



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:06 PM UTC

PDB ID : 7XZI / pdb_00007xzi
EMDB ID : EMD-33528
Title : Cryo-EM structure of TOC-TIC supercomplex from Chlamydomonas reinhardtii
Authors : Liu, H.; Li, A.J.; Liu, Z.F.
Deposited on : 2022-06-02
Resolution : 2.77 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

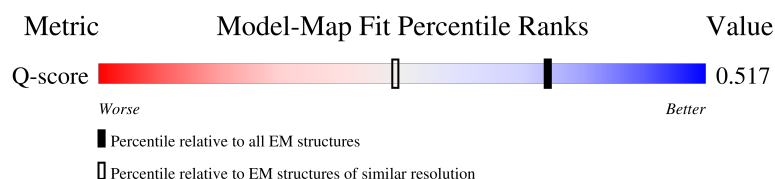
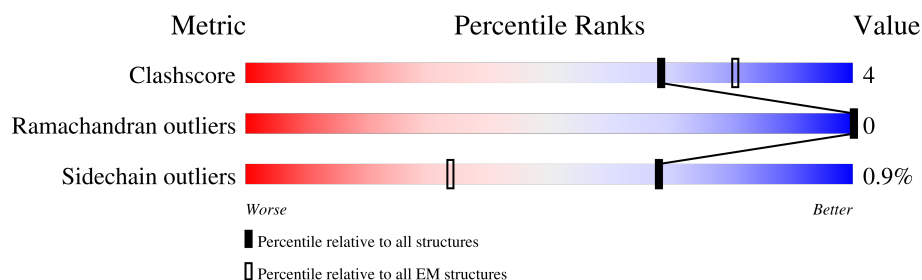
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 Å.

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



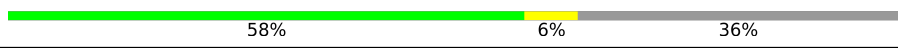
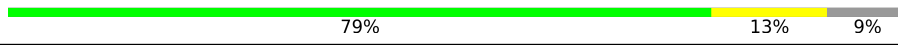
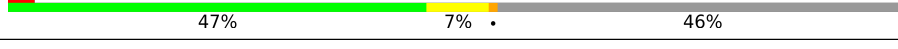
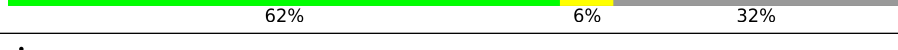
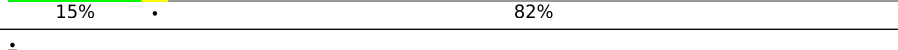
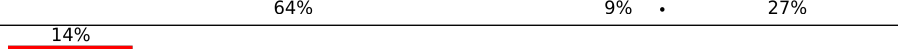
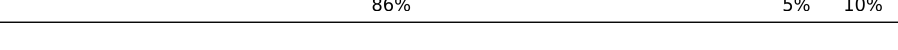
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10695 (2.27 - 3.27)

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

Mol	Chain	Length	Quality of chain
1	3	477	
2	4	363	
3	5	383	
4	7	798	

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Mol	Chain	Length	Quality of chain
5	9	967	
6	A	1995	
7	B	259	
8	C	127	
9	D	187	
10	E	955	
11	F	244	
12	G	397	
13	U	124	
14	X	21	

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 37365 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 Ctap3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	206	Total	C	N	O	S	0	0
			1528	965	271	286	6		

- Molecule 2 is a protein called Ctap4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	273	Total	C	N	O	S	0	0
			1734	1074	319	340	1		

- Molecule 3 is a protein called Ctap5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	196	Total	C	N	O		0	0
			1506	973	268	265			

- Molecule 4 is a protein called Toc75.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	616	Total	C	N	O	S	0	0
			4249	2674	761	800	14		

- Molecule 5 is a protein called Toc90.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	381	Total	C	N	O	S	0	0
			2800	1790	466	529	15		

- Molecule 6 is a protein called Tic214.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1598	Total	C	N	O	S	0	0
			12921	8361	2294	2239	27		

- Molecule 7 is a protein called Protein TIC 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	166	Total	C	N	O	S	0	0
			1409	964	206	227	12		

- Molecule 8 is a protein called Tic15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	116	Total	C	N	O	S	0	0
			947	615	170	156	6		

- Molecule 9 is a protein called Simp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	101	Total	C	N	O	S	0	0
			823	558	125	135	5		

- Molecule 10 is a protein called Tic100.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	770	Total	C	N	O	S	0	0
			6055	3784	1044	1196	31		

- Molecule 11 is a protein called Tic56.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	167	Total	C	N	O	S	0	0
			1361	877	245	230	9		

- Molecule 12 is a protein called Toc34.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	G	70	Total	C	N	O	0	0
			501	318	102	81		

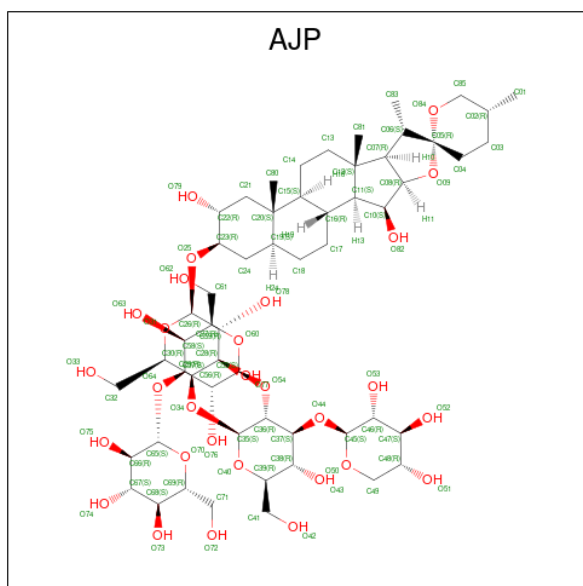
- Molecule 13 is a protein called Simp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	91	Total	C	N	O	S	0	0
			662	421	123	117	1		

- Molecule 14 is a protein called Unknown peptide.

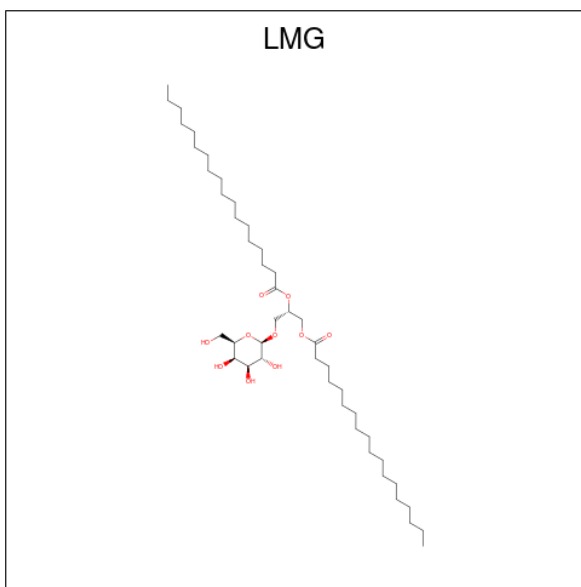
Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	19	Total	C	N	O	0	0
			93	55	19	19		

- Molecule 15 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



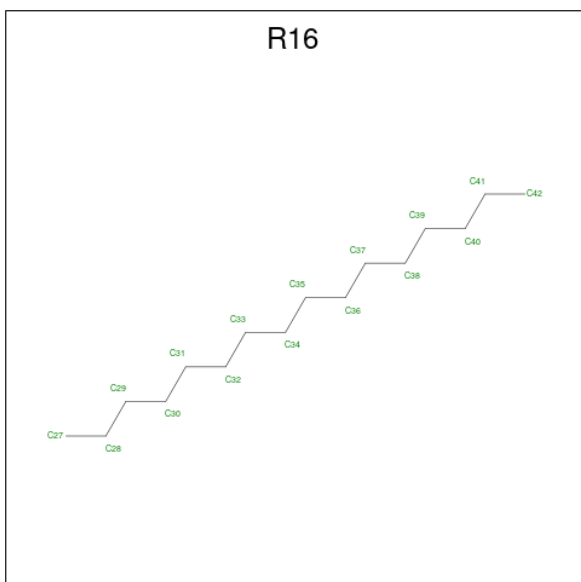
Mol	Chain	Residues	Atoms			AltConf
15	4	1	Total	C	O	0
			31	27	4	
15	5	1	Total	C	O	0
			43	33	10	
15	B	1	Total	C	O	0
			42	33	9	
15	D	1	Total	C	O	0
			32	27	5	
15	D	1	Total	C	O	0
			52	39	13	

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



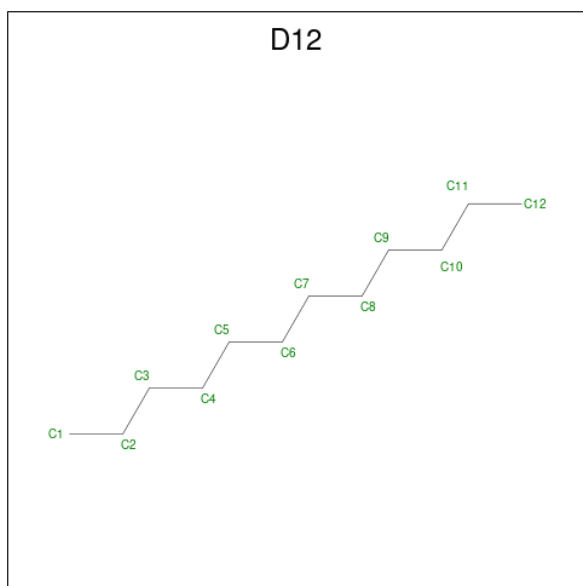
Mol	Chain	Residues	Atoms			AltConf
16	5	1	Total	C	O	0
			42	32	10	
16	A	1	Total	C	O	0
			52	42	10	
16	A	1	Total	C	O	0
			55	45	10	
16	A	1	Total	C	O	0
			39	29	10	
16	B	1	Total	C	O	0
			37	27	10	

- Molecule 17 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



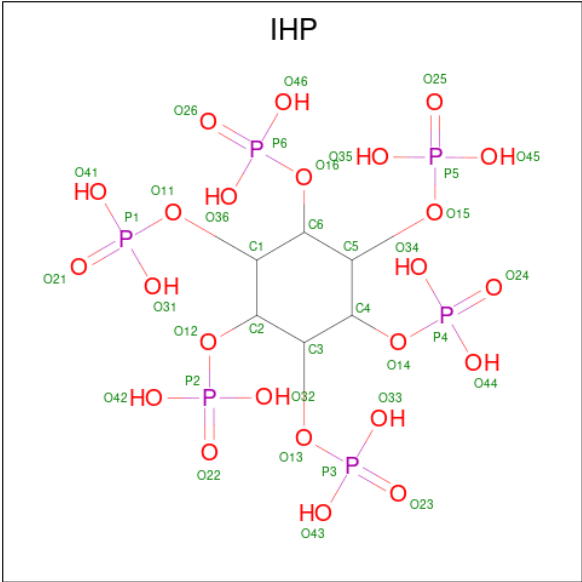
Mol	Chain	Residues	Atoms	AltConf
17	7	1	Total C 10 10	0

- Molecule 18 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



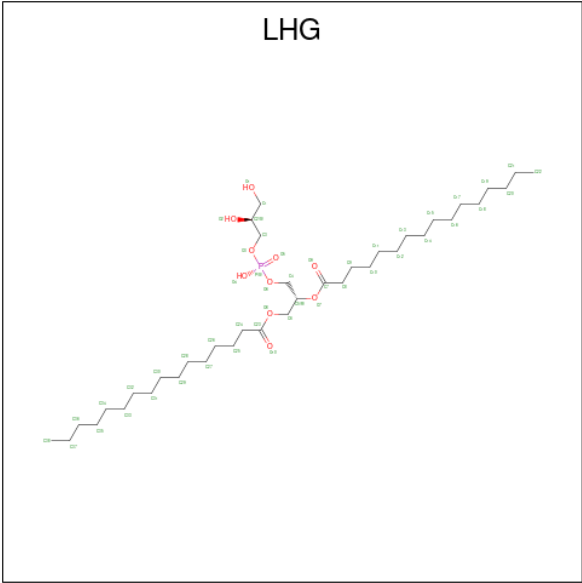
Mol	Chain	Residues	Atoms	AltConf
18	9	1	Total C 12 12	0
18	A	1	Total C 12 12	0
18	A	1	Total C 12 12	0
18	A	1	Total C 12 12	0
18	B	1	Total C 12 12	0
18	B	1	Total C 12 12	0
18	D	1	Total C 12 12	0

- Molecule 19 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			36	25	10	1	

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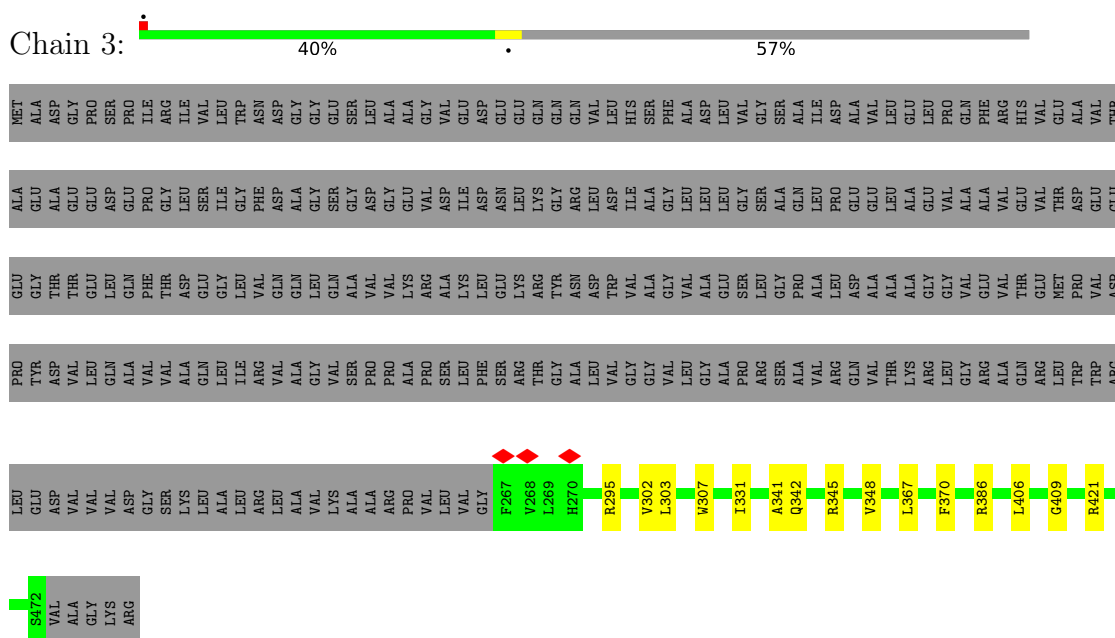
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Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	P	0
			45	34	10	1	
20	C	1	Total	C	O	P	0
			47	36	10	1	
20	F	1	Total	C	O	P	0
			44	33	10	1	

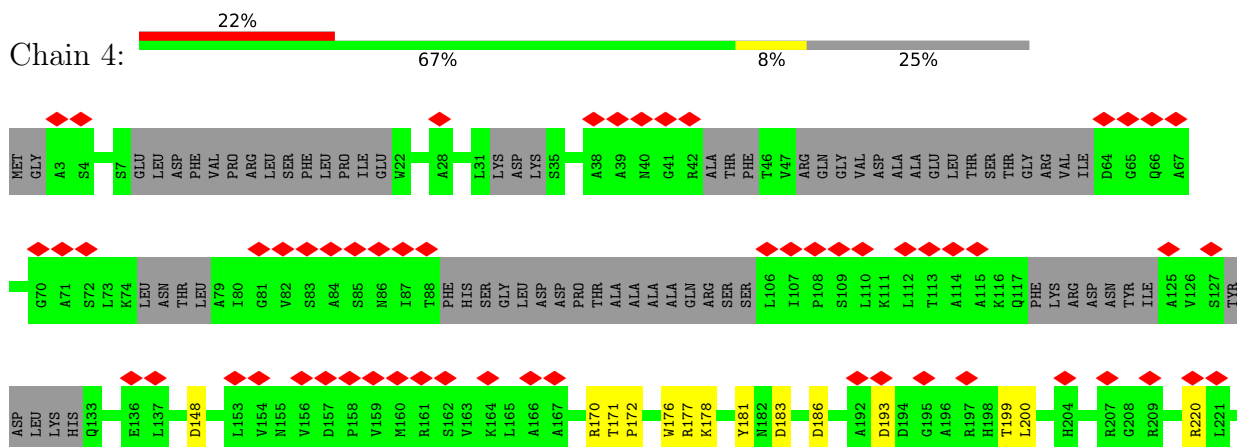
3 Residue-property plots

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.

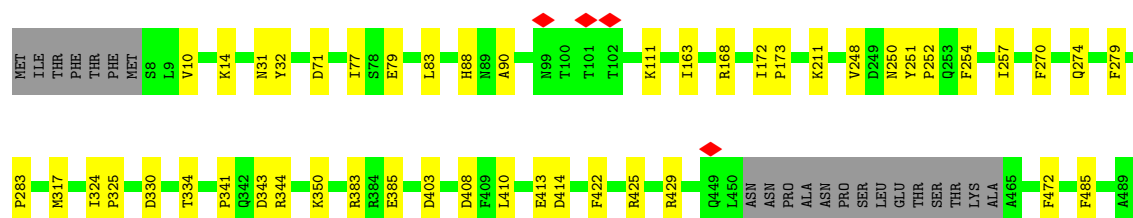
• Molecule 1: Ctap3



• Molecule 2: Ctap4



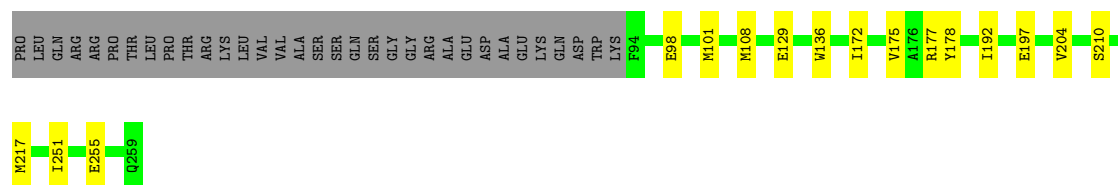
Chain 9: 34% 5% 61%





Device Type	Percentage
Smartphones	58%
Tablets	6%
Feature Phones	36%





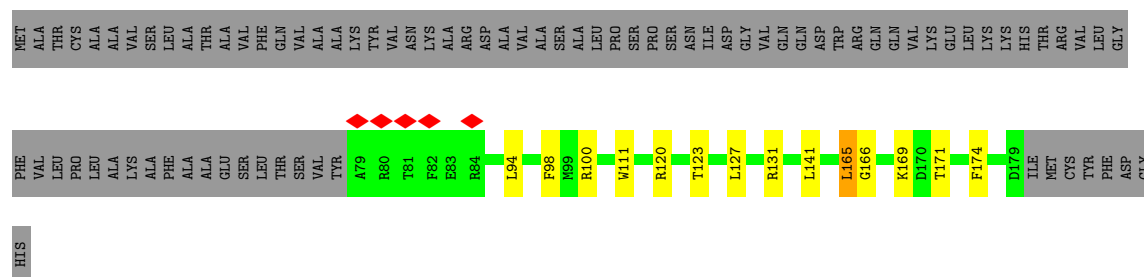
- Molecule 8: Tic15

Chain C: 79% 13% 9%



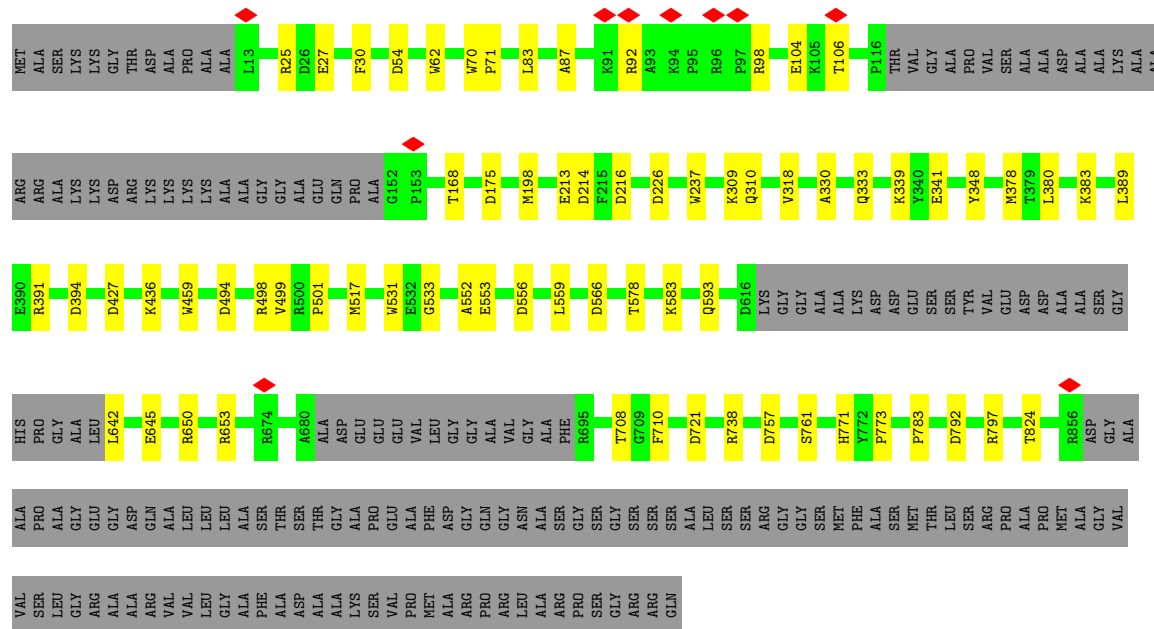
- Molecule 9: Simp3

Chain D: 47% 7% 46%



- Molecule 10: Tic100

Chain E: 73% 7% 19%



- Molecule 11: Tic56

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	796731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.956	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.675, 0.675, 0.675	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: IHP, R16, AJP, LHG, D12, LMG

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	3	0.09	0/1561	0.22	0/2125
2	4	0.13	0/1757	0.33	0/2398
3	5	0.10	0/1543	0.24	0/2100
4	7	0.11	0/4336	0.28	0/5910
5	9	0.10	0/2882	0.27	0/3934
6	A	0.14	0/13218	0.30	1/17847 (0.0%)
7	B	0.13	0/1467	0.29	0/2007
8	C	0.11	0/984	0.28	0/1338
9	D	0.10	0/854	0.25	0/1167
10	E	0.14	0/6198	0.30	0/8393
11	F	0.11	0/1400	0.29	0/1900
12	G	0.14	0/515	0.31	0/704
13	U	0.11	0/679	0.30	0/926
14	X	0.10	0/92	0.19	0/126
All	All	0.13	0/37486	0.29	1/50875 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1943	ASN	CB-CA-C	-5.14	110.67	116.63

There are no chirality outliers.

