLN:O	10:H:168:TYR:CD1	2.71	0.44
13:L:545:ALA:O	13:L:550:LEU:N	2.50	0.44
14:N:302:VAL:N	14:N:303:PRO:HD3	2.32	0.44
3:A:41:TYR:N	10:H:240:GLU:OE2	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:62:ILE:HG22	5:D:67:ILE:HD13	1.98	0.44
5:D:160:MET:CE	10:H:43:LEU:HD22	2.47	0.44
6:E:153:ASP:N	6:E:153:ASP:OD1	2.50	0.44
7:G:104:GLU:O	7:G:108:ILE:HG23	2.18	0.44
15:M:331:HIS:ND1	15:M:353:TYR:OH	2.45	0.44
17:D:501:MQ9:H451	10:H:64:LEU:HD12	1.99	0.44
8:F:103:ILE:HG23	8:F:140:VAL:CG2	2.45	0.44
13:L:557:GLU:HA	13:L:561:MET:HB3	1.99	0.44
14:N:347:GLY:O	14:N:351:THR:HG23	2.18	0.44
14:N:373:PHE:O	14:N:495:THR:CG2	2.65	0.44
13:L:188:ILE:HD12	13:L:191:MET:HE1	1.98	0.44
3:A:3:LEU:O	10:H:124:LEU:HD11	2.18	0.44
5:D:55:VAL:HG23	5:D:437:MET:HG3	1.99	0.44
5:D:365:THR:HB	9:I:62:TRP:CE2	2.53	0.44
7:G:391:LEU:HD22	7:G:452:MET:HE2	1.98	0.44
2:B:113:TYR:CZ	4:C:209:PRO:HB3	2.53	0.44
4:C:67:VAL:HG12	4:C:68:MET:HE2	1.99	0.44
5:D:257:ARG:NH2	5:D:299:GLU:OE2	2.51	0.44
7:G:274:CYS:SG	7:G:276:LYS:HB3	2.58	0.44
12:K:38:LEU:HD13	12:K:68:ALA:HB2	1.98	0.44
14:N:261:VAL:CA	14:N:264:HIS:HD1	2.31	0.44
17:D:501:MQ9:H353	17:D:501:MQ9:C40	2.44	0.44
17:D:501:MQ9:H371	10:H:67:GLY:HA2	2.00	0.44
7:G:242:CYS:HA	7:G:497:ARG:O	2.17	0.44
11:J:198:PHE:CD1	11:J:198:PHE:C	2.88	0.44
14:N:280:ALA:HB2	14:N:379:PHE:HB3	1.99	0.44
14:N:349:ILE:HG13	14:N:367:TYR:CE2	2.53	0.44
15:M:239:ALA:O	15:M:242:VAL:HG22	2.18	0.44
5:D:77:LEU:O	5:D:77:LEU:HG	2.17	0.44
6:E:224:LEU:O	6:E:228:ARG:HG2	2.17	0.44
8:F:32:LEU:HD11	8:F:118:ILE:CG2	2.48	0.44
8:F:137:VAL:O	8:F:140:VAL:N	2.50	0.44
15:M:186:MET:HE1	15:M:240:PHE:CE1	2.53	0.44
6:E:40:ILE:O	6:E:43:ARG:HG2	2.17	0.43
9:I:112:ARG:CG	9:I:112:ARG:O	2.65	0.43
14:N:239:ASN:OD1	14:N:241:SER:N	2.47	0.43
5:D:200:PRO:HG2	5:D:203:ALA:HB2	1.99	0.43
5:D:245:GLY:HA2	11:J:198:PHE:CZ	2.53	0.43
5:D:276:ASN:O	5:D:313:ARG:NH2	2.51	0.43
7:G:262:ALA:HA	7:G:273:ASN:OD1	2.18	0.43
13:L:78:LEU:HG	13:L:80:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:445:ILE:HG22	14:N:446:PRO:HD3	2.00	0.43
7:G:69:GLN:HG3	7:G:73:MET:SD	2.59	0.43
8:F:55:ARG:N	20:F:501:FMN:O3P	2.52	0.43
8:F:354:CYS:SG	8:F:396:PHE:CB	3.06	0.43
11:J:198:PHE:O	11:J:198:PHE:CG	2.71	0.43
3:A:60:ILE:HD12	5:D:41:ILE:HD11	1.99	0.43
5:D:255:ILE:HA	5:D:292:ARG:HD3	2.00	0.43
8:F:237:PHE:CZ	8:F:247:GLY:HA3	2.53	0.43
12:K:76:LEU:O	12:K:80:MET:HG2	2.18	0.43
12:K:60:VAL:HG21	14:N:224:LEU:HD11	2.01	0.43
4:C:144:MET:HG3	4:C:151:ARG:HG2	2.01	0.43
7:G:77:THR:HB	8:F:200:LEU:HD11	1.99	0.43
10:H:78:PRO:O	10:H:81:VAL:HG22	2.19	0.43
11:J:198:PHE:CD2	11:J:201:GLY:HA3	2.54	0.43
15:M:56:ASP:O	15:M:63:GLN:NE2	2.44	0.43
15:M:334:PHE:HZ	15:M:437:ALA:HB3	1.82	0.43
7:G:15:MET:HE1	7:G:28:PRO:HA	2.01	0.43
7:G:718:THR:HG22	7:G:718:THR:O	2.18	0.43
11:J:205:THR:CB	11:J:206:PRO:CD	2.96	0.43
13:L:193:MET:HE3	13:L:205:VAL:HG11	2.00	0.43
14:N:349:ILE:CG1	14:N:367:TYR:CD2	3.02	0.43
15:M:192:GLY:O	15:M:196:VAL:HG23	2.19	0.43
15:M:353:TYR:HB2	15:M:415:SER:HB3	2.01	0.43
3:A:23:GLY:O	3:A:27:VAL:HG22	2.19	0.43
8:F:383:LYS:O	8:F:384:LEU:C	2.57	0.43
6:E:154:TYR:O	6:E:155:ALA:O	2.37	0.43
3:A:109:ALA:HB2	11:J:169:ILE:HG12	2.01	0.42
10:H:103:VAL:HG23	10:H:131:ILE:HD11	2.02	0.42
5:D:390:MET:HG3	5:D:401:VAL:HG22	2.00	0.42
11:J:76:VAL:HG21	12:K:65:MET:HE2	2.01	0.42
14:N:41:VAL:HG13	14:N:42:THR:N	2.33	0.42
14:N:342:ALA:HA	14:N:371:TYR:OH	2.20	0.42
15:M:307:ILE:HD11	15:M:334:PHE:HA	2.01	0.42
4:C:74:VAL:HG11	4:C:109:VAL:HG13	2.01	0.42
14:N:17:VAL:HG21	14:N:156:LEU:CD1	2.49	0.42
14:N:176:LEU:HB2	14:N:177:PRO:HD3	2.00	0.42
9:I:105:CYS:HB3	16:I:201:SF4:S1	2.59	0.42
15:M:48:THR:HG21	15:M:91:VAL:HA	2.02	0.42
2:B:34:GLY:C	2:B:35:LEU:HD12	2.40	0.42
8:F:249:THR:HG21	8:F:267:LEU:HD21	2.02	0.42
10:H:164:GLN:OE1	10:H:226:LEU:HD12	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:233:LEU:O	10:H:235:GLY:N	2.53	0.42
4:C:124:VAL:HG22	4:C:141:TYR:CD2	2.55	0.42
7:G:160:ARG:NH1	7:G:192:GLN:OE1	2.44	0.42
10:H:219:THR:HG21	10:H:257:MET:HA	2.02	0.42
10:H:329:ILE:HB	10:H:330:PRO:HD3	2.01	0.42
14:N:157:LEU:CG	14:N:170:ALA:HB2	2.50	0.42
7:G:744:VAL:HG23	7:G:744:VAL:O	2.20	0.42
5:D:45:MET:HB3	5:D:58:LEU:HB2	2.00	0.42
14:N:377:GLY:N	14:N:495:THR:HG21	2.35	0.42
15:M:402:LEU:HA	15:M:405:LEU:HB3	2.01	0.42
3:A:84:TRP:HB2	11:J:154:PHE:CZ	2.55	0.42
9:I:17:SER:OG	10:H:46:MET:O	2.38	0.42
15:M:402:LEU:HD23	15:M:405:LEU:HD23	2.02	0.42
1:O:94:ARG:NH2	2:B:115:VAL:O	2.41	0.42
5:D:388:VAL:HG22	5:D:403:TYR:CD1	2.55	0.42
7:G:334:VAL:HG12	7:G:616:SER:O	2.19	0.42
8:F:377:THR:HG22	8:F:378:GLU:N	2.35	0.42
13:L:193:MET:CE	13:L:205:VAL:HG21	2.50	0.42
14:N:94:LEU:HB3	14:N:376:LEU:HD21	2.02	0.42
5:D:41:ILE:HG22	5:D:42:VAL:N	2.35	0.41
5:D:81:ILE:HG21	5:D:100:MET:HE3	2.02	0.41
8:F:295:SER:O	8:F:406:PRO:HG3	2.20	0.41
2:B:151:GLN:O	2:B:151:GLN:NE2	2.50	0.41
3:A:66:LEU:HD23	3:A:118:GLY:O	2.20	0.41
7:G:726:MET:CE	7:G:730:THR:HG22	2.50	0.41
8:F:5:THR:HG22	8:F:5:THR:O	2.20	0.41
14:N:73:GLY:O	14:N:74:ALA:HB3	2.20	0.41
2:B:52:ILE:HD12	2:B:52:ILE:HA	1.96	0.41
3:A:84:TRP:HH2	10:H:340:ALA:HB2	1.85	0.41
4:C:100:ARG:O	4:C:101:VAL:HB	2.20	0.41
6:E:199:THR:HG22	8:F:138:LEU:CD2	2.50	0.41
7:G:169:CYS:SG	7:G:170:THR:N	2.93	0.41
12:K:28:ILE:O	12:K:32:MET:HG3	2.19	0.41
13:L:342:HIS:HA	13:L:345:PHE:CZ	2.55	0.41
13:L:441:MET:O	13:L:448:ARG:NH2	2.52	0.41
5:D:110:THR:HG21	5:D:138:MET:SD	2.59	0.41
6:E:130:VAL:HG13	6:E:134:GLN:CB	2.50	0.41
14:N:84:LEU:HD13	14:N:292:GLY:HA3	2.03	0.41
4:C:58:ARG:NH1	4:C:65:ASP:OD1	2.44	0.41
8:F:317:VAL:O	8:F:317:VAL:HG12	2.21	0.41
9:I:148:PRO:O	9:I:150:HIS:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:209:ALA:N	13:L:210:PRO:CD	2.83	0.41
14:N:357:ASN:O	14:N:360:GLY:N	2.53	0.41
14:N:410:GLY:HA2	14:N:469:MET:HE1	2.03	0.41
6:E:14:GLU:OE1	7:G:160:ARG:NH1	2.52	0.41
8:F:405:SER:HB3	8:F:406:PRO:HD3	2.01	0.41
13:L:378:VAL:HG21	13:L:463:THR:CG2	2.51	0.41
15:M:143:LEU:O	15:M:147:VAL:HG23	2.21	0.41
4:C:124:VAL:HG22	4:C:141:TYR:CE2	2.56	0.41
7:G:639:LEU:HD21	7:G:657:THR:C	2.41	0.41
13:L:249:THR:HG21	13:L:354:GLY:CA	2.50	0.41
14:N:14:MET:CE	14:N:157:LEU:HB2	2.51	0.41
14:N:145:PHE:HB2	14:N:146:PRO:HD3	2.03	0.41
14:N:419:ALA:O	14:N:428:GLY:HA3	2.21	0.41
15:M:142:ILE:HD12	15:M:142:ILE:H	1.85	0.41
2:B:37:CYS:HB3	5:D:102:TYR:CG	2.56	0.41
2:B:68:ASP:OD1	10:H:73:LYS:NZ	2.40	0.41
8:F:231:VAL:O	8:F:232:ASN:HB2	2.21	0.41
10:H:265:THR:HA	10:H:269:LEU:HB2	2.03	0.41
3:A:72:ILE:HG22	12:K:69:ALA:HB1	2.03	0.41
5:D:119:LEU:CD1	5:D:390:MET:HE2	2.50	0.41
5:D:364:VAL:HG11	9:I:108:ALA:CB	2.51	0.41
17:D:501:MQ9:H303	17:D:501:MQ9:H321	1.66	0.41
7:G:111:PRO:HG3	7:G:161:GLU:HB3	2.01	0.41
8:F:218:ASN:HA	20:F:501:FMN:O1P	2.21	0.41
10:H:14:TRP:CG	10:H:15:TRP:N	2.89	0.41
10:H:226:LEU:HD13	10:H:317:TYR:HA	2.03	0.41
11:J:85:PHE:CZ	11:J:89:LEU:HD11	2.56	0.41
14:N:28:GLU:OE2	14:N:142:THR:OG1	2.34	0.41
15:M:154:ILE:CG1	15:M:155:PRO:HD3	2.51	0.41
10:H:211:TYR:HE2	10:H:264:ALA:HB2	1.86	0.41
13:L:38:CYS:SG	13:L:109:ILE:HD11	2.61	0.41
2:B:41:GLU:HG3	2:B:133:PRO:HB2	2.03	0.40
5:D:355:GLU:OE1	7:G:137:THR:HG22	2.21	0.40
6:E:114:ILE:HG22	8:F:337:ARG:CZ	2.51	0.40
6:E:115:MET:HE3	8:F:435:LEU:HD21	2.03	0.40
8:F:12:TRP:O	8:F:13:ASP:CB	2.69	0.40
14:N:255:LEU:HD11	14:N:316:ILE:HD13	2.04	0.40
2:B:72:VAL:HG21	2:B:119:VAL:HG11	2.03	0.40
14:N:155:MET:HE2	14:N:285:ALA:CB	2.50	0.40
14:N:185:ALA:HB3	14:N:192:SER:CB	2.51	0.40
1:O:117:ILE:HG21	7:G:644:TYR:CE2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:388:VAL:HG22	5:D:403:TYR:CE1	2.56	0.40
13:L:317:GLN:O	13:L:321:MET:HG2	2.20	0.40
14:N:155:MET:HE2	14:N:285:ALA:HB1	2.03	0.40
15:M:341:VAL:HG21	15:M:423:THR:HA	2.04	0.40
6:E:93:MET:HG3	8:F:177:GLY:N	2.36	0.40
7:G:402:PRO:O	7:G:405:PHE:HB3	2.21	0.40
7:G:514:LEU:HD13	7:G:529:VAL:HG11	2.03	0.40
10:H:226:LEU:HD13	10:H:317:TYR:CB	2.52	0.40
15:M:99:LEU:HD21	15:M:481:PRO:HB2	2.03	0.40
15:M:122:TYR:CE1	15:M:159:LEU:HD11	2.56	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	O	123/132 (93%)	121 (98%)	2 (2%)	0	100	100
2	B	181/184 (98%)	168 (93%)	13 (7%)	0	100	100
3	A	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
4	C	218/238 (92%)	209 (96%)	9 (4%)	0	100	100
5	D	405/442 (92%)	389 (96%)	16 (4%)	0	100	100
6	E	230/245 (94%)	219 (95%)	9 (4%)	2 (1%)	17	40
7	G	780/794 (98%)	755 (97%)	25 (3%)	0	100	100
8	F	434/443 (98%)	412 (95%)	22 (5%)	0	100	100
9	I	163/180 (91%)	158 (97%)	5 (3%)	0	100	100
10	H	393/408 (96%)	374 (95%)	17 (4%)	2 (0%)	29	54
11	J	229/252 (91%)	213 (93%)	12 (5%)	4 (2%)	9	23
12	K	97/99 (98%)	97 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	623/629 (99%)	602 (97%)	21 (3%)	0	100	100
14	N	517/521 (99%)	497 (96%)	20 (4%)	0	100	100
15	M	515/529 (97%)	494 (96%)	21 (4%)	0	100	100
All	All	5028/5218 (96%)	4825 (96%)	195 (4%)	8 (0%)	50	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	155	ALA
6	E	156	PRO
10	H	384	PRO
11	J	204	PRO
11	J	205	THR
11	J	199	GLN
10	H	234	VAL
11	J	197	ARG

