



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:13 PM UTC

PDB ID : 8QYY / pdb_00008qyy
EMDB ID : EMD-18766
Title : Zorya anti-bacteriophage defense system ZorAB, ZorA delta_435-729, ZorA tail tip deletion.
Authors : Hu, H.; Taylor, N.M.I.
Deposited on : 2023-10-26
Resolution : 2.56 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

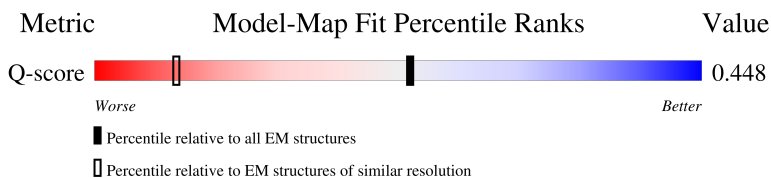
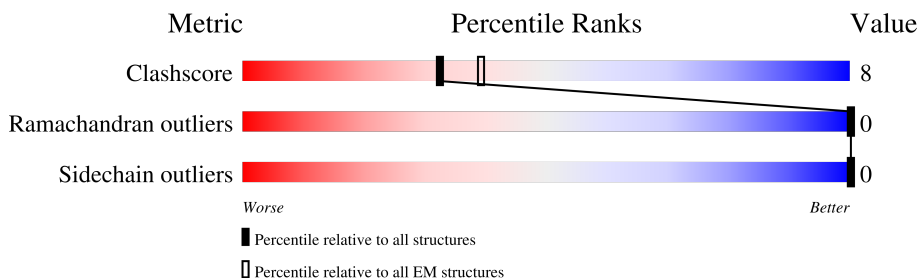
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.56 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7558 (2.06 - 3.06)

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	434	
1	B	434	
1	C	434	
1	D	434	

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Mol	Chain	Length	Quality of chain
1	E	434	
2	F	246	
2	G	246	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14829 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.

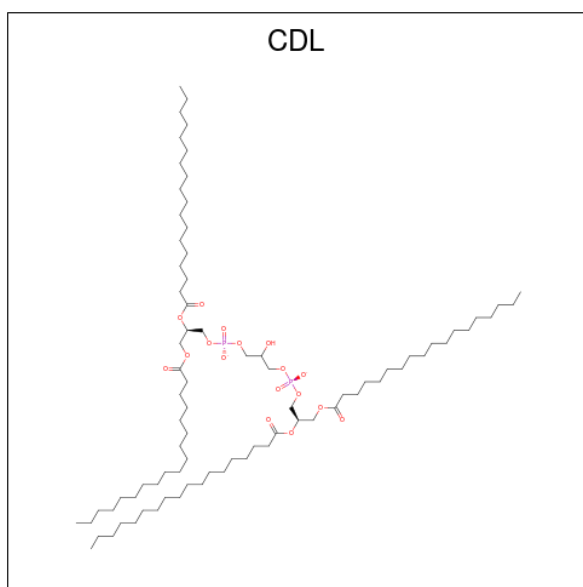
- Molecule 1 is a protein called Anti-phage defense ZorAB system ZorA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	245	Total	C	N	O	S	1	0
			1969	1284	317	364	4		
1	B	245	Total	C	N	O	S	0	0
			1960	1279	313	364	4		
1	C	245	Total	C	N	O	S	0	0
			1960	1279	313	364	4		
1	D	245	Total	C	N	O	S	0	0
			1960	1279	313	364	4		
1	E	245	Total	C	N	O	S	1	0
			1967	1284	315	364	4		

- Molecule 2 is a protein called Membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	246	Total	C	N	O	S	0	0
			1970	1241	353	364	12		
2	G	246	Total	C	N	O	S	0	0
			1970	1241	353	364	12		

- Molecule 3 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

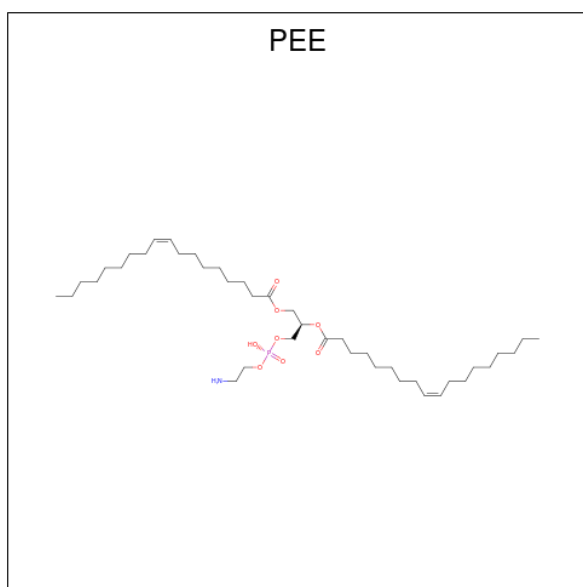


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			100	81	17	2	
3	B	1	Total	C	O	P	0
			100	81	17	2	
3	C	1	Total	C	O	P	0
			100	81	17	2	
3	D	1	Total	C	O	P	0
			100	81	17	2	
3	E	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	
4	E	1	Total	Ca	0
			1	1	

- Molecule 5 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	E	1	Total	C	N	O	P	0
			51	41	1	8	1	

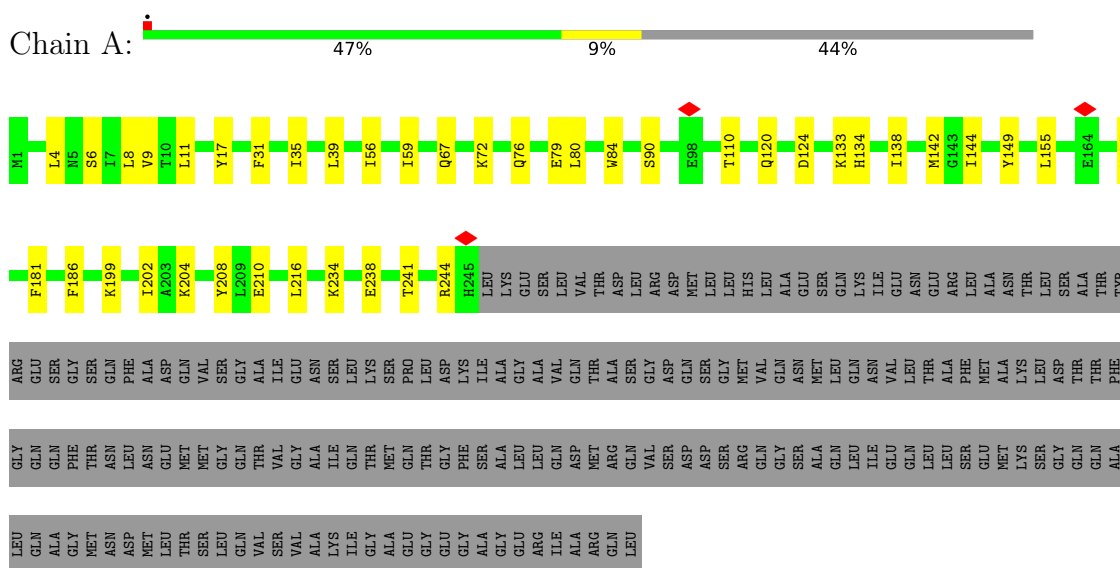
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	51	Total	O	0
			51	51	
6	B	65	Total	O	0
			65	65	
6	C	78	Total	O	0
			78	78	
6	D	60	Total	O	0
			60	60	
6	E	52	Total	O	0
			52	52	
6	F	4	Total	O	0
			4	4	
6	G	3	Total	O	0
			3	3	

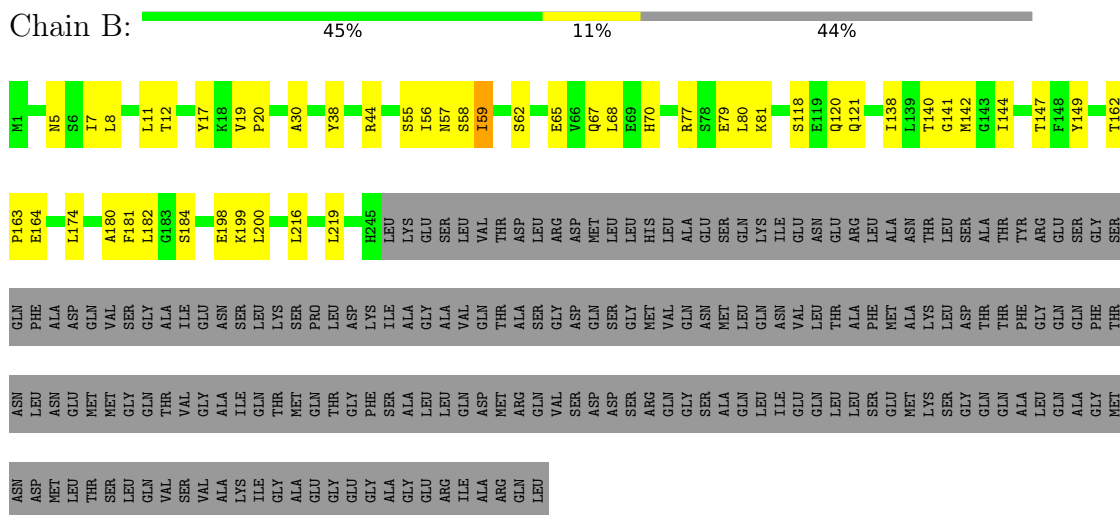
3 Residue-property plots

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.

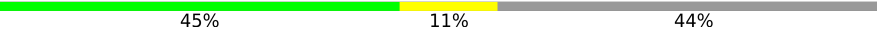
- Molecule 1: Anti-phage defense ZorAB system ZorA

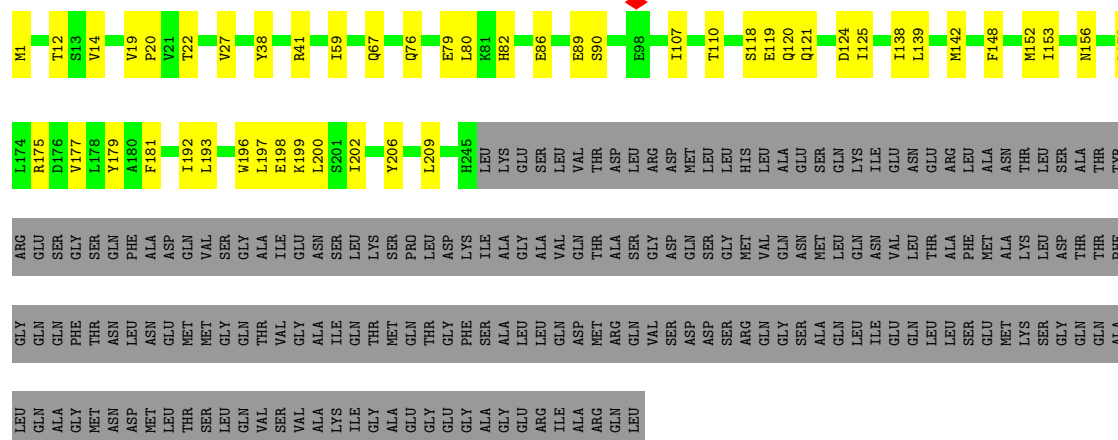


- Molecule 1: Anti-phage defense ZorAB system ZorA

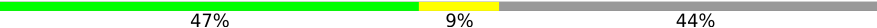


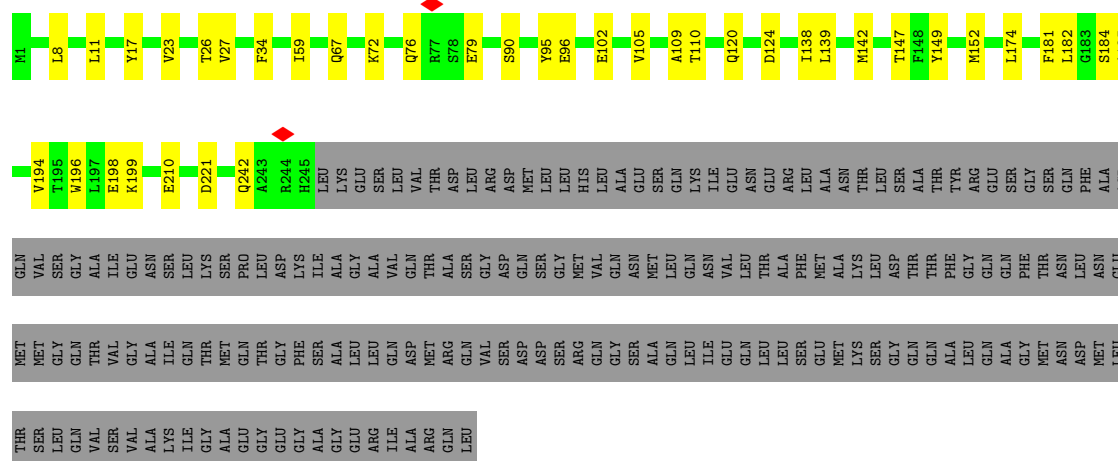
- Molecule 1: Anti-phage defense ZorAB system ZorA

Chain C:  45% 11% 44%



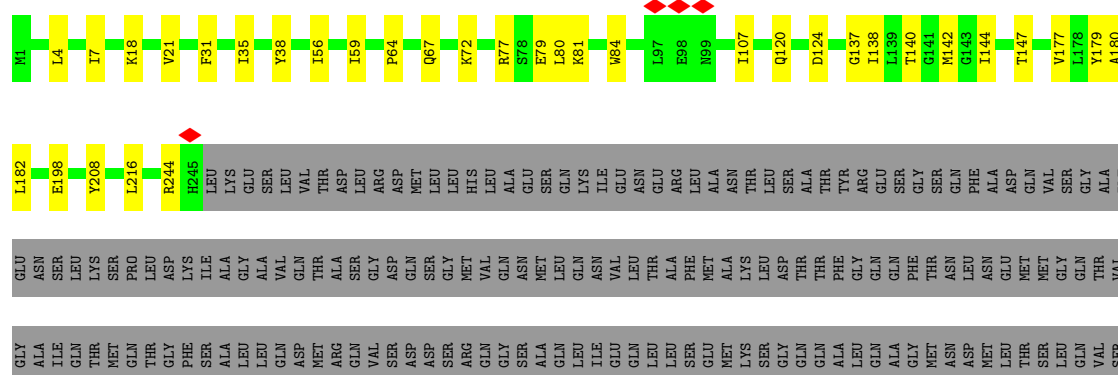
- Molecule 1: Anti-phage defense ZorAB system ZorA

Chain D:  47% 9% 44%



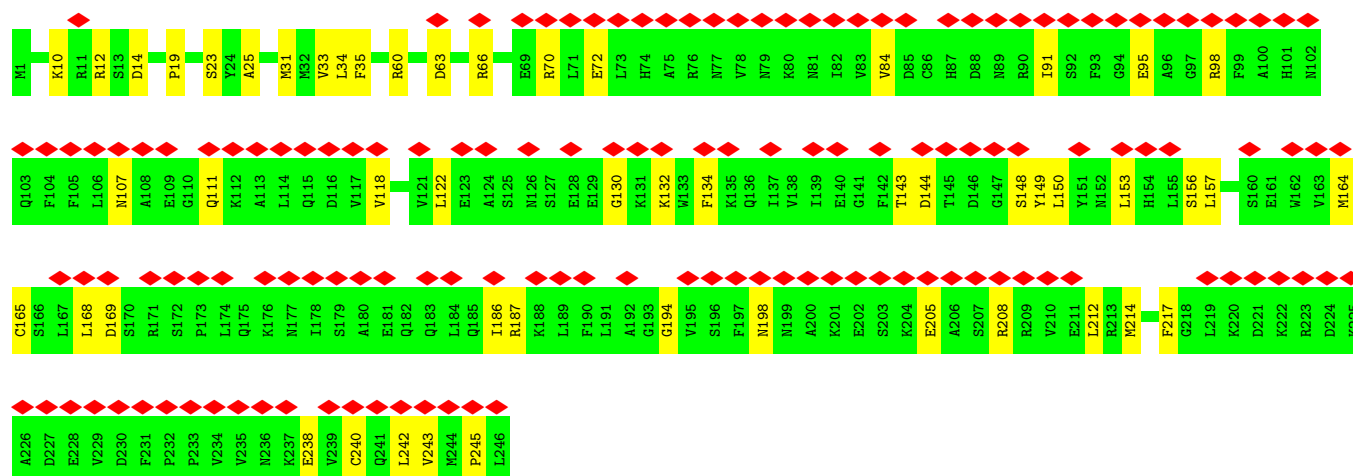
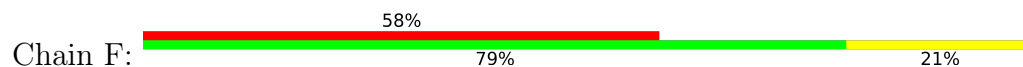
- Molecule 1: Anti-phage defense ZorAB system ZorA

