



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:45 PM JST

PDB ID : 7CP9
EMDB ID : EMD-30421
Title : Cryo-EM structure of human mitochondrial translocase TOM complex at 3.0 angstrom.
Authors : Guan, Z.; Yan, L.; Wang, Q.; Yan, C.; Yin, P.
Deposited on : 2020-08-06
Resolution : 3.00 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

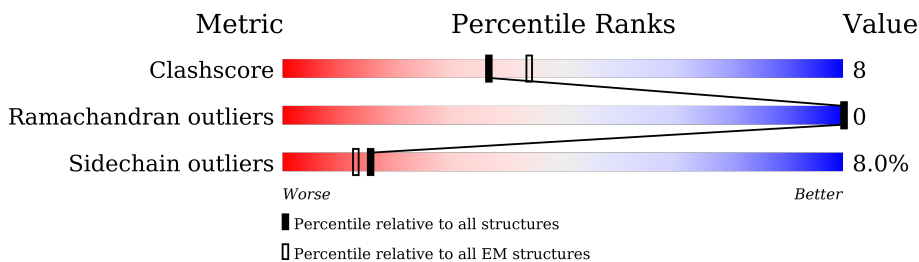
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
3	E	55	
3	F	55	
4	G	142	
4	H	142	

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Mol	Chain	Length	Quality of chain
5	I	361	
5	J	361	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8530 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	38	Total	C	N	O	S	0	0
			320	210	55	53	2		
1	B	37	Total	C	N	O	S	0	0
			312	204	54	52	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	49	Total	C	N	O	0	0
			400	254	75	71		
2	D	49	Total	C	N	O	0	0
			400	254	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	52	Total	C	N	O	S	0	0
			417	278	71	67	1		
3	F	52	Total	C	N	O	S	0	0
			417	278	71	67	1		

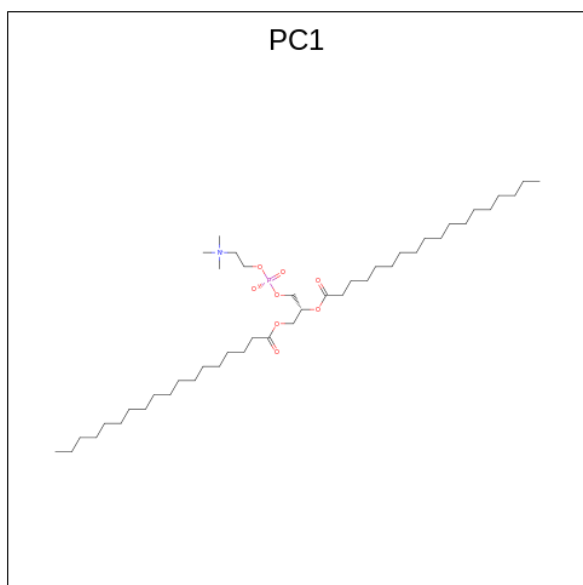
- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	86	Total	C	N	O	S	0	0
			646	412	113	117	4		
4	H	86	Total	C	N	O	S	0	0
			646	412	113	117	4		

- 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 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
6	E	1	Total	C	N	O	P	0
			108	88	2	16	2	
6	E	1	Total	C	N	O	P	0
			108	88	2	16	2	
6	F	1	Total	C	N	O	P	0
			108	88	2	16	2	
6	F	1	Total	C	N	O	P	0
			108	88	2	16	2	
6	G	1	Total	C	N	O	P	0
			162	132	3	24	3	
6	G	1	Total	C	N	O	P	0
			162	132	3	24	3	
6	G	1	Total	C	N	O	P	0
			162	132	3	24	3	
6	H	1	Total	C	N	O	P	0
			108	88	2	16	2	

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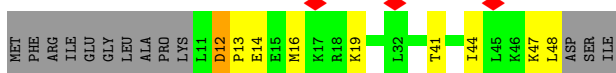
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Mol	Chain	Residues	Atoms					AltConf
6	H	1	Total	C	N	O	P	0
			108	88	2	16	2	
6	J	1	Total	C	N	O	P	0
			54	44	1	8	1	

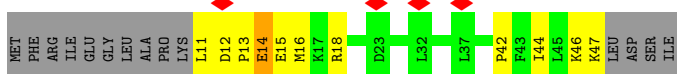
3 Residue-property plots

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.

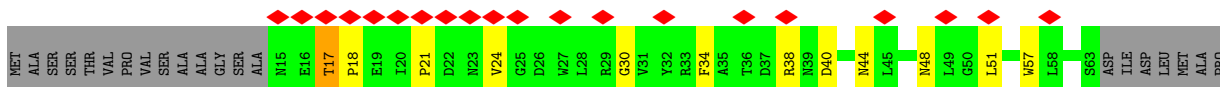
- Molecule 1: Mitochondrial import receptor subunit TOM5 homolog



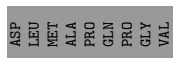
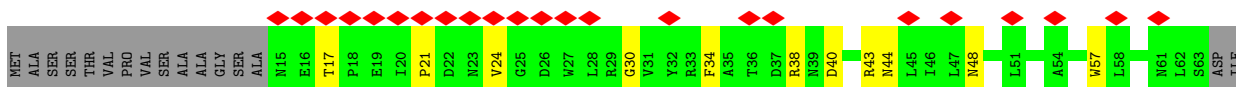
- Molecule 1: Mitochondrial import receptor subunit TOM5 homolog



- Molecule 2: Mitochondrial import receptor subunit TOM6 homolog



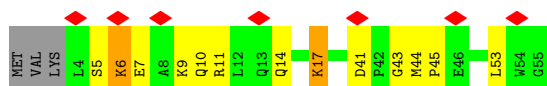
- Molecule 2: Mitochondrial import receptor subunit TOM6 homolog



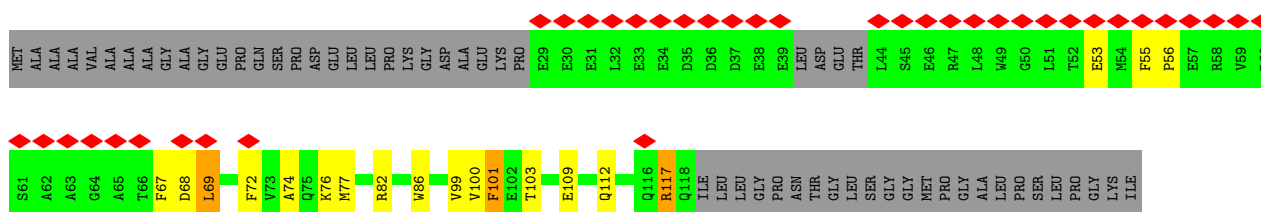
- Molecule 3: Mitochondrial import receptor subunit TOM7 homolog



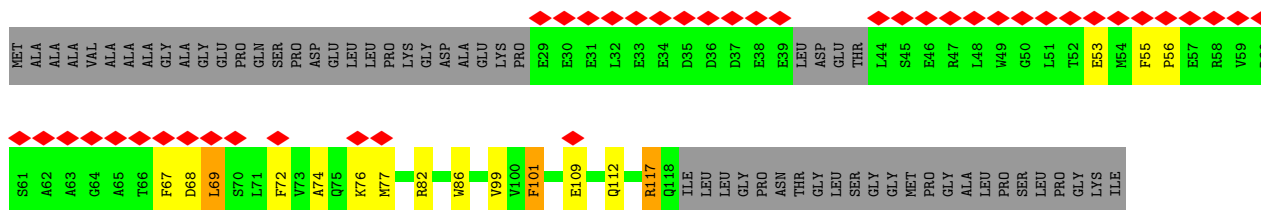
- Chain F:  13% 71% 20% 5%



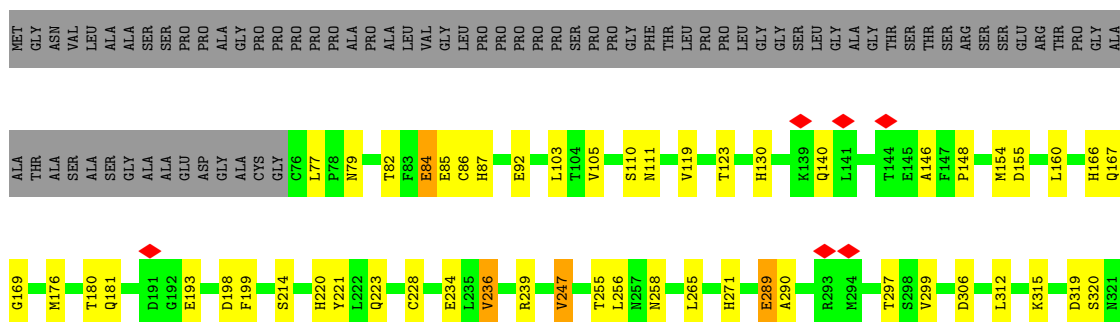
- Chain G: 



- Chain H: 30% 49% 10% . 39%



- Chain I:  62% 16% 21%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	360445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.017	Depositor
Minimum map value	-2.064	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.409	Depositor
Map size (\AA)	365.04, 365.04, 365.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.014, 1.014, 1.014	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.37	0/324	0.53	0/433
1	B	0.38	0/316	0.53	0/422
2	C	0.24	0/409	0.45	0/556
2	D	0.24	0/409	0.45	0/556
3	E	0.33	0/429	0.41	0/578
3	F	0.33	0/429	0.41	0/578
4	G	0.30	0/655	0.40	0/884
4	H	0.30	0/655	0.40	0/884
5	I	0.36	0/2239	0.48	0/3039
5	J	0.36	0/2239	0.48	0/3039
All	All	0.34	0/8104	0.46	0/10969

