



## Full wwPDB EM Validation Report ⓘ

Jul 1, 2025 – 05:27 pm BST

PDB ID : 9I6B / pdb\_00009i6b  
EMDB ID : EMD-52652  
Title : CryoEM structure of the Chaetomium thermophilum TOM core complex at 2.7 angstrom resolution (pALDH treated)  
Authors : Agip, A.N.A.; Ornelas, P.; Yang, T.J.; Ermanno, U.; Haeder, S.; McDowell, M.A.; Kuehlbrandt, W.  
Deposited on : 2025-01-29  
Resolution : 2.70 Å (reported)  
Based on initial model : .

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>.

---

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

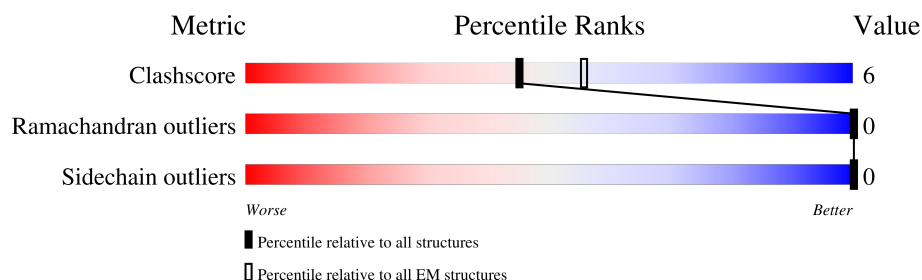
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	C	175	
1	D	175	
2	E	50	
2	F	50	
3	G	84	
3	H	84	
4	I	71	
4	J	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	347	<div><div><div>6%</div><div>84%</div><div>7%</div><div>8%</div></div></div>
5	B	347	<div><div><div>6%</div><div>85%</div><div>6%</div><div>8%</div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8644 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 Mitochondrial import receptor subunit tom22.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	57	Total	C	N	O	S	0	0
			451	289	77	84	1		
1	D	57	Total	C	N	O	S	0	0
			451	289	77	84	1		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	159	GLY	-	expression tag	UNP G0S6L5
C	160	SER	-	expression tag	UNP G0S6L5
C	161	ASP	-	expression tag	UNP G0S6L5
C	162	TYR	-	expression tag	UNP G0S6L5
C	163	LYS	-	expression tag	UNP G0S6L5
C	164	ASP	-	expression tag	UNP G0S6L5
C	165	HIS	-	expression tag	UNP G0S6L5
C	166	ASP	-	expression tag	UNP G0S6L5
C	167	GLY	-	expression tag	UNP G0S6L5
C	168	ASP	-	expression tag	UNP G0S6L5
C	169	TYR	-	expression tag	UNP G0S6L5
C	170	LYS	-	expression tag	UNP G0S6L5
C	171	ASP	-	expression tag	UNP G0S6L5
C	172	ASP	-	expression tag	UNP G0S6L5
C	173	ASP	-	expression tag	UNP G0S6L5
C	174	ASP	-	expression tag	UNP G0S6L5
C	175	LYS	-	expression tag	UNP G0S6L5
D	159	GLY	-	expression tag	UNP G0S6L5
D	160	SER	-	expression tag	UNP G0S6L5
D	161	ASP	-	expression tag	UNP G0S6L5
D	162	TYR	-	expression tag	UNP G0S6L5
D	163	LYS	-	expression tag	UNP G0S6L5
D	164	ASP	-	expression tag	UNP G0S6L5
D	165	HIS	-	expression tag	UNP G0S6L5
D	166	ASP	-	expression tag	UNP G0S6L5
D	167	GLY	-	expression tag	UNP G0S6L5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	168	ASP	-	expression tag	UNP G0S6L5
D	169	TYR	-	expression tag	UNP G0S6L5
D	170	LYS	-	expression tag	UNP G0S6L5
D	171	ASP	-	expression tag	UNP G0S6L5
D	172	ASP	-	expression tag	UNP G0S6L5
D	173	ASP	-	expression tag	UNP G0S6L5
D	174	ASP	-	expression tag	UNP G0S6L5
D	175	LYS	-	expression tag	UNP G0S6L5

- Molecule 2 is a protein called Mitochondrial import receptor subunit tom5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	43	Total	C	N	O	S	0	0
			326	211	52	62	1		
2	F	43	Total	C	N	O	S	0	0
			326	211	52	62	1		

- Molecule 3 is a protein called Mitochondrial import receptor subunit tom6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	41	Total	C	N	O	S	0	0
			298	196	47	55			
3	H	41	Total	C	N	O	S	0	0
			298	196	47	55			

- Molecule 4 is a protein called Import receptor subunit-like protein.

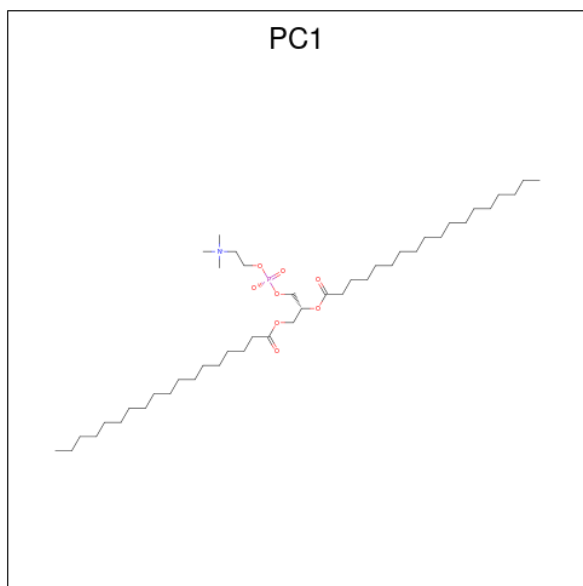
Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	51	Total	C	N	O	S	0	0
			410	267	69	73	1		
4	J	51	Total	C	N	O	S	0	0
			410	267	69	73	1		

- Molecule 5 is a protein called Mitochondrial import receptor subunit (Tom40)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	318	Total	C	N	O	S	0	0
			2466	1564	419	474	9		
5	B	318	Total	C	N	O	S	0	0
			2466	1564	419	474	9		

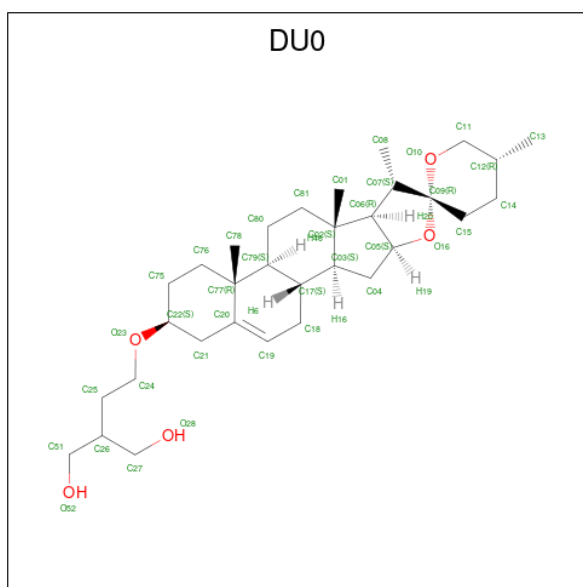
- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula:  $C_{44}H_{88}NO_8P$ ).



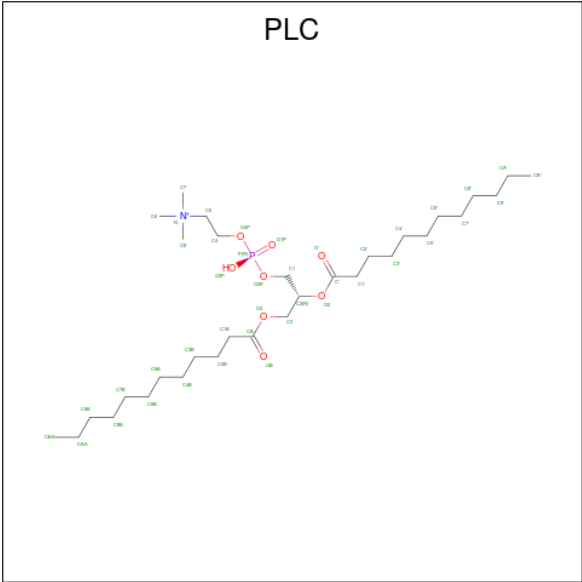
Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			48	38	1	8	1	
6	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
6	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	A	1	Total	C	N	O	P	0
			28	18	1	8	1	
6	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
6	D	1	Total	C	N	O	P	0
			48	38	1	8	1	
6	J	1	Total	C	N	O	P	0
			47	37	1	8	1	
6	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	B	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 7 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0<sup>2,9</sup>.0<sup>4,8</sup>.0<sup>13,18</sup>]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula:  $C_{32}H_{52}O_5$ ).



Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	C	O	0
			37	32	5	
7	A	1	Total	C	O	0
			37	32	5	
7	A	1	Total	C	O	0
			37	32	5	
7	A	1	Total	C	O	0
			37	32	5	
7	H	1	Total	C	O	0
			37	32	5	
7	B	1	Total	C	O	0
			37	32	5	
7	B	1	Total	C	O	0
			37	32	5	
7	B	1	Total	C	O	0
			37	32	5	

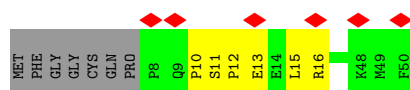
- Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula:  $C_{32}H_{65}NO_8P$ ).



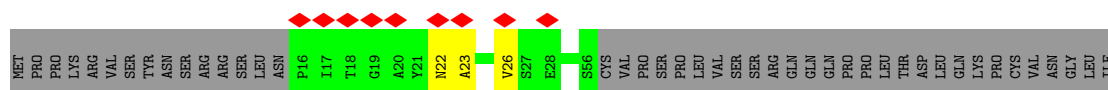
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			42	32	1	8	1	



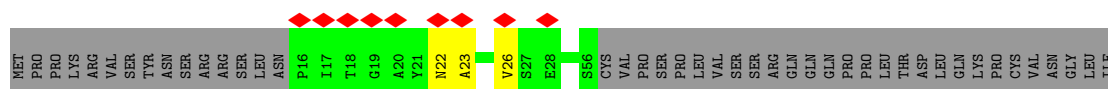




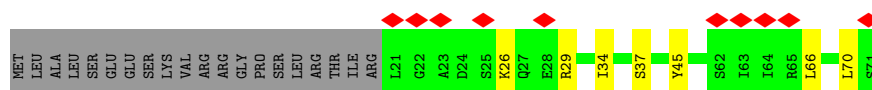
- Molecule 3: Mitochondrial import receptor subunit tom6



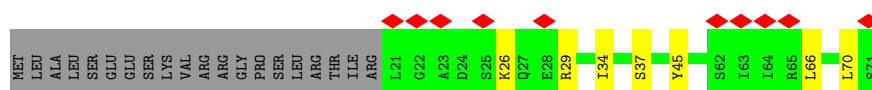
- Molecule 3: Mitochondrial import receptor subunit tom6



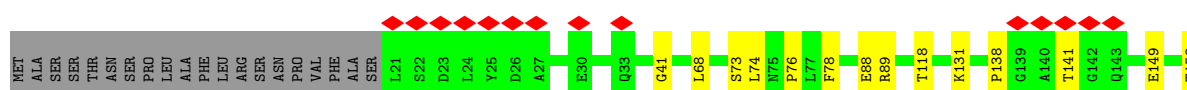
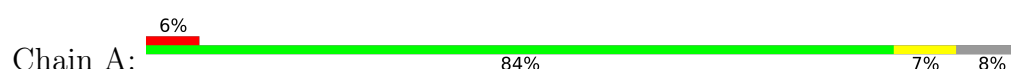
- Molecule 4: Import receptor subunit-like protein



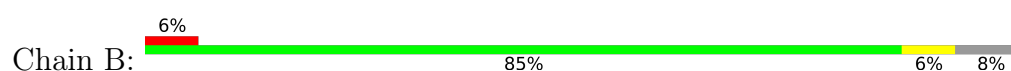
- Molecule 4: Import receptor subunit-like protein

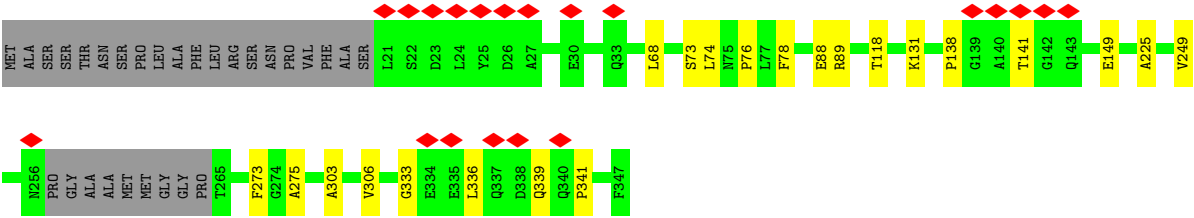


- Molecule 5: Mitochondrial import receptor subunit (Tom40)-like protein



- Molecule 5: Mitochondrial import receptor subunit (Tom40)-like protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	345380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.212	Depositor
Minimum map value	-0.913	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.103	Depositor
Map size (Å)	320.88, 320.88, 320.88	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLC, PC1, DU0

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	C	0.19	0/462	0.29	0/627
1	D	0.19	0/462	0.29	0/627
2	E	0.24	0/333	0.56	0/453
2	F	0.24	0/333	0.56	0/453
3	G	0.24	0/304	0.37	0/415
3	H	0.24	0/304	0.37	0/415
4	I	0.23	0/418	0.39	0/563
4	J	0.23	0/418	0.39	0/563
5	A	0.32	0/2517	0.51	0/3406
5	B	0.32	0/2517	0.51	0/3406
All	All	0.29	0/8068	0.48	0/10928

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
2	E	0	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	16	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	F	16	ARG	Sidechain

## 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	C	451	0	434	3	0
1	D	451	0	434	4	0
2	E	326	0	328	4	0
2	F	326	0	328	4	0
3	G	298	0	300	2	0
3	H	298	0	300	2	0
4	I	410	0	439	7	0
4	J	410	0	439	7	0
5	A	2466	0	2417	22	0
5	B	2466	0	2417	20	0
6	A	68	0	84	7	0
6	B	68	0	84	9	0
6	C	87	0	125	11	0
6	D	87	0	125	11	0
6	I	47	0	68	7	0
6	J	47	0	68	9	0
7	A	111	0	0	1	0
7	B	111	0	0	1	0
7	G	37	0	0	0	0
7	H	37	0	0	0	0
8	A	42	0	64	1	0
All	All	8644	0	8454	105	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 6.