Chain E:  49% 8% 44%

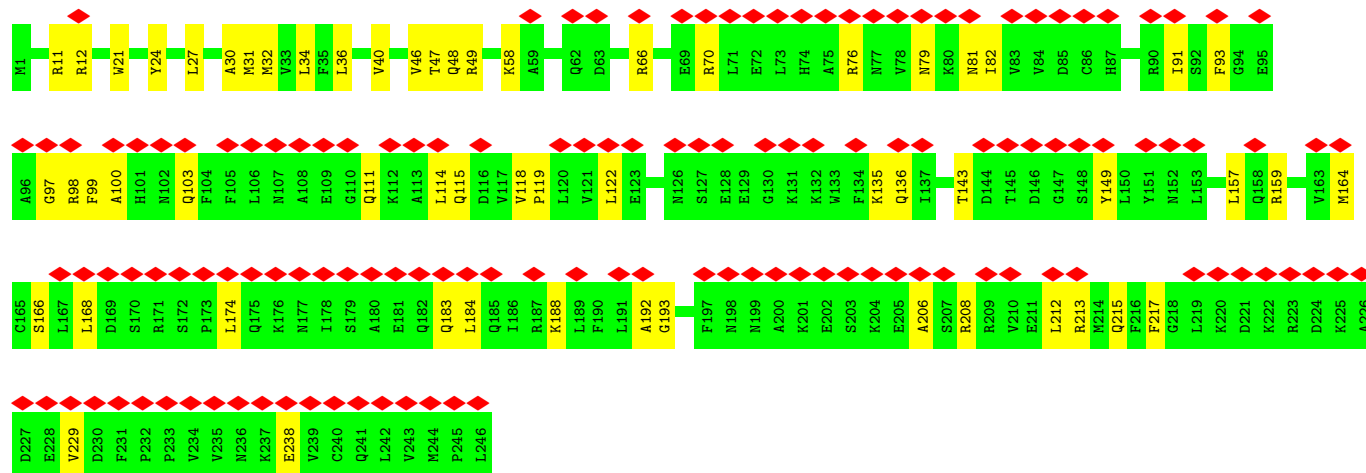
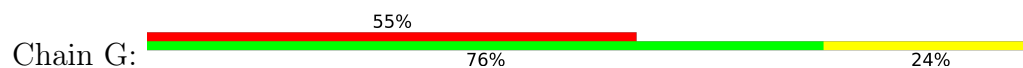


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• Molecule 2: Membrane protein



• Molecule 2: Membrane protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	3.594	Depositor
Minimum map value	-1.870	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	416.0, 416.0, 416.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CDL, PEE

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	0.19	0/2018	0.32	0/2736
1	B	0.34	1/2007 (0.0%)	0.45	2/2722 (0.1%)
1	C	0.18	0/2007	0.29	0/2722
1	D	0.18	0/2007	0.30	0/2722
1	E	0.18	0/2016	0.29	0/2733
2	F	0.13	0/2003	0.32	0/2690
2	G	0.13	0/2003	0.32	0/2690
All	All	0.20	1/14061 (0.0%)	0.33	2/19015 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	SER	C-O	5.02	1.29	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ASN	N-CA-C	-6.18	105.80	113.15
1	B	59	ILE	N-CA-C	-6.04	106.61	112.29

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	1969	0	1982	34	0
1	B	1960	0	1969	38	0
1	C	1960	0	1969	40	0
1	D	1960	0	1969	34	0
1	E	1967	0	1982	24	0
2	F	1970	0	1973	58	0
2	G	1970	0	1973	49	0
3	A	100	0	156	6	0
3	B	100	0	156	6	0
3	C	100	0	156	6	0
3	D	100	0	156	10	0
3	E	100	0	156	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	B	102	0	156	4	0
5	C	51	0	78	4	0
5	D	51	0	78	5	0
5	E	51	0	78	2	0
6	A	51	0	0	3	0
6	B	65	0	0	1	0
6	C	78	0	0	1	0
6	D	60	0	0	0	0
6	E	52	0	0	0	0
6	F	4	0	0	0	0
6	G	3	0	0	1	0
All	All	14829	0	14987	250	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 8.

All (250) 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)
2:F:95:GLU:OE2	2:F:98:ARG:HD2	1.59	1.00
2:F:95:GLU:CD	2:F:98:ARG:HE	1.69	0.99
2:F:95:GLU:OE2	2:F:98:ARG:CD	2.25	0.85
2:G:111:GLN:HE22	2:G:166:SER:HB2	1.41	0.84
2:F:98:ARG:NH1	2:F:205:GLU:CB	2.41	0.83
1:C:20:PRO:HG3	1:C:179:TYR:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:GLU:CD	2:F:98:ARG:NE	2.44	0.76
2:F:95:GLU:OE1	2:F:98:ARG:NE	2.15	0.74
2:F:98:ARG:NH1	2:F:205:GLU:HB3	2.02	0.74
1:D:147:THR:OG1	1:D:184:SER:HB2	1.87	0.73
2:G:76:ARG:NH2	2:G:82:ILE:O	2.21	0.73
1:A:72:LYS:HG2	1:A:84:TRP:HE1	1.53	0.72
1:B:59:ILE:HG21	1:B:70:HIS:CD2	2.26	0.71
1:E:79:GLU:HG3	1:E:80:LEU:HD12	1.73	0.70
1:A:181:PHE:HE2	2:F:33:VAL:HG21	1.55	0.70
2:F:98:ARG:NH1	2:F:205:GLU:C	2.49	0.70
1:E:72:LYS:HG2	1:E:84:TRP:HE1	1.57	0.70
2:G:111:GLN:NE2	2:G:166:SER:HB2	2.07	0.68
2:F:95:GLU:OE2	2:F:98:ARG:NE	2.27	0.68
2:F:157:LEU:HD11	2:G:157:LEU:HG	1.74	0.68
2:F:98:ARG:HH11	2:F:205:GLU:C	2.02	0.68
1:E:177:VAL:HG11	2:F:34:LEU:HD11	1.76	0.67
3:E:501:CDL:H572	3:E:501:CDL:H442	1.75	0.67
1:C:12:THR:HG21	1:C:156:ASN:HB3	1.78	0.66
1:D:26:THR:HG21	5:D:502:PEE:H76	1.77	0.66
2:F:165:CYS:O	2:F:169:ASP:N	2.29	0.65
1:B:44:ARG:NH1	6:B:603:HOH:O	2.30	0.64
1:B:120:GLN:NE2	1:C:119:GLU:OE2	2.30	0.64
1:E:120:GLN:HA	1:E:124:ASP:HB2	1.77	0.64
3:A:501:CDL:H631	3:A:501:CDL:H802	1.80	0.64
1:D:174:LEU:HD21	2:G:40:VAL:HG21	1.80	0.64
1:E:144:ILE:HD11	2:F:23:SER:HA	1.78	0.64
2:F:98:ARG:NH1	2:F:205:GLU:HB2	2.11	0.64
2:G:100:ALA:H	2:G:103:GLN:HE21	1.44	0.63
1:B:11:LEU:HB3	1:B:149:TYR:HE1	1.65	0.62
1:D:72:LYS:O	1:D:76:GLN:HB3	2.00	0.62
1:D:138:ILE:HG22	1:D:142:MET:HE3	1.82	0.61
2:G:46:VAL:HG23	2:G:47:THR:HG23	1.83	0.60
1:A:59:ILE:O	1:A:67:GLN:NE2	2.31	0.60
1:B:5:ASN:OD1	1:C:175:ARG:NH2	2.34	0.60
1:A:210:GLU:OE1	6:A:601:HOH:O	2.16	0.60
1:A:39:LEU:HD21	3:A:501:CDL:H391	1.83	0.59
2:F:143:THR:OG1	2:F:156:SER:OG	2.20	0.59
1:B:163:PRO:HD3	2:G:48:GLN:HE21	1.67	0.59
2:F:60:ARG:NH1	2:F:217:PHE:O	2.35	0.59
1:E:147:THR:HA	1:E:180:ALA:HB1	1.84	0.59
1:E:208:TYR:OH	3:E:501:CDL:OA4	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLN:NE2	6:A:609:HOH:O	2.34	0.59
1:A:181:PHE:CE2	2:F:33:VAL:HG21	2.36	0.59
2:F:243:VAL:HG22	2:F:245:PRO:HD2	1.85	0.59
2:G:188:LYS:NZ	2:G:229:VAL:O	2.35	0.59
1:C:121:GLN:NE2	1:D:210:GLU:OE2	2.30	0.59
2:F:187:ARG:NH2	2:F:238:GLU:OE2	2.35	0.58
1:B:79:GLU:HG3	1:B:80:LEU:HD12	1.84	0.58
1:C:19:VAL:HG13	5:C:502:PEE:H60	1.85	0.58
1:B:147:THR:OG1	1:B:184:SER:HB2	2.04	0.58
1:C:14:VAL:HG12	5:C:502:PEE:H1	1.86	0.57
2:F:84:VAL:HG22	2:F:91:ILE:HG23	1.86	0.57
1:A:234:LYS:O	1:A:238:GLU:HG3	2.04	0.57
2:G:93:PHE:O	2:G:97:GLY:N	2.37	0.57
2:F:35:PHE:HE1	2:G:36:LEU:HD13	1.70	0.56
2:F:98:ARG:HH11	2:F:205:GLU:CB	2.16	0.56
2:F:63:ASP:OD2	2:F:132:LYS:NZ	2.33	0.56
1:D:79:GLU:OE2	1:D:79:GLU:N	2.28	0.56
2:G:100:ALA:N	2:G:103:GLN:HE21	2.04	0.56
2:F:35:PHE:CE1	2:G:36:LEU:HD13	2.41	0.55
1:A:208:TYR:OH	3:A:501:CDL:OA4	2.22	0.55
2:F:98:ARG:HH11	2:F:205:GLU:HB3	1.67	0.55
2:F:187:ARG:HH12	2:G:149:TYR:HB2	1.71	0.55
1:B:147:THR:HG23	1:B:180:ALA:HB1	1.89	0.55
1:C:120:GLN:HA	1:C:124:ASP:HB2	1.88	0.54
2:G:135:LYS:HE2	2:G:217:PHE:CD2	2.43	0.54
1:B:38:TYR:CZ	1:B:198:GLU:HG2	2.42	0.54
1:A:124:ASP:OD2	2:F:10:LYS:NZ	2.33	0.54
2:F:84:VAL:HG13	2:F:91:ILE:HG12	1.90	0.54
2:F:194:GLY:HA2	2:G:193:GLY:HA3	1.90	0.54
1:B:7:ILE:O	1:B:11:LEU:HG	2.08	0.53
1:D:8:LEU:HD22	1:E:179:TYR:CZ	2.43	0.53
1:E:38:TYR:CZ	1:E:198:GLU:HG3	2.44	0.53
2:G:159:ARG:HH12	2:G:208:ARG:HE	1.57	0.52
1:C:107:ILE:O	6:C:601:HOH:O	2.19	0.52
1:D:242:GLN:HE21	1:E:244:ARG:HG3	1.75	0.52
2:G:82:ILE:HG12	2:G:93:PHE:HE1	1.75	0.52
1:A:142:MET:HE3	5:B:501:PEE:H70	1.91	0.52
1:B:138:ILE:O	1:B:142:MET:HG3	2.10	0.52
1:B:62:SER:HB2	1:B:67:GLN:HG3	1.92	0.52
1:A:8:LEU:HD21	1:B:182:LEU:HD22	1.90	0.51
1:D:198:GLU:OE2	1:D:199:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:ILE:HD13	1:E:216:LEU:HG	1.92	0.51
1:B:140:THR:O	1:B:144:ILE:HG12	2.10	0.51
1:C:41:ARG:NH2	3:D:501:CDL:OB3	2.35	0.51
1:B:162:THR:HG22	1:B:164:GLU:H	1.75	0.51
1:D:34:PHE:CE1	1:D:198:GLU:HB3	2.46	0.51
1:C:59:ILE:HG13	1:C:67:GLN:HG2	1.93	0.50
1:B:163:PRO:HD3	2:G:48:GLN:NE2	2.26	0.50
1:D:11:LEU:O	1:D:149:TYR:OH	2.20	0.50
2:F:240:CYS:SG	2:F:242:LEU:HD23	2.52	0.50
1:B:118:SER:OG	1:B:121:GLN:HG3	2.11	0.50
2:G:143:THR:HA	2:G:208:ARG:HH22	1.77	0.50
1:D:59:ILE:O	1:D:67:GLN:NE2	2.35	0.50
1:D:120:GLN:HA	1:D:124:ASP:HB2	1.93	0.50
1:C:82:HIS:O	1:C:86:GLU:HG2	2.12	0.49
2:G:91:ILE:HB	2:G:212:LEU:HB2	1.94	0.49
1:C:181:PHE:CE1	2:G:30:ALA:HB1	2.47	0.49
1:C:125:ILE:HD11	2:G:11:ARG:HH22	1.77	0.49
2:F:144:ASP:OD2	2:F:208:ARG:NH2	2.46	0.49
2:F:198:ASN:HA	2:G:229:VAL:HG11	1.94	0.49
2:G:119:PRO:HA	2:G:122:LEU:HD12	1.95	0.49
1:B:77:ARG:O	1:B:81:LYS:N	2.27	0.48
2:F:98:ARG:HH12	2:F:205:GLU:HB2	1.78	0.48
1:A:133:LYS:NZ	2:F:14:ASP:OD2	2.36	0.48
3:D:501:CDL:H161	3:D:501:CDL:H511	1.95	0.48
1:E:59:ILE:HD12	1:E:67:GLN:HB2	1.93	0.48
2:F:72:GLU:HG3	2:F:84:VAL:HB	1.95	0.48
1:E:138:ILE:HG22	1:E:142:MET:HE2	1.95	0.48
1:A:56:ILE:HD13	1:A:216:LEU:HG	1.96	0.48
2:F:25:ALA:HB1	2:G:24:TYR:CD2	2.48	0.48
1:B:56:ILE:HD13	1:B:216:LEU:HG	1.96	0.48
1:E:18:LYS:HA	1:E:21:VAL:HG22	1.95	0.47
1:E:64:PRO:HB3	1:E:107:ILE:HG13	1.96	0.47
1:A:204:LYS:HG3	3:A:501:CDL:H312	1.96	0.47
1:C:200:LEU:HD23	3:C:501:CDL:H371	1.97	0.47
2:G:114:LEU:O	2:G:118:VAL:HG23	2.15	0.47
1:E:138:ILE:O	1:E:142:MET:HG3	2.15	0.47
1:A:31:PHE:O	1:A:35:ILE:HG12	2.15	0.46
2:G:213:ARG:NH1	2:G:215:GLN:HB3	2.30	0.46
1:D:34:PHE:HE1	1:D:198:GLU:HB3	1.80	0.46
1:A:17:TYR:HB2	1:E:4:LEU:HD23	1.97	0.46
5:B:501:PEE:H75	3:B:502:CDL:H671	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG13	1:C:139:LEU:HD22	1.96	0.46
1:C:197:LEU:HD11	3:C:501:CDL:H472	1.98	0.46
2:F:153:LEU:HD11	2:G:192:ALA:HB3	1.96	0.46
1:C:90:SER:O	1:C:110:THR:OG1	2.33	0.46
1:A:4:LEU:HD23	1:B:17:TYR:HB2	1.98	0.46
1:A:241:THR:O	1:A:244:ARG:HG2	2.15	0.46
1:D:23:VAL:HG22	5:D:502:PEE:H70	1.97	0.46
2:G:49:ARG:NE	6:G:303:HOH:O	2.40	0.46
1:C:1:MET:HG3	1:D:17:TYR:HE2	1.81	0.46
1:D:27:VAL:HG13	1:D:139:LEU:HD22	1.96	0.46
1:C:193:LEU:HD13	3:C:501:CDL:H671	1.97	0.46
3:A:501:CDL:H552	3:A:501:CDL:H722	1.98	0.46
1:D:95:TYR:HB3	1:D:102:GLU:HG3	1.97	0.46
1:A:79:GLU:HG2	6:A:602:HOH:O	2.17	0.45
2:G:79:ASN:HD21	2:G:81:ASN:HB2	1.81	0.45
1:B:59:ILE:O	1:B:67:GLN:NE2	2.38	0.45
1:C:173:LEU:O	1:C:177:VAL:HG23	2.16	0.45
1:C:181:PHE:HZ	2:G:34:LEU:HB2	1.81	0.45
3:D:501:CDL:H391	3:D:501:CDL:H422	1.53	0.45
1:E:77:ARG:O	1:E:81:LYS:N	2.45	0.45
1:D:11:LEU:HD13	5:D:502:PEE:H42	1.99	0.45
1:D:152:MET:HA	1:D:152:MET:HE2	1.99	0.45
1:D:242:GLN:NE2	1:E:244:ARG:HG3	2.31	0.45
1:C:38:TYR:CZ	1:C:198:GLU:HG3	2.51	0.45
3:D:501:CDL:H592	3:D:501:CDL:H812	1.97	0.45
2:F:122:LEU:HD21	2:F:186:ILE:HG12	1.98	0.45
1:A:6:SER:HA	1:A:9:VAL:HG12	1.98	0.45
1:C:12:THR:HG23	1:C:153:ILE:HA	1.98	0.45
1:D:194:VAL:O	1:D:198:GLU:HG3	2.16	0.45
3:E:501:CDL:H511	3:E:501:CDL:H722	2.00	0.44
1:C:79:GLU:HG3	1:C:80:LEU:HD22	2.00	0.44
2:F:164:MET:HE2	2:G:149:TYR:CE1	2.53	0.44
2:G:98:ARG:HH12	2:G:206:ALA:HA	1.82	0.44
3:D:501:CDL:H371	3:D:501:CDL:H402	1.43	0.44
2:F:12:ARG:HG2	2:G:12:ARG:NH1	2.32	0.44
1:B:19:VAL:HB	1:B:20:PRO:HD3	1.98	0.44
1:B:56:ILE:HG23	1:B:219:LEU:HD11	1.99	0.44
1:C:138:ILE:HG22	1:C:142:MET:HE2	2.00	0.44
1:B:200:LEU:HD21	3:B:502:CDL:H122	1.99	0.44
3:D:501:CDL:H111	3:D:501:CDL:H141	1.81	0.44
3:E:501:CDL:H162	3:E:501:CDL:H191	1.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:136:GLN:OE1	2:G:136:GLN:N	2.42	0.44
2:G:184:LEU:O	2:G:188:LYS:HG2	2.18	0.43
5:D:502:PEE:H43	1:E:182:LEU:HA	1.99	0.43
2:F:130:GLY:HA2	2:F:134:PHE:HB2	2.00	0.43
1:A:155:LEU:HD22	1:B:174:LEU:HD22	2.01	0.43
1:E:140:THR:CG2	2:F:23:SER:HB3	2.47	0.43
5:E:502:PEE:H73	5:E:502:PEE:H79	1.93	0.43
1:A:199:LYS:HA	1:A:202:ILE:HG22	1.99	0.43
1:A:11:LEU:HB3	1:A:149:TYR:HE1	1.83	0.43
1:A:144:ILE:HD11	2:G:21:TRP:CH2	2.53	0.43
3:B:502:CDL:H711	3:B:502:CDL:H742	1.47	0.43
1:D:152:MET:HE3	2:F:31:MET:HE1	2.00	0.43
1:D:181:PHE:CE1	2:G:32:MET:HE1	2.54	0.43
2:F:148:SER:OG	2:G:238:GLU:OE1	2.28	0.43
3:A:501:CDL:HB61	3:A:501:CDL:H522	2.01	0.43
1:B:30:ALA:HB2	3:C:501:CDL:H781	2.00	0.43
2:F:134:PHE:CE1	2:F:214:MET:HB2	2.54	0.43
5:B:501:PEE:H78	3:B:502:CDL:H272	2.01	0.43
1:D:26:THR:HG23	3:E:501:CDL:H842	2.01	0.43
1:D:109:ALA:N	1:D:221:ASP:O	2.47	0.43
1:D:196:TRP:CZ2	3:D:501:CDL:H601	2.54	0.43
1:B:56:ILE:C	1:B:58:SER:H	2.26	0.43
1:B:144:ILE:HD12	2:G:27:LEU:HD22	2.01	0.42
1:B:141:GLY:HA3	1:C:192:ILE:HG21	2.00	0.42
1:C:148:PHE:O	1:C:152:MET:HG3	2.18	0.42
3:E:501:CDL:H311	3:E:501:CDL:H341	1.55	0.42
1:A:11:LEU:O	1:A:149:TYR:OH	2.27	0.42
1:A:177:VAL:HG11	2:F:33:VAL:HG11	2.00	0.42
1:A:138:ILE:O	1:A:142:MET:HG3	2.19	0.42
1:D:90:SER:O	1:D:110:THR:OG1	2.30	0.42
2:F:164:MET:HE3	2:F:168:LEU:HD23	2.01	0.42
1:B:77:ARG:HD3	1:B:80:LEU:HD13	2.02	0.42
1:E:4:LEU:HD12	1:E:7:ILE:HD11	2.02	0.42
1:C:148:PHE:HB3	1:D:185:ALA:HB2	2.01	0.42
1:A:4:LEU:HD11	1:B:182:LEU:HD21	2.01	0.42
1:C:199:LYS:HA	1:C:202:ILE:HG22	2.01	0.41
1:D:149:TYR:CD1	5:D:502:PEE:H41	2.55	0.41
2:F:107:ASN:O	2:F:111:GLN:HG3	2.20	0.41
1:B:181:PHE:CZ	2:G:31:MET:HE2	2.56	0.41
3:D:501:CDL:H442	3:D:501:CDL:H211	2.02	0.41
2:F:153:LEU:HD22	2:G:164:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:THR:HA	1:B:180:ALA:HB1	2.02	0.41
5:B:501:PEE:H75	3:B:502:CDL:H652	2.01	0.41
1:B:8:LEU:O	1:B:12:THR:OG1	2.25	0.41
1:E:137:GLY:HA2	2:F:19:PRO:HB3	2.01	0.41
1:A:79:GLU:HG3	1:A:80:LEU:HD12	2.02	0.41
1:A:134:HIS:CD2	1:B:199:LYS:HE3	2.55	0.41
1:C:118:SER:OG	1:C:121:GLN:HG2	2.20	0.41
2:G:58:LYS:HB3	2:G:58:LYS:HE2	1.93	0.41
2:G:66:ARG:NH1	2:G:70:ARG:HB2	2.36	0.41
1:C:22:THR:HG21	5:C:502:PEE:H59	2.03	0.41
1:C:89:GLU:OE1	1:D:221:ASP:HA	2.20	0.41
1:D:96:GLU:HG3	1:D:105:VAL:HG11	2.02	0.41
3:D:501:CDL:H332	3:D:501:CDL:H361	1.87	0.41
1:B:38:TYR:CE1	1:B:198:GLU:HG2	2.56	0.41
1:C:59:ILE:HG13	1:C:59:ILE:O	2.20	0.41
1:C:196:TRP:CZ2	3:C:501:CDL:H612	2.56	0.41
3:B:502:CDL:H772	3:B:502:CDL:H141	2.01	0.41
1:C:199:LYS:HA	1:C:199:LYS:HD3	1.75	0.41
5:C:502:PEE:H72	5:C:502:PEE:H79	1.81	0.41
1:A:120:GLN:HB2	2:F:10:LYS:HD3	2.02	0.41
3:C:501:CDL:H621	3:C:501:CDL:H652	1.88	0.41
2:F:66:ARG:O	2:F:70:ARG:HG2	2.21	0.41
2:F:149:TYR:HD2	2:F:150:LEU:HD22	1.85	0.41
2:G:115:GLN:HA	2:G:174:LEU:HD12	2.02	0.41
1:A:90:SER:O	1:A:110:THR:OG1	2.38	0.40
1:A:186:PHE:CD1	5:E:502:PEE:H41	2.56	0.40
1:C:152:MET:HE3	1:D:182:LEU:HB2	2.02	0.40
1:B:65:GLU:O	1:B:68:LEU:N	2.54	0.40
1:C:76:GLN:OE1	1:C:76:GLN:HA	2.20	0.40
3:D:501:CDL:H772	3:D:501:CDL:H801	1.82	0.40
1:E:31:PHE:O	1:E:35:ILE:HG12	2.21	0.40
2:G:168:LEU:HD11	2:G:183:GLN:HG3	2.03	0.40
1:C:119:GLU:HG2	1:C:206:TYR:CD1	2.56	0.40
2:F:134:PHE:HE1	2:F:214:MET:HB2	1.86	0.40
2:F:91:ILE:HD12	2:F:212:LEU:HD11	2.04	0.40
1:C:119:GLU:HG3	1:C:209:LEU:HD23	2.03	0.40
2:F:118:VAL:O	2:F:122:LEU:HD23	2.22	0.40
2:G:99:PHE:HB2	2:G:208:ARG:HB3	2.02	0.40
2:G:159:ARG:HH12	2:G:208:ARG:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	244/434 (56%)	239 (98%)	5 (2%)	0	100	100
1	B	243/434 (56%)	238 (98%)	5 (2%)	0	100	100
1	C	243/434 (56%)	240 (99%)	3 (1%)	0	100	100
1	D	243/434 (56%)	241 (99%)	2 (1%)	0	100	100
1	E	244/434 (56%)	238 (98%)	6 (2%)	0	100	100
2	F	244/246 (99%)	241 (99%)	3 (1%)	0	100	100
2	G	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
All	All	1705/2662 (64%)	1673 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	219/372 (59%)	219 (100%)	0	100	100
1	B	218/372 (59%)	218 (100%)	0	100	100
1	C	218/372 (59%)	218 (100%)	0	100	100
1	D	218/372 (59%)	218 (100%)	0	100	100
1	E	219/372 (59%)	219 (100%)	0	100	100
2	F	215/215 (100%)	215 (100%)	0	100	100
2	G	215/215 (100%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1522/2290 (66%)	1522 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	134	HIS
1	A	157	HIS
1	D	120	GLN
1	E	67	GLN
2	F	4	ASN
2	F	152	ASN
2	F	158	GLN
2	G	48	GLN
2	G	81	ASN
2	G	101	HIS
2	G	107	ASN
2	G	111	GLN
2	G	152	ASN
2	G	199	ASN
2	G	215	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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$
5	PEE	E	502	-	50,50,50	1.45	7 (14%)	53,55,55	1.63	7 (13%)
3	CDL	A	501	-	99,99,99	0.30	0	105,111,111	0.20	0
3	CDL	E	501	-	99,99,99	0.32	0	105,111,111	0.21	0
5	PEE	C	502	-	50,50,50	1.47	9 (18%)	53,55,55	1.65	7 (13%)
5	PEE	D	502	-	50,50,50	1.49	9 (18%)	53,55,55	1.66	6 (11%)
5	PEE	B	503	-	50,50,50	1.46	6 (12%)	53,55,55	1.62	7 (13%)
3	CDL	C	501	-	99,99,99	0.29	0	105,111,111	0.20	0
5	PEE	B	501	-	50,50,50	1.53	8 (16%)	53,55,55	1.65	6 (11%)
3	CDL	D	501	-	99,99,99	0.30	0	105,111,111	0.20	0
3	CDL	B	502	-	99,99,99	0.30	0	105,111,111	0.20	0