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

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	320	0	353	4	0
1	B	312	0	342	6	0
2	C	400	0	388	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	400	0	388	7	0
3	E	417	0	434	12	0
3	F	417	0	434	9	0
4	G	646	0	601	11	0
4	H	646	0	601	9	0
5	I	2189	0	2171	32	0
5	J	2189	0	2171	34	0
6	C	54	0	88	3	0
6	E	108	0	176	5	0
6	F	108	0	176	7	0
6	G	162	0	264	9	0
6	H	108	0	176	3	0
6	J	54	0	88	2	0
All	All	8530	0	8851	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (145) 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:30:GLY:O	2:D:34:PHE:HB2	1.49	1.12
2:C:30:GLY:O	2:C:34:PHE:HB2	1.49	1.11
5:I:236:VAL:HG13	5:I:247:VAL:HG13	1.67	0.77
2:C:30:GLY:O	2:C:34:PHE:CB	2.31	0.75
2:D:30:GLY:O	2:D:34:PHE:CB	2.31	0.75
5:J:236:VAL:HG13	5:J:247:VAL:HG13	1.67	0.74
6:F:102:PC1:H122	6:F:102:PC1:H372	1.72	0.71
4:H:86:TRP:HB2	6:H:201:PC1:H11	1.70	0.71
5:J:271:HIS:HD2	5:J:289:GLU:HG2	1.58	0.69
5:I:271:HIS:HD2	5:I:289:GLU:HG2	1.58	0.68
6:C:101:PC1:O32	5:I:322:TRP:NE1	2.27	0.66
5:J:319:ASP:OD1	5:J:320:SER:N	2.31	0.64
1:A:13:PRO:HA	1:A:16:MET:HG2	1.79	0.63
1:B:12:ASP:HB3	1:B:13:PRO:HD3	1.81	0.63
5:I:86:CYS:SG	5:I:87:HIS:N	2.71	0.63
5:J:86:CYS:SG	5:J:87:HIS:N	2.71	0.63
5:I:319:ASP:OD1	5:I:320:SER:N	2.31	0.63
1:B:13:PRO:HA	1:B:16:MET:HB3	1.81	0.63
5:J:140:GLN:HA	5:J:146:ALA:HA	1.82	0.61
5:I:140:GLN:HA	5:I:146:ALA:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:41:ASP:N	3:E:41:ASP:OD1	2.35	0.60
5:J:221:TYR:OH	5:J:223:GLN:OE1	2.18	0.60
6:F:102:PC1:H222	6:F:102:PC1:H121	1.84	0.59
2:C:44:ASN:O	2:C:48:ASN:ND2	2.27	0.59
4:G:86:TRP:HB2	6:G:202:PC1:H12	1.84	0.59
5:I:221:TYR:OH	5:I:223:GLN:OE1	2.18	0.58
5:J:167:GLN:NE2	5:J:169:GLY:O	2.37	0.58
5:I:167:GLN:NE2	5:I:169:GLY:O	2.37	0.58
3:F:41:ASP:OD1	3:F:41:ASP:N	2.35	0.57
5:J:148:PRO:HB3	5:J:166:HIS:HD2	1.70	0.57
5:I:148:PRO:HB3	5:I:166:HIS:HD2	1.70	0.57
2:C:40:ASP:O	2:C:44:ASN:ND2	2.38	0.57
3:F:44:MET:HG2	3:F:45:PRO:HD2	1.87	0.56
2:D:44:ASN:O	2:D:48:ASN:ND2	2.27	0.56
3:E:41:ASP:O	3:E:43:GLY:N	2.38	0.56
3:E:44:MET:HG2	3:E:45:PRO:HD2	1.87	0.55
3:F:41:ASP:O	3:F:43:GLY:N	2.39	0.55
2:D:40:ASP:O	2:D:44:ASN:ND2	2.38	0.55
5:I:289:GLU:OE1	5:I:290:ALA:N	2.40	0.55
4:H:55:PHE:HB3	4:H:56:PRO:HD3	1.88	0.55
5:J:289:GLU:OE1	5:J:290:ALA:N	2.40	0.55
4:G:82:ARG:NH1	6:G:203:PC1:O22	2.37	0.55
4:G:55:PHE:HB3	4:G:56:PRO:HD3	1.88	0.55
5:J:79:ASN:ND2	5:J:199:PHE:O	2.41	0.54
5:I:79:ASN:ND2	5:I:199:PHE:O	2.41	0.54
1:A:44:ILE:O	1:A:48:LEU:N	2.40	0.54
1:B:11:LEU:O	1:B:14:GLU:N	2.41	0.53
5:J:214:SER:HA	5:J:239:ARG:O	2.08	0.53
5:J:306:ASP:OD1	5:J:306:ASP:N	2.41	0.53
3:E:37:LYS:HE2	6:E:102:PC1:H131	1.91	0.53
4:H:82:ARG:NH1	6:H:202:PC1:O22	2.38	0.53
5:I:214:SER:HA	5:I:239:ARG:O	2.08	0.53
3:E:14:GLN:O	3:E:17:LYS:HG3	2.09	0.53
2:C:21:PRO:HA	2:C:24:VAL:HG22	1.91	0.53
3:F:14:GLN:O	3:F:17:LYS:HG3	2.09	0.53
5:J:105:VAL:HG22	5:J:360:ILE:HD12	1.90	0.53
5:I:105:VAL:HG22	5:I:360:ILE:HD12	1.90	0.52
5:I:306:ASP:OD1	5:I:306:ASP:N	2.41	0.52
2:C:48:ASN:HB3	5:I:299:VAL:HG23	1.91	0.52
2:D:21:PRO:HA	2:D:24:VAL:HG22	1.91	0.51
5:J:130:HIS:ND1	5:J:155:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:110:SER:OG	5:J:111:ASN:N	2.44	0.50
5:I:110:SER:OG	5:I:111:ASN:N	2.44	0.50
5:I:130:HIS:ND1	5:I:155:ASP:OD1	2.44	0.50
4:G:68:ASP:OD1	4:G:69:LEU:N	2.45	0.50
6:G:201:PC1:H3A1	5:J:358:LEU:HD22	1.94	0.50
5:I:84:GLU:OE2	5:I:85:GLU:N	2.45	0.49
6:H:202:PC1:H241	5:I:154:MET:HG2	1.95	0.48
4:H:68:ASP:OD1	4:H:69:LEU:N	2.45	0.48
5:J:84:GLU:OE2	5:J:85:GLU:N	2.45	0.48
5:I:220:HIS:CE1	5:I:234:GLU:HG3	2.50	0.47
5:J:322:TRP:HE3	5:J:348:ARG:HD3	1.79	0.47
6:F:102:PC1:H231	6:F:102:PC1:H261	1.56	0.47
6:F:102:PC1:H251	6:F:102:PC1:H3C2	1.95	0.47
3:E:54:TRP:HD1	5:J:107:LYS:HZ1	1.61	0.47
5:J:220:HIS:CE1	5:J:234:GLU:HG3	2.50	0.47
5:J:333:PRO:HG2	5:J:334:PRO:HD3	1.97	0.47
5:I:256:LEU:HD12	5:I:256:LEU:HA	1.77	0.47
6:G:202:PC1:H2E1	6:G:202:PC1:H2B1	1.80	0.47
5:I:322:TRP:HE3	5:I:348:ARG:HD3	1.79	0.46
5:J:91:LYS:HD3	5:J:91:LYS:HA	1.79	0.46
3:E:52:LEU:HD23	5:J:109:LEU:HD11	1.97	0.46
3:E:6:LYS:O	3:E:10:GLN:HG2	2.16	0.46
5:I:333:PRO:HG2	5:I:334:PRO:HD3	1.97	0.46
1:A:12:ASP:HB3	1:A:13:PRO:HD3	1.97	0.46
3:F:6:LYS:O	3:F:10:GLN:HG2	2.16	0.46
6:E:102:PC1:H133	6:E:102:PC1:H112	1.70	0.45
6:E:101:PC1:H352	5:J:208:PRO:HG2	1.99	0.45
1:B:42:PRO:O	1:B:44:ILE:N	2.50	0.45
4:H:69:LEU:O	4:H:72:PHE:HB3	2.17	0.44
5:I:258:ASN:OD1	5:I:258:ASN:N	2.50	0.44
4:H:101:PHE:HZ	5:I:360:ILE:HD13	1.83	0.44
4:H:109:GLU:HG3	4:H:112:GLN:HE21	1.82	0.44
1:B:46:LYS:HG3	1:B:47:LYS:N	2.32	0.44
4:G:109:GLU:HG3	4:G:112:GLN:HE21	1.82	0.44
4:G:69:LEU:O	4:G:72:PHE:HB3	2.17	0.43
6:F:102:PC1:H133	6:F:102:PC1:H112	1.71	0.43
5:I:92:GLU:O	5:I:315:LYS:NZ	2.43	0.43
5:J:258:ASN:OD1	5:J:258:ASN:N	2.50	0.43
3:F:10:GLN:O	3:F:14:GLN:HG3	2.19	0.43
5:J:352:PHE:CE2	5:J:354:CYS:HB3	2.53	0.43
5:J:92:GLU:O	5:J:315:LYS:NZ	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:256:LEU:HD12	5:J:256:LEU:HA	1.77	0.43
3:E:10:GLN:O	3:E:14:GLN:HG3	2.18	0.43
1:B:15:GLU:HA	1:B:18:ARG:HB3	2.00	0.43
6:F:101:PC1:H351	6:F:101:PC1:H321	1.92	0.43
5:I:312:LEU:HD11	5:I:328:LEU:HD11	2.01	0.43
6:G:201:PC1:H2G1	6:G:201:PC1:H2D2	1.90	0.43
6:G:202:PC1:H143	6:G:202:PC1:H112	1.70	0.43
5:I:352:PHE:CE2	5:I:354:CYS:HB3	2.53	0.43
5:I:228:CYS:HB3	5:I:255:THR:O	2.19	0.42
5:J:176:MET:SD	5:J:176:MET:N	2.92	0.42
4:G:117:ARG:HE	4:G:117:ARG:HB3	1.57	0.42
5:J:148:PRO:HB3	5:J:166:HIS:CD2	2.53	0.42
3:E:10:GLN:HG3	3:E:11:ARG:N	2.35	0.42
5:I:176:MET:N	5:I:176:MET:SD	2.92	0.42
5:J:228:CYS:HB3	5:J:255:THR:O	2.18	0.42
6:E:101:PC1:H31	6:E:101:PC1:H322	1.62	0.42
6:C:101:PC1:H252	6:C:101:PC1:H221	1.82	0.42
2:D:48:ASN:HB3	5:J:299:VAL:HG23	2.01	0.42
3:F:10:GLN:HG3	3:F:11:ARG:N	2.35	0.42
6:G:203:PC1:H251	6:G:203:PC1:H282	1.66	0.42
1:A:47:LYS:HB3	1:A:47:LYS:HE3	1.82	0.42
4:G:101:PHE:HD1	4:G:101:PHE:HA	1.77	0.41
5:J:312:LEU:HD11	5:J:328:LEU:HD11	2.01	0.41
3:E:5:SER:O	3:E:9:LYS:HG3	2.21	0.41
3:F:5:SER:O	3:F:9:LYS:HG3	2.21	0.41
4:G:100:VAL:HA	4:G:103:THR:HG22	2.03	0.41
5:I:220:HIS:ND1	5:I:234:GLU:HG3	2.36	0.41
2:C:17:THR:OG1	2:C:18:PRO:HD3	2.21	0.41
2:C:51:LEU:HD11	6:C:101:PC1:H31	2.02	0.41
5:I:148:PRO:HB3	5:I:166:HIS:CD2	2.53	0.41
6:J:401:PC1:H143	6:J:401:PC1:H112	1.66	0.41
4:H:74:ALA:O	4:H:77:MET:HG2	2.21	0.41
4:H:117:ARG:HE	4:H:117:ARG:HB3	1.57	0.41
6:J:401:PC1:H2I2	6:J:401:PC1:H2F1	1.94	0.41
6:E:101:PC1:H132	6:E:101:PC1:H111	1.60	0.41
3:F:6:LYS:HG3	3:F:7:GLU:H	1.86	0.41
4:G:69:LEU:HD22	4:G:69:LEU:HA	1.87	0.41
6:G:201:PC1:H2D2	6:G:201:PC1:H2A2	1.83	0.41
5:J:322:TRP:CE3	5:J:348:ARG:HD3	2.55	0.41
6:F:102:PC1:H2E2	6:F:102:PC1:H2B1	1.87	0.40
2:D:40:ASP:HB3	2:D:43:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:53:LEU:HD21	6:G:203:PC1:H2D1	2.03	0.40
4:G:74:ALA:O	4:G:77:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	36/51 (71%)	33 (92%)	3 (8%)	0	100	100
1	B	35/51 (69%)	33 (94%)	2 (6%)	0	100	100
2	C	47/74 (64%)	45 (96%)	2 (4%)	0	100	100
2	D	47/74 (64%)	45 (96%)	2 (4%)	0	100	100
3	E	50/55 (91%)	45 (90%)	5 (10%)	0	100	100
3	F	50/55 (91%)	45 (90%)	5 (10%)	0	100	100
4	G	82/142 (58%)	82 (100%)	0	0	100	100
4	H	82/142 (58%)	82 (100%)	0	0	100	100
5	I	284/361 (79%)	261 (92%)	23 (8%)	0	100	100
5	J	284/361 (79%)	261 (92%)	23 (8%)	0	100	100
All	All	997/1366 (73%)	932 (94%)	65 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	37/48 (77%)	33 (89%)	4 (11%)	6	26
1	B	36/48 (75%)	35 (97%)	1 (3%)	43	77
2	C	41/59 (70%)	38 (93%)	3 (7%)	14	44
2	D	41/59 (70%)	38 (93%)	3 (7%)	14	44
3	E	43/46 (94%)	40 (93%)	3 (7%)	15	47
3	F	43/46 (94%)	40 (93%)	3 (7%)	15	47
4	G	60/115 (52%)	53 (88%)	7 (12%)	5	22
4	H	60/115 (52%)	53 (88%)	7 (12%)	5	22
5	I	238/288 (83%)	220 (92%)	18 (8%)	13	43
5	J	238/288 (83%)	220 (92%)	18 (8%)	13	43
All	All	837/1112 (75%)	770 (92%)	67 (8%)	16	40

