Full wwPDB EM Validation Report ⓘ

Aug 20, 2021 – 11:24 AM EDT

PDB ID	:	7RWJ
EMDB ID	:	EMD-24717
Title	:	afTMEM16 in C22 lipid nanodiscs with MSP2N2 scaffold protein in the presnece of Ca2+
Deposited on	:	2021-08-20
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

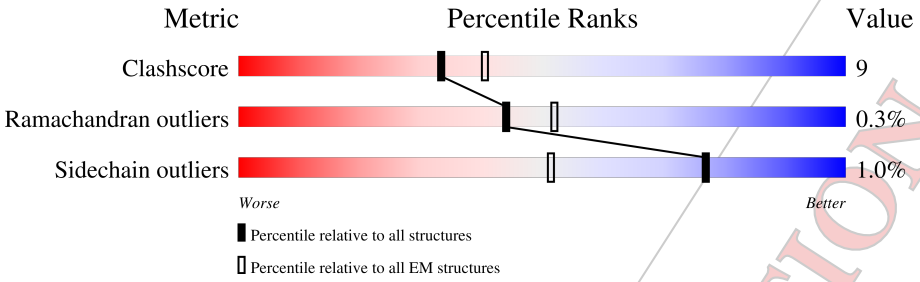
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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 <=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	735	71% 11% 18%
1	B	735	71% 11% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9906 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.

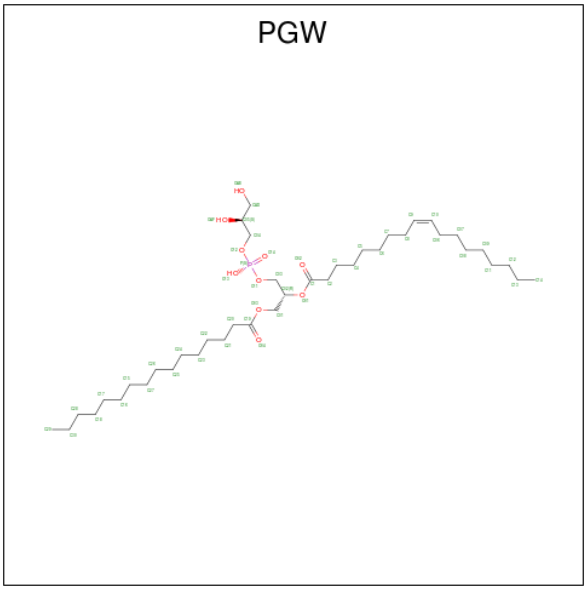
- Molecule 1 is a protein called Plasma membrane channel protein (Aqy1), putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	606	Total 4885	C 3197	N 814	O 855	S 19	0	0
1	A	606	Total 4885	C 3197	N 814	O 855	S 19	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	B	2	Total 2	Ca 2	0
2	A	2	Total 2	Ca 2	0

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



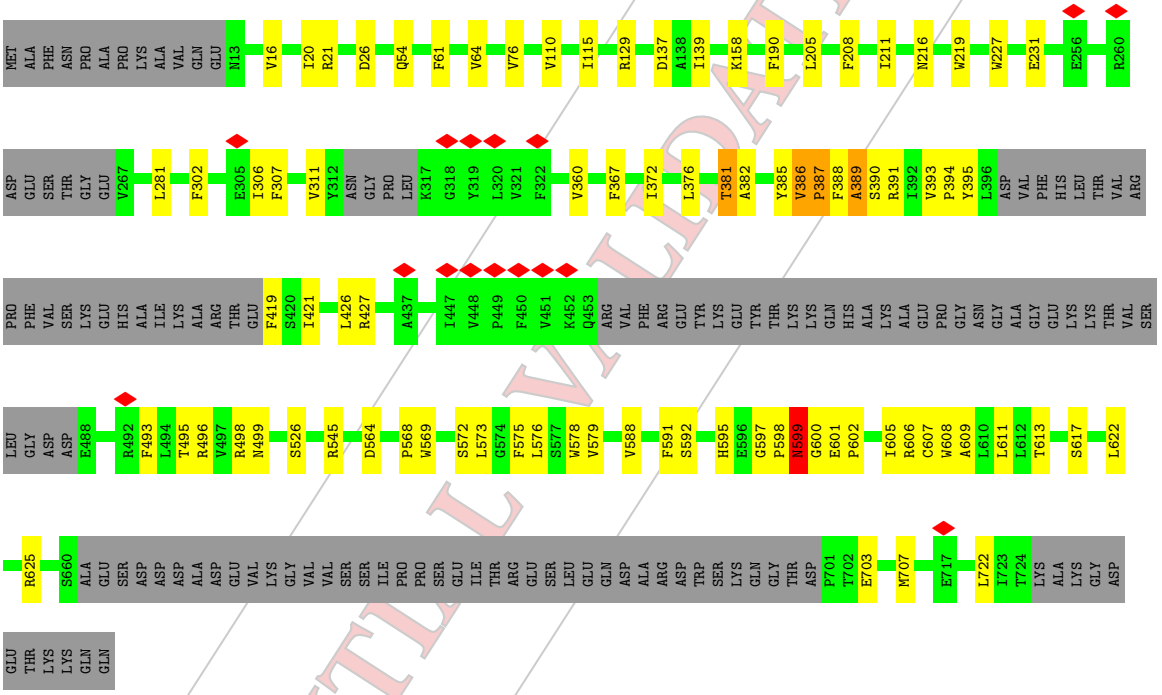
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	O	P	0
			66	46	18	2	
3	B	1	Total	C	O	P	0
			66	46	18	2	
3	A	1	Total	C	O	P	0
			66	46	18	2	
3	A	1	Total	C	O	P	0
			66	46	18	2	

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.

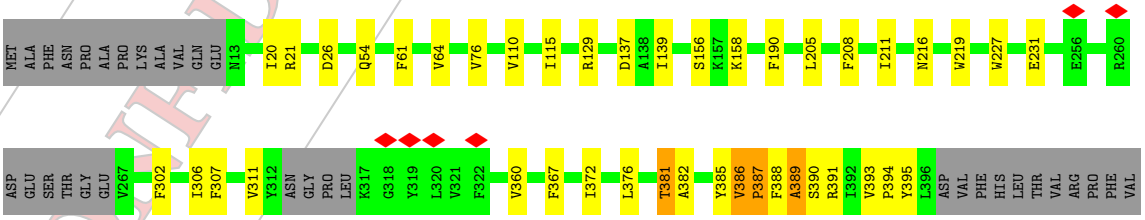
• Molecule 1: Plasma membrane channel protein (Aqy1), putative

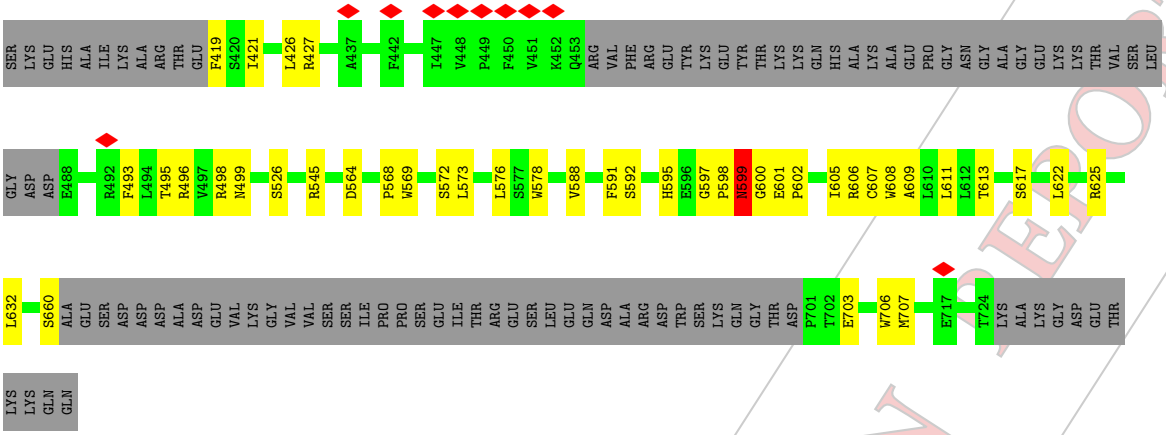
Chain B:



• Molecule 1: Plasma membrane channel protein (Aqy1), putative

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	31890	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 ($e^-/Å^2$)	44.4	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	3.084	Depositor
Minimum map value	-1.871	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.429	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.41	0/5014	0.57	0/6818
1	B	0.41	0/5014	0.57	0/6818
All	All	0.41	0/10028	0.57	0/13636

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	4885	0	4840	92	0
1	B	4885	0	4840	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	66	0	75	4	0
3	B	66	0	75	4	0
All	All	9906	0	9830	180	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 9.

All (180) 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:578:TRP:CH2	1:A:622:LEU:HD21	1.54	1.43
1:B:578:TRP:CZ3	1:B:622:LEU:HD21	1.56	1.40
1:B:578:TRP:CH2	1:B:622:LEU:HD21	1.54	1.39
1:A:578:TRP:CZ3	1:A:622:LEU:HD21	1.56	1.39
1:A:578:TRP:CZ3	1:A:622:LEU:CD2	2.34	1.11
1:B:578:TRP:CZ3	1:B:622:LEU:CD2	2.34	1.09
1:B:386:VAL:HG12	1:B:387:PRO:HD3	1.36	1.08
1:A:386:VAL:HG12	1:A:387:PRO:HD3	1.36	1.04
1:B:578:TRP:CH2	1:B:622:LEU:CD2	2.41	1.03
1:A:578:TRP:CH2	1:A:622:LEU:CD2	2.41	1.03
1:B:386:VAL:HG11	1:B:591:PHE:CZ	1.96	1.00
1:A:386:VAL:HG11	1:A:591:PHE:CZ	1.96	1.00
1:A:572:SER:O	1:A:576:LEU:HG	1.66	0.95
1:B:390:SER:HG	1:B:419:PHE:N	1.63	0.95
1:B:572:SER:O	1:B:576:LEU:HG	1.66	0.95
1:A:390:SER:HG	1:A:419:PHE:N	1.66	0.93
1:A:607:CYS:SG	1:A:607:CYS:O	2.26	0.93
1:B:607:CYS:SG	1:B:607:CYS:O	2.26	0.93
1:A:387:PRO:HG3	1:A:598:PRO:HG3	1.51	0.92
1:B:387:PRO:HG3	1:B:598:PRO:HG3	1.51	0.92
1:B:386:VAL:HG11	1:B:591:PHE:HZ	1.36	0.91
1:A:386:VAL:HG11	1:A:591:PHE:HZ	1.36	0.84
1:A:367:PHE:HZ	1:A:576:LEU:HD21	1.48	0.78
1:B:367:PHE:HZ	1:B:576:LEU:HD21	1.48	0.77
1:B:578:TRP:NE1	3:A:804:PGW:H3	2.02	0.73
1:A:573:LEU:HD23	1:A:576:LEU:HD12	1.70	0.73
1:B:573:LEU:HD23	1:B:576:LEU:HD12	1.70	0.73
3:B:804:PGW:H3	1:A:578:TRP:NE1	2.03	0.73
1:A:390:SER:OG	1:A:419:PHE:CB	2.39	0.71
1:B:390:SER:OG	1:B:419:PHE:CB	2.39	0.71
1:B:386:VAL:HG12	1:B:387:PRO:CD	2.19	0.70
1:B:703:GLU:O	1:B:707:MET:HG2	1.92	0.69
1:A:703:GLU:O	1:A:707:MET:HG2	1.92	0.69
1:B:386:VAL:CG1	1:B:387:PRO:HD3	2.20	0.68
1:B:601:GLU:OE2	1:B:601:GLU:N	2.26	0.67
1:A:390:SER:OG	1:A:419:PHE:HB3	1.95	0.67
1:A:386:VAL:CG1	1:A:387:PRO:HD3	2.20	0.67
1:B:390:SER:OG	1:B:419:PHE:HB3	1.95	0.66
1:A:601:GLU:OE2	1:A:601:GLU:N	2.26	0.65
1:B:388:PHE:HD1	1:B:602:PRO:HG3	1.62	0.65
1:A:388:PHE:HD1	1:A:602:PRO:HG3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PRO:HG3	1:B:598:PRO:CG	2.26	0.64
1:A:386:VAL:HG12	1:A:387:PRO:CD	2.19	0.64
1:A:421:ILE:HD11	1:A:600:GLY:H	1.63	0.64
1:B:421:ILE:HD11	1:B:600:GLY:H	1.63	0.63
1:A:387:PRO:HG3	1:A:598:PRO:CG	2.26	0.63
1:A:421:ILE:CD1	1:A:600:GLY:H	2.11	0.63
1:A:367:PHE:CZ	1:A:576:LEU:HD21	2.33	0.62
1:B:421:ILE:CD1	1:B:600:GLY:H	2.11	0.62
1:B:367:PHE:CZ	1:B:576:LEU:HD21	2.33	0.62
1:B:427:ARG:HD3	1:B:595:HIS:NE2	2.15	0.62
3:B:804:PGW:H3	1:A:578:TRP:CD1	2.35	0.61
1:A:427:ARG:HD3	1:A:595:HIS:NE2	2.15	0.61
1:B:578:TRP:CD1	3:A:804:PGW:H3	2.37	0.60
1:B:607:CYS:SG	1:B:611:LEU:CD1	2.91	0.59
1:B:208:PHE:HE2	1:B:595:HIS:HD1	1.50	0.58
1:A:208:PHE:HE2	1:A:595:HIS:HD1	1.50	0.58
1:A:607:CYS:SG	1:A:611:LEU:CD1	2.91	0.58
1:B:307:PHE:O	1:B:311:VAL:HB	2.04	0.57
1:B:591:PHE:CD1	1:B:597:GLY:HA3	2.40	0.57
1:A:307:PHE:O	1:A:311:VAL:HB	2.04	0.57
1:A:382:ALA:HB2	1:A:426:LEU:HD13	1.87	0.57
1:B:605:ILE:O	1:B:605:ILE:HG22	2.05	0.56
1:B:388:PHE:HA	1:B:602:PRO:HD3	1.87	0.56
1:B:395:TYR:CD2	1:B:395:TYR:N	2.71	0.56
1:A:388:PHE:HA	1:A:602:PRO:HD3	1.87	0.56
1:B:382:ALA:HB2	1:B:426:LEU:HD13	1.87	0.56
1:B:76:VAL:HG23	1:B:110:VAL:HG21	1.88	0.56
1:A:395:TYR:CD2	1:A:395:TYR:N	2.71	0.56
1:A:591:PHE:CD1	1:A:597:GLY:HA3	2.40	0.55
1:A:386:VAL:CG1	1:A:598:PRO:HD2	2.36	0.55
1:B:386:VAL:CG1	1:B:598:PRO:HD2	2.36	0.55
1:B:388:PHE:CD1	1:B:602:PRO:HG3	2.41	0.55
1:A:605:ILE:HG22	1:A:605:ILE:O	2.05	0.55
1:A:76:VAL:HG23	1:A:110:VAL:HG21	1.88	0.54
1:B:395:TYR:N	1:B:395:TYR:HD2	2.07	0.53
1:B:386:VAL:HG13	1:B:598:PRO:HD2	1.91	0.53
1:A:390:SER:OG	1:A:419:PHE:N	2.38	0.53
1:A:395:TYR:N	1:A:395:TYR:HD2	2.07	0.53
1:A:386:VAL:HG13	1:A:598:PRO:HD2	1.91	0.52
1:A:388:PHE:CD1	1:A:602:PRO:HG3	2.41	0.52
1:A:390:SER:O	1:A:394:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:TRP:HZ3	1:B:622:LEU:CD2	2.13	0.52
1:A:227:TRP:NE1	1:A:231:GLU:OE2	2.43	0.52
1:A:607:CYS:SG	1:A:611:LEU:HD12	2.49	0.52
1:B:227:TRP:NE1	1:B:231:GLU:OE2	2.43	0.52
1:A:495:THR:O	1:A:499:ASN:ND2	2.43	0.52
1:B:495:THR:O	1:B:499:ASN:ND2	2.43	0.51
1:A:54:GLN:O	1:A:498:ARG:NH1	2.43	0.51
1:B:607:CYS:SG	1:B:611:LEU:HD12	2.49	0.51
1:B:390:SER:O	1:B:394:PRO:HD2	2.09	0.51
1:B:54:GLN:O	1:B:498:ARG:NH1	2.43	0.51
1:A:129:ARG:NH2	1:A:137:ASP:O	2.41	0.51
1:A:591:PHE:CE1	1:A:597:GLY:HA3	2.46	0.51
1:B:564:ASP:N	1:B:564:ASP:OD1	2.44	0.51
1:B:216:ASN:ND2	1:B:526:SER:OG	2.44	0.51
1:B:591:PHE:CE1	1:B:597:GLY:HA3	2.46	0.50
1:A:578:TRP:HZ3	1:A:622:LEU:CD2	2.13	0.50
1:A:302:PHE:HZ	1:A:385:TYR:HB2	1.77	0.50
1:B:129:ARG:NH2	1:B:137:ASP:O	2.41	0.50
1:B:381:THR:HA	1:B:385:TYR:HB3	1.94	0.50
1:A:216:ASN:ND2	1:A:526:SER:OG	2.44	0.50
1:A:493:PHE:HA	1:A:496:ARG:HG2	1.94	0.50
1:B:493:PHE:HA	1:B:496:ARG:HG2	1.94	0.49
1:B:606:ARG:HB3	1:B:608:TRP:CD1	2.47	0.49
1:A:617:SER:HB2	3:A:803:PGW:H24A	1.95	0.49
1:B:302:PHE:HZ	1:B:385:TYR:HB2	1.77	0.49
1:A:381:THR:HA	1:A:385:TYR:HB3	1.94	0.49
1:B:21:ARG:HA	1:B:61:PHE:HB3	1.95	0.49
1:A:306:ILE:HD12	1:A:385:TYR:CE1	2.48	0.49
1:B:306:ILE:HD12	1:B:385:TYR:CE1	2.48	0.48
1:A:21:ARG:HA	1:A:61:PHE:HB3	1.95	0.48
1:B:617:SER:HB2	3:B:803:PGW:H24A	1.95	0.48
1:B:607:CYS:SG	1:B:611:LEU:HD11	2.54	0.48
1:B:16:VAL:HG22	1:A:706:TRP:HZ2	1.79	0.47
1:A:26:ASP:OD1	1:A:26:ASP:N	2.41	0.47
1:A:588:VAL:O	1:A:592:SER:OG	2.31	0.47
1:A:564:ASP:OD1	1:A:564:ASP:N	2.44	0.47
1:A:607:CYS:SG	1:A:611:LEU:HD11	2.54	0.47
1:A:208:PHE:HE2	1:A:595:HIS:ND1	2.12	0.47
1:A:606:ARG:HB3	1:A:608:TRP:CD1	2.47	0.47
1:A:381:THR:O	1:A:385:TYR:HB3	2.15	0.47
1:B:381:THR:O	1:B:385:TYR:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HD11	1:B:211:ILE:HD11	1.97	0.46
1:A:205:LEU:HD11	1:A:211:ILE:HD11	1.97	0.46
1:A:599:ASN:C	1:A:599:ASN:HD22	2.19	0.46
1:B:599:ASN:C	1:B:599:ASN:HD22	2.18	0.46
1:B:208:PHE:HE2	1:B:595:HIS:ND1	2.12	0.46
1:B:613:THR:HB	3:B:803:PGW:H4	1.97	0.46
1:A:306:ILE:HD12	1:A:385:TYR:HE1	1.81	0.46
1:B:306:ILE:HD12	1:B:385:TYR:HE1	1.81	0.45
1:A:607:CYS:HG	1:A:611:LEU:HD12	1.81	0.45
1:B:190:PHE:O	1:B:219:TRP:NE1	2.50	0.45
1:B:606:ARG:O	1:B:609:ALA:N	2.37	0.45
1:B:26:ASP:OD1	1:B:26:ASP:N	2.41	0.45
1:B:573:LEU:HA	1:B:576:LEU:HD12	1.99	0.45
1:A:573:LEU:HA	1:A:576:LEU:HD12	1.99	0.45
1:A:613:THR:HB	3:A:803:PGW:H4	1.98	0.45
1:B:385:TYR:O	1:B:389:ALA:HB2	2.17	0.45
1:A:387:PRO:O	1:A:602:PRO:HB3	2.17	0.45
1:B:387:PRO:O	1:B:602:PRO:HB3	2.17	0.45
1:A:372:ILE:O	1:A:376:LEU:HB2	2.16	0.44
1:B:360:VAL:HG22	1:B:568:PRO:HD3	2.00	0.44
1:B:372:ILE:O	1:B:376:LEU:HB2	2.16	0.44
1:A:606:ARG:O	1:A:609:ALA:N	2.37	0.44
1:B:390:SER:OG	1:B:419:PHE:N	2.38	0.44
1:A:569:TRP:HA	1:A:572:SER:HB3	1.99	0.44
1:A:385:TYR:O	1:A:389:ALA:HB2	2.17	0.44
1:A:360:VAL:HG22	1:A:568:PRO:HD3	2.00	0.43
1:B:607:CYS:HG	1:B:611:LEU:HD12	1.82	0.43
1:A:390:SER:O	1:A:394:PRO:CD	2.67	0.43
1:B:64:VAL:HG11	1:B:115:ILE:HD11	2.00	0.43
1:B:569:TRP:HA	1:B:572:SER:HB3	1.99	0.43
1:A:391:ARG:HG3	1:A:602:PRO:HD2	2.01	0.43
1:B:578:TRP:CE3	1:B:625:ARG:NH2	2.87	0.43
1:B:390:SER:O	1:B:394:PRO:CD	2.67	0.42
1:A:578:TRP:CE3	1:A:625:ARG:NH2	2.87	0.42
1:A:158:LYS:O	1:A:545:ARG:NH1	2.52	0.42
1:B:158:LYS:O	1:B:545:ARG:NH1	2.52	0.42
1:B:391:ARG:HG3	1:B:602:PRO:HD2	2.01	0.42
1:B:588:VAL:O	1:B:592:SER:OG	2.30	0.42
1:A:190:PHE:O	1:A:219:TRP:NE1	2.50	0.42
1:A:20:ILE:HG12	1:A:139:ILE:HG23	2.02	0.42
1:B:20:ILE:HG12	1:B:139:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:TRP:HZ3	1:B:625:ARG:NH1	2.17	0.42
1:A:382:ALA:HB2	1:A:426:LEU:CD1	2.50	0.42
1:A:388:PHE:HB2	1:A:389:ALA:H	1.68	0.41
1:A:578:TRP:HZ3	1:A:625:ARG:NH1	2.17	0.41
1:B:599:ASN:C	1:B:599:ASN:ND2	2.73	0.41
1:B:382:ALA:HB2	1:B:426:LEU:CD1	2.50	0.41
1:A:64:VAL:HG11	1:A:115:ILE:HD11	2.00	0.41
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.88	0.41
1:A:306:ILE:HD13	1:A:306:ILE:HA	1.87	0.41
1:A:599:ASN:C	1:A:599:ASN:ND2	2.73	0.41
1:B:575:PHE:O	1:B:579:VAL:HG23	2.22	0.40
1:A:156:SER:O	1:A:156:SER:OG	2.39	0.40
1:A:591:PHE:CD1	1:A:597:GLY:CA	3.04	0.40
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.94	0.40
1:B:722:LEU:HD23	1:B:722:LEU:HA	1.97	0.40
1:A:660:SER:O	1:A:660:SER:OG	2.36	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	594/735 (81%)	562 (95%)	30 (5%)	2 (0%)	41	75
1	B	594/735 (81%)	562 (95%)	30 (5%)	2 (0%)	41	75
All	All	1188/1470 (81%)	1124 (95%)	60 (5%)	4 (0%)	44	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	389	ALA
1	B	599	ASN

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Mol	Chain	Res	Type
1	A	389	ALA
1	A	599	ASN

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	519/646 (80%)	514 (99%)	5 (1%)	76	88
1	B	519/646 (80%)	514 (99%)	5 (1%)	76	88
All	All	1038/1292 (80%)	1028 (99%)	10 (1%)	77	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	381	THR
1	B	386	VAL
1	B	387	PRO
1	B	393	VAL
1	B	599	ASN
1	A	381	THR
1	A	386	VAL
1	A	387	PRO
1	A	393	VAL
1	A	599	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	ASN
1	B	171	ASN
1	B	216	ASN
1	B	230	GLN
1	B	499	ASN
1	B	599	ASN

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Mol	Chain	Res	Type
1	A	148	ASN
1	A	171	ASN
1	A	216	ASN
1	A	230	GLN
1	A	499	ASN
1	A	599	ASN

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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	PGW	A	803	-	37,37,50	1.08	3 (8%)	40,43,56	1.05	2 (5%)
3	PGW	B	804	-	27,27,50	1.26	4 (14%)	31,32,56	1.19	3 (9%)
3	PGW	B	803	-	37,37,50	1.08	3 (8%)	40,43,56	1.04	2 (5%)
3	PGW	A	804	-	27,27,50	1.26	4 (14%)	31,32,56	1.19	3 (9%)

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	PGW	A	803	-	-	15/42/42/55	-
3	PGW	B	804	-	-	11/29/29/55	-
3	PGW	B	803	-	-	15/42/42/55	-
3	PGW	A	804	-	-	11/29/29/55	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	PGW	O01-C1	3.30	1.43	1.34
3	A	804	PGW	O01-C1	3.30	1.43	1.34
3	B	803	PGW	O01-C1	2.94	1.42	1.34
3	A	803	PGW	O01-C1	2.92	1.42	1.34
3	B	803	PGW	O03-C19	2.53	1.40	1.33
3	A	803	PGW	O03-C19	2.53	1.40	1.33
3	A	804	PGW	O03-C01	-2.38	1.39	1.45
3	B	804	PGW	O03-C01	-2.37	1.39	1.45
3	B	804	PGW	O03-C19	2.32	1.40	1.33
3	A	804	PGW	O03-C19	2.32	1.40	1.33
3	B	804	PGW	P-O12	2.31	1.63	1.54
3	A	804	PGW	P-O12	2.29	1.63	1.54
3	B	803	PGW	O03-C01	-2.24	1.40	1.45
3	A	803	PGW	O03-C01	-2.22	1.40	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	PGW	O01-C1-C2	3.98	120.08	111.50
3	B	803	PGW	O01-C1-C2	3.97	120.06	111.50
3	B	804	PGW	O01-C1-C2	2.88	117.72	111.50
3	A	804	PGW	O01-C1-C2	2.88	117.71	111.50
3	A	804	PGW	C02-O01-C1	2.78	124.64	117.79
3	B	804	PGW	C02-O01-C1	2.78	124.63	117.79
3	A	803	PGW	O03-C19-C20	2.53	119.84	111.91
3	B	803	PGW	O03-C19-C20	2.52	119.83	111.91
3	B	804	PGW	O03-C19-C20	2.47	119.66	111.91
3	A	804	PGW	O03-C19-C20	2.46	119.61	111.91

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	PGW	C04-C05-CAD-OAE
3	B	803	PGW	C04-O12-P-O13
3	B	803	PGW	C04-O12-P-O14
3	B	803	PGW	O03-C01-C02-O01
3	B	804	PGW	C03-O11-P-O12
3	B	804	PGW	C03-O11-P-O13
3	A	803	PGW	C04-C05-CAD-OAE
3	A	803	PGW	C04-O12-P-O13
3	A	803	PGW	C04-O12-P-O14
3	A	803	PGW	O03-C01-C02-O01
3	A	804	PGW	C03-O11-P-O12
3	A	804	PGW	C03-O11-P-O13
3	B	804	PGW	C20-C19-O03-C01
3	A	804	PGW	C20-C19-O03-C01
3	B	804	PGW	O04-C19-O03-C01
3	A	804	PGW	O04-C19-O03-C01
3	B	803	PGW	OAF-C05-CAD-OAE
3	A	803	PGW	OAF-C05-CAD-OAE
3	B	803	PGW	C04-O12-P-O11
3	A	803	PGW	C04-O12-P-O11
3	A	804	PGW	C21-C22-C23-C24
3	B	804	PGW	C21-C22-C23-C24
3	B	803	PGW	C25-C26-C27-C15
3	A	803	PGW	C25-C26-C27-C15
3	B	804	PGW	C03-O11-P-O14
3	A	804	PGW	C03-O11-P-O14
3	B	803	PGW	O01-C02-C03-O11
3	A	803	PGW	O01-C02-C03-O11
3	B	803	PGW	O03-C01-C02-C03
3	A	803	PGW	O03-C01-C02-C03
3	B	804	PGW	O03-C01-C02-O01
3	A	804	PGW	O03-C01-C02-O01
3	B	803	PGW	C27-C15-C16-C17
3	A	803	PGW	C27-C15-C16-C17
3	B	803	PGW	C01-C02-C03-O11
3	A	803	PGW	C01-C02-C03-O11
3	B	804	PGW	C2-C3-C4-C5
3	A	804	PGW	C2-C3-C4-C5
3	B	804	PGW	O03-C01-C02-C03
3	A	804	PGW	O03-C01-C02-C03
3	B	803	PGW	C02-C03-O11-P
3	A	803	PGW	C02-C03-O11-P
3	B	803	PGW	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
3	A	803	PGW	C24-C25-C26-C27
3	B	804	PGW	C22-C23-C24-C25
3	A	804	PGW	C22-C23-C24-C25
3	B	803	PGW	O01-C1-C2-C3
3	A	803	PGW	O01-C1-C2-C3
3	B	803	PGW	O02-C1-C2-C3
3	A	803	PGW	O02-C1-C2-C3
3	B	804	PGW	C01-C02-O01-C1
3	A	804	PGW	C01-C02-O01-C1

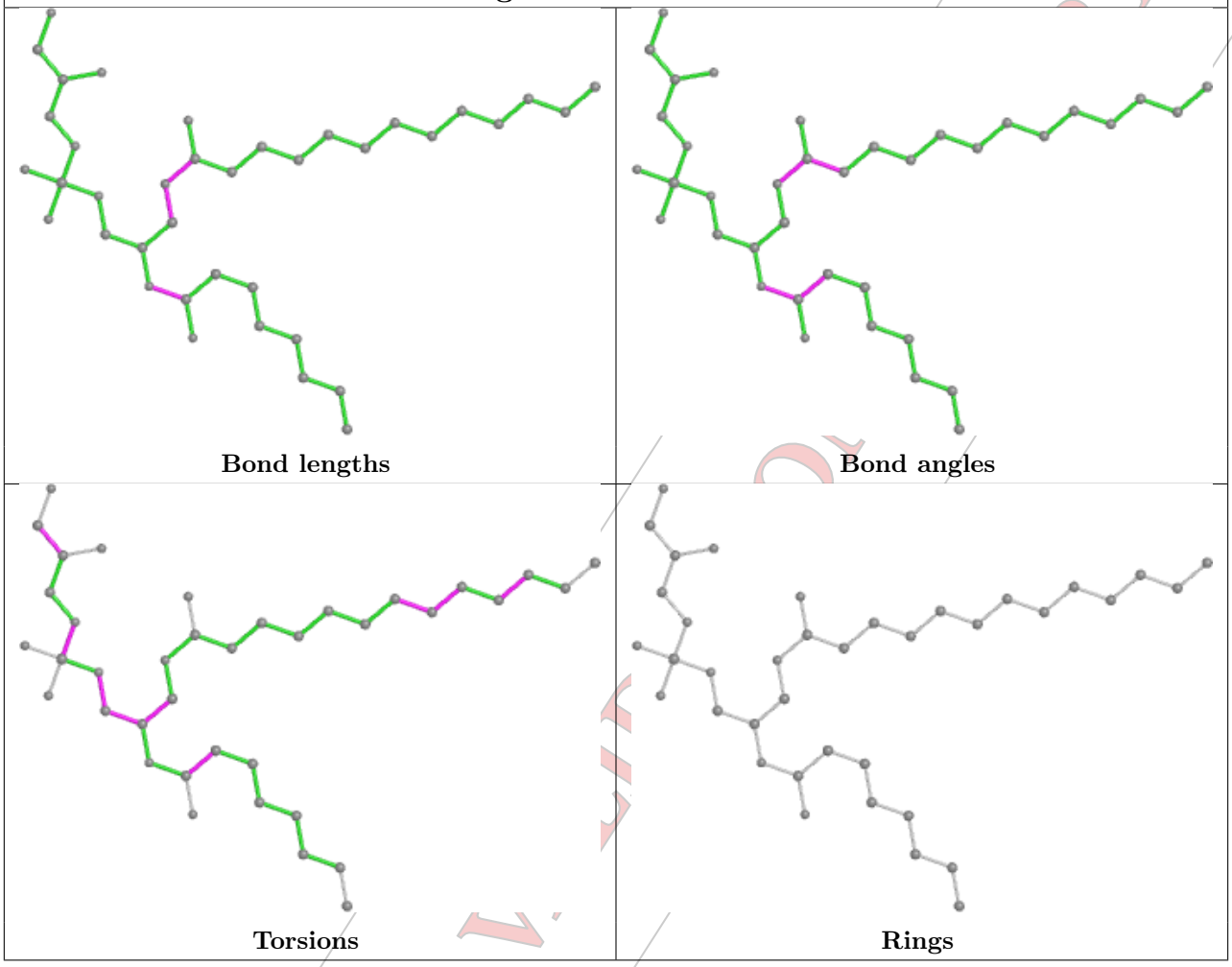
There are no ring outliers.

4 monomers are involved in 8 short contacts:

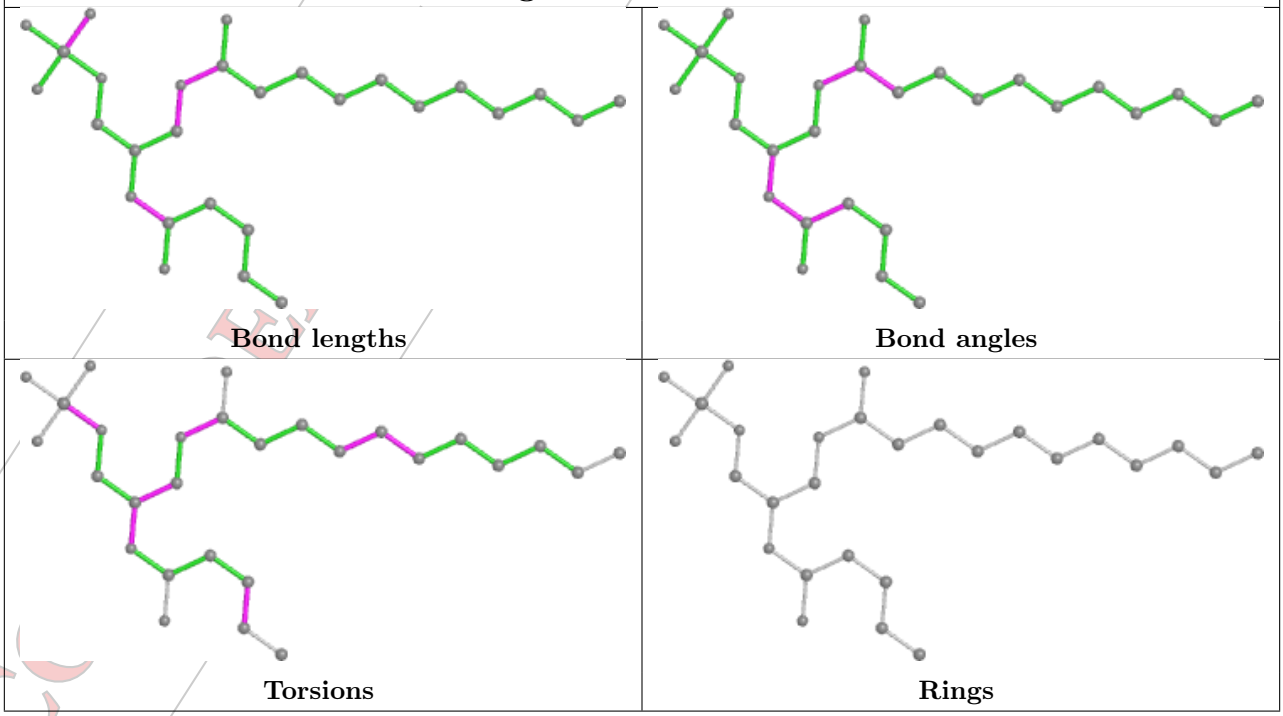
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	PGW	2	0
3	B	804	PGW	2	0
3	B	803	PGW	2	0
3	A	804	PGW	2	0

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 then 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.

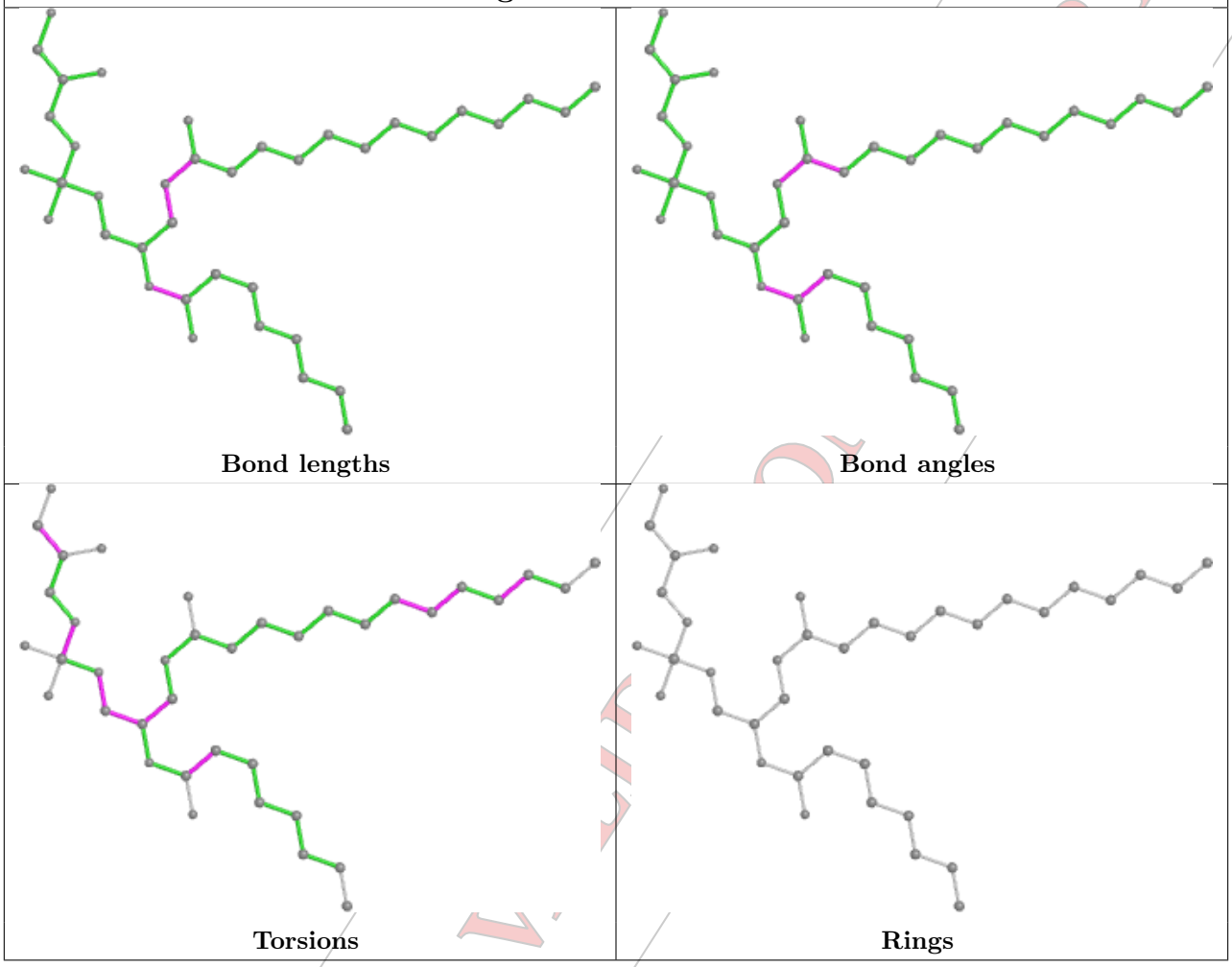
Ligand PGW A 803



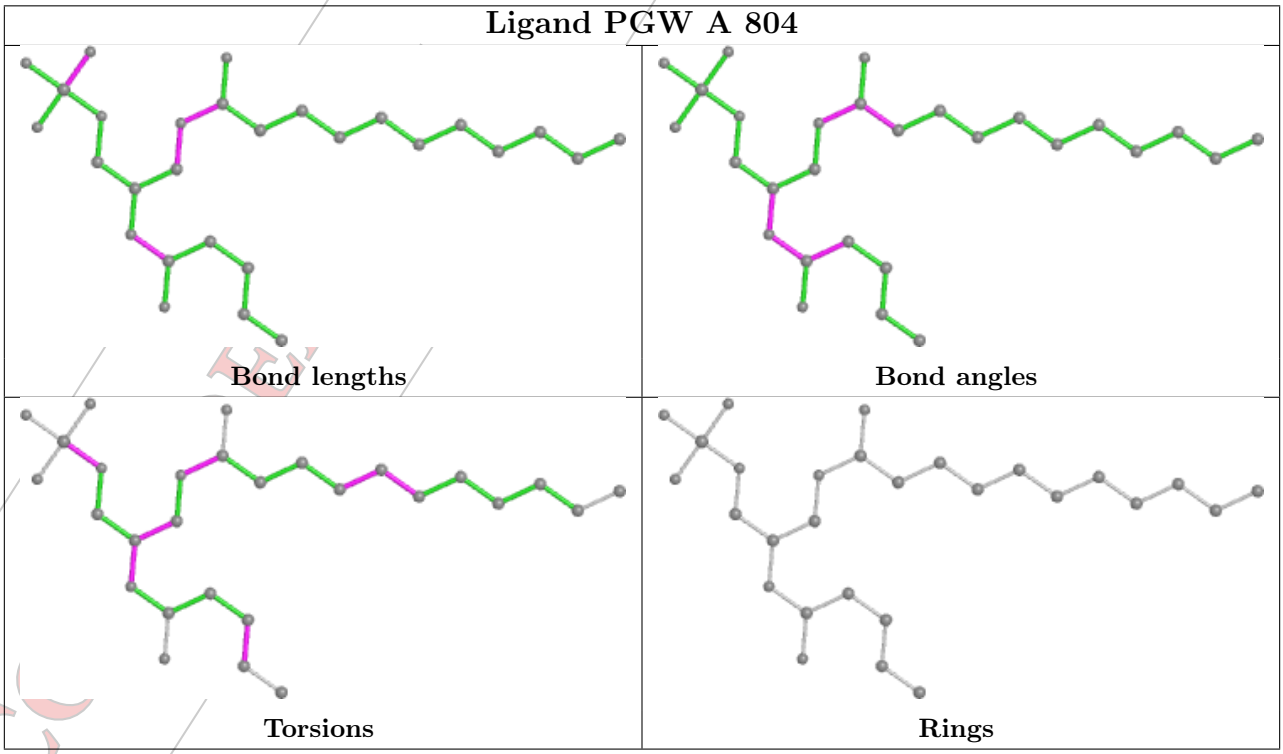
Ligand PGW B 804



Ligand PGW B 803



Ligand PGW A 804



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.

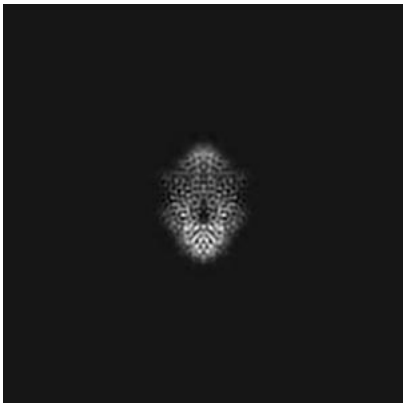
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24717. These allow visual inspection of the internal detail of the map and identification of artifacts.

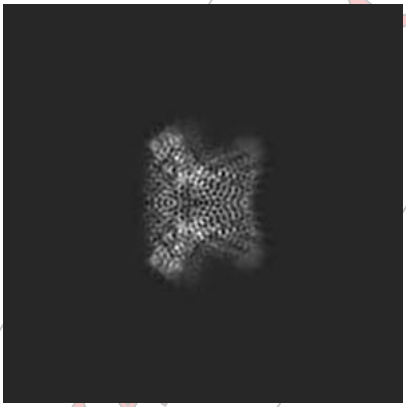
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

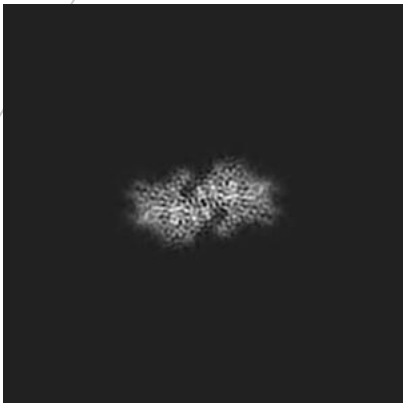
6.1.1 Primary map



X



Y



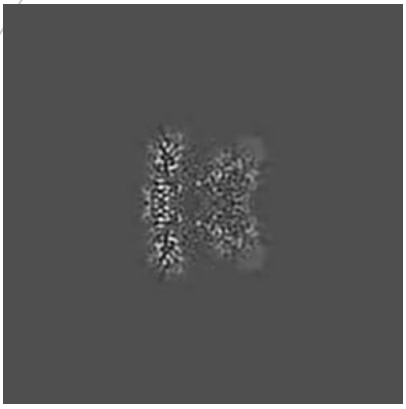
Z

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

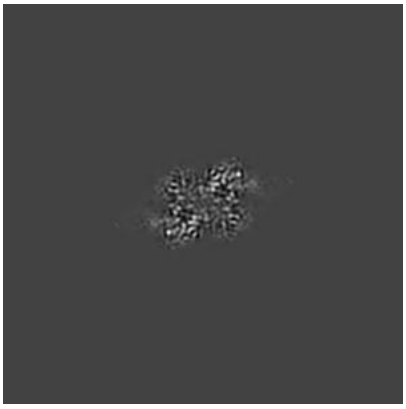
6.2 Central slices

6.2.1 Primary map

X Index: 144



Y Index: 144



Z Index: 144

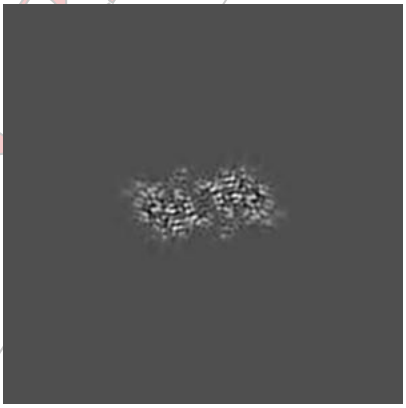
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 123

Y Index: 148

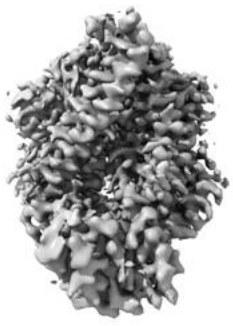


Z Index: 126

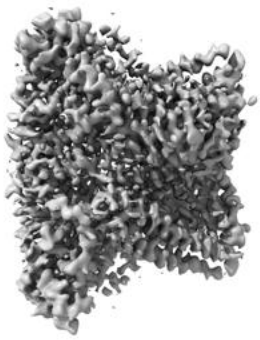
The images above show the largest variance slices of the map in three orthogonal directions.

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

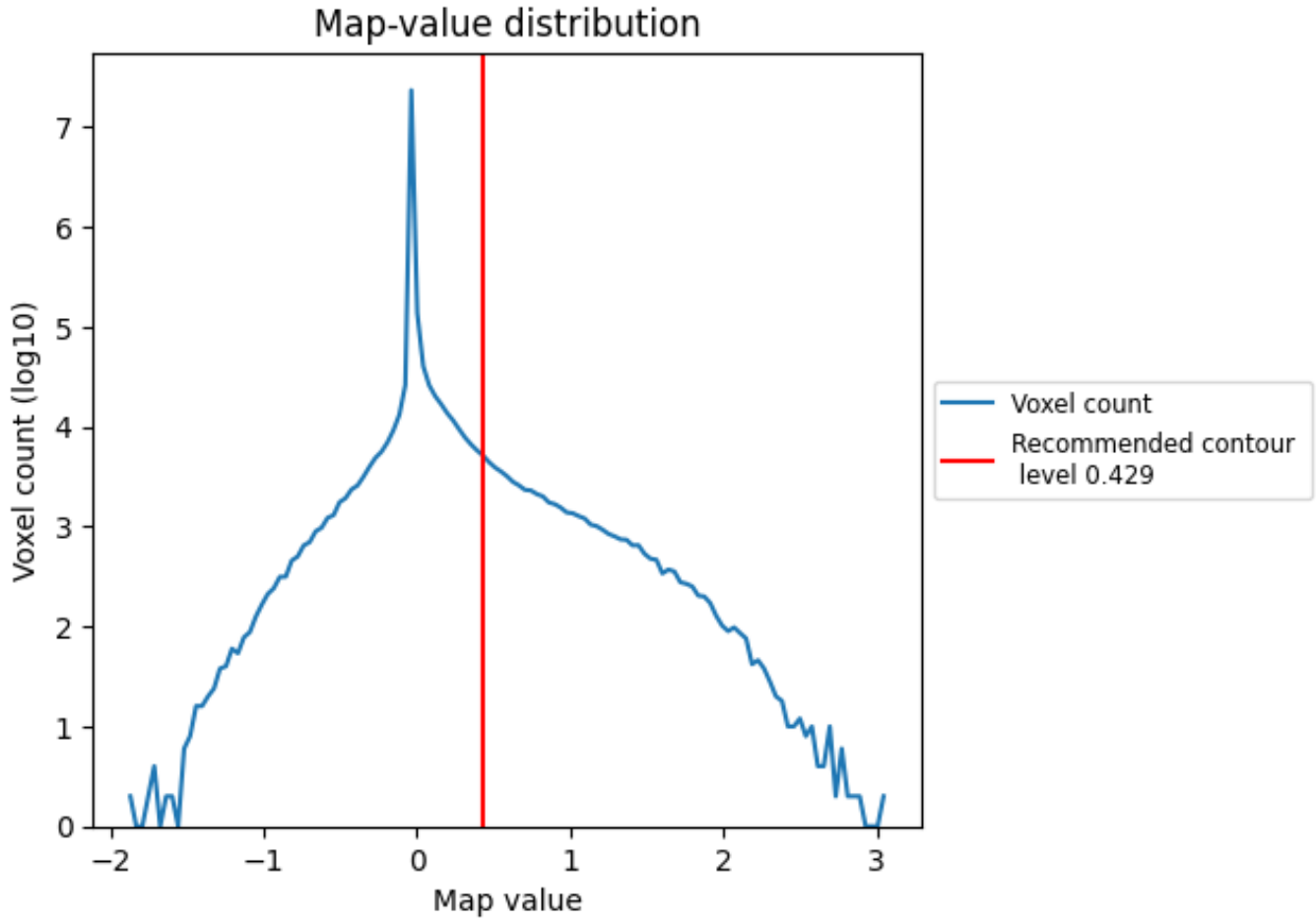
6.5 Mask visualisation (i)

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

7 Map analysis

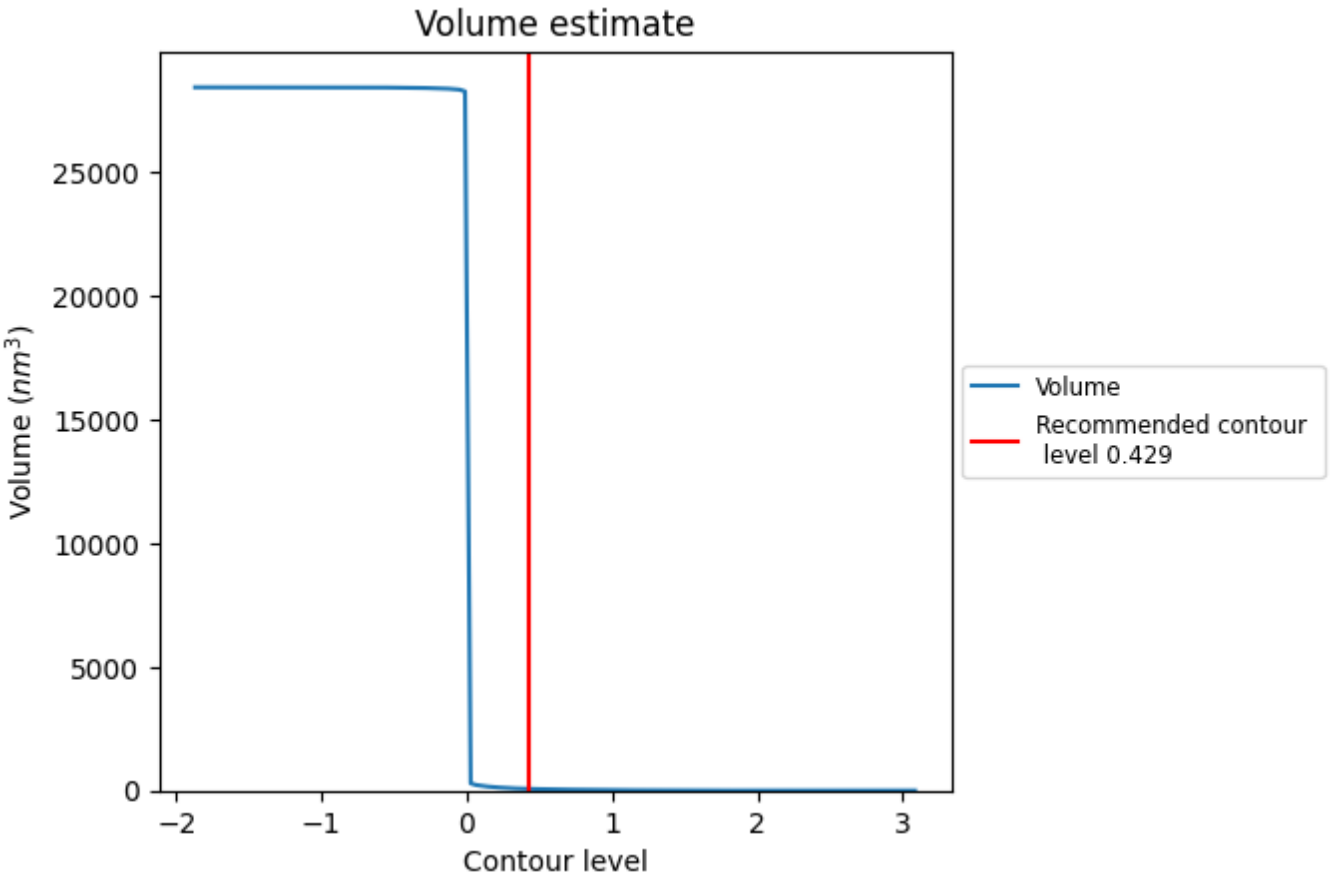
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

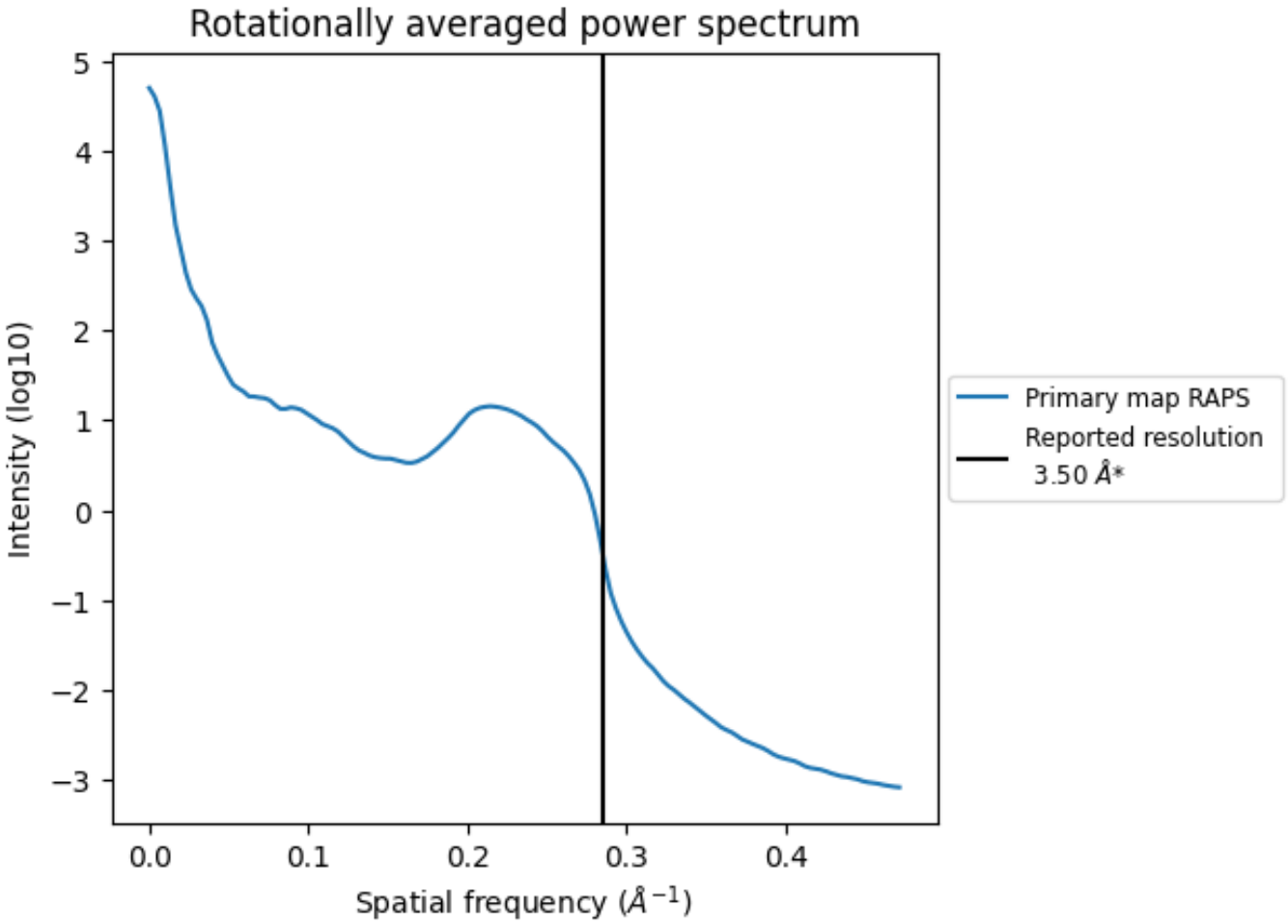
7.2 Volume estimate



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 62 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 0.286 Å^{-1}

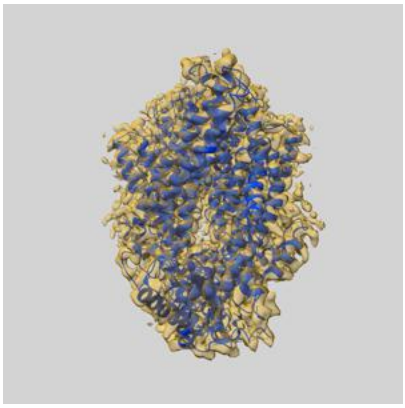
8 Fourier-Shell correlation (i)

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

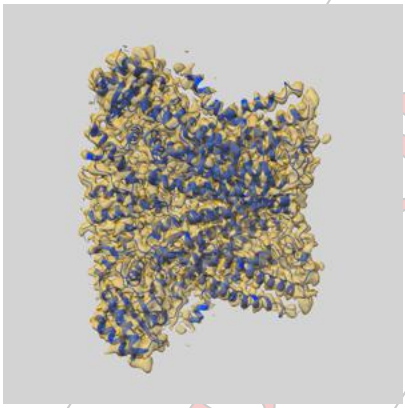
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24717 and PDB model 7RWJ. Per-residue inclusion information can be found in section 3 on page 5.

