



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 07:43 PM JST

PDB ID : 7DUW
EMDB ID : EMD-30869
Title : Cryo-EM structure of the multiple peptide resistance factor (MprF) loaded with two lysyl-phosphatidylglycerol molecules
Authors : Song, D.F.; Jiao, H.Z.; Liu, Z.F.
Deposited on : 2021-01-12
Resolution : 2.96 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

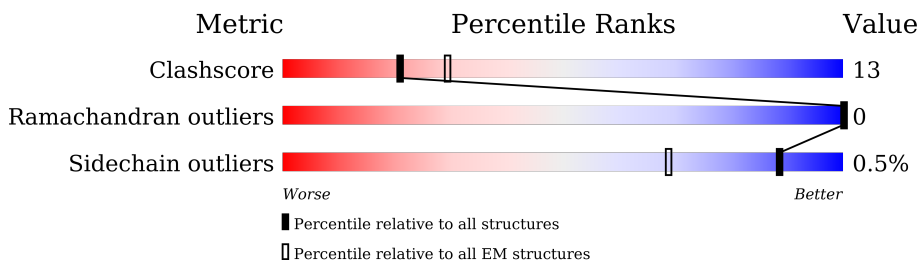
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	882	
1	B	882	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13276 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 Bifunctional lysylphosphatidylglycerol flippase/synthetase MprF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	820	6307	4128	1053	1106	20	0	0
1	B	820	6307	4128	1053	1106	20	0	0

There are 26 discrepancies between the modelled and reference sequences:

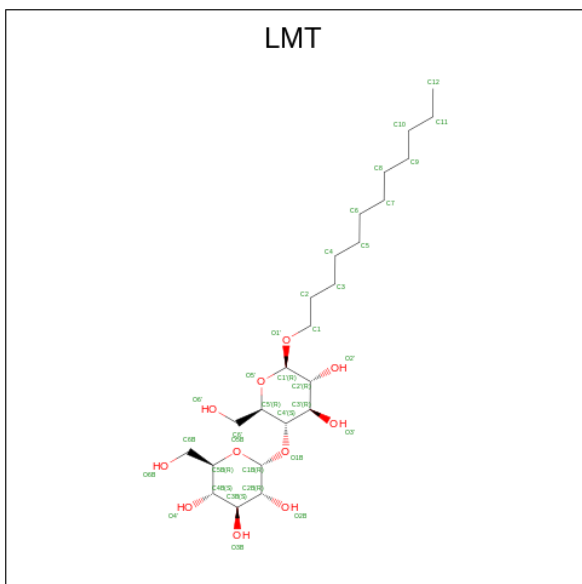
Chain	Residue	Modelled	Actual	Comment	Reference
A	870	LYS	-	expression tag	UNP A0A6P1C618
A	871	LEU	-	expression tag	UNP A0A6P1C618
A	872	ALA	-	expression tag	UNP A0A6P1C618
A	873	ALA	-	expression tag	UNP A0A6P1C618
A	874	ALA	-	expression tag	UNP A0A6P1C618
A	875	LEU	-	expression tag	UNP A0A6P1C618
A	876	GLU	-	expression tag	UNP A0A6P1C618
A	877	HIS	-	expression tag	UNP A0A6P1C618
A	878	HIS	-	expression tag	UNP A0A6P1C618
A	879	HIS	-	expression tag	UNP A0A6P1C618
A	880	HIS	-	expression tag	UNP A0A6P1C618
A	881	HIS	-	expression tag	UNP A0A6P1C618
A	882	HIS	-	expression tag	UNP A0A6P1C618
B	870	LYS	-	expression tag	UNP A0A6P1C618
B	871	LEU	-	expression tag	UNP A0A6P1C618
B	872	ALA	-	expression tag	UNP A0A6P1C618
B	873	ALA	-	expression tag	UNP A0A6P1C618
B	874	ALA	-	expression tag	UNP A0A6P1C618
B	875	LEU	-	expression tag	UNP A0A6P1C618
B	876	GLU	-	expression tag	UNP A0A6P1C618
B	877	HIS	-	expression tag	UNP A0A6P1C618
B	878	HIS	-	expression tag	UNP A0A6P1C618
B	879	HIS	-	expression tag	UNP A0A6P1C618
B	880	HIS	-	expression tag	UNP A0A6P1C618
B	881	HIS	-	expression tag	UNP A0A6P1C618

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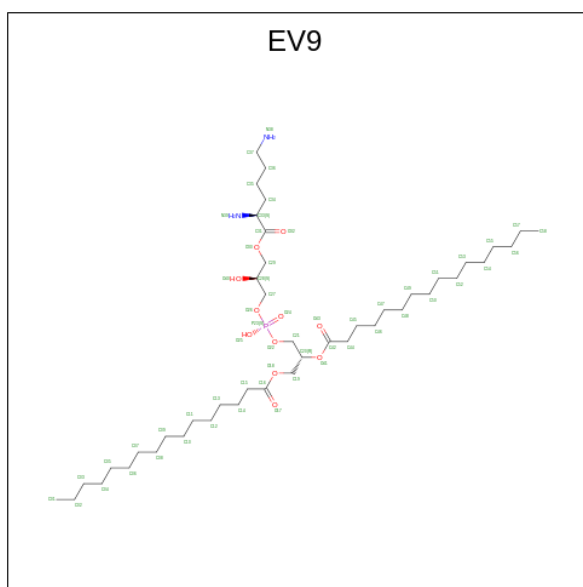
Chain	Residue	Modelled	Actual	Comment	Reference
B	882	HIS	-	expression tag	UNP A0A6P1C618

- Molecule 2 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



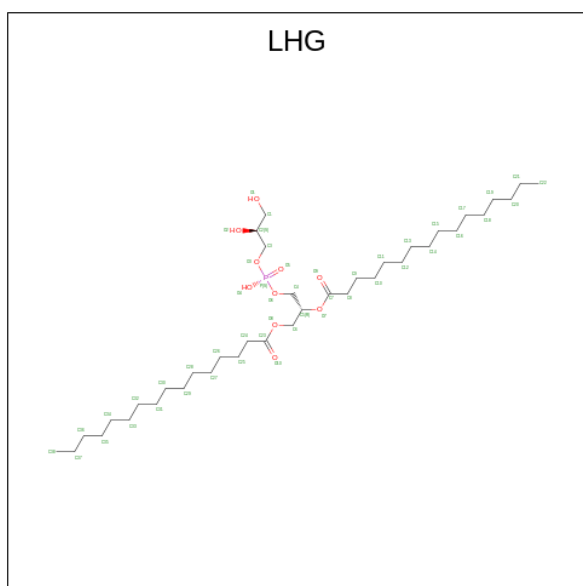
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	

- Molecule 3 is [(2 {R})-3-[(2 {S})-3-[(2 {S})-2,6-bis(azanyl)hexanoyl]oxy-2-oxidanyl-propoxy]-oxidanyl-phosphoryl]oxy-2-hexadecanoyloxy-propyl] hexadecanoate (three-letter code: EV9) (formula: $C_{44}H_{87}N_2O_{11}P$) (labeled as "Ligand of Interest" by depositor).



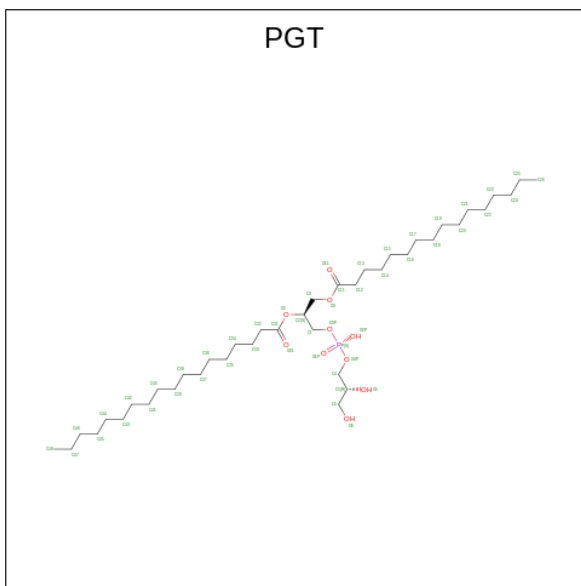
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
3	A	1	Total 116	88	4	22	2	0
3	A	1	Total 116	88	4	22	2	0
3	B	1	Total 116	88	4	22	2	0
3	B	1	Total 116	88	4	22	2	0

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



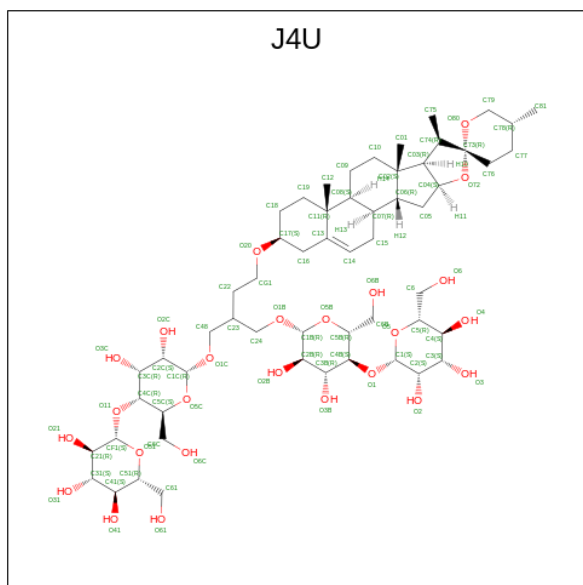
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			47	36	10	1	
4	B	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 5 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			51	40	10	1	
5	B	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 6 is (2 {R},3 {S},4 {S},5 {S},6 {S})-2-(hydroxymethyl)-6-[(2 {R},3 {S},4 {R},5 {R},6 {R})-2-(hydroxymethyl)-6-[2-[(2 {R},3 {S},4 {R},5 {R},6 {S})-6-(hydroxymethyl)-5-[(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]oxymethyl]-4-[(1 {R},2 {R},4 {S},5' {R},6 {R},7 {R},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxy-butoxy]-4,5-bis(oxidanyl)oxan-3-yl]oxy-oxane-3,4,5-triol (three-letter code: J4U) (formula: C₅₆H₉₂O₂₅).



Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C O	0
			81	56 25	
6	B	1	Total	C O	0
			81	56 25	

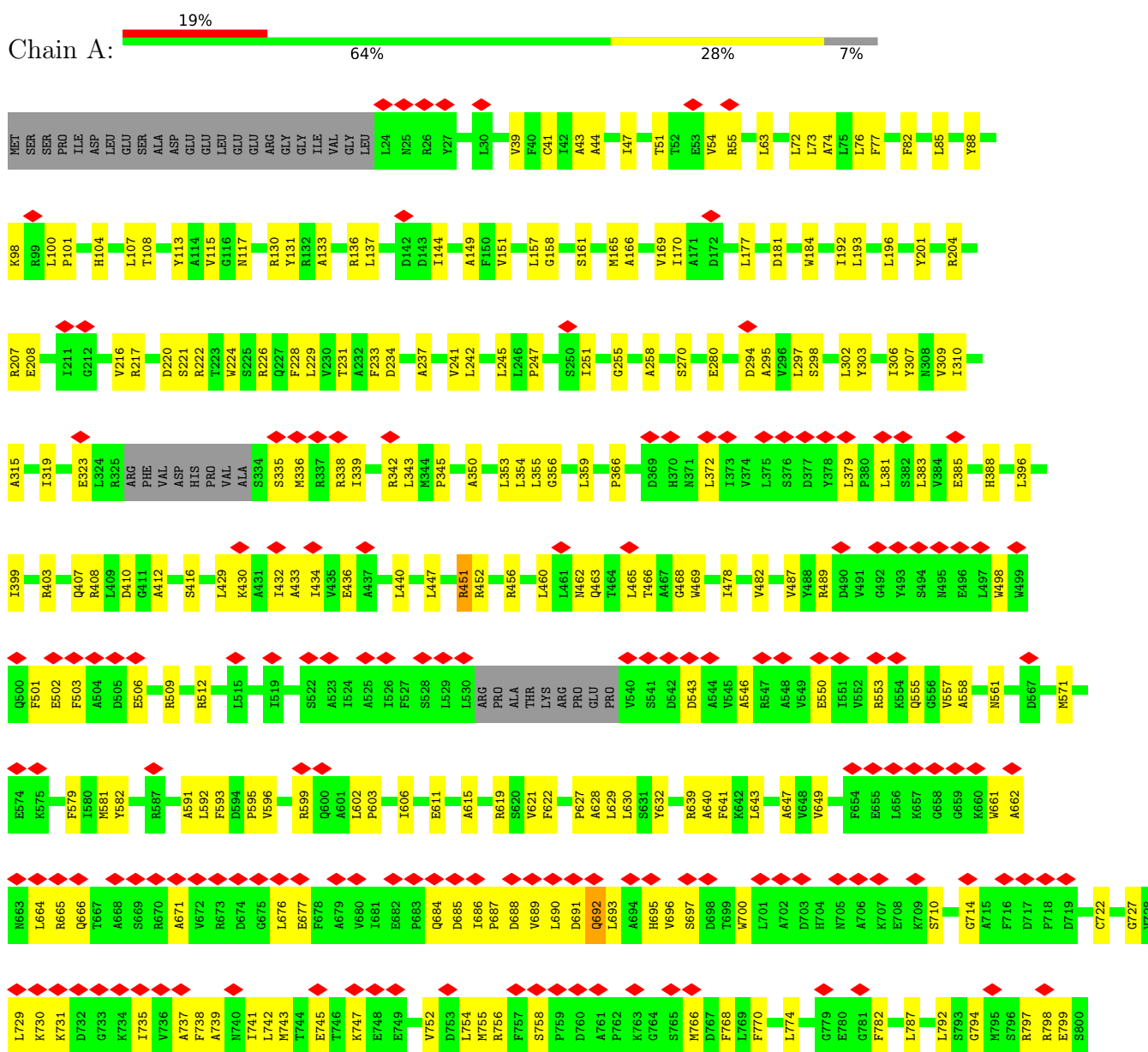
- Molecule 7 is water.

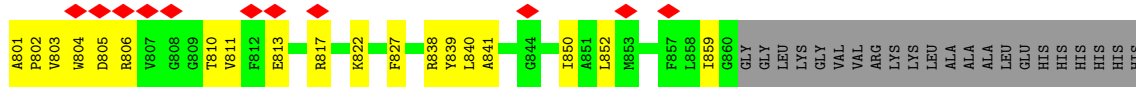
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

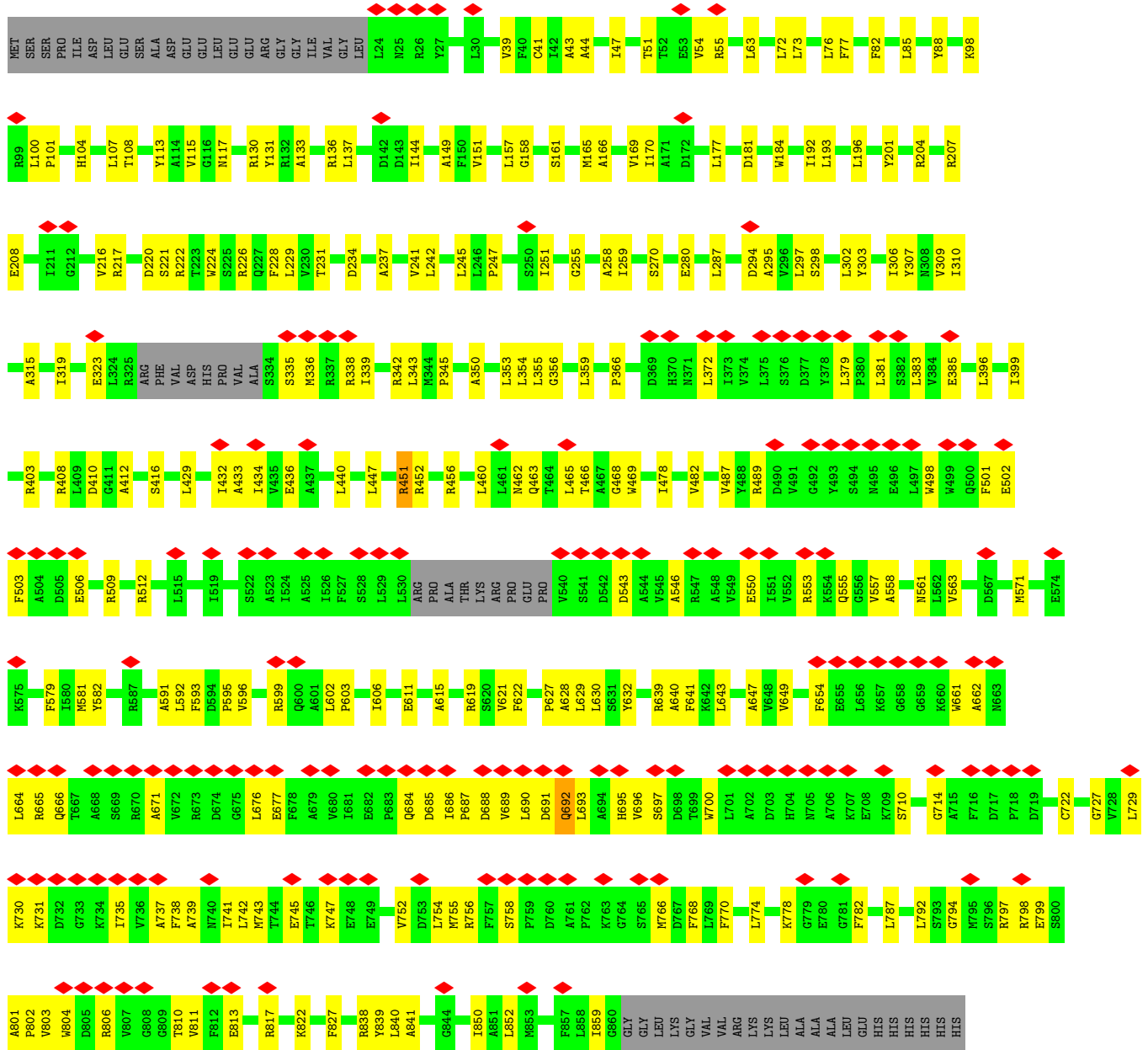
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bifunctional lysylphosphatidylglycerol flippase/synthetase MprF