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	O	86/103 (84%)	86 (100%)	0	100	100
2	B	135/149 (91%)	135 (100%)	0	100	100
3	A	94/98 (96%)	94 (100%)	0	100	100
4	C	167/201 (83%)	167 (100%)	0	100	100
5	D	308/361 (85%)	308 (100%)	0	100	100
6	E	153/190 (80%)	152 (99%)	1 (1%)	84	94
7	G	557/610 (91%)	557 (100%)	0	100	100
8	F	301/347 (87%)	301 (100%)	0	100	100
9	I	118/145 (81%)	118 (100%)	0	100	100
10	H	285/330 (86%)	285 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	156/191 (82%)	156 (100%)	0	100	100
12	K	77/80 (96%)	77 (100%)	0	100	100
13	L	320/452 (71%)	320 (100%)	0	100	100
14	N	350/387 (90%)	350 (100%)	0	100	100
15	M	361/412 (88%)	361 (100%)	0	100	100
All	All	3468/4056 (86%)	3467 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	E	156	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	187	HIS
7	G	248	GLN
7	G	643	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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
20	FMN	F	501	-	33,33,33	1.07	2 (6%)	48,50,50	1.22	6 (12%)
18	FES	E	1000	6	0,4,4	-	-	-	-	-
19	GTP	G	802	-	26,34,34	1.19	1 (3%)	32,54,54	1.63	8 (25%)
16	SF4	G	803	7	0,12,12	-	-	-	-	-
22	XP2	L	701	-	78,78,78	1.42	10 (12%)	101,103,103	1.10	7 (6%)
18	FES	G	801	7	0,4,4	-	-	-	-	-
16	SF4	G	804	7	0,12,12	-	-	-	-	-
17	MQ9	D	501	-	59,59,59	0.35	0	72,75,75	0.39	0
16	SF4	G	805	7	0,12,12	-	-	-	-	-
16	SF4	I	202	9	0,12,12	-	-	-	-	-
16	SF4	B	1000	2	0,12,12	-	-	-	-	-
16	SF4	I	201	9	0,12,12	-	-	-	-	-
16	SF4	F	503	8	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
20	FMN	F	501	-	-	6/18/18/18	0/3/3/3
19	GTP	G	802	-	-	6/18/38/38	0/3/3/3
18	FES	E	1000	6	-	-	0/1/1/1
22	XP2	L	701	-	-	25/62/126/126	0/3/3/3
16	SF4	G	803	7	-	-	0/6/5/5
18	FES	G	801	7	-	-	0/1/1/1
16	SF4	G	804	7	-	-	0/6/5/5
17	MQ9	D	501	-	-	13/53/73/73	0/2/2/2
16	SF4	G	805	7	-	-	0/6/5/5
16	SF4	I	202	9	-	-	0/6/5/5
16	SF4	B	1000	2	-	-	0/6/5/5
16	SF4	I	201	9	-	-	0/6/5/5
16	SF4	F	503	8	-	-	0/6/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	802	GTP	C5-C6	-4.25	1.38	1.47
22	L	701	XP2	O49-C50	3.71	1.44	1.33
22	L	701	XP2	O10-C09	3.66	1.51	1.41
22	L	701	XP2	O13-C14	3.62	1.43	1.33
20	F	501	FMN	C4A-N5	3.58	1.37	1.30
22	L	701	XP2	O38-C39	3.54	1.44	1.34
22	L	701	XP2	P34-O33	3.08	1.68	1.60
22	L	701	XP2	O38-C37	-3.03	1.39	1.46
22	L	701	XP2	O08-C09	-3.00	1.33	1.41
22	L	701	XP2	O76-C73	2.96	1.51	1.44
22	L	701	XP2	C71-C69	-2.57	1.45	1.52
20	F	501	FMN	C10-N1	2.35	1.38	1.33
22	L	701	XP2	C40-C39	2.06	1.56	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	701	XP2	O38-C39-C40	4.22	120.60	111.50
22	L	701	XP2	C09-O08-C07	-3.99	108.09	117.96
19	G	802	GTP	PA-O3A-PB	-3.68	120.19	132.83
22	L	701	XP2	C66-O65-C64	-3.36	109.65	117.96
19	G	802	GTP	C5-C6-N1	3.28	119.74	113.95
19	G	802	GTP	PB-O3B-PG	-3.22	121.78	132.83
20	F	501	FMN	C4-N3-C2	-3.16	119.80	125.64
19	G	802	GTP	C8-N7-C5	3.12	108.93	102.99
19	G	802	GTP	C2-N1-C6	-3.07	119.44	125.10
20	F	501	FMN	C4A-C4-N3	2.69	120.02	113.19
20	F	501	FMN	C4A-C10-N10	2.58	120.25	116.48
20	F	501	FMN	O4-C4-C4A	-2.58	119.76	126.60
22	L	701	XP2	C37-O38-C39	-2.49	111.66	117.79
22	L	701	XP2	O49-C50-C51	2.46	119.63	111.91
19	G	802	GTP	C3'-C2'-C1'	2.44	104.66	100.98
22	L	701	XP2	O13-C14-C15	2.44	119.55	111.91
19	G	802	GTP	O6-C6-C5	-2.22	120.04	124.37
20	F	501	FMN	C4A-C10-N1	-2.18	119.67	124.73
22	L	701	XP2	C09-O10-C11	-2.16	109.45	113.69
20	F	501	FMN	C10-C4A-N5	-2.10	120.41	124.86
19	G	802	GTP	O3G-PG-O3B	2.03	111.43	104.64

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	D	501	MQ9	C7-C8-C9-C10
17	D	501	MQ9	C7-C8-C9-C11
17	D	501	MQ9	C32-C33-C34-C35
17	D	501	MQ9	C32-C33-C34-C36
19	G	802	GTP	PB-O3B-PG-O3G
19	G	802	GTP	C5'-O5'-PA-O1A
19	G	802	GTP	C5'-O5'-PA-O2A
20	F	501	FMN	N10-C1'-C2'-O2'
20	F	501	FMN	N10-C1'-C2'-C3'
20	F	501	FMN	C5'-O5'-P-O2P
20	F	501	FMN	C5'-O5'-P-O3P
22	L	701	XP2	C15-C14-O13-C12
22	L	701	XP2	O25-C14-O13-C12
22	L	701	XP2	C51-C50-O49-C48
22	L	701	XP2	O61-C50-O49-C48
22	L	701	XP2	O10-C09-O08-C07
22	L	701	XP2	O76-C66-O65-C64
22	L	701	XP2	C30-C09-O08-C07
22	L	701	XP2	O10-C11-C12-O13
22	L	701	XP2	C40-C41-C42-C43
17	D	501	MQ9	C30-C29-C31-C32
17	D	501	MQ9	C35-C34-C36-C37
17	D	501	MQ9	C28-C29-C31-C32
17	D	501	MQ9	C33-C34-C36-C37
17	D	501	MQ9	C24-C26-C27-C28
17	D	501	MQ9	C9-C11-C12-C13
22	L	701	XP2	C40-C39-O38-C37
22	L	701	XP2	O47-C39-O38-C37
22	L	701	XP2	C16-C17-C18-C19
22	L	701	XP2	C42-C43-C44-C45
22	L	701	XP2	C26-C11-C12-O13
22	L	701	XP2	C56-C57-C58-C59
22	L	701	XP2	O38-C37-C48-O49
22	L	701	XP2	C32-C07-O08-C09
22	L	701	XP2	C05-C07-O08-C09
20	F	501	FMN	C5'-O5'-P-O1P
22	L	701	XP2	C54-C55-C56-C57
22	L	701	XP2	C19-C20-C21-C22
22	L	701	XP2	C36-C37-C48-O49
17	D	501	MQ9	C14-C16-C17-C18
22	L	701	XP2	O35-C36-C37-C48
22	L	701	XP2	O35-C36-C37-O38
19	G	802	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

