



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 07:21 AM UTC

PDB ID : 7VBY / pdb_00007vby
EMDB ID : EMD-31885
Title : Tom core complex with Tom20 and Tom22 subunits.
Authors : Liu, D.S.; Sui, S.F.
Deposited on : 2021-09-01
Resolution : 2.54 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

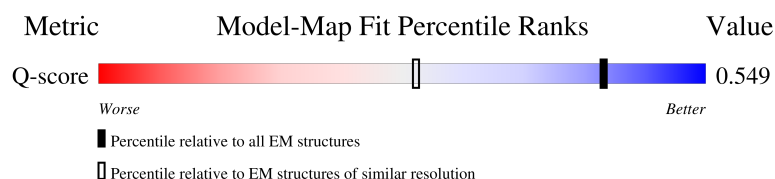
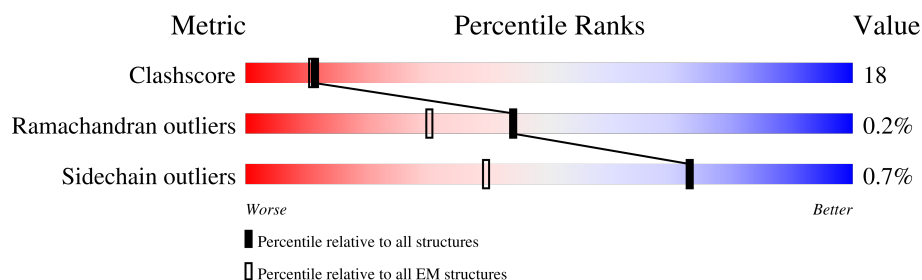
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.54 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	7403 (2.04 - 3.04)

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	B	828	 24% 10% 65%
1	I	828	 23% 11% 65%
2	A	74	 14% 32% 26% 42%
2	F	74	 14% 36% 22% 42%

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Mol	Chain	Length	Quality of chain
3	D	51	24%51%20%29%
3	E	51	22%41%29%29%
4	G	55	16%62%36%
4	J	55	20%58%40%
5	C	142	11%19%21%60%
5	H	142	11%23%17%61%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9463 atoms, of which 1256 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 Translocase of the Outer Membrane.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	43	Total	C	N	O	0	0
			354	227	67	60		
2	F	43	Total	C	N	O	0	0
			354	227	67	60		

- Molecule 3 is a protein called Mitochondrial import receptor subunit TOM5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	36	Total	C	N	O	S	0	0
			304	200	53	49	2		
3	E	36	Total	C	N	O	S	0	0
			304	200	53	49	2		

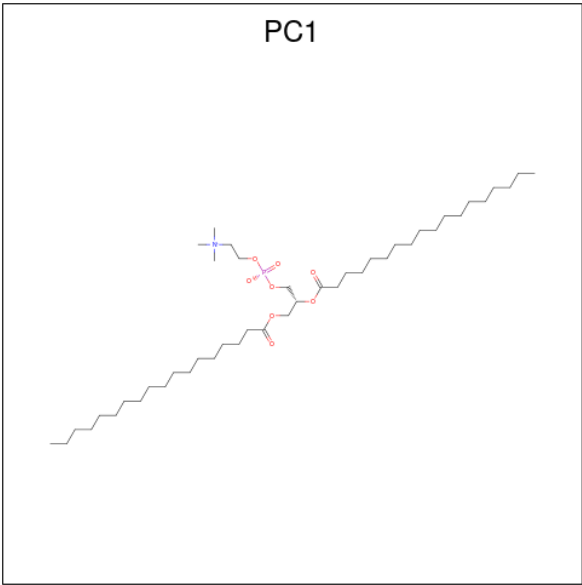
- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	54	Total	C	N	O	S	0	0
			433	289	74	69	1		
4	J	54	Total	C	N	O	S	0	0
			433	289	74	69	1		

- Molecule 5 is a protein called Mitochondrial import receptor subunit TOM22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	56	Total	C	N	O	S	0	0
			458	297	77	81	3		
5	C	57	Total	C	N	O	S	0	0
			463	300	78	82	3		

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



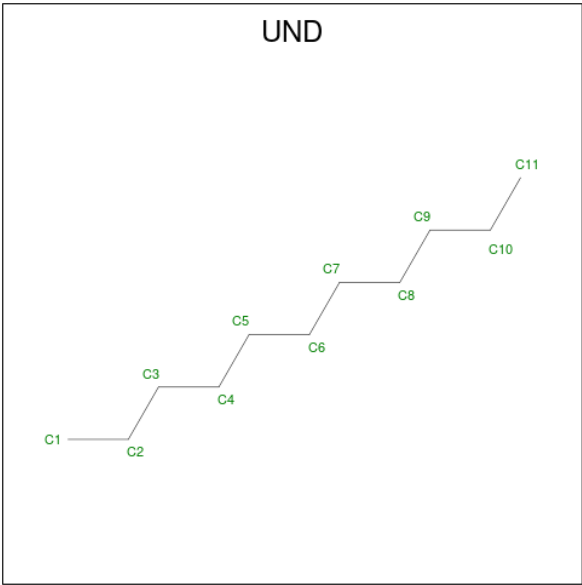
Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	I	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	I	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	I	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
6	H	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	H	N	O	P
			142	44	88	1	8	1
6	C	1	Total	C	H	N	O	P
			142	44	88	1	8	1

- Molecule 7 is UNDECANE (CCD ID: UND) (formula: C₁₁H₂₄).



Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	C	H	0
			35	11	24	
7	B	1	Total	C	H	0
			35	11	24	
7	A	1	Total	C	H	0
			35	11	24	
7	F	1	Total	C	H	0
			35	11	24	
7	G	1	Total	C	H	0
			35	11	24	
7	G	1	Total	C	H	0
			35	11	24	
7	I	1	Total	C	H	0
			35	11	24	
7	I	1	Total	C	H	0
			35	11	24	
7	I	1	Total	C	H	0
			35	11	24	

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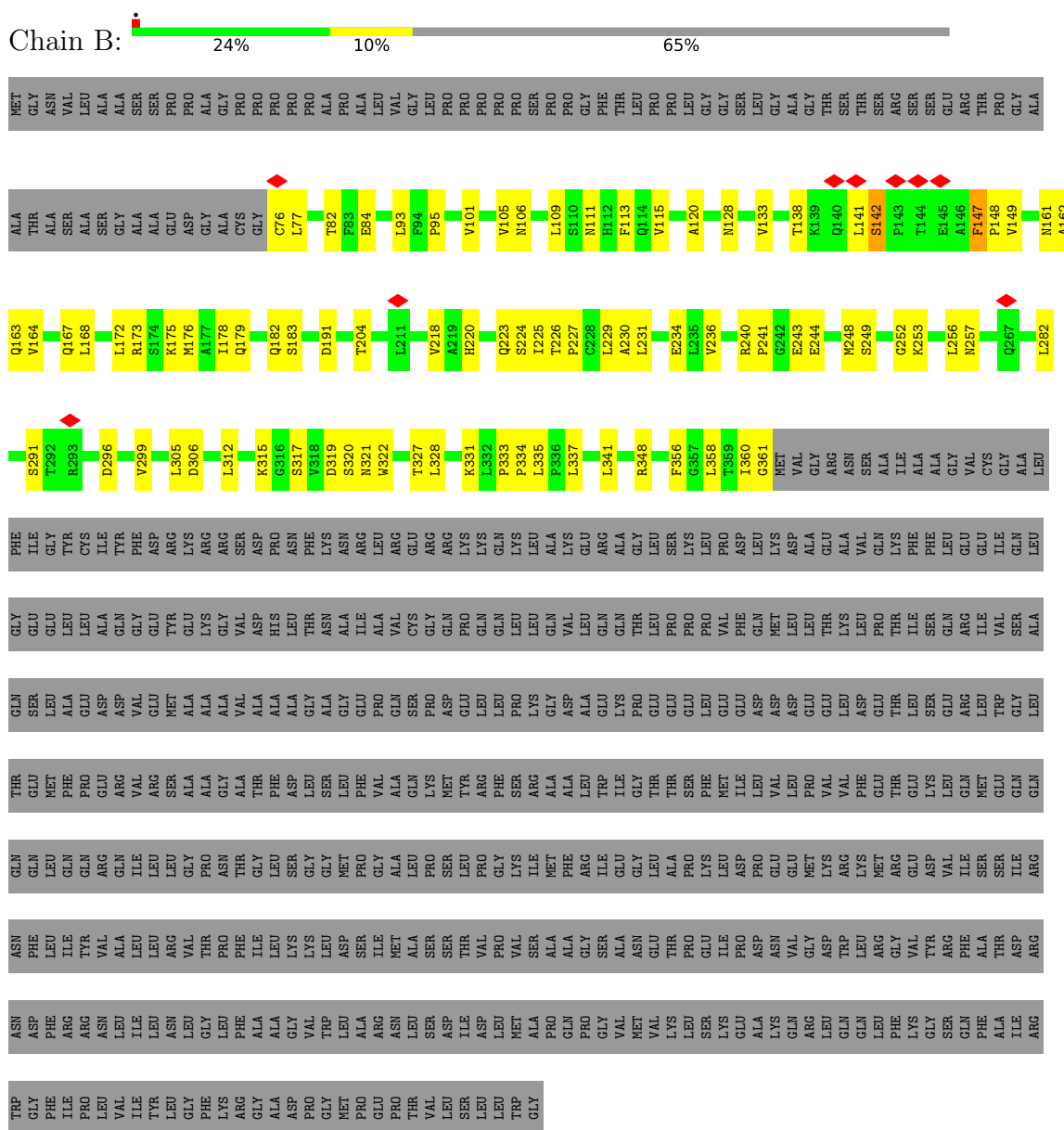
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Mol	Chain	Residues	Atoms			AltConf
7	H	1	Total	C	H	0
			35	11	24	
7	C	1	Total	C	H	0
			35	11	24	
7	J	1	Total	C	H	0
			35	11	24	

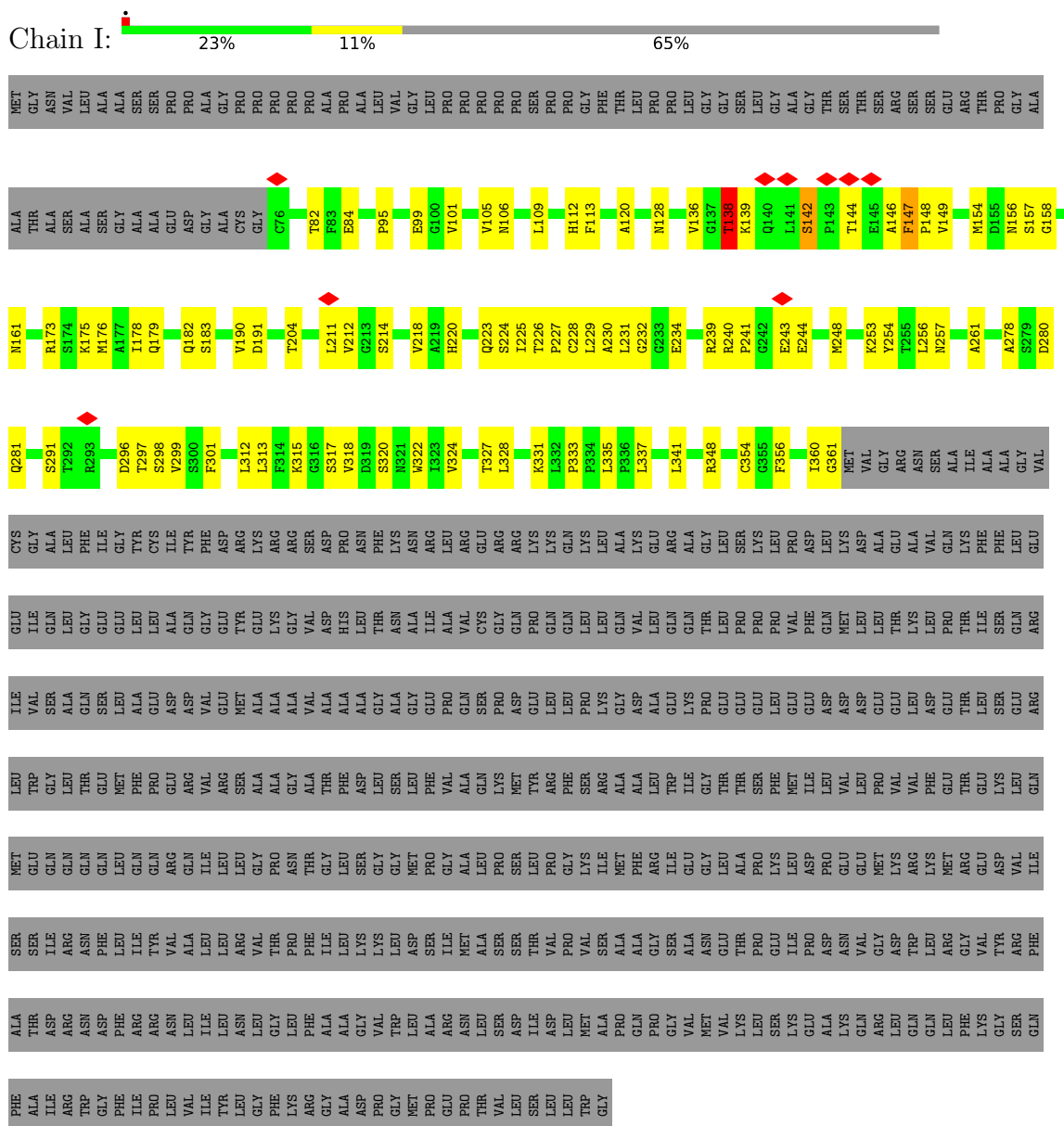
3 Residue-property plots

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.

