



## Full wwPDB EM Validation Report ⓘ

Oct 29, 2024 – 01:08 pm GMT

PDB ID : 8QYD  
EMDB ID : EMD-18751  
Title : Zorya anti-bacteriophage defense system ZorAB  
Authors : Hu, H.; Taylor, N.M.I.  
Deposited on : 2023-10-25  
Resolution : 2.67 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

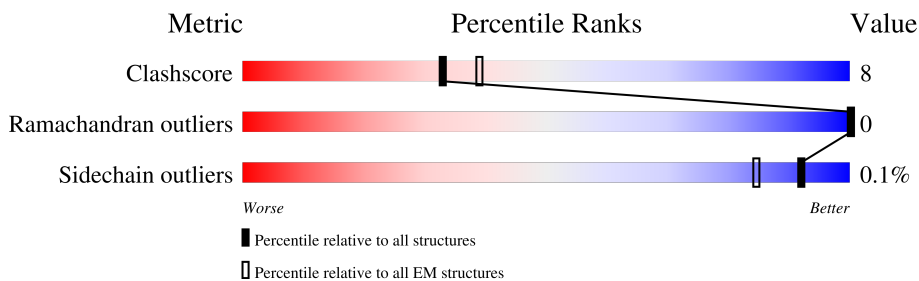
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.67 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	729	
1	B	729	
1	C	729	
1	D	729	
1	E	729	
2	F	246	
2	G	246	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16150 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.

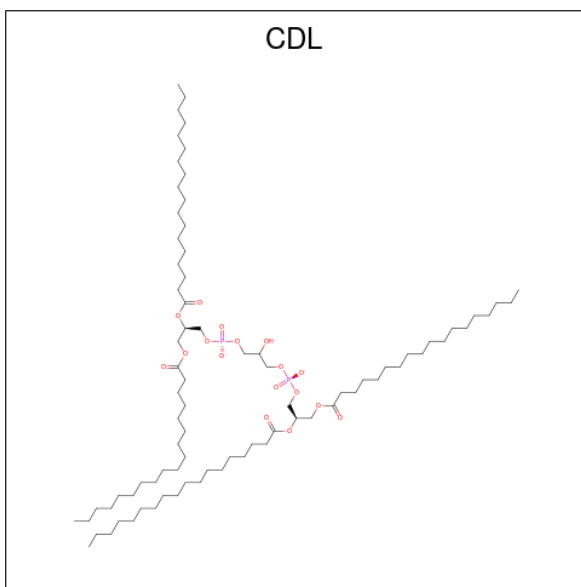
- Molecule 1 is a protein called Anti-phage defense ZorAB system ZorA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	280	2231	1446	364	416	5	1	0
1	B	280	2222	1441	360	416	5	0	0
1	C	280	2222	1441	360	416	5	0	0
1	D	280	2222	1441	360	416	5	0	0
1	E	280	2222	1441	360	416	5	0	0

- Molecule 2 is a protein called Membrane protein.

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

- Molecule 3 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).

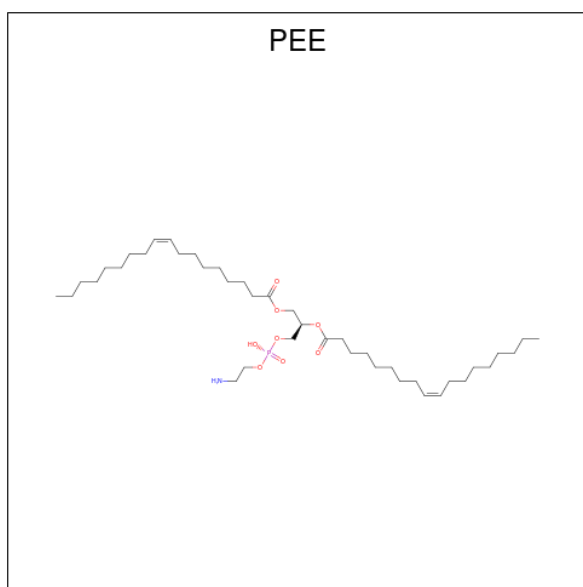


Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
3	A	1	100	81	17	2	0
3	B	1	100	81	17	2	0
3	C	1	100	81	17	2	0
3	D	1	100	81	17	2	0
3	E	1	100	81	17	2	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

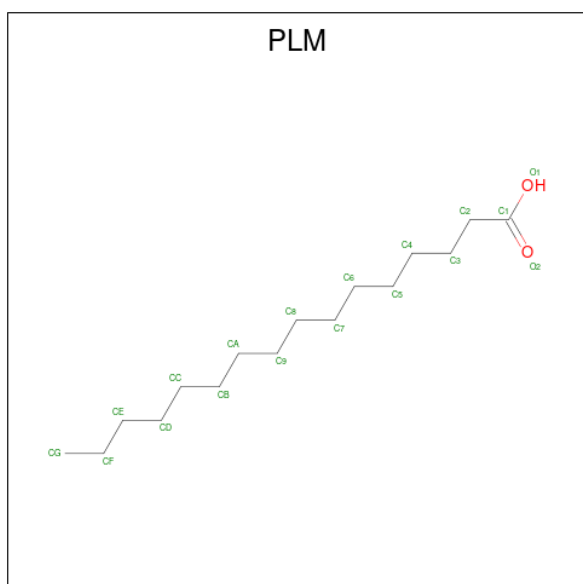
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	1	1	0
4	B	1	1	1	0
4	C	1	1	1	0
4	D	1	1	1	0
4	E	1	1	1	0

- Molecule 5 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	C	O	0
			18	16	2	

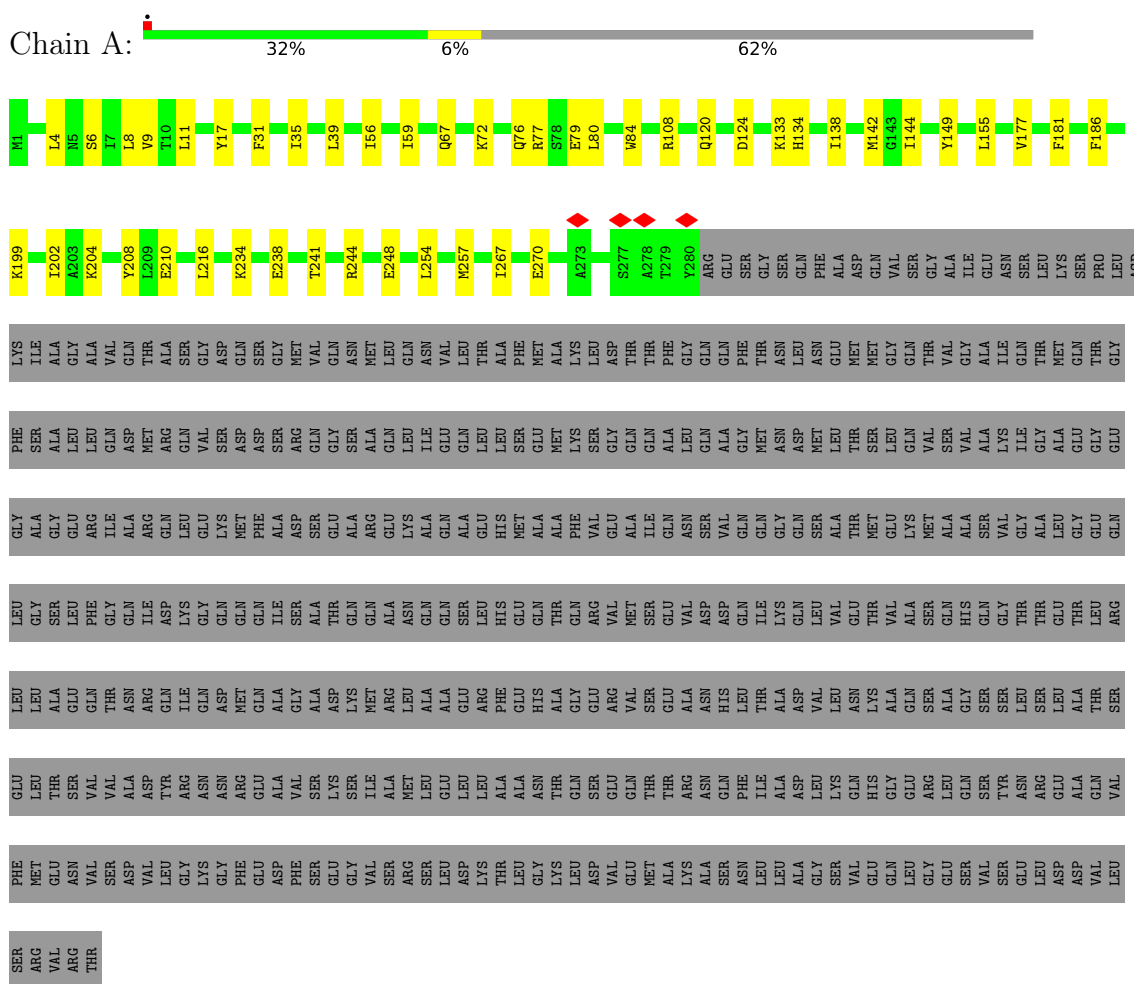
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	51	Total	O	0
			51	51	
7	B	65	Total	O	0
			65	65	
7	C	78	Total	O	0
			78	78	
7	D	61	Total	O	0
			61	61	
7	E	51	Total	O	0
			51	51	
7	F	4	Total	O	0
			4	4	
7	G	3	Total	O	0
			3	3	

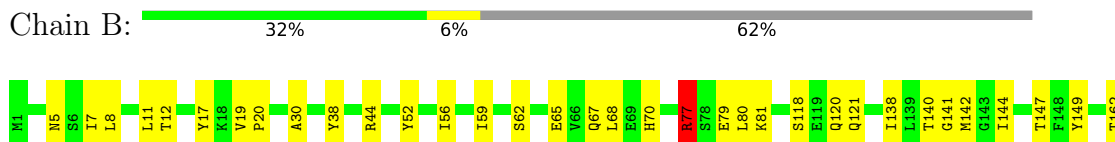
### 3 Residue-property plots

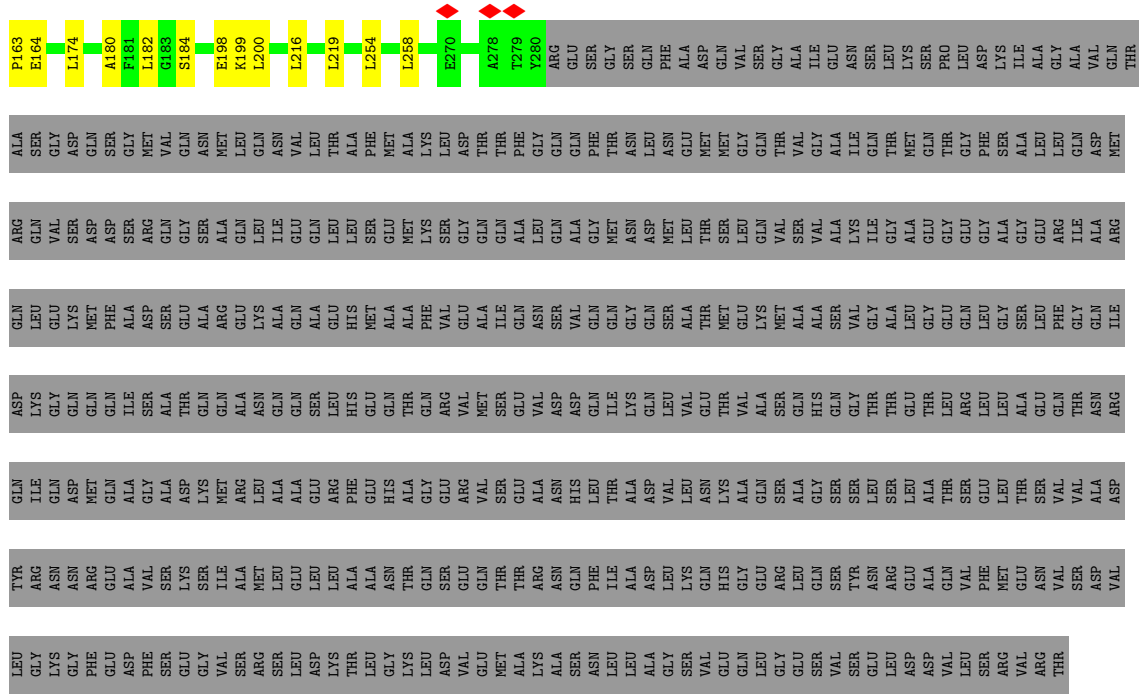
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

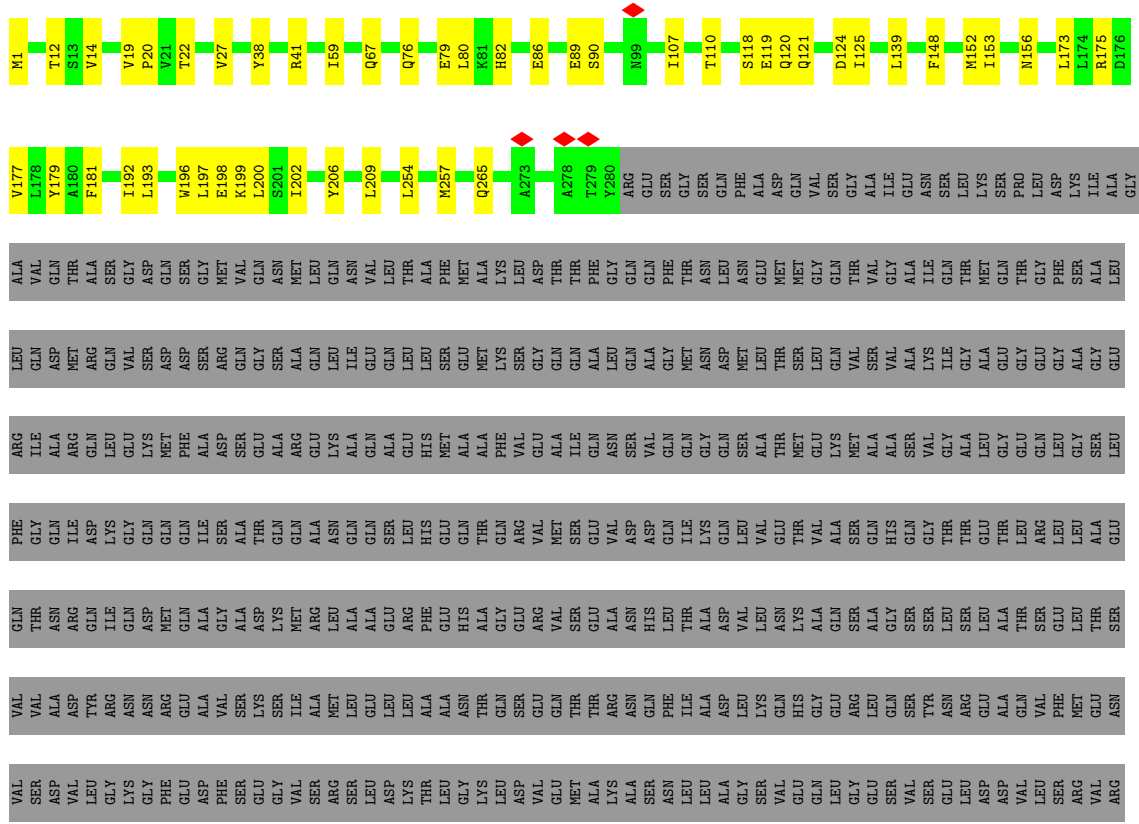


- Molecule 1: Anti-phage defense ZorAB system ZorA





● Molecule 1: Anti-phage defense ZorAB system ZorA



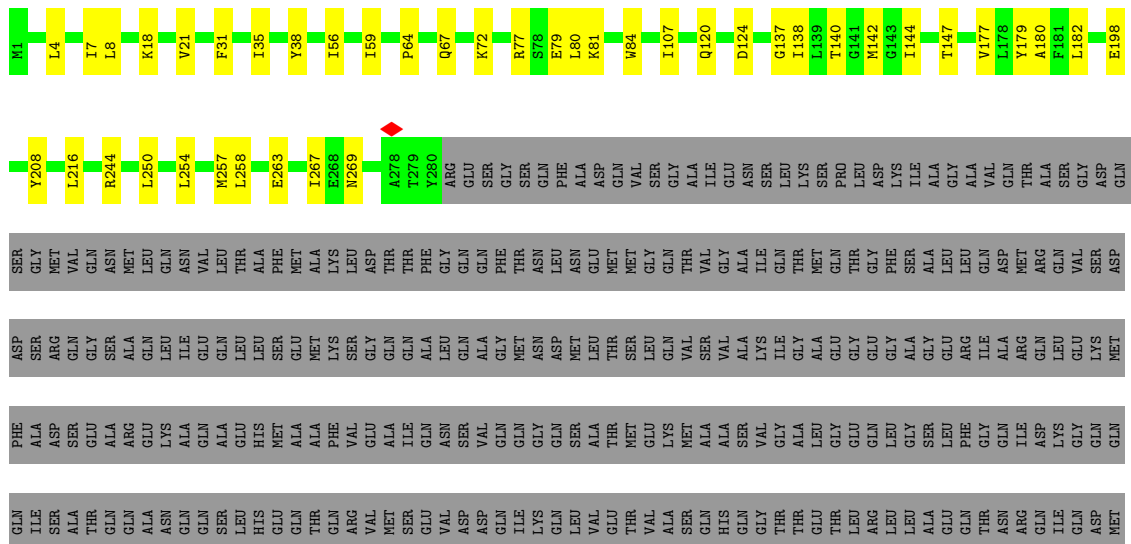


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• Molecule 1: Anti-phage defense ZorAB system ZorA