There are no planarity outliers.

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	3	1528	0	1393	13	0
2	4	1734	0	1366	18	0
3	5	1506	0	1443	8	0
4	7	4249	0	3621	34	0
5	9	2800	0	2476	27	0
6	A	12921	0	12873	117	0
7	B	1409	0	1368	11	0
8	C	947	0	910	12	0
9	D	823	0	790	9	0
10	E	6055	0	5642	53	0
11	F	1361	0	1362	11	0
12	G	501	0	410	7	0
13	U	662	0	650	7	0
14	X	93	0	75	2	0
15	4	31	0	0	0	0
15	5	43	0	0	0	0
15	B	42	0	0	2	0
15	D	84	0	0	0	0
16	5	42	0	57	2	0
16	A	146	0	211	5	0
16	B	37	0	44	0	0
17	7	10	0	16	0	0
18	9	12	0	26	0	0
18	A	36	0	78	0	0
18	B	24	0	52	0	0
18	D	12	0	26	0	0
19	A	36	0	6	0	0
20	A	49	0	74	1	0
20	B	81	0	105	0	0
20	C	47	0	67	3	0
20	F	44	0	61	1	0
All	All	37365	0	35202	265	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 4.

All (265) 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)
10:E:54:ASP:HB3	10:E:83:LEU:HD21	1.73	0.70
5:9:569:ALA:O	5:9:573:ASN:ND2	2.23	0.70
5:9:575:VAL:HG21	5:9:726:VAL:HG21	1.74	0.70
6:A:756:ILE:HD11	10:E:168:THR:HG21	1.76	0.68
1:3:406:LEU:HD13	6:A:928:LYS:HD3	1.77	0.67
6:A:665:TYR:OH	6:A:681:ARG:NH1	2.28	0.66
10:E:783:PRO:HG2	11:F:242:LEU:HD13	1.79	0.65
6:A:1087:GLN:HB3	10:E:501:PRO:HG3	1.79	0.63
8:C:13:VAL:HG13	8:C:15:LYS:HG3	1.81	0.63
3:5:293:ASP:OD2	10:E:391:ARG:NH2	2.33	0.62
4:7:792:VAL:HG22	5:9:707:LYS:HB3	1.80	0.61
6:A:1134:GLN:O	6:A:1138:ASN:ND2	2.33	0.61
6:A:168:ARG:HD3	8:C:68:ASN:HA	1.83	0.60
6:A:1153:LYS:NZ	10:E:226:ASP:O	2.34	0.60
4:7:245:GLY:O	6:A:1945:GLN:NE2	2.34	0.60
6:A:877:HIS:O	6:A:880:THR:OG1	2.18	0.60
6:A:1086:GLU:HG3	10:E:559:LEU:HD11	1.84	0.60
6:A:1763:TYR:O	6:A:1799:ARG:NH2	2.35	0.59
6:A:383:ARG:HG3	6:A:385:GLU:HG3	1.84	0.59
1:3:341:ALA:HB2	6:A:1143:LEU:HD21	1.85	0.59
4:7:606:LEU:HA	4:7:647:PHE:HB2	1.84	0.59
6:A:1058:GLU:HG3	6:A:1062:ARG:HD2	1.85	0.58
4:7:244:ARG:NH1	6:A:1946:PRO:O	2.36	0.58
6:A:1157:GLY:O	6:A:1161:ASN:ND2	2.27	0.58
6:A:77:ILE:HB	10:E:389:LEU:HD23	1.86	0.58
6:A:1799:ARG:NH1	10:E:213:GLU:OE2	2.35	0.58
10:E:330:ALA:HB3	10:E:333:GLN:HG3	1.86	0.58
10:E:378:MET:HE2	10:E:380:LEU:HD11	1.85	0.58
5:9:779:ARG:HG2	5:9:786:PRO:HG3	1.86	0.57
10:E:757:ASP:OD2	10:E:761:SER:OG	2.20	0.57
5:9:711:SER:HA	5:9:746:PRO:HG3	1.87	0.57
10:E:104:GLU:HG3	10:E:106:THR:H	1.69	0.57
6:A:756:ILE:HG13	10:E:168:THR:HB	1.85	0.57
6:A:1822:ARG:NH1	6:A:1823:THR:O	2.37	0.56
6:A:111:LYS:HG3	6:A:257:ILE:HG23	1.86	0.56
6:A:330:ASP:O	6:A:334:THR:OG1	2.24	0.56
6:A:853:GLN:HB3	11:F:197:PRO:HG3	1.87	0.56
3:5:196:PHE:HB3	13:U:97:VAL:HG22	1.87	0.56
6:A:1448:ARG:HD2	6:A:1450:ARG:HH12	1.71	0.56
4:7:185:ASP:O	5:9:600:ARG:NH1	2.39	0.55
5:9:800:THR:OG1	5:9:807:LYS:NZ	2.37	0.55
1:3:367:LEU:HD12	1:3:370:PHE:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:418:MET:HE3	5:9:904:TYR:HD1	1.72	0.55
11:F:160:LEU:HG	11:F:164:LYS:HE3	1.89	0.55
6:A:79:GLU:OE2	10:E:339:LYS:NZ	2.41	0.54
6:A:248:VAL:HG21	6:A:254:PHE:HB2	1.90	0.54
6:A:83:LEU:HB3	6:A:1544:ASN:HB2	1.89	0.54
10:E:783:PRO:O	11:F:239:GLN:NE2	2.39	0.54
6:A:1476:GLN:OE1	6:A:1480:ASN:ND2	2.40	0.53
6:A:324:ILE:HD12	16:A:2006:LMG:H261	1.90	0.53
6:A:1736:THR:O	10:E:531:TRP:NE1	2.35	0.53
4:7:691:SER:HA	4:7:708:ALA:HA	1.90	0.53
6:A:568:ARG:HG2	6:A:687:LEU:HD13	1.91	0.53
5:9:724:HIS:HB2	5:9:733:HIS:HB3	1.90	0.52
5:9:580:MET:HE3	5:9:591:ALA:HA	1.91	0.52
6:A:720:LEU:HD12	10:E:348:TYR:HE2	1.74	0.52
6:A:317:MET:HG2	8:C:31:PHE:HA	1.90	0.52
6:A:1965:LYS:HG2	6:A:1977:LEU:HD11	1.90	0.52
2:4:244:SER:HA	2:4:247:TRP:HD1	1.75	0.52
6:A:168:ARG:NH1	8:C:83:ASN:O	2.40	0.52
6:A:422:PHE:O	6:A:429:ARG:NH2	2.43	0.52
6:A:1827:THR:O	10:E:98:ARG:NH1	2.41	0.52
4:7:331:VAL:HG21	4:7:409:ARG:HE	1.74	0.52
6:A:1671:TRP:O	10:E:642:LEU:N	2.43	0.52
13:U:34:ILE:HG13	13:U:35:VAL:HG13	1.91	0.52
4:7:680:ALA:HB3	4:7:710:ARG:HB2	1.91	0.52
6:A:748:ARG:HH12	9:D:174:PHE:HD2	1.57	0.52
6:A:1238:LYS:HE3	6:A:1242:ILE:HD11	1.93	0.51
10:E:645:GLU:OE1	10:E:645:GLU:N	2.42	0.51
4:7:604:ASN:ND2	4:7:668:PRO:O	2.44	0.51
10:E:650:ARG:HG3	10:E:653:ARG:HH21	1.75	0.51
11:F:140:MET:HE1	11:F:194:LEU:HB2	1.91	0.51
4:7:388:GLU:HB2	4:7:413:VAL:HB	1.91	0.51
3:5:290:LEU:HD13	10:E:383:LYS:HE2	1.92	0.51
4:7:686:ALA:HA	4:7:689:TYR:CG	2.46	0.51
6:A:172:ILE:HG23	8:C:87:LEU:HD23	1.93	0.51
10:E:578:THR:O	10:E:593:GLN:NE2	2.42	0.51
13:U:42:VAL:HB	13:U:54:PRO:HG3	1.93	0.51
9:D:100:ARG:HH21	9:D:120:ARG:HA	1.76	0.51
12:G:385:ASP:HA	12:G:388:TRP:CD1	2.46	0.51
4:7:544:MET:HE2	4:7:588:SER:HB3	1.93	0.51
4:7:604:ASN:HB2	4:7:667:ALA:HB1	1.92	0.51
6:A:343:ASP:OD1	6:A:344:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:752:ARG:HH22	6:A:1804:ARG:HE	1.58	0.50
6:A:1231:ASP:OD1	6:A:1232:LEU:N	2.44	0.50
3:5:248:LEU:HD21	3:5:287:LEU:HD11	1.94	0.50
5:9:572:PHE:HD1	5:9:728:PRO:HG3	1.76	0.50
4:7:282:MET:HB3	4:7:314:LEU:HD11	1.93	0.50
8:C:51:SER:OG	8:C:52:GLU:N	2.43	0.49
7:B:204:VAL:O	7:B:210:SER:OG	2.26	0.49
5:9:744:LEU:HD23	5:9:748:ILE:HG12	1.94	0.49
16:A:2007:LMG:H242	16:A:2007:LMG:H362	1.94	0.49
9:D:111:TRP:HB3	9:D:120:ARG:HD2	1.93	0.49
4:7:738:TYR:HD1	4:7:763:MET:HB2	1.77	0.49
6:A:1780:LEU:HD21	10:E:198:MET:HE1	1.94	0.49
10:E:771:HIS:CE1	10:E:773:PRO:HB3	2.47	0.49
6:A:1813:LYS:NZ	10:E:175:ASP:OD1	2.46	0.49
12:G:331:PRO:O	12:G:334:ILE:HB	2.13	0.49
2:4:316:ARG:HH11	2:4:335:ARG:HH22	1.60	0.49
6:A:414:ASP:OD1	6:A:918:LYS:NZ	2.42	0.49
6:A:654:LYS:HD3	10:E:436:LYS:HG3	1.94	0.49
6:A:1073:ILE:HD11	6:A:1463:LYS:HG3	1.95	0.49
6:A:1635:MET:HE3	6:A:1636:PRO:HD2	1.94	0.49
4:7:414:GLN:OE1	4:7:414:GLN:N	2.46	0.48
5:9:564:THR:HB	6:A:1070:LYS:HD3	1.94	0.48
5:9:663:ILE:HB	5:9:681:VAL:HG13	1.94	0.48
4:7:797:ARG:O	4:7:797:ARG:NH1	2.42	0.48
6:A:1082:GLN:O	6:A:1086:GLU:HG2	2.14	0.48
4:7:499:ASN:HB3	4:7:523:PHE:HD1	1.78	0.48
9:D:165:LEU:HD23	9:D:166:GLY:H	1.78	0.48
10:E:25:ARG:NH1	10:E:27:GLU:OE2	2.46	0.48
3:5:267:ARG:NH2	3:5:274:ASP:OD2	2.43	0.48
2:4:186:ASP:OD1	6:A:1976:GLN:NE2	2.44	0.48
3:5:259:ALA:HB2	3:5:275:VAL:HG11	1.96	0.48
6:A:408:ASP:C	6:A:410:LEU:H	2.20	0.48
10:E:553:GLU:HA	10:E:556:ASP:OD2	2.12	0.48
1:3:386:ARG:NH2	6:A:706:ARG:O	2.47	0.48
6:A:32:TYR:CZ	6:A:1920:LEU:HB2	2.49	0.48
7:B:178:TYR:HA	7:B:251:ILE:HD11	1.96	0.48
6:A:862:ASN:OD1	6:A:865:ARG:NH2	2.44	0.47
10:E:309:LYS:HG2	10:E:310:GLN:HG2	1.95	0.47
1:3:303:LEU:HD21	6:A:578:LEU:HD12	1.97	0.47
4:7:273:GLN:HG2	4:7:275:TYR:H	1.79	0.47
6:A:1377:VAL:HG23	6:A:1380:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:177:ARG:NH1	7:B:255:GLU:OE2	2.48	0.47
1:3:345:ARG:HA	1:3:348:VAL:HG22	1.95	0.47
6:A:1062:ARG:HD3	6:A:1474:LEU:HD13	1.95	0.47
5:9:828:TRP:HZ2	14:X:4:ALA:HB2	1.80	0.47
6:A:1439:GLN:NE2	6:A:1443:ASN:OD1	2.48	0.47
10:E:566:ASP:HA	10:E:583:LYS:HD2	1.97	0.47
10:E:394:ASP:OD1	10:E:394:ASP:N	2.48	0.47
7:B:192:ILE:HG23	9:D:98:PHE:HZ	1.80	0.47
6:A:425:ARG:NH2	7:B:129:GLU:OE2	2.41	0.46
6:A:597:GLN:O	6:A:656:ARG:NH1	2.48	0.46
11:F:101:HIS:HE1	11:F:103:LEU:HD13	1.80	0.46
6:A:756:ILE:HD11	10:E:168:THR:CG2	2.45	0.46
10:E:30:PHE:CG	11:F:131:GLU:HG3	2.51	0.46
10:E:214:ASP:HB3	10:E:216:ASP:OD1	2.16	0.46
4:7:678:GLY:O	4:7:711:ARG:HA	2.16	0.46
6:A:168:ARG:NH2	8:C:75:GLU:OE2	2.49	0.46
6:A:413:GLU:HB2	6:A:918:LYS:HD3	1.97	0.46
6:A:1643:ASP:OD2	6:A:1748:TYR:OH	2.34	0.46
6:A:629:VAL:HG21	6:A:1052:PHE:HE1	1.81	0.45
5:9:576:TYR:O	5:9:580:MET:HG2	2.15	0.45
6:A:748:ARG:HH22	9:D:174:PHE:HD2	1.65	0.45
6:A:1727:MET:HA	6:A:1731:LEU:HB3	1.98	0.45
12:G:340:PHE:O	12:G:344:PHE:HB3	2.16	0.45
1:3:331:ILE:HG23	10:E:459:TRP:CD1	2.51	0.45
2:4:199:THR:O	2:4:220:ARG:N	2.45	0.45
1:3:459:ALA:HB2	11:F:92:ALA:HA	1.98	0.45
2:4:252:LEU:HB3	2:4:253:PRO:HD3	1.99	0.45
4:7:286:ARG:O	4:7:290:GLU:HG2	2.16	0.45
5:9:536:PHE:HB3	5:9:776:MET:HE1	1.98	0.45
1:3:409:GLY:O	1:3:421:ARG:NH1	2.50	0.45
20:C:201:LHG:H262	20:C:201:LHG:H291	1.77	0.45
2:4:265:ASP:O	6:A:605:LYS:NZ	2.50	0.45
3:5:137:ILE:HG12	6:A:211:LYS:HE2	1.98	0.45
6:A:904:ALA:O	10:E:738:ARG:NH2	2.50	0.45
5:9:541:SER:O	5:9:831:ARG:NH1	2.46	0.45
7:B:98:GLU:OE1	8:C:14:TYR:OH	2.34	0.45
7:B:172:ILE:HD11	15:B:305:AJP:C80	2.46	0.44
6:A:869:ILE:HA	6:A:872:PHE:HD2	1.82	0.44
6:A:1617:ASN:HB3	6:A:1915:GLY:HA3	1.99	0.44
2:4:177:ARG:NH2	2:4:193:ASP:O	2.51	0.44
6:A:756:ILE:CG1	10:E:168:THR:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:202:PRO:HG3	11:F:205:ARG:HH21	1.82	0.44
2:4:228:ASN:HA	2:4:231:VAL:HG22	2.00	0.44
6:A:279:PHE:O	6:A:283:PRO:HD2	2.17	0.44
6:A:1359:TYR:HB3	6:A:1456:GLY:HA3	1.98	0.44
1:3:295:ARG:HD3	1:3:295:ARG:H	1.82	0.44
2:4:178:LYS:HD2	6:A:600:TYR:CE1	2.52	0.44
5:9:688:PRO:HD2	5:9:697:VAL:O	2.18	0.44
11:F:212:ARG:HB2	11:F:242:LEU:HD23	1.98	0.44
1:3:302:VAL:HG13	1:3:303:LEU:HG	1.98	0.44
4:7:357:ILE:HG23	4:7:381:ILE:HD12	2.00	0.44
5:9:581:TYR:HB2	5:9:595:TYR:CE1	2.53	0.43
6:A:1710:LYS:HE2	6:A:1710:LYS:HB2	1.81	0.43
4:7:544:MET:HE1	4:7:590:GLN:HB2	1.99	0.43
6:A:251:TYR:HB3	6:A:252:PRO:HD3	2.00	0.43
6:A:341:PRO:HD3	8:C:111:TRP:CE2	2.52	0.43
7:B:101:MET:HE3	7:B:175:VAL:HG12	2.00	0.43
16:5:502:LMG:H453	16:A:2007:LMG:H262	2.01	0.43
6:A:88:HIS:CE1	6:A:90:ALA:HB3	2.53	0.43
6:A:869:ILE:HA	6:A:872:PHE:CD2	2.52	0.43
7:B:197:GLU:HB2	7:B:217:MET:HE1	1.99	0.43
13:U:50:TYR:CE2	13:U:61:GLU:HB3	2.54	0.43
2:4:261:PRO:HG2	2:4:269:ARG:HB3	2.01	0.43
6:A:1091:LEU:HD11	10:E:499:VAL:HG12	2.00	0.43
4:7:250:ASP:O	4:7:315:ARG:HA	2.19	0.43
16:A:2007:LMG:H142	7:B:136:TRP:CE3	2.53	0.43
13:U:98:ASN:HB2	13:U:99:PRO:HD3	2.01	0.43
6:A:472:PHE:HZ	6:A:825:TYR:HB2	1.84	0.43
6:A:250:ASN:OD1	6:A:250:ASN:N	2.51	0.43
6:A:1556:THR:O	6:A:1559:VAL:HG12	2.19	0.43
1:3:342:GLN:HG3	6:A:1140:SER:OG	2.19	0.43
2:4:171:THR:N	2:4:172:PRO:HD3	2.34	0.43
2:4:181:TYR:OH	6:A:1976:GLN:NE2	2.49	0.42
4:7:547:LEU:HD12	4:7:584:ASP:O	2.18	0.42
10:E:792:ASP:HA	10:E:797:ARG:HH21	1.84	0.42
12:G:341:TYR:O	12:G:345:LEU:N	2.50	0.42
1:3:307:TRP:CD1	1:3:307:TRP:H	2.37	0.42
2:4:172:PRO:HD2	2:4:200:LEU:H	1.84	0.42
13:U:49:ILE:HG23	13:U:50:TYR:CD2	2.54	0.42
10:E:494:ASP:OD1	10:E:498:ARG:N	2.52	0.42
2:4:224:GLY:HA2	2:4:227:VAL:HG22	2.01	0.42
6:A:1658:TRP:CD2	10:E:517:MET:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:708:THR:HG22	10:E:710:PHE:H	1.84	0.42
3:5:164:PHE:HD1	16:5:502:LMG:H291	1.85	0.42
6:A:1955:LEU:HD11	10:E:533:GLY:H	1.84	0.42
2:4:176:TRP:CZ2	2:4:268:VAL:HG12	2.54	0.42
6:A:867:LEU:HD13	6:A:940:PRO:HB2	2.01	0.42
6:A:350:LYS:HE3	6:A:350:LYS:HB2	1.88	0.42
10:E:83:LEU:HA	10:E:87:ALA:HB2	2.02	0.41
4:7:244:ARG:HH12	6:A:1944:VAL:HG22	1.85	0.41
6:A:10:VAL:HG12	6:A:14:LYS:HE3	2.01	0.41
6:A:485:PHE:HE2	6:A:831:HIS:CG	2.38	0.41
7:B:108:MET:HE1	15:B:305:AJP:O82	2.20	0.41
10:E:62:TRP:CE2	10:E:71:PRO:HB3	2.54	0.41
2:4:183:ASP:OD1	2:4:183:ASP:N	2.53	0.41
2:4:186:ASP:OD2	6:A:662:ARG:NH1	2.53	0.41
4:7:179:THR:OG1	4:7:180:ALA:N	2.53	0.41
5:9:836:TYR:CE2	5:9:838:TRP:HB2	2.55	0.41
4:7:274:PRO:HG3	6:A:1930:SER:HA	2.01	0.41
6:A:1075:HIS:HB2	10:E:552:ALA:HB2	2.02	0.41
20:C:201:LHG:HC62	20:C:201:LHG:H241	1.95	0.41
4:7:499:ASN:HB3	4:7:523:PHE:CD1	2.55	0.41
5:9:642:PRO:HB2	5:9:645:MET:HB2	2.03	0.41
6:A:71:ASP:OD1	6:A:71:ASP:N	2.53	0.41
5:9:743:VAL:HG13	5:9:751:VAL:HG12	2.03	0.41
10:E:318:VAL:HG13	10:E:341:GLU:HG2	2.03	0.41
4:7:601:ILE:HD11	4:7:606:LEU:HD21	2.03	0.41
6:A:485:PHE:O	10:E:70:TRP:HB2	2.20	0.41
6:A:607:ILE:HG23	6:A:1044:LEU:HD13	2.02	0.41
6:A:1690:SER:HB3	6:A:1693:ASN:OD1	2.21	0.41
6:A:1856:ARG:HG3	6:A:1858:LYS:H	1.85	0.41
20:F:301:LHG:H142	20:F:301:LHG:H111	1.82	0.41
12:G:342:ARG:HA	12:G:342:ARG:HD3	1.93	0.41
2:4:148:ASP:HA	2:4:170:ARG:O	2.21	0.41
4:7:489:PRO:HA	12:G:388:TRP:CE3	2.56	0.41
5:9:828:TRP:CZ2	14:X:4:ALA:HB2	2.56	0.41
6:A:270:PHE:HE1	6:A:274:GLN:HE21	1.68	0.41
6:A:1437:ARG:HG3	6:A:1438:HIS:CD2	2.56	0.41
9:D:127:LEU:O	9:D:131:ARG:HG3	2.21	0.41
9:D:165:LEU:HA	9:D:169:LYS:HB2	2.02	0.41
10:E:436:LYS:HE2	10:E:436:LYS:HB3	1.87	0.41
6:A:403:ASP:OD1	6:A:403:ASP:N	2.54	0.41
20:A:2002:LHG:H262	20:A:2002:LHG:H291	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:193:LYS:HD2	11:F:193:LYS:HA	1.95	0.41
5:9:871:ASP:OD1	5:9:872:TRP:N	2.54	0.40
6:A:31:ASN:ND2	16:A:2008:LMG:O3	2.54	0.40
9:D:94:LEU:HD23	9:D:94:LEU:HA	1.88	0.40
10:E:721:ASP:OD1	10:E:721:ASP:N	2.51	0.40
4:7:242:GLN:HA	4:7:278:ASP:HA	2.04	0.40
5:9:715:GLN:HE22	6:A:1262:ASN:HD22	1.68	0.40
6:A:869:ILE:HG23	6:A:872:PHE:HE2	1.85	0.40
4:7:385:GLY:H	12:G:389:ARG:NH2	2.20	0.40
6:A:172:ILE:HB	6:A:173:PRO:HD3	2.01	0.40
6:A:754:GLN:HG2	10:E:237:TRP:CH2	2.56	0.40
6:A:1245:ARG:HH12	6:A:1273:GLU:HG3	1.86	0.40
8:C:36:ASN:ND2	20:C:201:LHG:H223	2.36	0.40
5:9:530:LEU:HA	5:9:531:PRO:HD3	1.95	0.40
13:U:58:LEU:HG	13:U:59:PRO:HD2	2.03	0.40
6:A:163:ILE:HD13	8:C:63:LEU:HD22	2.03	0.40
6:A:324:ILE:HB	6:A:325:PRO:HD3	2.04	0.40
6:A:842:MET:HA	8:C:127:GLN:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	204/477 (43%)	203 (100%)	1 (0%)	0	100	100
2	4	253/363 (70%)	244 (96%)	9 (4%)	0	100	100
3	5	194/383 (51%)	191 (98%)	3 (2%)	0	100	100
4	7	600/798 (75%)	587 (98%)	13 (2%)	0	100	100
5	9	375/967 (39%)	368 (98%)	7 (2%)	0	100	100
6	A	1570/1995 (79%)	1523 (97%)	47 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B	164/259 (63%)	160 (98%)	4 (2%)	0	100	100
8	C	114/127 (90%)	113 (99%)	1 (1%)	0	100	100
9	D	99/187 (53%)	96 (97%)	3 (3%)	0	100	100
10	E	762/955 (80%)	731 (96%)	31 (4%)	0	100	100
11	F	165/244 (68%)	162 (98%)	3 (2%)	0	100	100
12	G	68/397 (17%)	63 (93%)	5 (7%)	0	100	100
13	U	89/124 (72%)	87 (98%)	2 (2%)	0	100	100
14	X	17/21 (81%)	17 (100%)	0	0	100	100
All	All	4674/7297 (64%)	4545 (97%)	129 (3%)	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	3	134/373 (36%)	134 (100%)	0	100	100
2	4	115/287 (40%)	115 (100%)	0	100	100
3	5	135/308 (44%)	135 (100%)	0	100	100
4	7	349/653 (53%)	341 (98%)	8 (2%)	44	75
5	9	256/713 (36%)	252 (98%)	4 (2%)	55	81
6	A	1349/1848 (73%)	1343 (100%)	6 (0%)	84	93
7	B	149/223 (67%)	149 (100%)	0	100	100
8	C	96/106 (91%)	94 (98%)	2 (2%)	47	76
9	D	84/158 (53%)	80 (95%)	4 (5%)	23	53
10	E	613/755 (81%)	610 (100%)	3 (0%)	81	92
11	F	143/213 (67%)	141 (99%)	2 (1%)	59	82
12	G	33/336 (10%)	33 (100%)	0	100	100
13	U	64/97 (66%)	63 (98%)	1 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3520/6070 (58%)	3490 (99%)	30 (1%)	68	87