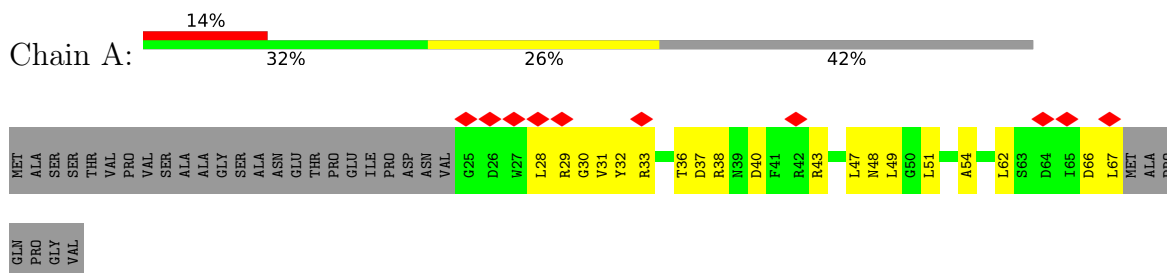
• Molecule 1: Translocase of the Outer Membrane



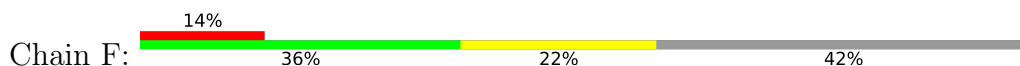
• Molecule 1: Translocase of the Outer Membrane

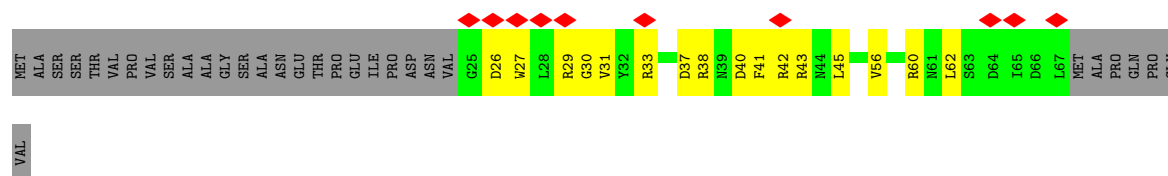


- Molecule 2: Mitochondrial import receptor subunit TOM6 homolog



- Molecule 2: Mitochondrial import receptor subunit TOM6 homolog





- Molecule 3: Mitochondrial import receptor subunit TOM5 homolog



- Molecule 3: Mitochondrial import receptor subunit TOM5 homolog



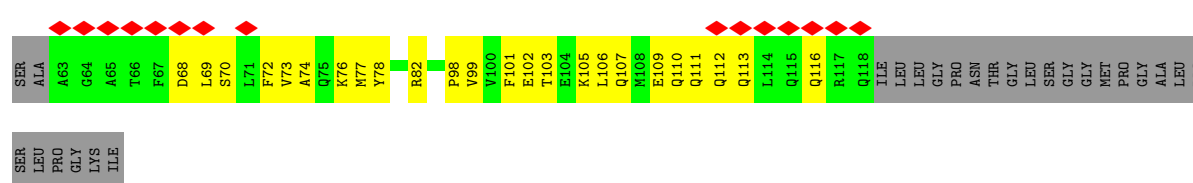
- Molecule 4: Mitochondrial import receptor subunit TOM7 homolog



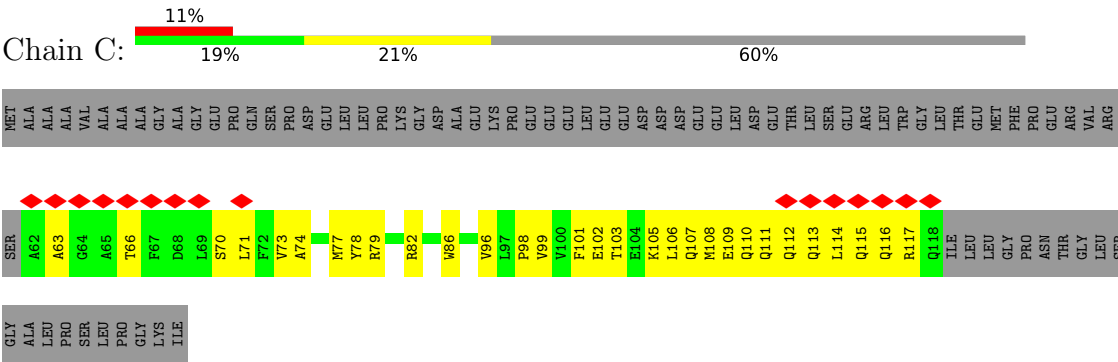
- Molecule 4: Mitochondrial import receptor subunit TOM7 homolog



- Molecule 5: Mitochondrial import receptor subunit TOM22 homolog



- Molecule 5: Mitochondrial import receptor subunit TOM22 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288736	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.107	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.302	Depositor
Map size ($\text{\AA}$)	269.856, 269.856, 269.856	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8433, 0.8433, 0.8433	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, UND

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	B	0.29	0/2239	0.44	3/3039 (0.1%)
1	I	0.32	0/2239	0.52	5/3039 (0.2%)
2	A	0.20	0/361	0.44	0/488
2	F	0.21	0/361	0.49	0/488
3	D	0.20	0/308	0.48	0/410
3	E	0.15	0/308	0.33	0/410
4	G	0.19	0/445	0.32	0/599
4	J	0.19	0/445	0.29	0/599
5	C	0.18	0/471	0.29	0/634
5	H	0.20	0/466	0.35	0/627
All	All	0.26	0/7643	0.44	8/10333 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	147	PHE	CA-CB-CG	-6.14	107.66	113.80
1	I	147	PHE	CA-C-O	-5.80	112.22	120.16
1	I	147	PHE	N-CA-C	5.71	122.43	109.81
1	B	147	PHE	N-CA-C	5.69	122.39	109.81
1	B	147	PHE	CA-C-O	-5.56	112.54	120.16
1	B	147	PHE	CA-CB-CG	-5.29	108.51	113.80
1	I	138	THR	CB-CA-C	-5.24	104.15	111.85
1	I	147	PHE	CB-CA-C	5.03	120.07	110.17

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	B	2189	0	2171	83	0
1	I	2189	0	2171	83	0
2	A	354	0	349	19	0
2	F	354	0	349	12	0
3	D	304	0	339	10	0
3	E	304	0	339	19	0
4	G	433	0	456	21	0
4	J	433	0	456	27	0
5	C	463	0	470	33	0
5	H	458	0	465	21	0
6	A	54	88	88	8	0
6	B	162	264	264	16	0
6	C	108	176	176	15	0
6	D	54	88	88	0	0
6	H	54	88	88	10	0
6	I	162	264	264	17	0
7	A	11	24	24	0	0
7	B	22	48	48	0	0
7	C	11	24	24	0	0
7	F	11	24	24	0	0
7	G	22	48	48	0	0
7	H	11	24	24	0	0
7	I	33	72	72	1	0
7	J	11	24	24	0	0
All	All	8207	1256	8821	304	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 18.