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
5	PEE	E	502	-	-	25/54/54/54	-
3	CDL	A	501	-	-	64/110/110/110	-
3	CDL	E	501	-	-	67/110/110/110	-
5	PEE	C	502	-	-	28/54/54/54	-
5	PEE	D	502	-	-	22/54/54/54	-
5	PEE	B	503	-	-	19/54/54/54	-
3	CDL	C	501	-	-	67/110/110/110	-
5	PEE	B	501	-	-	30/54/54/54	-
3	CDL	D	501	-	-	67/110/110/110	-
3	CDL	B	502	-	-	67/110/110/110	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	PEE	C3-C2	3.98	1.63	1.50
5	D	502	PEE	C3-C2	3.90	1.63	1.50
5	C	502	PEE	C3-C2	3.79	1.62	1.50
5	B	503	PEE	C3-C2	3.76	1.62	1.50
5	E	502	PEE	C3-C2	3.64	1.62	1.50
5	B	501	PEE	P-O4P	3.28	1.72	1.59
5	E	502	PEE	P-O3P	3.24	1.72	1.59
5	C	502	PEE	P-O3P	3.22	1.72	1.59
5	D	502	PEE	P-O3P	3.22	1.72	1.59
5	C	502	PEE	P-O4P	3.21	1.72	1.59
5	B	501	PEE	P-O3P	3.21	1.71	1.59
5	D	502	PEE	P-O4P	3.19	1.71	1.59
5	B	503	PEE	P-O3P	3.17	1.71	1.59
5	B	503	PEE	P-O4P	3.16	1.71	1.59
5	E	502	PEE	P-O4P	3.13	1.71	1.59
5	B	501	PEE	C31-C30	2.62	1.58	1.50
5	B	501	PEE	O3-C30	2.32	1.40	1.33
5	C	502	PEE	C12-C11	2.26	1.60	1.52
5	D	502	PEE	C12-C11	2.23	1.60	1.52
5	D	502	PEE	C11-C10	2.21	1.57	1.50
5	C	502	PEE	C11-C10	2.18	1.57	1.50
5	D	502	PEE	C31-C30	2.17	1.57	1.50
5	C	502	PEE	O2-C10	2.16	1.40	1.34
5	E	502	PEE	C12-C11	2.16	1.60	1.52
5	D	502	PEE	O2-C10	2.14	1.40	1.34
5	D	502	PEE	O3-C30	2.14	1.39	1.33
5	C	502	PEE	C5-C4	2.12	1.58	1.49
5	E	502	PEE	O2-C10	2.12	1.40	1.34
5	B	501	PEE	C5-C4	2.11	1.58	1.49
5	C	502	PEE	C31-C30	2.10	1.56	1.50
5	B	503	PEE	O3-C30	2.10	1.39	1.33
5	B	501	PEE	C12-C11	2.09	1.59	1.52
5	D	502	PEE	C5-C4	2.07	1.58	1.49
5	B	503	PEE	C5-C4	2.07	1.58	1.49
5	B	503	PEE	C12-C11	2.05	1.59	1.52
5	E	502	PEE	C5-C4	2.05	1.58	1.49
5	C	502	PEE	O3-C30	2.04	1.39	1.33
5	B	501	PEE	O2-C10	2.03	1.40	1.34
5	E	502	PEE	O3-C30	2.03	1.39	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	PEE	O2-C10-C11	6.03	124.54	111.48
5	C	502	PEE	O2-C10-C11	5.95	124.35	111.48
5	B	501	PEE	O2-C10-C11	5.87	124.19	111.48
5	E	502	PEE	O2-C10-C11	5.72	123.86	111.48
5	B	503	PEE	O2-C10-C11	5.59	123.58	111.48
5	B	501	PEE	C40-C39-C38	5.31	164.60	124.83
5	D	502	PEE	C40-C39-C38	5.30	164.54	124.83
5	D	502	PEE	C37-C38-C39	5.25	164.18	124.83
5	E	502	PEE	C40-C39-C38	5.23	164.03	124.83
5	B	501	PEE	C37-C38-C39	5.21	163.89	124.83
5	C	502	PEE	C40-C39-C38	5.21	163.86	124.83
5	B	503	PEE	C40-C39-C38	5.20	163.82	124.83
5	C	502	PEE	C37-C38-C39	5.19	163.72	124.83
5	E	502	PEE	C37-C38-C39	5.17	163.56	124.83
5	B	503	PEE	C37-C38-C39	5.15	163.39	124.83
5	B	501	PEE	O3-C30-C31	3.95	123.88	111.83
5	D	502	PEE	O3-C30-C31	3.89	123.69	111.83
5	C	502	PEE	O3-C30-C31	3.87	123.62	111.83
5	B	503	PEE	O3-C30-C31	3.86	123.61	111.83
5	E	502	PEE	O3-C30-C31	3.82	123.48	111.83
5	B	501	PEE	O3-C30-O5	-2.64	117.02	123.63
5	D	502	PEE	O2-C10-O4	-2.62	117.57	123.70
5	B	503	PEE	O3-C30-O5	-2.61	117.10	123.63
5	C	502	PEE	O3-C30-O5	-2.58	117.16	123.63
5	E	502	PEE	O3-C30-O5	-2.55	117.25	123.63
5	C	502	PEE	O2-C10-O4	-2.54	117.77	123.70
5	D	502	PEE	O3-C30-O5	-2.52	117.32	123.63
5	B	501	PEE	O2-C10-O4	-2.52	117.82	123.70
5	E	502	PEE	O2-C10-O4	-2.44	118.00	123.70
5	B	503	PEE	O2-C10-O4	-2.42	118.05	123.70
5	E	502	PEE	C3-C2-C1	-2.22	106.61	111.78
5	B	503	PEE	C3-C2-C1	-2.18	106.69	111.78
5	C	502	PEE	C3-C2-C1	-2.08	106.93	111.78

There are no chirality outliers.