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	7	345	VAL
4	7	420	LEU
4	7	544	MET
4	7	606	LEU
4	7	614	VAL
4	7	703	HIS
4	7	717	THR
4	7	782	ASP
5	9	537	VAL
5	9	798	GLN
5	9	803	VAL
5	9	886	VAL
6	A	860	THR
6	A	1225	ARG
6	A	1629	LEU
6	A	1942	ILE
6	A	1944	VAL
6	A	1964	LEU
8	C	54	HIS
8	C	126	TRP
9	D	123	THR
9	D	141	LEU
9	D	165	LEU
9	D	171	THR
10	E	92	ARG
10	E	427	ASP
10	E	824	THR
11	F	181	HIS
11	F	239	GLN
13	U	42	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	332	ASN
2	4	213	HIS

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Mol	Chain	Res	Type
2	4	228	ASN
2	4	264	ASN
2	4	267	GLN
3	5	154	ASN
4	7	232	GLN
4	7	379	ASN
4	7	450	HIS
4	7	471	ASN
4	7	613	GLN
5	9	715	GLN
5	9	733	HIS
6	A	31	ASN
6	A	89	ASN
6	A	335	ASN
6	A	366	ASN
6	A	389	GLN
6	A	416	ASN
6	A	484	ASN
6	A	688	GLN
6	A	800	ASN
6	A	822	HIS
6	A	877	HIS
6	A	1087	GLN
6	A	1176	ASN
6	A	1180	GLN
6	A	1430	HIS
6	A	1438	HIS
6	A	1439	GLN
6	A	1443	ASN
6	A	1444	HIS
6	A	1480	ASN
6	A	1489	ASN
6	A	1491	GLN
6	A	1546	ASN
6	A	1761	ASN
6	A	1945	GLN
6	A	1959	HIS
7	B	174	HIS
9	D	114	GLN
9	D	128	GLN
9	D	167	HIS
10	E	480	GLN

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Mol	Chain	Res	Type
10	E	575	ASN
10	E	657	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](#)

24 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	$\# Z > 2$
18	D12	D	202	-	11,11,11	0.23	0	10,10,10	0.21	0
20	LHG	C	201	-	46,46,48	0.66	1 (2%)	49,52,54	1.29	6 (12%)
15	AJP	5	501	-	49,49,95	1.15	7 (14%)	75,80,149	1.71	15 (20%)
19	IHP	A	2001	-	36,36,36	0.86	0	60,60,60	0.52	0
17	R16	7	801	-	9,9,15	0.25	0	8,8,14	0.19	0
20	LHG	F	301	-	43,43,48	0.66	2 (4%)	46,49,54	1.24	4 (8%)
18	D12	B	302	-	11,11,11	0.24	0	10,10,10	0.19	0
15	AJP	D	203	-	59,59,95	1.05	4 (6%)	90,95,149	1.63	19 (21%)
16	LMG	A	2006	-	52,52,55	0.72	1 (1%)	60,60,63	1.38	7 (11%)
15	AJP	B	305	-	48,48,95	1.06	5 (10%)	74,79,149	1.67	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LHG	A	2002	-	48,48,48	0.62	1 (2%)	51,54,54	1.29	6 (11%)
18	D12	9	1001	-	11,11,11	0.24	0	10,10,10	0.19	0
16	LMG	A	2008	-	39,39,55	0.82	1 (2%)	47,47,63	1.29	6 (12%)
15	AJP	D	201	-	37,37,95	1.20	5 (13%)	58,62,149	1.78	12 (20%)
18	D12	A	2003	-	11,11,11	0.24	0	10,10,10	0.19	0
15	AJP	4	401	-	36,36,95	1.18	4 (11%)	56,60,149	1.85	12 (21%)
18	D12	A	2004	-	11,11,11	0.24	0	10,10,10	0.19	0
16	LMG	B	301	-	37,37,55	0.84	1 (2%)	45,45,63	1.34	7 (15%)
20	LHG	B	304	-	35,35,48	0.73	1 (2%)	38,41,54	1.29	4 (10%)
16	LMG	5	502	-	42,42,55	0.80	1 (2%)	50,50,63	1.34	7 (14%)
18	D12	A	2005	-	11,11,11	0.24	0	10,10,10	0.20	0
16	LMG	A	2007	-	55,55,55	0.68	0	63,63,63	1.38	7 (11%)
20	LHG	B	306	-	44,44,48	0.66	2 (4%)	47,50,54	1.31	7 (14%)
18	D12	B	303	-	11,11,11	0.24	0	10,10,10	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
18	D12	D	202	-	-	3/9/9/9	-
20	LHG	C	201	-	-	15/51/51/53	-
15	AJP	5	501	-	-	2/6/121/220	0/7/7/11
19	IHP	A	2001	-	-	6/30/54/54	0/1/1/1
17	R16	7	801	-	-	0/7/7/13	-
20	LHG	F	301	-	-	18/48/48/53	-
18	D12	B	302	-	-	2/9/9/9	-
15	AJP	D	203	-	-	5/10/141/220	1/8/8/11
16	LMG	A	2006	-	-	24/47/67/70	0/1/1/1
15	AJP	B	305	-	-	3/4/119/220	0/7/7/11
20	LHG	A	2002	-	-	18/53/53/53	-
18	D12	9	1001	-	-	3/9/9/9	-
16	LMG	A	2008	-	-	12/34/54/70	0/1/1/1
15	AJP	D	201	-	-	-	1/6/6/11
18	D12	A	2003	-	-	0/9/9/9	-
15	AJP	4	401	-	-	-	0/6/6/11
18	D12	A	2004	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMG	B	301	-	-	5/32/52/70	0/1/1/1
20	LHG	B	304	-	-	13/40/40/53	-
16	LMG	5	502	-	-	20/37/57/70	0/1/1/1
18	D12	A	2005	-	-	4/9/9/9	-
16	LMG	A	2007	-	-	16/50/70/70	0/1/1/1
20	LHG	B	306	-	-	23/49/49/53	-
18	D12	B	303	-	-	3/9/9/9	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	203	AJP	C16-C11	-3.44	1.49	1.54
15	5	501	AJP	C12-C11	-2.90	1.50	1.56
15	5	501	AJP	C20-C15	-2.85	1.51	1.56
15	4	401	AJP	C16-C11	-2.84	1.50	1.54
15	4	401	AJP	C20-C15	-2.79	1.51	1.56
15	D	203	AJP	C12-C11	-2.77	1.50	1.56
15	5	501	AJP	C12-C07	-2.75	1.50	1.56
15	B	305	AJP	C16-C11	-2.75	1.50	1.54
15	B	305	AJP	C20-C15	-2.72	1.51	1.56
15	D	201	AJP	C20-C15	-2.63	1.51	1.56
15	B	305	AJP	C12-C11	-2.61	1.51	1.56
15	D	203	AJP	C20-C15	-2.60	1.51	1.56
15	D	201	AJP	C16-C11	-2.54	1.50	1.54
15	5	501	AJP	C16-C11	-2.53	1.51	1.54
20	C	201	LHG	O7-C5	-2.46	1.40	1.46
15	D	201	AJP	C12-C11	-2.45	1.51	1.56
15	D	201	AJP	C20-C19	-2.36	1.51	1.55
15	5	501	AJP	C13-C12	-2.34	1.50	1.54
15	5	501	AJP	C20-C19	-2.27	1.51	1.55
15	4	401	AJP	C12-C07	-2.23	1.51	1.56
20	B	306	LHG	O7-C5	-2.22	1.41	1.46
20	A	2002	LHG	O7-C5	-2.21	1.41	1.46
15	B	305	AJP	C12-C07	-2.20	1.51	1.56
15	D	201	AJP	C12-C07	-2.19	1.51	1.56
20	F	301	LHG	O7-C5	-2.18	1.41	1.46
15	4	401	AJP	C12-C11	-2.17	1.52	1.56
16	B	301	LMG	O7-C8	-2.15	1.41	1.46
16	5	502	LMG	O7-C8	-2.15	1.41	1.46
20	B	304	LHG	O7-C5	-2.14	1.41	1.46
16	A	2008	LMG	O7-C8	-2.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	5	501	AJP	C21-C20	-2.07	1.51	1.54
20	B	306	LHG	P-O6	2.06	1.67	1.59
20	F	301	LHG	P-O6	2.05	1.67	1.59
15	D	203	AJP	C12-C07	-2.05	1.52	1.56
16	A	2006	LMG	O7-C8	-2.02	1.41	1.46
15	B	305	AJP	C13-C12	-2.00	1.50	1.54