All (105) 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)
5:A:88:GLU:OE2	5:A:89:ARG:NH1	2.29	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:88:GLU:OE2	5:B:89:ARG:NH1	2.29	0.63
2:E:10:PRO:HG2	2:E:15:LEU:HD21	1.82	0.62
2:F:10:PRO:HG2	2:F:15:LEU:HD21	1.82	0.60
2:E:11:SER:HB2	2:E:12:PRO:HD3	1.87	0.56
2:F:11:SER:HB2	2:F:12:PRO:HD3	1.87	0.56
1:C:82:PHE:HA	6:A:405:PC1:H151	1.89	0.54
6:D:202:PC1:H2B2	5:B:275:ALA:HB3	1.88	0.54
4:J:34:ILE:HG23	6:B:402:PC1:H351	1.90	0.54
6:C:201:PC1:H2B2	5:A:275:ALA:HB3	1.88	0.54
1:D:82:PHE:HA	6:B:405:PC1:H151	1.89	0.53
5:B:74:LEU:HG	5:B:336:LEU:HD13	1.91	0.53
5:A:141:THR:HG22	6:A:401:PC1:H151	1.91	0.52
5:B:141:THR:HG22	6:B:402:PC1:H151	1.91	0.52
5:A:74:LEU:HG	5:A:336:LEU:HD13	1.91	0.52
4:I:34:ILE:HG23	6:A:401:PC1:H351	1.90	0.52
5:A:249:VAL:HG22	5:A:273:PHE:HD1	1.75	0.52
5:A:131:LYS:HB2	5:A:149:GLU:HB2	1.92	0.51
5:B:249:VAL:HG22	5:B:273:PHE:HD1	1.75	0.51
5:B:131:LYS:HB2	5:B:149:GLU:HB2	1.92	0.51
6:J:401:PC1:H121	5:B:138:PRO:HB2	1.93	0.51
5:A:74:LEU:CG	5:A:336:LEU:HD13	2.41	0.51
6:J:401:PC1:H31	5:B:138:PRO:HG3	1.92	0.51
6:C:202:PC1:H231	6:C:202:PC1:H351	1.93	0.51
5:B:74:LEU:CG	5:B:336:LEU:HD13	2.41	0.50
6:I:401:PC1:H143	6:I:401:PC1:H32	1.93	0.50
6:I:401:PC1:H31	5:A:138:PRO:HG3	1.92	0.50
3:H:22:ASN:OD1	3:H:23:ALA:N	2.45	0.50
6:I:401:PC1:H121	5:A:138:PRO:HB2	1.93	0.49
6:D:201:PC1:H231	6:D:201:PC1:H351	1.93	0.49
6:J:401:PC1:H2B1	6:J:401:PC1:H2E1	1.51	0.48
6:J:401:PC1:H32	6:J:401:PC1:H143	1.93	0.48
5:A:333:GLY:HA2	5:A:336:LEU:HD11	1.96	0.48
5:B:74:LEU:HB3	5:B:341:PRO:HA	1.96	0.48
5:A:74:LEU:HB3	5:A:341:PRO:HA	1.96	0.47
3:G:22:ASN:OD1	3:G:23:ALA:N	2.45	0.47
4:I:26:LYS:HG3	4:I:29:ARG:NH2	2.29	0.47
4:J:26:LYS:HG3	4:J:29:ARG:NH2	2.29	0.47
5:B:333:GLY:HA2	5:B:336:LEU:HD11	1.96	0.47
6:B:402:PC1:H341	6:B:402:PC1:H372	1.50	0.47
5:B:73:SER:OG	5:B:76:PRO:O	2.30	0.47
6:J:401:PC1:H271	6:J:401:PC1:H2A2	1.59	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:303:ALA:HB3	5:A:306:VAL:HB	1.97	0.46
6:D:201:PC1:H371	6:D:201:PC1:H342	1.57	0.46
6:I:401:PC1:H271	6:I:401:PC1:H2A2	1.59	0.46
5:B:303:ALA:HB3	5:B:306:VAL:HB	1.97	0.46
4:I:45:TYR:CE2	5:A:118:THR:HB	2.51	0.46
6:A:401:PC1:H372	6:A:401:PC1:H341	1.50	0.46
4:J:45:TYR:CE2	5:B:118:THR:HB	2.51	0.46
5:B:225:ALA:HB3	7:B:404:DU0:C11	2.46	0.45
5:A:225:ALA:HB3	7:A:403:DU0:C11	2.46	0.45
6:B:402:PC1:H291	6:B:402:PC1:H261	1.67	0.45
6:D:202:PC1:H142	6:D:202:PC1:H111	1.79	0.45
6:B:402:PC1:H242	6:B:402:PC1:H272	1.65	0.45
3:G:22:ASN:HA	3:G:26:VAL:HG22	1.99	0.45
4:J:70:LEU:HD11	5:B:68:LEU:HD22	1.99	0.45
5:A:73:SER:OG	5:A:76:PRO:O	2.30	0.45
3:H:22:ASN:HA	3:H:26:VAL:HG22	1.99	0.44
6:I:401:PC1:H142	6:I:401:PC1:H112	1.82	0.44
6:D:201:PC1:H143	6:D:201:PC1:H112	1.79	0.44
6:D:201:PC1:H391	6:D:201:PC1:H362	1.50	0.44
6:D:201:PC1:H242	6:D:201:PC1:H271	1.35	0.44
2:F:11:SER:HB2	2:F:12:PRO:CD	2.48	0.44
6:B:405:PC1:H321	6:B:405:PC1:H31	1.51	0.44
6:C:202:PC1:H351	6:C:202:PC1:H321	1.90	0.43
6:C:202:PC1:H271	6:C:202:PC1:H242	1.35	0.43
2:E:11:SER:HB2	2:E:12:PRO:CD	2.48	0.43
1:D:99:VAL:HB	1:D:100:PRO:HD3	2.00	0.43
6:J:401:PC1:H142	6:J:401:PC1:H112	1.82	0.43
1:C:77:ARG:HH11	6:C:202:PC1:H151	1.84	0.43
1:D:77:ARG:HH11	6:D:201:PC1:H151	1.84	0.43
6:B:405:PC1:H361	6:B:405:PC1:H331	1.74	0.43
1:C:99:VAL:HB	1:C:100:PRO:HD3	2.00	0.43
6:C:202:PC1:H2A1	6:C:202:PC1:H272	1.78	0.43
4:I:70:LEU:HD11	5:A:68:LEU:HD22	1.99	0.43
6:J:401:PC1:H32	6:J:401:PC1:H132	2.01	0.43
4:I:66:LEU:HD11	5:A:78:PHE:CE2	2.54	0.42
6:A:401:PC1:H261	6:A:401:PC1:H291	1.67	0.42
6:D:201:PC1:H2A1	6:D:201:PC1:H272	1.78	0.42
6:C:202:PC1:H371	6:C:202:PC1:H342	1.57	0.42
5:A:249:VAL:HG22	5:A:273:PHE:CD1	2.54	0.42
6:J:401:PC1:H2C2	6:J:401:PC1:H291	1.83	0.42
6:C:201:PC1:H142	6:C:201:PC1:H111	1.79	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:PRO:HD2	2:E:13:GLU:H	1.84	0.42
4:I:66:LEU:HD11	5:A:78:PHE:HE2	1.84	0.42
4:J:66:LEU:HD11	5:B:78:PHE:CE2	2.54	0.42
6:D:202:PC1:H2B1	6:D:202:PC1:H2E1	1.88	0.41
6:C:202:PC1:H362	6:C:202:PC1:H391	1.50	0.41
5:A:74:LEU:HD12	5:A:339:GLN:O	2.20	0.41
4:J:66:LEU:HD11	5:B:78:PHE:HE2	1.84	0.41
6:I:401:PC1:H32	6:I:401:PC1:H132	2.01	0.41
6:J:401:PC1:H252	6:J:401:PC1:H282	1.79	0.41
4:I:37:SER:HB2	6:A:401:PC1:H362	2.02	0.41
5:B:74:LEU:HD12	5:B:339:GLN:O	2.20	0.41
6:A:405:PC1:H331	6:A:405:PC1:H361	1.74	0.41
2:F:12:PRO:HD2	2:F:13:GLU:H	1.84	0.41
6:C:202:PC1:H231	6:C:202:PC1:H321	2.03	0.41
5:B:249:VAL:HG22	5:B:273:PHE:CD1	2.54	0.41
5:A:41:GLY:O	5:A:158:THR:HG21	2.21	0.41
6:D:201:PC1:H231	6:D:201:PC1:H321	2.03	0.41
6:C:202:PC1:H143	6:C:202:PC1:H112	1.79	0.40
6:I:401:PC1:H252	6:I:401:PC1:H282	1.79	0.40
8:A:404:PLC:H52	1:D:107:GLU:OE2	2.21	0.40
4:J:37:SER:HB2	6:B:402:PC1:H362	2.02	0.40
5:A:41:GLY:O	5:A:182:LEU:HD23	2.22	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	C	55/175 (31%)	55 (100%)	0	0	100	100
1	D	55/175 (31%)	55 (100%)	0	0	100	100
2	E	41/50 (82%)	41 (100%)	0	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	41/50 (82%)	41 (100%)	0	0	100	100
3	G	39/84 (46%)	38 (97%)	1 (3%)	0	100	100
3	H	39/84 (46%)	38 (97%)	1 (3%)	0	100	100
4	I	49/71 (69%)	47 (96%)	2 (4%)	0	100	100
4	J	49/71 (69%)	47 (96%)	2 (4%)	0	100	100
5	A	314/347 (90%)	312 (99%)	2 (1%)	0	100	100
5	B	314/347 (90%)	312 (99%)	2 (1%)	0	100	100
All	All	996/1454 (68%)	986 (99%)	10 (1%)	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	C	44/141 (31%)	44 (100%)	0	100	100
1	D	44/141 (31%)	44 (100%)	0	100	100
2	E	32/37 (86%)	32 (100%)	0	100	100
2	F	32/37 (86%)	32 (100%)	0	100	100
3	G	30/72 (42%)	30 (100%)	0	100	100
3	H	30/72 (42%)	30 (100%)	0	100	100
4	I	47/65 (72%)	47 (100%)	0	100	100
4	J	47/65 (72%)	47 (100%)	0	100	100
5	A	259/280 (92%)	259 (100%)	0	100	100
5	B	259/280 (92%)	259 (100%)	0	100	100
All	All	824/1190 (69%)	824 (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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
4	I	27	GLN
5	A	29	GLN
5	A	226	GLN
5	A	316	HIS
4	J	27	GLN
5	B	29	GLN
5	B	226	GLN
5	B	316	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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	$\# Z  > 2$
6	PC1	A	405	-	27,27,53	0.66	0	33,35,61	0.57	1 (3%)
6	PC1	B	402	-	39,39,53	0.60	0	45,47,61	0.64	1 (2%)
8	PLC	A	404	-	41,41,41	0.49	0	47,49,49	0.52	0
6	PC1	D	202	-	47,47,53	0.51	0	53,55,61	0.49	1 (1%)
7	DU0	A	403	-	42,42,42	0.69	0	66,66,66	1.19	6 (9%)
6	PC1	C	202	-	38,38,53	0.57	0	44,46,61	0.51	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PC1	J	401	-	46,46,53	0.53	0	52,54,61	0.47	1 (1%)
6	PC1	C	201	-	47,47,53	0.51	0	53,55,61	0.49	1 (1%)
6	PC1	A	401	-	39,39,53	0.60	0	45,47,61	0.64	1 (2%)
6	PC1	I	401	-	46,46,53	0.53	0	52,54,61	0.47	1 (1%)
6	PC1	B	405	-	27,27,53	0.66	0	33,35,61	0.57	1 (3%)
7	DU0	A	402	-	42,42,42	0.78	0	66,66,66	0.88	2 (3%)
7	DU0	G	101	-	42,42,42	0.68	0	66,66,66	0.86	1 (1%)
7	DU0	B	401	-	42,42,42	0.70	0	66,66,66	1.06	6 (9%)
7	DU0	A	406	-	42,42,42	0.70	0	66,66,66	1.06	6 (9%)
7	DU0	B	404	-	42,42,42	0.69	0	66,66,66	1.19	6 (9%)
7	DU0	H	101	-	42,42,42	0.68	0	66,66,66	0.86	1 (1%)
7	DU0	B	403	-	42,42,42	0.78	0	66,66,66	0.88	2 (3%)
6	PC1	D	201	-	38,38,53	0.57	0	44,46,61	0.51	1 (2%)

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
6	PC1	A	405	-	-	17/30/30/57	-
6	PC1	B	402	-	-	26/43/43/57	-
8	PLC	A	404	-	-	15/45/45/45	-
6	PC1	D	202	-	-	33/51/51/57	-
7	DU0	A	403	-	-	4/10/98/98	0/6/6/6
6	PC1	C	202	-	-	29/42/42/57	-
6	PC1	J	401	-	-	35/50/50/57	-
6	PC1	C	201	-	-	33/51/51/57	-
6	PC1	A	401	-	-	26/43/43/57	-
6	PC1	I	401	-	-	35/50/50/57	-
6	PC1	B	405	-	-	17/30/30/57	-
7	DU0	A	402	-	-	9/10/98/98	0/6/6/6
7	DU0	G	101	-	-	2/10/98/98	0/6/6/6
7	DU0	B	401	-	-	1/10/98/98	0/6/6/6
7	DU0	A	406	-	-	1/10/98/98	0/6/6/6
7	DU0	B	404	-	-	4/10/98/98	0/6/6/6

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DU0	H	101	-	-	2/10/98/98	0/6/6/6
7	DU0	B	403	-	-	9/10/98/98	0/6/6/6
6	PC1	D	201	-	-	29/42/42/57	-

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	403	DU0	O16-C05-C06	3.31	109.95	105.07
7	B	404	DU0	O16-C05-C06	3.31	109.95	105.07
7	A	406	DU0	C08-C07-C06	-2.96	107.93	114.50
7	B	401	DU0	C08-C07-C06	-2.96	107.93	114.50
7	A	403	DU0	C03-C04-C05	-2.93	96.74	102.37
7	B	404	DU0	C03-C04-C05	-2.93	96.74	102.37
7	A	403	DU0	O10-C09-O16	-2.90	101.70	109.78
7	B	404	DU0	O10-C09-O16	-2.90	101.70	109.78
7	A	406	DU0	O10-C09-O16	-2.69	102.27	109.78
7	B	401	DU0	O10-C09-O16	-2.69	102.27	109.78
7	A	402	DU0	O10-C09-O16	-2.66	102.38	109.78
7	B	403	DU0	O10-C09-O16	-2.66	102.38	109.78
7	A	402	DU0	C80-C79-C77	-2.60	109.66	113.08
7	B	403	DU0	C80-C79-C77	-2.60	109.66	113.08
7	A	403	DU0	C08-C07-C06	-2.57	108.78	114.50
7	B	404	DU0	C08-C07-C06	-2.57	108.78	114.50
7	A	403	DU0	O16-C09-C07	2.48	108.14	104.47
7	B	404	DU0	O16-C09-C07	2.48	108.14	104.47
6	A	405	PC1	O12-P-O14	2.40	124.11	112.24
6	B	405	PC1	O12-P-O14	2.40	124.11	112.24
7	A	406	DU0	C11-O10-C09	2.33	118.13	113.72
7	B	401	DU0	C11-O10-C09	2.33	118.13	113.72
7	A	406	DU0	O10-C09-C15	2.33	112.93	110.77
7	B	401	DU0	O10-C09-C15	2.33	112.93	110.77
6	C	201	PC1	O12-P-O14	2.28	123.50	112.24
6	D	202	PC1	O12-P-O14	2.28	123.50	112.24
7	A	406	DU0	C24-C25-C26	-2.27	111.01	113.88
7	B	401	DU0	C24-C25-C26	-2.27	111.01	113.88
6	I	401	PC1	O12-P-O14	2.25	123.37	112.24
6	J	401	PC1	O12-P-O14	2.25	123.37	112.24
6	C	202	PC1	O12-P-O14	2.21	123.15	112.24
6	D	201	PC1	O12-P-O14	2.21	123.15	112.24
7	G	101	DU0	O10-C09-C15	2.21	112.82	110.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	101	DU0	O10-C09-C15	2.21	112.82	110.77
7	A	406	DU0	C14-C12-C11	-2.12	105.62	108.56
7	B	401	DU0	C14-C12-C11	-2.12	105.62	108.56
6	A	401	PC1	O12-P-O14	2.11	122.66	112.24
6	B	402	PC1	O12-P-O14	2.11	122.66	112.24
7	A	403	DU0	C76-C77-C20	2.05	112.52	108.75
7	B	404	DU0	C76-C77-C20	2.05	112.52	108.75

There are no chirality outliers.

All (327) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	PC1	C11-O13-P-O14
6	C	201	PC1	C1-O11-P-O13
6	C	201	PC1	O13-C11-C12-N
6	C	202	PC1	C11-O13-P-O12
6	C	202	PC1	C11-O13-P-O11
6	C	202	PC1	C22-C21-O21-C2
6	I	401	PC1	C11-O13-P-O12
6	I	401	PC1	C11-O13-P-O14
6	I	401	PC1	C1-O11-P-O12
6	I	401	PC1	C1-O11-P-O14
6	I	401	PC1	O13-C11-C12-N
6	A	401	PC1	C11-O13-P-O14
6	A	401	PC1	C1-O11-P-O12
6	A	401	PC1	C1-O11-P-O14
6	A	401	PC1	C1-O11-P-O13
6	A	401	PC1	C22-C21-O21-C2
6	A	401	PC1	C32-C31-O31-C3
6	A	405	PC1	C12-C11-O13-P
6	D	201	PC1	C11-O13-P-O12
6	D	201	PC1	C11-O13-P-O11
6	D	201	PC1	C22-C21-O21-C2
6	D	202	PC1	C11-O13-P-O14
6	D	202	PC1	C1-O11-P-O13
6	D	202	PC1	O13-C11-C12-N
6	J	401	PC1	C11-O13-P-O12
6	J	401	PC1	C11-O13-P-O14
6	J	401	PC1	C1-O11-P-O12
6	J	401	PC1	C1-O11-P-O14
6	J	401	PC1	O13-C11-C12-N
6	B	402	PC1	C11-O13-P-O14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	B	402	PC1	C1-O11-P-O12
6	B	402	PC1	C1-O11-P-O14
6	B	402	PC1	C1-O11-P-O13
6	B	402	PC1	C22-C21-O21-C2
6	B	402	PC1	C32-C31-O31-C3
6	B	405	PC1	C12-C11-O13-P
7	G	101	DU0	C25-C26-C27-O28
7	A	402	DU0	C25-C24-O23-C22
7	A	402	DU0	C25-C26-C27-O28
7	A	402	DU0	C25-C26-C51-O52
7	A	403	DU0	C27-C26-C51-O52
7	H	101	DU0	C25-C26-C27-O28
7	B	403	DU0	C25-C24-O23-C22
7	B	403	DU0	C25-C26-C27-O28
7	B	403	DU0	C25-C26-C51-O52
7	B	404	DU0	C27-C26-C51-O52
8	A	404	PLC	C1-O3P-P-O1P
8	A	404	PLC	C1-O3P-P-O2P
8	A	404	PLC	C1-O3P-P-O4P
8	A	404	PLC	C4-O4P-P-O1P
8	A	404	PLC	C4-O4P-P-O2P
8	A	404	PLC	C4-O4P-P-O3P
6	A	405	PC1	C22-C21-O21-C2
6	B	405	PC1	C22-C21-O21-C2
6	A	401	PC1	O32-C31-O31-C3
6	A	405	PC1	O32-C31-O31-C3
6	B	402	PC1	O32-C31-O31-C3
6	B	405	PC1	O32-C31-O31-C3
6	A	405	PC1	C32-C31-O31-C3
6	B	405	PC1	C32-C31-O31-C3
6	C	202	PC1	O22-C21-O21-C2
6	A	401	PC1	O22-C21-O21-C2
6	D	201	PC1	O22-C21-O21-C2
6	B	402	PC1	O22-C21-O21-C2
6	C	202	PC1	C32-C31-O31-C3
6	D	201	PC1	C32-C31-O31-C3
6	C	202	PC1	C24-C25-C26-C27
6	D	201	PC1	C24-C25-C26-C27
6	C	201	PC1	C32-C31-O31-C3
6	D	202	PC1	C32-C31-O31-C3
6	C	202	PC1	C34-C35-C36-C37
6	D	201	PC1	C34-C35-C36-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	C	201	PC1	C29-C2A-C2B-C2C
6	A	405	PC1	O22-C21-O21-C2
6	D	202	PC1	C29-C2A-C2B-C2C
6	B	405	PC1	O22-C21-O21-C2
6	C	201	PC1	O32-C31-O31-C3
6	C	202	PC1	O32-C31-O31-C3
6	D	201	PC1	O32-C31-O31-C3
6	D	202	PC1	O32-C31-O31-C3
6	I	401	PC1	C2B-C2C-C2D-C2E
6	J	401	PC1	C2B-C2C-C2D-C2E
6	I	401	PC1	C3A-C3B-C3C-C3D
6	A	401	PC1	C24-C25-C26-C27
6	J	401	PC1	C3A-C3B-C3C-C3D
6	B	402	PC1	C24-C25-C26-C27
6	C	201	PC1	C2B-C2C-C2D-C2E
6	C	202	PC1	C32-C33-C34-C35
6	A	401	PC1	C34-C35-C36-C37
6	D	201	PC1	C32-C33-C34-C35
6	D	202	PC1	C2B-C2C-C2D-C2E
6	B	402	PC1	C34-C35-C36-C37
6	I	401	PC1	C23-C24-C25-C26
6	J	401	PC1	C23-C24-C25-C26
6	I	401	PC1	C35-C36-C37-C38
6	J	401	PC1	C35-C36-C37-C38
6	C	202	PC1	C36-C37-C38-C39
6	D	201	PC1	C36-C37-C38-C39
6	A	401	PC1	C28-C29-C2A-C2B
6	B	402	PC1	C28-C29-C2A-C2B
6	I	401	PC1	C29-C2A-C2B-C2C
6	J	401	PC1	C29-C2A-C2B-C2C
6	A	405	PC1	C33-C34-C35-C36
6	B	405	PC1	C33-C34-C35-C36
6	I	401	PC1	C25-C26-C27-C28
6	J	401	PC1	C25-C26-C27-C28
6	I	401	PC1	C31-C32-C33-C34
6	J	401	PC1	C31-C32-C33-C34
6	C	202	PC1	C21-C22-C23-C24
6	D	201	PC1	C21-C22-C23-C24
6	A	401	PC1	C26-C27-C28-C29
6	B	402	PC1	C26-C27-C28-C29
6	I	401	PC1	C27-C28-C29-C2A
6	J	401	PC1	C27-C28-C29-C2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	C	201	PC1	C11-O13-P-O11
6	I	401	PC1	C11-O13-P-O11
6	I	401	PC1	C1-O11-P-O13
6	A	405	PC1	C11-O13-P-O11
6	D	202	PC1	C11-O13-P-O11
6	J	401	PC1	C11-O13-P-O11
6	J	401	PC1	C1-O11-P-O13
6	B	405	PC1	C11-O13-P-O11
6	C	201	PC1	C2D-C2E-C2F-C2G
6	D	202	PC1	C2D-C2E-C2F-C2G
6	C	201	PC1	C36-C37-C38-C39
6	C	202	PC1	C25-C26-C27-C28
6	D	201	PC1	C25-C26-C27-C28
6	D	202	PC1	C36-C37-C38-C39
6	C	201	PC1	C35-C36-C37-C38
6	I	401	PC1	C33-C34-C35-C36
6	D	202	PC1	C35-C36-C37-C38
6	J	401	PC1	C33-C34-C35-C36
6	A	401	PC1	C1-C2-O21-C21
6	B	402	PC1	C1-C2-O21-C21
6	A	401	PC1	C35-C36-C37-C38
6	B	402	PC1	C35-C36-C37-C38
6	C	201	PC1	C32-C33-C34-C35
6	A	401	PC1	C25-C26-C27-C28
6	D	202	PC1	C32-C33-C34-C35
6	B	402	PC1	C25-C26-C27-C28
7	A	402	DU0	C21-C22-O23-C24
7	A	406	DU0	C21-C22-O23-C24
7	B	401	DU0	C21-C22-O23-C24
7	B	403	DU0	C21-C22-O23-C24
6	I	401	PC1	C38-C39-C3A-C3B
6	J	401	PC1	C38-C39-C3A-C3B
6	I	401	PC1	C39-C3A-C3B-C3C
6	A	401	PC1	C33-C34-C35-C36
6	J	401	PC1	C39-C3A-C3B-C3C
6	B	402	PC1	C33-C34-C35-C36
6	C	201	PC1	C31-C32-C33-C34
6	D	202	PC1	C31-C32-C33-C34
6	C	201	PC1	C2C-C2D-C2E-C2F
6	C	202	PC1	C33-C34-C35-C36
6	D	201	PC1	C33-C34-C35-C36
6	D	202	PC1	C2C-C2D-C2E-C2F