• Molecule 1: Bifunctional lysylphosphatidylglycerol flippase/synthetase MprF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	144479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	320.0, 320.0, 320.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMT, PGT, J4U, EV9

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	0.29	0/6452	0.44	0/8776
1	B	0.29	0/6452	0.44	0/8776
All	All	0.29	0/12904	0.44	0/17552

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	6307	0	6445	174	0
1	B	6307	0	6445	174	0
2	A	35	0	45	1	0
2	B	35	0	45	1	0
3	A	116	0	0	4	0
3	B	116	0	0	4	0
4	A	47	0	67	5	0
4	B	47	0	67	4	0
5	A	51	0	78	5	0
5	B	51	0	78	4	0
6	A	81	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	81	0	0	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	13276	0	13270	349	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 13.

All (349) 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:A:222:ARG:HB3	1:B:222:ARG:HB3	1.60	0.83
1:B:687:PRO:HA	1:B:690:LEU:HB3	1.65	0.79
1:A:687:PRO:HA	1:A:690:LEU:HB3	1.66	0.78
1:B:714:GLY:HA3	1:B:754:LEU:HB3	1.68	0.75
1:A:714:GLY:HA3	1:A:754:LEU:HB3	1.68	0.74
1:A:247:PRO:HG3	1:A:295:ALA:HB1	1.74	0.70
1:B:599:ARG:HH22	1:B:628:ALA:HB1	1.57	0.69
1:B:247:PRO:HG3	1:B:295:ALA:HB1	1.74	0.69
1:A:599:ARG:HH22	1:A:628:ALA:HB1	1.57	0.69
1:A:385:GLU:OE1	1:A:512:ARG:NH2	2.26	0.69
1:B:385:GLU:OE1	1:B:512:ARG:NH2	2.26	0.69
1:A:403:ARG:NH1	1:A:463:GLN:OE1	2.28	0.67
1:B:170:ILE:HD12	1:B:255:GLY:HA2	1.75	0.67
1:B:403:ARG:NH1	1:B:463:GLN:OE1	2.28	0.67
1:A:170:ILE:HD12	1:A:255:GLY:HA2	1.75	0.66
1:A:356:GLY:HA3	1:A:399:ILE:HG23	1.78	0.66
1:A:622:PHE:HB2	1:A:841:ALA:HB3	1.78	0.66
1:A:381:LEU:HD21	1:A:501:PHE:HB3	1.78	0.66
1:B:356:GLY:HA3	1:B:399:ILE:HG23	1.78	0.66
1:B:622:PHE:HB2	1:B:841:ALA:HB3	1.78	0.65
1:A:100:LEU:HD13	1:A:137:LEU:HD23	1.79	0.65
1:B:100:LEU:HD13	1:B:137:LEU:HD23	1.79	0.65
1:B:381:LEU:HD21	1:B:501:PHE:HB3	1.78	0.64
1:B:44:ALA:HB1	1:B:482:VAL:HG21	1.80	0.64
1:B:381:LEU:HD11	1:B:502:GLU:HA	1.80	0.64
1:A:104:HIS:HB3	1:A:137:LEU:HD21	1.80	0.63
1:B:104:HIS:HB3	1:B:137:LEU:HD21	1.80	0.63
1:B:558:ALA:O	1:B:561:ASN:ND2	2.30	0.63
1:B:684:GLN:NE2	1:B:685:ASP:OD2	2.31	0.63
1:A:44:ALA:HB1	1:A:482:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HD11	1:A:502:GLU:HA	1.80	0.63
1:A:684:GLN:NE2	1:A:685:ASP:OD2	2.31	0.63
1:B:792:LEU:O	1:B:797:ARG:NH1	2.33	0.62
1:A:792:LEU:O	1:A:797:ARG:NH1	2.33	0.62
1:A:606:ILE:HD11	1:A:629:LEU:HD13	1.82	0.62
1:B:359:LEU:HD21	1:B:440:LEU:HD11	1.82	0.62
1:B:149:ALA:HB1	1:B:803:VAL:HG12	1.82	0.61
1:A:558:ALA:O	1:A:561:ASN:ND2	2.30	0.61
1:A:359:LEU:HD21	1:A:440:LEU:HD11	1.82	0.61
1:B:466:THR:HG22	1:B:468:GLY:H	1.66	0.61
1:B:730:LYS:HB3	1:B:735:ILE:HG22	1.83	0.61
1:A:730:LYS:HB3	1:A:735:ILE:HG22	1.83	0.60
1:A:85:LEU:HB3	1:A:113:TYR:CD2	2.36	0.60
1:B:465:LEU:O	1:B:466:THR:OG1	2.16	0.60
1:A:466:THR:HG22	1:A:468:GLY:H	1.66	0.60
1:B:85:LEU:HB3	1:B:113:TYR:CD2	2.36	0.60
1:A:383:LEU:HD21	1:A:429:LEU:HD13	1.83	0.60
1:A:170:ILE:HD11	1:A:258:ALA:HB3	1.83	0.60
1:B:383:LEU:HD21	1:B:429:LEU:HD13	1.83	0.60
1:B:606:ILE:HD11	1:B:629:LEU:HD13	1.82	0.60
1:A:149:ALA:HB1	1:A:803:VAL:HG12	1.82	0.59
1:B:410:ASP:OD1	1:B:451:ARG:NH1	2.33	0.59
1:B:177:LEU:HD11	1:B:251:ILE:HG21	1.84	0.59
1:B:170:ILE:HD11	1:B:258:ALA:HB3	1.83	0.59
1:B:208:GLU:HG2	1:B:217:ARG:HE	1.66	0.59
1:B:307:TYR:OH	3:B:903:EV9:N38	2.36	0.59
1:A:166:ALA:O	1:A:170:ILE:HG12	2.03	0.59
1:A:177:LEU:HD11	1:A:251:ILE:HG21	1.84	0.59
1:B:166:ALA:O	1:B:170:ILE:HG12	2.03	0.59
1:A:208:GLU:HG2	1:A:217:ARG:HE	1.66	0.58
1:A:465:LEU:O	1:A:466:THR:OG1	2.16	0.58
1:A:697:SER:HA	1:A:756:ARG:HG2	1.86	0.57
1:A:43:ALA:O	1:A:47:ILE:HG13	2.05	0.57
1:A:307:TYR:OH	3:A:902:EV9:N38	2.36	0.57
1:B:43:ALA:O	1:B:47:ILE:HG13	2.05	0.57
1:A:366:PRO:HD3	1:A:487:VAL:HG11	1.87	0.57
1:B:671:ALA:HB1	1:B:676:LEU:HD12	1.87	0.57
1:B:697:SER:HA	1:B:756:ARG:HG2	1.86	0.57
1:A:671:ALA:HB1	1:A:676:LEU:HD12	1.87	0.57
1:A:136:ARG:HG2	1:A:342:ARG:HG3	1.86	0.56
1:B:649:VAL:HG11	1:B:774:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:HG2	1:B:342:ARG:HG3	1.86	0.56
1:B:366:PRO:HD3	1:B:487:VAL:HG11	1.87	0.56
1:A:355:LEU:HD21	1:A:440:LEU:HD23	1.88	0.56
1:B:161:SER:O	1:B:165:MET:HG3	2.06	0.56
1:B:555:GLN:OE1	1:B:557:VAL:N	2.39	0.56
1:A:85:LEU:O	1:A:88:TYR:HB2	2.05	0.56
1:B:85:LEU:O	1:B:88:TYR:HB2	2.05	0.56
1:A:161:SER:O	1:A:165:MET:HG3	2.06	0.55
1:A:730:LYS:HA	1:A:735:ILE:HA	1.88	0.55
1:A:555:GLN:OE1	1:A:557:VAL:N	2.39	0.55
1:A:649:VAL:HG11	1:A:774:LEU:HD11	1.87	0.55
1:A:170:ILE:CD1	1:A:255:GLY:HA2	2.36	0.55
1:B:115:VAL:HG13	1:B:350:ALA:HB2	1.89	0.55
1:B:355:LEU:HD21	1:B:440:LEU:HD23	1.87	0.55
1:B:591:ALA:N	1:B:621:VAL:O	2.36	0.55
1:A:770:PHE:HZ	1:A:822:LYS:HG2	1.71	0.55
1:B:170:ILE:CD1	1:B:255:GLY:HA2	2.36	0.55
1:B:770:PHE:HZ	1:B:822:LYS:HG2	1.71	0.55
1:A:410:ASP:OD1	1:A:451:ARG:NH1	2.33	0.54
1:A:661:TRP:HB3	1:A:664:LEU:HB2	1.89	0.54
1:B:245:LEU:HD22	1:B:302:LEU:HD23	1.89	0.54
1:A:591:ALA:N	1:A:621:VAL:O	2.35	0.54
1:A:729:LEU:HB3	1:A:737:ALA:HB3	1.90	0.54
1:B:131:TYR:HA	1:B:144:ILE:HG21	1.90	0.54
1:B:456:ARG:NE	1:B:611:GLU:OE2	2.33	0.54
1:B:730:LYS:HA	1:B:735:ILE:HA	1.88	0.54
1:A:546:ALA:O	1:A:550:GLU:HG2	2.08	0.54
1:B:335:SER:O	1:B:338:ARG:HG2	2.08	0.54
1:A:662:ALA:O	1:A:665:ARG:HG2	2.08	0.54
1:B:546:ALA:O	1:B:550:GLU:HG2	2.08	0.54
1:A:690:LEU:HA	1:A:693:LEU:HD12	1.90	0.54
1:A:335:SER:O	1:A:338:ARG:HG2	2.08	0.53
1:A:353:LEU:HA	1:A:399:ILE:HG22	1.89	0.53
1:B:353:LEU:HA	1:B:399:ILE:HG22	1.89	0.53
1:A:115:VAL:HG13	1:A:350:ALA:HB2	1.89	0.53
1:A:131:TYR:HA	1:A:144:ILE:HG21	1.90	0.53
1:A:245:LEU:HD22	1:A:302:LEU:HD23	1.89	0.53
1:B:661:TRP:HB3	1:B:664:LEU:HB2	1.90	0.53
1:B:729:LEU:HB3	1:B:737:ALA:HB3	1.90	0.53
1:B:690:LEU:HA	1:B:693:LEU:HD12	1.90	0.53
1:B:662:ALA:O	1:B:665:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ASP:OD1	1:B:692:GLN:N	2.42	0.53
1:A:739:ALA:HB1	1:A:752:VAL:HG21	1.92	0.52
1:A:456:ARG:NE	1:A:611:GLU:OE2	2.33	0.52
1:B:412:ALA:N	1:B:460:LEU:HD11	2.24	0.52
1:A:412:ALA:N	1:A:460:LEU:HD11	2.24	0.52
1:A:133:ALA:HB2	1:A:343:LEU:HD21	1.92	0.52
1:A:840:LEU:HD22	1:A:852:LEU:HD13	1.91	0.52
1:B:840:LEU:HD22	1:B:852:LEU:HD13	1.91	0.52
1:A:39:VAL:HG11	1:A:270:SER:HB2	1.92	0.52
1:B:571:MET:HB2	1:B:582:TYR:HE1	1.75	0.52
1:B:688:ASP:N	1:B:688:ASP:OD1	2.43	0.52
1:A:691:ASP:OD1	1:A:692:GLN:N	2.42	0.51
1:B:39:VAL:HG11	1:B:270:SER:HB2	1.92	0.51
2:A:901:LMT:O6'	3:A:903:EV9:O43	2.28	0.51
1:A:543:ASP:N	1:A:543:ASP:OD2	2.44	0.51
1:A:571:MET:HB2	1:A:582:TYR:HE1	1.75	0.51
1:A:595:PRO:HB2	1:A:602:LEU:HD22	1.93	0.51
1:B:739:ALA:HB1	1:B:752:VAL:HG21	1.91	0.51
1:B:686:ILE:HG21	1:B:722:CYS:HA	1.93	0.51
2:B:902:LMT:O6'	3:B:904:EV9:O43	2.28	0.51
1:B:619:ARG:CZ	1:B:850:ILE:HD12	2.41	0.51
1:A:498:TRP:O	1:A:512:ARG:NH1	2.43	0.51
1:B:133:ALA:HB2	1:B:343:LEU:HD21	1.92	0.51
1:B:216:VAL:HG12	1:B:803:VAL:HG23	1.93	0.51
1:B:543:ASP:OD2	1:B:543:ASP:N	2.44	0.51
1:B:595:PRO:HB2	1:B:602:LEU:HD22	1.92	0.51
1:A:234:ASP:OD2	3:A:902:EV9:N38	2.43	0.51
1:A:553:ARG:HB3	1:A:745:GLU:HG2	1.93	0.51
1:B:498:TRP:O	1:B:512:ARG:NH1	2.43	0.51
1:A:619:ARG:CZ	1:A:850:ILE:HD12	2.41	0.50
1:A:688:ASP:OD1	1:A:688:ASP:N	2.43	0.50
1:A:192:ILE:O	1:A:196:LEU:HG	2.12	0.50
1:B:234:ASP:OD2	3:B:903:EV9:N38	2.43	0.50
1:B:710:SER:O	1:B:859:ILE:HA	2.12	0.50
1:B:280:GLU:N	1:B:280:GLU:OE1	2.45	0.50
1:B:662:ALA:O	1:B:666:GLN:HG2	2.11	0.50
1:A:710:SER:O	1:A:859:ILE:HA	2.12	0.50
1:A:201:TYR:O	1:A:204:ARG:NE	2.43	0.50
1:A:229:LEU:HB3	5:B:906:PGT:H142	1.94	0.50
1:A:686:ILE:HG21	1:A:722:CYS:HA	1.93	0.50
1:A:627:PRO:HA	1:A:630:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HD11	1:B:258:ALA:CB	2.42	0.50
1:A:130:ARG:NH2	1:A:151:VAL:HG11	2.27	0.49
1:A:662:ALA:O	1:A:666:GLN:HG2	2.11	0.49
1:B:563:VAL:HB	1:B:581:MET:HE2	1.94	0.49
1:B:130:ARG:NH2	1:B:151:VAL:HG11	2.27	0.49
1:B:221:SER:HA	1:B:224:TRP:NE1	2.27	0.49
1:B:627:PRO:HA	1:B:630:LEU:HG	1.94	0.49
1:A:379:LEU:HD12	1:A:383:LEU:HD22	1.94	0.49
1:B:553:ARG:HB3	1:B:745:GLU:HG2	1.93	0.49
1:A:82:PHE:HA	1:A:85:LEU:HD12	1.95	0.49
1:A:766:MET:HG2	1:A:827:PHE:CZ	2.48	0.49
1:B:82:PHE:HA	1:B:85:LEU:HD12	1.94	0.49
1:A:170:ILE:HD11	1:A:258:ALA:CB	2.42	0.49
1:A:221:SER:HA	1:A:224:TRP:NE1	2.27	0.49
1:B:738:PHE:CE1	1:B:756:ARG:HB2	2.48	0.49
1:B:766:MET:HG2	1:B:827:PHE:CZ	2.48	0.49
1:A:216:VAL:HG12	1:A:803:VAL:HG23	1.93	0.49
1:A:799:GLU:HG2	1:A:799:GLU:O	2.13	0.49
1:B:192:ILE:O	1:B:196:LEU:HG	2.12	0.49
1:A:433:ALA:HB1	1:A:436:GLU:HB3	1.94	0.49
1:A:738:PHE:CE1	1:A:756:ARG:HB2	2.48	0.49
1:A:169:VAL:HG12	1:A:170:ILE:HG23	1.95	0.49
1:A:220:ASP:HB2	5:A:905:PGT:H41	1.95	0.49
1:B:433:ALA:HB1	1:B:436:GLU:HB3	1.94	0.48
1:A:54:VAL:O	1:A:489:ARG:NH2	2.46	0.48
5:A:905:PGT:H142	1:B:229:LEU:HB3	1.94	0.48
1:A:149:ALA:HB3	1:A:802:PRO:HD2	1.96	0.48