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	14	GLU
1	A	19	LYS
1	A	41	THR
1	B	14	GLU
2	C	17	THR
2	C	38	ARG
2	C	57	TRP
2	D	17	THR
2	D	38	ARG
2	D	57	TRP
3	E	6	LYS
3	E	17	LYS
3	E	53	LEU
3	F	6	LYS
3	F	17	LYS
3	F	53	LEU
4	G	53	GLU
4	G	67	PHE
4	G	69	LEU
4	G	76	LYS
4	G	99	VAL

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Mol	Chain	Res	Type
4	G	101	PHE
4	G	117	ARG
4	H	53	GLU
4	H	67	PHE
4	H	69	LEU
4	H	76	LYS
4	H	99	VAL
4	H	101	PHE
4	H	117	ARG
5	I	77	LEU
5	I	82	THR
5	I	84	GLU
5	I	103	LEU
5	I	119	VAL
5	I	123	THR
5	I	160	LEU
5	I	180	THR
5	I	181	GLN
5	I	193	GLU
5	I	198	ASP
5	I	236	VAL
5	I	247	VAL
5	I	265	LEU
5	I	289	GLU
5	I	297	THR
5	I	338	THR
5	I	345	LEU
5	J	77	LEU
5	J	82	THR
5	J	84	GLU
5	J	103	LEU
5	J	119	VAL
5	J	123	THR
5	J	160	LEU
5	J	180	THR
5	J	181	GLN
5	J	193	GLU
5	J	198	ASP
5	J	236	VAL
5	J	247	VAL
5	J	265	LEU
5	J	289	GLU

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Mol	Chain	Res	Type
5	J	297	THR
5	J	338	THR
5	J	345	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PC1	F	101	-	53,53,53	0.96	3 (5%)	59,61,61	1.07	2 (3%)
6	PC1	F	102	-	53,53,53	0.95	3 (5%)	59,61,61	1.06	3 (5%)
6	PC1	C	101	-	53,53,53	0.96	4 (7%)	59,61,61	1.05	2 (3%)
6	PC1	H	201	-	53,53,53	0.97	3 (5%)	59,61,61	1.09	2 (3%)
6	PC1	H	202	-	53,53,53	0.95	3 (5%)	59,61,61	1.11	2 (3%)
6	PC1	J	401	-	53,53,53	0.96	4 (7%)	59,61,61	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PC1	G	201	-	53,53,53	0.92	4 (7%)	59,61,61	1.06	2 (3%)
6	PC1	G	202	-	53,53,53	0.97	4 (7%)	59,61,61	1.08	2 (3%)
6	PC1	E	102	-	53,53,53	0.95	4 (7%)	59,61,61	1.10	2 (3%)
6	PC1	G	203	-	53,53,53	0.95	3 (5%)	59,61,61	1.07	2 (3%)
6	PC1	E	101	-	53,53,53	0.96	4 (7%)	59,61,61	1.07	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PC1	F	101	-	-	20/57/57/57	-
6	PC1	F	102	-	-	31/57/57/57	-
6	PC1	C	101	-	-	22/57/57/57	-
6	PC1	H	201	-	-	15/57/57/57	-
6	PC1	H	202	-	-	26/57/57/57	-
6	PC1	J	401	-	-	20/57/57/57	-
6	PC1	G	201	-	-	23/57/57/57	-
6	PC1	G	202	-	-	11/57/57/57	-
6	PC1	E	102	-	-	21/57/57/57	-
6	PC1	G	203	-	-	27/57/57/57	-
6	PC1	E	101	-	-	20/57/57/57	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	201	PC1	O21-C2	-2.82	1.39	1.46
6	F	101	PC1	O21-C2	-2.77	1.39	1.46
6	F	102	PC1	O21-C2	-2.73	1.39	1.46
6	G	203	PC1	O21-C2	-2.71	1.39	1.46
6	H	202	PC1	O21-C2	-2.70	1.39	1.46
6	J	401	PC1	O21-C2	-2.65	1.40	1.46
6	E	101	PC1	O21-C2	-2.63	1.40	1.46
6	G	202	PC1	O21-C2	-2.58	1.40	1.46
6	C	101	PC1	O21-C2	-2.57	1.40	1.46
6	E	102	PC1	O31-C31	2.52	1.40	1.33
6	E	102	PC1	O21-C2	-2.44	1.40	1.46
6	G	201	PC1	O21-C2	-2.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	202	PC1	O31-C31	2.39	1.40	1.33
6	F	102	PC1	O31-C31	2.38	1.40	1.33
6	J	401	PC1	O31-C31	2.36	1.40	1.33
6	G	203	PC1	O31-C31	2.35	1.40	1.33
6	H	201	PC1	O31-C31	2.32	1.40	1.33
6	C	101	PC1	O31-C3	-2.32	1.39	1.45
6	J	401	PC1	O31-C3	-2.31	1.39	1.45
6	H	201	PC1	O31-C3	-2.29	1.39	1.45
6	H	202	PC1	O31-C31	2.29	1.40	1.33
6	E	101	PC1	O31-C3	-2.27	1.40	1.45
6	C	101	PC1	O31-C31	2.27	1.40	1.33
6	E	102	PC1	O21-C21	2.27	1.40	1.34
6	F	101	PC1	O31-C31	2.26	1.39	1.33
6	G	201	PC1	O31-C3	-2.26	1.40	1.45
6	F	101	PC1	O31-C3	-2.25	1.40	1.45
6	G	203	PC1	O31-C3	-2.23	1.40	1.45
6	G	201	PC1	O31-C31	2.21	1.39	1.33
6	G	202	PC1	O31-C3	-2.20	1.40	1.45
6	E	101	PC1	O31-C31	2.20	1.39	1.33
6	H	202	PC1	O31-C3	-2.16	1.40	1.45
6	C	101	PC1	O21-C21	2.15	1.40	1.34
6	G	201	PC1	O21-C21	2.13	1.40	1.34
6	J	401	PC1	O21-C21	2.12	1.40	1.34
6	G	202	PC1	O21-C21	2.10	1.40	1.34
6	E	101	PC1	O21-C21	2.09	1.40	1.34
6	E	102	PC1	O31-C3	-2.07	1.40	1.45
6	F	102	PC1	O31-C3	-2.06	1.40	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	202	PC1	O21-C21-C22	4.28	120.72	111.50
6	G	202	PC1	O21-C21-C22	4.23	120.63	111.50
6	F	101	PC1	O21-C21-C22	4.23	120.61	111.50
6	E	102	PC1	O21-C21-C22	4.22	120.60	111.50
6	E	101	PC1	O21-C21-C22	4.18	120.51	111.50
6	C	101	PC1	O21-C21-C22	4.14	120.42	111.50
6	J	401	PC1	O21-C21-C22	4.10	120.34	111.50
6	G	201	PC1	O21-C21-C22	4.00	120.11	111.50
6	G	203	PC1	O21-C21-C22	3.92	119.94	111.50
6	F	102	PC1	O21-C21-C22	3.83	119.76	111.50
6	H	201	PC1	O21-C21-C22	3.79	119.68	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	102	PC1	O31-C31-C32	3.08	121.57	111.91
6	G	202	PC1	O31-C31-C32	2.81	120.72	111.91
6	H	202	PC1	O31-C31-C32	2.72	120.43	111.91
6	E	101	PC1	O31-C31-C32	2.69	120.35	111.91
6	C	101	PC1	O31-C31-C32	2.66	120.25	111.91
6	H	201	PC1	O31-C31-C32	2.64	120.18	111.91
6	F	101	PC1	O31-C31-C32	2.61	120.10	111.91
6	G	201	PC1	O31-C31-C32	2.58	120.00	111.91
6	G	203	PC1	O31-C31-C32	2.55	119.91	111.91
6	F	102	PC1	O31-C31-C32	2.54	119.86	111.91
6	J	401	PC1	O31-C31-C32	2.52	119.81	111.91
6	F	102	PC1	C2-O21-C21	-2.14	112.52	117.79