• Molecule 1: Anti-phage defense ZorAB system ZorA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227728	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	4.140	Depositor
Minimum map value	-2.414	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.068	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, 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	0.29	0/2281	0.46	0/3091
1	B	0.35	0/2270	0.53	2/3077 (0.1%)
1	C	0.29	0/2270	0.44	0/3077
1	D	0.29	0/2270	0.43	0/3077
1	E	0.28	0/2270	0.44	0/3077
2	F	0.26	0/2003	0.51	0/2690
2	G	0.26	0/2003	0.49	0/2690
All	All	0.29	0/15367	0.47	2/20779 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	CB-CA-C	10.96	132.32	110.40
1	B	77	ARG	N-CA-C	-6.92	92.33	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	ARG	Sidechain
1	B	77	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2231	0	2237	41	0
1	B	2222	0	2224	42	0
1	C	2222	0	2224	42	0
1	D	2222	0	2224	33	0
1	E	2222	0	2224	31	0
2	F	1970	0	1973	54	0
2	G	1970	0	1973	47	0
3	A	100	0	156	7	0
3	B	100	0	156	7	0
3	C	100	0	156	6	0
3	D	100	0	156	9	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	3	0
5	C	51	0	78	4	0
5	D	51	0	78	5	0
5	E	51	0	78	2	0
6	D	18	0	31	6	0
7	A	51	0	0	3	0
7	B	65	0	0	1	0
7	C	78	0	0	1	0
7	D	61	0	0	0	0
7	E	51	0	0	0	0
7	F	4	0	0	0	0
7	G	3	0	0	1	0
All	All	16150	0	16280	262	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 (262) 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	1.01
2:F:95:GLU:CD	2:F:98:ARG:HE	1.69	0.94
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	0.85
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
2:F:98:ARG:NH1	2:F:205:GLU:HB3	2.02	0.75
1:D:147:THR:OG1	1:D:184:SER:HB2	1.87	0.74
2:F:95:GLU:OE1	2:F:98:ARG:NE	2.15	0.74
1:A:72:LYS:HG2	1:A:84:TRP:HE1	1.53	0.73
2:G:76:ARG:NH2	2:G:82:ILE:O	2.21	0.73
2:F:95:GLU:CD	2:F:98:ARG:NE	2.44	0.71
1:B:59:ILE:HG21	1:B:70:HIS:CD2	2.26	0.70
1:E:79:GLU:HG3	1:E:80:LEU:HD12	1.73	0.70
1:E:72:LYS:HG2	1:E:84:TRP:HE1	1.57	0.69
1:A:181:PHE:HE2	2:F:33:VAL:HG21	1.55	0.69
2:F:95:GLU:OE2	2:F:98:ARG:NE	2.27	0.68
2:G:111:GLN:NE2	2:G:166:SER:HB2	2.07	0.68
1:E:177:VAL:HG11	2:F:34:LEU:HD11	1.76	0.68
2:F:157:LEU:HD11	2:G:157:LEU:HG	1.74	0.68
3:E:801:CDL:H572	3:E:801:CDL:H442	1.75	0.67
1:D:26:THR:HG21	5:D:802:PEE:H76	1.77	0.66
1:C:12:THR:HG21	1:C:156:ASN:HB3	1.78	0.66
2:F:98:ARG:NH1	2:F:205:GLU:C	2.50	0.65
1:E:120:GLN:HA	1:E:124:ASP:HB2	1.77	0.65
1:B:120:GLN:NE2	1:C:119:GLU:OE2	2.30	0.64
1:B:52:TYR:HE2	1:B:77:ARG:HH22	1.43	0.64
2:F:98:ARG:NH1	2:F:205:GLU:HB2	2.11	0.64
1:B:44:ARG:NH1	7:B:903:HOH:O	2.30	0.64
1:E:144:ILE:HD11	2:F:23:SER:HA	1.78	0.64
3:A:801:CDL:H631	3:A:801:CDL:H802	1.80	0.64
1:D:174:LEU:HD21	2:G:40:VAL:HG21	1.80	0.64
2:G:100:ALA:H	2:G:103:GLN:HE21	1.45	0.63
2:F:98:ARG:HH11	2:F:205:GLU:C	2.02	0.63
2:F:165:CYS:O	2:F:169:ASP:N	2.29	0.62
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:B:77:ARG:O	1:B:81:LYS:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:O	1:A:67:GLN:NE2	2.31	0.61
1:A:210:GLU:OE1	7:A:901:HOH:O	2.16	0.60
2:G:46:VAL:HG23	2:G:47:THR:HG23	1.83	0.60
1:B:5:ASN:OD1	1:C:175:ARG:NH2	2.34	0.60
6:D:803:PLM:HD1	1:E:258:LEU:HD21	1.84	0.60
1:A:39:LEU:HD21	3:A:801:CDL:H391	1.83	0.59
1:A:181:PHE:CE2	2:F:33:VAL:HG21	2.36	0.59
2:F:143:THR:OG1	2:F:156:SER:OG	2.20	0.59
2:F:60:ARG:NH1	2:F:217:PHE:O	2.35	0.59
1:B:163:PRO:HD3	2:G:48:GLN:HE21	1.67	0.59
1:C:121:GLN:NE2	1:D:210:GLU:OE2	2.30	0.59
1:E:147:THR:HA	1:E:180:ALA:HB1	1.84	0.59
1:A:76:GLN:NE2	7:A:909:HOH:O	2.34	0.59
1:E:208:TYR:OH	3:E:801:CDL:OA4	2.17	0.59
2:F:243:VAL:HG22	2:F:245:PRO:HD2	1.85	0.59
1:C:19:VAL:HG13	5:C:802:PEE:H60	1.85	0.59
1:B:79:GLU:HG3	1:B:80:LEU:HD12	1.84	0.58
2:F:187:ARG:NH2	2:F:238:GLU:OE2	2.35	0.58
1:B:147:THR:OG1	1:B:184:SER:HB2	2.04	0.58
1:C:254:LEU:HD21	6:D:803:PLM:H72	1.86	0.58
1:C:14:VAL:HG12	5:C:802:PEE:H1	1.86	0.58
1:A:234:LYS:O	1:A:238:GLU:HG3	2.04	0.57
2:F:84:VAL:HG22	2:F:91:ILE:HG23	1.86	0.57
2:G:93:PHE:O	2:G:97:GLY:N	2.37	0.57
2:F:98:ARG:HH11	2:F:205:GLU:CB	2.16	0.57
1:B:77:ARG:O	1:B:81:LYS:CB	2.52	0.56
1:D:59:ILE:O	1:D:67:GLN:NE2	2.35	0.56
2:F:35:PHE:HE1	2:G:36:LEU:HD13	1.71	0.56
2:G:100:ALA:N	2:G:103:GLN:HE21	2.04	0.56
2:F:63:ASP:OD2	2:F:132:LYS:NZ	2.33	0.56
2:F:35:PHE:CE1	2:G:36:LEU:HD13	2.41	0.55
1:A:208:TYR:OH	3:A:801:CDL:OA4	2.22	0.55
1:C:120:GLN:HA	1:C:124:ASP:HB2	1.88	0.55
1:A:257:MET:HB3	1:B:258:LEU:HD12	1.89	0.55
1:B:147:THR:HG23	1:B:180:ALA:HB1	1.89	0.55
2:F:98:ARG:HH11	2:F:205:GLU:HB3	1.67	0.55
1:A:124:ASP:OD2	2:F:10:LYS:NZ	2.33	0.54
1:D:79:GLU:OE2	1:D:79:GLU:N	2.28	0.54
2:F:187:ARG:HH12	2:G:149:TYR:HB2	1.71	0.54
2:G:188:LYS:NZ	2:G:229:VAL:O	2.35	0.54
1:B:38:TYR:CZ	1:B:198:GLU:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:135:LYS:HE2	2:G:217:PHE:CD2	2.43	0.54
2:F:194:GLY:HA2	2:G:193:GLY:HA3	1.90	0.54
2:F:84:VAL:HG13	2:F:91:ILE:HG12	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:49:ARG:NE	7:G:303:HOH:O	2.40	0.53
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
2:G:159:ARG:HH12	2:G:208:ARG:HE	1.57	0.52
1:A:254:LEU:HD13	1:E:254:LEU:HD21	1.92	0.52
1:B:138:ILE:O	1:B:142:MET:HG3	2.10	0.52
1:C:107:ILE:O	7:C:901:HOH:O	2.19	0.52
1:B:62:SER:HB2	1:B:67:GLN:HG3	1.92	0.51
1:B:140:THR:O	1:B:144:ILE:HG12	2.10	0.51
1:D:11:LEU:O	1:D:149:TYR:OH	2.20	0.51
1:D:198:GLU:OE2	1:D:199:LYS:HE2	2.10	0.51
1:E:56:ILE:HD13	1:E:216:LEU:HG	1.92	0.51
1:A:8:LEU:HD21	1:B:182:LEU:HD22	1.90	0.51
1:C:41:ARG:NH2	3:D:801:CDL:OB3	2.35	0.51
1:D:34:PHE:CE1	1:D:198:GLU:HB3	2.46	0.51
1:A:254:LEU:HB3	1:E:257:MET:HE3	1.93	0.51
1:B:162:THR:HG22	1:B:164:GLU:H	1.75	0.51
1:B:163:PRO:HD3	2:G:48:GLN:NE2	2.27	0.50
1:C:59:ILE:HG13	1:C:67:GLN:HG2	1.94	0.50
2:F:240:CYS:SG	2:F:242:LEU:HD23	2.51	0.50
2:G:143:THR:HA	2:G:208:ARG:HH22	1.77	0.50
1:B:118:SER:OG	1:B:121:GLN:HG3	2.11	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:D:120:GLN:HA	1:D:124:ASP:HB2	1.93	0.49
2:F:198:ASN:HA	2:G:229:VAL:HG11	1.94	0.49
1:A:133:LYS:NZ	2:F:14:ASP:OD2	2.36	0.49
1:D:250:LEU:HD21	6:D:803:PLM:H42	1.95	0.49
2:F:144:ASP:OD2	2:F:208:ARG:NH2	2.46	0.49
1:C:125:ILE:HD11	2:G:11:ARG:HH22	1.78	0.49
1:E:59:ILE:HD12	1:E:67:GLN:HB2	1.93	0.49
2:F:72:GLU:HG3	2:F:84:VAL:HB	1.95	0.49
2:G:119:PRO:HA	2:G:122:LEU:HD12	1.95	0.49
3:D:801:CDL:H161	3:D:801:CDL:H511	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HD13	1:A:216:LEU:HG	1.96	0.48
2:F:98:ARG:HH12	2:F:205:GLU:HB2	1.78	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:64:PRO:HB3	1:E:107:ILE:HG13	1.96	0.47
1:C:200:LEU:HD23	3:C:801:CDL:H371	1.97	0.47
1:E:18:LYS:HA	1:E:21:VAL:HG22	1.95	0.47
1:D:34:PHE:HE1	1:D:198:GLU:HB3	1.80	0.47
2:G:114:LEU:O	2:G:118:VAL:HG23	2.15	0.47
5:B:801:PEE:H75	3:B:802:CDL:H671	1.97	0.47
1:A:204:LYS:HG3	3:A:801:CDL:H312	1.96	0.47
1:C:27:VAL:HG13	1:C:139:LEU:HD22	1.96	0.47
3:D:801:CDL:H422	3:D:801:CDL:H391	1.52	0.47
1:A:31:PHE:O	1:A:35:ILE:HG12	2.15	0.46
1:A:241:THR:O	1:A:244:ARG:HG2	2.15	0.46
1:C:90:SER:O	1:C:110:THR:OG1	2.33	0.46
1:E:138:ILE:O	1:E:142:MET:HG3	2.15	0.46
2:G:213:ARG:NH1	2:G:215:GLN:HB3	2.30	0.46
1:B:59:ILE:O	1:B:67:GLN:NE2	2.38	0.46
1:C:197:LEU:HD11	3:C:801:CDL:H472	1.98	0.46
1:A:17:TYR:HB2	1:E:4:LEU:HD23	1.97	0.46
1:D:27:VAL:HG13	1:D:139:LEU:HD22	1.96	0.46
2:F:153:LEU:HD11	2:G:192:ALA:HB3	1.96	0.46
6:D:803:PLM:H41	1:E:250:LEU:HD21	1.97	0.46
1:A:4:LEU:HD23	1:B:17:TYR:HB2	1.98	0.46
1:C:193:LEU:HD13	3:C:801:CDL:H671	1.97	0.46
1:C:1:MET:HG3	1:D:17:TYR:HE2	1.80	0.46
1:C:254:LEU:HA	1:C:257:MET:HE3	1.96	0.46
1:D:152:MET:HA	1:D:152:MET:HE2	1.98	0.46
3:A:801:CDL:H722	3:A:801:CDL:H552	1.98	0.46
1:D:95:TYR:HB3	1:D:102:GLU:HG3	1.97	0.46
1:A:79:GLU:HG2	7:A:902:HOH:O	2.17	0.46
1:D:23:VAL:HG22	5:D:802:PEE:H70	1.97	0.46
1:A:254:LEU:HD23	1:A:257:MET:HE3	1.98	0.45
3:B:802:CDL:H422	3:B:802:CDL:H452	1.79	0.45
1:C:181:PHE:HZ	2:G:34:LEU:HB2	1.82	0.45
1:C:38:TYR:CZ	1:C:198:GLU:HG3	2.51	0.45
2:G:79:ASN:HD21	2:G:81:ASN:HB2	1.81	0.45
3:D:801:CDL:H812	3:D:801:CDL:H592	1.97	0.45
1:C:12:THR:HG23	1:C:153:ILE:HA	1.98	0.45
1:C:173:LEU:O	1:C:177:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ARG:O	1:E:81:LYS:N	2.45	0.45
1:D:11:LEU:HD13	5:D:802:PEE:H42	1.98	0.45
2:F:122:LEU:HD21	2:F:186:ILE:HG12	1.98	0.45
3:B:802:CDL:H742	3:B:802:CDL:H711	1.46	0.45
1:D:242:GLN:NE2	1:E:244:ARG:HG3	2.31	0.45
1:D:194:VAL:O	1:D:198:GLU:HG3	2.16	0.45
3:D:801:CDL:H371	3:D:801:CDL:H402	1.43	0.45
1:A:6:SER:HA	1:A:9:VAL:HG12	1.98	0.45
1:B:254:LEU:HD21	1:C:254:LEU:HD23	1.98	0.45
3:E:801:CDL:H722	3:E:801:CDL:H511	2.00	0.44
1:B:200:LEU:HD21	3:B:802:CDL:H122	1.99	0.44
1:C:79:GLU:HG3	1:C:80:LEU:HD22	2.00	0.44
2:G:98:ARG:HH12	2:G:206:ALA:HA	1.82	0.44
1:A:254:LEU:HD21	1:B:254:LEU:HD13	2.00	0.44
1:B:19:VAL:HB	1:B:20:PRO:HD3	1.98	0.44
2:F:148:SER:OG	2:G:238:GLU:OE1	2.28	0.44
1:B:56:ILE:HG23	1:B:219:LEU:HD11	1.99	0.44
3:D:801:CDL:H141	3:D:801:CDL:H111	1.81	0.44
2:F:12:ARG:HG2	2:G:12:ARG:NH1	2.32	0.44
1:E:140:THR:CG2	2:F:23:SER:HB3	2.47	0.44
1:C:265:GLN:NE2	1:D:265:GLN:OE1	2.51	0.44
2:G:184:LEU:O	2:G:188:LYS:HG2	2.18	0.44
2:F:130:GLY:HA2	2:F:134:PHE:HB2	2.00	0.43
1:A:144:ILE:HD11	2:G:21:TRP:CH2	2.53	0.43
1:A:155:LEU:HD22	1:B:174:LEU:HD22	2.00	0.43
1:A:199:LYS:HA	1:A:202:ILE:HG22	1.99	0.43
1:E:263:GLU:O	1:E:267:ILE:HG12	2.18	0.43
1:A:244:ARG:O	1:A:248:GLU:HG2	2.18	0.43
1:B:30:ALA:HB2	3:C:801:CDL:H781	2.00	0.43
1:A:11:LEU:HB3	1:A:149:TYR:HE1	1.84	0.43
2:F:134:PHE:CE1	2:F:214:MET:HB2	2.54	0.43
2:G:136:GLN:OE1	2:G:136:GLN:N	2.42	0.43
1:B:141:GLY:HA3	1:C:192:ILE:HG21	2.00	0.43
1:D:26:THR:HG23	3:E:801:CDL:H842	2.01	0.43
1:D:196:TRP:CZ2	3:D:801:CDL:H601	2.54	0.43
5:D:802:PEE:H43	1:E:182:LEU:HA	1.99	0.43
3:A:801:CDL:H522	3:A:801:CDL:HB61	2.01	0.43
1:B:144:ILE:HD12	2:G:27:LEU:HD22	2.01	0.43
5:B:801:PEE:H78	3:B:802:CDL:H272	2.01	0.43
1:D:109:ALA:N	1:D:221:ASP:O	2.47	0.43
1:D:272:LEU:HD13	1:E:269:ASN:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:O	1:B:12:THR:OG1	2.25	0.42
1:C:148:PHE:O	1:C:152:MET:HG3	2.18	0.42
1:C:199:LYS:HA	1:C:199:LYS:HD3	1.75	0.42
1:C:148:PHE:HB3	1:D:185:ALA:HB2	2.01	0.42
5:C:802:PEE:H72	5:C:802:PEE:H79	1.81	0.42
1:A:4:LEU:HD11	1:B:182:LEU:HD21	2.01	0.42
5:B:801:PEE:H75	3:B:802:CDL:H652	2.01	0.42
1:C:199:LYS:HA	1:C:202:ILE:HG22	2.01	0.42
1:A:11:LEU:O	1:A:149:TYR:OH	2.27	0.42
5:E:802:PEE:H73	5:E:802:PEE:H79	1.93	0.42
1:A:177:VAL:HG11	2:F:33:VAL:HG11	2.00	0.42
1:E:4:LEU:HD12	1:E:7:ILE:HD11	2.02	0.42
2:F:107:ASN:O	2:F:111:GLN:HG3	2.20	0.42
1:A:138:ILE:O	1:A:142:MET:HG3	2.19	0.41
1:A:267:ILE:O	1:A:270:GLU:HG3	2.19	0.41
1:D:96:GLU:HG3	1:D:105:VAL:HG11	2.02	0.41
1:E:137:GLY:HA2	2:F:19:PRO:HB3	2.01	0.41
2:G:66:ARG:NH1	2:G:70:ARG:HB2	2.36	0.41
1:B:147:THR:HA	1:B:180:ALA:HB1	2.02	0.41
1:C:76:GLN:HA	1:C:76:GLN:OE1	2.20	0.41
2:G:58:LYS:HB3	2:G:58:LYS:HE2	1.93	0.41
1:A:79:GLU:HG3	1:A:80:LEU:HD12	2.02	0.41
1:E:8:LEU:HD23	1:E:8:LEU:HA	1.91	0.41
1:A:134:HIS:CD2	1:B:199:LYS:HE3	2.55	0.41
3:A:801:CDL:H242	3:A:801:CDL:H271	1.82	0.41
1:C:22:THR:HG21	5:C:802:PEE:H59	2.03	0.41
1:D:149:TYR:CD1	5:D:802:PEE:H41	2.55	0.41
3:D:801:CDL:H442	3:D:801:CDL:H211	2.02	0.41
2:F:153:LEU:HD22	2:G:164:MET:HG2	2.02	0.41
1:B:38:TYR:CE1	1:B:198:GLU:HG2	2.56	0.41
1:C:118:SER:OG	1:C:121:GLN:HG2	2.20	0.41
3:B:802:CDL:H141	3:B:802:CDL:H772	2.01	0.41
1:C:59:ILE:HG13	1:C:59:ILE:O	2.20	0.41
1:C:89:GLU:OE1	1:D:221:ASP:HA	2.20	0.41
1:C:196:TRP:CZ2	3:C:801:CDL:H612	2.56	0.41
3:D:801:CDL:H332	3:D:801:CDL:H361	1.87	0.41
2:G:115:GLN:HA	2:G:174:LEU:HD12	2.02	0.41
1:A:254:LEU:HD11	6:D:803:PLM:H61	2.03	0.41
3:C:801:CDL:H242	3:C:801:CDL:H211	1.97	0.41
1:D:199:LYS:HA	1:D:199:LYS:HD3	1.78	0.41
2:G:31:MET:HB3	2:G:31:MET:HE2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HA	1:A:108:ARG:HD2	1.94	0.41
1:A:186:PHE:CD1	5:E:802:PEE:H41	2.56	0.41
1:C:119:GLU:HG2	1:C:206:TYR:CD1	2.56	0.41
2:F:66:ARG:O	2:F:70:ARG:HG2	2.21	0.40
2:F:149:TYR:HD2	2:F:150:LEU:HD22	1.85	0.40
1:A:120:GLN:HB2	2:F:10:LYS:HD3	2.02	0.40
1:B:65:GLU:O	1:B:68:LEU:N	2.54	0.40
1:E:31:PHE:O	1:E:35:ILE:HG12	2.21	0.40
3:E:801:CDL:H191	3:E:801:CDL:H162	1.47	0.40
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.92	0.40
6:D:803:PLM:C4	1:E:250:LEU:HD21	2.51	0.40
3:E:801:CDL:H311	3:E:801:CDL:H341	1.55	0.40
2:G:70:ARG:HH22	2:G:127:SER:HB3	1.86	0.40
1:B:59:ILE:HG21	1:B:70:HIS:CG	2.55	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:F:134:PHE:HE1	2:F:214:MET:HB2	1.86	0.40
2:G:69:GLU:HA	2:G:72:GLU:HG3	2.04	0.40
2:G:135:LYS:HD2	2:G:215:GLN:HE22	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/729 (38%)	274 (98%)	5 (2%)	0	100	100
1	B	278/729 (38%)	273 (98%)	5 (2%)	0	100	100
1	C	278/729 (38%)	275 (99%)	3 (1%)	0	100	100
1	D	278/729 (38%)	276 (99%)	2 (1%)	0	100	100
1	E	278/729 (38%)	272 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	1879/4137 (45%)	1847 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [\(i\)](#)