1:A:280:GLU:N	1:A:280:GLU:OE1	2.45	0.48
1:A:193:LEU:HD13	4:B:905:LHG:H332	1.95	0.48
1:B:396:LEU:HD12	1:B:399:ILE:HD11	1.96	0.48
1:B:41:CYS:SG	1:B:478:ILE:HD13	2.54	0.48
1:B:379:LEU:HD12	1:B:383:LEU:HD22	1.94	0.48
1:B:799:GLU:O	1:B:799:GLU:HG2	2.13	0.48
1:A:396:LEU:HD12	1:A:399:ILE:HD11	1.96	0.48
6:A:906:J4U:O6C	4:B:905:LHG:O5	2.31	0.47
1:B:54:VAL:O	1:B:489:ARG:NH2	2.46	0.47
1:B:700:TRP:CE3	1:B:756:ARG:HG3	2.49	0.47
1:A:700:TRP:CE3	1:A:756:ARG:HG3	2.49	0.47
1:B:169:VAL:HG12	1:B:170:ILE:HG23	1.95	0.47
1:B:220:ASP:HB2	5:B:906:PGT:H41	1.95	0.47
1:B:654:PHE:O	1:B:778:LYS:NZ	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD23	1:A:339:ILE:HG23	1.96	0.47
1:B:738:PHE:HE1	1:B:756:ARG:HB2	1.79	0.47
4:A:904:LHG:O5	6:B:901:J4U:O6C	2.31	0.47
1:B:677:GLU:O	1:B:730:LYS:N	2.41	0.47
1:B:149:ALA:HB3	1:B:802:PRO:HD2	1.96	0.47
1:A:181:ASP:OD2	6:A:906:J4U:O3C	2.33	0.47
4:A:904:LHG:H332	1:B:193:LEU:HD13	1.95	0.47
1:B:181:ASP:OD2	6:B:901:J4U:O3C	2.33	0.47
1:B:416:SER:OG	1:B:447:LEU:HD21	2.15	0.47
1:A:41:CYS:SG	1:A:478:ILE:HD13	2.54	0.47
1:B:107:LEU:HD23	1:B:339:ILE:HG23	1.96	0.47
1:B:201:TYR:O	1:B:204:ARG:NE	2.43	0.47
1:A:738:PHE:HE1	1:A:756:ARG:HB2	1.79	0.46
1:A:592:LEU:HG	1:A:593:PHE:H	1.81	0.46
1:A:690:LEU:HA	1:A:693:LEU:HB2	1.98	0.46
1:B:561:ASN:HB2	1:B:742:LEU:HG	1.96	0.46
1:A:416:SER:OG	1:A:447:LEU:HD21	2.15	0.46
1:B:676:LEU:HD23	1:B:731:LYS:HB2	1.97	0.46
1:B:794:GLY:O	1:B:798:ARG:HG2	2.16	0.46
1:A:157:LEU:HD23	5:A:905:PGT:H462	1.98	0.46
1:A:581:MET:SD	1:A:592:LEU:HD23	2.55	0.46
1:A:104:HIS:O	1:A:108:THR:HG22	2.16	0.46
1:B:640:ALA:HB1	1:B:839:TYR:HB3	1.98	0.46
1:A:794:GLY:O	1:A:798:ARG:HG2	2.16	0.46
1:B:581:MET:SD	1:B:592:LEU:HD23	2.55	0.46
1:A:676:LEU:HD23	1:A:731:LYS:HB2	1.97	0.45
1:B:104:HIS:O	1:B:108:THR:HG22	2.16	0.45
1:A:104:HIS:NE2	1:A:335:SER:HB3	2.30	0.45
1:B:104:HIS:NE2	1:B:335:SER:HB3	2.30	0.45
1:B:158:GLY:HA3	1:B:231:THR:HG21	1.98	0.45
1:A:561:ASN:HB2	1:A:742:LEU:HG	1.96	0.45
1:B:686:ILE:HG12	1:B:690:LEU:HB2	1.98	0.45
1:B:323:GLU:OE1	1:B:452:ARG:NH1	2.49	0.45
1:A:640:ALA:HB1	1:A:839:TYR:HB3	1.98	0.45
1:B:157:LEU:HD23	5:B:906:PGT:H462	1.98	0.45
1:B:690:LEU:HA	1:B:693:LEU:HB2	1.98	0.45
1:A:228:PHE:HA	1:A:231:THR:HG22	1.99	0.45
1:A:599:ARG:NH2	1:A:628:ALA:HB1	2.30	0.45
5:A:905:PGT:H171	1:B:229:LEU:HB3	1.98	0.44
1:B:592:LEU:HG	1:B:593:PHE:H	1.81	0.44
1:A:686:ILE:HG12	1:A:690:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HB3	4:A:904:LHG:H122	1.99	0.44
1:A:117:ASN:OD1	3:A:902:EV9:O40	2.36	0.44
1:A:204:ARG:HB2	1:A:207:ARG:HH12	1.83	0.44
1:A:741:ILE:HG22	1:A:743:MET:HG3	2.00	0.44
1:B:432:ILE:HG22	1:B:434:ILE:HG12	2.00	0.44
1:A:55:ARG:HD3	1:A:55:ARG:HA	1.75	0.44
1:A:229:LEU:HB3	5:B:906:PGT:H171	1.99	0.44
1:A:323:GLU:OE1	1:A:452:ARG:NH1	2.49	0.44
1:B:117:ASN:OD1	3:B:903:EV9:O40	2.36	0.44
1:B:381:LEU:HA	1:B:503:PHE:CZ	2.53	0.44
1:B:755:MET:C	1:B:756:ARG:HD2	2.38	0.44
1:A:158:GLY:HA3	1:A:231:THR:HG21	1.98	0.44
1:A:169:VAL:HA	6:A:906:J4U:C05	2.47	0.44
1:B:101:PRO:HG2	1:B:104:HIS:ND1	2.33	0.44
1:B:204:ARG:HB2	1:B:207:ARG:HH12	1.83	0.44
1:A:692:GLN:HA	1:A:695:HIS:HB3	2.00	0.44
1:A:107:LEU:HD22	1:A:336:MET:HG3	2.00	0.43
1:B:72:LEU:HB3	4:B:905:LHG:H122	1.99	0.43
1:A:381:LEU:HA	1:A:503:PHE:CZ	2.53	0.43
1:A:432:ILE:HG22	1:A:434:ILE:HG12	2.00	0.43
1:B:63:LEU:HG	1:B:298:SER:HB2	2.00	0.43
1:B:237:ALA:O	1:B:241:VAL:HG23	2.18	0.43
1:B:741:ILE:HG22	1:B:743:MET:HG3	2.00	0.43
1:A:805:ASP:OD1	1:A:805:ASP:N	2.50	0.43
1:B:169:VAL:HA	6:B:901:J4U:C05	2.48	0.43
1:B:315:ALA:O	1:B:319:ILE:HG12	2.19	0.43
1:B:107:LEU:HD22	1:B:336:MET:HG3	2.00	0.43
1:A:73:LEU:HG	1:A:77:PHE:CE2	2.54	0.43
1:A:237:ALA:O	1:A:241:VAL:HG23	2.18	0.43
1:A:755:MET:C	1:A:756:ARG:HD2	2.38	0.43
1:B:76:LEU:HA	4:B:905:LHG:H182	2.01	0.43
1:B:228:PHE:HA	1:B:231:THR:HG22	1.99	0.43
1:B:403:ARG:NE	1:B:465:LEU:O	2.52	0.43
1:B:627:PRO:HG3	1:B:839:TYR:HE2	1.84	0.43
1:B:639:ARG:HG2	1:B:641:PHE:CZ	2.54	0.43
1:A:372:LEU:HD23	1:A:372:LEU:HA	1.90	0.43
1:A:403:ARG:NE	1:A:465:LEU:O	2.52	0.43
1:B:73:LEU:HG	1:B:77:PHE:CE2	2.54	0.42
1:B:242:LEU:HD13	1:B:303:TYR:HB2	2.01	0.42
1:A:63:LEU:HG	1:A:298:SER:HB2	2.00	0.42
1:A:101:PRO:HG2	1:A:104:HIS:ND1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:PRO:HG3	1:B:606:ILE:HG13	2.01	0.42
1:A:342:ARG:HD3	1:A:342:ARG:HA	1.83	0.42
1:A:677:GLU:O	1:A:730:LYS:N	2.41	0.42
1:B:181:ASP:HB3	1:B:184:TRP:CD1	2.54	0.42
1:B:309:VAL:HG22	1:B:354:LEU:HD13	2.02	0.42
1:A:181:ASP:HB3	1:A:184:TRP:CD1	2.54	0.42
1:A:462:ASN:O	1:A:615:ALA:HA	2.20	0.42
1:A:639:ARG:HG2	1:A:641:PHE:CZ	2.54	0.42
1:B:55:ARG:HA	1:B:55:ARG:HD3	1.75	0.42
1:B:592:LEU:HD12	1:B:592:LEU:HA	1.81	0.42
1:B:355:LEU:HD11	1:B:440:LEU:HG	2.02	0.42
1:B:462:ASN:O	1:B:615:ALA:HA	2.20	0.42
1:A:466:THR:HB	1:A:469:TRP:H	1.85	0.42
1:A:506:GLU:HG2	1:A:509:ARG:CZ	2.50	0.42
1:A:627:PRO:HG3	1:A:839:TYR:HE2	1.84	0.42
1:B:466:THR:HB	1:B:469:TRP:H	1.85	0.42
1:B:692:GLN:HA	1:B:695:HIS:HB3	2.00	0.42
1:A:595:PRO:HG3	1:A:606:ILE:HG13	2.01	0.42
1:A:647:ALA:HB3	1:A:787:LEU:HB2	2.02	0.42
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.90	0.42
1:B:810:THR:HG23	1:B:852:LEU:HD23	2.02	0.42
1:A:315:ALA:O	1:A:319:ILE:HG12	2.19	0.41
1:B:51:THR:HG21	1:B:297:LEU:HD11	2.02	0.41
1:B:661:TRP:CD1	1:B:664:LEU:HD12	2.55	0.41
1:B:294:ASP:OD1	1:B:295:ALA:N	2.53	0.41
1:B:647:ALA:HB3	1:B:787:LEU:HB2	2.02	0.41
1:B:813:GLU:O	1:B:817:ARG:HG3	2.20	0.41
1:A:242:LEU:HD13	1:A:303:TYR:HB2	2.01	0.41
1:A:810:THR:HG23	1:A:852:LEU:HD23	2.02	0.41
1:B:98:LYS:HA	1:B:98:LYS:HD3	1.74	0.41
1:B:579:PHE:CE1	1:B:596:VAL:HB	2.56	0.41
1:A:838:ARG:HA	1:A:838:ARG:HD3	1.89	0.41
1:B:643:LEU:HA	1:B:811:VAL:HG13	2.03	0.41
1:B:664:LEU:HD23	1:B:664:LEU:HA	1.88	0.41
1:A:579:PHE:CE1	1:A:596:VAL:HB	2.56	0.41
1:B:838:ARG:HD3	1:B:838:ARG:HA	1.89	0.41
1:A:661:TRP:CD1	1:A:664:LEU:HD12	2.55	0.41
1:A:801:ALA:HB3	1:A:804:TRP:HD1	1.86	0.41
1:A:76:LEU:HA	4:A:904:LHG:H182	2.01	0.41
1:A:309:VAL:HG22	1:A:354:LEU:HD13	2.02	0.41
1:B:506:GLU:HG2	1:B:509:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HD2	1:B:222:ARG:CG	2.50	0.41
1:A:388:HIS:ND1	1:A:430:LYS:HD2	2.36	0.41
1:B:603:PRO:HG3	1:B:632:TYR:CE2	2.56	0.41
1:B:729:LEU:HD11	1:B:768:PHE:CD2	2.56	0.41
1:A:689:VAL:O	1:A:693:LEU:HG	2.21	0.41
1:B:259:ILE:HD13	1:B:287:LEU:HD21	2.03	0.41
1:B:696:VAL:HG23	1:B:758:SER:OG	2.21	0.41
1:B:801:ALA:HB3	1:B:804:TRP:HD1	1.86	0.41
1:A:51:THR:HG21	1:A:297:LEU:HD11	2.03	0.41
1:A:355:LEU:HD11	1:A:440:LEU:HG	2.02	0.41
1:A:603:PRO:HG3	1:A:632:TYR:CE2	2.56	0.41
1:A:643:LEU:HA	1:A:811:VAL:HG13	2.02	0.41
1:A:729:LEU:HD11	1:A:768:PHE:CD2	2.56	0.41
1:A:222:ARG:CG	1:B:226:ARG:HD2	2.51	0.40
1:A:233:PHE:HE1	4:A:904:LHG:H322	1.87	0.40
1:A:345:PRO:HG2	1:A:408:ARG:CZ	2.51	0.40
1:A:747:LYS:HA	1:A:782:PHE:CE1	2.56	0.40
1:B:599:ARG:NH2	1:B:628:ALA:HB1	2.30	0.40
1:B:747:LYS:HA	1:B:782:PHE:CE1	2.56	0.40
1:A:294:ASP:OD1	1:A:295:ALA:N	2.53	0.40
1:A:696:VAL:HG23	1:A:758:SER:OG	2.21	0.40
1:A:727:GLY:H	1:A:741:ILE:HG13	1.86	0.40
1:A:813:GLU:O	1:A:817:ARG:HG3	2.20	0.40
5:A:905:PGT:H171	1:B:229:LEU:HD23	2.03	0.40
1:B:306:ILE:O	1:B:310:ILE:HB	2.21	0.40
1:B:345:PRO:HG2	1:B:408:ARG:CZ	2.51	0.40
1:B:727:GLY:H	1:B:741:ILE:HG13	1.86	0.40
1:A:98:LYS:HA	1:A:98:LYS:HD3	1.74	0.40
1:A:306:ILE:O	1:A:310:ILE:HB	2.21	0.40
1:A:74:ALA:HB1	1:A:241:VAL:HG13	2.04	0.40
1:A:403:ARG:CZ	1:A:407:GLN:HE22	2.34	0.40
1:B:689:VAL:O	1:B:693:LEU:HG	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	814/882 (92%)	782 (96%)	32 (4%)	0	100	100
1	B	814/882 (92%)	781 (96%)	33 (4%)	0	100	100
All	All	1628/1764 (92%)	1563 (96%)	65 (4%)	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	654/705 (93%)	651 (100%)	3 (0%)	88	95
1	B	654/705 (93%)	651 (100%)	3 (0%)	88	95
All	All	1308/1410 (93%)	1302 (100%)	6 (0%)	89	95

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

Mol	Chain	Res	Type
1	A	451	ARG
1	A	692	GLN
1	A	806	ARG
1	B	451	ARG
1	B	692	GLN
1	B	806	ARG

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](#)

12 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
3	EV9	B	904	-	57,57,57	1.04	4 (7%)	61,65,65	1.02	4 (6%)
2	LMT	A	901	-	36,36,36	1.15	5 (13%)	47,47,47	1.01	2 (4%)
6	J4U	A	906	-	90,90,90	1.79	15 (16%)	136,138,138	1.90	25 (18%)
3	EV9	A	902	-	57,57,57	1.04	4 (7%)	61,65,65	1.00	4 (6%)
5	PGT	A	905	-	50,50,50	0.91	2 (4%)	53,56,56	1.05	3 (5%)
6	J4U	B	901	-	90,90,90	1.79	14 (15%)	136,138,138	1.90	25 (18%)
3	EV9	B	903	-	57,57,57	1.04	4 (7%)	61,65,65	1.00	4 (6%)
4	LHG	B	905	-	46,46,48	0.95	2 (4%)	49,52,54	1.09	4 (8%)
3	EV9	A	903	-	57,57,57	1.04	4 (7%)	61,65,65	1.02	4 (6%)
2	LMT	B	902	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
4	LHG	A	904	-	46,46,48	0.95	2 (4%)	49,52,54	1.08	4 (8%)
5	PGT	B	906	-	50,50,50	0.92	2 (4%)	53,56,56	1.05	3 (5%)