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	5	501	AJP	C12-C11-C16	-5.48	106.26	113.90
15	D	203	AJP	C12-C11-C16	-5.47	106.28	113.90
15	B	305	AJP	C12-C11-C16	-5.19	106.66	113.90
15	4	401	AJP	C12-C11-C16	-5.16	106.71	113.90
15	4	401	AJP	C20-C21-C22	-4.94	109.15	113.94
15	D	201	AJP	C12-C11-C16	-4.82	107.18	113.90
15	5	501	AJP	C14-C15-C20	-4.76	108.55	113.91
15	D	201	AJP	C19-C24-C23	-4.57	108.97	114.40
20	A	2002	LHG	O4-P-O5	4.46	133.17	112.44
20	F	301	LHG	O4-P-O5	4.42	133.01	112.44
20	C	201	LHG	O4-P-O5	4.42	133.00	112.44
15	B	305	AJP	C20-C15-C16	-4.39	107.97	112.43
20	B	304	LHG	O4-P-O5	4.39	132.87	112.44
20	B	306	LHG	O4-P-O5	4.37	132.76	112.44
15	B	305	AJP	C14-C15-C20	-4.25	109.12	113.91
15	4	401	AJP	C14-C15-C20	-4.20	109.17	113.91
15	D	201	AJP	C24-C19-C20	-4.18	108.22	112.66
15	5	501	AJP	C26-O25-C23	-4.08	108.45	115.27
15	B	305	AJP	C24-C19-C20	-4.02	108.39	112.66
15	D	203	AJP	C24-C19-C20	-3.98	108.43	112.66
15	D	203	AJP	C14-C15-C20	-3.94	109.47	113.91
15	5	501	AJP	C12-C07-C06	-3.78	109.31	120.50
15	D	201	AJP	C20-C15-C16	-3.73	108.64	112.43
15	5	501	AJP	C24-C19-C20	-3.54	108.89	112.66
15	4	401	AJP	C12-C07-C06	-3.52	110.07	120.50
15	D	203	AJP	C35-O34-C29	-3.52	107.71	114.72
15	5	501	AJP	C14-C13-C12	-3.51	106.81	112.74
15	B	305	AJP	C14-C13-C12	-3.51	106.81	112.74
15	D	203	AJP	C12-C07-C06	-3.45	110.31	120.50
15	D	203	AJP	C26-O25-C23	-3.44	109.51	115.27
15	4	401	AJP	C14-C13-C12	-3.43	106.95	112.74
15	D	201	AJP	C14-C15-C20	-3.41	110.07	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	305	AJP	C12-C07-C06	-3.37	110.54	120.50
15	B	305	AJP	C20-C21-C22	-3.35	108.65	114.17
15	D	203	AJP	C83-C06-C05	-3.27	109.67	114.94
15	D	201	AJP	C12-C07-C06	-3.25	110.88	120.50
15	5	501	AJP	C20-C21-C22	-3.22	108.87	114.17
15	5	501	AJP	C20-C15-C16	-3.22	109.16	112.43
15	D	201	AJP	C14-C13-C12	-3.20	107.34	112.74
15	D	201	AJP	C83-C06-C05	-3.20	109.78	114.94
15	D	201	AJP	C21-C20-C19	3.17	110.26	107.23
15	4	401	AJP	C83-C06-C05	-3.08	109.97	114.94
15	B	305	AJP	C83-C06-C05	-3.07	109.99	114.94
15	D	203	AJP	C14-C13-C12	-3.07	107.57	112.74
15	4	401	AJP	C05-C06-C07	-2.96	99.00	103.37
15	D	203	AJP	C18-C17-C16	-2.89	107.55	112.16
15	4	401	AJP	C20-C15-C16	-2.86	109.52	112.43
16	B	301	LMG	O6-C1-O1	-2.86	103.30	110.04
20	A	2002	LHG	O8-C23-C24	2.86	120.54	111.83
20	C	201	LHG	O8-C23-C24	2.84	120.51	111.83
15	D	203	AJP	C83-C06-C07	-2.84	108.81	114.50
20	B	306	LHG	O8-C23-C24	2.81	120.40	111.83
16	A	2007	LMG	O6-C1-O1	-2.81	103.41	110.04
16	A	2006	LMG	O6-C1-O1	-2.75	103.55	110.04
15	5	501	AJP	C83-C06-C07	-2.74	109.02	114.50
15	D	203	AJP	C20-C21-C22	-2.72	109.70	114.17
15	B	305	AJP	C18-C17-C16	-2.66	107.92	112.16
15	5	501	AJP	C83-C06-C05	-2.65	110.67	114.94
15	D	203	AJP	C85-O84-C05	-2.64	109.14	113.69
20	B	304	LHG	O8-C23-C24	2.63	119.86	111.83
20	F	301	LHG	O8-C23-C24	2.61	119.80	111.83
20	C	201	LHG	C11-C10-C9	-2.58	101.31	114.37
15	4	401	AJP	C21-C20-C19	2.53	109.65	107.23
15	D	203	AJP	C26-O31-C30	-2.53	108.79	113.72
15	B	305	AJP	C85-O84-C05	-2.51	109.35	113.69
15	5	501	AJP	C21-C20-C19	2.50	109.62	107.23
20	A	2002	LHG	C11-C10-C9	-2.48	101.83	114.37
16	A	2006	LMG	O1-C7-C8	-2.48	104.78	110.82
15	5	501	AJP	O84-C85-C02	-2.47	109.00	112.17
20	B	306	LHG	C11-C10-C9	-2.47	101.91	114.37
15	B	305	AJP	C83-C06-C07	-2.45	109.60	114.50
16	A	2006	LMG	C40-C39-C38	-2.45	101.99	114.37
15	D	201	AJP	C83-C06-C07	-2.44	109.61	114.50
20	B	306	LHG	C20-C19-C18	-2.42	102.12	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	2006	LMG	C38-C37-C36	-2.42	102.13	114.37
20	F	301	LHG	C11-C10-C9	-2.42	102.14	114.37
16	A	2007	LMG	C38-C37-C36	-2.41	102.18	114.37
16	5	502	LMG	C40-C39-C38	-2.40	102.21	114.37
16	B	301	LMG	C38-C37-C36	-2.40	102.24	114.37
16	A	2008	LMG	C38-C37-C36	-2.40	102.26	114.37
20	B	304	LHG	C11-C10-C9	-2.40	102.26	114.37
16	A	2007	LMG	C40-C39-C38	-2.38	102.34	114.37
16	B	301	LMG	O1-C7-C8	-2.36	105.07	110.82
20	C	201	LHG	C20-C19-C18	-2.36	102.42	114.37
16	A	2007	LMG	O1-C7-C8	-2.36	105.08	110.82
20	A	2002	LHG	C20-C19-C18	-2.34	102.52	114.37
15	D	203	AJP	C20-C15-C16	-2.32	110.07	112.43
16	5	502	LMG	C38-C37-C36	-2.32	102.62	114.37
16	A	2008	LMG	O2-C2-C1	-2.31	104.57	110.08
16	5	502	LMG	O1-C7-C8	-2.30	105.22	110.82
15	5	501	AJP	C85-O84-C05	-2.30	109.71	113.69
16	A	2008	LMG	O1-C7-C8	-2.30	105.22	110.82
15	D	201	AJP	C04-C05-C06	-2.30	111.50	115.66
16	A	2006	LMG	O2-C2-C1	-2.30	104.60	110.08
16	5	502	LMG	O6-C1-O1	-2.30	104.62	110.04
15	4	401	AJP	C83-C06-C07	-2.29	109.91	114.50
16	5	502	LMG	O2-C2-C1	-2.28	104.65	110.08
20	B	306	LHG	C27-C26-C25	-2.28	102.86	114.37
20	A	2002	LHG	C27-C26-C25	-2.25	103.00	114.37
15	5	501	AJP	C18-C17-C16	-2.24	108.59	112.16
16	B	301	LMG	O2-C2-C1	-2.22	104.77	110.08
20	C	201	LHG	C18-C17-C16	-2.22	103.13	114.37
16	A	2008	LMG	O3-C3-C2	-2.22	105.14	110.38
16	A	2007	LMG	C42-C41-C40	-2.20	103.22	114.37
16	A	2007	LMG	O2-C2-C1	-2.20	104.83	110.08
15	B	305	AJP	O84-C85-C02	-2.20	109.34	112.17
16	5	502	LMG	C42-C41-C40	-2.20	103.27	114.37
16	B	301	LMG	O3-C3-C2	-2.18	105.24	110.38
15	D	203	AJP	C05-C06-C07	-2.18	100.16	103.37
20	B	306	LHG	C18-C17-C16	-2.17	103.38	114.37
20	A	2002	LHG	C18-C17-C16	-2.17	103.39	114.37
20	F	301	LHG	C27-C26-C25	-2.16	103.45	114.37
16	A	2008	LMG	O6-C1-O1	-2.16	104.95	110.04
15	D	203	AJP	C11-C16-C15	-2.15	105.36	109.17
15	4	401	AJP	C18-C17-C16	-2.15	108.73	112.16
16	5	502	LMG	O3-C3-C2	-2.15	105.31	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	201	LHG	C27-C26-C25	-2.14	103.56	114.37
15	B	305	AJP	C80-C20-C15	-2.13	108.31	111.18
16	A	2007	LMG	O3-C3-C2	-2.13	105.36	110.38
15	D	203	AJP	O84-C85-C02	-2.12	109.45	112.17
16	A	2006	LMG	O3-C3-C2	-2.11	105.40	110.38
16	A	2006	LMG	O1-C1-C2	-2.11	105.07	108.27
16	B	301	LMG	O7-C10-O9	-2.11	118.78	123.70
20	B	304	LHG	C27-C26-C25	-2.11	103.72	114.37
15	5	501	AJP	C24-C23-C22	-2.08	108.89	111.07
15	4	401	AJP	C03-C04-C05	-2.07	108.69	111.93
16	B	301	LMG	O1-C1-C2	-2.06	105.14	108.27
15	D	203	AJP	C17-C16-C11	-2.06	109.38	112.29
15	D	201	AJP	C18-C19-C20	-2.05	108.87	112.31
16	A	2008	LMG	O1-C1-C2	-2.04	105.17	108.27
20	B	306	LHG	C5-O7-C7	-2.04	112.91	117.80
15	D	203	AJP	C80-C20-C15	-2.02	108.47	111.18

There are no chirality outliers.

All (197) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	5	502	LMG	C2-C1-O1-C7
16	5	502	LMG	O6-C1-O1-C7
16	5	502	LMG	C11-C10-O7-C8
16	A	2008	LMG	O6-C1-O1-C7
20	A	2002	LHG	C3-O3-P-O5
20	A	2002	LHG	C3-O3-P-O6
20	B	304	LHG	C3-O3-P-O6
20	B	304	LHG	O9-C7-O7-C5
20	B	306	LHG	C2-C3-O3-P
20	B	306	LHG	C3-O3-P-O4
20	B	306	LHG	C3-O3-P-O6
20	C	201	LHG	C4-O6-P-O3
20	C	201	LHG	C4-O6-P-O5
20	C	201	LHG	C24-C23-O8-C6
20	F	301	LHG	O1-C1-C2-C3
20	F	301	LHG	C4-O6-P-O5
15	5	501	AJP	O31-C26-O25-C23
15	5	501	AJP	C27-C26-O25-C23
20	C	201	LHG	O10-C23-O8-C6
16	A	2006	LMG	C29-C28-O8-C9
16	5	502	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
16	A	2006	LMG	O10-C28-O8-C9
20	B	306	LHG	O10-C23-O8-C6
15	D	203	AJP	O31-C26-O25-C23
16	5	502	LMG	O9-C10-O7-C8
20	B	306	LHG	O9-C7-O7-C5
20	B	306	LHG	C24-C23-O8-C6
20	B	304	LHG	C8-C7-O7-C5
15	D	203	AJP	C27-C26-O25-C23
16	5	502	LMG	C29-C28-O8-C9
20	A	2002	LHG	C24-C23-O8-C6
20	A	2002	LHG	O10-C23-O8-C6
20	B	304	LHG	O2-C2-C3-O3
16	A	2008	LMG	O6-C5-C6-O5
20	B	304	LHG	C1-C2-C3-O3
16	A	2008	LMG	C2-C1-O1-C7
20	C	201	LHG	C23-C24-C25-C26
16	A	2008	LMG	C4-C5-C6-O5
20	B	306	LHG	C8-C7-O7-C5
20	F	301	LHG	O1-C1-C2-O2
16	A	2007	LMG	C28-C29-C30-C31
16	5	502	LMG	C10-C11-C12-C13
16	B	301	LMG	O6-C5-C6-O5
20	B	306	LHG	O2-C2-C3-O3
20	B	306	LHG	C23-C24-C25-C26
20	B	306	LHG	C7-C8-C9-C10
20	B	306	LHG	C1-C2-C3-O3
20	F	301	LHG	O2-C2-C3-O3
20	A	2002	LHG	O1-C1-C2-C3
20	F	301	LHG	C29-C30-C31-C32
20	B	304	LHG	C7-C8-C9-C10
20	F	301	LHG	C23-C24-C25-C26
18	B	302	D12	C6-C7-C8-C9
20	B	306	LHG	C27-C28-C29-C30
16	A	2006	LMG	C17-C18-C19-C20
16	A	2006	LMG	C31-C32-C33-C34
16	A	2007	LMG	C37-C38-C39-C40
20	A	2002	LHG	C12-C13-C14-C15
20	B	304	LHG	C24-C25-C26-C27
16	5	502	LMG	C29-C30-C31-C32
20	F	301	LHG	C1-C2-C3-O3
20	B	304	LHG	C24-C23-O8-C6
16	A	2006	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
16	A	2007	LMG	C13-C14-C15-C16
16	5	502	LMG	C35-C36-C37-C38
20	A	2002	LHG	C24-C25-C26-C27
20	F	301	LHG	C32-C33-C34-C35
16	A	2007	LMG	C32-C33-C34-C35
16	A	2008	LMG	C34-C35-C36-C37
16	A	2006	LMG	C33-C34-C35-C36
20	A	2002	LHG	C32-C33-C34-C35
18	9	1001	D12	C7-C8-C9-C10
16	A	2007	LMG	C31-C32-C33-C34
16	A	2008	LMG	C33-C34-C35-C36
16	5	502	LMG	O6-C5-C6-O5
19	A	2001	IHP	C4-C3-O13-P3
16	A	2007	LMG	O6-C5-C6-O5
16	A	2007	LMG	C33-C34-C35-C36
15	D	203	AJP	C36-C35-O34-C29
16	5	502	LMG	C34-C35-C36-C37
16	A	2006	LMG	C15-C16-C17-C18
20	C	201	LHG	C32-C33-C34-C35
20	A	2002	LHG	C8-C7-O7-C5
20	A	2002	LHG	C28-C29-C30-C31
20	F	301	LHG	C27-C28-C29-C30
20	A	2002	LHG	C23-C24-C25-C26
16	A	2007	LMG	C41-C42-C43-C44
20	F	301	LHG	C24-C23-O8-C6
16	B	301	LMG	C30-C31-C32-C33
15	D	203	AJP	O31-C30-C32-O33
16	A	2007	LMG	C14-C15-C16-C17
20	F	301	LHG	O6-C4-C5-O7
16	A	2006	LMG	C34-C35-C36-C37
18	9	1001	D12	C1-C2-C3-C4
20	B	304	LHG	C27-C28-C29-C30
16	A	2008	LMG	C31-C32-C33-C34
16	A	2007	LMG	C29-C30-C31-C32
19	A	2001	IHP	C2-C3-O13-P3
20	A	2002	LHG	O1-C1-C2-O2
18	B	302	D12	C5-C6-C7-C8
18	A	2004	D12	C5-C6-C7-C8
20	A	2002	LHG	O6-C4-C5-C6
20	A	2002	LHG	C15-C16-C17-C18
16	A	2007	LMG	C30-C31-C32-C33
15	D	203	AJP	O40-C35-O34-C29

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Mol	Chain	Res	Type	Atoms
16	5	502	LMG	C38-C39-C40-C41
20	A	2002	LHG	C33-C34-C35-C36
16	5	502	LMG	C7-C8-C9-O8
16	A	2006	LMG	O1-C7-C8-C9
20	B	306	LHG	C4-C5-C6-O8
20	A	2002	LHG	O6-C4-C5-O7
20	C	201	LHG	O6-C4-C5-O7
16	B	301	LMG	C31-C32-C33-C34
16	A	2008	LMG	C32-C33-C34-C35
16	A	2006	LMG	O1-C7-C8-O7
20	B	306	LHG	O7-C5-C6-O8
20	A	2002	LHG	C27-C28-C29-C30
20	B	306	LHG	C11-C12-C13-C14
16	A	2006	LMG	C23-C24-C25-C26
20	B	306	LHG	C24-C25-C26-C27
16	A	2006	LMG	C28-C29-C30-C31
20	B	306	LHG	O1-C1-C2-O2
20	C	201	LHG	O6-C4-C5-C6
20	F	301	LHG	O6-C4-C5-C6
16	A	2007	LMG	C18-C19-C20-C21
18	D	202	D12	C7-C8-C9-C10
18	A	2005	D12	C2-C3-C4-C5
16	A	2007	LMG	C11-C10-O7-C8
18	D	202	D12	C6-C7-C8-C9
20	B	304	LHG	C12-C13-C14-C15
16	5	502	LMG	O1-C7-C8-O7
16	5	502	LMG	O7-C8-C9-O8
20	F	301	LHG	O7-C5-C6-O8
18	B	303	D12	C6-C7-C8-C9
20	B	306	LHG	C12-C13-C14-C15
16	A	2006	LMG	C38-C39-C40-C41
16	A	2006	LMG	C29-C30-C31-C32
18	A	2005	D12	C4-C5-C6-C7
20	F	301	LHG	C28-C29-C30-C31
18	9	1001	D12	C9-C10-C11-C12
20	B	306	LHG	C30-C31-C32-C33
20	A	2002	LHG	C11-C10-C9-C8
20	B	304	LHG	C3-O3-P-O5
20	B	306	LHG	C5-C4-O6-P
20	B	304	LHG	O1-C1-C2-O2
16	A	2006	LMG	C10-C11-C12-C13
16	A	2006	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
20	C	201	LHG	C17-C18-C19-C20
19	A	2001	IHP	C3-C4-O14-P4
19	A	2001	IHP	C4-O14-P4-O44
20	C	201	LHG	C27-C28-C29-C30
16	5	502	LMG	C42-C43-C44-C45
16	B	301	LMG	C36-C37-C38-C39
16	A	2006	LMG	C18-C19-C20-C21
16	A	2006	LMG	C16-C17-C18-C19
20	C	201	LHG	O1-C1-C2-C3
15	B	305	AJP	O31-C26-O25-C23
16	A	2008	LMG	C37-C38-C39-C40
20	B	306	LHG	O6-C4-C5-O7
20	C	201	LHG	C29-C30-C31-C32
20	C	201	LHG	C5-C4-O6-P
19	A	2001	IHP	C5-C4-O14-P4
18	A	2005	D12	C1-C2-C3-C4
19	A	2001	IHP	C4-O14-P4-O24
16	A	2006	LMG	C35-C36-C37-C38
20	B	304	LHG	O10-C23-O8-C6
18	B	303	D12	C7-C8-C9-C10
18	B	303	D12	C2-C3-C4-C5
20	B	306	LHG	O6-C4-C5-C6
16	B	301	LMG	O7-C10-C11-C12
18	A	2004	D12	C1-C2-C3-C4
16	A	2007	LMG	C35-C36-C37-C38
16	A	2006	LMG	C4-C5-C6-O5
18	A	2005	D12	C5-C6-C7-C8
16	A	2006	LMG	O7-C10-C11-C12
16	A	2008	LMG	O7-C10-C11-C12
16	5	502	LMG	C33-C34-C35-C36
20	F	301	LHG	C7-C8-C9-C10
20	F	301	LHG	C8-C7-O7-C5
15	B	305	AJP	C27-C26-O25-C23
16	A	2006	LMG	C37-C38-C39-C40
16	A	2007	LMG	C20-C21-C22-C23
16	5	502	LMG	O7-C10-C11-C12
20	C	201	LHG	C33-C34-C35-C36
16	A	2007	LMG	C19-C20-C21-C22
15	B	305	AJP	C22-C23-O25-C26
16	5	502	LMG	C37-C38-C39-C40
16	5	502	LMG	O10-C28-C29-C30
16	A	2006	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	A	2008	LMG	O9-C10-C11-C12
20	F	301	LHG	O10-C23-C24-C25
16	A	2006	LMG	C21-C22-C23-C24
18	D	202	D12	C5-C6-C7-C8
16	A	2008	LMG	O8-C28-C29-C30
20	C	201	LHG	C26-C27-C28-C29
20	B	306	LHG	O9-C7-C8-C9
20	F	301	LHG	C30-C31-C32-C33

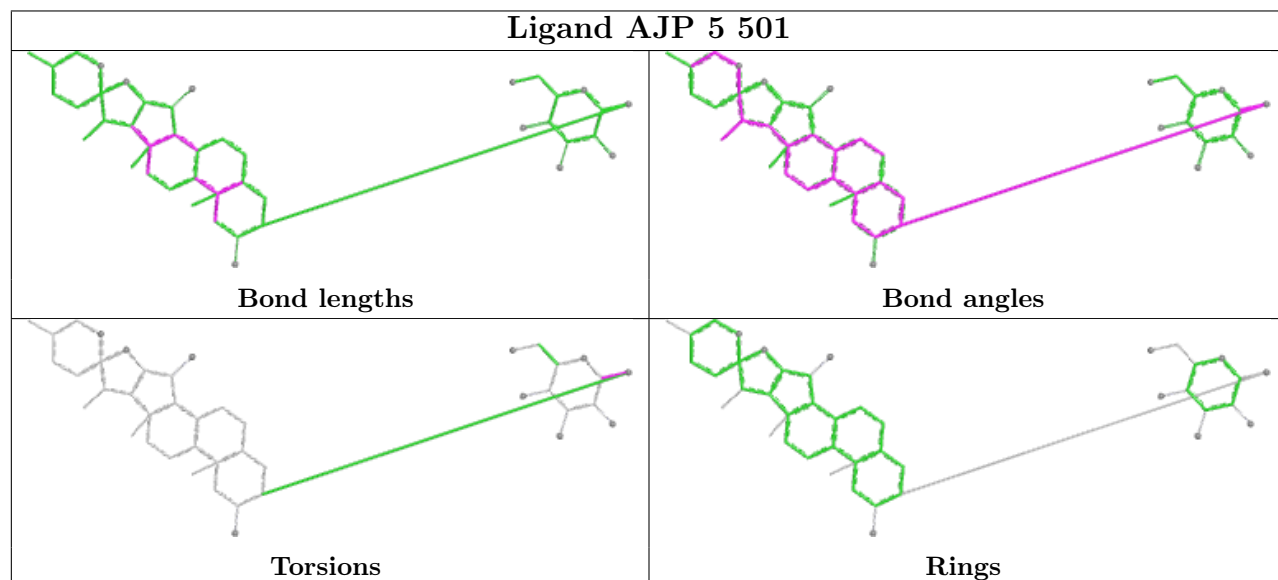
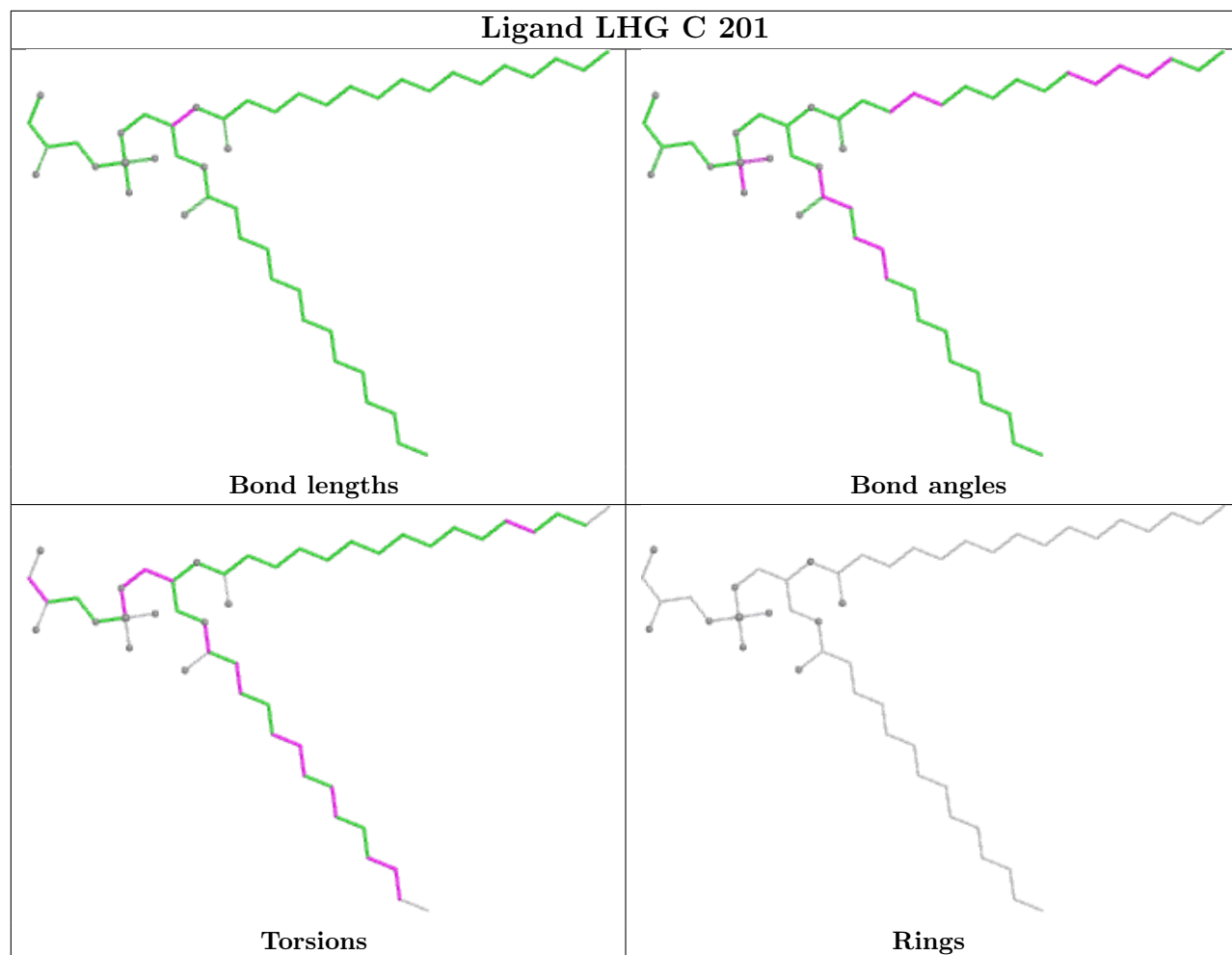
All (2) ring outliers are listed below:

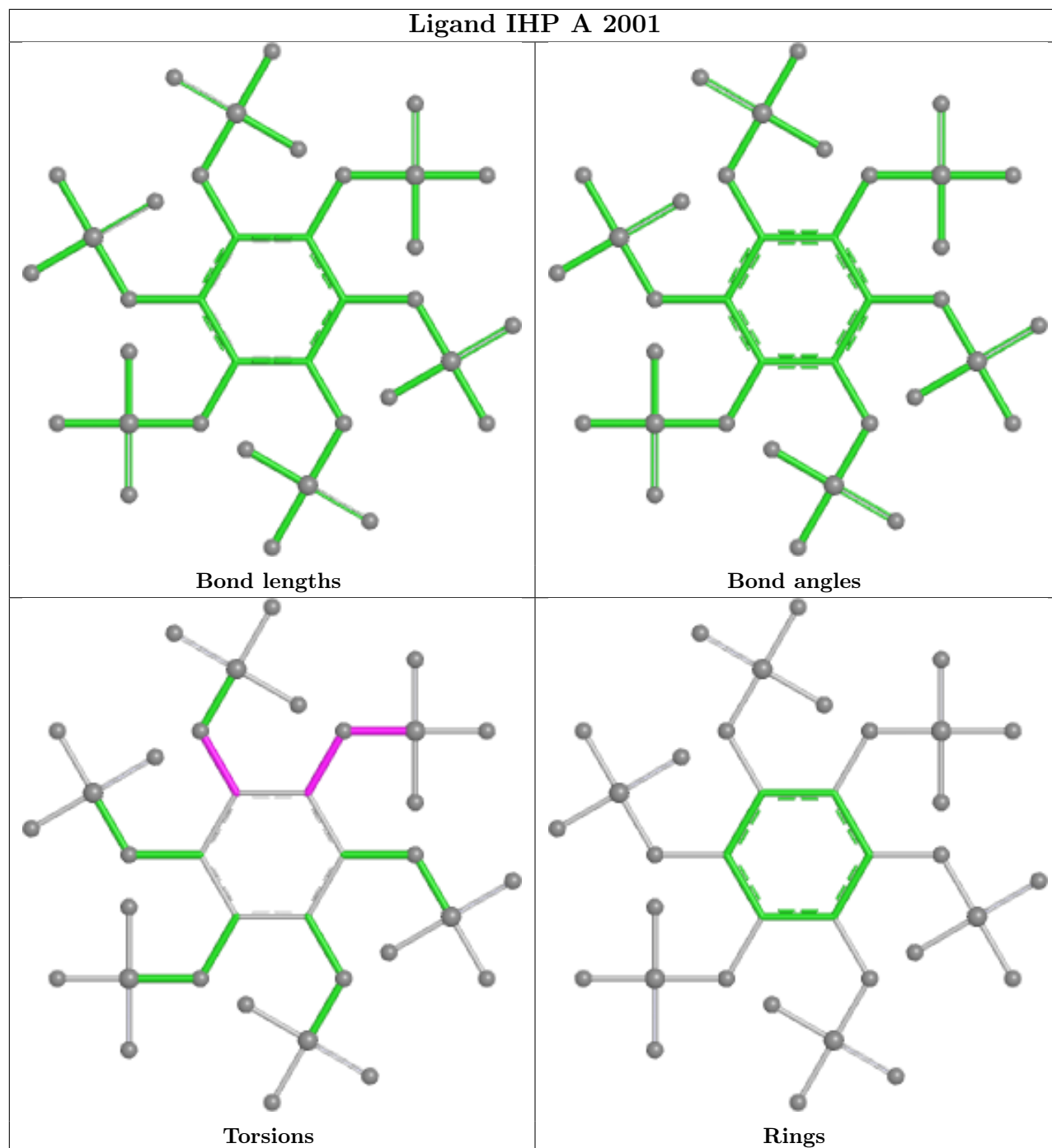
Mol	Chain	Res	Type	Atoms
15	D	201	AJP	C19-C20-C21-C22-C23-C24
15	D	203	AJP	C35-C36-C37-C38-C39-O40

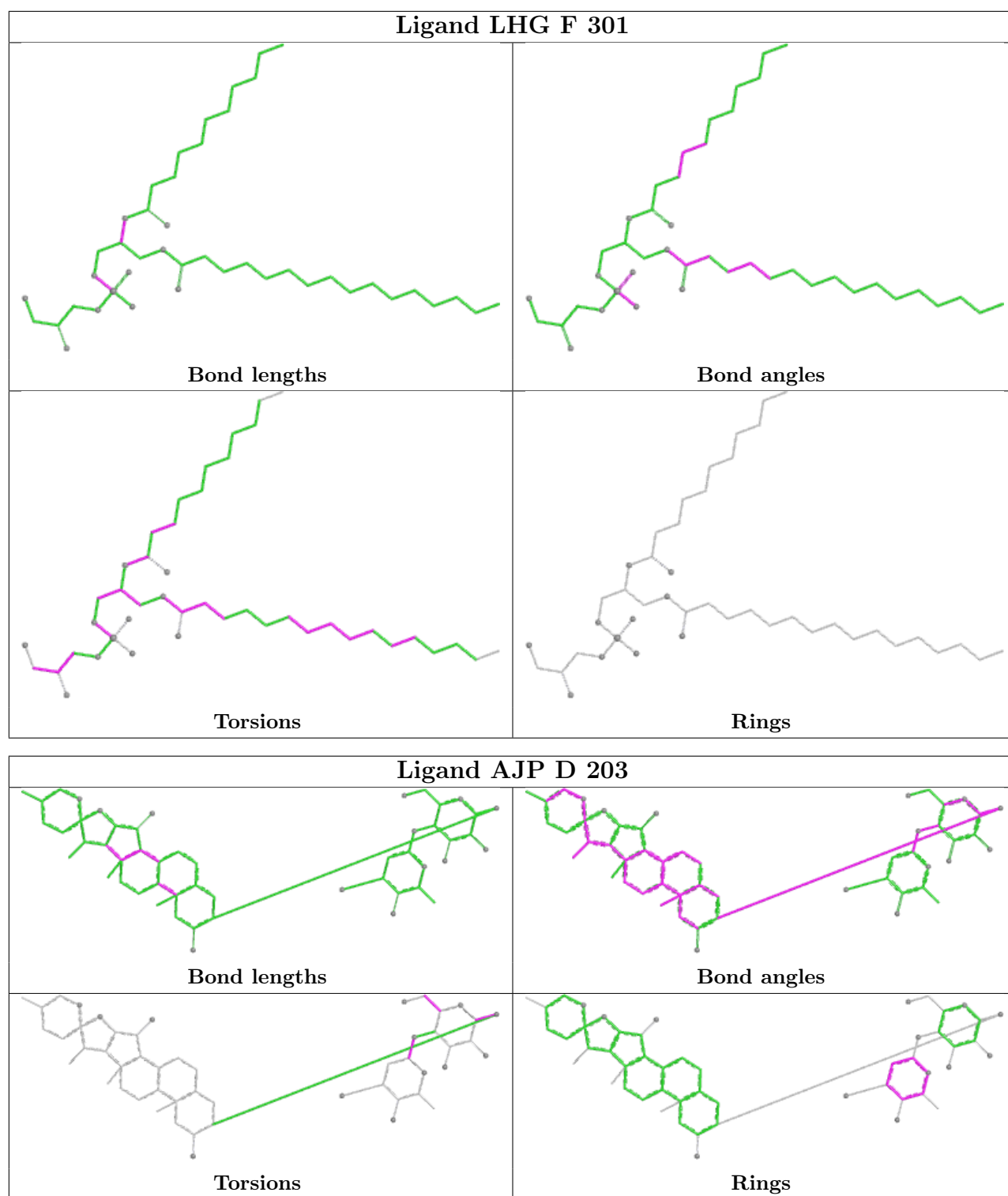
8 monomers are involved in 13 short contacts:

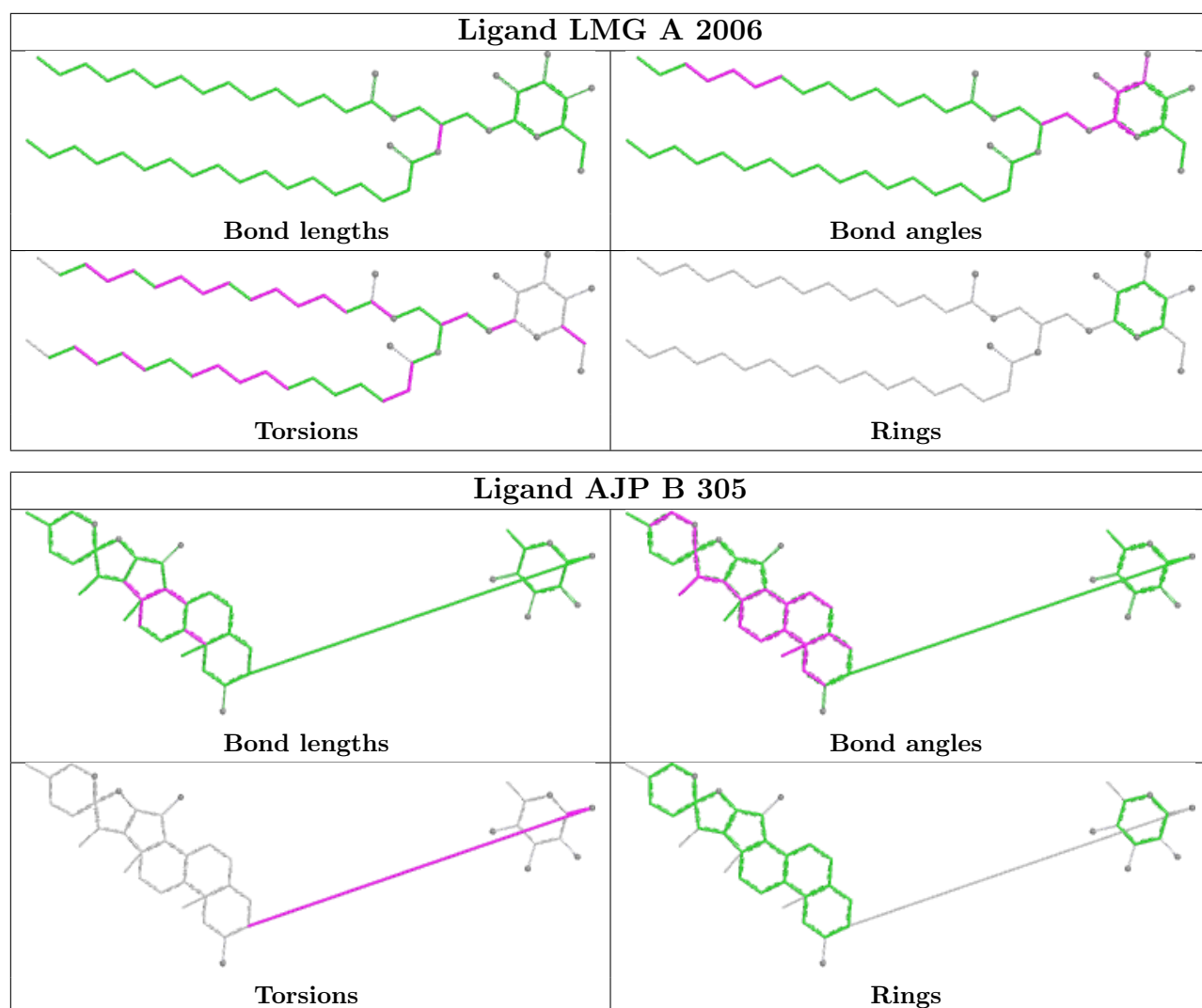
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	201	LHG	3	0
20	F	301	LHG	1	0
16	A	2006	LMG	1	0
15	B	305	AJP	2	0
20	A	2002	LHG	1	0
16	A	2008	LMG	1	0
16	5	502	LMG	2	0
16	A	2007	LMG	3	0

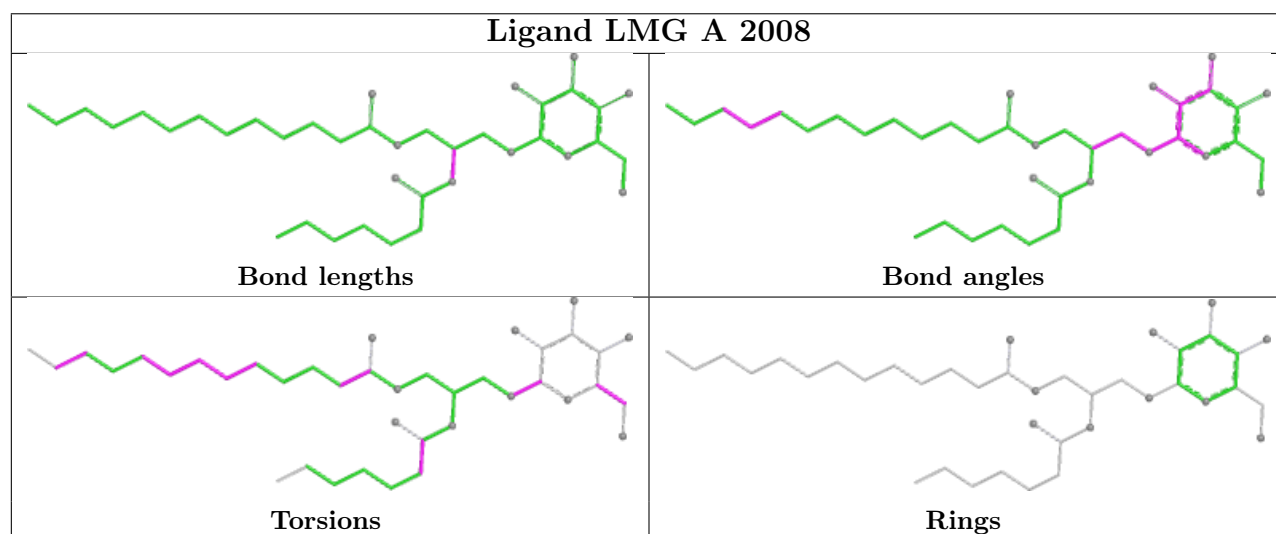
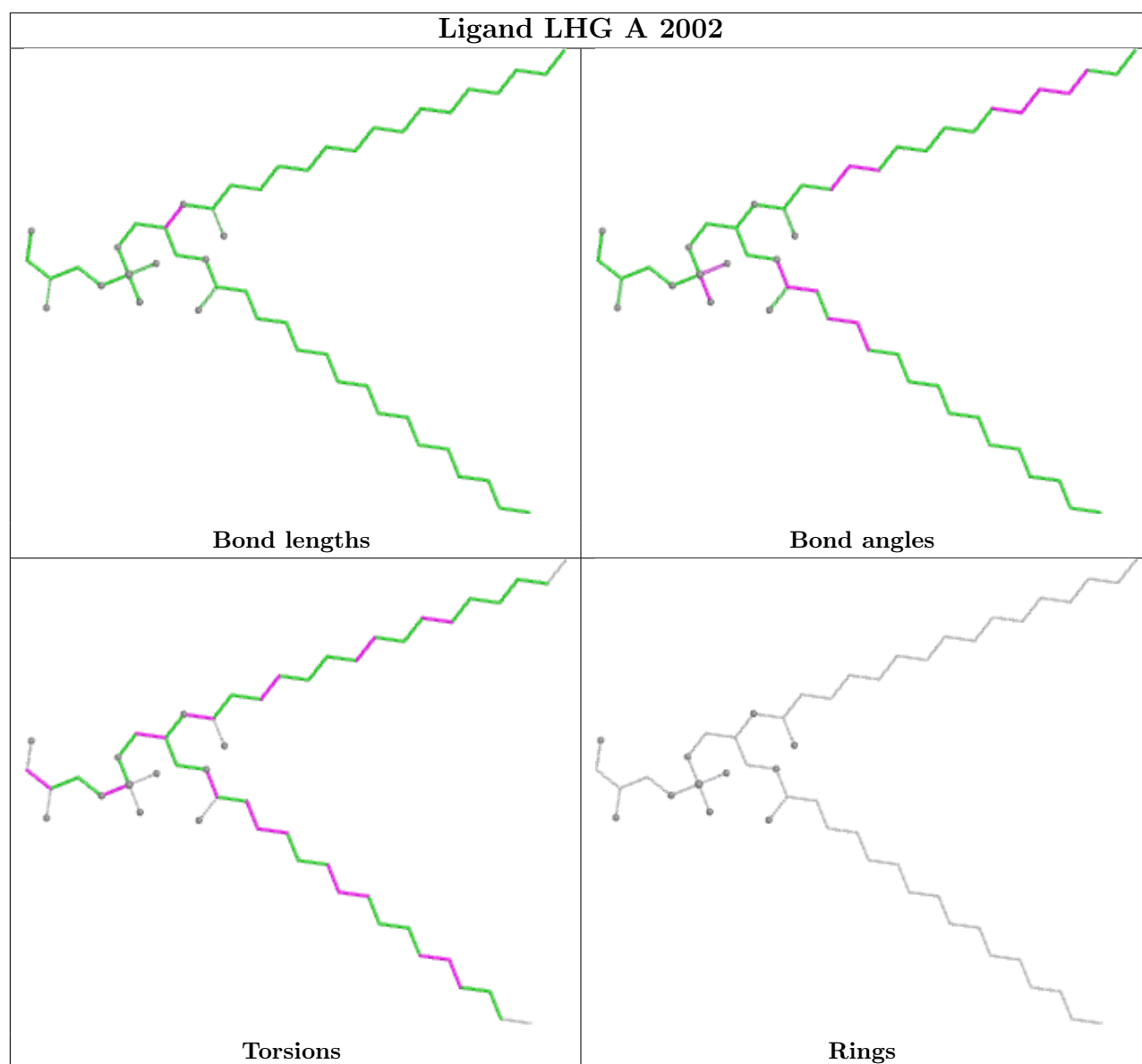
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