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	245/615 (40%)	245 (100%)	0	100	100
1	B	244/615 (40%)	243 (100%)	1 (0%)	89	96
1	C	244/615 (40%)	244 (100%)	0	100	100
1	D	244/615 (40%)	243 (100%)	1 (0%)	89	96
1	E	244/615 (40%)	244 (100%)	0	100	100
2	F	215/215 (100%)	215 (100%)	0	100	100
2	G	215/215 (100%)	215 (100%)	0	100	100
All	All	1651/3505 (47%)	1649 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	ARG
1	D	234	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	48	GLN
2	G	103	GLN
2	G	111	GLN

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Mol	Chain	Res	Type
2	G	215	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEE	B	803	-	50,50,50	1.42	7 (14%)	53,55,55	1.60	7 (13%)
5	PEE	B	801	-	50,50,50	1.50	8 (16%)	53,55,55	1.63	6 (11%)
5	PEE	E	802	-	50,50,50	1.42	7 (14%)	53,55,55	1.61	7 (13%)
3	CDL	E	801	-	99,99,99	0.32	0	105,111,111	0.20	0
3	CDL	C	801	-	99,99,99	0.29	0	105,111,111	0.20	0
5	PEE	C	802	-	50,50,50	1.44	9 (18%)	53,55,55	1.63	7 (13%)
3	CDL	A	801	-	99,99,99	0.30	0	105,111,111	0.19	0
3	CDL	B	802	-	99,99,99	0.29	0	105,111,111	0.20	0
6	PLM	D	803	-	17,17,17	0.57	0	17,17,17	0.56	0
5	PEE	D	802	-	50,50,50	1.46	9 (18%)	53,55,55	1.64	6 (11%)
3	CDL	D	801	-	99,99,99	0.30	0	105,111,111	0.19	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	B	803	-	-	20/54/54/54	-
5	PEE	B	801	-	-	30/54/54/54	-
5	PEE	E	802	-	-	26/54/54/54	-
3	CDL	E	801	-	-	67/110/110/110	-
3	CDL	C	801	-	-	67/110/110/110	-
5	PEE	C	802	-	-	29/54/54/54	-
3	CDL	A	801	-	-	64/110/110/110	-
3	CDL	B	802	-	-	67/110/110/110	-
6	PLM	D	803	-	-	9/15/15/15	-
5	PEE	D	802	-	-	26/54/54/54	-
3	CDL	D	801	-	-	70/110/110/110	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	PEE	C3-C2	4.09	1.63	1.50
5	D	802	PEE	C3-C2	4.01	1.63	1.50
5	C	802	PEE	C3-C2	3.88	1.62	1.50
5	B	803	PEE	C3-C2	3.85	1.62	1.50
5	E	802	PEE	C3-C2	3.76	1.62	1.50
5	B	801	PEE	P-O4P	3.19	1.72	1.59
5	E	802	PEE	P-O3P	3.14	1.72	1.59
5	C	802	PEE	P-O4P	3.14	1.72	1.59
5	D	802	PEE	P-O3P	3.13	1.72	1.59
5	C	802	PEE	P-O3P	3.12	1.71	1.59
5	B	801	PEE	P-O3P	3.11	1.71	1.59
5	B	803	PEE	P-O4P	3.10	1.71	1.59
5	D	802	PEE	P-O4P	3.09	1.71	1.59
5	B	803	PEE	P-O3P	3.09	1.71	1.59
5	E	802	PEE	P-O4P	3.05	1.71	1.59
5	B	801	PEE	C31-C30	2.62	1.58	1.50
5	B	801	PEE	O3-C30	2.33	1.40	1.33
5	C	802	PEE	C12-C11	2.25	1.60	1.52
5	D	802	PEE	C12-C11	2.21	1.60	1.52
5	D	802	PEE	C11-C10	2.20	1.57	1.50
5	D	802	PEE	C31-C30	2.18	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	802	PEE	O3-C30	2.15	1.39	1.33
5	C	802	PEE	C11-C10	2.14	1.57	1.50
5	C	802	PEE	O2-C10	2.14	1.40	1.34
5	E	802	PEE	C12-C11	2.13	1.60	1.52
5	D	802	PEE	O2-C10	2.12	1.40	1.34
5	E	802	PEE	O2-C10	2.11	1.40	1.34
5	C	802	PEE	C5-C4	2.10	1.58	1.50
5	B	801	PEE	C5-C4	2.09	1.58	1.50
5	B	801	PEE	C12-C11	2.08	1.59	1.52
5	B	803	PEE	O3-C30	2.07	1.39	1.33
5	C	802	PEE	C31-C30	2.07	1.56	1.50
5	D	802	PEE	C5-C4	2.06	1.58	1.50
5	C	802	PEE	O3-C30	2.03	1.39	1.33
5	E	802	PEE	C5-C4	2.03	1.58	1.50
5	B	801	PEE	O2-C10	2.03	1.40	1.34
5	B	803	PEE	C12-C11	2.03	1.59	1.52
5	B	803	PEE	C5-C4	2.02	1.58	1.50
5	E	802	PEE	O3-C30	2.01	1.39	1.33
5	B	803	PEE	C31-C30	2.00	1.56	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	802	PEE	O2-C10-C11	6.05	124.54	111.50
5	C	802	PEE	O2-C10-C11	5.97	124.36	111.50
5	B	801	PEE	O2-C10-C11	5.90	124.22	111.50
5	E	802	PEE	O2-C10-C11	5.73	123.86	111.50
5	B	803	PEE	O2-C10-C11	5.63	123.63	111.50
5	B	801	PEE	C40-C39-C38	5.19	164.56	124.73
5	D	802	PEE	C40-C39-C38	5.19	164.55	124.73
5	D	802	PEE	C37-C38-C39	5.14	164.18	124.73
5	E	802	PEE	C40-C39-C38	5.13	164.06	124.73
5	B	801	PEE	C37-C38-C39	5.11	163.96	124.73
5	C	802	PEE	C40-C39-C38	5.10	163.89	124.73
5	B	803	PEE	C40-C39-C38	5.09	163.82	124.73
5	C	802	PEE	C37-C38-C39	5.08	163.69	124.73
5	E	802	PEE	C37-C38-C39	5.06	163.54	124.73
5	B	803	PEE	C37-C38-C39	5.04	163.41	124.73
5	B	801	PEE	O3-C30-C31	3.82	123.88	111.91
5	C	802	PEE	O3-C30-C31	3.74	123.65	111.91
5	D	802	PEE	O3-C30-C31	3.74	123.65	111.91
5	B	803	PEE	O3-C30-C31	3.73	123.62	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	802	PEE	O3-C30-C31	3.68	123.46	111.91
5	B	801	PEE	O3-C30-O5	-2.60	117.03	123.59
5	C	802	PEE	O3-C30-O5	-2.56	117.12	123.59
5	B	803	PEE	O3-C30-O5	-2.56	117.13	123.59
5	D	802	PEE	O2-C10-O4	-2.54	117.57	123.70
5	D	802	PEE	O3-C30-O5	-2.49	117.30	123.59
5	E	802	PEE	O3-C30-O5	-2.49	117.31	123.59
5	C	802	PEE	O2-C10-O4	-2.46	117.76	123.70
5	B	801	PEE	O2-C10-O4	-2.45	117.79	123.70
5	B	803	PEE	O2-C10-O4	-2.36	118.00	123.70
5	E	802	PEE	O2-C10-O4	-2.35	118.01	123.70
5	E	802	PEE	C3-C2-C1	-2.20	106.58	111.79
5	B	803	PEE	C3-C2-C1	-2.15	106.71	111.79
5	C	802	PEE	C3-C2-C1	-2.05	106.95	111.79

There are no chirality outliers.