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
3	EV9	B	904	-	-	36/65/65/65	-
2	LMT	A	901	-	-	13/21/61/61	0/2/2/2
6	J4U	A	906	-	-	19/32/200/200	0/10/10/10
3	EV9	A	902	-	-	35/65/65/65	-
5	PGT	A	905	-	-	6/55/55/55	-
6	J4U	B	901	-	-	19/32/200/200	0/10/10/10
3	EV9	B	903	-	-	35/65/65/65	-
4	LHG	B	905	-	-	4/51/51/53	-
3	EV9	A	903	-	-	36/65/65/65	-
2	LMT	B	902	-	-	13/21/61/61	0/2/2/2
4	LHG	A	904	-	-	4/51/51/53	-
5	PGT	B	906	-	-	6/55/55/55	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	J4U	O72-C73	8.54	1.61	1.42
6	A	906	J4U	O72-C73	8.50	1.61	1.42
6	A	906	J4U	C09-C08	-5.32	1.44	1.53
6	B	901	J4U	C09-C08	-5.28	1.44	1.53
6	A	906	J4U	C11-C13	-4.40	1.44	1.52
6	B	901	J4U	C11-C13	-4.40	1.44	1.52
6	A	906	J4U	C03-C04	-4.32	1.45	1.54
6	B	901	J4U	C03-C04	-4.30	1.45	1.54
4	B	905	LHG	O8-C23	4.22	1.45	1.33
4	A	904	LHG	O8-C23	4.20	1.45	1.33
5	B	906	PGT	O3-C11	4.19	1.45	1.33
6	A	906	J4U	C10-C09	-4.16	1.44	1.53
6	B	901	J4U	C10-C09	-4.16	1.44	1.53
5	A	905	PGT	O3-C11	4.15	1.45	1.33
5	A	905	PGT	O2-C31	4.10	1.45	1.34
5	B	906	PGT	O2-C31	4.10	1.45	1.34
4	A	904	LHG	O7-C7	4.08	1.45	1.34
4	B	905	LHG	O7-C7	4.08	1.45	1.34
6	B	901	J4U	C14-C13	-3.69	1.24	1.33
6	A	906	J4U	C14-C13	-3.68	1.24	1.33
3	A	903	EV9	O30-C31	3.61	1.40	1.33
3	B	904	EV9	O30-C31	3.61	1.40	1.33
3	B	903	EV9	O30-C31	3.61	1.40	1.33
3	A	902	EV9	O30-C31	3.59	1.40	1.33
6	A	906	J4U	C11-C08	3.38	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	J4U	C11-C08	3.38	1.61	1.56
6	A	906	J4U	C02-C06	-3.32	1.48	1.55
6	B	901	J4U	C02-C06	-3.32	1.48	1.55
3	A	902	EV9	O18-C16	2.94	1.41	1.33
3	B	903	EV9	O18-C16	2.94	1.41	1.33
3	A	903	EV9	O18-C16	2.90	1.41	1.33
3	B	904	EV9	O18-C16	2.88	1.41	1.33
3	B	903	EV9	O41-C20	-2.80	1.39	1.46
3	A	902	EV9	O41-C20	-2.79	1.39	1.46
3	A	903	EV9	O41-C20	-2.70	1.39	1.46
2	B	902	LMT	O3'-C3'	-2.66	1.36	1.43
3	B	904	EV9	O41-C20	-2.66	1.39	1.46
2	A	901	LMT	O3'-C3'	-2.64	1.36	1.43
6	A	906	J4U	C10-C02	-2.60	1.49	1.54
6	B	901	J4U	C10-C02	-2.57	1.49	1.54
6	A	906	J4U	C05-C04	2.53	1.58	1.52
6	A	906	J4U	O72-C04	2.53	1.49	1.43
6	B	901	J4U	C05-C04	2.51	1.58	1.52
6	B	901	J4U	O72-C04	2.49	1.49	1.43
3	A	903	EV9	O41-C42	2.43	1.41	1.34
3	B	904	EV9	O41-C42	2.40	1.41	1.34
6	A	906	J4U	C75-C74	2.35	1.58	1.53
6	B	901	J4U	C75-C74	2.35	1.58	1.53
2	A	901	LMT	O2'-C2'	-2.30	1.37	1.43
6	A	906	J4U	C19-C18	2.30	1.58	1.53
3	A	902	EV9	O41-C42	2.29	1.40	1.34
3	B	903	EV9	O41-C42	2.29	1.40	1.34
2	A	901	LMT	O3B-C3B	-2.29	1.37	1.43
2	B	902	LMT	O2'-C2'	-2.28	1.37	1.43
6	B	901	J4U	C19-C18	2.28	1.58	1.53
2	B	902	LMT	O3B-C3B	-2.26	1.37	1.43
2	A	901	LMT	O4'-C4B	-2.15	1.37	1.43
2	B	902	LMT	O4'-C4B	-2.15	1.37	1.43
6	A	906	J4U	C22-CG1	2.10	1.58	1.50
6	B	901	J4U	C22-CG1	2.10	1.58	1.50
2	A	901	LMT	O2B-C2B	-2.08	1.38	1.43
2	B	902	LMT	O2B-C2B	-2.08	1.38	1.43
6	A	906	J4U	C48-C23	2.01	1.58	1.51

All (84) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	906	J4U	C76-C73-C74	11.62	139.60	115.69
6	B	901	J4U	C76-C73-C74	11.62	139.60	115.69
6	B	901	J4U	C05-C06-C07	-5.37	107.99	119.48
6	A	906	J4U	C05-C06-C07	-5.36	108.00	119.48
6	B	901	J4U	C03-C02-C06	4.71	107.16	100.23
6	A	906	J4U	C03-C02-C06	4.70	107.14	100.23
6	B	901	J4U	C09-C08-C11	-4.54	107.10	113.08
6	A	906	J4U	C09-C08-C11	-4.52	107.12	113.08
5	A	905	PGT	O2-C31-C32	4.23	120.61	111.50
5	B	906	PGT	O2-C31-C32	4.22	120.59	111.50
4	B	905	LHG	O7-C7-C8	4.16	120.48	111.50
3	A	903	EV9	O41-C42-C44	4.16	120.47	111.50
3	B	904	EV9	O41-C42-C44	4.16	120.46	111.50
4	A	904	LHG	O7-C7-C8	4.14	120.42	111.50
6	A	906	J4U	C09-C10-C02	4.14	119.88	112.78
6	B	901	J4U	C09-C10-C02	4.12	119.85	112.78
6	B	901	J4U	O72-C73-C76	-3.98	99.36	108.60
6	A	906	J4U	C08-C07-C06	3.98	114.42	109.09
6	A	906	J4U	O72-C73-C76	-3.97	99.40	108.60
6	B	901	J4U	C08-C07-C06	3.97	114.40	109.09
6	B	901	J4U	C10-C02-C03	-3.96	109.13	115.46
6	A	906	J4U	C10-C02-C03	-3.95	109.15	115.46
3	B	903	EV9	O41-C42-C44	3.94	120.00	111.50
3	A	902	EV9	O41-C42-C44	3.92	119.95	111.50
3	B	903	EV9	O30-C31-C33	3.72	120.56	111.59
6	A	906	J4U	C01-C02-C06	-3.72	104.78	111.71
6	B	901	J4U	C01-C02-C06	-3.71	104.80	111.71
3	A	902	EV9	O30-C31-C33	3.71	120.53	111.59
6	B	901	J4U	C1-O1-C4B	-3.48	109.36	117.96
6	A	906	J4U	C1-O1-C4B	-3.46	109.39	117.96
3	A	903	EV9	O30-C31-C33	3.45	119.91	111.59
3	B	904	EV9	O30-C31-C33	3.45	119.90	111.59
6	A	906	J4U	CG1-C22-C23	-3.24	109.78	113.88
6	B	901	J4U	CG1-C22-C23	-3.24	109.78	113.88
6	B	901	J4U	C73-C74-C03	3.19	108.56	103.37
6	A	906	J4U	C73-C74-C03	3.19	108.56	103.37
6	A	906	J4U	C16-C13-C11	3.07	120.49	116.42
6	B	901	J4U	C16-C13-C11	3.07	120.49	116.42
5	A	905	PGT	C2-O2-C31	-3.01	110.37	117.79
5	B	906	PGT	C2-O2-C31	-2.99	110.42	117.79
2	A	901	LMT	C3'-C4'-C5'	-2.97	104.12	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	LMT	C3'-C4'-C5'	-2.96	104.15	110.93
4	B	905	LHG	O8-C23-C24	2.90	121.01	111.91
4	A	904	LHG	O8-C23-C24	2.89	120.98	111.91
6	A	906	J4U	O11-C4C-C3C	2.80	114.73	107.28
6	B	901	J4U	O11-C4C-C3C	2.80	114.72	107.28
6	A	906	J4U	C17-C16-C13	2.78	115.83	111.52
6	B	901	J4U	O80-C73-O72	-2.75	102.12	109.78
6	B	901	J4U	C17-C16-C13	2.74	115.77	111.52
6	A	906	J4U	O80-C73-O72	-2.73	102.17	109.78
6	A	906	J4U	C1B-O5B-C5B	2.66	118.92	113.69
6	A	906	J4U	O80-C79-C78	-2.66	108.35	112.18
6	B	901	J4U	O80-C79-C78	-2.65	108.36	112.18
6	B	901	J4U	C1B-O5B-C5B	2.65	118.90	113.69
6	A	906	J4U	O80-C73-C74	-2.58	98.31	107.38
6	B	901	J4U	O80-C73-C74	-2.58	98.34	107.38
3	B	904	EV9	O18-C16-C15	2.49	119.73	111.91
3	A	903	EV9	O18-C16-C15	2.49	119.71	111.91
3	A	902	EV9	O18-C16-C15	2.43	119.54	111.91
3	B	903	EV9	O18-C16-C15	2.43	119.54	111.91
6	B	901	J4U	O5B-C5B-C6B	2.38	112.34	106.44
6	A	906	J4U	O5B-C5B-C6B	2.36	112.30	106.44
4	A	904	LHG	C5-O7-C7	-2.36	111.99	117.79
6	A	906	J4U	C15-C07-C06	-2.35	107.49	110.91
4	B	905	LHG	C5-O7-C7	-2.35	112.02	117.79
3	B	903	EV9	O30-C31-O32	-2.34	119.70	124.13
6	B	901	J4U	C15-C07-C06	-2.34	107.52	110.91
3	A	902	EV9	O30-C31-O32	-2.29	119.78	124.13
2	B	902	LMT	C1'-O5'-C5'	-2.26	109.25	113.69
2	A	901	LMT	C1'-O5'-C5'	-2.25	109.28	113.69
6	A	906	J4U	C01-C02-C03	2.18	116.94	111.63
6	B	901	J4U	C01-C02-C03	2.18	116.93	111.63
6	B	901	J4U	O72-C04-C03	2.16	108.26	105.07
3	A	903	EV9	O30-C31-O32	-2.16	120.05	124.13
3	B	904	EV9	O30-C31-O32	-2.16	120.05	124.13
5	A	905	PGT	O3-C11-C12	2.15	118.64	111.91
5	B	906	PGT	O3-C11-C12	2.14	118.62	111.91
6	A	906	J4U	O72-C04-C03	2.14	108.22	105.07
6	A	906	J4U	O80-C73-C76	-2.07	108.85	110.77
6	B	901	J4U	O80-C73-C76	-2.06	108.85	110.77
6	B	901	J4U	C81-C78-C79	-2.05	107.58	111.18
6	A	906	J4U	C81-C78-C79	-2.02	107.62	111.18
4	B	905	LHG	O8-C23-O10	-2.01	118.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	LHG	O8-C23-O10	-2.01	118.53	123.59

There are no chirality outliers.

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	LMT	O5'-C1'-O1'-C1
2	B	902	LMT	O5'-C1'-O1'-C1
3	A	902	EV9	O26-C27-C28-O40
3	A	902	EV9	C27-C28-C29-O30
3	A	902	EV9	C33-C31-O30-C29
3	A	902	EV9	C44-C42-O41-C20
3	A	902	EV9	C21-O22-P23-O24
3	A	902	EV9	C27-O26-P23-O24
3	A	903	EV9	O30-C31-C33-C34
3	A	903	EV9	C31-C33-C34-C35
3	A	903	EV9	N39-C33-C34-C35
3	A	903	EV9	C21-O22-P23-O24
3	A	903	EV9	C27-O26-P23-O22
3	B	903	EV9	O26-C27-C28-O40
3	B	903	EV9	C27-C28-C29-O30
3	B	903	EV9	C33-C31-O30-C29
3	B	903	EV9	C44-C42-O41-C20
3	B	903	EV9	C21-O22-P23-O24
3	B	903	EV9	C27-O26-P23-O24
3	B	904	EV9	O30-C31-C33-C34
3	B	904	EV9	C31-C33-C34-C35
3	B	904	EV9	N39-C33-C34-C35
3	B	904	EV9	C21-O22-P23-O24
3	B	904	EV9	C27-O26-P23-O22
6	A	906	J4U	O5C-C1C-O1C-C48
6	B	901	J4U	O5C-C1C-O1C-C48
3	A	902	EV9	O17-C16-O18-C19
3	B	903	EV9	O17-C16-O18-C19
3	A	902	EV9	C15-C16-O18-C19
3	B	903	EV9	C15-C16-O18-C19
6	A	906	J4U	C4B-C5B-C6B-O6B
6	B	901	J4U	C4B-C5B-C6B-O6B
3	A	902	EV9	O43-C42-O41-C20
3	B	903	EV9	O43-C42-O41-C20
2	A	901	LMT	C2B-C1B-O1B-C4'
2	B	902	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
2	A	901	LMT	O5B-C1B-O1B-C4'
2	B	902	LMT	O5B-C1B-O1B-C4'
3	A	902	EV9	O32-C31-O30-C29
3	B	903	EV9	O32-C31-O30-C29
6	A	906	J4U	O5B-C5B-C6B-O6B
6	B	901	J4U	O5B-C5B-C6B-O6B
6	A	906	J4U	O5-C1-O1-C4B
6	B	901	J4U	O5-C1-O1-C4B
2	A	901	LMT	O5B-C5B-C6B-O6B
2	B	902	LMT	O5B-C5B-C6B-O6B
6	A	906	J4U	O5-C5-C6-O6
6	B	901	J4U	O5-C5-C6-O6
3	A	903	EV9	C15-C16-O18-C19
3	B	904	EV9	C15-C16-O18-C19
2	A	901	LMT	C4B-C5B-C6B-O6B
3	A	902	EV9	C10-C11-C12-C13
3	B	903	EV9	C10-C11-C12-C13
2	B	902	LMT	C4B-C5B-C6B-O6B
6	A	906	J4U	C4-C5-C6-O6
6	B	901	J4U	C4-C5-C6-O6
3	A	902	EV9	C12-C13-C14-C15
3	B	903	EV9	C12-C13-C14-C15
6	A	906	J4U	C2-C1-O1-C4B
6	B	901	J4U	C2-C1-O1-C4B
6	A	906	J4U	O5C-C5C-C6C-O6C
6	B	901	J4U	O5C-C5C-C6C-O6C
3	A	902	EV9	O40-C28-C29-O30
3	B	903	EV9	O40-C28-C29-O30
2	A	901	LMT	O5'-C5'-C6'-O6'
2	B	902	LMT	O5'-C5'-C6'-O6'
3	A	902	EV9	C04-C05-C06-C07
3	B	903	EV9	C04-C05-C06-C07
3	A	902	EV9	C02-C03-C04-C05
3	B	903	EV9	C02-C03-C04-C05
6	A	906	J4U	C5C-C4C-O11-CF1
6	B	901	J4U	C5C-C4C-O11-CF1
3	A	903	EV9	O17-C16-O18-C19
3	B	904	EV9	O17-C16-O18-C19
3	A	903	EV9	O40-C28-C29-O30
3	B	904	EV9	O40-C28-C29-O30
3	A	902	EV9	C21-O22-P23-O26
3	A	903	EV9	C21-O22-P23-O26