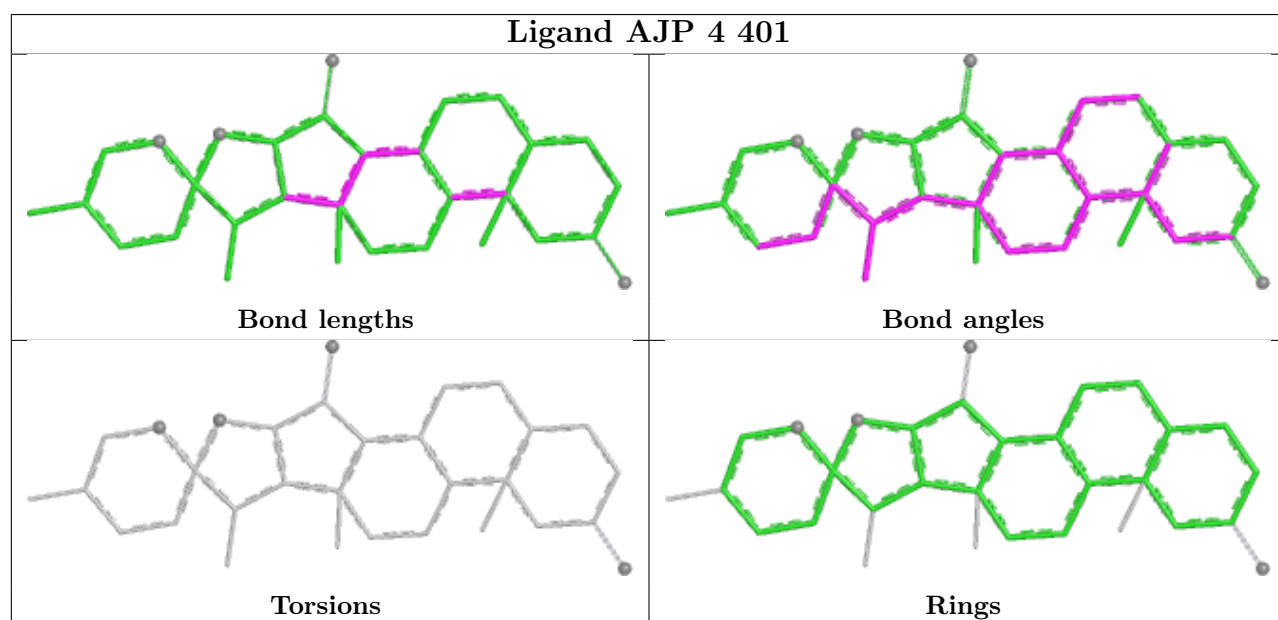
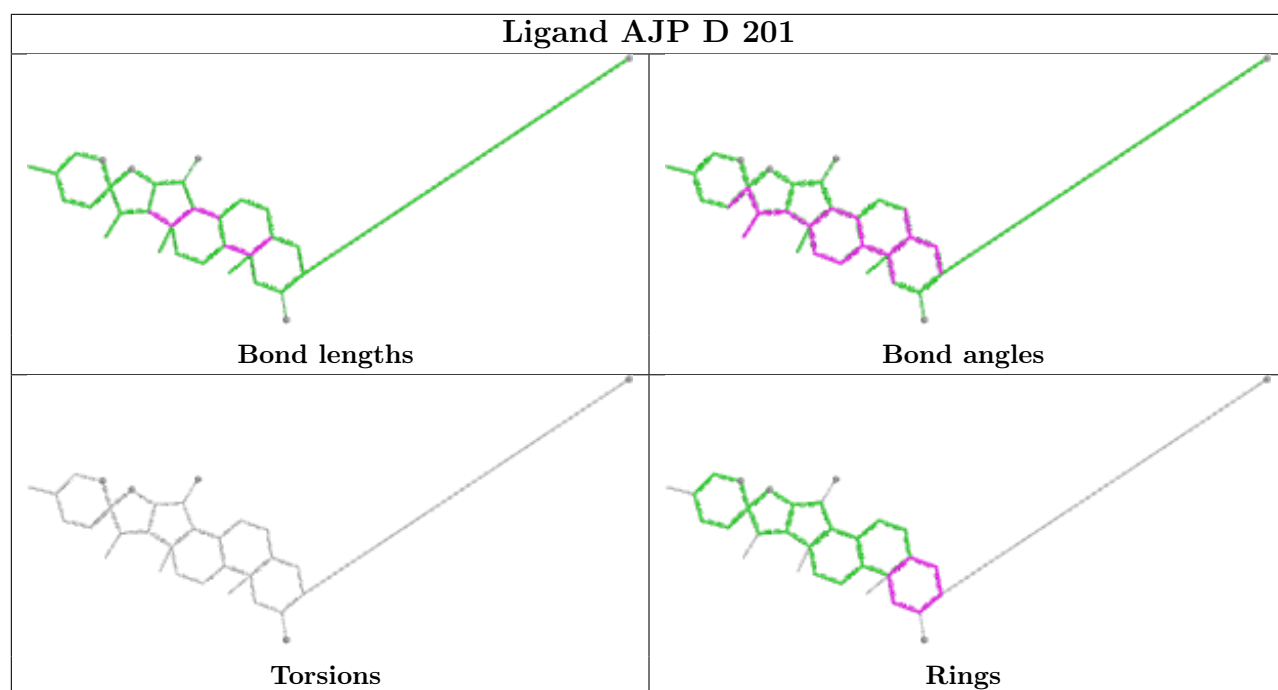


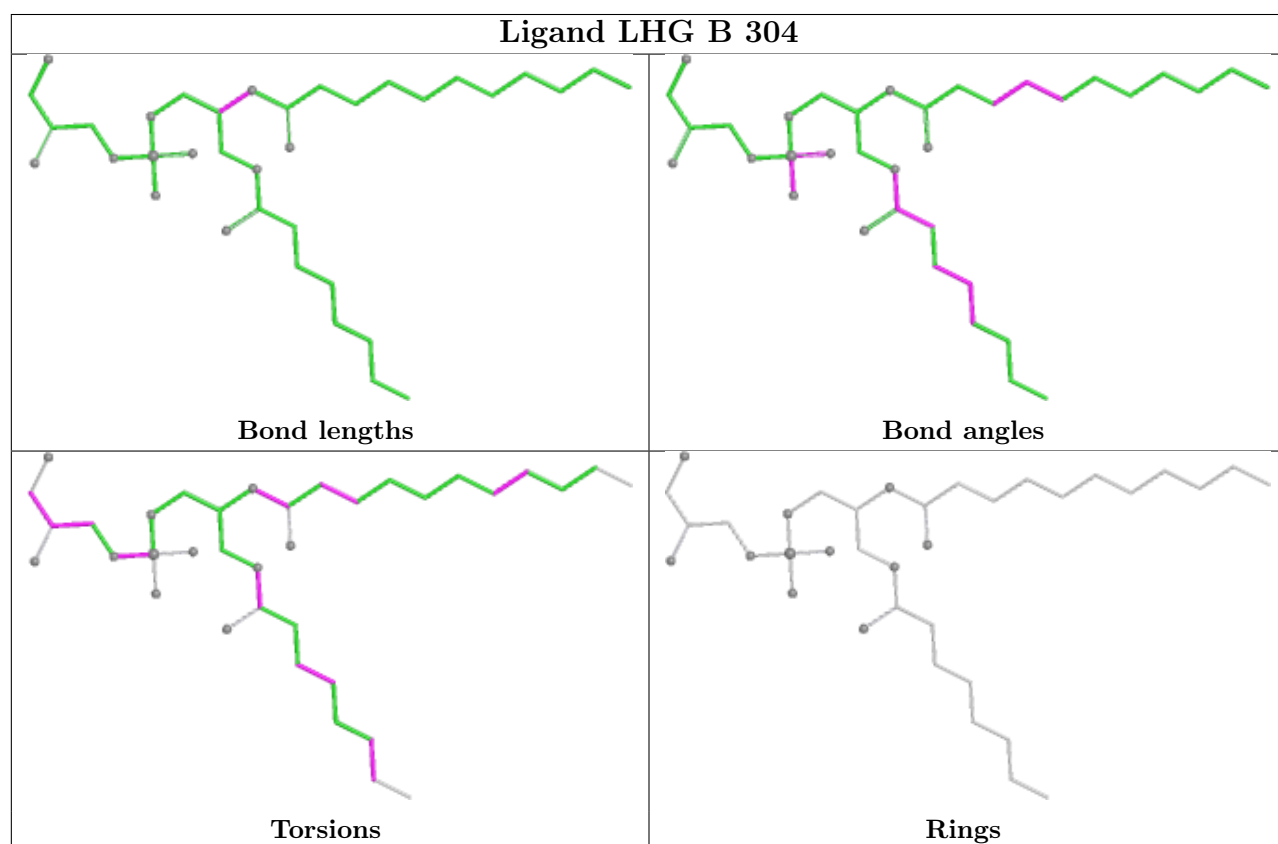
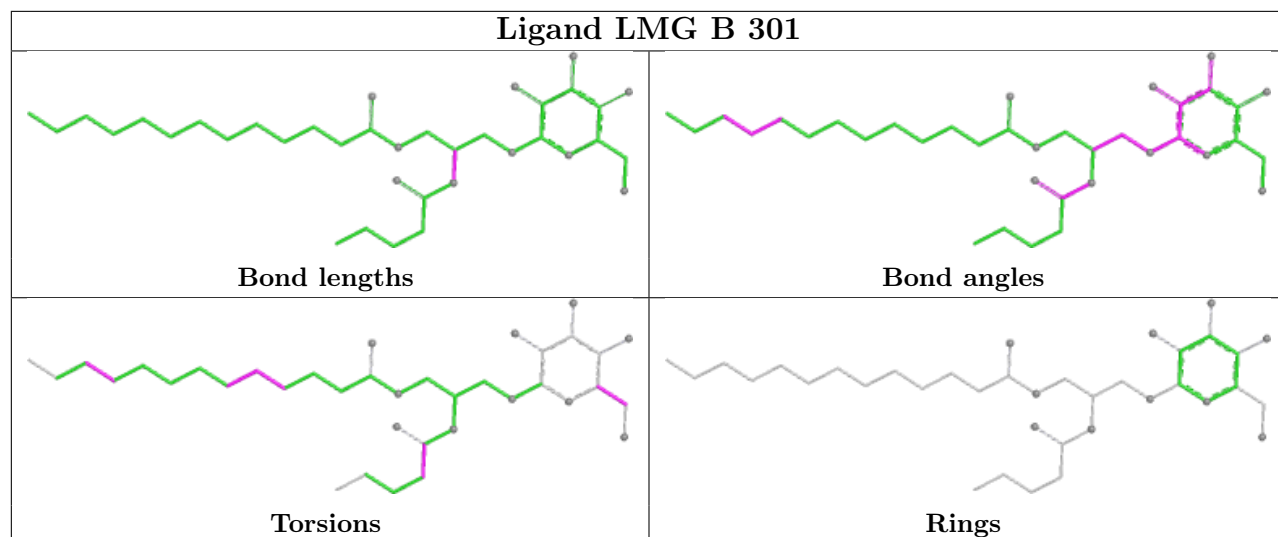


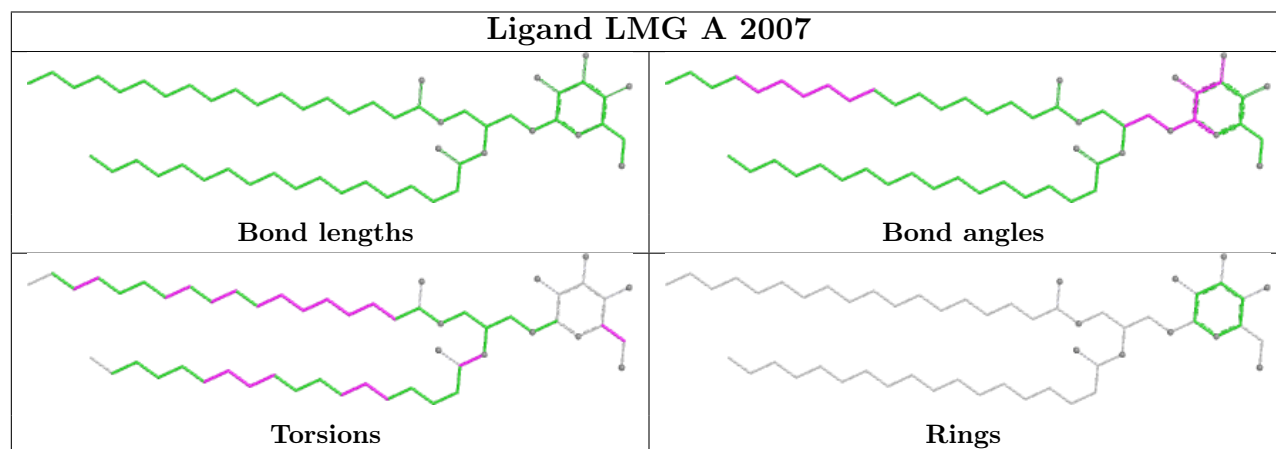
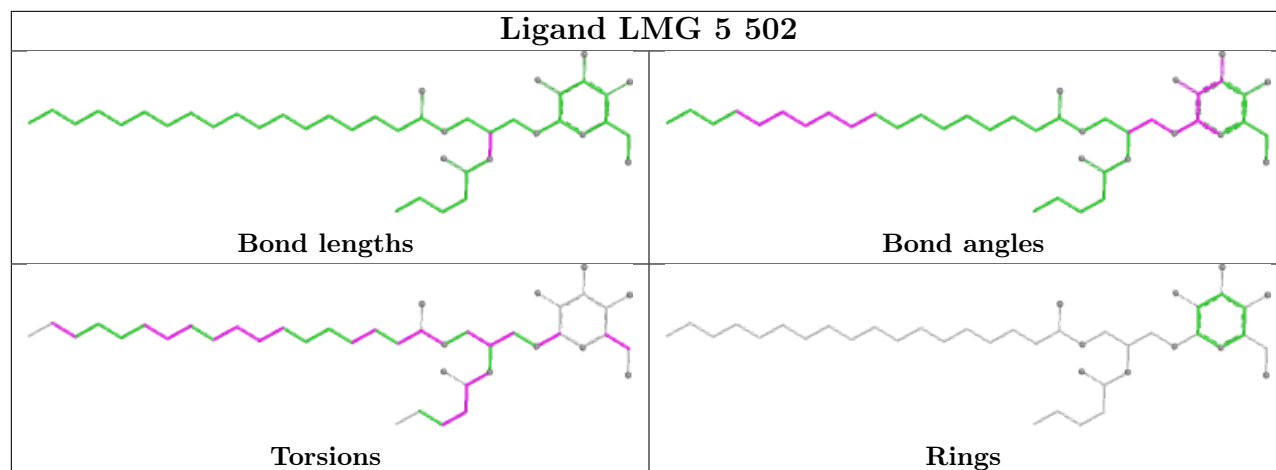


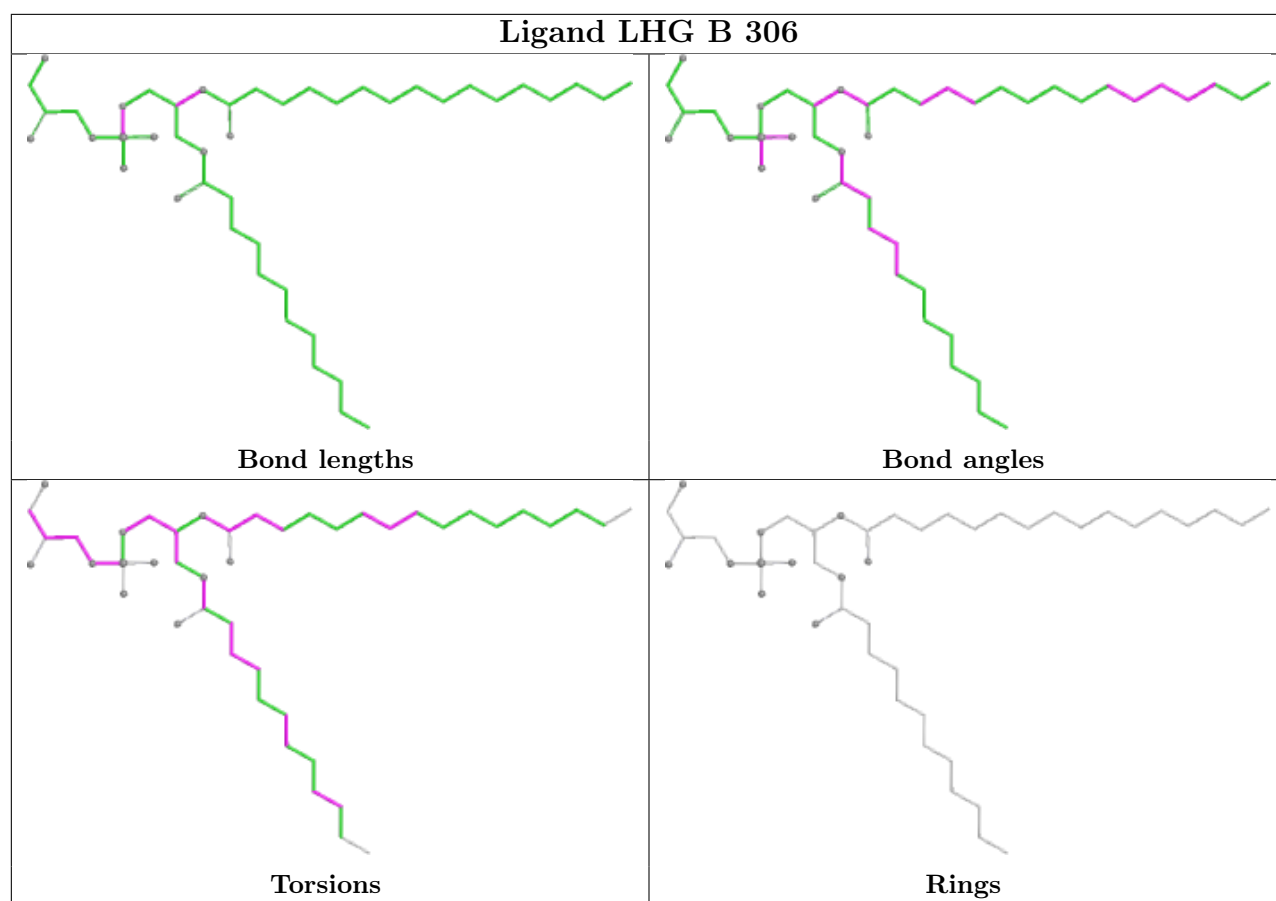












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

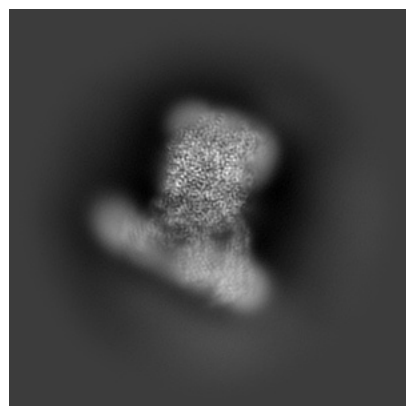
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33528. These allow visual inspection of the internal detail of the map and identification of artifacts.