All (456) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CDL	CA2-OA2-PA1-OA3
3	A	501	CDL	CA2-OA2-PA1-OA4
3	A	501	CDL	CA2-OA2-PA1-OA5
3	A	501	CDL	CB2-OB2-PB2-OB4
3	A	501	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
3	B	502	CDL	CA2-OA2-PA1-OA3
3	B	502	CDL	CA2-OA2-PA1-OA4
3	B	502	CDL	CA2-OA2-PA1-OA5
3	B	502	CDL	CA3-OA5-PA1-OA2
3	B	502	CDL	CA3-OA5-PA1-OA4
3	B	502	CDL	CB2-OB2-PB2-OB3
3	B	502	CDL	CB2-OB2-PB2-OB5
3	B	502	CDL	CB3-OB5-PB2-OB2
3	B	502	CDL	CB3-OB5-PB2-OB3
3	C	501	CDL	CA3-OA5-PA1-OA3
3	C	501	CDL	CB2-OB2-PB2-OB3
3	C	501	CDL	CB2-OB2-PB2-OB5
3	C	501	CDL	CB3-OB5-PB2-OB3
3	C	501	CDL	CB3-OB5-PB2-OB4
3	D	501	CDL	CA2-OA2-PA1-OA3
3	D	501	CDL	CA2-OA2-PA1-OA5
3	D	501	CDL	CA3-OA5-PA1-OA3
3	D	501	CDL	C11-CA5-OA6-CA4
3	D	501	CDL	CB2-OB2-PB2-OB3
3	D	501	CDL	CB2-OB2-PB2-OB4
3	D	501	CDL	CB2-OB2-PB2-OB5
3	D	501	CDL	CB3-OB5-PB2-OB2
3	D	501	CDL	CB3-OB5-PB2-OB3
3	E	501	CDL	CA2-OA2-PA1-OA3
3	E	501	CDL	CA2-OA2-PA1-OA4
3	E	501	CDL	CA2-OA2-PA1-OA5
3	E	501	CDL	CB2-OB2-PB2-OB3
3	E	501	CDL	CB2-OB2-PB2-OB4
3	E	501	CDL	CB2-OB2-PB2-OB5
5	B	501	PEE	C11-C10-O2-C2
5	B	501	PEE	O4-C10-O2-C2
5	B	501	PEE	O3P-C1-C2-O2
5	C	502	PEE	O4-C10-O2-C2
5	C	502	PEE	C1-O3P-P-O2P
5	C	502	PEE	C4-O4P-P-O1P
5	D	502	PEE	C11-C10-O2-C2
5	D	502	PEE	O4-C10-O2-C2
5	D	502	PEE	C4-O4P-P-O1P
5	E	502	PEE	C11-C10-O2-C2
5	E	502	PEE	O4-C10-O2-C2
5	E	502	PEE	O4P-C4-C5-N
3	A	501	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
3	B	502	CDL	OB9-CB7-OB8-CB6
3	D	501	CDL	OB9-CB7-OB8-CB6
3	E	501	CDL	OA9-CA7-OA8-CA6
5	D	502	PEE	O5-C30-O3-C3
3	D	501	CDL	OA7-CA5-OA6-CA4
3	B	502	CDL	C71-CB7-OB8-CB6
3	D	501	CDL	C71-CB7-OB8-CB6
3	E	501	CDL	C31-CA7-OA8-CA6
5	D	502	PEE	C31-C30-O3-C3
5	C	502	PEE	C11-C10-O2-C2
3	A	501	CDL	OA9-CA7-OA8-CA6
3	A	501	CDL	C71-CB7-OB8-CB6
5	B	503	PEE	C43-C44-C45-C46
3	D	501	CDL	O1-C1-CB2-OB2
3	A	501	CDL	C51-CB5-OB6-CB4
3	A	501	CDL	C31-CA7-OA8-CA6
5	E	502	PEE	C43-C44-C45-C46
3	D	501	CDL	C37-C38-C39-C40
5	B	501	PEE	C43-C44-C45-C46
3	A	501	CDL	C37-C38-C39-C40
5	C	502	PEE	C43-C44-C45-C46
3	E	501	CDL	C16-C17-C18-C19
3	D	501	CDL	CA2-C1-CB2-OB2
3	B	502	CDL	C59-C60-C61-C62
3	B	502	CDL	C71-C72-C73-C74
3	D	501	CDL	C11-C12-C13-C14
5	D	502	PEE	C43-C44-C45-C46
3	E	501	CDL	C40-C41-C42-C43
3	D	501	CDL	C77-C78-C79-C80
3	C	501	CDL	C58-C59-C60-C61
3	C	501	CDL	C62-C63-C64-C65
3	D	501	CDL	C39-C40-C41-C42
3	D	501	CDL	C82-C83-C84-C85
3	B	502	CDL	C42-C43-C44-C45
3	A	501	CDL	CB7-C71-C72-C73
3	A	501	CDL	OB7-CB5-OB6-CB4
3	B	502	CDL	C11-CA5-OA6-CA4
5	C	502	PEE	C31-C30-O3-C3
3	C	501	CDL	CB7-C71-C72-C73
3	B	502	CDL	CB7-C71-C72-C73
3	E	501	CDL	CB5-C51-C52-C53
3	E	501	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
5	B	503	PEE	C30-C31-C32-C33
3	E	501	CDL	C51-CB5-OB6-CB4
3	E	501	CDL	CA5-C11-C12-C13
3	E	501	CDL	C31-C32-C33-C34
3	E	501	CDL	CA7-C31-C32-C33
3	D	501	CDL	C33-C34-C35-C36
3	A	501	CDL	CA7-C31-C32-C33
5	C	502	PEE	C40-C41-C42-C43
3	B	502	CDL	OA7-CA5-OA6-CA4
3	E	501	CDL	OB7-CB5-OB6-CB4
5	C	502	PEE	O5-C30-O3-C3
3	A	501	CDL	C11-CA5-OA6-CA4
3	C	501	CDL	C31-CA7-OA8-CA6
3	D	501	CDL	C15-C16-C17-C18
3	E	501	CDL	C38-C39-C40-C41
5	D	502	PEE	C40-C41-C42-C43
3	C	501	CDL	C57-C58-C59-C60
5	B	503	PEE	C13-C14-C15-C16
5	D	502	PEE	C34-C35-C36-C37
3	B	502	CDL	C63-C64-C65-C66
3	B	502	CDL	C11-C12-C13-C14
3	C	501	CDL	C37-C38-C39-C40
3	A	501	CDL	C74-C75-C76-C77
5	B	503	PEE	C40-C41-C42-C43
5	E	502	PEE	C12-C13-C14-C15
3	A	501	CDL	OA7-CA5-OA6-CA4
3	C	501	CDL	C75-C76-C77-C78
3	E	501	CDL	C11-C12-C13-C14
5	B	503	PEE	C34-C35-C36-C37
3	A	501	CDL	C52-C53-C54-C55
3	D	501	CDL	C40-C41-C42-C43
3	D	501	CDL	C13-C14-C15-C16
5	B	503	PEE	C11-C12-C13-C14
3	C	501	CDL	C11-C12-C13-C14
3	D	501	CDL	C38-C39-C40-C41
5	B	501	PEE	C13-C14-C15-C16
3	E	501	CDL	C61-C62-C63-C64
5	B	501	PEE	C22-C23-C24-C25
5	B	501	PEE	C21-C22-C23-C24
5	B	501	PEE	C20-C21-C22-C23
3	B	502	CDL	C17-C18-C19-C20
3	B	502	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
3	C	501	CDL	C33-C34-C35-C36
3	C	501	CDL	C63-C64-C65-C66
3	E	501	CDL	C20-C21-C22-C23
5	E	502	PEE	C31-C32-C33-C34
3	B	502	CDL	C78-C79-C80-C81
3	D	501	CDL	C16-C17-C18-C19
3	D	501	CDL	C61-C62-C63-C64
5	C	502	PEE	C13-C14-C15-C16
3	A	501	CDL	C32-C33-C34-C35
3	B	502	CDL	C34-C35-C36-C37
3	D	501	CDL	C19-C20-C21-C22
3	D	501	CDL	C78-C79-C80-C81
3	C	501	CDL	C35-C36-C37-C38
3	C	501	CDL	C74-C75-C76-C77
3	E	501	CDL	C51-C52-C53-C54
3	E	501	CDL	C55-C56-C57-C58
5	D	502	PEE	C21-C22-C23-C24
3	E	501	CDL	C17-C18-C19-C20
5	B	501	PEE	C40-C41-C42-C43
3	E	501	CDL	C71-C72-C73-C74
3	B	502	CDL	C61-C62-C63-C64
3	D	501	CDL	C53-C54-C55-C56
3	D	501	CDL	C73-C74-C75-C76
3	C	501	CDL	OA9-CA7-OA8-CA6
3	C	501	CDL	C32-C33-C34-C35
5	B	501	PEE	C11-C12-C13-C14
3	C	501	CDL	C44-C45-C46-C47
3	B	502	CDL	C13-C14-C15-C16
3	B	502	CDL	C20-C21-C22-C23
3	C	501	CDL	C55-C56-C57-C58
3	D	501	CDL	C60-C61-C62-C63
3	E	501	CDL	C15-C16-C17-C18
3	A	501	CDL	C20-C21-C22-C23
3	A	501	CDL	C31-C32-C33-C34
3	D	501	CDL	CA7-C31-C32-C33
3	A	501	CDL	C39-C40-C41-C42
3	A	501	CDL	C57-C58-C59-C60
3	A	501	CDL	C17-C18-C19-C20
3	B	502	CDL	C37-C38-C39-C40
3	B	502	CDL	C77-C78-C79-C80
5	C	502	PEE	C34-C35-C36-C37
3	C	501	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
3	B	502	CDL	C44-C45-C46-C47
3	A	501	CDL	C35-C36-C37-C38
3	C	501	CDL	OB7-CB5-OB6-CB4
5	C	502	PEE	C15-C16-C17-C18
5	E	502	PEE	C19-C20-C21-C22
3	B	502	CDL	C52-C53-C54-C55
5	B	503	PEE	C20-C21-C22-C23
5	E	502	PEE	C11-C12-C13-C14
3	A	501	CDL	C12-C13-C14-C15
3	E	501	CDL	C58-C59-C60-C61
3	E	501	CDL	OA6-CA4-CA6-OA8
3	E	501	CDL	OB6-CB4-CB6-OB8
5	B	501	PEE	C15-C16-C17-C18
3	B	502	CDL	C32-C33-C34-C35
5	B	501	PEE	C31-C32-C33-C34
3	D	501	CDL	C17-C18-C19-C20
3	D	501	CDL	C57-C58-C59-C60
3	D	501	CDL	C1-CA2-OA2-PA1
3	A	501	CDL	C54-C55-C56-C57
3	B	502	CDL	C76-C77-C78-C79
5	B	501	PEE	C41-C42-C43-C44
3	A	501	CDL	C36-C37-C38-C39
3	B	502	CDL	C72-C73-C74-C75
5	B	503	PEE	C31-C32-C33-C34
5	B	503	PEE	C32-C33-C34-C35
5	E	502	PEE	C34-C35-C36-C37
5	E	502	PEE	C32-C33-C34-C35
3	D	501	CDL	C20-C21-C22-C23
3	B	502	CDL	C40-C41-C42-C43
3	D	501	CDL	C72-C73-C74-C75
5	C	502	PEE	C36-C37-C38-C39
5	B	501	PEE	C19-C20-C21-C22
5	B	503	PEE	C19-C20-C21-C22
5	E	502	PEE	C39-C40-C41-C42
3	E	501	CDL	C77-C78-C79-C80
3	C	501	CDL	OA5-CA3-CA4-CA6
3	C	501	CDL	OB5-CB3-CB4-CB6
5	B	501	PEE	O3P-C1-C2-C3
3	C	501	CDL	C39-C40-C41-C42
3	E	501	CDL	C59-C60-C61-C62
3	D	501	CDL	C36-C37-C38-C39
5	E	502	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	A	501	CDL	C23-C24-C25-C26
3	D	501	CDL	C54-C55-C56-C57
3	E	501	CDL	C19-C20-C21-C22
3	A	501	CDL	C55-C56-C57-C58
3	C	501	CDL	CB3-CB4-CB6-OB8
3	E	501	CDL	CB3-CB4-CB6-OB8
3	A	501	CDL	C24-C25-C26-C27
3	E	501	CDL	C63-C64-C65-C66
5	B	501	PEE	C39-C40-C41-C42
3	C	501	CDL	C80-C81-C82-C83
3	B	502	CDL	C33-C34-C35-C36
3	D	501	CDL	C59-C60-C61-C62
3	D	501	CDL	CB5-C51-C52-C53
3	E	501	CDL	C12-C13-C14-C15
5	C	502	PEE	C39-C40-C41-C42
5	D	502	PEE	C39-C40-C41-C42
5	E	502	PEE	C15-C16-C17-C18
3	B	502	CDL	C55-C56-C57-C58
5	D	502	PEE	C11-C12-C13-C14
5	C	502	PEE	C11-C12-C13-C14
3	C	501	CDL	C24-C25-C26-C27
3	E	501	CDL	C71-CB7-OB8-CB6
3	C	501	CDL	C20-C21-C22-C23
3	D	501	CDL	C63-C64-C65-C66
5	B	501	PEE	C32-C33-C34-C35
3	A	501	CDL	C18-C19-C20-C21
3	B	502	CDL	C12-C13-C14-C15
3	D	501	CDL	C22-C23-C24-C25
3	E	501	CDL	C76-C77-C78-C79
3	C	501	CDL	C78-C79-C80-C81
3	C	501	CDL	C18-C19-C20-C21
3	B	502	CDL	C74-C75-C76-C77
3	E	501	CDL	C22-C23-C24-C25
5	B	501	PEE	C38-C39-C40-C41
3	C	501	CDL	C84-C85-C86-C87
3	B	502	CDL	C84-C85-C86-C87
5	C	502	PEE	C31-C32-C33-C34
5	B	501	PEE	C44-C45-C46-C47
3	C	501	CDL	C60-C61-C62-C63
3	A	501	CDL	C76-C77-C78-C79
3	E	501	CDL	C32-C33-C34-C35
3	E	501	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
3	D	501	CDL	CB7-C71-C72-C73
3	C	501	CDL	C59-C60-C61-C62
3	A	501	CDL	C84-C85-C86-C87
3	C	501	CDL	C41-C42-C43-C44
5	D	502	PEE	C13-C14-C15-C16
3	B	502	CDL	C1-CB2-OB2-PB2
3	C	501	CDL	C1-CA2-OA2-PA1
3	E	501	CDL	CB4-CB3-OB5-PB2
3	B	502	CDL	C54-C55-C56-C57
3	D	501	CDL	C44-C45-C46-C47
3	C	501	CDL	C19-C20-C21-C22
3	E	501	CDL	C78-C79-C80-C81
5	E	502	PEE	C41-C42-C43-C44
3	A	501	CDL	C79-C80-C81-C82
3	E	501	CDL	C18-C19-C20-C21
3	E	501	CDL	C24-C25-C26-C27
5	D	502	PEE	O3P-C1-C2-C3
5	D	502	PEE	C31-C32-C33-C34
3	A	501	CDL	C44-C45-C46-C47
3	C	501	CDL	C36-C37-C38-C39
5	C	502	PEE	C44-C45-C46-C47
3	D	501	CDL	C74-C75-C76-C77
5	E	502	PEE	C1-C2-C3-O3
3	A	501	CDL	CA5-C11-C12-C13
3	A	501	CDL	C59-C60-C61-C62
3	E	501	CDL	C57-C58-C59-C60
3	B	502	CDL	C73-C74-C75-C76
3	E	501	CDL	C62-C63-C64-C65
3	D	501	CDL	CA4-CA3-OA5-PA1
3	D	501	CDL	C51-C52-C53-C54
3	A	501	CDL	C64-C65-C66-C67
5	B	501	PEE	C31-C30-O3-C3
5	E	502	PEE	C31-C30-O3-C3
3	B	502	CDL	C60-C61-C62-C63
5	B	501	PEE	C33-C34-C35-C36
3	D	501	CDL	C32-C33-C34-C35
3	E	501	CDL	C74-C75-C76-C77
3	C	501	CDL	C64-C65-C66-C67
3	B	502	CDL	C41-C42-C43-C44
5	E	502	PEE	C33-C34-C35-C36
3	B	502	CDL	C24-C25-C26-C27
3	E	501	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
3	E	501	CDL	C37-C38-C39-C40
3	E	501	CDL	C75-C76-C77-C78
3	A	501	CDL	C72-C73-C74-C75
3	B	502	CDL	C36-C37-C38-C39
3	D	501	CDL	C62-C63-C64-C65
3	D	501	CDL	C42-C43-C44-C45
3	A	501	CDL	C75-C76-C77-C78
3	E	501	CDL	OB9-CB7-OB8-CB6
3	B	502	CDL	C16-C17-C18-C19
3	B	502	CDL	C56-C57-C58-C59
3	B	502	CDL	C14-C15-C16-C17
5	D	502	PEE	C35-C36-C37-C38
5	E	502	PEE	C44-C45-C46-C47
3	C	501	CDL	C38-C39-C40-C41
5	E	502	PEE	O5-C30-O3-C3
5	E	502	PEE	C13-C14-C15-C16
3	C	501	CDL	C71-C72-C73-C74
3	C	501	CDL	OA5-CA3-CA4-OA6
3	C	501	CDL	OB5-CB3-CB4-OB6
5	D	502	PEE	O3P-C1-C2-O2
5	C	502	PEE	C23-C24-C25-C26
3	A	501	CDL	C60-C61-C62-C63
5	E	502	PEE	O2-C2-C3-O3
3	B	502	CDL	C31-CA7-OA8-CA6
5	B	501	PEE	O5-C30-O3-C3
3	A	501	CDL	C33-C34-C35-C36
3	E	501	CDL	C80-C81-C82-C83
5	B	503	PEE	C41-C42-C43-C44
5	C	502	PEE	C12-C13-C14-C15
3	D	501	CDL	C71-C72-C73-C74
3	E	501	CDL	C34-C35-C36-C37
5	C	502	PEE	C20-C21-C22-C23
3	A	501	CDL	C13-C14-C15-C16
3	A	501	CDL	C41-C42-C43-C44
3	D	501	CDL	C80-C81-C82-C83
3	E	501	CDL	C43-C44-C45-C46
3	E	501	CDL	C23-C24-C25-C26
3	A	501	CDL	CB4-CB3-OB5-PB2
3	B	502	CDL	C1-CA2-OA2-PA1
3	C	501	CDL	CA4-CA3-OA5-PA1
3	C	501	CDL	C1-CB2-OB2-PB2
3	B	502	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
5	E	502	PEE	C20-C21-C22-C23
3	B	502	CDL	OA9-CA7-OA8-CA6
5	D	502	PEE	C41-C42-C43-C44
3	A	501	CDL	OB6-CB4-CB6-OB8
3	C	501	CDL	OB6-CB4-CB6-OB8
3	D	501	CDL	C84-C85-C86-C87
3	E	501	CDL	CA3-CA4-CA6-OA8
5	E	502	PEE	C36-C37-C38-C39
3	A	501	CDL	CB3-OB5-PB2-OB3
3	B	502	CDL	CA3-OA5-PA1-OA3
3	B	502	CDL	CB2-OB2-PB2-OB4
3	B	502	CDL	CB3-OB5-PB2-OB4
3	C	501	CDL	CA2-OA2-PA1-OA5
3	C	501	CDL	CA3-OA5-PA1-OA2
3	C	501	CDL	CA3-OA5-PA1-OA4
3	C	501	CDL	CB2-OB2-PB2-OB4
3	C	501	CDL	CB3-OB5-PB2-OB2
3	E	501	CDL	CA3-OA5-PA1-OA3
3	E	501	CDL	CB3-OB5-PB2-OB2
3	E	501	CDL	CB3-OB5-PB2-OB3
3	E	501	CDL	CB3-OB5-PB2-OB4
5	B	501	PEE	C1-O3P-P-O1P
5	B	503	PEE	C1-O3P-P-O1P
5	B	503	PEE	C4-O4P-P-O3P
5	B	503	PEE	C4-O4P-P-O2P
5	B	503	PEE	C4-O4P-P-O1P
5	C	502	PEE	C1-O3P-P-O1P
5	C	502	PEE	C1-O3P-P-O4P
5	C	502	PEE	C22-C23-C24-C25
3	A	501	CDL	C1-CB2-OB2-PB2
3	E	501	CDL	C1-CA2-OA2-PA1
3	E	501	CDL	CA4-CA3-OA5-PA1
3	B	502	CDL	C19-C20-C21-C22
5	C	502	PEE	C32-C33-C34-C35
3	B	502	CDL	CA5-C11-C12-C13
5	C	502	PEE	C3-C2-O2-C10
3	A	501	CDL	C34-C35-C36-C37
3	A	501	CDL	C71-C72-C73-C74
3	C	501	CDL	C15-C16-C17-C18
3	C	501	CDL	C34-C35-C36-C37
3	D	501	CDL	C18-C19-C20-C21
3	C	501	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	D	501	CDL	C75-C76-C77-C78
5	D	502	PEE	C2-C1-O3P-P
3	C	501	CDL	C23-C24-C25-C26
5	B	501	PEE	C24-C25-C26-C27
3	A	501	CDL	CB3-CB4-CB6-OB8
3	C	501	CDL	C11-CA5-OA6-CA4
3	D	501	CDL	C43-C44-C45-C46
3	C	501	CDL	OA7-CA5-OA6-CA4
3	D	501	CDL	OB7-CB5-OB6-CB4
3	A	501	CDL	C77-C78-C79-C80
5	B	501	PEE	C16-C17-C18-C19
3	B	502	CDL	C38-C39-C40-C41
3	B	502	CDL	C32-C31-CA7-OA8
3	D	501	CDL	CB4-CB3-OB5-PB2
3	E	501	CDL	C1-CB2-OB2-PB2
3	D	501	CDL	C12-C13-C14-C15
5	B	503	PEE	C16-C17-C18-C19
3	C	501	CDL	C13-C14-C15-C16
3	E	501	CDL	C13-C14-C15-C16
5	B	503	PEE	C44-C45-C46-C47
5	B	501	PEE	C1-C2-O2-C10
5	D	502	PEE	C3-C2-O2-C10
3	A	501	CDL	C19-C20-C21-C22
3	A	501	CDL	C15-C16-C17-C18
5	C	502	PEE	C18-C19-C20-C21
3	C	501	CDL	C43-C44-C45-C46
3	B	502	CDL	OB5-CB3-CB4-CB6
5	B	501	PEE	C12-C13-C14-C15
3	D	501	CDL	C51-CB5-OB6-CB4
3	E	501	CDL	C14-C15-C16-C17
5	B	503	PEE	C21-C22-C23-C24
3	B	502	CDL	C75-C76-C77-C78
3	A	501	CDL	C22-C23-C24-C25
3	C	501	CDL	C54-C55-C56-C57
3	D	501	CDL	C23-C24-C25-C26
3	C	501	CDL	C73-C74-C75-C76
3	C	501	CDL	C72-C71-CB7-OB8
3	A	501	CDL	OB5-CB3-CB4-OB6
3	C	501	CDL	C21-C22-C23-C24
5	B	503	PEE	O3P-C1-C2-C3
5	D	502	PEE	C16-C17-C18-C19
3	B	502	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
5	D	502	PEE	C38-C39-C40-C41
3	A	501	CDL	C83-C84-C85-C86
5	C	502	PEE	O2-C10-C11-C12
5	B	501	PEE	C3-C2-O2-C10
5	C	502	PEE	C16-C17-C18-C19
5	C	502	PEE	C1-C2-C3-O3
3	E	501	CDL	C52-C53-C54-C55
3	C	501	CDL	C32-C31-CA7-OA8
3	A	501	CDL	OB5-CB3-CB4-CB6
3	A	501	CDL	C82-C83-C84-C85
3	D	501	CDL	C52-C51-CB5-OB6
3	B	502	CDL	C52-C51-CB5-OB6
3	B	502	CDL	OB5-CB3-CB4-OB6
3	A	501	CDL	C16-C17-C18-C19
3	D	501	CDL	C81-C82-C83-C84
5	B	501	PEE	O3-C30-C31-C32
3	A	501	CDL	C42-C43-C44-C45
5	D	502	PEE	C24-C25-C26-C27
3	D	501	CDL	C52-C53-C54-C55
5	B	501	PEE	C2-C1-O3P-P
3	B	502	CDL	C52-C51-CB5-OB7
3	D	501	CDL	C14-C15-C16-C17
5	E	502	PEE	O2-C10-C11-C12
3	C	501	CDL	C32-C31-CA7-OA9
3	A	501	CDL	C52-C51-CB5-OB6
3	D	501	CDL	C52-C51-CB5-OB7
3	B	502	CDL	CA3-CA4-CA6-OA8
3	A	501	CDL	CA4-CA3-OA5-PA1
3	E	501	CDL	C42-C43-C44-C45
3	C	501	CDL	C16-C17-C18-C19
5	E	502	PEE	O4-C10-C11-C12

