



Full wwPDB EM Validation Report ⓘ

Aug 16, 2026 – 01:16 AM JST

PDB ID : 9WV3 / pdb_00009wv3
EMDB ID : EMD-66281
Title : Human TOM complex with substrate Tim22-GGC1-sfGFP
Authors : Liu, X.L.; Cai, H.J.; Li, L.
Deposited on : 2025-09-19
Resolution : 2.98 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

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

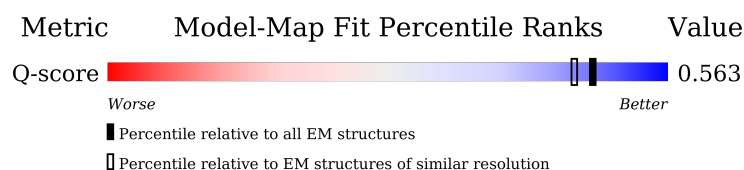
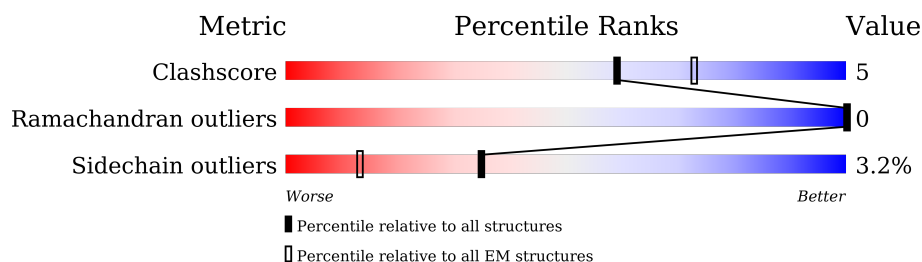
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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	13236 (2.48 - 3.48)

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

Mol	Chain	Length	Quality of chain
1	A	51	
1	B	51	
2	C	74	
2	D	74	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	55	16%82%11%7%
3	F	55	15%82%11%7%
4	G	142	6%34%.65%
4	H	142	.33%.65%
5	I	361	.67%12%.21%
5	J	361	.66%13%21%
6	K	300	.7%..92%
6	L	300	.7%.92%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8800 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 TOM5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	36	Total	C	N	O	S	0	0
			304	200	53	49	2		
1	B	36	Total	C	N	O	S	0	0
			304	200	53	49	2		

- Molecule 2 is a protein called Mitochondrial import receptor subunit TOM6 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	45	Total	C	N	O	S	0	0
			367	235	69	62	1		
2	D	45	Total	C	N	O	S	0	0
			367	235	69	62	1		

- Molecule 3 is a protein called Mitochondrial import receptor subunit TOM7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	51	Total	C	N	O	S	0	0
			409	272	70	66	1		
3	F	51	Total	C	N	O	S	0	0
			409	272	70	66	1		

- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	50	Total	C	N	O	S	0	0
			417	271	70	73	3		
4	H	50	Total	C	N	O	S	0	0
			417	271	70	73	3		

- Molecule 5 is a protein called Mitochondrial import receptor subunit TOM40 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	286	Total	C	N	O	S	0	0
			2189	1393	376	409	11		
5	J	286	Total	C	N	O	S	0	0
			2189	1393	376	409	11		

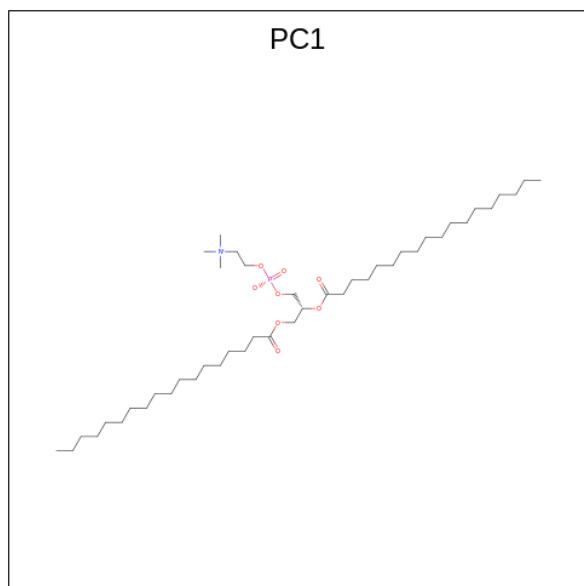
- Molecule 6 is a protein called Mitochondrial GTP/GDP carrier protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	25	Total	C	N	O	0	0
			187	129	28	30		
6	L	25	Total	C	N	O	0	0
			187	129	28	30		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	222	SER	CYS	engineered mutation	UNP P38988
L	222	SER	CYS	engineered mutation	UNP P38988

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



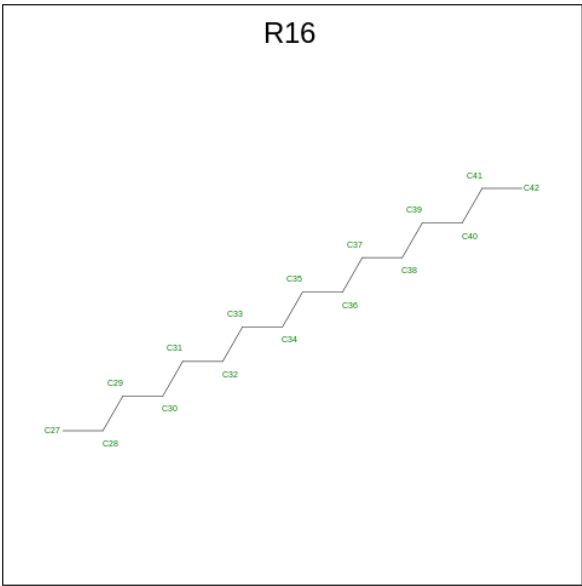
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
7	B	1	Total	C	N	O	P	0
			50	40	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total 44	C 35	O 8	P 1	0	
7	D	1	Total 44	C 35	O 8	P 1	0	
7	E	1	Total 31	C 22	N 1	O 7	P 1	0
7	E	1	Total 35	C 26	N 1	O 7	P 1	0
7	E	1	Total 33	C 23	N 1	O 8	P 1	0
7	F	1	Total 31	C 22	N 1	O 7	P 1	0
7	F	1	Total 35	C 26	N 1	O 7	P 1	0
7	F	1	Total 33	C 23	N 1	O 8	P 1	0
7	G	1	Total 44	C 34	N 1	O 8	P 1	0
7	G	1	Total 54	C 44	N 1	O 8	P 1	0
7	H	1	Total 44	C 34	N 1	O 8	P 1	0
7	I	1	Total 41	C 31	N 1	O 8	P 1	0
7	I	1	Total 40	C 30	N 1	O 8	P 1	0
7	I	1	Total 50	C 40	N 1	O 8	P 1	0
7	I	1	Total 35	C 25	N 1	O 8	P 1	0
7	J	1	Total 41	C 31	N 1	O 8	P 1	0
7	J	1	Total 50	C 40	N 1	O 8	P 1	0
7	J	1	Total 35	C 25	N 1	O 8	P 1	0
7	J	1	Total 40	C 30	N 1	O 8	P 1	0
7	K	1	Total 27	C 18	N 1	O 7	P 1	0
7	L	1	Total 27	C 18	N 1	O 7	P 1	0

- Molecule 8 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).

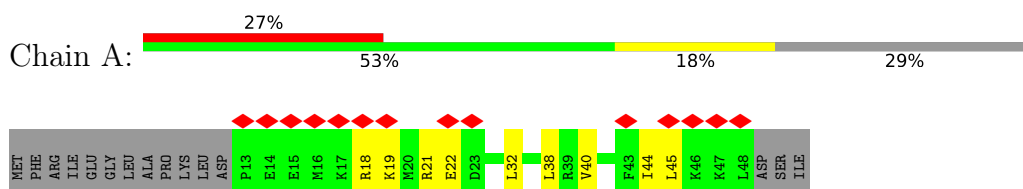


Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total	C	0
			12	12	
8	C	1	Total	C	0
			14	14	
8	C	1	Total	C	0
			16	16	
8	D	1	Total	C	0
			12	12	
8	D	1	Total	C	0
			16	16	
8	D	1	Total	C	0
			14	14	
8	E	1	Total	C	0
			16	16	
8	F	1	Total	C	0
			16	16	
8	I	1	Total	C	0
			12	12	
8	J	1	Total	C	0
			12	12	

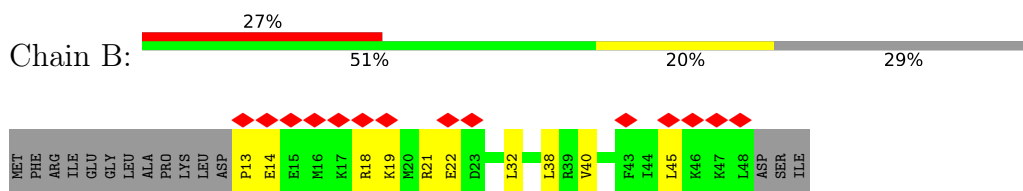
3 Residue-property plots [i](#)

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.

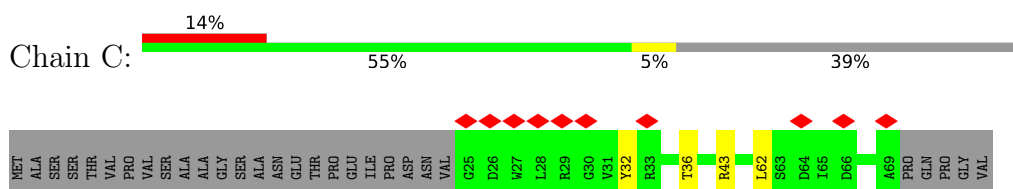
- Molecule 1: Mitochondrial import receptor subunit TOM5 homolog



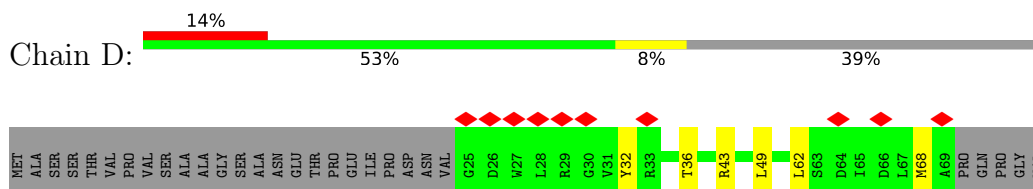
- Molecule 1: Mitochondrial import receptor subunit TOM5 homolog



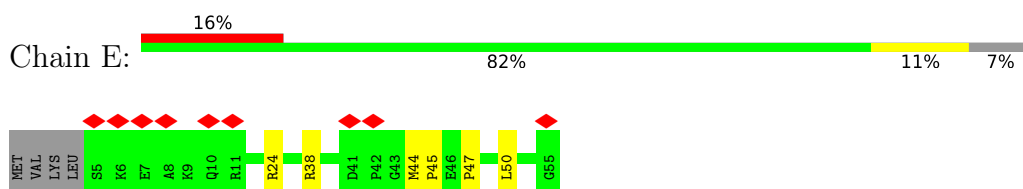
- Molecule 2: Mitochondrial import receptor subunit TOM6 homolog



- Molecule 2: Mitochondrial import receptor subunit TOM6 homolog



- Molecule 3: Mitochondrial import receptor subunit TOM7 homolog

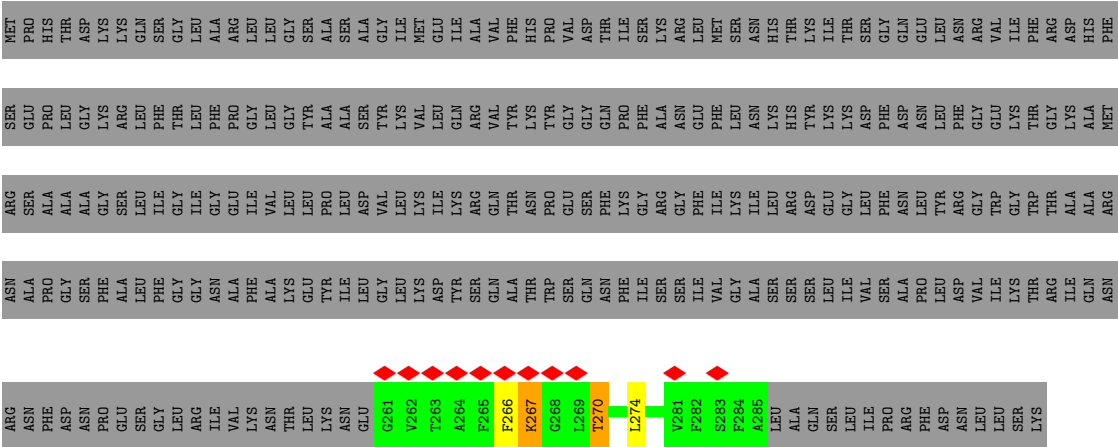


- | | | | |
|-----|-----|------|-----|
| ALA | THR | ALA | MET |
| THR | THR | THR | GLY |
| ALA | THR | THR | ASN |
| SER | SER | SER | VAL |
| ALA | SER | ALA | LEU |
| SER | GLY | ALA | ALA |
| ALA | ALA | SER | SER |
| ALA | ALA | GLU | PRO |
| GLU | GLU | GLU | PRO |
| ASP | ASP | GLY | ALA |
| GLY | GLY | ALA | GLY |
| ALA | ALA | ALA | PRO |
| CYS | CYS | GLY | PRO |
| GLY | GLY | C76 | PRO |
| | | | PRO |
| | | T82 | ALA |
| | | E85 | ALA |
| | | P95 | ALA |
| | | E99 | VAL |
| | | L103 | GLY |
| | | T104 | LEU |
| | | | LEU |
| | | L109 | VAL |
| | | | GLY |
| | | V115 | LEU |
| | | S122 | PRO |
| | | S127 | PRO |
| | | V133 | PRO |
| | | T138 | PRO |
| | | | LEU |
| | | L141 | GLY |
| | | S157 | GLY |
| | | G158 | SER |
| | | S159 | LEU |
| | | L160 | GLY |
| | | L178 | GLY |
| | | Q179 | THR |
| | | T180 | THR |
| | | Q181 | SER |
| | | K184 | ARG |
| | | | SER |
| | | N187 | SER |
| | | W188 | GLU |
| | | | THR |
| | | G206 | PRO |
| | | N207 | GLY |



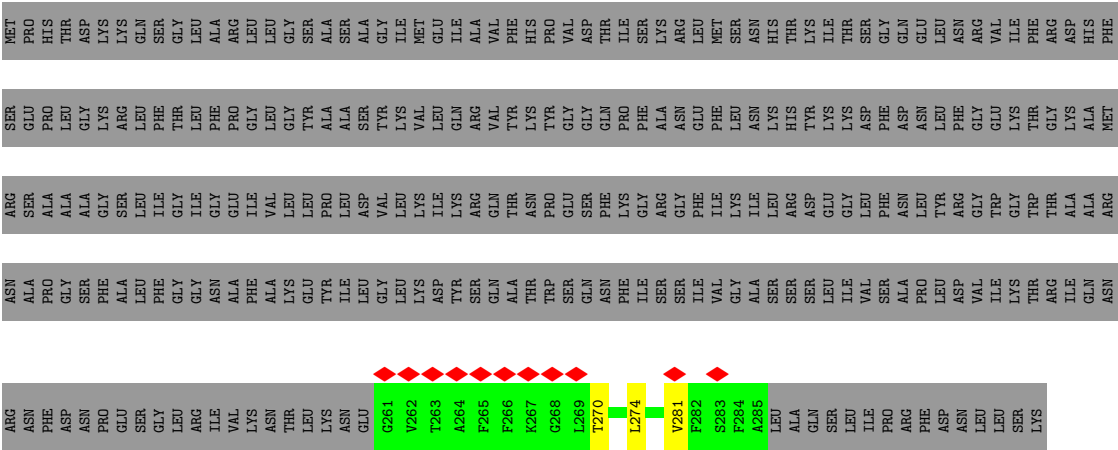
• Molecule 6: Mitochondrial GTP/GDP carrier protein 1

Chain K: 7% .. 92%



• Molecule 6: Mitochondrial GTP/GDP carrier protein 1

Chain L: 7% . 92%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	614218	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.739	Depositor
Minimum map value	-1.767	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	273.6, 273.6, 273.6	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95000005, 0.95000005, 0.95000005	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: PC1, R16

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/308	0.22	0/410
1	B	0.08	0/308	0.22	0/410
2	C	0.08	0/374	0.16	0/505
2	D	0.08	0/374	0.16	0/505
3	E	0.10	0/421	0.21	0/567
3	F	0.10	0/421	0.21	0/567
4	G	0.11	0/424	0.22	0/570
4	H	0.11	0/424	0.25	0/570
5	I	0.12	0/2239	0.26	0/3039
5	J	0.11	0/2239	0.26	0/3039
6	K	0.16	0/192	0.35	0/259
6	L	0.11	0/192	0.24	0/259
All	All	0.11	0/7916	0.24	0/10700

There are no bond length outliers.