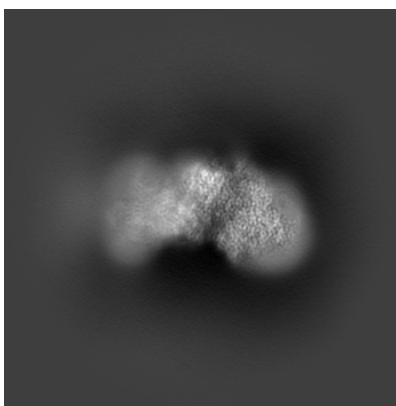
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

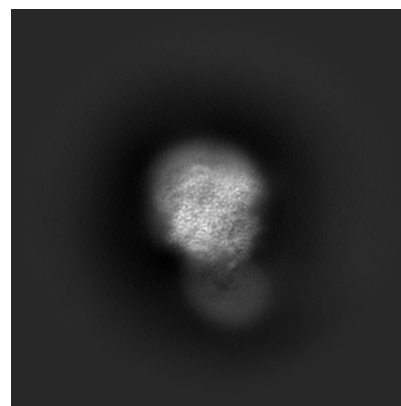
6.1.1 Primary map



X

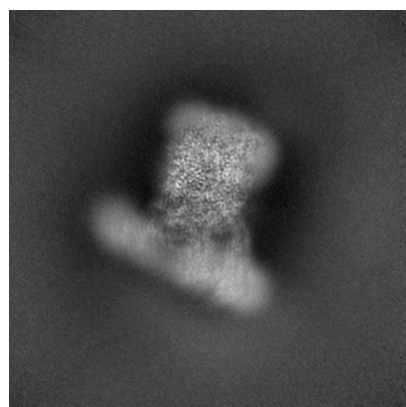


Y

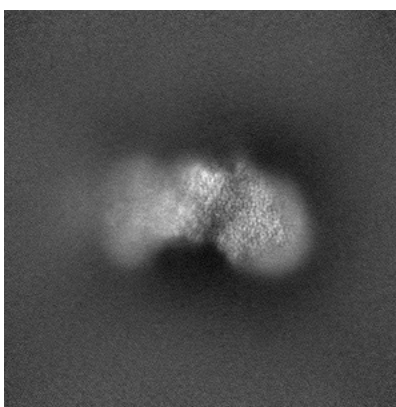


Z

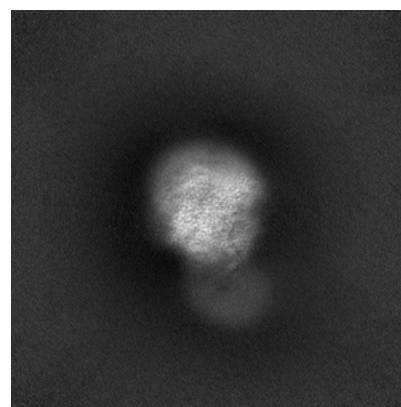
6.1.2 Raw map



X



Y

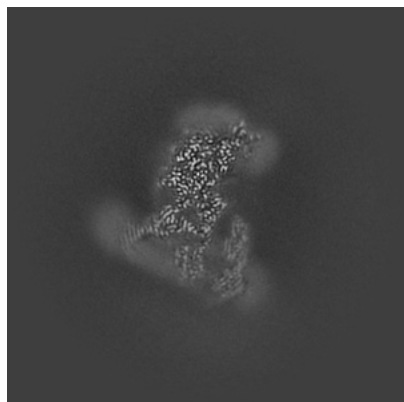


Z

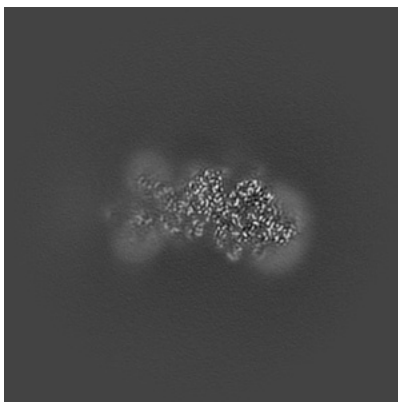
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

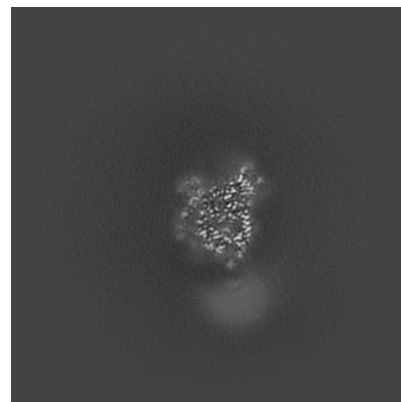
6.2.1 Primary map



X Index: 320

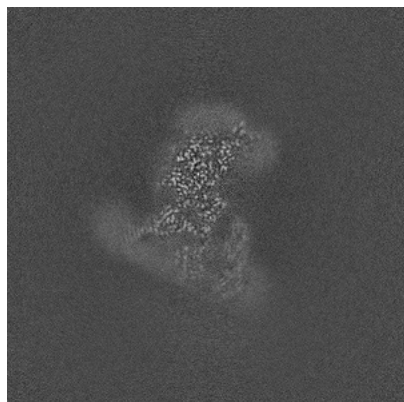


Y Index: 320

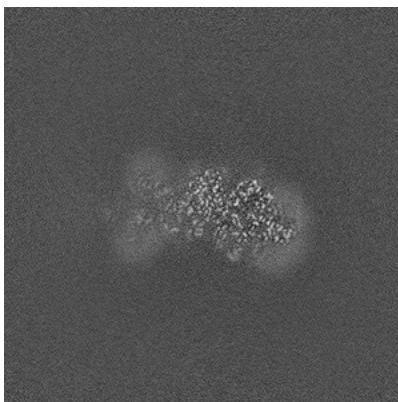


Z Index: 320

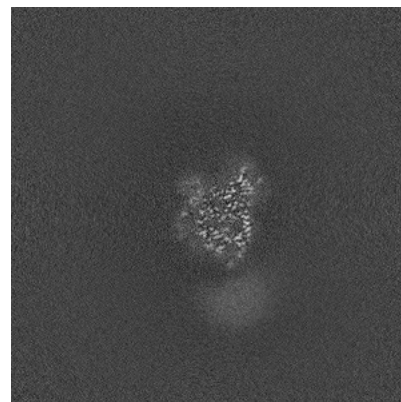
6.2.2 Raw map



X Index: 320



Y Index: 320

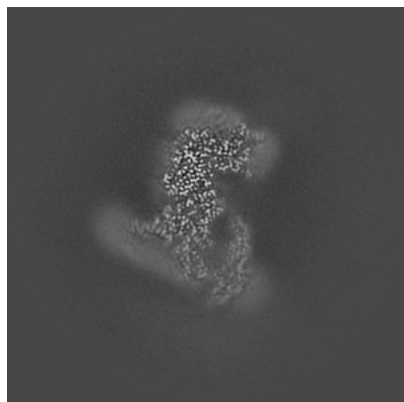


Z Index: 320

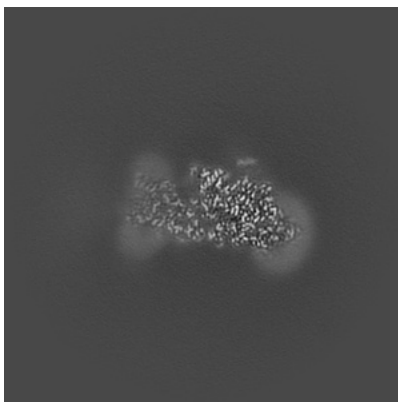
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

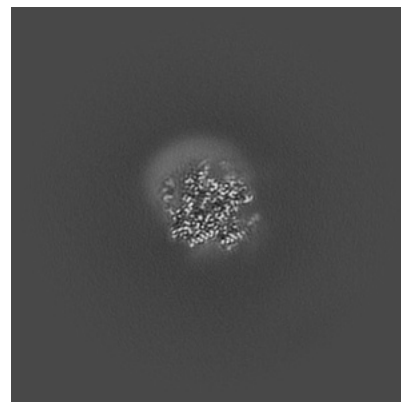
6.3.1 Primary map



X Index: 312

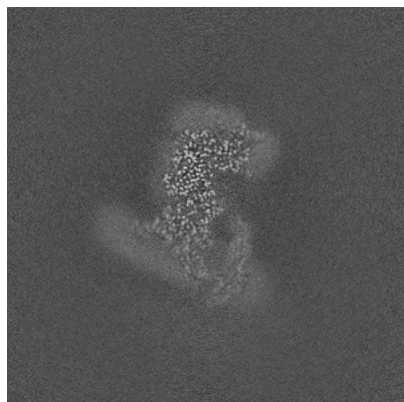


Y Index: 305

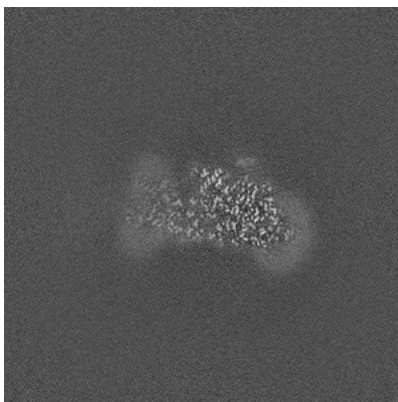


Z Index: 397

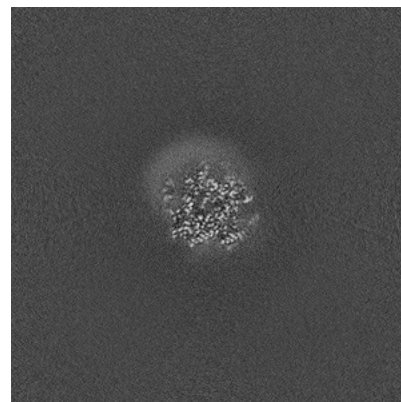
6.3.2 Raw map



X Index: 312



Y Index: 304

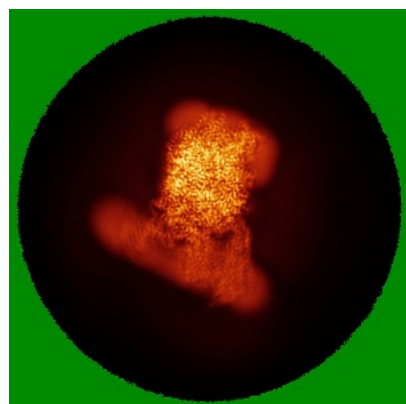


Z Index: 397

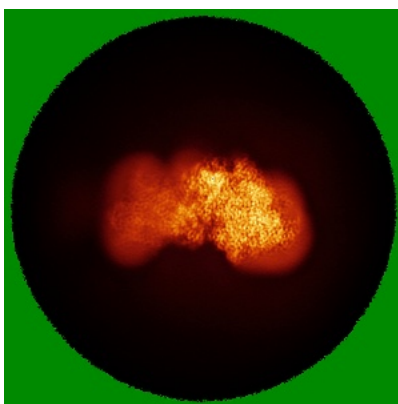
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

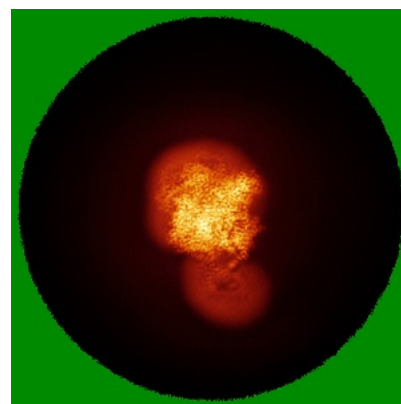
6.4.1 Primary map



X

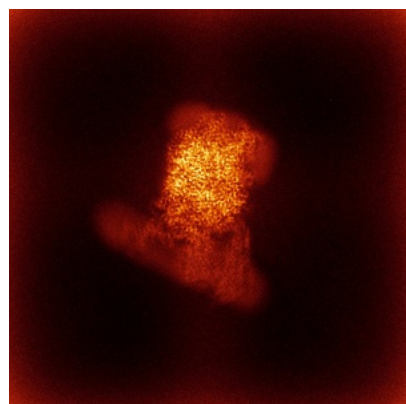


Y

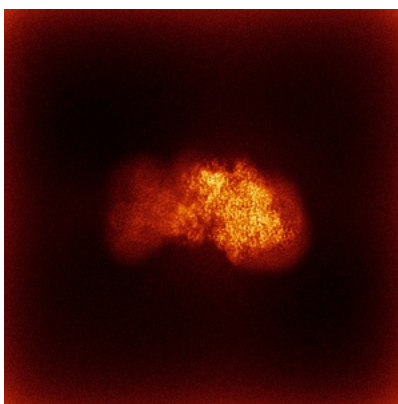


Z

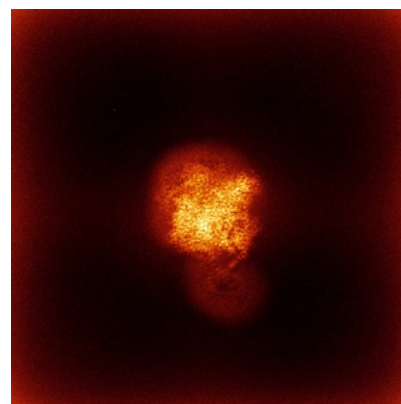
6.4.2 Raw map



X



Y

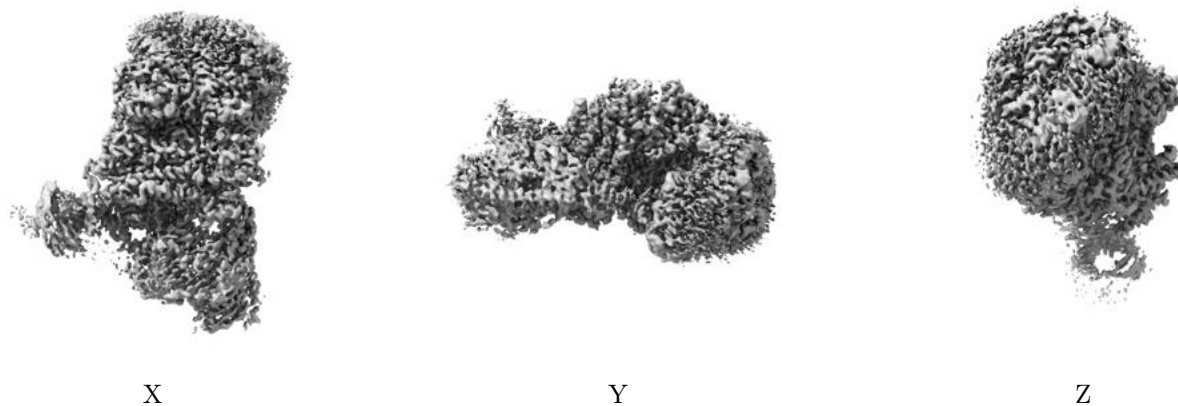


Z

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.

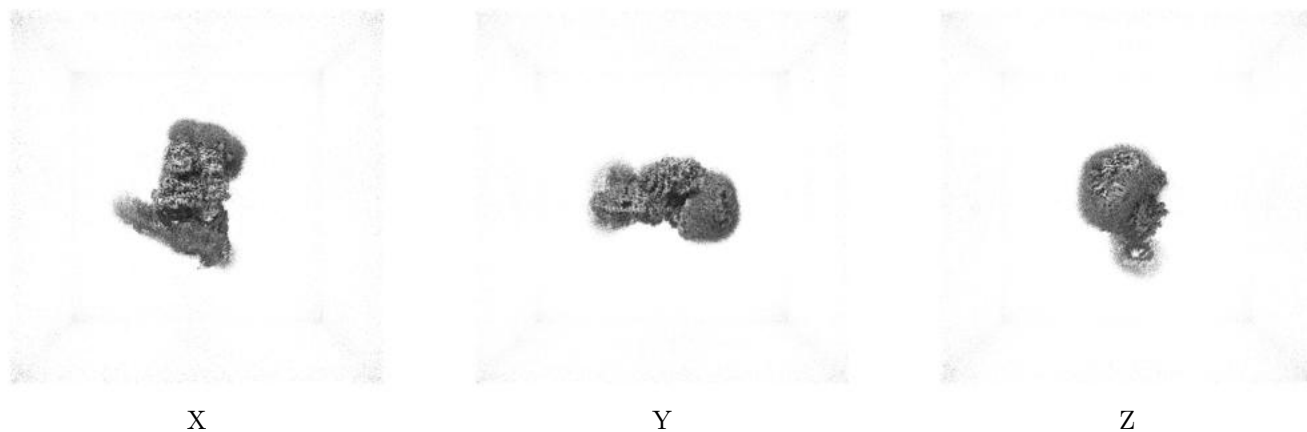
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

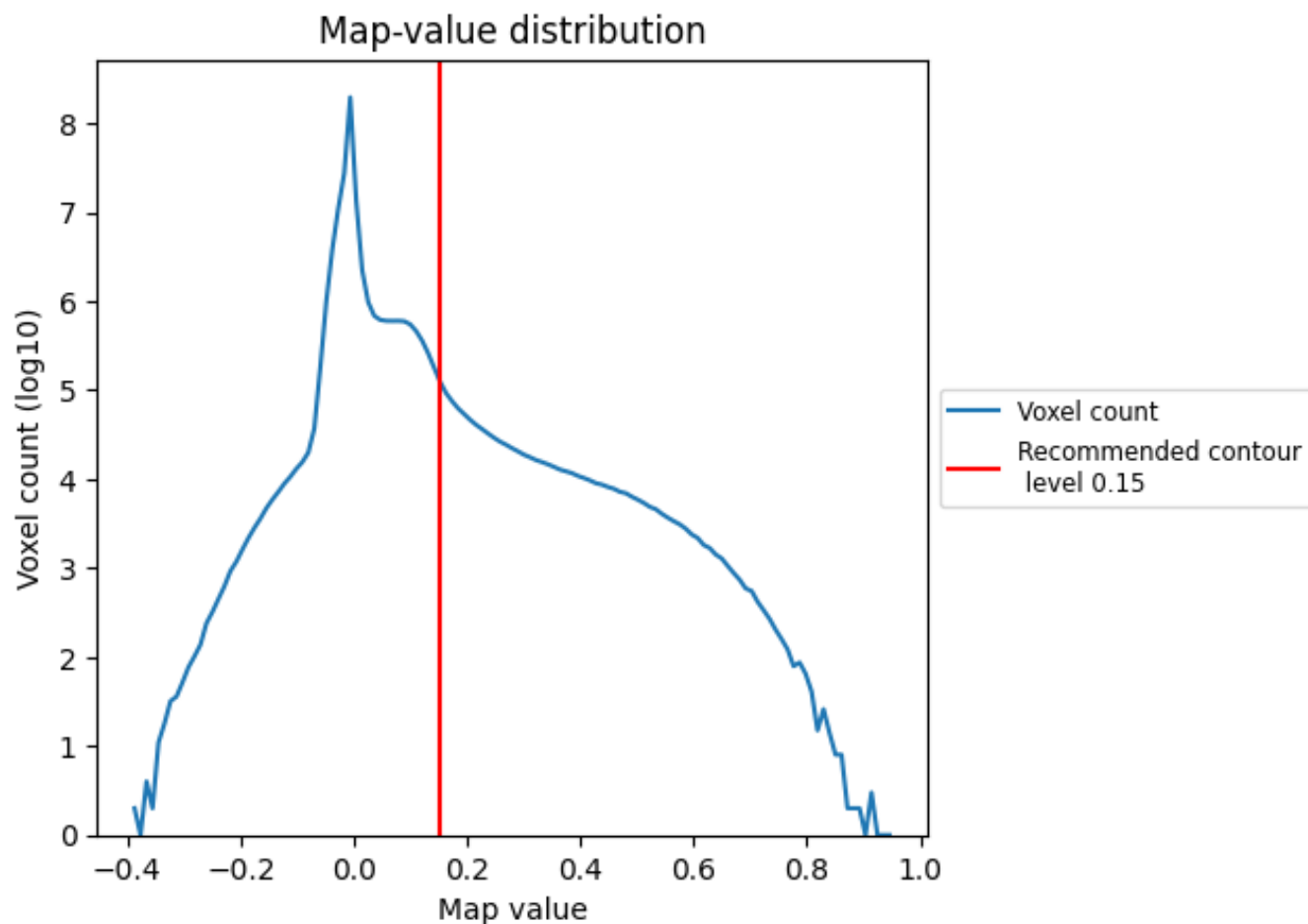
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