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	101	PC1	O13-C11-C12-N
6	C	101	PC1	O22-C21-O21-C2
6	E	101	PC1	O22-C21-O21-C2
6	E	101	PC1	C22-C21-O21-C2
6	E	101	PC1	O32-C31-O31-C3
6	E	101	PC1	C32-C31-O31-C3
6	E	102	PC1	C11-O13-P-O14
6	E	102	PC1	C11-O13-P-O11
6	E	102	PC1	C2-C1-O11-P
6	E	102	PC1	C22-C21-O21-C2
6	F	101	PC1	C22-C21-O21-C2
6	F	102	PC1	C11-O13-P-O12
6	F	102	PC1	O22-C21-O21-C2
6	G	201	PC1	C22-C21-O21-C2
6	G	202	PC1	O32-C31-O31-C3
6	G	202	PC1	C32-C31-O31-C3
6	G	203	PC1	C2-C1-O11-P
6	H	201	PC1	C11-O13-P-O14
6	H	201	PC1	C11-O13-P-O11
6	H	201	PC1	O32-C31-O31-C3
6	H	201	PC1	C32-C31-O31-C3
6	H	202	PC1	C22-C21-O21-C2
6	J	401	PC1	O22-C21-O21-C2
6	E	102	PC1	O32-C31-O31-C3
6	J	401	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
6	E	102	PC1	C32-C31-O31-C3
6	C	101	PC1	O32-C31-O31-C3
6	E	102	PC1	O22-C21-O21-C2
6	F	101	PC1	O22-C21-O21-C2
6	G	201	PC1	O22-C21-O21-C2
6	H	202	PC1	O22-C21-O21-C2
6	C	101	PC1	C32-C31-O31-C3
6	J	401	PC1	C32-C31-O31-C3
6	C	101	PC1	C22-C21-O21-C2
6	F	102	PC1	C22-C21-O21-C2
6	J	401	PC1	C22-C21-O21-C2
6	G	201	PC1	C32-C31-O31-C3
6	G	201	PC1	O32-C31-O31-C3
6	G	203	PC1	C32-C31-O31-C3
6	G	203	PC1	O32-C31-O31-C3
6	E	102	PC1	C21-C22-C23-C24
6	G	203	PC1	C21-C22-C23-C24
6	F	102	PC1	C31-C32-C33-C34
6	G	201	PC1	C31-C32-C33-C34
6	C	101	PC1	C11-O13-P-O11
6	F	102	PC1	C11-O13-P-O11
6	G	203	PC1	C1-O11-P-O13
6	H	202	PC1	C11-O13-P-O11
6	F	101	PC1	C32-C31-O31-C3
6	F	102	PC1	C32-C31-O31-C3
6	H	202	PC1	C22-C23-C24-C25
6	E	101	PC1	C34-C35-C36-C37
6	G	203	PC1	C2E-C2F-C2G-C2H
6	J	401	PC1	C23-C24-C25-C26
6	C	101	PC1	C32-C33-C34-C35
6	F	101	PC1	C28-C29-C2A-C2B
6	F	102	PC1	C28-C29-C2A-C2B
6	C	101	PC1	C2A-C2B-C2C-C2D
6	C	101	PC1	C2E-C2F-C2G-C2H
6	E	102	PC1	C27-C28-C29-C2A
6	G	202	PC1	C3B-C3C-C3D-C3E
6	H	201	PC1	C2E-C2F-C2G-C2H
6	F	101	PC1	C2E-C2F-C2G-C2H
6	G	202	PC1	C32-C33-C34-C35
6	G	203	PC1	C28-C29-C2A-C2B
6	H	202	PC1	C33-C34-C35-C36
6	H	202	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
6	J	401	PC1	C27-C28-C29-C2A
6	E	102	PC1	C26-C27-C28-C29
6	H	202	PC1	C23-C24-C25-C26
6	J	401	PC1	C34-C35-C36-C37
6	H	202	PC1	C24-C25-C26-C27
6	G	203	PC1	C34-C35-C36-C37
6	H	201	PC1	C34-C35-C36-C37
6	J	401	PC1	C3C-C3D-C3E-C3F
6	J	401	PC1	C25-C26-C27-C28
6	G	201	PC1	C3D-C3E-C3F-C3G
6	G	203	PC1	C2C-C2D-C2E-C2F
6	F	101	PC1	O32-C31-O31-C3
6	F	102	PC1	O32-C31-O31-C3
6	G	203	PC1	C37-C38-C39-C3A
6	G	203	PC1	C38-C39-C3A-C3B
6	J	401	PC1	C21-C22-C23-C24
6	E	102	PC1	C2A-C2B-C2C-C2D
6	C	101	PC1	C26-C27-C28-C29
6	E	101	PC1	C35-C36-C37-C38
6	H	202	PC1	C28-C29-C2A-C2B
6	J	401	PC1	C2E-C2F-C2G-C2H
6	G	201	PC1	C3E-C3F-C3G-C3H
6	E	102	PC1	C38-C39-C3A-C3B
6	F	102	PC1	C24-C25-C26-C27
6	G	203	PC1	C3B-C3C-C3D-C3E
6	F	102	PC1	C3E-C3F-C3G-C3H
6	F	102	PC1	C26-C27-C28-C29
6	E	101	PC1	C22-C23-C24-C25
6	C	101	PC1	C34-C35-C36-C37
6	G	203	PC1	C35-C36-C37-C38
6	G	203	PC1	C29-C2A-C2B-C2C
6	E	101	PC1	C23-C24-C25-C26
6	G	203	PC1	C23-C24-C25-C26
6	E	101	PC1	C31-C32-C33-C34
6	G	201	PC1	C2B-C2C-C2D-C2E
6	G	203	PC1	C3E-C3F-C3G-C3H
6	G	203	PC1	C1-C2-C3-O31
6	F	102	PC1	C21-C22-C23-C24
6	H	202	PC1	C38-C39-C3A-C3B
6	J	401	PC1	C33-C34-C35-C36
6	G	201	PC1	C3-C2-O21-C21
6	C	101	PC1	C2-C3-O31-C31

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Mol	Chain	Res	Type	Atoms
6	E	102	PC1	O11-C1-C2-O21
6	G	203	PC1	O21-C2-C3-O31
6	J	401	PC1	O21-C2-C3-O31
6	H	201	PC1	C2D-C2E-C2F-C2G
6	G	202	PC1	C2A-C2B-C2C-C2D
6	J	401	PC1	C26-C27-C28-C29
6	G	203	PC1	C3D-C3E-C3F-C3G
6	E	101	PC1	C25-C26-C27-C28
6	F	101	PC1	O11-C1-C2-C3
6	H	202	PC1	O11-C1-C2-C3
6	F	102	PC1	C25-C26-C27-C28
6	J	401	PC1	C24-C25-C26-C27
6	H	202	PC1	C32-C31-O31-C3
6	G	201	PC1	C36-C37-C38-C39
6	C	101	PC1	C1-C2-C3-O31
6	F	101	PC1	C1-C2-C3-O31
6	E	101	PC1	C36-C37-C38-C39
6	E	101	PC1	O11-C1-C2-O21
6	E	101	PC1	C2B-C2C-C2D-C2E
6	F	101	PC1	C2D-C2E-C2F-C2G
6	G	201	PC1	C2-C1-O11-P
6	G	201	PC1	C23-C24-C25-C26
6	G	201	PC1	C32-C33-C34-C35
6	F	102	PC1	C23-C24-C25-C26
6	G	201	PC1	C39-C3A-C3B-C3C
6	C	101	PC1	C23-C24-C25-C26
6	E	101	PC1	O11-C1-C2-C3
6	G	201	PC1	O11-C1-C2-C3
6	F	101	PC1	C2B-C2C-C2D-C2E
6	H	201	PC1	C3C-C3D-C3E-C3F
6	H	202	PC1	C3A-C3B-C3C-C3D
6	F	102	PC1	C22-C23-C24-C25
6	H	202	PC1	C2-C1-O11-P
6	H	202	PC1	O11-C1-C2-O21
6	G	203	PC1	C2F-C2G-C2H-C2I
6	H	201	PC1	C37-C38-C39-C3A
6	E	101	PC1	C2A-C2B-C2C-C2D
6	H	202	PC1	O32-C31-O31-C3
6	C	101	PC1	O21-C2-C3-O31
6	E	102	PC1	C39-C3A-C3B-C3C
6	F	102	PC1	C2-C1-O11-P
6	F	101	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
6	F	102	PC1	C2E-C2F-C2G-C2H
6	C	101	PC1	C11-O13-P-O12
6	F	102	PC1	C11-O13-P-O14
6	G	203	PC1	C1-O11-P-O14
6	H	202	PC1	C11-O13-P-O12
6	H	202	PC1	C11-O13-P-O14
6	G	202	PC1	O11-C1-C2-C3
6	F	102	PC1	C29-C2A-C2B-C2C
6	G	201	PC1	C12-C11-O13-P
6	H	201	PC1	C3B-C3C-C3D-C3E
6	F	101	PC1	O11-C1-C2-O21
6	G	202	PC1	O11-C1-C2-O21
6	F	101	PC1	C11-C12-N-C13
6	F	102	PC1	C1-C2-C3-O31
6	H	201	PC1	O13-C11-C12-N
6	H	202	PC1	O13-C11-C12-N
6	J	401	PC1	C1-C2-C3-O31
6	F	101	PC1	O21-C2-C3-O31
6	F	102	PC1	O21-C2-C3-O31
6	H	201	PC1	O21-C2-C3-O31
6	G	203	PC1	C2A-C2B-C2C-C2D
6	E	102	PC1	C32-C33-C34-C35
6	F	101	PC1	C26-C27-C28-C29
6	F	102	PC1	C2-C3-O31-C31
6	G	201	PC1	C24-C25-C26-C27
6	G	202	PC1	C31-C32-C33-C34
6	G	203	PC1	C2B-C2C-C2D-C2E
6	J	401	PC1	C2D-C2E-C2F-C2G
6	F	102	PC1	C2D-C2E-C2F-C2G
6	E	102	PC1	O11-C1-C2-C3
6	H	202	PC1	C35-C36-C37-C38
6	E	101	PC1	C2E-C2F-C2G-C2H
6	F	101	PC1	C11-C12-N-C15
6	C	101	PC1	C1-O11-P-O13
6	G	201	PC1	C11-O13-P-O11
6	G	201	PC1	C1-O11-P-O13
6	G	202	PC1	C11-O13-P-O11
6	H	202	PC1	C1-O11-P-O13
6	J	401	PC1	C11-O13-P-O11
6	H	201	PC1	C1-C2-C3-O31
6	E	101	PC1	C33-C34-C35-C36
6	H	202	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
6	G	201	PC1	C11-C12-N-C14
6	F	102	PC1	C2A-C2B-C2C-C2D
6	H	202	PC1	O31-C31-C32-C33
6	F	102	PC1	C33-C34-C35-C36
6	H	202	PC1	C32-C33-C34-C35
6	F	101	PC1	C11-C12-N-C14
6	H	201	PC1	C3A-C3B-C3C-C3D
6	E	101	PC1	C26-C27-C28-C29
6	G	202	PC1	C36-C37-C38-C39
6	G	201	PC1	C11-C12-N-C15
6	H	202	PC1	C3D-C3E-C3F-C3G
6	G	201	PC1	C26-C27-C28-C29
6	G	203	PC1	C25-C26-C27-C28
6	F	101	PC1	C31-C32-C33-C34
6	E	101	PC1	C11-O13-P-O11
6	F	101	PC1	C24-C25-C26-C27
6	G	203	PC1	O31-C31-C32-C33
6	J	401	PC1	C31-C32-C33-C34
6	E	102	PC1	C2C-C2D-C2E-C2F
6	H	201	PC1	C38-C39-C3A-C3B
6	G	201	PC1	C11-C12-N-C13
6	H	202	PC1	C2D-C2E-C2F-C2G
6	F	102	PC1	C34-C35-C36-C37
6	G	203	PC1	O32-C31-C32-C33
6	C	101	PC1	C1-O11-P-O14
6	F	101	PC1	C11-O13-P-O14
6	G	202	PC1	C1-O11-P-O14
6	G	203	PC1	C1-O11-P-O12
6	J	401	PC1	C1-O11-P-O12
6	F	102	PC1	O11-C1-C2-C3
6	E	102	PC1	C2B-C2C-C2D-C2E
6	C	101	PC1	C1-C2-O21-C21
6	C	101	PC1	C3-C2-O21-C21
6	F	102	PC1	C32-C33-C34-C35
6	F	102	PC1	C39-C3A-C3B-C3C
6	C	101	PC1	O21-C21-C22-C23
6	F	102	PC1	O21-C21-C22-C23
6	C	101	PC1	C3D-C3E-C3F-C3G
6	E	102	PC1	C33-C34-C35-C36
6	E	102	PC1	O32-C31-C32-C33
6	F	102	PC1	O22-C21-C22-C23
6	E	102	PC1	O31-C31-C32-C33