There are no bond angle outliers.

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	A	304	0	339	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	304	0	339	6	0
2	C	367	0	363	2	0
2	D	367	0	363	5	0
3	E	409	0	423	4	0
3	F	409	0	423	5	0
4	G	417	0	428	1	0
4	H	417	0	428	4	0
5	I	2189	0	2171	27	0
5	J	2189	0	2171	26	0
6	K	187	0	202	3	0
6	L	187	0	202	1	0
7	A	50	0	77	1	0
7	B	50	0	77	1	0
7	C	44	0	64	0	0
7	D	44	0	64	0	0
7	E	99	0	135	4	0
7	F	99	0	135	3	0
7	G	98	0	153	3	0
7	H	44	0	65	1	0
7	I	166	0	231	3	0
7	J	166	0	231	3	0
7	K	27	0	34	0	0
7	L	27	0	34	0	0
8	C	42	0	84	0	0
8	D	42	0	84	0	0
8	E	16	0	34	0	0
8	F	16	0	34	1	0
8	I	12	0	23	0	0
8	J	12	0	23	0	0
All	All	8800	0	9434	84	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 5.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:ARG:NH2	7:J:401:PC1:O12	2.31	0.63
2:C:43:ARG:NH2	7:I:401:PC1:O12	2.32	0.61
1:A:18:ARG:HH22	1:A:22:GLU:HB2	1.65	0.60
1:B:18:ARG:HH22	1:B:22:GLU:HB2	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:115:VAL:HG12	5:I:133:VAL:HG12	1.86	0.58
7:G:202:PC1:H382	4:H:98:PRO:HG3	1.87	0.57
5:I:335:LEU:HD22	6:K:274:LEU:HD22	1.87	0.57
5:J:115:VAL:HG12	5:J:133:VAL:HG12	1.86	0.57
2:D:68:MET:HE2	4:H:106:LEU:HD22	1.86	0.56
3:F:47:PRO:HB3	5:J:109:LEU:HD23	1.89	0.55
5:I:95:PRO:HD2	5:I:317:SER:HB3	1.89	0.54
3:E:47:PRO:HB3	5:I:109:LEU:HD23	1.89	0.54
1:A:38:LEU:HD22	5:I:225:ILE:HD11	1.90	0.53
5:J:95:PRO:HD2	5:J:317:SER:HB3	1.90	0.53
5:J:225:ILE:HG13	5:J:231:LEU:HD12	1.91	0.52
5:J:312:LEU:HD11	5:J:328:LEU:HD11	1.90	0.52
5:J:335:LEU:HD22	6:L:274:LEU:HD22	1.92	0.52
5:I:103:LEU:HD11	5:I:360:ILE:HD11	1.92	0.51
1:A:32:LEU:HB3	7:A:101:PC1:H2E2	1.93	0.51
3:F:44:MET:HE3	3:F:45:PRO:HD2	1.92	0.51
1:B:32:LEU:HB3	7:B:101:PC1:H2E2	1.92	0.51
5:I:226:THR:HG22	5:I:229:LEU:HB3	1.93	0.51
5:I:312:LEU:HD11	5:I:328:LEU:HD11	1.93	0.50
5:J:160:LEU:HD23	5:J:178:ILE:HD11	1.93	0.50
5:I:160:LEU:HD23	5:I:178:ILE:HD11	1.93	0.50
5:J:103:LEU:HD11	5:J:360:ILE:HD11	1.91	0.50
5:I:206:GLY:N	5:I:216:ILE:O	2.45	0.50
5:J:226:THR:HG22	5:J:229:LEU:HB3	1.94	0.49
1:B:21:ARG:NH1	5:J:244:GLU:OE1	2.44	0.49
5:J:206:GLY:N	5:J:216:ILE:O	2.45	0.49
5:J:82:THR:HB	5:J:85:GLU:HG2	1.95	0.49
6:K:266:PHE:O	6:K:270:THR:OG1	2.29	0.48
1:A:21:ARG:NH1	5:I:244:GLU:OE1	2.44	0.48
5:J:271:HIS:HE1	5:J:287:GLU:HG3	1.78	0.48
2:D:32:TYR:O	2:D:36:THR:OG1	2.30	0.48
5:I:304:GLN:NE2	5:I:306:ASP:OD2	2.47	0.48
2:C:32:TYR:O	2:C:36:THR:OG1	2.30	0.48
3:E:44:MET:HE3	3:E:45:PRO:HD2	1.96	0.47
4:G:88:GLY:HA3	7:G:201:PC1:H292	1.97	0.47
4:H:88:GLY:HA3	7:H:201:PC1:H292	1.96	0.47
6:K:267:LYS:HA	6:K:267:LYS:HD2	1.59	0.46
3:E:38:ARG:HH22	5:I:138:THR:HB	1.80	0.46
3:E:24:ARG:HD2	5:I:180:THR:HG21	1.97	0.46
5:I:296:ASP:OD1	5:I:296:ASP:N	2.47	0.45
5:I:206:GLY:O	5:I:208:PRO:HD3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:206:GLY:O	5:J:208:PRO:HD3	2.16	0.45
5:I:91:LYS:HE3	5:I:91:LYS:HB3	1.76	0.45
5:J:304:GLN:NE2	5:J:306:ASP:OD2	2.49	0.45
5:J:296:ASP:N	5:J:296:ASP:OD1	2.49	0.45
5:I:104:THR:HB	5:I:359:THR:HG23	2.00	0.44
3:F:38:ARG:HH22	5:J:138:THR:HB	1.82	0.44
5:J:309:LYS:HE3	5:J:309:LYS:HB2	1.67	0.44
5:I:184:LYS:HB3	5:I:184:LYS:HE3	1.62	0.44
5:J:104:THR:HB	5:J:359:THR:HG23	2.00	0.44
7:E:101:PC1:H131	5:I:182:GLN:HB3	1.99	0.44
3:F:24:ARG:HD2	5:J:180:THR:HG21	1.99	0.44
2:D:68:MET:HE1	4:H:106:LEU:HD13	2.00	0.43
5:I:222:LEU:HD12	5:I:232:GLY:HA3	1.99	0.43
5:I:319:ASP:OD1	5:I:320:SER:N	2.52	0.43
5:I:187:ASN:OD1	5:I:188:TRP:N	2.51	0.43
5:J:187:ASN:OD1	5:J:188:TRP:N	2.52	0.43
5:J:319:ASP:OD1	5:J:320:SER:N	2.52	0.43
7:F:101:PC1:H121	7:J:404:PC1:H12	2.01	0.43
8:F:103:R16:H331	8:F:103:R16:H302	1.87	0.43
1:B:38:LEU:HD22	5:J:225:ILE:HD11	1.99	0.43
2:D:49:LEU:HD23	2:D:49:LEU:HA	1.88	0.43
1:A:19:LYS:HB3	1:A:19:LYS:HE2	1.81	0.42
7:E:104:PC1:H251	7:E:104:PC1:H222	1.82	0.42
5:I:271:HIS:HE1	5:I:287:GLU:HG3	1.85	0.42
7:I:405:PC1:H152	7:I:405:PC1:H111	1.85	0.42
5:J:184:LYS:HE2	5:J:184:LYS:HB2	1.80	0.42
1:B:13:PRO:HB2	1:B:14:GLU:H	1.66	0.42
7:E:104:PC1:H143	5:I:184:LYS:HG2	2.01	0.42
1:B:19:LYS:HB3	1:B:19:LYS:HE2	1.82	0.41
7:G:202:PC1:H143	7:G:202:PC1:H112	1.82	0.41
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.92	0.41
7:E:101:PC1:H121	7:I:402:PC1:H12	2.01	0.41
5:I:290:ALA:HB2	5:I:297:THR:HG23	2.02	0.41
5:J:159:SER:OG	5:J:181:GLN:O	2.32	0.41
5:I:225:ILE:HG13	5:I:231:LEU:HD12	2.02	0.41
5:J:99:GLU:OE2	5:J:122:SER:OG	2.34	0.41
7:J:401:PC1:H133	7:J:401:PC1:H111	1.78	0.41
7:F:104:PC1:H251	7:F:104:PC1:H222	1.81	0.41
3:F:46:GLU:HB3	7:F:102:PC1:H142	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	34/51 (67%)	33 (97%)	1 (3%)	0	100	100
1	B	34/51 (67%)	33 (97%)	1 (3%)	0	100	100
2	C	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
2	D	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
3	E	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
3	F	49/55 (89%)	47 (96%)	2 (4%)	0	100	100
4	G	48/142 (34%)	48 (100%)	0	0	100	100
4	H	48/142 (34%)	48 (100%)	0	0	100	100
5	I	284/361 (79%)	272 (96%)	12 (4%)	0	100	100
5	J	284/361 (79%)	272 (96%)	12 (4%)	0	100	100
6	K	23/300 (8%)	23 (100%)	0	0	100	100
6	L	23/300 (8%)	22 (96%)	1 (4%)	0	100	100
All	All	962/1966 (49%)	928 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	35/48 (73%)	32 (91%)	3 (9%)	10	34
1	B	35/48 (73%)	33 (94%)	2 (6%)	18	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	36/59 (61%)	35 (97%)	1 (3%)	38	69
2	D	36/59 (61%)	35 (97%)	1 (3%)	38	69
3	E	42/46 (91%)	41 (98%)	1 (2%)	43	72
3	F	42/46 (91%)	42 (100%)	0	100	100
4	G	46/115 (40%)	45 (98%)	1 (2%)	45	73
4	H	46/115 (40%)	46 (100%)	0	100	100
5	I	238/288 (83%)	231 (97%)	7 (3%)	37	68
5	J	238/288 (83%)	231 (97%)	7 (3%)	37	68
6	K	20/249 (8%)	18 (90%)	2 (10%)	7	27
6	L	20/249 (8%)	18 (90%)	2 (10%)	7	27
All	All	834/1610 (52%)	807 (97%)	27 (3%)	35	65

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	44	ILE
1	A	45	LEU
1	B	40	VAL
1	B	45	LEU
2	C	62	LEU
2	D	62	LEU
3	E	50	LEU
4	G	114	LEU
5	I	76	CYS
5	I	127	SER
5	I	157	SER
5	I	168	LEU
5	I	174	SER
5	I	180	THR
5	I	297	THR
5	J	76	CYS
5	J	127	SER
5	J	157	SER
5	J	180	THR
5	J	224	SER
5	J	286	VAL
5	J	297	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	K	267	LYS
6	K	270	THR
6	L	270	THR
6	L	281	VAL

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

Mol	Chain	Res	Type
5	I	283	GLN
5	I	346	ASN
5	J	223	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](#)

33 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	$\# Z > 2$
7	PC1	I	405	-	34,34,53	0.60	0	40,42,61	0.52	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PC1	J	402	-	49,49,53	0.50	0	55,57,61	0.47	1 (1%)
8	R16	C	101	-	11,11,15	0.24	0	10,10,14	0.21	0
7	PC1	D	104	-	43,43,53	0.62	1 (2%)	47,48,61	0.74	2 (4%)
7	PC1	G	201	-	43,43,53	0.54	0	49,51,61	0.49	1 (2%)
8	R16	J	405	-	11,11,15	0.24	0	10,10,14	0.17	0
8	R16	D	102	-	15,15,15	0.23	0	14,14,14	0.22	0
7	PC1	K	401	-	26,26,53	0.63	0	31,33,61	0.67	1 (3%)
7	PC1	A	101	-	49,49,53	0.50	0	55,57,61	0.48	1 (1%)
7	PC1	I	402	-	39,39,53	0.55	0	45,47,61	0.57	1 (2%)
7	PC1	F	102	-	34,34,53	0.54	0	39,41,61	0.75	2 (5%)
7	PC1	E	103	-	34,34,53	0.54	0	39,41,61	0.75	2 (5%)
8	R16	C	103	-	15,15,15	0.23	0	14,14,14	0.22	0
7	PC1	C	104	-	43,43,53	0.62	1 (2%)	47,48,61	0.74	2 (4%)
7	PC1	J	403	-	34,34,53	0.60	0	40,42,61	0.52	1 (2%)
7	PC1	H	201	-	43,43,53	0.54	0	49,51,61	0.49	1 (2%)
7	PC1	I	404	-	49,49,53	0.50	0	55,57,61	0.47	1 (1%)
7	PC1	I	401	-	40,40,53	0.56	0	46,48,61	0.51	1 (2%)
7	PC1	B	101	-	49,49,53	0.50	0	55,57,61	0.48	1 (1%)
7	PC1	L	401	-	26,26,53	0.63	0	31,33,61	0.67	1 (3%)
8	R16	I	403	-	11,11,15	0.24	0	10,10,14	0.18	0
7	PC1	F	101	-	30,30,53	0.59	0	35,37,61	0.64	1 (2%)
7	PC1	J	401	-	40,40,53	0.55	0	46,48,61	0.51	1 (2%)
7	PC1	E	104	-	32,32,53	0.62	0	38,40,61	0.56	1 (2%)
8	R16	D	101	-	11,11,15	0.24	0	10,10,14	0.21	0
8	R16	E	102	-	15,15,15	0.24	0	14,14,14	0.22	0
8	R16	F	103	-	15,15,15	0.24	0	14,14,14	0.22	0
7	PC1	E	101	-	30,30,53	0.59	0	35,37,61	0.64	1 (2%)
7	PC1	J	404	-	39,39,53	0.55	0	45,47,61	0.57	1 (2%)
8	R16	C	102	-	13,13,15	0.24	0	12,12,14	0.20	0
8	R16	D	103	-	13,13,15	0.24	0	12,12,14	0.20	0
7	PC1	G	202	-	53,53,53	0.49	0	59,61,61	0.45	1 (1%)
7	PC1	F	104	-	32,32,53	0.61	0	38,40,61	0.56	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
7	PC1	I	405	-	-	14/38/38/57	-
7	PC1	J	402	-	-	18/53/53/57	-
8	R16	C	101	-	-	0/9/9/13	-
7	PC1	D	104	-	-	12/45/45/57	-
7	PC1	G	201	-	-	13/47/47/57	-
8	R16	J	405	-	-	2/9/9/13	-
8	R16	D	102	-	-	2/13/13/13	-
7	PC1	K	401	-	-	13/29/29/57	-
7	PC1	A	101	-	-	21/53/53/57	-
7	PC1	I	402	-	-	17/43/43/57	-
7	PC1	F	102	-	-	17/37/37/57	-
7	PC1	E	103	-	-	18/37/37/57	-
8	R16	C	103	-	-	2/13/13/13	-
7	PC1	C	104	-	-	12/45/45/57	-
7	PC1	J	403	-	-	14/38/38/57	-
7	PC1	H	201	-	-	13/47/47/57	-
7	PC1	I	404	-	-	18/53/53/57	-
7	PC1	I	401	-	-	26/44/44/57	-
7	PC1	B	101	-	-	21/53/53/57	-
7	PC1	L	401	-	-	13/29/29/57	-
8	R16	I	403	-	-	2/9/9/13	-
7	PC1	F	101	-	-	16/33/33/57	-
7	PC1	J	401	-	-	26/44/44/57	-
7	PC1	E	104	-	-	19/36/36/57	-
8	R16	D	101	-	-	0/9/9/13	-
8	R16	E	102	-	-	1/13/13/13	-
8	R16	F	103	-	-	1/13/13/13	-
7	PC1	E	101	-	-	16/33/33/57	-
7	PC1	J	404	-	-	17/43/43/57	-
8	R16	C	102	-	-	3/11/11/13	-
8	R16	D	103	-	-	3/11/11/13	-
7	PC1	G	202	-	-	24/57/57/57	-
7	PC1	F	104	-	-	19/36/36/57	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	104	PC1	P-O13	2.79	1.65	1.54
7	C	104	PC1	P-O13	2.78	1.65	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	104	PC1	O12-P-O14	3.31	123.65	110.68
7	D	104	PC1	O12-P-O14	3.31	123.64	110.68
7	E	103	PC1	C2-O21-C21	2.42	123.76	117.79
7	F	102	PC1	C2-O21-C21	2.40	123.70	117.79
7	F	101	PC1	O12-P-O14	2.34	123.81	112.24
7	E	101	PC1	O12-P-O14	2.33	123.77	112.24
7	E	103	PC1	O12-P-O14	2.32	123.72	112.24
7	H	201	PC1	O12-P-O14	2.32	123.70	112.24
7	J	404	PC1	O12-P-O14	2.32	123.70	112.24
7	I	402	PC1	O12-P-O14	2.32	123.69	112.24
7	F	102	PC1	O12-P-O14	2.31	123.68	112.24
7	E	104	PC1	O12-P-O14	2.31	123.66	112.24
7	J	402	PC1	O12-P-O14	2.31	123.65	112.24
7	I	404	PC1	O12-P-O14	2.31	123.65	112.24
7	A	101	PC1	O12-P-O14	2.31	123.65	112.24
7	F	104	PC1	O12-P-O14	2.31	123.64	112.24
7	G	201	PC1	O12-P-O14	2.30	123.63	112.24
7	I	405	PC1	O12-P-O14	2.30	123.63	112.24
7	B	101	PC1	O12-P-O14	2.30	123.62	112.24
7	K	401	PC1	O12-P-O14	2.30	123.62	112.24
7	L	401	PC1	O12-P-O14	2.29	123.58	112.24
7	J	403	PC1	O12-P-O14	2.29	123.54	112.24
7	G	202	PC1	O12-P-O14	2.27	123.46	112.24
7	J	401	PC1	O12-P-O14	2.27	123.46	112.24
7	D	104	PC1	O13-P-O11	-2.26	100.71	106.73
7	I	401	PC1	O12-P-O14	2.25	123.38	112.24
7	C	104	PC1	O13-P-O11	-2.25	100.75	106.73

There are no chirality outliers.