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Mol	Chain	Res	Type	Atoms
3	B	903	EV9	C21-O22-P23-O26
3	B	904	EV9	C21-O22-P23-O26
3	A	902	EV9	C33-C34-C35-C36
3	B	903	EV9	C33-C34-C35-C36
3	A	902	EV9	O26-C27-C28-C29
3	B	903	EV9	O26-C27-C28-C29
3	A	903	EV9	C06-C07-C08-C09
3	A	903	EV9	C52-C53-C54-C55
3	B	904	EV9	C06-C07-C08-C09
3	B	904	EV9	C52-C53-C54-C55
3	A	903	EV9	C27-C28-C29-O30
3	B	904	EV9	C27-C28-C29-O30
2	A	901	LMT	C7-C8-C9-C10
2	B	902	LMT	C7-C8-C9-C10
3	A	903	EV9	C46-C47-C48-C49
3	B	904	EV9	C46-C47-C48-C49
6	A	906	J4U	C4C-C5C-C6C-O6C
6	B	901	J4U	C4C-C5C-C6C-O6C
6	A	906	J4U	C2B-C1B-O1B-C24
6	B	901	J4U	C2B-C1B-O1B-C24
2	A	901	LMT	C11-C10-C9-C8
2	B	902	LMT	C11-C10-C9-C8
3	A	902	EV9	C49-C50-C51-C52
3	A	903	EV9	C04-C05-C06-C07
3	B	903	EV9	C49-C50-C51-C52
3	B	904	EV9	C04-C05-C06-C07
6	A	906	J4U	O5B-C1B-O1B-C24
6	B	901	J4U	O5B-C1B-O1B-C24
3	A	903	EV9	C12-C13-C14-C15
3	B	904	EV9	C12-C13-C14-C15
3	A	903	EV9	C48-C49-C50-C51
3	A	903	EV9	C50-C51-C52-C53
3	B	904	EV9	C48-C49-C50-C51
3	B	904	EV9	C50-C51-C52-C53
2	A	901	LMT	C3-C4-C5-C6
2	B	902	LMT	C3-C4-C5-C6
3	A	902	EV9	C50-C51-C52-C53
3	B	903	EV9	C50-C51-C52-C53
3	B	904	EV9	C49-C50-C51-C52
3	A	903	EV9	C49-C50-C51-C52
3	A	903	EV9	C44-C45-C46-C47
3	B	904	EV9	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
2	A	901	LMT	C2-C3-C4-C5
2	B	902	LMT	C2-C3-C4-C5
6	A	906	J4U	C2C-C1C-O1C-C48
6	B	901	J4U	C2C-C1C-O1C-C48
3	A	903	EV9	O18-C19-C20-O41
3	B	904	EV9	O18-C19-C20-O41
3	A	902	EV9	C51-C52-C53-C54
3	B	903	EV9	C51-C52-C53-C54
5	A	905	PGT	C33-C34-C35-C36
5	B	906	PGT	C33-C34-C35-C36
3	A	903	EV9	C11-C12-C13-C14
3	B	904	EV9	C11-C12-C13-C14
3	A	903	EV9	O18-C19-C20-C21
3	B	904	EV9	O18-C19-C20-C21
3	A	903	EV9	C05-C06-C07-C08
3	B	904	EV9	C05-C06-C07-C08
3	A	903	EV9	C01-C02-C03-C04
3	B	904	EV9	C01-C02-C03-C04
3	A	903	EV9	O32-C31-C33-C34
3	B	904	EV9	O32-C31-C33-C34
6	B	901	J4U	O51-C51-C61-O61
6	A	906	J4U	C3C-C4C-O11-CF1
6	B	901	J4U	C3C-C4C-O11-CF1
6	A	906	J4U	O51-C51-C61-O61
3	B	903	EV9	C01-C02-C03-C04
3	A	902	EV9	C01-C02-C03-C04
3	A	902	EV9	O18-C19-C20-O41
3	B	903	EV9	O18-C19-C20-O41
3	A	903	EV9	C10-C11-C12-C13
3	B	904	EV9	C10-C11-C12-C13
3	A	902	EV9	C53-C54-C55-C56
3	B	903	EV9	C53-C54-C55-C56
3	A	902	EV9	C27-O26-P23-O22
3	B	903	EV9	C27-O26-P23-O22
6	A	906	J4U	C24-C23-C48-O1C
6	B	901	J4U	C24-C23-C48-O1C
3	A	903	EV9	C28-C27-O26-P23
3	B	904	EV9	C28-C27-O26-P23
3	B	903	EV9	C05-C06-C07-C08
2	A	901	LMT	C4'-C5'-C6'-O6'
3	A	902	EV9	C05-C06-C07-C08
2	B	902	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
6	A	906	J4U	C22-C23-C48-O1C
6	B	901	J4U	C22-C23-C48-O1C
3	A	902	EV9	C47-C48-C49-C50
3	B	903	EV9	C47-C48-C49-C50
3	B	904	EV9	C42-C44-C45-C46
3	A	903	EV9	C42-C44-C45-C46
4	A	904	LHG	C29-C30-C31-C32
4	B	905	LHG	C29-C30-C31-C32
6	A	906	J4U	C23-C22-CG1-O20
6	B	901	J4U	C23-C22-CG1-O20
5	A	905	PGT	C1-O3P-P-O4P
5	B	906	PGT	C1-O3P-P-O4P
3	A	902	EV9	C21-O22-P23-O25
3	A	903	EV9	C27-O26-P23-O25
3	B	903	EV9	C21-O22-P23-O25
3	B	904	EV9	C27-O26-P23-O25
3	A	903	EV9	C03-C04-C05-C06
3	B	904	EV9	C03-C04-C05-C06
6	A	906	J4U	C23-C24-O1B-C1B
6	B	901	J4U	C23-C24-O1B-C1B
3	A	902	EV9	O18-C19-C20-C21
3	B	903	EV9	O18-C19-C20-C21
3	B	903	EV9	C07-C08-C09-C10
3	A	902	EV9	C07-C08-C09-C10
2	A	901	LMT	O1'-C1-C2-C3
2	B	902	LMT	O1'-C1-C2-C3
4	A	904	LHG	C3-O3-P-O6
4	A	904	LHG	C4-O6-P-O3
4	B	905	LHG	C3-O3-P-O6
4	B	905	LHG	C4-O6-P-O3
5	A	905	PGT	C4-O4P-P-O3P
5	B	906	PGT	C4-O4P-P-O3P
3	B	903	EV9	C13-C14-C15-C16
3	B	903	EV9	C45-C46-C47-C48
3	A	902	EV9	C13-C14-C15-C16
3	A	902	EV9	C45-C46-C47-C48
3	A	903	EV9	C54-C55-C56-C57
3	B	904	EV9	C54-C55-C56-C57
5	A	905	PGT	C13-C14-C15-C16
5	B	906	PGT	C13-C14-C15-C16
4	A	904	LHG	O7-C5-C6-O8
4	B	905	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
3	B	903	EV9	C06-C07-C08-C09
3	A	902	EV9	C06-C07-C08-C09
3	A	903	EV9	C45-C46-C47-C48
3	A	903	EV9	C53-C54-C55-C56
3	B	904	EV9	C45-C46-C47-C48
3	B	904	EV9	C53-C54-C55-C56
3	A	903	EV9	O43-C42-O41-C20
3	B	904	EV9	O43-C42-O41-C20
3	B	903	EV9	C09-C10-C11-C12
3	A	902	EV9	C09-C10-C11-C12
3	A	903	EV9	C44-C42-O41-C20
5	A	905	PGT	C34-C35-C36-C37
5	B	906	PGT	C34-C35-C36-C37
5	A	905	PGT	C37-C38-C39-C40
5	B	906	PGT	C37-C38-C39-C40
3	B	904	EV9	C44-C42-O41-C20
3	A	902	EV9	C35-C36-C37-N38
3	B	903	EV9	C35-C36-C37-N38
2	A	901	LMT	C1-C2-C3-C4
2	B	902	LMT	C1-C2-C3-C4
3	A	903	EV9	C08-C09-C10-C11
3	B	904	EV9	C08-C09-C10-C11

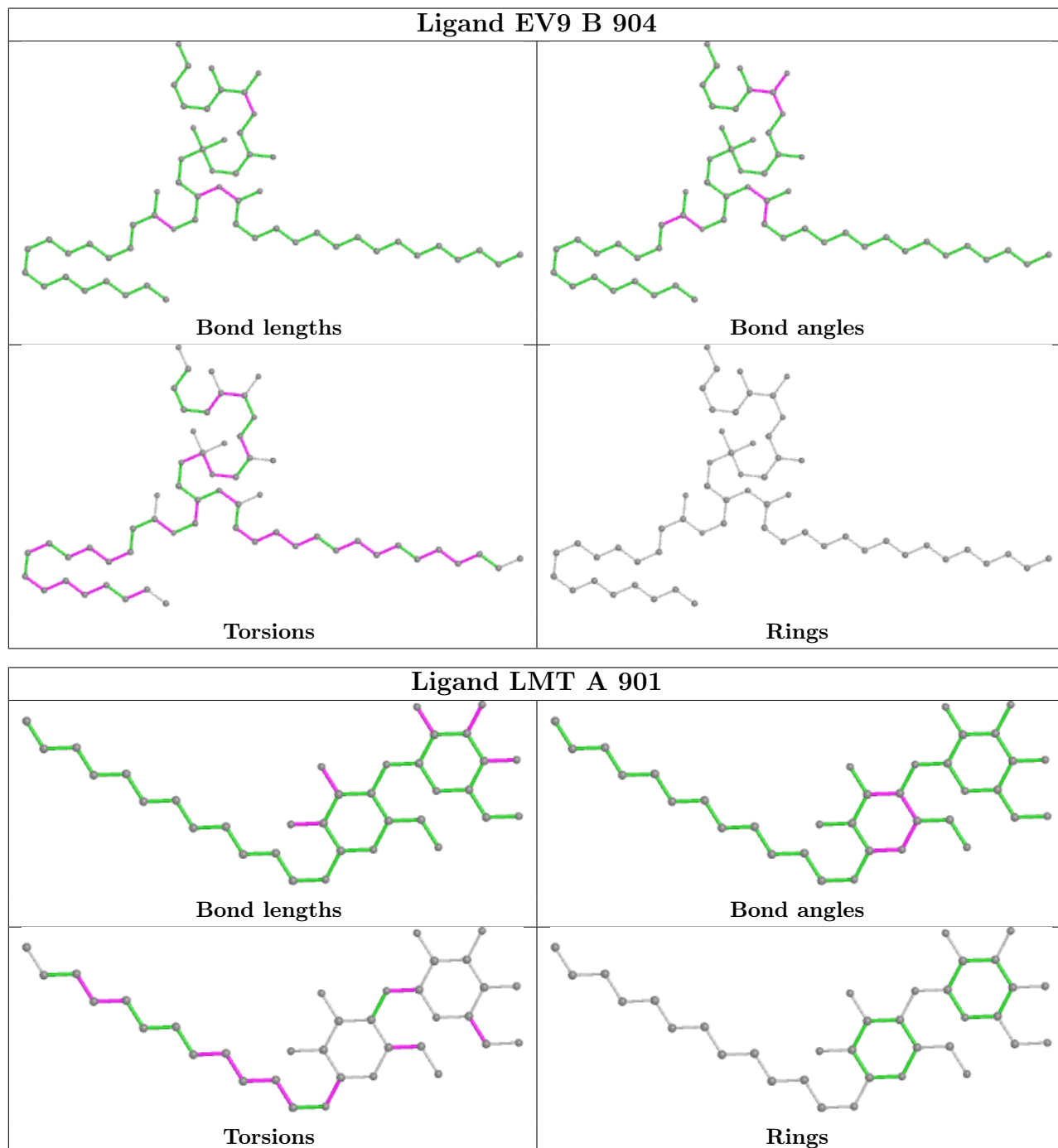
There are no ring outliers.

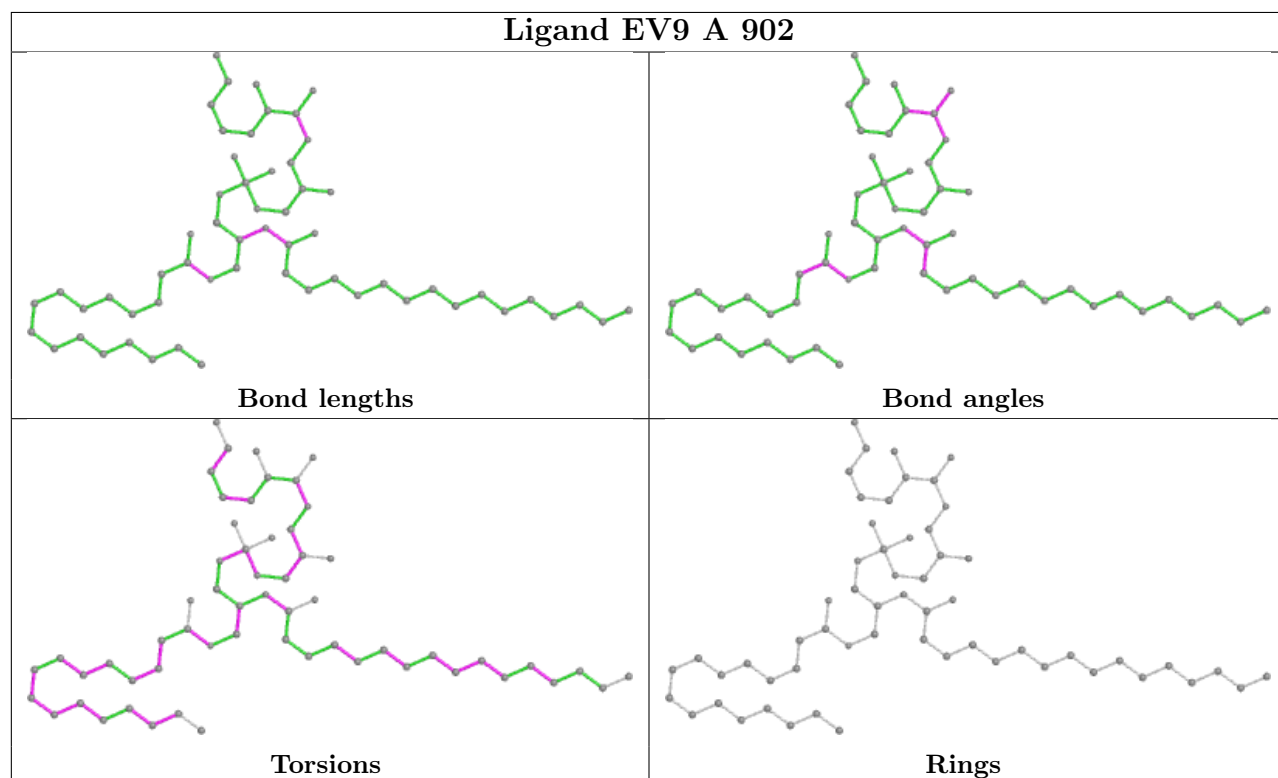
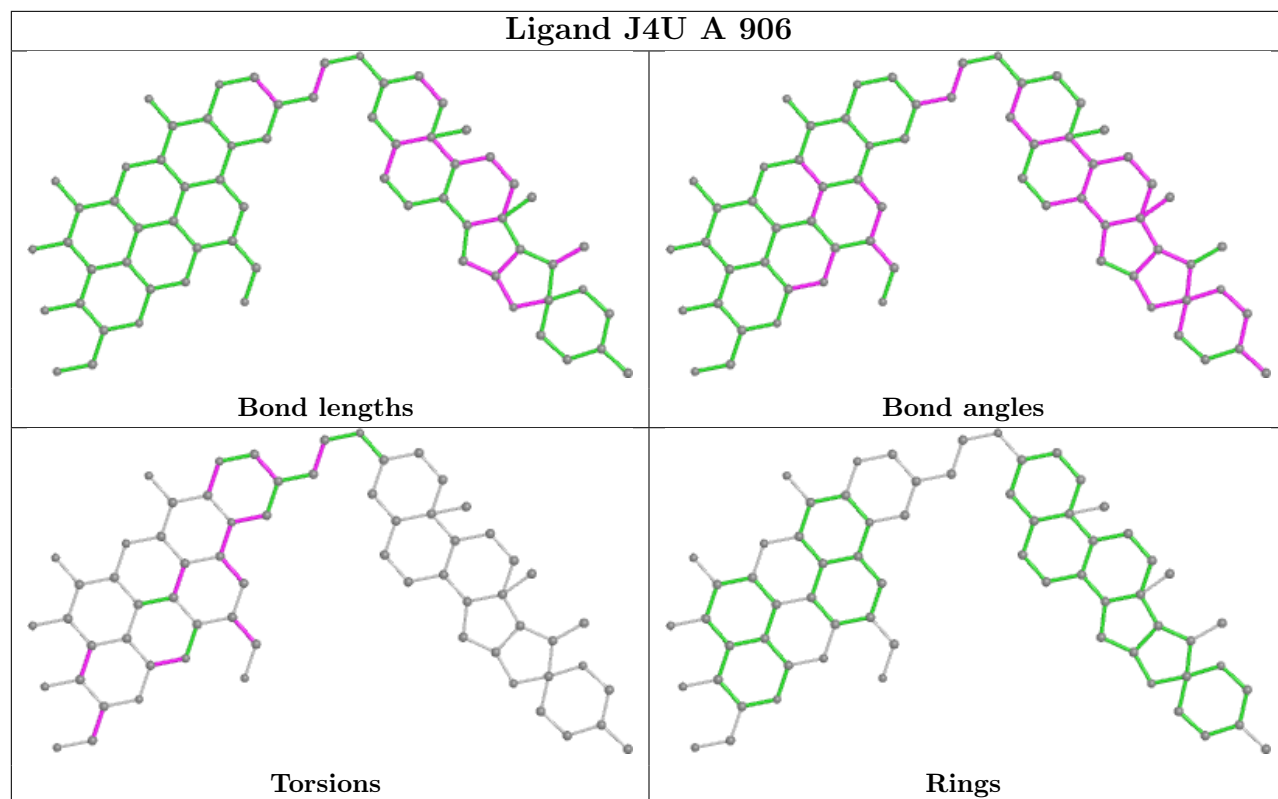
12 monomers are involved in 30 short contacts:

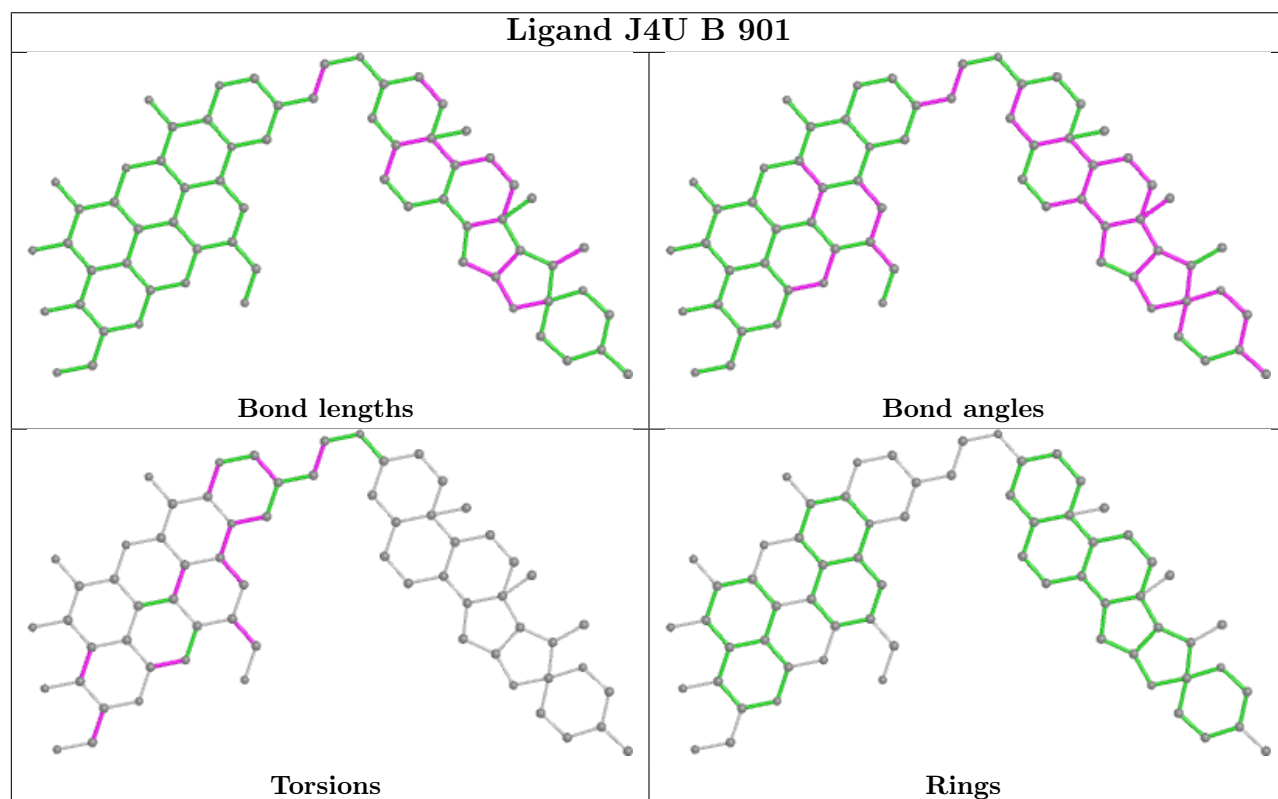
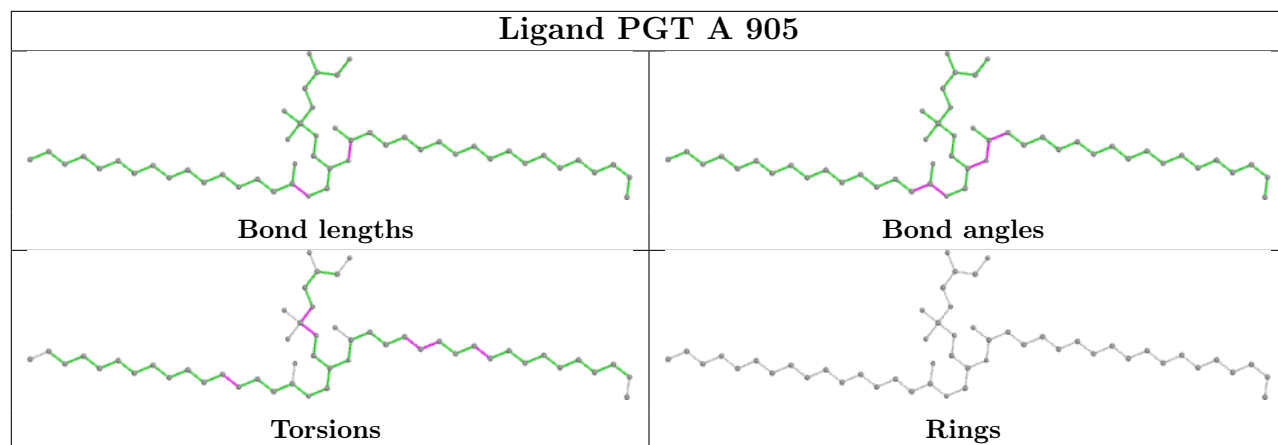
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	904	EV9	1	0
2	A	901	LMT	1	0
6	A	906	J4U	3	0
3	A	902	EV9	3	0
5	A	905	PGT	5	0
6	B	901	J4U	3	0
3	B	903	EV9	3	0
4	B	905	LHG	4	0
3	A	903	EV9	1	0
2	B	902	LMT	1	0
4	A	904	LHG	5	0
5	B	906	PGT	4	0

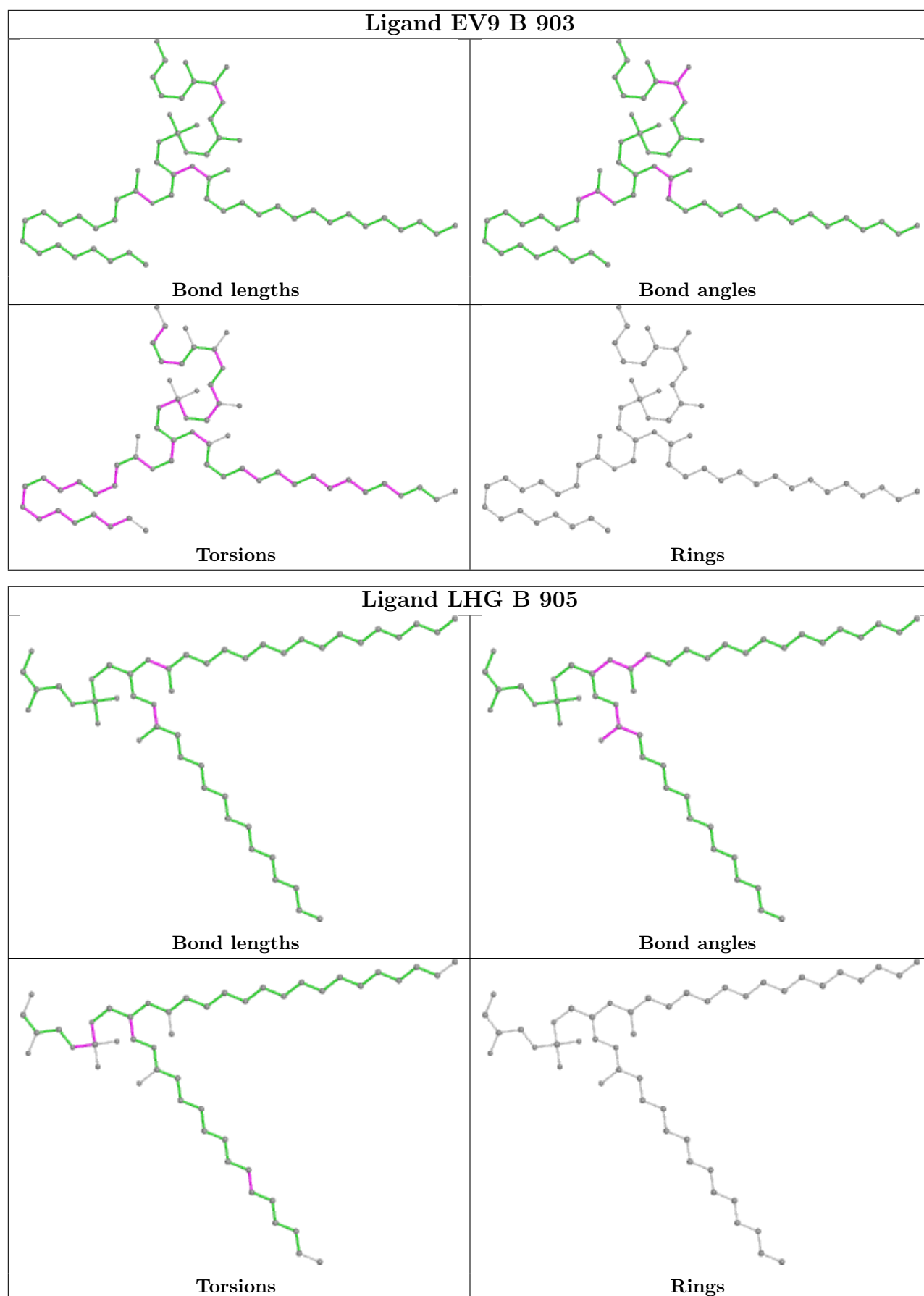
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

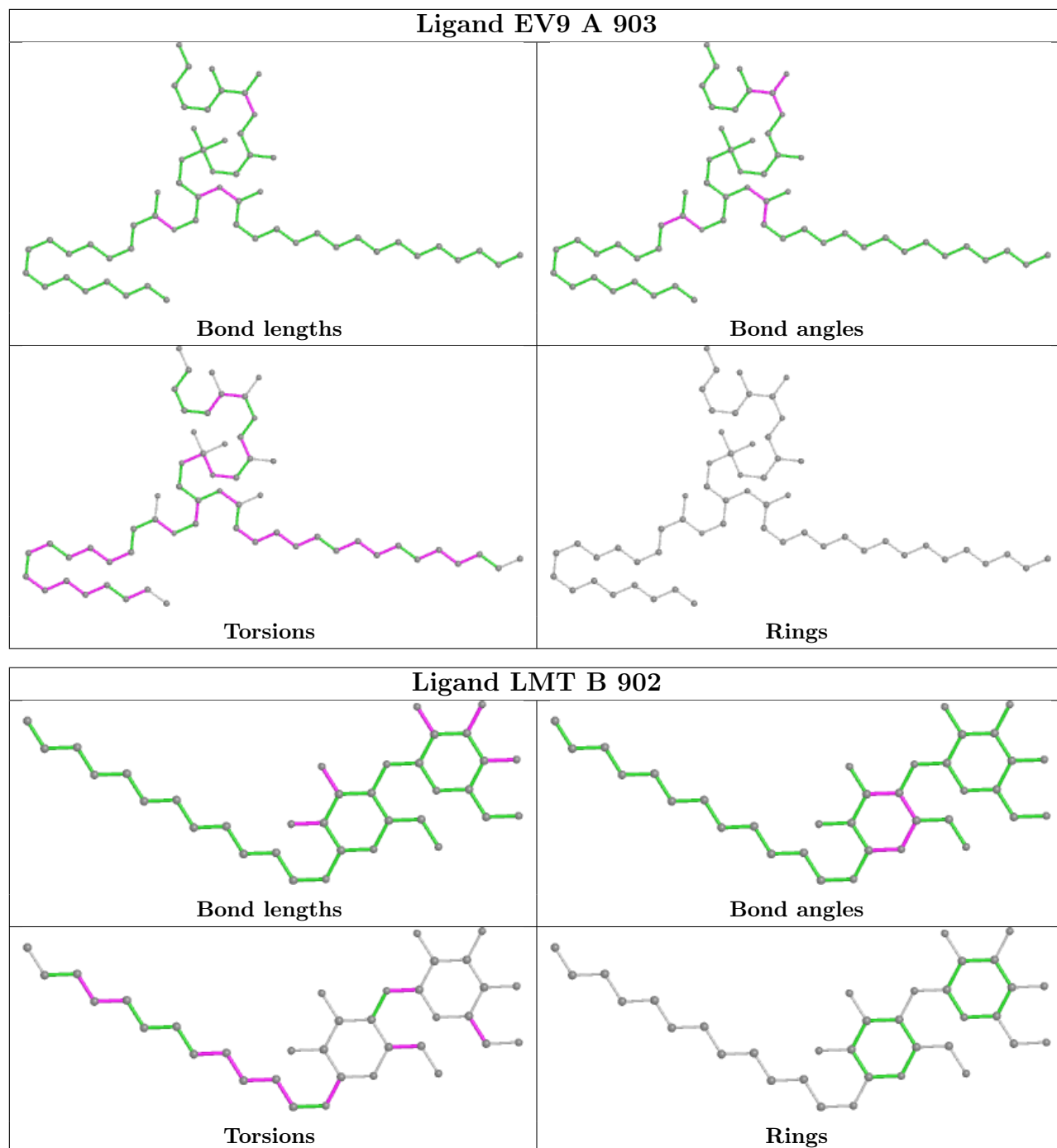
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