All (304) 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)
1:B:243:GLU:HA	3:E:20:MET:HE1	1.30	1.06
1:I:312:LEU:HD11	1:I:328:LEU:HD11	1.44	0.99
2:A:29:ARG:HG3	2:A:33:ARG:HH21	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:903:PC1:H332	6:H:201:PC1:C32	1.93	0.98
2:F:29:ARG:HG3	2:F:33:ARG:HH11	1.30	0.95
1:I:328:LEU:CD2	6:I:901:PC1:H2I1	1.98	0.93
1:I:328:LEU:HD22	6:I:901:PC1:H2I1	1.48	0.93
1:B:312:LEU:HD11	1:B:328:LEU:HD11	1.47	0.93
4:G:40:ALA:HB2	4:G:47:PRO:HD3	1.51	0.89
1:B:106:ASN:HB2	1:B:361:GLY:HA3	1.53	0.89
1:I:328:LEU:HB2	6:I:901:PC1:H2H1	1.55	0.89
1:I:226:THR:HG22	1:I:229:LEU:HB3	1.54	0.88
1:B:204:THR:HB	1:B:218:VAL:HG22	1.55	0.88
1:B:226:THR:HG22	1:B:229:LEU:HB3	1.55	0.88
4:J:40:ALA:HB2	4:J:47:PRO:HD3	1.55	0.87
2:F:29:ARG:HG3	2:F:33:ARG:NH1	1.91	0.86
4:G:12:LEU:HD23	1:I:211:LEU:HD21	1.59	0.84
1:I:312:LEU:CD1	1:I:328:LEU:HD11	2.08	0.83
1:I:106:ASN:HB2	1:I:361:GLY:HA3	1.59	0.82
6:B:903:PC1:H332	6:H:201:PC1:H321	1.60	0.81
1:B:322:TRP:CE3	6:B:902:PC1:H331	2.15	0.81
1:B:312:LEU:CD1	1:B:328:LEU:HD11	2.10	0.80
5:C:82:ARG:NH1	6:C:201:PC1:H143	1.95	0.80
1:B:204:THR:HB	1:B:218:VAL:CG2	2.13	0.79
1:I:204:THR:HG22	1:I:218:VAL:HB	1.64	0.78
1:I:226:THR:OG1	1:I:227:PRO:HD2	1.84	0.78
2:A:29:ARG:HG3	2:A:33:ARG:NH2	1.98	0.77
4:J:41:ASP:HB2	4:J:44:MET:HE2	1.67	0.77
1:B:226:THR:OG1	1:B:227:PRO:HD2	1.84	0.77
2:A:48:ASN:HD22	1:I:297:THR:HG22	1.50	0.77
4:G:41:ASP:HB2	4:G:44:MET:HE2	1.68	0.75
6:B:903:PC1:C33	6:H:201:PC1:H321	2.17	0.75
6:A:101:PC1:H11	1:I:322:TRP:NE1	2.00	0.75
3:E:29:ARG:HG2	3:E:29:ARG:HH11	1.52	0.74
5:C:82:ARG:HH11	6:C:201:PC1:H143	1.50	0.73
5:C:86:TRP:HB2	6:C:202:PC1:H11	1.70	0.73
6:B:903:PC1:C33	6:H:201:PC1:C32	2.66	0.73
6:B:903:PC1:H332	6:H:201:PC1:H322	1.70	0.73
1:B:167:GLN:OE1	1:B:173:ARG:NE	2.20	0.72
1:I:204:THR:CG2	1:I:218:VAL:HB	2.19	0.72
2:F:30:GLY:HA2	2:F:33:ARG:CZ	2.19	0.72
4:G:53:LEU:HD21	6:C:201:PC1:H3C2	1.72	0.72
3:E:15:GLU:OE2	3:E:18:ARG:HB2	1.90	0.71
1:I:240:ARG:HB3	1:I:241:PRO:HD2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:30:GLY:HA2	2:A:33:ARG:CZ	2.20	0.71
1:I:328:LEU:HB2	6:I:901:PC1:C2H	2.20	0.70
2:A:66:ASP:O	2:A:67:LEU:HD23	1.91	0.70
3:D:13:PRO:HB2	3:D:15:GLU:OE1	1.92	0.70
3:D:34:TYR:CE1	3:D:38:LEU:HD11	2.27	0.69
1:B:223:GLN:NE2	3:E:38:LEU:O	2.25	0.69
4:G:25:TRP:CZ3	1:I:154:MET:HE1	2.27	0.69
1:I:225:ILE:HG13	1:I:231:LEU:HD12	1.74	0.69
6:I:901:PC1:H2I3	5:H:98:PRO:CG	2.21	0.69
1:I:138:THR:OG1	7:I:906:UND:H111	1.92	0.69
1:I:256:LEU:HG	1:I:257:ASN:H	1.57	0.69
1:B:111:ASN:HB2	4:J:41:ASP:OD2	1.92	0.69
5:C:86:TRP:HE3	6:C:202:PC1:H31	1.57	0.69
1:B:225:ILE:HG13	1:B:231:LEU:HD12	1.74	0.68
4:J:8:ALA:O	4:J:12:LEU:HD23	1.93	0.68
1:B:348:ARG:HH12	6:B:902:PC1:H111	1.57	0.68
1:B:183:SER:HA	4:J:24:ARG:HD2	1.76	0.68
3:E:34:TYR:O	3:E:38:LEU:HD13	1.93	0.68
4:J:5:SER:O	4:J:9:LYS:NZ	2.25	0.68
1:B:256:LEU:HG	1:B:257:ASN:H	1.59	0.67
3:E:34:TYR:CE1	3:E:38:LEU:HD11	2.30	0.67
1:I:315:LYS:HB2	1:I:327:THR:HG22	1.75	0.67
1:I:136:VAL:HG12	1:I:146:ALA:HB3	1.76	0.67
5:C:113:GLN:O	5:C:116:GLN:HG3	1.95	0.66
4:J:16:PHE:O	4:J:20:GLN:HG3	1.96	0.65
5:C:105:LYS:HG2	5:C:109:GLU:OE2	1.96	0.65
6:A:101:PC1:H281	1:I:301:PHE:HB2	1.79	0.65
4:G:16:PHE:O	4:G:20:GLN:HG3	1.97	0.65
6:B:903:PC1:C13	6:H:201:PC1:O14	2.45	0.64
4:G:5:SER:O	4:G:8:ALA:N	2.31	0.64
6:I:901:PC1:H2I3	5:H:98:PRO:CB	2.27	0.64
5:H:68:ASP:OD1	5:H:69:LEU:N	2.30	0.64
2:A:47:LEU:HD21	6:A:101:PC1:H31	1.79	0.64
6:A:101:PC1:H11	1:I:322:TRP:HE1	1.61	0.63
2:F:37:ASP:OD1	2:F:40:ASP:N	2.29	0.63
4:G:12:LEU:HD23	1:I:211:LEU:CD2	2.28	0.63
4:G:40:ALA:HB2	4:G:47:PRO:CD	2.27	0.63
4:G:38:ARG:HH21	1:I:112:HIS:CE1	2.18	0.62
4:J:10:GLN:HA	4:J:13:GLN:OE1	1.98	0.62
1:B:183:SER:HA	4:J:24:ARG:CD	2.29	0.62
5:H:105:LYS:HG2	5:H:109:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:O	1:B:183:SER:OG	2.12	0.62
3:D:31:PHE:HB2	1:I:248:MET:HE2	1.82	0.62
4:J:7:GLU:HA	4:J:10:GLN:HE22	1.65	0.62
3:E:22:GLU:O	3:E:25:ILE:HG22	1.99	0.61
1:I:214:SER:HA	1:I:239:ARG:O	2.01	0.61
1:I:175:LYS:HB3	1:I:191:ASP:OD1	2.00	0.61
5:C:78:TYR:CZ	5:C:82:ARG:HD2	2.35	0.61
1:I:328:LEU:CB	6:I:901:PC1:C2H	2.77	0.61
2:A:28:LEU:O	2:A:31:VAL:HG12	2.01	0.60
1:B:248:MET:HE2	3:E:31:PHE:HB2	1.83	0.60
5:H:78:TYR:CZ	5:H:82:ARG:HD2	2.36	0.60
1:B:95:PRO:HD2	1:B:317:SER:HB3	1.83	0.60
6:B:903:PC1:C33	6:H:201:PC1:H322	2.31	0.60
4:G:46:GLU:CD	4:G:47:PRO:HD2	2.27	0.60
1:B:230:ALA:HB3	1:B:253:LYS:HG2	1.83	0.59
2:F:27:TRP:O	2:F:31:VAL:HG23	2.01	0.59
1:I:154:MET:HE2	6:C:201:PC1:H322	1.84	0.59
5:C:79:ARG:HH22	6:C:201:PC1:H112	1.68	0.59
5:C:99:VAL:O	5:C:103:THR:HG23	2.03	0.58
1:B:141:LEU:HD12	1:B:142:SER:HB3	1.84	0.58
1:B:218:VAL:HG12	1:B:236:VAL:HG22	1.86	0.58
1:I:328:LEU:HD23	6:I:901:PC1:H2I1	1.82	0.58
1:B:163:GLN:OE1	1:B:175:LYS:HD2	2.04	0.58
1:B:82:THR:CG2	1:B:84:GLU:HG2	2.34	0.58
1:B:77:LEU:HD13	1:B:224:SER:O	2.04	0.58
3:E:15:GLU:O	3:E:15:GLU:HG3	2.04	0.57
5:C:82:ARG:NH1	6:C:201:PC1:C14	2.68	0.57
1:B:282:LEU:HD13	1:B:305:LEU:HD21	1.87	0.57
1:B:291:SER:HB3	1:B:296:ASP:OD1	2.04	0.56
1:B:105:VAL:HG22	1:B:360:ILE:HD12	1.87	0.56
1:B:168:LEU:HB2	1:B:172:LEU:HB3	1.87	0.56
1:I:230:ALA:HB3	1:I:253:LYS:HG2	1.88	0.56
5:H:99:VAL:O	5:H:103:THR:HG23	2.05	0.56
4:J:46:GLU:CD	4:J:47:PRO:HD2	2.29	0.56
1:B:141:LEU:CD2	1:B:167:GLN:HG3	2.35	0.56
1:B:321:ASN:OD1	6:B:902:PC1:H142	2.06	0.56
1:I:120:ALA:HB3	1:I:128:ASN:OD1	2.05	0.56
1:B:282:LEU:HD13	1:B:305:LEU:CD2	2.35	0.56
4:G:44:MET:HB3	4:G:45:PRO:HD2	1.88	0.56
3:E:15:GLU:HG3	3:E:18:ARG:HB3	1.88	0.55
1:I:299:VAL:HG12	1:I:320:SER:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:312:LEU:HD13	5:H:102:GLU:HG3	1.87	0.55
1:B:321:ASN:OD1	6:B:902:PC1:C14	2.55	0.55
2:A:32:TYR:O	2:A:36:THR:HG23	2.07	0.54
1:B:141:LEU:HD12	1:B:142:SER:N	2.22	0.54
6:I:901:PC1:H2I3	5:H:98:PRO:HB3	1.89	0.54
4:J:41:ASP:HB2	4:J:44:MET:CE	2.37	0.54
6:B:903:PC1:H133	6:H:201:PC1:O14	2.07	0.54
4:G:23:ILE:HG21	1:I:178:ILE:HD13	1.90	0.54
1:I:318:VAL:HG23	1:I:324:VAL:HG12	1.88	0.54
5:C:110:GLN:O	5:C:113:GLN:HG3	2.07	0.54
1:I:95:PRO:HD2	1:I:317:SER:HB3	1.90	0.54
1:I:291:SER:HB3	1:I:296:ASP:OD1	2.08	0.53
1:B:109:LEU:HD12	1:B:113:PHE:CE2	2.43	0.53
5:C:112:GLN:O	5:C:115:GLN:HG3	2.08	0.53
3:D:21:ARG:O	3:D:25:ILE:HG12	2.08	0.53
5:C:86:TRP:NE1	6:C:202:PC1:H132	2.24	0.53
1:B:93:LEU:O	1:B:315:LYS:HG2	2.09	0.52
2:F:40:ASP:OD2	2:F:42:ARG:HB2	2.09	0.52
5:C:113:GLN:O	5:C:117:ARG:HG3	2.10	0.52
2:F:38:ARG:HA	2:F:43:ARG:NH1	2.24	0.52
1:I:220:HIS:CE1	1:I:234:GLU:HG3	2.45	0.52
1:I:328:LEU:HB3	6:I:901:PC1:H2H2	1.91	0.52
1:B:240:ARG:HB3	1:B:241:PRO:HD2	1.91	0.52
4:J:38:ARG:HG2	4:J:38:ARG:HH11	1.76	0.51
1:B:191:ASP:OD1	1:B:204:THR:HG23	2.11	0.51
4:J:44:MET:HB3	4:J:45:PRO:HD2	1.92	0.51
1:B:82:THR:HG22	1:B:84:GLU:HG2	1.91	0.51
3:E:28:ILE:O	3:E:32:LEU:HD13	2.11	0.51
1:B:109:LEU:HD22	4:J:51:SER:HB3	1.91	0.51
5:H:112:GLN:O	5:H:116:GLN:OE1	2.28	0.51
3:D:21:ARG:HA	3:D:21:ARG:HE	1.76	0.51
4:J:5:SER:HB3	4:J:8:ALA:CB	2.41	0.51
1:B:120:ALA:HB3	1:B:128:ASN:OD1	2.11	0.50
2:A:54:ALA:HB1	6:A:101:PC1:H2D1	1.92	0.50
1:B:220:HIS:HD2	1:B:234:GLU:CB	2.24	0.50
5:C:86:TRP:CE3	6:C:202:PC1:H31	2.44	0.50
4:G:51:SER:HB3	1:I:109:LEU:HD22	1.94	0.50
1:I:254:TYR:HB2	6:I:902:PC1:H2B2	1.94	0.50
3:D:28:ILE:O	3:D:32:LEU:HD13	2.11	0.50
1:B:133:VAL:HG23	4:J:31:VAL:HG11	1.93	0.50
1:B:312:LEU:HD13	5:C:102:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:86:TRP:HB2	6:C:202:PC1:C1	2.42	0.50
4:J:38:ARG:HG2	4:J:38:ARG:NH1	2.26	0.49
4:G:15:LEU:C	4:G:15:LEU:HD23	2.37	0.49
1:B:178:ILE:HD13	4:J:23:ILE:HG21	1.95	0.49
5:H:110:GLN:O	5:H:113:GLN:HG3	2.12	0.49
1:B:226:THR:HG22	1:B:229:LEU:CB	2.36	0.49
2:A:30:GLY:HA2	2:A:33:ARG:NH1	2.27	0.49
1:B:243:GLU:HA	3:E:20:MET:CE	2.22	0.49
5:C:79:ARG:NH2	6:C:201:PC1:H112	2.27	0.49
1:B:252:GLY:HA3	6:B:901:PC1:H3E2	1.94	0.48
1:B:348:ARG:NH1	6:B:902:PC1:H111	2.26	0.48
3:D:13:PRO:HD2	3:D:15:GLU:OE2	2.13	0.48
3:D:15:GLU:HG2	3:D:16:MET:N	2.27	0.48
6:I:901:PC1:H2I3	5:H:98:PRO:HG2	1.95	0.48
1:B:335:LEU:HB3	1:B:337:LEU:HD13	1.95	0.48
4:G:40:ALA:HB2	4:G:46:GLU:HA	1.95	0.48
2:A:47:LEU:HD21	6:A:101:PC1:C3	2.44	0.48
5:C:86:TRP:CE2	6:C:202:PC1:H132	2.48	0.48
5:H:74:ALA:HA	5:H:77:MET:HE3	1.95	0.48
1:I:142:SER:C	1:I:144:THR:H	2.21	0.48
1:B:226:THR:HG23	1:B:229:LEU:H	1.77	0.48
1:B:360:ILE:CD1	5:H:101:PHE:HZ	2.27	0.48
2:A:38:ARG:HH21	1:I:348:ARG:CZ	2.27	0.47
4:G:23:ILE:HG21	1:I:178:ILE:CD1	2.45	0.47
1:I:156:ASN:O	6:C:201:PC1:H141	2.13	0.47
4:G:41:ASP:CB	4:G:44:MET:HE2	2.41	0.47
1:B:306:ASP:OD1	1:B:306:ASP:O	2.31	0.47
4:G:7:GLU:HG2	4:G:8:ALA:N	2.28	0.47
1:I:161:ASN:OD1	1:I:179:GLN:HG3	2.14	0.47
1:I:299:VAL:CG1	1:I:320:SER:HB3	2.45	0.47
5:C:63:ALA:O	5:C:66:THR:HG22	2.14	0.47
1:I:261:ALA:HB1	6:I:902:PC1:H391	1.96	0.47
1:B:319:ASP:OD1	1:B:320:SER:N	2.48	0.46
1:B:358:LEU:HD22	6:I:901:PC1:H282	1.96	0.46
1:I:341:LEU:HD23	1:I:356:PHE:HB3	1.97	0.46
1:B:162:ALA:HB3	1:B:178:ILE:HG12	1.98	0.46
1:I:147:PHE:O	1:I:149:VAL:N	2.49	0.46
1:I:280:ASP:OD1	1:I:281:GLN:HG3	2.15	0.46
5:C:107:GLN:O	5:C:110:GLN:HG3	2.16	0.46
2:F:56:VAL:O	2:F:60:ARG:HG3	2.16	0.46
1:I:176:MET:HG2	1:I:190:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASN:OD1	1:B:179:GLN:HG3	2.16	0.46
1:B:220:HIS:HD2	1:B:234:GLU:HB3	1.81	0.46
3:D:34:TYR:O	3:D:38:LEU:HD13	2.15	0.46
1:I:82:THR:HG22	1:I:84:GLU:H	1.81	0.46
1:I:105:VAL:HG22	1:I:360:ILE:HD12	1.97	0.46
1:B:82:THR:HG21	1:B:84:GLU:HG2	1.98	0.46
4:J:40:ALA:HB2	4:J:47:PRO:CD	2.36	0.46
3:E:15:GLU:HG3	3:E:18:ARG:CB	2.46	0.45
1:I:154:MET:CE	1:I:158:GLY:HA2	2.46	0.45
1:B:138:THR:HG22	4:J:38:ARG:CZ	2.46	0.45
1:B:244:GLU:OE2	3:E:21:ARG:NH2	2.47	0.45
2:A:49:LEU:HD11	6:I:902:PC1:H3I2	1.97	0.45
1:I:157:SER:HA	6:C:201:PC1:H141	1.98	0.45
5:H:70:SER:O	5:H:73:VAL:HG22	2.16	0.45
1:I:99:GLU:HA	1:I:354:CYS:O	2.17	0.45
1:I:331:LYS:O	1:I:333:PRO:HD3	2.16	0.45
5:C:74:ALA:HA	5:C:77:MET:HE3	1.99	0.45
4:G:4:LEU:HD12	4:G:4:LEU:O	2.17	0.45
1:I:223:GLN:HG2	1:I:224:SER:N	2.32	0.45
4:J:7:GLU:HA	4:J:10:GLN:NE2	2.32	0.45
1:I:226:THR:HG23	1:I:229:LEU:H	1.81	0.45
5:C:96:VAL:O	5:C:99:VAL:HG12	2.17	0.45
1:B:147:PHE:O	1:B:149:VAL:N	2.50	0.45
1:B:341:LEU:HD23	1:B:356:PHE:HB3	1.97	0.45
1:I:335:LEU:HB3	1:I:337:LEU:HD13	1.99	0.45
5:C:116:GLN:NE2	5:C:117:ARG:HG3	2.32	0.45
1:B:164:VAL:CG1	1:B:176:MET:HB2	2.47	0.44
2:A:37:ASP:O	2:A:43:ARG:HD2	2.17	0.44
1:I:182:GLN:O	1:I:183:SER:HB3	2.16	0.44
1:I:106:ASN:HB2	1:I:361:GLY:CA	2.38	0.44
1:I:154:MET:HE3	1:I:158:GLY:HA2	2.00	0.44
1:B:106:ASN:CB	1:B:361:GLY:HA3	2.37	0.44
1:I:360:ILE:CD1	5:C:101:PHE:HZ	2.30	0.44
1:I:360:ILE:HD11	5:C:101:PHE:HZ	1.82	0.44
1:B:95:PRO:HB2	1:B:327:THR:HG23	1.99	0.44
1:B:253:LYS:O	1:B:253:LYS:HG3	2.17	0.44
6:A:101:PC1:H11	1:I:322:TRP:CE2	2.53	0.44
1:I:101:VAL:HA	1:I:356:PHE:O	2.18	0.44
4:J:7:GLU:HG2	4:J:10:GLN:NE2	2.32	0.44
1:B:331:LYS:O	1:B:333:PRO:HD3	2.17	0.44
1:B:101:VAL:HA	1:B:356:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:OH	1:I:232:GLY:O	2.29	0.43
3:E:37:LEU:HD23	3:E:37:LEU:HA	1.80	0.43
1:B:164:VAL:HG12	1:B:176:MET:HB2	1.99	0.43
1:B:333:PRO:N	1:B:334:PRO:CD	2.81	0.43
1:I:253:LYS:O	1:I:253:LYS:HG3	2.17	0.43
6:I:901:PC1:C39	5:C:98:PRO:HG3	2.48	0.43
6:B:903:PC1:H133	5:H:82:ARG:HH11	1.83	0.43
5:H:72:PHE:O	5:H:76:LYS:HG2	2.17	0.43
2:A:37:ASP:OD1	2:A:40:ASP:N	2.51	0.43
3:E:29:ARG:HG2	3:E:29:ARG:NH1	2.25	0.43
6:H:201:PC1:H292	4:J:53:LEU:O	2.19	0.43
1:I:226:THR:HG23	1:I:228:CYS:H	1.84	0.43
1:I:297:THR:HG22	1:I:298:SER:N	2.34	0.43
5:H:111:GLN:OE1	5:H:112:GLN:N	2.52	0.42
1:I:212:VAL:O	1:I:212:VAL:HG12	2.18	0.42
5:C:70:SER:O	5:C:73:VAL:HG22	2.19	0.42
1:B:244:GLU:CD	3:E:21:ARG:HH21	2.28	0.42
1:B:230:ALA:HB3	1:B:253:LYS:CG	2.49	0.42
1:I:313:LEU:HD21	1:I:315:LYS:HE3	2.00	0.42
5:C:106:LEU:C	5:C:106:LEU:HD23	2.45	0.42
4:J:5:SER:HB3	4:J:8:ALA:HB2	2.02	0.42
6:B:903:PC1:H331	6:H:201:PC1:H321	1.99	0.42
2:F:62:LEU:HD12	2:F:62:LEU:HA	1.83	0.42
4:G:5:SER:O	4:G:6:LYS:C	2.63	0.42
1:I:256:LEU:O	1:I:257:ASN:C	2.63	0.42
1:I:112:HIS:HB3	1:I:136:VAL:O	2.20	0.41
3:E:29:ARG:NH1	3:E:29:ARG:CG	2.83	0.41
5:H:69:LEU:HD12	5:H:69:LEU:HA	1.88	0.41
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.89	0.41
2:A:29:ARG:O	2:A:32:TYR:HB3	2.21	0.41
1:B:234:GLU:HG2	1:B:249:SER:HB3	2.03	0.41
2:A:62:LEU:O	1:I:278:ALA:HB1	2.21	0.41
2:F:41:PHE:CE2	2:F:45:LEU:HD11	2.55	0.41
5:H:106:LEU:C	5:H:106:LEU:HD23	2.45	0.41
1:B:360:ILE:HD11	5:H:101:PHE:HZ	1.85	0.41
5:C:70:SER:HA	5:C:73:VAL:HG22	2.02	0.41
5:C:108:MET:O	5:C:111:GLN:HG3	2.20	0.41
1:B:76:CYS:HB3	1:B:77:LEU:H	1.58	0.41
1:B:299:VAL:HG12	1:B:320:SER:HB3	2.02	0.41
1:I:109:LEU:HD12	1:I:113:PHE:CE2	2.55	0.41
1:I:142:SER:C	1:I:144:THR:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:HG21	4:J:52:LEU:HD23	2.02	0.41
2:A:51:LEU:HD11	6:A:101:PC1:H32	2.03	0.41
1:B:256:LEU:O	1:B:257:ASN:C	2.64	0.41
2:A:29:ARG:CG	2:A:33:ARG:NH2	2.78	0.41
2:F:30:GLY:HA2	2:F:33:ARG:NH2	2.35	0.41
1:I:173:ARG:HE	1:I:173:ARG:HB2	1.57	0.41
1:I:328:LEU:HB3	6:I:901:PC1:C2H	2.47	0.41
2:F:26:ASP:OD1	2:F:27:TRP:N	2.54	0.41
5:H:107:GLN:O	5:H:110:GLN:HG3	2.21	0.41
5:C:114:LEU:C	5:C:114:LEU:HD23	2.46	0.41
1:B:162:ALA:HB3	1:B:178:ILE:CG1	2.52	0.40
1:B:178:ILE:CD1	4:J:23:ILE:HG21	2.51	0.40
3:E:41:THR:HB	3:E:42:PRO:HD3	2.03	0.40
5:C:71:LEU:C	5:C:71:LEU:HD23	2.46	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	B	284/828 (34%)	275 (97%)	8 (3%)	1 (0%)	30	39
1	I	284/828 (34%)	276 (97%)	7 (2%)	1 (0%)	30	39
2	A	41/74 (55%)	40 (98%)	1 (2%)	0	100	100
2	F	41/74 (55%)	40 (98%)	1 (2%)	0	100	100
3	D	34/51 (67%)	34 (100%)	0	0	100	100
3	E	34/51 (67%)	34 (100%)	0	0	100	100
4	G	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
4	J	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
5	C	55/142 (39%)	55 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	54/142 (38%)	54 (100%)	0	0	100	100
All	All	931/2300 (40%)	908 (98%)	21 (2%)	2 (0%)	44	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	PRO
1	I	148	PRO