All (475) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	CDL	CA2-OA2-PA1-OA3
3	A	801	CDL	CA2-OA2-PA1-OA4
3	A	801	CDL	CB2-OB2-PB2-OB5
3	B	802	CDL	CA2-OA2-PA1-OA3
3	B	802	CDL	CA2-OA2-PA1-OA4
3	B	802	CDL	CA3-OA5-PA1-OA4
3	B	802	CDL	CB2-OB2-PB2-OB3
3	B	802	CDL	CB3-OB5-PB2-OB3
3	C	801	CDL	CA2-OA2-PA1-OA5
3	C	801	CDL	CA3-OA5-PA1-OA3
3	C	801	CDL	CB2-OB2-PB2-OB3
3	C	801	CDL	CB3-OB5-PB2-OB3
3	C	801	CDL	CB3-OB5-PB2-OB4
3	D	801	CDL	CA2-OA2-PA1-OA3
3	D	801	CDL	CA3-OA5-PA1-OA3
3	D	801	CDL	C11-CA5-OA6-CA4
3	D	801	CDL	CB2-OB2-PB2-OB3
3	D	801	CDL	CB2-OB2-PB2-OB4
3	D	801	CDL	CB3-OB5-PB2-OB3
3	E	801	CDL	CA2-OA2-PA1-OA3
3	E	801	CDL	CA2-OA2-PA1-OA4
3	E	801	CDL	CA2-OA2-PA1-OA5
3	E	801	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
3	E	801	CDL	CB2-OB2-PB2-OB4
3	E	801	CDL	CB2-OB2-PB2-OB5
5	B	801	PEE	C11-C10-O2-C2
5	B	801	PEE	O4-C10-O2-C2
5	B	801	PEE	O3P-C1-C2-O2
5	C	802	PEE	O4-C10-O2-C2
5	C	802	PEE	C4-O4P-P-O1P
5	D	802	PEE	C11-C10-O2-C2
5	D	802	PEE	O4-C10-O2-C2
5	D	802	PEE	C4-O4P-P-O1P
5	E	802	PEE	C11-C10-O2-C2
5	E	802	PEE	O4-C10-O2-C2
5	E	802	PEE	O4P-C4-C5-N
3	A	801	CDL	OB9-CB7-OB8-CB6
3	B	802	CDL	OB9-CB7-OB8-CB6
3	D	801	CDL	OB9-CB7-OB8-CB6
3	E	801	CDL	OA9-CA7-OA8-CA6
5	D	802	PEE	O5-C30-O3-C3
3	D	801	CDL	OA7-CA5-OA6-CA4
3	B	802	CDL	C71-CB7-OB8-CB6
3	D	801	CDL	C71-CB7-OB8-CB6
3	E	801	CDL	C31-CA7-OA8-CA6
5	D	802	PEE	C31-C30-O3-C3
5	C	802	PEE	C11-C10-O2-C2
3	A	801	CDL	OA9-CA7-OA8-CA6
5	B	803	PEE	C43-C44-C45-C46
3	A	801	CDL	C71-CB7-OB8-CB6
3	D	801	CDL	C37-C38-C39-C40
5	E	802	PEE	C43-C44-C45-C46
3	D	801	CDL	O1-C1-CB2-OB2
3	A	801	CDL	C37-C38-C39-C40
5	B	801	PEE	C43-C44-C45-C46
3	A	801	CDL	C51-CB5-OB6-CB4
3	E	801	CDL	C16-C17-C18-C19
3	E	801	CDL	C40-C41-C42-C43
3	D	801	CDL	C77-C78-C79-C80
5	C	802	PEE	C43-C44-C45-C46
3	A	801	CDL	C31-CA7-OA8-CA6
3	B	802	CDL	C71-C72-C73-C74
5	D	802	PEE	C43-C44-C45-C46
3	B	802	CDL	C59-C60-C61-C62
3	C	801	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
3	D	801	CDL	C11-C12-C13-C14
3	C	801	CDL	C58-C59-C60-C61
3	D	801	CDL	C39-C40-C41-C42
3	D	801	CDL	C82-C83-C84-C85
3	B	802	CDL	C42-C43-C44-C45
3	D	801	CDL	CA2-C1-CB2-OB2
3	E	801	CDL	C31-C32-C33-C34
3	A	801	CDL	CB7-C71-C72-C73
3	A	801	CDL	OB7-CB5-OB6-CB4
3	B	802	CDL	C11-CA5-OA6-CA4
3	D	801	CDL	C33-C34-C35-C36
5	C	802	PEE	C31-C30-O3-C3
3	C	801	CDL	CB7-C71-C72-C73
3	E	801	CDL	CB5-C51-C52-C53
5	B	803	PEE	C30-C31-C32-C33
3	B	802	CDL	CB7-C71-C72-C73
3	E	801	CDL	CA5-C11-C12-C13
3	E	801	CDL	CB7-C71-C72-C73
6	D	803	PLM	C1-C2-C3-C4
5	C	802	PEE	C40-C41-C42-C43
3	E	801	CDL	CA7-C31-C32-C33
3	E	801	CDL	C51-CB5-OB6-CB4
3	A	801	CDL	CA7-C31-C32-C33
3	A	801	CDL	CA2-OA2-PA1-OA5
3	B	802	CDL	CA2-OA2-PA1-OA5
3	B	802	CDL	CA3-OA5-PA1-OA2
3	B	802	CDL	CB2-OB2-PB2-OB5
3	C	801	CDL	CB2-OB2-PB2-OB5
3	C	801	CDL	CB3-OB5-PB2-OB2
3	D	801	CDL	CB2-OB2-PB2-OB5
3	E	801	CDL	CB3-OB5-PB2-OB2
5	B	803	PEE	C4-O4P-P-O3P
3	B	802	CDL	OA7-CA5-OA6-CA4
3	E	801	CDL	OB7-CB5-OB6-CB4
3	D	801	CDL	C15-C16-C17-C18
3	E	801	CDL	C38-C39-C40-C41
5	D	802	PEE	C40-C41-C42-C43
5	D	802	PEE	C34-C35-C36-C37
3	B	802	CDL	C11-C12-C13-C14
3	B	802	CDL	C63-C64-C65-C66
3	C	801	CDL	C57-C58-C59-C60
5	B	803	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	A	801	CDL	C74-C75-C76-C77
3	C	801	CDL	C37-C38-C39-C40
5	B	803	PEE	C34-C35-C36-C37
5	B	803	PEE	C40-C41-C42-C43
3	D	801	CDL	C13-C14-C15-C16
3	E	801	CDL	C11-C12-C13-C14
5	E	802	PEE	C12-C13-C14-C15
3	C	801	CDL	C11-C12-C13-C14
3	D	801	CDL	C40-C41-C42-C43
3	C	801	CDL	C63-C64-C65-C66
5	B	801	PEE	C22-C23-C24-C25
3	A	801	CDL	C52-C53-C54-C55
3	B	802	CDL	C17-C18-C19-C20
3	B	802	CDL	C78-C79-C80-C81
3	C	801	CDL	C75-C76-C77-C78
3	D	801	CDL	C61-C62-C63-C64
5	B	803	PEE	C11-C12-C13-C14
5	E	802	PEE	C31-C32-C33-C34
5	C	802	PEE	O5-C30-O3-C3
3	A	801	CDL	C32-C33-C34-C35
3	C	801	CDL	C33-C34-C35-C36
3	C	801	CDL	C74-C75-C76-C77
3	D	801	CDL	C38-C39-C40-C41
3	E	801	CDL	C20-C21-C22-C23
5	B	801	PEE	C13-C14-C15-C16
3	D	801	CDL	C16-C17-C18-C19
3	D	801	CDL	C73-C74-C75-C76
3	E	801	CDL	C51-C52-C53-C54
5	B	801	PEE	C40-C41-C42-C43
3	C	801	CDL	C32-C33-C34-C35
3	D	801	CDL	C60-C61-C62-C63
3	E	801	CDL	C61-C62-C63-C64
3	A	801	CDL	OA7-CA5-OA6-CA4
3	A	801	CDL	C11-CA5-OA6-CA4
5	B	801	PEE	C21-C22-C23-C24
5	B	801	PEE	C20-C21-C22-C23
5	E	802	PEE	C19-C20-C21-C22
3	A	801	CDL	C17-C18-C19-C20
3	A	801	CDL	C20-C21-C22-C23
3	A	801	CDL	C39-C40-C41-C42
3	A	801	CDL	C57-C58-C59-C60
3	B	802	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
3	C	801	CDL	C35-C36-C37-C38
3	B	802	CDL	C37-C38-C39-C40
5	C	802	PEE	C34-C35-C36-C37
3	B	802	CDL	C34-C35-C36-C37
3	B	802	CDL	C52-C53-C54-C55
3	D	801	CDL	C19-C20-C21-C22
3	D	801	CDL	C78-C79-C80-C81
5	B	803	PEE	C20-C21-C22-C23
5	E	802	PEE	C11-C12-C13-C14
3	A	801	CDL	C12-C13-C14-C15
3	C	801	CDL	C31-CA7-OA8-CA6
3	B	802	CDL	C62-C63-C64-C65
3	E	801	CDL	C55-C56-C57-C58
5	D	802	PEE	C21-C22-C23-C24
3	E	801	CDL	C17-C18-C19-C20
5	C	802	PEE	C13-C14-C15-C16
3	B	802	CDL	C61-C62-C63-C64
3	D	801	CDL	C53-C54-C55-C56
3	E	801	CDL	C71-C72-C73-C74
3	B	802	CDL	C20-C21-C22-C23
3	B	802	CDL	C32-C33-C34-C35
5	B	801	PEE	C11-C12-C13-C14
5	B	801	PEE	C31-C32-C33-C34
3	A	801	CDL	C54-C55-C56-C57
3	E	801	CDL	C15-C16-C17-C18
3	B	802	CDL	C13-C14-C15-C16
3	C	801	CDL	C55-C56-C57-C58
3	D	801	CDL	C57-C58-C59-C60
3	A	801	CDL	C31-C32-C33-C34
5	C	802	PEE	C15-C16-C17-C18
3	A	801	CDL	C35-C36-C37-C38
3	D	801	CDL	C17-C18-C19-C20
3	A	801	CDL	C36-C37-C38-C39
5	B	801	PEE	C41-C42-C43-C44
5	B	803	PEE	C32-C33-C34-C35
3	D	801	CDL	CA7-C31-C32-C33
3	B	802	CDL	C72-C73-C74-C75
5	E	802	PEE	C32-C33-C34-C35
3	D	801	CDL	C20-C21-C22-C23
3	B	802	CDL	C40-C41-C42-C43
3	D	801	CDL	C72-C73-C74-C75
3	E	801	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
3	C	801	CDL	C39-C40-C41-C42
3	E	801	CDL	C59-C60-C61-C62
3	C	801	CDL	OA9-CA7-OA8-CA6
3	D	801	CDL	C36-C37-C38-C39
5	B	801	PEE	C19-C20-C21-C22
5	B	801	PEE	C15-C16-C17-C18
3	C	801	CDL	OB7-CB5-OB6-CB4
3	B	802	CDL	C44-C45-C46-C47
3	C	801	CDL	C44-C45-C46-C47
3	E	801	CDL	C58-C59-C60-C61
5	E	802	PEE	C21-C22-C23-C24
3	D	801	CDL	C54-C55-C56-C57
3	A	801	CDL	C23-C24-C25-C26
3	E	801	CDL	C63-C64-C65-C66
5	B	803	PEE	C31-C32-C33-C34
3	A	801	CDL	C55-C56-C57-C58
3	B	802	CDL	C76-C77-C78-C79
3	C	801	CDL	C80-C81-C82-C83
5	E	802	PEE	C34-C35-C36-C37
3	C	801	CDL	C51-CB5-OB6-CB4
3	B	802	CDL	C33-C34-C35-C36
3	D	801	CDL	C59-C60-C61-C62
3	E	801	CDL	OA6-CA4-CA6-OA8
3	E	801	CDL	OB6-CB4-CB6-OB8
5	B	801	PEE	C39-C40-C41-C42
5	B	803	PEE	C19-C20-C21-C22
5	E	802	PEE	C39-C40-C41-C42
3	D	801	CDL	CB5-C51-C52-C53
3	B	802	CDL	C55-C56-C57-C58
5	D	802	PEE	C11-C12-C13-C14
5	C	802	PEE	C36-C37-C38-C39
3	D	801	CDL	CA2-OA2-PA1-OA5
3	D	801	CDL	CB3-OB5-PB2-OB2
5	C	802	PEE	C1-O3P-P-O4P
5	C	802	PEE	C11-C12-C13-C14
3	D	801	CDL	C1-CA2-OA2-PA1
3	E	801	CDL	C19-C20-C21-C22
3	C	801	CDL	OA5-CA3-CA4-CA6
3	C	801	CDL	OB5-CB3-CB4-CB6
5	B	801	PEE	O3P-C1-C2-C3
3	C	801	CDL	C20-C21-C22-C23
5	B	801	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	A	801	CDL	C18-C19-C20-C21
3	D	801	CDL	C63-C64-C65-C66
3	C	801	CDL	C78-C79-C80-C81
3	C	801	CDL	CB3-CB4-CB6-OB8
3	E	801	CDL	CB3-CB4-CB6-OB8
3	C	801	CDL	C18-C19-C20-C21
3	B	802	CDL	C74-C75-C76-C77
3	B	802	CDL	C84-C85-C86-C87
3	E	801	CDL	C44-C45-C46-C47
3	E	801	CDL	C76-C77-C78-C79
3	E	801	CDL	C12-C13-C14-C15
5	C	802	PEE	C31-C32-C33-C34
3	A	801	CDL	C24-C25-C26-C27
3	C	801	CDL	C84-C85-C86-C87
5	C	802	PEE	C39-C40-C41-C42
5	D	802	PEE	C39-C40-C41-C42
5	E	802	PEE	C15-C16-C17-C18
3	C	801	CDL	C60-C61-C62-C63
3	E	801	CDL	C22-C23-C24-C25
3	E	801	CDL	C32-C33-C34-C35
3	C	801	CDL	C59-C60-C61-C62
3	D	801	CDL	CB7-C71-C72-C73
3	A	801	CDL	C76-C77-C78-C79
3	D	801	CDL	C22-C23-C24-C25
3	A	801	CDL	C84-C85-C86-C87
3	B	802	CDL	C12-C13-C14-C15
5	B	801	PEE	C44-C45-C46-C47
5	B	801	PEE	C38-C39-C40-C41
3	B	802	CDL	C54-C55-C56-C57
3	E	801	CDL	C78-C79-C80-C81
5	D	802	PEE	C13-C14-C15-C16
5	E	802	PEE	C41-C42-C43-C44
3	C	801	CDL	C41-C42-C43-C44
3	A	801	CDL	C79-C80-C81-C82
3	E	801	CDL	C18-C19-C20-C21
3	A	801	CDL	CA5-C11-C12-C13
3	C	801	CDL	C24-C25-C26-C27
3	D	801	CDL	C44-C45-C46-C47
5	D	802	PEE	C31-C32-C33-C34
3	C	801	CDL	C36-C37-C38-C39
3	A	801	CDL	C44-C45-C46-C47
3	E	801	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
3	C	801	CDL	C19-C20-C21-C22
3	E	801	CDL	C71-CB7-OB8-CB6
3	D	801	CDL	C74-C75-C76-C77
5	C	802	PEE	C44-C45-C46-C47
5	D	802	PEE	O3P-C1-C2-C3
3	A	801	CDL	C59-C60-C61-C62
3	E	801	CDL	C57-C58-C59-C60
3	B	802	CDL	C73-C74-C75-C76
3	E	801	CDL	C62-C63-C64-C65
3	B	802	CDL	C1-CB2-OB2-PB2
3	C	801	CDL	C1-CA2-OA2-PA1
3	E	801	CDL	CB4-CB3-OB5-PB2
3	D	801	CDL	C51-C52-C53-C54
5	E	802	PEE	C1-C2-C3-O3
3	B	802	CDL	CB3-OB5-PB2-OB2
5	D	802	PEE	C1-O3P-P-O4P
5	B	801	PEE	C33-C34-C35-C36
3	B	802	CDL	C60-C61-C62-C63
3	D	801	CDL	C32-C33-C34-C35
3	E	801	CDL	C74-C75-C76-C77
3	B	802	CDL	C41-C42-C43-C44
3	E	801	CDL	C84-C85-C86-C87
5	E	802	PEE	C33-C34-C35-C36
3	E	801	CDL	C37-C38-C39-C40
3	E	801	CDL	C75-C76-C77-C78
3	A	801	CDL	C72-C73-C74-C75
3	B	802	CDL	C36-C37-C38-C39
3	D	801	CDL	C62-C63-C64-C65
3	A	801	CDL	C75-C76-C77-C78
3	C	801	CDL	C64-C65-C66-C67
3	D	801	CDL	C42-C43-C44-C45
3	A	801	CDL	C1-CB2-OB2-PB2
3	D	801	CDL	CA4-CA3-OA5-PA1
3	E	801	CDL	C1-CA2-OA2-PA1
3	E	801	CDL	CA4-CA3-OA5-PA1
3	A	801	CDL	C64-C65-C66-C67
5	E	802	PEE	C44-C45-C46-C47
6	D	803	PLM	C5-C6-C7-C8
3	B	802	CDL	C24-C25-C26-C27
3	B	802	CDL	C56-C57-C58-C59
3	B	802	CDL	C14-C15-C16-C17
3	B	802	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	C	801	CDL	C38-C39-C40-C41
5	E	802	PEE	C13-C14-C15-C16
3	C	801	CDL	C71-C72-C73-C74
5	C	802	PEE	C23-C24-C25-C26
5	B	801	PEE	C31-C30-O3-C3
5	E	802	PEE	C31-C30-O3-C3
3	A	801	CDL	C60-C61-C62-C63
3	A	801	CDL	C33-C34-C35-C36
3	E	801	CDL	C80-C81-C82-C83
5	D	802	PEE	C35-C36-C37-C38
3	B	802	CDL	C1-CA2-OA2-PA1
3	C	801	CDL	CA4-CA3-OA5-PA1
5	D	802	PEE	C2-C1-O3P-P
3	C	801	CDL	OA5-CA3-CA4-OA6
3	C	801	CDL	OB5-CB3-CB4-OB6
5	D	802	PEE	O3P-C1-C2-O2
5	C	802	PEE	C12-C13-C14-C15
3	E	801	CDL	OB9-CB7-OB8-CB6
5	E	802	PEE	O5-C30-O3-C3
5	B	803	PEE	C41-C42-C43-C44
5	E	802	PEE	O2-C2-C3-O3
3	E	801	CDL	C34-C35-C36-C37
5	C	802	PEE	C20-C21-C22-C23
3	D	801	CDL	C71-C72-C73-C74
5	B	801	PEE	O5-C30-O3-C3
3	B	802	CDL	C31-CA7-OA8-CA6
3	A	801	CDL	C13-C14-C15-C16
3	A	801	CDL	C41-C42-C43-C44
3	E	801	CDL	C43-C44-C45-C46
3	D	801	CDL	C80-C81-C82-C83
3	C	801	CDL	CA3-OA5-PA1-OA2
3	D	801	CDL	CA3-OA5-PA1-OA2
5	D	802	PEE	C4-O4P-P-O3P
3	B	802	CDL	C80-C81-C82-C83
3	E	801	CDL	C23-C24-C25-C26
3	A	801	CDL	CB4-CB3-OB5-PB2
3	C	801	CDL	C1-CB2-OB2-PB2
6	D	803	PLM	C9-CA-CB-CC
3	A	801	CDL	CB2-OB2-PB2-OB4
3	B	802	CDL	CA3-OA5-PA1-OA3
3	B	802	CDL	CB2-OB2-PB2-OB4
3	B	802	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
3	C	801	CDL	CA3-OA5-PA1-OA4
3	C	801	CDL	CB2-OB2-PB2-OB4
3	E	801	CDL	CB3-OB5-PB2-OB3
3	E	801	CDL	CB3-OB5-PB2-OB4
5	B	803	PEE	C4-O4P-P-O2P
5	B	803	PEE	C4-O4P-P-O1P
5	C	802	PEE	C1-O3P-P-O2P
5	C	802	PEE	C1-O3P-P-O1P
3	D	801	CDL	C84-C85-C86-C87
5	E	802	PEE	C20-C21-C22-C23
5	D	802	PEE	C41-C42-C43-C44
6	D	803	PLM	CB-CC-CD-CE
3	B	802	CDL	CA5-C11-C12-C13
3	E	801	CDL	CA3-CA4-CA6-OA8
3	A	801	CDL	OB6-CB4-CB6-OB8
3	C	801	CDL	OB6-CB4-CB6-OB8
5	C	802	PEE	C22-C23-C24-C25
3	B	802	CDL	C19-C20-C21-C22
3	B	802	CDL	OA9-CA7-OA8-CA6
5	E	802	PEE	C36-C37-C38-C39
3	D	801	CDL	CB4-CB3-OB5-PB2
3	E	801	CDL	C1-CB2-OB2-PB2
5	C	802	PEE	C32-C33-C34-C35
3	C	801	CDL	C34-C35-C36-C37
3	A	801	CDL	C34-C35-C36-C37
3	C	801	CDL	C15-C16-C17-C18
3	A	801	CDL	C71-C72-C73-C74
3	D	801	CDL	C18-C19-C20-C21
3	C	801	CDL	C17-C18-C19-C20
3	D	801	CDL	C75-C76-C77-C78
3	C	801	CDL	C23-C24-C25-C26
5	C	802	PEE	C3-C2-O2-C10
5	B	801	PEE	C24-C25-C26-C27
3	D	801	CDL	C43-C44-C45-C46
3	C	801	CDL	OA7-CA5-OA6-CA4
3	D	801	CDL	OB7-CB5-OB6-CB4
3	E	801	CDL	CA3-OA5-PA1-OA2
5	B	803	PEE	C1-O3P-P-O4P
5	C	802	PEE	C4-O4P-P-O3P
5	E	802	PEE	C1-O3P-P-O4P
3	A	801	CDL	C77-C78-C79-C80
3	A	801	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
6	D	803	PLM	C2-C3-C4-C5
3	C	801	CDL	C11-CA5-OA6-CA4
3	B	802	CDL	C38-C39-C40-C41
3	B	802	CDL	OB5-CB3-CB4-CB6
3	B	802	CDL	C32-C31-CA7-OA8
3	D	801	CDL	C12-C13-C14-C15
5	C	802	PEE	C18-C19-C20-C21
3	E	801	CDL	C13-C14-C15-C16
5	B	803	PEE	C44-C45-C46-C47
3	A	801	CDL	C19-C20-C21-C22
3	C	801	CDL	C13-C14-C15-C16
3	C	801	CDL	C43-C44-C45-C46
5	B	801	PEE	C12-C13-C14-C15
5	C	802	PEE	C1-C2-C3-O3
3	A	801	CDL	C15-C16-C17-C18
5	B	801	PEE	C1-C2-O2-C10
5	D	802	PEE	C3-C2-O2-C10
5	B	803	PEE	C21-C22-C23-C24
5	B	801	PEE	C16-C17-C18-C19
3	A	801	CDL	C22-C23-C24-C25
3	E	801	CDL	C14-C15-C16-C17
3	D	801	CDL	C51-CB5-OB6-CB4
3	C	801	CDL	C73-C74-C75-C76
3	D	801	CDL	C23-C24-C25-C26
3	B	802	CDL	C75-C76-C77-C78
5	D	802	PEE	C38-C39-C40-C41
3	C	801	CDL	C54-C55-C56-C57
5	B	803	PEE	C16-C17-C18-C19
3	C	801	CDL	C72-C71-CB7-OB8
3	C	801	CDL	C21-C22-C23-C24
6	D	803	PLM	C4-C5-C6-C7
5	D	802	PEE	C16-C17-C18-C19
3	A	801	CDL	OB5-CB3-CB4-OB6
5	B	803	PEE	O3P-C1-C2-C3
3	A	801	CDL	C83-C84-C85-C86
3	B	802	CDL	C82-C83-C84-C85
6	D	803	PLM	CA-CB-CC-CD
3	C	801	CDL	C32-C31-CA7-OA8
3	D	801	CDL	C52-C51-CB5-OB6
5	C	802	PEE	O2-C10-C11-C12
5	B	801	PEE	C3-C2-O2-C10
3	B	802	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
5	C	802	PEE	C16-C17-C18-C19
3	E	801	CDL	C52-C53-C54-C55
3	A	801	CDL	C82-C83-C84-C85
6	D	803	PLM	O2-C1-C2-C3
6	D	803	PLM	O1-C1-C2-C3
3	A	801	CDL	OB5-CB3-CB4-CB6
3	A	801	CDL	C16-C17-C18-C19
3	D	801	CDL	C81-C82-C83-C84
3	B	802	CDL	C52-C51-CB5-OB7
3	C	801	CDL	C32-C31-CA7-OA9
3	B	802	CDL	OB5-CB3-CB4-OB6
3	A	801	CDL	C42-C43-C44-C45
3	B	802	CDL	CA3-CA4-CA6-OA8
3	D	801	CDL	C52-C51-CB5-OB7
3	D	801	CDL	C52-C53-C54-C55
5	E	802	PEE	O2-C10-C11-C12
5	B	801	PEE	C2-C1-O3P-P
3	D	801	CDL	C14-C15-C16-C17
5	D	802	PEE	C24-C25-C26-C27
3	A	801	CDL	CB3-OB5-PB2-OB3
5	B	801	PEE	C1-O3P-P-O1P
5	B	803	PEE	C1-O3P-P-O1P
5	B	801	PEE	O3-C30-C31-C32
3	A	801	CDL	C52-C51-CB5-OB6
5	D	802	PEE	C18-C19-C20-C21
5	D	802	PEE	O3-C30-C31-C32
3	C	801	CDL	C16-C17-C18-C19
3	E	801	CDL	C42-C43-C44-C45
3	A	801	CDL	CA4-CA3-OA5-PA1
3	D	801	CDL	C32-C31-CA7-OA8
5	E	802	PEE	O4-C10-C11-C12
3	D	801	CDL	C32-C31-CA7-OA9

There are no ring outliers.