There are no ring outliers.

9 monomers are involved in 46 short contacts:

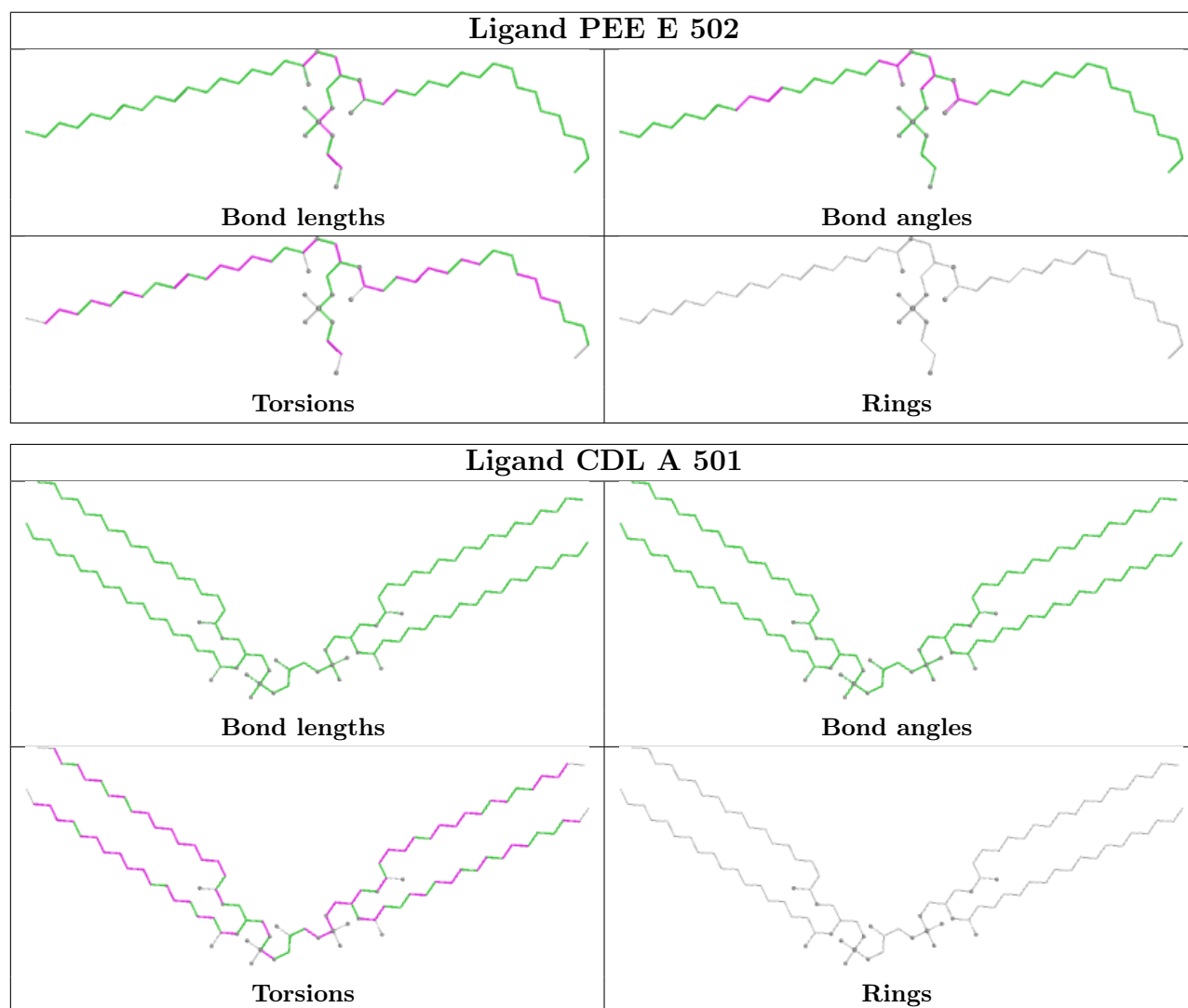
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	502	PEE	2	0
3	A	501	CDL	6	0
3	E	501	CDL	6	0
5	C	502	PEE	4	0
5	D	502	PEE	5	0
3	C	501	CDL	6	0