All (413) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	101	PC1	C11-O13-P-O14
7	A	101	PC1	C1-O11-P-O12
7	B	101	PC1	C11-O13-P-O14
7	B	101	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	104	PC1	C1-O11-P-O12
7	C	104	PC1	C1-O11-P-O13
7	C	104	PC1	O22-C21-O21-C2
7	C	104	PC1	C22-C21-O21-C2
7	D	104	PC1	C1-O11-P-O12
7	D	104	PC1	C1-O11-P-O13
7	D	104	PC1	O22-C21-O21-C2
7	D	104	PC1	C22-C21-O21-C2
7	E	101	PC1	C11-O13-P-O14
7	E	101	PC1	C11-O13-P-O11
7	E	101	PC1	C1-O11-P-O13
7	E	103	PC1	C1-O11-P-O14
7	E	103	PC1	O21-C2-C3-O31
7	E	104	PC1	C11-O13-P-O12
7	E	104	PC1	C11-O13-P-O14
7	E	104	PC1	C11-O13-P-O11
7	E	104	PC1	O22-C21-O21-C2
7	E	104	PC1	C22-C21-O21-C2
7	F	101	PC1	C11-O13-P-O14
7	F	101	PC1	C11-O13-P-O11
7	F	101	PC1	C1-O11-P-O13
7	F	102	PC1	C1-O11-P-O14
7	F	102	PC1	O21-C2-C3-O31
7	F	104	PC1	C11-O13-P-O12
7	F	104	PC1	C11-O13-P-O14
7	F	104	PC1	C11-O13-P-O11
7	F	104	PC1	O22-C21-O21-C2
7	F	104	PC1	C22-C21-O21-C2
7	G	201	PC1	C11-O13-P-O12
7	G	201	PC1	C11-O13-P-O14
7	G	201	PC1	C11-O13-P-O11
7	G	202	PC1	C11-O13-P-O12
7	G	202	PC1	C11-O13-P-O14
7	G	202	PC1	C1-O11-P-O12
7	G	202	PC1	C1-O11-P-O14
7	G	202	PC1	C1-O11-P-O13
7	H	201	PC1	C11-O13-P-O12
7	H	201	PC1	C11-O13-P-O14
7	H	201	PC1	C11-O13-P-O11
7	I	401	PC1	C11-O13-P-O12
7	I	401	PC1	C11-O13-P-O14
7	I	401	PC1	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	I	401	PC1	C22-C21-O21-C2
7	I	402	PC1	C11-O13-P-O14
7	I	402	PC1	C1-O11-P-O14
7	I	402	PC1	O13-C11-C12-N
7	I	404	PC1	O13-C11-C12-N
7	I	404	PC1	O22-C21-O21-C2
7	I	405	PC1	C11-O13-P-O14
7	J	401	PC1	C11-O13-P-O12
7	J	401	PC1	C11-O13-P-O14
7	J	401	PC1	O13-C11-C12-N
7	J	401	PC1	C22-C21-O21-C2
7	J	402	PC1	O13-C11-C12-N
7	J	402	PC1	O22-C21-O21-C2
7	J	403	PC1	C11-O13-P-O14
7	J	404	PC1	C11-O13-P-O14
7	J	404	PC1	C1-O11-P-O14
7	J	404	PC1	O13-C11-C12-N
7	K	401	PC1	C11-O13-P-O12
7	K	401	PC1	C11-O13-P-O14
7	K	401	PC1	C11-O13-P-O11
7	K	401	PC1	C1-O11-P-O12
7	K	401	PC1	C1-O11-P-O14
7	K	401	PC1	C1-O11-P-O13
7	K	401	PC1	O13-C11-C12-N
7	L	401	PC1	C11-O13-P-O12
7	L	401	PC1	C11-O13-P-O14
7	L	401	PC1	C11-O13-P-O11
7	L	401	PC1	C1-O11-P-O12
7	L	401	PC1	C1-O11-P-O14
7	L	401	PC1	C1-O11-P-O13
7	L	401	PC1	O13-C11-C12-N
7	A	101	PC1	O32-C31-O31-C3
7	B	101	PC1	O32-C31-O31-C3
7	I	401	PC1	O32-C31-O31-C3
7	J	401	PC1	O32-C31-O31-C3
7	I	401	PC1	O22-C21-O21-C2
7	J	401	PC1	O22-C21-O21-C2
7	A	101	PC1	C32-C31-O31-C3
7	B	101	PC1	C32-C31-O31-C3
7	I	401	PC1	C32-C31-O31-C3
7	J	401	PC1	C32-C31-O31-C3
7	I	404	PC1	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	J	402	PC1	C22-C21-O21-C2
7	G	201	PC1	O32-C31-O31-C3
7	H	201	PC1	O32-C31-O31-C3
7	G	201	PC1	C32-C31-O31-C3
7	H	201	PC1	C32-C31-O31-C3
7	A	101	PC1	O21-C2-C3-O31
7	B	101	PC1	O21-C2-C3-O31
7	E	103	PC1	C27-C28-C29-C2A
7	F	102	PC1	C27-C28-C29-C2A
7	I	401	PC1	C21-C22-C23-C24
7	I	405	PC1	C21-C22-C23-C24
7	J	401	PC1	C21-C22-C23-C24
7	I	402	PC1	C21-C22-C23-C24
7	J	403	PC1	C21-C22-C23-C24
7	J	404	PC1	C21-C22-C23-C24
7	J	403	PC1	C31-C32-C33-C34
7	I	402	PC1	C22-C21-O21-C2
7	J	404	PC1	C22-C21-O21-C2
7	A	101	PC1	C1-O11-P-O13
7	B	101	PC1	C1-O11-P-O13
7	E	103	PC1	C1-O11-P-O13
7	E	104	PC1	C1-O11-P-O13
7	F	102	PC1	C1-O11-P-O13
7	F	104	PC1	C1-O11-P-O13
7	G	202	PC1	C11-O13-P-O11
7	I	401	PC1	C11-O13-P-O11
7	I	402	PC1	C1-O11-P-O13
7	I	404	PC1	C1-O11-P-O13
7	I	405	PC1	C11-O13-P-O11
7	J	401	PC1	C11-O13-P-O11
7	J	402	PC1	C1-O11-P-O13
7	J	403	PC1	C11-O13-P-O11
7	J	404	PC1	C1-O11-P-O13
7	I	405	PC1	C31-C32-C33-C34
7	I	402	PC1	O22-C21-O21-C2
7	J	404	PC1	O22-C21-O21-C2
7	C	104	PC1	C32-C31-O31-C3
7	D	104	PC1	C32-C31-O31-C3
8	C	102	R16	C35-C36-C37-C38
8	D	103	R16	C35-C36-C37-C38
7	G	201	PC1	C25-C26-C27-C28
7	G	202	PC1	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	G	202	PC1	C22-C23-C24-C25
7	G	202	PC1	C37-C38-C39-C3A
7	I	401	PC1	C3C-C3D-C3E-C3F
7	J	401	PC1	C3C-C3D-C3E-C3F
7	A	101	PC1	C24-C25-C26-C27
7	B	101	PC1	C24-C25-C26-C27
7	B	101	PC1	C35-C36-C37-C38
7	H	201	PC1	C25-C26-C27-C28
7	A	101	PC1	C2B-C2C-C2D-C2E
7	F	101	PC1	C2A-C2B-C2C-C2D
7	B	101	PC1	C2B-C2C-C2D-C2E
7	E	101	PC1	C2A-C2B-C2C-C2D
7	F	102	PC1	C25-C26-C27-C28
7	A	101	PC1	C35-C36-C37-C38
7	E	103	PC1	C25-C26-C27-C28
7	I	404	PC1	C39-C3A-C3B-C3C
7	J	402	PC1	C39-C3A-C3B-C3C
7	I	402	PC1	C32-C33-C34-C35
7	J	404	PC1	C32-C33-C34-C35
7	A	101	PC1	C25-C26-C27-C28
7	B	101	PC1	C25-C26-C27-C28
7	G	202	PC1	C25-C26-C27-C28
7	I	402	PC1	C31-C32-C33-C34
7	C	104	PC1	O32-C31-O31-C3
7	D	104	PC1	O32-C31-O31-C3
7	G	202	PC1	C34-C35-C36-C37
7	G	202	PC1	C27-C28-C29-C2A
7	I	401	PC1	C3E-C3F-C3G-C3H
7	J	404	PC1	C31-C32-C33-C34
7	G	202	PC1	C33-C34-C35-C36
7	J	401	PC1	C3E-C3F-C3G-C3H
7	C	104	PC1	C32-C33-C34-C35
7	D	104	PC1	C32-C33-C34-C35
7	J	401	PC1	C39-C3A-C3B-C3C
7	E	104	PC1	C11-C12-N-C15
7	I	401	PC1	C39-C3A-C3B-C3C
7	F	102	PC1	C24-C25-C26-C27
7	E	103	PC1	C24-C25-C26-C27
8	I	403	R16	C32-C33-C34-C35
7	J	402	PC1	C36-C37-C38-C39
8	J	405	R16	C32-C33-C34-C35
7	G	202	PC1	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	I	404	PC1	C36-C37-C38-C39
7	E	104	PC1	C11-C12-N-C13
7	I	401	PC1	C33-C34-C35-C36
7	A	101	PC1	C11-O13-P-O11
7	B	101	PC1	C11-O13-P-O11
7	E	103	PC1	O11-C1-C2-C3
7	F	102	PC1	O11-C1-C2-C3
7	G	202	PC1	O11-C1-C2-C3
7	J	401	PC1	C33-C34-C35-C36
7	L	401	PC1	C22-C21-O21-C2
7	A	101	PC1	C1-C2-C3-O31
7	B	101	PC1	C1-C2-C3-O31
7	I	405	PC1	C32-C33-C34-C35
7	I	404	PC1	C35-C36-C37-C38
7	J	403	PC1	C32-C33-C34-C35
7	J	402	PC1	C35-C36-C37-C38
7	J	402	PC1	C33-C34-C35-C36
7	E	104	PC1	C11-C12-N-C14
7	F	101	PC1	C11-C12-N-C15
7	F	104	PC1	C11-C12-N-C14
7	F	104	PC1	C11-C12-N-C15
7	C	104	PC1	C34-C35-C36-C37
7	I	401	PC1	C34-C35-C36-C37
7	I	401	PC1	C38-C39-C3A-C3B
7	I	404	PC1	C29-C2A-C2B-C2C
7	D	104	PC1	C34-C35-C36-C37
7	J	401	PC1	C34-C35-C36-C37
7	J	401	PC1	C38-C39-C3A-C3B
7	E	103	PC1	C23-C24-C25-C26
7	G	202	PC1	C29-C2A-C2B-C2C
7	I	404	PC1	C33-C34-C35-C36
7	J	402	PC1	C29-C2A-C2B-C2C
7	I	401	PC1	C3D-C3E-C3F-C3G
7	J	401	PC1	C3D-C3E-C3F-C3G
7	E	101	PC1	O11-C1-C2-C3
7	F	101	PC1	O11-C1-C2-C3
7	I	401	PC1	O11-C1-C2-C3
7	J	401	PC1	O11-C1-C2-C3
7	F	102	PC1	C23-C24-C25-C26
7	C	104	PC1	C33-C34-C35-C36
7	D	104	PC1	C33-C34-C35-C36
7	I	401	PC1	C3A-C3B-C3C-C3D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	E	101	PC1	C22-C23-C24-C25
7	I	401	PC1	C1-C2-C3-O31
7	I	404	PC1	C1-C2-C3-O31
7	J	401	PC1	C1-C2-C3-O31
7	J	402	PC1	C1-C2-C3-O31
7	G	202	PC1	C39-C3A-C3B-C3C
7	F	101	PC1	C22-C23-C24-C25
7	F	104	PC1	C11-C12-N-C13
7	F	101	PC1	C23-C24-C25-C26
7	J	401	PC1	C3A-C3B-C3C-C3D
7	I	401	PC1	O11-C1-C2-O21
7	J	401	PC1	O11-C1-C2-O21
7	E	101	PC1	C23-C24-C25-C26
7	I	404	PC1	C34-C35-C36-C37
7	I	401	PC1	O21-C2-C3-O31
7	I	405	PC1	O21-C2-C3-O31
7	J	401	PC1	O21-C2-C3-O31
7	J	402	PC1	C24-C25-C26-C27
7	E	101	PC1	C1-C2-C3-O31
7	F	101	PC1	C1-C2-C3-O31
7	A	101	PC1	C34-C35-C36-C37
7	L	401	PC1	O22-C21-O21-C2
7	E	101	PC1	C11-C12-N-C15
7	B	101	PC1	C34-C35-C36-C37
7	J	402	PC1	C34-C35-C36-C37
7	K	401	PC1	C22-C21-O21-C2
7	I	404	PC1	O11-C1-C2-C3
7	J	402	PC1	O11-C1-C2-C3
8	D	102	R16	C29-C30-C31-C32
7	I	404	PC1	C24-C25-C26-C27
8	C	103	R16	C29-C30-C31-C32
7	E	103	PC1	C1-C2-O21-C21
7	F	102	PC1	C1-C2-O21-C21
7	I	405	PC1	C1-C2-C3-O31
7	E	101	PC1	O11-C1-C2-O21
7	G	201	PC1	O11-C1-C2-O21
7	H	201	PC1	O11-C1-C2-O21
7	G	202	PC1	C28-C29-C2A-C2B
7	J	403	PC1	O21-C2-C3-O31
7	I	404	PC1	C32-C33-C34-C35
7	G	202	PC1	C3F-C3G-C3H-C3I
7	K	401	PC1	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	J	402	PC1	C32-C33-C34-C35
7	G	202	PC1	C2F-C2G-C2H-C2I
7	H	201	PC1	C24-C25-C26-C27
7	G	201	PC1	C24-C25-C26-C27
7	A	101	PC1	C2-C1-O11-P
7	B	101	PC1	C2-C1-O11-P
7	E	101	PC1	C2-C1-O11-P
7	A	101	PC1	C11-O13-P-O12
7	B	101	PC1	C11-O13-P-O12
7	E	101	PC1	C1-O11-P-O14
7	E	103	PC1	C1-O11-P-O12
7	E	104	PC1	C1-O11-P-O14
7	F	101	PC1	C1-O11-P-O14
7	F	102	PC1	C1-O11-P-O12
7	F	104	PC1	C1-O11-P-O14
7	I	402	PC1	C1-O11-P-O12
7	I	404	PC1	C1-O11-P-O14
7	I	405	PC1	C11-O13-P-O12
7	J	402	PC1	C1-O11-P-O14
7	J	403	PC1	C11-O13-P-O12
7	J	404	PC1	C1-O11-P-O12
7	G	202	PC1	C38-C39-C3A-C3B
7	J	402	PC1	C2B-C2C-C2D-C2E
7	G	201	PC1	O11-C1-C2-C3
7	H	201	PC1	O11-C1-C2-C3
7	I	404	PC1	C2B-C2C-C2D-C2E
7	B	101	PC1	C2A-C2B-C2C-C2D
7	A	101	PC1	O11-C1-C2-O21
7	B	101	PC1	O11-C1-C2-O21
7	E	103	PC1	O11-C1-C2-O21
7	F	101	PC1	O11-C1-C2-O21
7	F	102	PC1	O11-C1-C2-O21
7	I	404	PC1	O11-C1-C2-O21
7	J	402	PC1	O11-C1-C2-O21
7	A	101	PC1	C2A-C2B-C2C-C2D
7	A	101	PC1	O13-C11-C12-N
7	B	101	PC1	O13-C11-C12-N
7	G	201	PC1	O13-C11-C12-N
7	H	201	PC1	O13-C11-C12-N
7	I	404	PC1	O21-C2-C3-O31
7	J	402	PC1	O21-C2-C3-O31
7	F	101	PC1	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	G	201	PC1	C29-C2A-C2B-C2C
7	H	201	PC1	C29-C2A-C2B-C2C
7	C	104	PC1	C3-C2-O21-C21
7	D	104	PC1	C3-C2-O21-C21
7	I	402	PC1	C3-C2-O21-C21
7	J	404	PC1	C3-C2-O21-C21
7	I	405	PC1	C22-C23-C24-C25
7	C	104	PC1	C1-O11-P-O14
7	D	104	PC1	C1-O11-P-O14
7	K	401	PC1	C2-C1-O11-P
7	L	401	PC1	C2-C1-O11-P
7	J	403	PC1	C22-C23-C24-C25
7	E	101	PC1	C11-C12-N-C13
7	F	101	PC1	C11-C12-N-C13
7	G	202	PC1	C2B-C2C-C2D-C2E
7	I	401	PC1	C1-O11-P-O13
7	E	104	PC1	C1-C2-C3-O31
7	F	104	PC1	C1-C2-C3-O31
7	J	403	PC1	C1-C2-C3-O31
7	E	103	PC1	C11-C12-N-C14
7	F	102	PC1	C11-C12-N-C14
7	E	104	PC1	C32-C31-O31-C3
7	F	104	PC1	C32-C31-O31-C3
7	G	201	PC1	C2D-C2E-C2F-C2G
7	F	102	PC1	C26-C27-C28-C29
7	E	104	PC1	O11-C1-C2-O21
7	F	104	PC1	O11-C1-C2-O21
7	E	103	PC1	C26-C27-C28-C29
7	F	101	PC1	C11-C12-N-C14
7	I	405	PC1	C33-C34-C35-C36
7	H	201	PC1	C2D-C2E-C2F-C2G
7	F	104	PC1	O32-C31-O31-C3
7	E	101	PC1	C11-C12-N-C14
7	J	401	PC1	C11-C12-N-C13
7	E	104	PC1	O32-C31-O31-C3
7	I	402	PC1	C11-O13-P-O11
7	J	404	PC1	C11-O13-P-O11
7	F	101	PC1	C25-C26-C27-C28
7	J	403	PC1	C33-C34-C35-C36
7	J	404	PC1	C24-C25-C26-C27
7	I	402	PC1	C24-C25-C26-C27
7	J	401	PC1	C11-C12-N-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	E	101	PC1	C25-C26-C27-C28
7	F	102	PC1	C11-C12-N-C15
7	L	401	PC1	C22-C23-C24-C25
7	E	103	PC1	C2F-C2G-C2H-C2I
7	K	401	PC1	C22-C23-C24-C25
7	F	102	PC1	C2F-C2G-C2H-C2I
7	J	404	PC1	C37-C38-C39-C3A
7	I	402	PC1	C37-C38-C39-C3A
7	G	202	PC1	C3C-C3D-C3E-C3F
7	E	104	PC1	C21-C22-C23-C24
7	F	104	PC1	C21-C22-C23-C24
7	E	103	PC1	C11-C12-N-C15
7	I	401	PC1	C11-C12-N-C13
7	A	101	PC1	O11-C1-C2-C3
7	B	101	PC1	O11-C1-C2-C3
8	D	102	R16	C30-C31-C32-C33
8	C	103	R16	C30-C31-C32-C33
7	E	101	PC1	O21-C2-C3-O31
7	F	101	PC1	O21-C2-C3-O31
7	J	403	PC1	O21-C21-C22-C23
8	E	102	R16	C32-C33-C34-C35
7	I	405	PC1	O21-C21-C22-C23
8	F	103	R16	C32-C33-C34-C35
7	J	401	PC1	C1-O11-P-O13
7	I	401	PC1	C11-C12-N-C15
7	J	401	PC1	C11-C12-N-C14
7	E	104	PC1	C22-C23-C24-C25
7	F	104	PC1	C22-C23-C24-C25
7	H	201	PC1	C2-C1-O11-P
7	J	404	PC1	C26-C27-C28-C29
8	J	405	R16	C29-C30-C31-C32
7	E	104	PC1	O31-C31-C32-C33
7	I	402	PC1	C26-C27-C28-C29
8	I	403	R16	C29-C30-C31-C32
7	F	104	PC1	O31-C31-C32-C33
7	K	401	PC1	O21-C21-C22-C23
7	F	104	PC1	C25-C26-C27-C28
7	E	104	PC1	C25-C26-C27-C28
8	D	103	R16	C31-C32-C33-C34
7	G	201	PC1	C2-C1-O11-P
8	C	102	R16	C31-C32-C33-C34
7	L	401	PC1	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	I	401	PC1	C11-C12-N-C14
7	D	104	PC1	C3A-C3B-C3C-C3D
7	B	101	PC1	C38-C39-C3A-C3B
7	I	405	PC1	O22-C21-C22-C23
7	J	403	PC1	C24-C25-C26-C27
7	J	403	PC1	O22-C21-C22-C23
7	L	401	PC1	O22-C21-C22-C23
7	C	104	PC1	C3A-C3B-C3C-C3D
7	I	405	PC1	O22-C21-O21-C2
7	G	202	PC1	C21-C22-C23-C24
7	J	404	PC1	C33-C34-C35-C36
7	A	101	PC1	C38-C39-C3A-C3B
7	I	402	PC1	C33-C34-C35-C36
7	I	405	PC1	C24-C25-C26-C27
7	I	401	PC1	C1-O11-P-O14
7	J	401	PC1	C1-O11-P-O14
8	C	102	R16	C30-C31-C32-C33
8	D	103	R16	C30-C31-C32-C33
7	A	101	PC1	C12-C11-O13-P
7	B	101	PC1	C12-C11-O13-P
7	E	103	PC1	C12-C11-O13-P
7	F	102	PC1	C12-C11-O13-P
7	E	103	PC1	C11-C12-N-C13
7	F	102	PC1	C11-C12-N-C13
7	I	402	PC1	C39-C3A-C3B-C3C
7	J	404	PC1	C39-C3A-C3B-C3C
7	F	104	PC1	O32-C31-C32-C33
7	E	104	PC1	O32-C31-C32-C33
7	J	403	PC1	O22-C21-O21-C2
7	K	401	PC1	O22-C21-C22-C23
7	E	103	PC1	C2B-C2C-C2D-C2E