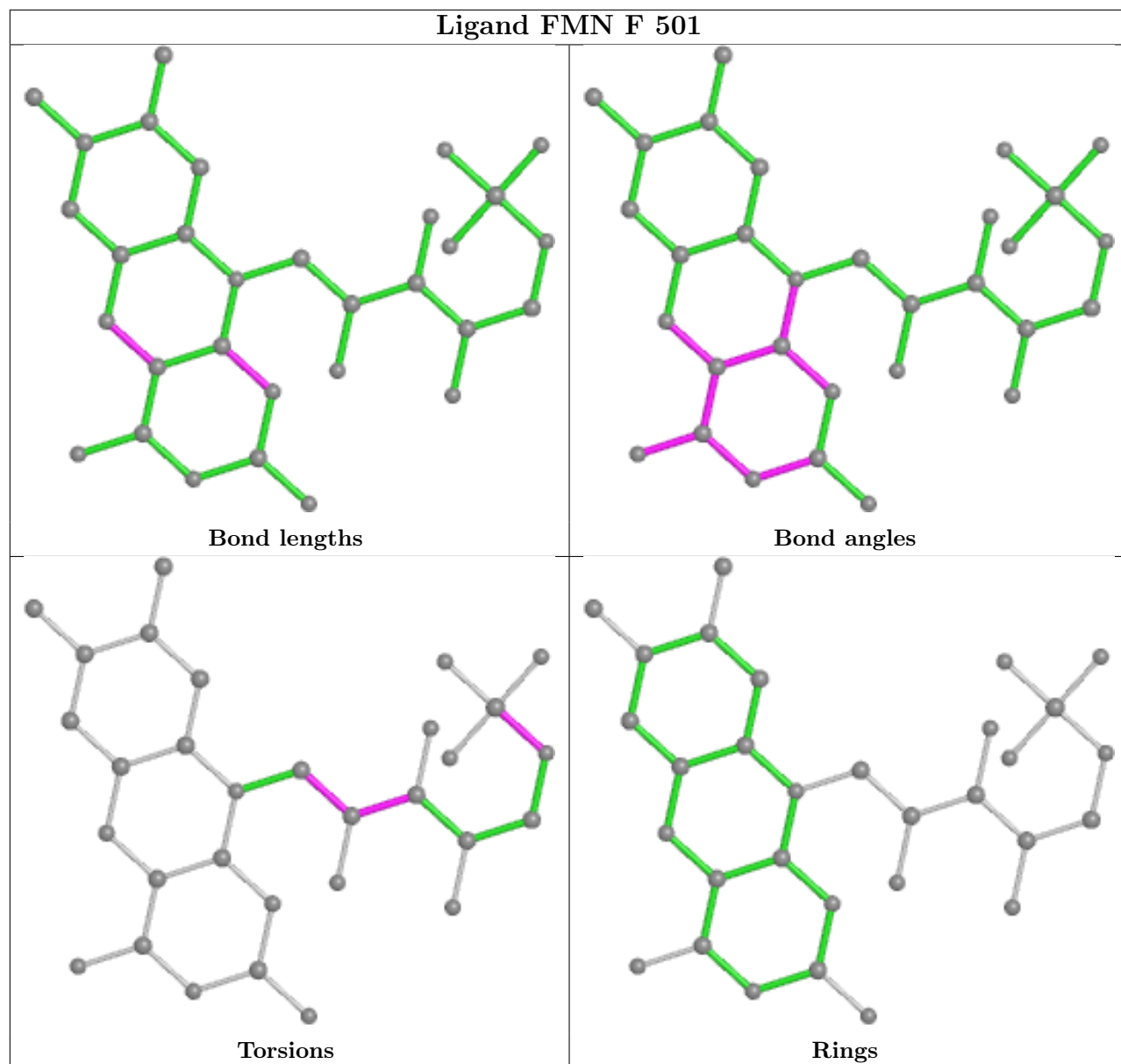
Mol	Chain	Res	Type	Atoms
17	D	501	MQ9	C26-C27-C28-C29
22	L	701	XP2	C36-O35-P34-O33
22	L	701	XP2	C51-C52-C53-C54
19	G	802	GTP	PB-O3B-PG-O2G
19	G	802	GTP	PB-O3A-PA-O2A
17	D	501	MQ9	C41-C42-C43-C44
20	F	501	FMN	O2'-C2'-C3'-O3'

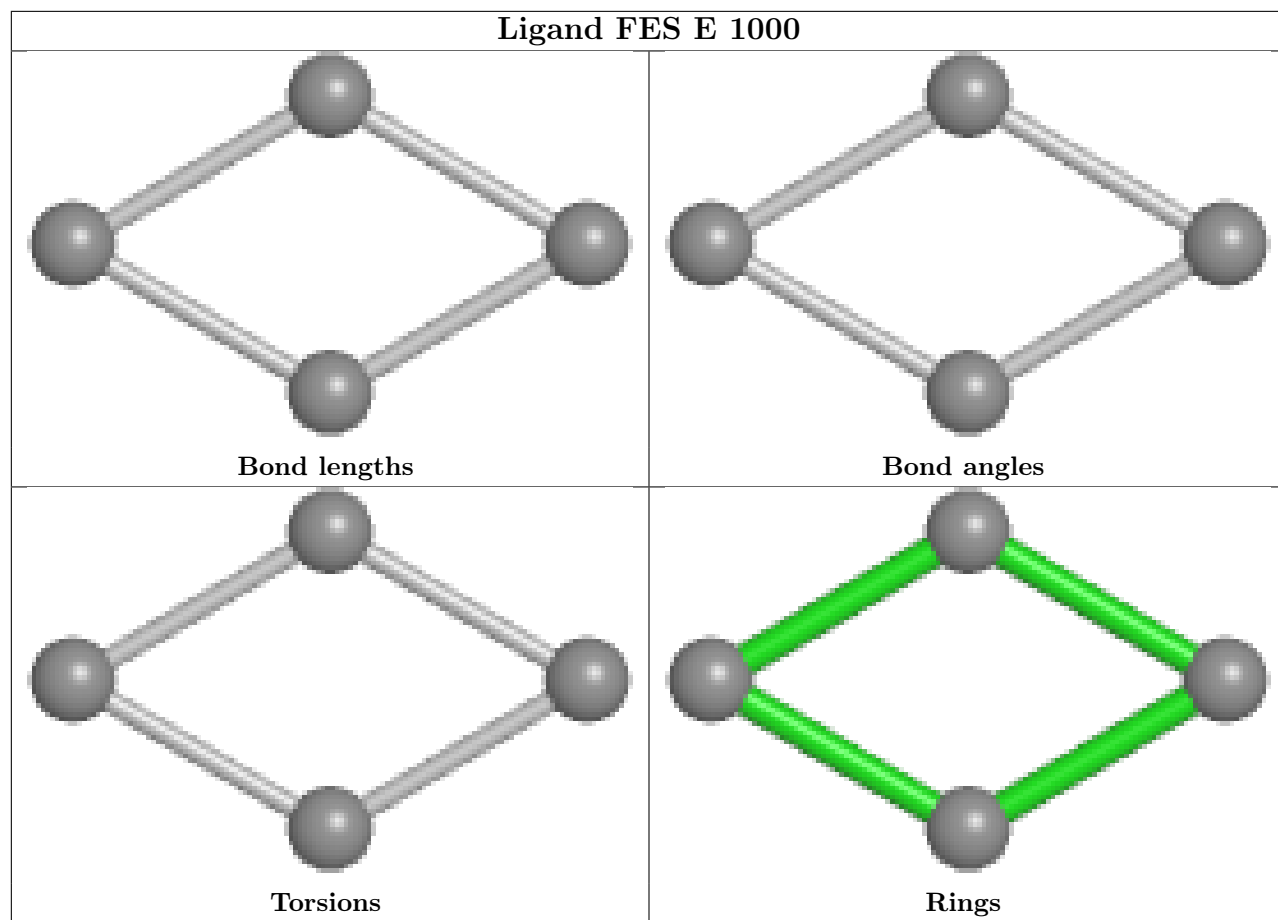
There are no ring outliers.

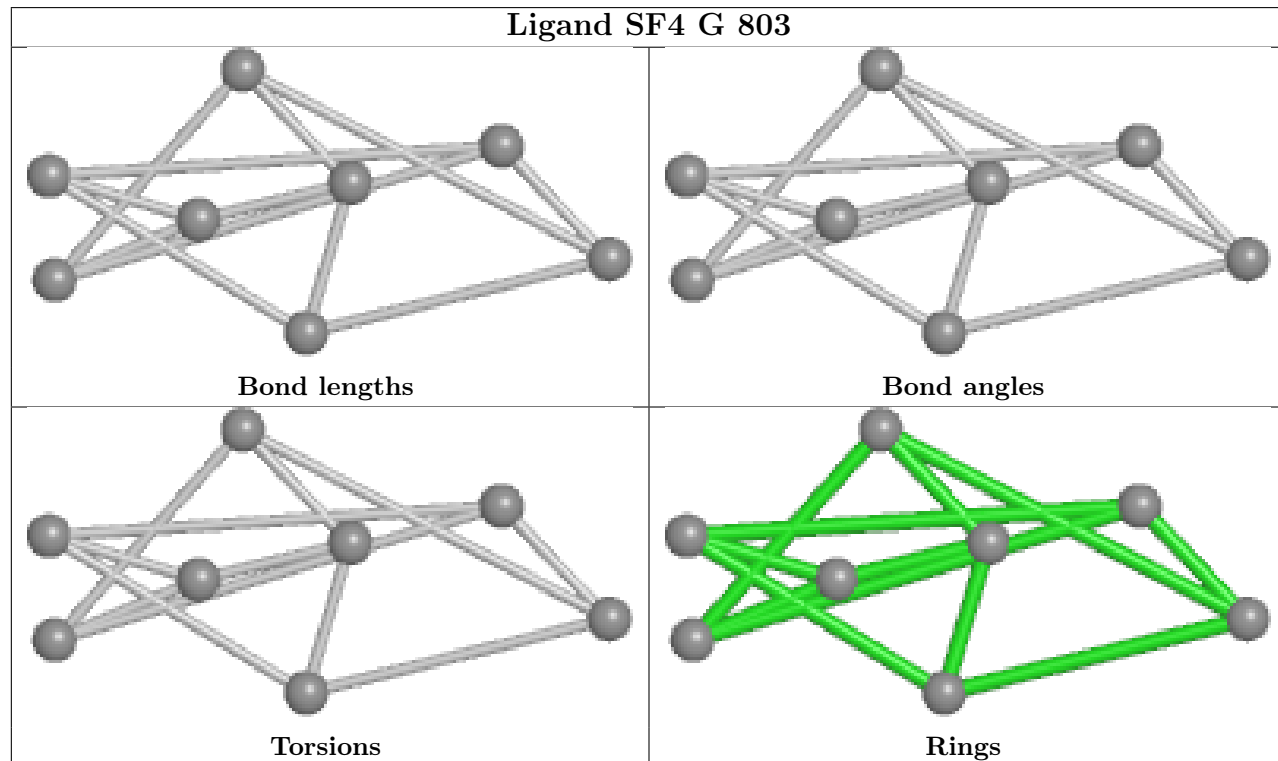
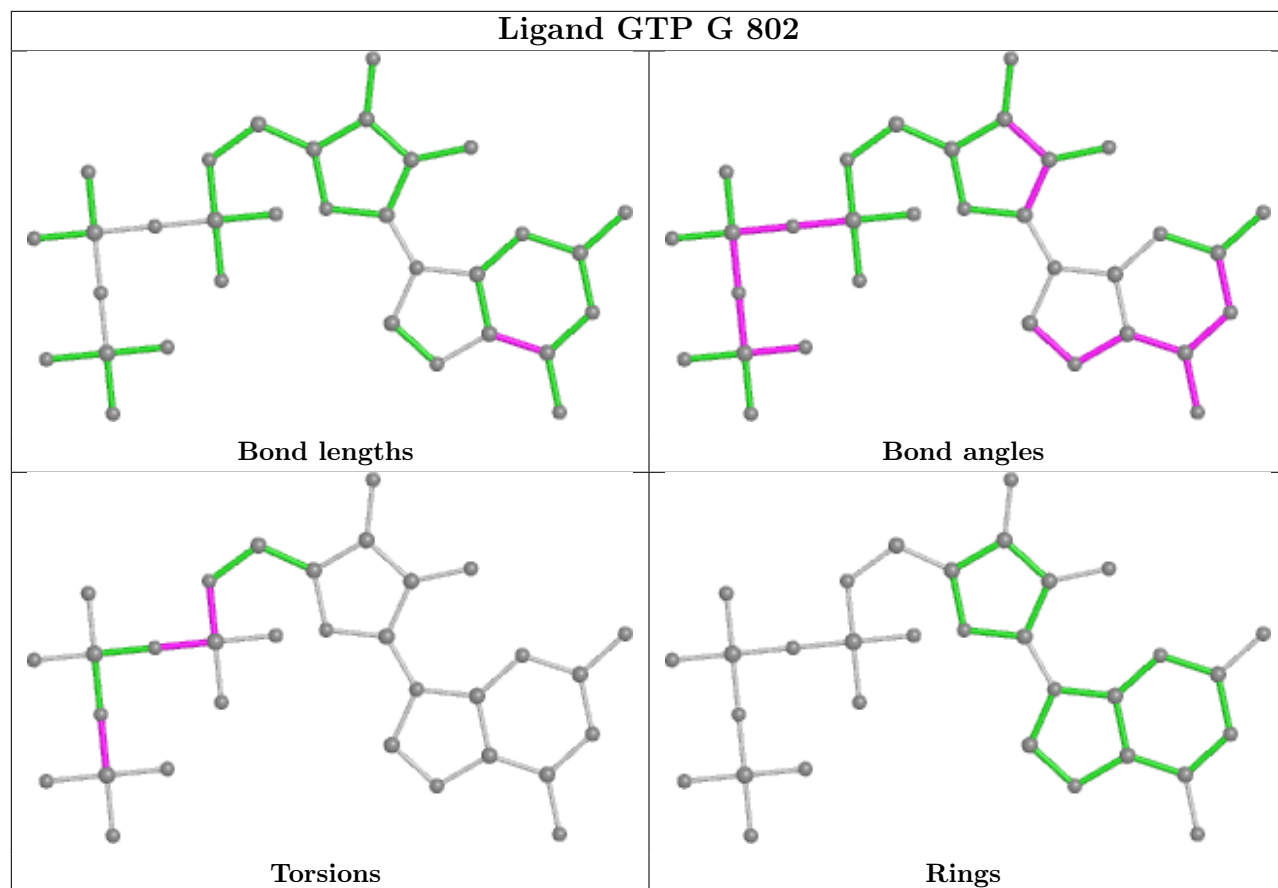
6 monomers are involved in 21 short contacts:

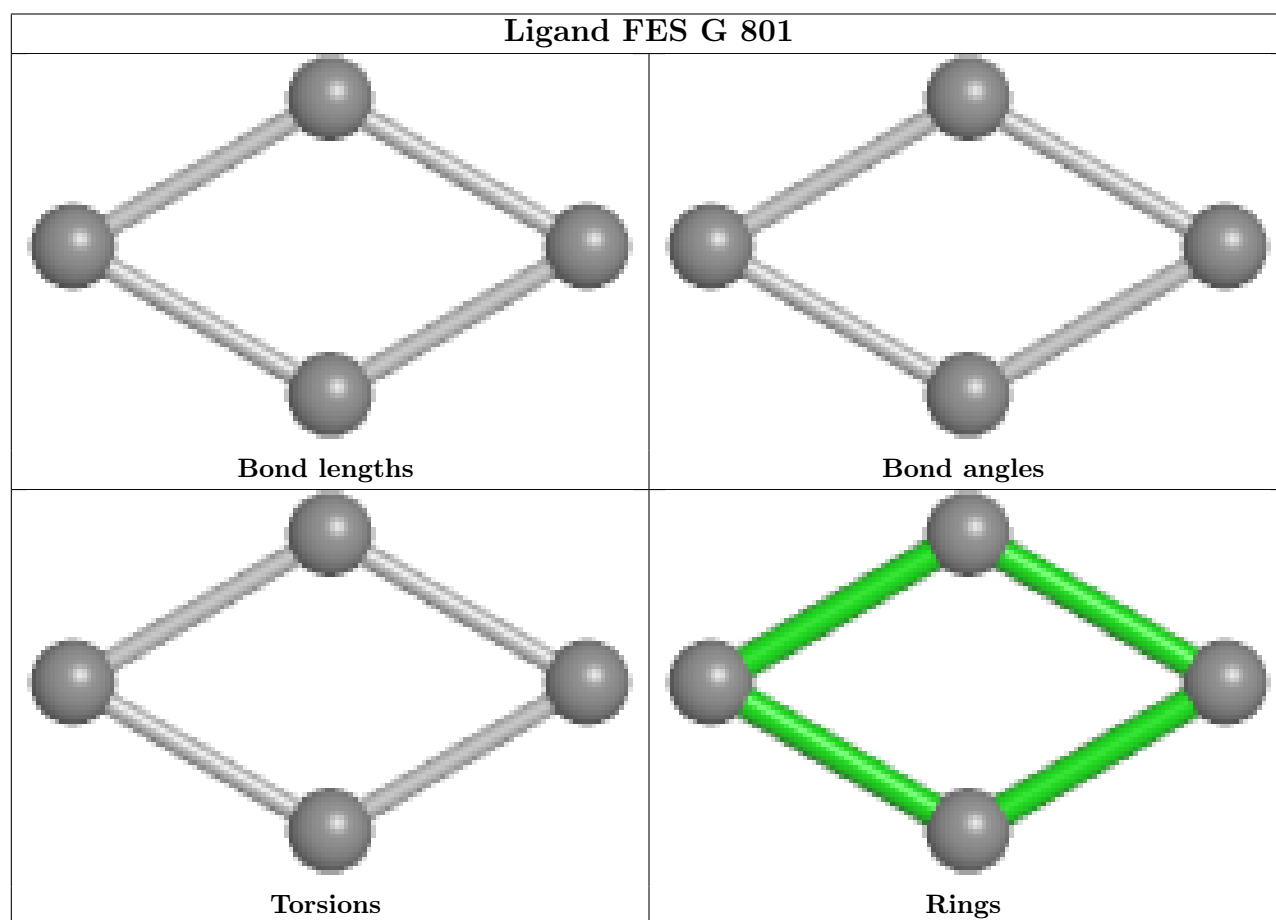
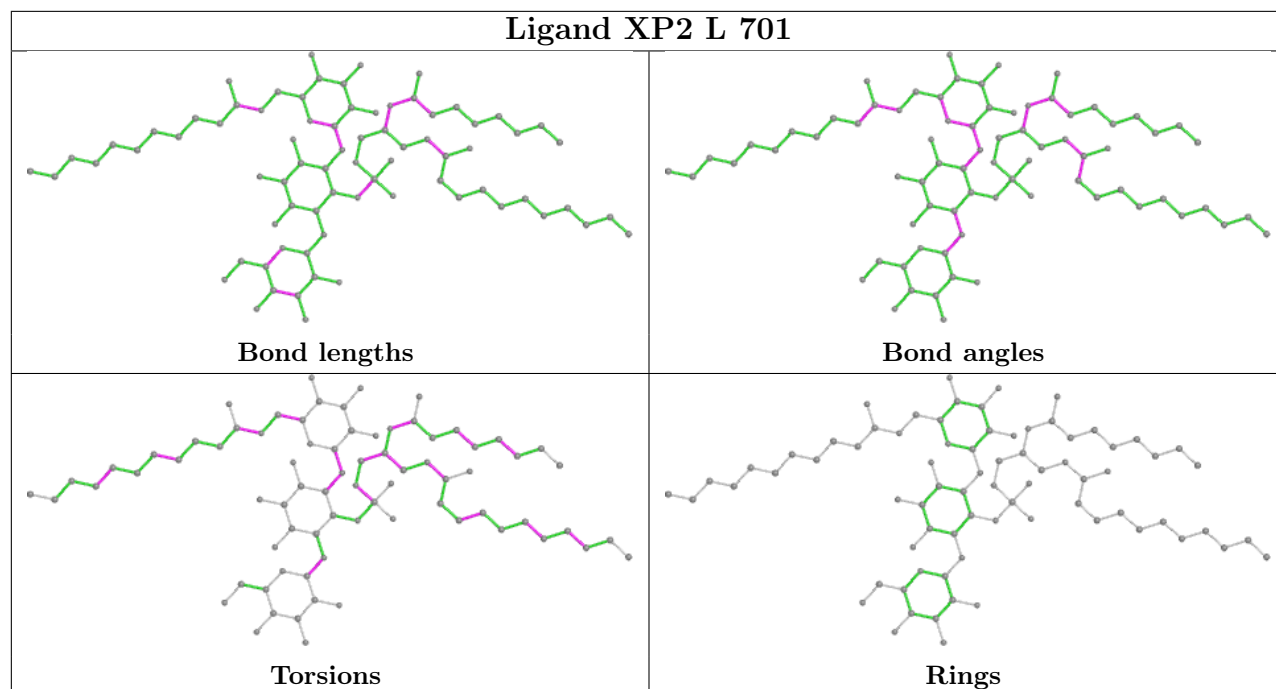
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	F	501	FMN	3	0
19	G	802	GTP	5	0
22	L	701	XP2	1	0
17	D	501	MQ9	9	0
16	I	201	SF4	2	0
16	F	503	SF4	1	0

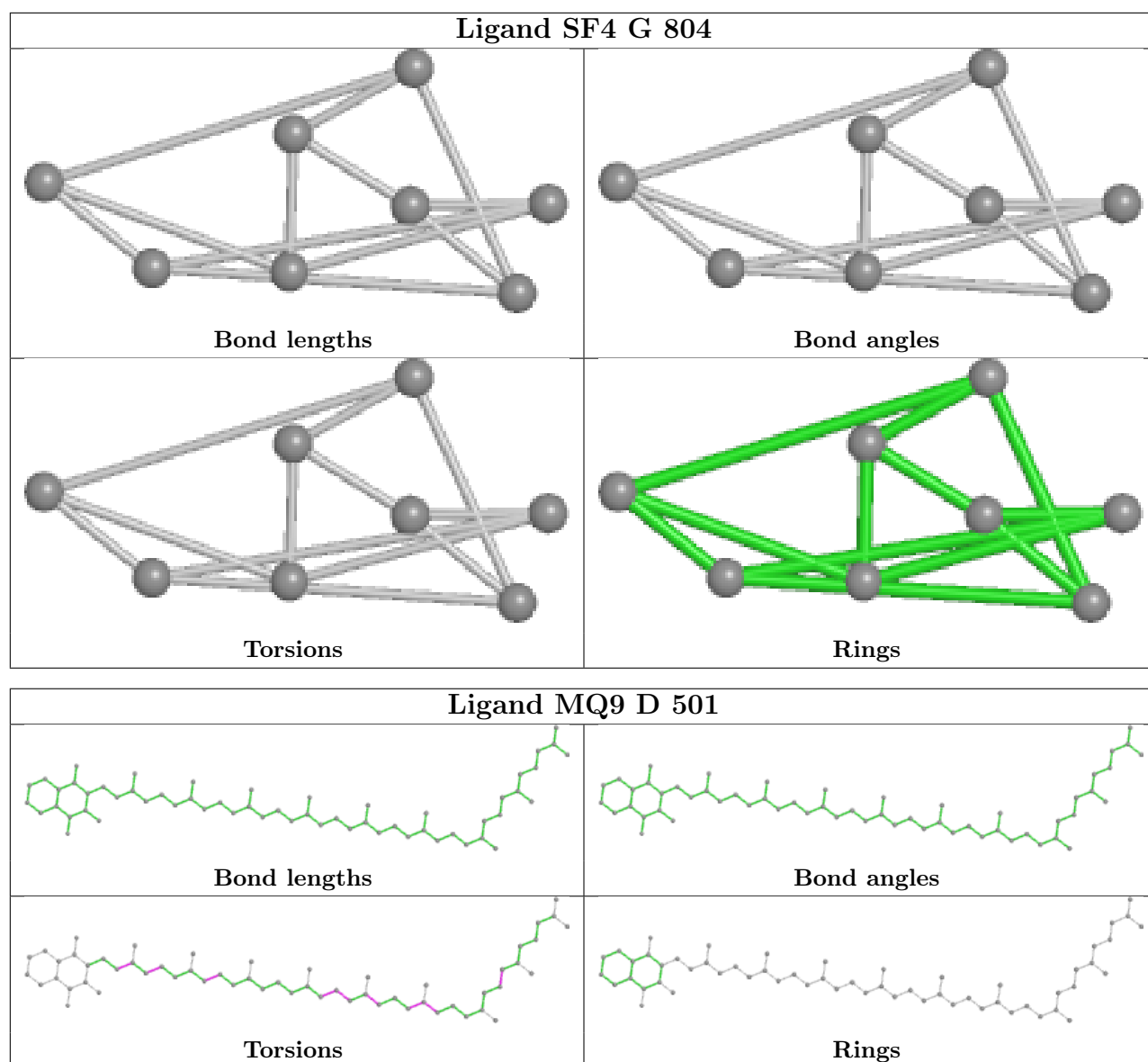
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