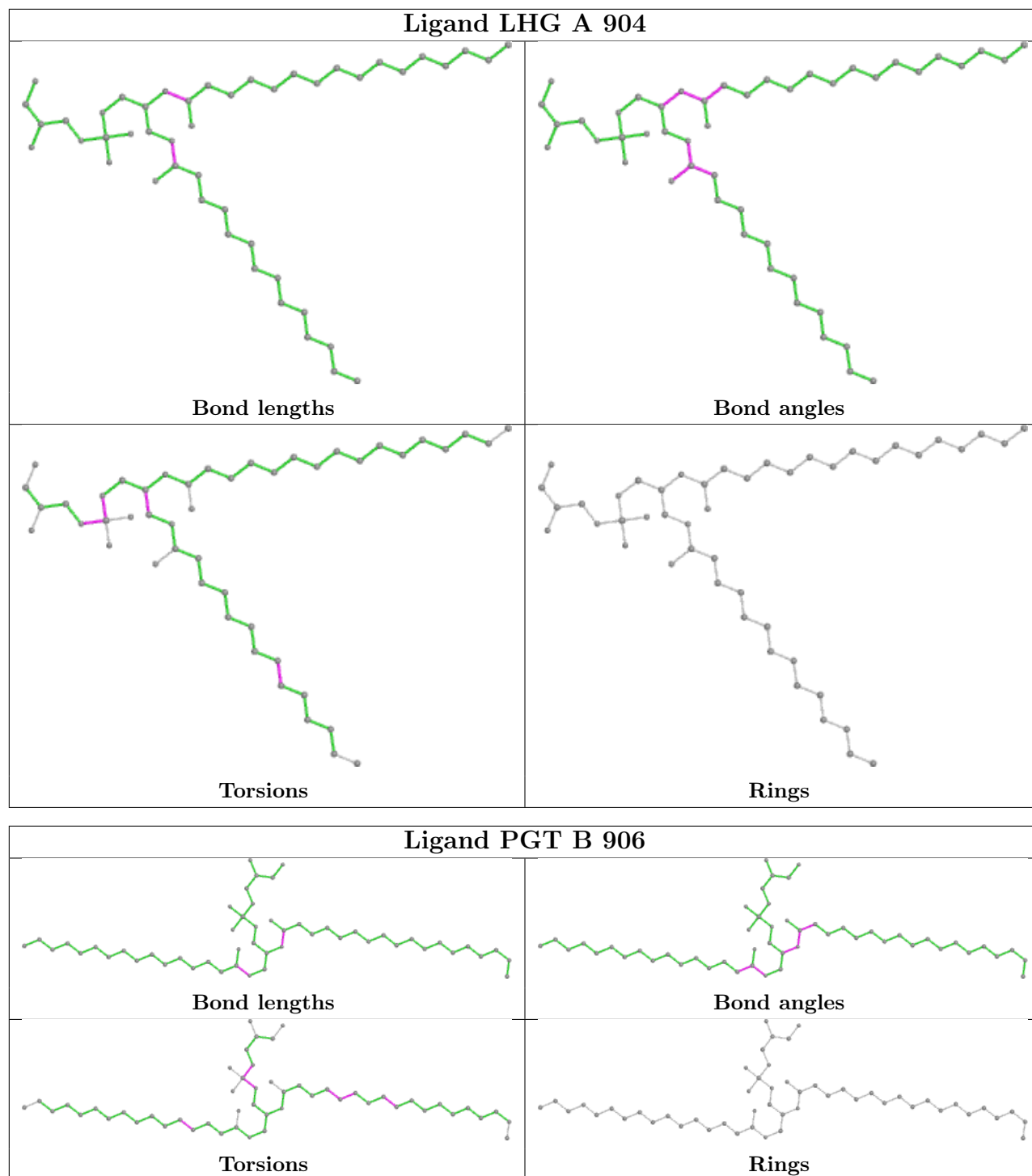












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

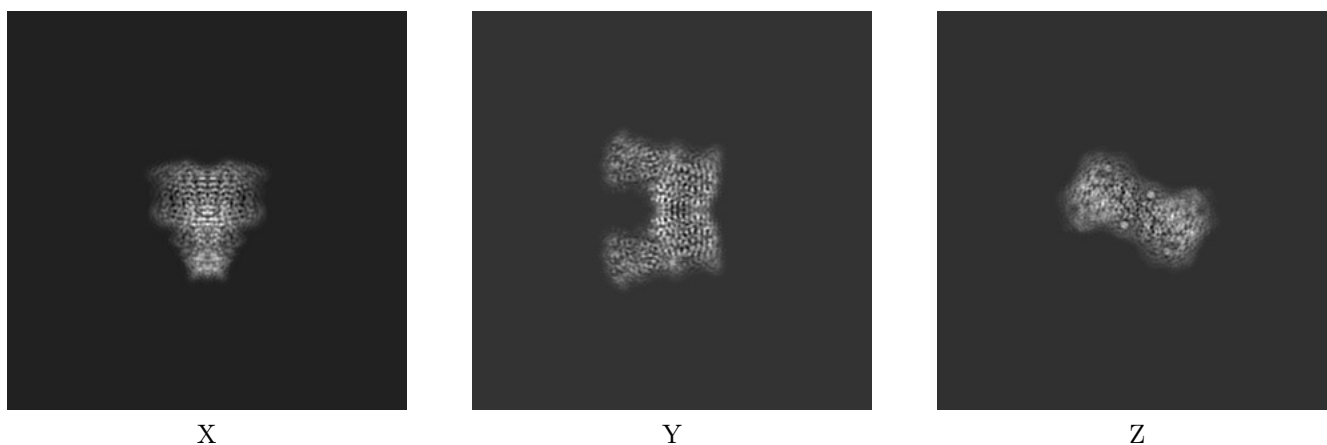
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30869. 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](#)

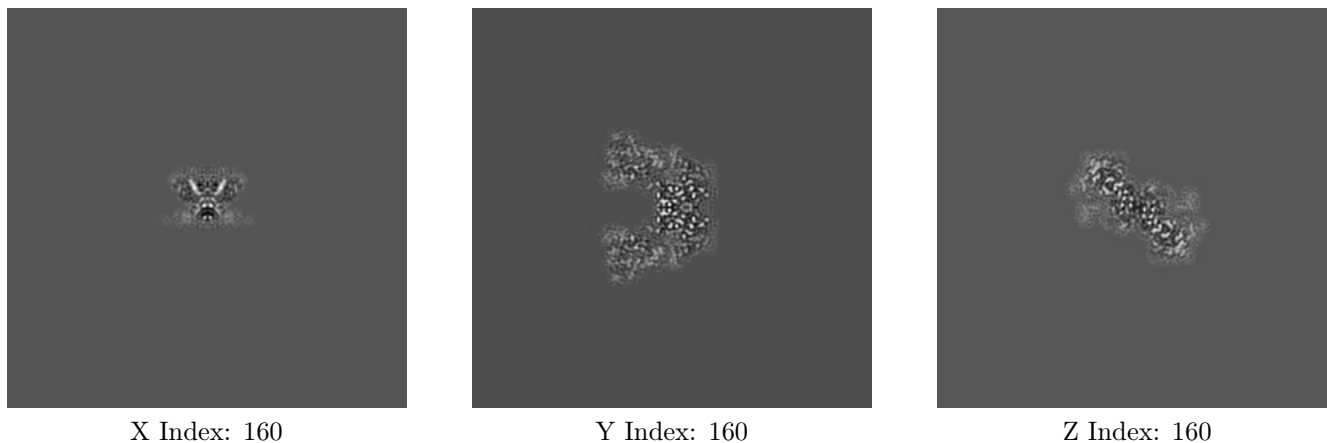
6.1.1 Primary map



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

6.2 Central slices [i](#)

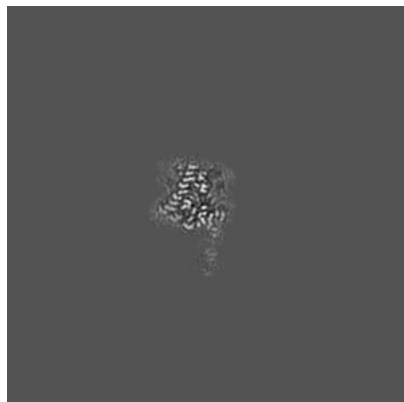
6.2.1 Primary map



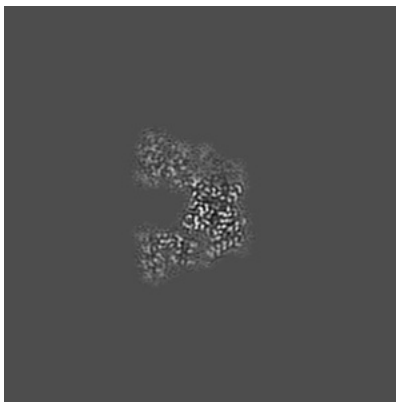
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

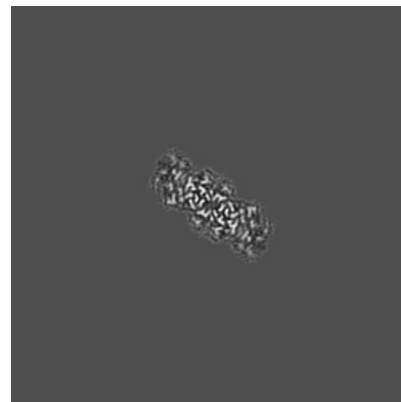
6.3.1 Primary map



X Index: 177



Y Index: 163

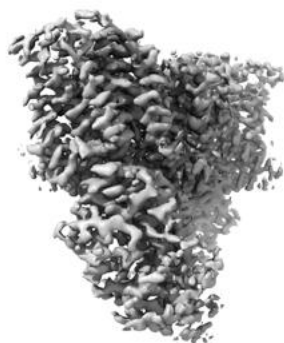


Z Index: 176

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

6.4 Orthogonal surface views [i](#)

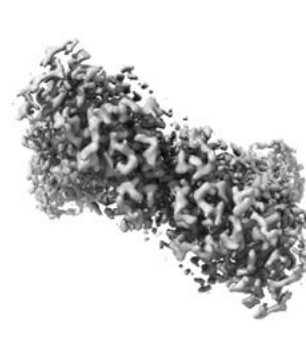
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

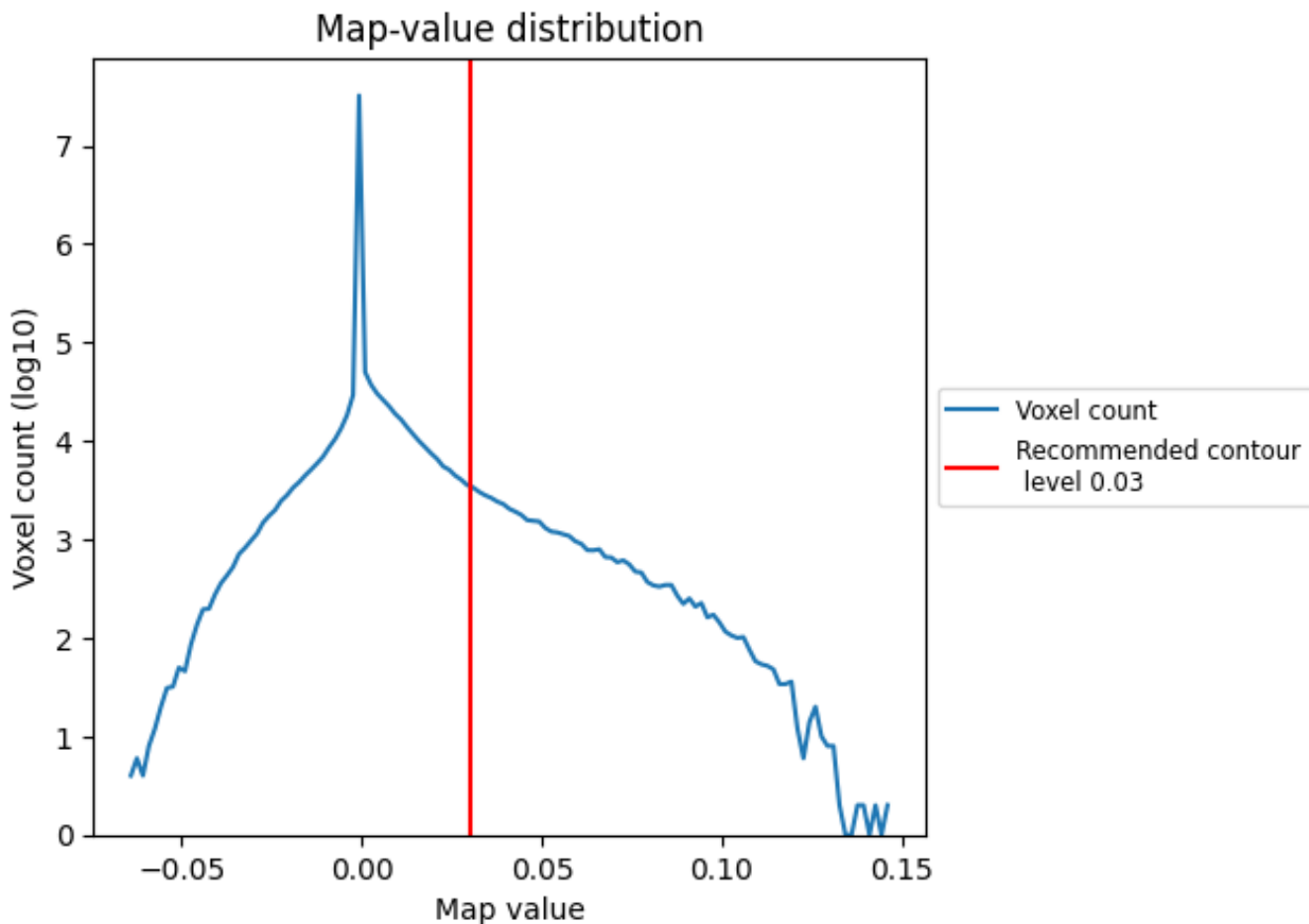
6.5 Mask visualisation

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

7 Map analysis [i](#)

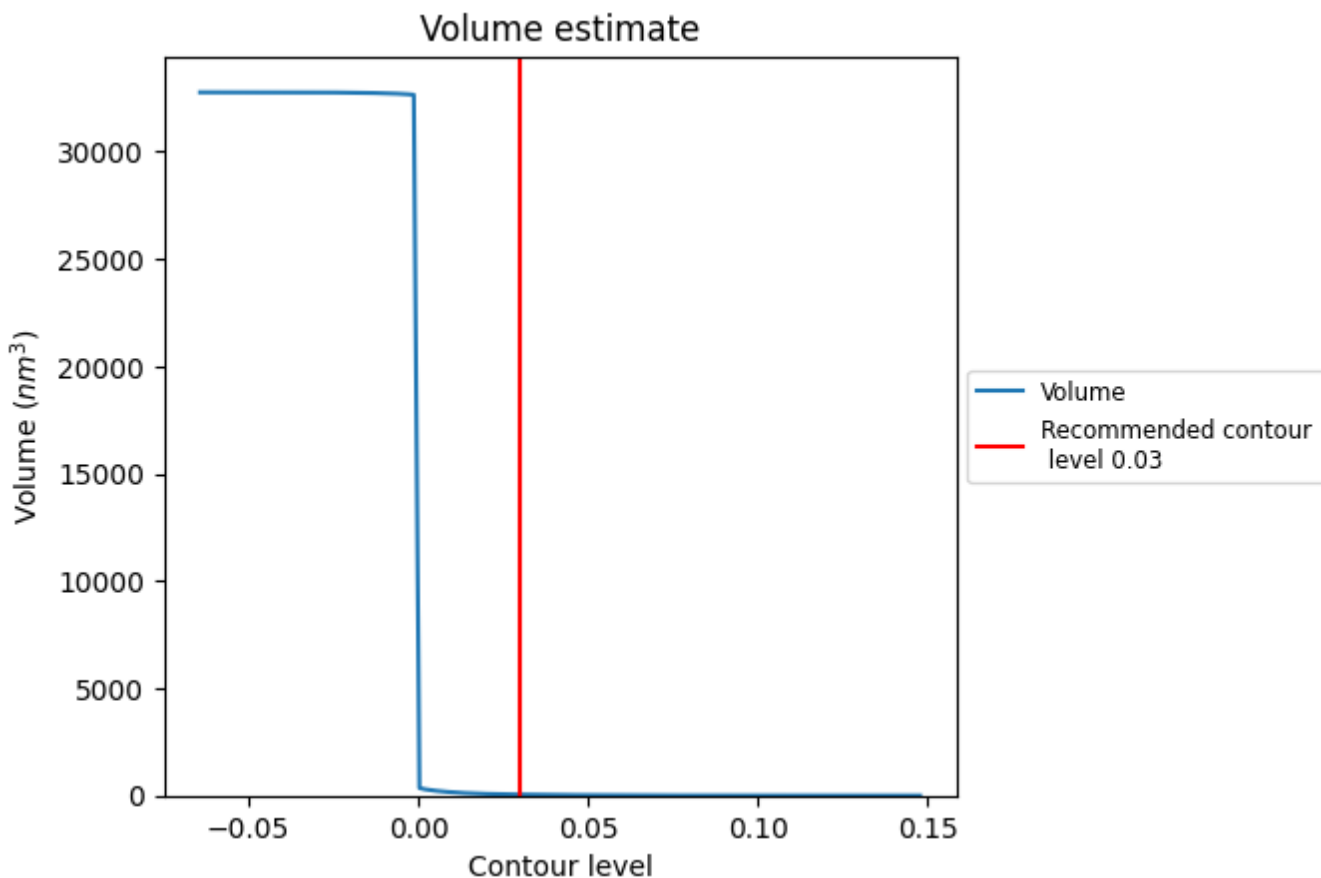
This section contains the results of statistical analysis of the map.

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.