10 monomers are involved in 52 short contacts:

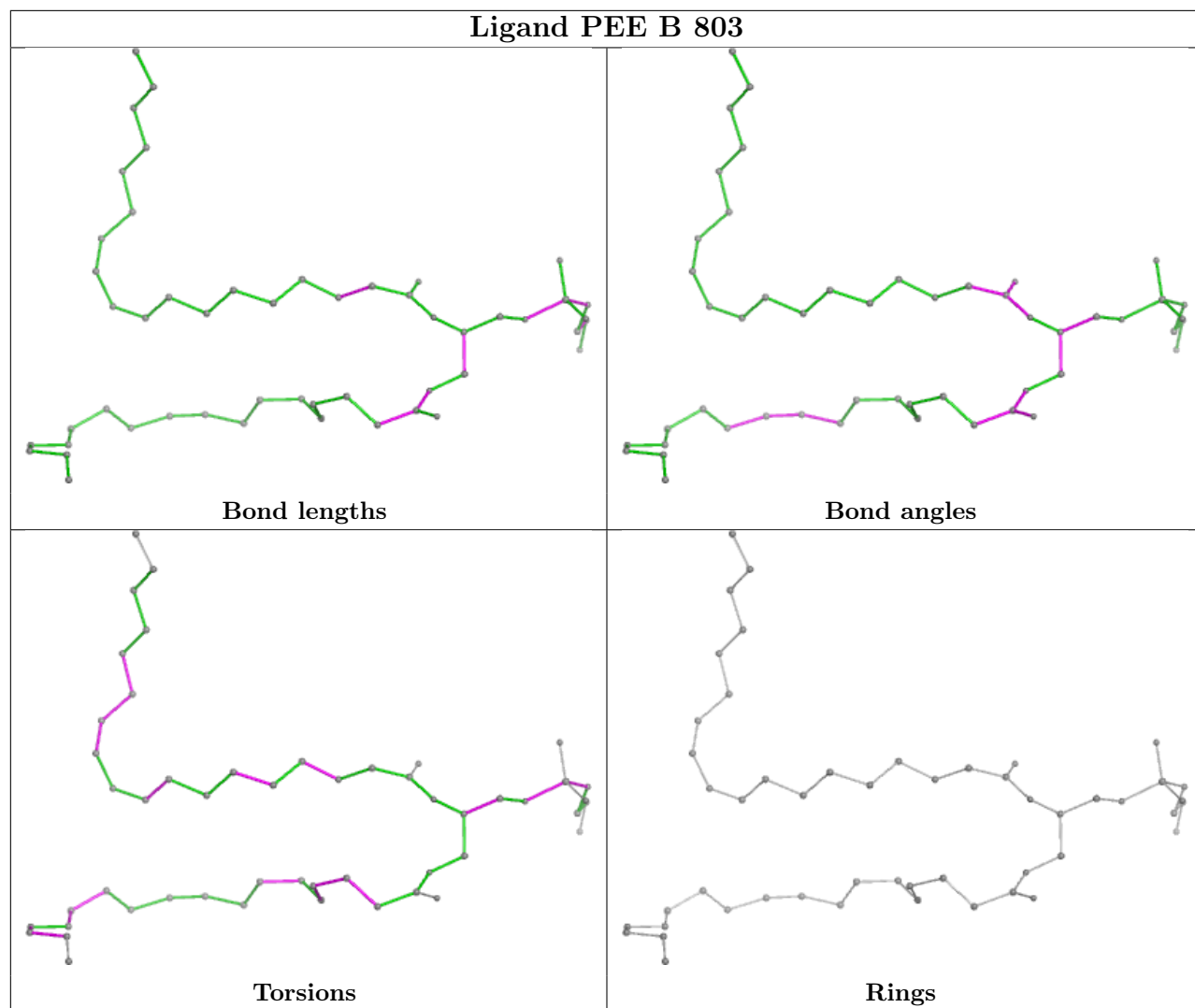
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	PEE	3	0
5	E	802	PEE	2	0
3	E	801	CDL	6	0
3	C	801	CDL	6	0
5	C	802	PEE	4	0

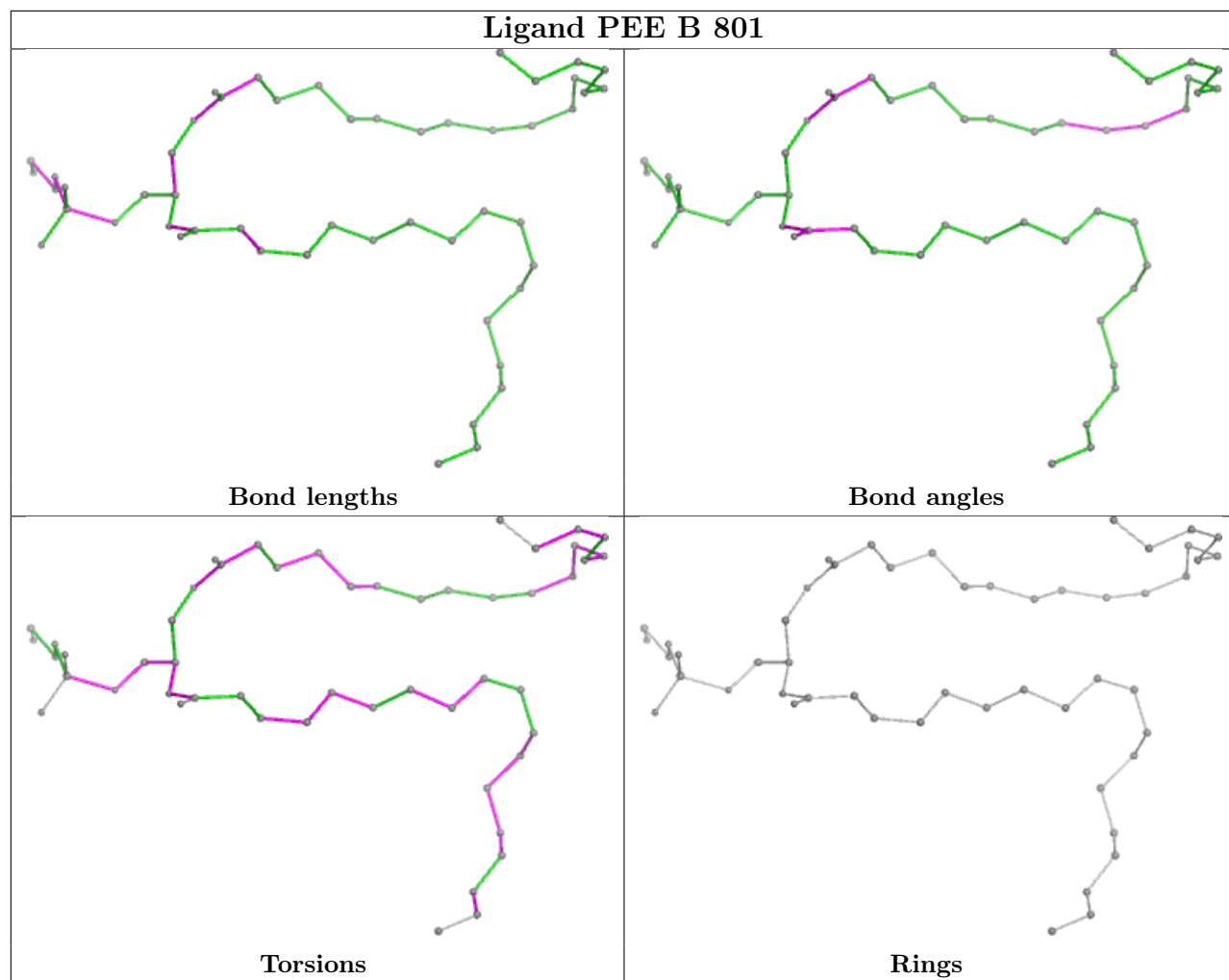
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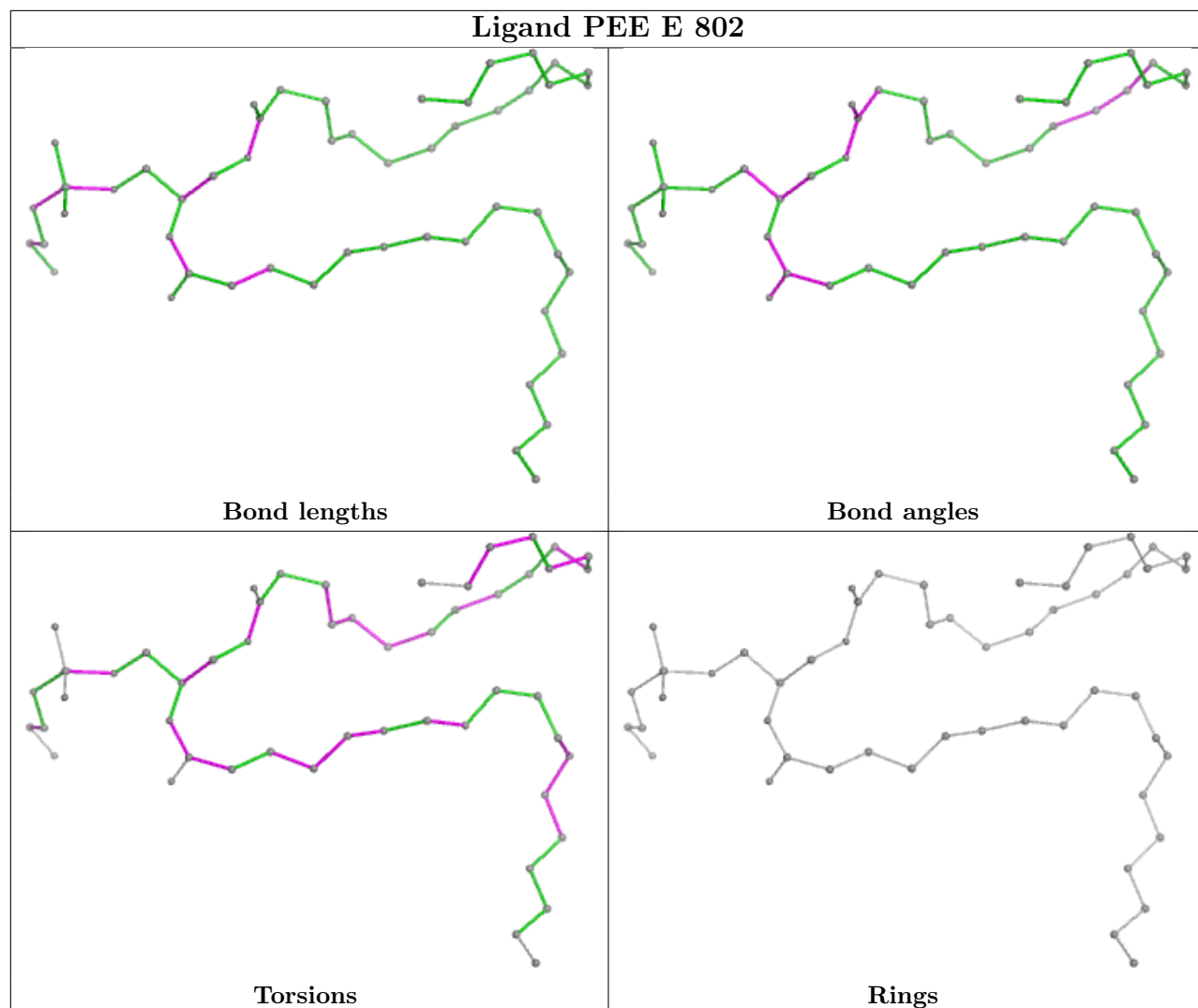
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	CDL	7	0
3	B	802	CDL	7	0
6	D	803	PLM	6	0
5	D	802	PEE	5	0
3	D	801	CDL	9	0

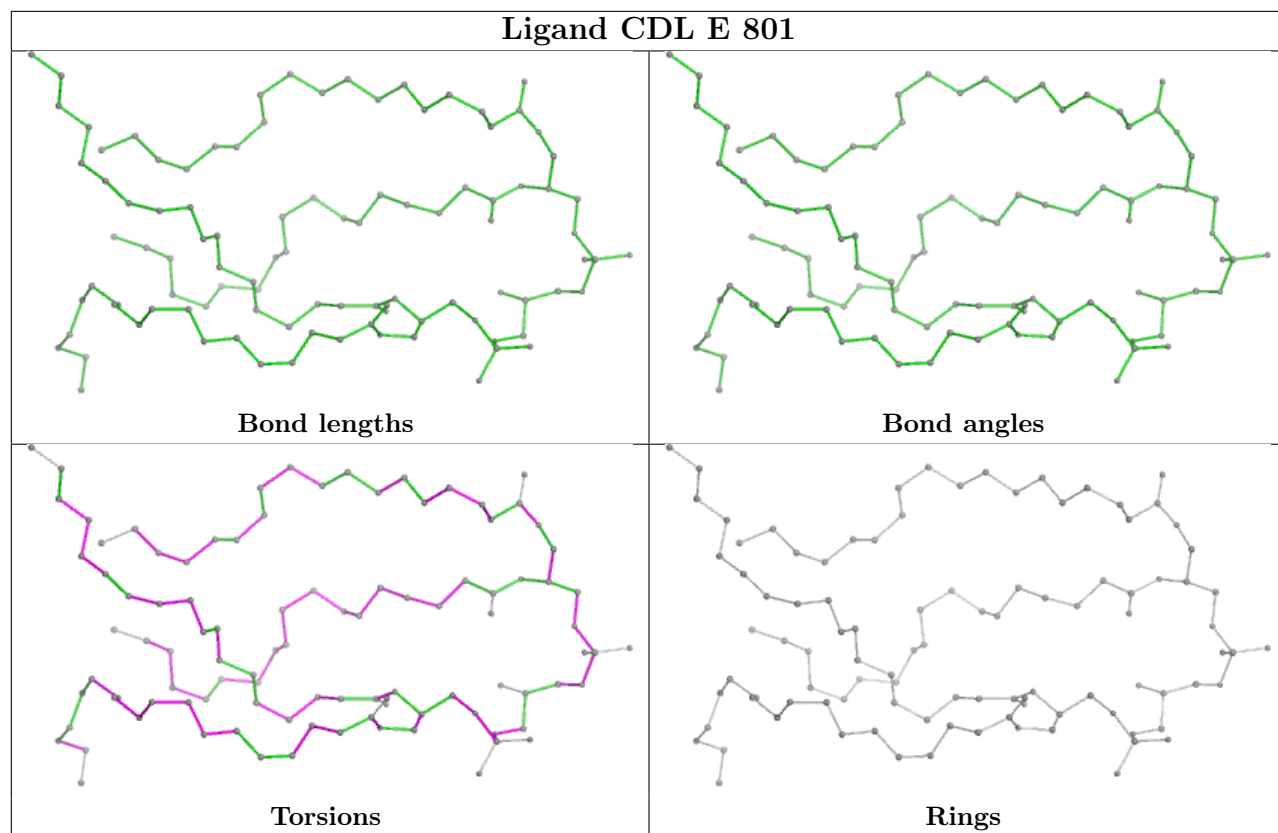
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