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	I	401	PC1	C28-C29-C2A-C2B
6	J	401	PC1	C28-C29-C2A-C2B
7	A	403	DU0	C24-C25-C26-C51
7	B	404	DU0	C24-C25-C26-C51
6	C	202	PC1	C11-C12-N-C14
6	D	201	PC1	C11-C12-N-C14
6	A	405	PC1	C35-C36-C37-C38
6	B	405	PC1	C35-C36-C37-C38
6	I	401	PC1	C37-C38-C39-C3A
6	J	401	PC1	C37-C38-C39-C3A
6	C	202	PC1	O21-C2-C3-O31
6	D	201	PC1	O21-C2-C3-O31
6	C	202	PC1	C11-C12-N-C15
6	D	201	PC1	C11-C12-N-C15
6	C	201	PC1	C37-C38-C39-C3A
6	D	202	PC1	C37-C38-C39-C3A
6	I	401	PC1	C22-C21-O21-C2
6	J	401	PC1	C22-C21-O21-C2
6	C	202	PC1	C26-C27-C28-C29
6	D	201	PC1	C26-C27-C28-C29
6	C	201	PC1	C2-C1-O11-P
6	D	202	PC1	C2-C1-O11-P
6	C	202	PC1	C22-C23-C24-C25
6	D	201	PC1	C22-C23-C24-C25
6	C	201	PC1	C33-C34-C35-C36
6	D	202	PC1	C33-C34-C35-C36
6	I	401	PC1	C34-C35-C36-C37
6	J	401	PC1	C34-C35-C36-C37
6	A	401	PC1	C23-C24-C25-C26
6	B	402	PC1	C23-C24-C25-C26
6	C	201	PC1	C21-C22-C23-C24
6	D	202	PC1	C21-C22-C23-C24
6	I	401	PC1	C26-C27-C28-C29
6	J	401	PC1	C26-C27-C28-C29
6	C	201	PC1	C2F-C2G-C2H-C2I
6	D	202	PC1	C2F-C2G-C2H-C2I
6	C	201	PC1	C2E-C2F-C2G-C2H
6	D	202	PC1	C2E-C2F-C2G-C2H
6	I	401	PC1	O21-C2-C3-O31
6	J	401	PC1	O21-C2-C3-O31
6	I	401	PC1	C2C-C2D-C2E-C2F
6	J	401	PC1	C2C-C2D-C2E-C2F

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	C	202	PC1	C37-C38-C39-C3A
6	D	201	PC1	C37-C38-C39-C3A
7	A	402	DU0	C75-C22-O23-C24
7	B	403	DU0	C75-C22-O23-C24
6	C	201	PC1	C38-C39-C3A-C3B
6	D	202	PC1	C38-C39-C3A-C3B
6	A	401	PC1	O11-C1-C2-C3
6	A	405	PC1	O11-C1-C2-C3
6	B	402	PC1	O11-C1-C2-C3
6	B	405	PC1	O11-C1-C2-C3
7	A	402	DU0	C51-C26-C27-O28
7	B	403	DU0	C51-C26-C27-O28
6	C	202	PC1	C1-C2-C3-O31
6	I	401	PC1	C1-C2-C3-O31
6	A	405	PC1	C1-C2-C3-O31
6	D	201	PC1	C1-C2-C3-O31
6	J	401	PC1	C1-C2-C3-O31
6	B	405	PC1	C1-C2-C3-O31
6	C	201	PC1	C34-C35-C36-C37
6	D	202	PC1	C34-C35-C36-C37
6	A	401	PC1	C11-O13-P-O11
6	B	402	PC1	C11-O13-P-O11
7	A	403	DU0	C25-C26-C51-O52
7	B	404	DU0	C25-C26-C51-O52
7	A	403	DU0	C24-C25-C26-C27
7	B	404	DU0	C24-C25-C26-C27
6	A	401	PC1	O11-C1-C2-O21
6	B	402	PC1	O11-C1-C2-O21
6	A	405	PC1	C32-C33-C34-C35
6	B	405	PC1	C32-C33-C34-C35
6	I	401	PC1	O22-C21-O21-C2
6	J	401	PC1	O22-C21-O21-C2
6	I	401	PC1	C36-C37-C38-C39
6	J	401	PC1	C36-C37-C38-C39
6	C	202	PC1	C23-C24-C25-C26
6	D	201	PC1	C23-C24-C25-C26
7	G	101	DU0	O23-C24-C25-C26
7	A	402	DU0	O23-C24-C25-C26
7	H	101	DU0	O23-C24-C25-C26
7	B	403	DU0	O23-C24-C25-C26
6	C	201	PC1	O11-C1-C2-C3
6	I	401	PC1	O11-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	D	202	PC1	O11-C1-C2-C3
6	J	401	PC1	O11-C1-C2-C3
8	A	404	PLC	O3P-C1-C2-C3
6	C	201	PC1	C1-C2-C3-O31
6	D	202	PC1	C1-C2-C3-O31
8	A	404	PLC	C2-C1-O3P-P
6	C	201	PC1	O11-C1-C2-O21
6	D	202	PC1	O11-C1-C2-O21
6	C	202	PC1	C28-C29-C2A-C2B
6	D	201	PC1	C28-C29-C2A-C2B
6	A	401	PC1	O21-C2-C3-O31
6	A	405	PC1	O21-C2-C3-O31
6	B	402	PC1	O21-C2-C3-O31
6	B	405	PC1	O21-C2-C3-O31
6	C	202	PC1	C1-O11-P-O13
6	D	201	PC1	C1-O11-P-O13
6	I	401	PC1	C32-C33-C34-C35
6	J	401	PC1	C32-C33-C34-C35
6	A	405	PC1	C2-C1-O11-P
6	B	405	PC1	C2-C1-O11-P
6	C	201	PC1	C11-O13-P-O12
6	C	201	PC1	C1-O11-P-O14
6	C	202	PC1	C11-O13-P-O14
6	A	405	PC1	C11-O13-P-O14
6	D	201	PC1	C11-O13-P-O14
6	D	202	PC1	C11-O13-P-O12
6	D	202	PC1	C1-O11-P-O14
6	B	405	PC1	C11-O13-P-O14
6	C	201	PC1	C25-C26-C27-C28
6	D	202	PC1	C25-C26-C27-C28
8	A	404	PLC	C5-C4-O4P-P
6	C	202	PC1	O11-C1-C2-O21
6	I	401	PC1	O11-C1-C2-O21
6	A	405	PC1	O11-C1-C2-O21
6	D	201	PC1	O11-C1-C2-O21
6	J	401	PC1	O11-C1-C2-O21
6	B	405	PC1	O11-C1-C2-O21
8	A	404	PLC	O3P-C1-C2-O2
6	C	202	PC1	C11-C12-N-C13
6	D	201	PC1	C11-C12-N-C13
8	A	404	PLC	O4P-C4-C5-N
6	C	201	PC1	O21-C2-C3-O31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	D	202	PC1	O21-C2-C3-O31
7	A	402	DU0	C24-C25-C26-C27
7	A	402	DU0	C24-C25-C26-C51
7	B	403	DU0	C24-C25-C26-C27
7	B	403	DU0	C24-C25-C26-C51
6	I	401	PC1	C2A-C2B-C2C-C2D
6	J	401	PC1	C2A-C2B-C2C-C2D
6	C	202	PC1	O11-C1-C2-C3
6	D	201	PC1	O11-C1-C2-C3
6	C	201	PC1	C39-C3A-C3B-C3C
6	D	202	PC1	C39-C3A-C3B-C3C
6	C	201	PC1	C22-C23-C24-C25
6	D	202	PC1	C22-C23-C24-C25
6	I	401	PC1	C21-C22-C23-C24
6	J	401	PC1	C21-C22-C23-C24
6	C	202	PC1	C35-C36-C37-C38
6	D	201	PC1	C35-C36-C37-C38
6	A	405	PC1	C11-C12-N-C14
6	B	405	PC1	C11-C12-N-C14
6	C	201	PC1	O21-C21-C22-C23
6	D	202	PC1	O21-C21-C22-C23
6	I	401	PC1	C2-C1-O11-P
6	J	401	PC1	C2-C1-O11-P
6	A	401	PC1	O31-C31-C32-C33
6	B	402	PC1	O31-C31-C32-C33
8	A	404	PLC	C1B-C2B-C3B-C4B
6	C	201	PC1	O22-C21-C22-C23
6	D	202	PC1	O22-C21-C22-C23
6	A	401	PC1	O32-C31-C32-C33
6	B	402	PC1	O32-C31-C32-C33
8	A	404	PLC	O2-C'-C1'-C2'
6	A	401	PC1	C11-O13-P-O12
6	B	402	PC1	C11-O13-P-O12
6	A	401	PC1	C12-C11-O13-P
6	B	402	PC1	C12-C11-O13-P
8	A	404	PLC	C1-C2-O2-C'
6	A	405	PC1	C11-C12-N-C13
6	B	405	PC1	C11-C12-N-C13
6	C	202	PC1	O21-C21-C22-C23
6	D	201	PC1	O21-C21-C22-C23
6	I	401	PC1	O21-C21-C22-C23
6	J	401	PC1	O21-C21-C22-C23

*Continued on next page...*

*Continued from previous page...*

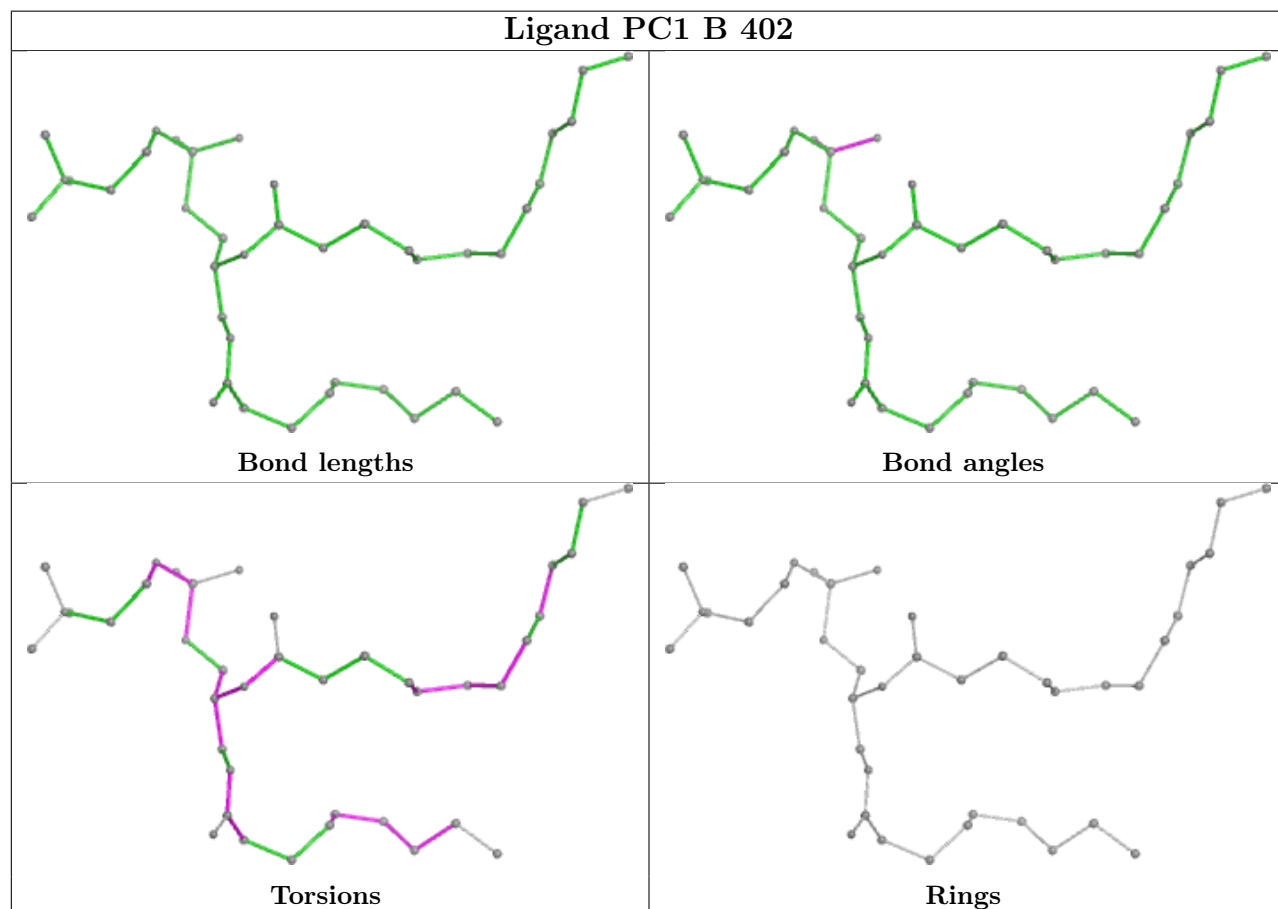
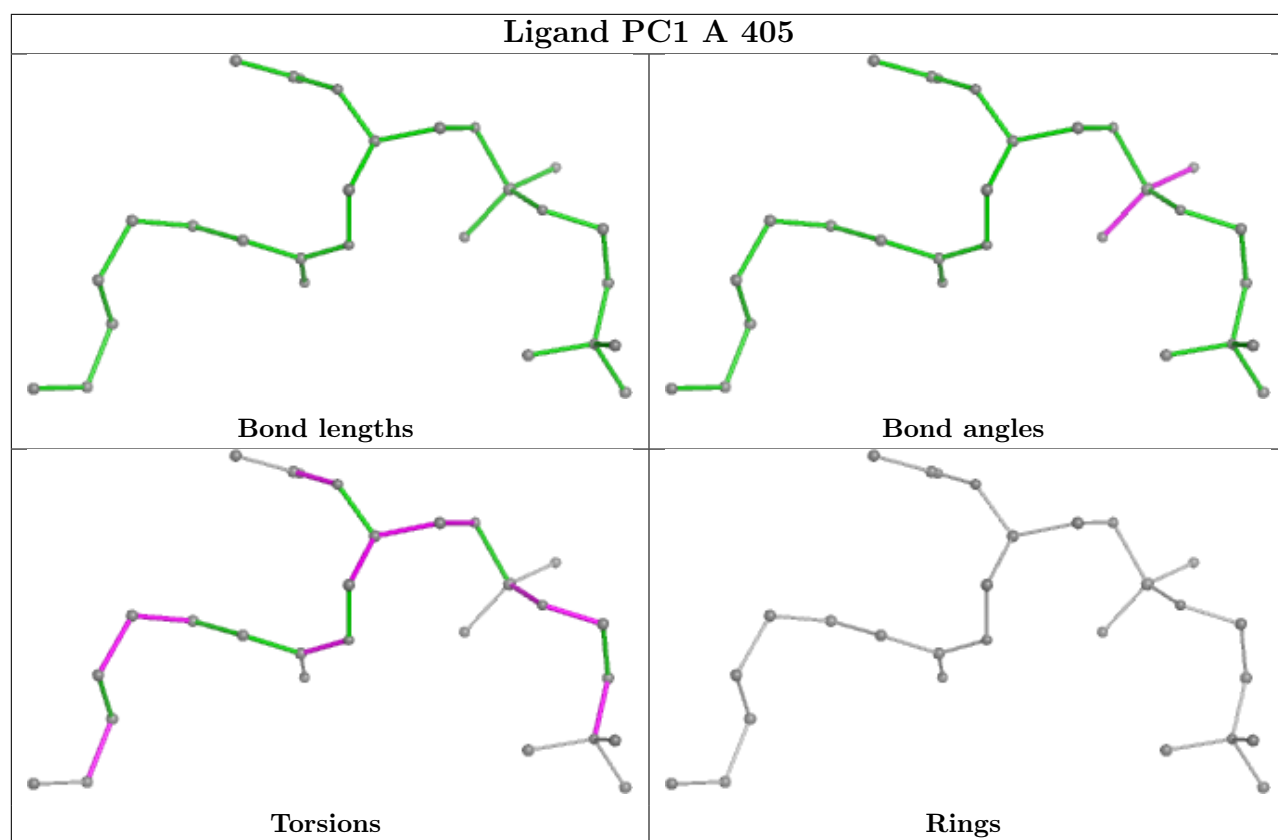
Mol	Chain	Res	Type	Atoms
8	A	404	PLC	O'-C'-C1'-C2'
6	A	401	PC1	C36-C37-C38-C39
6	B	402	PC1	C36-C37-C38-C39