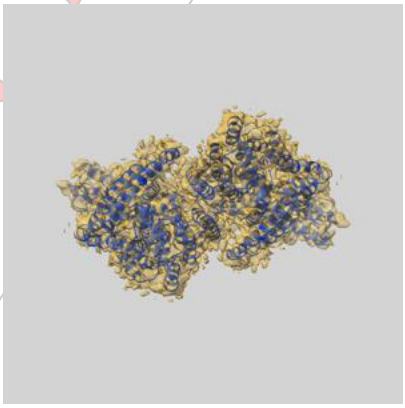
9.1 Map-model overlay



X



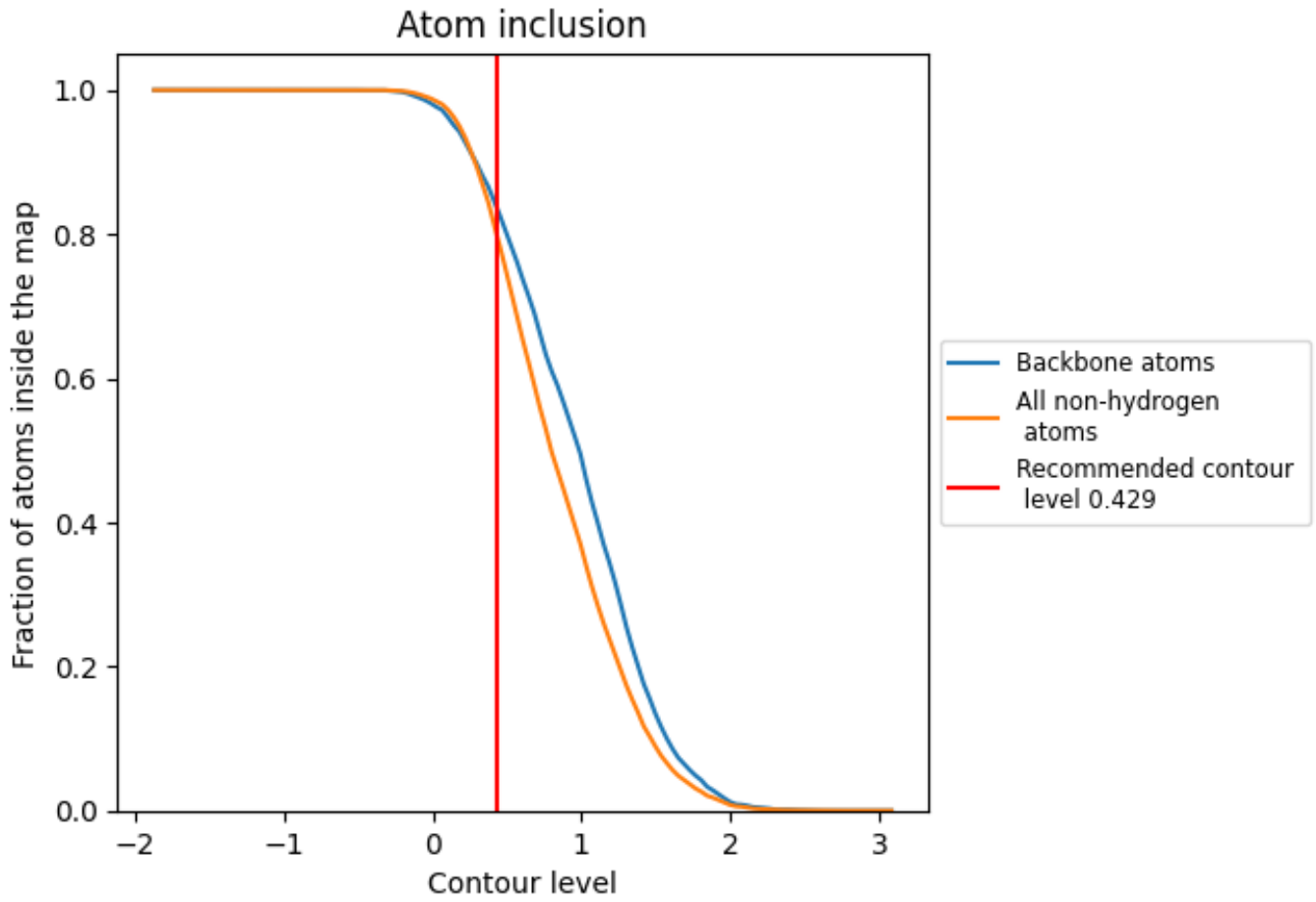
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.429 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 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

Full wwPDB EM Validation Report ⓘ

Aug 30, 2021 – 10:19 AM EDT

PDB ID	:	7RXG
EMDB ID	:	EMD-24730
Title	:	afTMEM16 in C18 lipid nanodiscs with MSP1E3 scaffold protein in the presence of Ca2+, full dimer
Deposited on	:	2021-08-23
Resolution	:	2.28 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

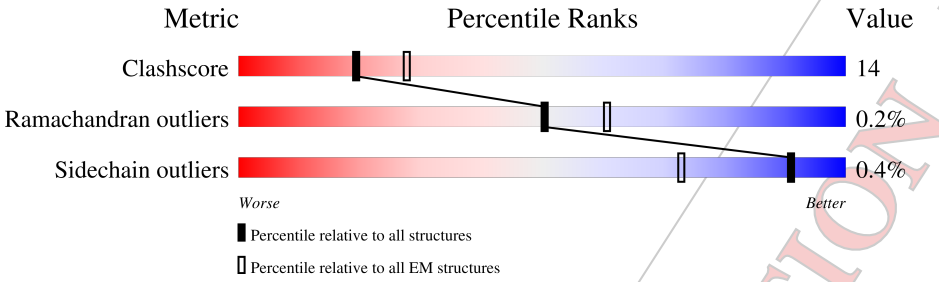
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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 <=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	735	7% 64% 24% 12%
1	B	735	7% 65% 24% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11380 atoms, of which 96 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.

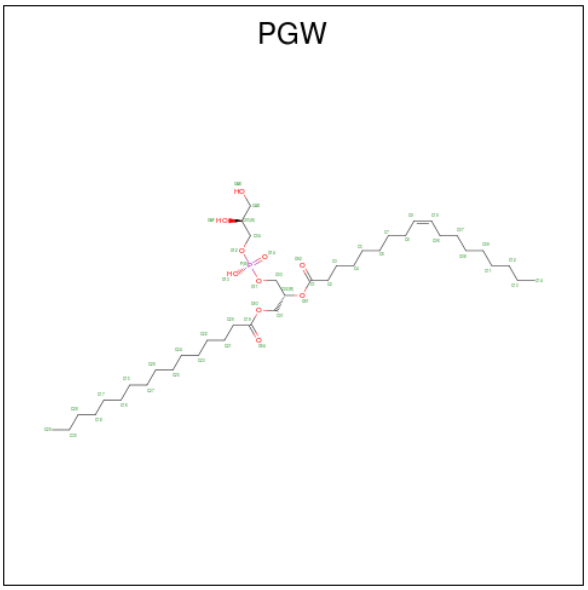
- Molecule 1 is a protein called afTMEM16 lipid scramblase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	650	Total	C	N	O	S	0	0
			5258	3429	883	927	19		
1	A	650	Total	C	N	O	S	0	0
			5258	3429	883	927	19		

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	B	2	Total	Ca	0
			2	2	
2	A	2	Total	Ca	0
			2	2	

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	B	1	Total 324	C 233	O 82	P 9	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0
3	A	1	Total 392	C 283	O 98	P 11	0

- Molecule 4 is water.

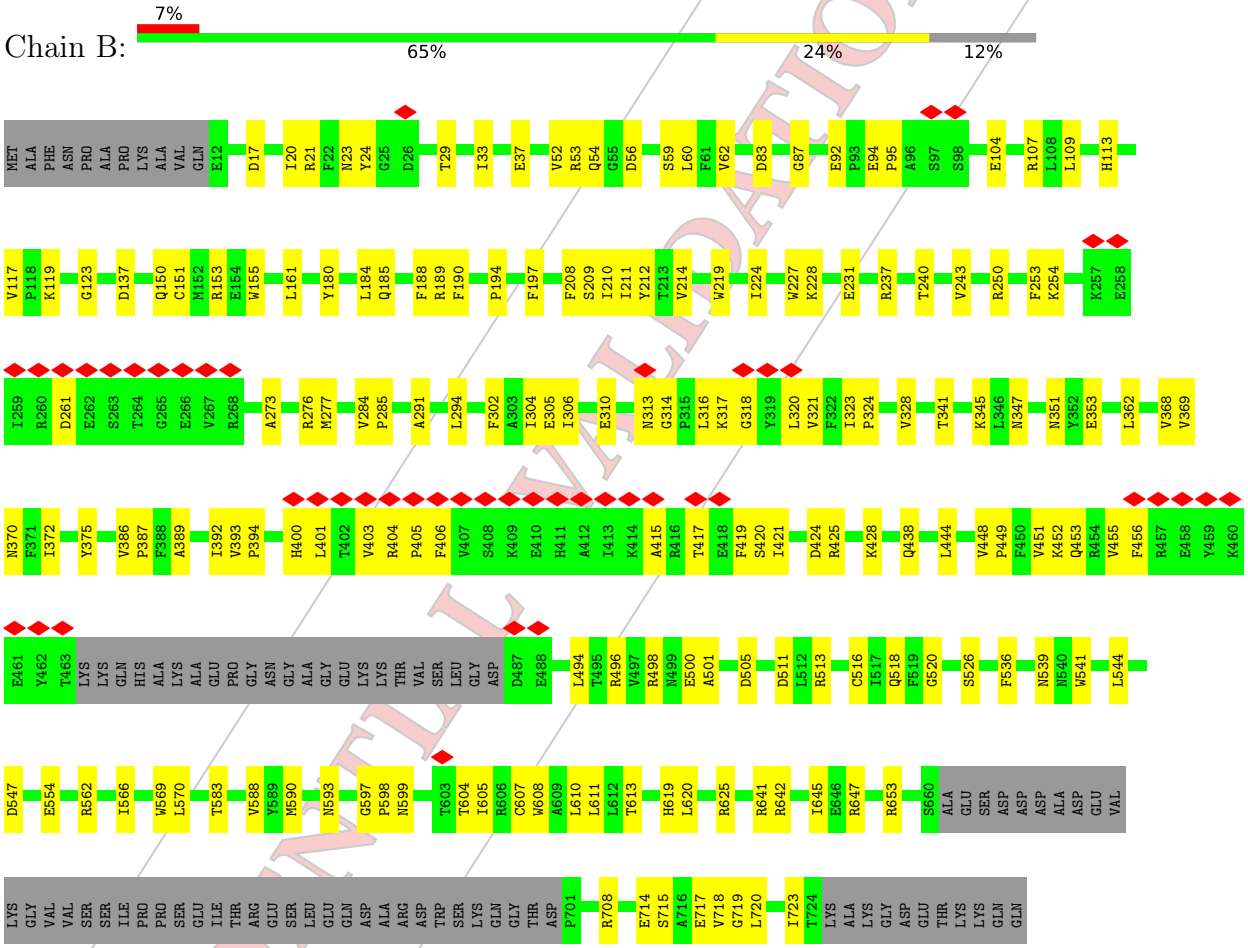
Mol	Chain	Residues	Atoms			AltConf
4	B	24	Total	H	O	0
			72	48	24	
4	A	24	Total	H	O	0
			72	48	24	

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.

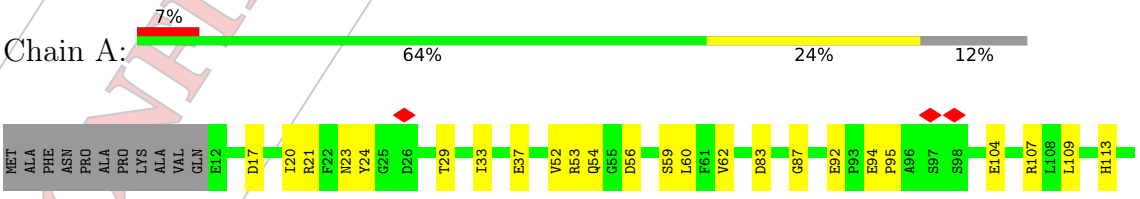
• Molecule 1: afTMEM16 lipid scramblase

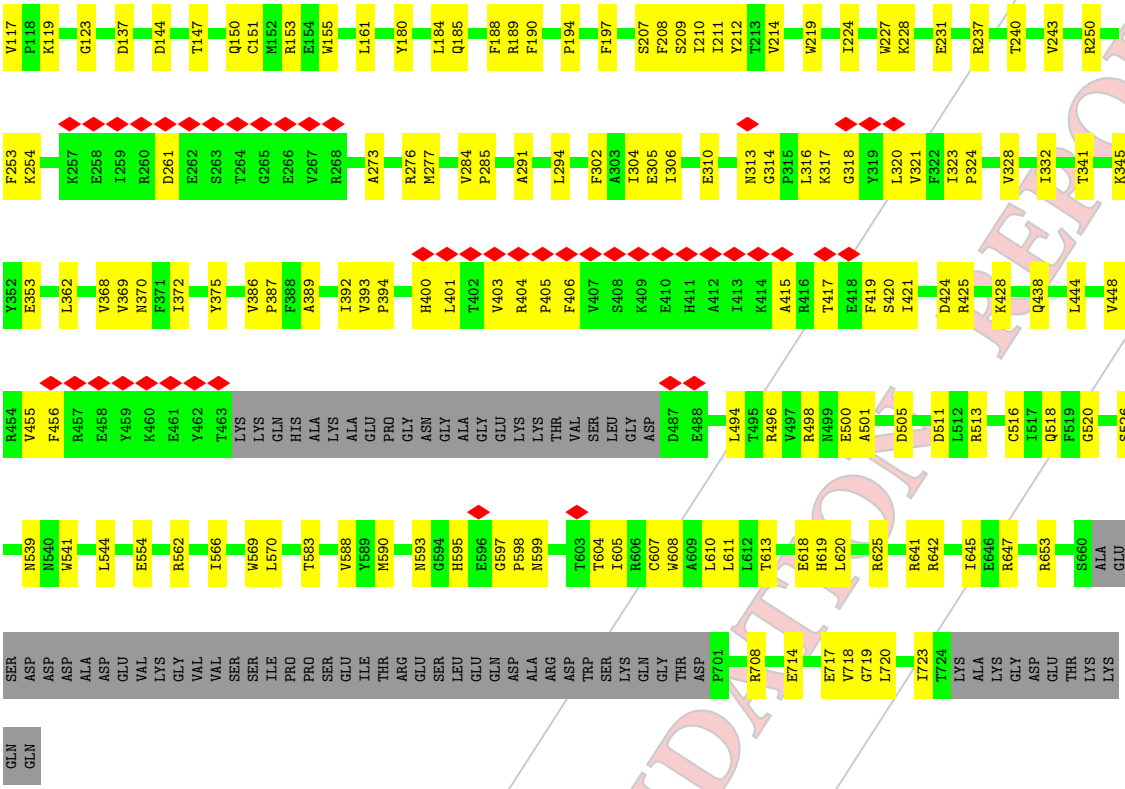
Chain B:



• Molecule 1: afTMEM16 lipid scramblase

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	994187	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 ($e^-/Å^2$)	42.8227	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	0.139	Depositor
Minimum map value	-0.072	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0169	Depositor
Map size (Å)	271.3728, 271.3728, 271.3728	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7067, 0.7067, 0.7067	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/5398	0.43	0/7340
1	B	0.32	0/5398	0.43	0/7340
All	All	0.31	0/10796	0.43	0/14680

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	5258	0	5207	165	0
1	B	5258	0	5207	157	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	392	0	462	39	0
3	B	324	0	380	27	0
4	A	24	48	0	4	0
4	B	24	48	0	3	0
All	All	11284	96	11256	316	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 14.

All (316) 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:33:ILE:CD1	1:A:723:ILE:HD12	1.71	1.20
1:B:33:ILE:HD13	1:A:723:ILE:HD12	1.12	1.05
1:B:33:ILE:HD13	1:A:723:ILE:CD1	1.85	1.05
1:A:719:GLY:O	1:A:723:ILE:HG13	1.67	0.94
1:B:604:THR:HG22	3:B:803:PGW:HAD	1.56	0.87
1:A:604:THR:HG22	3:A:1105:PGW:HAD	1.56	0.86
1:A:401:LEU:HA	1:A:404:ARG:HB2	1.60	0.84
1:B:401:LEU:HA	1:B:404:ARG:HB2	1.60	0.83
1:A:109:LEU:HD21	1:A:562:ARG:HD2	1.60	0.83
1:B:368:VAL:HG13	3:B:812:PGW:H16	1.61	0.82
1:B:109:LEU:HD21	1:B:562:ARG:HD2	1.60	0.82
1:A:368:VAL:HG13	3:A:1102:PGW:H16	1.63	0.80
1:A:304:ILE:HG22	1:A:324:PRO:HG3	1.65	0.78
1:B:393:VAL:HG23	1:B:394:PRO:HD3	1.65	0.78
1:A:320:LEU:HD13	1:A:403:VAL:HG12	1.66	0.77
1:B:320:LEU:HD13	1:B:403:VAL:HG12	1.66	0.77
1:A:393:VAL:HG23	1:A:394:PRO:HD3	1.65	0.77
1:A:452:LYS:HE2	1:A:456:PHE:CE2	2.20	0.77
1:B:304:ILE:HG22	1:B:324:PRO:HG3	1.65	0.77
1:B:452:LYS:HE2	1:B:456:PHE:CE2	2.20	0.76
1:A:389:ALA:HA	1:A:392:ILE:HB	1.70	0.74
1:B:389:ALA:HA	1:B:392:ILE:HB	1.69	0.74
1:A:598:PRO:HG3	1:A:605:ILE:HD11	1.72	0.71
1:B:598:PRO:HG3	1:B:605:ILE:HD11	1.72	0.70
1:A:313:ASN:H	1:A:415:ALA:HB1	1.57	0.70
1:A:17:ASP:OD1	1:A:107:ARG:NH1	2.25	0.69
1:B:209:SER:HA	3:B:807:PGW:H04	1.75	0.69
1:A:209:SER:HA	3:A:1110:PGW:H04	1.75	0.69
1:A:452:LYS:HE2	1:A:456:PHE:HE2	1.56	0.69
1:B:17:ASP:OD1	1:B:107:ARG:NH1	2.25	0.69
1:B:184:LEU:HD23	1:B:544:LEU:HD23	1.75	0.69
1:B:452:LYS:HE2	1:B:456:PHE:HE2	1.56	0.68
1:B:313:ASN:H	1:B:415:ALA:HB1	1.57	0.68
1:A:184:LEU:HD23	1:A:544:LEU:HD23	1.75	0.68
1:B:720:LEU:HA	1:A:33:ILE:HD12	1.75	0.67
1:B:291:ALA:HA	1:B:372:ILE:HD13	1.77	0.67
1:B:496:ARG:NH1	1:B:500:GLU:OE2	2.28	0.66
1:A:291:ALA:HA	1:A:372:ILE:HD13	1.77	0.66
3:B:805:PGW:H01A	3:A:1101:PGW:H02	1.78	0.66
1:A:496:ARG:NH1	1:A:500:GLU:OE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:NH2	1:B:501:ALA:O	2.29	0.66
3:A:1107:PGW:H02	3:A:1108:PGW:H01A	1.78	0.66
1:A:318:GLY:HA2	1:A:321:VAL:HG22	1.78	0.65
1:A:21:ARG:NH2	1:A:501:ALA:O	2.29	0.65
1:B:189:ARG:HD3	3:B:809:PGW:H03A	1.79	0.65
1:B:228:LYS:HG2	1:B:570:LEU:HD21	1.79	0.65
1:B:318:GLY:HA2	1:B:321:VAL:HG22	1.78	0.65
1:B:723:ILE:HD12	1:A:33:ILE:HD13	1.78	0.65
1:A:294:LEU:HD11	1:A:369:VAL:HG13	1.80	0.64
1:A:189:ARG:HD3	3:A:1112:PGW:H03A	1.79	0.63
1:B:539:ASN:HB2	3:B:806:PGW:H09	1.80	0.63
1:A:228:LYS:HG2	1:A:570:LEU:HD21	1.79	0.63
1:B:310:GLU:OE2	1:B:425:ARG:NH2	2.31	0.63
1:B:294:LEU:HD11	1:B:369:VAL:HG13	1.80	0.63
1:A:539:ASN:HB2	3:A:1109:PGW:H09	1.80	0.62
1:A:452:LYS:CE	1:A:456:PHE:CE2	2.83	0.62
1:A:310:GLU:OE2	1:A:425:ARG:NH2	2.31	0.62
1:A:52:VAL:CG1	1:A:60:LEU:HD23	2.30	0.62
1:A:109:LEU:CD2	1:A:562:ARG:HD2	2.28	0.62
1:B:33:ILE:HG13	1:A:720:LEU:HD13	1.82	0.61
1:B:52:VAL:CG1	1:B:60:LEU:HD23	2.30	0.61
1:B:109:LEU:CD2	1:B:562:ARG:HD2	2.28	0.61
1:B:452:LYS:CE	1:B:456:PHE:CE2	2.83	0.61
1:A:714:GLU:O	1:A:718:VAL:HG23	2.01	0.60
1:A:313:ASN:N	1:A:415:ALA:O	2.34	0.60
1:B:714:GLU:O	1:B:718:VAL:HG23	2.01	0.60
1:B:313:ASN:N	1:B:415:ALA:O	2.34	0.60
1:B:404:ARG:N	1:B:405:PRO:HD2	2.17	0.59
1:B:583:THR:HG22	3:B:805:PGW:H18A	1.84	0.59
1:A:404:ARG:N	1:A:405:PRO:HD2	2.17	0.59
1:B:610:LEU:HD21	3:B:805:PGW:H25A	1.84	0.59
1:A:610:LEU:HD21	3:A:1108:PGW:H25A	1.84	0.59
1:B:305:GLU:OE1	1:B:425:ARG:NH1	2.36	0.58
1:A:119:LYS:HA	1:A:123:GLY:O	2.03	0.58
1:A:583:THR:HG22	3:A:1108:PGW:H18A	1.84	0.58
1:B:33:ILE:HD12	1:A:720:LEU:HA	1.84	0.58
1:B:119:LYS:HA	1:B:123:GLY:O	2.03	0.58
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.86	0.58
1:B:401:LEU:HD23	1:B:404:ARG:HG2	1.86	0.58
1:A:29:THR:O	1:A:33:ILE:HG12	2.04	0.57
1:B:29:THR:O	1:B:33:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:CD1	1:A:723:ILE:CD1	2.57	0.57
1:B:719:GLY:HA2	1:A:60:LEU:HD21	1.86	0.57
1:A:273:ALA:O	1:A:277:MET:HG3	2.04	0.57
1:B:273:ALA:O	1:B:277:MET:HG3	2.04	0.56
1:B:720:LEU:HA	1:A:33:ILE:CD1	2.35	0.56
1:B:253:PHE:CZ	1:B:353:GLU:HG2	2.41	0.56
1:B:284:VAL:HB	1:B:285:PRO:HD3	1.86	0.56
1:B:320:LEU:HD13	1:B:403:VAL:CG1	2.36	0.56
1:B:419:PHE:HE2	1:B:421:ILE:HG22	1.71	0.56
1:A:401:LEU:HD23	1:A:404:ARG:HG2	1.86	0.56
1:A:305:GLU:OE1	1:A:425:ARG:NH1	2.36	0.55
1:A:320:LEU:HD13	1:A:403:VAL:CG1	2.36	0.55
1:A:419:PHE:HE2	1:A:421:ILE:HG22	1.71	0.55
1:A:253:PHE:CZ	1:A:353:GLU:HG2	2.41	0.55
1:B:151:CYS:HB3	1:B:155:TRP:CZ2	2.42	0.55
1:A:151:CYS:HB3	1:A:155:TRP:CZ2	2.42	0.54
1:B:593:ASN:HD21	1:B:597:GLY:HA2	1.73	0.54
1:A:593:ASN:HD21	1:A:597:GLY:HA2	1.73	0.53
1:B:393:VAL:HG11	1:B:419:PHE:CD1	2.44	0.53
1:B:188:PHE:CE1	1:B:541:TRP:HB2	2.44	0.53
1:B:33:ILE:CD1	1:A:720:LEU:HA	2.39	0.53
1:A:393:VAL:HG11	1:A:419:PHE:CD1	2.44	0.53
3:B:811:PGW:O14	3:B:811:PGW:H01A	2.09	0.52
1:B:494:LEU:O	1:B:498:ARG:HG3	2.10	0.52
1:A:323:ILE:HB	1:A:324:PRO:HD3	1.92	0.52
1:B:323:ILE:HB	1:B:324:PRO:HD3	1.92	0.52
1:A:386:VAL:HG12	1:A:598:PRO:HG2	1.91	0.52
1:A:607:CYS:O	1:A:611:LEU:HD23	2.10	0.52
1:A:188:PHE:CE1	1:A:541:TRP:HB2	2.44	0.51
1:B:60:LEU:HD21	1:A:719:GLY:HA2	1.91	0.51
1:B:607:CYS:O	1:B:611:LEU:HD23	2.10	0.51
1:A:494:LEU:O	1:A:498:ARG:HG3	2.10	0.51
3:A:1114:PGW:O14	3:A:1114:PGW:H01A	2.09	0.51
1:B:386:VAL:HG12	1:B:598:PRO:HG2	1.91	0.51
1:A:21:ARG:NH1	1:A:137:ASP:OD2	2.43	0.51
1:B:620:LEU:HG	3:B:803:PGW:H28	1.93	0.51
1:A:54:GLN:NE2	1:A:56:ASP:O	2.28	0.51
1:A:620:LEU:HG	3:A:1105:PGW:H28	1.93	0.51
1:B:180:TYR:CZ	1:B:511:ASP:HB3	2.46	0.51
1:B:52:VAL:HG11	1:B:60:LEU:HD23	1.93	0.50
1:B:444:LEU:HA	1:B:448:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HD2	1:A:137:ASP:HB3	1.93	0.50
1:A:448:VAL:CG2	1:A:449:PRO:HD3	2.41	0.50
1:B:94:GLU:HB3	1:B:95:PRO:HD2	1.93	0.50
1:B:317:LYS:O	1:B:321:VAL:HG13	2.12	0.50
1:B:448:VAL:CG2	1:B:449:PRO:HD3	2.41	0.50
1:A:180:TYR:CZ	1:A:511:ASP:HB3	2.46	0.50
1:A:316:LEU:O	1:A:320:LEU:HG	2.11	0.50
1:A:607:CYS:SG	3:A:1107:PGW:H2A	2.52	0.50
1:B:24:TYR:CE2	1:B:60:LEU:HD12	2.47	0.49
1:B:21:ARG:NH1	1:B:137:ASP:OD2	2.42	0.49
1:B:21:ARG:HD2	1:B:137:ASP:HB3	1.93	0.49
3:B:808:PGW:H24A	3:B:809:PGW:O04	2.13	0.49
1:A:94:GLU:HB3	1:A:95:PRO:HD2	1.93	0.49
1:B:607:CYS:SG	3:A:1101:PGW:H2A	2.52	0.49
1:A:317:LYS:O	1:A:321:VAL:HG13	2.12	0.49
3:A:1111:PGW:H24A	3:A:1112:PGW:O04	2.13	0.49
1:B:316:LEU:O	1:B:320:LEU:HG	2.11	0.49
1:A:24:TYR:CE2	1:A:60:LEU:HD12	2.47	0.49
1:A:52:VAL:HG11	1:A:60:LEU:HD23	1.93	0.49
1:A:161:LEU:N	1:A:185:GLN:OE1	2.43	0.49
1:B:708:ARG:HG3	1:A:53:ARG:NH2	2.27	0.49
1:A:227:TRP:CE2	1:A:231:GLU:HG3	2.48	0.49
1:B:250:ARG:HD3	4:B:2701:HOH:O	2.12	0.49
1:A:211:ILE:HD13	3:A:1110:PGW:H6A	1.95	0.49
1:A:313:ASN:N	1:A:415:ALA:HB1	2.27	0.49
1:B:211:ILE:HD13	3:B:807:PGW:H6A	1.95	0.49
1:A:444:LEU:HA	1:A:448:VAL:HG22	1.94	0.49
1:B:87:GLY:HA3	1:A:647:ARG:HH12	1.77	0.49
1:B:368:VAL:CG1	3:B:812:PGW:H16	2.38	0.49
1:B:151:CYS:HB3	1:B:155:TRP:CH2	2.48	0.48
1:A:250:ARG:HD3	4:A:2701:HOH:O	2.12	0.48
1:B:227:TRP:CE2	1:B:231:GLU:HG3	2.47	0.48
1:B:386:VAL:HB	1:B:387:PRO:HD3	1.95	0.48
1:A:393:VAL:CG2	1:A:394:PRO:HD3	2.40	0.48
1:B:33:ILE:HD11	1:A:723:ILE:HB	1.96	0.48
1:B:208:PHE:O	3:B:807:PGW:HADA	2.14	0.48
1:B:516:CYS:SG	1:B:569:TRP:HB3	2.54	0.48
1:A:386:VAL:HB	1:A:387:PRO:HD3	1.95	0.48
1:A:613:THR:CG2	3:A:1105:PGW:H22	2.43	0.48
1:B:276:ARG:HH11	1:B:351:ASN:HB3	1.79	0.48
1:B:613:THR:CG2	3:B:803:PGW:H22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:HG3	1:A:107:ARG:NH2	2.29	0.48
1:A:516:CYS:SG	1:A:569:TRP:HB3	2.54	0.48
1:A:208:PHE:O	3:A:1110:PGW:HADA	2.14	0.48
1:B:619:HIS:NE2	1:A:618:GLU:OE2	2.35	0.48
1:A:151:CYS:HB3	1:A:155:TRP:CH2	2.48	0.48
1:A:368:VAL:CG1	3:A:1102:PGW:H16	2.40	0.48
1:B:393:VAL:CG2	1:B:394:PRO:HD3	2.40	0.47
1:A:375:TYR:OH	1:A:520:GLY:HA3	2.14	0.47
1:B:104:GLU:HG3	1:B:107:ARG:NH2	2.29	0.47
1:B:161:LEU:N	1:B:185:GLN:OE1	2.43	0.47
1:B:150:GLN:OE1	1:B:153:ARG:NH1	2.41	0.47
1:B:313:ASN:N	1:B:415:ALA:HB1	2.27	0.47
1:B:708:ARG:HG3	1:A:53:ARG:HH22	1.79	0.47
1:A:190:PHE:O	1:A:194:PRO:HD2	2.14	0.47
1:B:190:PHE:O	1:B:194:PRO:HD2	2.14	0.47
1:A:419:PHE:CE2	1:A:421:ILE:HG22	2.50	0.47
1:B:647:ARG:HH12	1:A:87:GLY:HA3	1.79	0.47
1:B:419:PHE:CE2	1:B:421:ILE:HG22	2.50	0.46
1:A:224:ILE:HG22	1:A:228:LYS:HE2	1.97	0.46
1:B:224:ILE:HG22	1:B:228:LYS:HE2	1.97	0.46
1:B:375:TYR:OH	1:B:520:GLY:HA3	2.14	0.46
1:A:276:ARG:HH11	1:A:351:ASN:HB3	1.79	0.46
1:A:387:PRO:HG3	1:A:590:MET:HE1	1.98	0.46
1:B:714:GLU:HA	1:B:717:GLU:HG2	1.98	0.46
1:A:453:GLN:HE22	1:A:554:GLU:HA	1.81	0.46
1:B:641:ARG:O	1:B:645:ILE:HG12	2.16	0.46
1:A:320:LEU:HD22	1:A:323:ILE:HD11	1.97	0.46
1:B:611:LEU:HD21	3:A:1101:PGW:H6A	1.98	0.45
1:B:619:HIS:HB3	3:A:1102:PGW:H06A	1.98	0.45
1:B:453:GLN:HE22	1:B:554:GLU:HA	1.81	0.45
1:A:611:LEU:HD21	3:A:1107:PGW:H6A	1.98	0.45
1:B:53:ARG:NH2	1:A:708:ARG:HG3	2.32	0.45
1:B:320:LEU:HD22	1:B:323:ILE:HD11	1.97	0.45
1:A:714:GLU:HA	1:A:717:GLU:HG2	1.98	0.45
1:A:641:ARG:O	1:A:645:ILE:HG12	2.16	0.45
1:B:197:PHE:HD1	3:B:808:PGW:H30A	1.81	0.45
1:A:421:ILE:HD11	1:A:599:ASN:HA	1.99	0.45
1:B:608:TRP:CZ2	3:A:1107:PGW:H21	2.52	0.45
1:B:720:LEU:HD13	1:A:33:ILE:HG13	1.98	0.45
1:B:604:THR:CG2	3:B:803:PGW:HAD	2.37	0.44
3:B:812:PGW:H06A	1:A:619:HIS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:SER:CA	3:B:807:PGW:H04	2.45	0.44
1:B:421:ILE:HD11	1:B:599:ASN:HA	1.99	0.44
1:B:613:THR:HG23	3:B:803:PGW:H22	2.00	0.44
3:B:803:PGW:H17	3:B:803:PGW:H30	1.71	0.44
1:A:254:LYS:O	1:A:351:ASN:ND2	2.48	0.44
1:A:302:PHE:O	1:A:306:ILE:HG12	2.17	0.44
1:B:593:ASN:ND2	1:B:597:GLY:HA2	2.32	0.44
1:B:625:ARG:NH2	4:B:2705:HOH:O	2.29	0.44
1:A:197:PHE:HD1	3:A:1111:PGW:H30A	1.81	0.44
1:A:294:LEU:CD1	1:A:369:VAL:HG13	2.46	0.44
1:A:425:ARG:HD2	4:A:2722:HOH:O	2.17	0.44
1:B:180:TYR:OH	1:B:547:ASP:OD2	2.31	0.44
1:B:212:TYR:OH	1:B:526:SER:HB2	2.17	0.44
1:A:212:TYR:OH	1:A:526:SER:HB2	2.17	0.44
1:A:613:THR:HG23	3:A:1105:PGW:H22	2.00	0.44
1:B:254:LYS:O	1:B:351:ASN:ND2	2.48	0.44
1:B:302:PHE:O	1:B:306:ILE:HG12	2.18	0.44
1:A:240:THR:O	1:A:243:VAL:HB	2.18	0.44
1:A:438:GLN:HE22	1:A:518:GLN:HE21	1.66	0.44
1:A:593:ASN:ND2	1:A:597:GLY:HA2	2.32	0.44
1:A:324:PRO:O	1:A:328:VAL:HG23	2.18	0.44
1:A:604:THR:CG2	3:A:1105:PGW:HAD	2.37	0.44
1:B:425:ARG:HD2	4:B:2722:HOH:O	2.17	0.43
1:A:424:ASP:HB3	1:A:428:LYS:HE2	1.99	0.43
1:B:194:PRO:HD3	1:B:219:TRP:CD1	2.53	0.43
1:B:387:PRO:HG3	1:B:590:MET:HE1	2.00	0.43
1:B:33:ILE:O	1:B:37:GLU:HG3	2.18	0.43
1:B:53:ARG:HH22	1:A:708:ARG:HG3	1.83	0.43
1:B:424:ASP:HB3	1:B:428:LYS:HE2	1.99	0.43
1:A:261:ASP:N	1:A:261:ASP:OD1	2.51	0.43
1:B:240:THR:O	1:B:243:VAL:HB	2.18	0.43
1:B:318:GLY:HA2	1:B:321:VAL:CG2	2.48	0.43
1:B:438:GLN:HE22	1:B:518:GLN:HE21	1.66	0.43
1:B:715:SER:HB3	1:A:52:VAL:HG23	2.00	0.43
1:A:150:GLN:OE1	1:A:153:ARG:NH1	2.41	0.43
1:A:194:PRO:HD3	1:A:219:TRP:CD1	2.53	0.43
1:A:231:GLU:OE2	1:A:566:ILE:HG12	2.18	0.43
1:B:54:GLN:NE2	1:B:56:ASP:O	2.28	0.43
1:B:210:ILE:HG12	1:B:588:VAL:HG11	2.01	0.43
1:A:92:GLU:OE2	1:A:653:ARG:HD2	2.19	0.43
1:A:318:GLY:HA2	1:A:321:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1101:PGW:H03	3:A:1101:PGW:O04	2.19	0.43
1:A:209:SER:CA	3:A:1110:PGW:H04	2.45	0.43
1:A:237:ARG:HA	1:A:642:ARG:HH12	1.84	0.43
1:A:625:ARG:NH2	4:A:2705:HOH:O	2.29	0.43
1:B:231:GLU:OE2	1:B:566:ILE:HG12	2.18	0.43
1:B:324:PRO:O	1:B:328:VAL:HG23	2.18	0.43
1:B:92:GLU:OE2	1:B:653:ARG:HD2	2.19	0.42
1:B:237:ARG:HA	1:B:642:ARG:HH12	1.84	0.42
1:A:23:ASN:HD22	1:A:59:SER:HB3	1.84	0.42
1:A:83:ASP:OD2	1:A:562:ARG:NH2	2.52	0.42
1:A:318:GLY:CA	1:A:321:VAL:HG22	2.49	0.42
1:A:113:HIS:O	1:A:117:VAL:HG22	2.19	0.42
1:A:347:ASN:ND2	1:A:362:LEU:HB2	2.34	0.42
1:B:83:ASP:OD2	1:B:562:ARG:NH2	2.52	0.42
3:B:808:PGW:H01	3:B:808:PGW:C2	2.49	0.42
1:A:210:ILE:HG12	1:A:588:VAL:HG11	2.01	0.42
1:B:113:HIS:O	1:B:117:VAL:HG22	2.19	0.42
1:A:451:VAL:O	1:A:455:VAL:HG23	2.20	0.42
3:A:1107:PGW:H03	3:A:1107:PGW:O04	2.19	0.42
1:B:23:ASN:HD22	1:B:59:SER:HB3	1.84	0.42
1:B:294:LEU:CD1	1:B:369:VAL:HG13	2.46	0.42
3:A:1107:PGW:H01A	3:A:1108:PGW:H02	2.01	0.42
1:A:291:ALA:HA	1:A:372:ILE:CD1	2.48	0.42
1:B:619:HIS:CB	3:A:1102:PGW:H06A	2.49	0.42
1:A:33:ILE:O	1:A:37:GLU:HG3	2.18	0.42
3:A:1111:PGW:C2	3:A:1111:PGW:H01	2.49	0.42
3:B:812:PGW:H06A	1:A:619:HIS:CB	2.49	0.42
3:B:812:PGW:H6	1:A:619:HIS:CD2	2.55	0.42
1:B:347:ASN:ND2	1:B:362:LEU:HB2	2.34	0.42
1:A:314:GLY:N	1:A:415:ALA:HB1	2.35	0.42
1:A:405:PRO:HG2	1:A:406:PHE:CD2	2.55	0.42
1:B:314:GLY:N	1:B:415:ALA:HB1	2.35	0.41
1:B:405:PRO:HG2	1:B:406:PHE:CD2	2.55	0.41
1:B:400:HIS:O	1:B:403:VAL:HG22	2.20	0.41
1:A:144:ASP:OD2	1:A:147:THR:OG1	2.31	0.41
3:B:805:PGW:H02	3:A:1101:PGW:H01A	2.01	0.41
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.86	0.41
1:B:451:VAL:O	1:B:455:VAL:HG23	2.20	0.41
1:A:54:GLN:O	1:A:498:ARG:NH1	2.48	0.41
3:A:1108:PGW:H26A	3:A:1108:PGW:H16	1.83	0.41
1:B:54:GLN:O	1:B:498:ARG:NH1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:HIS:CD2	3:A:1102:PGW:H6	2.55	0.41
1:A:209:SER:OG	1:A:211:ILE:HG22	2.21	0.41
1:B:291:ALA:HA	1:B:372:ILE:CD1	2.48	0.41
3:B:805:PGW:H02	3:A:1101:PGW:C01	2.51	0.41
1:B:209:SER:OG	1:B:211:ILE:HG22	2.21	0.41
1:B:261:ASP:OD1	1:B:261:ASP:N	2.51	0.41
3:A:1107:PGW:C01	3:A:1108:PGW:H02	2.51	0.41
1:A:341:THR:O	1:A:345:LYS:HD3	2.20	0.41
1:A:518:GLN:HG2	1:A:536:PHE:CE2	2.56	0.41
1:A:608:TRP:CZ2	3:A:1101:PGW:H21	2.56	0.41
1:B:341:THR:O	1:B:345:LYS:HD3	2.20	0.41
1:B:370:ASN:HD21	1:B:513:ARG:HE	1.69	0.41
1:A:400:HIS:O	1:A:403:VAL:HG22	2.20	0.41
1:B:214:VAL:HG22	3:B:803:PGW:H15	2.03	0.40
1:A:332:ILE:HD13	1:A:332:ILE:HA	1.88	0.40
1:A:20:ILE:HB	1:A:62:VAL:HB	2.03	0.40
1:A:214:VAL:HG22	3:A:1105:PGW:H15	2.03	0.40
1:A:370:ASN:HD21	1:A:513:ARG:HE	1.69	0.40
1:B:452:LYS:HE3	1:B:456:PHE:CZ	2.57	0.40
1:B:518:GLN:HG2	1:B:536:PHE:CE2	2.56	0.40
1:A:23:ASN:ND2	1:A:59:SER:HB3	2.37	0.40
1:A:207:SER:OG	1:A:595:HIS:NE2	2.51	0.40
1:A:444:LEU:HA	1:A:448:VAL:CG2	2.51	0.40
1:A:448:VAL:HG23	1:A:449:PRO:HD3	2.03	0.40
3:A:1113:PGW:H20A	3:A:1113:PGW:H01A	1.86	0.40
1:B:20:ILE:HB	1:B:62:VAL:HB	2.03	0.40
1:B:23:ASN:ND2	1:B:59:SER:HB3	2.37	0.40
1:B:33:ILE:HD11	1:A:723:ILE:HD12	1.85	0.40
1:A:305:GLU:HA	1:A:324:PRO:HG2	2.04	0.40
1:A:425:ARG:HD3	4:A:2717:HOH:O	2.22	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	644/735 (88%)	627 (97%)	16 (2%)	1 (0%)	47 57
1	B	644/735 (88%)	627 (97%)	16 (2%)	1 (0%)	47 57
All	All	1288/1470 (88%)	1254 (97%)	32 (2%)	2 (0%)	50 57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	420	SER
1	A	420	SER

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	560/646 (87%)	558 (100%)	2 (0%)	91 95
1	B	560/646 (87%)	558 (100%)	2 (0%)	91 95
All	All	1120/1292 (87%)	1116 (100%)	4 (0%)	91 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	417	THR
1	B	505	ASP
1	A	417	THR
1	A	505	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	ASN
1	B	78	GLN

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Mol	Chain	Res	Type
1	B	148	ASN
1	B	171	ASN
1	B	283	GLN
1	B	370	ASN
1	B	438	GLN
1	B	453	GLN
1	B	593	ASN
1	A	23	ASN
1	A	78	GLN
1	A	148	ASN
1	A	171	ASN
1	A	283	GLN
1	A	370	ASN
1	A	400	HIS
1	A	438	GLN
1	A	453	GLN
1	A	593	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

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	PGW	A	1107	-	33,33,50	1.14	4 (12%)	37,38,56	1.18	2 (5%)
3	PGW	A	1101	-	33,33,50	1.14	4 (12%)	37,38,56	1.18	2 (5%)
3	PGW	B	804	-	24,24,50	1.31	4 (16%)	28,29,56	1.30	3 (10%)
3	PGW	B	808	-	31,31,50	1.16	4 (12%)	35,36,56	1.20	2 (5%)
3	PGW	A	1109	-	30,30,50	1.22	4 (13%)	34,35,56	1.20	2 (5%)
3	PGW	A	1106	-	24,24,50	1.32	4 (16%)	28,29,56	1.31	3 (10%)
3	PGW	A	1113	-	27,27,50	1.24	5 (18%)	31,32,56	1.23	2 (6%)
3	PGW	B	806	-	30,30,50	1.22	4 (13%)	34,35,56	1.20	2 (5%)
3	PGW	A	1105	-	44,44,50	0.98	3 (6%)	46,50,56	1.12	2 (4%)
3	PGW	A	1102	-	43,43,50	1.00	4 (9%)	46,49,56	1.09	2 (4%)
3	PGW	A	1114	-	28,28,50	1.25	5 (17%)	32,33,56	1.23	2 (6%)
3	PGW	B	809	-	26,26,50	1.29	4 (15%)	30,31,56	1.28	2 (6%)
3	PGW	B	805	-	37,37,50	0.98	3 (8%)	39,39,56	1.19	2 (5%)
3	PGW	B	811	-	28,28,50	1.25	5 (17%)	32,33,56	1.23	2 (6%)
3	PGW	B	803	-	44,44,50	0.98	3 (6%)	46,50,56	1.12	2 (4%)
3	PGW	B	807	-	24,24,50	1.06	1 (4%)	26,29,56	1.03	1 (3%)
3	PGW	B	812	-	43,43,50	1.01	4 (9%)	46,49,56	1.09	2 (4%)
3	PGW	A	1111	-	31,31,50	1.16	4 (12%)	35,36,56	1.20	2 (5%)
3	PGW	A	1108	-	37,37,50	0.98	3 (8%)	39,39,56	1.20	2 (5%)
3	PGW	A	1112	-	26,26,50	1.29	4 (15%)	30,31,56	1.28	2 (6%)
3	PGW	A	1110	-	24,24,50	1.06	1 (4%)	26,29,56	1.03	1 (3%)
3	PGW	B	810	-	27,27,50	1.24	5 (18%)	31,32,56	1.23	2 (6%)

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	PGW	A	1107	-	-	16/35/35/55	-
3	PGW	A	1101	-	-	16/35/35/55	-
3	PGW	B	804	-	-	11/26/26/55	-
3	PGW	B	808	-	-	17/33/33/55	-
3	PGW	A	1109	-	-	10/32/32/55	-
3	PGW	A	1106	-	-	11/26/26/55	-
3	PGW	A	1113	-	-	17/29/29/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGW	B	806	-	-	10/32/32/55	-
3	PGW	A	1105	-	-	23/49/49/55	-
3	PGW	A	1102	-	-	23/48/48/55	-
3	PGW	A	1114	-	-	18/30/30/55	-
3	PGW	B	809	-	-	16/28/28/55	-
3	PGW	B	805	-	-	14/39/39/55	-
3	PGW	B	811	-	-	18/30/30/55	-
3	PGW	B	803	-	-	23/49/49/55	-
3	PGW	B	807	-	-	12/28/28/55	-
3	PGW	B	812	-	-	23/48/48/55	-
3	PGW	A	1111	-	-	17/33/33/55	-
3	PGW	A	1108	-	-	14/39/39/55	-
3	PGW	A	1112	-	-	16/28/28/55	-
3	PGW	A	1110	-	-	12/28/28/55	-
3	PGW	B	810	-	-	17/29/29/55	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	809	PGW	O01-C1	3.09	1.43	1.34
3	A	1112	PGW	O01-C1	3.09	1.43	1.34
3	A	1109	PGW	O01-C1	2.97	1.42	1.34
3	B	806	PGW	O01-C1	2.95	1.42	1.34
3	A	1111	PGW	O01-C1	2.95	1.42	1.34
3	B	808	PGW	O01-C1	2.94	1.42	1.34
3	A	1108	PGW	O01-C1	2.92	1.42	1.34
3	B	805	PGW	O01-C1	2.89	1.42	1.34
3	A	1101	PGW	O01-C1	2.85	1.42	1.34
3	A	1107	PGW	O01-C1	2.84	1.42	1.34
3	A	1113	PGW	O01-C1	2.80	1.42	1.34
3	B	803	PGW	O01-C1	2.80	1.42	1.34
3	A	1110	PGW	O01-C1	2.79	1.42	1.34
3	A	1105	PGW	O01-C1	2.79	1.42	1.34
3	B	810	PGW	O01-C1	2.79	1.42	1.34
3	B	804	PGW	O01-C1	2.78	1.42	1.34
3	B	807	PGW	O01-C1	2.77	1.42	1.34
3	A	1106	PGW	O01-C1	2.76	1.42	1.34
3	A	1114	PGW	O01-C1	2.75	1.42	1.34
3	B	811	PGW	O01-C1	2.75	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	812	PGW	O01-C1	2.68	1.41	1.34
3	A	1102	PGW	O01-C1	2.67	1.41	1.34
3	B	812	PGW	O03-C19	2.56	1.40	1.33
3	A	1102	PGW	O03-C19	2.56	1.40	1.33
3	A	1112	PGW	O03-C19	2.47	1.40	1.33
3	A	1109	PGW	O03-C19	2.46	1.40	1.33
3	B	806	PGW	O03-C19	2.45	1.40	1.33
3	B	809	PGW	O03-C19	2.45	1.40	1.33
3	B	808	PGW	O03-C19	2.44	1.40	1.33
3	A	1111	PGW	O03-C19	2.42	1.40	1.33
3	A	1101	PGW	O03-C19	2.41	1.40	1.33
3	A	1106	PGW	O03-C01	-2.38	1.39	1.45
3	A	1114	PGW	O03-C19	2.38	1.40	1.33
3	B	803	PGW	O03-C19	2.38	1.40	1.33
3	B	811	PGW	O03-C19	2.38	1.40	1.33
3	A	1107	PGW	O03-C19	2.38	1.40	1.33
3	A	1105	PGW	O03-C19	2.37	1.40	1.33
3	A	1106	PGW	P-O12	2.37	1.64	1.54
3	A	1114	PGW	P-O12	2.37	1.64	1.54
3	B	806	PGW	P-O12	2.37	1.64	1.54
3	A	1109	PGW	P-O12	2.37	1.64	1.54
3	A	1106	PGW	O03-C19	2.37	1.40	1.33
3	B	804	PGW	O03-C01	-2.36	1.39	1.45
3	B	804	PGW	P-O12	2.36	1.63	1.54
3	B	804	PGW	O03-C19	2.35	1.40	1.33
3	A	1101	PGW	P-O12	2.35	1.63	1.54
3	B	811	PGW	P-O12	2.35	1.63	1.54
3	B	810	PGW	O03-C19	2.34	1.40	1.33
3	A	1107	PGW	P-O12	2.34	1.63	1.54
3	A	1113	PGW	O03-C19	2.34	1.40	1.33
3	A	1111	PGW	P-O12	2.33	1.63	1.54
3	A	1112	PGW	P-O12	2.33	1.63	1.54
3	B	808	PGW	P-O12	2.32	1.63	1.54
3	B	805	PGW	O03-C19	2.31	1.40	1.33
3	A	1111	PGW	O03-C01	-2.31	1.39	1.45
3	B	805	PGW	O03-C01	-2.31	1.39	1.45
3	A	1108	PGW	O03-C19	2.31	1.40	1.33
3	B	810	PGW	P-O12	2.30	1.63	1.54
3	B	809	PGW	P-O12	2.30	1.63	1.54
3	B	808	PGW	O03-C01	-2.30	1.39	1.45
3	B	811	PGW	O03-C01	-2.30	1.39	1.45
3	B	810	PGW	O03-C01	-2.30	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1113	PGW	P-O12	2.29	1.63	1.54
3	A	1101	PGW	O03-C01	-2.29	1.39	1.45
3	A	1108	PGW	O03-C01	-2.29	1.39	1.45
3	A	1113	PGW	O03-C01	-2.29	1.39	1.45
3	A	1109	PGW	O03-C01	-2.28	1.39	1.45
3	A	1107	PGW	O03-C01	-2.28	1.40	1.45
3	B	806	PGW	O03-C01	-2.27	1.40	1.45
3	A	1114	PGW	O03-C01	-2.27	1.40	1.45
3	B	803	PGW	O03-C01	-2.25	1.40	1.45
3	A	1105	PGW	O03-C01	-2.24	1.40	1.45
3	A	1102	PGW	O03-C01	-2.22	1.40	1.45
3	B	812	PGW	O03-C01	-2.21	1.40	1.45
3	B	809	PGW	O03-C01	-2.21	1.40	1.45
3	A	1112	PGW	O03-C01	-2.21	1.40	1.45
3	B	812	PGW	O01-C02	-2.08	1.41	1.46
3	A	1102	PGW	O01-C02	-2.05	1.41	1.46
3	B	811	PGW	O01-C02	-2.03	1.41	1.46
3	A	1114	PGW	O01-C02	-2.02	1.41	1.46
3	A	1113	PGW	O01-C02	-2.01	1.41	1.46
3	B	810	PGW	O01-C02	-2.01	1.41	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	809	PGW	O01-C1-C2	4.18	120.51	111.50
3	A	1112	PGW	O01-C1-C2	4.18	120.50	111.50
3	A	1106	PGW	O01-C1-C2	4.16	120.46	111.50
3	B	804	PGW	O01-C1-C2	4.14	120.43	111.50
3	A	1108	PGW	O01-C1-C2	4.13	120.40	111.50
3	B	805	PGW	O01-C1-C2	4.11	120.36	111.50
3	A	1101	PGW	O01-C1-C2	4.09	120.31	111.50
3	A	1107	PGW	O01-C1-C2	4.08	120.30	111.50
3	A	1102	PGW	O01-C1-C2	4.06	120.25	111.50
3	B	812	PGW	O01-C1-C2	4.06	120.25	111.50
3	A	1109	PGW	O01-C1-C2	4.04	120.21	111.50
3	B	806	PGW	O01-C1-C2	4.04	120.20	111.50
3	B	811	PGW	O01-C1-C2	4.03	120.19	111.50
3	A	1114	PGW	O01-C1-C2	4.03	120.19	111.50
3	B	803	PGW	O01-C1-C2	4.01	120.15	111.50
3	A	1105	PGW	O01-C1-C2	4.01	120.15	111.50
3	A	1111	PGW	O01-C1-C2	3.98	120.07	111.50
3	B	810	PGW	O01-C1-C2	3.97	120.06	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	808	PGW	O01-C1-C2	3.97	120.06	111.50
3	A	1113	PGW	O01-C1-C2	3.96	120.03	111.50
3	B	807	PGW	O01-C1-C2	3.80	119.68	111.50
3	A	1110	PGW	O01-C1-C2	3.78	119.65	111.50
3	B	809	PGW	O03-C19-C20	2.83	120.78	111.91
3	A	1112	PGW	O03-C19-C20	2.82	120.76	111.91
3	A	1109	PGW	O03-C19-C20	2.73	120.48	111.91
3	B	806	PGW	O03-C19-C20	2.73	120.47	111.91
3	A	1102	PGW	O03-C19-C20	2.72	120.45	111.91
3	B	812	PGW	O03-C19-C20	2.71	120.41	111.91
3	A	1105	PGW	O03-C19-C20	2.64	120.19	111.91
3	B	803	PGW	O03-C19-C20	2.64	120.18	111.91
3	B	805	PGW	O03-C19-C20	2.62	120.14	111.91
3	A	1108	PGW	O03-C19-C20	2.61	120.11	111.91
3	A	1113	PGW	O03-C19-C20	2.56	119.94	111.91
3	B	810	PGW	O03-C19-C20	2.55	119.92	111.91
3	A	1106	PGW	O03-C19-C20	2.54	119.89	111.91
3	B	804	PGW	O03-C19-C20	2.54	119.89	111.91
3	A	1107	PGW	O03-C19-C20	2.54	119.86	111.91
3	A	1101	PGW	O03-C19-C20	2.54	119.86	111.91
3	A	1111	PGW	O03-C19-C20	2.53	119.85	111.91
3	B	808	PGW	O03-C19-C20	2.52	119.83	111.91
3	A	1114	PGW	O03-C19-C20	2.45	119.59	111.91
3	B	811	PGW	O03-C19-C20	2.45	119.58	111.91
3	B	804	PGW	C02-O01-C1	-2.11	112.59	117.79
3	A	1106	PGW	C02-O01-C1	-2.10	112.62	117.79

There are no chirality outliers.