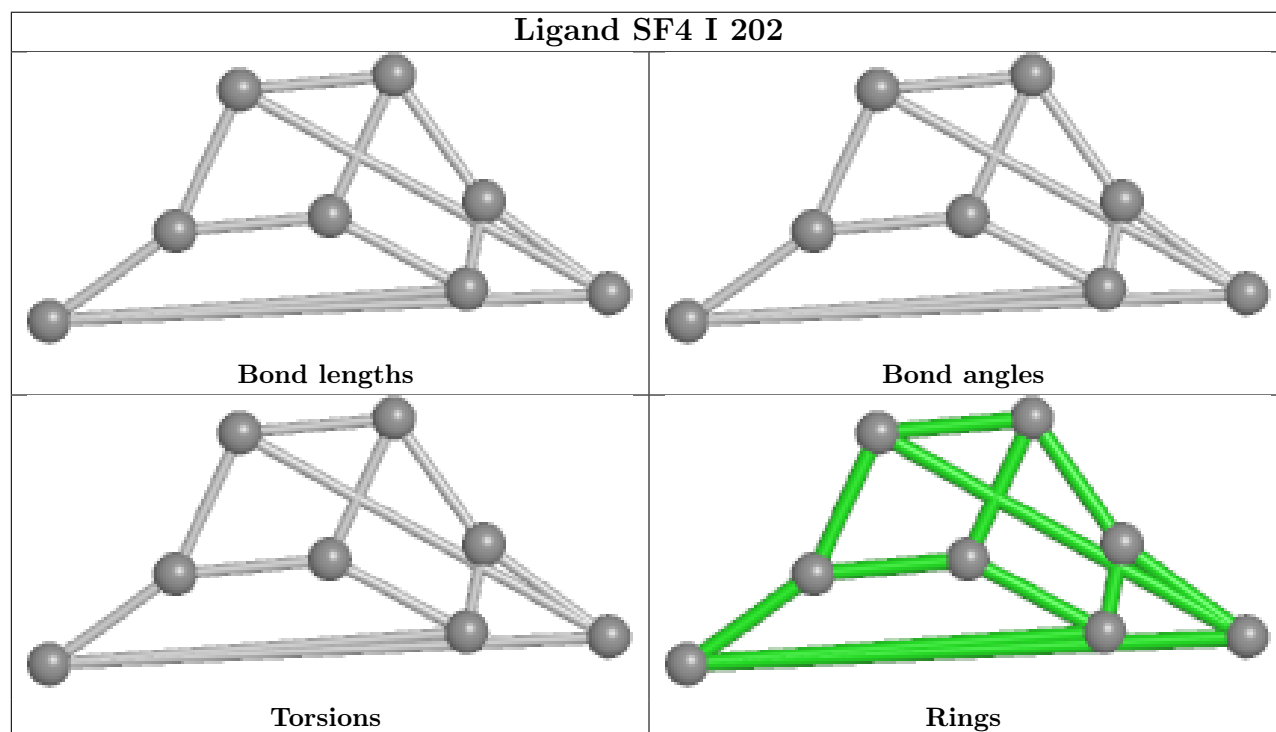
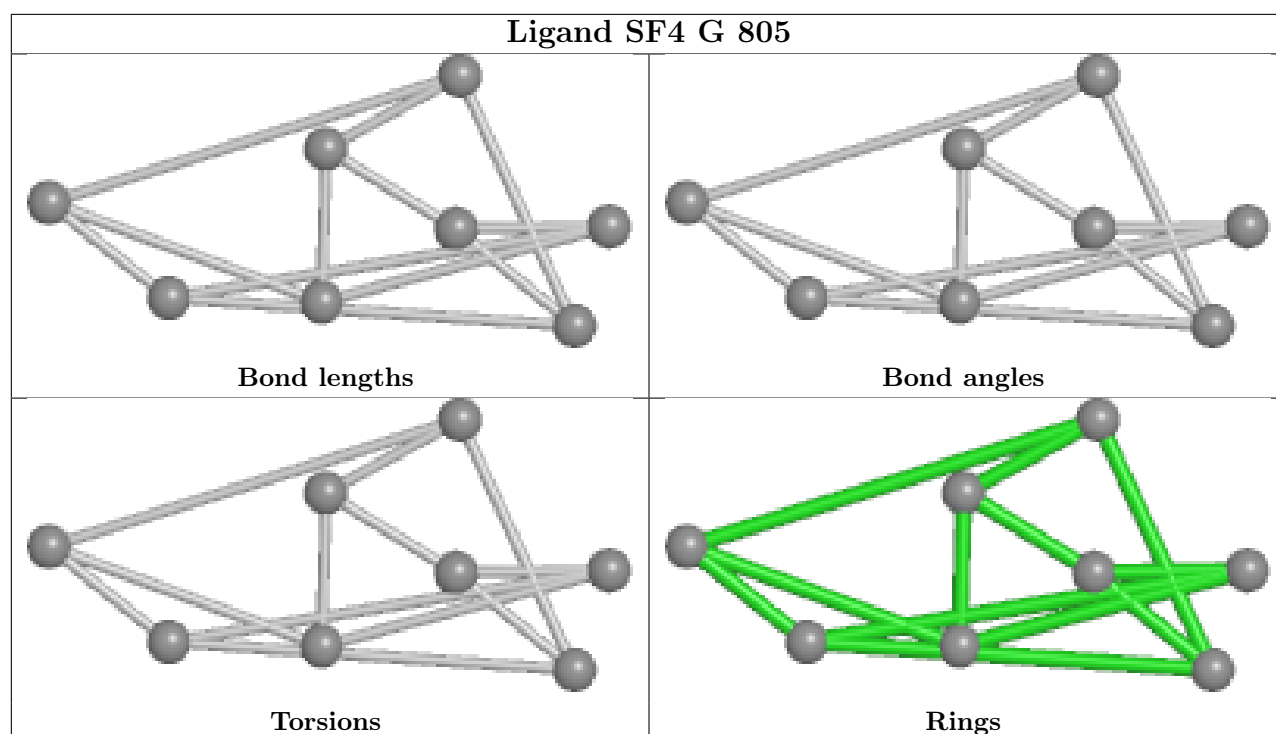


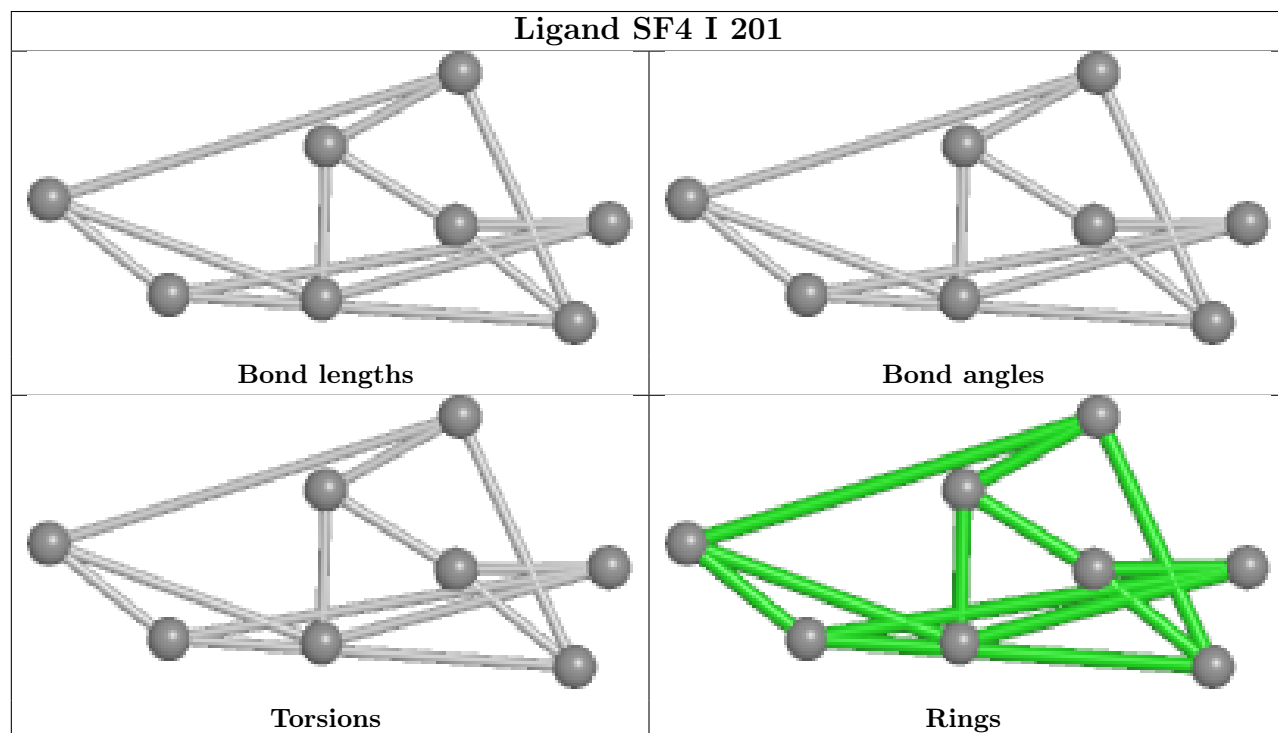
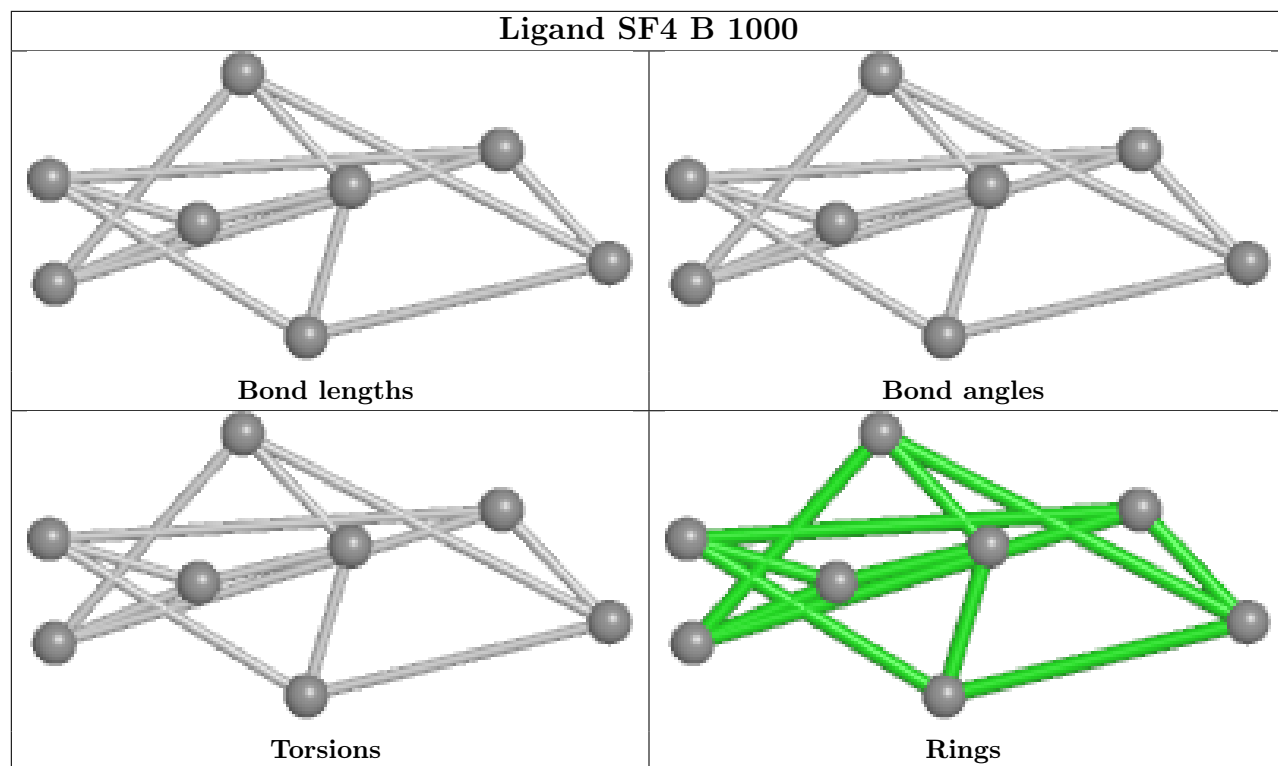


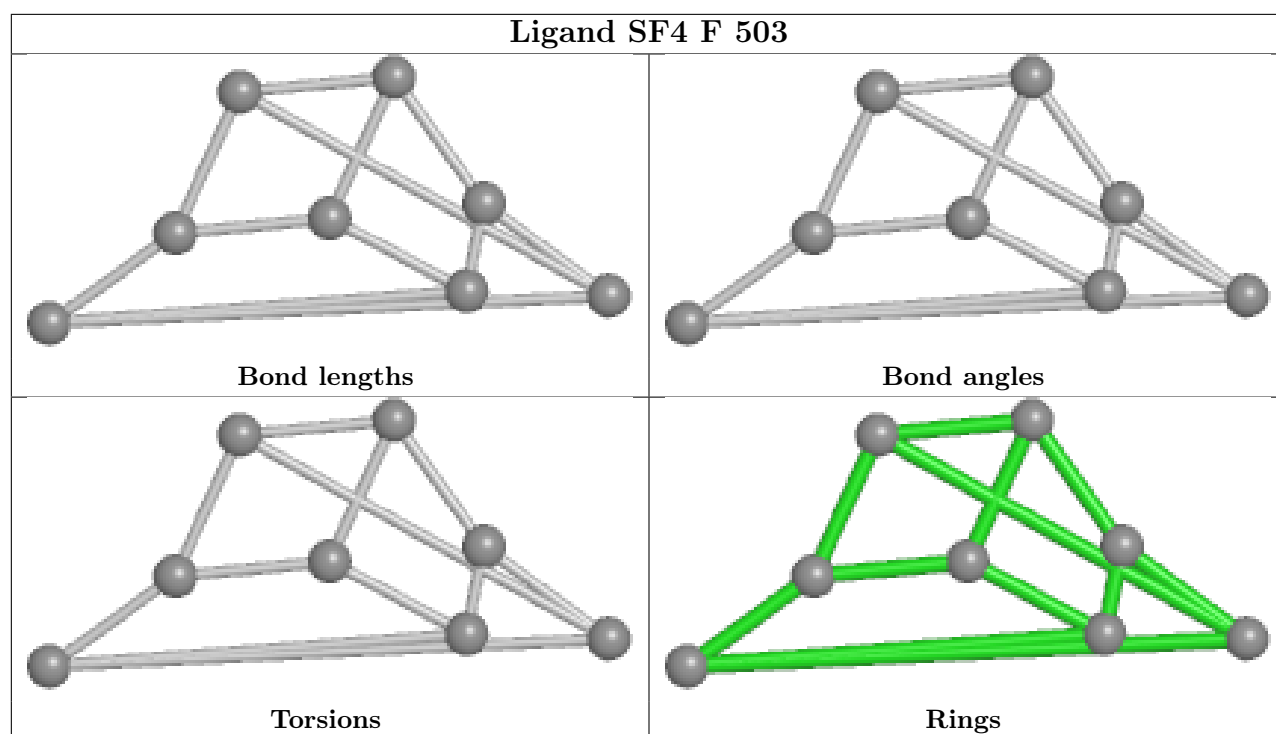












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

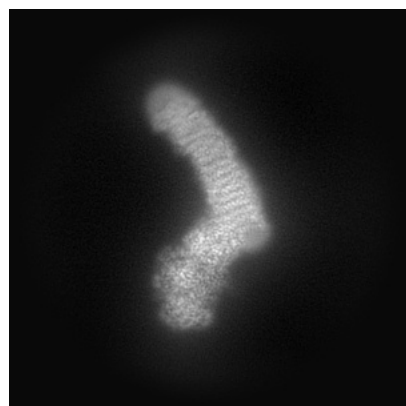
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27964. These allow visual inspection of the internal detail of the map and identification of artifacts.