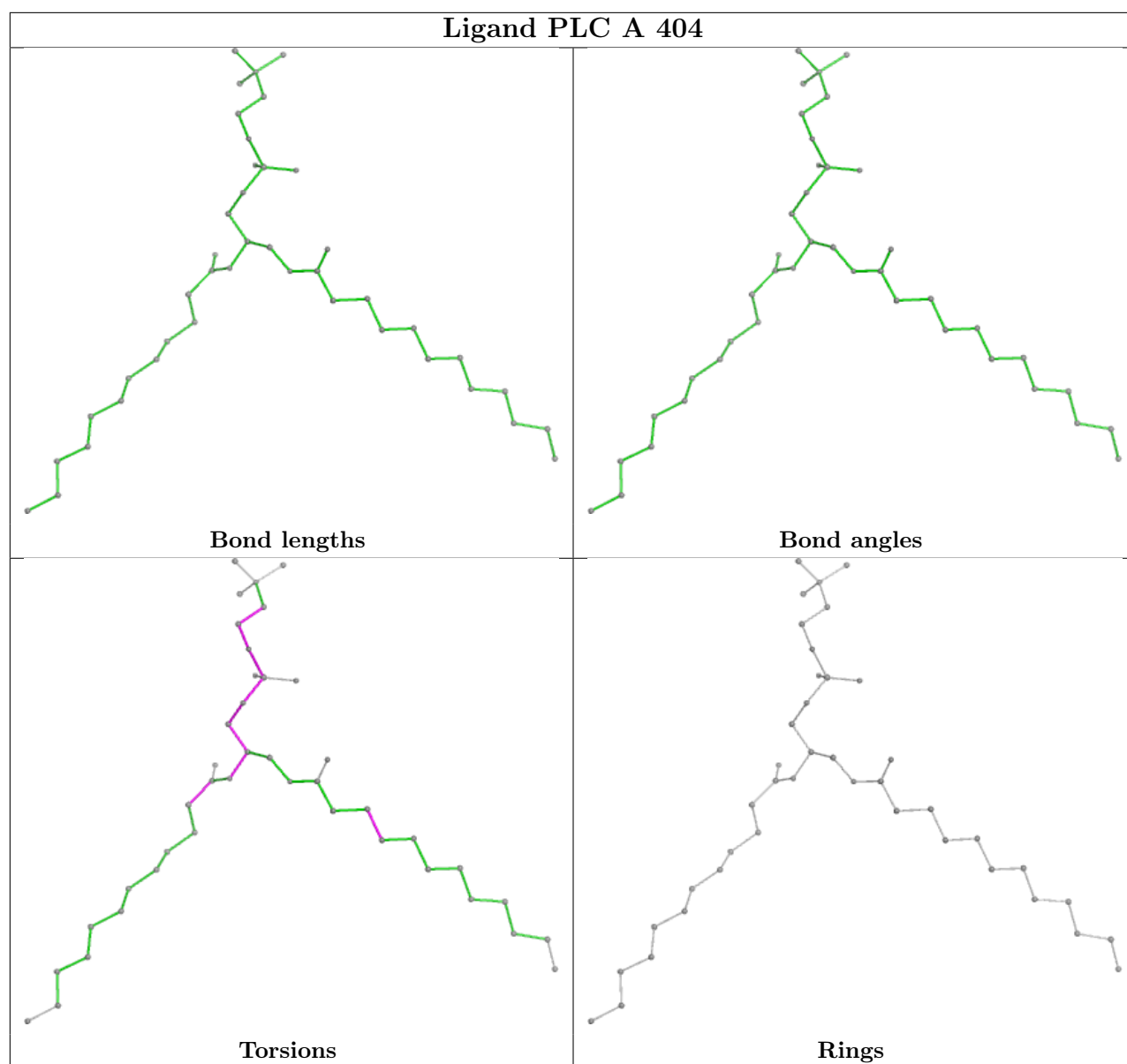
There are no ring outliers.

13 monomers are involved in 57 short contacts:

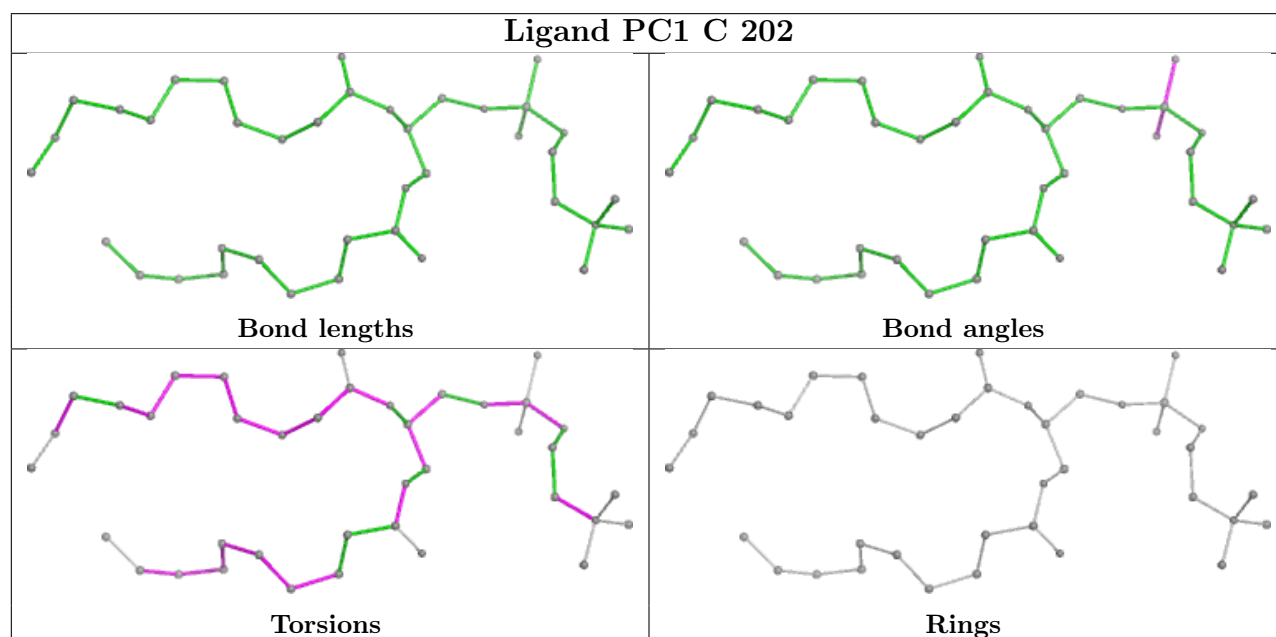
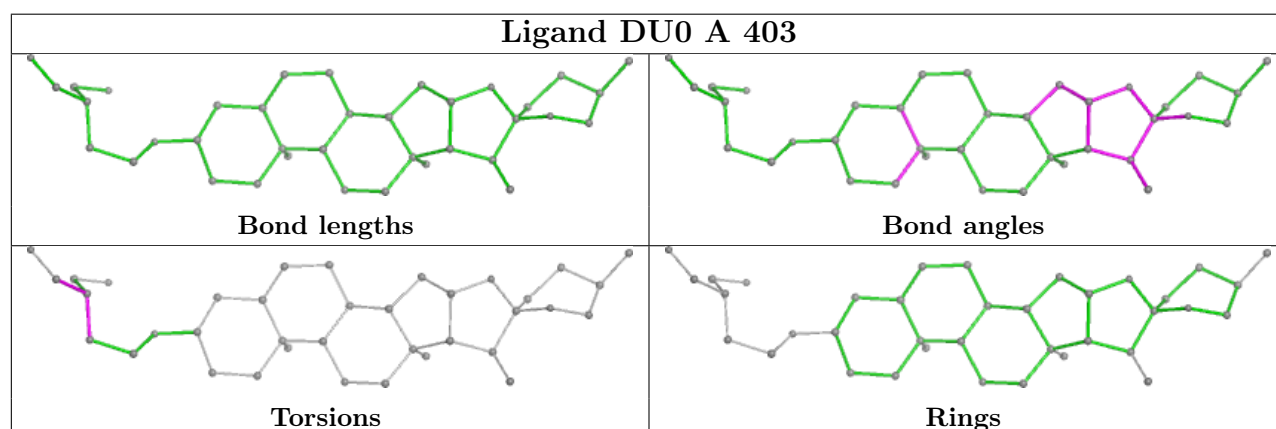
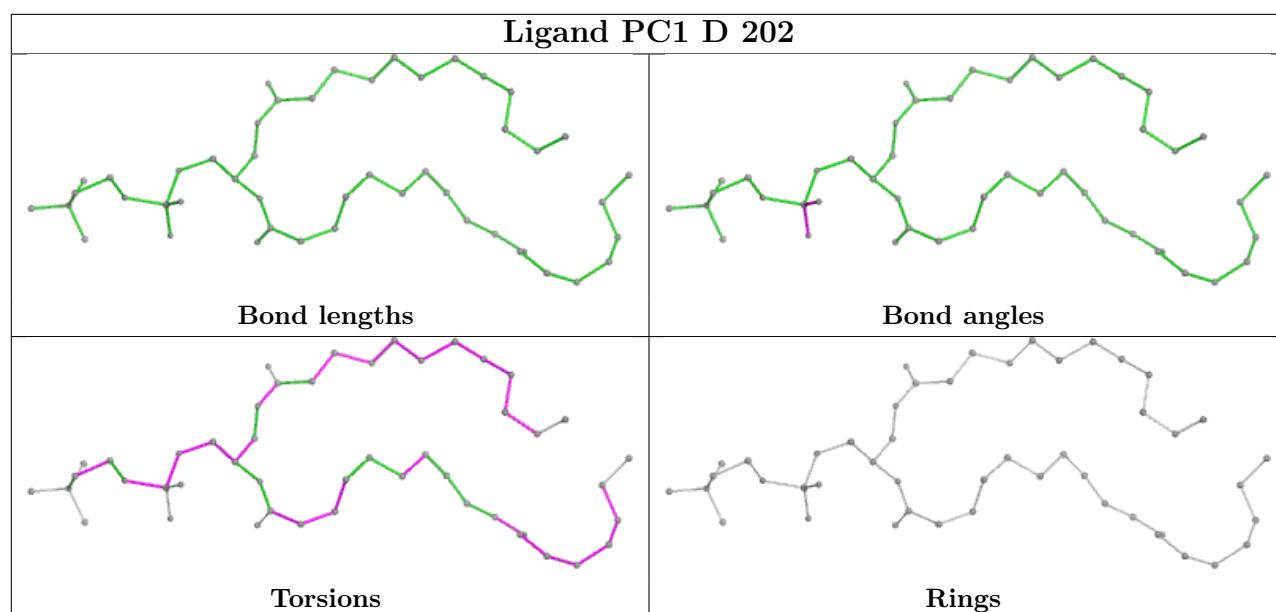
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	405	PC1	2	0
6	B	402	PC1	6	0
8	A	404	PLC	1	0
6	D	202	PC1	3	0
7	A	403	DU0	1	0
6	C	202	PC1	9	0
6	J	401	PC1	9	0
6	C	201	PC1	2	0
6	A	401	PC1	5	0
6	I	401	PC1	7	0
6	B	405	PC1	3	0
7	B	404	DU0	1	0
6	D	201	PC1	8	0

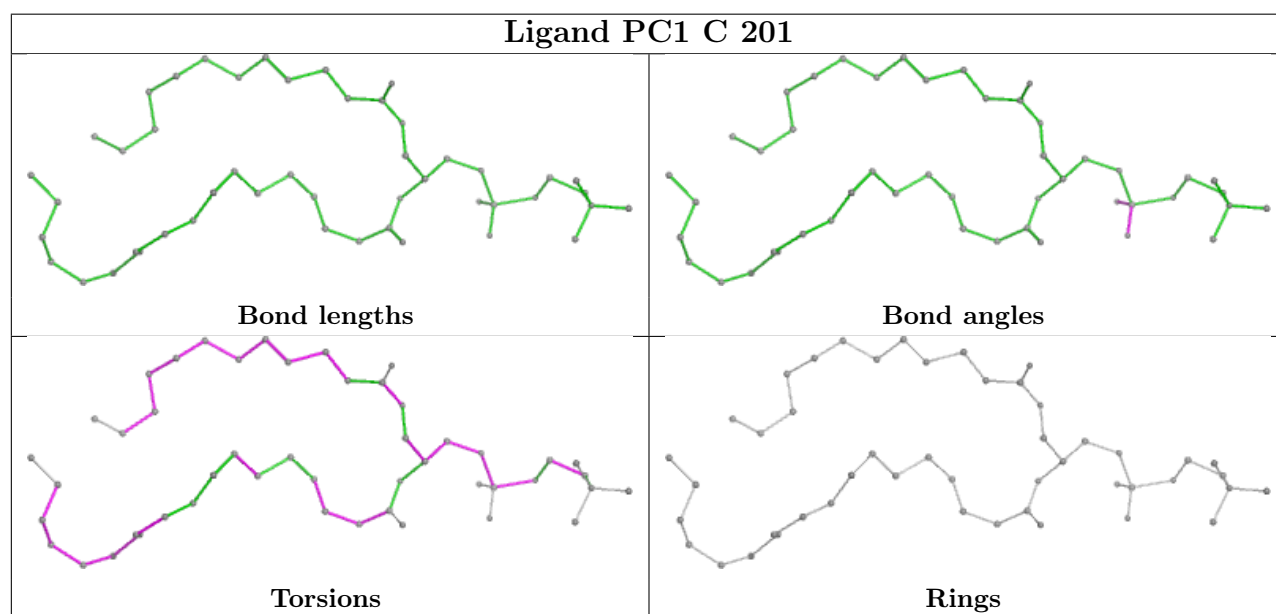
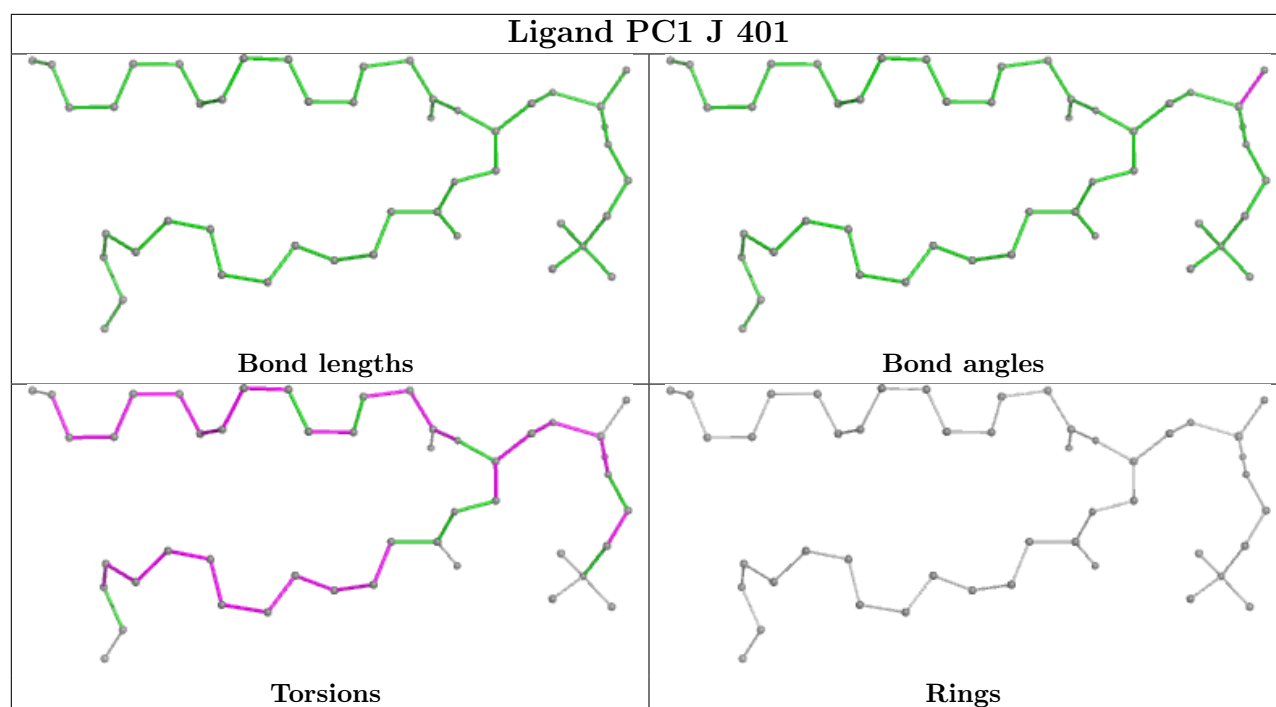
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