There are no ring outliers.

16 monomers are involved in 18 short contacts:

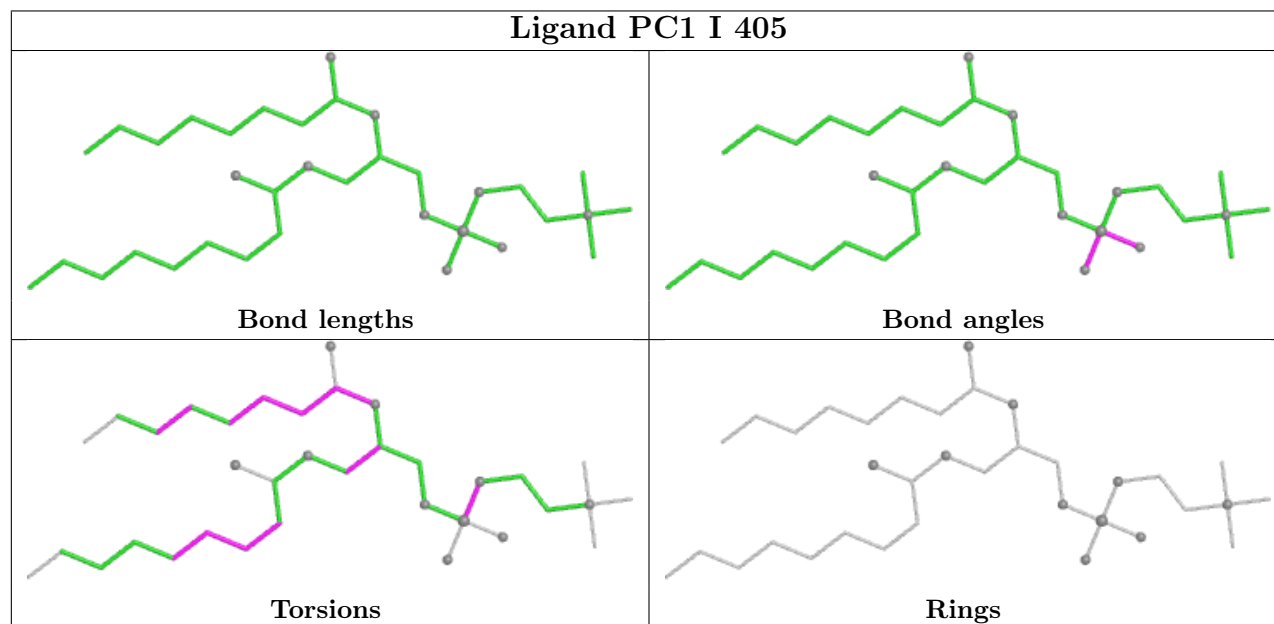
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	405	PC1	1	0
7	G	201	PC1	1	0
7	A	101	PC1	1	0
7	I	402	PC1	1	0
7	F	102	PC1	1	0
7	H	201	PC1	1	0

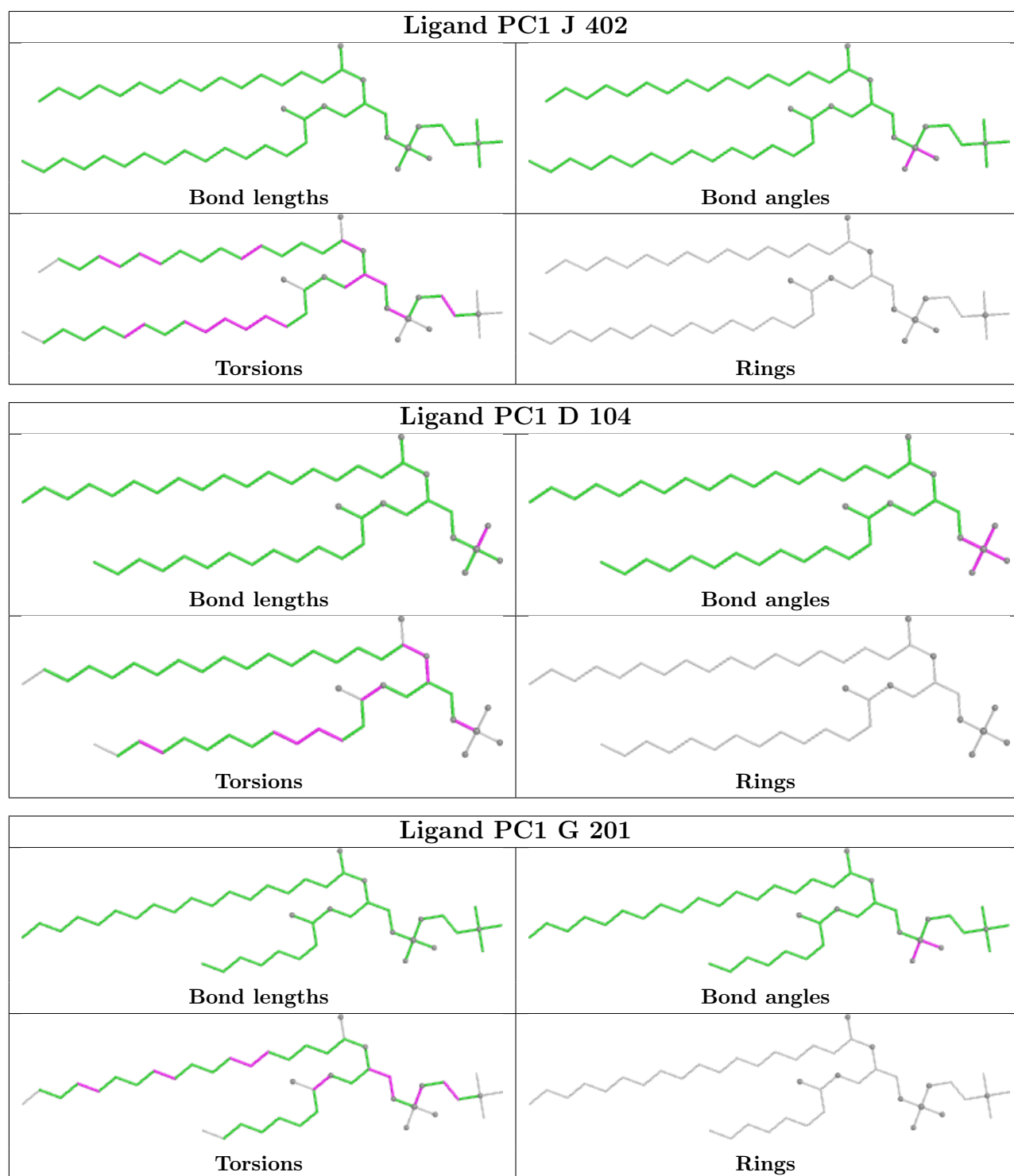
Continued on next page...

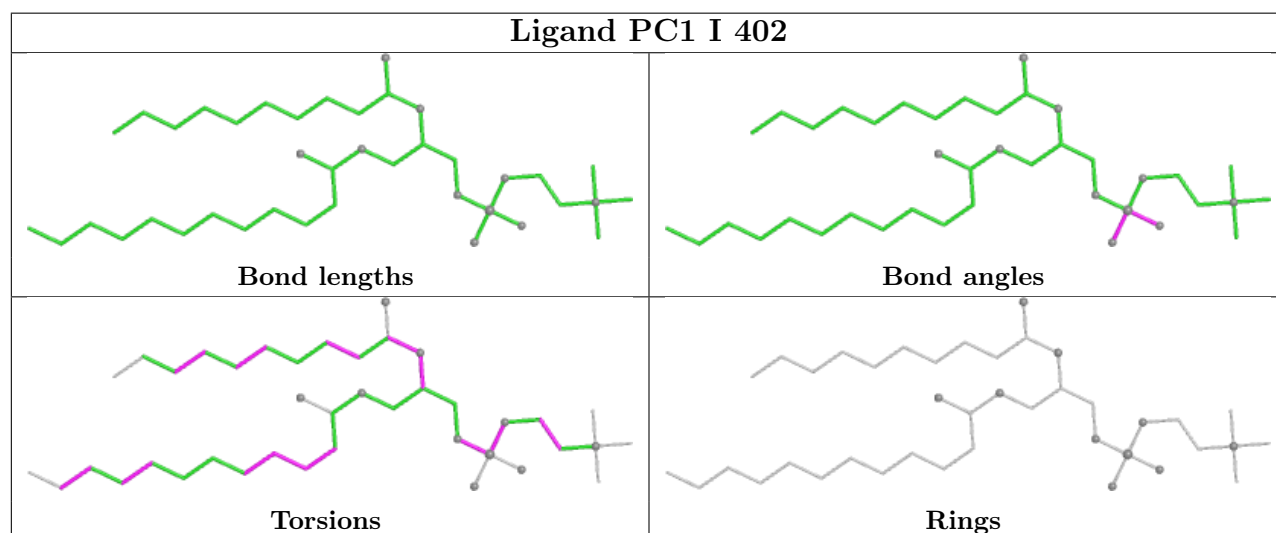
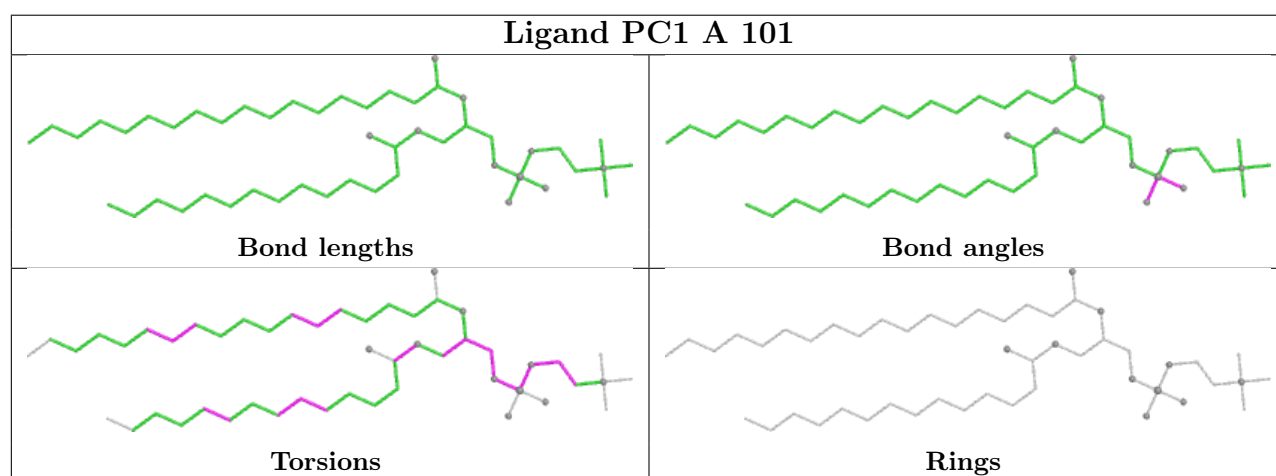
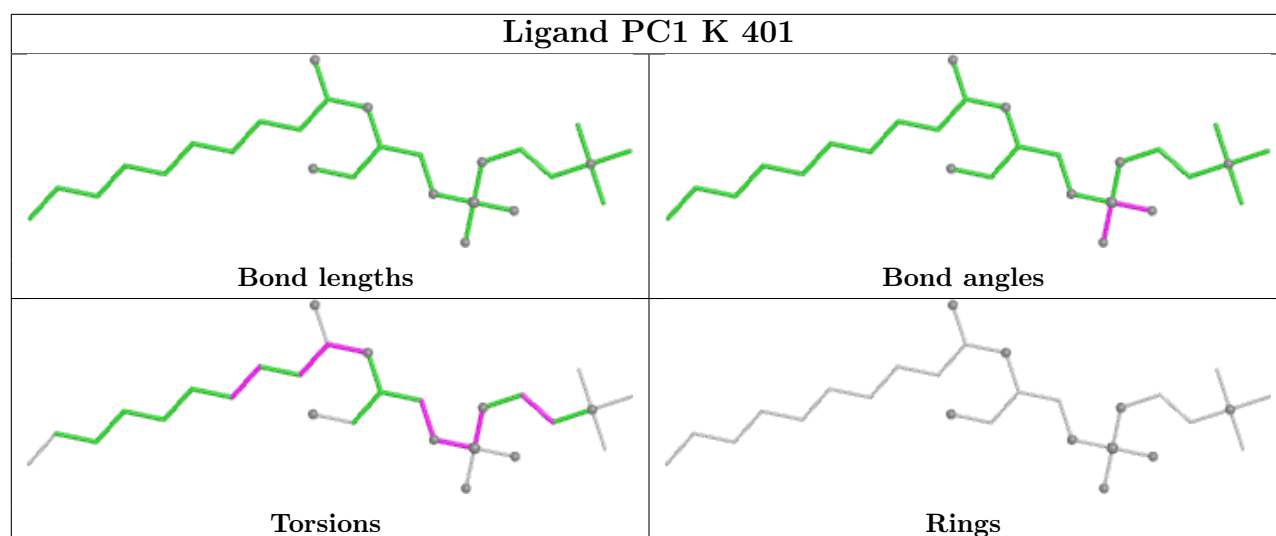
Continued from previous page...