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	B	238/679 (35%)	237 (100%)	1 (0%)	84	90
1	I	238/679 (35%)	233 (98%)	5 (2%)	47	66
2	A	35/59 (59%)	35 (100%)	0	100	100
2	F	35/59 (59%)	35 (100%)	0	100	100
3	D	35/48 (73%)	35 (100%)	0	100	100
3	E	35/48 (73%)	35 (100%)	0	100	100
4	G	45/46 (98%)	45 (100%)	0	100	100
4	J	45/46 (98%)	45 (100%)	0	100	100
5	C	49/115 (43%)	49 (100%)	0	100	100
5	H	49/115 (43%)	49 (100%)	0	100	100
All	All	804/1894 (42%)	798 (99%)	6 (1%)	73	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	142	SER
1	I	138	THR
1	I	139	LYS
1	I	142	SER

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Mol	Chain	Res	Type
1	I	243	GLU
1	I	244	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	HIS
1	B	130	HIS
1	B	257	ASN
2	A	48	ASN
1	I	130	HIS
1	I	271	HIS
1	I	281	GLN
1	I	353	GLN
5	C	115	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](#)

23 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	C	201	-	53,53,53	0.28	0	59,61,61	0.46	0
7	UND	I	904	-	10,10,10	0.15	0	9,9,9	0.07	0
6	PC1	H	201	-	53,53,53	0.28	0	59,61,61	0.38	0
7	UND	B	904	-	10,10,10	0.15	0	9,9,9	0.07	0
6	PC1	B	901	-	53,53,53	0.27	0	59,61,61	0.33	0
6	PC1	I	903	-	53,53,53	0.32	0	59,61,61	0.38	0
7	UND	G	101	-	10,10,10	0.17	0	9,9,9	0.07	0
6	PC1	D	101	-	53,53,53	0.26	0	59,61,61	0.33	0
7	UND	F	101	-	10,10,10	0.13	0	9,9,9	0.06	0
7	UND	I	906	-	10,10,10	0.15	0	9,9,9	0.07	0
6	PC1	B	902	-	53,53,53	0.27	0	59,61,61	0.34	0
7	UND	G	102	-	10,10,10	0.14	0	9,9,9	0.07	0
6	PC1	B	903	-	53,53,53	0.27	0	59,61,61	0.48	1 (1%)
7	UND	J	101	-	10,10,10	0.17	0	9,9,9	0.08	0
6	PC1	I	902	-	53,53,53	0.28	0	59,61,61	0.39	0
7	UND	B	905	-	10,10,10	0.16	0	9,9,9	0.08	0
7	UND	C	203	-	10,10,10	0.14	0	9,9,9	0.06	0
6	PC1	C	202	-	53,53,53	0.28	0	59,61,61	0.32	0
7	UND	H	202	-	10,10,10	0.14	0	9,9,9	0.09	0
6	PC1	A	101	-	53,53,53	0.26	0	59,61,61	0.36	0
6	PC1	I	901	-	53,53,53	0.28	0	59,61,61	0.40	0
7	UND	I	905	-	10,10,10	0.14	0	9,9,9	0.05	0
7	UND	A	102	-	10,10,10	0.14	0	9,9,9	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PC1	C	201	-	-	23/57/57/57	-
7	UND	I	904	-	-	3/8/8/8	-
6	PC1	H	201	-	-	21/57/57/57	-
7	UND	B	904	-	-	1/8/8/8	-
6	PC1	B	901	-	-	22/57/57/57	-
6	PC1	I	903	-	-	18/57/57/57	-
7	UND	G	101	-	-	0/8/8/8	-
6	PC1	D	101	-	-	26/57/57/57	-
7	UND	F	101	-	-	3/8/8/8	-
7	UND	I	906	-	-	2/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PC1	B	902	-	-	24/57/57/57	-
7	UND	G	102	-	-	1/8/8/8	-
6	PC1	B	903	-	-	23/57/57/57	-
7	UND	J	101	-	-	0/8/8/8	-
6	PC1	I	902	-	-	33/57/57/57	-
7	UND	B	905	-	-	2/8/8/8	-
7	UND	C	203	-	-	0/8/8/8	-
6	PC1	C	202	-	-	20/57/57/57	-
7	UND	H	202	-	-	1/8/8/8	-
6	PC1	A	101	-	-	16/57/57/57	-
6	PC1	I	901	-	-	25/57/57/57	-
7	UND	I	905	-	-	5/8/8/8	-
7	UND	A	102	-	-	3/8/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	903	PC1	O21-C21-C22	2.04	115.90	111.48

There are no chirality outliers.