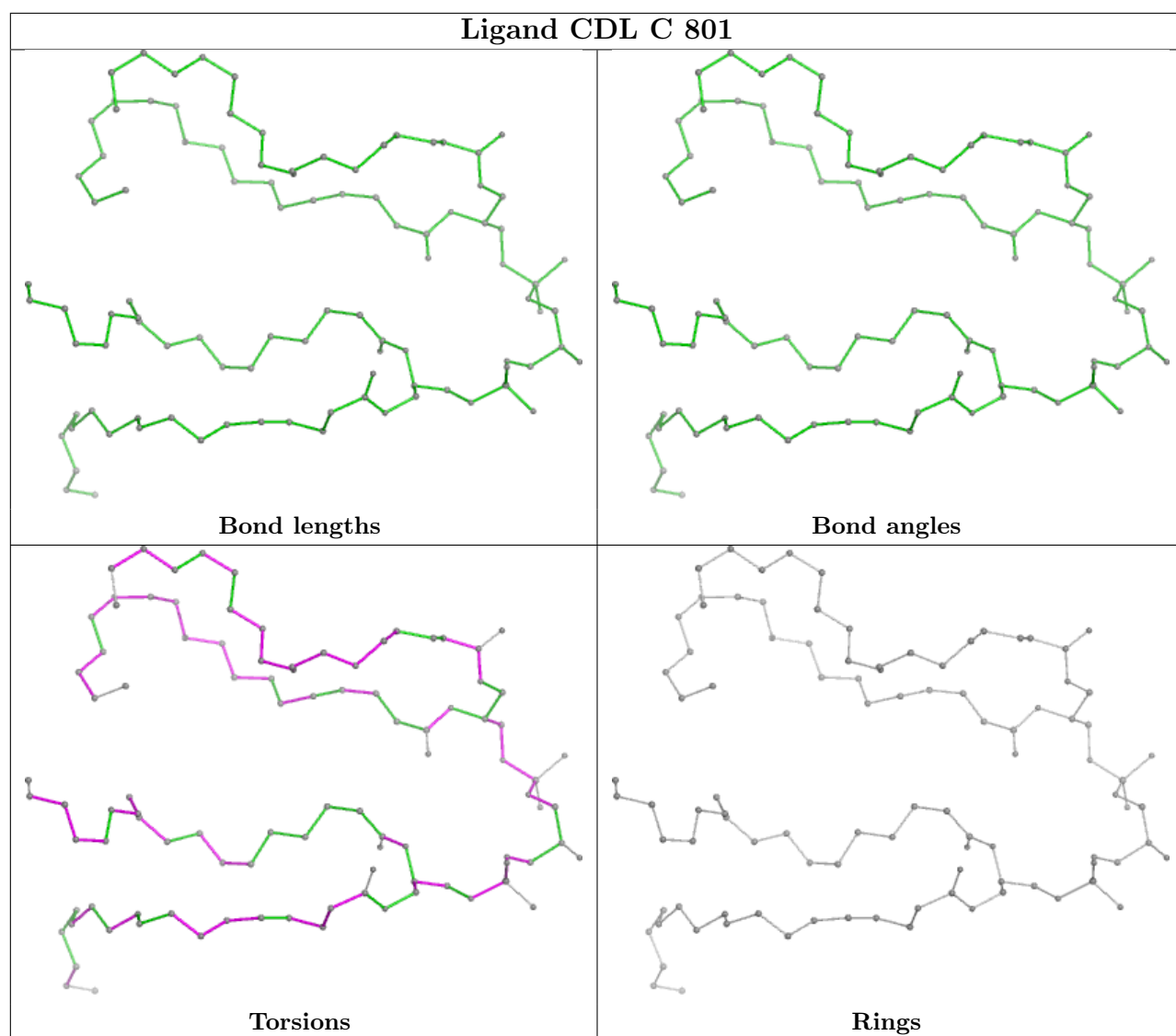


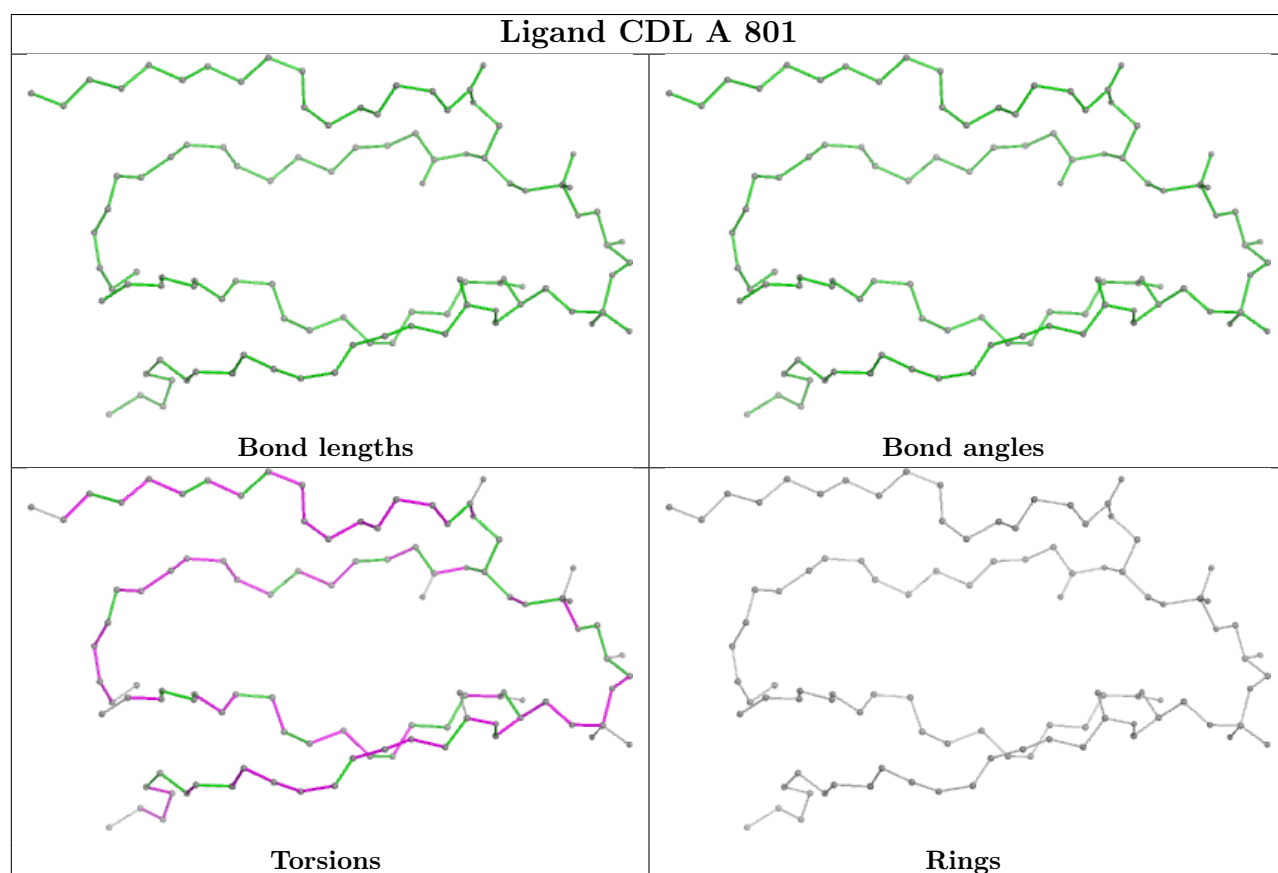
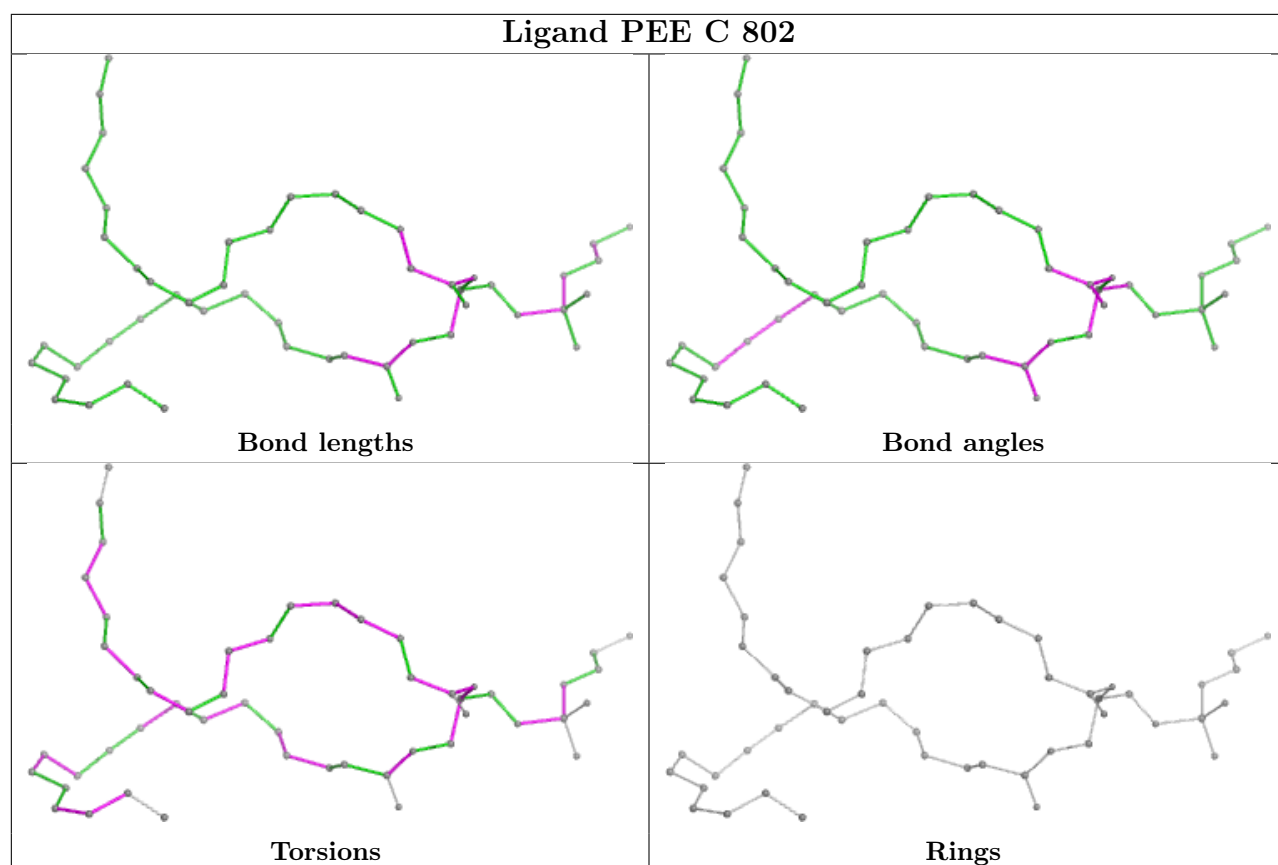


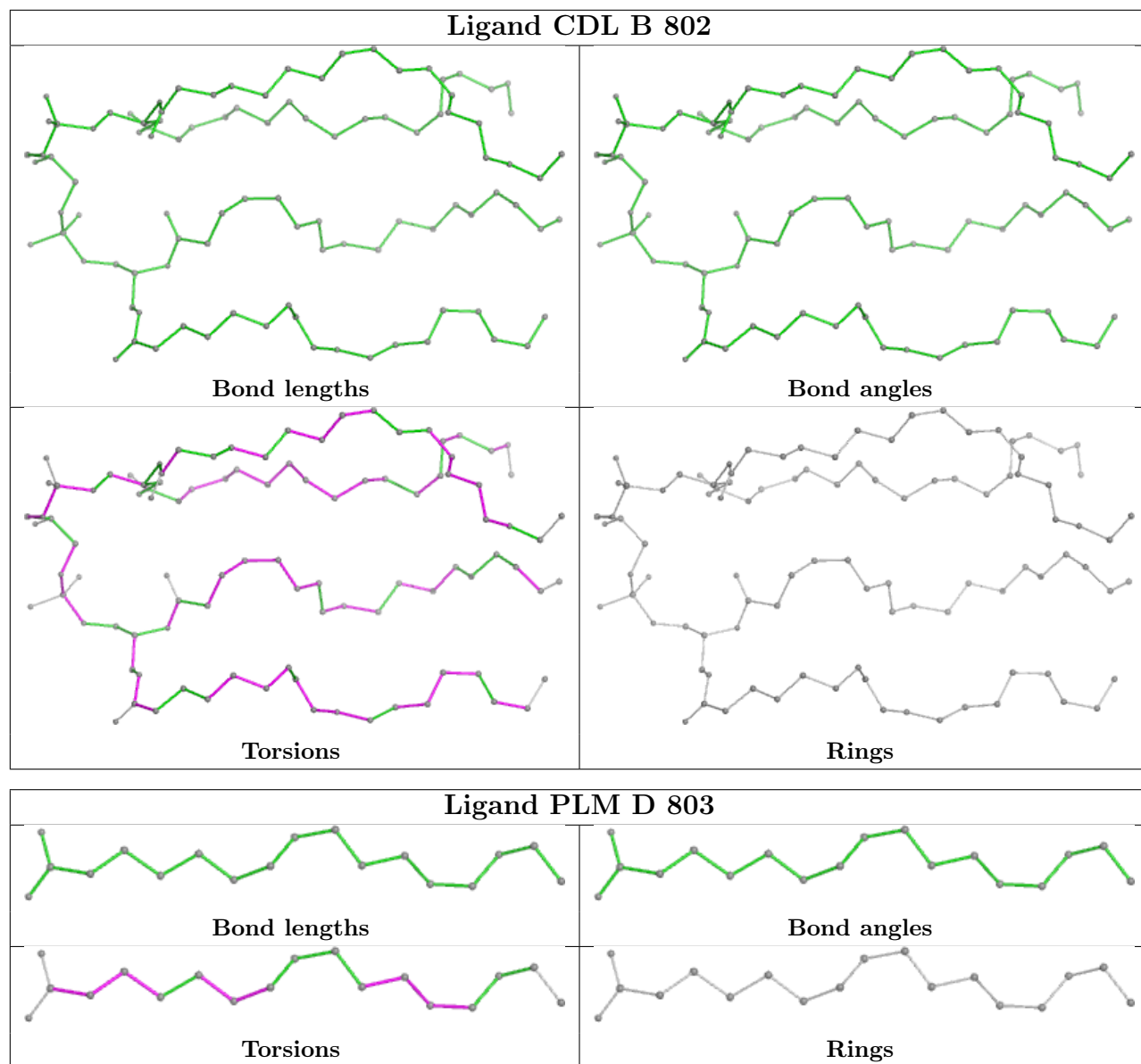


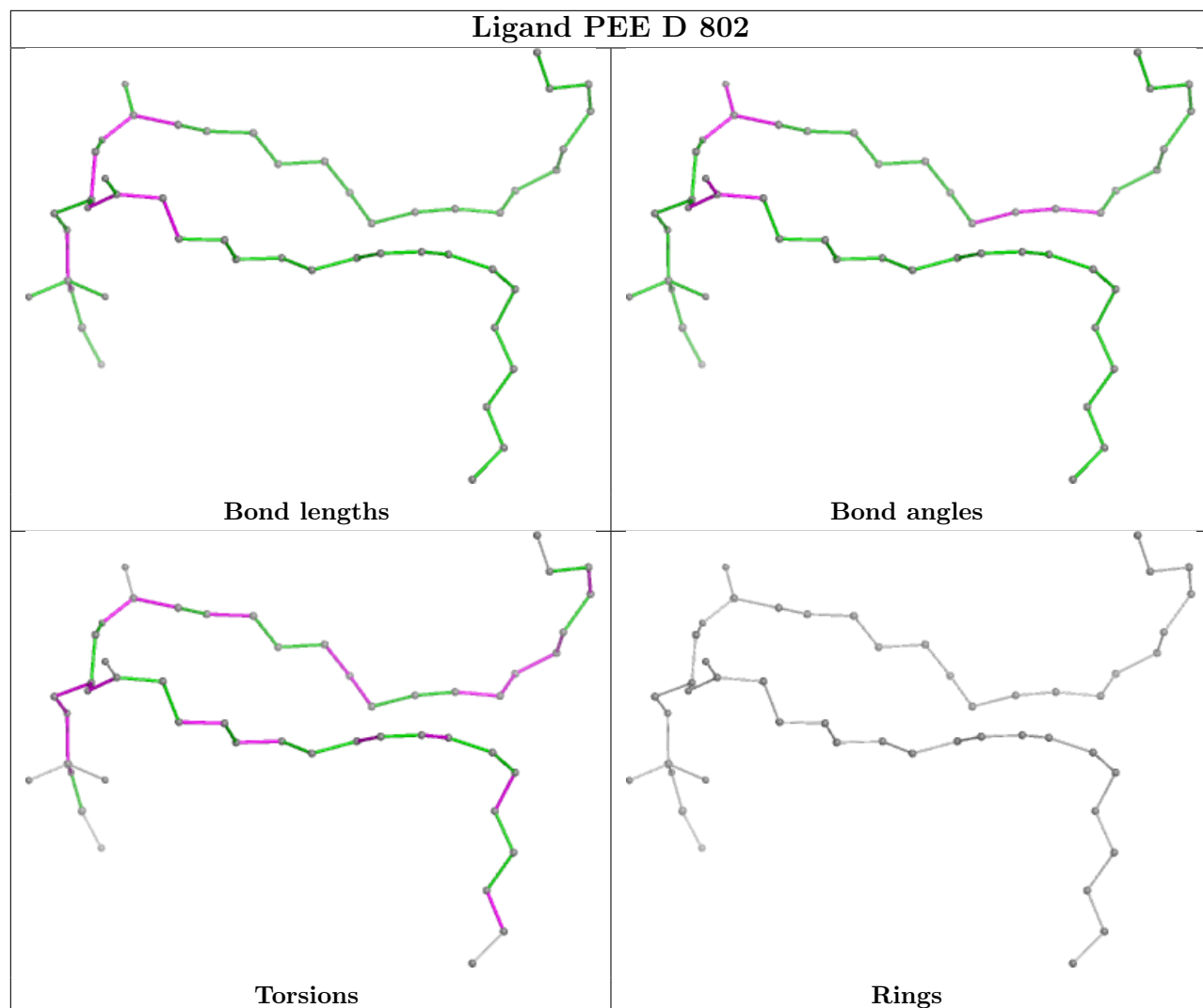


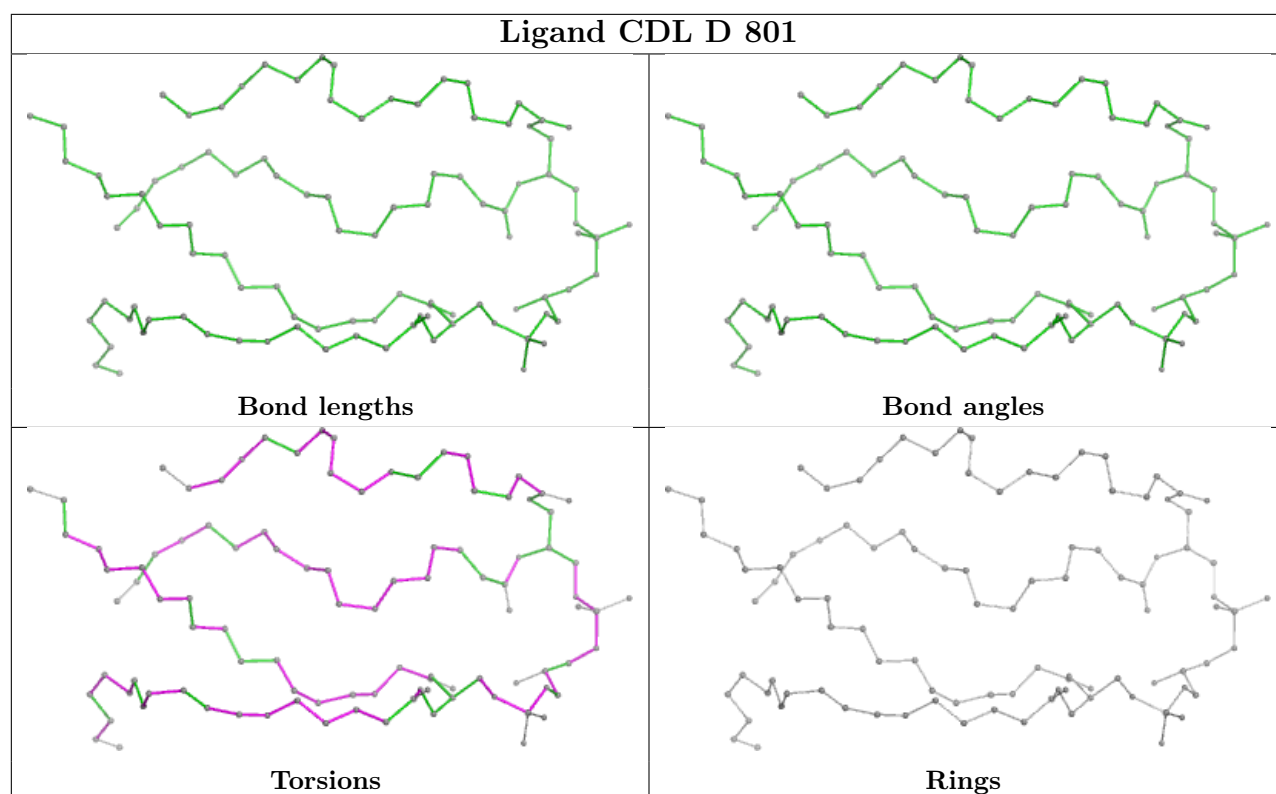












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

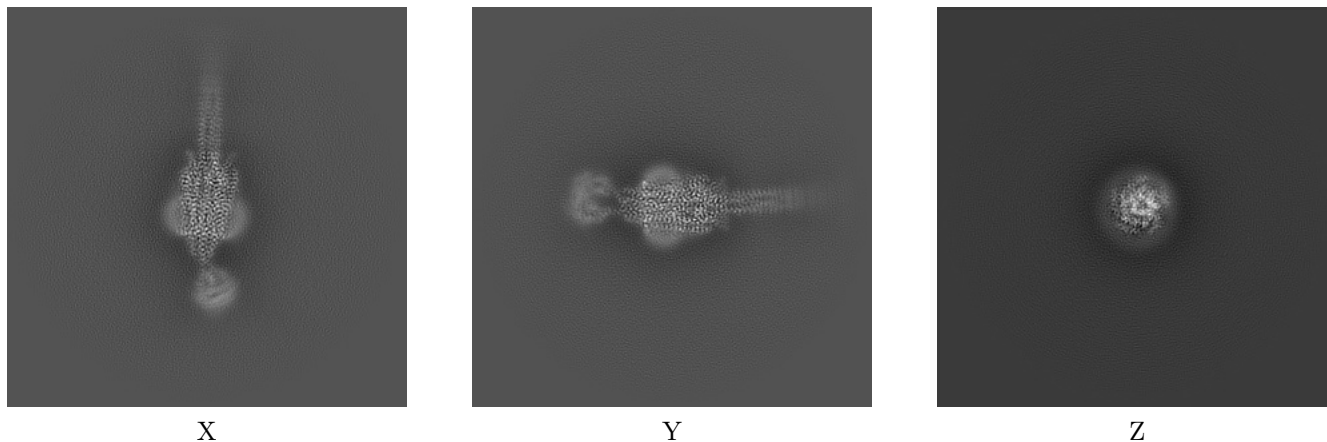
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18751. These allow visual inspection of the internal detail of the map and identification of artifacts.