All (354) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	PGW	C04-C05-CAD-OAE
3	B	803	PGW	O03-C01-C02-O01
3	B	804	PGW	C03-O11-P-O12
3	B	804	PGW	C03-O11-P-O14
3	B	805	PGW	C01-C02-C03-O11
3	B	805	PGW	O01-C02-C03-O11
3	B	808	PGW	C2-C1-O01-C02
3	B	809	PGW	C03-O11-P-O13
3	B	809	PGW	C03-O11-P-O14
3	B	809	PGW	C2-C1-O01-C02
3	B	810	PGW	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	B	810	PGW	C03-O11-P-O13
3	B	810	PGW	C03-O11-P-O14
3	B	810	PGW	O04-C19-O03-C01
3	B	810	PGW	C20-C19-O03-C01
3	B	812	PGW	OAF-C05-CAD-OAE
3	B	812	PGW	C04-C05-CAD-OAE
3	B	812	PGW	O12-C04-C05-CAD
3	A	1101	PGW	C03-O11-P-O12
3	A	1101	PGW	C03-O11-P-O13
3	A	1101	PGW	C03-O11-P-O14
3	A	1101	PGW	C2-C1-O01-C02
3	A	1102	PGW	OAF-C05-CAD-OAE
3	A	1102	PGW	C04-C05-CAD-OAE
3	A	1102	PGW	O12-C04-C05-CAD
3	A	1105	PGW	C04-C05-CAD-OAE
3	A	1105	PGW	O03-C01-C02-O01
3	A	1106	PGW	C03-O11-P-O12
3	A	1106	PGW	C03-O11-P-O14
3	A	1107	PGW	C03-O11-P-O12
3	A	1107	PGW	C03-O11-P-O13
3	A	1107	PGW	C03-O11-P-O14
3	A	1107	PGW	C2-C1-O01-C02
3	A	1108	PGW	C01-C02-C03-O11
3	A	1108	PGW	O01-C02-C03-O11
3	A	1111	PGW	C2-C1-O01-C02
3	A	1112	PGW	C03-O11-P-O13
3	A	1112	PGW	C03-O11-P-O14
3	A	1112	PGW	C2-C1-O01-C02
3	A	1113	PGW	C03-O11-P-O12
3	A	1113	PGW	C03-O11-P-O13
3	A	1113	PGW	C03-O11-P-O14
3	A	1113	PGW	O04-C19-O03-C01
3	A	1113	PGW	C20-C19-O03-C01
3	B	811	PGW	O04-C19-O03-C01
3	A	1114	PGW	O04-C19-O03-C01
3	B	808	PGW	O02-C1-O01-C02
3	B	809	PGW	O02-C1-O01-C02
3	A	1111	PGW	O02-C1-O01-C02
3	A	1112	PGW	O02-C1-O01-C02
3	B	808	PGW	C20-C19-O03-C01
3	B	811	PGW	C20-C19-O03-C01
3	A	1111	PGW	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
3	A	1114	PGW	C20-C19-O03-C01
3	A	1101	PGW	O02-C1-O01-C02
3	A	1107	PGW	O02-C1-O01-C02
3	B	808	PGW	O04-C19-O03-C01
3	A	1111	PGW	O04-C19-O03-C01
3	B	803	PGW	C2-C1-O01-C02
3	A	1105	PGW	C2-C1-O01-C02
3	B	803	PGW	C17-C18-C28-C30
3	A	1105	PGW	C17-C18-C28-C30
3	B	812	PGW	O12-C04-C05-OAF
3	A	1102	PGW	O12-C04-C05-OAF
3	B	812	PGW	C19-C20-C21-C22
3	A	1102	PGW	C19-C20-C21-C22
3	B	804	PGW	C1-C2-C3-C4
3	A	1106	PGW	C1-C2-C3-C4
3	B	805	PGW	C16-C15-C27-C26
3	A	1108	PGW	C16-C15-C27-C26
3	B	805	PGW	C19-C20-C21-C22
3	B	807	PGW	C1-C2-C3-C4
3	A	1108	PGW	C19-C20-C21-C22
3	A	1110	PGW	C1-C2-C3-C4
3	B	808	PGW	C19-C20-C21-C22
3	A	1111	PGW	C19-C20-C21-C22
3	B	810	PGW	C1-C2-C3-C4
3	A	1113	PGW	C1-C2-C3-C4
3	B	803	PGW	O02-C1-O01-C02
3	A	1105	PGW	O02-C1-O01-C02
3	B	812	PGW	C10-C06-C07-C08
3	A	1102	PGW	C10-C06-C07-C08
3	B	804	PGW	C21-C22-C23-C24
3	A	1106	PGW	C21-C22-C23-C24
3	B	810	PGW	C24-C25-C26-C27
3	A	1113	PGW	C24-C25-C26-C27
3	B	805	PGW	C2-C1-O01-C02
3	A	1108	PGW	C2-C1-O01-C02
3	B	809	PGW	C2-C3-C4-C5
3	A	1101	PGW	C23-C24-C25-C26
3	A	1107	PGW	C23-C24-C25-C26
3	A	1112	PGW	C2-C3-C4-C5
3	B	812	PGW	C24-C25-C26-C27
3	A	1101	PGW	C2-C3-C4-C5
3	A	1102	PGW	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
3	A	1107	PGW	C2-C3-C4-C5
3	B	805	PGW	O02-C1-O01-C02
3	A	1108	PGW	O02-C1-O01-C02
3	B	812	PGW	C16-C15-C27-C26
3	A	1102	PGW	C16-C15-C27-C26
3	B	810	PGW	C22-C23-C24-C25
3	A	1113	PGW	C22-C23-C24-C25
3	A	1101	PGW	C16-C15-C27-C26
3	A	1107	PGW	C16-C15-C27-C26
3	B	809	PGW	C20-C21-C22-C23
3	A	1112	PGW	C20-C21-C22-C23
3	B	803	PGW	C23-C24-C25-C26
3	B	805	PGW	C22-C23-C24-C25
3	B	808	PGW	C21-C22-C23-C24
3	A	1101	PGW	C21-C22-C23-C24
3	A	1105	PGW	C23-C24-C25-C26
3	A	1107	PGW	C21-C22-C23-C24
3	A	1108	PGW	C22-C23-C24-C25
3	A	1111	PGW	C21-C22-C23-C24
3	A	1102	PGW	C25-C26-C27-C15
3	B	812	PGW	C5-C6-C7-C8
3	B	812	PGW	C22-C23-C24-C25
3	B	812	PGW	C25-C26-C27-C15
3	A	1102	PGW	C5-C6-C7-C8
3	A	1102	PGW	C22-C23-C24-C25
3	B	803	PGW	C24-C25-C26-C27
3	B	810	PGW	C23-C24-C25-C26
3	A	1105	PGW	C24-C25-C26-C27
3	A	1113	PGW	C23-C24-C25-C26
3	B	809	PGW	C1-C2-C3-C4
3	A	1112	PGW	C1-C2-C3-C4
3	B	807	PGW	C3-C4-C5-C6
3	A	1110	PGW	C3-C4-C5-C6
3	A	1114	PGW	O02-C1-O01-C02
3	B	809	PGW	C19-C20-C21-C22
3	B	811	PGW	C1-C2-C3-C4
3	A	1112	PGW	C19-C20-C21-C22
3	A	1114	PGW	C1-C2-C3-C4
3	B	810	PGW	C21-C22-C23-C24
3	A	1113	PGW	C21-C22-C23-C24
3	B	807	PGW	C2-C1-O01-C02
3	B	811	PGW	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
3	A	1110	PGW	C2-C1-O01-C02
3	A	1114	PGW	C2-C1-O01-C02
3	B	811	PGW	C7-C8-C9-C10
3	A	1114	PGW	C7-C8-C9-C10
3	B	811	PGW	O02-C1-O01-C02
3	B	803	PGW	C19-C20-C21-C22
3	A	1105	PGW	C19-C20-C21-C22
3	B	807	PGW	C4-C5-C6-C7
3	A	1110	PGW	C4-C5-C6-C7
3	B	810	PGW	O03-C01-C02-O01
3	A	1113	PGW	O03-C01-C02-O01
3	B	808	PGW	C20-C21-C22-C23
3	B	803	PGW	C6-C7-C8-C9
3	B	805	PGW	C6-C7-C8-C9
3	A	1105	PGW	C6-C7-C8-C9
3	A	1108	PGW	C6-C7-C8-C9
3	A	1111	PGW	C20-C21-C22-C23
3	B	806	PGW	C5-C6-C7-C8
3	A	1109	PGW	C5-C6-C7-C8
3	B	807	PGW	O02-C1-O01-C02
3	A	1110	PGW	O02-C1-O01-C02
3	A	1105	PGW	C16-C15-C27-C26
3	B	806	PGW	C02-C03-O11-P
3	A	1109	PGW	C02-C03-O11-P
3	B	803	PGW	C16-C15-C27-C26
3	B	804	PGW	C01-C02-C03-O11
3	A	1101	PGW	C01-C02-C03-O11
3	A	1106	PGW	C01-C02-C03-O11
3	A	1107	PGW	C01-C02-C03-O11
3	B	812	PGW	C23-C24-C25-C26
3	A	1102	PGW	C23-C24-C25-C26
3	B	808	PGW	O03-C01-C02-C03
3	A	1111	PGW	O03-C01-C02-C03
3	B	804	PGW	C20-C21-C22-C23
3	A	1106	PGW	C20-C21-C22-C23
3	B	804	PGW	C22-C23-C24-C25
3	A	1106	PGW	C22-C23-C24-C25
3	B	803	PGW	OAF-C05-CAD-OAE
3	A	1105	PGW	OAF-C05-CAD-OAE
3	B	805	PGW	C10-C06-C07-C08
3	A	1108	PGW	C10-C06-C07-C08
3	B	805	PGW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	A	1108	PGW	C21-C22-C23-C24
3	A	1111	PGW	C15-C16-C17-C18
3	B	804	PGW	C3-C4-C5-C6
3	B	808	PGW	C15-C16-C17-C18
3	A	1105	PGW	C18-C28-C30-C29
3	A	1106	PGW	C3-C4-C5-C6
3	B	803	PGW	C18-C28-C30-C29
3	B	808	PGW	C23-C24-C25-C26
3	B	809	PGW	C24-C25-C26-C27
3	A	1111	PGW	C23-C24-C25-C26
3	A	1112	PGW	C24-C25-C26-C27
3	B	808	PGW	C01-C02-C03-O11
3	A	1111	PGW	C01-C02-C03-O11
3	B	803	PGW	C22-C23-C24-C25
3	A	1105	PGW	C22-C23-C24-C25
3	B	803	PGW	O03-C01-C02-C03
3	B	810	PGW	O03-C01-C02-C03
3	A	1105	PGW	O03-C01-C02-C03
3	A	1113	PGW	O03-C01-C02-C03
3	B	808	PGW	O01-C02-C03-O11
3	B	809	PGW	O01-C02-C03-O11
3	A	1101	PGW	O01-C02-C03-O11
3	A	1107	PGW	O01-C02-C03-O11
3	A	1111	PGW	O01-C02-C03-O11
3	A	1112	PGW	O01-C02-C03-O11
3	B	810	PGW	C3-C4-C5-C6
3	A	1113	PGW	C3-C4-C5-C6
3	B	805	PGW	C15-C16-C17-C18
3	B	808	PGW	C16-C17-C18-C28
3	A	1111	PGW	C16-C17-C18-C28
3	A	1108	PGW	C15-C16-C17-C18
3	A	1114	PGW	C19-C20-C21-C22
3	B	809	PGW	C03-O11-P-O12
3	A	1112	PGW	C03-O11-P-O12
3	B	811	PGW	C19-C20-C21-C22
3	A	1110	PGW	C2-C3-C4-C5
3	B	807	PGW	C2-C3-C4-C5
3	B	808	PGW	C03-C02-O01-C1
3	A	1111	PGW	C03-C02-O01-C1
3	B	812	PGW	C21-C22-C23-C24
3	A	1102	PGW	C21-C22-C23-C24
3	A	1101	PGW	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	1107	PGW	C6-C7-C8-C9
3	B	807	PGW	O03-C01-C02-C03
3	B	808	PGW	C02-C03-O11-P
3	B	809	PGW	O03-C01-C02-C03
3	B	812	PGW	O03-C01-C02-C03
3	A	1102	PGW	O03-C01-C02-C03
3	A	1110	PGW	O03-C01-C02-C03
3	A	1111	PGW	C02-C03-O11-P
3	A	1112	PGW	O03-C01-C02-C03
3	B	807	PGW	O03-C01-C02-O01
3	B	809	PGW	O03-C01-C02-O01
3	A	1110	PGW	O03-C01-C02-O01
3	A	1112	PGW	O03-C01-C02-O01
3	B	806	PGW	C19-C20-C21-C22
3	A	1109	PGW	C19-C20-C21-C22
3	B	809	PGW	C22-C23-C24-C25
3	A	1112	PGW	C22-C23-C24-C25
3	B	812	PGW	C1-C2-C3-C4
3	A	1102	PGW	C1-C2-C3-C4
3	B	806	PGW	C06-C07-C08-C09
3	A	1109	PGW	C06-C07-C08-C09
3	B	812	PGW	C03-O11-P-O14
3	A	1102	PGW	C03-O11-P-O14
3	B	810	PGW	C01-C02-C03-O11
3	A	1113	PGW	C01-C02-C03-O11
3	B	811	PGW	C2-C3-C4-C5
3	A	1114	PGW	C2-C3-C4-C5
3	B	803	PGW	C20-C21-C22-C23
3	A	1105	PGW	C20-C21-C22-C23
3	B	806	PGW	C10-C06-C07-C08
3	B	811	PGW	C6-C7-C8-C9
3	A	1109	PGW	C10-C06-C07-C08
3	A	1114	PGW	C6-C7-C8-C9
3	B	810	PGW	O01-C02-C03-O11
3	A	1113	PGW	O01-C02-C03-O11
3	A	1101	PGW	O03-C19-C20-C21
3	A	1101	PGW	C22-C23-C24-C25
3	A	1107	PGW	C22-C23-C24-C25
3	A	1107	PGW	O03-C19-C20-C21
3	B	811	PGW	O03-C01-C02-C03
3	A	1114	PGW	O03-C01-C02-C03
3	B	808	PGW	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
3	B	811	PGW	O03-C01-C02-O01
3	A	1111	PGW	O03-C01-C02-O01
3	A	1114	PGW	O03-C01-C02-O01
3	A	1105	PGW	C15-C16-C17-C18
3	B	803	PGW	C15-C16-C17-C18
3	B	804	PGW	C19-C20-C21-C22
3	A	1106	PGW	C19-C20-C21-C22
3	B	811	PGW	C20-C21-C22-C23
3	A	1114	PGW	C20-C21-C22-C23
3	B	809	PGW	C01-C02-C03-O11
3	A	1112	PGW	C01-C02-C03-O11
3	A	1101	PGW	C3-C4-C5-C6
3	A	1107	PGW	C3-C4-C5-C6
3	B	804	PGW	O01-C02-C03-O11
3	B	806	PGW	O01-C02-C03-O11
3	A	1106	PGW	O01-C02-C03-O11
3	A	1109	PGW	O01-C02-C03-O11
3	B	812	PGW	O03-C01-C02-O01
3	A	1102	PGW	O03-C01-C02-O01
3	B	803	PGW	C04-O12-P-O11
3	B	807	PGW	C04-O12-P-O11
3	A	1105	PGW	C04-O12-P-O11
3	A	1110	PGW	C04-O12-P-O11
3	A	1105	PGW	C21-C22-C23-C24
3	B	803	PGW	C21-C22-C23-C24
3	B	805	PGW	C17-C18-C28-C30
3	A	1108	PGW	C17-C18-C28-C30
3	A	1109	PGW	C4-C5-C6-C7
3	B	806	PGW	C4-C5-C6-C7
3	A	1105	PGW	C2-C3-C4-C5
3	B	803	PGW	C2-C3-C4-C5
3	B	811	PGW	C02-C03-O11-P
3	A	1114	PGW	C02-C03-O11-P
3	B	803	PGW	O03-C19-C20-C21
3	A	1105	PGW	O03-C19-C20-C21
3	B	806	PGW	C2-C3-C4-C5
3	B	812	PGW	C03-O11-P-O12
3	A	1109	PGW	C2-C3-C4-C5
3	B	812	PGW	C15-C16-C17-C18
3	A	1102	PGW	C15-C16-C17-C18
3	B	807	PGW	C02-C01-O03-C19
3	A	1110	PGW	C02-C01-O03-C19

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Mol	Chain	Res	Type	Atoms
3	B	812	PGW	O01-C02-C03-O11
3	A	1102	PGW	O01-C02-C03-O11
3	B	805	PGW	C4-C5-C6-C7
3	A	1108	PGW	C4-C5-C6-C7
3	B	805	PGW	C7-C8-C9-C10
3	A	1108	PGW	C7-C8-C9-C10
3	B	804	PGW	C03-O11-P-O13
3	A	1106	PGW	C03-O11-P-O13
3	A	1102	PGW	C03-O11-P-O12
3	B	803	PGW	C5-C6-C7-C8
3	A	1105	PGW	C5-C6-C7-C8
3	B	808	PGW	C22-C23-C24-C25
3	A	1111	PGW	C22-C23-C24-C25
3	B	811	PGW	O01-C1-C2-C3
3	A	1114	PGW	O01-C1-C2-C3
3	B	806	PGW	C01-C02-C03-O11
3	A	1109	PGW	C01-C02-C03-O11
3	B	812	PGW	C7-C8-C9-C10
3	A	1102	PGW	C7-C8-C9-C10
3	B	810	PGW	O01-C1-C2-C3
3	A	1113	PGW	O01-C1-C2-C3
3	A	1101	PGW	C4-C5-C6-C7
3	A	1107	PGW	C4-C5-C6-C7
3	B	811	PGW	C3-C4-C5-C6
3	A	1114	PGW	C3-C4-C5-C6
3	A	1114	PGW	O02-C1-C2-C3
3	B	811	PGW	O02-C1-C2-C3
3	B	803	PGW	C03-O11-P-O14
3	B	807	PGW	C03-O11-P-O14
3	B	807	PGW	C04-O12-P-O14
3	B	812	PGW	C04-O12-P-O14
3	A	1102	PGW	C04-O12-P-O14
3	A	1105	PGW	C03-O11-P-O14
3	A	1110	PGW	C03-O11-P-O14
3	A	1110	PGW	C04-O12-P-O14
3	A	1105	PGW	C1-C2-C3-C4
3	B	803	PGW	C1-C2-C3-C4
3	B	806	PGW	C07-C06-C10-C9
3	A	1109	PGW	C07-C06-C10-C9
3	B	811	PGW	O03-C19-C20-C21
3	A	1114	PGW	O03-C19-C20-C21
3	B	812	PGW	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
3	A	1102	PGW	O03-C19-C20-C21
3	B	810	PGW	O02-C1-C2-C3
3	A	1113	PGW	O02-C1-C2-C3
3	A	1114	PGW	O04-C19-C20-C21
3	B	809	PGW	O03-C19-C20-C21
3	A	1112	PGW	O03-C19-C20-C21
3	B	811	PGW	O04-C19-C20-C21

There are no ring outliers.

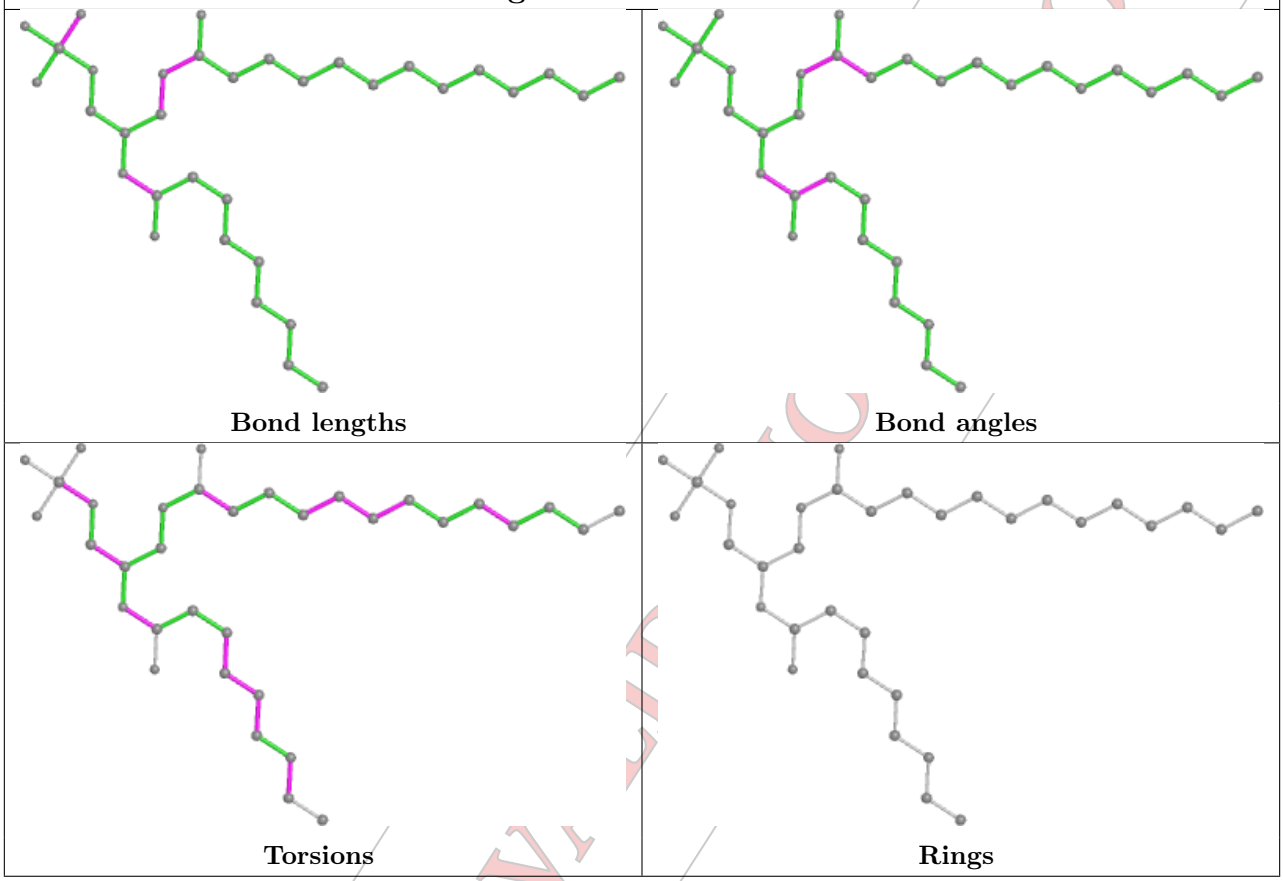
19 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1107	PGW	7	0
3	A	1101	PGW	7	0
3	B	808	PGW	3	0
3	A	1109	PGW	1	0
3	A	1113	PGW	1	0
3	B	806	PGW	1	0
3	A	1105	PGW	6	0
3	A	1102	PGW	5	0
3	A	1114	PGW	1	0
3	B	809	PGW	2	0
3	B	805	PGW	5	0
3	B	811	PGW	1	0
3	B	803	PGW	7	0
3	B	807	PGW	4	0
3	B	812	PGW	5	0
3	A	1111	PGW	3	0
3	A	1108	PGW	6	0
3	A	1112	PGW	2	0
3	A	1110	PGW	4	0

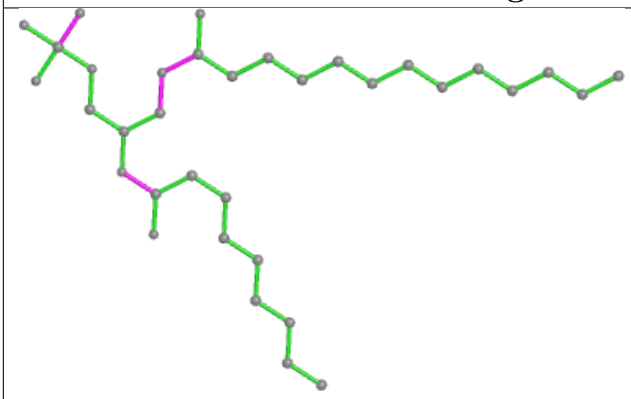
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

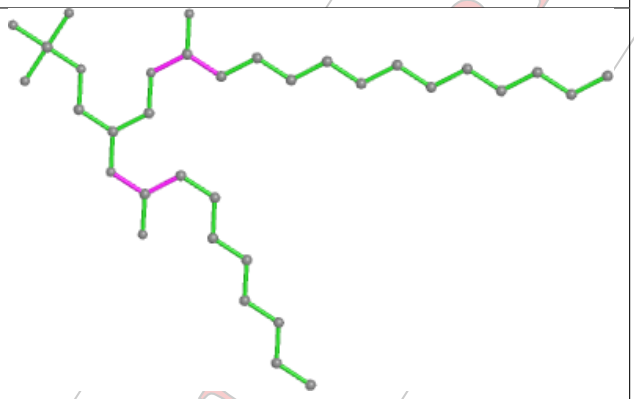
Ligand PGW A 1107



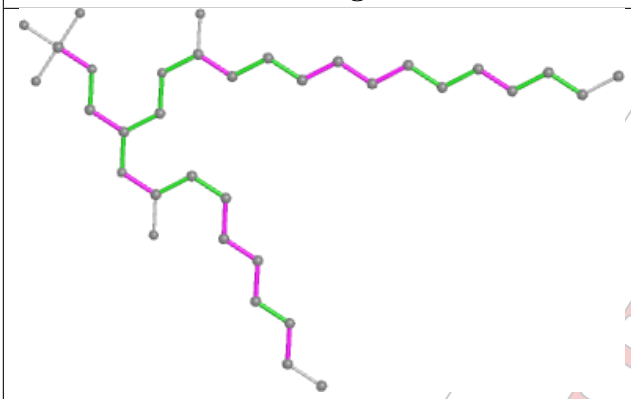
Ligand PGW A 1101



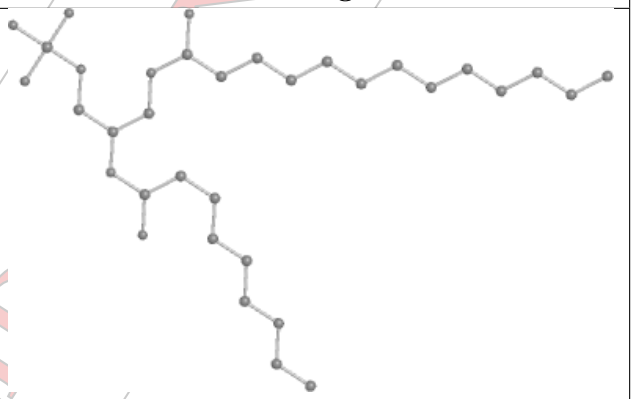
Bond lengths



Bond angles

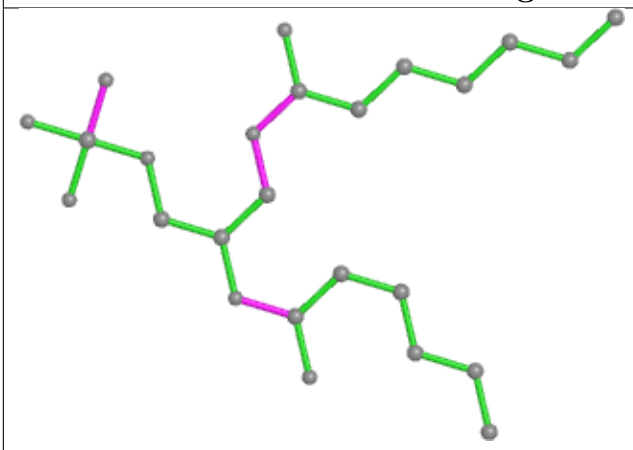


Torsions

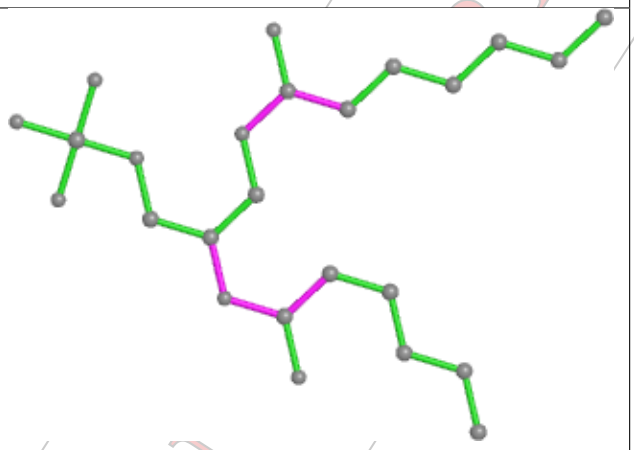


Rings

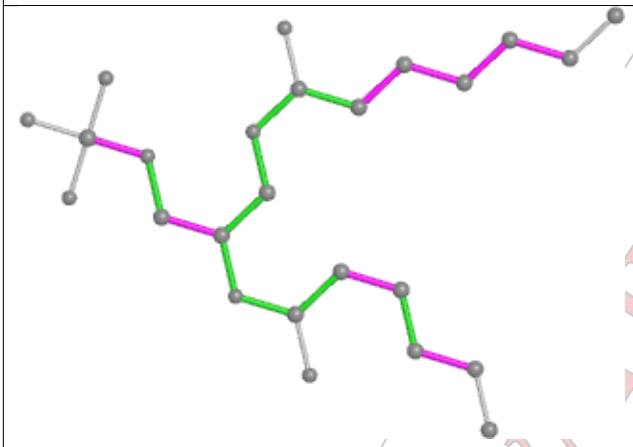
Ligand PGW B 804



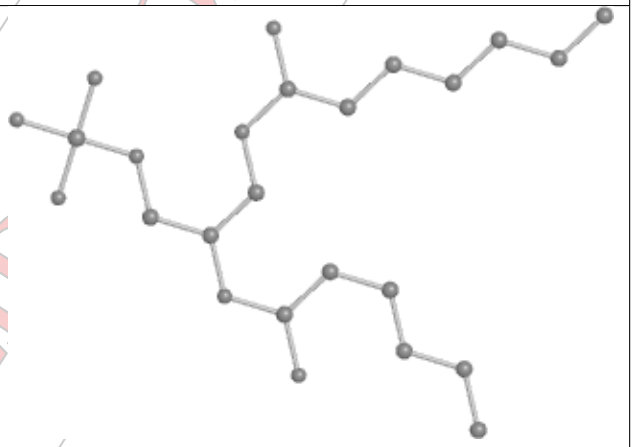
Bond lengths



Bond angles

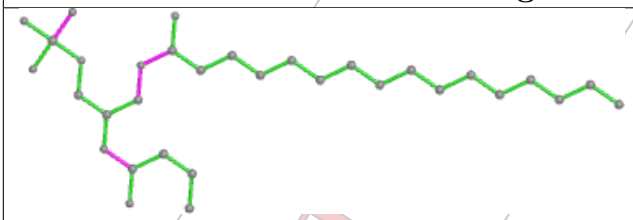


Torsions

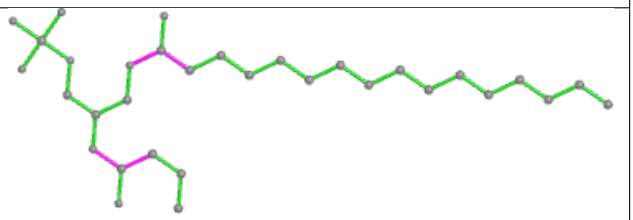


Rings

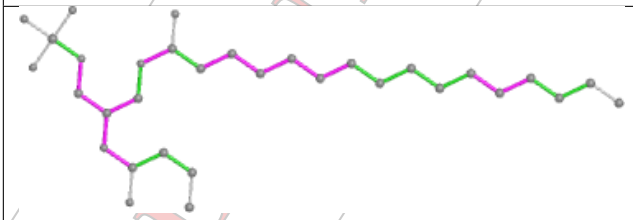
Ligand PGW B 808



Bond lengths



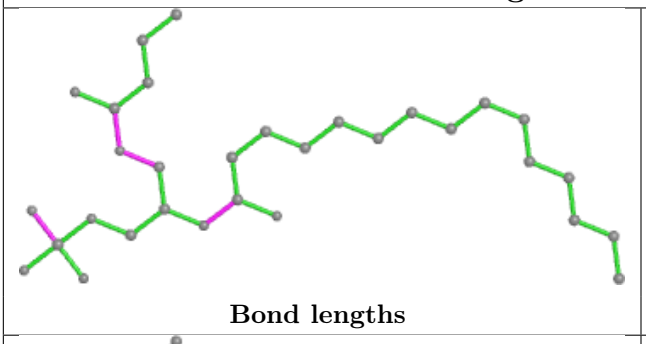
Bond angles



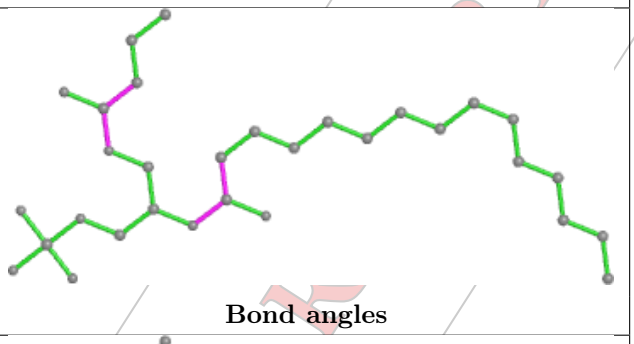
Torsions

Rings

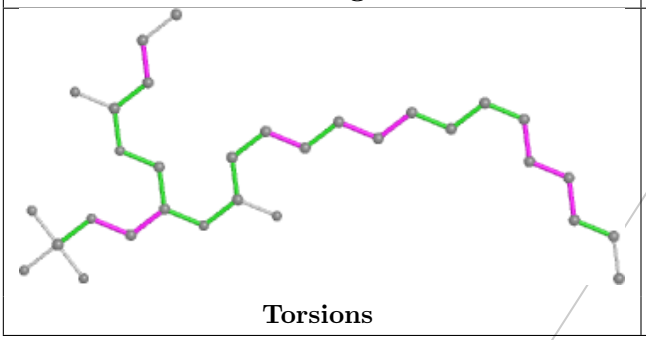
Ligand PGW A 1109



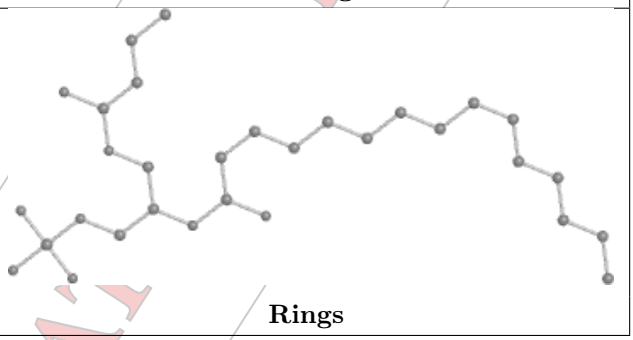
Bond lengths



Bond angles

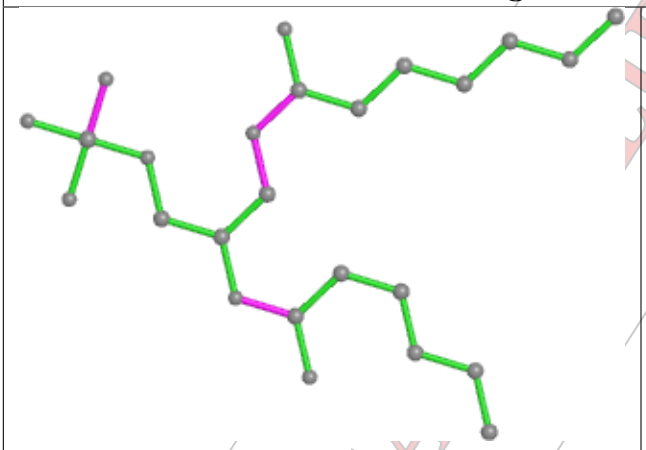


Torsions

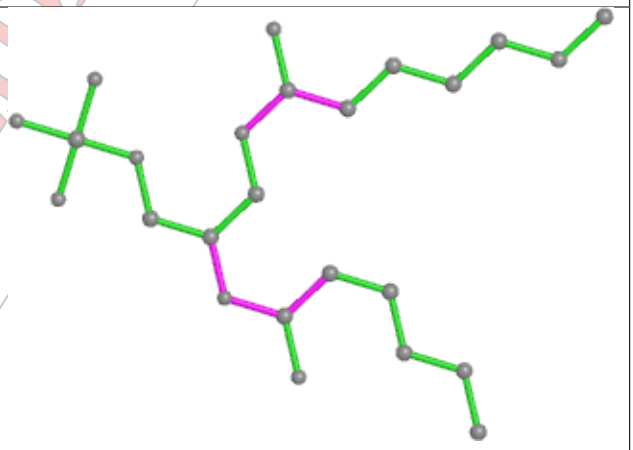


Rings

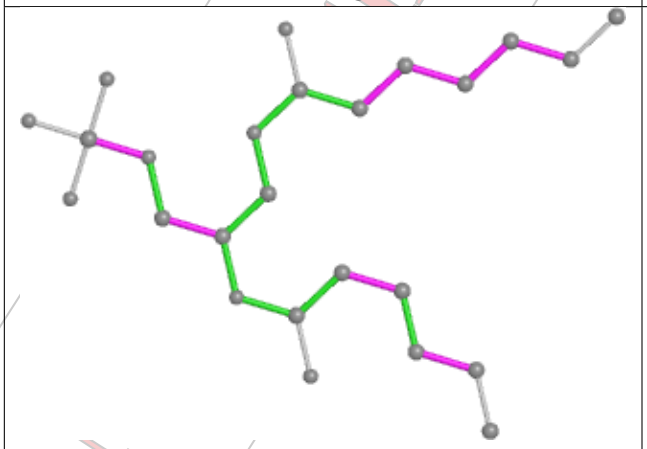
Ligand PGW A 1106



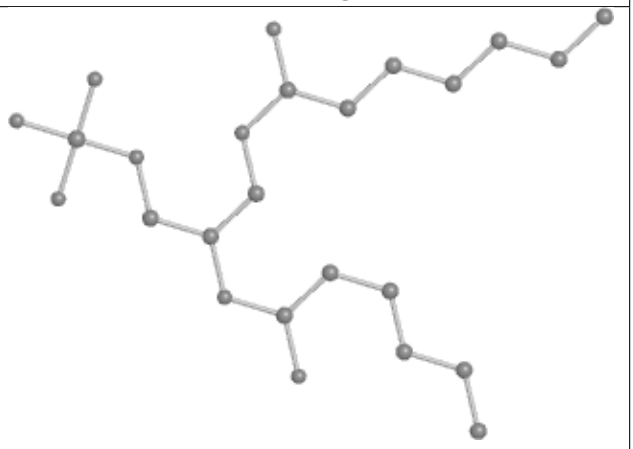
Bond lengths



Bond angles

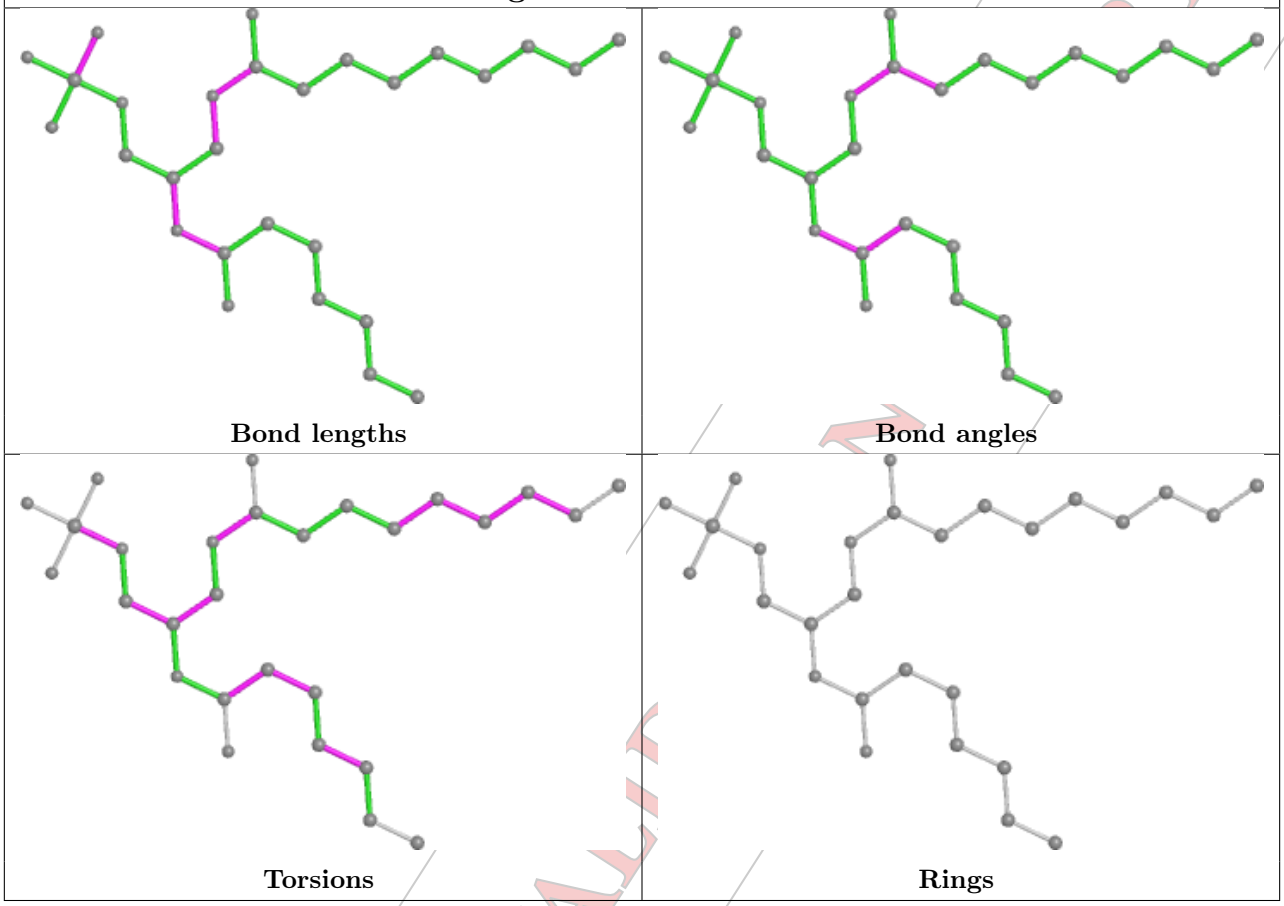


Torsions

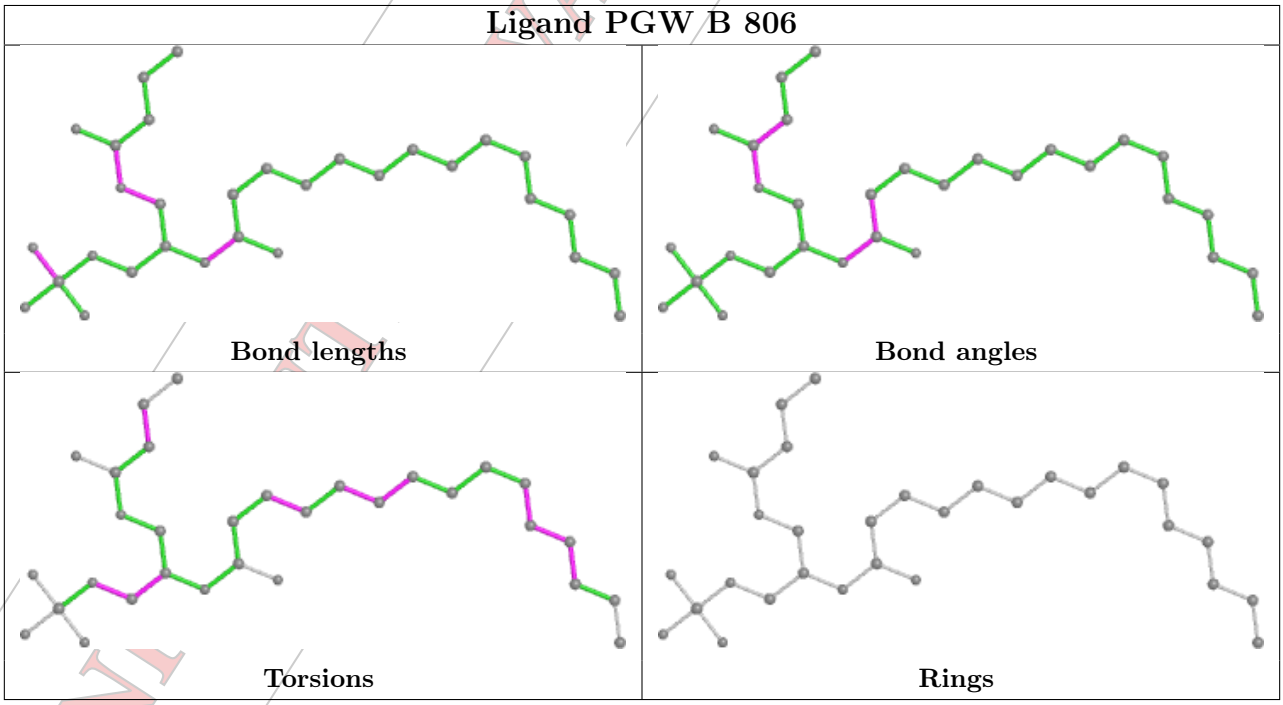


Rings

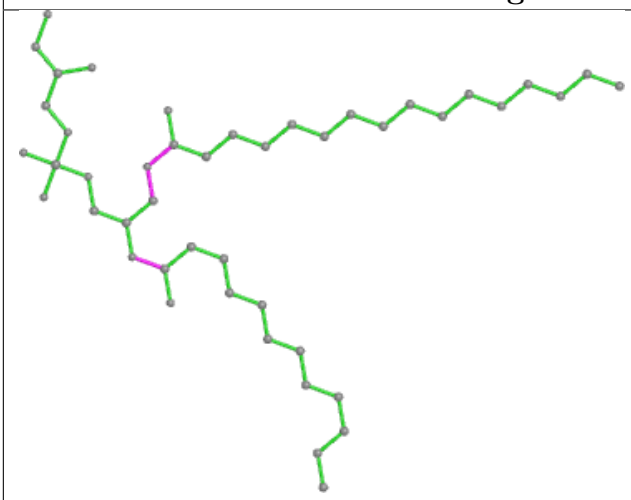
Ligand PGW A 1113



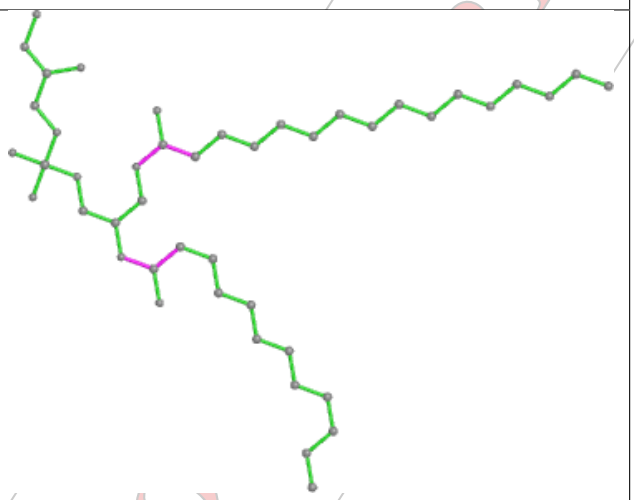
Ligand PGW B 806



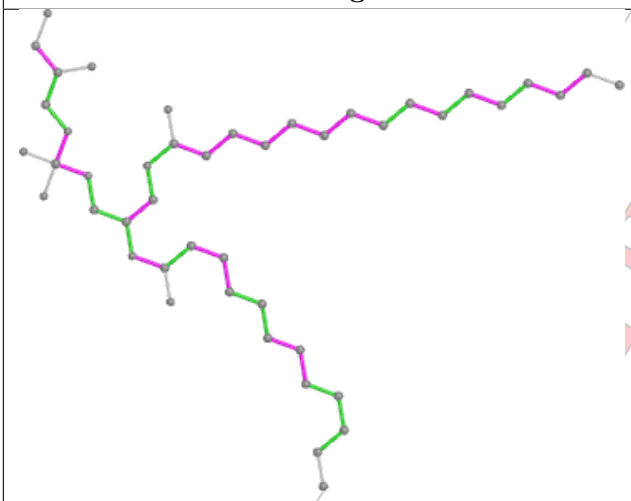
Ligand PGW A 1105



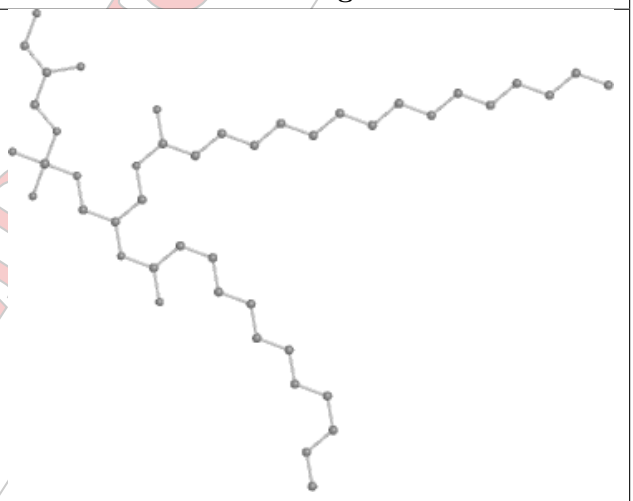
Bond lengths



Bond angles

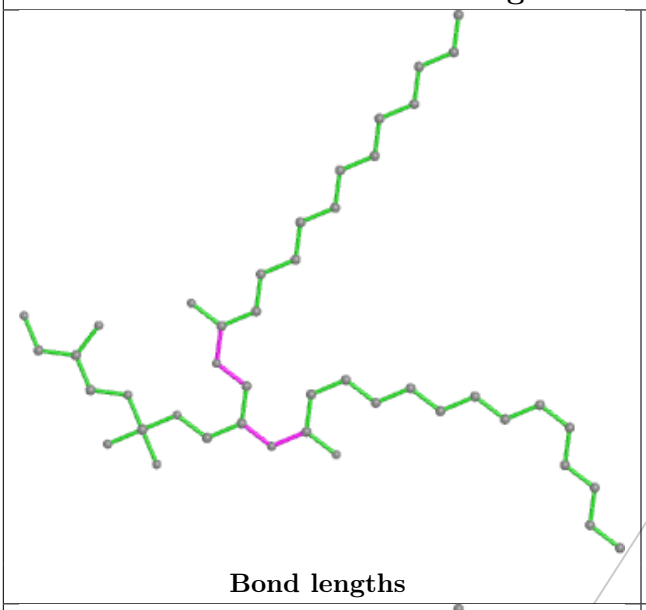


Torsions

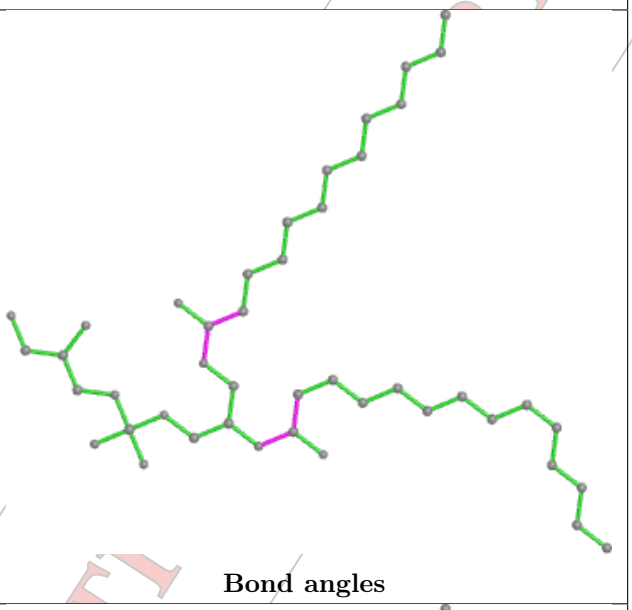


Rings

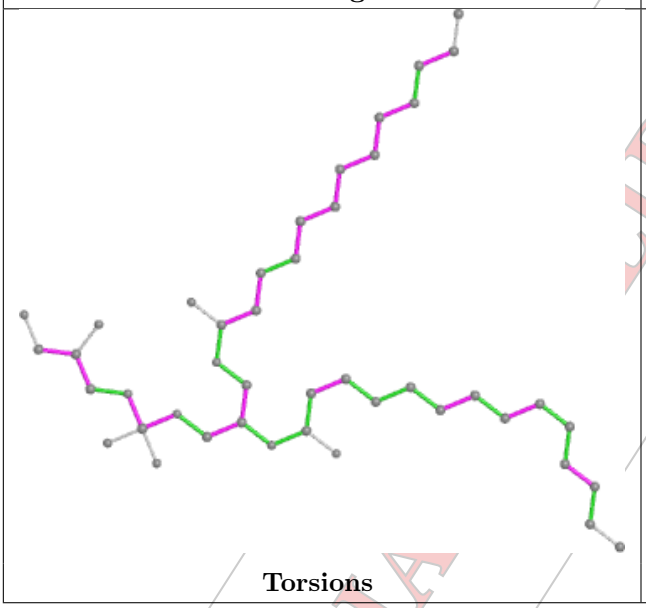
Ligand PGW A 1102



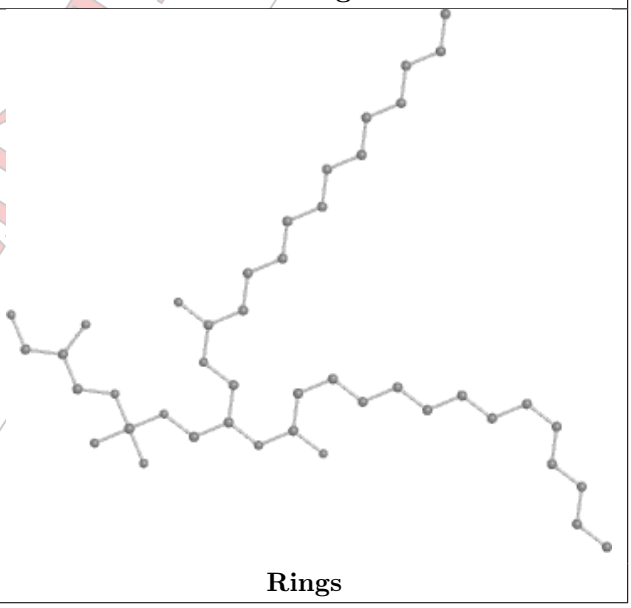
Bond lengths



Bond angles

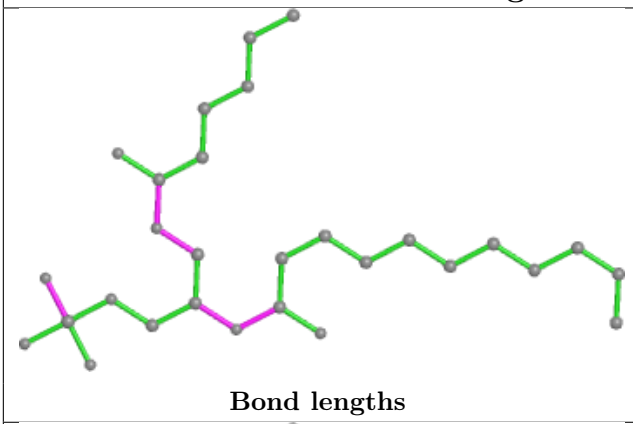


Torsions

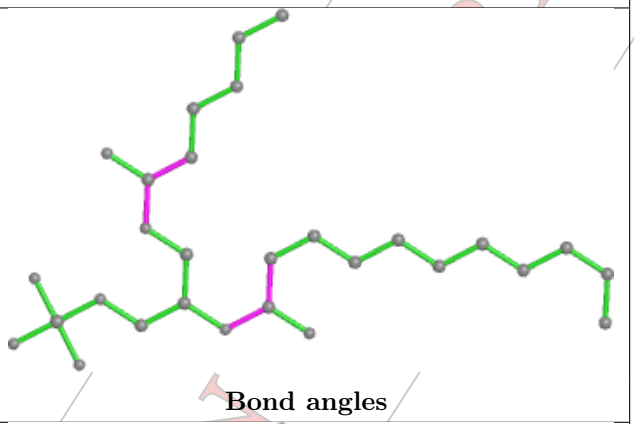


Rings

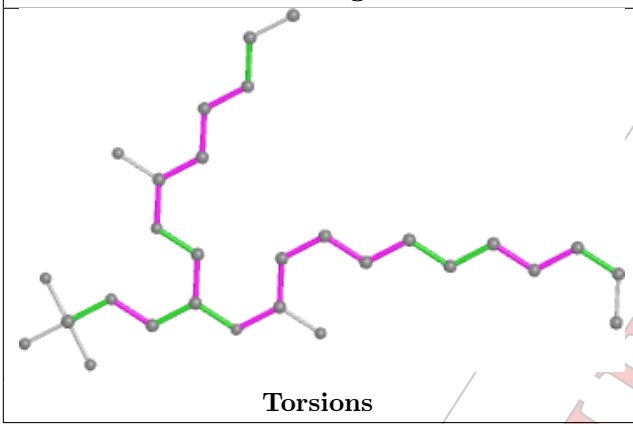
Ligand PGW A 1114



Bond lengths



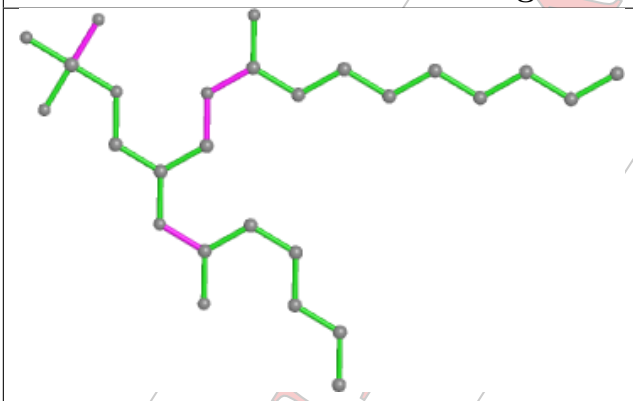
Bond angles



Torsions

Rings

Ligand PGW B 809



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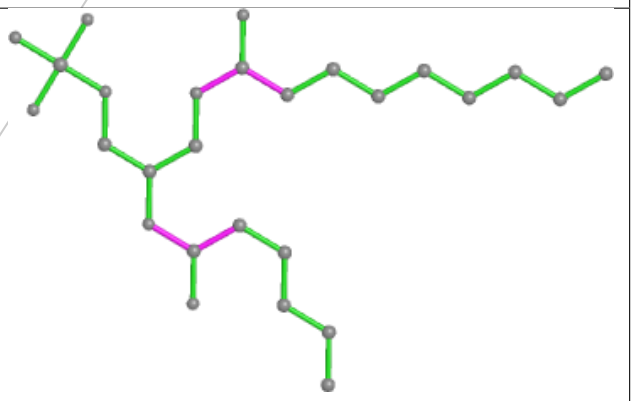
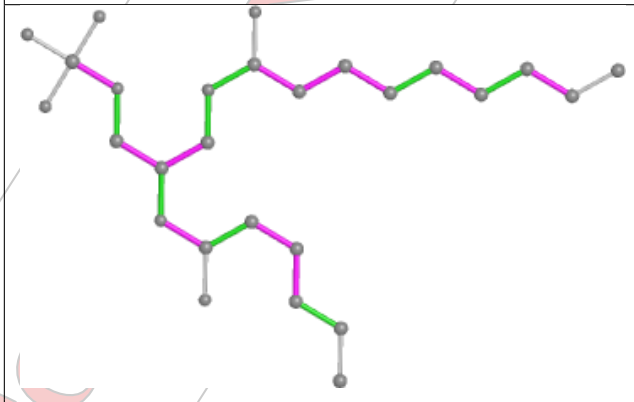
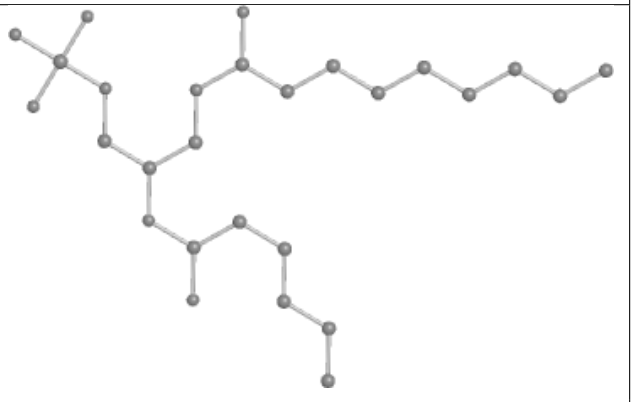