All (272) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	901	PC1	O13-C11-C12-N
6	B	902	PC1	C1-O11-P-O14
6	B	902	PC1	C1-O11-P-O13
6	B	903	PC1	O13-C11-C12-N
6	B	903	PC1	C22-C21-O21-C2
6	A	101	PC1	C22-C21-O21-C2
6	D	101	PC1	C11-O13-P-O14
6	D	101	PC1	C11-O13-P-O11
6	D	101	PC1	O13-C11-C12-N
6	D	101	PC1	C22-C21-O21-C2
6	I	901	PC1	C1-O11-P-O12
6	I	901	PC1	C1-O11-P-O13
6	I	901	PC1	O13-C11-C12-N
6	I	902	PC1	C11-O13-P-O14
6	I	902	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
6	I	902	PC1	O13-C11-C12-N
6	I	902	PC1	C22-C21-O21-C2
6	I	903	PC1	C11-O13-P-O12
6	I	903	PC1	C11-O13-P-O14
6	I	903	PC1	C11-O13-P-O11
6	I	903	PC1	C22-C21-O21-C2
6	H	201	PC1	C11-O13-P-O14
6	H	201	PC1	C11-O13-P-O11
6	H	201	PC1	C22-C21-O21-C2
6	C	201	PC1	C1-O11-P-O14
6	C	201	PC1	C22-C21-O21-C2
6	B	903	PC1	O22-C21-O21-C2
6	I	902	PC1	O22-C21-O21-C2
6	I	903	PC1	O22-C21-O21-C2
6	H	201	PC1	O22-C21-O21-C2
6	C	201	PC1	O22-C21-O21-C2
6	B	902	PC1	C32-C31-O31-C3
6	H	201	PC1	C32-C31-O31-C3
6	B	903	PC1	O32-C31-O31-C3
6	I	901	PC1	O32-C31-O31-C3
6	C	202	PC1	O32-C31-O31-C3
6	D	101	PC1	C32-C31-O31-C3
6	B	902	PC1	O32-C31-O31-C3
6	I	902	PC1	O32-C31-O31-C3
6	A	101	PC1	O22-C21-O21-C2
6	D	101	PC1	O22-C21-O21-C2
6	I	901	PC1	C32-C31-O31-C3
6	H	201	PC1	O32-C31-O31-C3
6	B	903	PC1	C32-C31-O31-C3
6	I	902	PC1	C32-C31-O31-C3
6	C	202	PC1	C32-C31-O31-C3
6	D	101	PC1	O32-C31-O31-C3
6	B	901	PC1	C32-C31-O31-C3
6	B	901	PC1	O32-C31-O31-C3
6	B	903	PC1	O11-C1-C2-O21
6	B	902	PC1	C22-C21-O21-C2
6	A	101	PC1	O21-C2-C3-O31
6	C	201	PC1	C32-C31-O31-C3
6	D	101	PC1	C31-C32-C33-C34
6	B	902	PC1	O22-C21-O21-C2
6	B	901	PC1	C22-C21-O21-C2
6	C	201	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
6	B	901	PC1	O22-C21-O21-C2
6	I	903	PC1	C32-C31-O31-C3
6	I	903	PC1	O32-C31-O31-C3
6	I	901	PC1	C22-C21-O21-C2
6	D	101	PC1	C39-C3A-C3B-C3C
6	B	901	PC1	C3A-C3B-C3C-C3D
6	B	901	PC1	C3E-C3F-C3G-C3H
6	I	901	PC1	C39-C3A-C3B-C3C
6	B	901	PC1	C2E-C2F-C2G-C2H
6	I	901	PC1	O22-C21-O21-C2
6	B	903	PC1	C39-C3A-C3B-C3C
6	B	903	PC1	C2E-C2F-C2G-C2H
6	C	201	PC1	C29-C2A-C2B-C2C
6	I	902	PC1	C29-C2A-C2B-C2C
6	A	101	PC1	C26-C27-C28-C29
6	A	101	PC1	C34-C35-C36-C37
6	I	901	PC1	C29-C2A-C2B-C2C
6	I	901	PC1	C3A-C3B-C3C-C3D
6	I	903	PC1	C2E-C2F-C2G-C2H
6	A	101	PC1	C28-C29-C2A-C2B
6	D	101	PC1	C2B-C2C-C2D-C2E
6	I	902	PC1	C2C-C2D-C2E-C2F
6	I	902	PC1	C38-C39-C3A-C3B
6	B	901	PC1	C37-C38-C39-C3A
6	B	902	PC1	C2E-C2F-C2G-C2H
6	D	101	PC1	C28-C29-C2A-C2B
6	D	101	PC1	C2E-C2F-C2G-C2H
6	D	101	PC1	C21-C22-C23-C24
6	I	902	PC1	C2E-C2F-C2G-C2H
6	B	903	PC1	C29-C2A-C2B-C2C
6	B	902	PC1	C37-C38-C39-C3A
6	C	202	PC1	C22-C21-O21-C2
6	C	202	PC1	O22-C21-O21-C2
6	C	202	PC1	C35-C36-C37-C38
6	C	201	PC1	C24-C25-C26-C27
6	C	201	PC1	C3D-C3E-C3F-C3G
6	D	101	PC1	C3E-C3F-C3G-C3H
6	A	101	PC1	C2B-C2C-C2D-C2E
6	H	201	PC1	C29-C2A-C2B-C2C
6	I	901	PC1	C24-C25-C26-C27
6	I	902	PC1	C3A-C3B-C3C-C3D
6	I	901	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
6	B	901	PC1	C31-C32-C33-C34
6	B	902	PC1	C21-C22-C23-C24
6	B	902	PC1	C1-C2-C3-O31
6	B	903	PC1	C1-C2-C3-O31
6	A	101	PC1	C1-C2-C3-O31
6	B	903	PC1	C32-C33-C34-C35
6	A	101	PC1	C22-C23-C24-C25
6	H	201	PC1	C2C-C2D-C2E-C2F
6	D	101	PC1	C3C-C3D-C3E-C3F
6	D	101	PC1	C37-C38-C39-C3A
6	C	202	PC1	C3F-C3G-C3H-C3I
7	I	904	UND	C2-C3-C4-C5
6	B	902	PC1	C31-C32-C33-C34
6	I	901	PC1	C31-C32-C33-C34
6	B	902	PC1	O11-C1-C2-O21
6	I	902	PC1	O11-C1-C2-O21
6	A	101	PC1	C32-C31-O31-C3
7	F	101	UND	C6-C7-C8-C9
6	I	902	PC1	C2A-C2B-C2C-C2D
7	G	102	UND	C6-C7-C8-C9
6	B	903	PC1	C3F-C3G-C3H-C3I
6	C	202	PC1	C24-C25-C26-C27
7	I	905	UND	C6-C7-C8-C9
6	I	901	PC1	C2E-C2F-C2G-C2H
6	I	902	PC1	C27-C28-C29-C2A
6	I	901	PC1	C33-C34-C35-C36
7	I	906	UND	C6-C7-C8-C9
6	B	902	PC1	O11-C1-C2-C3
6	B	903	PC1	O11-C1-C2-C3
6	C	201	PC1	C3F-C3G-C3H-C3I
6	A	101	PC1	O32-C31-O31-C3
6	B	902	PC1	C39-C3A-C3B-C3C
6	B	902	PC1	C2A-C2B-C2C-C2D
6	D	101	PC1	C34-C35-C36-C37
6	I	902	PC1	C26-C27-C28-C29
6	I	902	PC1	C35-C36-C37-C38
6	C	201	PC1	C38-C39-C3A-C3B
6	D	101	PC1	C26-C27-C28-C29
6	B	902	PC1	O21-C2-C3-O31
6	B	903	PC1	O21-C2-C3-O31
6	C	202	PC1	O21-C2-C3-O31
7	B	904	UND	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	I	903	PC1	C36-C37-C38-C39
6	I	902	PC1	C39-C3A-C3B-C3C
7	F	101	UND	C5-C6-C7-C8
7	A	102	UND	C1-C2-C3-C4
6	B	902	PC1	C35-C36-C37-C38
6	B	902	PC1	C33-C34-C35-C36
6	I	903	PC1	O11-C1-C2-C3
6	C	202	PC1	C38-C39-C3A-C3B
6	C	202	PC1	C36-C37-C38-C39
6	A	101	PC1	C37-C38-C39-C3A
6	A	101	PC1	C3F-C3G-C3H-C3I
6	I	902	PC1	C2B-C2C-C2D-C2E
6	B	901	PC1	C34-C35-C36-C37
6	B	902	PC1	C34-C35-C36-C37
6	D	101	PC1	C12-C11-O13-P
6	I	902	PC1	C12-C11-O13-P
6	I	903	PC1	C23-C24-C25-C26
7	F	101	UND	C7-C8-C9-C10
6	B	901	PC1	C33-C34-C35-C36
6	H	201	PC1	C3A-C3B-C3C-C3D
7	I	904	UND	C1-C2-C3-C4
6	C	201	PC1	C32-C33-C34-C35
6	H	201	PC1	C27-C28-C29-C2A
6	I	902	PC1	C36-C37-C38-C39
6	I	903	PC1	C35-C36-C37-C38
6	H	201	PC1	C3D-C3E-C3F-C3G
6	I	902	PC1	O11-C1-C2-C3
6	C	202	PC1	C28-C29-C2A-C2B
7	A	102	UND	C3-C4-C5-C6
6	I	903	PC1	O11-C1-C2-O21
6	B	903	PC1	C26-C27-C28-C29
6	I	901	PC1	C22-C23-C24-C25
6	C	202	PC1	C27-C28-C29-C2A
6	B	903	PC1	C2A-C2B-C2C-C2D
7	I	905	UND	C7-C8-C9-C10
6	B	902	PC1	C1-O11-P-O12
6	D	101	PC1	C11-O13-P-O12
6	I	902	PC1	C11-O13-P-O12
6	I	903	PC1	C1-O11-P-O14
6	H	201	PC1	C11-O13-P-O12
6	C	201	PC1	C1-O11-P-O12
6	C	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
6	B	901	PC1	C28-C29-C2A-C2B
6	D	101	PC1	C22-C23-C24-C25
6	B	902	PC1	C2-C1-O11-P
6	B	903	PC1	C2D-C2E-C2F-C2G
6	I	901	PC1	C2D-C2E-C2F-C2G
6	I	902	PC1	C28-C29-C2A-C2B
6	B	901	PC1	C35-C36-C37-C38
6	C	201	PC1	O11-C1-C2-O21
6	I	902	PC1	C34-C35-C36-C37
6	B	903	PC1	C3D-C3E-C3F-C3G
6	A	101	PC1	C2A-C2B-C2C-C2D
6	H	201	PC1	C11-C12-N-C14
6	B	901	PC1	C21-C22-C23-C24
6	B	903	PC1	C24-C25-C26-C27
6	C	201	PC1	C2A-C2B-C2C-C2D
6	C	202	PC1	C26-C27-C28-C29
6	B	901	PC1	C24-C25-C26-C27
6	I	903	PC1	C3B-C3C-C3D-C3E
6	A	101	PC1	C29-C2A-C2B-C2C
6	B	901	PC1	C1-C2-C3-O31
7	A	102	UND	C6-C7-C8-C9
6	C	201	PC1	C3-C2-O21-C21
6	C	201	PC1	C2D-C2E-C2F-C2G
6	D	101	PC1	C3B-C3C-C3D-C3E
6	I	901	PC1	C38-C39-C3A-C3B
6	B	901	PC1	C3B-C3C-C3D-C3E
6	I	901	PC1	C2F-C2G-C2H-C2I
7	B	905	UND	C4-C5-C6-C7
6	I	901	PC1	C26-C27-C28-C29
6	C	201	PC1	C22-C23-C24-C25
6	C	201	PC1	C3C-C3D-C3E-C3F
6	D	101	PC1	O21-C2-C3-O31
6	I	903	PC1	C3C-C3D-C3E-C3F
6	B	903	PC1	C3B-C3C-C3D-C3E
6	H	201	PC1	C11-C12-N-C15
6	C	201	PC1	C39-C3A-C3B-C3C
6	H	201	PC1	C34-C35-C36-C37
6	B	903	PC1	C3E-C3F-C3G-C3H
6	I	901	PC1	C23-C24-C25-C26
6	I	902	PC1	C24-C25-C26-C27
6	B	901	PC1	C26-C27-C28-C29
6	H	201	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
6	B	901	PC1	C22-C23-C24-C25
6	C	202	PC1	C2-C1-O11-P
7	I	905	UND	C2-C3-C4-C5
6	C	202	PC1	C3C-C3D-C3E-C3F
6	I	901	PC1	C25-C26-C27-C28
7	I	905	UND	C4-C5-C6-C7
6	A	101	PC1	C36-C37-C38-C39
6	H	201	PC1	C36-C37-C38-C39
6	C	202	PC1	C1-C2-C3-O31
6	C	202	PC1	C33-C34-C35-C36
6	I	902	PC1	C32-C33-C34-C35
7	B	905	UND	C6-C7-C8-C9
6	I	901	PC1	C11-C12-N-C13
6	B	901	PC1	O31-C31-C32-C33
7	H	202	UND	C2-C3-C4-C5
6	I	902	PC1	C31-C32-C33-C34
6	C	202	PC1	C3A-C3B-C3C-C3D
6	I	903	PC1	O31-C31-C32-C33
6	C	201	PC1	C25-C26-C27-C28
6	B	903	PC1	C38-C39-C3A-C3B
6	B	902	PC1	O31-C31-C32-C33
6	I	901	PC1	C11-C12-N-C15
6	H	201	PC1	C3E-C3F-C3G-C3H
6	B	903	PC1	C31-C32-C33-C34
6	H	201	PC1	C28-C29-C2A-C2B
6	C	202	PC1	O21-C21-C22-C23
6	I	902	PC1	O21-C21-C22-C23
6	I	901	PC1	C11-C12-N-C14
6	B	902	PC1	C23-C24-C25-C26
6	H	201	PC1	C25-C26-C27-C28
6	I	902	PC1	C3B-C3C-C3D-C3E
6	I	902	PC1	C3F-C3G-C3H-C3I
6	B	901	PC1	O32-C31-C32-C33
6	D	101	PC1	O31-C31-C32-C33
6	C	201	PC1	C34-C35-C36-C37
6	D	101	PC1	O21-C21-C22-C23
6	I	903	PC1	O32-C31-C32-C33
7	I	904	UND	C4-C5-C6-C7
7	I	906	UND	C4-C5-C6-C7
6	I	902	PC1	O22-C21-C22-C23
6	D	101	PC1	C3D-C3E-C3F-C3G
6	C	202	PC1	O22-C21-C22-C23

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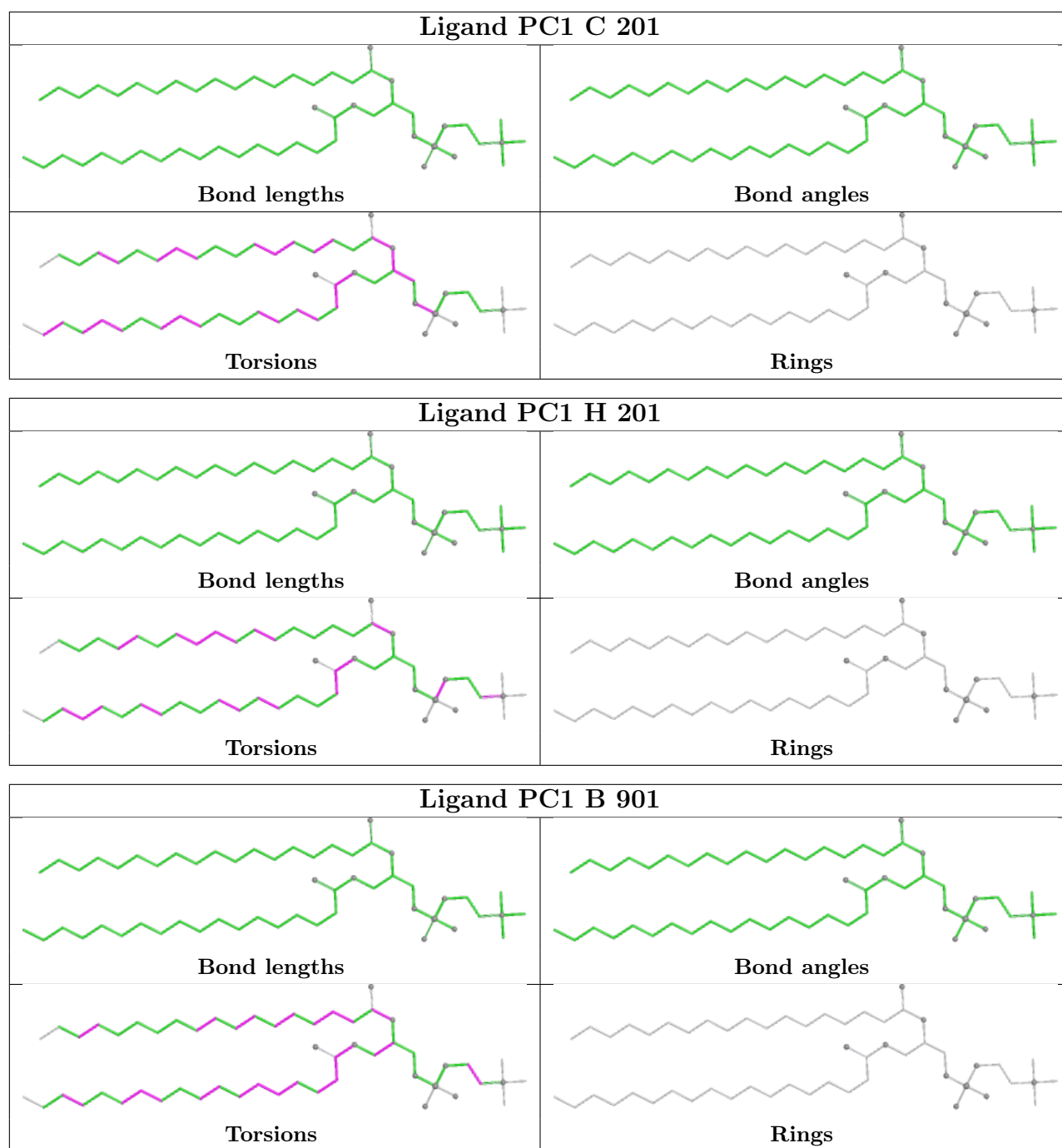
Mol	Chain	Res	Type	Atoms
6	B	902	PC1	O32-C31-C32-C33
7	I	905	UND	C11-C10-C9-C8
6	I	902	PC1	C37-C38-C39-C3A
6	H	201	PC1	O31-C31-C32-C33
6	C	201	PC1	O31-C31-C32-C33

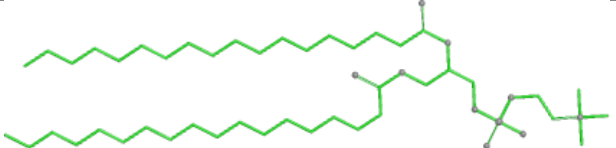
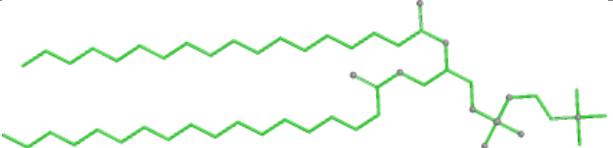
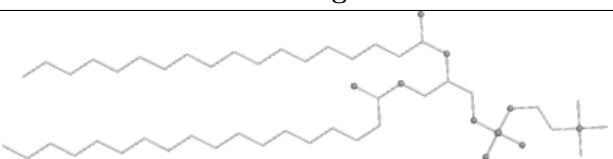
There are no ring outliers.