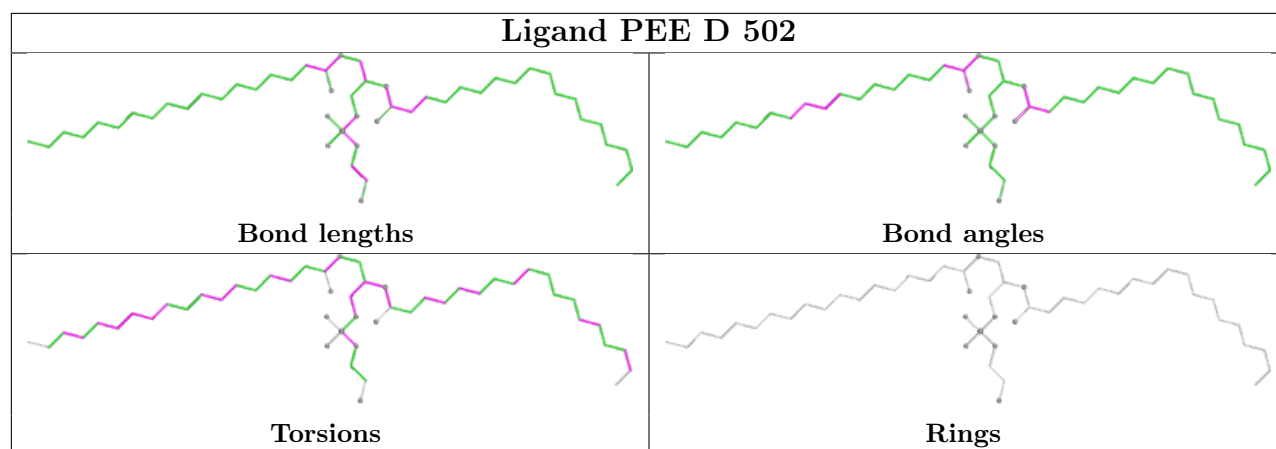
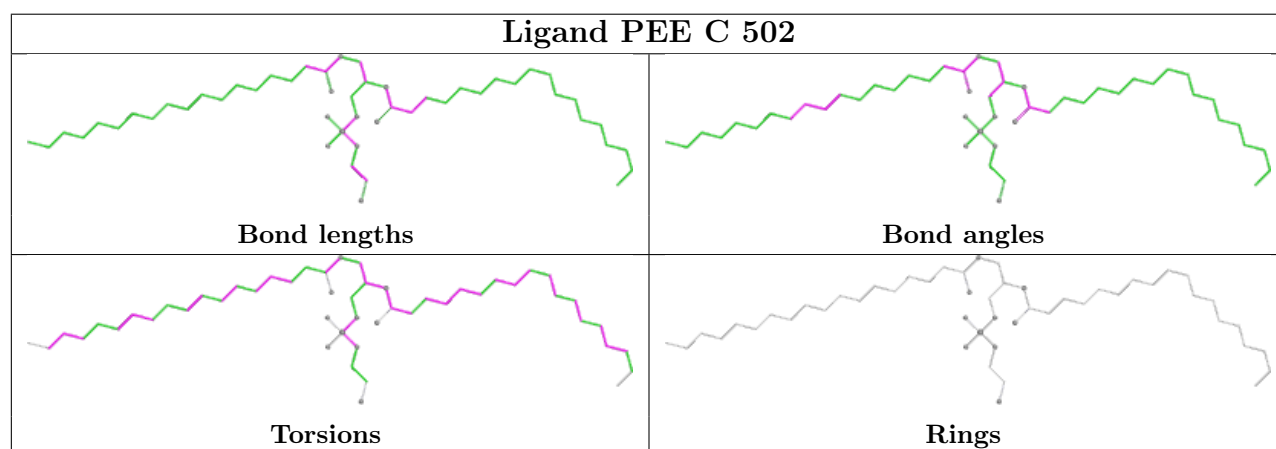
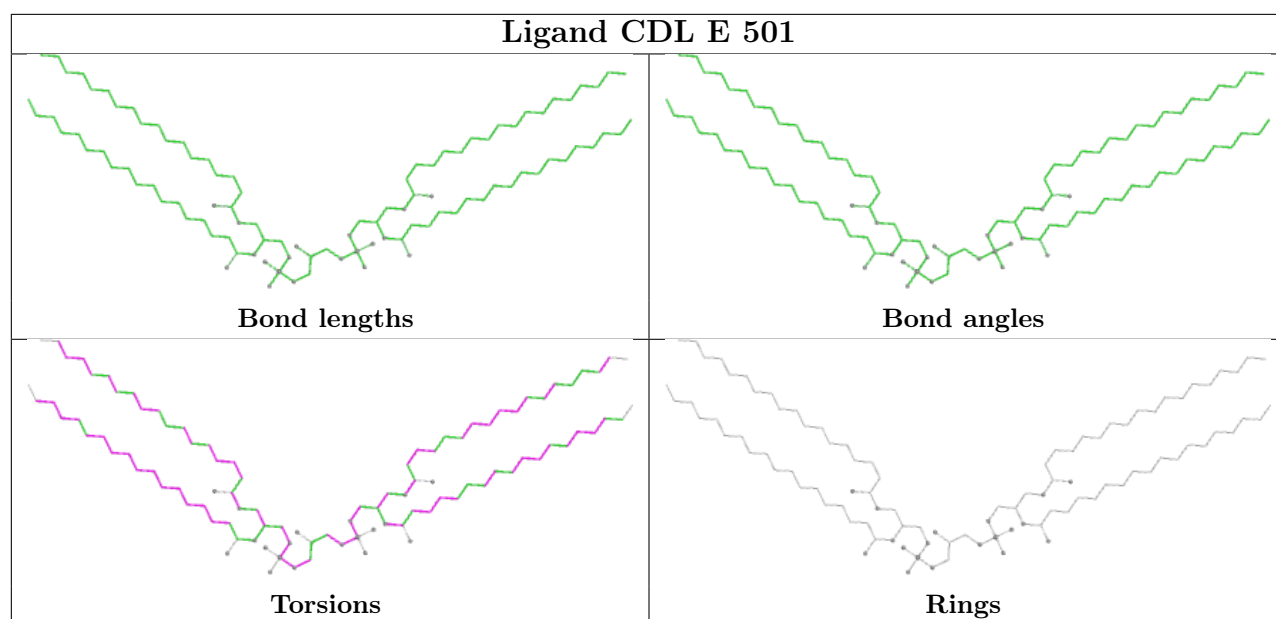
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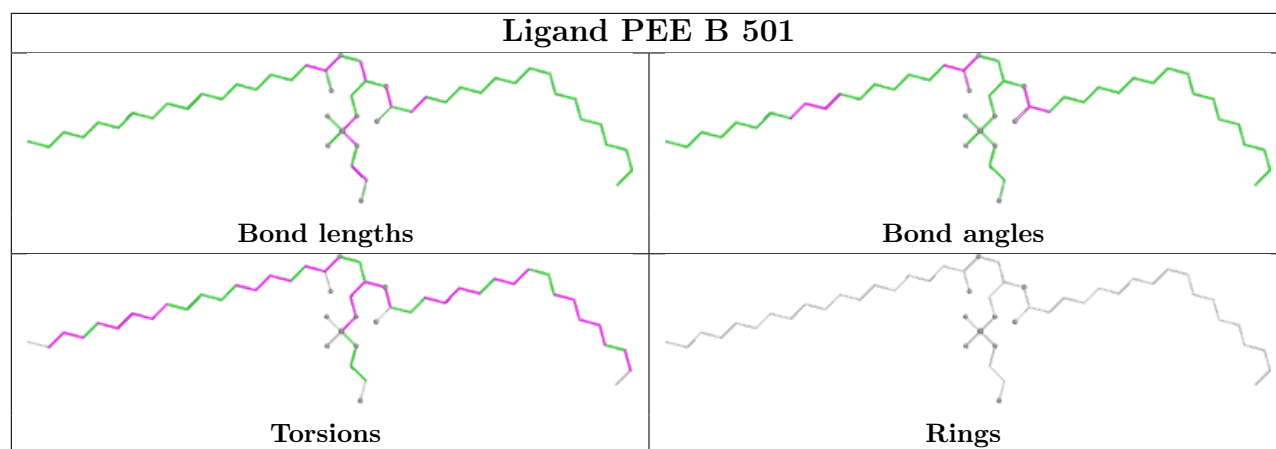
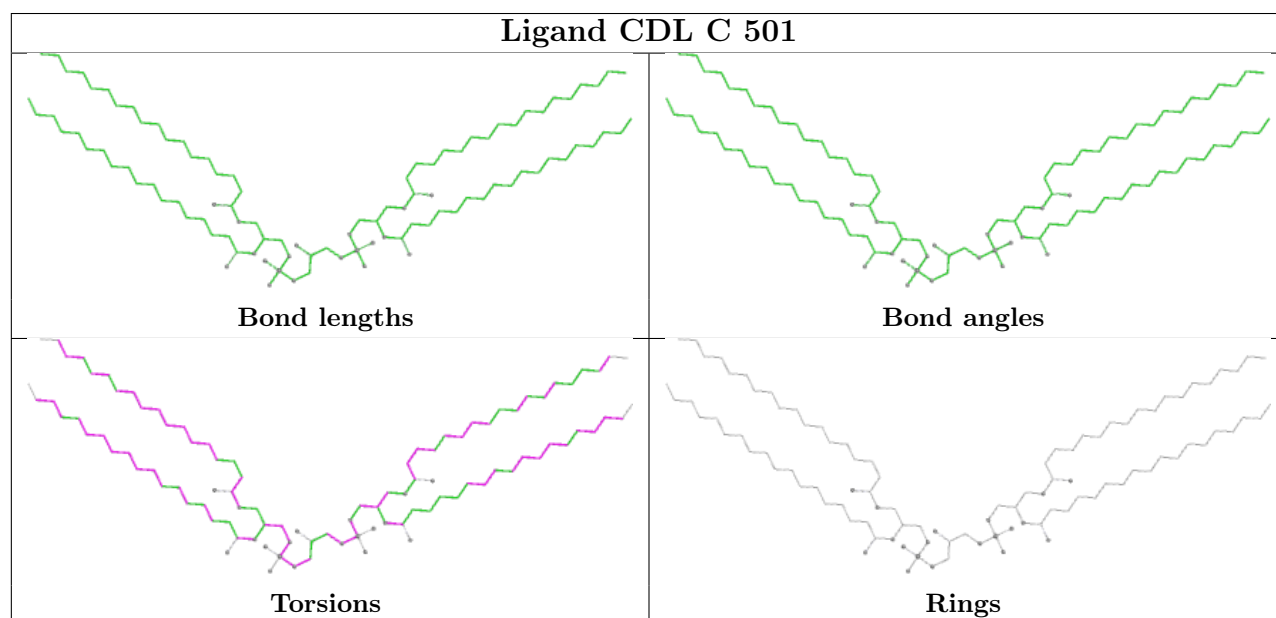
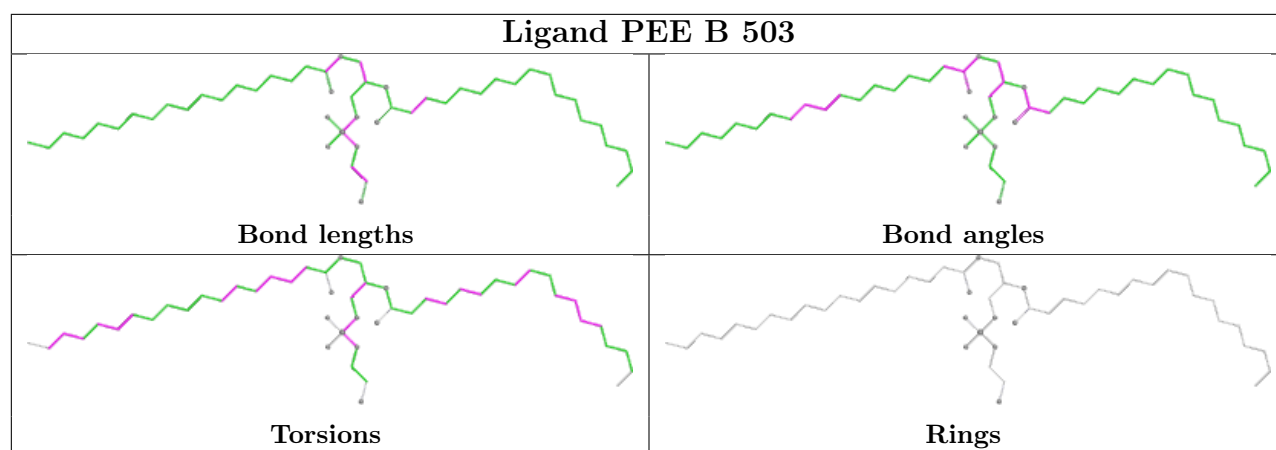
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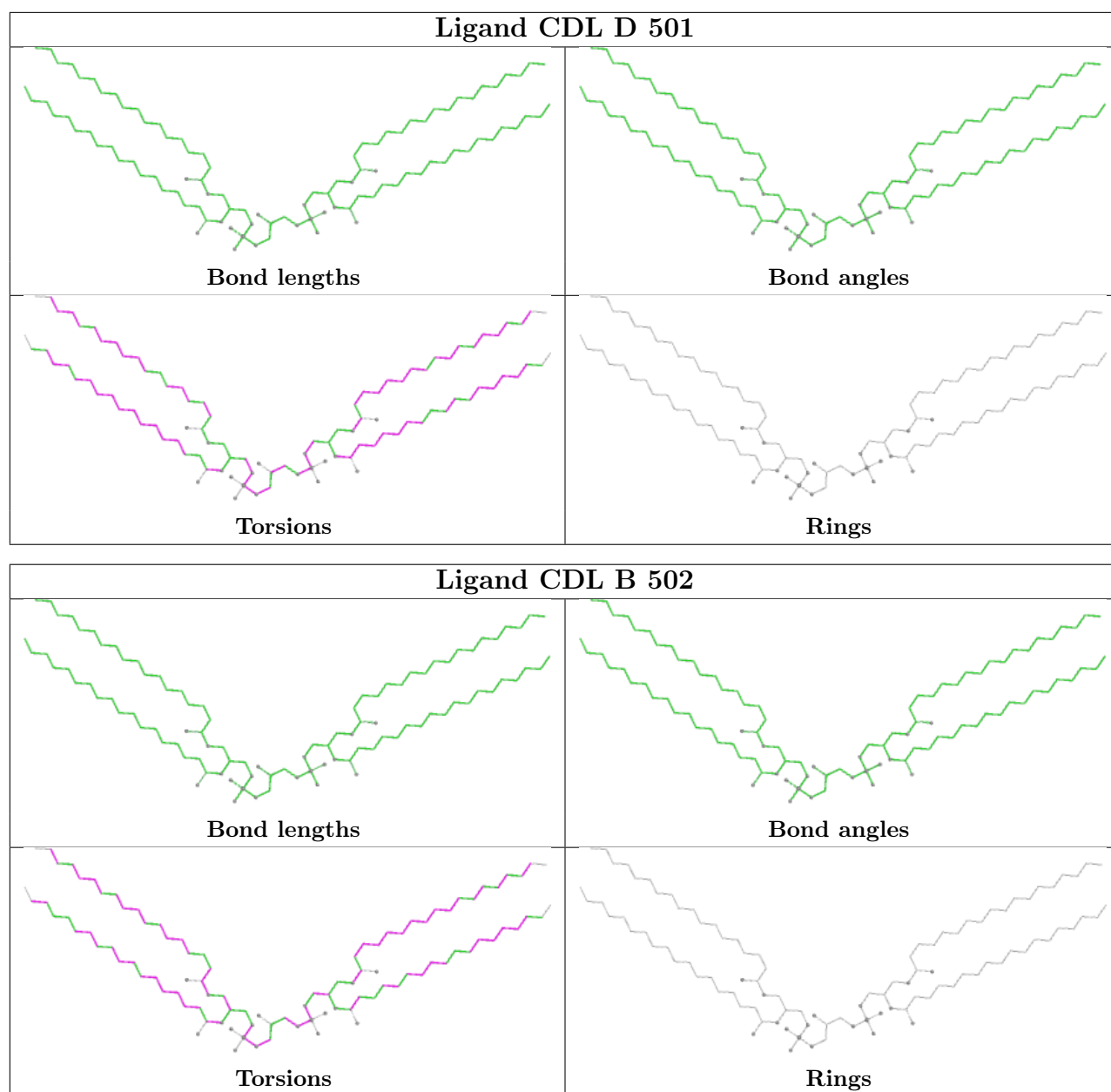
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	PEE	4	0
3	D	501	CDL	10	0
3	B	502	CDL	6	0

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.

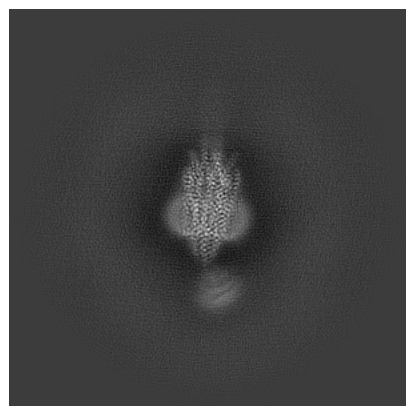
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18766. These allow visual inspection of the internal detail of the map and identification of artifacts.

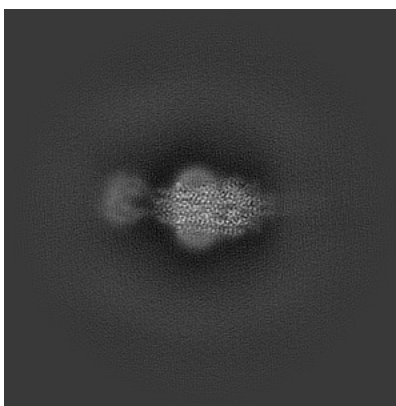
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

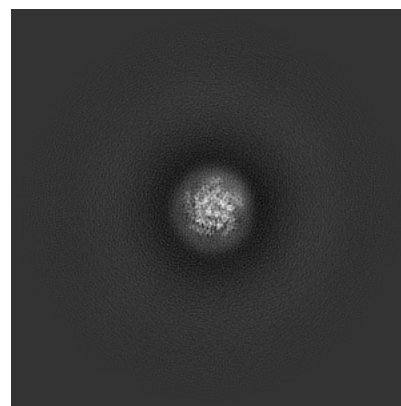
6.1.1 Primary map



X

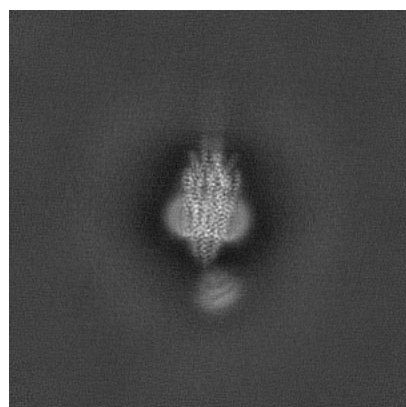


Y

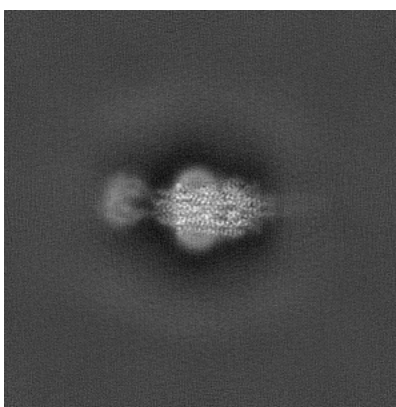


Z

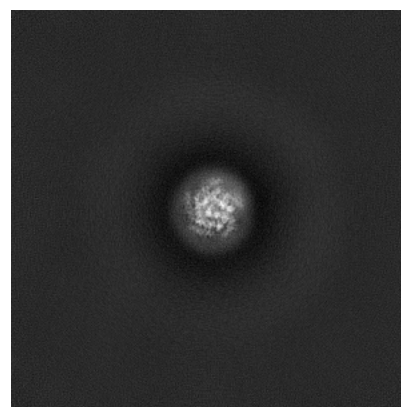
6.1.2 Raw map



X



Y

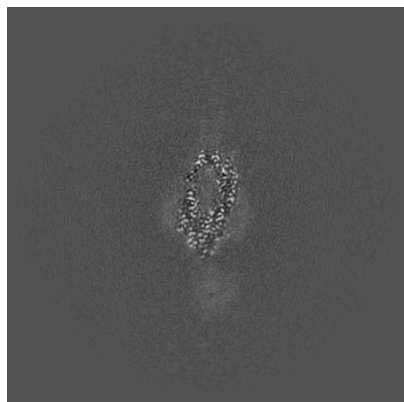


Z

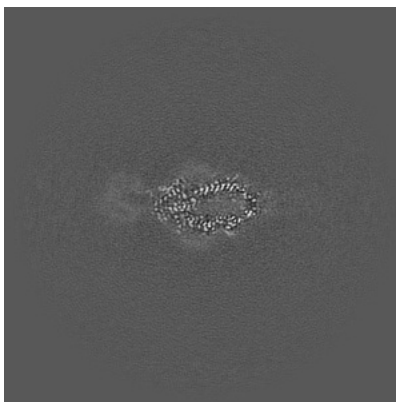
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

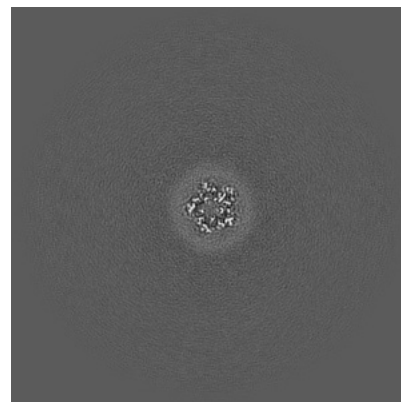
6.2.1 Primary map



X Index: 250

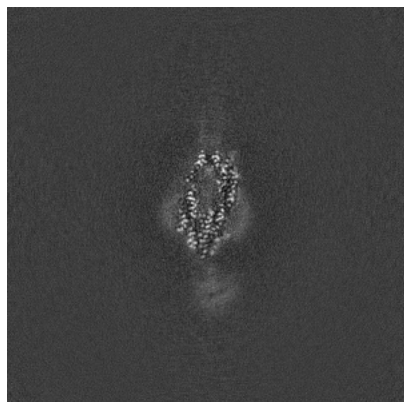


Y Index: 250

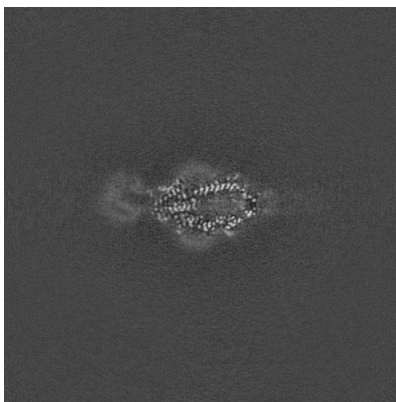


Z Index: 250

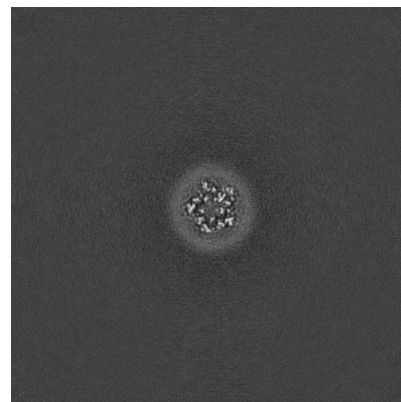
6.2.2 Raw map



X Index: 250



Y Index: 250

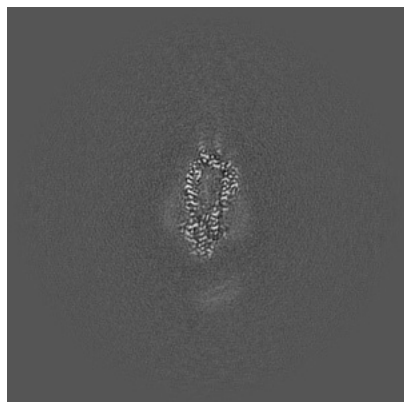


Z Index: 250

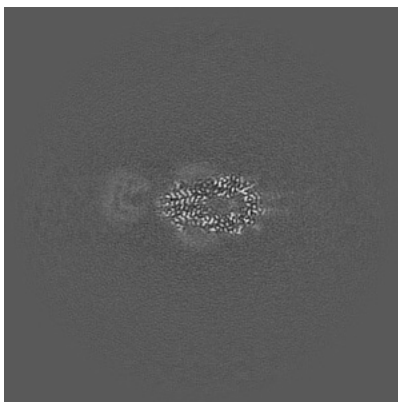
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