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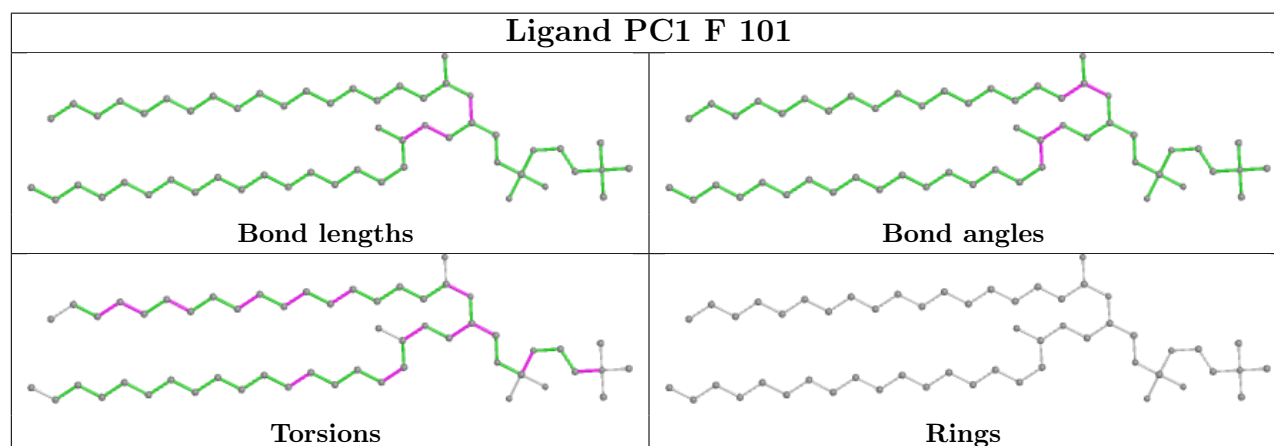
Mol	Chain	Res	Type	Atoms
6	E	101	PC1	C28-C29-C2A-C2B

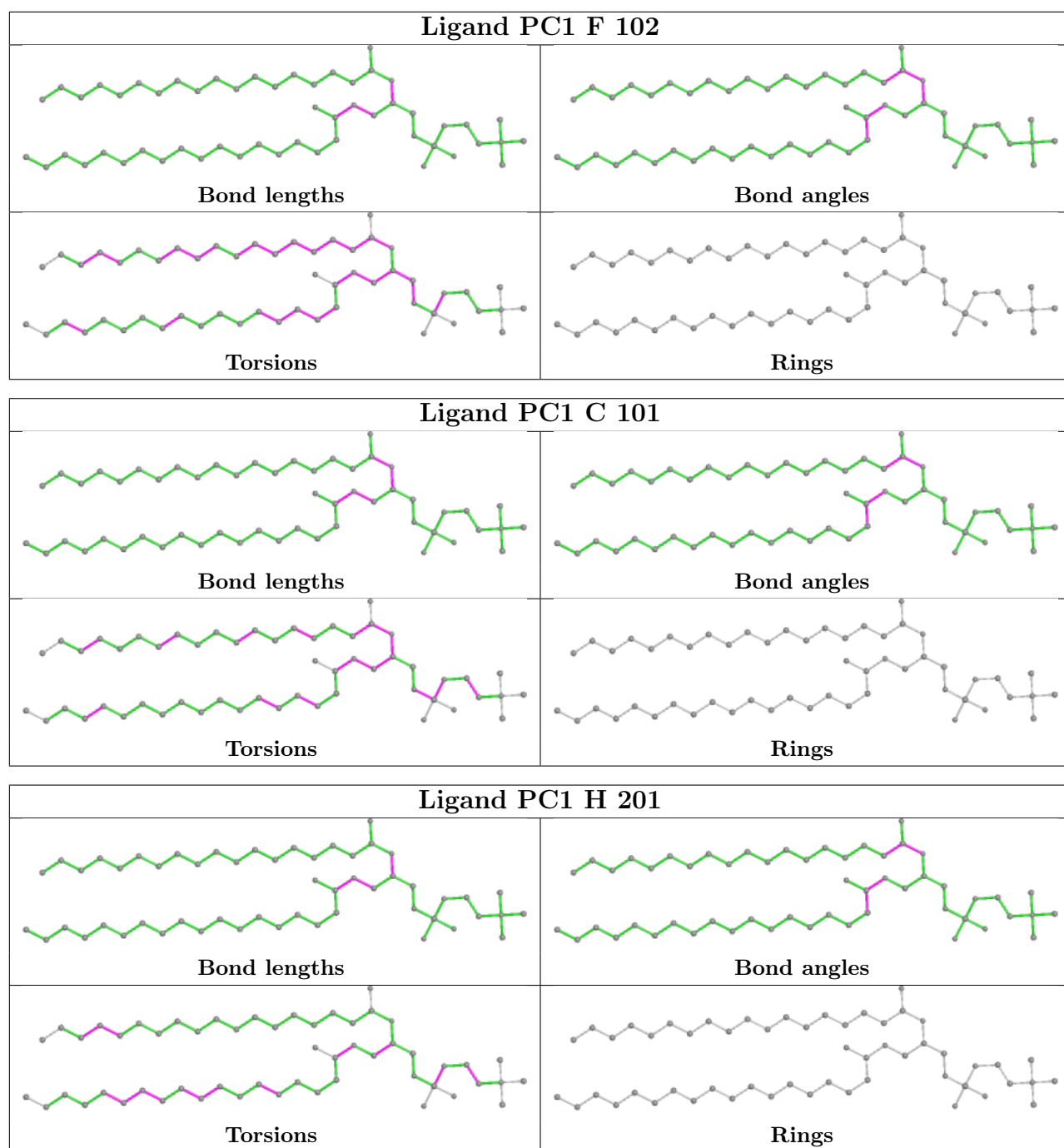
There are no ring outliers.

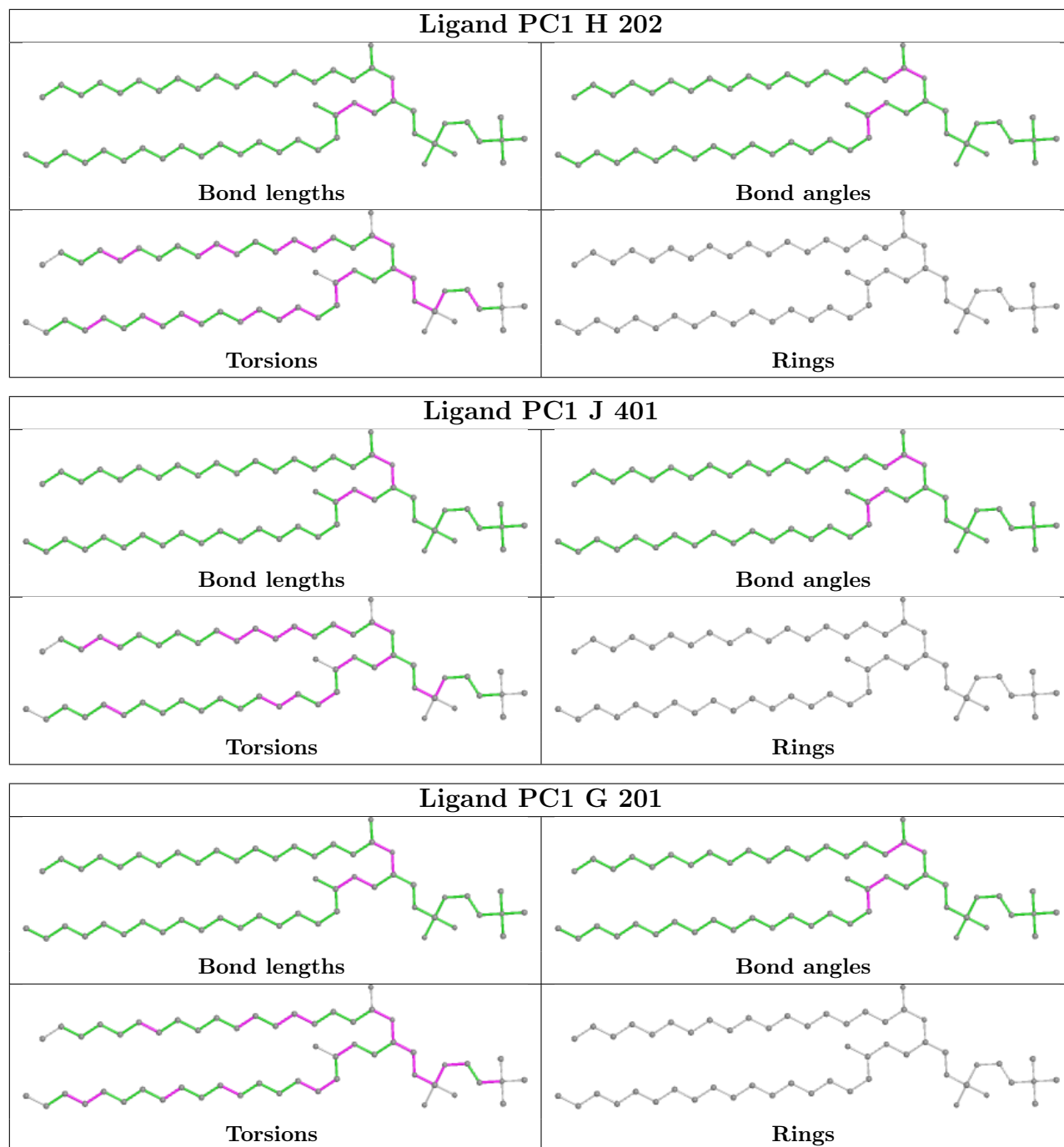
11 monomers are involved in 29 short contacts:

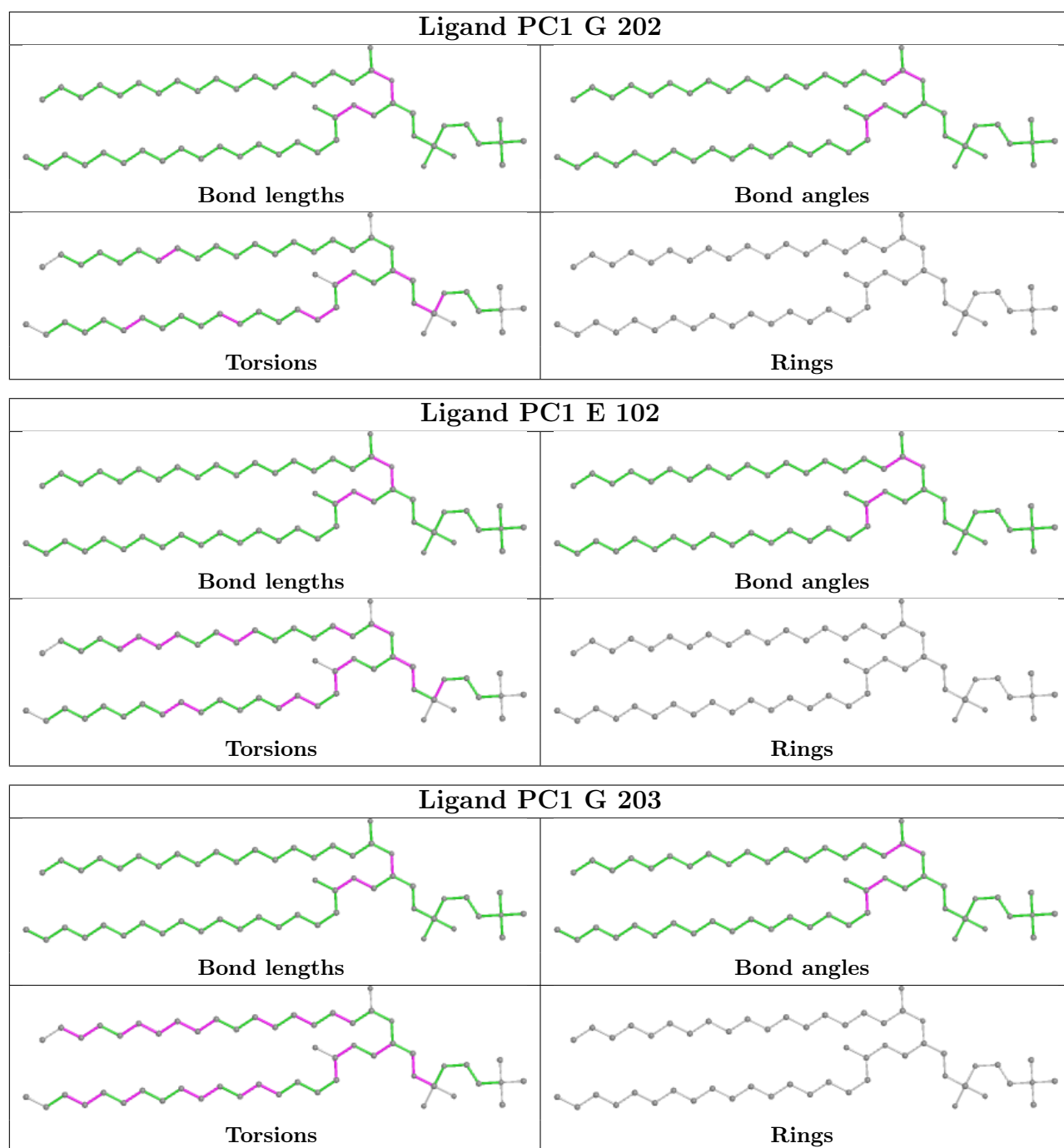
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	101	PC1	1	0
6	F	102	PC1	6	0
6	C	101	PC1	3	0
6	H	201	PC1	1	0
6	H	202	PC1	2	0
6	J	401	PC1	2	0
6	G	201	PC1	3	0
6	G	202	PC1	3	0
6	E	102	PC1	2	0
6	G	203	PC1	3	0
6	E	101	PC1	3	0

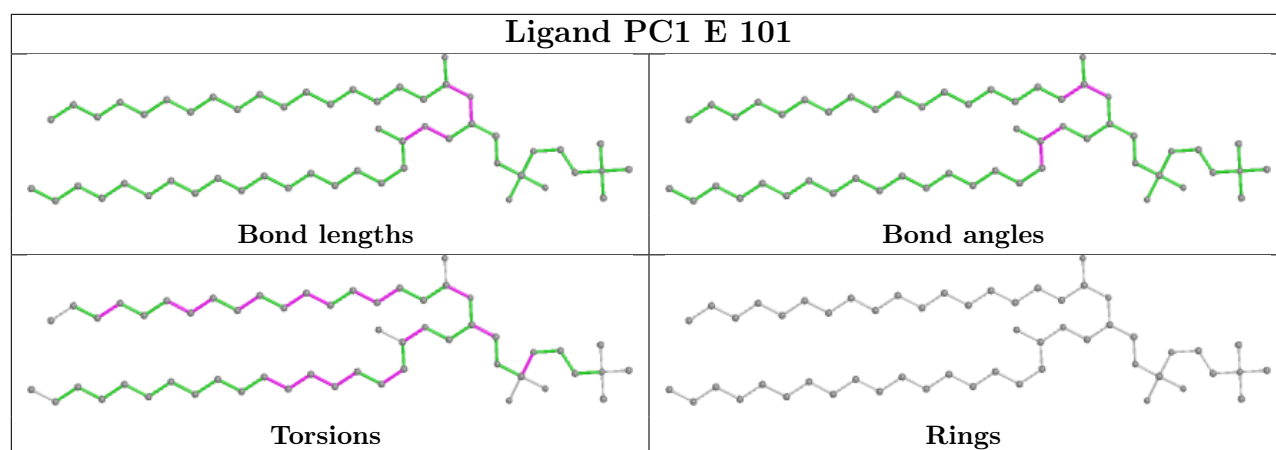
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

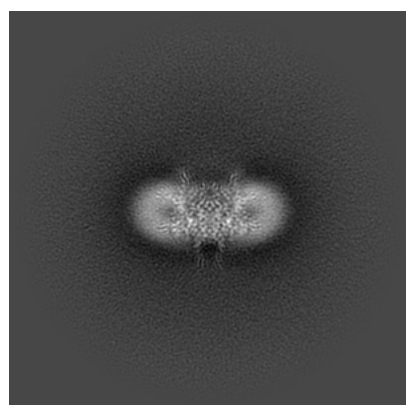
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30421. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

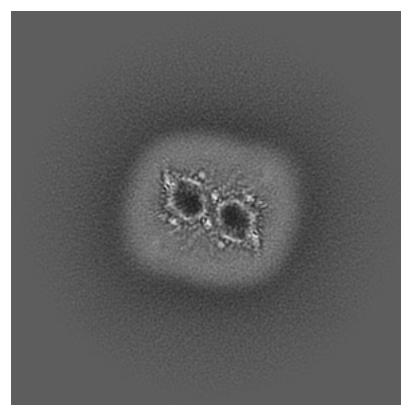
6.1.1 Primary map



X



Y

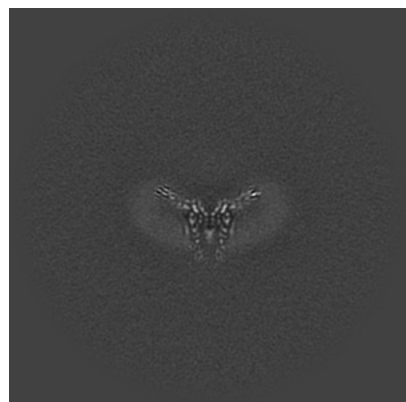


Z

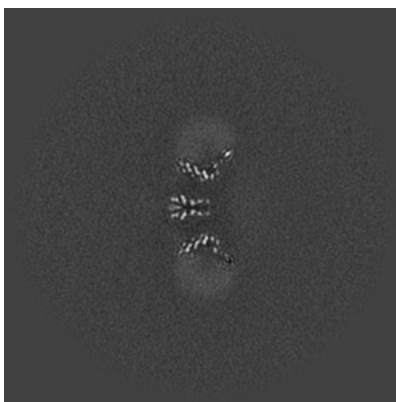
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

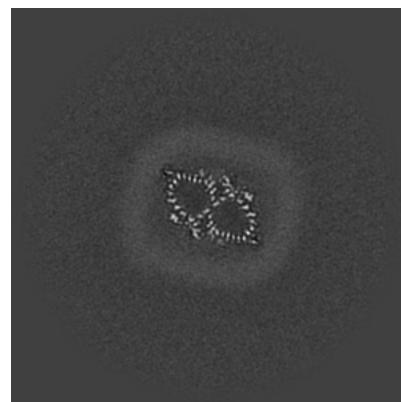
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

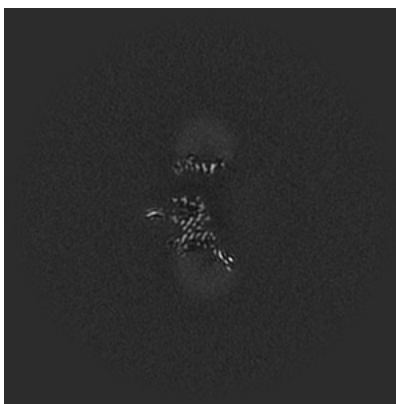
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

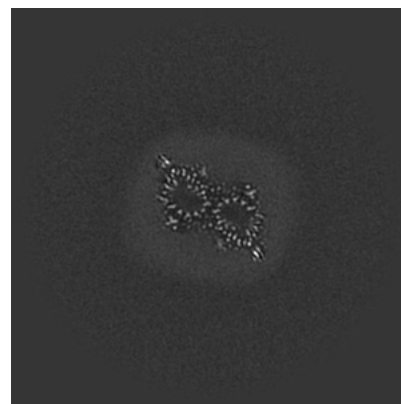
6.3.1 Primary map



X Index: 140



Y Index: 174



Z Index: 166

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.409. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