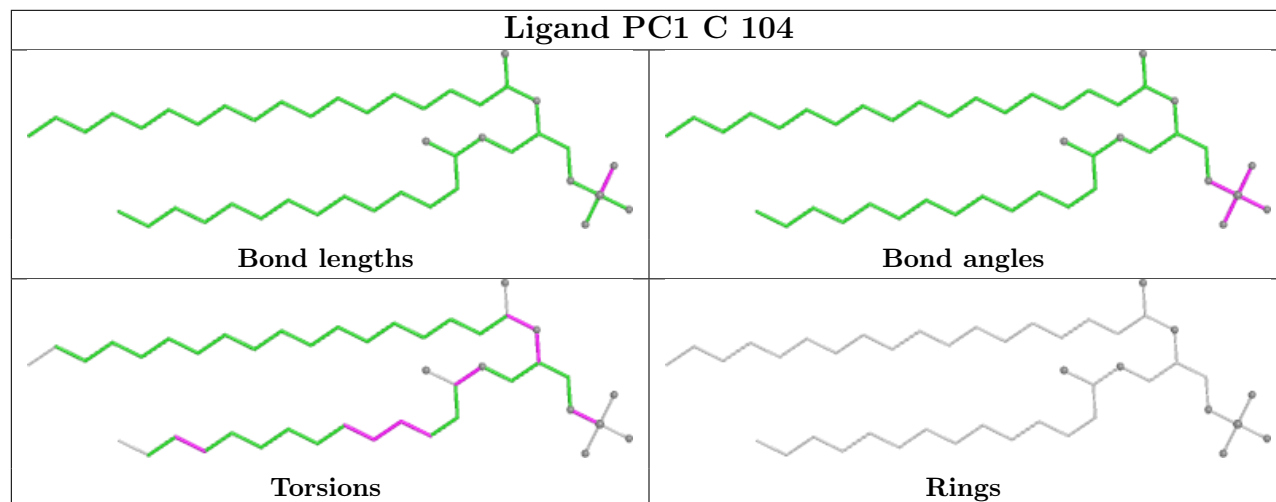
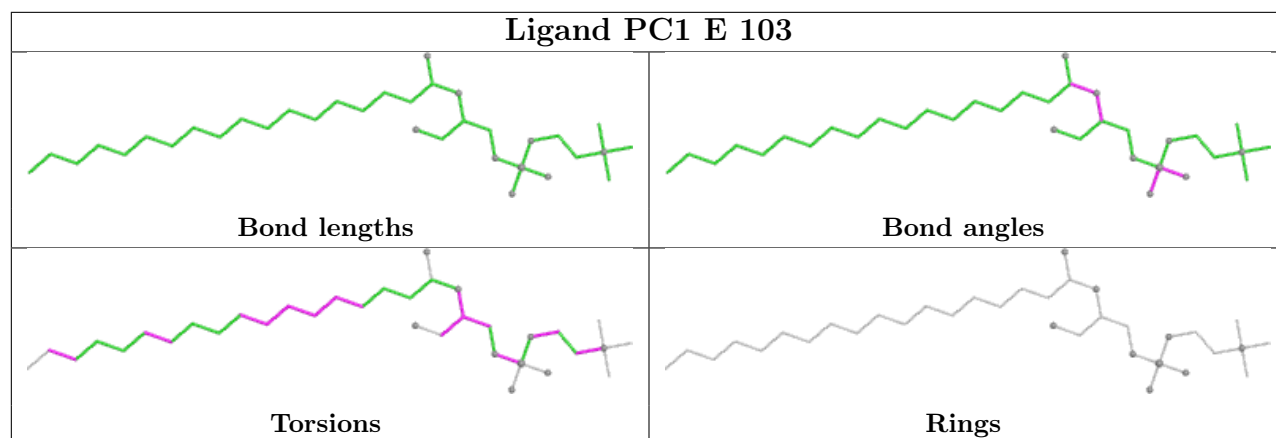
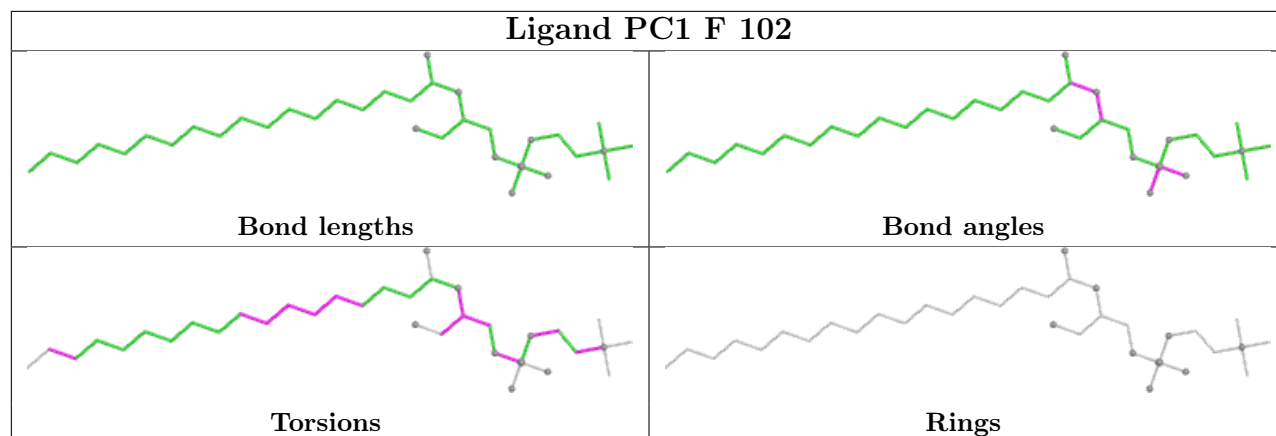
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	401	PC1	1	0
7	B	101	PC1	1	0
7	F	101	PC1	1	0
7	J	401	PC1	2	0
7	E	104	PC1	2	0
8	F	103	R16	1	0
7	E	101	PC1	2	0
7	J	404	PC1	1	0
7	G	202	PC1	2	0
7	F	104	PC1	1	0

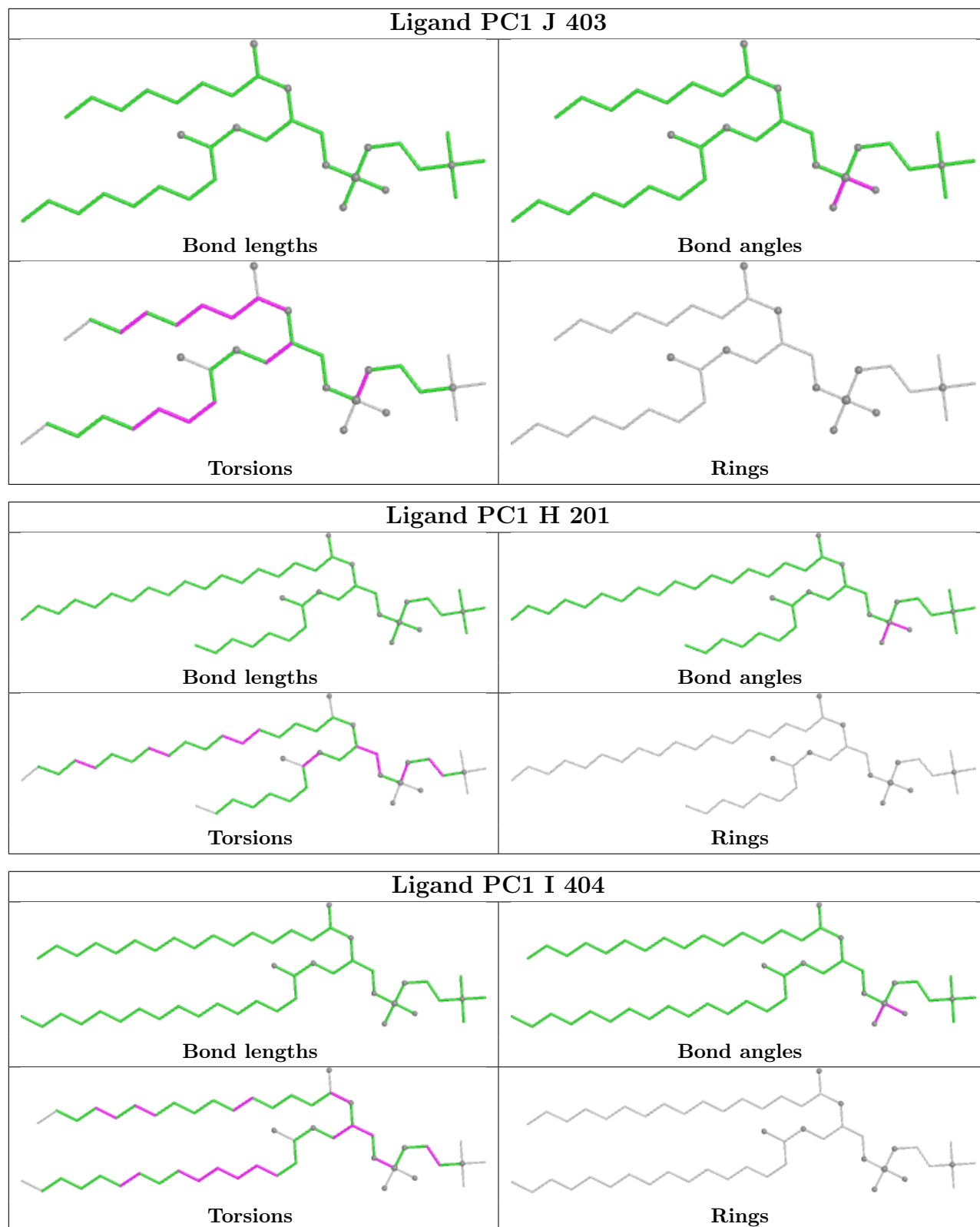
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

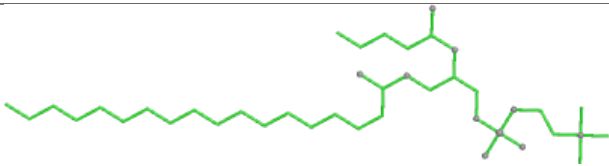
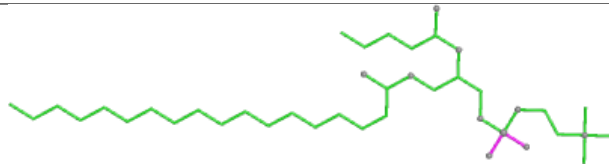
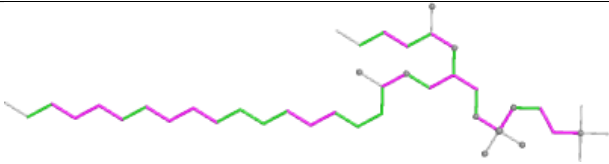
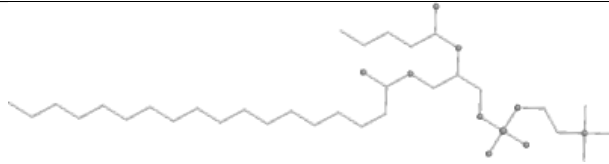
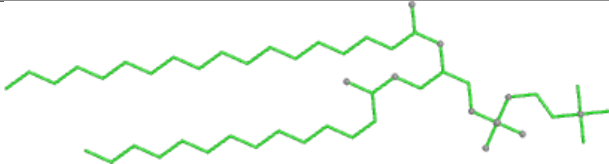
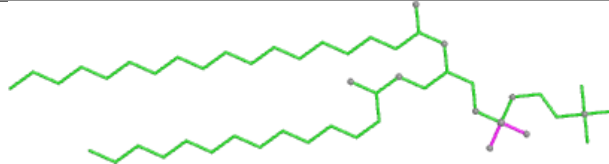
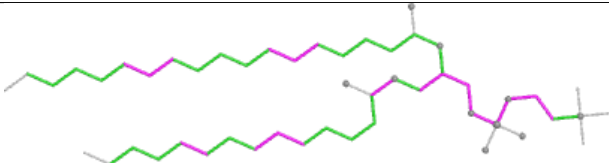
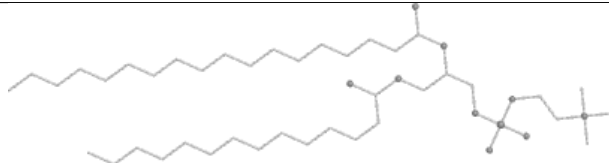
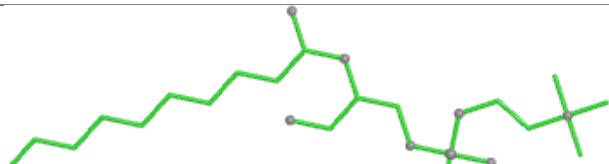
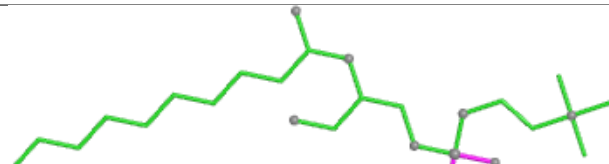
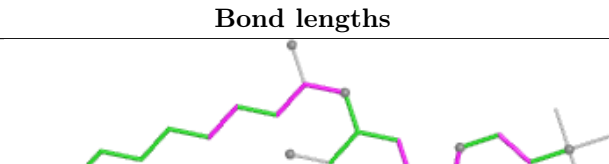
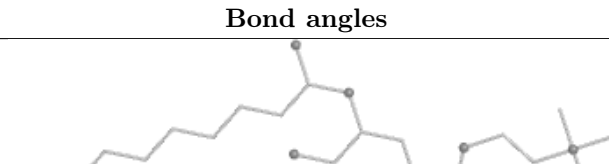