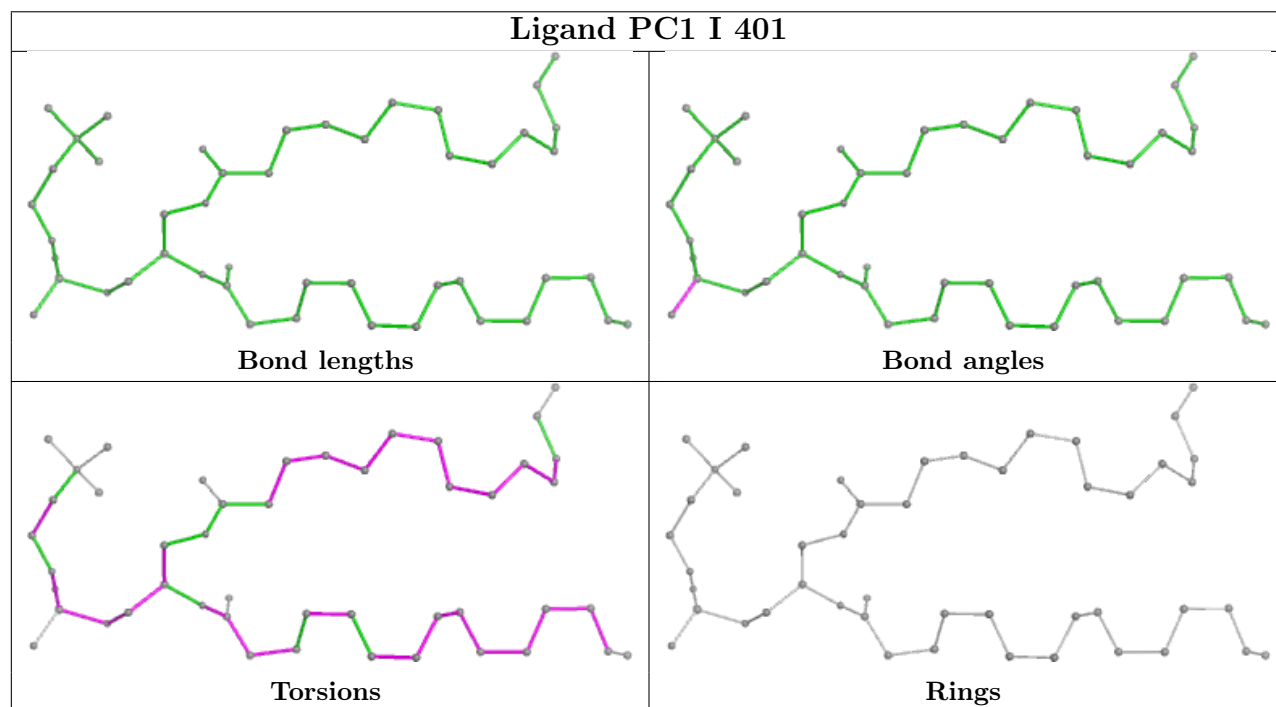
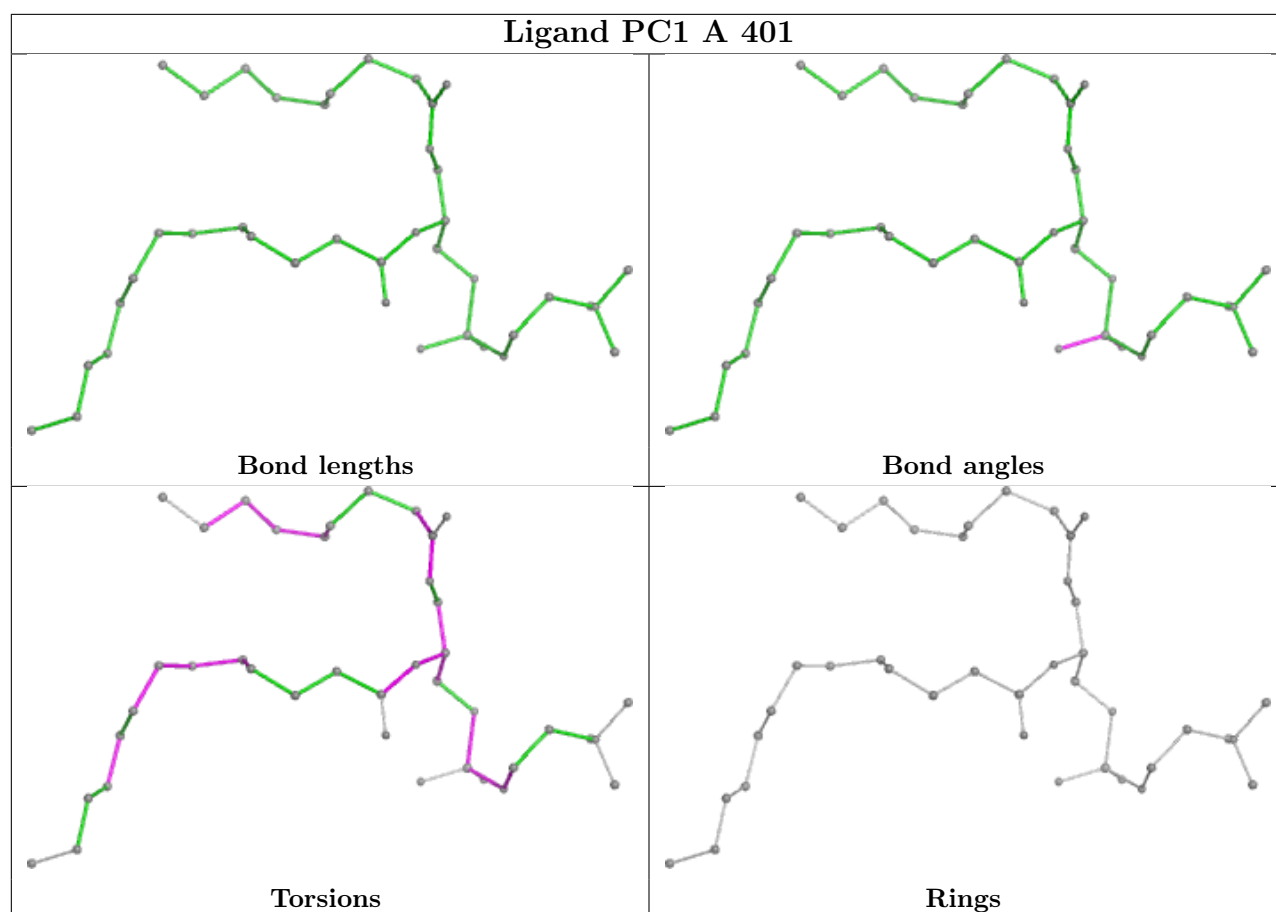


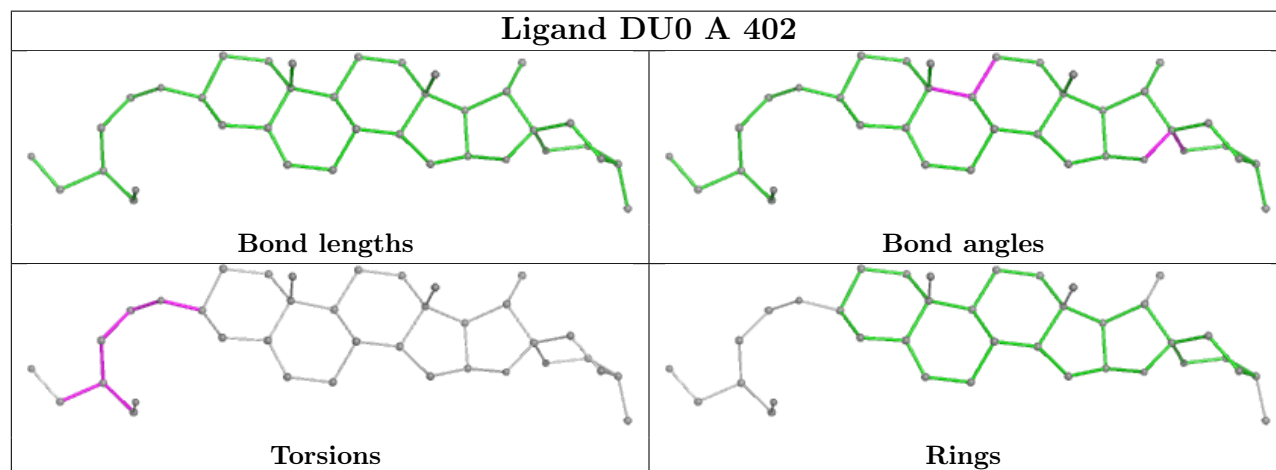
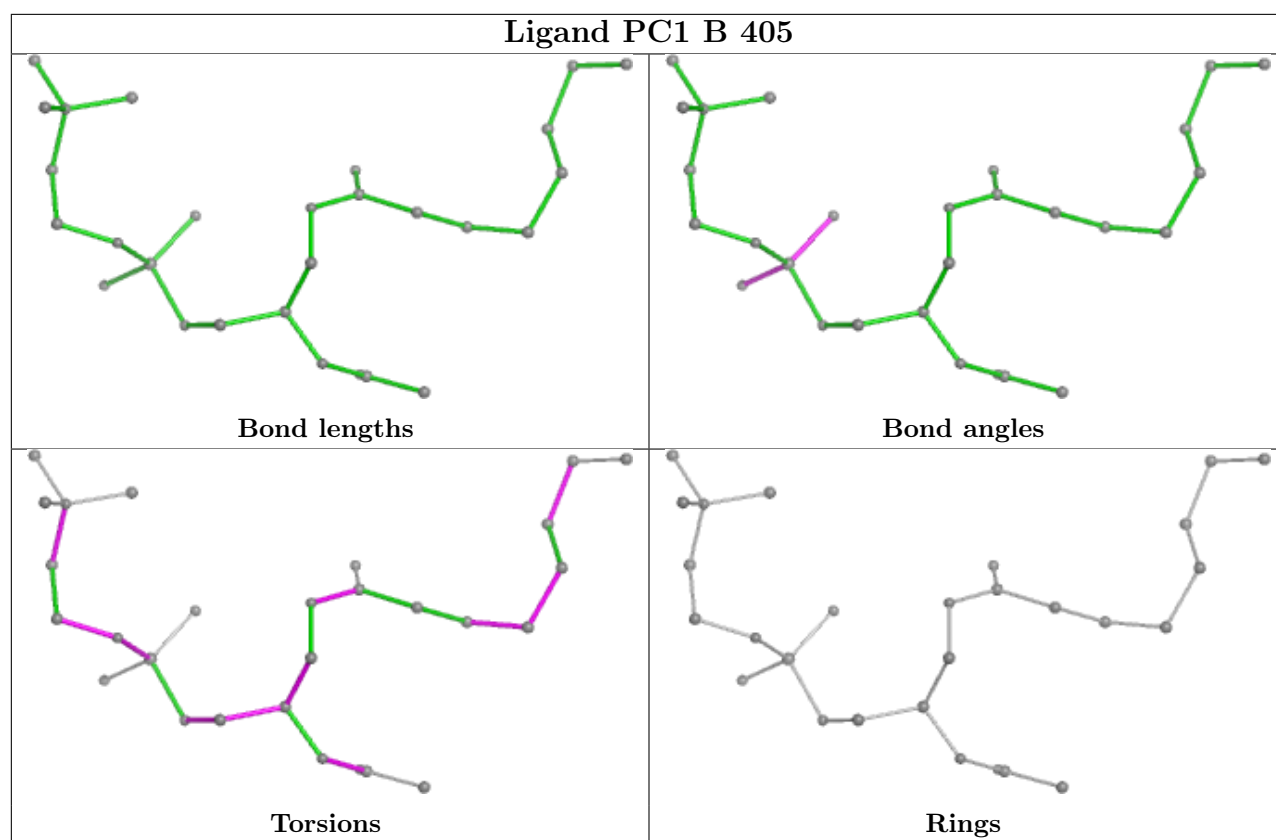