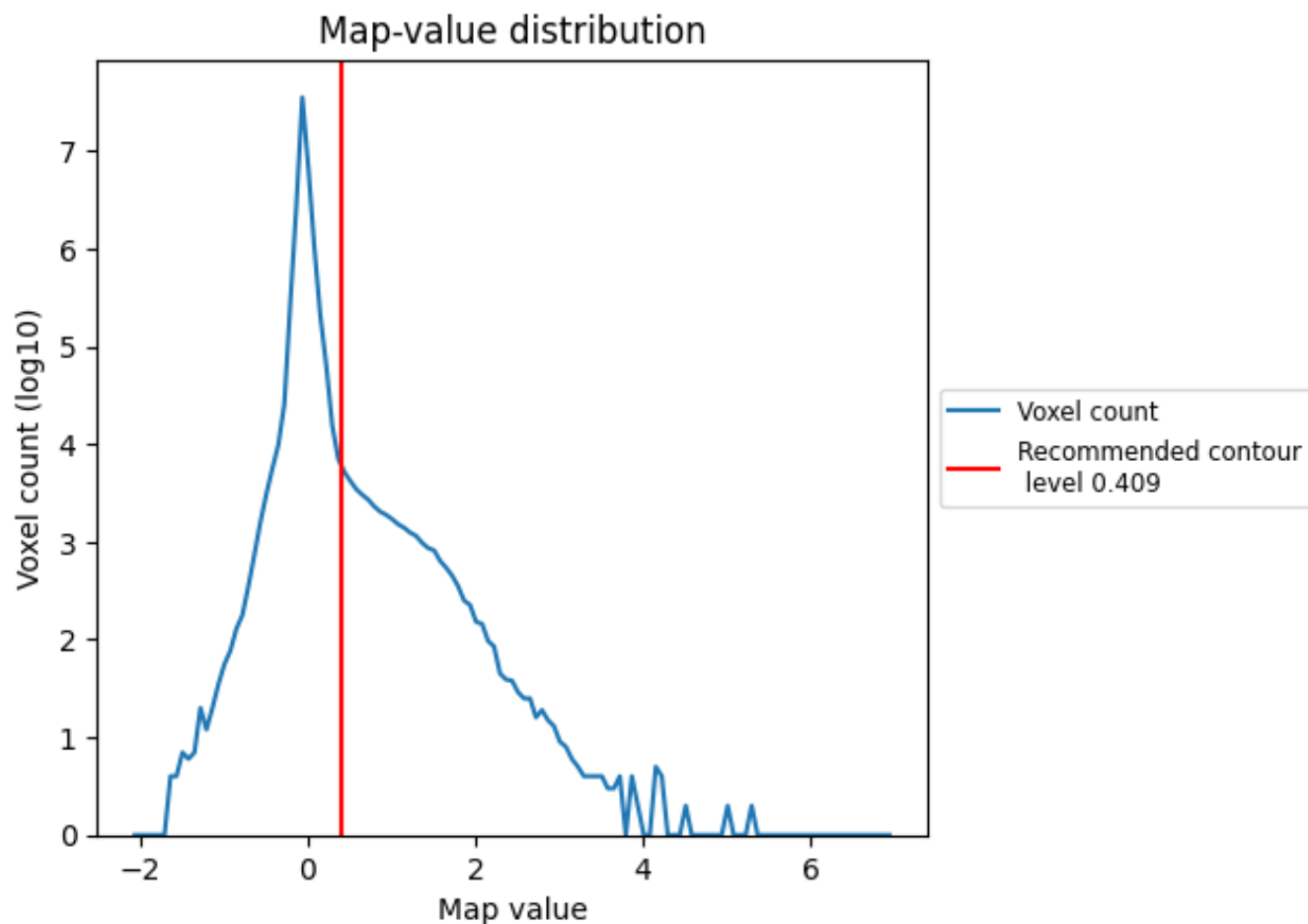
6.5 Mask visualisation

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

7 Map analysis [i](#)

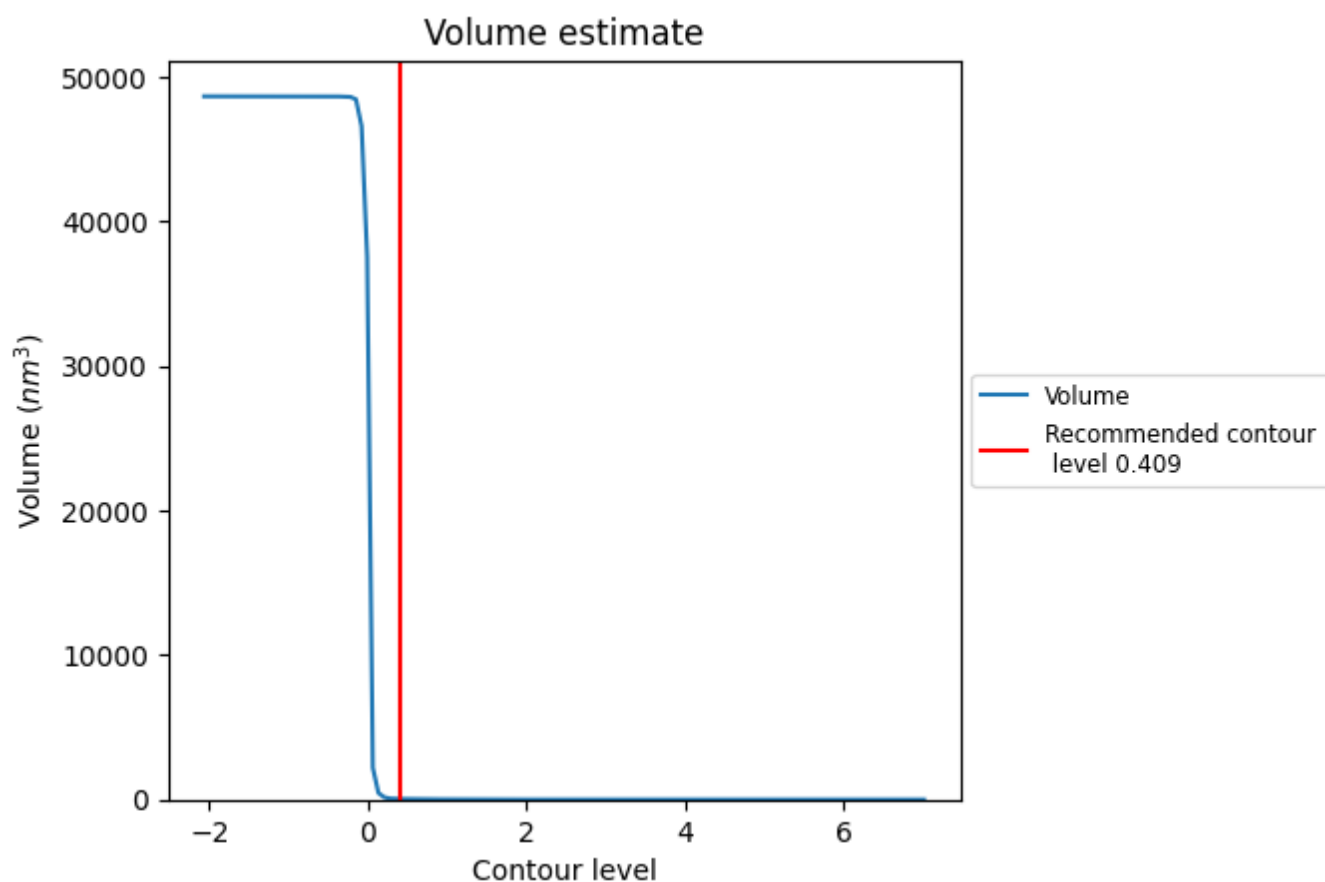
This section contains the results of statistical analysis of the map.

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.

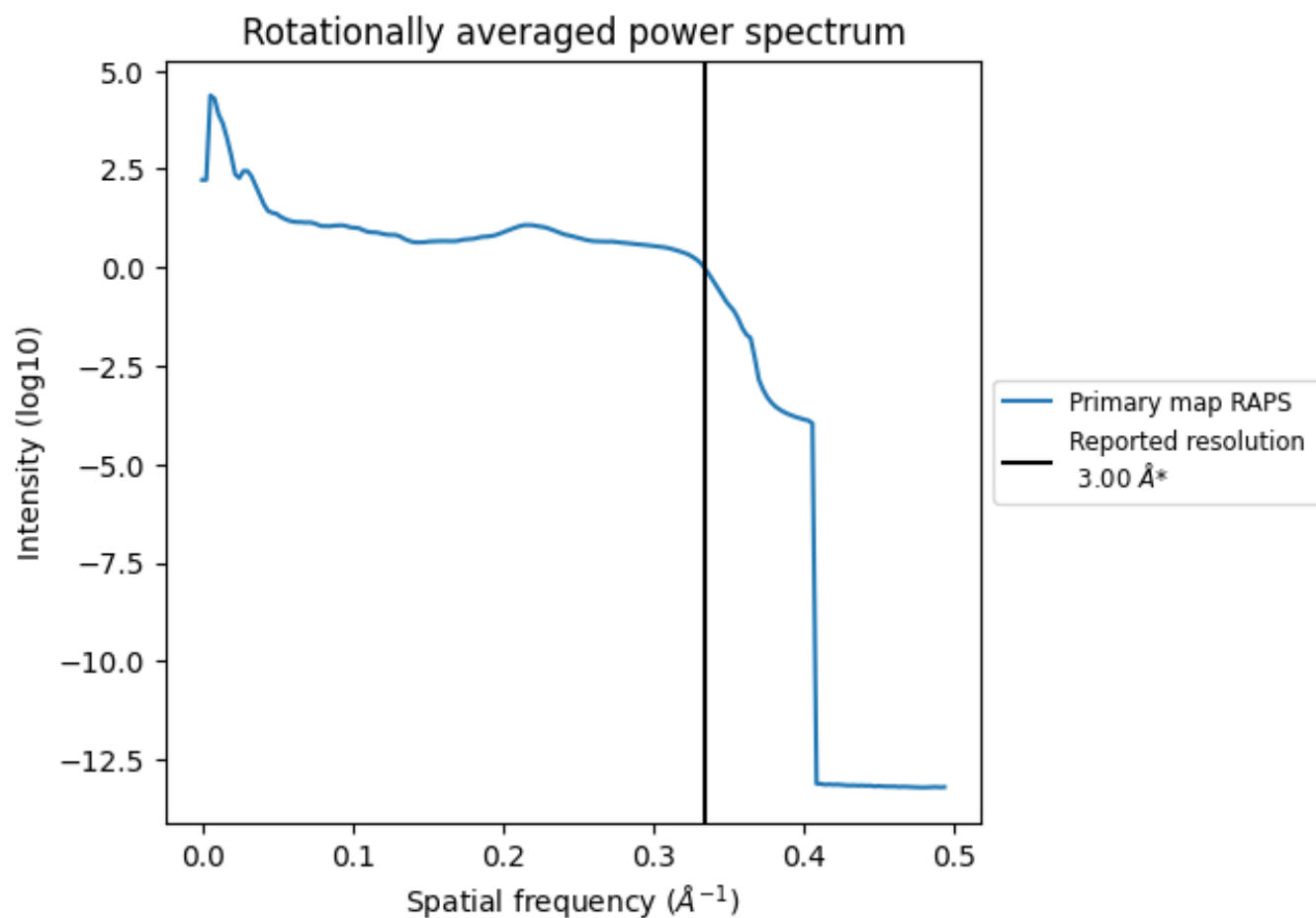
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm^3 ; this corresponds to an approximate mass of 38 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 0.333 Å⁻¹