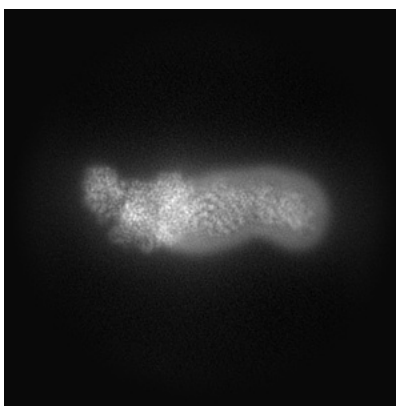
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

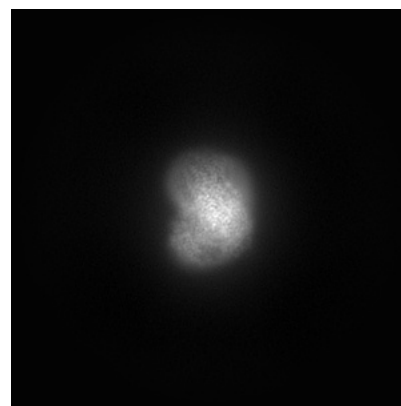
6.1.1 Primary map



X

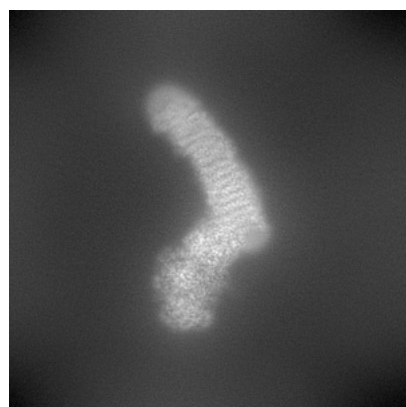


Y

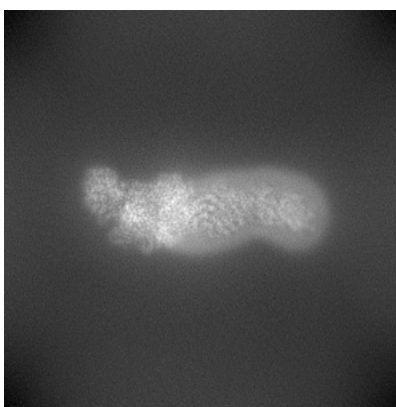


Z

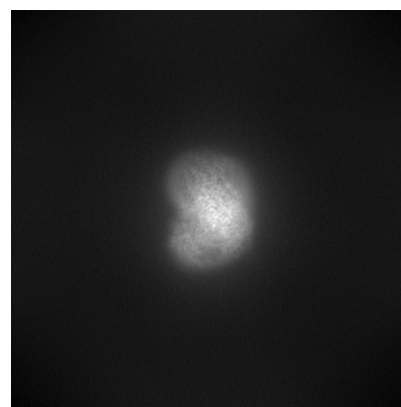
6.1.2 Raw map



X



Y

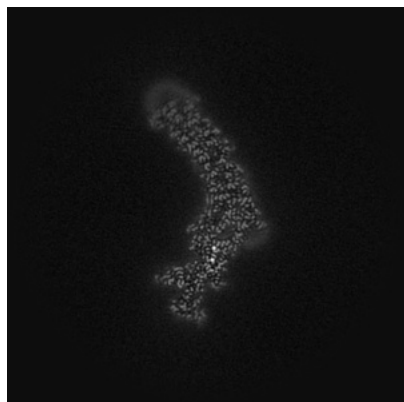


Z

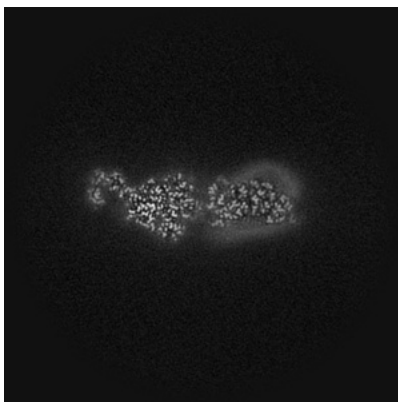
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

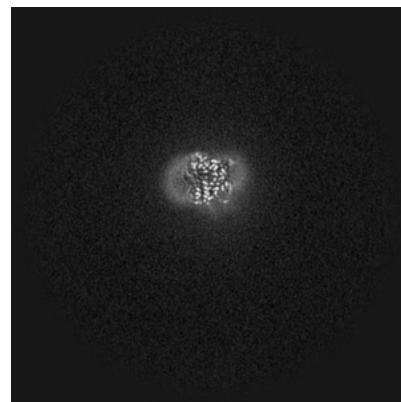
6.2.1 Primary map



X Index: 192

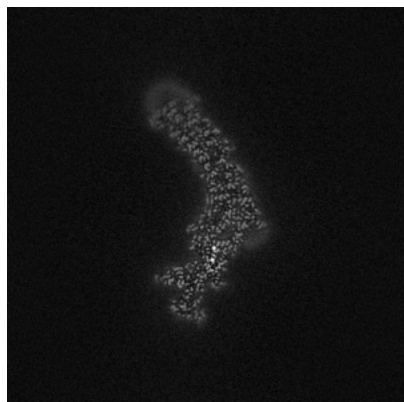


Y Index: 192

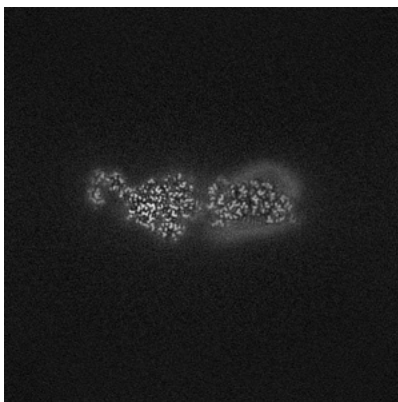


Z Index: 192

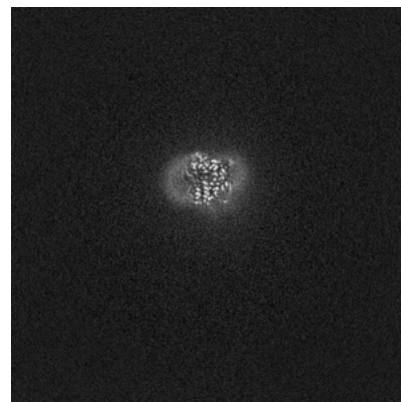
6.2.2 Raw map



X Index: 192



Y Index: 192

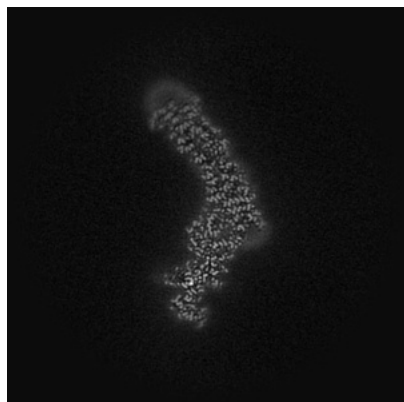


Z Index: 192

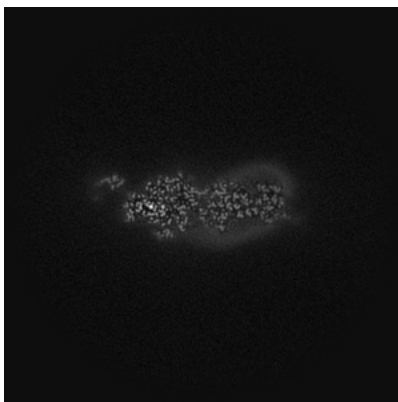
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

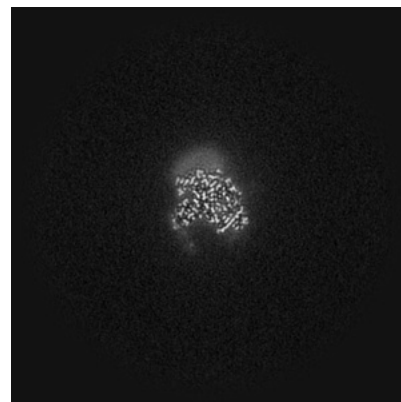
6.3.1 Primary map



X Index: 194

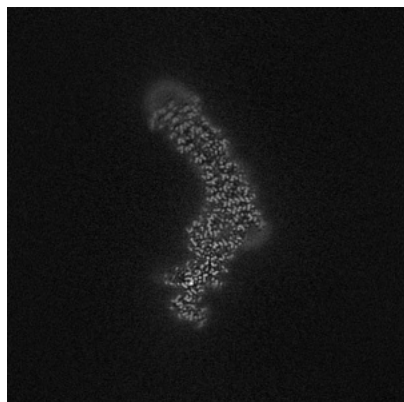


Y Index: 197

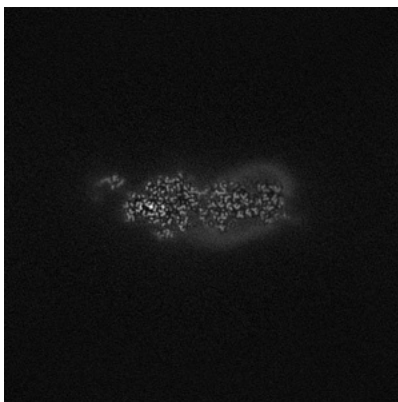


Z Index: 158

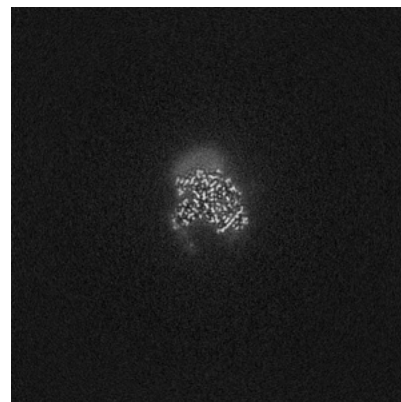
6.3.2 Raw map



X Index: 194



Y Index: 197

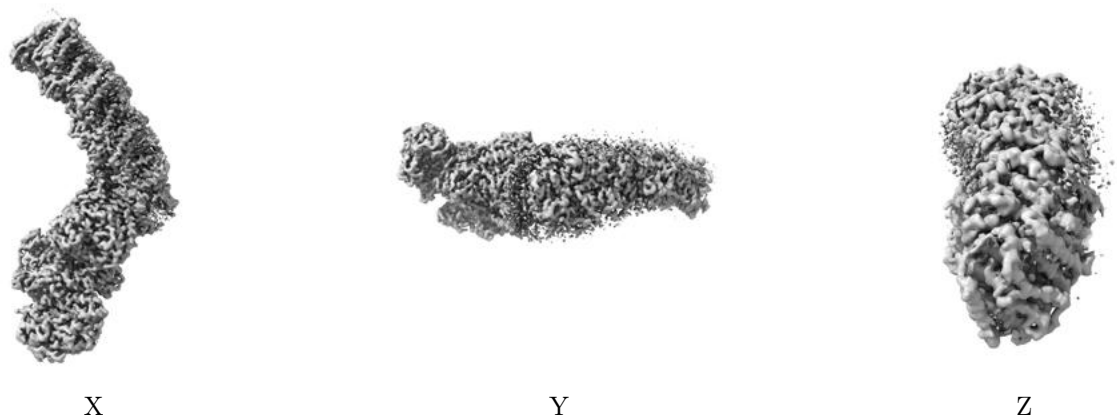


Z Index: 158

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

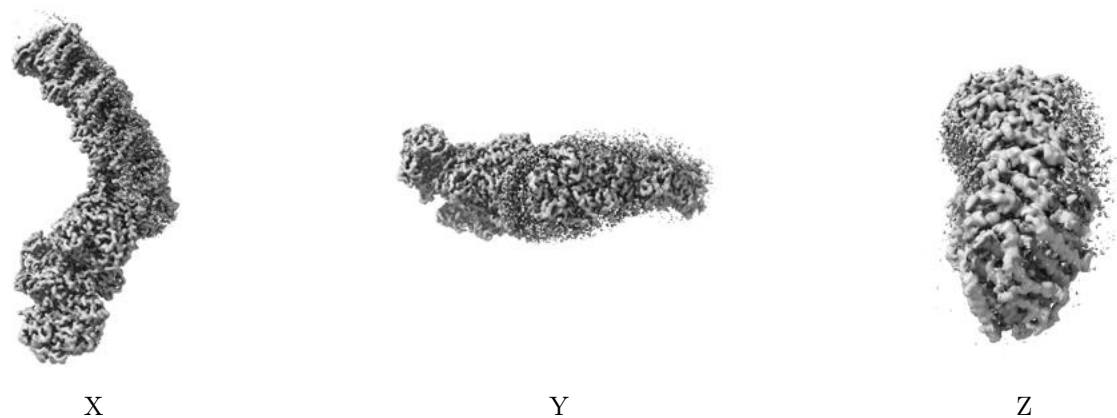
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. 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.