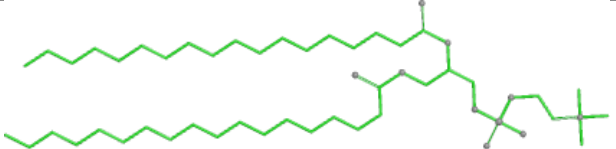
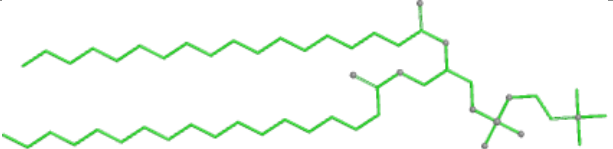
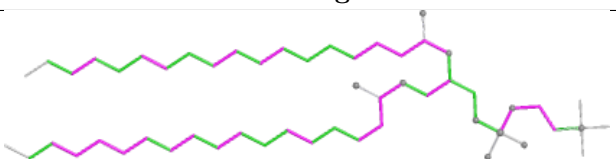
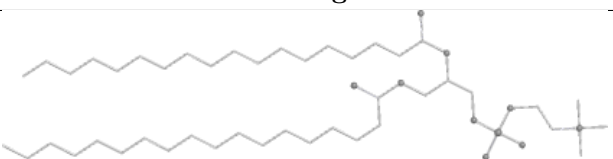
10 monomers are involved in 58 short contacts:

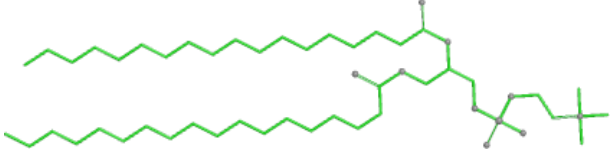
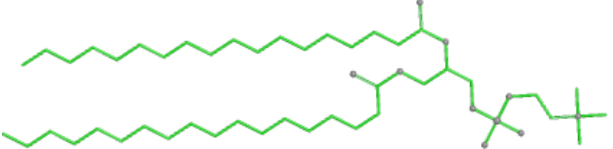
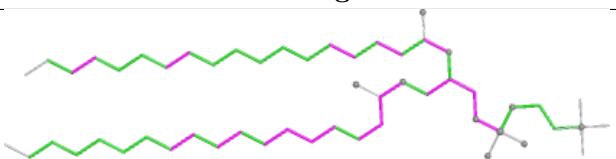
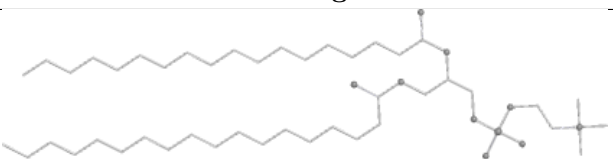
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	PC1	9	0
6	H	201	PC1	10	0
6	B	901	PC1	1	0
7	I	906	UND	1	0
6	B	902	PC1	5	0
6	B	903	PC1	10	0
6	I	902	PC1	3	0
6	C	202	PC1	6	0
6	A	101	PC1	8	0
6	I	901	PC1	14	0

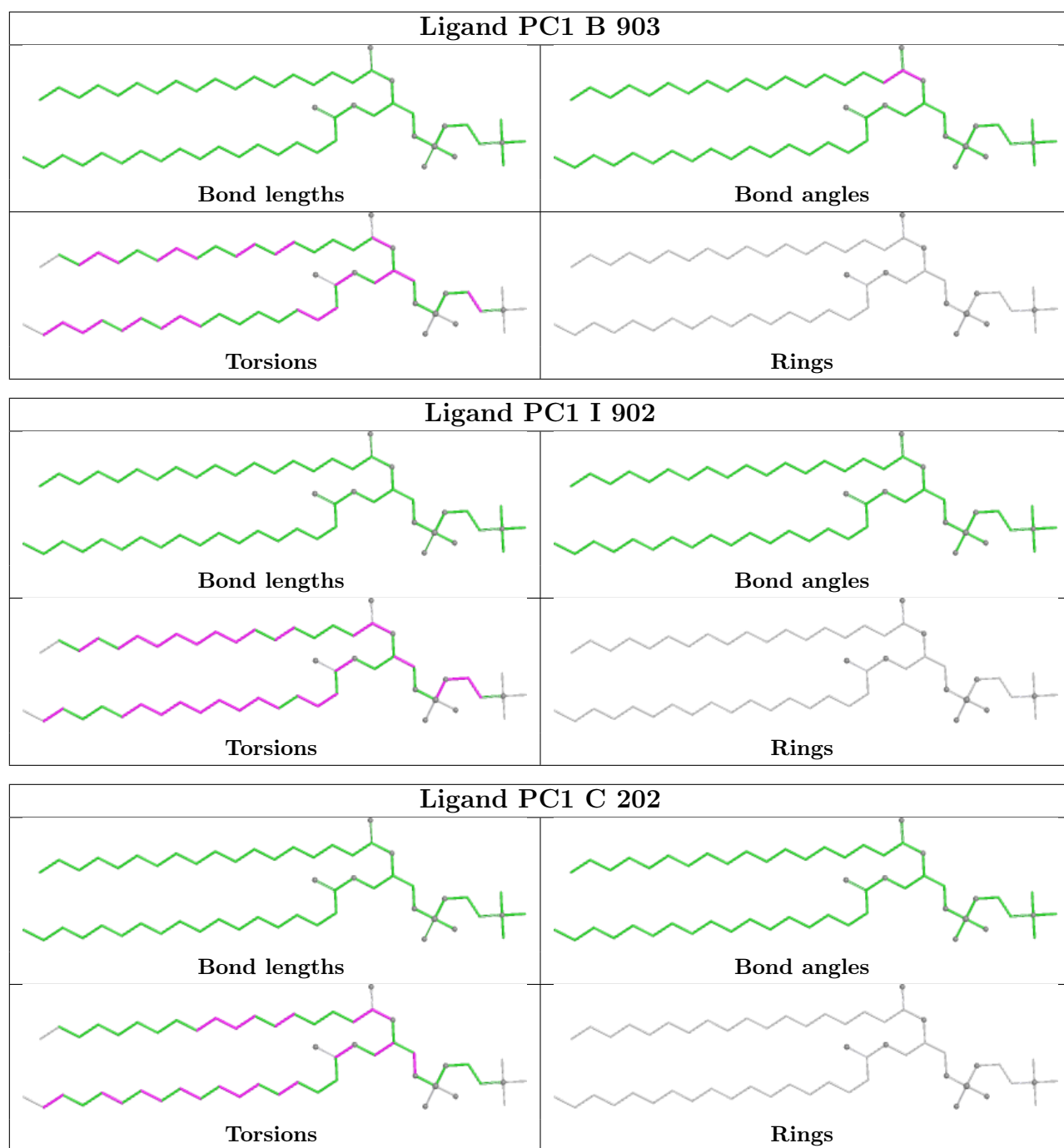
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

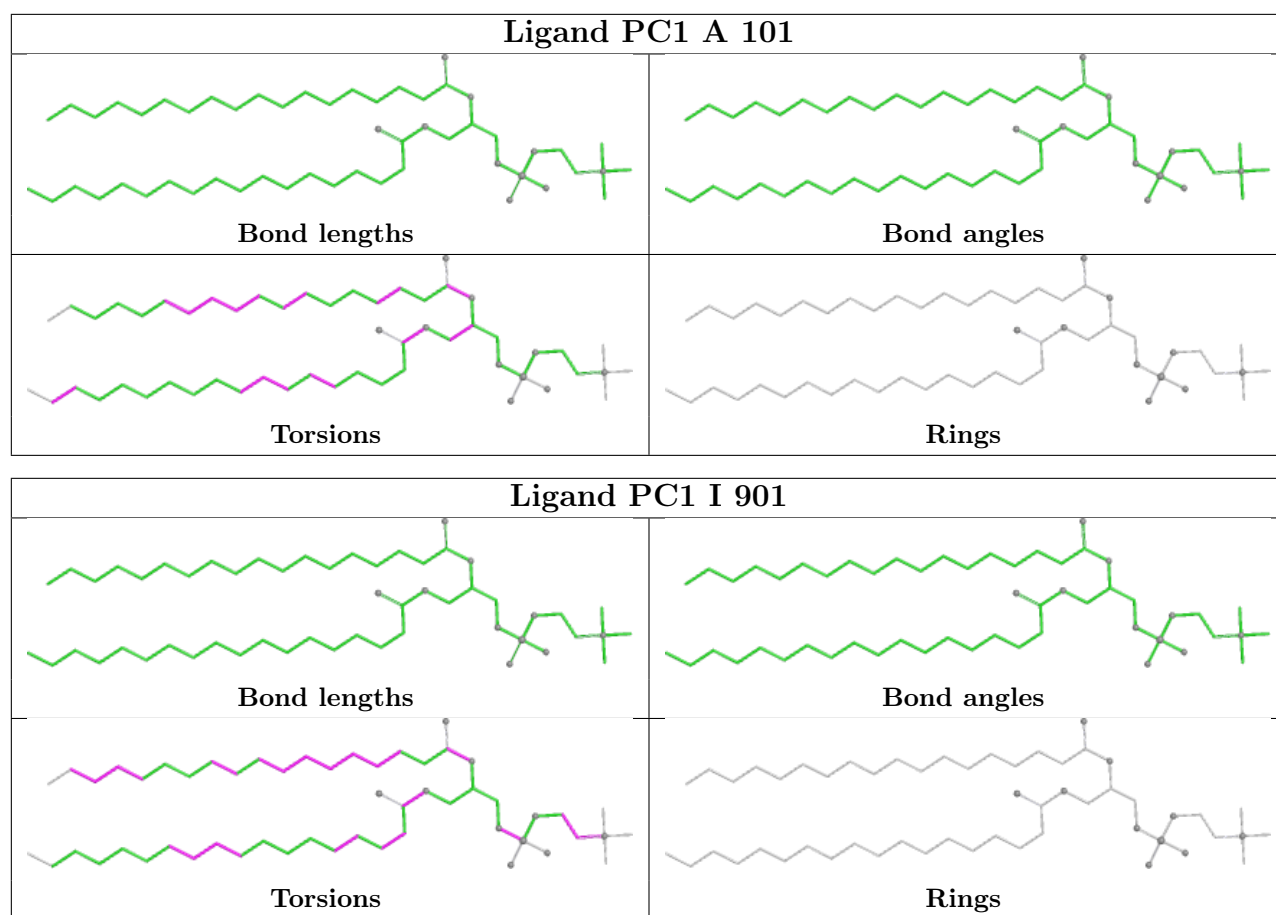


Ligand PC1 I 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 D 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 B 902	
 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.

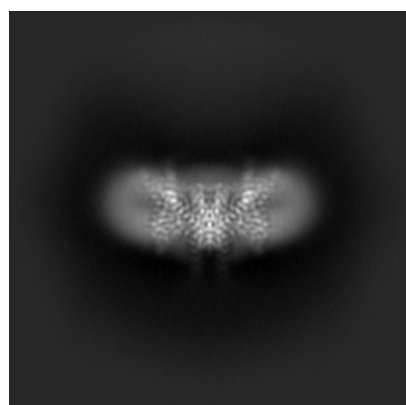
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31885. These allow visual inspection of the internal detail of the map and identification of artifacts.