Bond angles

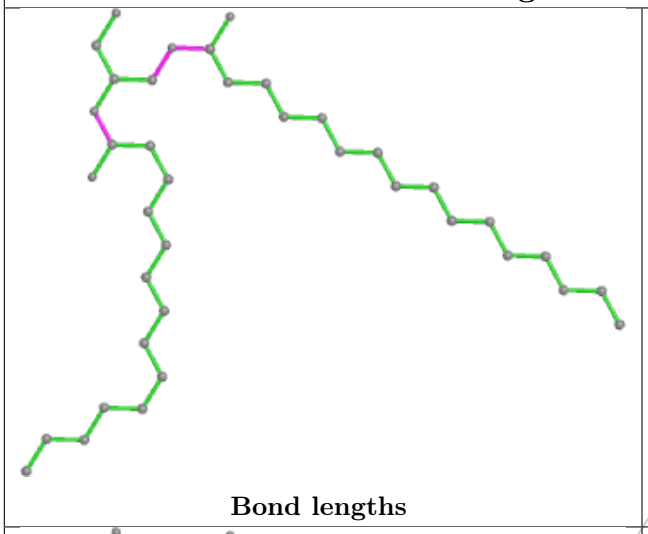


Torsions

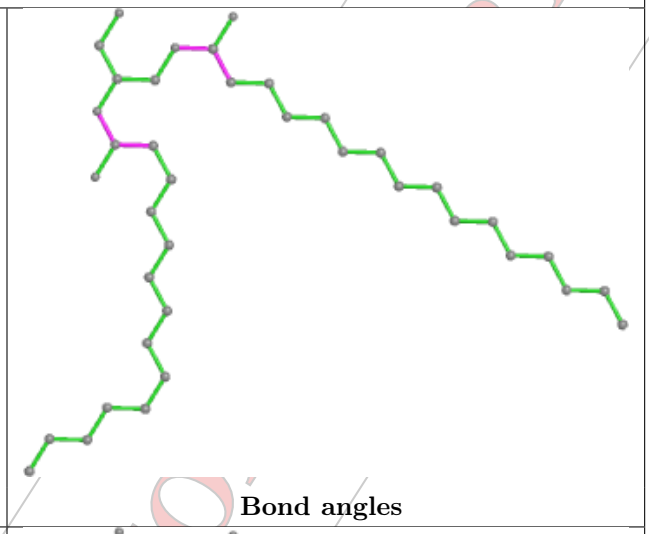


Rings

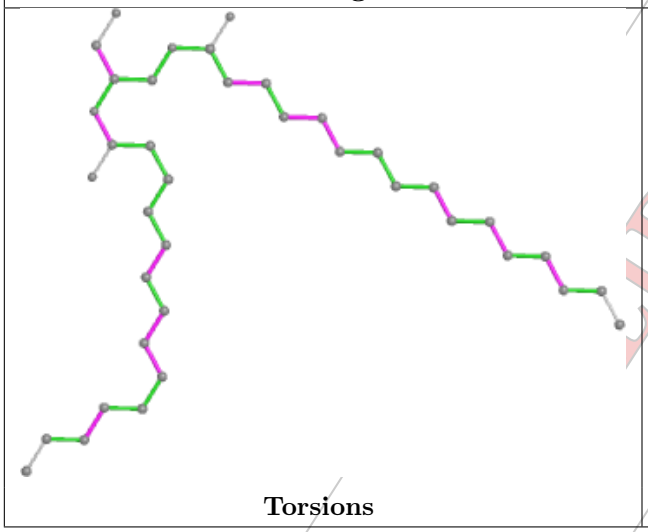
Ligand PGW B 805



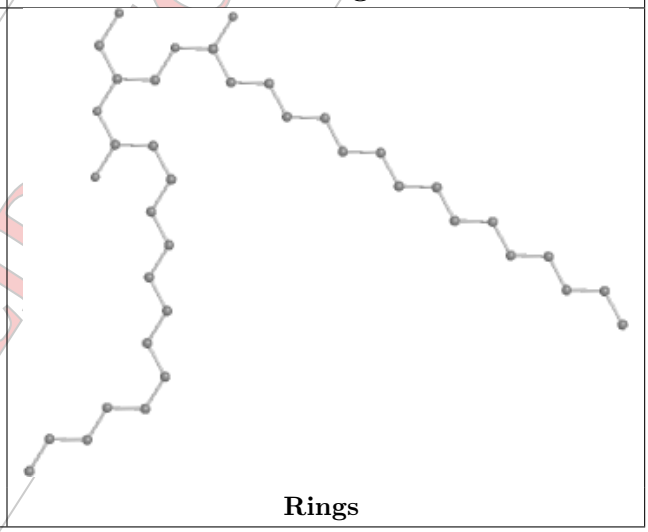
Bond lengths



Bond angles

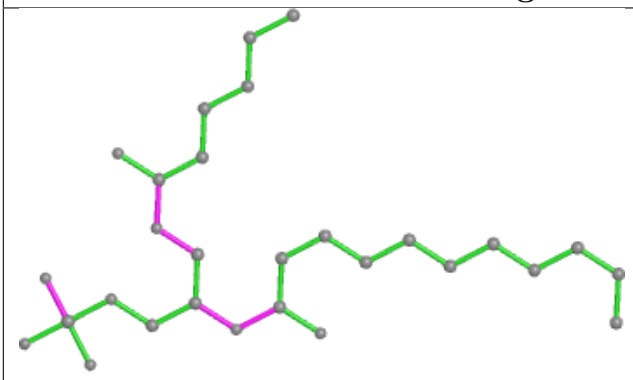


Torsions

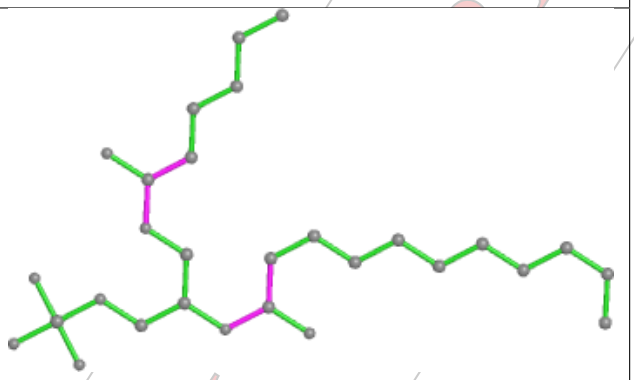


Rings

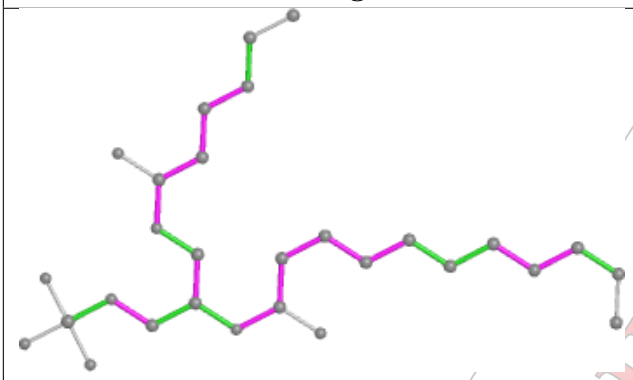
Ligand PGW B 811



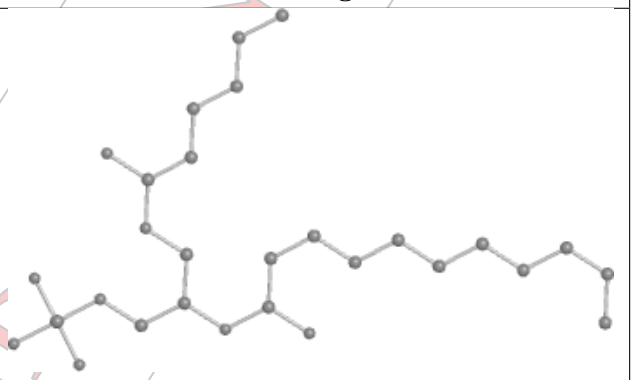
Bond lengths



Bond angles

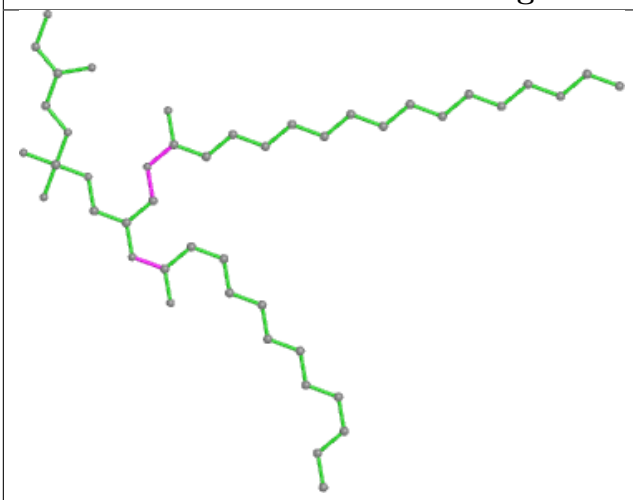


Torsions

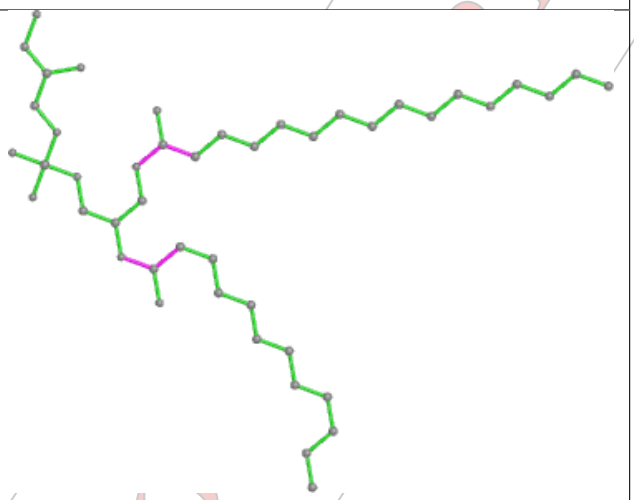


Rings

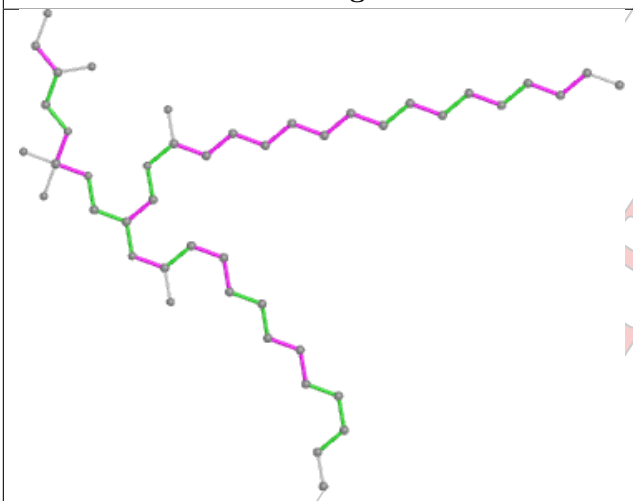
Ligand PGW B 803



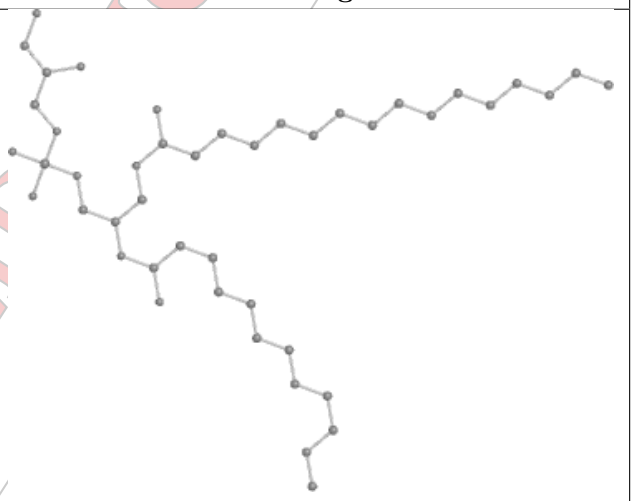
Bond lengths



Bond angles

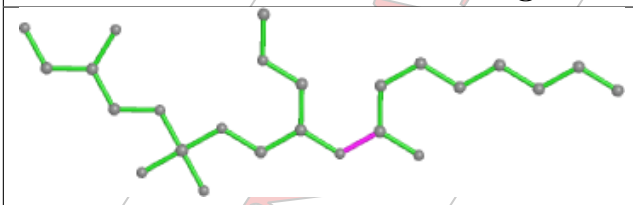


Torsions

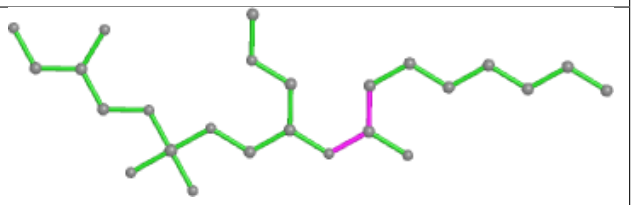


Rings

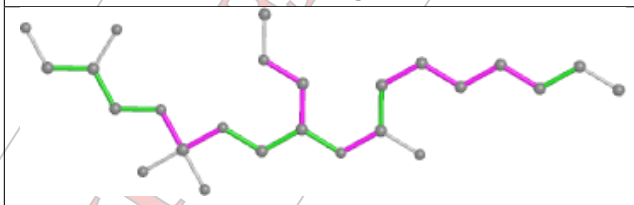
Ligand PGW B 807



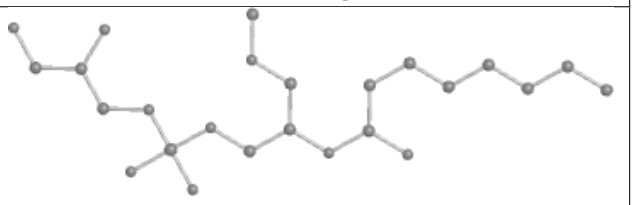
Bond lengths



Bond angles

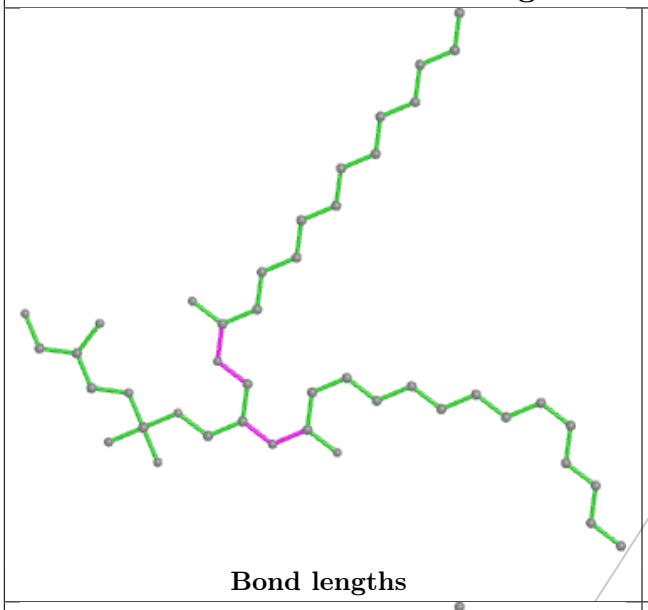


Torsions

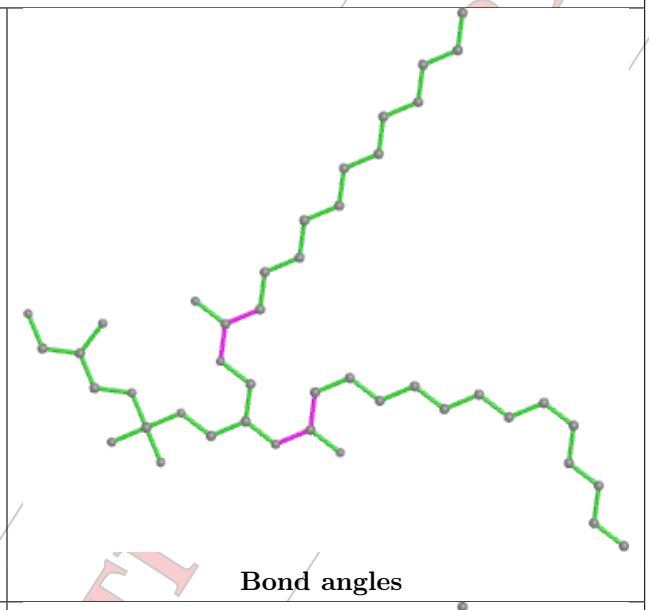


Rings

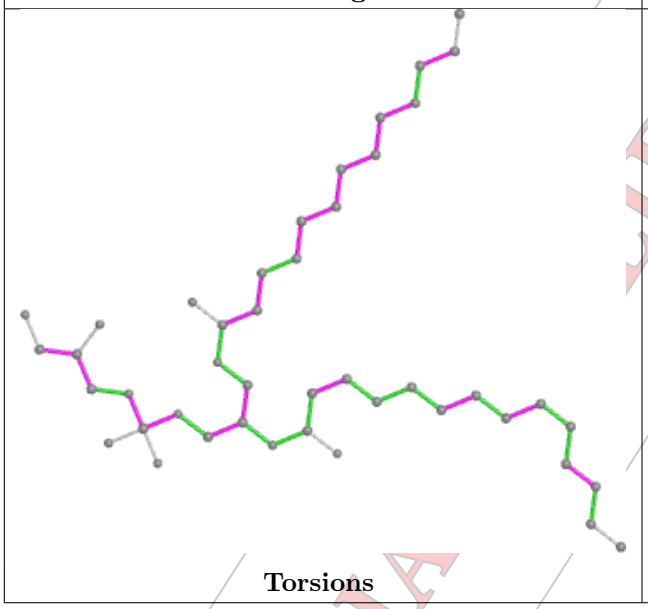
Ligand PGW B 812



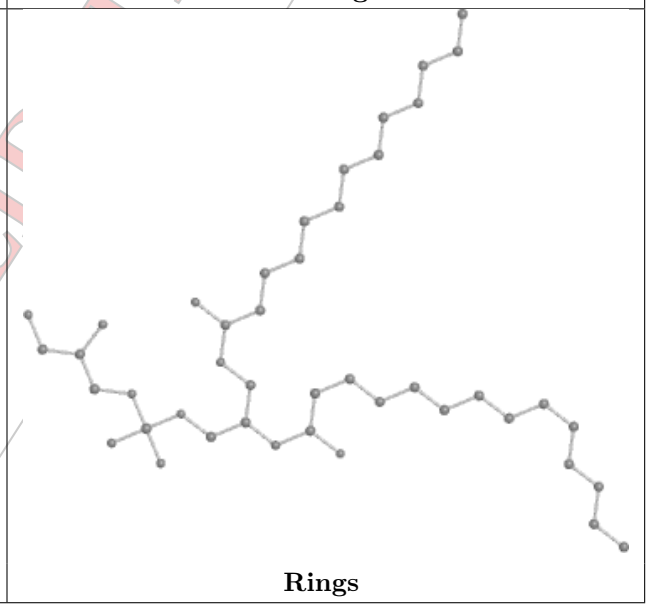
Bond lengths



Bond angles

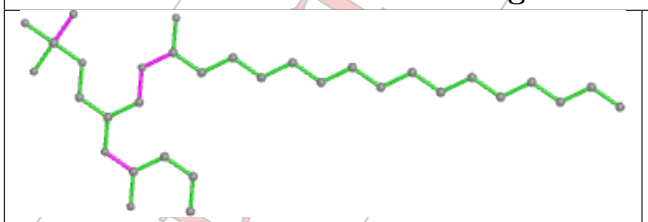


Torsions

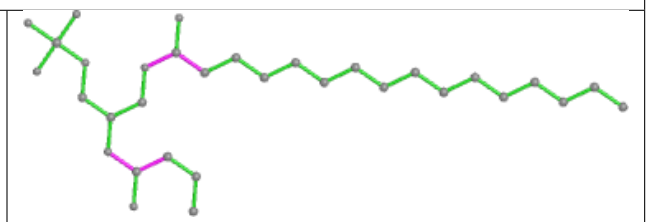


Rings

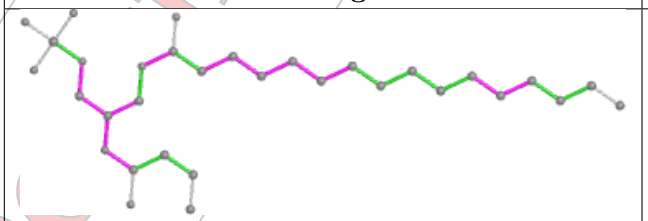
Ligand PGW A 1111



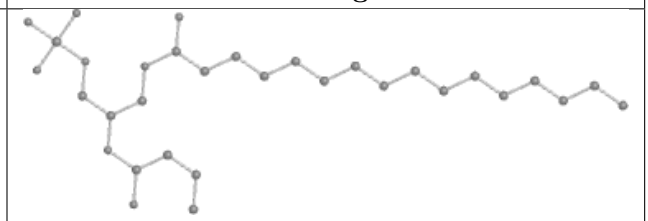
Bond lengths



Bond angles

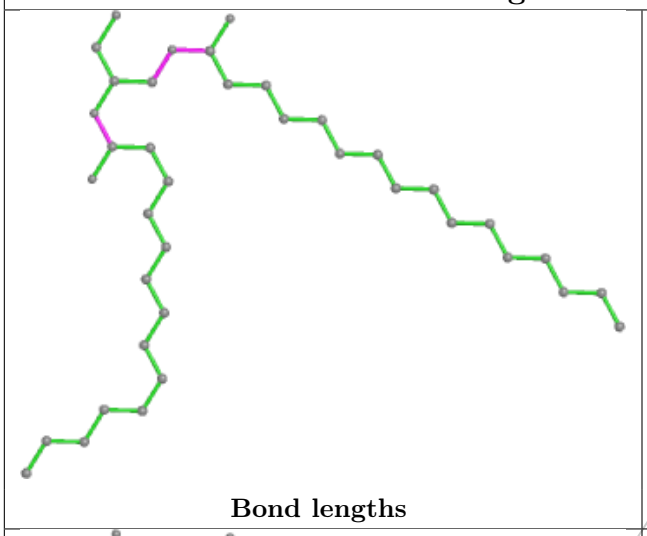


Torsions

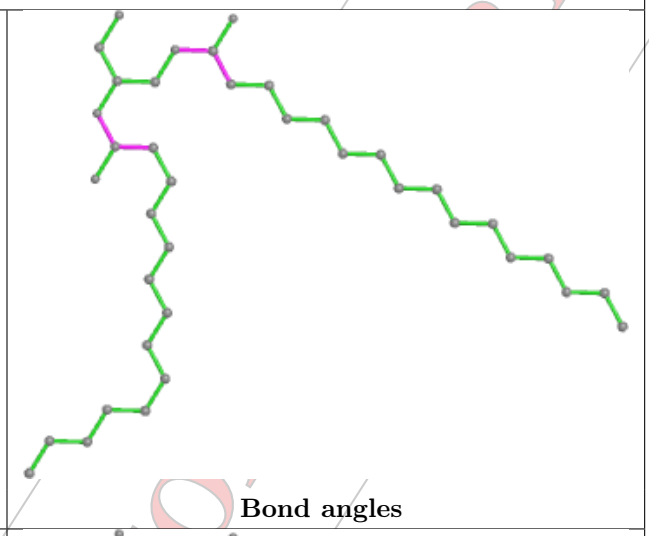


Rings

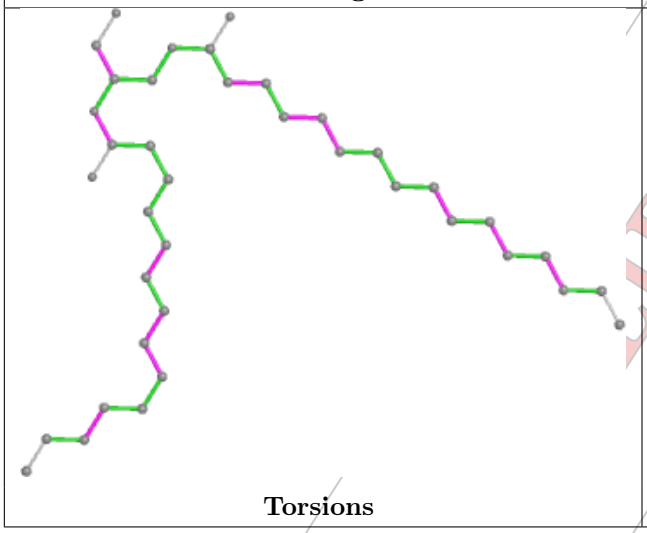
Ligand PGW A 1108



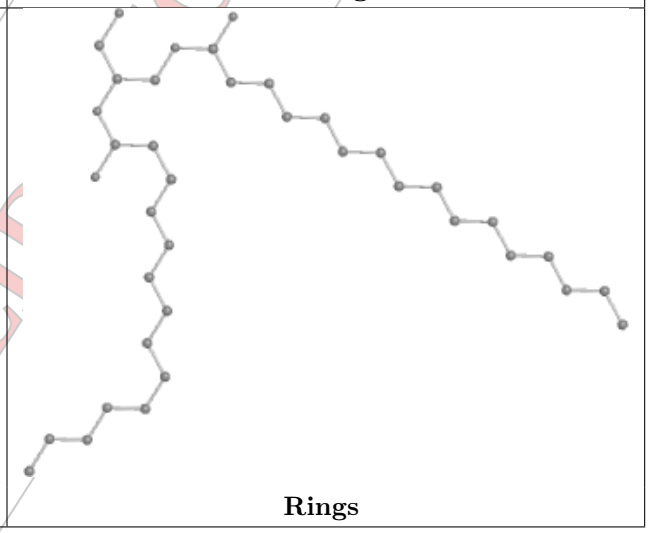
Bond lengths



Bond angles

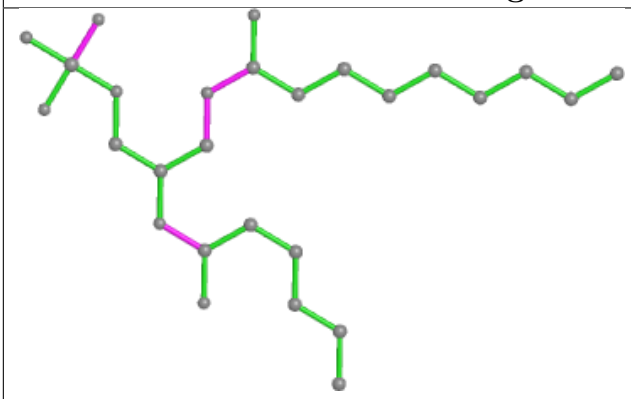


Torsions

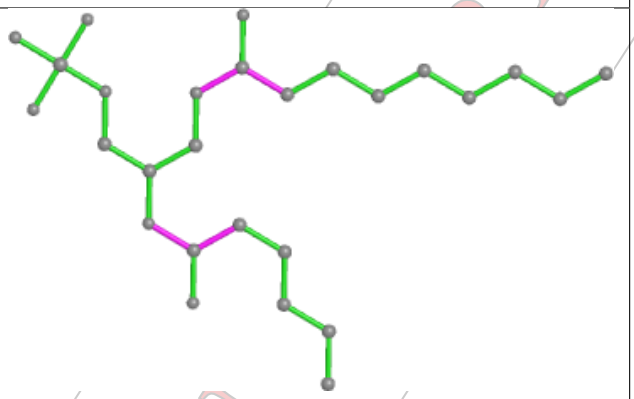


Rings

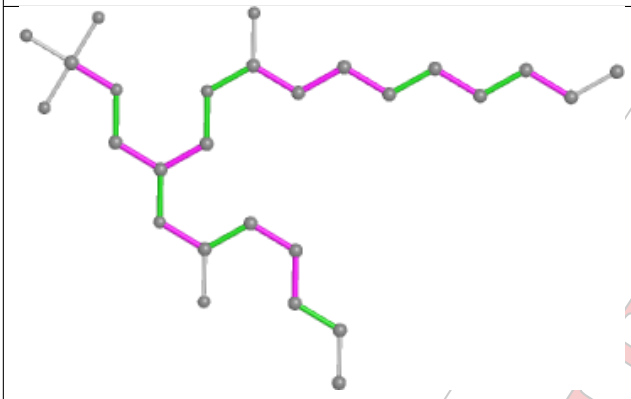
Ligand PGW A 1112



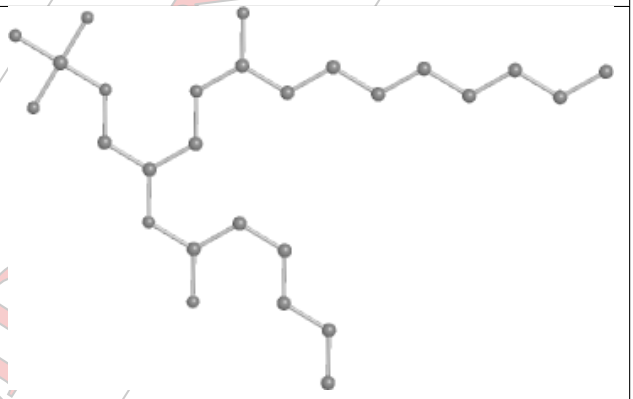
Bond lengths



Bond angles

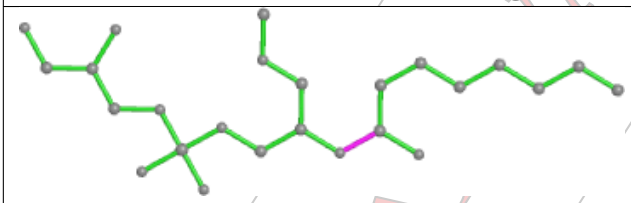


Torsions

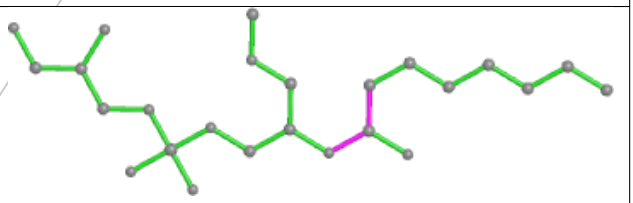


Rings

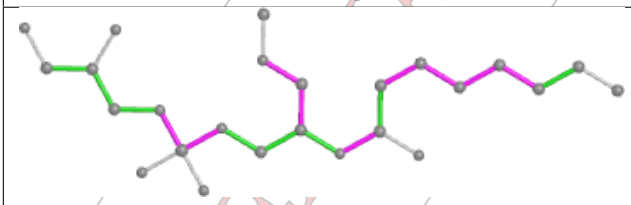
Ligand PGW A 1110



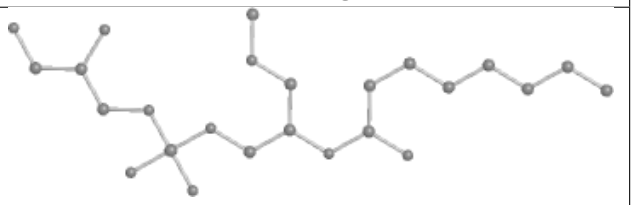
Bond lengths



Bond angles

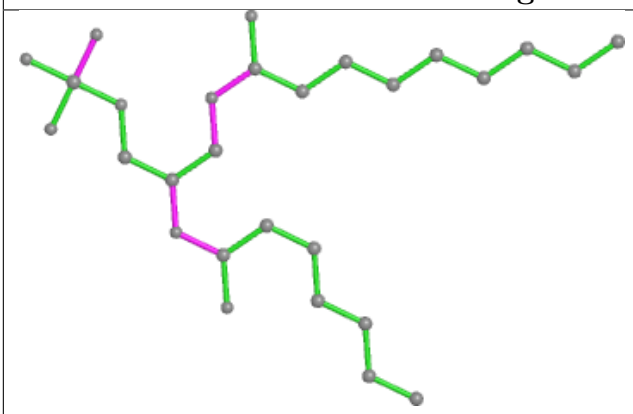


Torsions

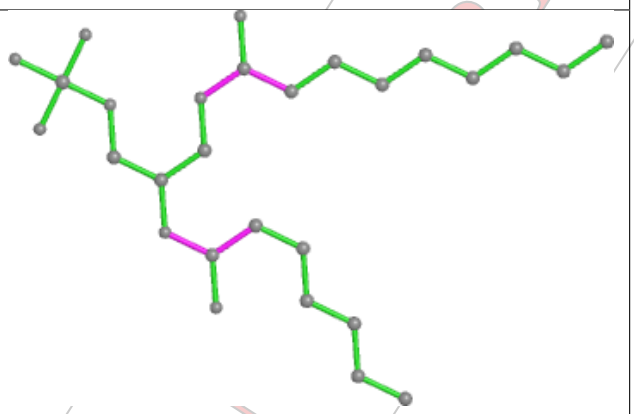


Rings

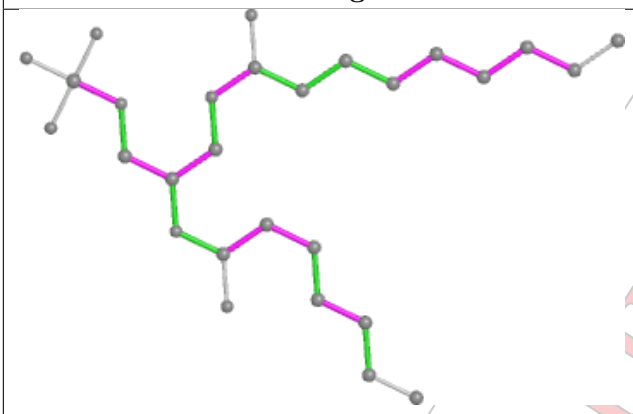
Ligand PGW B 810



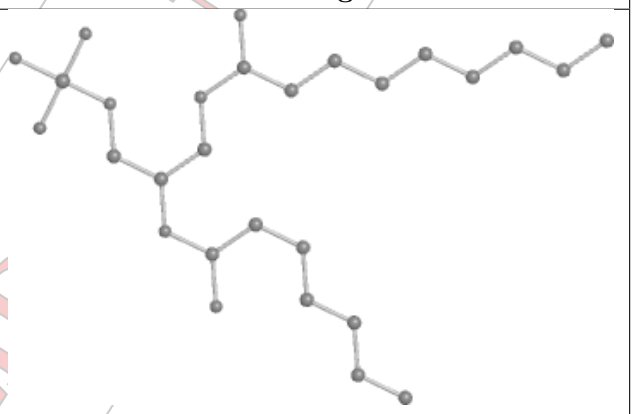
Bond lengths



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.

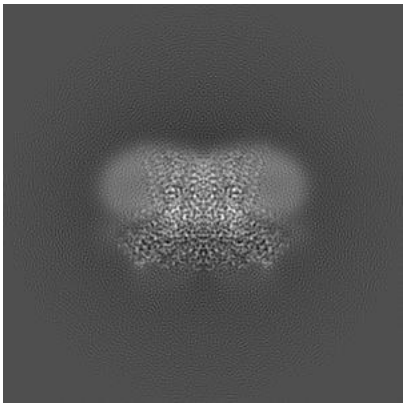
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24730. These allow visual inspection of the internal detail of the map and identification of artifacts.

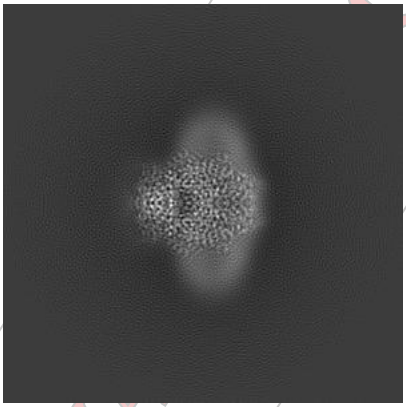
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

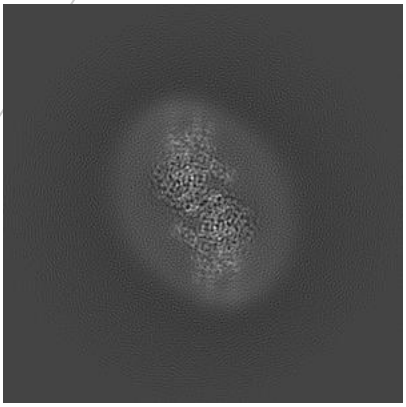
6.1.1 Primary map



X



Y

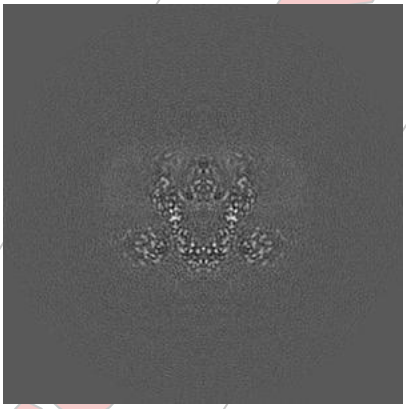


Z

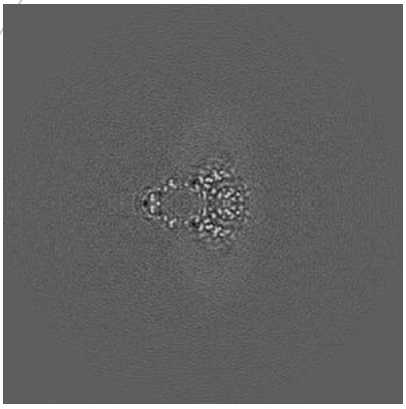
The images above show the map projected in three orthogonal directions.

6.2 Central slices

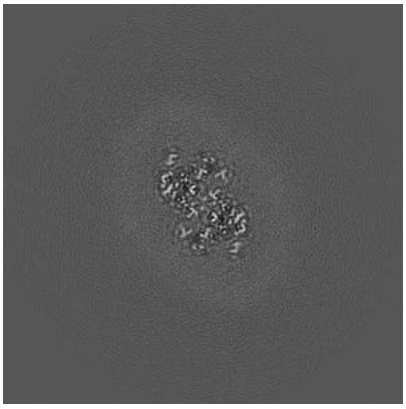
6.2.1 Primary map



X Index: 192



Y Index: 192

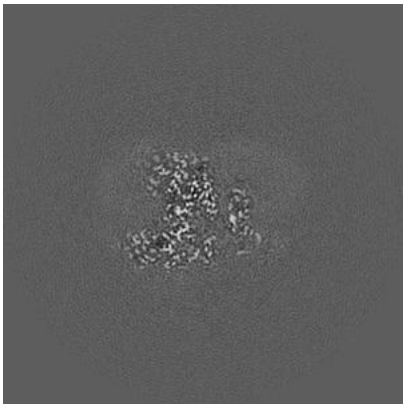


Z Index: 192

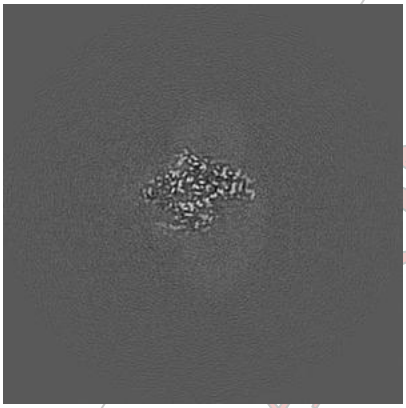
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

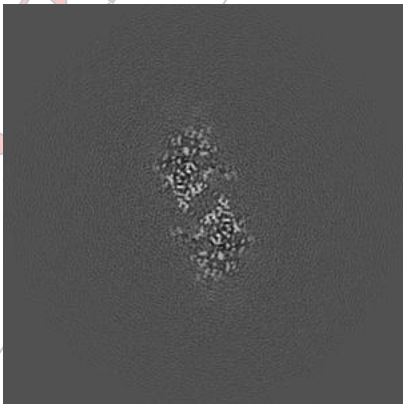
6.3.1 Primary map



X Index: 203



Y Index: 165



Z Index: 161

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 0.0169. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

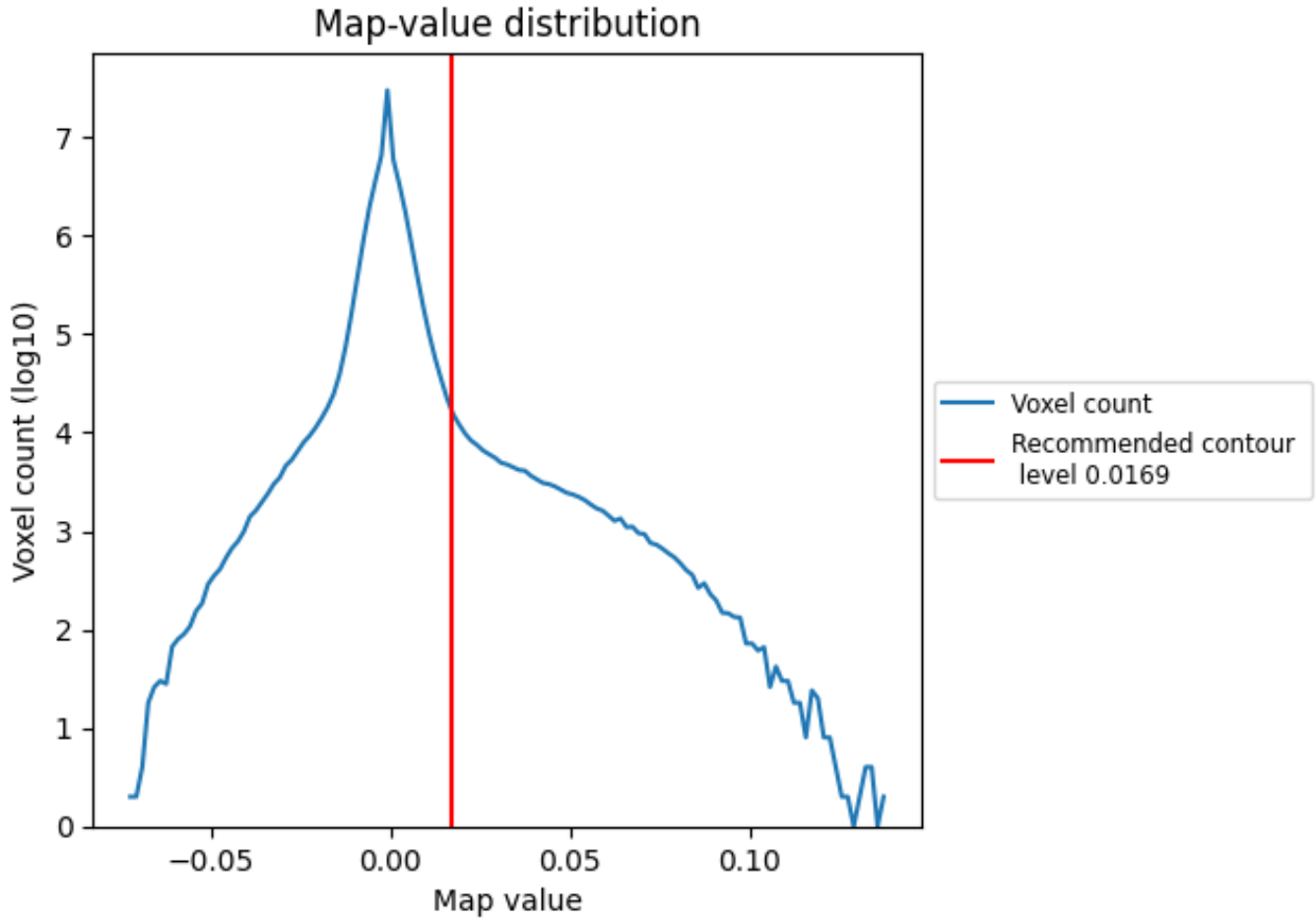
6.5 Mask visualisation (i)

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

7 Map analysis

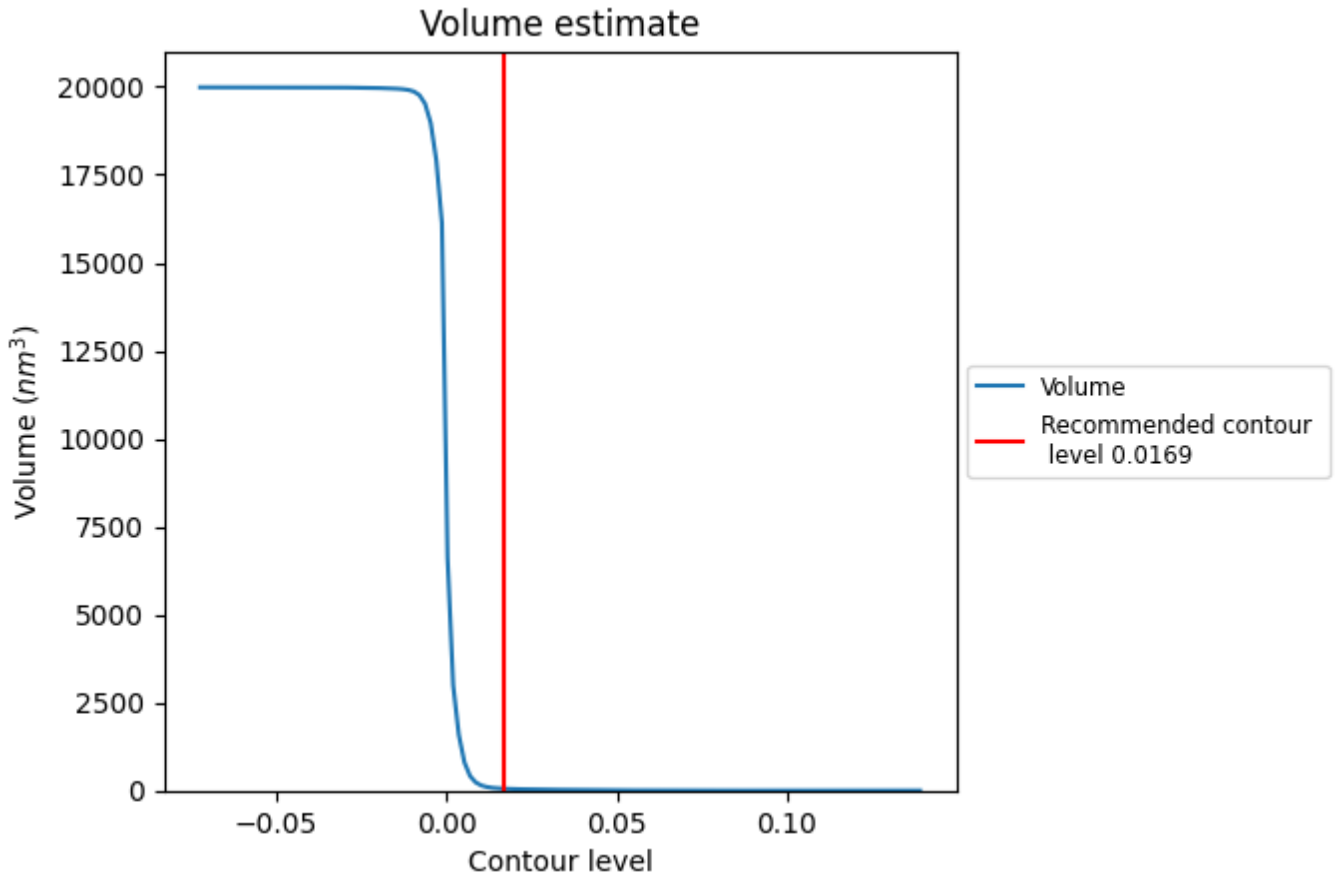
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

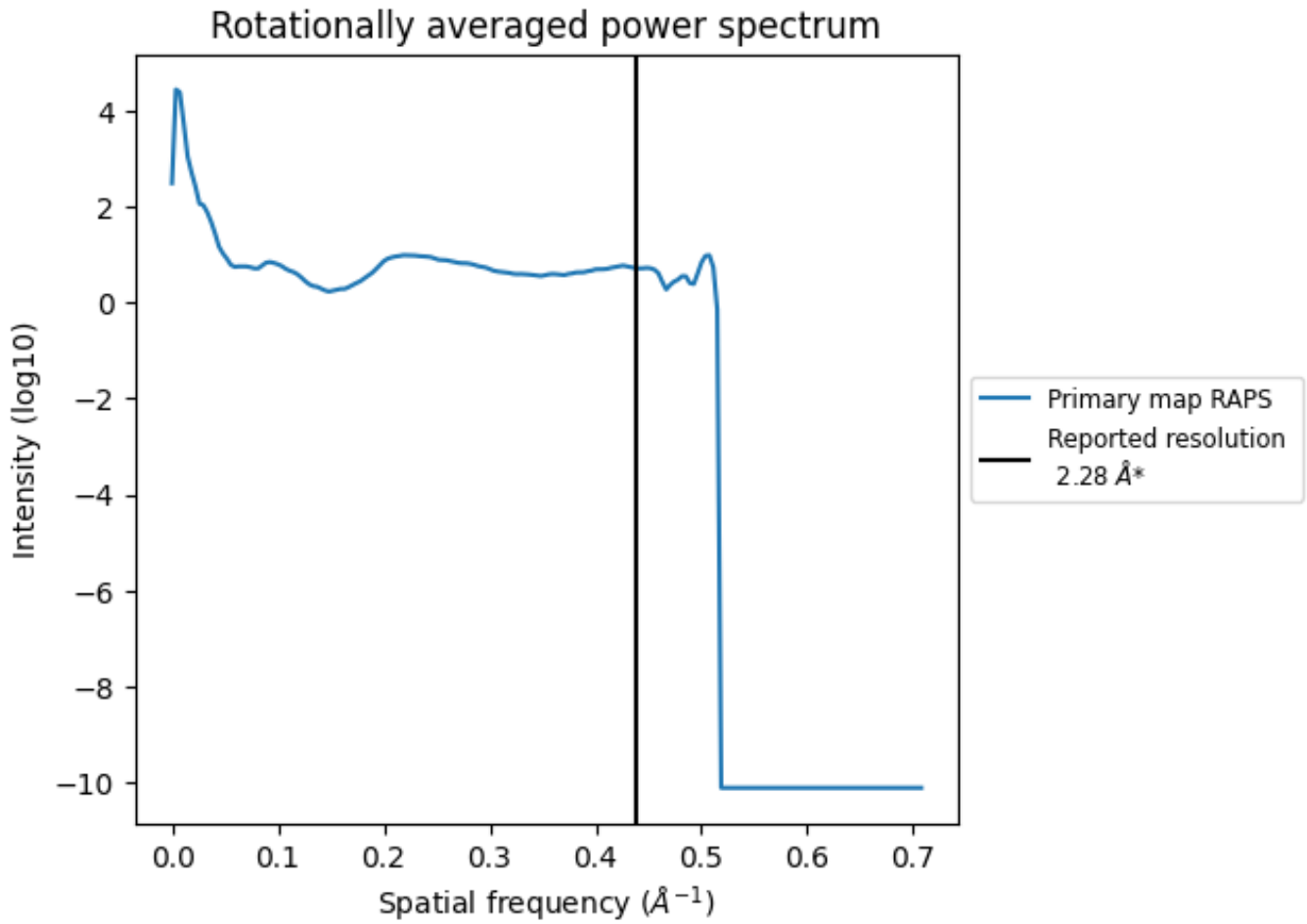
7.2 Volume estimate



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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)

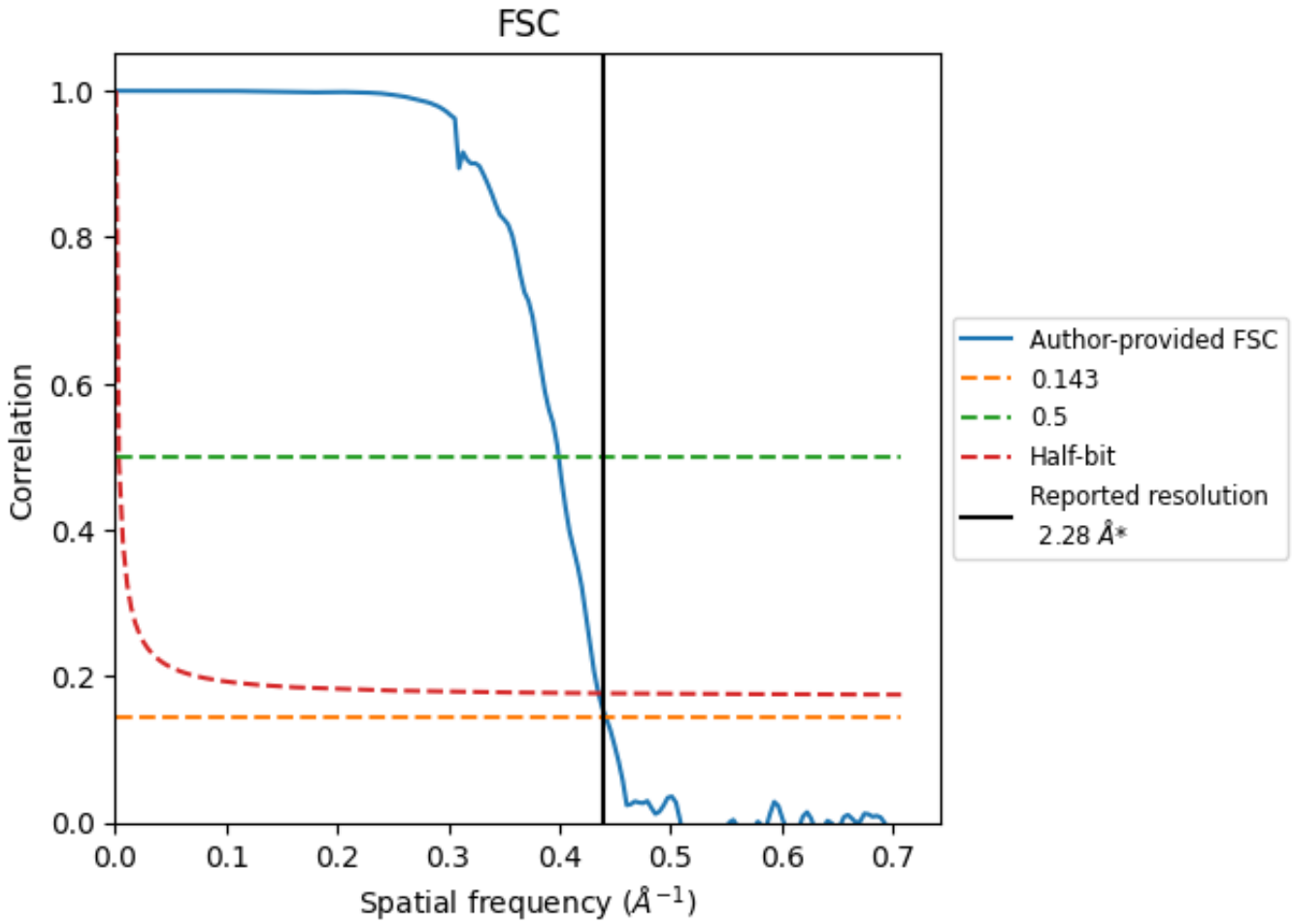


*Reported resolution corresponds to spatial frequency of 0.439 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.439 Å^{-1}

8.2 Resolution estimates (i)

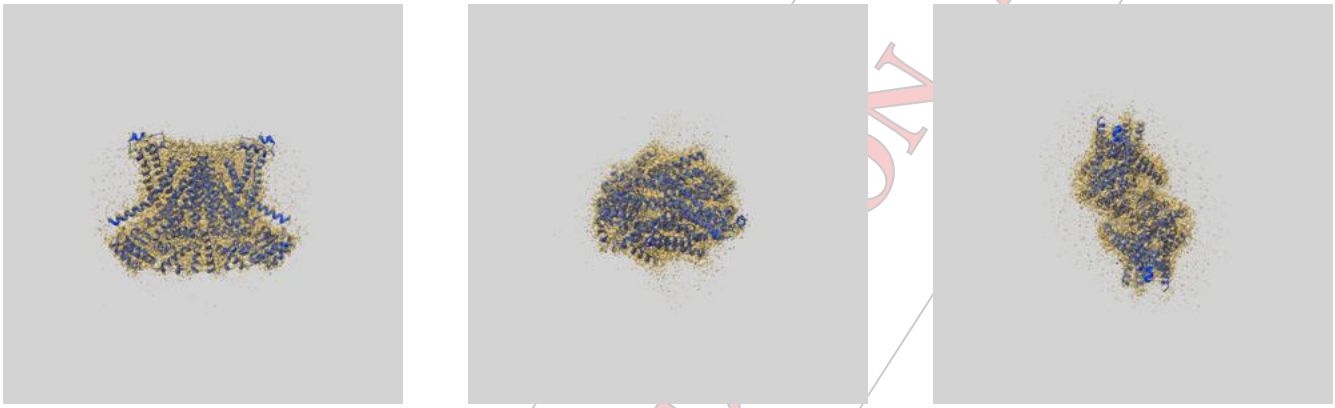
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.28	-	-
Author-provided FSC curve	2.26	2.50	2.30
Unmasked-calculated*	-	-	-

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24730 and PDB model 7RXG. Per-residue inclusion information can be found in section 3 on page 6.