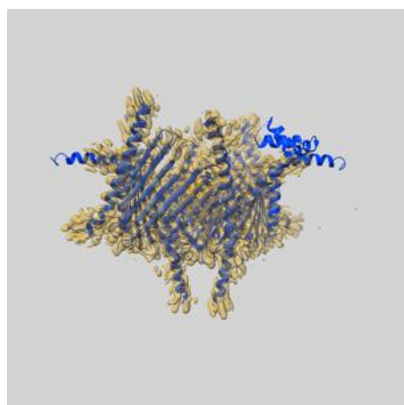
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

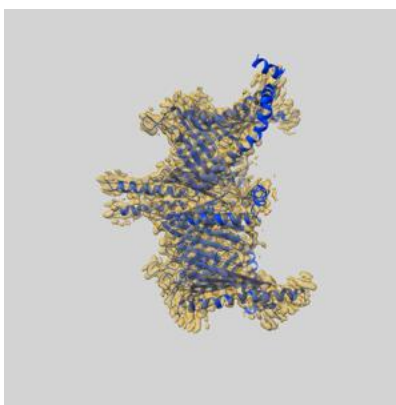
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30421 and PDB model 7CP9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

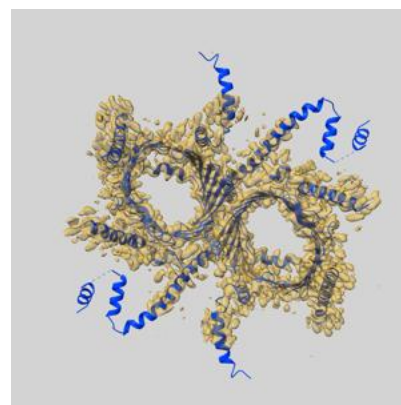
9.1 Map-model overlay [i](#)



X



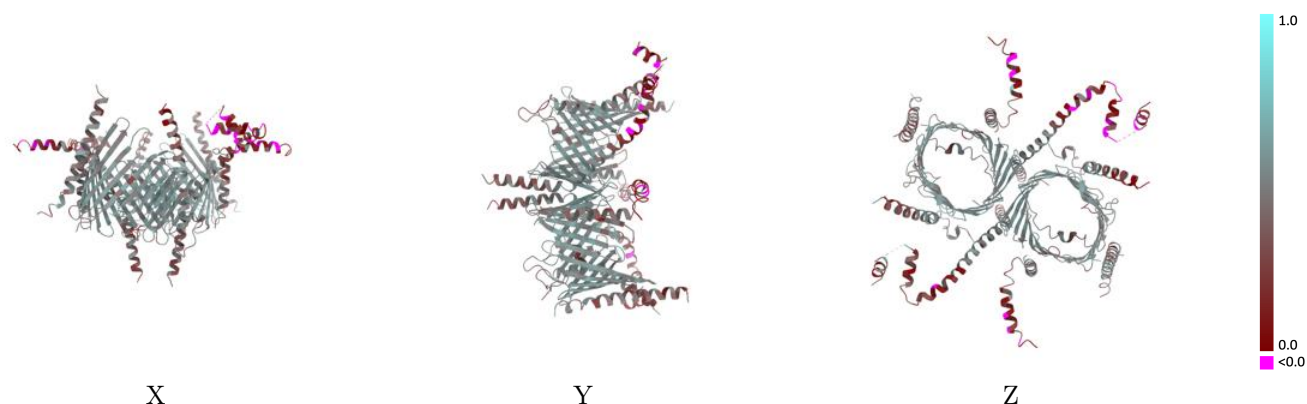
Y



Z

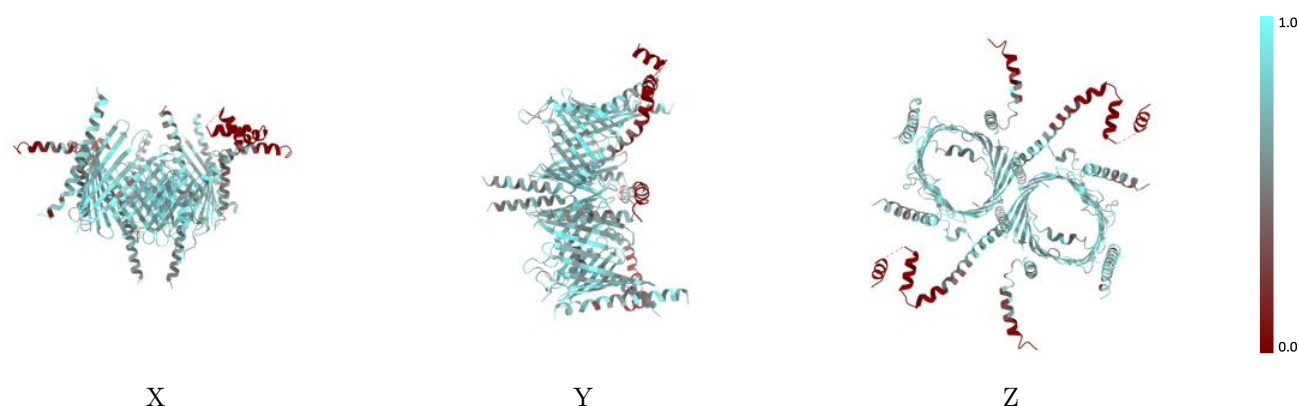
The images above show the 3D surface view of the map at the recommended contour level 0.409 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



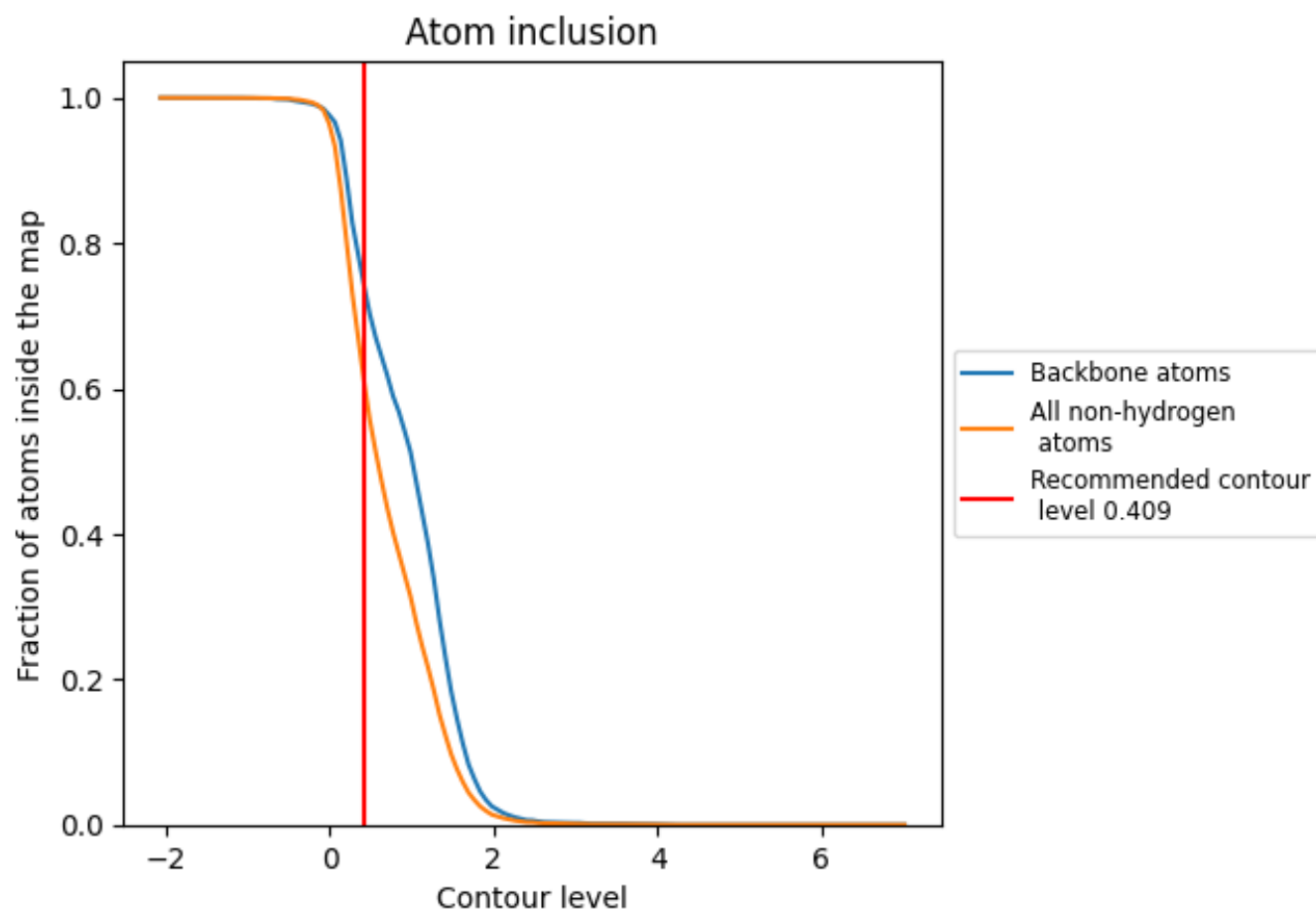
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.409).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 62% 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 (0.409) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6171	<div></div> 0.4490
A	<div></div> 0.6817	<div></div> 0.4420
B	<div></div> 0.6667	<div></div> 0.4100
C	<div></div> 0.4119	<div></div> 0.3280
D	<div></div> 0.3870	<div></div> 0.2760
E	<div></div> 0.6465	<div></div> 0.4500
F	<div></div> 0.6230	<div></div> 0.4280
G	<div></div> 0.4241	<div></div> 0.3970
H	<div></div> 0.3984	<div></div> 0.3350
I	<div></div> 0.7240	<div></div> 0.5080
J	<div></div> 0.7111	<div></div> 0.5160

1.0

0.0

<0.0