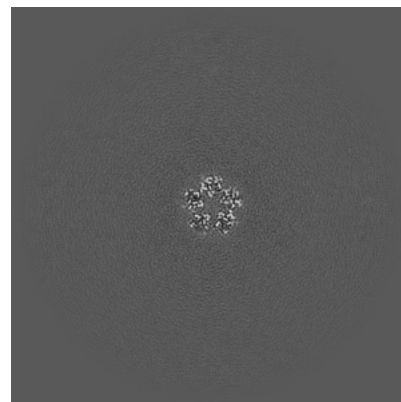
6.3.1 Primary map



X Index: 258

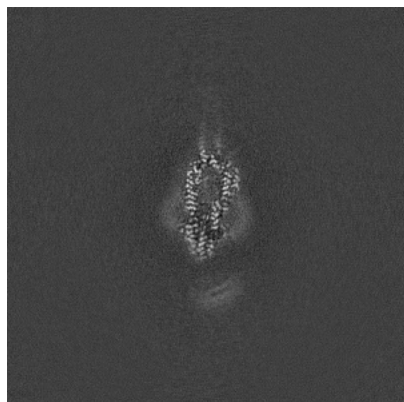


Y Index: 258

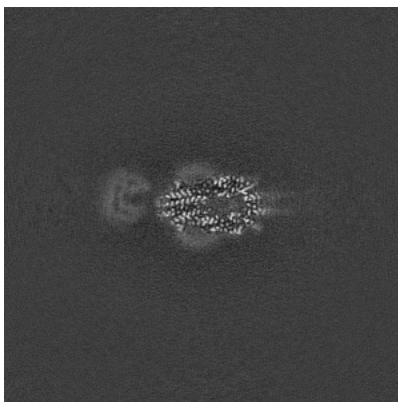


Z Index: 281

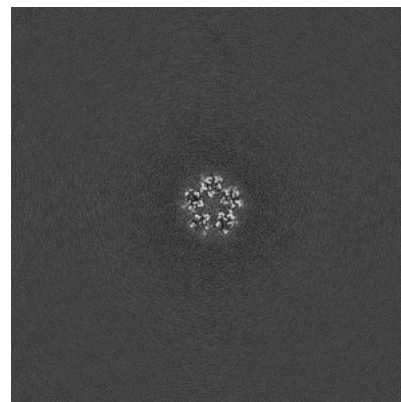
6.3.2 Raw map



X Index: 259



Y Index: 258

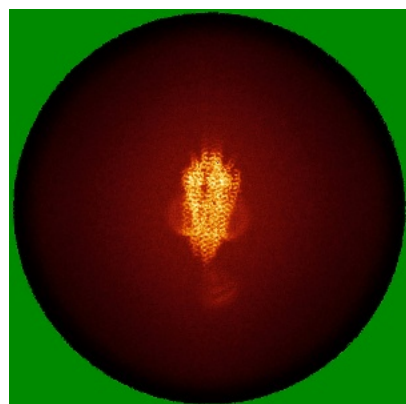


Z Index: 281

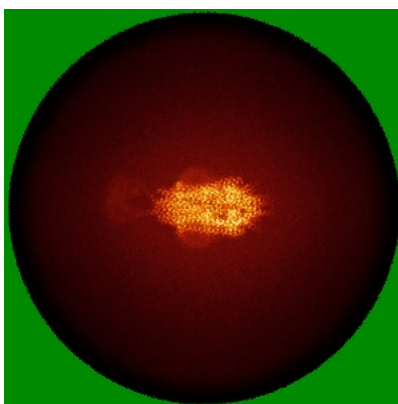
The images above show the largest variance slices of the map in three orthogonal directions.

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

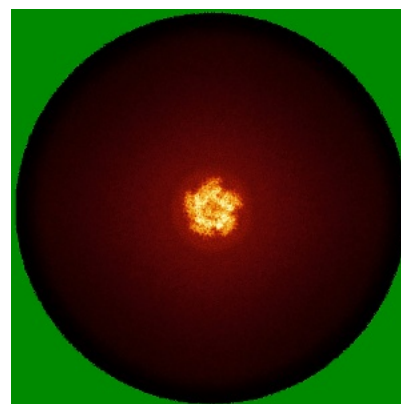
6.4.1 Primary map



X

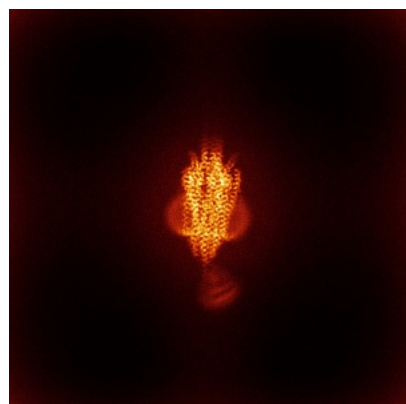


Y

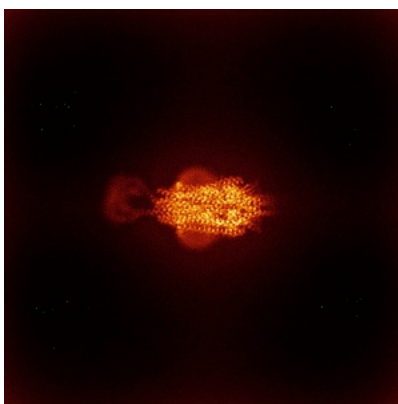


Z

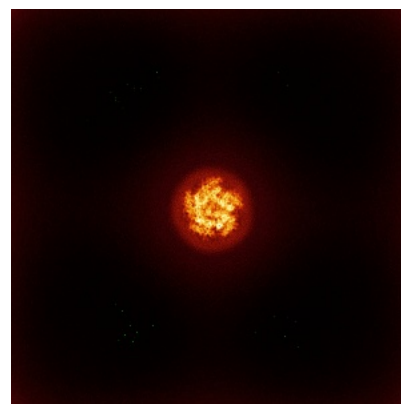
6.4.2 Raw map



X



Y

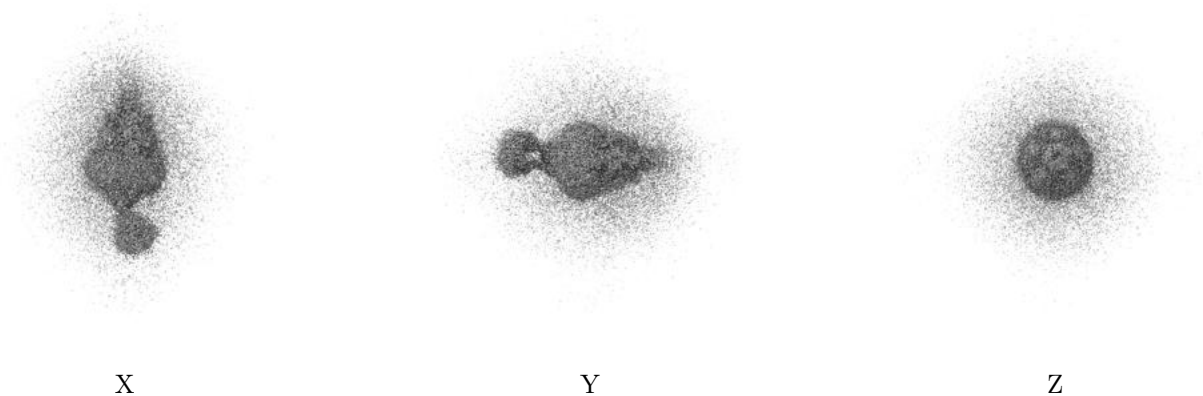


Z

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

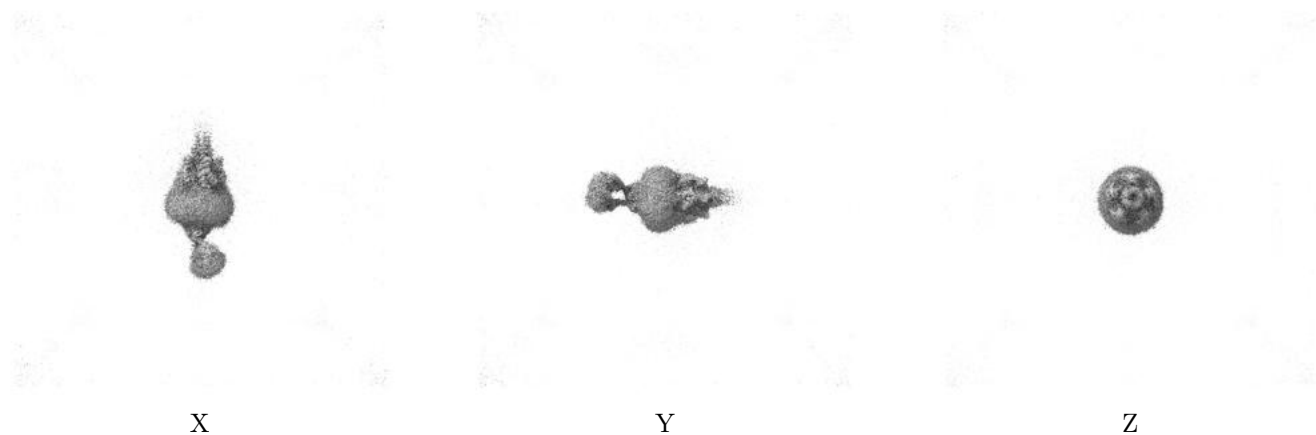
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

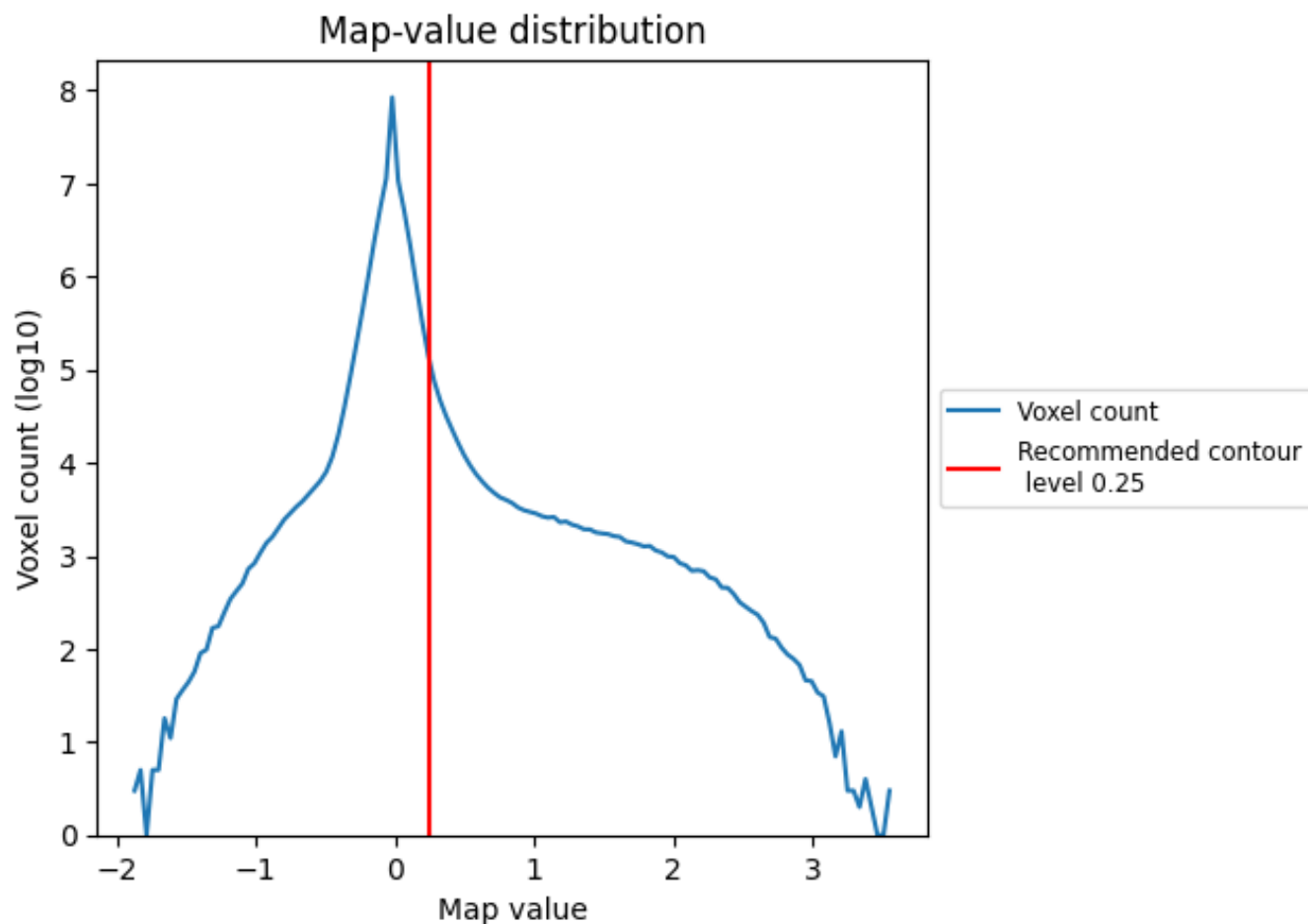
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

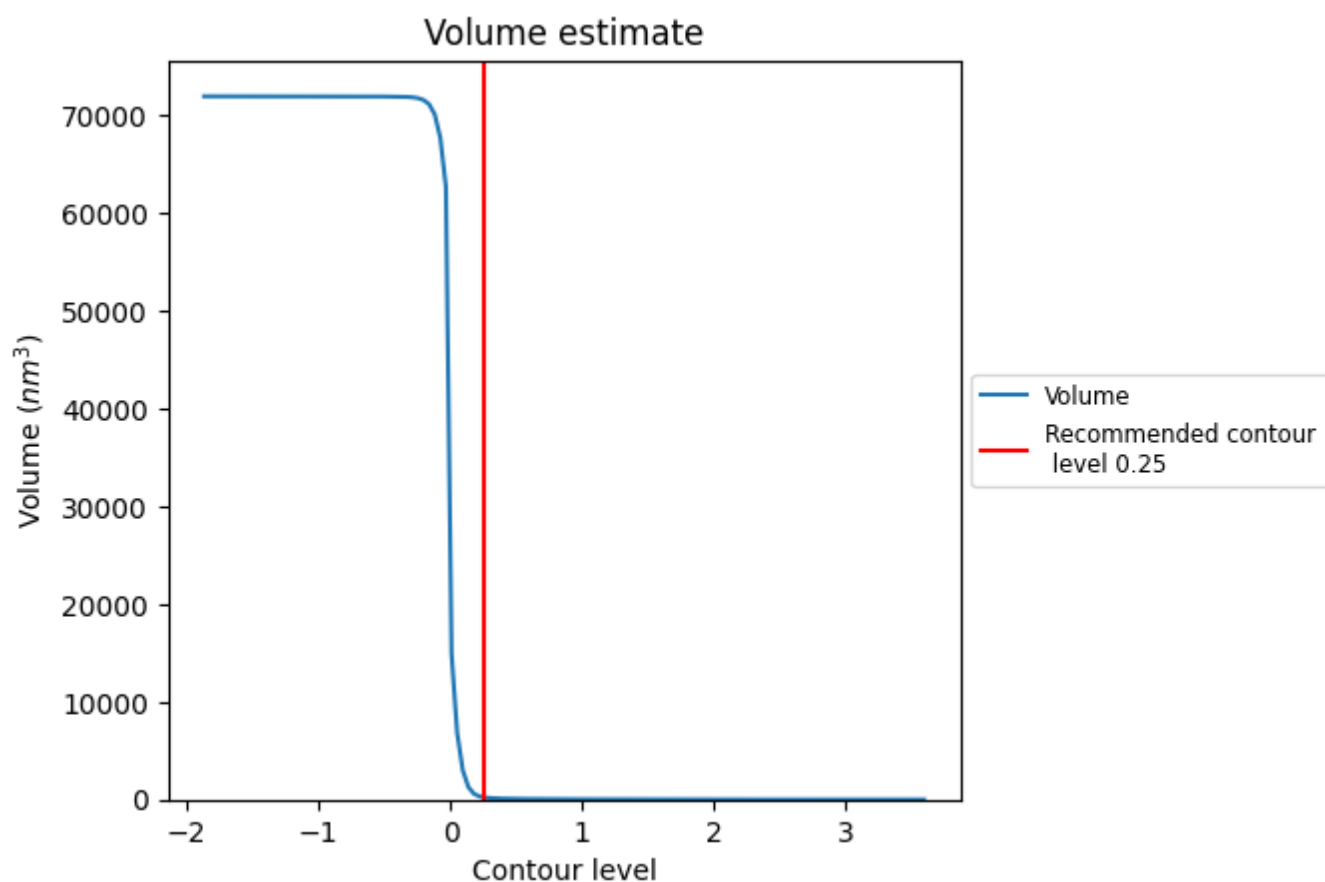
This section contains the results of statistical analysis of the map.