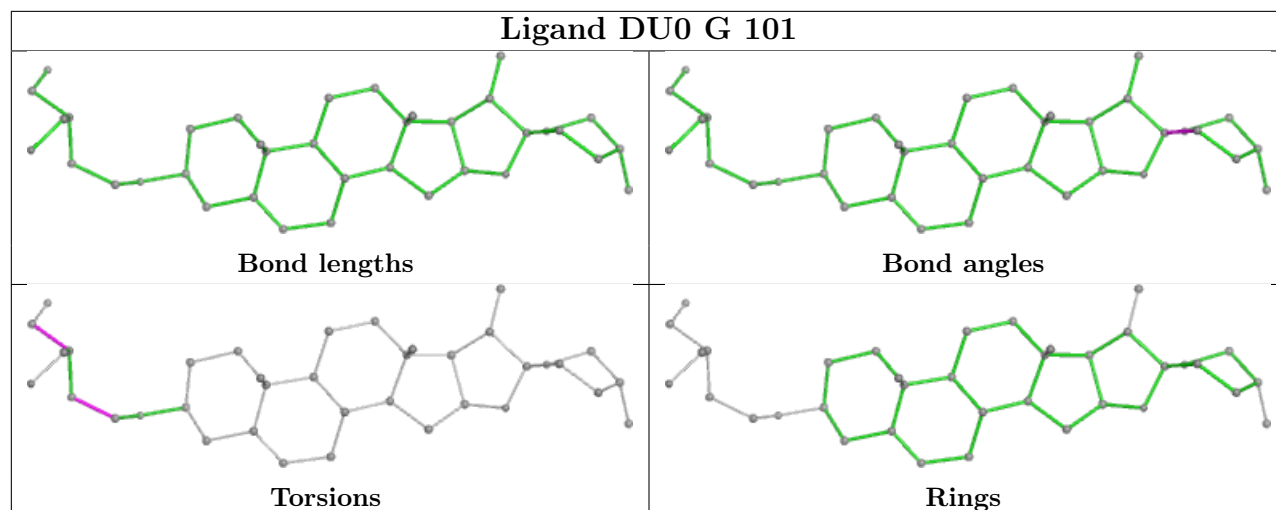




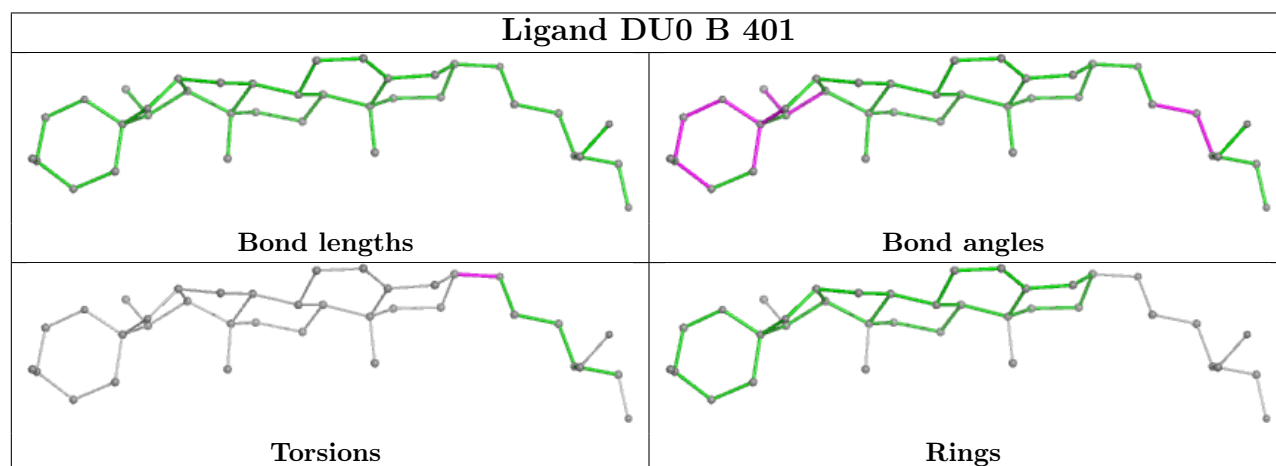




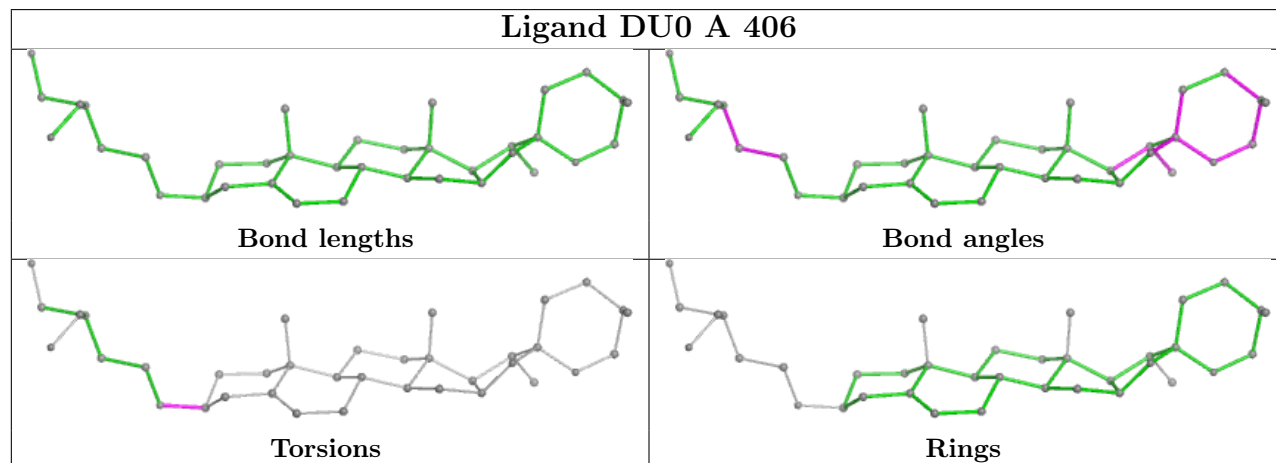
## Ligand DU0 G 101

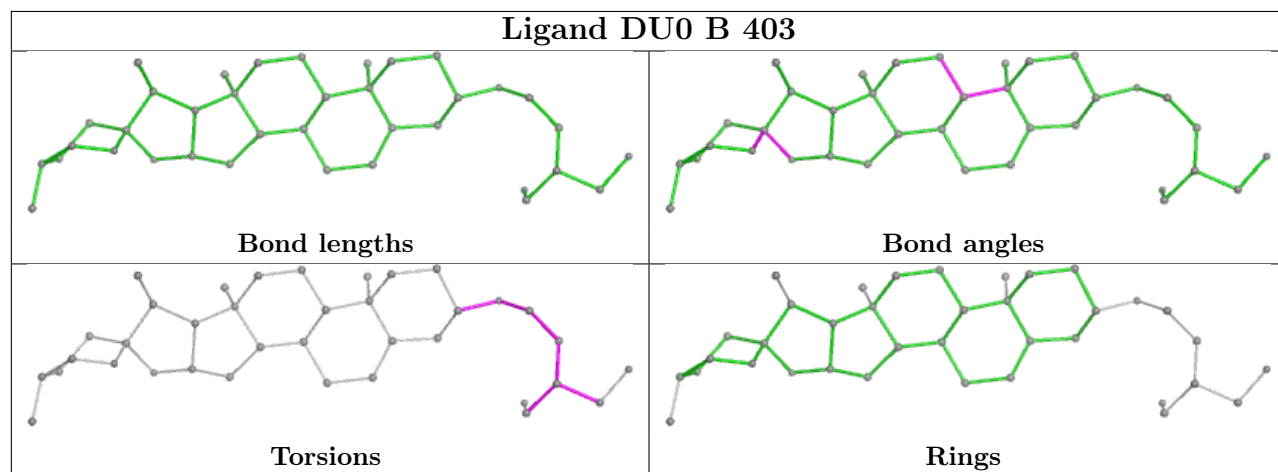
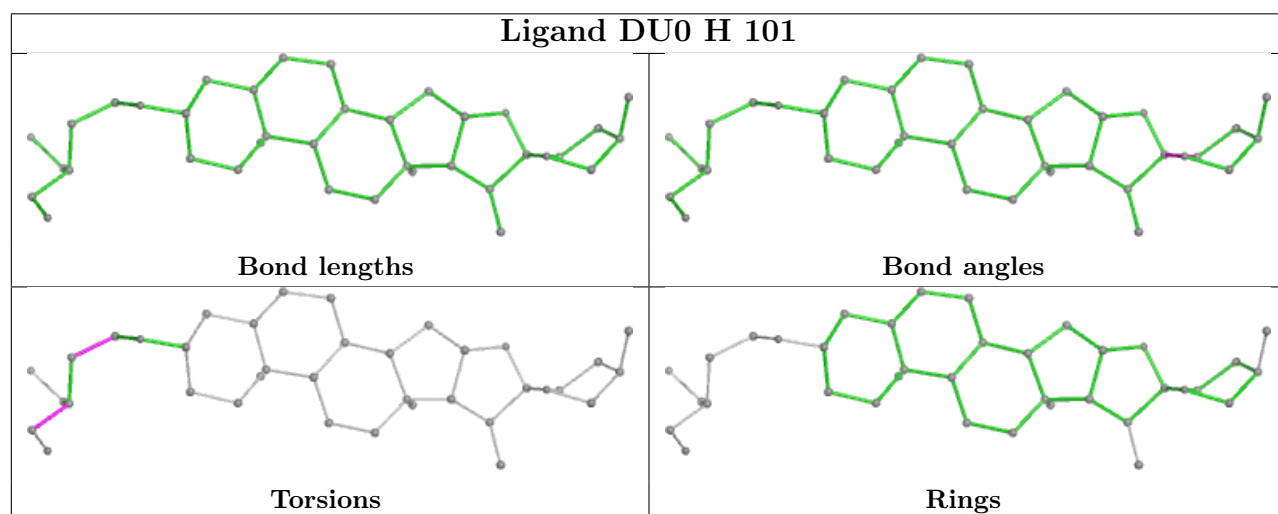
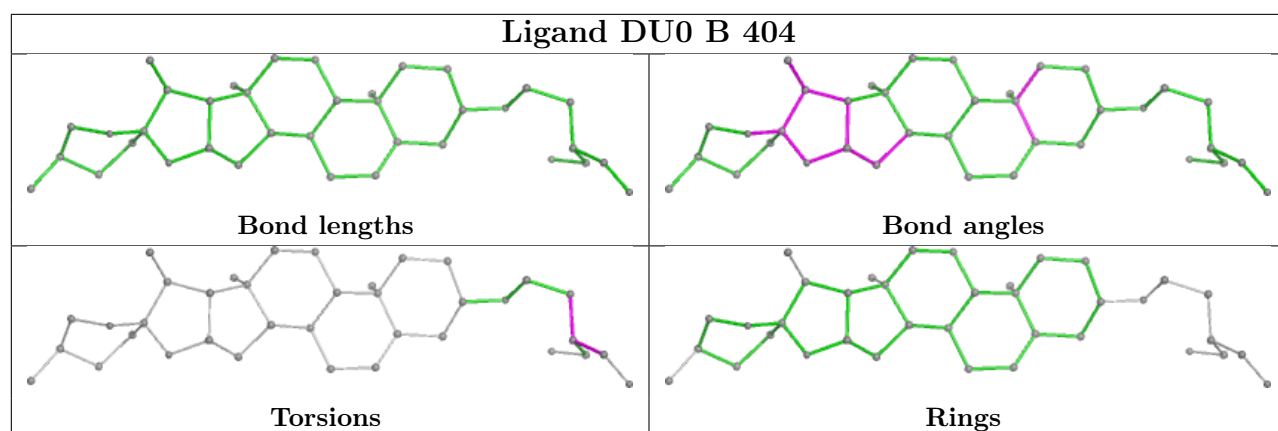


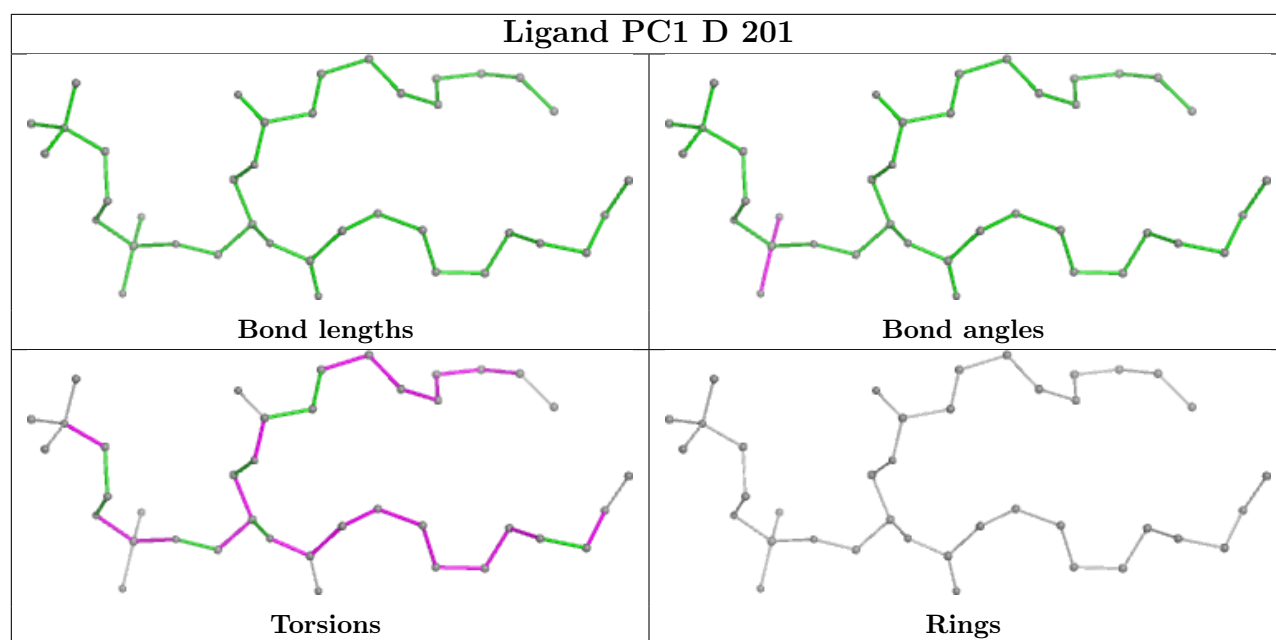
## Ligand DU0 B 401



## Ligand DU0 A 406







## 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.

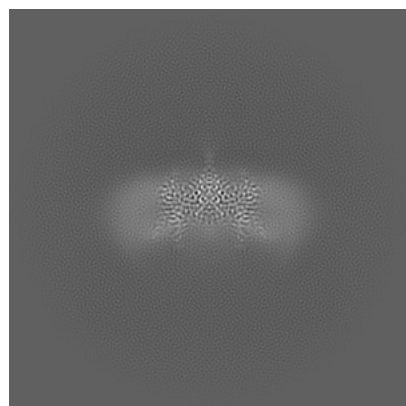
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52652. These allow visual inspection of the internal detail of the map and identification of artifacts.

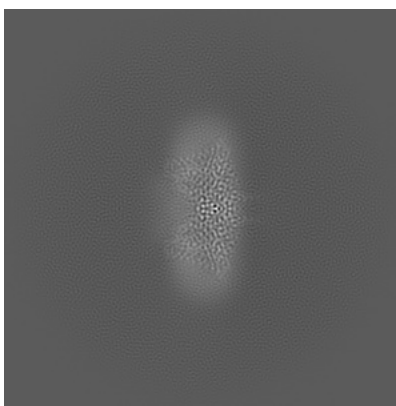
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

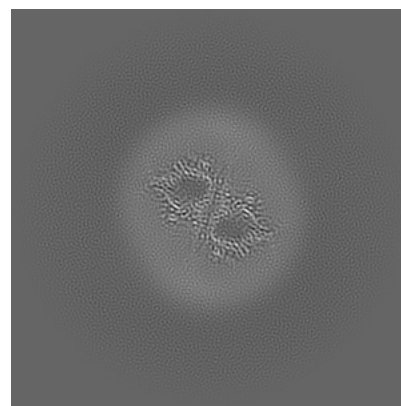
#### 6.1.1 Primary map



X

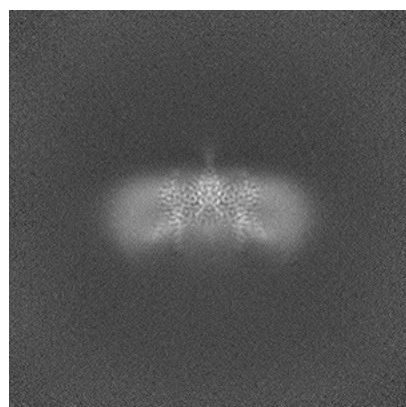


Y

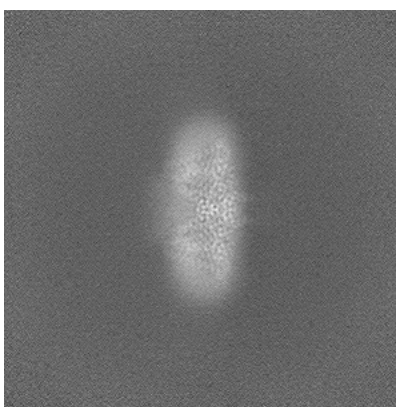


Z

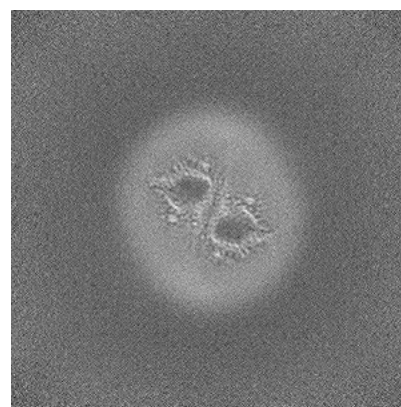
#### 6.1.2 Raw map



X



Y



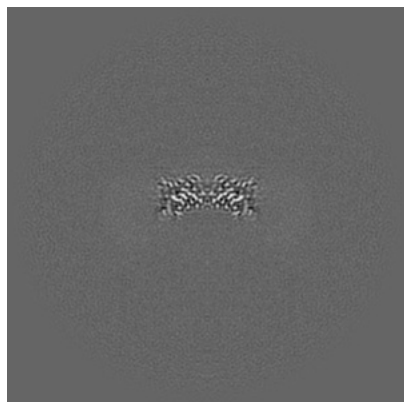
Z

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

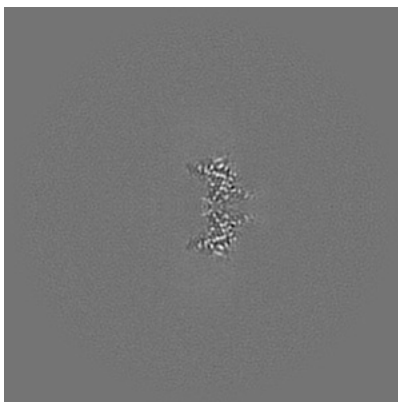


## 6.2 Central slices [i](#)

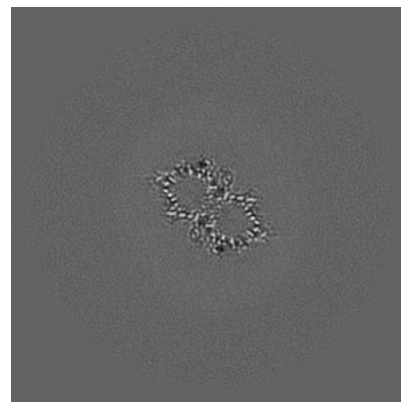
### 6.2.1 Primary map



X Index: 280

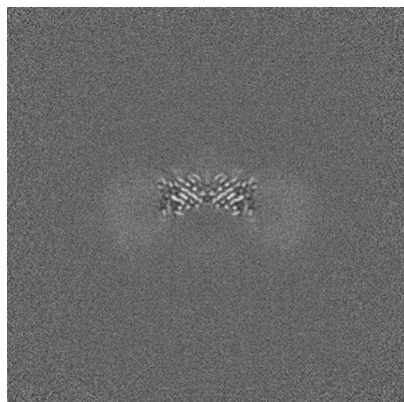


Y Index: 280

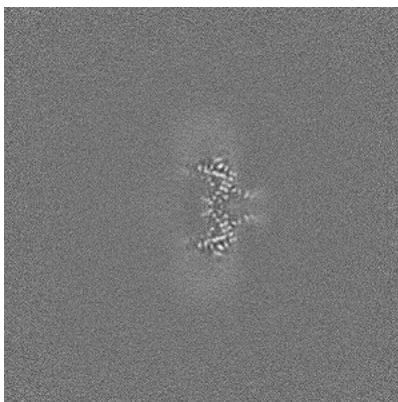


Z Index: 280

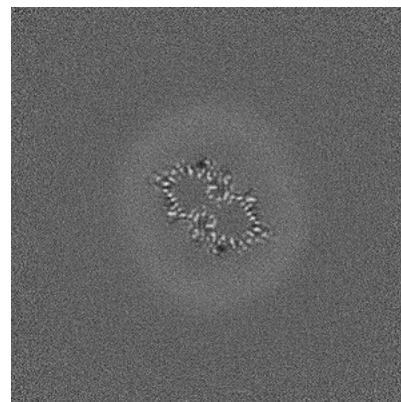
### 6.2.2 Raw map



X Index: 280



Y Index: 280

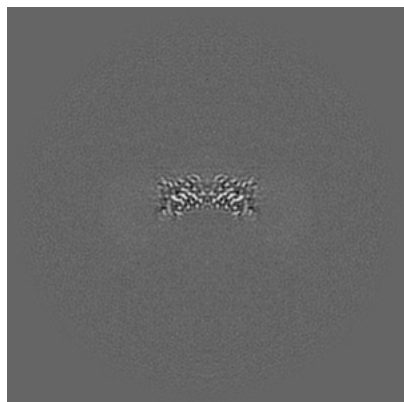


Z Index: 280

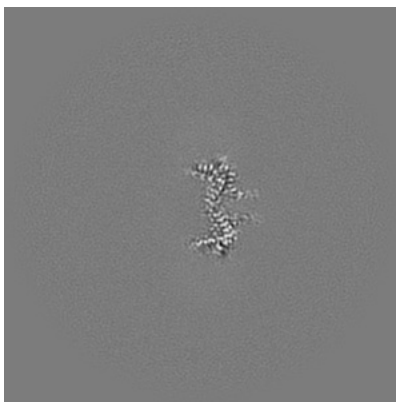
The images above show central slices of the map in three orthogonal directions.