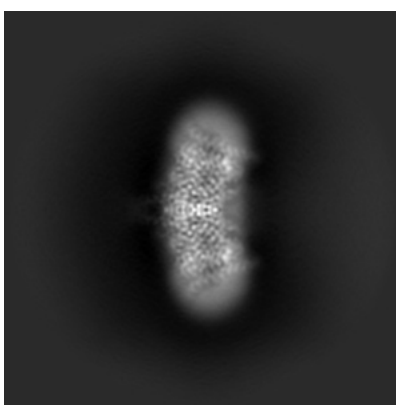
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

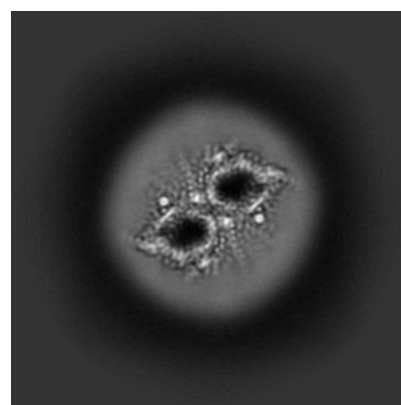
6.1.1 Primary map



X



Y

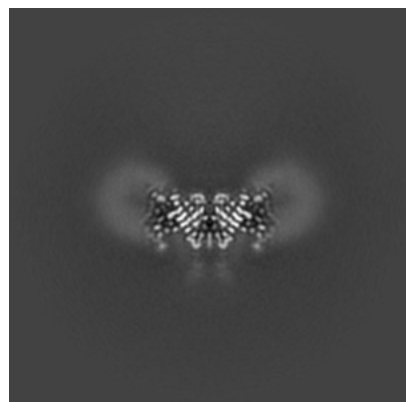


Z

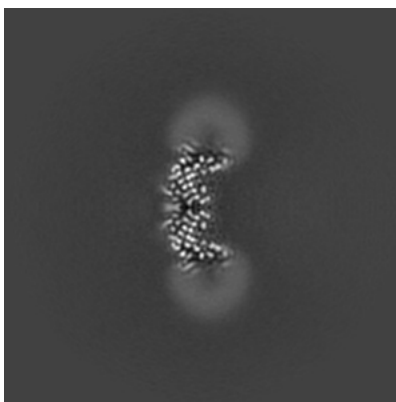
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

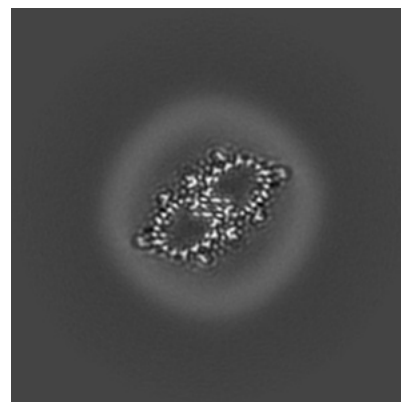
6.2.1 Primary map



X Index: 160



Y Index: 160

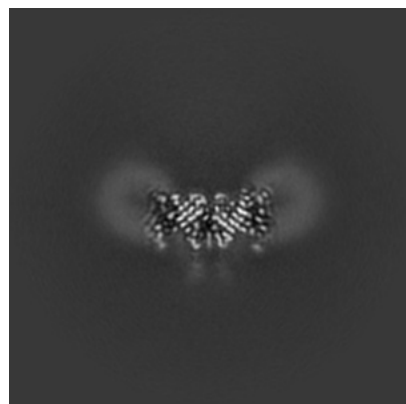


Z Index: 160

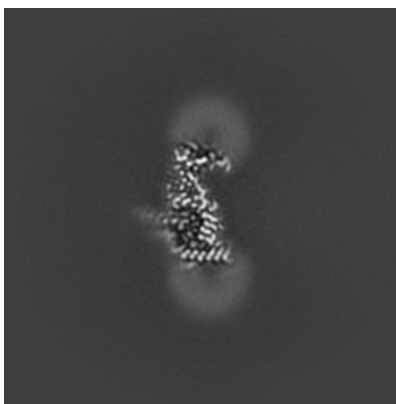
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

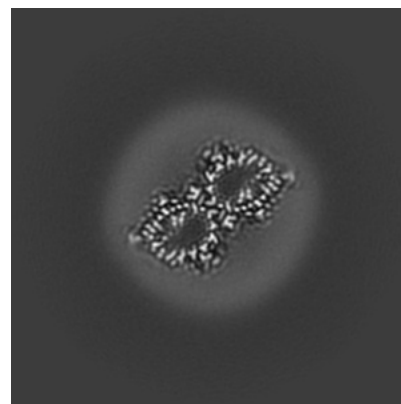
6.3.1 Primary map



X Index: 161



Y Index: 166



Z Index: 151

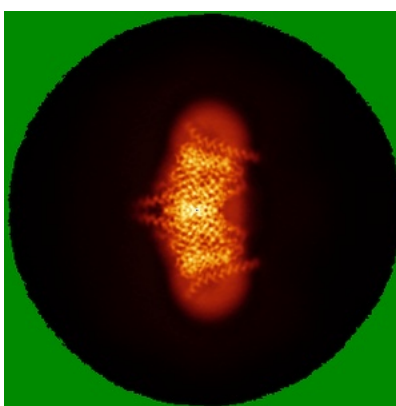
The images above show the largest variance slices of the map in three orthogonal directions.

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

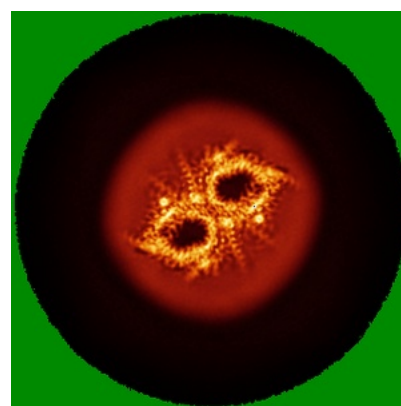
6.4.1 Primary map



X



Y

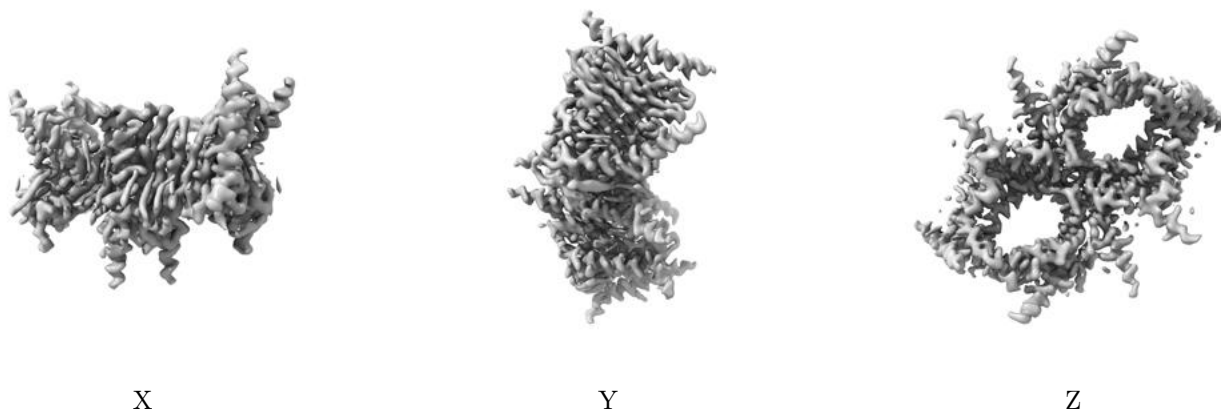


Z

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 0.302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

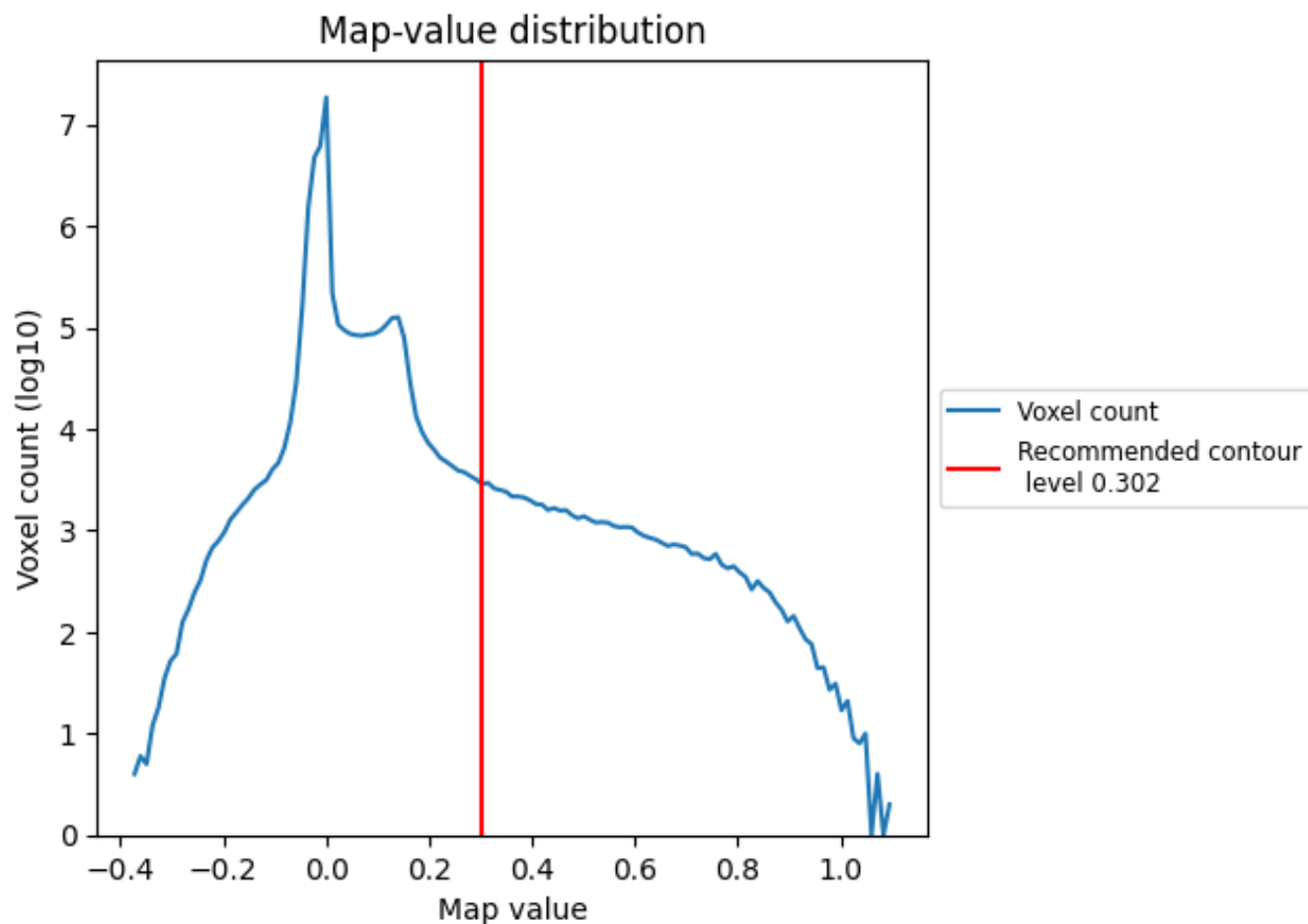
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

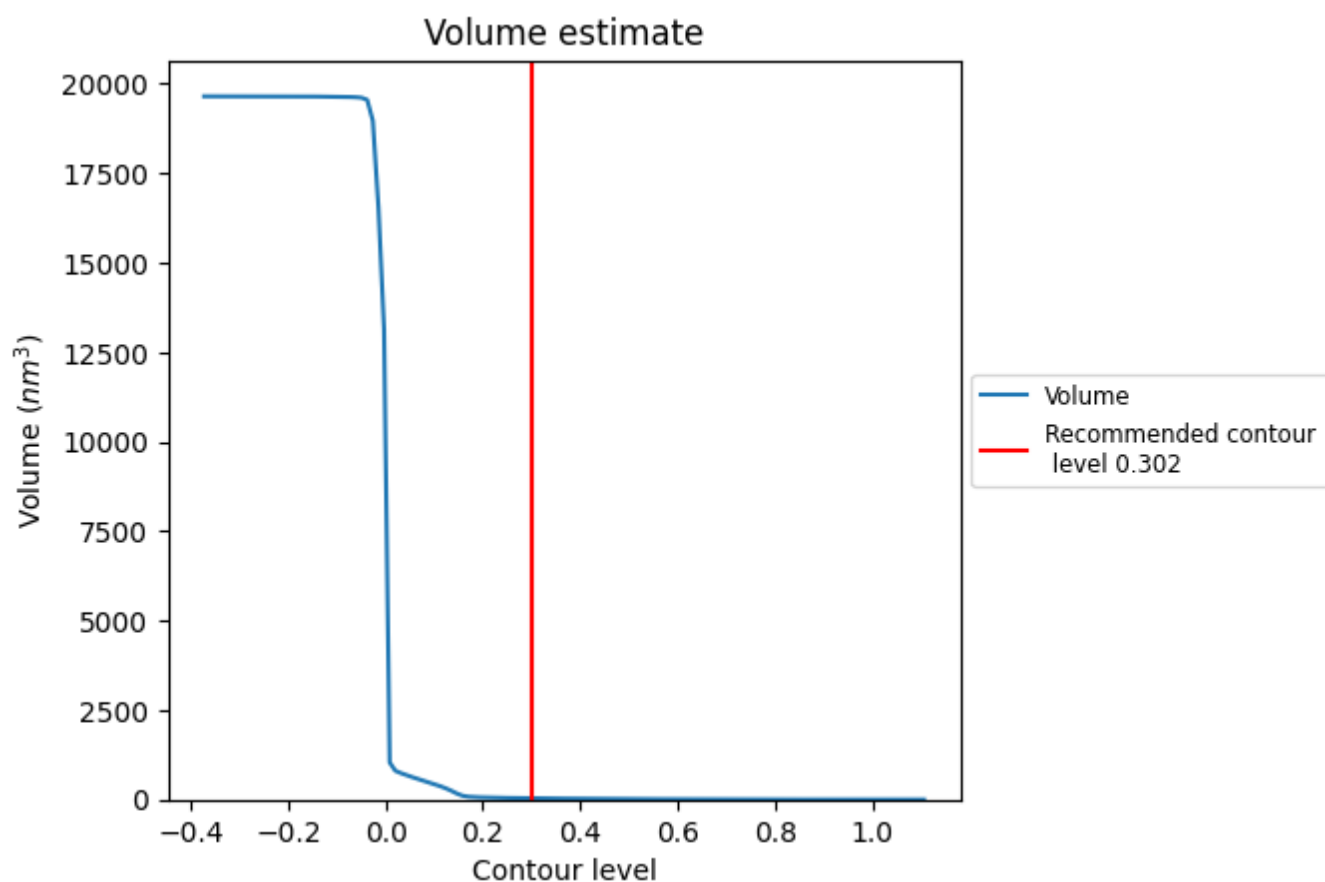
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