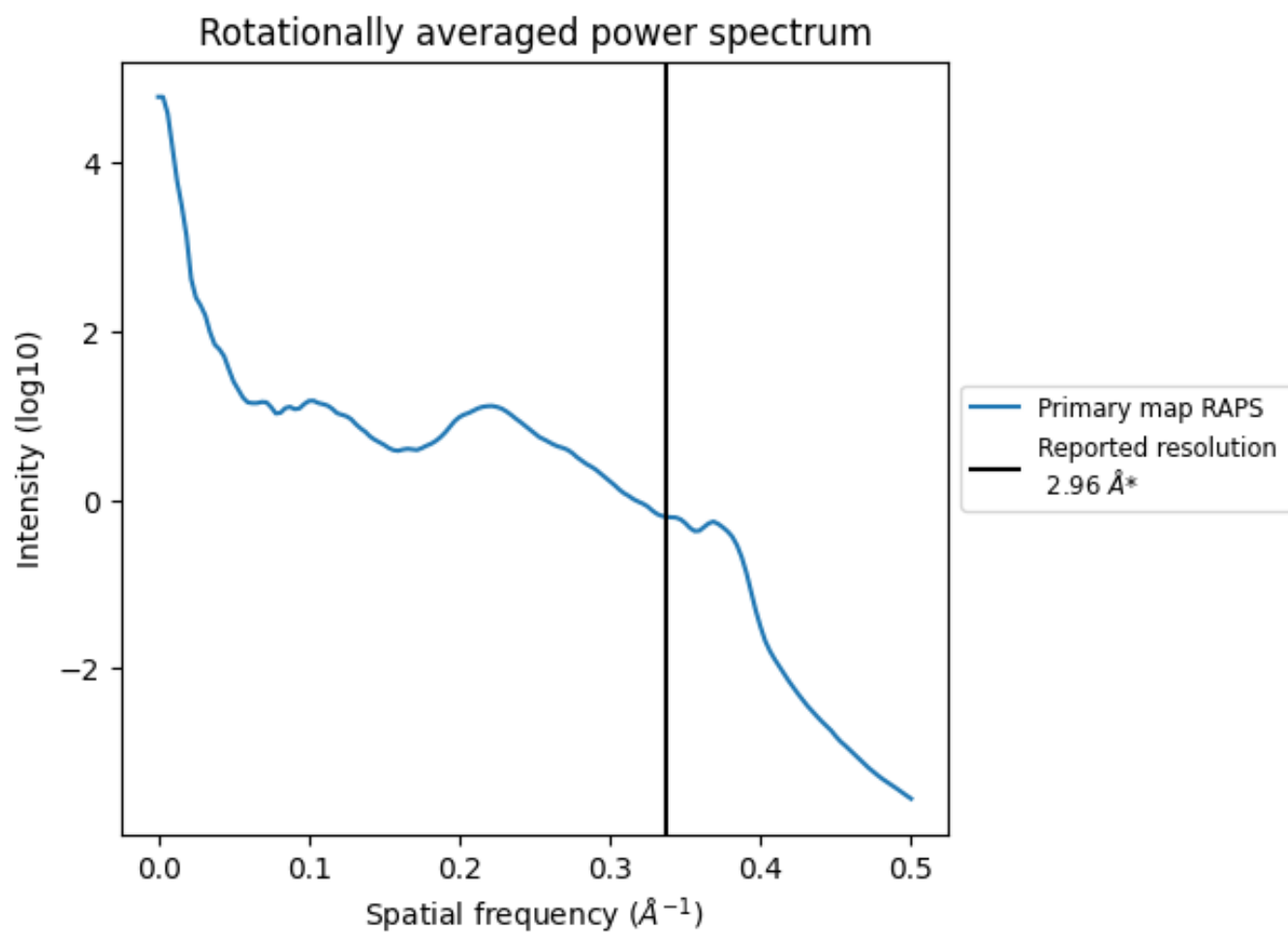
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm³; this corresponds to an approximate mass of 43 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 [i](#)

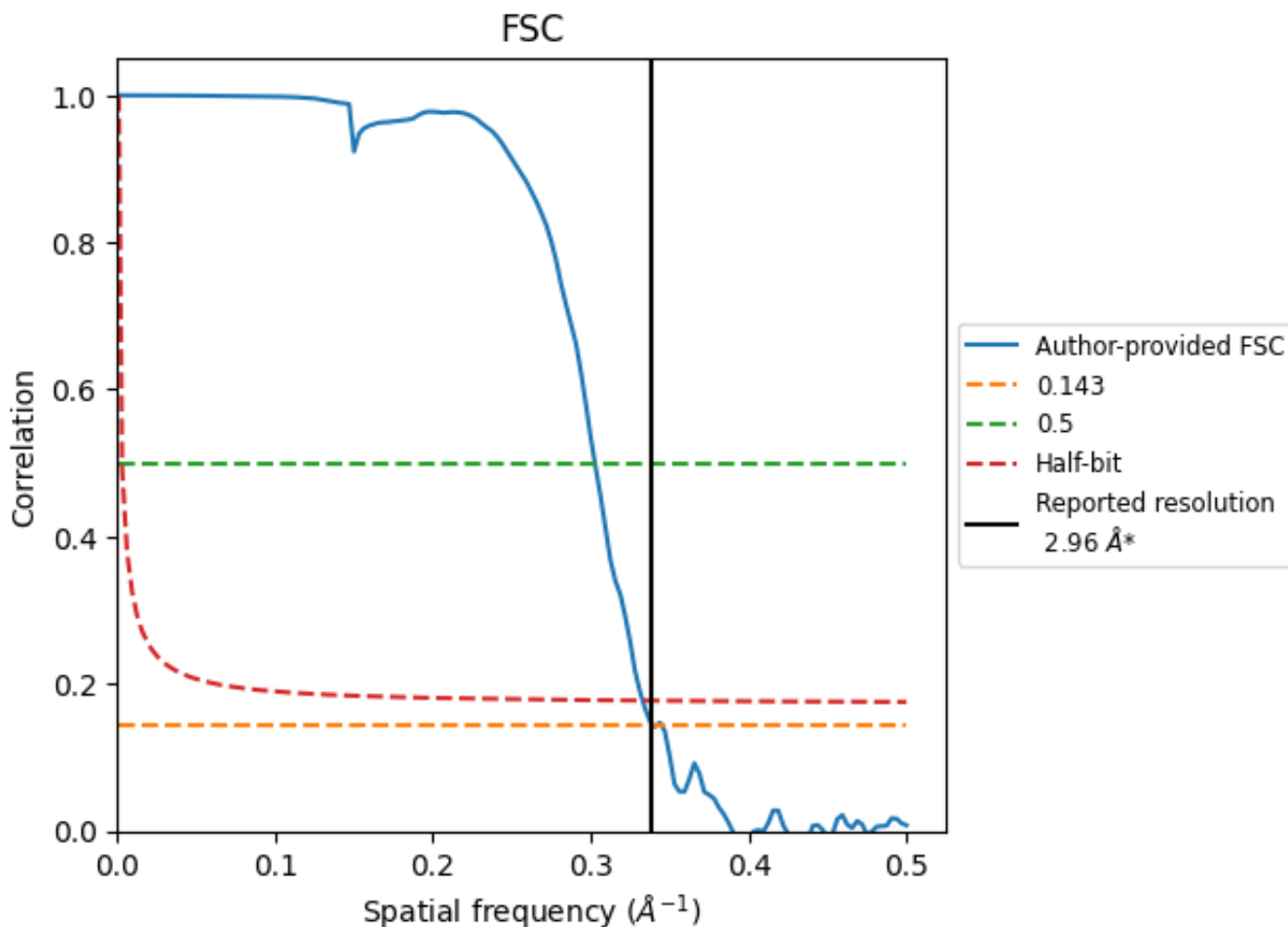


*Reported resolution corresponds to spatial frequency of 0.338\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

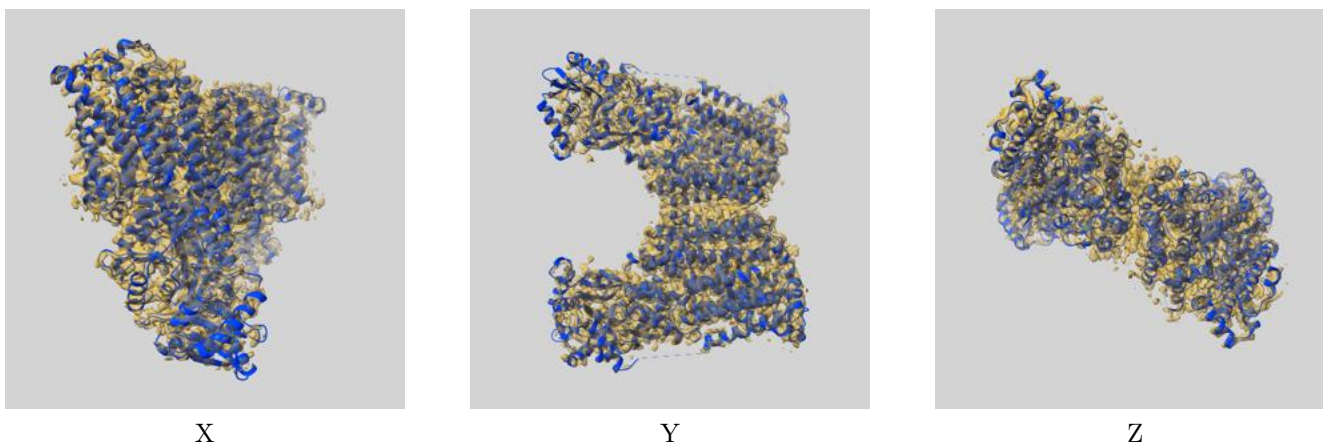
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.94	3.30	3.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

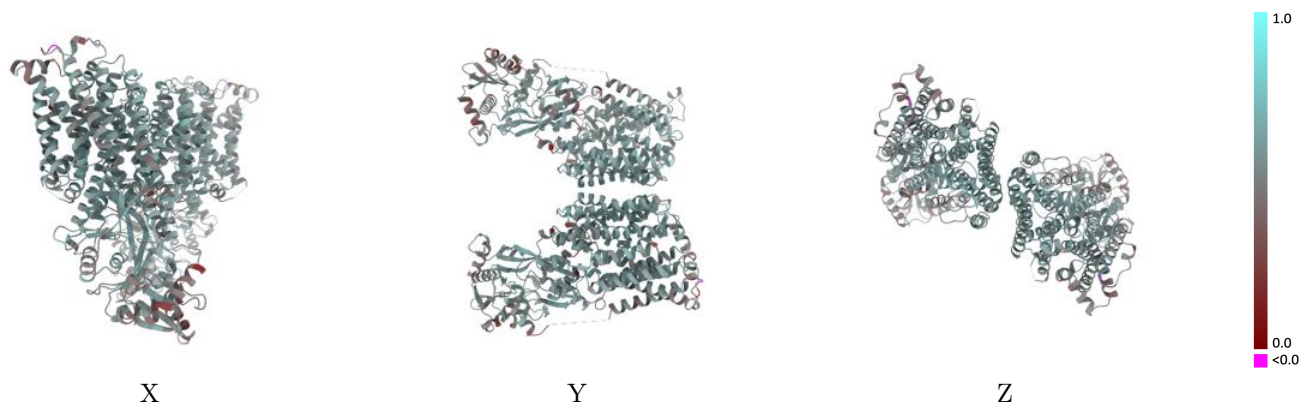
This section contains information regarding the fit between EMDB map EMD-30869 and PDB model 7DUW. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



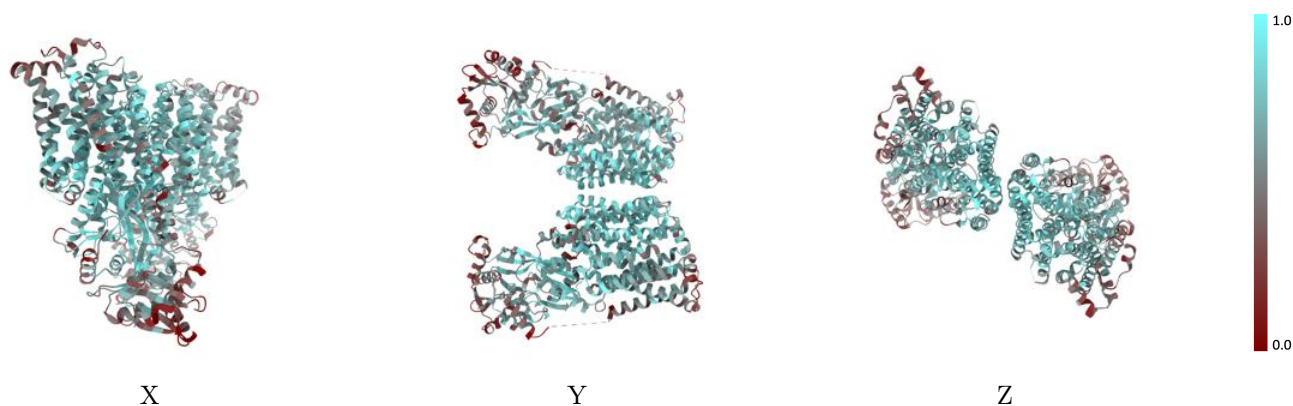
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



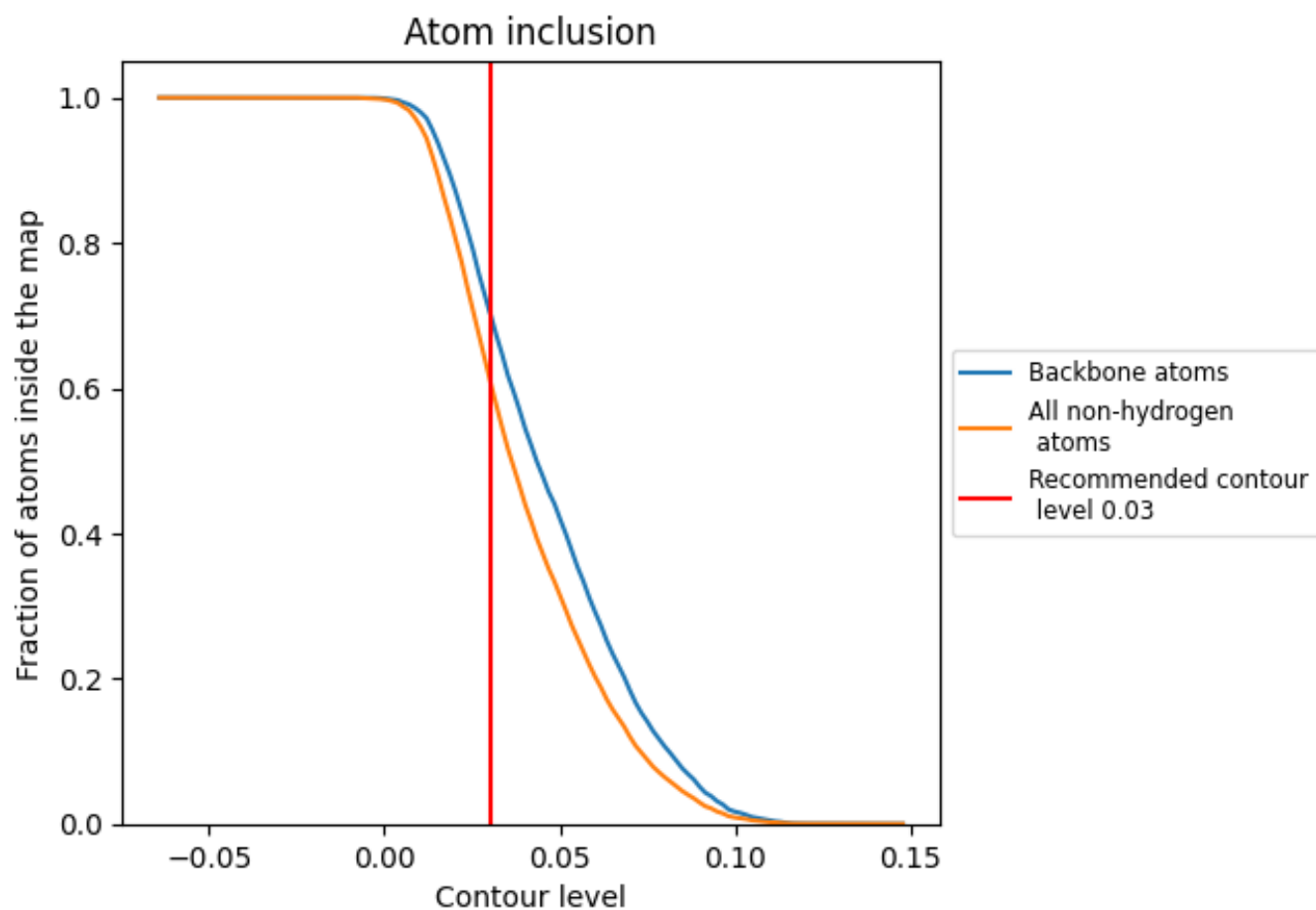
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).






9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 61% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6113	 0.5430
A	 0.6155	 0.5430
B	 0.6160	 0.5430