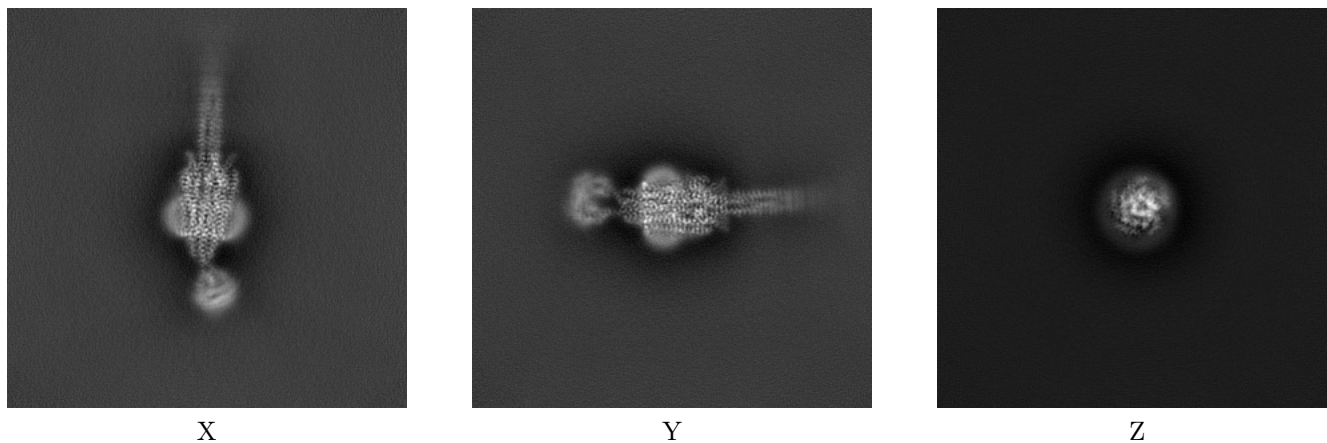
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



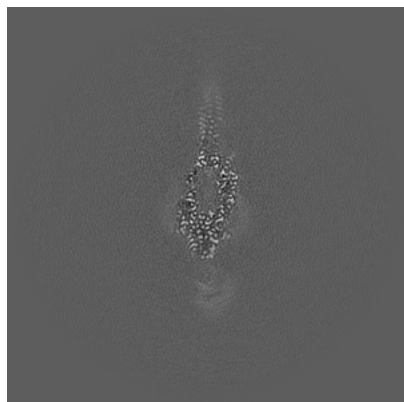
#### 6.1.2 Raw map



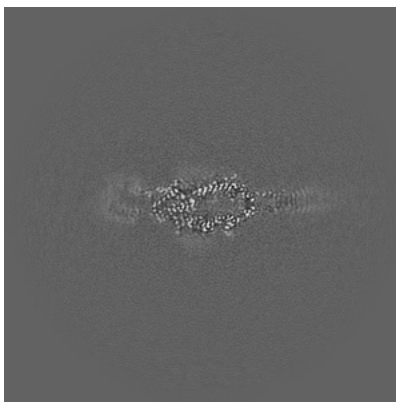
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

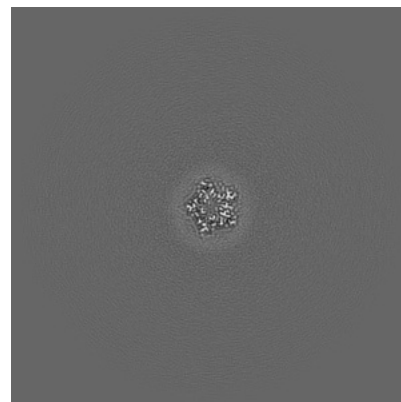
### 6.2.1 Primary map



X Index: 250

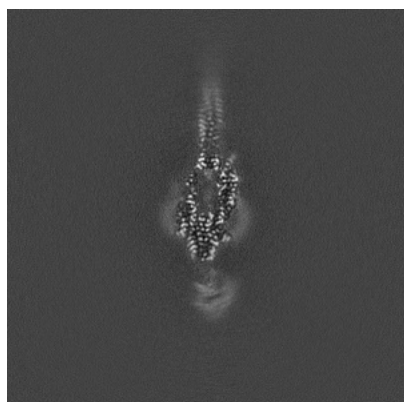


Y Index: 250

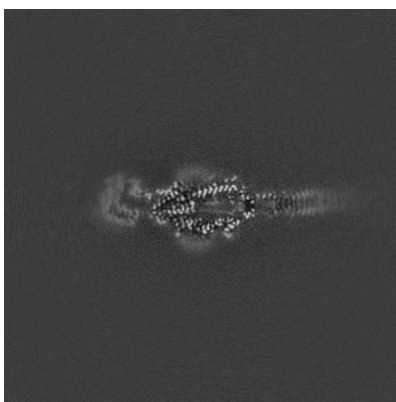


Z Index: 250

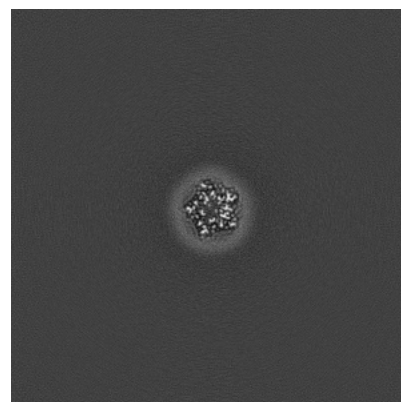
### 6.2.2 Raw map



X Index: 250



Y Index: 250



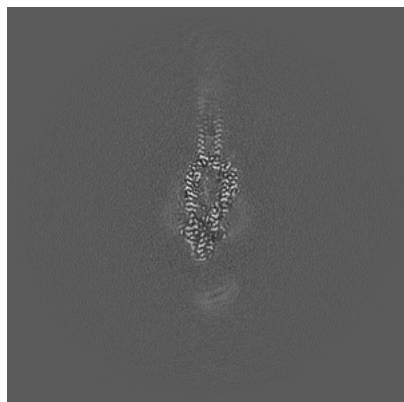
Z Index: 250

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



## 6.3 Largest variance slices [i](#)

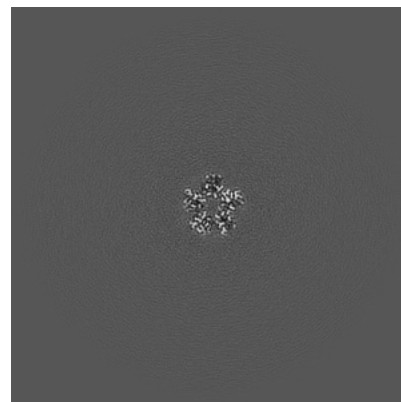
### 6.3.1 Primary map



X Index: 258

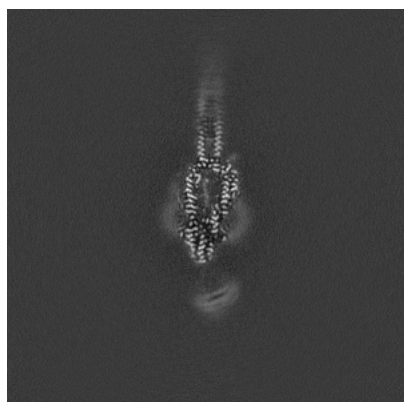


Y Index: 259

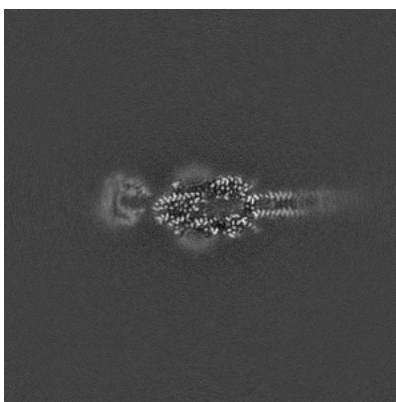


Z Index: 283

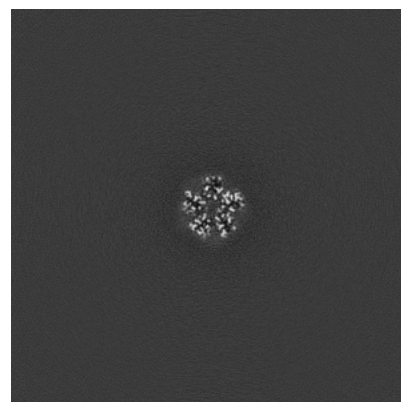
### 6.3.2 Raw map



X Index: 258



Y Index: 256

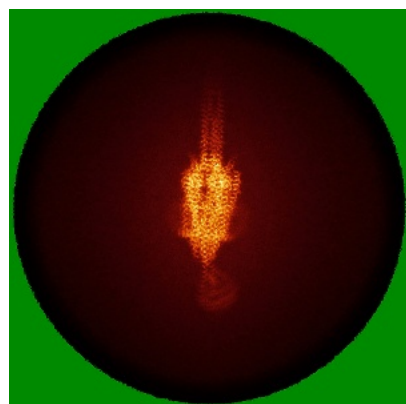


Z Index: 283

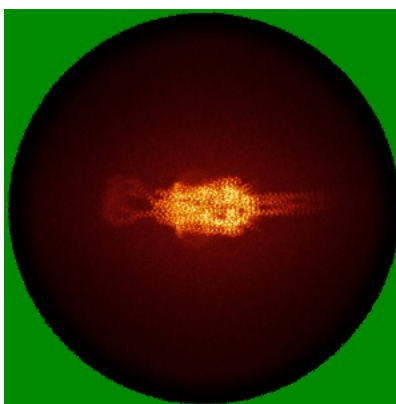
The images above show the largest variance slices of the map in three orthogonal directions.

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

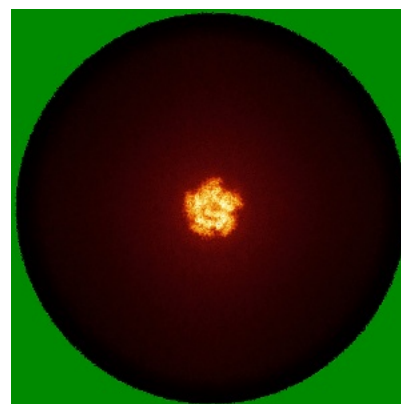
### 6.4.1 Primary map



X

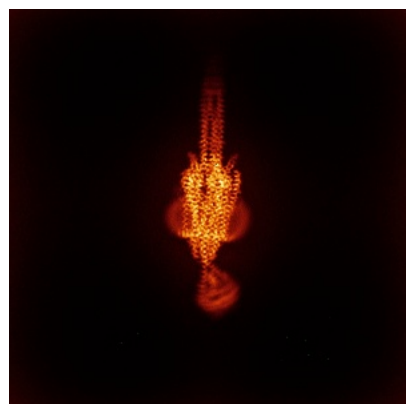


Y

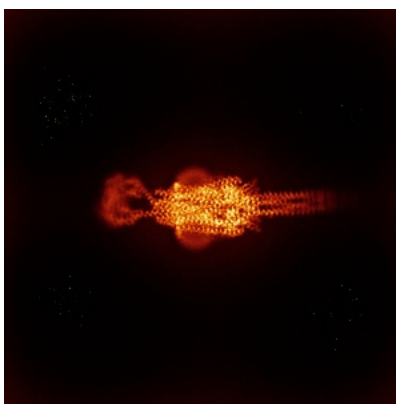


Z

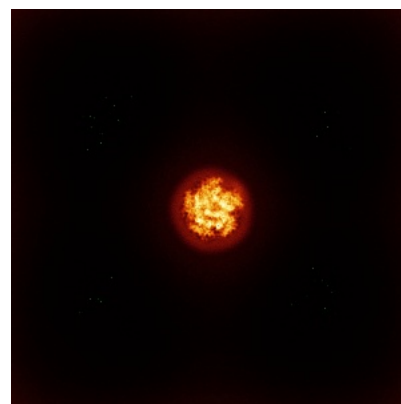
### 6.4.2 Raw map



X



Y

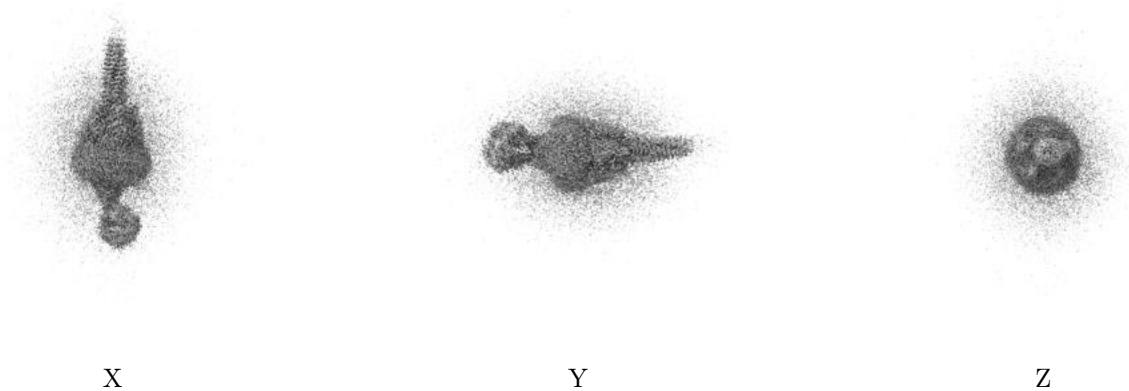


Z

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.

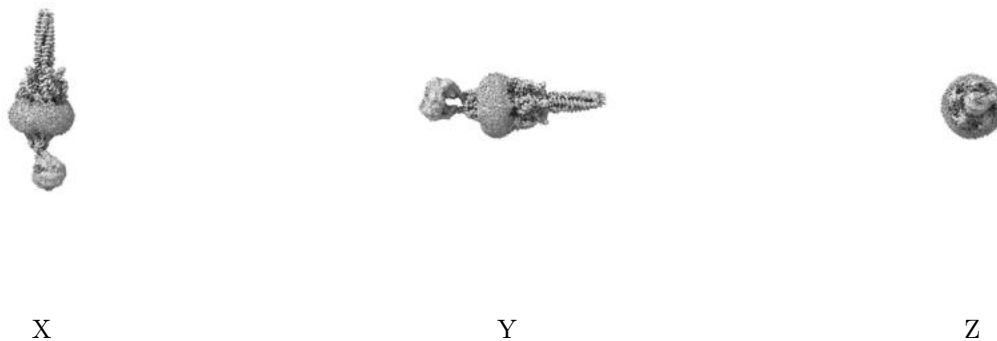
## 6.5 Orthogonal surface views [i](#)

### 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.

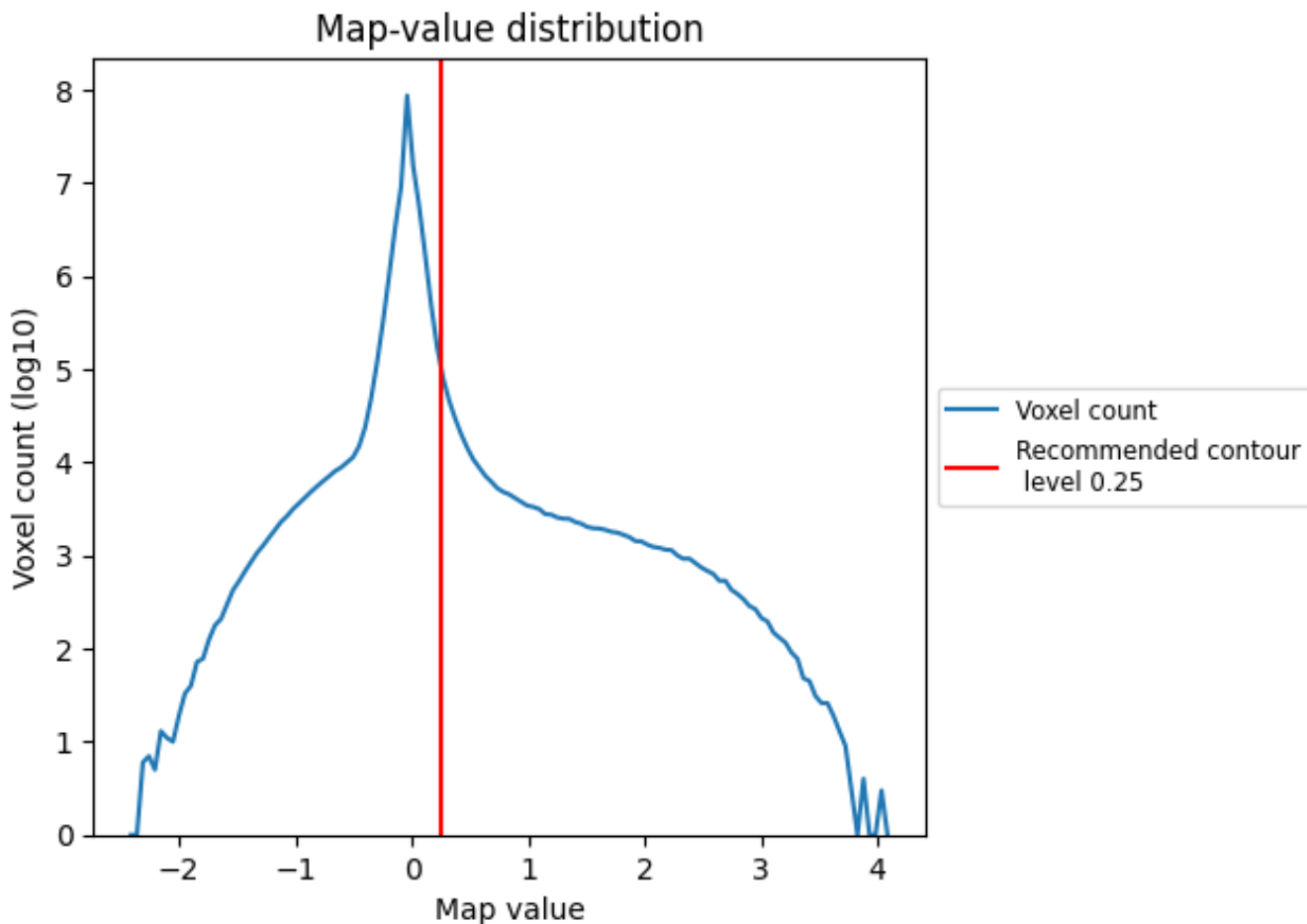
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

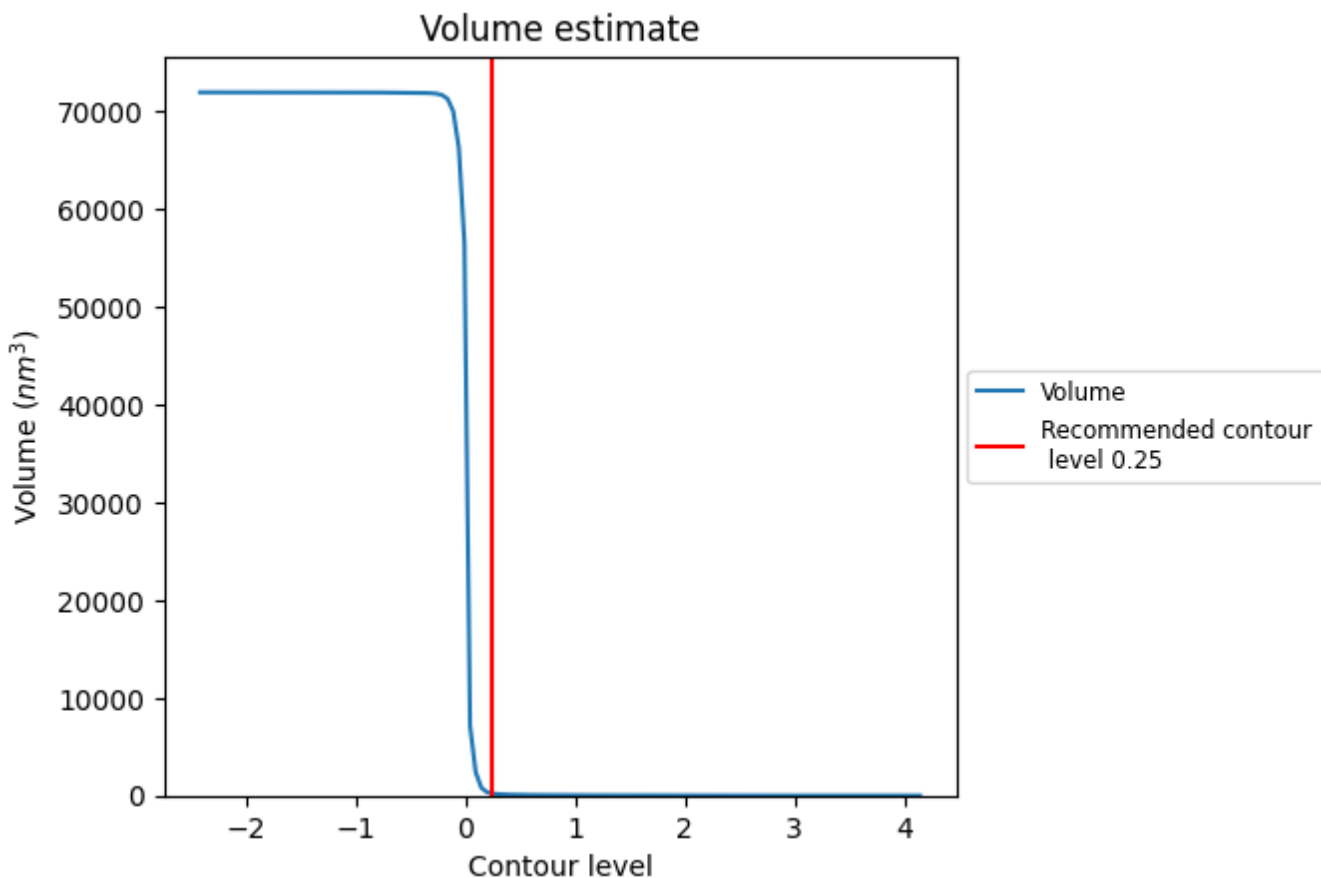
This section contains the results of statistical analysis of the map.