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.

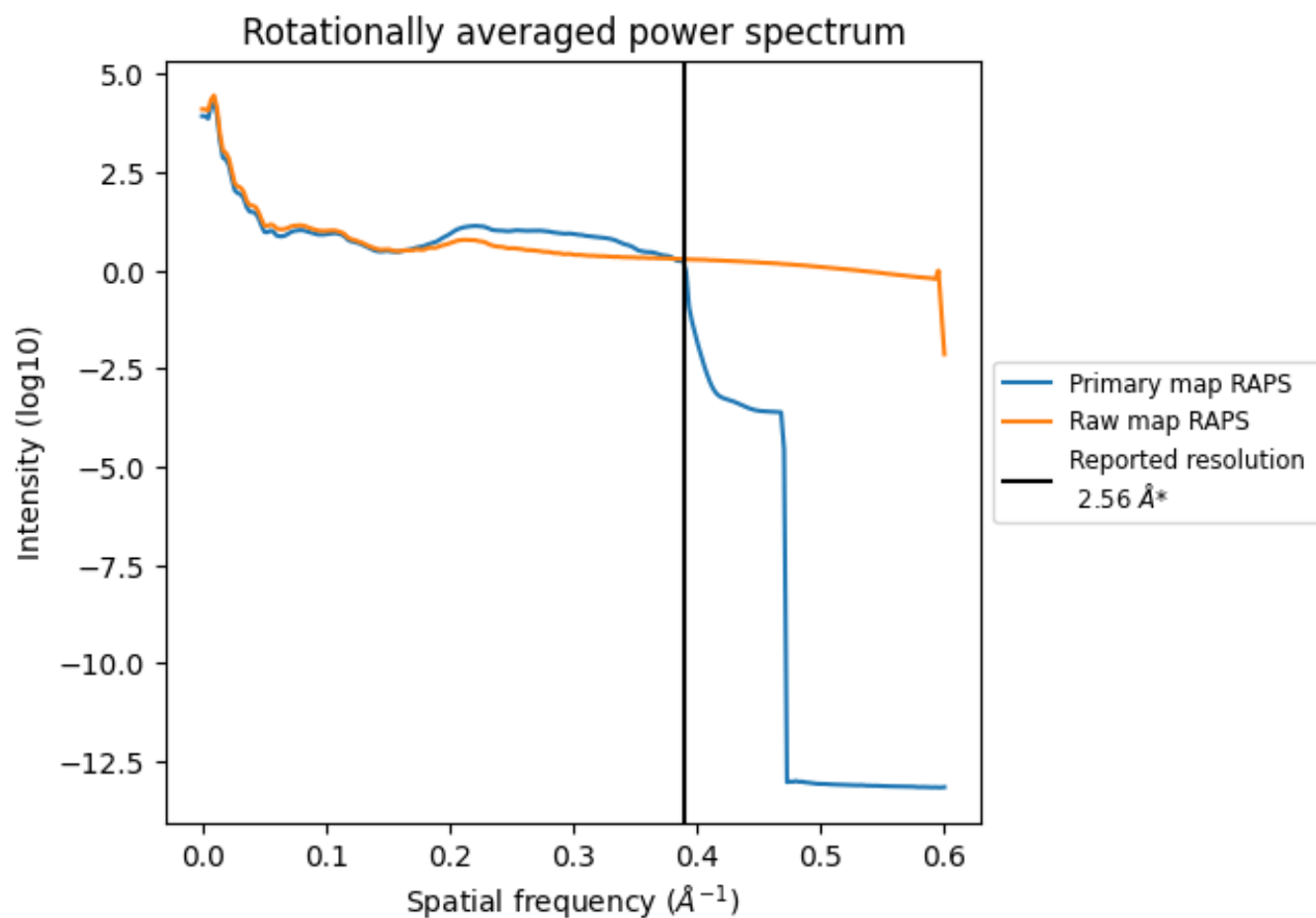
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm^3 ; this corresponds to an approximate mass of 220 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 ⓘ

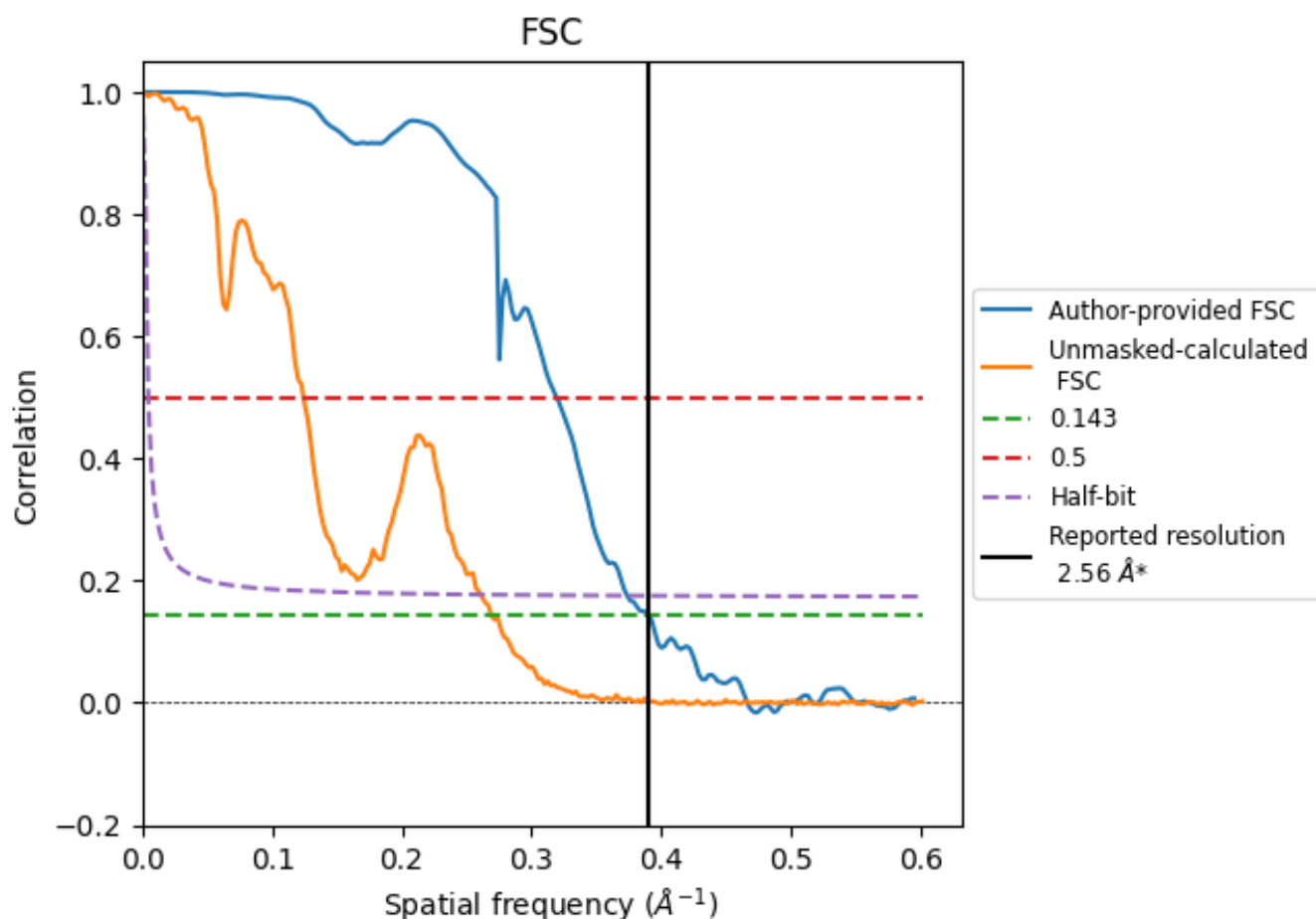


*Reported resolution corresponds to spatial frequency of 0.391 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.391 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

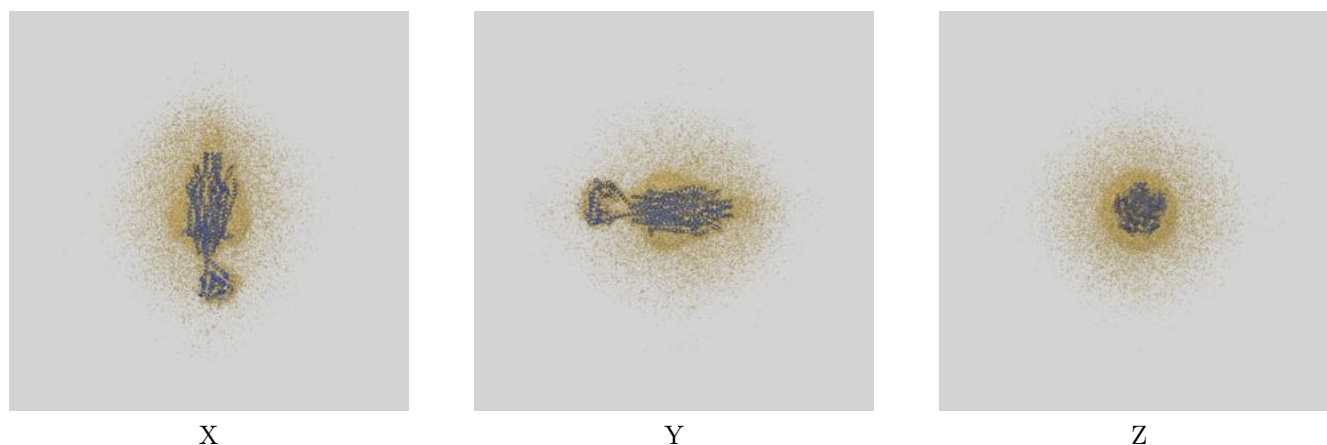
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.56	3.13	2.68
Unmasked-calculated*	3.72	8.05	3.83

*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 3.72 differs from the reported value 2.56 by more than 10 %

9 Map-model fit [i](#)

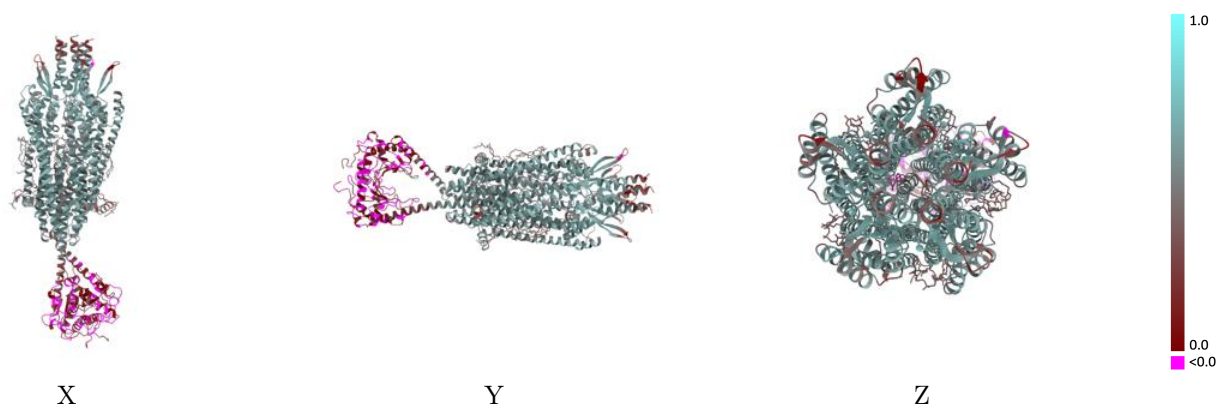
This section contains information regarding the fit between EMDB map EMD-18766 and PDB model 8QYY. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



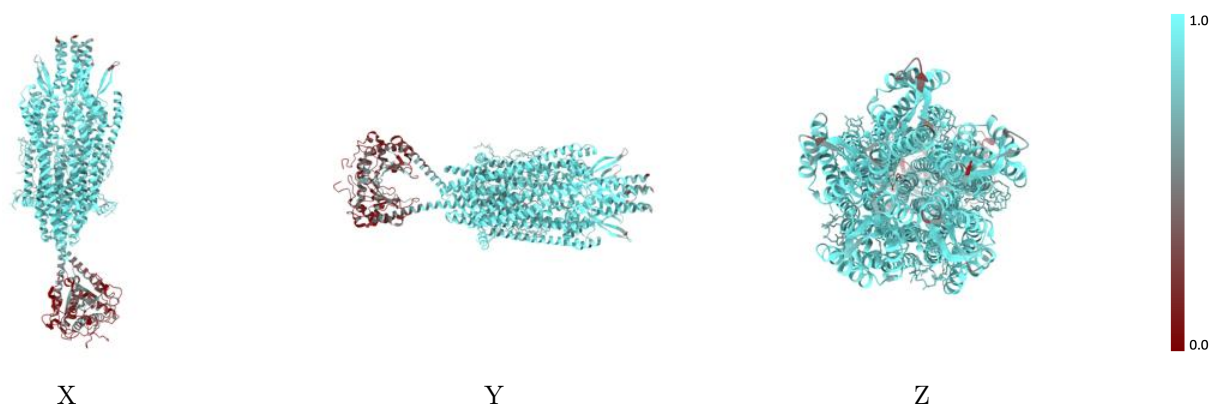
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



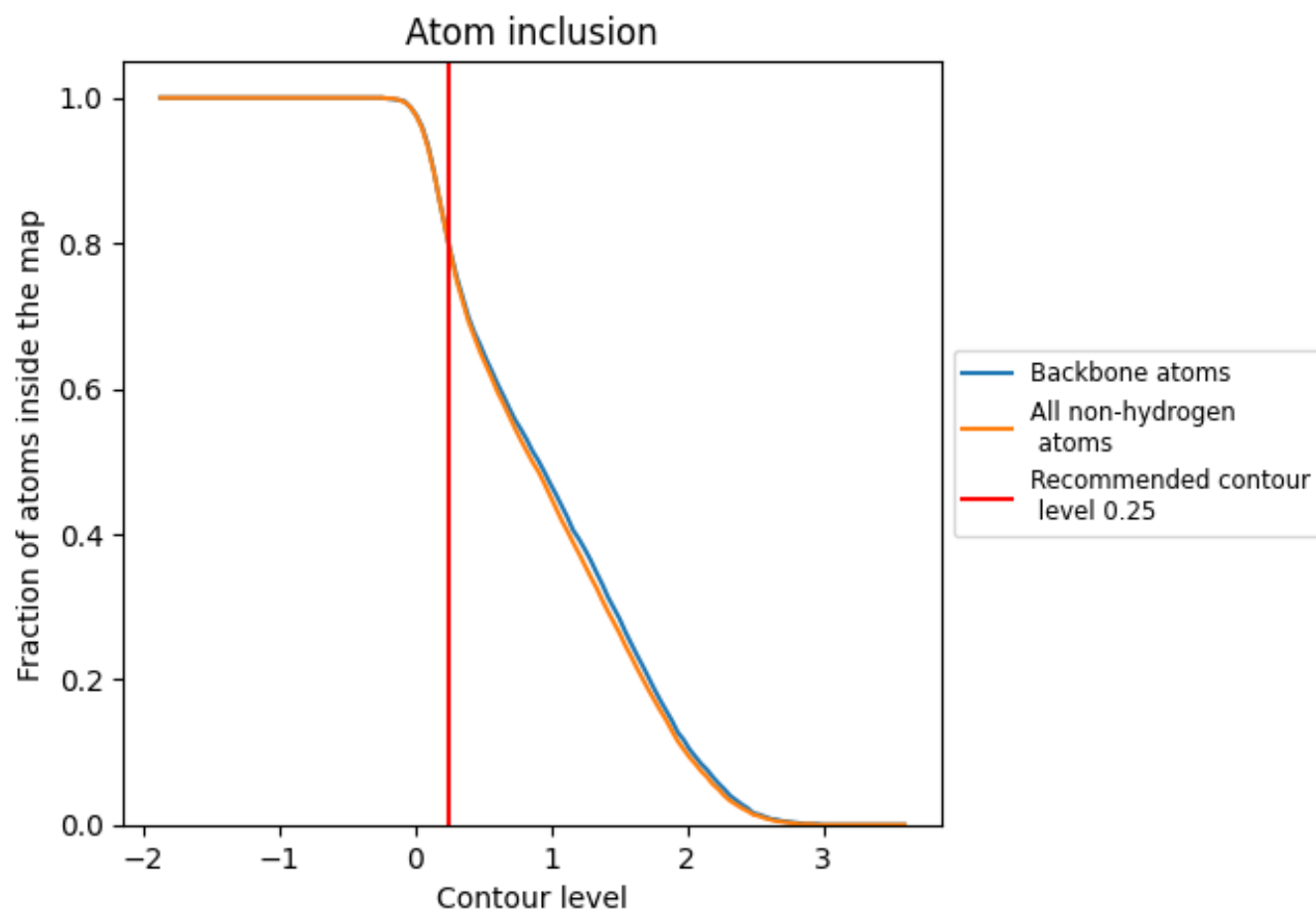
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.4480
A	0.9340	0.5590
B	0.9330	0.5560
C	0.9400	0.5640
D	0.9320	0.5470
E	0.9400	0.5640
F	0.4050	0.1460
G	0.4370	0.1630

1.0

0.0

<0.0