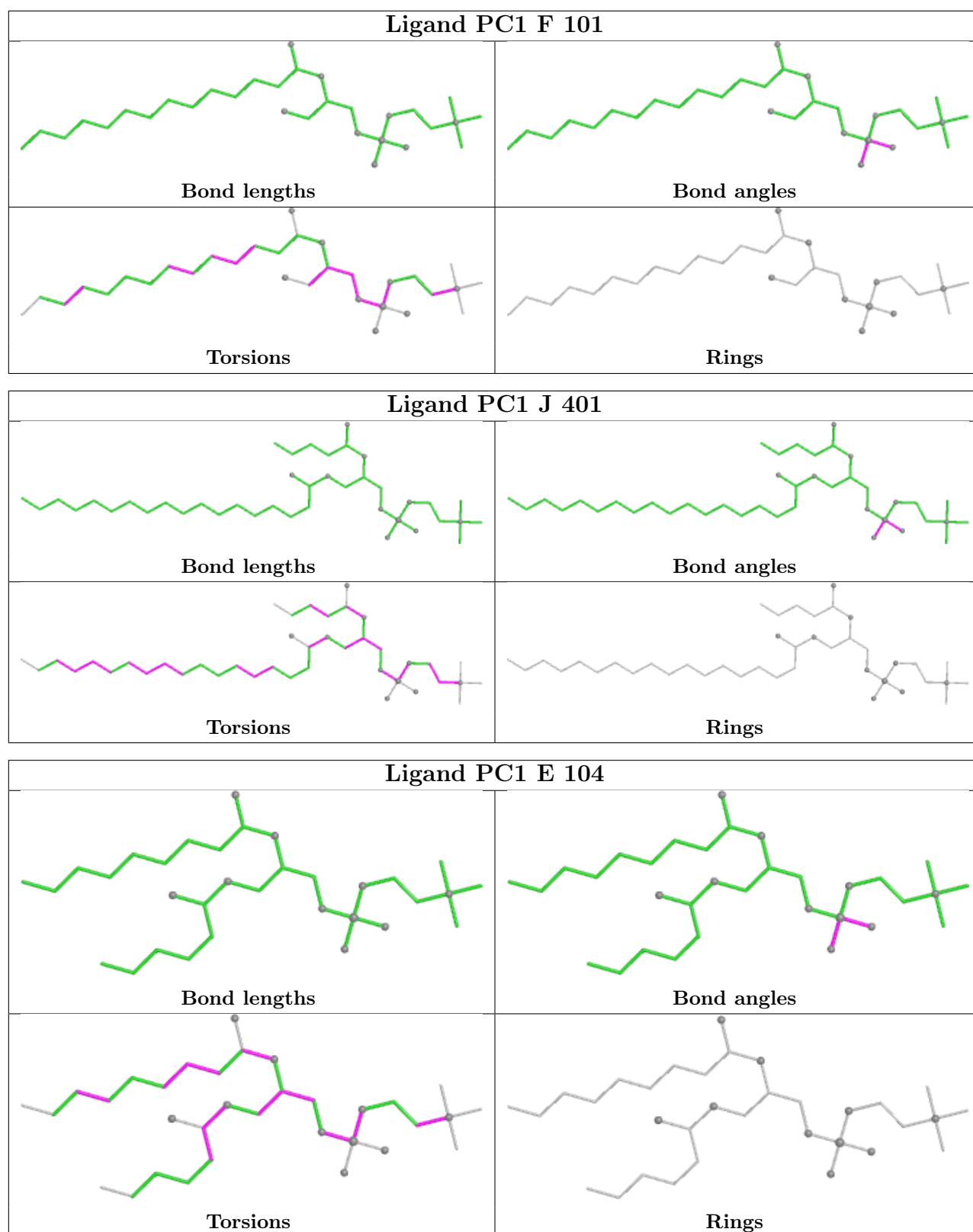


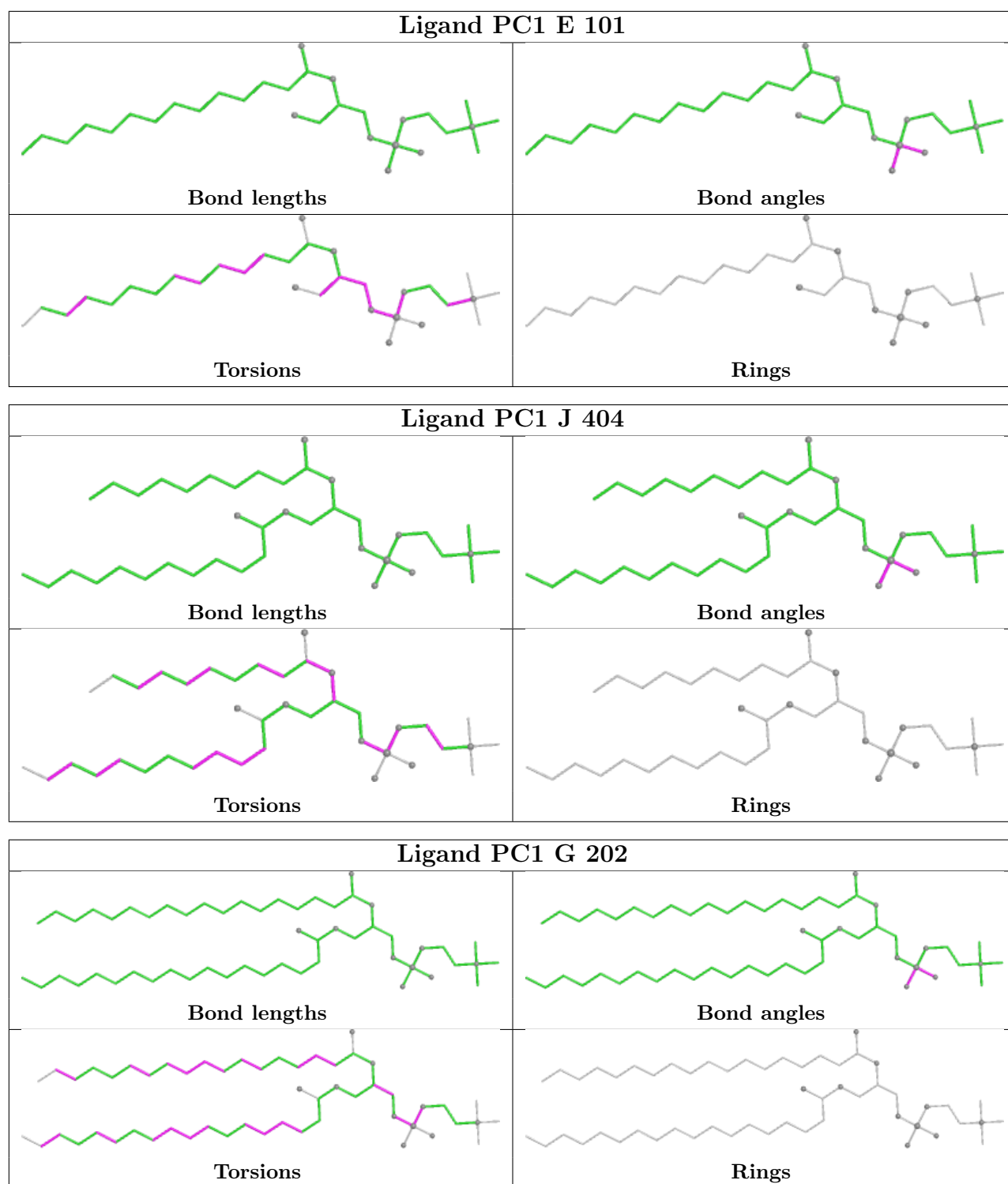


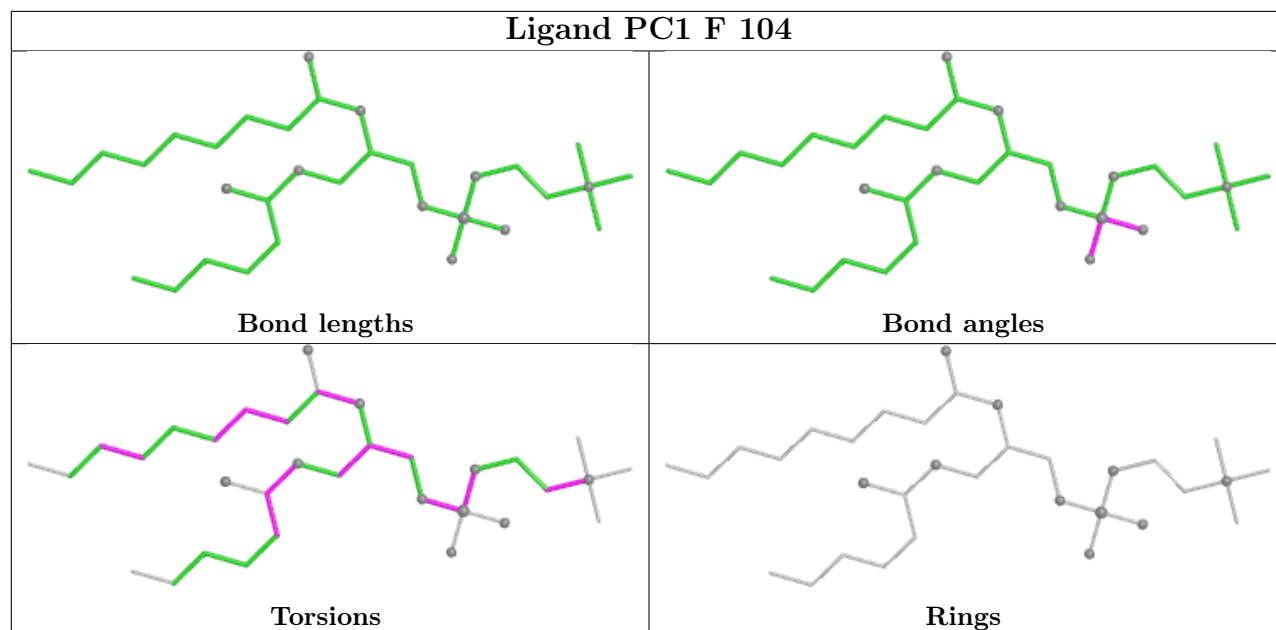




Ligand PC1 I 401	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 B 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 L 401	
 Bond lengths	 Bond angles
 Torsions	 Rings







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.

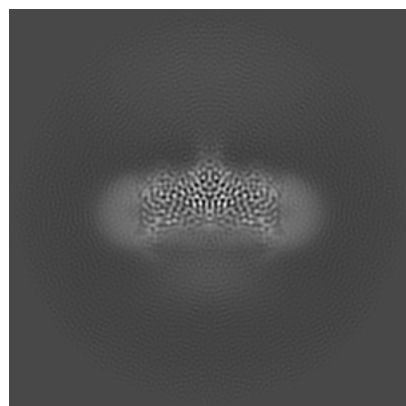
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66281. These allow visual inspection of the internal detail of the map and identification of artifacts.

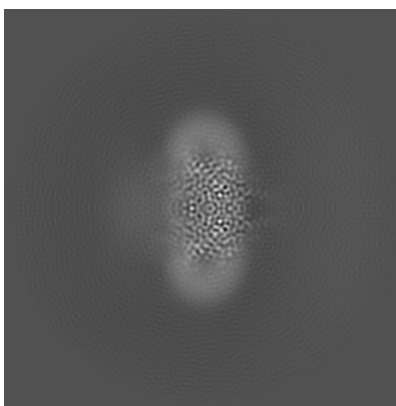
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

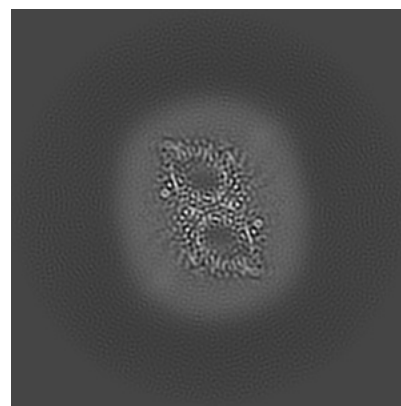
6.1.1 Primary map



X

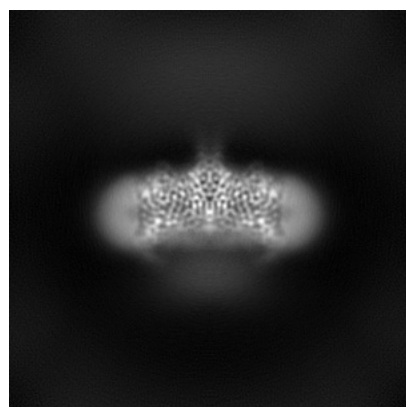


Y

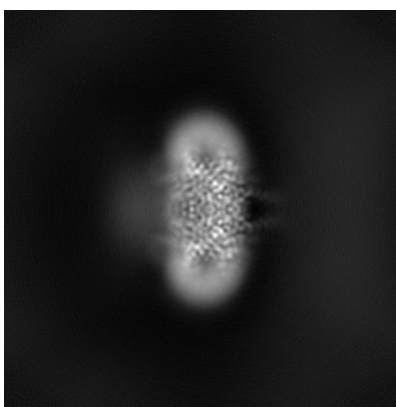


Z

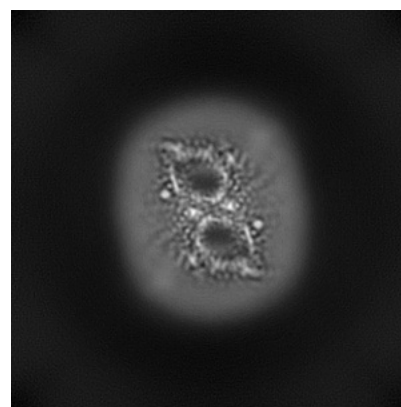
6.1.2 Raw map



X



Y

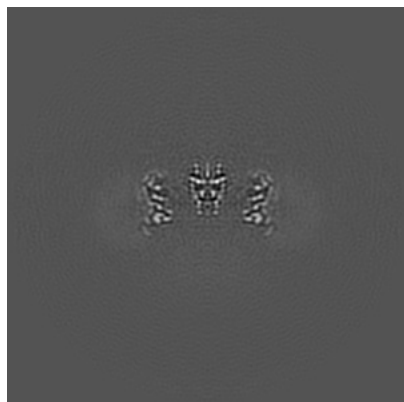


Z

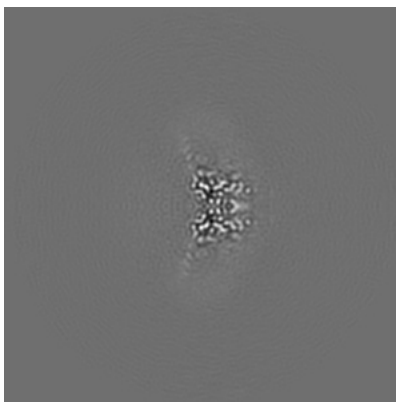
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

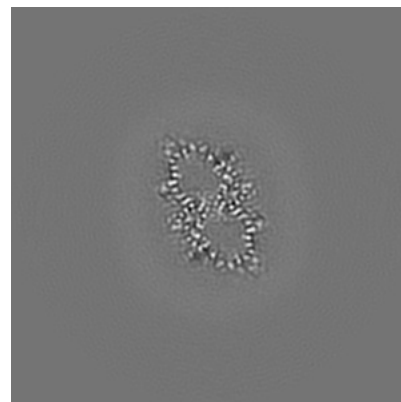
6.2.1 Primary map



X Index: 144

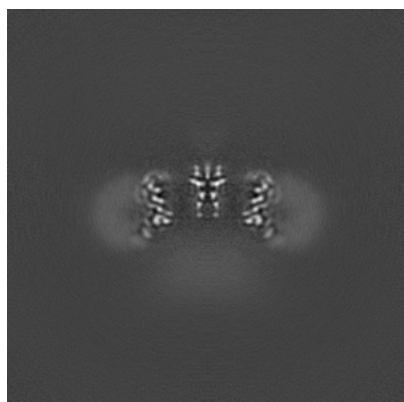


Y Index: 144

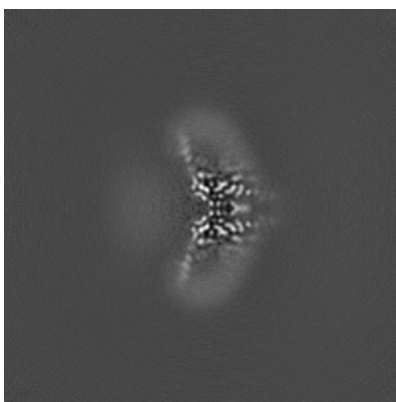


Z Index: 144

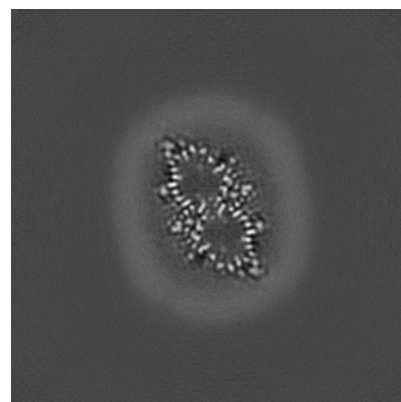
6.2.2 Raw map



X Index: 144



Y Index: 144

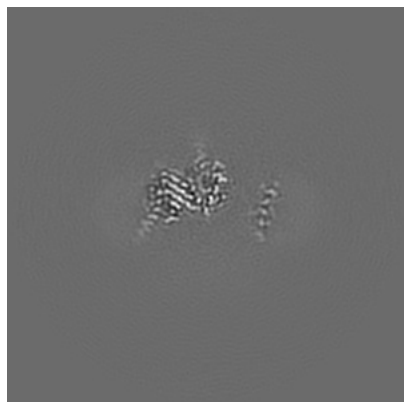


Z Index: 144

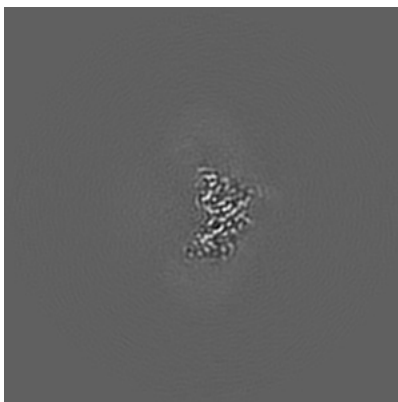
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