### 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.

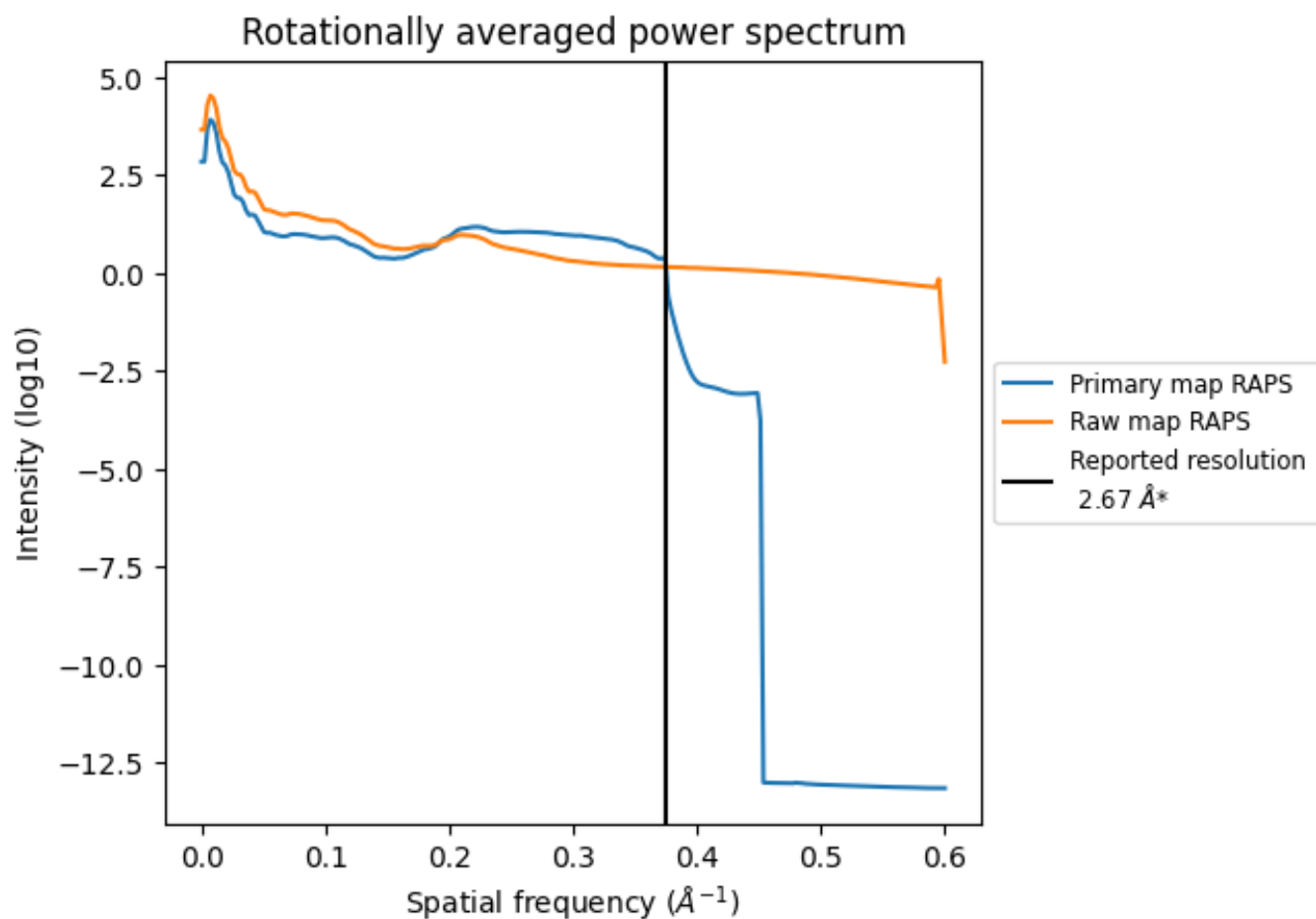
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 205 nm<sup>3</sup>; this corresponds to an approximate mass of 185 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

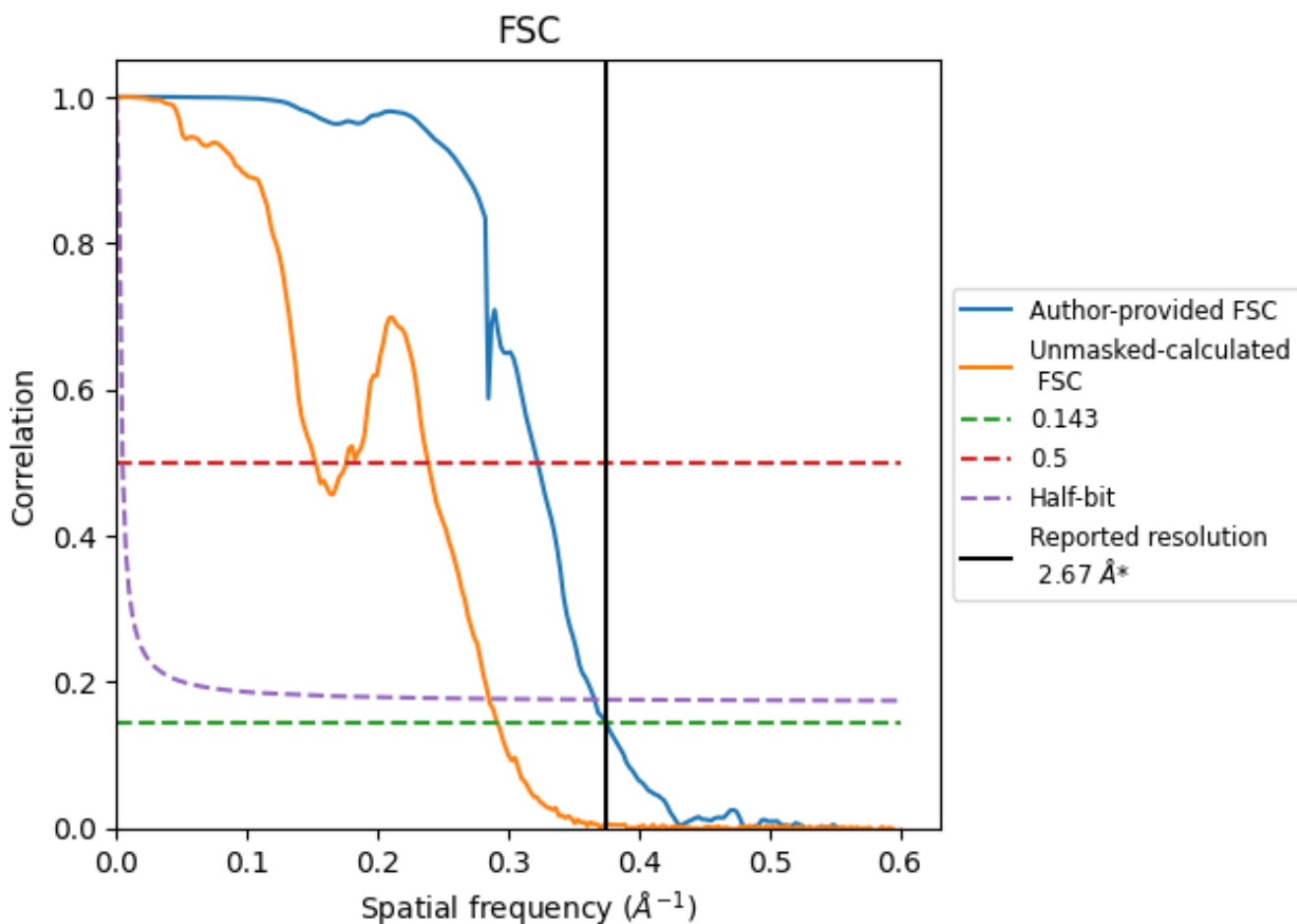


\*Reported resolution corresponds to spatial frequency of 0.375 Å<sup>-1</sup>

## 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 0.375 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.10	2.73
Unmasked-calculated*	3.43	6.56	3.51

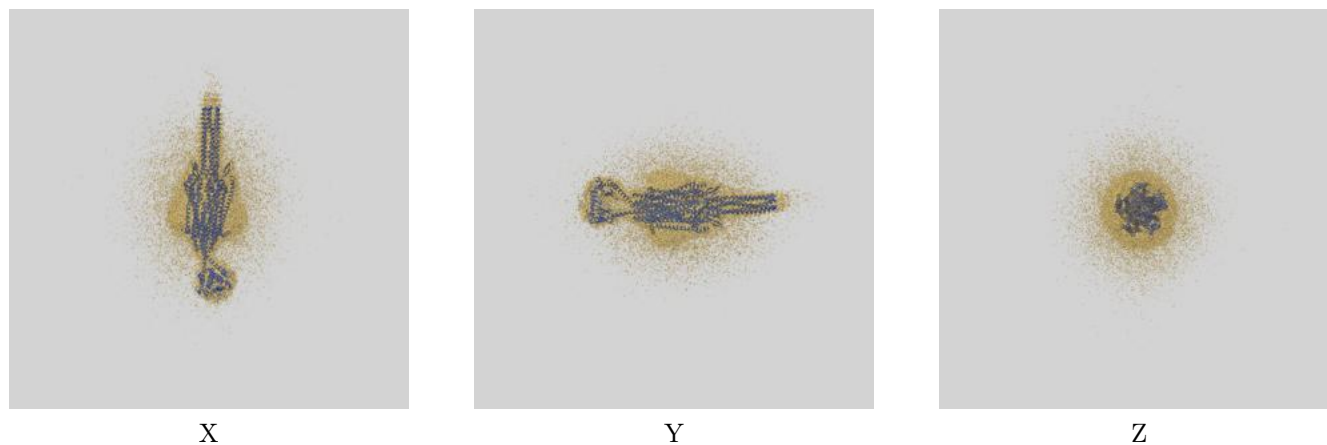
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 2.67 by more than 10 %



## 9 Map-model fit [i](#)

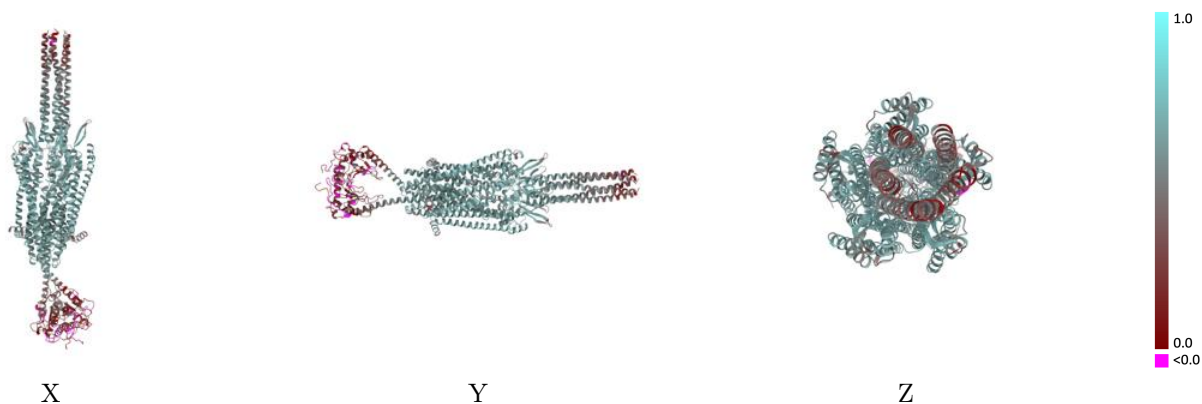
This section contains information regarding the fit between EMDB map EMD-18751 and PDB model 8QYD. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



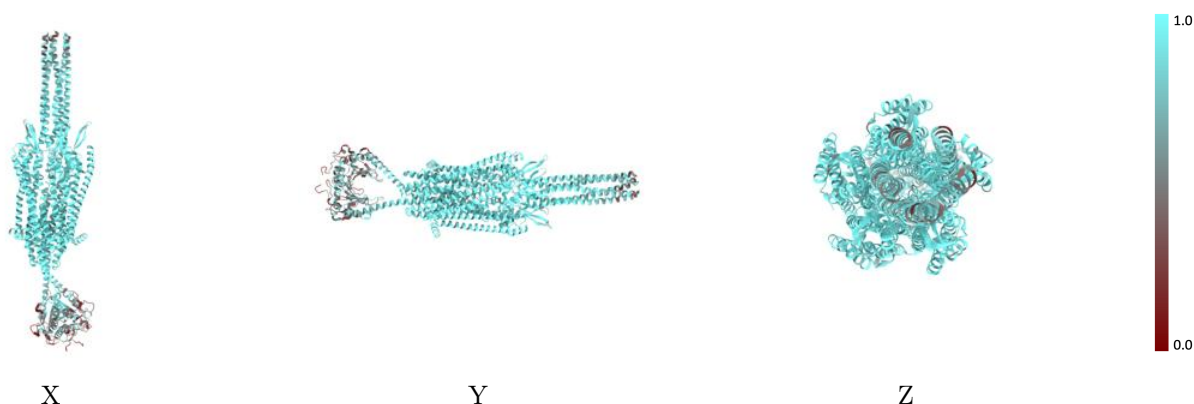
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



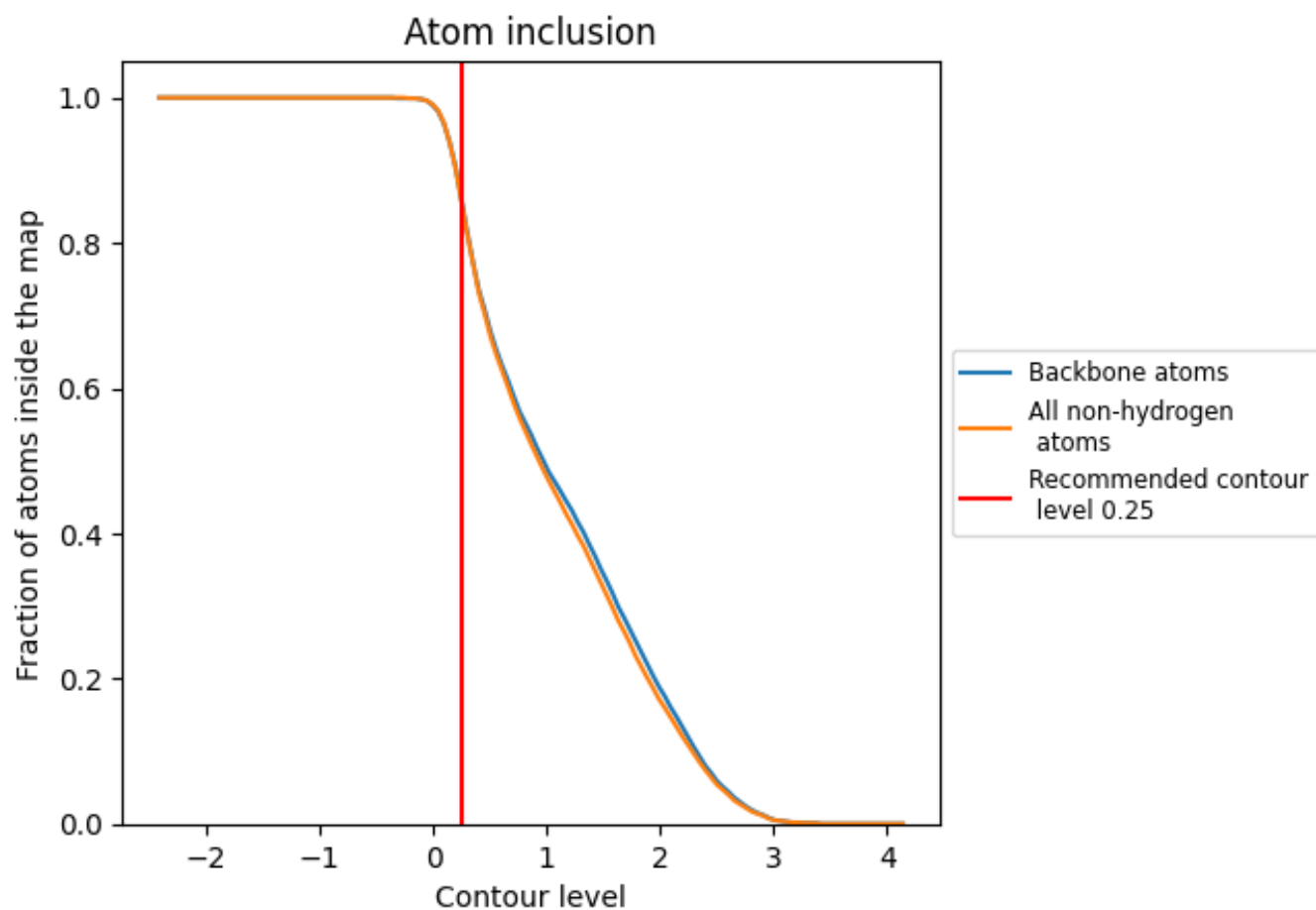
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 86% 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	 0.8560	 0.5070
A	 0.9300	 0.5790
B	 0.9340	 0.5830
C	 0.9370	 0.5830
D	 0.9280	 0.5760
E	 0.9460	 0.5910
F	 0.6320	 0.2790
G	 0.6160	 0.2750