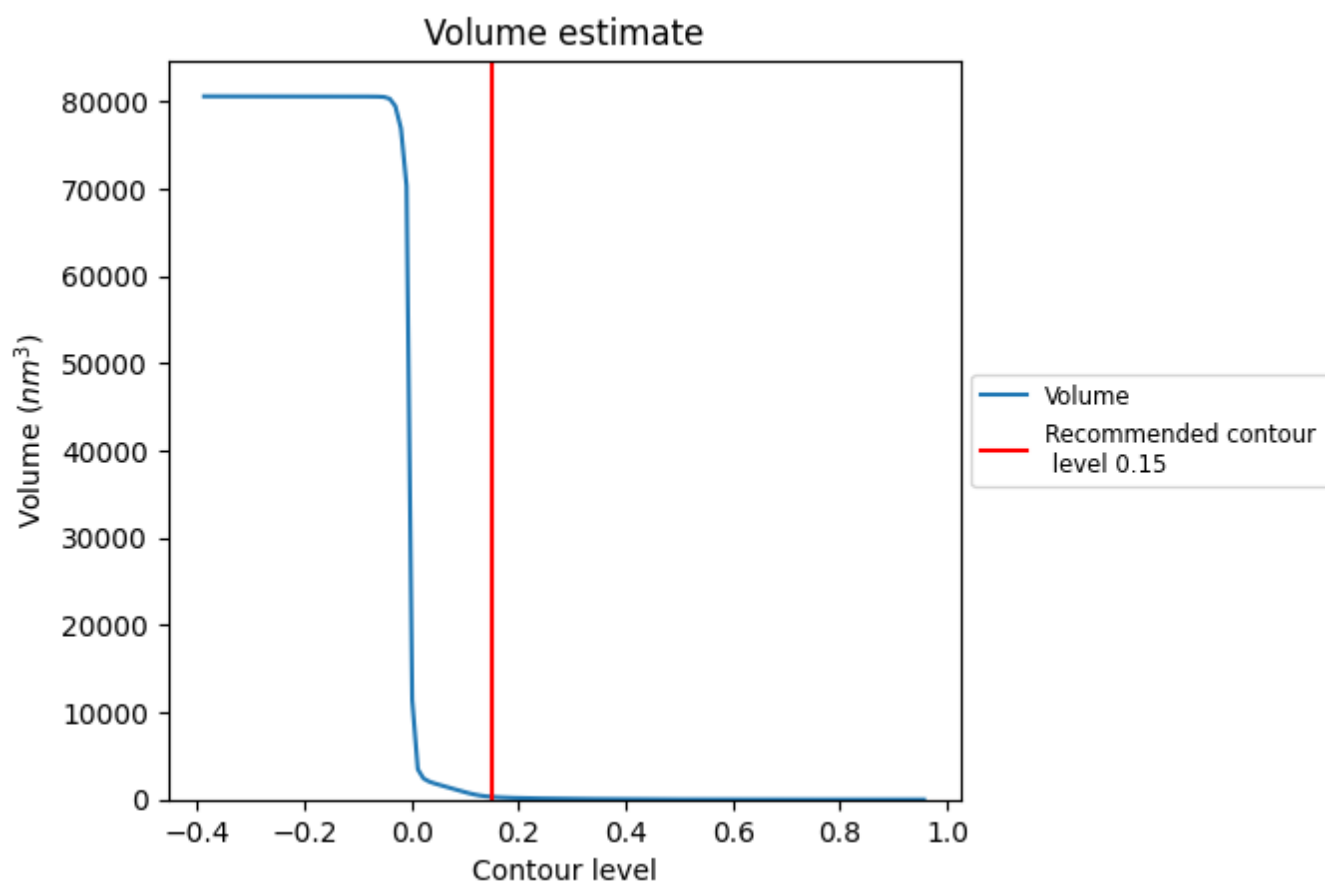
This section contains the results of statistical analysis of the map.

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.

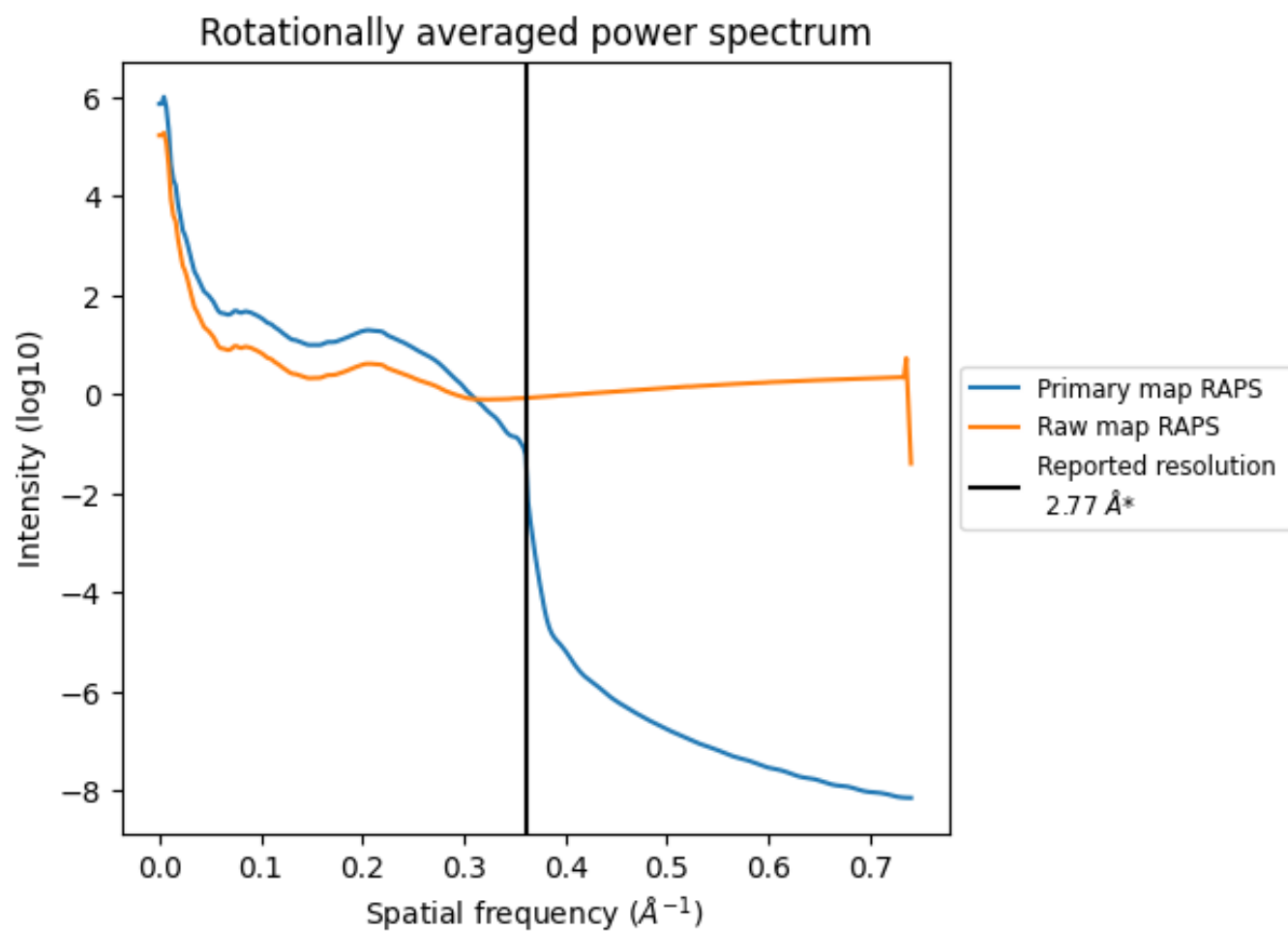
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; this corresponds to an approximate mass of 278 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 ⓘ

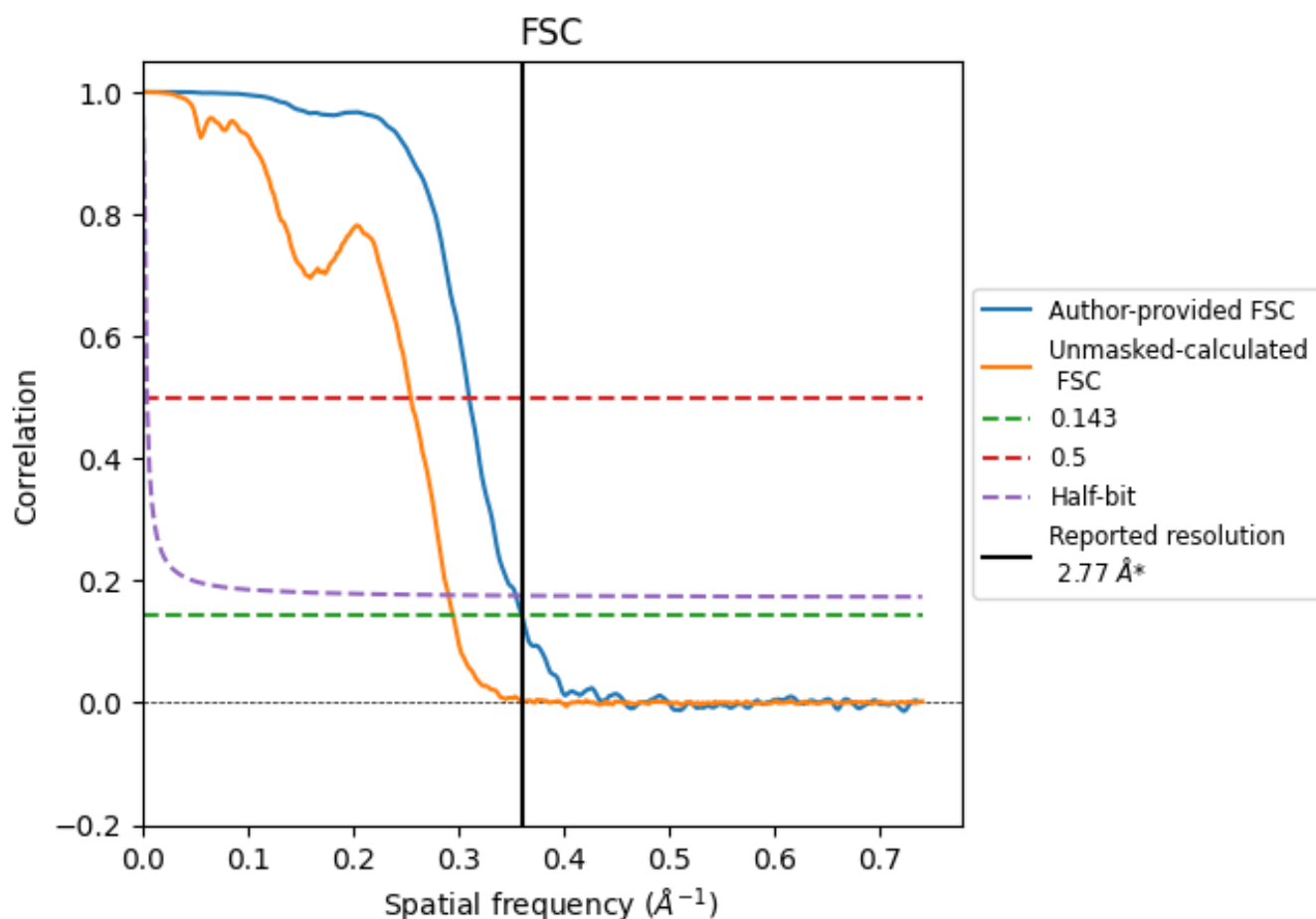


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.361 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

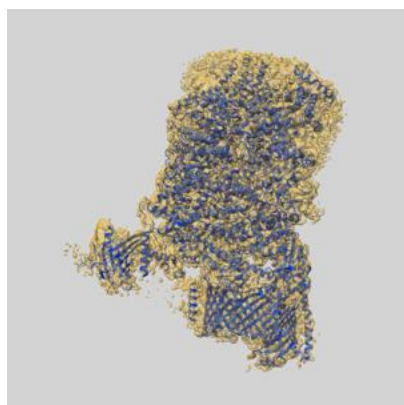
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.22	2.82
Unmasked-calculated*	3.39	3.92	3.44

*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 3.39 differs from the reported value 2.77 by more than 10 %

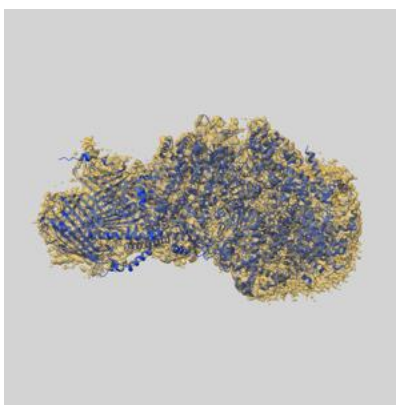
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33528 and PDB model 7XZI. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

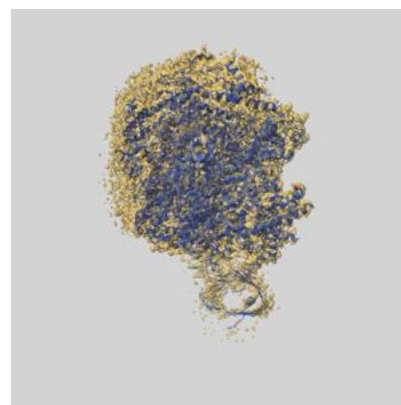
9.1 Map-model overlay [i](#)



X



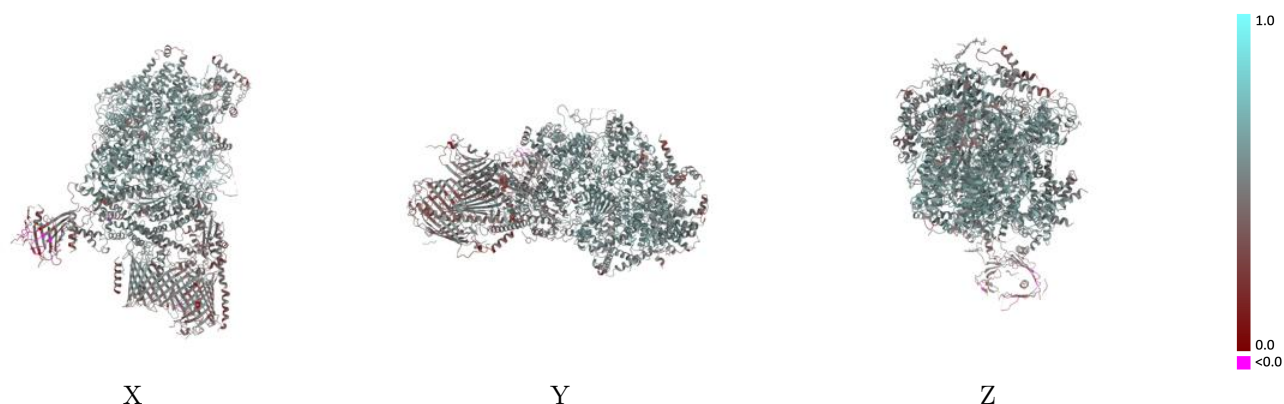
Y



Z

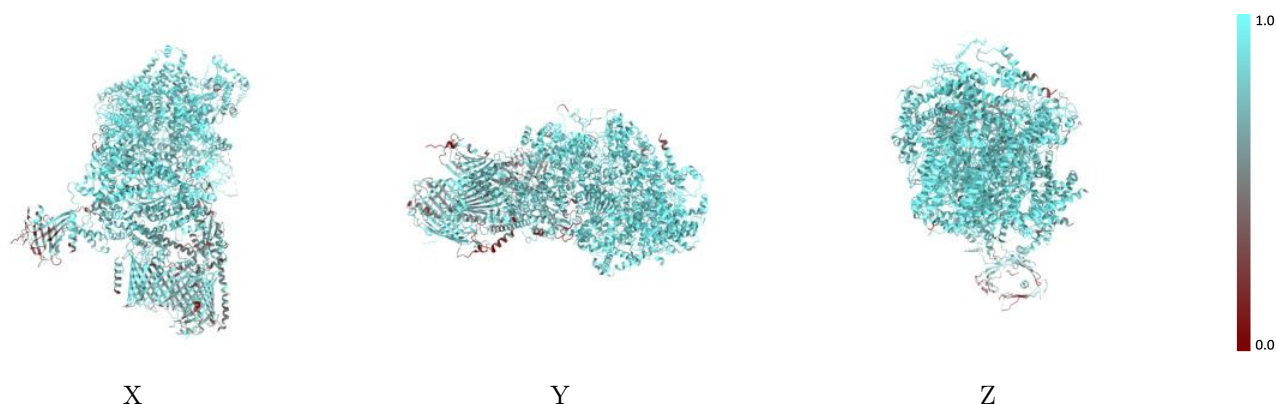
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



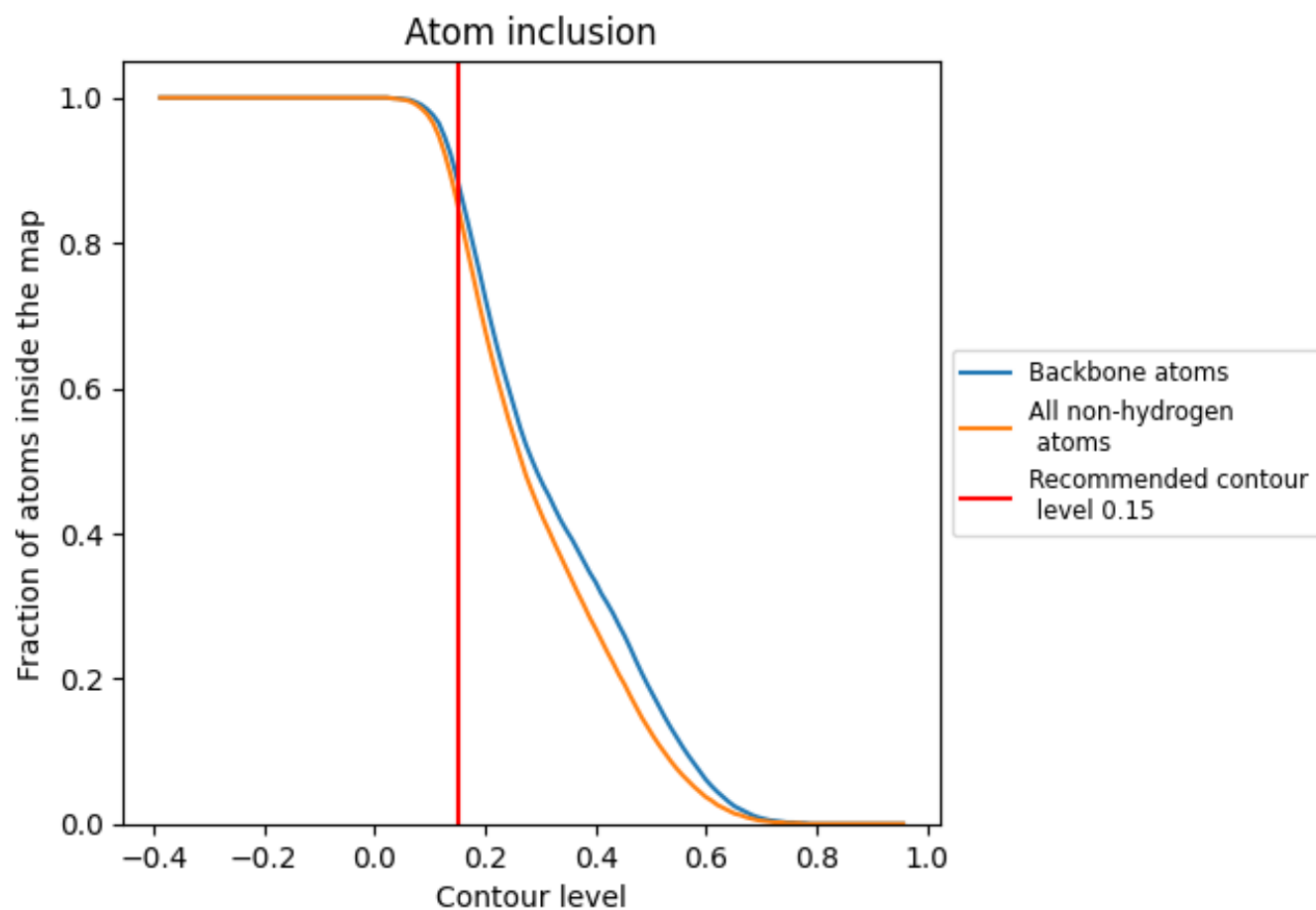
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8550	0.5170
3	0.8970	0.5330
4	0.6490	0.3700
5	0.9160	0.5440
7	0.7240	0.4460
9	0.7700	0.4760
A	0.8820	0.5400
B	0.9510	0.5620
C	0.9510	0.5850
D	0.8490	0.4460
E	0.9310	0.5610
F	0.9170	0.5670
G	0.6400	0.3790
U	0.8560	0.4860
X	0.6880	0.3600

1.0

0.0

<0.0