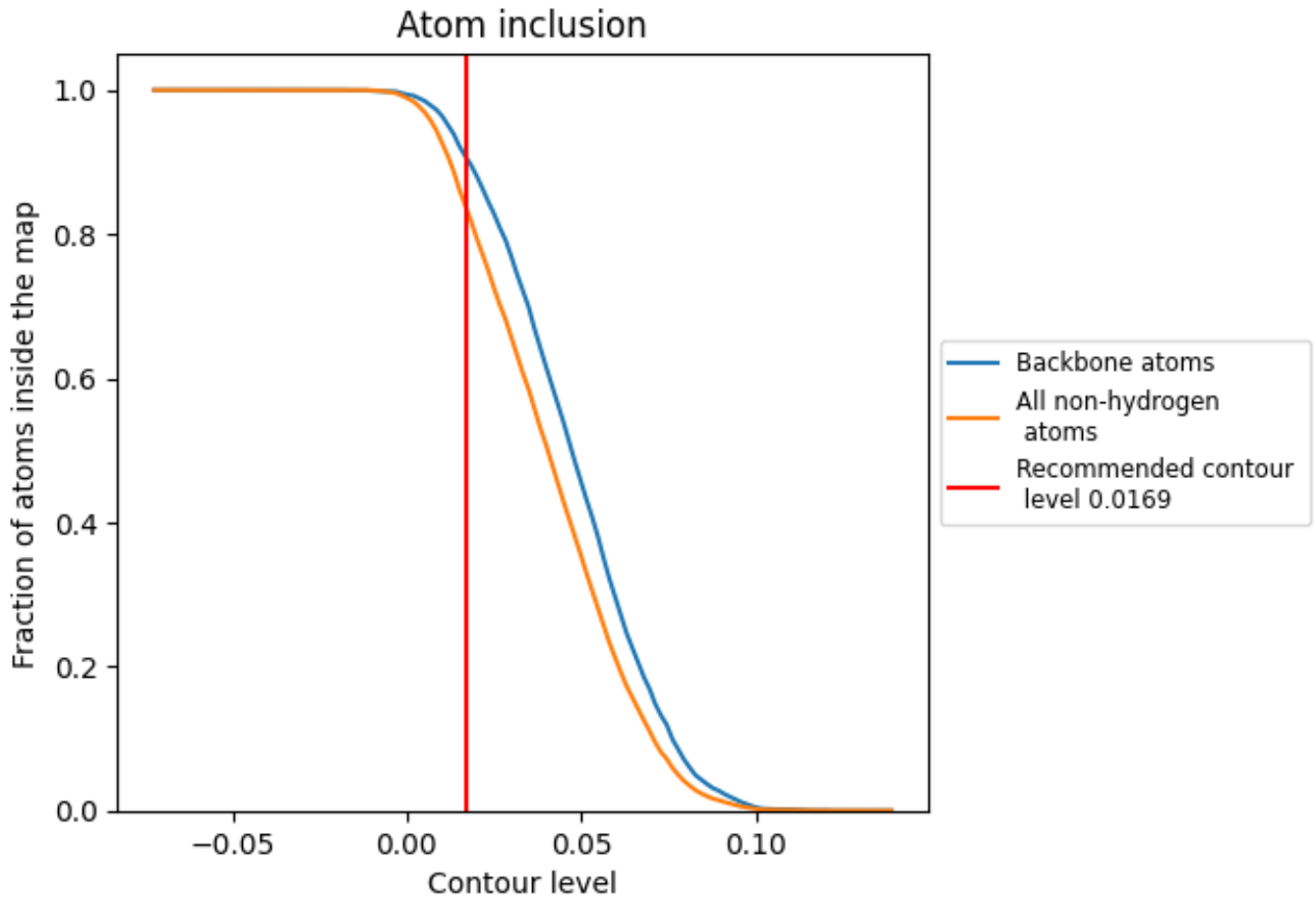
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0169 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 Atom inclusion



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

Full wwPDB EM Validation Report ⓘ

Aug 30, 2021 – 10:18 AM EDT

PDB ID	:	7RX2
EMDB ID	:	EMD-24722
Title	:	afTMEM16 in C22 lipid nanodiscs with MSP1E3 scaffold protein in the presnece of Ca2+
Deposited on	:	2021-08-21
Resolution	:	2.70 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

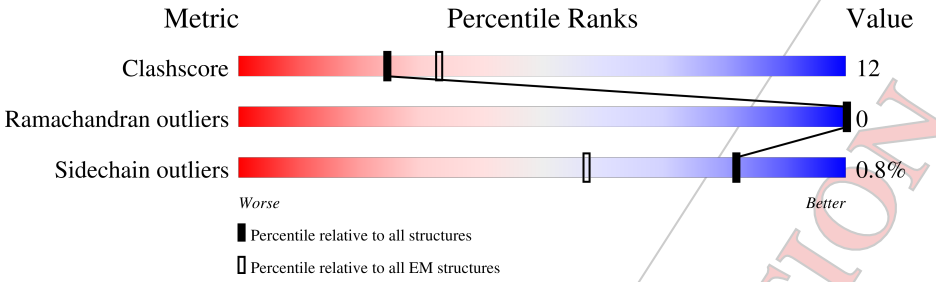
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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 <=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	735	61% 22% 16%
1	B	735	61% 22% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10390 atoms, of which 12 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.

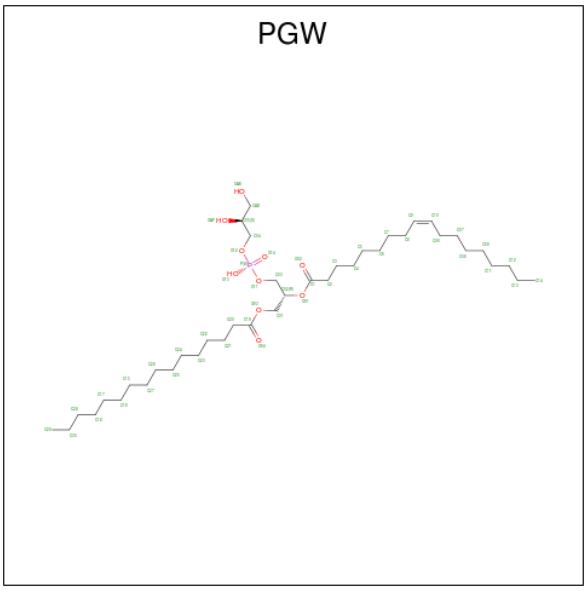
- Molecule 1 is a protein called afTMEM16 lipid scramblase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	615	Total 4969	C 3251	N 832	O 867	S 19	0	0
1	A	615	Total 4969	C 3251	N 832	O 867	S 19	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	B	2	Total 2	Ca 2	0
2	A	2	Total 2	Ca 2	0

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 215	C 154	O 55	P 6	0
3	B	1	Total 215	C 154	O 55	P 6	0
3	B	1	Total 215	C 154	O 55	P 6	0
3	B	1	Total 215	C 154	O 55	P 6	0
3	B	1	Total 215	C 154	O 55	P 6	0
3	B	1	Total 215	C 154	O 55	P 6	0
3	B	1	Total 215	C 154	O 55	P 6	0
3	A	1	Total 215	C 154	O 55	P 6	0
3	A	1	Total 215	C 154	O 55	P 6	0
3	A	1	Total 215	C 154	O 55	P 6	0
3	A	1	Total 215	C 154	O 55	P 6	0
3	A	1	Total 215	C 154	O 55	P 6	0
3	A	1	Total 215	C 154	O 55	P 6	0
3	A	1	Total 215	C 154	O 55	P 6	0

- Molecule 4 is water.

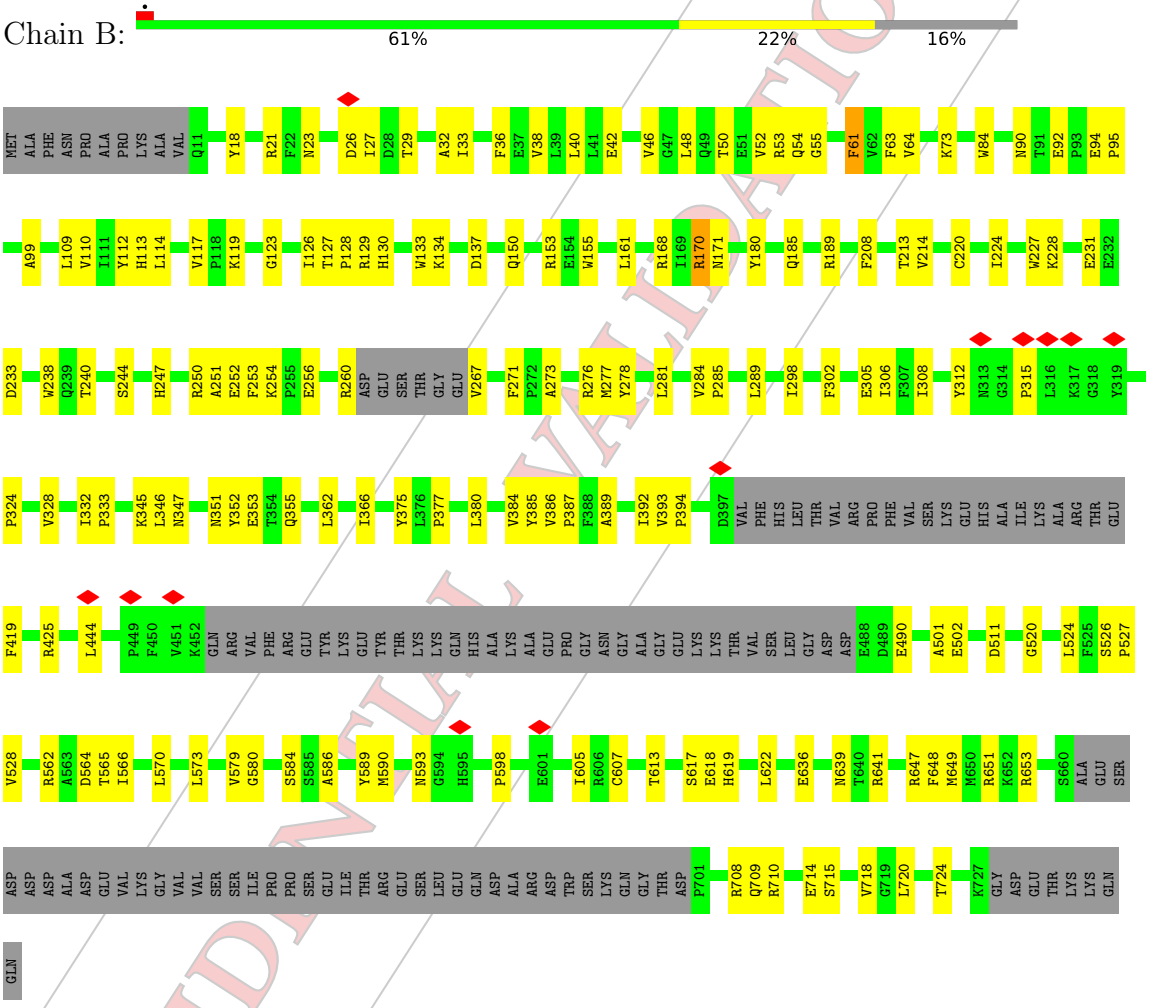
Mol	Chain	Residues	Atoms			AltConf
4	B	3	Total 9	H 6	O 3	0
4	A	3	Total 9	H 6	O 3	0

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.

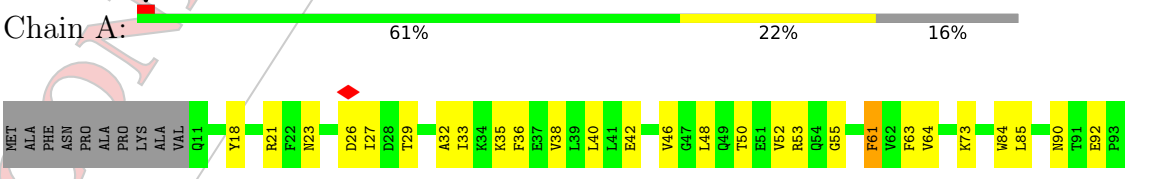
• Molecule 1: afTMEM16 lipid scramblase

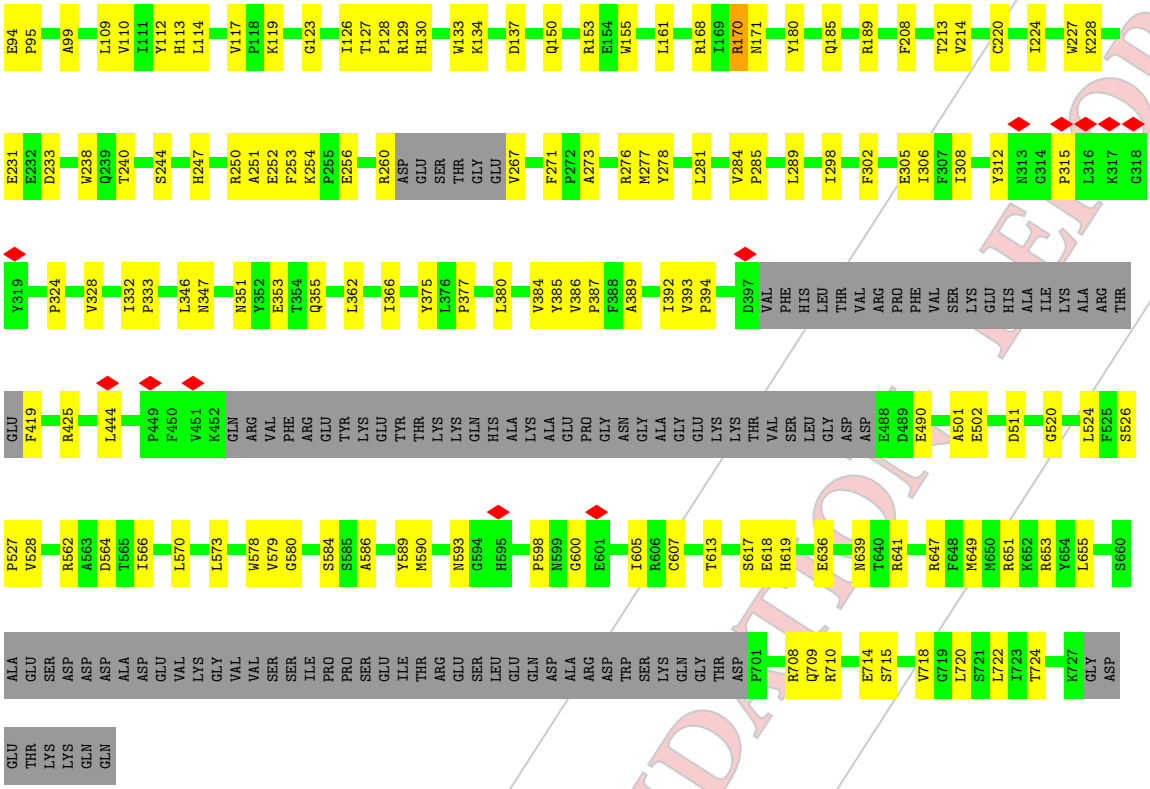
Chain B:



• Molecule 1: afTMEM16 lipid scramblase

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132332	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 ($e^-/Å^2$)	42.7884	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	0.087	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	271.3728, 271.3728, 271.3728	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7067, 0.7067, 0.7067	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.44	0/5101	0.47	0/6933
1	B	0.44	0/5101	0.47	0/6933
All	All	0.44	0/10202	0.47	0/13866

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	4969	0	4947	122	0
1	B	4969	0	4947	125	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	215	0	239	17	0
3	B	215	0	239	15	0
4	A	3	6	0	0	0
4	B	3	6	0	0	0
All	All	10378	12	10372	244	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 12.

All (244) 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:129:ARG:HA	1:A:134:LYS:HA	1.40	1.03
1:B:129:ARG:HA	1:B:134:LYS:HA	1.40	0.98
1:B:189:ARG:HD3	3:B:805:PGW:H03A	1.47	0.96
1:A:189:ARG:HD3	3:A:1506:PGW:H03A	1.47	0.94
1:A:524:LEU:HD23	1:A:580:GLY:HA2	1.62	0.82
1:B:524:LEU:HD23	1:B:580:GLY:HA2	1.62	0.81
1:A:380:LEU:O	1:A:384:VAL:HG22	1.82	0.80
1:B:380:LEU:O	1:B:384:VAL:HG22	1.82	0.79
1:A:109:LEU:HD21	1:A:562:ARG:HD2	1.70	0.73
1:B:598:PRO:HG3	1:B:605:ILE:HD11	1.71	0.73
1:A:598:PRO:HG3	1:A:605:ILE:HD11	1.71	0.73
1:B:109:LEU:HD21	1:B:562:ARG:HD2	1.70	0.73
1:B:21:ARG:HA	1:B:61:PHE:HB3	1.72	0.72
1:A:21:ARG:HA	1:A:61:PHE:HB3	1.72	0.72
1:B:380:LEU:O	1:B:384:VAL:CG2	2.38	0.71
1:A:393:VAL:HG23	1:A:394:PRO:HD3	1.73	0.71
1:A:380:LEU:O	1:A:384:VAL:CG2	2.38	0.70
1:B:21:ARG:NH2	1:B:501:ALA:O	2.24	0.70
1:A:617:SER:HB2	3:A:1505:PGW:H16	1.72	0.70
1:B:617:SER:HB2	3:B:804:PGW:H16	1.72	0.70
1:A:21:ARG:NH2	1:A:501:ALA:O	2.24	0.70
1:B:393:VAL:HG23	1:B:394:PRO:HD3	1.73	0.70
1:A:90:ASN:HD21	1:A:647:ARG:HB2	1.58	0.69
3:B:806:PGW:C30	3:A:1501:PGW:C9	2.72	0.68
3:B:809:PGW:C9	3:A:1507:PGW:C30	2.71	0.68
1:B:619:HIS:NE2	1:A:618:GLU:OE2	2.27	0.68
1:B:90:ASN:HD21	1:B:647:ARG:HB2	1.58	0.67
1:B:490:GLU:OE1	1:A:708:ARG:NH2	2.27	0.65
1:A:21:ARG:HH21	1:A:501:ALA:HB1	1.64	0.63
1:B:21:ARG:HH21	1:B:501:ALA:HB1	1.64	0.61
1:B:586:ALA:O	1:B:590:MET:HG2	2.03	0.59
1:B:240:THR:O	1:B:564:ASP:HB3	2.03	0.59
1:A:586:ALA:O	1:A:590:MET:HG2	2.03	0.59
1:B:710:ARG:N	1:B:714:GLU:OE2	2.34	0.58
1:A:240:THR:O	1:A:564:ASP:HB3	2.02	0.58
1:B:618:GLU:OE2	1:A:619:HIS:NE2	2.34	0.58
1:B:651:ARG:NH2	1:A:84:TRP:O	2.33	0.57
1:A:110:VAL:O	1:A:114:LEU:HD13	2.04	0.57
1:B:110:VAL:O	1:B:114:LEU:HD13	2.05	0.57
1:A:129:ARG:HA	1:A:134:LYS:CA	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:ARG:N	1:A:714:GLU:OE2	2.34	0.56
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.89	0.55
1:B:254:LYS:O	1:B:351:ASN:ND2	2.40	0.55
1:B:385:TYR:CE2	1:B:425:ARG:HD2	2.42	0.55
1:A:714:GLU:O	1:A:718:VAL:HG23	2.07	0.55
1:B:273:ALA:O	1:B:277:MET:HG3	2.07	0.55
1:B:284:VAL:HB	1:B:285:PRO:HD3	1.88	0.55
3:B:805:PGW:H3	3:B:805:PGW:H20A	1.89	0.55
1:A:273:ALA:O	1:A:277:MET:HG3	2.07	0.55
3:A:1506:PGW:H3	3:A:1506:PGW:H20A	1.89	0.55
1:B:619:HIS:HD2	3:A:1507:PGW:H5	1.72	0.55
1:A:254:LYS:O	1:A:351:ASN:ND2	2.40	0.54
1:B:129:ARG:HA	1:B:134:LYS:CA	2.25	0.54
1:A:385:TYR:CE2	1:A:425:ARG:HD2	2.42	0.54
1:A:48:LEU:HD13	1:A:64:VAL:HG11	1.89	0.54
1:B:48:LEU:HD13	1:B:64:VAL:HG11	1.89	0.54
1:B:589:TYR:HD1	3:B:804:PGW:H20A	1.73	0.54
1:A:109:LEU:CD2	1:A:562:ARG:HD2	2.38	0.53
1:A:208:PHE:CE1	1:A:528:VAL:HG22	2.43	0.53
1:B:346:LEU:HB2	3:B:808:PGW:H5	1.91	0.53
1:B:129:ARG:CA	1:B:134:LYS:HA	2.28	0.53
1:B:231:GLU:OE2	1:B:566:ILE:HG12	2.08	0.53
1:B:714:GLU:O	1:B:718:VAL:HG23	2.07	0.53
1:A:231:GLU:OE2	1:A:566:ILE:HG12	2.08	0.53
1:A:524:LEU:HD23	1:A:580:GLY:CA	2.38	0.53
1:B:84:TRP:O	1:A:651:ARG:NH2	2.37	0.53
1:B:127:THR:HG21	1:B:251:ALA:HB2	1.90	0.53
1:A:589:TYR:HD1	3:A:1505:PGW:H20A	1.73	0.53
1:B:224:ILE:HD12	1:B:573:LEU:HB3	1.91	0.53
1:A:46:VAL:HG21	1:A:123:GLY:HA2	1.91	0.53
1:A:253:PHE:CZ	1:A:353:GLU:HG2	2.44	0.53
1:B:208:PHE:CE1	1:B:528:VAL:HG22	2.43	0.53
1:B:393:VAL:HG21	1:B:419:PHE:CG	2.44	0.53
1:B:253:PHE:CZ	1:B:353:GLU:HG2	2.44	0.52
1:A:127:THR:HG21	1:A:251:ALA:HB2	1.90	0.52
1:A:393:VAL:HG21	1:A:419:PHE:CG	2.44	0.52
1:A:214:VAL:HG22	3:A:1505:PGW:H15A	1.91	0.52
1:B:46:VAL:HG21	1:B:123:GLY:HA2	1.91	0.52
1:A:636:GLU:OE1	1:A:641:ARG:HG3	2.10	0.52
1:A:129:ARG:CA	1:A:134:LYS:HA	2.28	0.52
1:A:224:ILE:HD12	1:A:573:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG22	3:B:804:PGW:H15A	1.91	0.52
1:B:636:GLU:OE1	1:B:641:ARG:HG3	2.10	0.52
1:A:250:ARG:HB3	1:A:355:GLN:HG3	1.92	0.51
1:B:54:GLN:OE1	1:A:722:LEU:HD22	2.11	0.51
1:A:308:ILE:HA	1:A:312:TYR:HB3	1.92	0.51
1:A:346:LEU:HB2	3:A:1509:PGW:H5	1.91	0.51
1:B:389:ALA:HA	1:B:392:ILE:HB	1.93	0.51
1:B:524:LEU:HD23	1:B:580:GLY:CA	2.38	0.51
1:A:389:ALA:HA	1:A:392:ILE:HB	1.93	0.51
1:B:649:MET:O	1:B:653:ARG:HG3	2.11	0.51
1:A:23:ASN:ND2	1:A:137:ASP:HB2	2.27	0.50
1:A:393:VAL:CG2	1:A:394:PRO:HD3	2.39	0.50
1:B:622:LEU:HD13	1:A:578:TRP:CH2	2.47	0.50
1:B:23:ASN:ND2	1:B:137:ASP:HB2	2.27	0.50
1:A:393:VAL:HG11	1:A:419:PHE:CE1	2.46	0.50
1:A:48:LEU:HD13	1:A:64:VAL:CG1	2.42	0.50
1:B:393:VAL:HG21	1:B:419:PHE:CD1	2.47	0.50
1:B:393:VAL:HG11	1:B:419:PHE:CE1	2.46	0.50
1:A:393:VAL:HG21	1:A:419:PHE:CD1	2.47	0.50
1:A:649:MET:O	1:A:653:ARG:HG3	2.11	0.50
1:B:113:HIS:O	1:B:117:VAL:HG22	2.12	0.49
1:A:180:TYR:CZ	1:A:511:ASP:HB3	2.48	0.49
1:B:48:LEU:HD13	1:B:64:VAL:CG1	2.42	0.49
1:B:109:LEU:CD2	1:B:562:ARG:HD2	2.38	0.49
1:B:250:ARG:HB3	1:B:355:GLN:HG3	1.92	0.49
1:A:332:ILE:HB	1:A:333:PRO:HD3	1.94	0.49
1:B:220:CYS:O	1:B:224:ILE:HG12	2.12	0.49
1:A:128:PRO:O	1:A:129:ARG:HG2	2.12	0.49
1:B:180:TYR:CZ	1:B:511:ASP:HB3	2.48	0.49
1:B:308:ILE:HA	1:B:312:TYR:HB3	1.92	0.49
1:B:524:LEU:HD21	1:B:579:VAL:HG12	1.93	0.49
1:B:128:PRO:O	1:B:129:ARG:HG2	2.12	0.49
1:B:332:ILE:HB	1:B:333:PRO:HD3	1.94	0.49
1:A:220:CYS:O	1:A:224:ILE:HG12	2.12	0.49
1:B:227:TRP:CE2	1:B:231:GLU:HG3	2.49	0.48
1:B:393:VAL:CG2	1:B:394:PRO:HD3	2.39	0.48
1:B:27:ILE:HG22	1:B:32:ALA:HB2	1.96	0.48
1:B:52:VAL:O	1:B:53:ARG:HD3	2.14	0.48
1:B:362:LEU:O	1:B:366:ILE:HG13	2.13	0.48
1:A:113:HIS:O	1:A:117:VAL:HG22	2.12	0.48
1:A:524:LEU:HD21	1:A:579:VAL:HG12	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:HE2	1:B:276:ARG:HB2	1.78	0.48
1:A:52:VAL:O	1:A:53:ARG:HD3	2.14	0.48
1:B:170:ARG:HD2	1:B:238:TRP:CD2	2.49	0.48
1:A:27:ILE:HG22	1:A:32:ALA:HB2	1.96	0.48
1:A:170:ARG:HD2	1:A:238:TRP:CD2	2.49	0.48
1:A:227:TRP:CE2	1:A:231:GLU:HG3	2.49	0.48
1:A:324:PRO:O	1:A:328:VAL:HG13	2.13	0.48
1:B:305:GLU:OE1	1:B:425:ARG:NH1	2.40	0.48
1:B:260:ARG:HA	1:B:267:VAL:HA	1.96	0.48
1:A:36:PHE:CE2	1:A:40:LEU:HD11	2.49	0.48
1:A:271:PHE:HE2	1:A:276:ARG:HB2	1.77	0.48
1:B:233:ASP:OD1	1:B:639:ASN:HB2	2.14	0.47
1:B:324:PRO:O	1:B:328:VAL:HG13	2.13	0.47
1:B:29:THR:O	1:B:33:ILE:HG22	2.15	0.47
1:A:362:LEU:O	1:A:366:ILE:HG13	2.13	0.47
1:B:84:TRP:HZ3	1:A:655:LEU:HB2	1.79	0.47
1:B:380:LEU:HA	1:B:384:VAL:HG22	1.97	0.47
1:B:90:ASN:ND2	1:B:647:ARG:HB2	2.27	0.47
1:B:94:GLU:HB3	1:B:95:PRO:HD2	1.97	0.47
1:B:150:GLN:NE2	1:B:168:ARG:HH12	2.13	0.47
1:B:347:ASN:ND2	1:B:362:LEU:HB2	2.30	0.47
1:A:29:THR:O	1:A:33:ILE:HG22	2.15	0.47
1:A:233:ASP:OD1	1:A:639:ASN:HB2	2.14	0.47
1:A:347:ASN:ND2	1:A:362:LEU:HB2	2.30	0.47
1:B:36:PHE:CE2	1:B:40:LEU:HD11	2.49	0.47
1:A:386:VAL:HB	1:A:387:PRO:HD3	1.97	0.47
1:A:73:LYS:HG2	1:A:99:ALA:O	2.15	0.46
1:A:260:ARG:HA	1:A:267:VAL:HA	1.96	0.46
1:A:380:LEU:HA	1:A:384:VAL:HG22	1.96	0.46
1:A:150:GLN:NE2	1:A:168:ARG:HH12	2.13	0.46
1:A:305:GLU:OE1	1:A:425:ARG:NH1	2.40	0.46
1:A:607:CYS:HB2	3:A:1504:PGW:H02	1.97	0.46
1:B:298:ILE:HD13	1:B:377:PRO:HD3	1.98	0.46
1:A:42:GLU:CD	1:A:119:LYS:HE2	2.36	0.46
1:A:94:GLU:HB3	1:A:95:PRO:HD2	1.97	0.46
1:B:73:LYS:HG2	1:B:99:ALA:O	2.16	0.46
1:A:90:ASN:ND2	1:A:647:ARG:HB2	2.27	0.46
1:A:709:GLN:OE1	1:A:715:SER:HA	2.16	0.46
1:B:42:GLU:CD	1:B:119:LYS:HE2	2.36	0.46
1:B:130:HIS:CD2	1:B:252:GLU:HG3	2.51	0.46
1:B:386:VAL:HB	1:B:387:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:HIS:CD2	1:A:252:GLU:HG3	2.51	0.45
1:A:256:GLU:HG2	1:A:271:PHE:HD1	1.81	0.45
1:B:607:CYS:HB2	3:B:803:PGW:H02	1.97	0.45
1:A:298:ILE:HD13	1:A:377:PRO:HD3	1.98	0.45
1:B:380:LEU:O	1:B:384:VAL:HG23	2.17	0.45
1:B:590:MET:HA	3:B:804:PGW:HADA	1.99	0.45
1:B:613:THR:HB	3:B:804:PGW:H4A	1.99	0.45
1:A:256:GLU:HG2	1:A:271:PHE:CD1	2.52	0.45
1:B:170:ARG:HD2	1:B:238:TRP:CE2	2.52	0.45
3:B:806:PGW:H15	3:B:806:PGW:H18	1.62	0.45
1:B:709:GLN:OE1	1:B:715:SER:HA	2.16	0.45
1:A:613:THR:HB	3:A:1505:PGW:H4A	1.99	0.45
1:B:244:SER:HA	1:B:247:HIS:CE1	2.52	0.44
1:A:170:ARG:HD2	1:A:238:TRP:CE2	2.52	0.44
1:B:720:LEU:O	1:B:724:THR:HG23	2.17	0.44
1:A:302:PHE:O	1:A:306:ILE:HG12	2.17	0.44
1:B:256:GLU:HG2	1:B:271:PHE:CD1	2.52	0.44
1:B:302:PHE:O	1:B:306:ILE:HG12	2.17	0.44
1:A:18:TYR:OH	1:A:112:TYR:HB2	2.17	0.44
1:A:214:VAL:CG2	3:A:1505:PGW:H15A	2.48	0.44
1:A:244:SER:HA	1:A:247:HIS:CE1	2.52	0.44
1:A:312:TYR:OH	1:A:315:PRO:O	2.20	0.44
1:B:18:TYR:OH	1:B:112:TYR:HB2	2.17	0.44
1:A:38:VAL:O	1:A:42:GLU:HG2	2.18	0.44
1:A:590:MET:HA	3:A:1505:PGW:HADA	1.99	0.44
1:B:38:VAL:O	1:B:42:GLU:HG2	2.18	0.44
1:B:256:GLU:HG2	1:B:271:PHE:HD1	1.81	0.44
1:B:708:ARG:NH2	1:A:490:GLU:OE1	2.46	0.44
1:B:170:ARG:HG3	1:B:171:ASN:N	2.32	0.44
1:B:55:GLY:HA2	1:B:61:PHE:CE2	2.53	0.43
1:A:170:ARG:HG3	1:A:171:ASN:N	2.32	0.43
1:A:224:ILE:CD1	1:A:573:LEU:HB3	2.48	0.43
1:B:312:TYR:OH	1:B:315:PRO:O	2.20	0.43
1:A:289:LEU:HD13	3:A:1509:PGW:C10	2.49	0.43
1:A:55:GLY:HA2	1:A:61:PHE:CE2	2.53	0.43
1:A:720:LEU:O	1:A:724:THR:HG23	2.18	0.43
1:B:289:LEU:HD13	3:B:808:PGW:C10	2.49	0.43
1:A:278:TYR:O	1:A:281:LEU:HB2	2.19	0.43
1:B:214:VAL:CG2	3:B:804:PGW:H15A	2.48	0.43
1:A:127:THR:O	1:A:133:TRP:HB2	2.19	0.43
1:B:50:THR:HA	1:B:63:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TYR:O	1:B:281:LEU:HB2	2.19	0.43
1:B:127:THR:O	1:B:133:TRP:HB2	2.19	0.43
1:B:161:LEU:HB2	1:B:185:GLN:OE1	2.19	0.43
1:B:224:ILE:CD1	1:B:573:LEU:HB3	2.48	0.43
1:B:648:PHE:CE1	1:A:85:LEU:HB3	2.54	0.43
1:B:26:ASP:O	1:B:27:ILE:HD13	2.19	0.42
1:B:213:THR:HG23	1:B:584:SER:HB3	2.01	0.42
1:A:213:THR:HG23	1:A:584:SER:HB3	2.01	0.42
1:A:26:ASP:O	1:A:27:ILE:HD13	2.19	0.42
1:A:380:LEU:O	1:A:384:VAL:HG23	2.16	0.42
1:A:598:PRO:O	1:A:600:GLY:N	2.50	0.42
1:A:50:THR:HA	1:A:63:PHE:O	2.19	0.42
1:A:502:GLU:HA	1:A:502:GLU:OE2	2.19	0.42
1:B:502:GLU:OE2	1:B:502:GLU:HA	2.19	0.42
1:A:161:LEU:HB2	1:A:185:GLN:OE1	2.19	0.42
1:B:150:GLN:HG3	1:B:153:ARG:NH2	2.35	0.42
1:B:155:TRP:CG	1:B:161:LEU:HD11	2.55	0.42
1:A:150:GLN:HG3	1:A:153:ARG:NH2	2.35	0.42
1:A:393:VAL:HG11	1:A:419:PHE:CZ	2.55	0.42
1:B:526:SER:N	1:B:527:PRO:HD2	2.35	0.42
1:A:155:TRP:CG	1:A:161:LEU:HD11	2.55	0.42
3:A:1507:PGW:H18	3:A:1507:PGW:H15	1.62	0.42
1:A:526:SER:N	1:A:527:PRO:HD2	2.35	0.42
1:B:375:TYR:OH	1:B:520:GLY:HA3	2.20	0.41
3:A:1501:PGW:H5	3:A:1501:PGW:H2	1.78	0.41
1:A:126:ILE:HA	1:A:133:TRP:CD1	2.56	0.41
1:A:228:LYS:HG2	1:A:570:LEU:HD21	2.02	0.41
1:B:393:VAL:HG11	1:B:419:PHE:CZ	2.55	0.41
1:B:345:LYS:HD3	1:B:345:LYS:HA	1.90	0.41
1:B:126:ILE:HA	1:B:133:TRP:CD1	2.56	0.41
1:B:92:GLU:OE1	1:B:653:ARG:NH1	2.54	0.41
1:B:278:TYR:HB3	3:B:807:PGW:H2A	2.03	0.41
1:A:92:GLU:OE1	1:A:653:ARG:NH1	2.54	0.41
1:A:375:TYR:OH	1:A:520:GLY:HA3	2.20	0.41
1:B:228:LYS:HG2	1:B:570:LEU:HD21	2.02	0.41
1:B:305:GLU:HB2	1:B:324:PRO:HG2	2.03	0.41
1:A:35:LYS:HA	1:A:38:VAL:HG22	2.03	0.40
1:B:250:ARG:HD3	1:B:352:TYR:O	2.21	0.40
1:B:231:GLU:OE1	1:B:565:THR:OG1	2.37	0.40
1:A:278:TYR:HB3	3:A:1508:PGW:H2A	2.03	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	605/735 (82%)	571 (94%)	34 (6%)	0	100	100
1	B	605/735 (82%)	571 (94%)	34 (6%)	0	100	100
All	All	1210/1470 (82%)	1142 (94%)	68 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	529/646 (82%)	525 (99%)	4 (1%)	81	93
1	B	529/646 (82%)	525 (99%)	4 (1%)	81	93
All	All	1058/1292 (82%)	1050 (99%)	8 (1%)	82	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	PHE
1	B	170	ARG
1	B	444	LEU
1	B	593	ASN
1	A	61	PHE
1	A	170	ARG
1	A	444	LEU
1	A	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	ASN
1	B	150	GLN
1	B	283	GLN
1	B	370	ASN
1	B	438	GLN
1	B	499	ASN
1	A	148	ASN
1	A	150	GLN
1	A	283	GLN
1	A	370	ASN
1	A	438	GLN
1	A	499	ASN

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)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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	PGW	A	1505	-	40,40,50	0.29	0	43,46,56	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PGW	B	807	-	29,29,50	1.21	4 (13%)	33,34,56	1.07	2 (6%)
3	PGW	A	1501	-	23,23,50	0.49	0	27,28,56	0.64	1 (3%)
3	PGW	A	1507	-	37,37,50	1.09	5 (13%)	41,42,56	1.23	3 (7%)
3	PGW	B	806	-	37,37,50	1.09	5 (13%)	41,42,56	1.23	3 (7%)
3	PGW	B	804	-	40,40,50	0.29	0	43,46,56	0.34	0
3	PGW	A	1506	-	25,25,50	1.30	4 (16%)	29,30,56	1.44	3 (10%)
3	PGW	B	803	-	25,25,50	1.18	3 (12%)	27,27,56	1.38	2 (7%)
3	PGW	B	808	-	28,28,50	1.24	5 (17%)	30,32,56	1.28	2 (6%)
3	PGW	A	1509	-	28,28,50	1.24	5 (17%)	30,32,56	1.28	2 (6%)
3	PGW	A	1508	-	29,29,50	1.21	4 (13%)	33,34,56	1.07	2 (6%)
3	PGW	B	805	-	25,25,50	1.30	4 (16%)	29,30,56	1.44	3 (10%)
3	PGW	A	1504	-	25,25,50	1.18	3 (12%)	27,27,56	1.38	2 (7%)
3	PGW	B	809	-	23,23,50	0.48	0	27,28,56	0.64	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGW	A	1505	-	-	22/45/45/55	-
3	PGW	B	807	-	-	8/31/31/55	-
3	PGW	A	1501	-	-	8/25/25/55	-
3	PGW	A	1507	-	-	18/39/39/55	-
3	PGW	B	806	-	-	18/39/39/55	-
3	PGW	B	804	-	-	22/45/45/55	-
3	PGW	A	1506	-	-	8/27/27/55	-
3	PGW	B	803	-	-	9/27/27/55	-
3	PGW	B	808	-	-	15/28/28/55	-
3	PGW	A	1509	-	-	15/28/28/55	-
3	PGW	A	1508	-	-	8/31/31/55	-
3	PGW	B	805	-	-	8/27/27/55	-
3	PGW	A	1504	-	-	9/27/27/55	-
3	PGW	B	809	-	-	8/25/25/55	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1508	PGW	O01-C1	2.95	1.42	1.34
3	B	807	PGW	O01-C1	2.94	1.42	1.34
3	A	1504	PGW	O01-C1	2.89	1.42	1.34
3	B	803	PGW	O01-C1	2.87	1.42	1.34
3	B	805	PGW	O01-C1	2.86	1.42	1.34
3	A	1506	PGW	O01-C1	2.85	1.42	1.34
3	B	808	PGW	O01-C1	2.70	1.41	1.34
3	A	1509	PGW	O01-C1	2.69	1.41	1.34
3	A	1507	PGW	O01-C1	2.66	1.41	1.34
3	B	806	PGW	O01-C1	2.65	1.41	1.34
3	A	1507	PGW	O03-C01	-2.47	1.39	1.45
3	A	1506	PGW	O03-C19	2.45	1.40	1.33
3	B	805	PGW	O03-C19	2.45	1.40	1.33
3	B	806	PGW	O03-C01	-2.43	1.39	1.45
3	B	803	PGW	O03-C19	2.43	1.40	1.33
3	A	1504	PGW	O03-C19	2.42	1.40	1.33
3	B	805	PGW	O03-C01	-2.42	1.39	1.45
3	A	1506	PGW	O03-C01	-2.42	1.39	1.45
3	A	1509	PGW	O03-C19	2.39	1.40	1.33
3	A	1508	PGW	P-O12	2.39	1.64	1.54
3	B	807	PGW	P-O12	2.37	1.64	1.54
3	B	808	PGW	O03-C19	2.37	1.40	1.33
3	A	1509	PGW	O03-C01	-2.36	1.39	1.45
3	B	808	PGW	O03-C01	-2.34	1.39	1.45
3	B	805	PGW	P-O12	2.34	1.63	1.54
3	A	1506	PGW	P-O12	2.34	1.63	1.54
3	A	1508	PGW	O03-C19	2.31	1.40	1.33
3	B	807	PGW	O03-C19	2.30	1.40	1.33
3	A	1509	PGW	P-O12	2.29	1.63	1.54
3	B	808	PGW	P-O12	2.29	1.63	1.54
3	A	1507	PGW	P-O12	2.27	1.63	1.54
3	B	806	PGW	O03-C19	2.26	1.39	1.33
3	B	806	PGW	P-O12	2.26	1.63	1.54
3	A	1507	PGW	O03-C19	2.25	1.39	1.33
3	B	807	PGW	O03-C01	-2.24	1.40	1.45
3	A	1508	PGW	O03-C01	-2.23	1.40	1.45
3	B	806	PGW	O01-C02	-2.23	1.41	1.46
3	A	1507	PGW	O01-C02	-2.20	1.41	1.46
3	B	808	PGW	O01-C02	-2.16	1.41	1.46
3	A	1509	PGW	O01-C02	-2.15	1.41	1.46
3	A	1504	PGW	O03-C01	-2.15	1.40	1.45
3	B	803	PGW	O03-C01	-2.15	1.40	1.45

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	805	PGW	O01-C1-C2	4.93	122.12	111.50
3	A	1506	PGW	O01-C1-C2	4.93	122.12	111.50
3	A	1504	PGW	O01-C1-C2	4.27	120.70	111.50
3	B	803	PGW	O01-C1-C2	4.27	120.70	111.50
3	B	806	PGW	O01-C1-C2	3.88	119.87	111.50
3	B	808	PGW	O01-C1-C2	3.88	119.87	111.50
3	A	1509	PGW	O01-C1-C2	3.88	119.87	111.50
3	A	1507	PGW	O01-C1-C2	3.88	119.86	111.50
3	B	807	PGW	O01-C1-C2	3.26	118.53	111.50
3	A	1508	PGW	O01-C1-C2	3.26	118.52	111.50
3	B	803	PGW	O03-C19-C20	2.76	120.58	111.91
3	A	1504	PGW	O03-C19-C20	2.76	120.57	111.91
3	A	1507	PGW	O03-C19-C20	2.71	120.40	111.91
3	B	806	PGW	O03-C19-C20	2.70	120.37	111.91
3	B	805	PGW	O03-C19-C20	2.60	120.07	111.91
3	A	1506	PGW	O03-C19-C20	2.59	120.04	111.91
3	B	808	PGW	O03-C19-C20	2.55	119.90	111.91
3	A	1509	PGW	O03-C19-C20	2.54	119.89	111.91
3	B	807	PGW	O03-C19-C20	2.48	119.70	111.91
3	A	1508	PGW	O03-C19-C20	2.48	119.68	111.91
3	A	1501	PGW	O13-P-O14	2.33	119.78	110.68
3	B	809	PGW	O13-P-O14	2.32	119.76	110.68
3	A	1507	PGW	C02-O01-C1	-2.23	112.30	117.79
3	B	806	PGW	C02-O01-C1	-2.22	112.33	117.79
3	B	805	PGW	O01-C1-O02	-2.18	118.43	123.70
3	A	1506	PGW	O01-C1-O02	-2.17	118.45	123.70

There are no chirality outliers.

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	PGW	C01-C02-C03-O11
3	B	803	PGW	O01-C02-C03-O11
3	B	804	PGW	C03-O11-P-O13
3	B	804	PGW	C03-O11-P-O14
3	B	805	PGW	C03-O11-P-O12
3	B	805	PGW	C03-O11-P-O13
3	B	805	PGW	C03-O11-P-O14
3	B	805	PGW	O03-C01-C02-O01
3	B	806	PGW	C03-O11-P-O12
3	B	806	PGW	C03-O11-P-O13
3	B	806	PGW	C03-O11-P-O14
3	B	807	PGW	C10-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
3	B	808	PGW	C2-C1-O01-C02
3	B	808	PGW	O02-C1-O01-C02
3	A	1504	PGW	C01-C02-C03-O11
3	A	1504	PGW	O01-C02-C03-O11
3	A	1505	PGW	C03-O11-P-O13
3	A	1505	PGW	C03-O11-P-O14
3	A	1506	PGW	C03-O11-P-O12
3	A	1506	PGW	C03-O11-P-O13
3	A	1506	PGW	C03-O11-P-O14
3	A	1506	PGW	O03-C01-C02-O01
3	A	1507	PGW	C03-O11-P-O12
3	A	1507	PGW	C03-O11-P-O13
3	A	1507	PGW	C03-O11-P-O14
3	A	1508	PGW	C10-C06-C07-C08
3	A	1509	PGW	C2-C1-O01-C02
3	A	1509	PGW	O02-C1-O01-C02
3	B	809	PGW	C2-C3-C4-C5
3	A	1501	PGW	C2-C3-C4-C5
3	B	807	PGW	C2-C3-C4-C5
3	A	1508	PGW	C2-C3-C4-C5
3	B	806	PGW	C1-C2-C3-C4
3	B	806	PGW	C19-C20-C21-C22
3	A	1507	PGW	C1-C2-C3-C4
3	A	1507	PGW	C19-C20-C21-C22
3	B	806	PGW	C20-C19-O03-C01
3	A	1507	PGW	C20-C19-O03-C01
3	B	804	PGW	C20-C19-O03-C01
3	A	1505	PGW	C20-C19-O03-C01
3	B	804	PGW	C1-C2-C3-C4
3	B	809	PGW	C1-C2-C3-C4
3	A	1501	PGW	C1-C2-C3-C4
3	A	1505	PGW	C1-C2-C3-C4
3	B	806	PGW	O04-C19-O03-C01
3	A	1507	PGW	O04-C19-O03-C01
3	B	804	PGW	C03-O11-P-O12
3	A	1505	PGW	C03-O11-P-O12
3	B	806	PGW	C20-C21-C22-C23
3	A	1505	PGW	C16-C15-C27-C26
3	A	1507	PGW	C20-C21-C22-C23
3	B	803	PGW	C2-C1-O01-C02
3	A	1504	PGW	C2-C1-O01-C02
3	B	804	PGW	C16-C15-C27-C26

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Mol	Chain	Res	Type	Atoms
3	B	804	PGW	O04-C19-O03-C01
3	A	1505	PGW	O04-C19-O03-C01
3	B	803	PGW	O02-C1-O01-C02
3	A	1504	PGW	O02-C1-O01-C02
3	B	804	PGW	C21-C22-C23-C24
3	A	1505	PGW	C21-C22-C23-C24
3	B	804	PGW	C25-C26-C27-C15
3	A	1505	PGW	C25-C26-C27-C15
3	B	803	PGW	C6-C7-C8-C9
3	A	1504	PGW	C6-C7-C8-C9
3	B	803	PGW	C22-C23-C24-C25
3	B	804	PGW	C24-C25-C26-C27
3	A	1504	PGW	C22-C23-C24-C25
3	A	1505	PGW	C24-C25-C26-C27
3	B	803	PGW	C19-C20-C21-C22
3	A	1504	PGW	C19-C20-C21-C22
3	B	804	PGW	C15-C16-C17-C18
3	A	1505	PGW	C15-C16-C17-C18
3	B	806	PGW	C24-C25-C26-C27
3	A	1507	PGW	C24-C25-C26-C27
3	B	806	PGW	C21-C22-C23-C24
3	A	1507	PGW	C21-C22-C23-C24
3	B	806	PGW	C15-C16-C17-C18
3	A	1507	PGW	C15-C16-C17-C18
3	B	808	PGW	C6-C7-C8-C9
3	A	1509	PGW	C6-C7-C8-C9
3	B	804	PGW	C17-C18-C28-C30
3	A	1505	PGW	C17-C18-C28-C30
3	B	808	PGW	C7-C8-C9-C10
3	A	1509	PGW	C7-C8-C9-C10
3	A	1505	PGW	C5-C6-C7-C8
3	B	804	PGW	C5-C6-C7-C8
3	B	804	PGW	C4-C5-C6-C7
3	A	1505	PGW	C4-C5-C6-C7
3	B	804	PGW	O01-C02-C03-O11
3	A	1505	PGW	O01-C02-C03-O11
3	B	808	PGW	C01-C02-C03-O11
3	A	1509	PGW	C01-C02-C03-O11
3	B	806	PGW	C22-C23-C24-C25
3	A	1507	PGW	C22-C23-C24-C25
3	B	808	PGW	C20-C19-O03-C01
3	A	1509	PGW	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
3	B	805	PGW	C02-C03-O11-P
3	A	1506	PGW	C02-C03-O11-P
3	B	804	PGW	C19-C20-C21-C22
3	A	1505	PGW	C19-C20-C21-C22
3	B	808	PGW	O01-C02-C03-O11
3	A	1509	PGW	O01-C02-C03-O11
3	B	808	PGW	C4-C5-C6-C7
3	A	1509	PGW	C4-C5-C6-C7
3	B	805	PGW	C5-C6-C7-C8
3	A	1506	PGW	C5-C6-C7-C8
3	B	807	PGW	C6-C7-C8-C9
3	A	1508	PGW	C6-C7-C8-C9
3	B	807	PGW	C01-C02-C03-O11
3	A	1508	PGW	C01-C02-C03-O11
3	B	805	PGW	O03-C01-C02-C03
3	A	1506	PGW	O03-C01-C02-C03
3	B	807	PGW	O01-C02-C03-O11
3	A	1508	PGW	O01-C02-C03-O11
3	B	808	PGW	O03-C01-C02-O01
3	A	1509	PGW	O03-C01-C02-O01
3	B	808	PGW	O04-C19-O03-C01
3	A	1509	PGW	O04-C19-O03-C01
3	B	804	PGW	C04-C05-CAD-OAE
3	A	1505	PGW	C04-C05-CAD-OAE
3	B	804	PGW	C23-C24-C25-C26
3	A	1505	PGW	C23-C24-C25-C26
3	B	804	PGW	C01-C02-C03-O11
3	A	1505	PGW	C01-C02-C03-O11
3	B	809	PGW	O04-C19-C20-C21
3	A	1501	PGW	O04-C19-C20-C21
3	B	809	PGW	C6-C7-C8-C9
3	A	1501	PGW	C6-C7-C8-C9
3	B	808	PGW	O03-C19-C20-C21
3	A	1509	PGW	O03-C19-C20-C21
3	B	804	PGW	C2-C3-C4-C5
3	A	1508	PGW	C4-C5-C6-C7
3	A	1505	PGW	C2-C3-C4-C5
3	B	807	PGW	C4-C5-C6-C7
3	B	804	PGW	C04-O12-P-O11
3	A	1505	PGW	C04-O12-P-O11
3	B	808	PGW	O03-C01-C02-C03
3	A	1509	PGW	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
3	B	805	PGW	C1-C2-C3-C4
3	A	1506	PGW	C1-C2-C3-C4
3	B	808	PGW	C19-C20-C21-C22
3	A	1509	PGW	C19-C20-C21-C22
3	B	804	PGW	C03-C02-O01-C1
3	B	807	PGW	C01-C02-O01-C1
3	A	1505	PGW	C03-C02-O01-C1
3	A	1508	PGW	C01-C02-O01-C1
3	B	809	PGW	O03-C19-C20-C21
3	A	1501	PGW	O03-C19-C20-C21
3	A	1507	PGW	C27-C15-C16-C17
3	B	806	PGW	C27-C15-C16-C17
3	B	809	PGW	O03-C01-C02-O01
3	A	1501	PGW	O03-C01-C02-O01
3	B	809	PGW	O01-C1-C2-C3
3	A	1501	PGW	O01-C1-C2-C3
3	B	807	PGW	C07-C06-C10-C9
3	A	1508	PGW	C07-C06-C10-C9
3	B	803	PGW	O03-C19-C20-C21
3	A	1504	PGW	O03-C19-C20-C21
3	B	808	PGW	C2-C3-C4-C5
3	A	1509	PGW	C2-C3-C4-C5
3	B	806	PGW	O01-C1-C2-C3
3	A	1507	PGW	O01-C1-C2-C3
3	B	806	PGW	C7-C8-C9-C10
3	A	1507	PGW	C7-C8-C9-C10
3	B	806	PGW	O03-C19-C20-C21
3	A	1507	PGW	O03-C19-C20-C21
3	B	803	PGW	O04-C19-C20-C21
3	A	1504	PGW	O04-C19-C20-C21
3	B	806	PGW	O02-C1-C2-C3
3	A	1507	PGW	O02-C1-C2-C3
3	B	806	PGW	O04-C19-C20-C21
3	A	1507	PGW	O04-C19-C20-C21
3	B	809	PGW	C5-C6-C7-C8
3	A	1501	PGW	C5-C6-C7-C8
3	B	808	PGW	O01-C1-C2-C3
3	A	1509	PGW	O01-C1-C2-C3

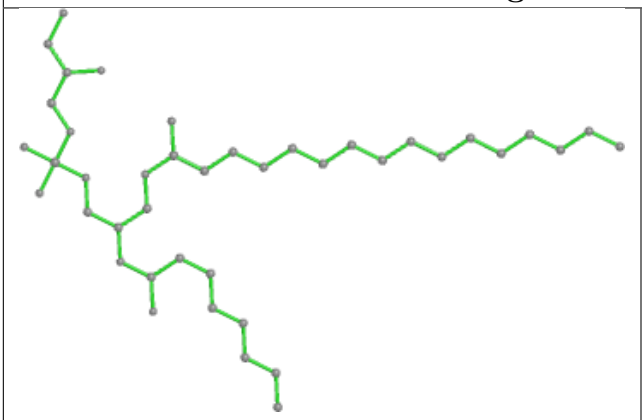
There are no ring outliers.