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

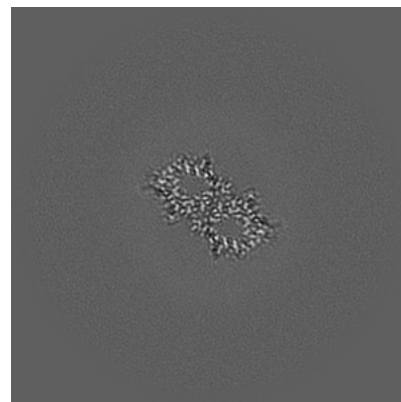
### 6.3.1 Primary map



X Index: 280

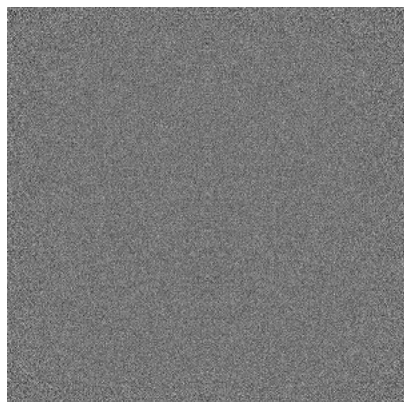


Y Index: 282

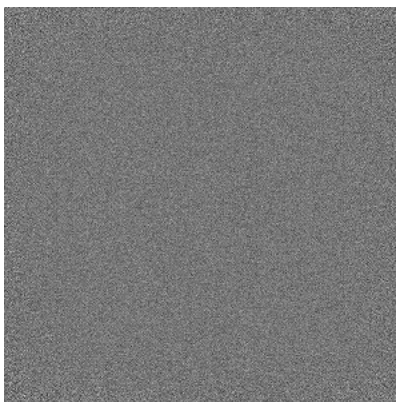


Z Index: 294

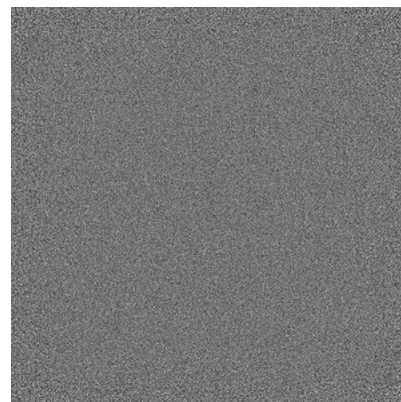
### 6.3.2 Raw map



X Index: 0



Y Index: 0

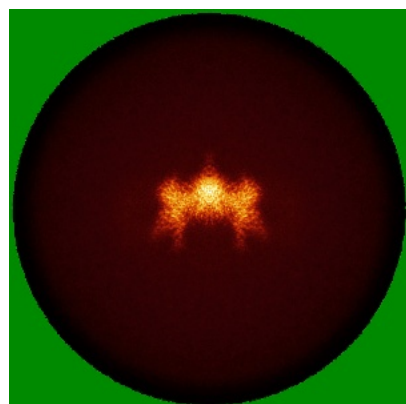


Z Index: 559

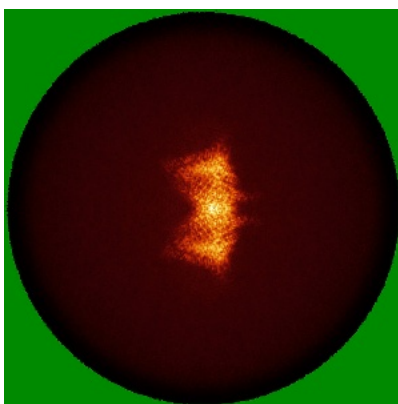
The images above show the largest variance slices of the map in three orthogonal directions.

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

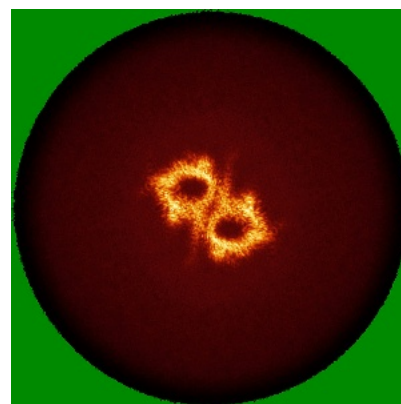
### 6.4.1 Primary map



X

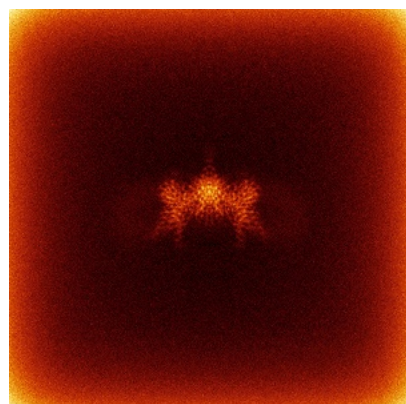


Y

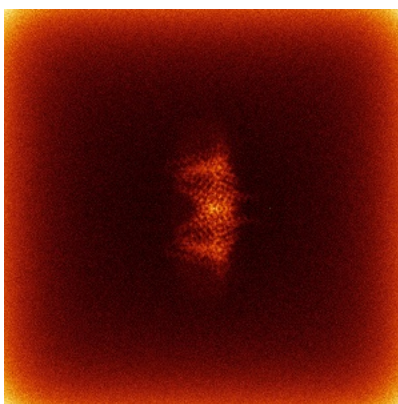


Z

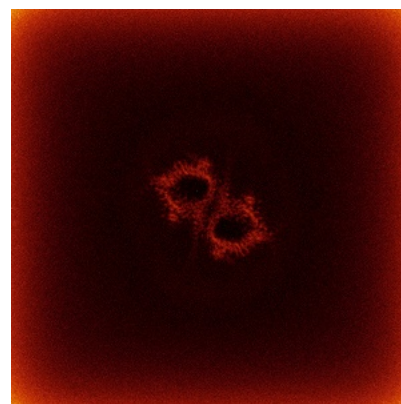
### 6.4.2 Raw map



X



Y

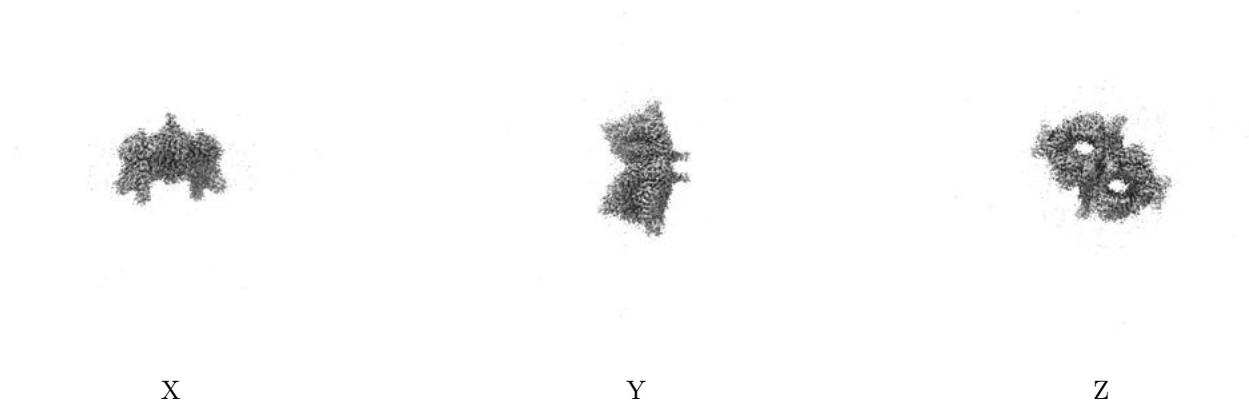


Z

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.

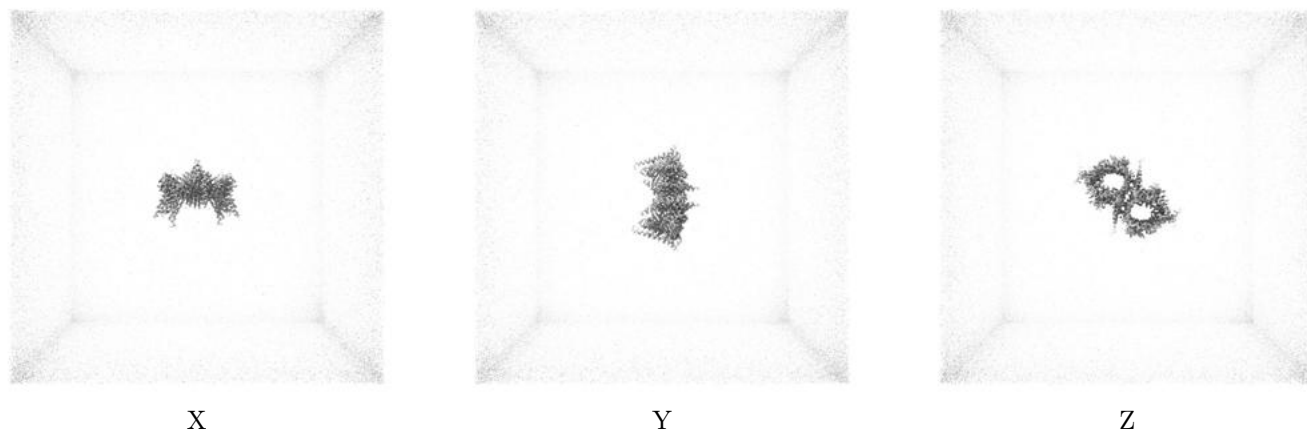
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.103. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

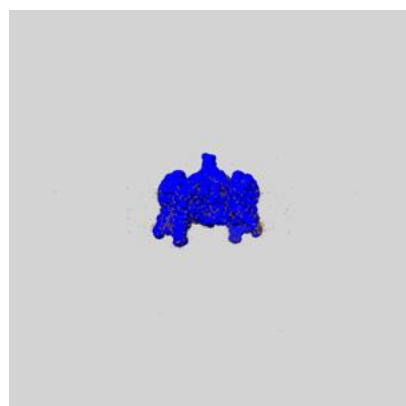
## 6.6 Mask visualisation [i](#)

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

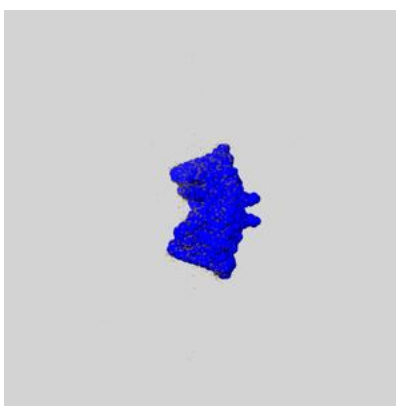
A mask typically either:

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

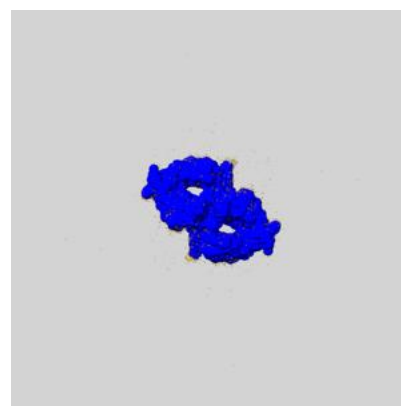
### 6.6.1 emd\_52652\_msk\_1.map [i](#)



X



Y



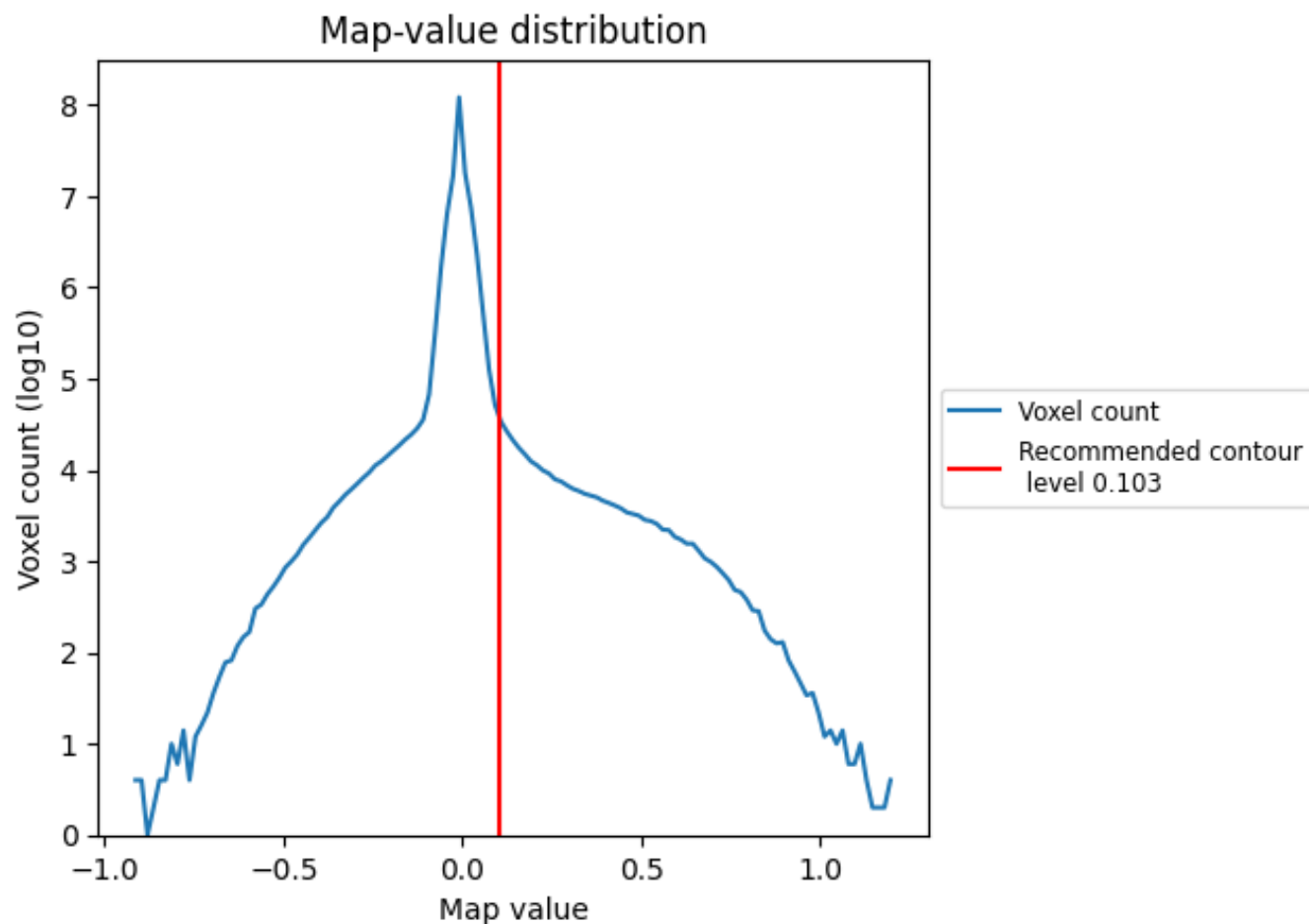
Z



## 7 Map analysis [i](#)

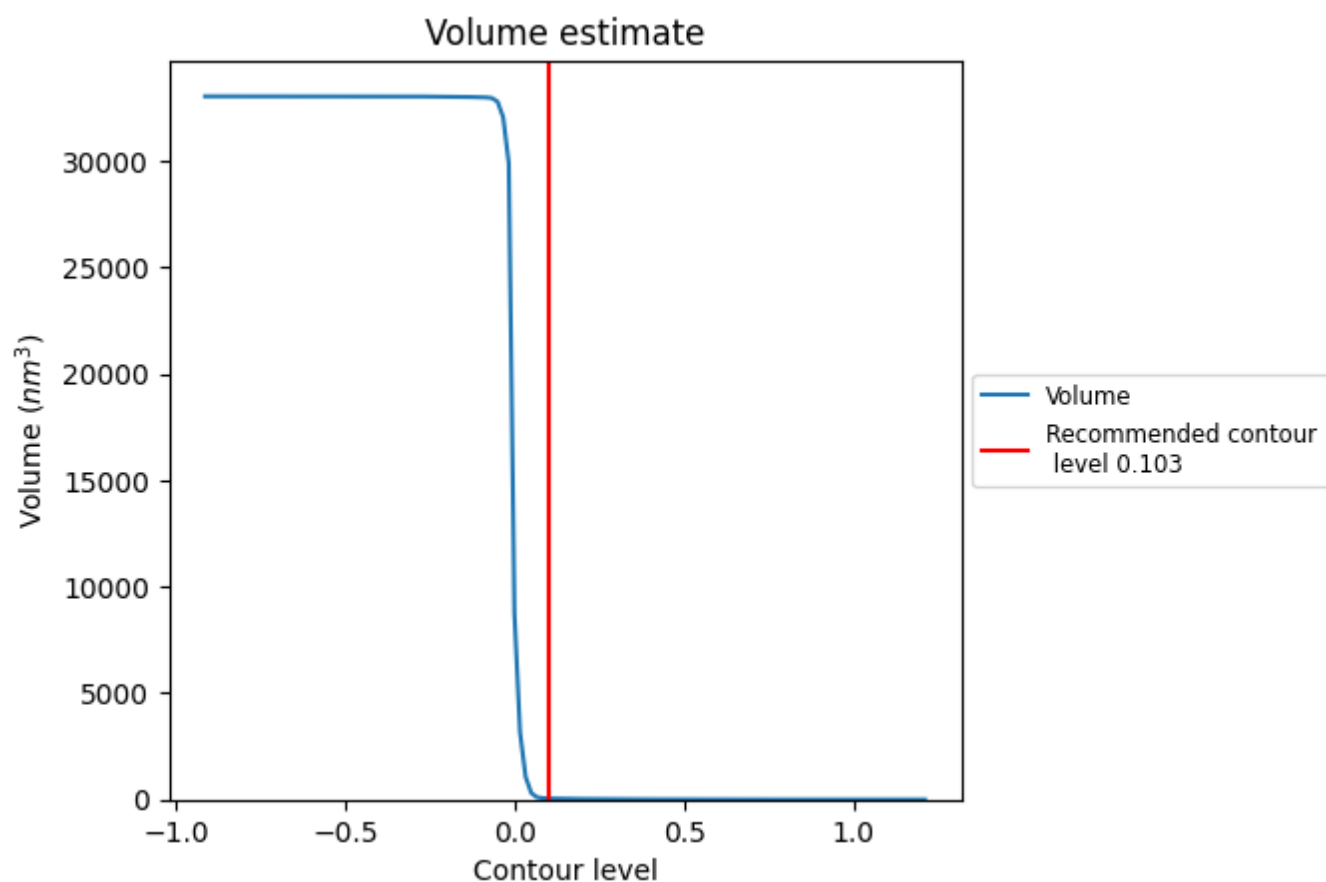
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