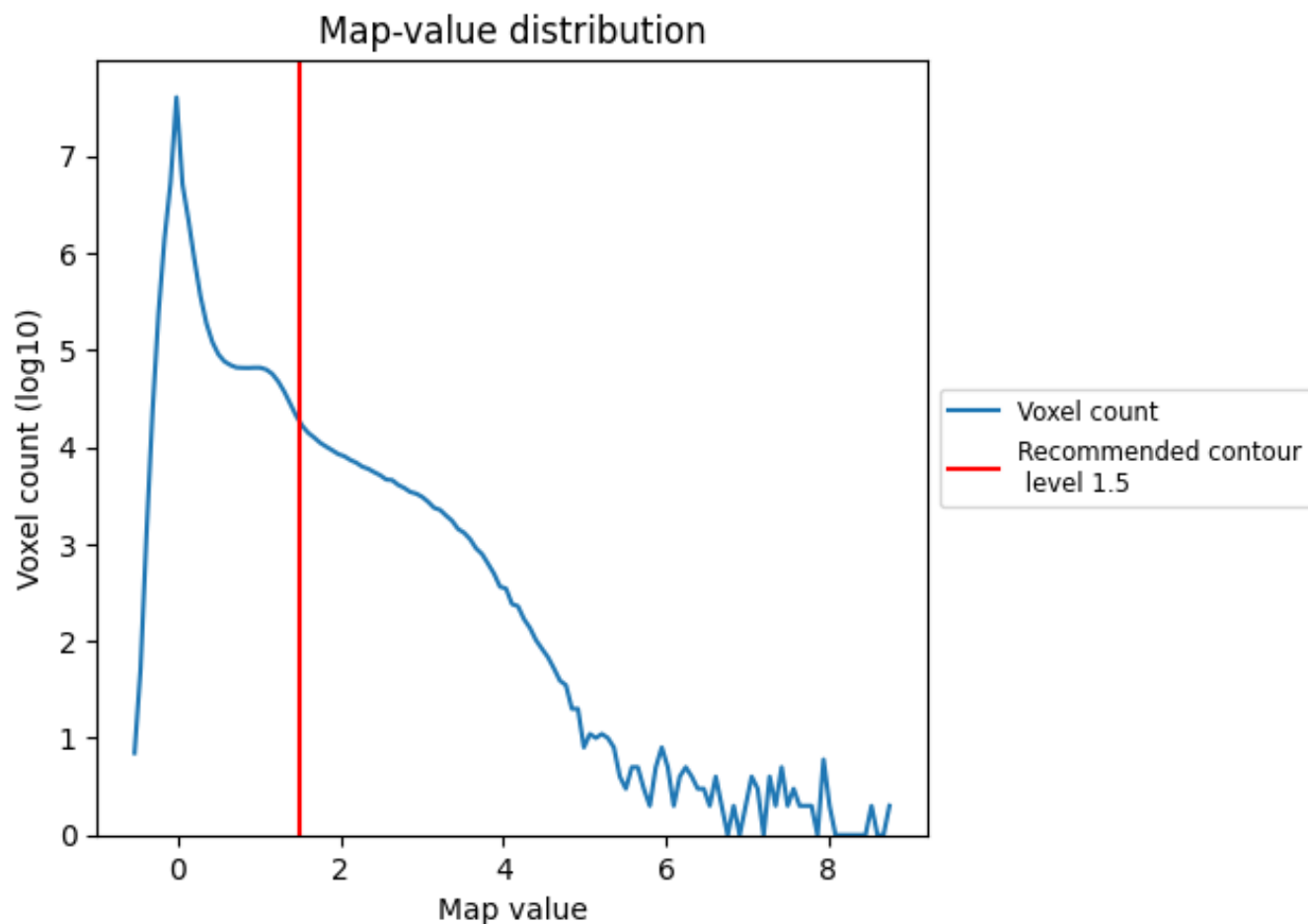
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

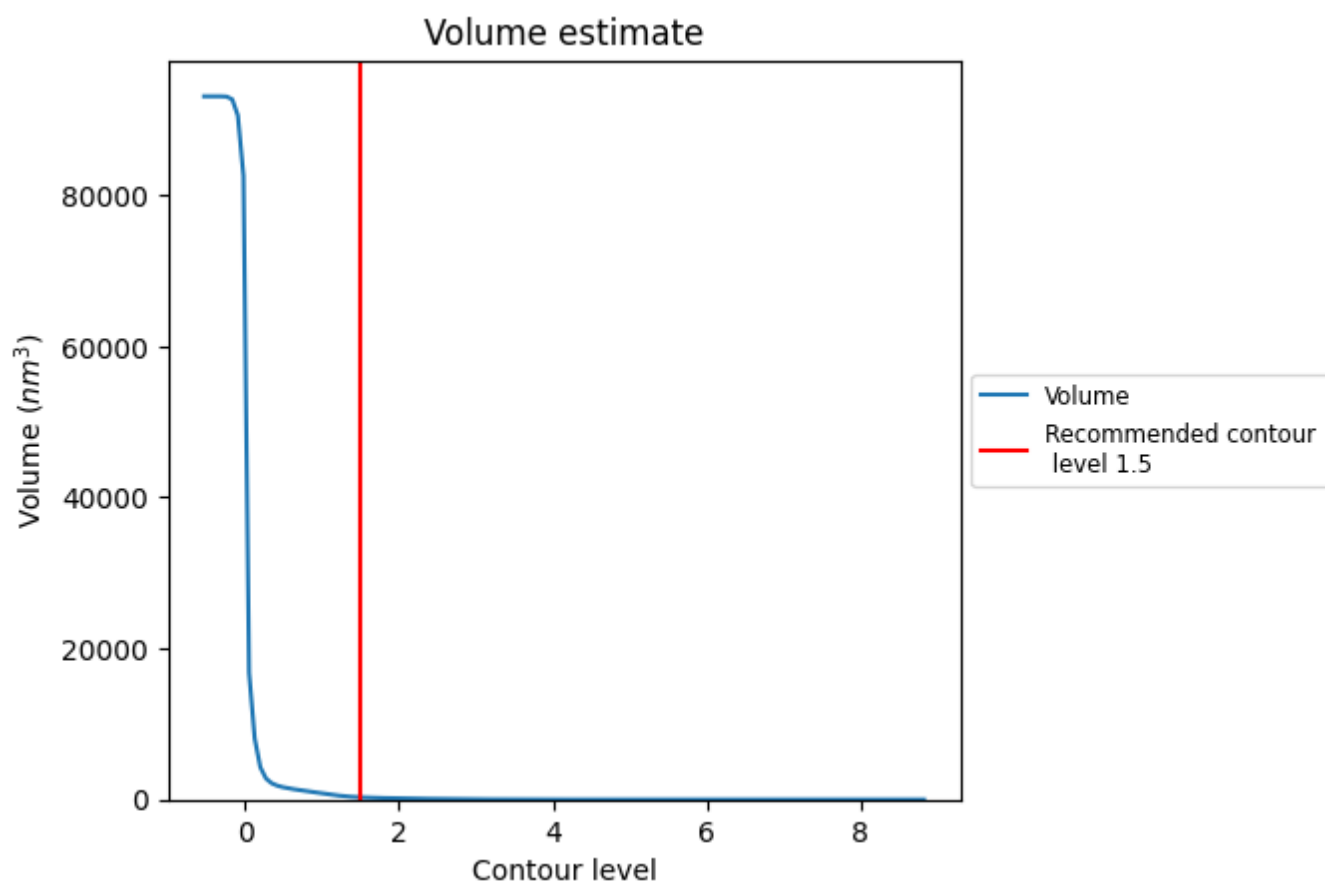
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

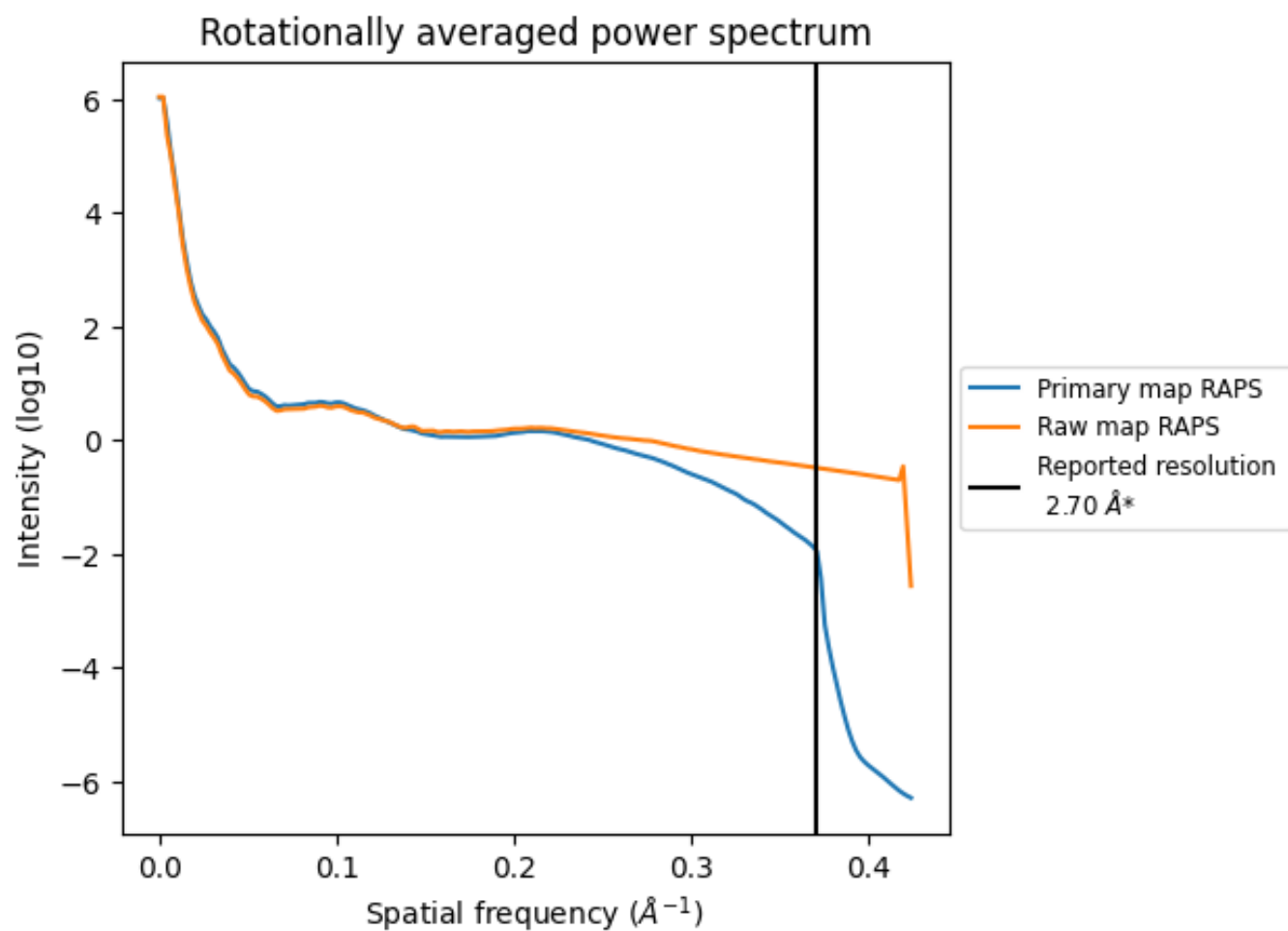
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm^3 ; this corresponds to an approximate mass of 269 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 ⓘ