14 monomers are involved in 30 short contacts:

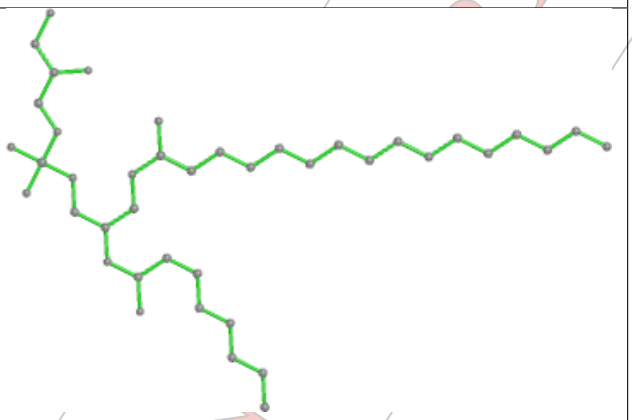
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1505	PGW	6	0
3	B	807	PGW	1	0
3	A	1501	PGW	2	0
3	A	1507	PGW	3	0
3	B	806	PGW	2	0
3	B	804	PGW	6	0
3	A	1506	PGW	2	0
3	B	803	PGW	1	0
3	B	808	PGW	2	0
3	A	1509	PGW	2	0
3	A	1508	PGW	1	0
3	B	805	PGW	2	0
3	A	1504	PGW	1	0
3	B	809	PGW	1	0

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

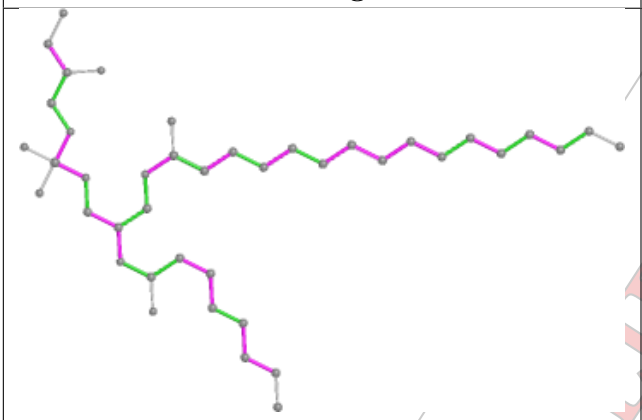
Ligand PGW A 1505



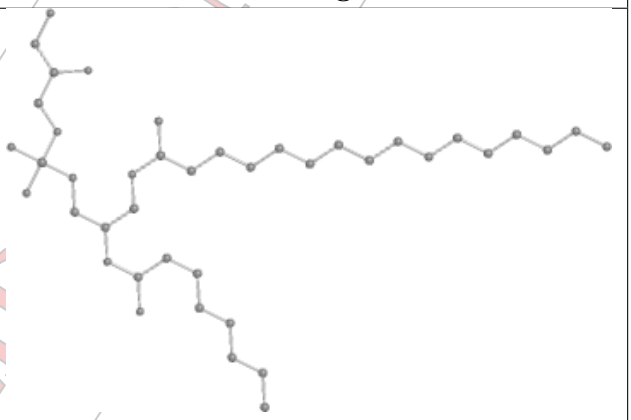
Bond lengths



Bond angles

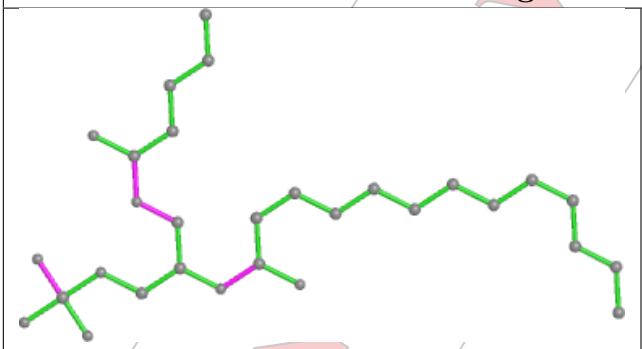


Torsions

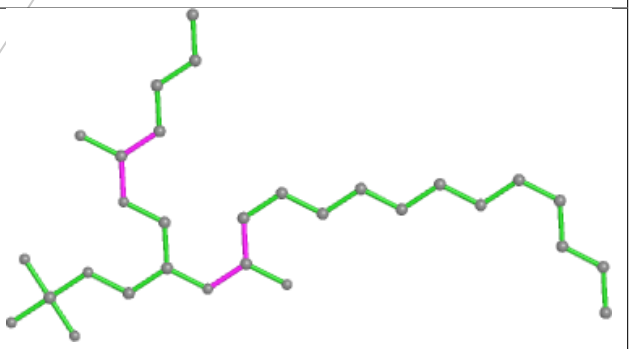


Rings

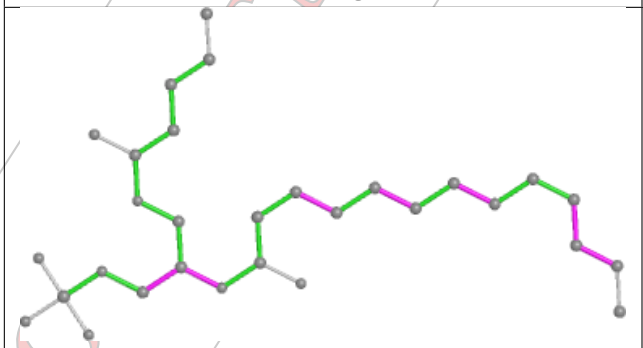
Ligand PGW B 807



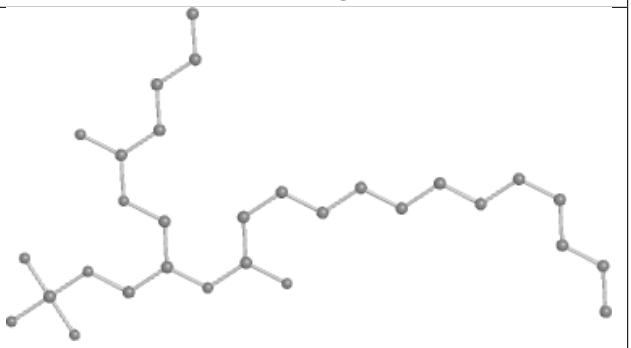
Bond lengths



Bond angles

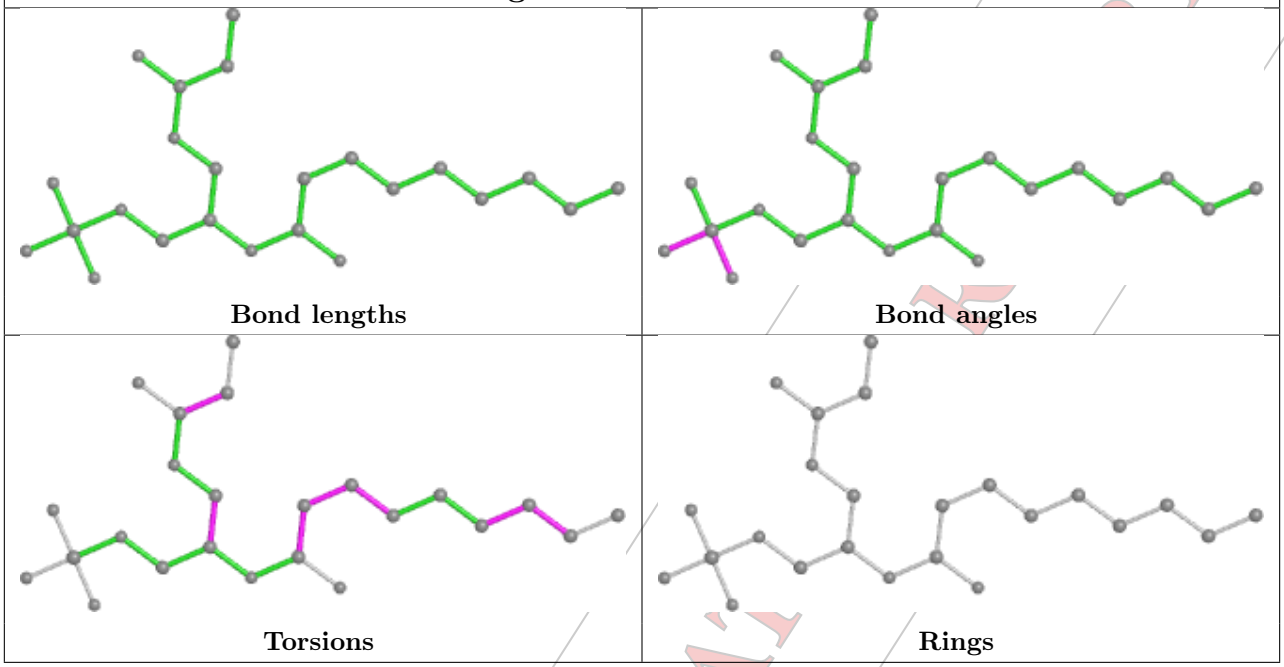


Torsions

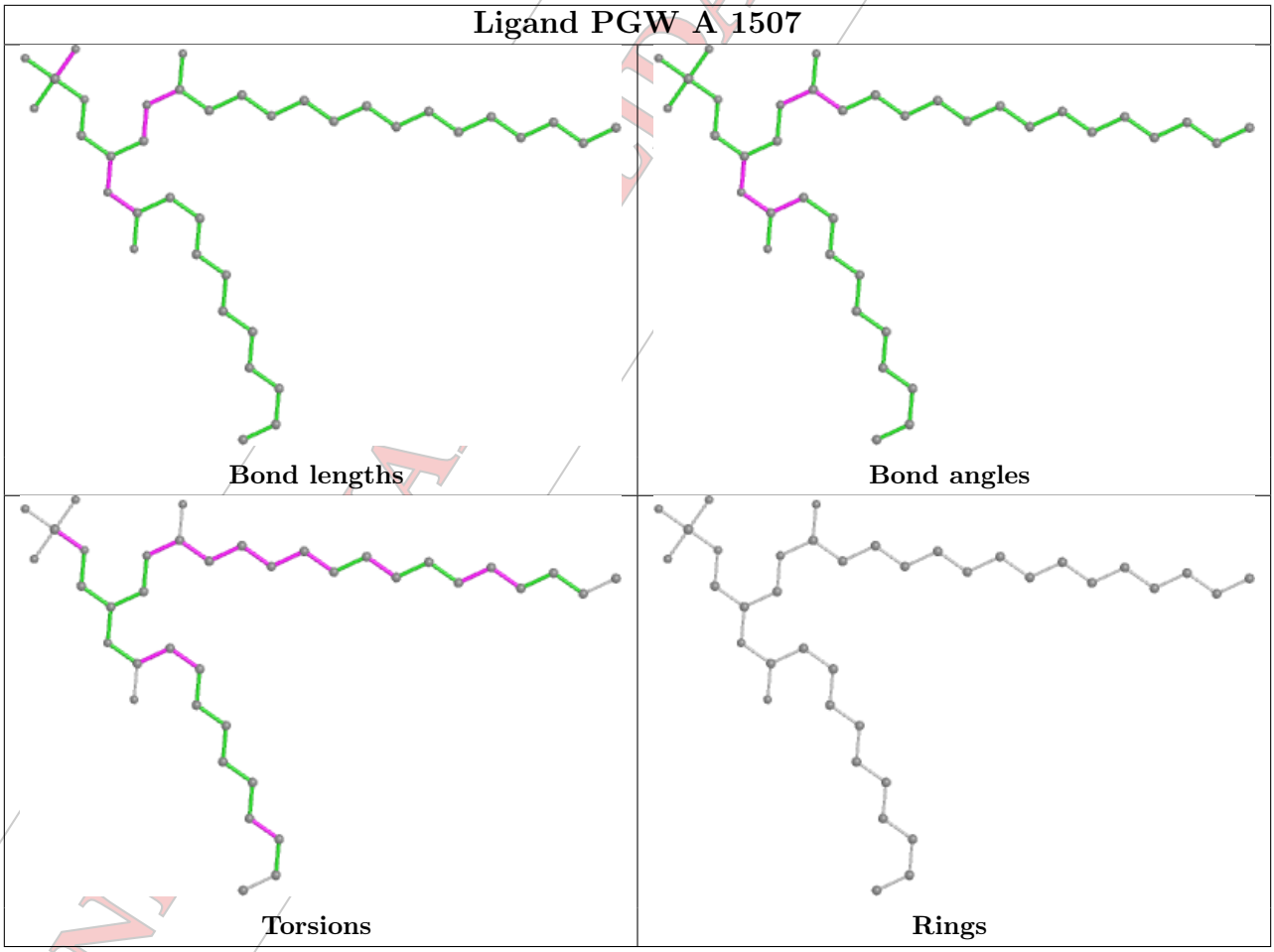


Rings

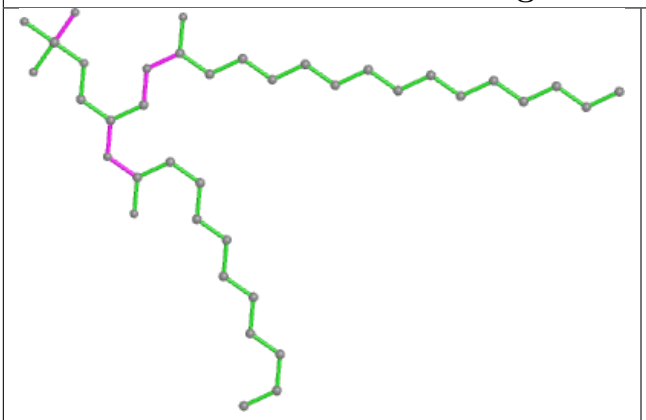
Ligand PGW A 1501



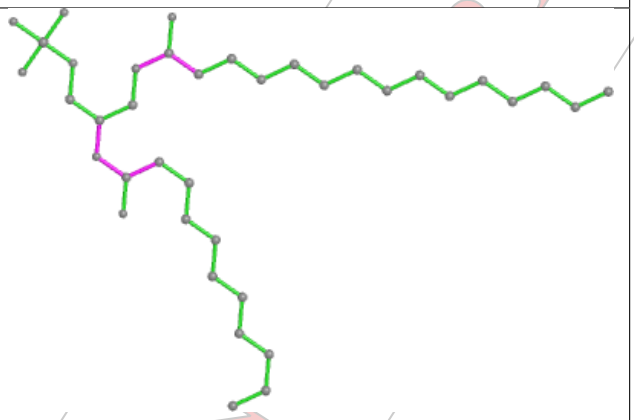
Ligand PGW A 1507



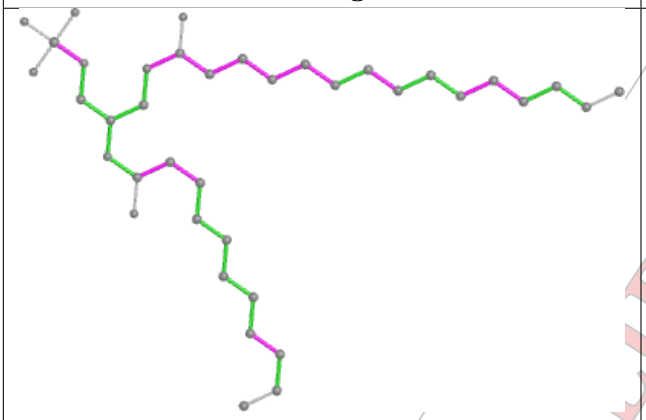
Ligand PGW B 806



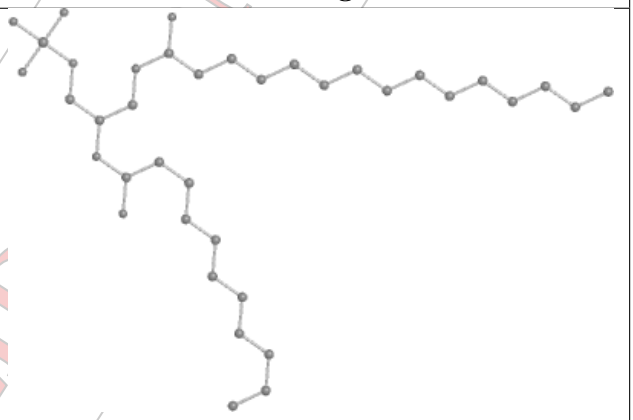
Bond lengths



Bond angles

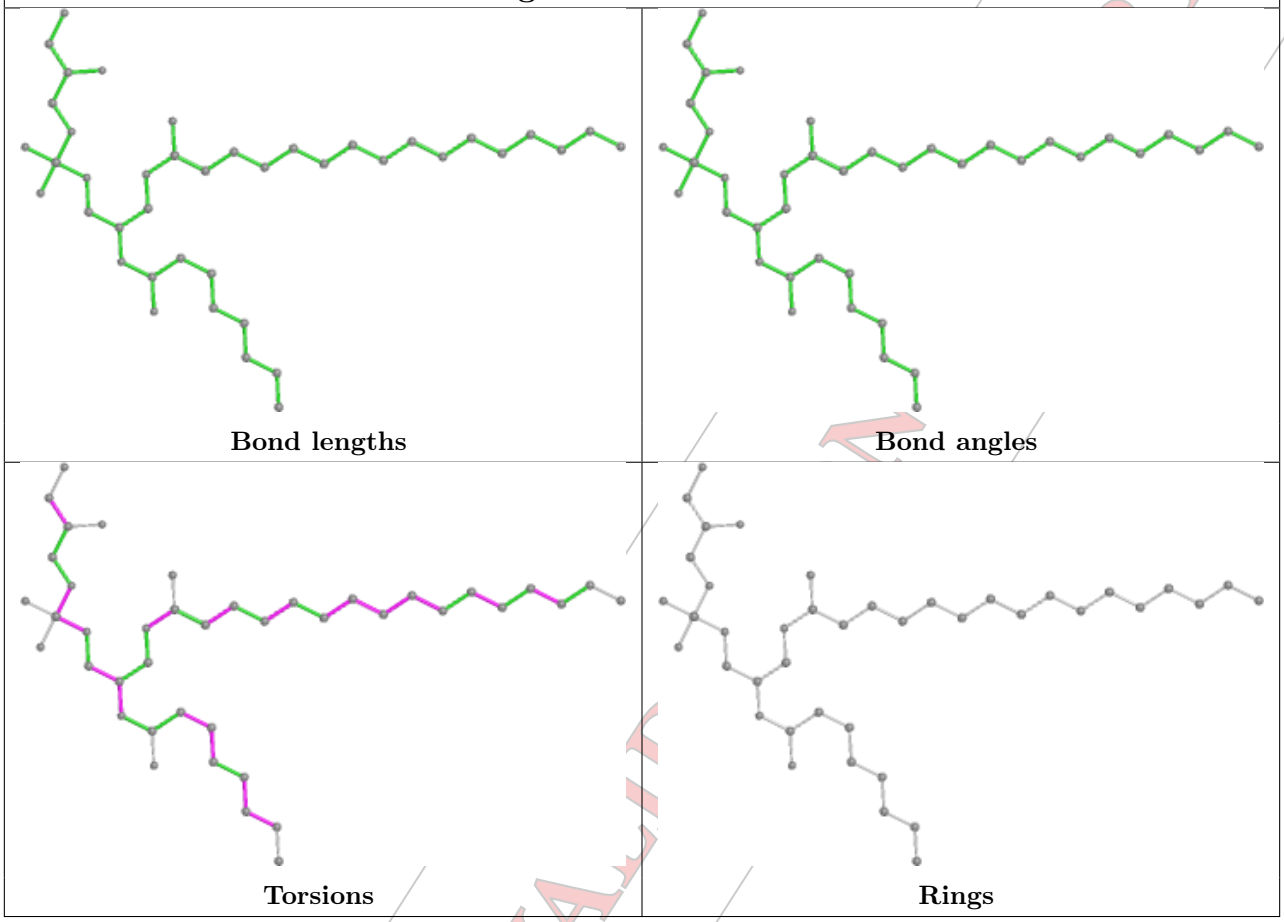


Torsions

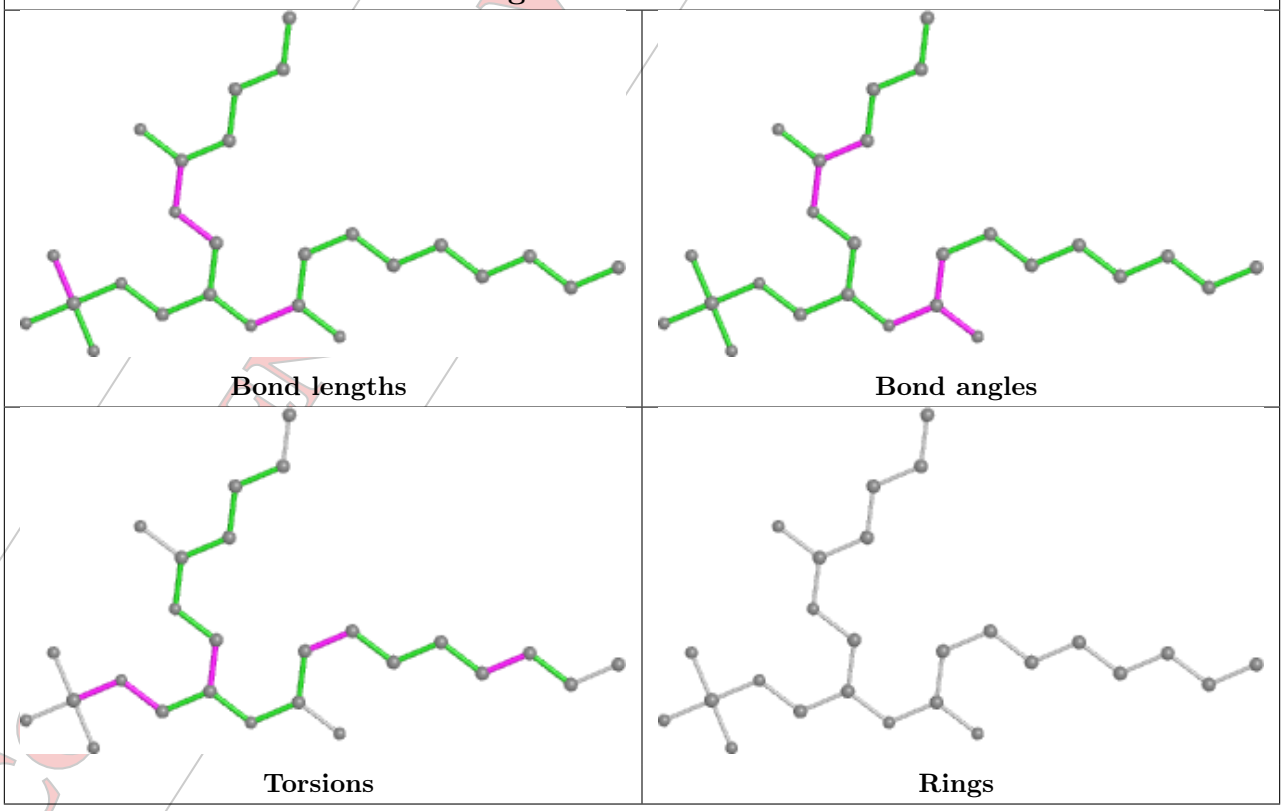


Rings

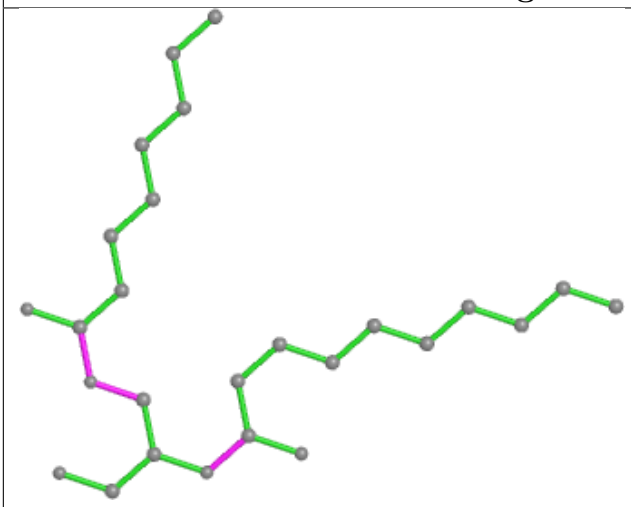
Ligand PGW B 804



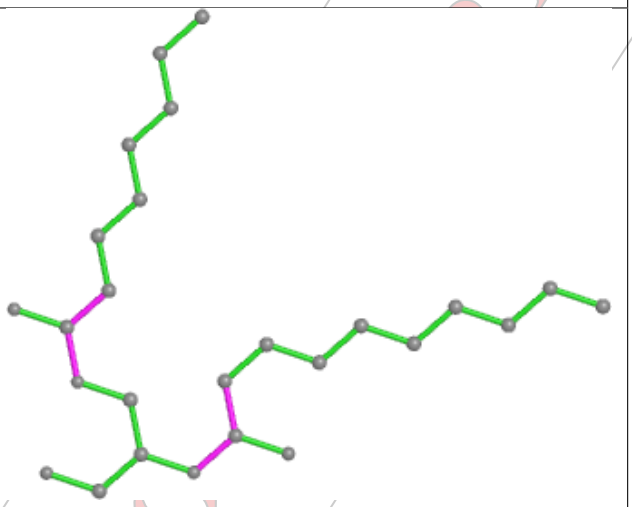
Ligand PGW A 1506



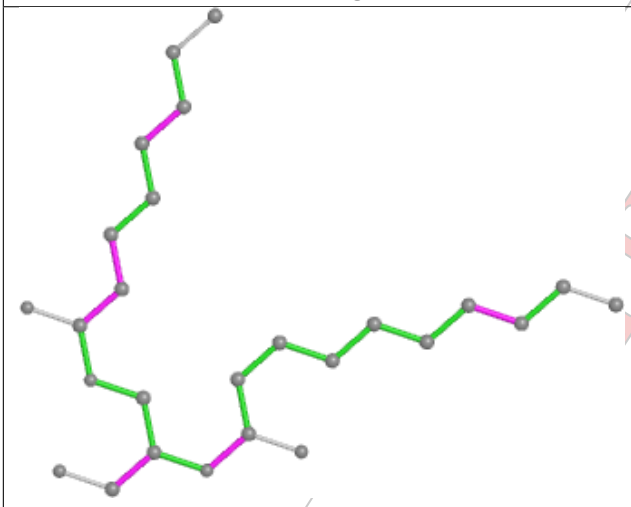
Ligand PGW B 803



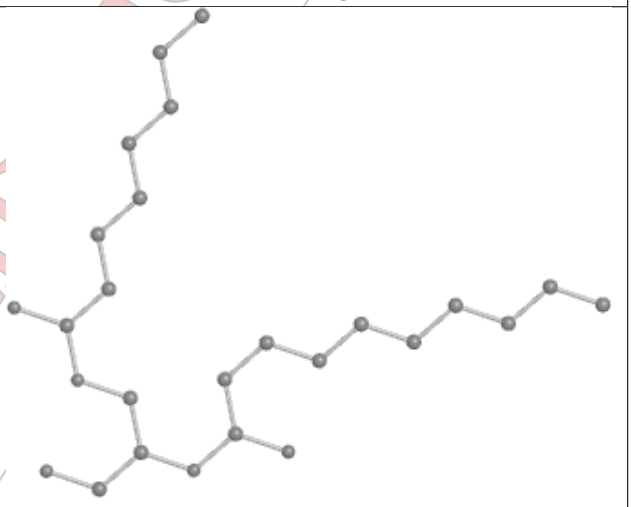
Bond lengths



Bond angles

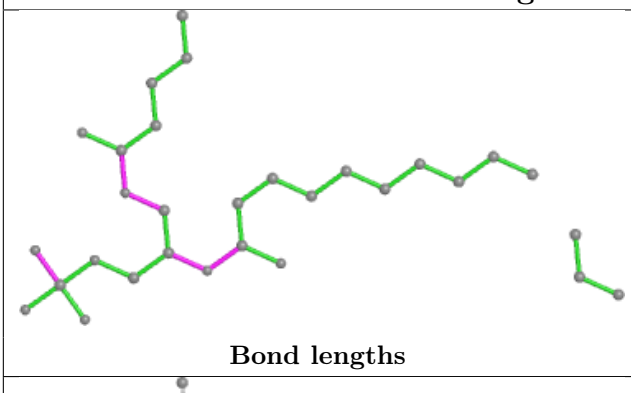


Torsions

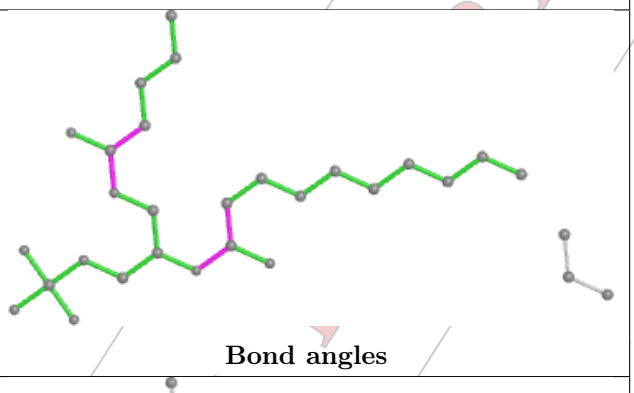


Rings

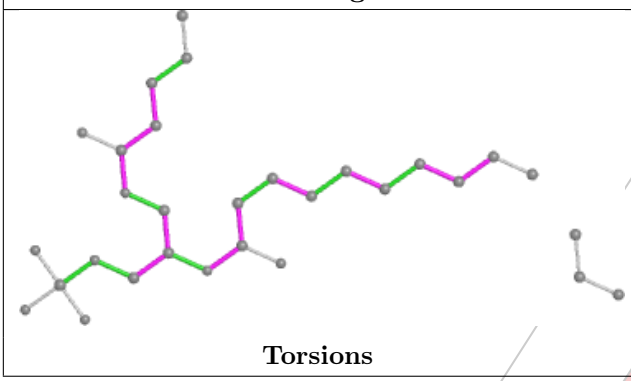
Ligand PGW B 808



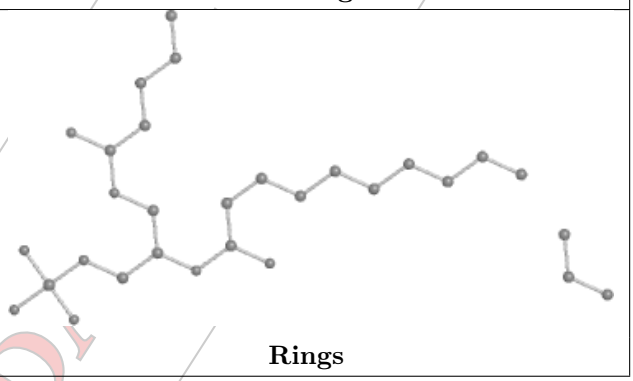
Bond lengths



Bond angles

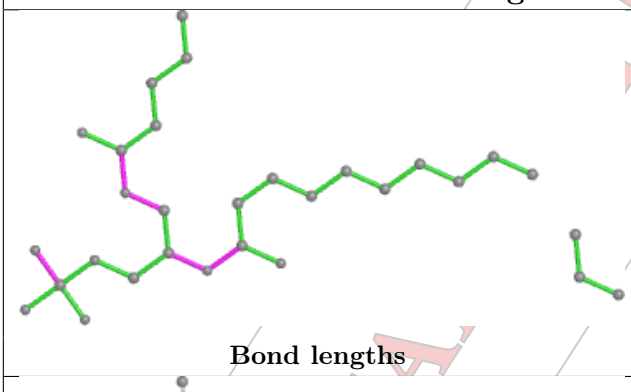


Torsions

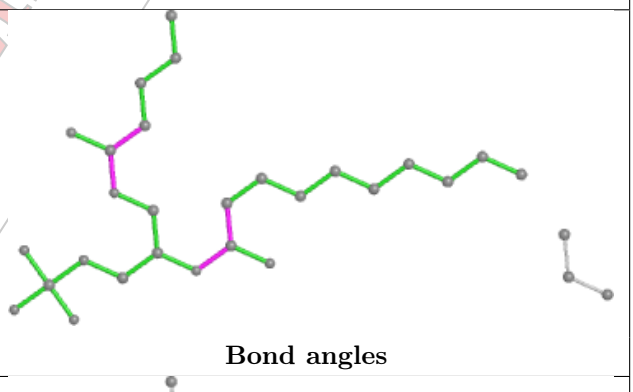


Rings

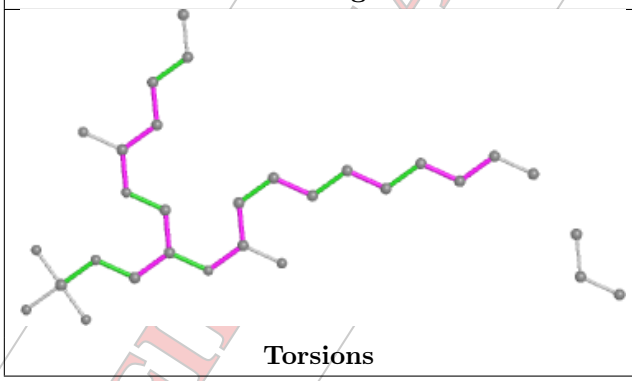
Ligand PGW A 1509



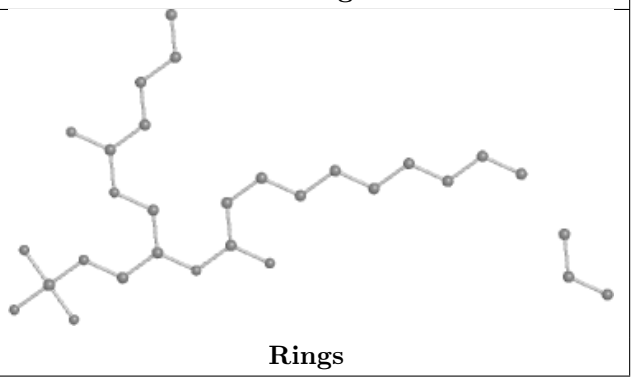
Bond lengths



Bond angles

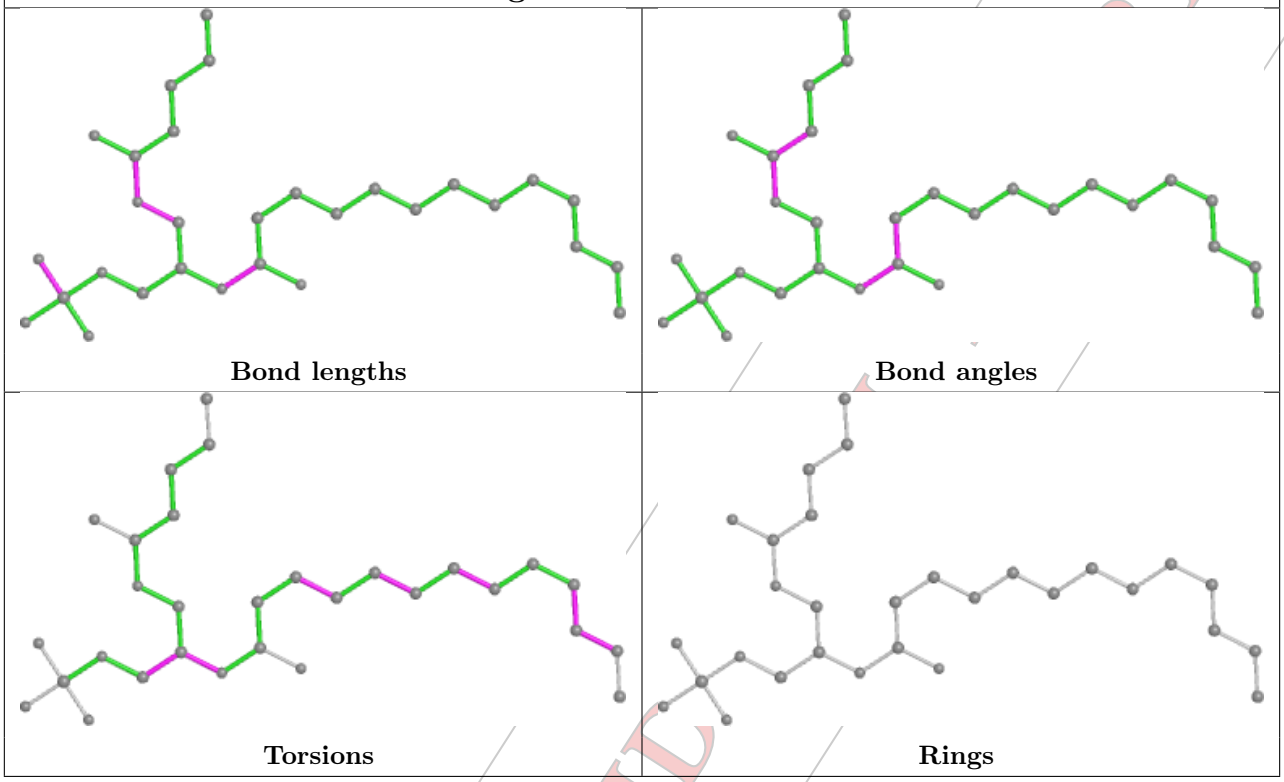


Torsions

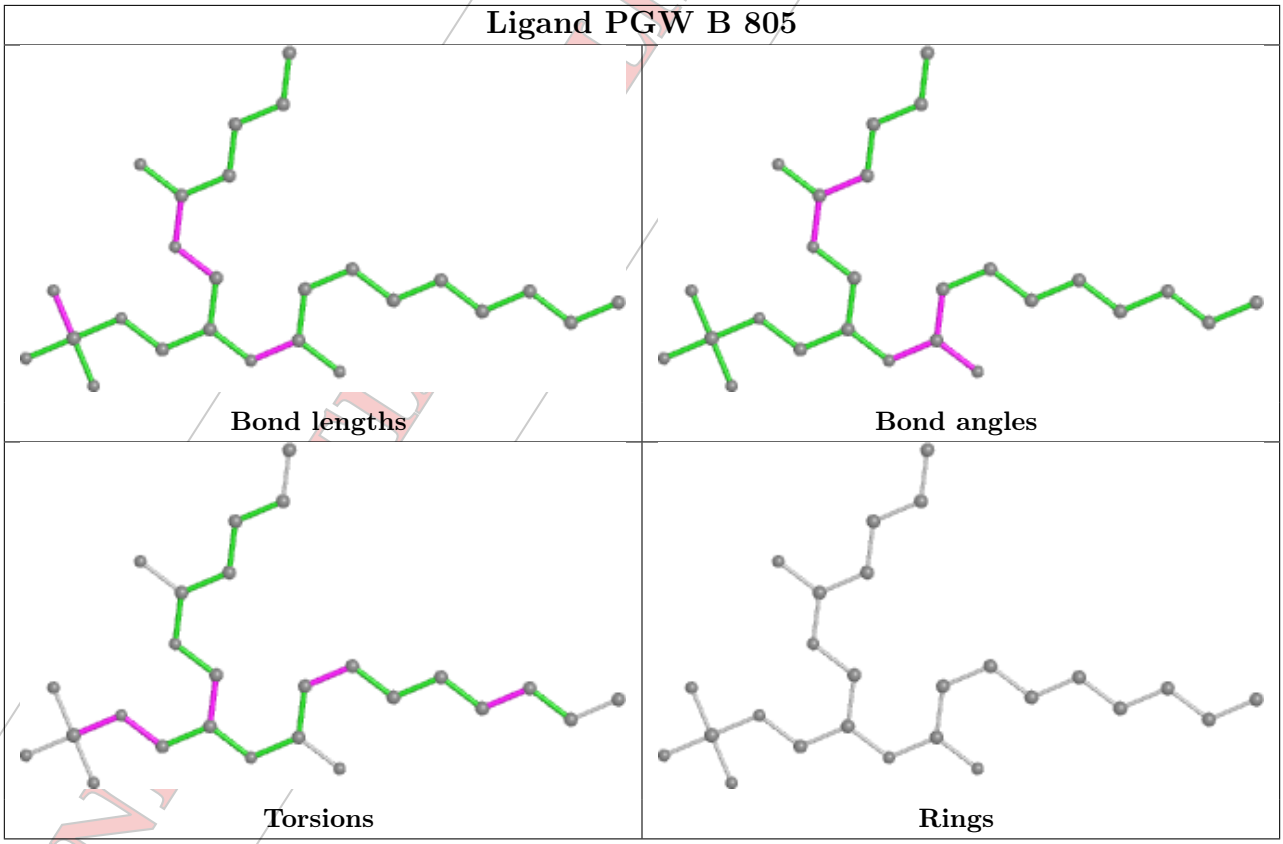


Rings

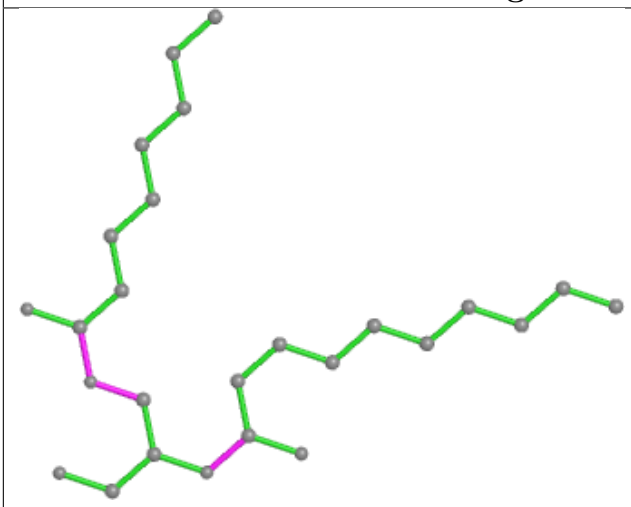
Ligand PGW A 1508



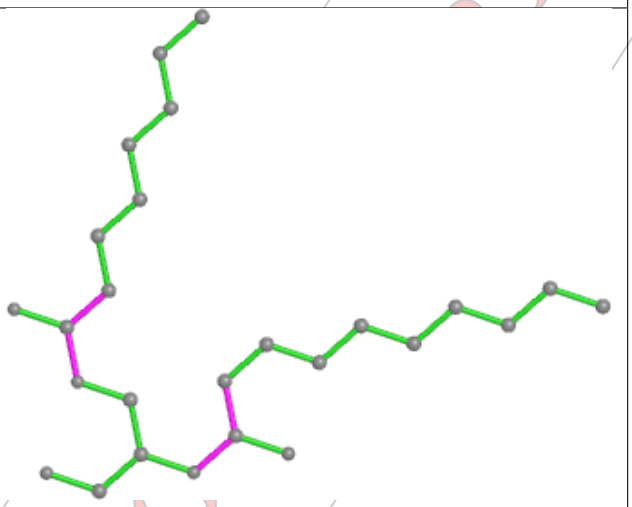
Ligand PGW B 805



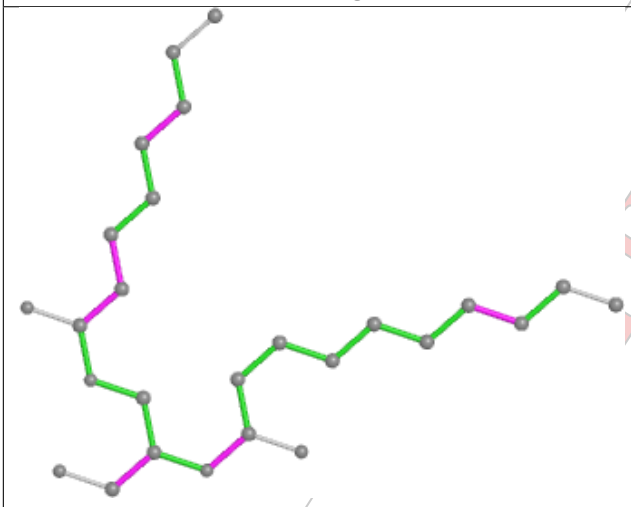
Ligand PGW A 1504



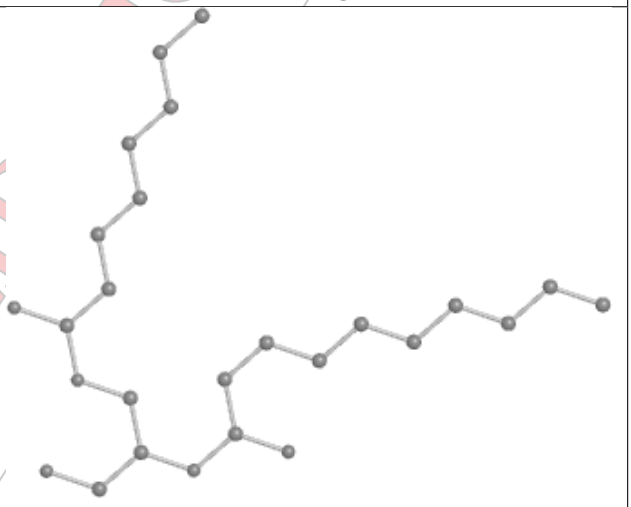
Bond lengths



Bond angles

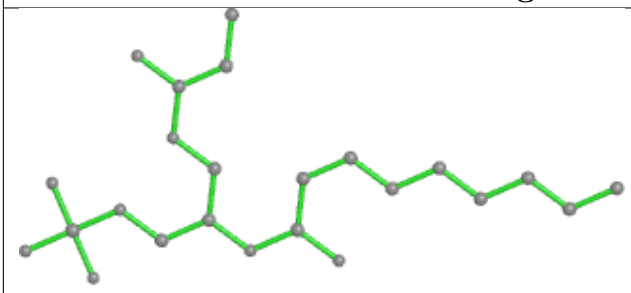


Torsions

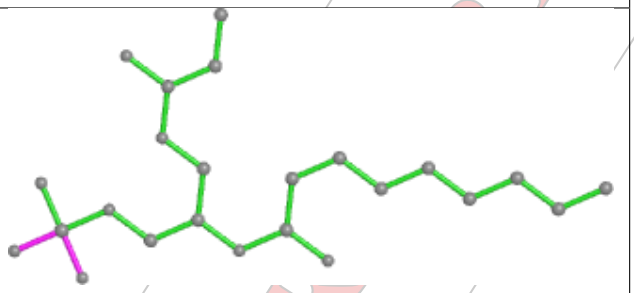


Rings

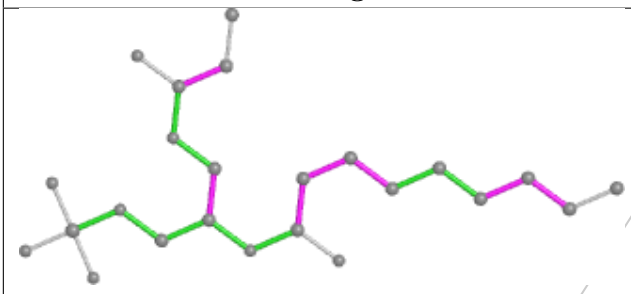
Ligand PGW B 809



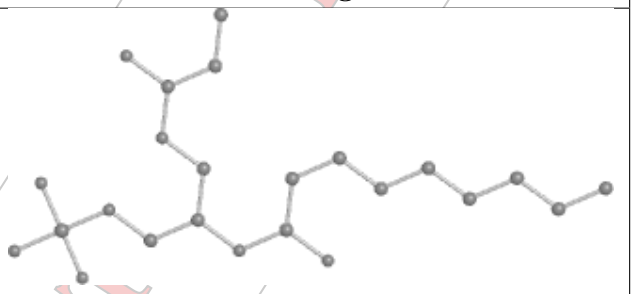
Bond lengths



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.

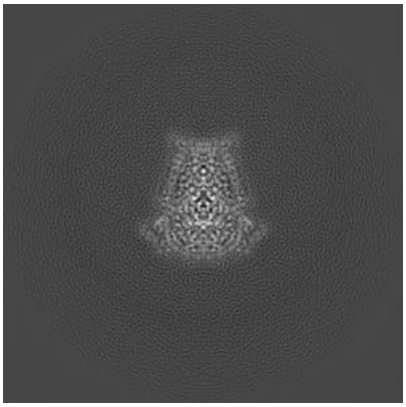
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24722. These allow visual inspection of the internal detail of the map and identification of artifacts.

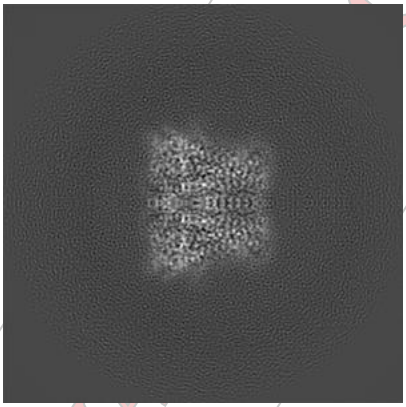
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

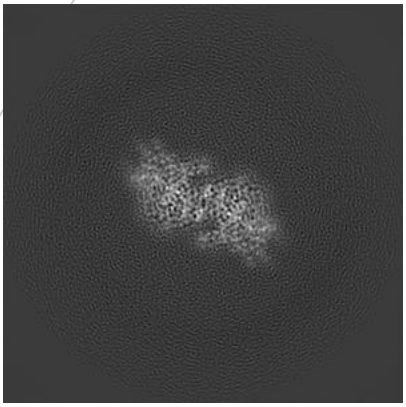
6.1.1 Primary map



X



Y

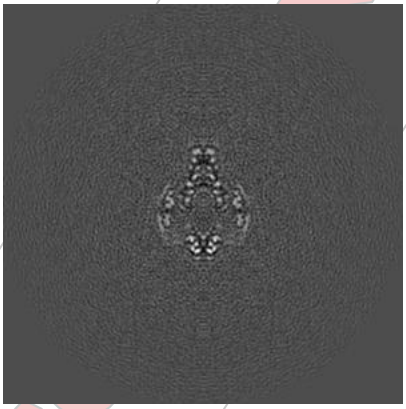


Z

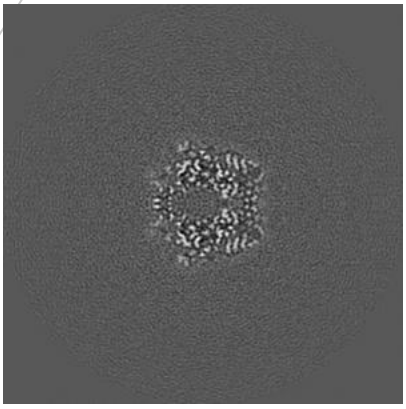
The images above show the map projected in three orthogonal directions.