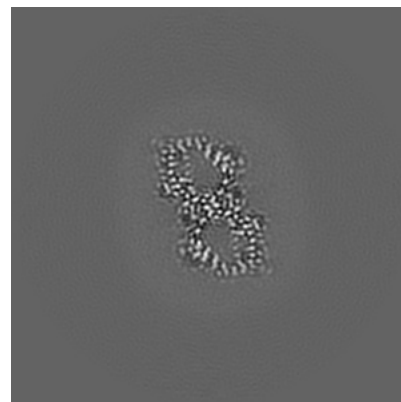
6.3.1 Primary map



X Index: 134

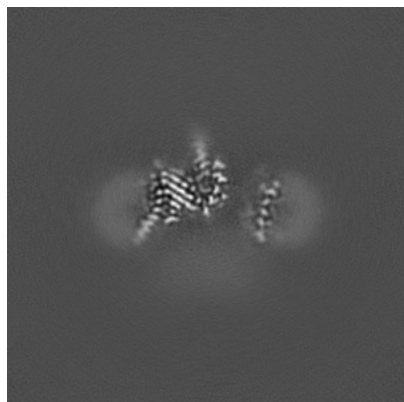


Y Index: 151

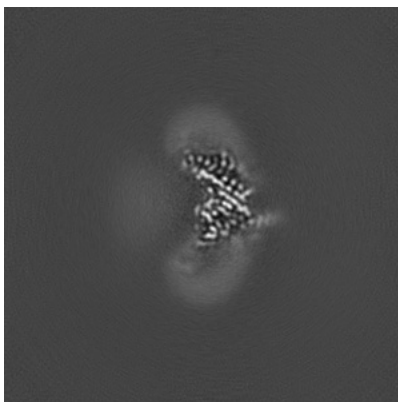


Z Index: 154

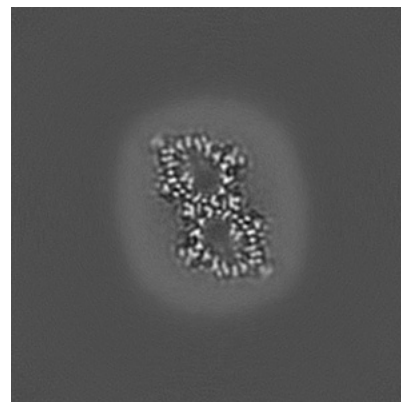
6.3.2 Raw map



X Index: 134



Y Index: 137

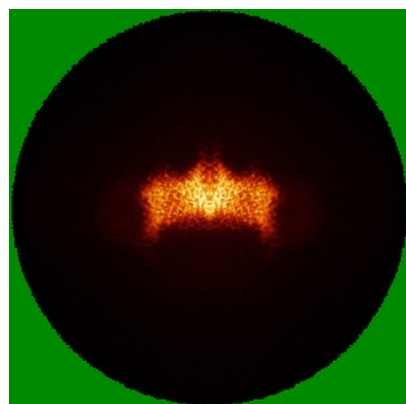


Z Index: 155

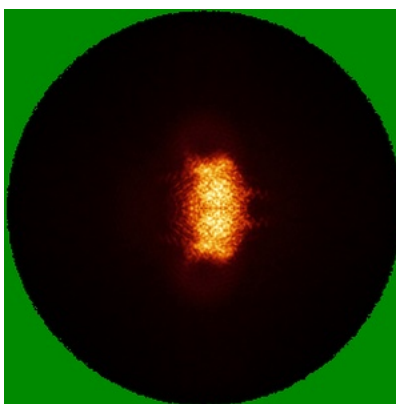
The images above show the largest variance slices of the map in three orthogonal directions.

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

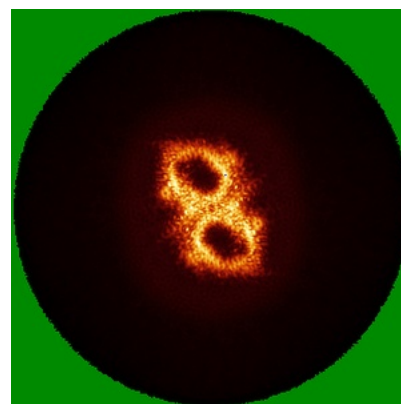
6.4.1 Primary map



X

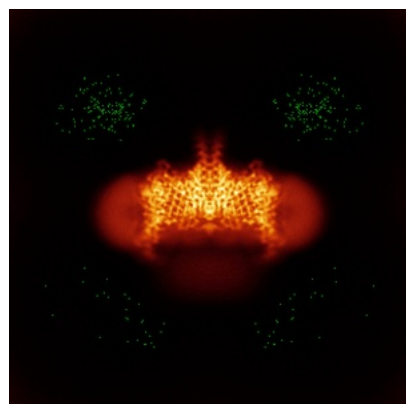


Y

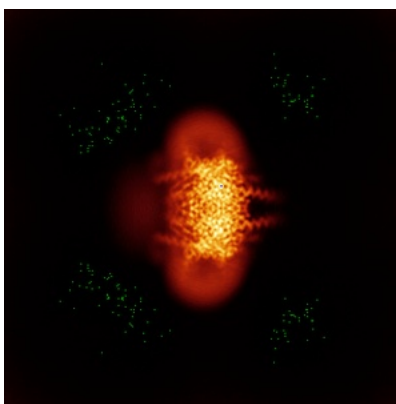


Z

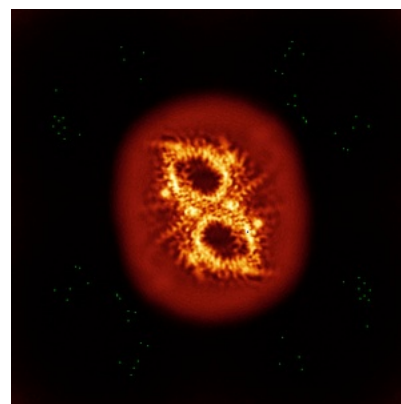
6.4.2 Raw map



X



Y

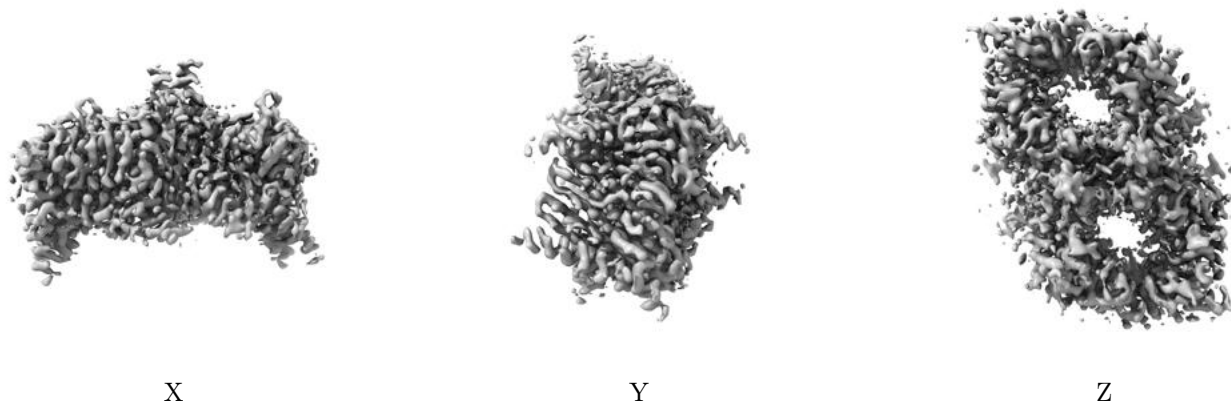


Z

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 0.2. 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.

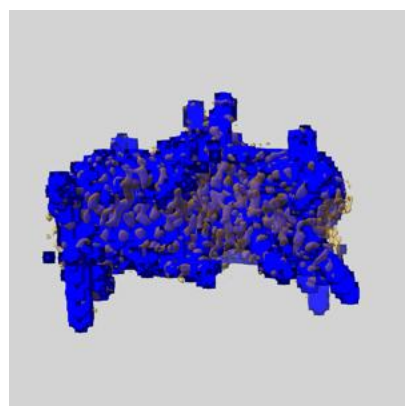
6.6 Mask visualisation [i](#)

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

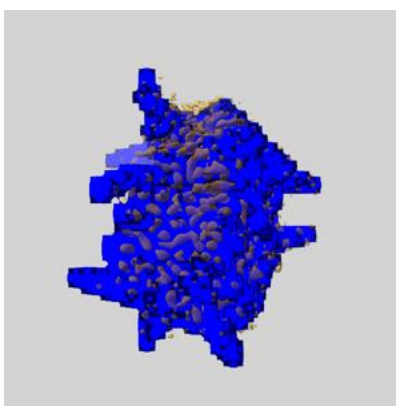
A mask typically either:

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

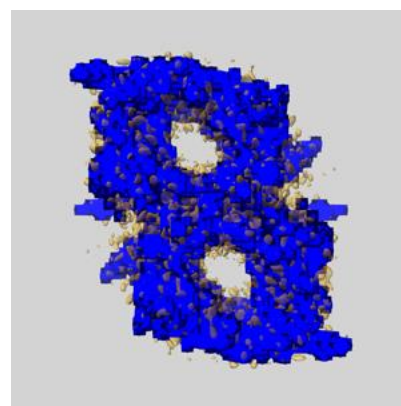
6.6.1 emd_66281_msk_1.map [i](#)



X



Y

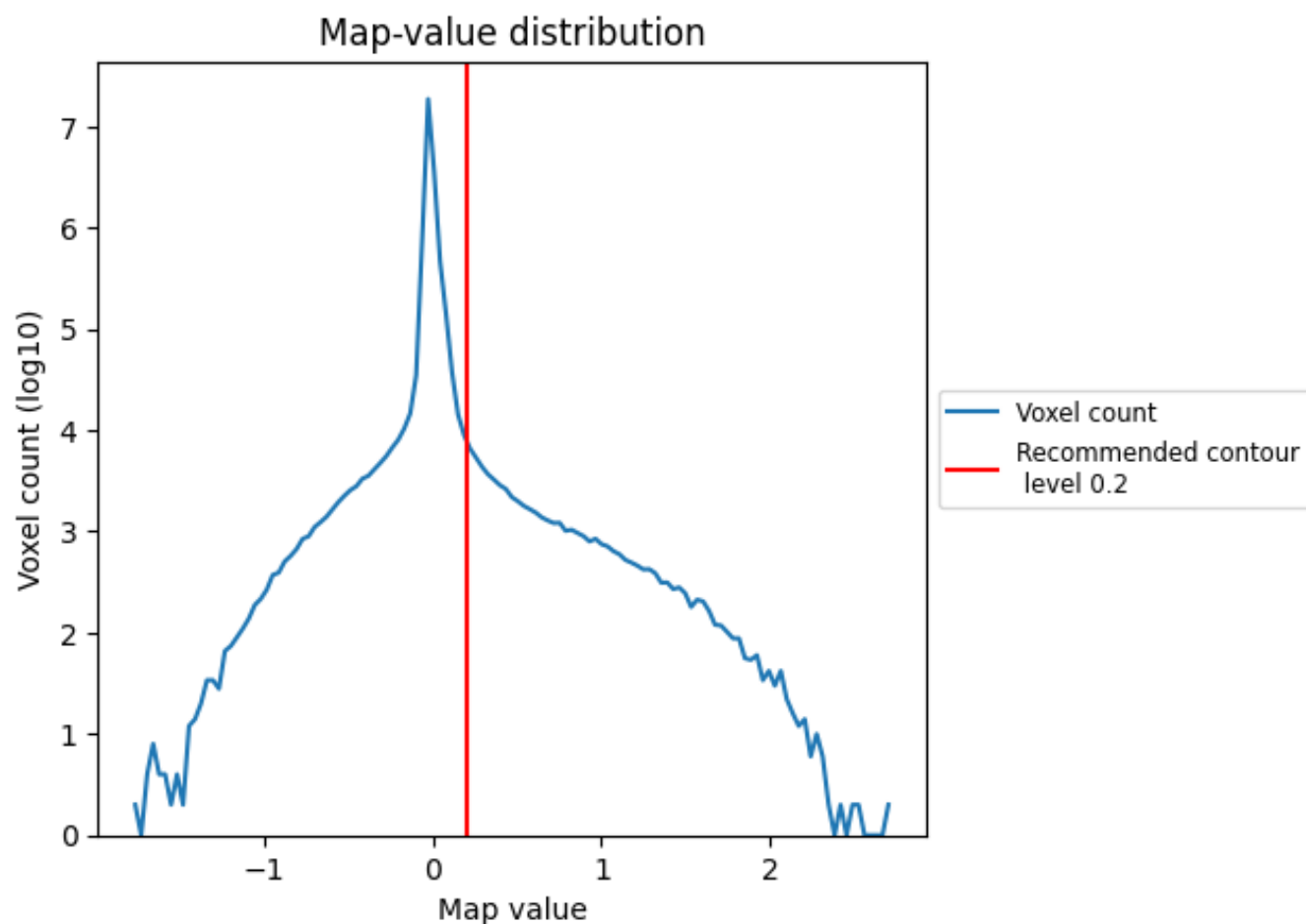


Z

7 Map analysis [i](#)

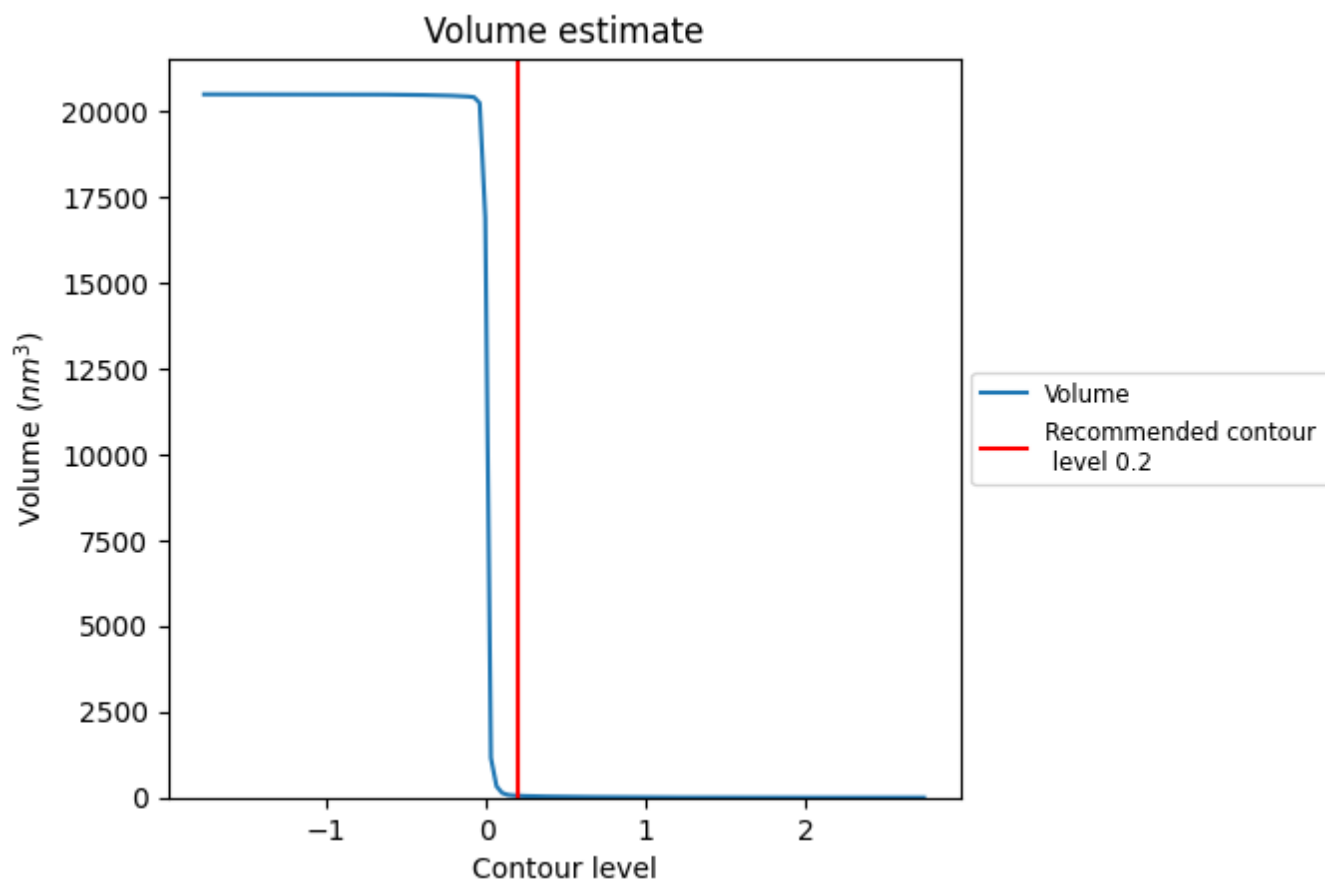
This section contains the results of statistical analysis of the map.

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.