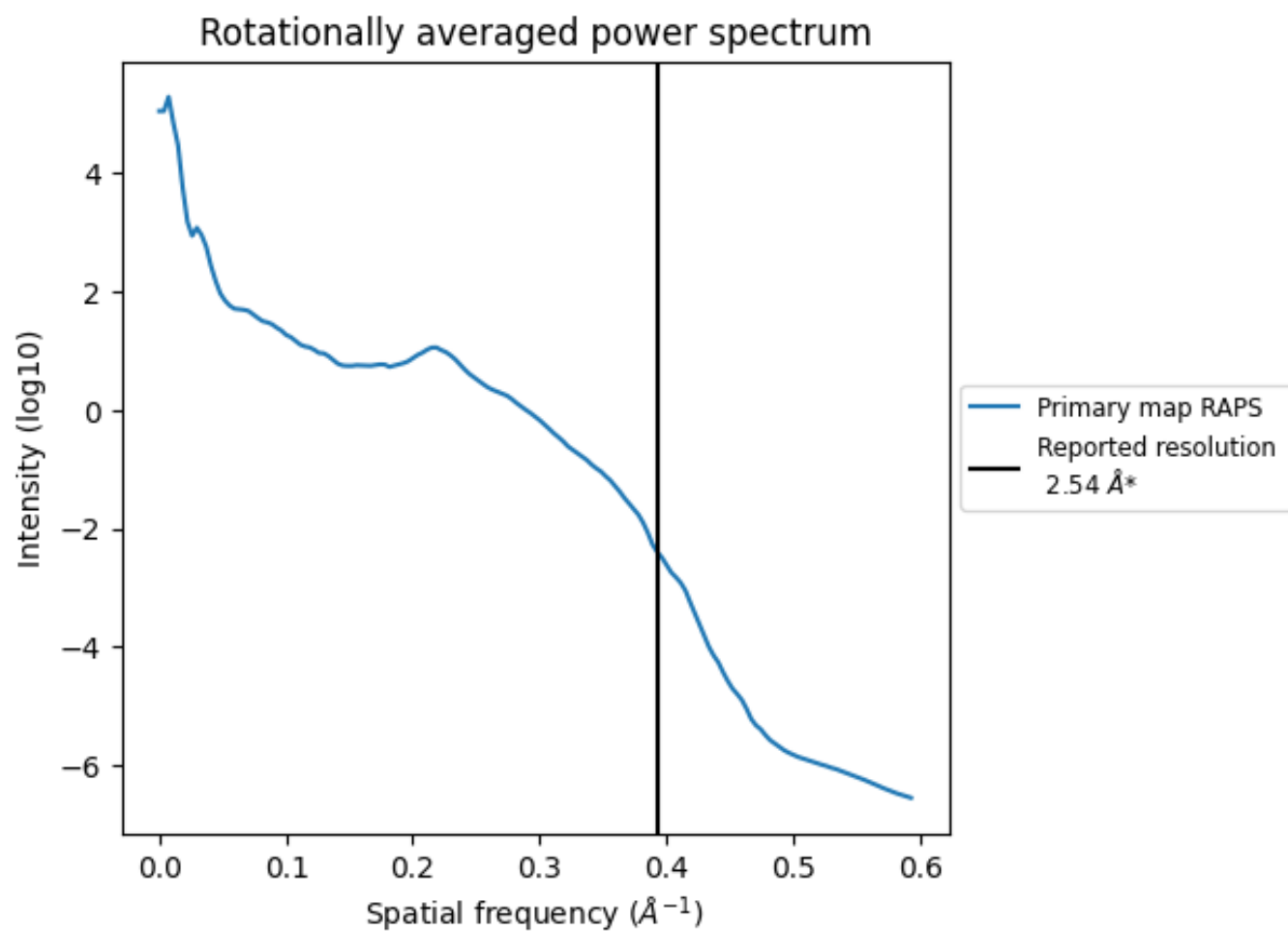
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm³; this corresponds to an approximate mass of 32 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 0.394 Å⁻¹

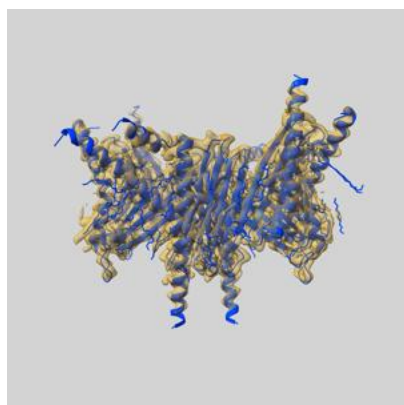
8 Fourier-Shell correlation ⓘ

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

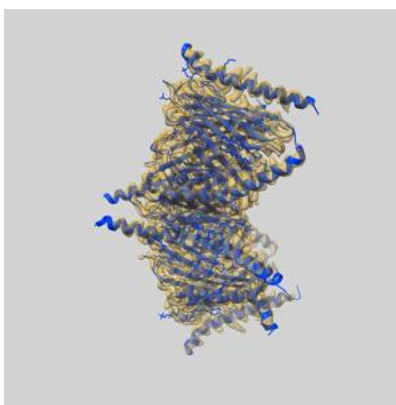
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31885 and PDB model 7VBY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

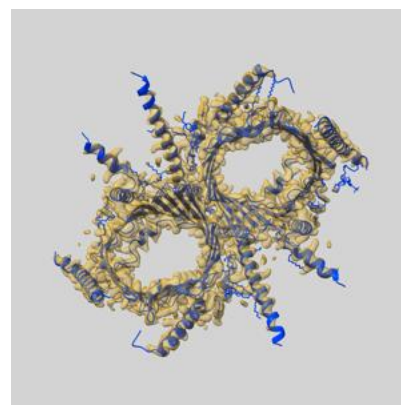
9.1 Map-model overlay [i](#)



X



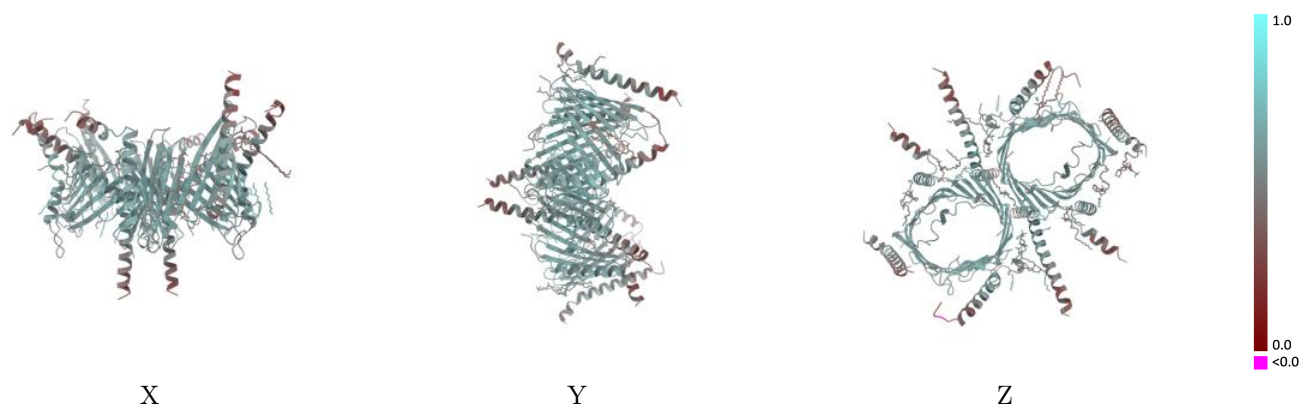
Y



Z

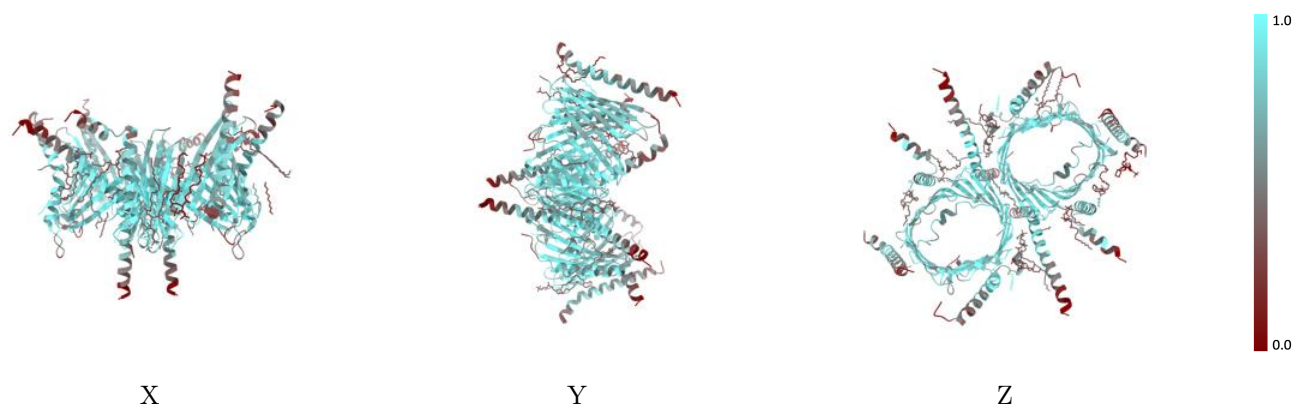
The images above show the 3D surface view of the map at the recommended contour level 0.302 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



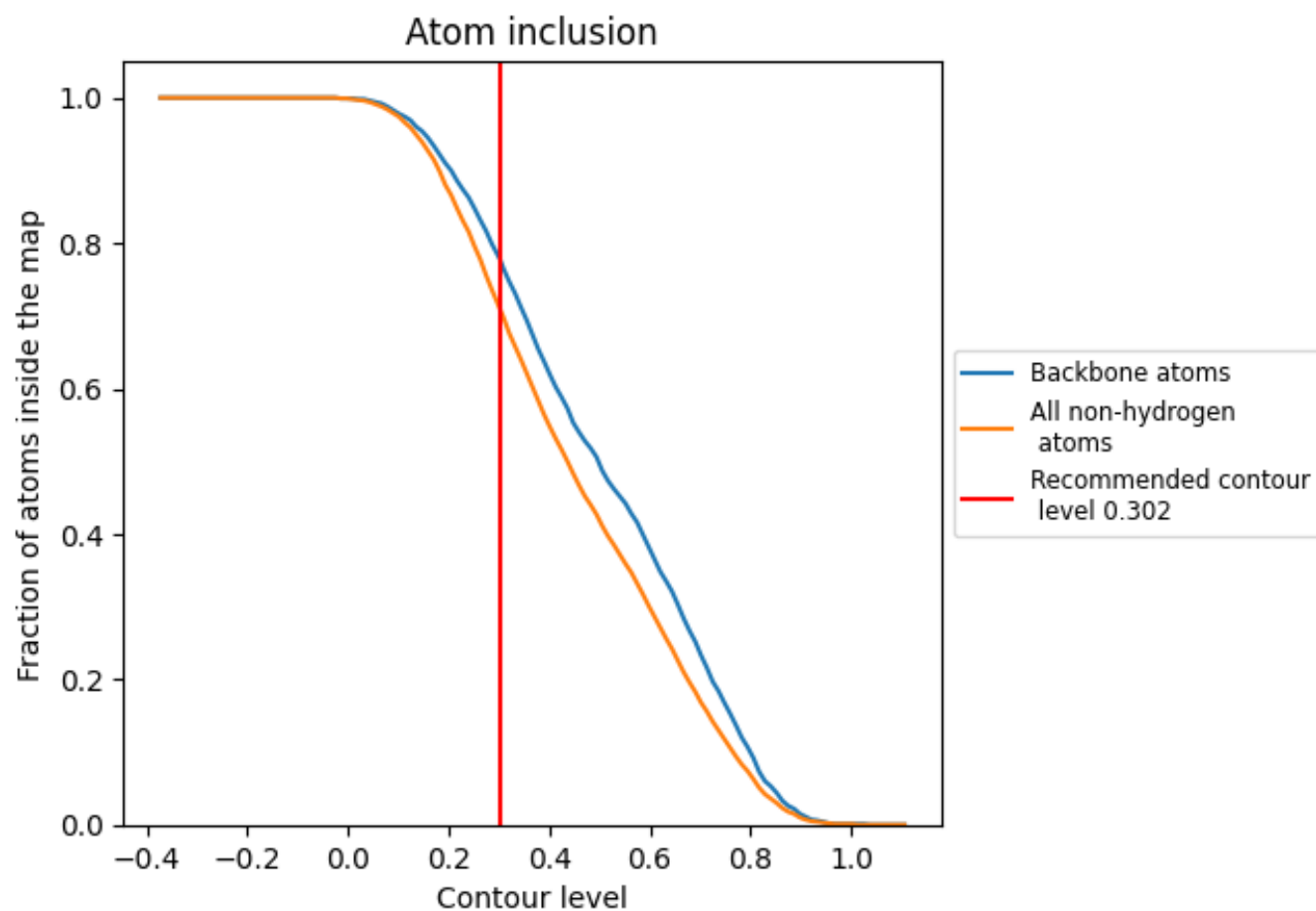
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.302).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.302) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.5490
A	0.5820	0.5190
B	0.7850	0.5860
C	0.5350	0.4910
D	0.4520	0.4550
E	0.5320	0.4690
F	0.6290	0.5190
G	0.6340	0.5170
H	0.5650	0.5090
I	0.7850	0.5840
J	0.6460	0.5110

1.0

0.0

<0.0