6.2 Central slices

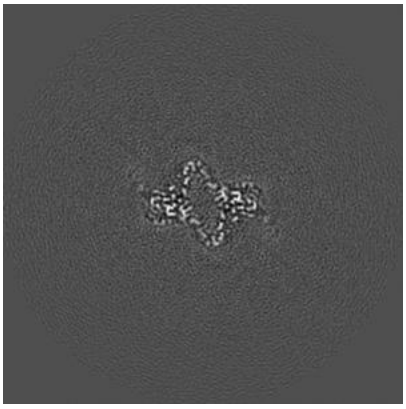
6.2.1 Primary map



X Index: 192



Y Index: 192

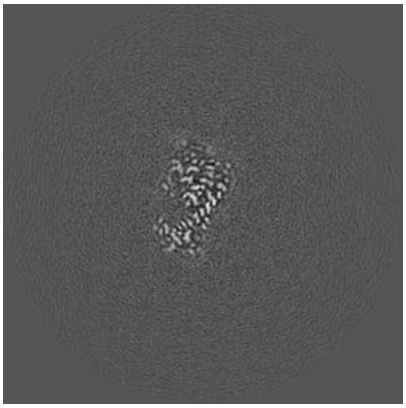


Z Index: 192

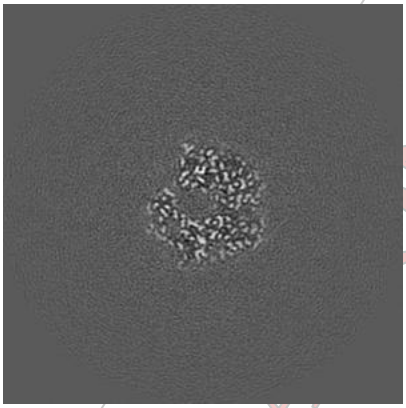
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

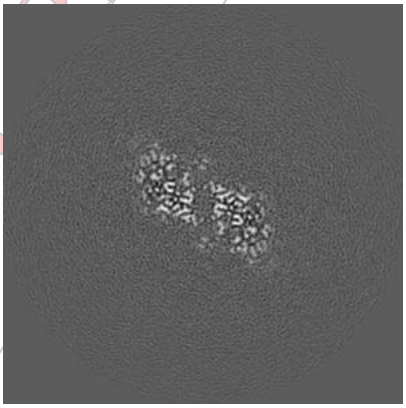
6.3.1 Primary map



X Index: 222



Y Index: 196



Z Index: 172

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

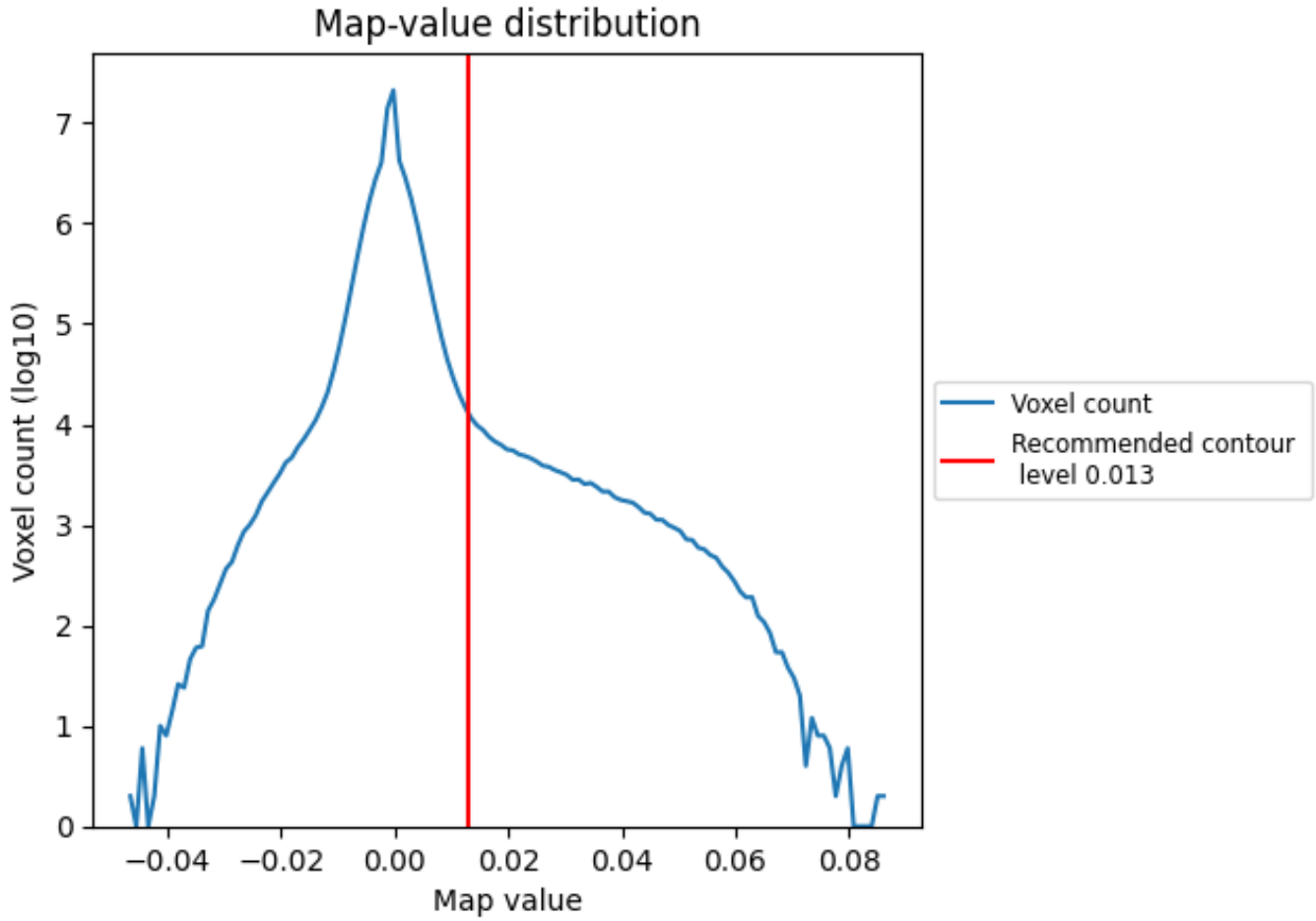
6.5 Mask visualisation (i)

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

7 Map analysis

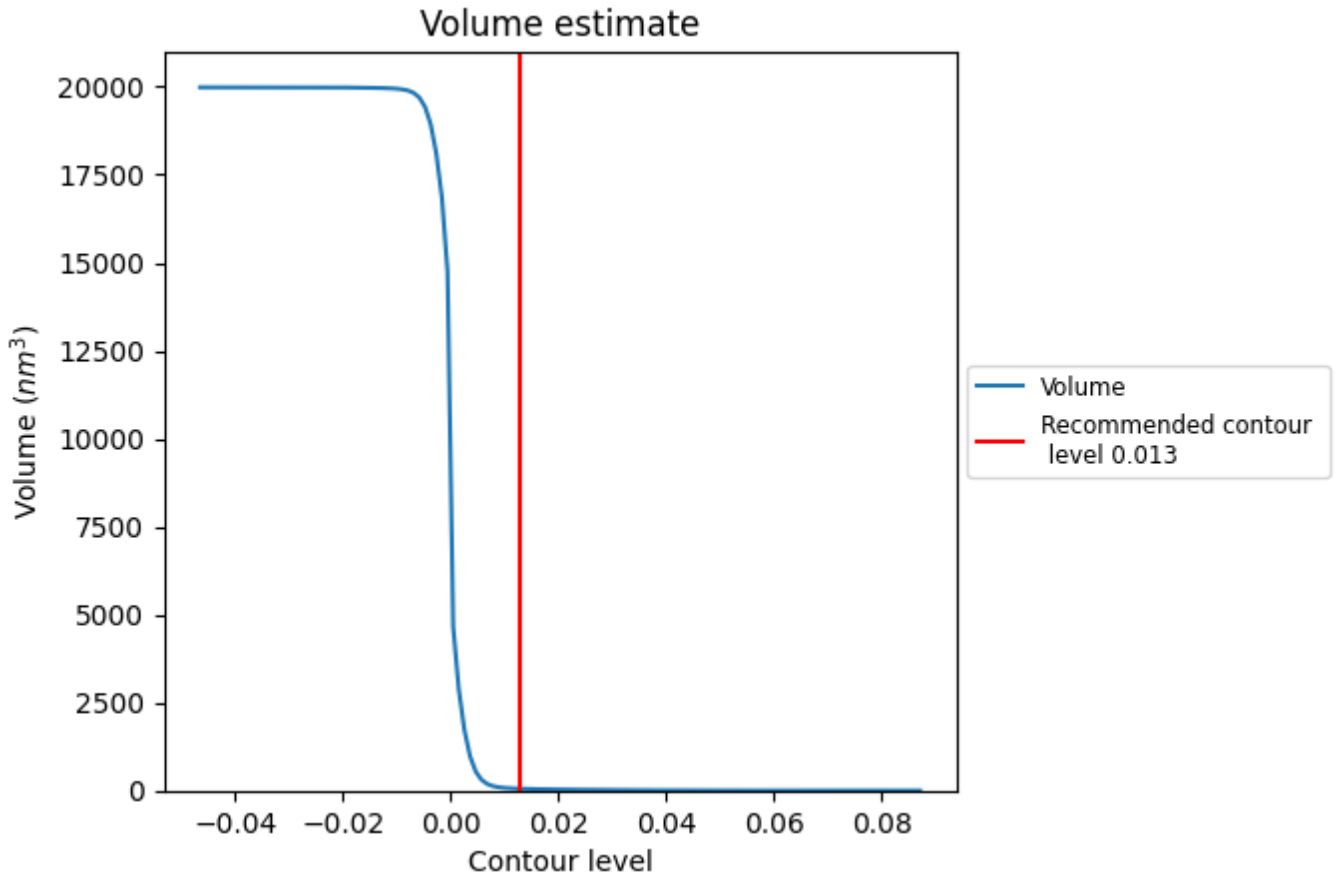
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

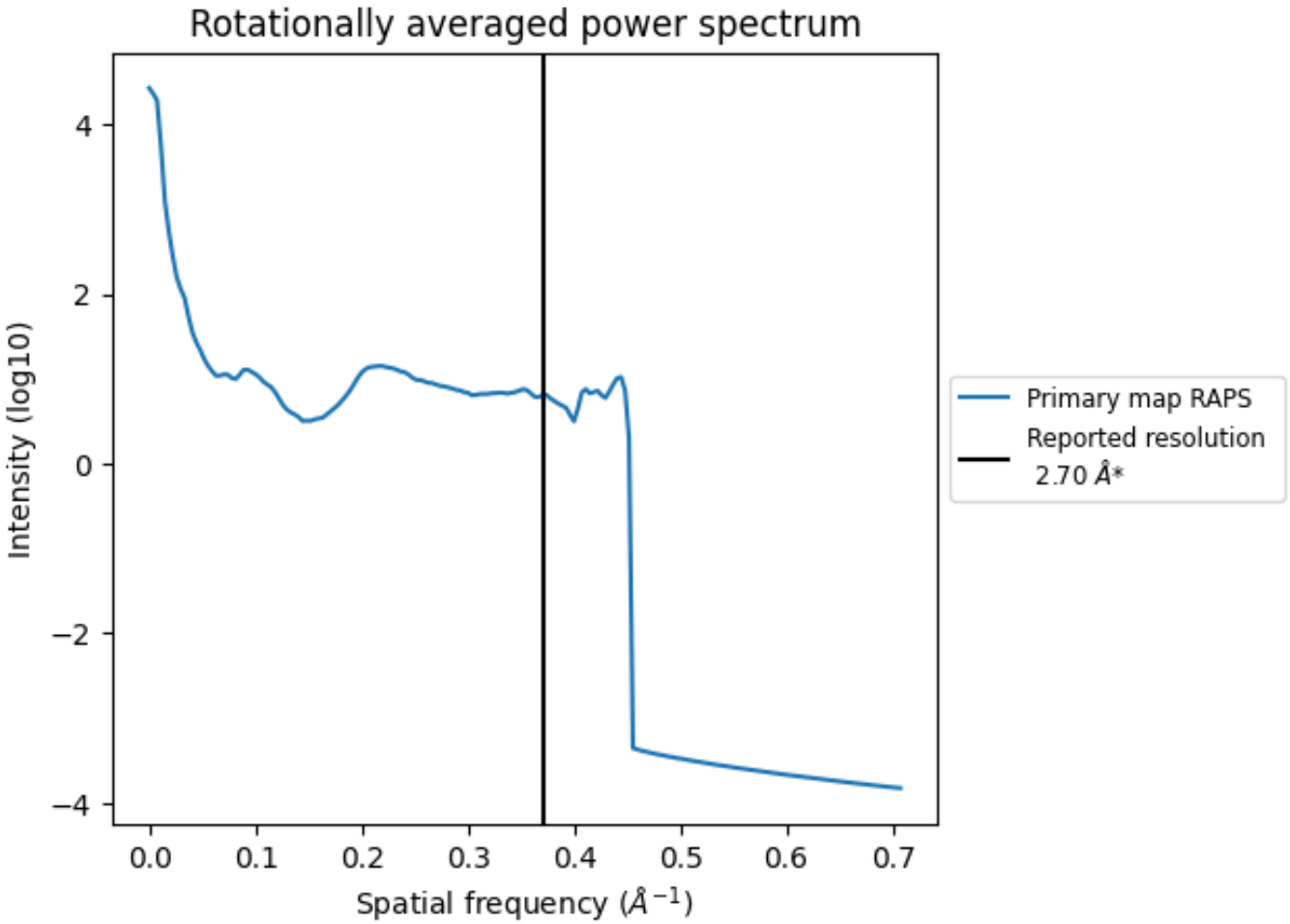
7.2 Volume estimate



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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)

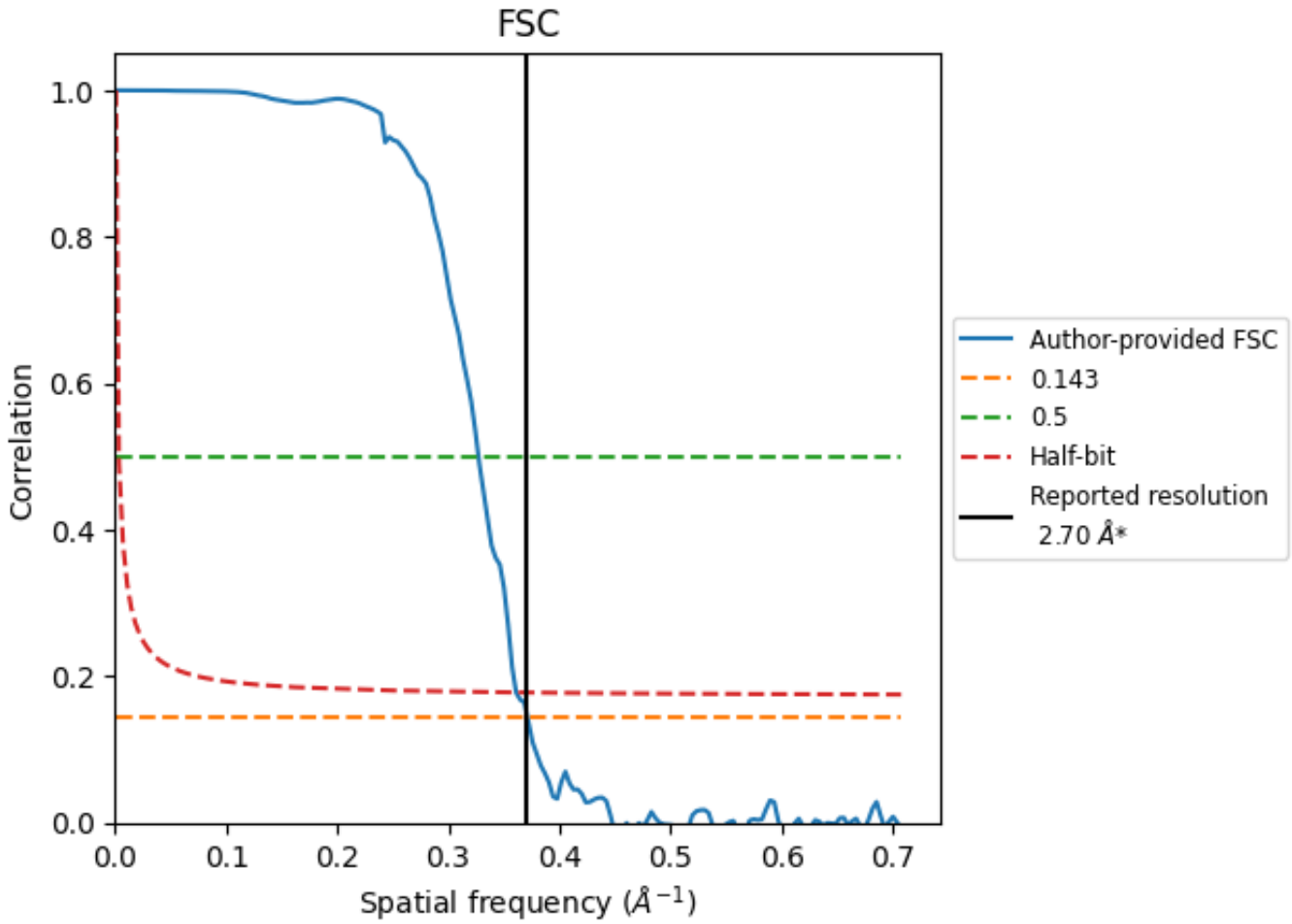


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

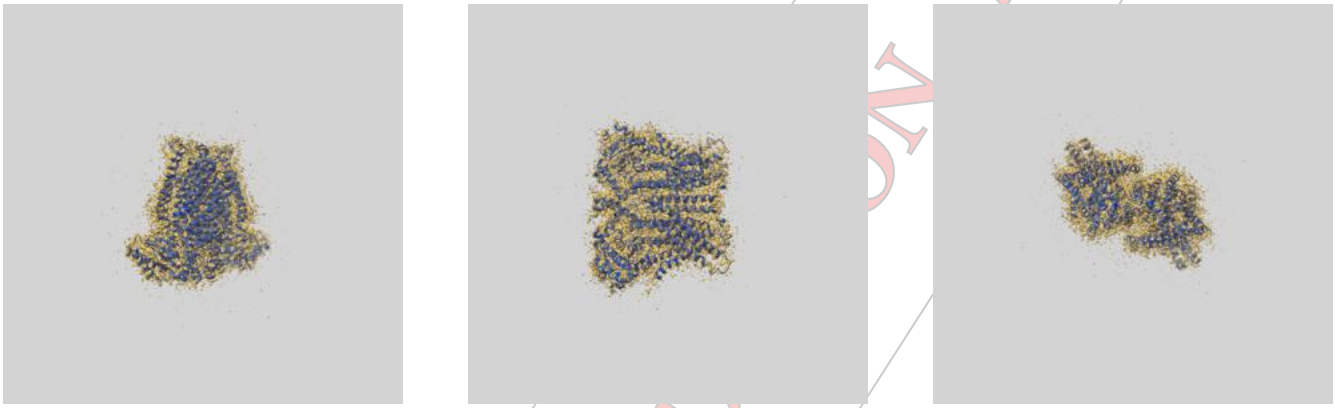
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.06	2.77
Unmasked-calculated*	-	-	-

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24722 and PDB model 7RX2. Per-residue inclusion information can be found in section 3 on page 5.

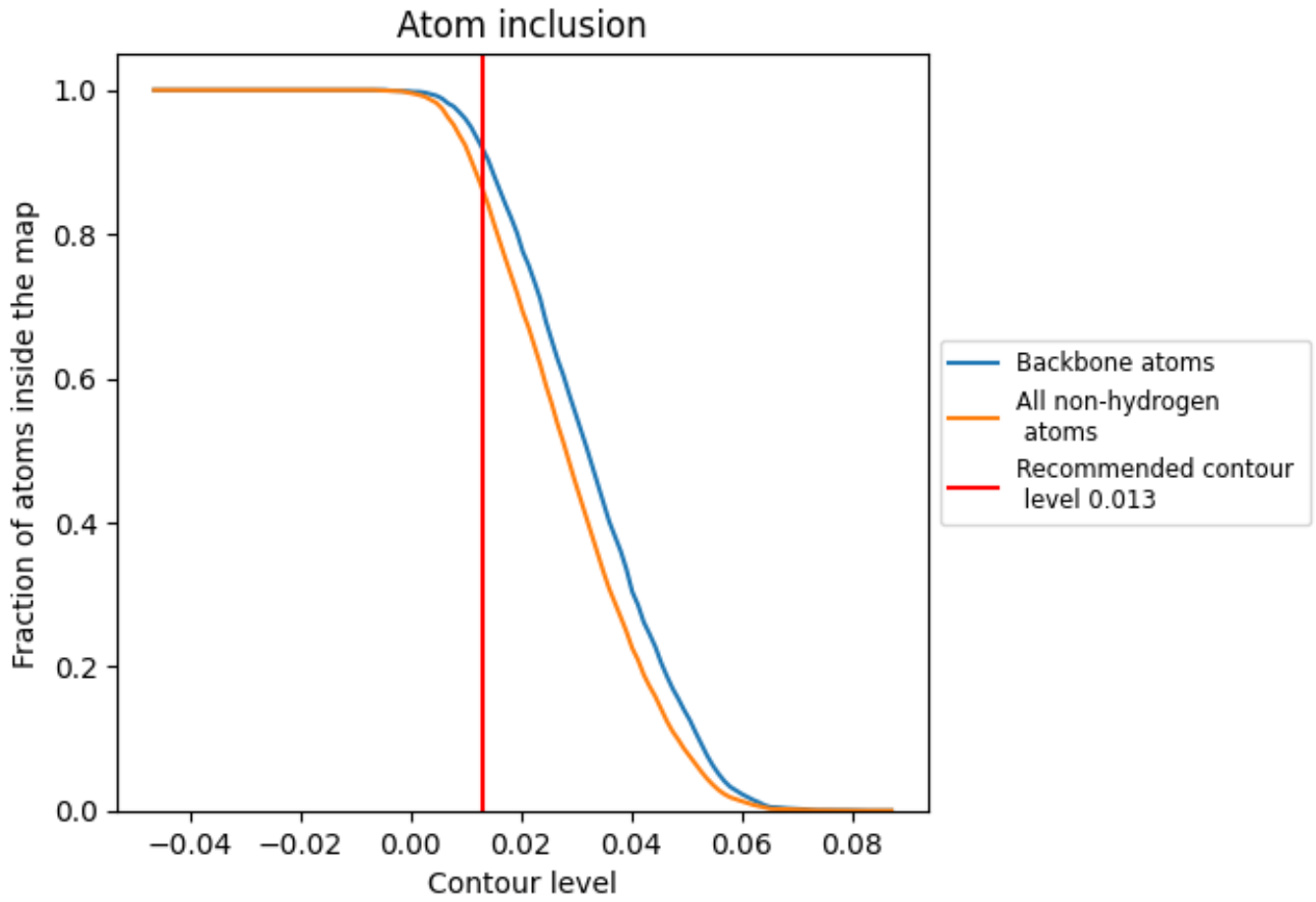
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

Full wwPDB EM Validation Report ⓘ

Aug 30, 2021 – 10:15 AM EDT

PDB ID	:	7RX3
EMDB ID	:	EMD-24723
Title	:	afTMEM16 in C14 lipid nanodiscs with MSP1E3 scaffold protein in the absence of Ca2+
Deposited on	:	2021-08-21
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

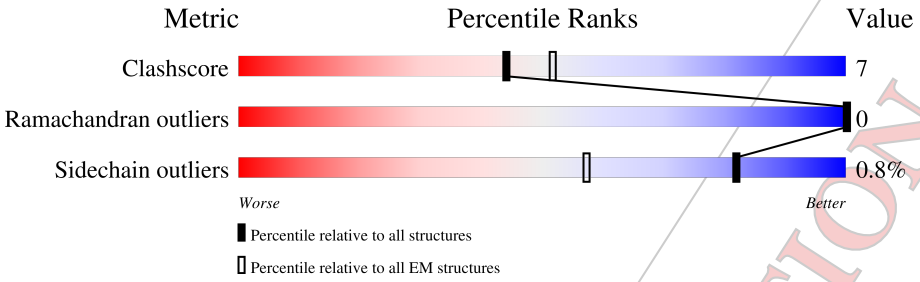
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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 <=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	735	71% 10% 20%
1	B	735	71% 9% 20%

2 Entry composition

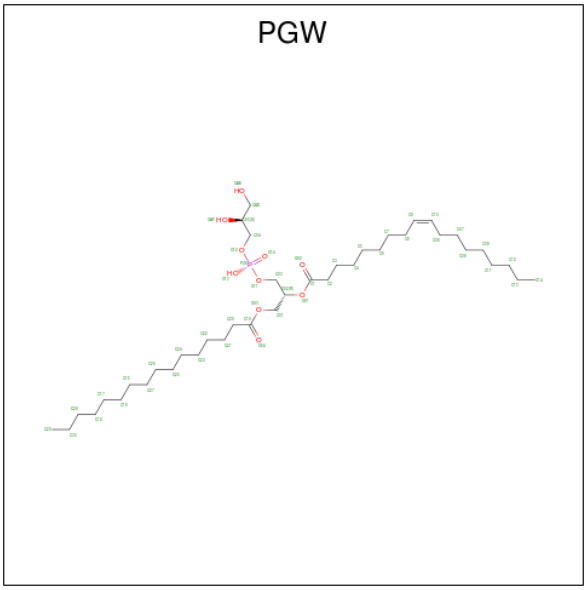
There are 2 unique types of molecules in this entry. The entry contains 10130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 afTMEM16 lipid scramblase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	591	Total	C	N	O	S	0	0
			4786	3135	800	832	19		
1	A	591	Total	C	N	O	S	0	0
			4786	3135	800	832	19		

- Molecule 2 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	O	P	0
			279	207	65	7	
2	B	1	Total	C	O	P	0
			279	207	65	7	
2	B	1	Total	C	O	P	0
			279	207	65	7	
2	B	1	Total	C	O	P	0
			279	207	65	7	

Continued on next page...

Continued from previous page...

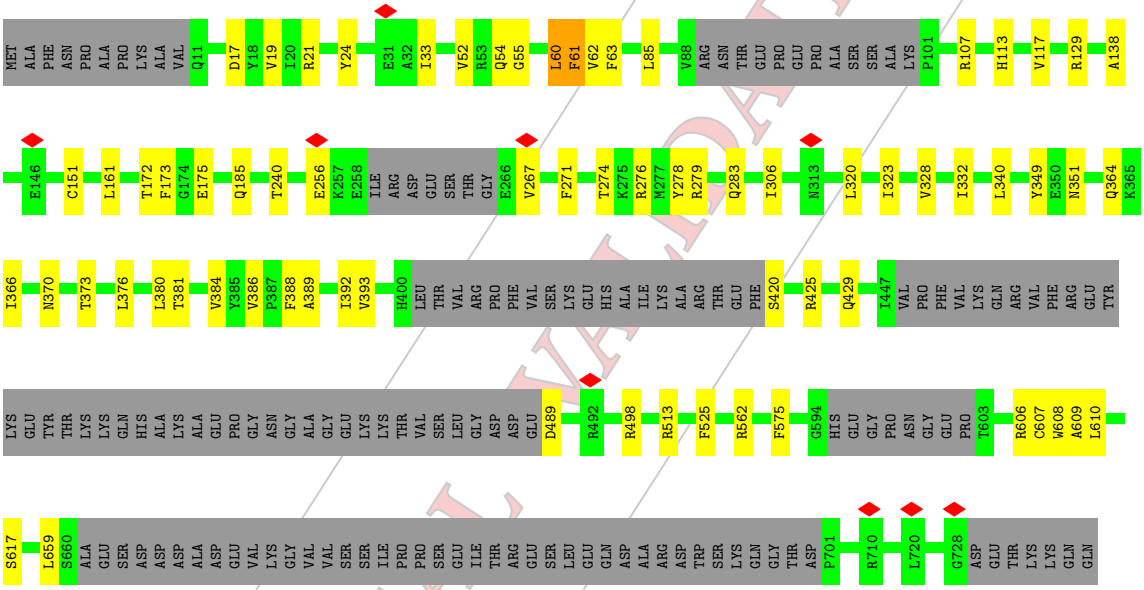
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 279	C 207	O 65	P 7	0
2	B	1	Total 279	C 207	O 65	P 7	0
2	B	1	Total 279	C 207	O 65	P 7	0
2	B	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0
2	A	1	Total 279	C 207	O 65	P 7	0

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.

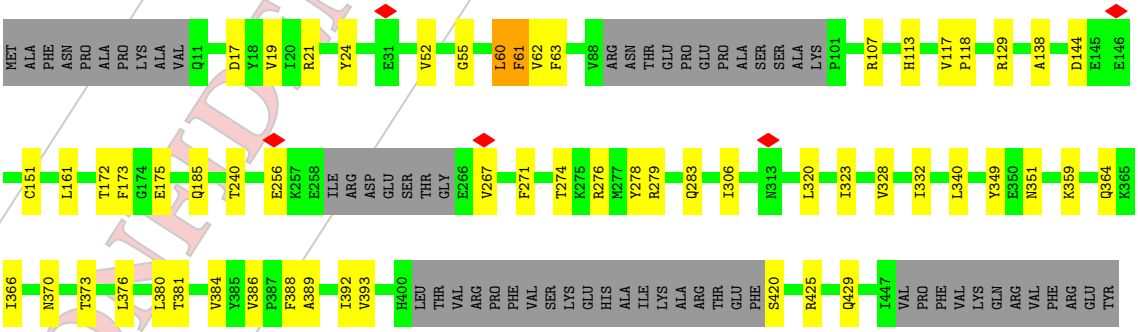
- Molecule 1: afTMEM16 lipid scramblase

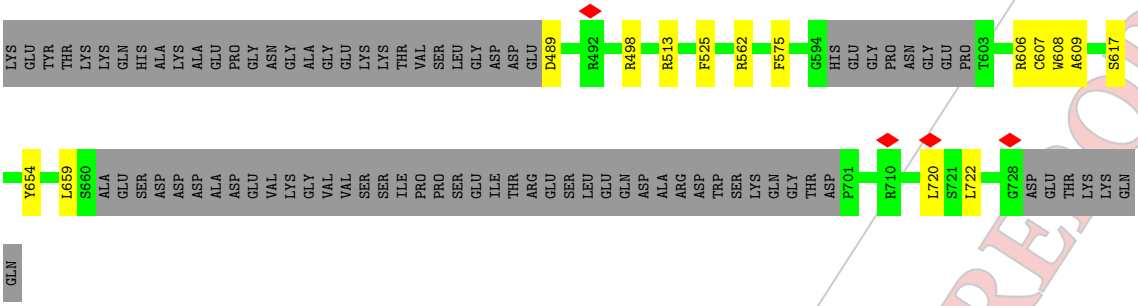
Chain B:



- Molecule 1: afTMEM16 lipid scramblase

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	244507	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 ($e^-/Å^2$)	71.68	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.39	0/4909	0.55	0/6667
1	B	0.38	0/4909	0.55	0/6667
All	All	0.39	0/9818	0.55	0/13334

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	4786	0	4763	72	0
1	B	4786	0	4763	65	0
2	A	279	0	342	12	0
2	B	279	0	342	11	0
All	All	10130	0	10210	140	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 7.

All (140) 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:328:VAL:O	1:B:332:ILE:HG13	1.82	0.79
1:B:21:ARG:HA	1:B:61:PHE:HB3	1.65	0.79
1:A:328:VAL:O	1:A:332:ILE:HG13	1.83	0.78
1:A:175:GLU:OE2	1:A:240:THR:HG21	1.84	0.78
1:A:21:ARG:HA	1:A:61:PHE:HB3	1.65	0.77
1:B:175:GLU:OE2	1:B:240:THR:HG21	1.84	0.77
1:B:659:LEU:HD12	1:B:659:LEU:O	1.87	0.74
1:A:659:LEU:HD12	1:A:659:LEU:O	1.87	0.74
1:B:332:ILE:HG23	1:B:373:THR:HG22	1.71	0.73
1:A:60:LEU:HD22	1:A:60:LEU:O	1.89	0.73
1:A:332:ILE:HG23	1:A:373:THR:HG22	1.71	0.72
1:B:60:LEU:HD22	1:B:60:LEU:O	1.89	0.72
1:A:60:LEU:HD13	1:A:60:LEU:H	1.56	0.71
1:B:60:LEU:H	1:B:60:LEU:HD13	1.56	0.71
1:A:60:LEU:H	1:A:60:LEU:CD1	2.07	0.67
1:A:24:TYR:CE2	1:A:60:LEU:HD12	2.30	0.67
1:B:271:PHE:HZ	1:B:279:ARG:NH1	1.93	0.67
1:A:52:VAL:CG2	1:A:60:LEU:HD23	2.25	0.66
1:B:24:TYR:CE2	1:B:60:LEU:HD12	2.30	0.66
1:A:388:PHE:O	1:A:392:ILE:HG13	1.96	0.66
1:B:370:ASN:HD21	1:B:513:ARG:HG3	1.60	0.66
1:A:271:PHE:HZ	1:A:279:ARG:NH1	1.93	0.66
1:A:370:ASN:HD21	1:A:513:ARG:HG3	1.60	0.66
1:B:60:LEU:H	1:B:60:LEU:CD1	2.07	0.66
1:B:52:VAL:CG2	1:B:60:LEU:HD23	2.25	0.66
1:B:388:PHE:O	1:B:392:ILE:HG13	1.96	0.65
1:B:24:TYR:HE2	1:B:60:LEU:HD12	1.65	0.61
1:A:24:TYR:HE2	1:A:60:LEU:HD12	1.65	0.61
1:A:332:ILE:HG23	1:A:373:THR:CG2	2.31	0.60
1:B:384:VAL:O	1:B:388:PHE:HB2	2.02	0.59
1:A:384:VAL:O	1:A:388:PHE:HB2	2.02	0.59
1:B:332:ILE:HG23	1:B:373:THR:CG2	2.31	0.59
1:A:606:ARG:NH2	2:A:904:PGW:C1	2.66	0.59
1:B:606:ARG:NH2	2:B:801:PGW:C1	2.66	0.59
1:A:381:THR:HG21	1:A:429:GLN:HG3	1.85	0.58
1:A:19:VAL:HG22	1:A:63:PHE:CD2	2.38	0.58
1:B:19:VAL:HG22	1:B:63:PHE:CD2	2.38	0.58
1:B:381:THR:HG21	1:B:429:GLN:HG3	1.85	0.58
1:B:606:ARG:HH22	2:B:801:PGW:C1	2.17	0.58
1:A:271:PHE:CZ	1:A:279:ARG:NH1	2.71	0.57
1:B:271:PHE:CZ	1:B:279:ARG:NH1	2.71	0.57
1:A:606:ARG:HH22	2:A:904:PGW:C1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:OE2	1:B:240:THR:CG2	2.54	0.56
1:A:17:ASP:OD1	1:A:107:ARG:NH2	2.39	0.55
1:B:17:ASP:OD1	1:B:107:ARG:NH2	2.39	0.55
1:A:274:THR:O	1:A:278:TYR:CD2	2.59	0.55
1:B:256:GLU:OE2	1:B:267:VAL:CG2	2.55	0.55
1:A:489:ASP:N	1:A:489:ASP:OD1	2.40	0.55
1:B:384:VAL:O	1:B:388:PHE:HD2	1.90	0.54
1:A:256:GLU:OE2	1:A:267:VAL:CG2	2.55	0.54
1:A:55:GLY:HA2	1:A:498:ARG:HE	1.72	0.54
1:B:274:THR:O	1:B:278:TYR:CD2	2.59	0.54
1:B:306:ILE:HD13	1:B:393:VAL:HG13	1.90	0.54
1:A:384:VAL:O	1:A:388:PHE:HD2	1.90	0.54
1:A:175:GLU:OE2	1:A:240:THR:CG2	2.54	0.53
1:A:306:ILE:HD13	1:A:393:VAL:HG13	1.90	0.53
1:B:55:GLY:HA2	1:B:498:ARG:HE	1.71	0.53
1:A:256:GLU:OE2	1:A:267:VAL:HG22	2.09	0.52
1:A:60:LEU:CD1	1:A:60:LEU:N	2.73	0.52
1:B:489:ASP:N	1:B:489:ASP:OD1	2.40	0.52
1:B:340:LEU:HG	1:B:366:ILE:HD12	1.92	0.52
1:A:340:LEU:HG	1:A:366:ILE:HD12	1.92	0.51
1:A:389:ALA:O	1:A:393:VAL:HG23	2.10	0.51
1:B:256:GLU:OE2	1:B:267:VAL:HG22	2.09	0.51
1:A:161:LEU:O	1:A:185:GLN:NE2	2.42	0.51
2:B:806:PGW:H23	1:A:608:TRP:CH2	2.46	0.51
1:A:60:LEU:O	1:A:60:LEU:HD13	2.11	0.51
1:B:389:ALA:O	1:B:393:VAL:HG23	2.10	0.50
1:B:60:LEU:O	1:B:60:LEU:HD13	2.11	0.50
1:B:608:TRP:CH2	2:A:901:PGW:H23	2.46	0.50
1:B:276:ARG:NH1	1:B:351:ASN:O	2.45	0.50
1:B:384:VAL:O	1:B:388:PHE:CD2	2.65	0.50
1:A:276:ARG:NH1	1:A:351:ASN:O	2.45	0.49
1:B:161:LEU:O	1:B:185:GLN:NE2	2.42	0.49
1:B:60:LEU:HD22	1:B:60:LEU:C	2.34	0.48
1:A:384:VAL:O	1:A:388:PHE:CD2	2.65	0.48
1:A:283:GLN:HE22	1:A:364:GLN:HE21	1.62	0.48
1:B:283:GLN:HE22	1:B:364:GLN:HE21	1.62	0.47
1:A:60:LEU:HD22	1:A:60:LEU:C	2.34	0.47
1:B:60:LEU:CD1	1:B:60:LEU:N	2.73	0.47
1:B:52:VAL:HB	1:B:62:VAL:HG12	1.97	0.47
1:A:420:SER:O	1:A:420:SER:OG	2.33	0.47
1:B:320:LEU:HA	1:B:323:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:PHE:HE1	2:A:903:PGW:H2	1.81	0.46
1:B:52:VAL:HG23	1:B:60:LEU:HD23	1.98	0.45
1:A:52:VAL:HB	1:A:62:VAL:HG12	1.97	0.45
1:B:607:CYS:C	1:B:609:ALA:N	2.70	0.45
1:A:129:ARG:HH21	1:A:138:ALA:HB2	1.82	0.45
2:B:808:PGW:H2	1:A:575:PHE:HE1	1.81	0.45
1:A:52:VAL:HG23	1:A:60:LEU:HD23	1.98	0.45
1:A:320:LEU:HA	1:A:323:ILE:HG12	1.97	0.45
1:B:425:ARG:NH1	1:B:429:GLN:OE1	2.50	0.45
1:A:332:ILE:CG2	1:A:373:THR:HG22	2.46	0.45
1:B:608:TRP:O	1:B:608:TRP:CE3	2.70	0.45
1:A:607:CYS:C	1:A:609:ALA:N	2.70	0.45
1:B:54:GLN:HG2	1:A:722:LEU:HD22	1.99	0.44
1:B:129:ARG:HH21	1:B:138:ALA:HB2	1.82	0.44
1:A:172:THR:HG22	1:A:173:PHE:N	2.33	0.44
1:A:271:PHE:HZ	1:A:279:ARG:HH11	1.64	0.44
1:B:607:CYS:C	1:B:609:ALA:H	2.21	0.44
1:A:607:CYS:C	1:A:609:ALA:H	2.21	0.44
1:A:608:TRP:CE3	1:A:608:TRP:O	2.70	0.44
1:A:425:ARG:NH1	1:A:429:GLN:OE1	2.50	0.44
1:B:85:LEU:HD11	1:A:654:TYR:HD2	1.83	0.43
2:A:903:PGW:H10	2:A:903:PGW:H08A	1.71	0.43
1:A:381:THR:O	1:A:386:VAL:HG23	2.19	0.43
2:B:808:PGW:H08A	2:B:808:PGW:H10	1.71	0.43
2:B:806:PGW:H5	2:B:807:PGW:H5	2.01	0.43
1:A:606:ARG:NH2	2:A:904:PGW:O01	2.52	0.42
1:A:617:SER:HB2	2:A:904:PGW:H16	2.02	0.42
1:B:172:THR:HG22	1:B:173:PHE:N	2.33	0.42
1:A:388:PHE:CZ	2:A:902:PGW:H22A	2.54	0.42
1:B:381:THR:O	1:B:386:VAL:HG23	2.19	0.42
1:A:144:ASP:OD1	1:A:144:ASP:N	2.50	0.42
1:B:19:VAL:CG2	1:B:63:PHE:CD2	3.03	0.42
1:B:388:PHE:CZ	2:B:807:PGW:H22A	2.55	0.42
1:B:606:ARG:NH2	2:B:801:PGW:O01	2.52	0.42
2:B:806:PGW:H7	2:B:807:PGW:H7	2.02	0.42
1:B:376:LEU:O	1:B:380:LEU:HB2	2.20	0.42
1:B:610:LEU:HD21	2:B:807:PGW:H6A	2.01	0.42
1:A:19:VAL:CG2	1:A:63:PHE:CD2	3.03	0.42
1:A:359:LYS:HD3	1:A:359:LYS:HA	1.93	0.42
1:B:113:HIS:O	1:B:117:VAL:HB	2.20	0.42
1:B:617:SER:HB2	2:B:801:PGW:H16	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:HIS:O	1:A:117:VAL:HB	2.20	0.41
2:A:901:PGW:H7	2:A:902:PGW:H7	2.02	0.41
1:A:117:VAL:HA	1:A:118:PRO:HD3	1.85	0.41
1:A:376:LEU:O	1:A:380:LEU:HB2	2.20	0.41
1:A:607:CYS:SG	2:A:902:PGW:H03	2.59	0.41
2:A:901:PGW:H5	2:A:902:PGW:H5	2.01	0.41
1:A:60:LEU:HD13	1:A:60:LEU:N	2.26	0.41
1:B:33:ILE:HG12	1:A:720:LEU:HD13	2.03	0.41
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.95	0.41
1:A:388:PHE:HZ	2:A:902:PGW:H22A	1.86	0.41
1:B:332:ILE:CG2	1:B:373:THR:HG22	2.46	0.40
1:B:420:SER:O	1:B:420:SER:OG	2.33	0.40
1:B:279:ARG:HG2	1:B:349:TYR:CE2	2.56	0.40
1:A:240:THR:CG2	1:A:562:ARG:HG2	2.51	0.40
1:A:279:ARG:HG2	1:A:349:TYR:CE2	2.57	0.40
1:B:240:THR:CG2	1:B:562:ARG:HG2	2.51	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	577/735 (78%)	534 (92%)	43 (8%)	0	100	100
1	B	577/735 (78%)	533 (92%)	44 (8%)	0	100	100
All	All	1154/1470 (78%)	1067 (92%)	87 (8%)	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	508/646 (79%)	504 (99%)	4 (1%)	81	89
1	B	508/646 (79%)	504 (99%)	4 (1%)	81	89
All	All	1016/1292 (79%)	1008 (99%)	8 (1%)	82	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60	LEU
1	B	61	PHE
1	B	151	CYS
1	B	525	PHE
1	A	60	LEU
1	A	61	PHE
1	A	151	CYS
1	A	525	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	280	GLN
1	B	283	GLN
1	B	364	GLN
1	B	370	ASN
1	B	518	GLN
1	A	280	GLN
1	A	283	GLN
1	A	364	GLN
1	A	370	ASN
1	A	518	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
2	PGW	B	802	-	31,31,50	1.16	3 (9%)	34,37,56	1.15	2 (5%)
2	PGW	A	906	-	30,30,50	1.20	4 (13%)	34,35,56	1.20	2 (5%)
2	PGW	B	807	-	30,30,50	1.09	3 (10%)	32,32,56	1.20	2 (6%)
2	PGW	B	803	-	30,30,50	1.20	4 (13%)	34,35,56	1.20	2 (5%)
2	PGW	A	904	-	40,40,50	1.04	4 (10%)	44,45,56	1.09	2 (4%)
2	PGW	B	805	-	33,33,50	1.11	3 (9%)	36,39,56	1.13	2 (5%)
2	PGW	B	808	-	34,34,50	1.14	5 (14%)	38,39,56	1.12	2 (5%)
2	PGW	A	901	-	36,36,50	1.09	4 (11%)	40,41,56	1.15	2 (5%)
2	PGW	A	908	-	33,33,50	1.12	3 (9%)	36,39,56	1.13	2 (5%)
2	PGW	B	806	-	36,36,50	1.09	4 (11%)	40,41,56	1.15	2 (5%)
2	PGW	A	902	-	30,30,50	1.09	3 (10%)	32,32,56	1.20	2 (6%)
2	PGW	B	804	-	37,37,50	1.07	5 (13%)	41,42,56	1.13	2 (4%)
2	PGW	A	903	-	34,34,50	1.15	5 (14%)	38,39,56	1.12	2 (5%)
2	PGW	B	801	-	40,40,50	1.04	4 (10%)	44,45,56	1.09	2 (4%)
2	PGW	A	905	-	31,31,50	1.16	3 (9%)	34,37,56	1.15	2 (5%)
2	PGW	A	907	-	37,37,50	1.07	5 (13%)	41,42,56	1.13	2 (4%)

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
2	PGW	B	802	-	-	17/36/36/55	-
2	PGW	A	906	-	-	17/32/32/55	-
2	PGW	B	807	-	-	16/32/32/55	-
2	PGW	B	803	-	-	17/32/32/55	-
2	PGW	A	904	-	-	23/42/42/55	-
2	PGW	B	805	-	-	20/38/38/55	-
2	PGW	B	808	-	-	23/36/36/55	-
2	PGW	A	901	-	-	18/38/38/55	-
2	PGW	A	908	-	-	20/38/38/55	-
2	PGW	B	806	-	-	18/38/38/55	-
2	PGW	A	902	-	-	16/32/32/55	-
2	PGW	B	804	-	-	20/39/39/55	-
2	PGW	A	903	-	-	23/36/36/55	-
2	PGW	B	801	-	-	23/42/42/55	-
2	PGW	A	905	-	-	17/36/36/55	-
2	PGW	A	907	-	-	20/39/39/55	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	807	PGW	O01-C1	3.04	1.42	1.34
2	A	902	PGW	O01-C1	3.03	1.42	1.34
2	B	803	PGW	O01-C1	3.02	1.42	1.34
2	A	906	PGW	O01-C1	3.02	1.42	1.34
2	A	901	PGW	O01-C1	2.99	1.42	1.34
2	B	806	PGW	O01-C1	2.98	1.42	1.34
2	A	904	PGW	O01-C1	2.97	1.42	1.34
2	B	801	PGW	O01-C1	2.97	1.42	1.34
2	B	802	PGW	O01-C1	2.92	1.42	1.34
2	A	905	PGW	O01-C1	2.92	1.42	1.34
2	B	805	PGW	O01-C1	2.90	1.42	1.34
2	A	908	PGW	O01-C1	2.89	1.42	1.34
2	A	903	PGW	O01-C1	2.83	1.42	1.34
2	B	808	PGW	O01-C1	2.83	1.42	1.34
2	A	907	PGW	O01-C1	2.83	1.42	1.34
2	B	804	PGW	O01-C1	2.82	1.42	1.34
2	B	806	PGW	O03-C19	2.51	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	903	PGW	O03-C01	-2.50	1.39	1.45
2	A	901	PGW	O03-C19	2.50	1.40	1.33
2	B	808	PGW	O03-C01	-2.47	1.39	1.45
2	A	907	PGW	O03-C19	2.47	1.40	1.33
2	A	905	PGW	O03-C19	2.47	1.40	1.33
2	B	804	PGW	O03-C19	2.46	1.40	1.33
2	B	802	PGW	O03-C19	2.46	1.40	1.33
2	B	801	PGW	O03-C19	2.43	1.40	1.33
2	A	908	PGW	O03-C19	2.43	1.40	1.33
2	A	904	PGW	O03-C19	2.42	1.40	1.33
2	B	805	PGW	O03-C19	2.41	1.40	1.33
2	A	906	PGW	O03-C19	2.40	1.40	1.33
2	B	803	PGW	O03-C19	2.39	1.40	1.33
2	B	807	PGW	O03-C19	2.38	1.40	1.33
2	A	902	PGW	O03-C19	2.36	1.40	1.33
2	B	804	PGW	P-O12	2.35	1.63	1.54
2	B	806	PGW	P-O12	2.34	1.63	1.54
2	A	907	PGW	P-O12	2.34	1.63	1.54
2	A	901	PGW	P-O12	2.32	1.63	1.54
2	B	803	PGW	O03-C01	-2.29	1.39	1.45
2	A	902	PGW	O03-C01	-2.29	1.39	1.45
2	B	803	PGW	P-O12	2.29	1.63	1.54
2	B	807	PGW	O03-C01	-2.29	1.39	1.45
2	A	903	PGW	O03-C19	2.29	1.40	1.33
2	A	908	PGW	O03-C01	-2.28	1.39	1.45
2	A	906	PGW	O03-C01	-2.28	1.40	1.45
2	B	808	PGW	O03-C19	2.28	1.40	1.33
2	A	906	PGW	P-O12	2.27	1.63	1.54
2	B	805	PGW	O03-C01	-2.27	1.40	1.45
2	B	806	PGW	O03-C01	-2.27	1.40	1.45
2	A	901	PGW	O03-C01	-2.27	1.40	1.45
2	B	802	PGW	O03-C01	-2.26	1.40	1.45
2	A	905	PGW	O03-C01	-2.26	1.40	1.45
2	B	808	PGW	P-O12	2.25	1.63	1.54
2	A	903	PGW	P-O12	2.25	1.63	1.54
2	B	801	PGW	O03-C01	-2.23	1.40	1.45
2	A	904	PGW	O03-C01	-2.23	1.40	1.45
2	B	801	PGW	P-O12	2.13	1.63	1.54
2	A	904	PGW	P-O12	2.12	1.63	1.54
2	B	804	PGW	O03-C01	-2.08	1.40	1.45
2	A	907	PGW	O03-C01	-2.08	1.40	1.45
2	A	903	PGW	O01-C02	-2.05	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	804	PGW	O01-C02	-2.04	1.41	1.46
2	A	907	PGW	O01-C02	-2.04	1.41	1.46
2	B	808	PGW	O01-C02	-2.03	1.41	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	905	PGW	O01-C1-C2	4.20	120.55	111.50
2	B	802	PGW	O01-C1-C2	4.19	120.52	111.50
2	B	805	PGW	O01-C1-C2	4.10	120.34	111.50
2	A	908	PGW	O01-C1-C2	4.10	120.34	111.50
2	A	903	PGW	O01-C1-C2	4.05	120.24	111.50
2	B	808	PGW	O01-C1-C2	4.04	120.21	111.50
2	B	803	PGW	O01-C1-C2	3.96	120.04	111.50
2	A	906	PGW	O01-C1-C2	3.96	120.04	111.50
2	B	806	PGW	O01-C1-C2	3.95	120.02	111.50
2	A	901	PGW	O01-C1-C2	3.93	119.97	111.50
2	B	801	PGW	O01-C1-C2	3.82	119.73	111.50
2	A	904	PGW	O01-C1-C2	3.82	119.73	111.50
2	A	907	PGW	O01-C1-C2	3.71	119.49	111.50
2	B	804	PGW	O01-C1-C2	3.69	119.46	111.50
2	A	902	PGW	O01-C1-C2	3.43	118.88	111.50
2	B	807	PGW	O01-C1-C2	3.42	118.87	111.50
2	B	803	PGW	O03-C19-C20	2.64	120.20	111.91
2	A	901	PGW	O03-C19-C20	2.64	120.18	111.91
2	A	906	PGW	O03-C19-C20	2.64	120.18	111.91
2	B	806	PGW	O03-C19-C20	2.62	120.13	111.91
2	A	903	PGW	O03-C19-C20	2.60	120.06	111.91
2	B	808	PGW	O03-C19-C20	2.59	120.05	111.91
2	A	907	PGW	O03-C19-C20	2.55	119.92	111.91
2	B	804	PGW	O03-C19-C20	2.55	119.91	111.91
2	A	904	PGW	O03-C19-C20	2.53	119.83	111.91
2	B	801	PGW	O03-C19-C20	2.52	119.81	111.91
2	B	802	PGW	O03-C19-C20	2.49	119.71	111.91
2	A	902	PGW	O03-C19-C20	2.48	119.70	111.91
2	A	905	PGW	O03-C19-C20	2.48	119.68	111.91
2	B	807	PGW	O03-C19-C20	2.48	119.68	111.91
2	B	805	PGW	O03-C19-C20	2.47	119.64	111.91
2	A	908	PGW	O03-C19-C20	2.46	119.61	111.91

There are no chirality outliers.

All (308) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	PGW	C03-O11-P-O12
2	B	801	PGW	C03-O11-P-O13
2	B	802	PGW	C2-C1-O01-C02
2	B	802	PGW	O12-C04-C05-OAF
2	B	803	PGW	C03-O11-P-O12
2	B	806	PGW	C03-O11-P-O12
2	B	806	PGW	C03-O11-P-O13
2	B	806	PGW	C2-C1-O01-C02
2	B	808	PGW	C03-O11-P-O12
2	B	808	PGW	O03-C01-C02-O01
2	A	901	PGW	C03-O11-P-O12
2	A	901	PGW	C03-O11-P-O13
2	A	901	PGW	C2-C1-O01-C02
2	A	903	PGW	C03-O11-P-O12
2	A	903	PGW	O03-C01-C02-O01
2	A	904	PGW	C03-O11-P-O12
2	A	904	PGW	C03-O11-P-O13
2	A	905	PGW	C2-C1-O01-C02
2	A	905	PGW	O12-C04-C05-OAF
2	A	906	PGW	C03-O11-P-O12
2	B	806	PGW	O04-C19-O03-C01
2	A	901	PGW	O04-C19-O03-C01
2	B	802	PGW	O02-C1-O01-C02
2	B	806	PGW	O02-C1-O01-C02
2	A	901	PGW	O02-C1-O01-C02
2	A	905	PGW	O02-C1-O01-C02
2	B	806	PGW	C20-C19-O03-C01
2	A	901	PGW	C20-C19-O03-C01
2	B	802	PGW	O12-C04-C05-CAD
2	B	805	PGW	O12-C04-C05-CAD
2	A	905	PGW	O12-C04-C05-CAD
2	A	908	PGW	O12-C04-C05-CAD
2	B	801	PGW	C20-C19-O03-C01
2	A	904	PGW	C20-C19-O03-C01
2	B	804	PGW	O03-C01-C02-O01
2	A	907	PGW	O03-C01-C02-O01
2	B	807	PGW	C19-C20-C21-C22
2	A	902	PGW	C19-C20-C21-C22
2	B	802	PGW	OAF-C05-CAD-OAE
2	A	905	PGW	OAF-C05-CAD-OAE
2	B	801	PGW	C19-C20-C21-C22
2	B	804	PGW	C19-C20-C21-C22
2	B	806	PGW	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	901	PGW	C1-C2-C3-C4
2	A	904	PGW	C19-C20-C21-C22
2	A	907	PGW	C19-C20-C21-C22
2	B	805	PGW	C02-C03-O11-P
2	A	908	PGW	C02-C03-O11-P
2	B	805	PGW	C19-C20-C21-C22
2	A	908	PGW	C19-C20-C21-C22
2	B	805	PGW	O12-C04-C05-OAF
2	A	908	PGW	O12-C04-C05-OAF
2	B	801	PGW	O04-C19-O03-C01
2	A	904	PGW	O04-C19-O03-C01
2	B	805	PGW	C2-C1-O01-C02
2	A	908	PGW	C2-C1-O01-C02
2	B	802	PGW	C04-O12-P-O11
2	B	805	PGW	C03-O11-P-O12
2	B	805	PGW	C04-O12-P-O11
2	A	905	PGW	C04-O12-P-O11
2	A	908	PGW	C03-O11-P-O12
2	A	908	PGW	C04-O12-P-O11
2	B	805	PGW	O02-C1-O01-C02
2	A	908	PGW	O02-C1-O01-C02
2	B	806	PGW	C3-C4-C5-C6
2	A	901	PGW	C3-C4-C5-C6
2	B	801	PGW	C21-C22-C23-C24
2	A	904	PGW	C21-C22-C23-C24
2	B	803	PGW	C21-C22-C23-C24
2	B	808	PGW	C21-C22-C23-C24
2	A	903	PGW	C21-C22-C23-C24
2	A	906	PGW	C21-C22-C23-C24
2	B	806	PGW	C21-C22-C23-C24
2	B	801	PGW	C5-C6-C7-C8
2	B	803	PGW	C23-C24-C25-C26
2	B	804	PGW	C22-C23-C24-C25
2	B	808	PGW	C5-C6-C7-C8
2	A	901	PGW	C21-C22-C23-C24
2	A	903	PGW	C5-C6-C7-C8
2	A	904	PGW	C5-C6-C7-C8
2	A	906	PGW	C23-C24-C25-C26
2	A	907	PGW	C22-C23-C24-C25
2	B	808	PGW	C2-C3-C4-C5
2	A	903	PGW	C2-C3-C4-C5
2	B	802	PGW	C04-C05-CAD-OAE

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Mol	Chain	Res	Type	Atoms
2	B	805	PGW	C04-C05-CAD-OAE
2	A	905	PGW	C04-C05-CAD-OAE
2	A	908	PGW	C04-C05-CAD-OAE
2	A	906	PGW	C24-C25-C26-C27
2	B	801	PGW	C25-C26-C27-C15
2	B	802	PGW	C21-C22-C23-C24
2	B	803	PGW	C2-C3-C4-C5
2	B	803	PGW	C22-C23-C24-C25
2	B	803	PGW	C24-C25-C26-C27
2	B	808	PGW	C22-C23-C24-C25
2	A	903	PGW	C22-C23-C24-C25
2	A	905	PGW	C21-C22-C23-C24
2	A	906	PGW	C2-C3-C4-C5
2	A	906	PGW	C22-C23-C24-C25
2	A	904	PGW	C25-C26-C27-C15
2	B	801	PGW	C10-C06-C07-C08
2	A	904	PGW	C10-C06-C07-C08
2	B	807	PGW	C20-C19-O03-C01
2	A	902	PGW	C20-C19-O03-C01
2	B	806	PGW	C20-C21-C22-C23
2	A	901	PGW	C20-C21-C22-C23
2	B	803	PGW	C5-C6-C7-C8
2	A	906	PGW	C5-C6-C7-C8
2	A	902	PGW	C23-C24-C25-C26
2	B	807	PGW	C23-C24-C25-C26
2	B	801	PGW	C17-C18-C28-C30
2	B	808	PGW	C3-C4-C5-C6
2	A	903	PGW	C3-C4-C5-C6
2	A	904	PGW	C17-C18-C28-C30
2	B	807	PGW	O04-C19-O03-C01
2	A	902	PGW	O04-C19-O03-C01
2	B	801	PGW	C20-C21-C22-C23
2	B	808	PGW	C23-C24-C25-C26
2	A	904	PGW	C20-C21-C22-C23
2	A	903	PGW	C23-C24-C25-C26
2	B	803	PGW	C2-C1-O01-C02
2	A	906	PGW	C2-C1-O01-C02
2	B	805	PGW	O03-C01-C02-O01
2	A	908	PGW	O03-C01-C02-O01
2	B	807	PGW	C25-C26-C27-C15
2	A	902	PGW	C25-C26-C27-C15
2	B	804	PGW	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	A	907	PGW	C6-C7-C8-C9
2	B	803	PGW	O02-C1-O01-C02
2	A	906	PGW	O02-C1-O01-C02
2	B	807	PGW	C2-C1-O01-C02
2	A	902	PGW	C2-C1-O01-C02
2	B	802	PGW	C23-C24-C25-C26
2	A	905	PGW	C23-C24-C25-C26
2	B	801	PGW	C01-C02-C03-O11
2	A	904	PGW	C01-C02-C03-O11
2	B	802	PGW	O03-C01-C02-C03
2	B	804	PGW	O03-C01-C02-C03
2	B	807	PGW	O03-C01-C02-C03
2	B	808	PGW	O03-C01-C02-C03
2	A	902	PGW	O03-C01-C02-C03
2	A	903	PGW	O03-C01-C02-C03
2	A	905	PGW	O03-C01-C02-C03
2	A	907	PGW	O03-C01-C02-C03
2	B	807	PGW	C24-C25-C26-C27
2	A	902	PGW	C24-C25-C26-C27
2	B	807	PGW	C6-C7-C8-C9
2	A	902	PGW	C6-C7-C8-C9
2	B	801	PGW	C03-O11-P-O14
2	B	806	PGW	C03-O11-P-O14
2	A	901	PGW	C03-O11-P-O14
2	A	904	PGW	C03-O11-P-O14
2	B	806	PGW	C22-C23-C24-C25
2	A	901	PGW	C22-C23-C24-C25
2	A	904	PGW	C24-C25-C26-C27
2	B	801	PGW	C24-C25-C26-C27
2	B	807	PGW	O02-C1-O01-C02
2	A	902	PGW	O02-C1-O01-C02
2	B	805	PGW	O03-C01-C02-C03
2	A	908	PGW	O03-C01-C02-C03
2	B	805	PGW	OAF-C05-CAD-OAE
2	A	908	PGW	OAF-C05-CAD-OAE
2	B	801	PGW	O01-C02-C03-O11
2	B	808	PGW	O01-C02-C03-O11
2	A	903	PGW	O01-C02-C03-O11
2	A	904	PGW	O01-C02-C03-O11
2	B	804	PGW	O03-C19-C20-C21
2	A	907	PGW	O03-C19-C20-C21
2	B	801	PGW	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	904	PGW	C3-C4-C5-C6
2	B	801	PGW	C27-C15-C16-C17
2	A	904	PGW	C27-C15-C16-C17
2	B	808	PGW	C19-C20-C21-C22
2	A	903	PGW	C19-C20-C21-C22
2	B	803	PGW	C03-O11-P-O13
2	B	808	PGW	C03-O11-P-O13
2	A	903	PGW	C03-O11-P-O13
2	A	906	PGW	C03-O11-P-O13
2	B	802	PGW	C24-C25-C26-C27
2	A	905	PGW	C24-C25-C26-C27
2	B	806	PGW	C16-C17-C18-C28
2	A	901	PGW	C16-C17-C18-C28
2	B	806	PGW	C24-C25-C26-C27
2	A	901	PGW	C24-C25-C26-C27
2	B	806	PGW	O01-C02-C03-O11
2	A	901	PGW	O01-C02-C03-O11
2	B	802	PGW	O03-C01-C02-O01
2	B	807	PGW	O03-C01-C02-O01
2	A	902	PGW	O03-C01-C02-O01
2	A	905	PGW	O03-C01-C02-O01
2	B	808	PGW	C20-C21-C22-C23
2	A	903	PGW	C20-C21-C22-C23
2	B	803	PGW	C20-C19-O03-C01
2	A	906	PGW	C20-C19-O03-C01
2	B	802	PGW	C04-O12-P-O13
2	B	805	PGW	C03-O11-P-O13
2	B	805	PGW	C03-O11-P-O14
2	B	805	PGW	C04-O12-P-O14
2	A	905	PGW	C04-O12-P-O13
2	A	908	PGW	C03-O11-P-O13
2	A	908	PGW	C03-O11-P-O14
2	A	908	PGW	C04-O12-P-O14
2	B	808	PGW	C01-C02-C03-O11
2	A	903	PGW	C01-C02-C03-O11
2	B	805	PGW	C21-C22-C23-C24
2	A	908	PGW	C21-C22-C23-C24
2	B	807	PGW	C16-C15-C27-C26
2	A	902	PGW	C16-C15-C27-C26
2	B	804	PGW	O01-C02-C03-O11
2	A	907	PGW	O01-C02-C03-O11
2	B	806	PGW	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	A	901	PGW	C6-C7-C8-C9
2	B	808	PGW	C24-C25-C26-C27
2	B	803	PGW	O04-C19-O03-C01
2	B	806	PGW	C2-C3-C4-C5
2	A	901	PGW	C2-C3-C4-C5
2	A	903	PGW	C24-C25-C26-C27
2	A	906	PGW	O04-C19-O03-C01
2	B	804	PGW	C01-C02-C03-O11
2	B	806	PGW	C01-C02-C03-O11
2	A	901	PGW	C01-C02-C03-O11
2	A	907	PGW	C01-C02-C03-O11
2	B	802	PGW	C22-C23-C24-C25
2	B	807	PGW	C7-C8-C9-C10
2	A	902	PGW	C7-C8-C9-C10
2	B	803	PGW	C03-O11-P-O14
2	B	808	PGW	C03-O11-P-O14
2	A	903	PGW	C03-O11-P-O14
2	A	906	PGW	C03-O11-P-O14
2	A	905	PGW	C22-C23-C24-C25
2	A	908	PGW	C23-C24-C25-C26
2	B	805	PGW	C23-C24-C25-C26
2	B	804	PGW	C16-C15-C27-C26
2	A	907	PGW	C16-C15-C27-C26
2	B	801	PGW	C4-C5-C6-C7
2	A	904	PGW	C4-C5-C6-C7
2	A	903	PGW	C7-C8-C9-C10
2	B	804	PGW	C21-C22-C23-C24
2	A	907	PGW	C21-C22-C23-C24
2	B	805	PGW	C2-C3-C4-C5
2	B	807	PGW	C22-C23-C24-C25
2	A	902	PGW	C22-C23-C24-C25
2	A	908	PGW	C2-C3-C4-C5
2	B	803	PGW	O03-C01-C02-C03
2	A	906	PGW	O03-C01-C02-C03
2	B	808	PGW	C7-C8-C9-C10
2	B	804	PGW	C20-C21-C22-C23
2	A	907	PGW	C20-C21-C22-C23
2	B	804	PGW	O02-C1-O01-C02
2	A	907	PGW	O02-C1-O01-C02
2	B	804	PGW	C10-C06-C07-C08
2	A	907	PGW	C10-C06-C07-C08
2	A	907	PGW	C27-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	B	804	PGW	C27-C15-C16-C17
2	B	808	PGW	O03-C19-C20-C21
2	A	903	PGW	O03-C19-C20-C21
2	B	803	PGW	C3-C4-C5-C6
2	A	906	PGW	C3-C4-C5-C6
2	B	808	PGW	O01-C1-C2-C3
2	A	903	PGW	O01-C1-C2-C3
2	B	804	PGW	C07-C06-C10-C9
2	A	907	PGW	C07-C06-C10-C9
2	B	801	PGW	O01-C1-C2-C3
2	A	904	PGW	O01-C1-C2-C3
2	B	805	PGW	O01-C1-C2-C3
2	A	908	PGW	O01-C1-C2-C3
2	B	801	PGW	C16-C15-C27-C26
2	A	904	PGW	C16-C15-C27-C26
2	B	804	PGW	O04-C19-C20-C21
2	A	907	PGW	O04-C19-C20-C21
2	B	802	PGW	O03-C19-C20-C21
2	A	905	PGW	O03-C19-C20-C21
2	A	907	PGW	C2-C1-O01-C02
2	B	804	PGW	C2-C3-C4-C5
2	B	808	PGW	C07-C06-C10-C9
2	A	903	PGW	C07-C06-C10-C9
2	B	804	PGW	C24-C25-C26-C27
2	A	907	PGW	C2-C3-C4-C5
2	A	907	PGW	C24-C25-C26-C27
2	B	804	PGW	C2-C1-O01-C02
2	B	801	PGW	O02-C1-C2-C3
2	A	904	PGW	O02-C1-C2-C3
2	B	808	PGW	C6-C7-C8-C9
2	A	903	PGW	C6-C7-C8-C9
2	B	805	PGW	O02-C1-C2-C3
2	A	908	PGW	O02-C1-C2-C3
2	B	808	PGW	O04-C19-C20-C21
2	A	903	PGW	O04-C19-C20-C21
2	B	808	PGW	O02-C1-C2-C3
2	A	903	PGW	O02-C1-C2-C3
2	A	905	PGW	O04-C19-C20-C21
2	B	802	PGW	O04-C19-C20-C21
2	B	801	PGW	C23-C24-C25-C26
2	A	904	PGW	C23-C24-C25-C26
2	B	801	PGW	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	904	PGW	C7-C8-C9-C10
2	A	905	PGW	O01-C1-C2-C3
2	B	802	PGW	O01-C1-C2-C3
2	B	803	PGW	O01-C1-C2-C3
2	B	807	PGW	O01-C1-C2-C3
2	A	902	PGW	O01-C1-C2-C3
2	A	906	PGW	O01-C1-C2-C3
2	B	807	PGW	O02-C1-C2-C3
2	A	902	PGW	O02-C1-C2-C3
2	A	907	PGW	C06-C07-C08-C09
2	B	804	PGW	C06-C07-C08-C09
2	B	803	PGW	O03-C19-C20-C21
2	A	906	PGW	O03-C19-C20-C21

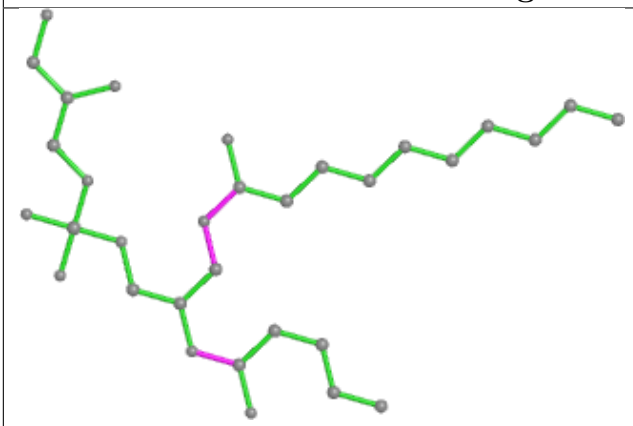
There are no ring outliers.