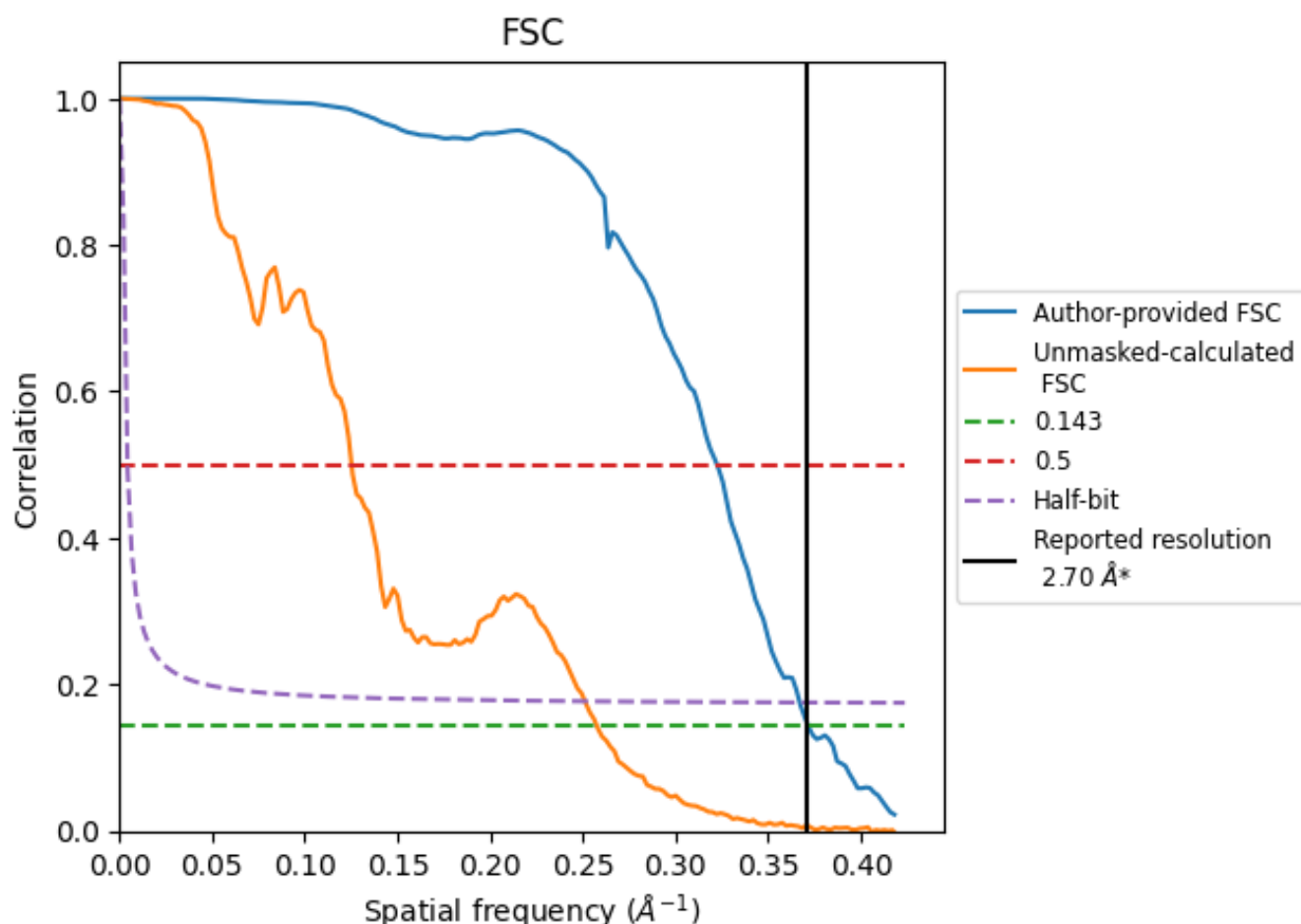


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

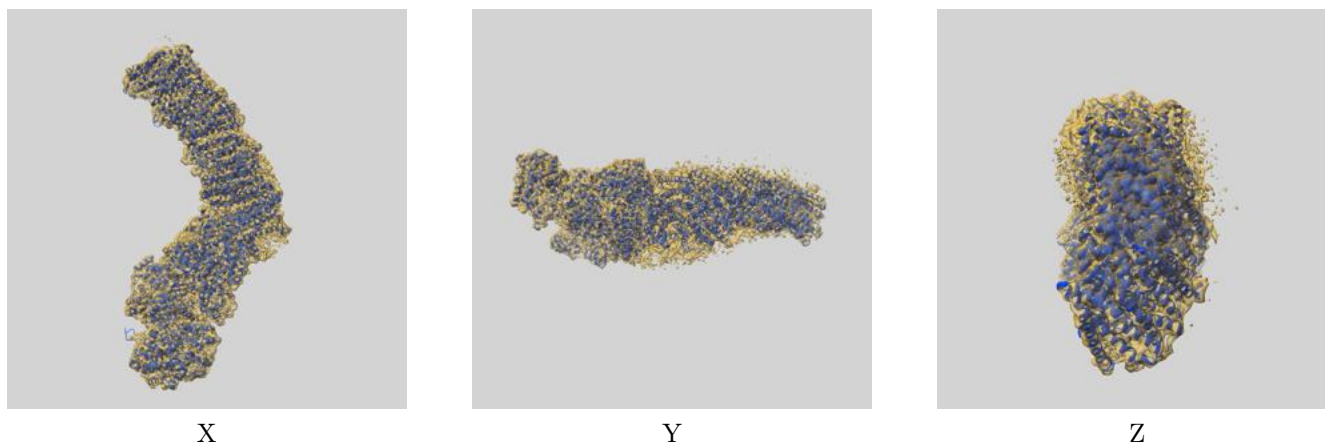
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.10	2.72
Unmasked-calculated*	3.88	7.99	3.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

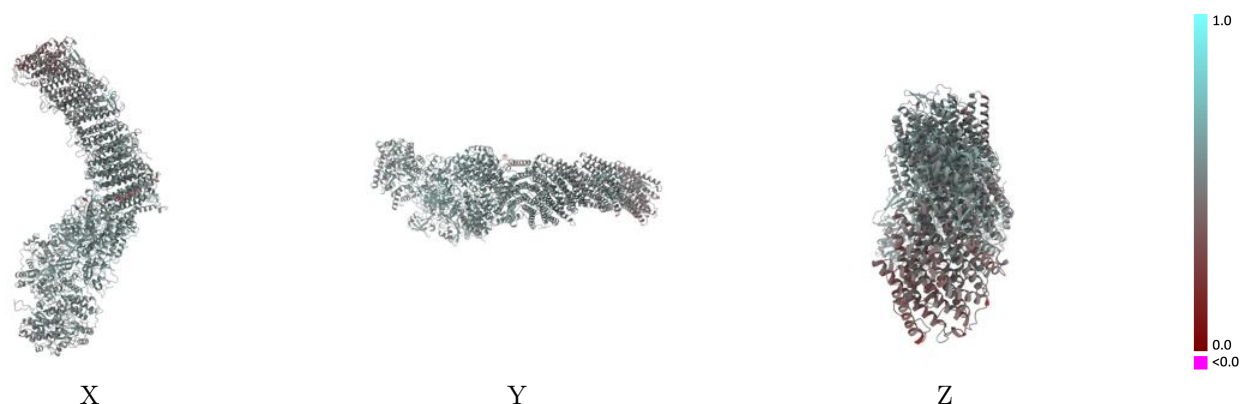
This section contains information regarding the fit between EMDB map EMD-27964 and PDB model 8E9H. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



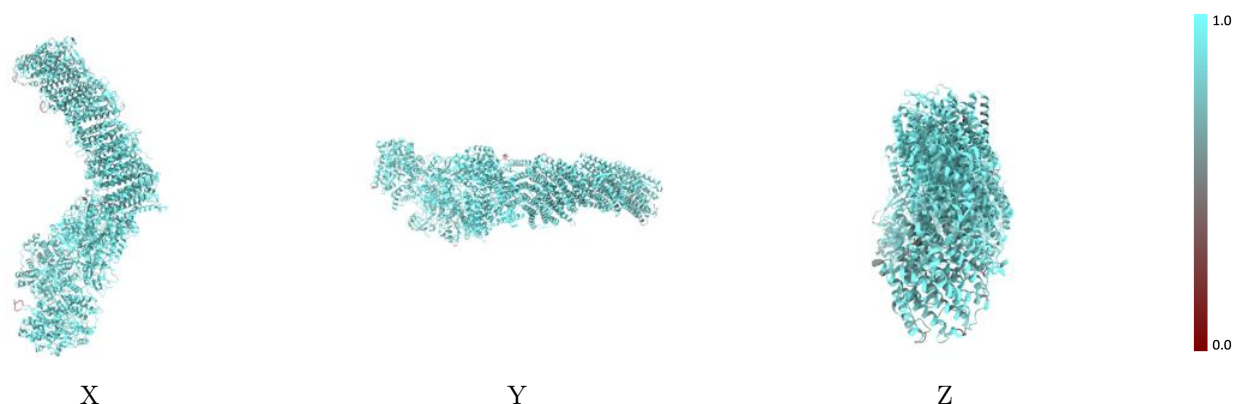
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



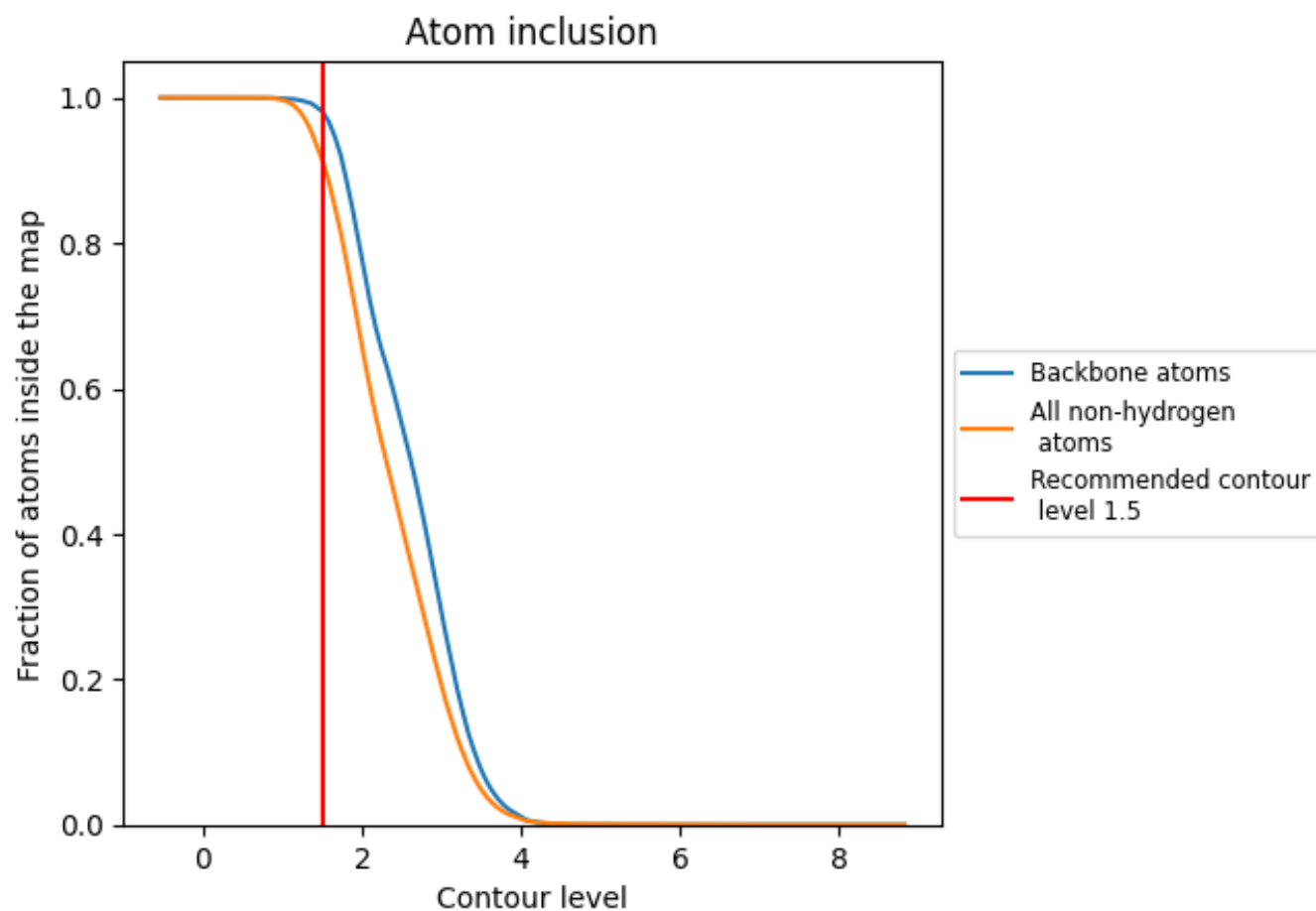
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9143	 0.5330
A	 0.9137	 0.5290
B	 0.9697	 0.5600
C	 0.9594	 0.5630
D	 0.9641	 0.5690
E	 0.9142	 0.5260
F	 0.8987	 0.5310
G	 0.9135	 0.5530
H	 0.9335	 0.5390
I	 0.9694	 0.5740
J	 0.9463	 0.5390
K	 0.9578	 0.5430
L	 0.8179	 0.4500
M	 0.8832	 0.5190
N	 0.9290	 0.5340
O	 0.9304	 0.5510