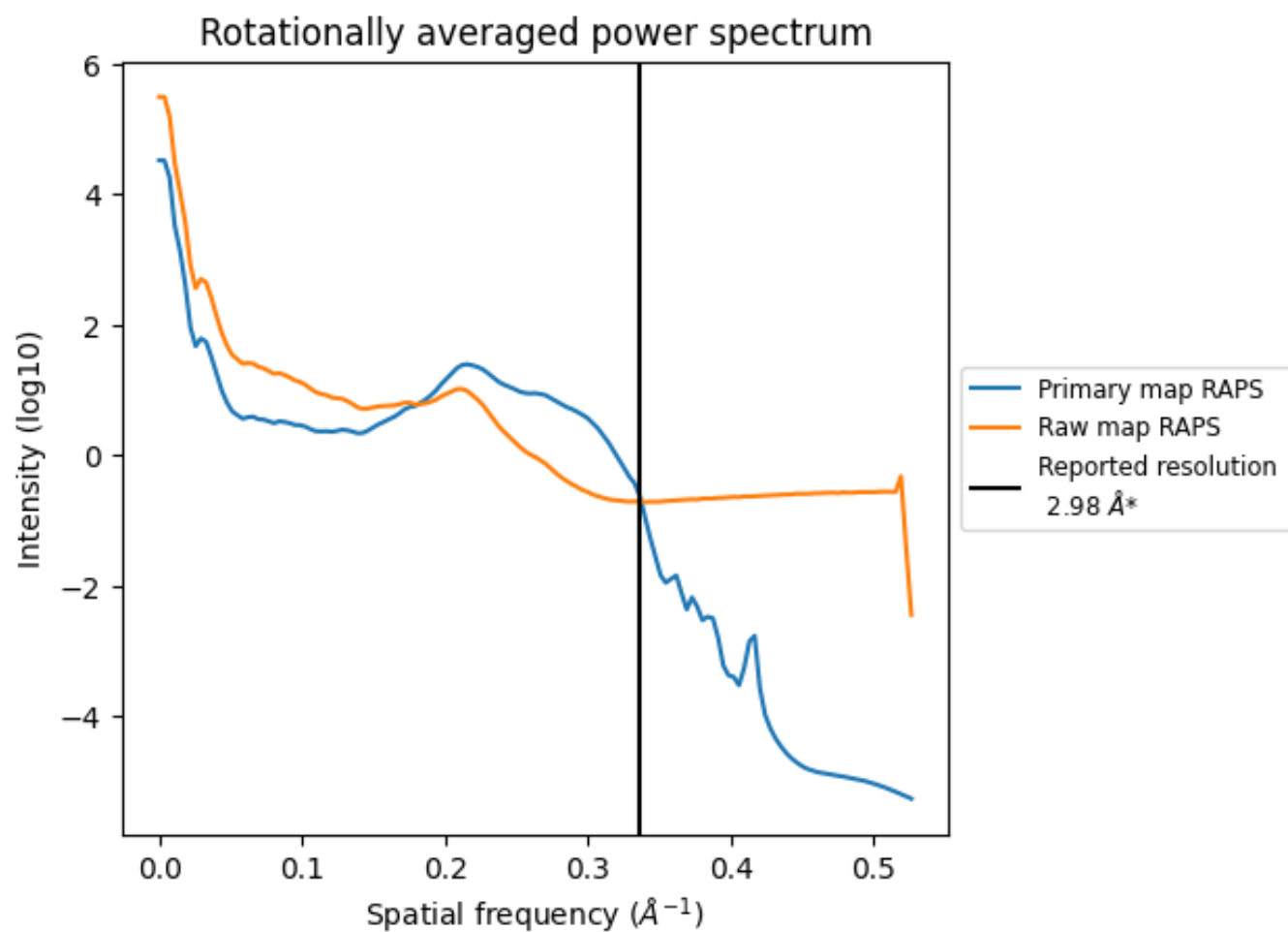
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm^3 ; this corresponds to an approximate mass of 48 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 ⓘ

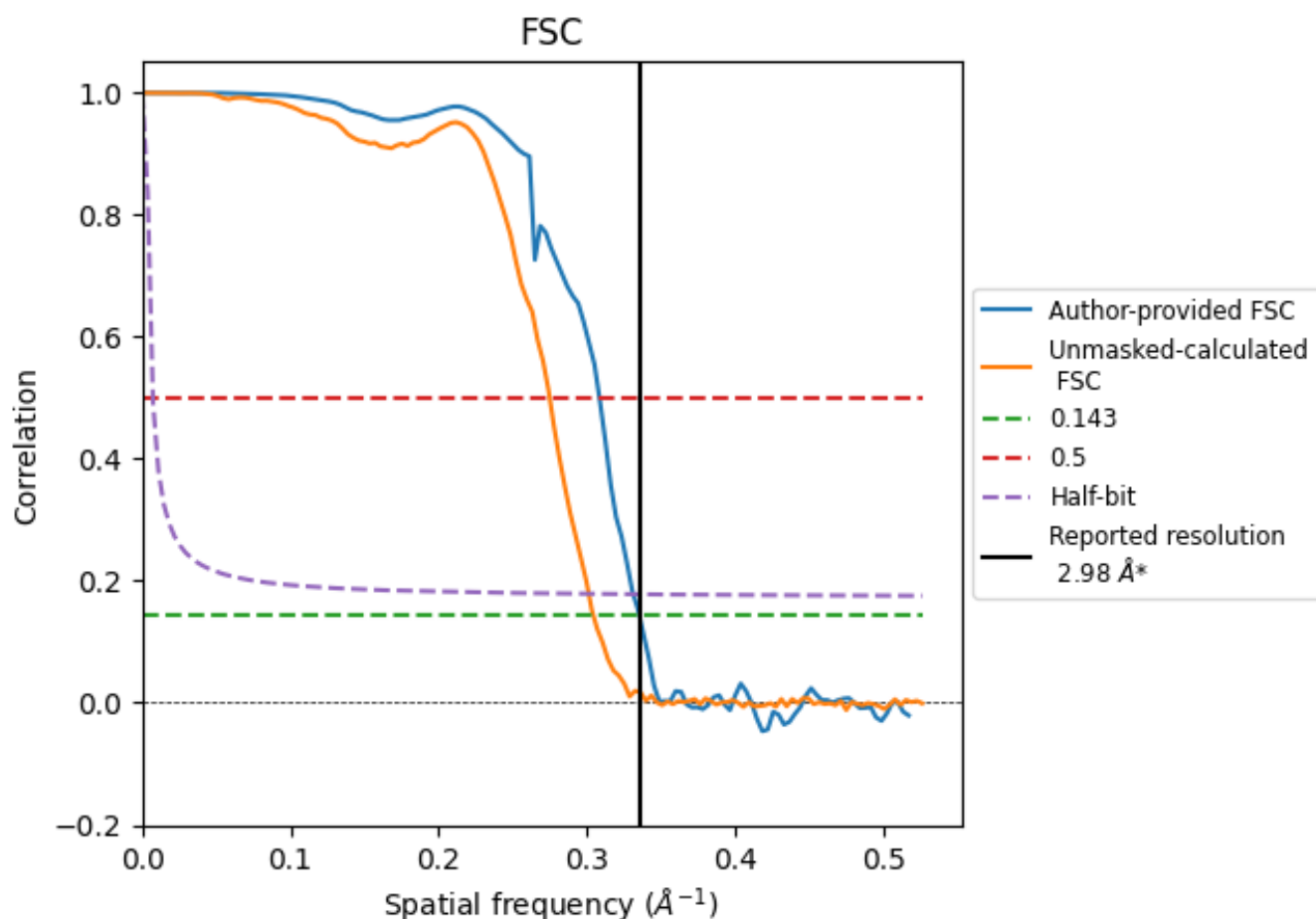


*Reported resolution corresponds to spatial frequency of 0.336 $\text{\AA}^{-1}$

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 0.336 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

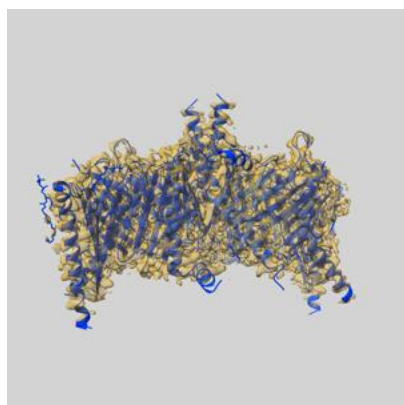
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.24	3.02
Unmasked-calculated*	3.29	3.64	3.32

*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 3.29 differs from the reported value 2.98 by more than 10 %

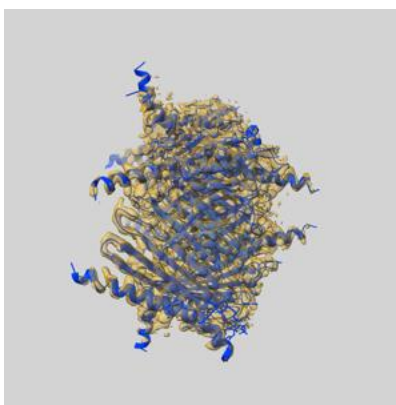
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66281 and PDB model 9WV3. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

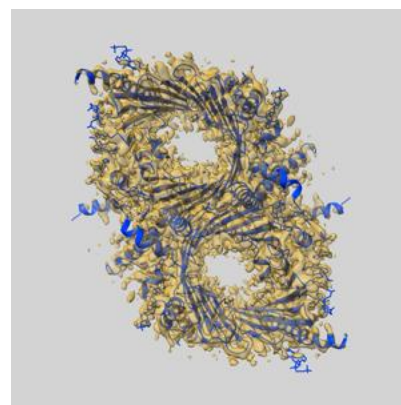
9.1 Map-model overlay [i](#)



X



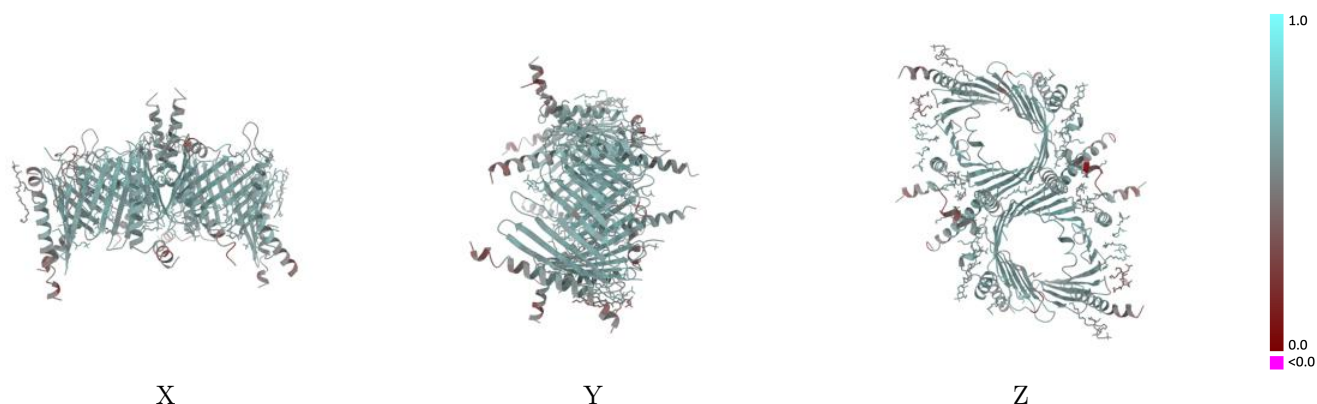
Y



Z

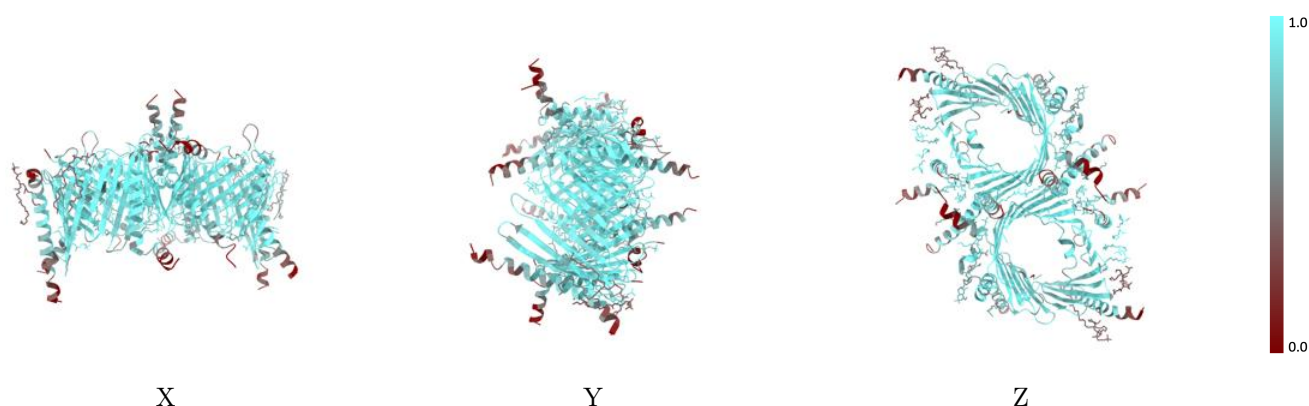
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



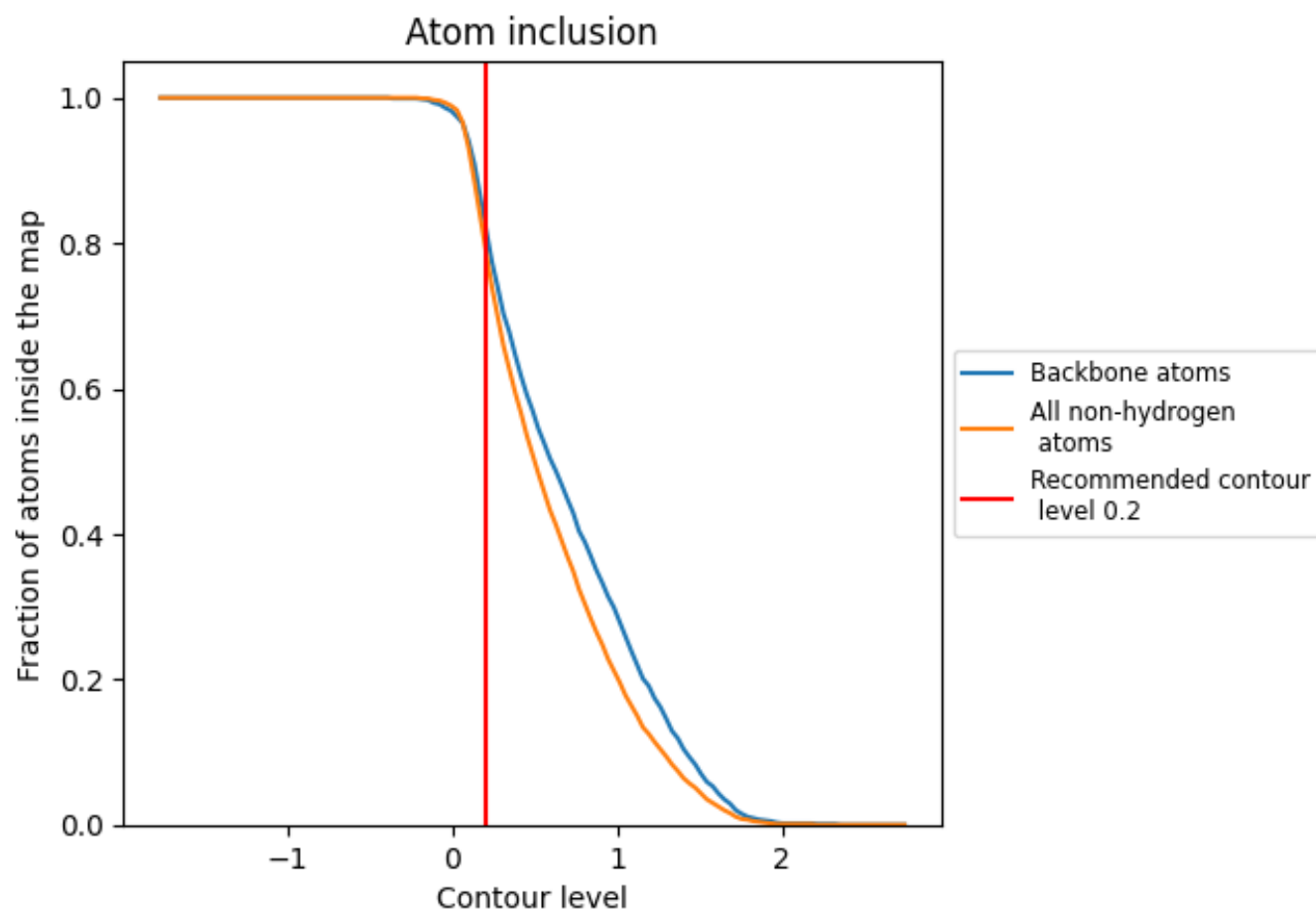
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.5630
A	0.5140	0.4790
B	0.5170	0.4800
C	0.7210	0.5360
D	0.7190	0.5400
E	0.7280	0.5470
F	0.7300	0.5490
G	0.7140	0.5480
H	0.7080	0.5470
I	0.9040	0.5950
J	0.9050	0.5970
K	0.5230	0.4730
L	0.5090	0.4630

1.0

0.0

<0.0