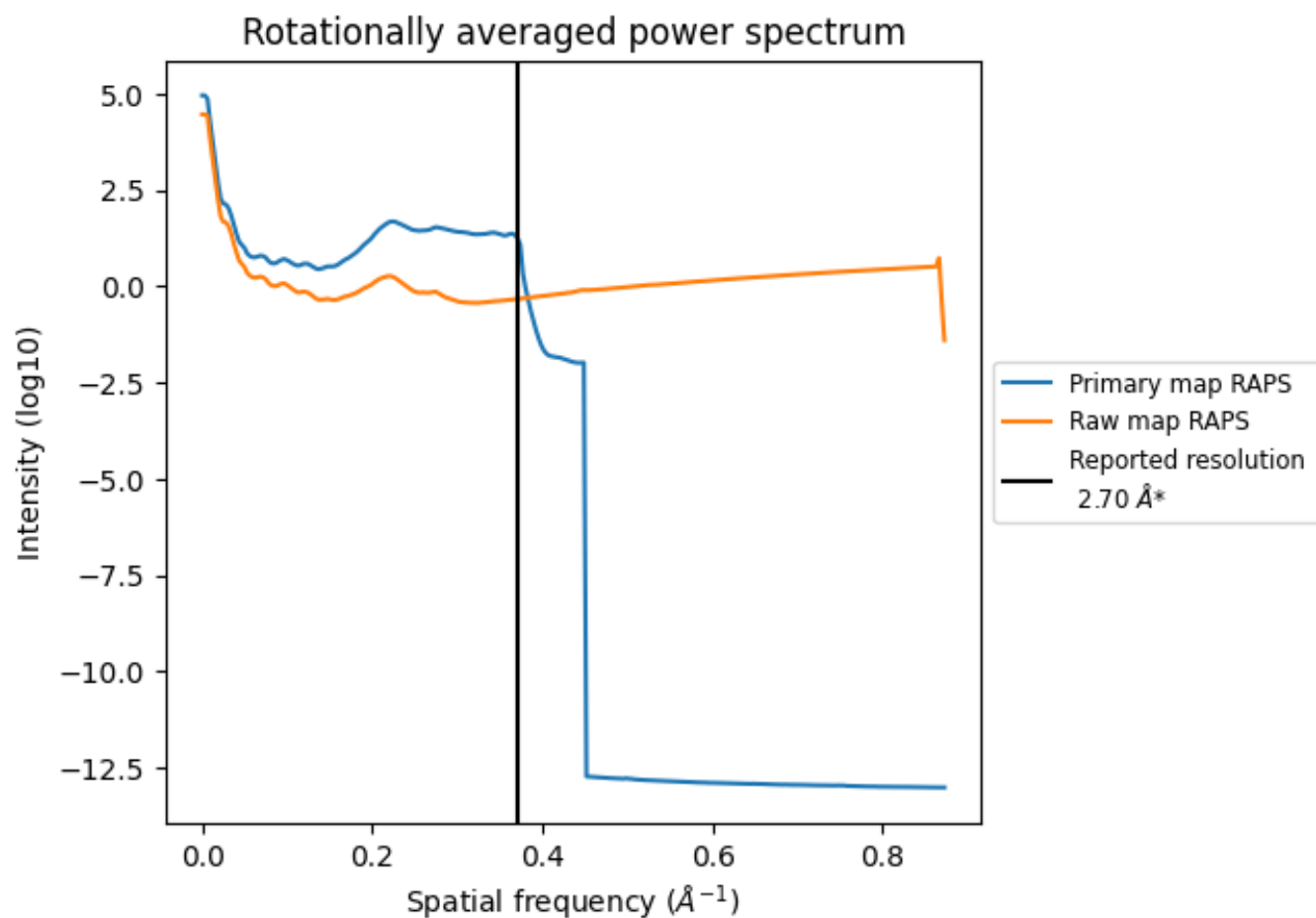
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm<sup>3</sup>; this corresponds to an approximate mass of 47 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



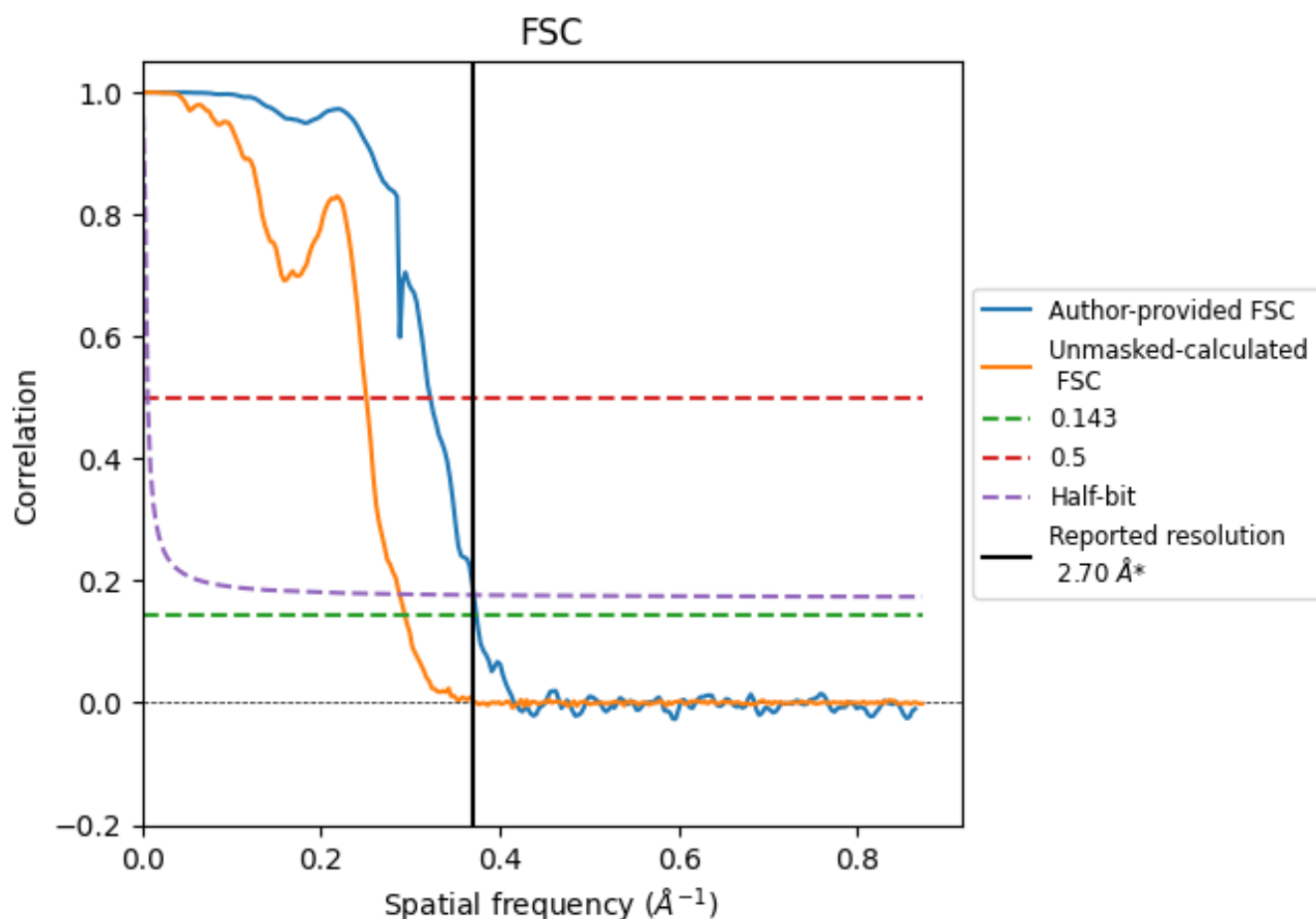
\*Reported resolution corresponds to spatial frequency of 0.370  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

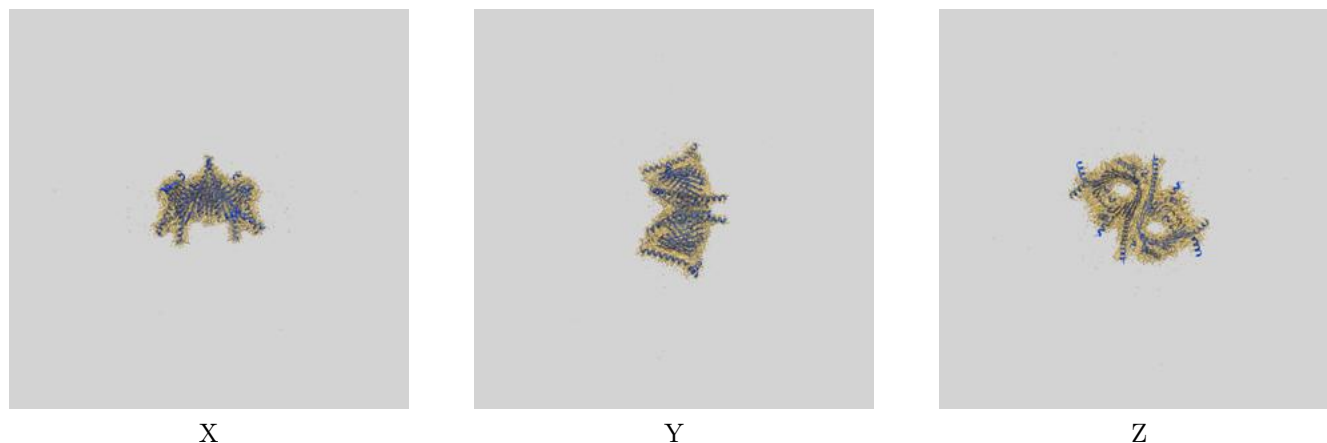
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.10	2.70
Unmasked-calculated*	3.40	3.99	3.47

\*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 3.40 differs from the reported value 2.7 by more than 10 %

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

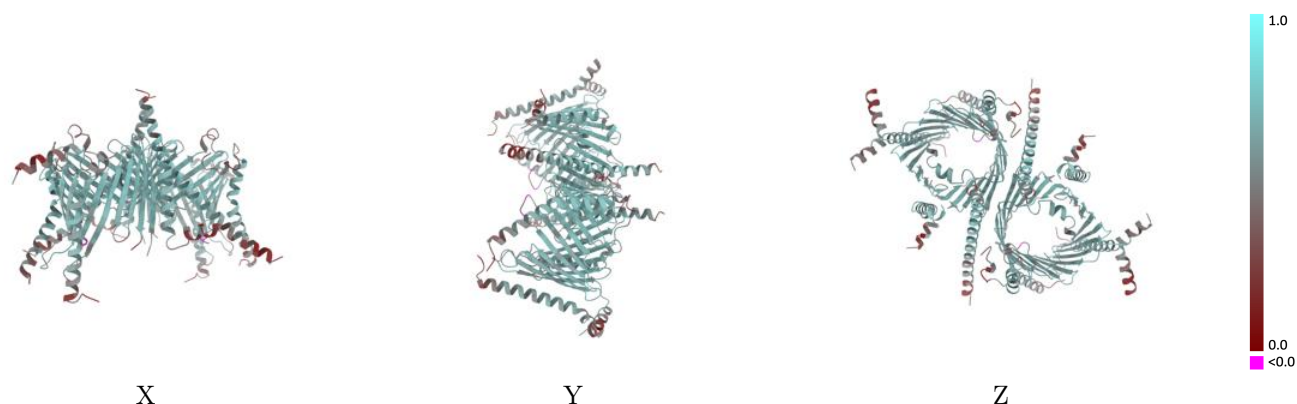
This section contains information regarding the fit between EMDB map EMD-52652 and PDB model 9I6B. Per-residue inclusion information can be found in section 3 on page 9.

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



The images above show the 3D surface view of the map at the recommended contour level 0.103 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](#)



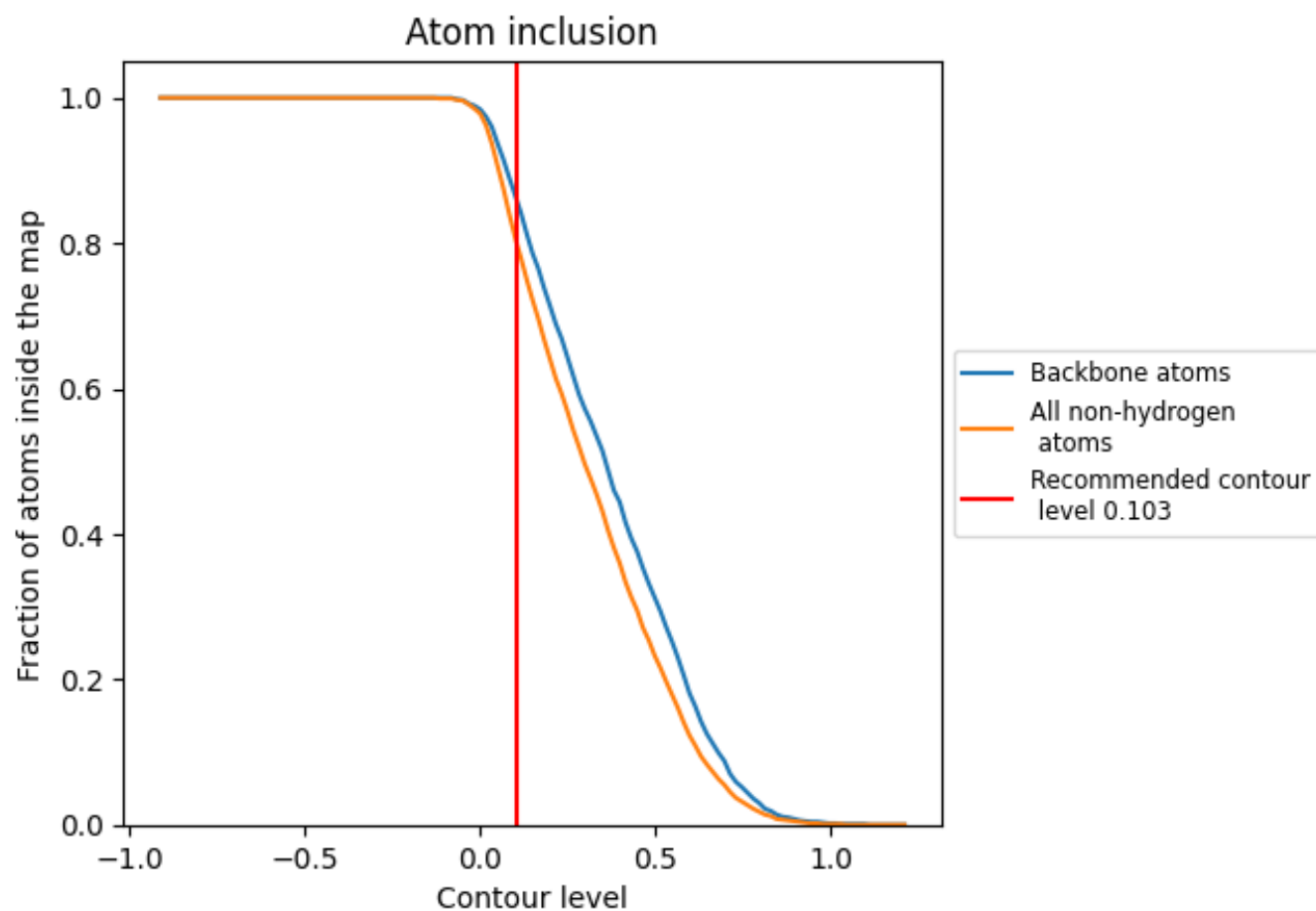
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.103).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8020</div>	<div><div></div>0.5580</div>
A	<div><div></div>0.8610</div>	<div><div></div>0.5880</div>
B	<div><div></div>0.8640</div>	<div><div></div>0.5910</div>
C	<div><div></div>0.7030</div>	<div><div></div>0.5130</div>
D	<div><div></div>0.7030</div>	<div><div></div>0.5140</div>
E	<div><div></div>0.6780</div>	<div><div></div>0.4880</div>
F	<div><div></div>0.6780</div>	<div><div></div>0.4900</div>
G	<div><div></div>0.7310</div>	<div><div></div>0.5130</div>
H	<div><div></div>0.7310</div>	<div><div></div>0.5160</div>
I	<div><div></div>0.7030</div>	<div><div></div>0.5110</div>
J	<div><div></div>0.7030</div>	<div><div></div>0.5070</div>

1.0

0.0

<0.0