8 monomers are involved in 23 short contacts:

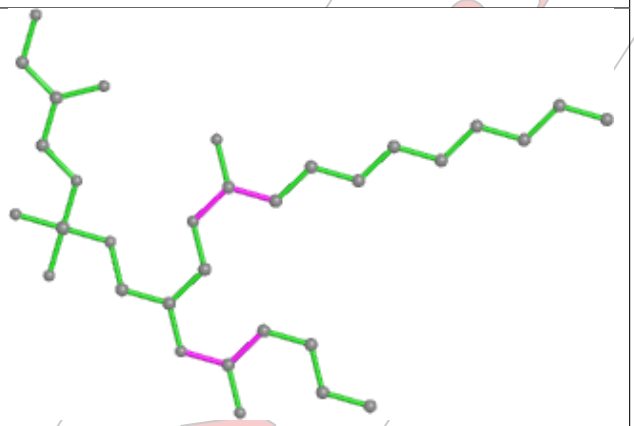
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	807	PGW	4	0
2	A	904	PGW	4	0
2	B	808	PGW	2	0
2	A	901	PGW	3	0
2	B	806	PGW	3	0
2	A	902	PGW	5	0
2	A	903	PGW	2	0
2	B	801	PGW	4	0

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 then 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.

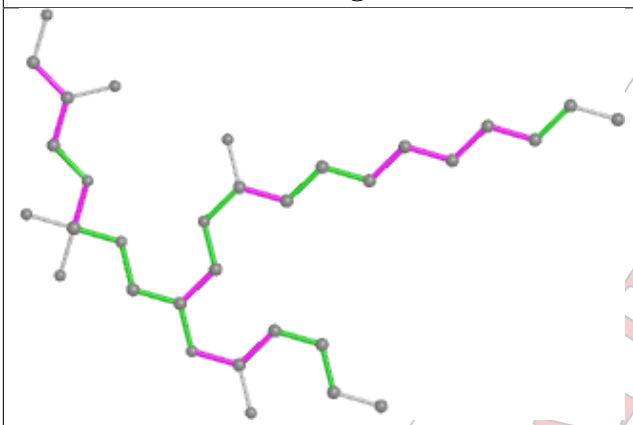
Ligand PGW B 802



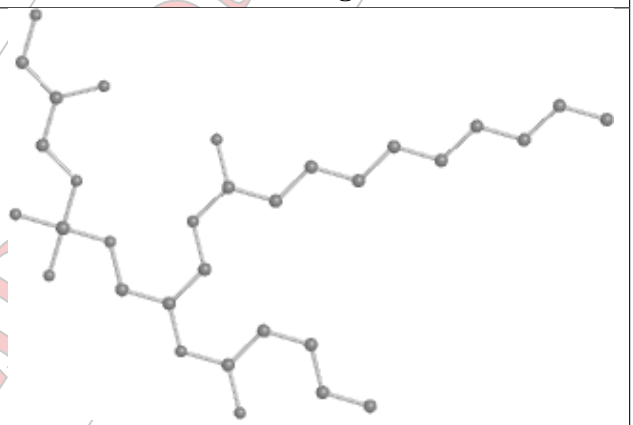
Bond lengths



Bond angles

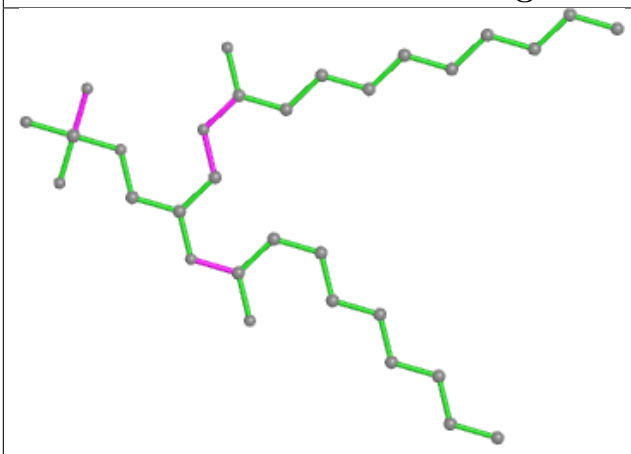


Torsions

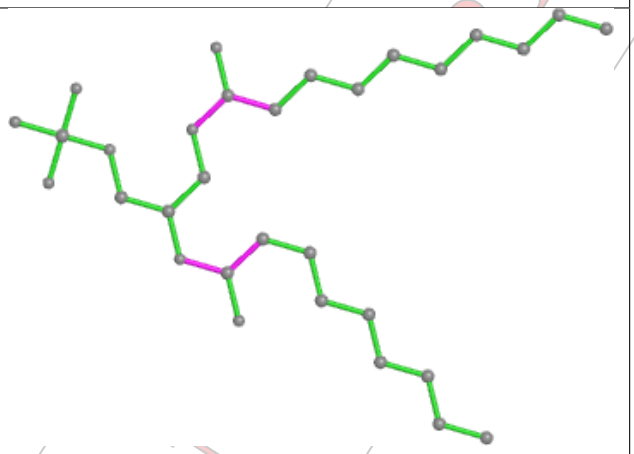


Rings

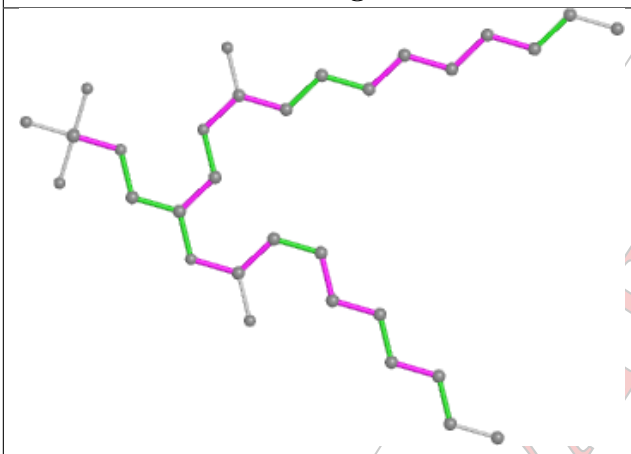
Ligand PGW A 906



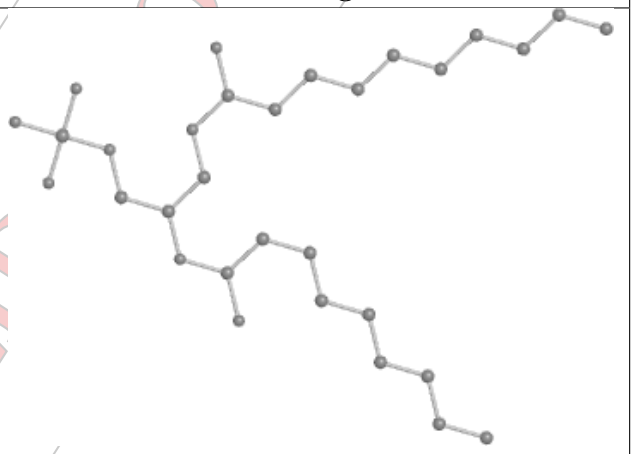
Bond lengths



Bond angles

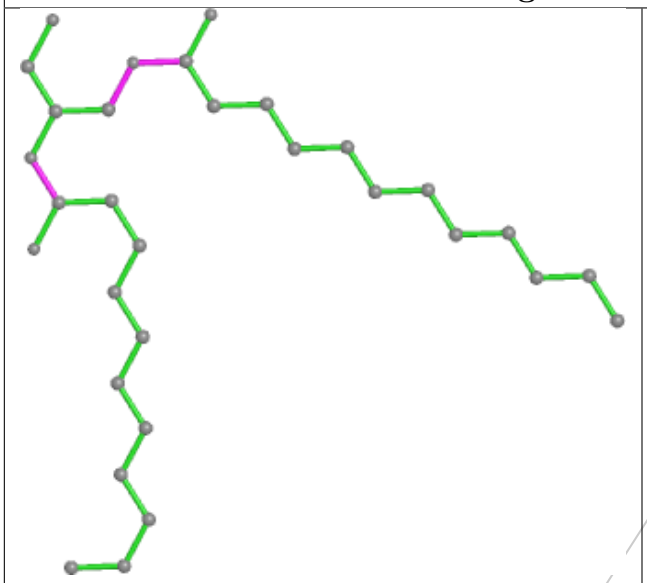


Torsions

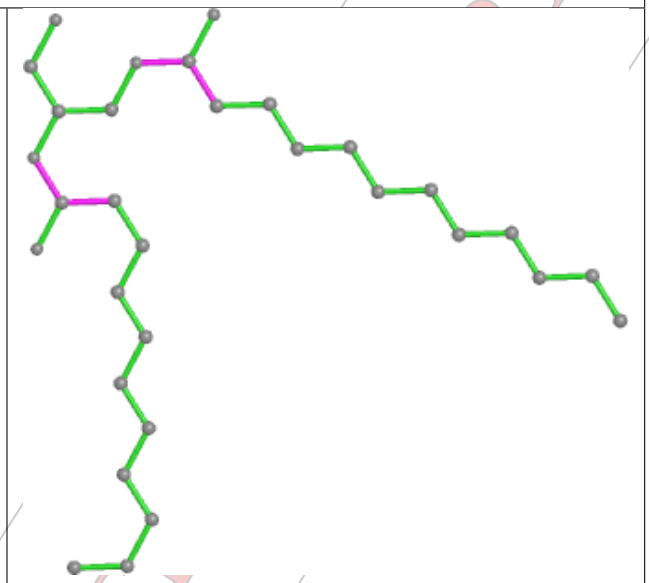


Rings

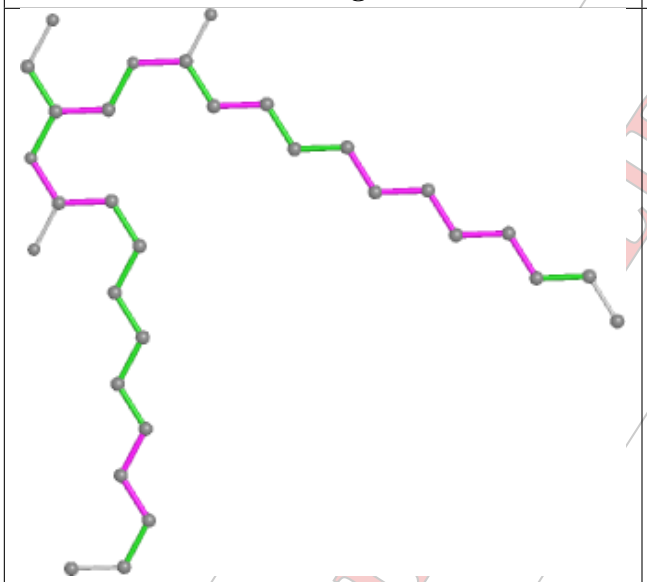
Ligand PGW B 807



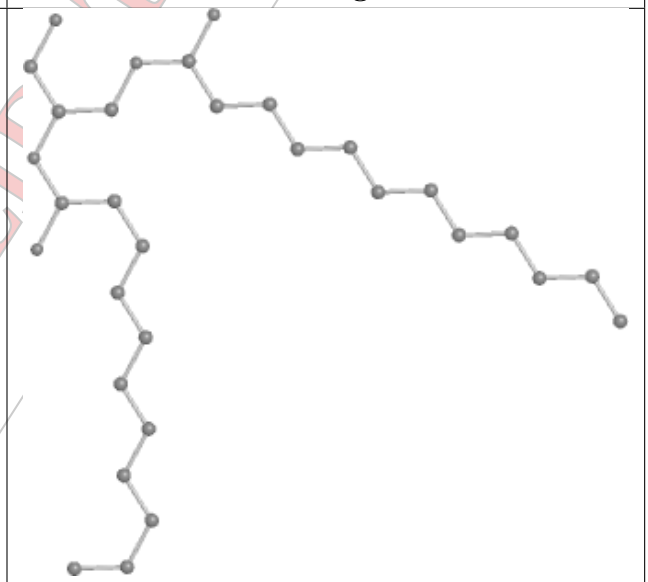
Bond lengths



Bond angles

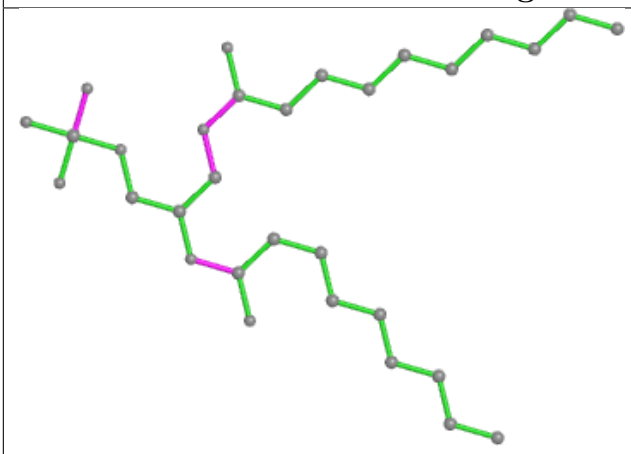


Torsions

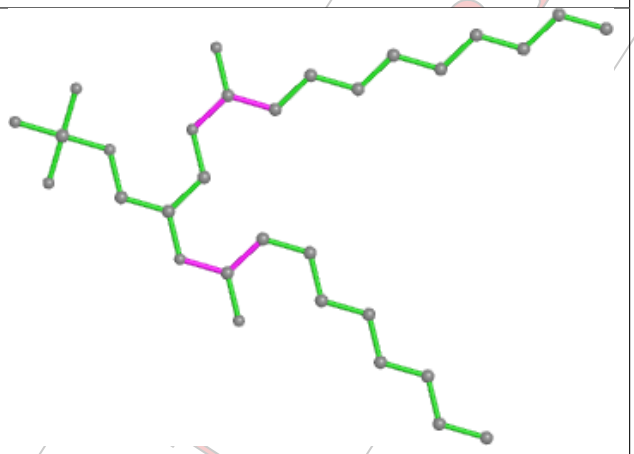


Rings

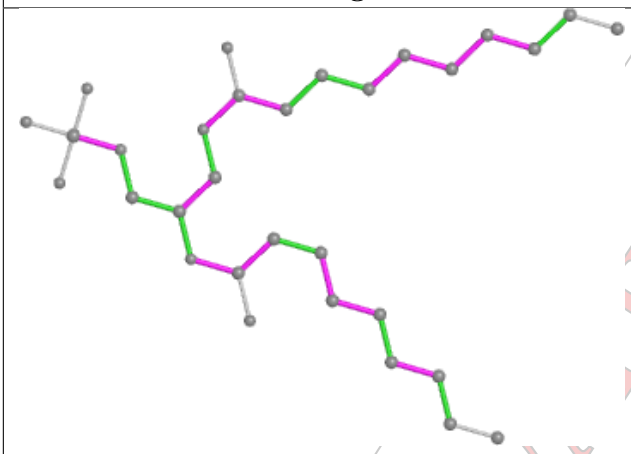
Ligand PGW B 803



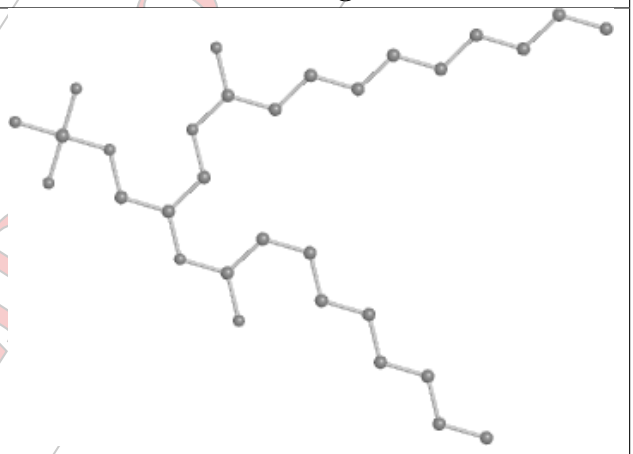
Bond lengths



Bond angles

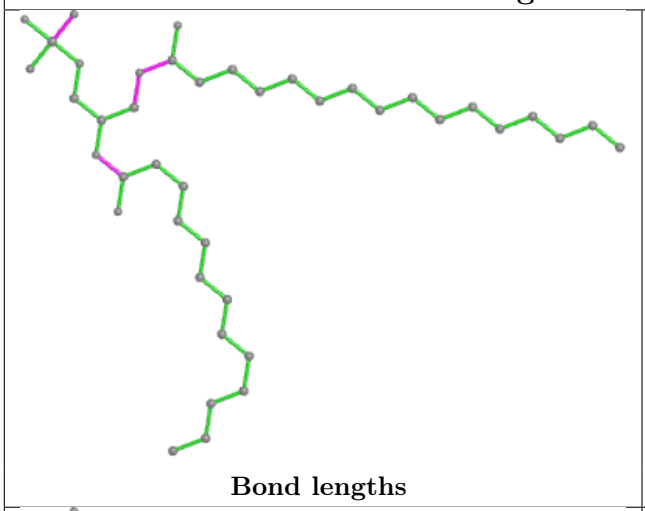


Torsions

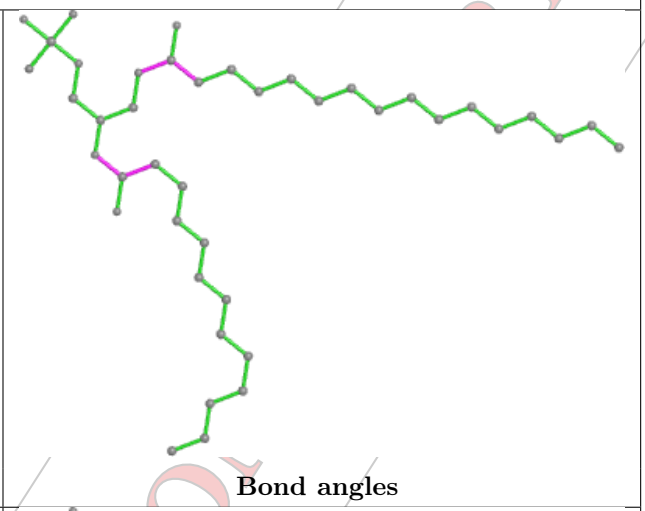


Rings

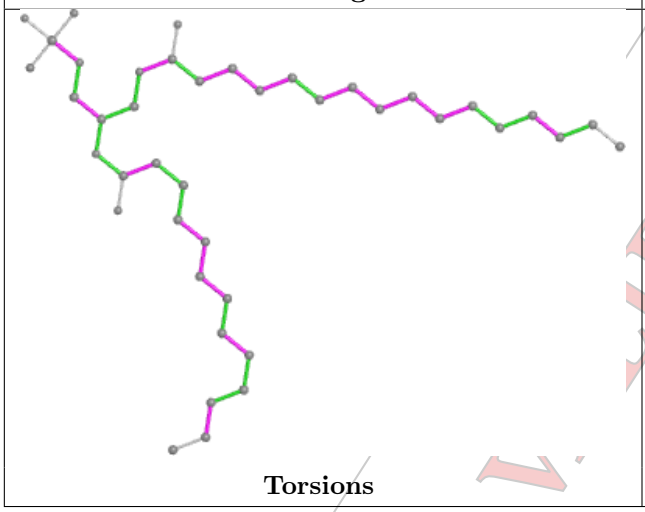
Ligand PGW A 904



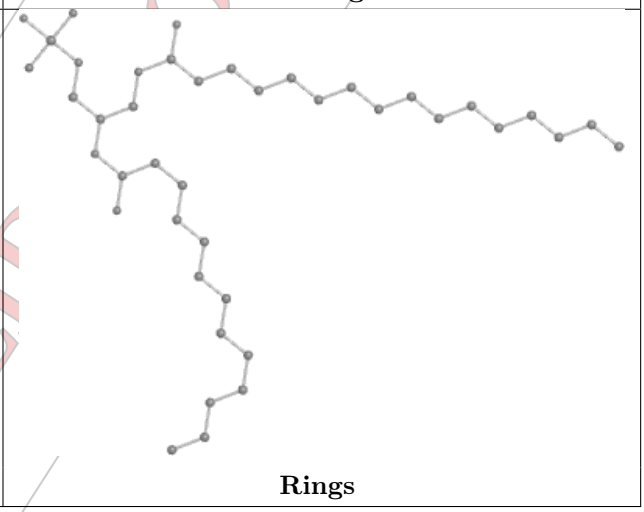
Bond lengths



Bond angles

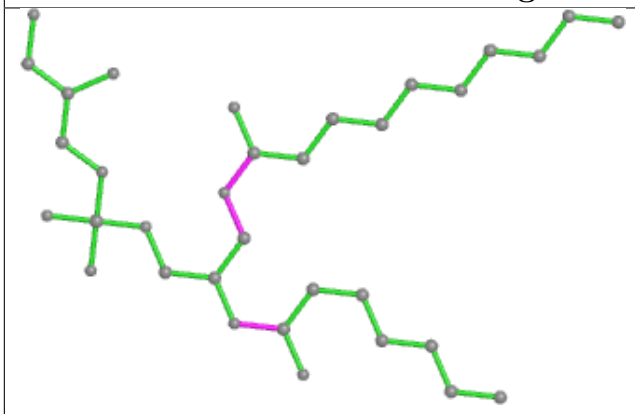


Torsions

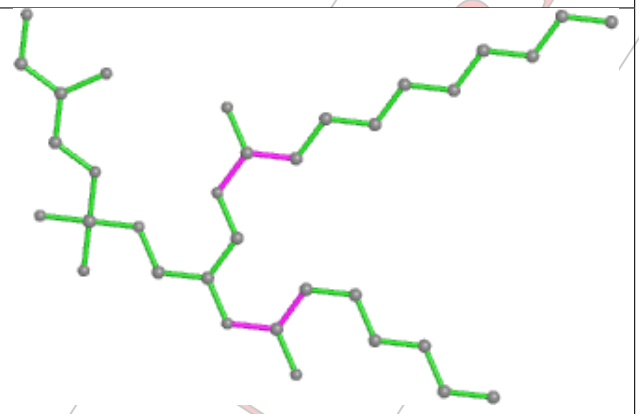


Rings

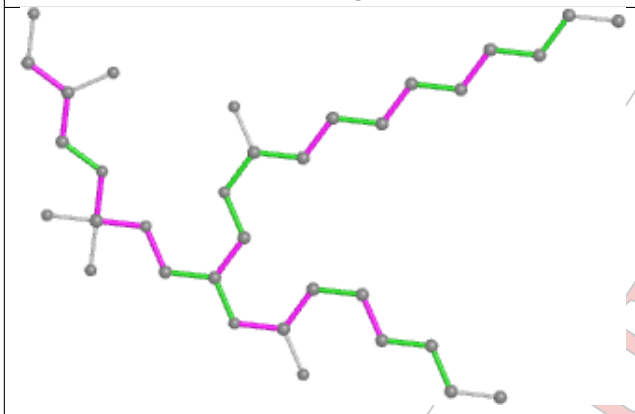
Ligand PGW B 805



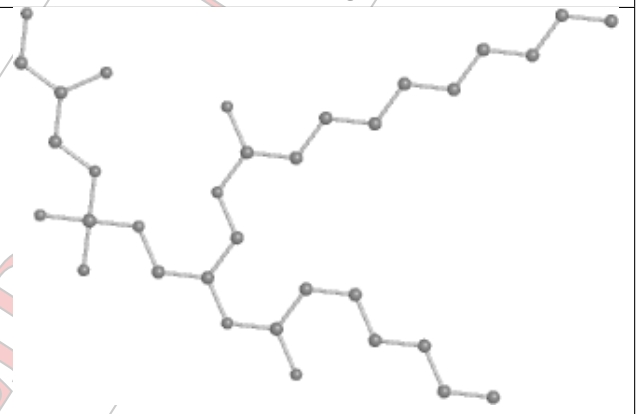
Bond lengths



Bond angles

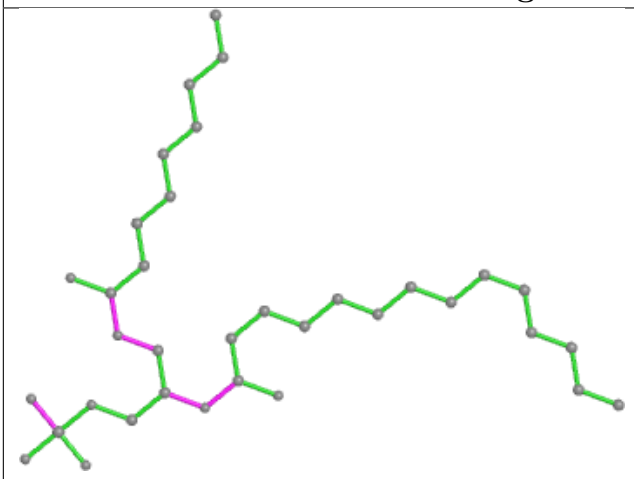


Torsions

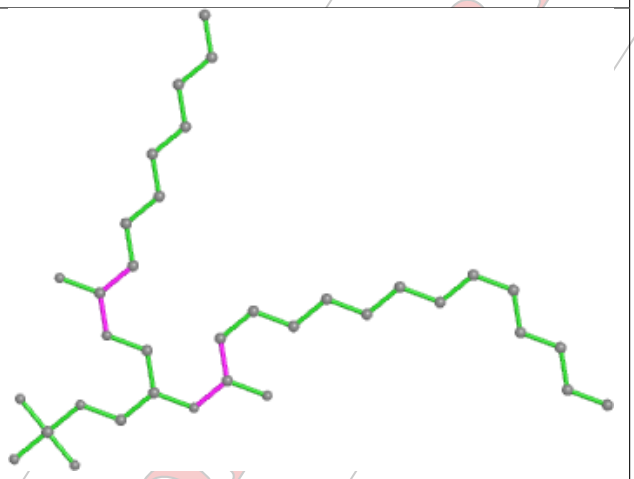


Rings

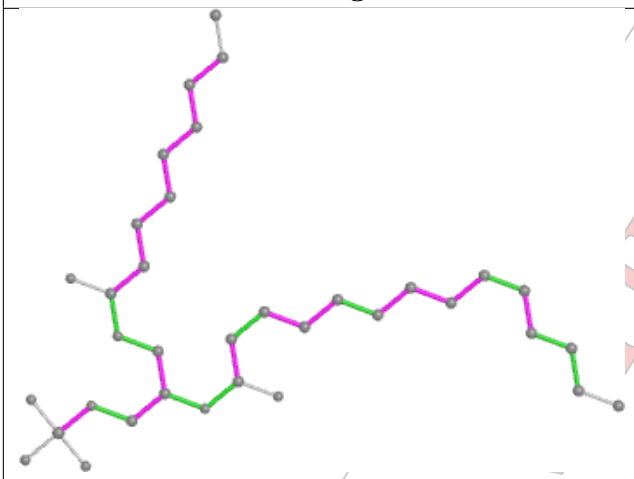
Ligand PGW B 808



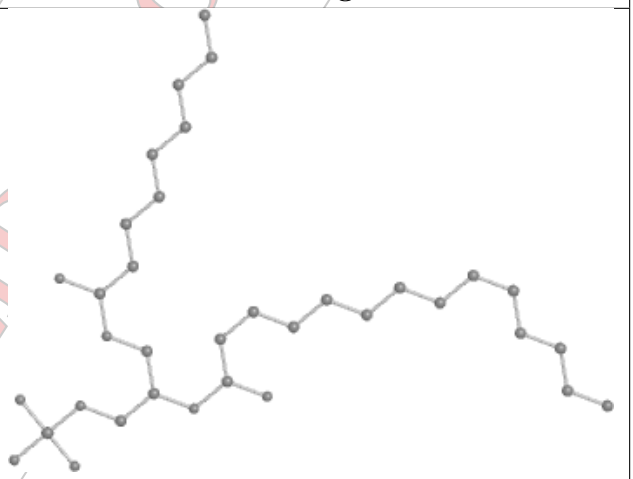
Bond lengths



Bond angles

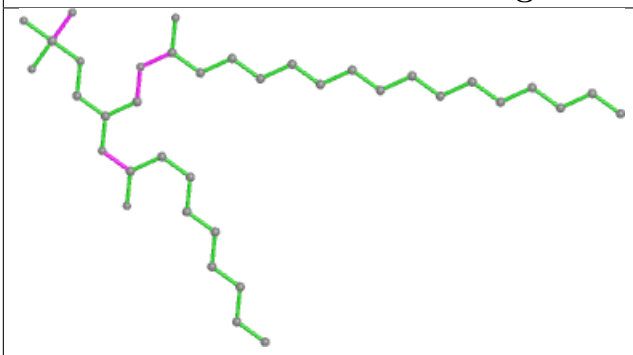


Torsions

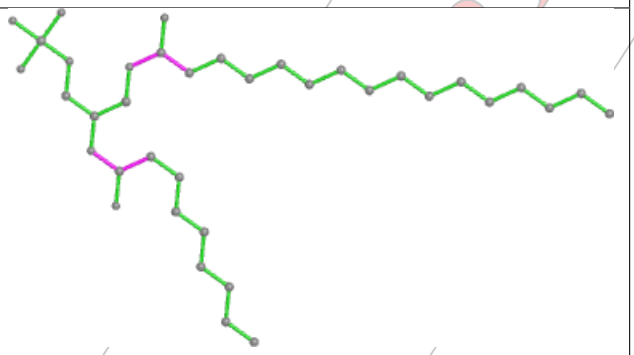


Rings

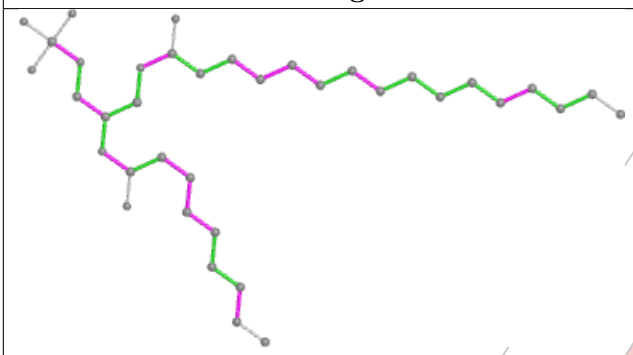
Ligand PGW A 901



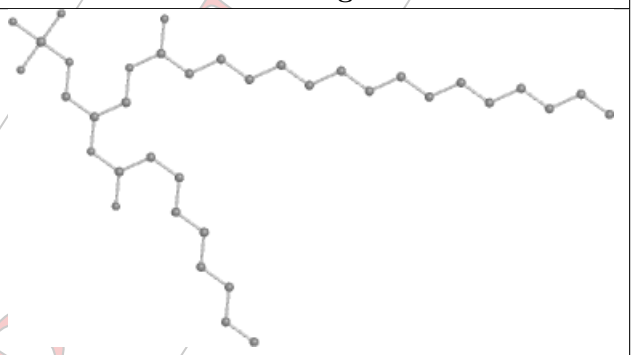
Bond lengths



Bond angles

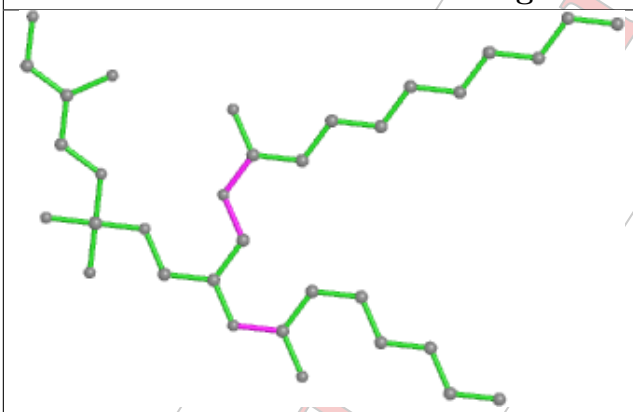


Torsions

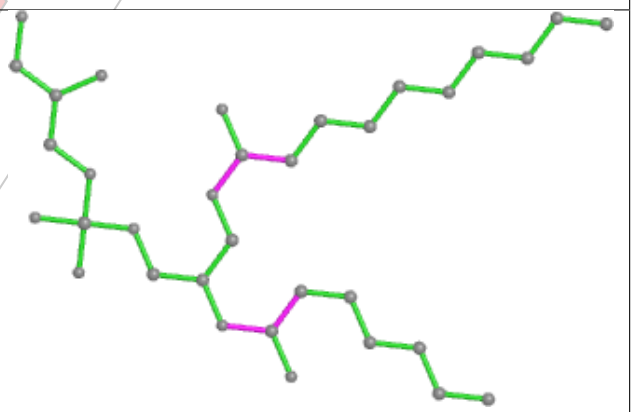


Rings

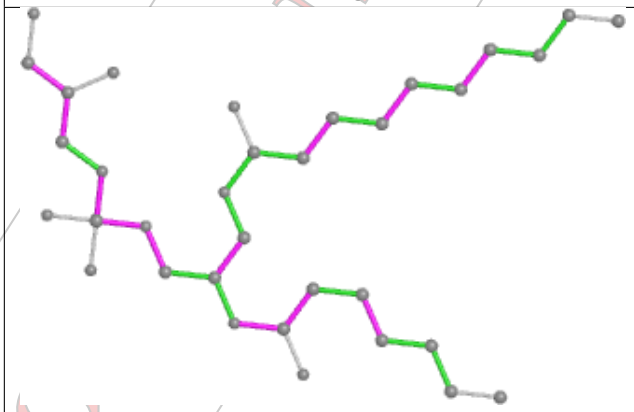
Ligand PGW A 908



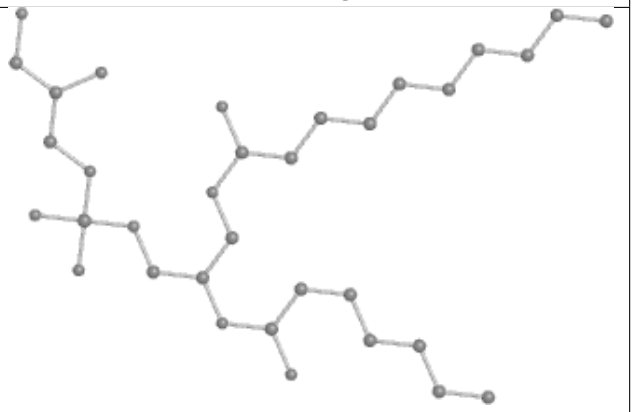
Bond lengths



Bond angles

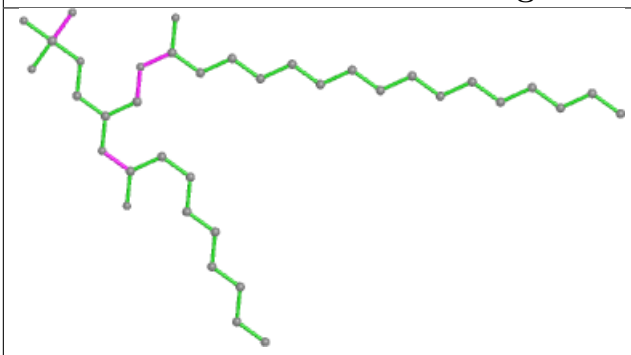


Torsions

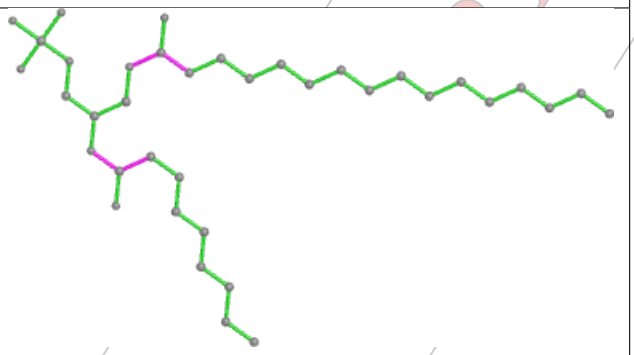


Rings

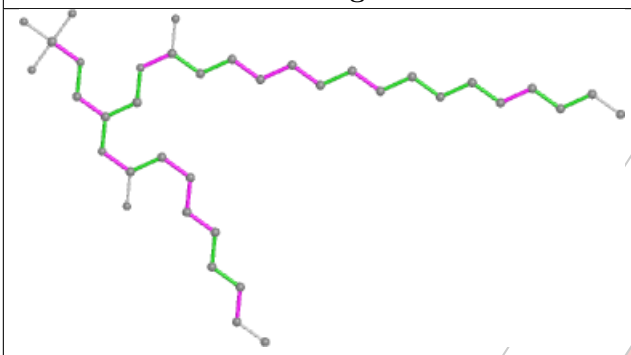
Ligand PGW B 806



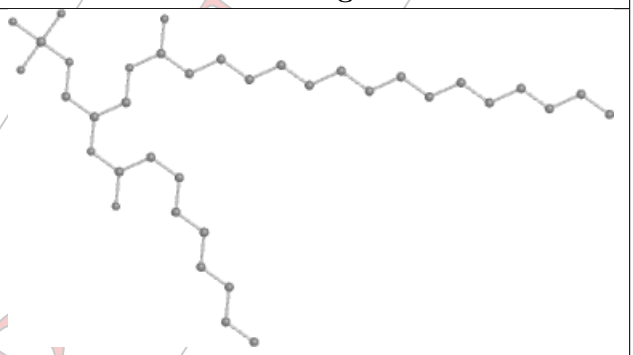
Bond lengths



Bond angles

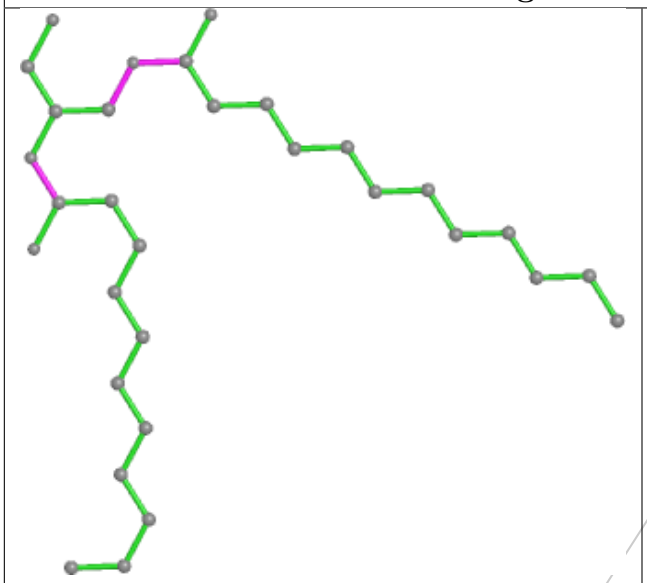


Torsions

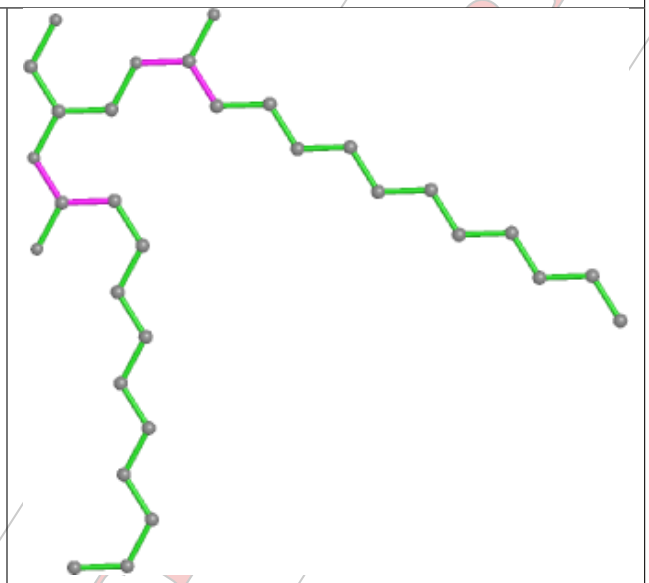


Rings

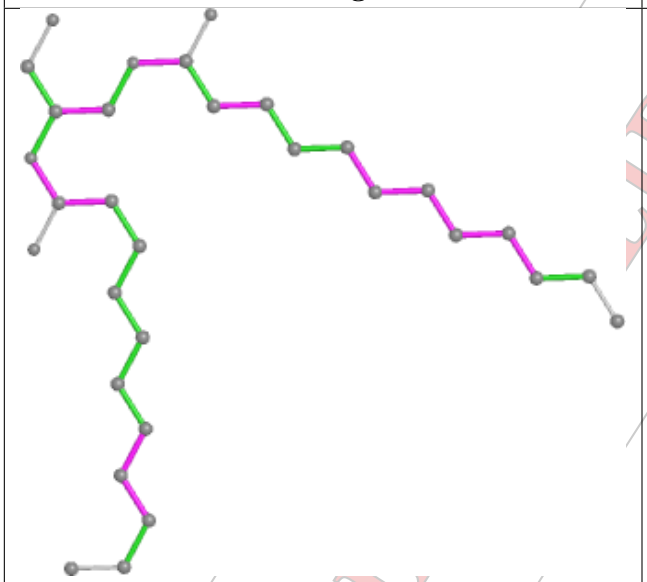
Ligand PGW A 902



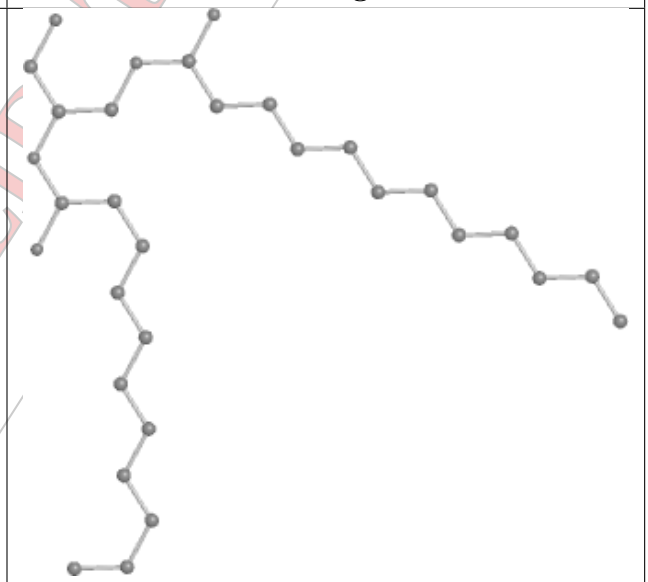
Bond lengths



Bond angles

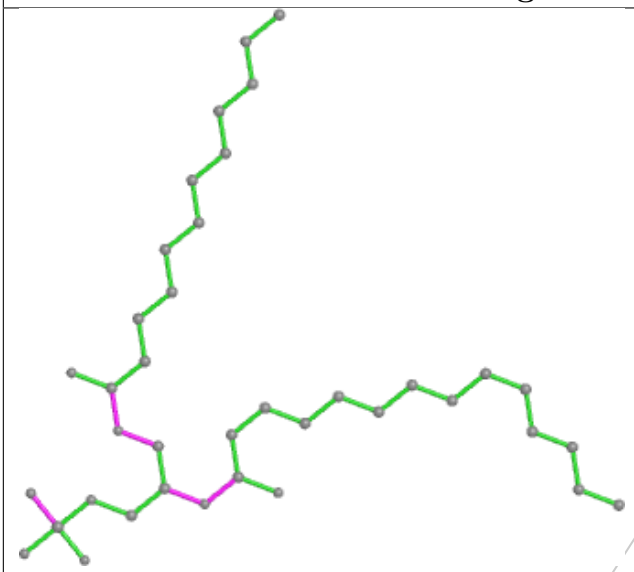


Torsions

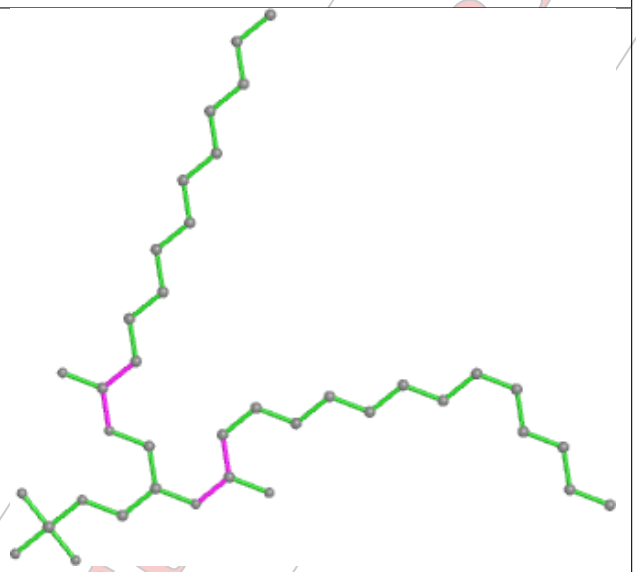


Rings

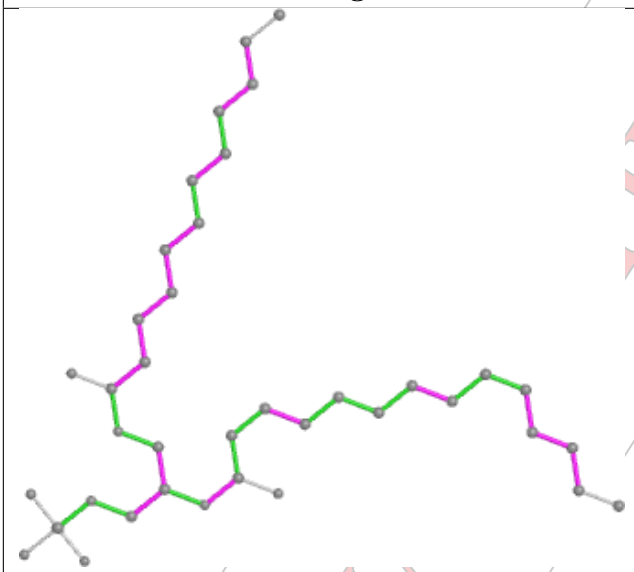
Ligand PGW B 804



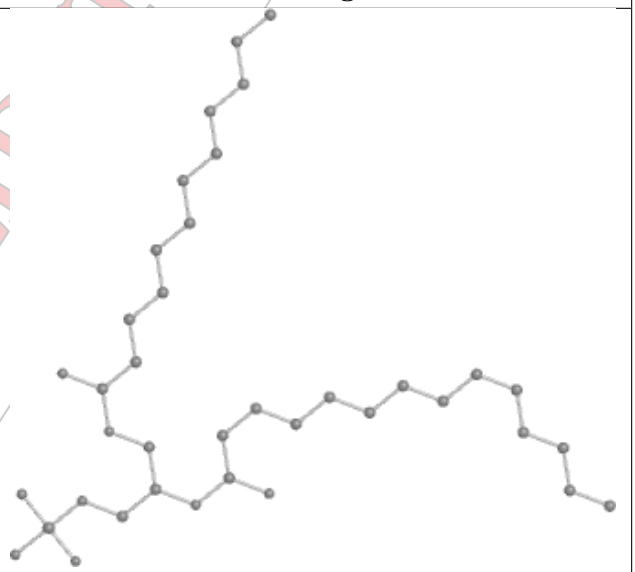
Bond lengths



Bond angles

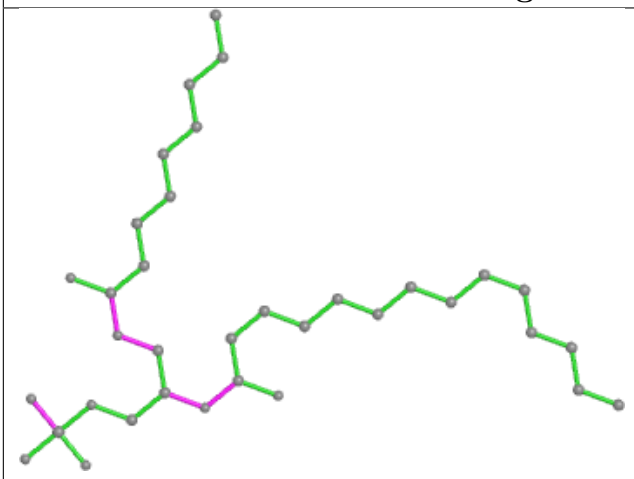


Torsions

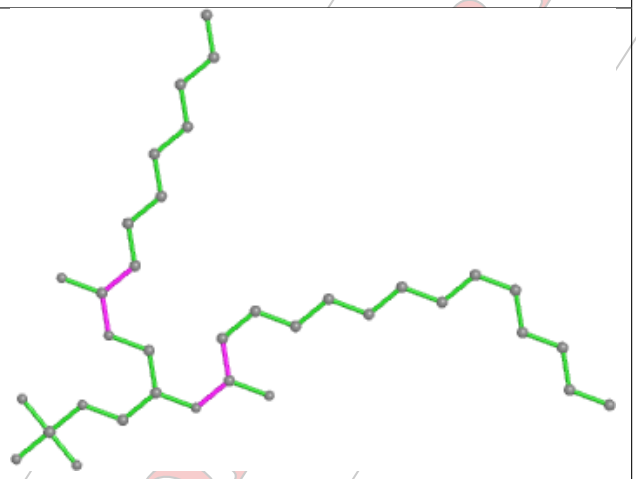


Rings

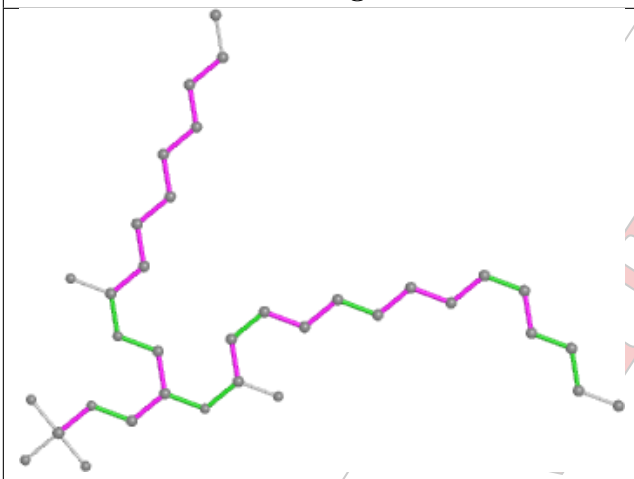
Ligand PGW A 903



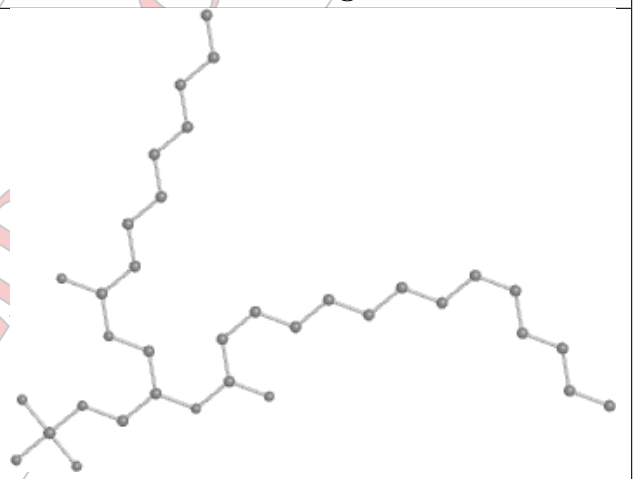
Bond lengths



Bond angles

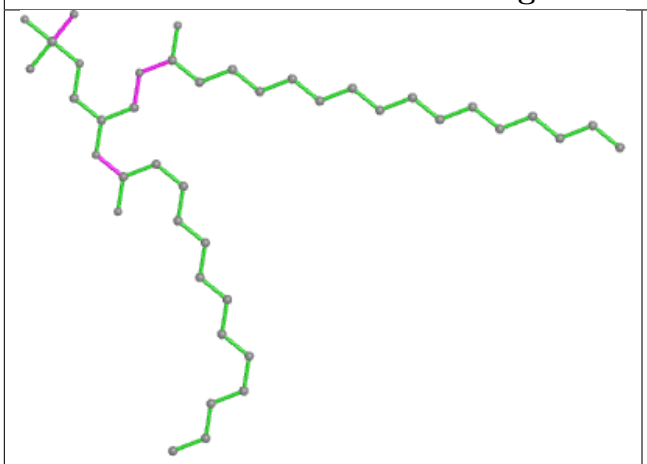


Torsions

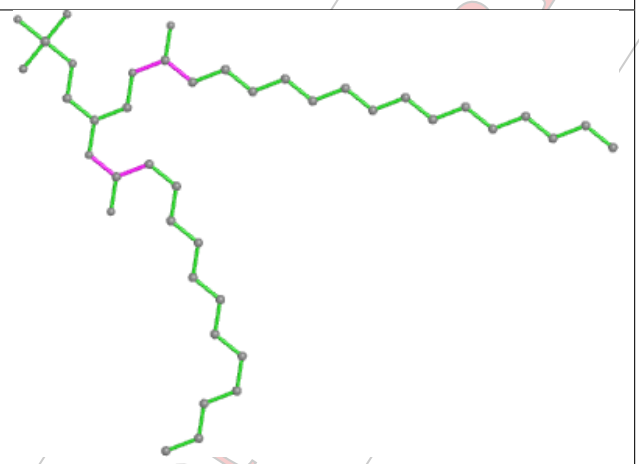


Rings

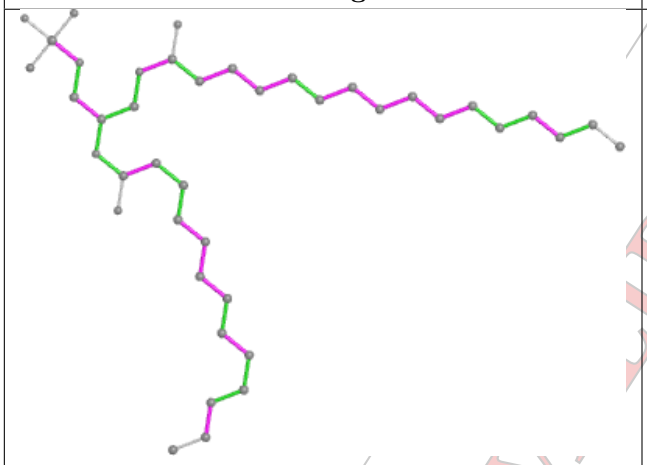
Ligand PGW B 801



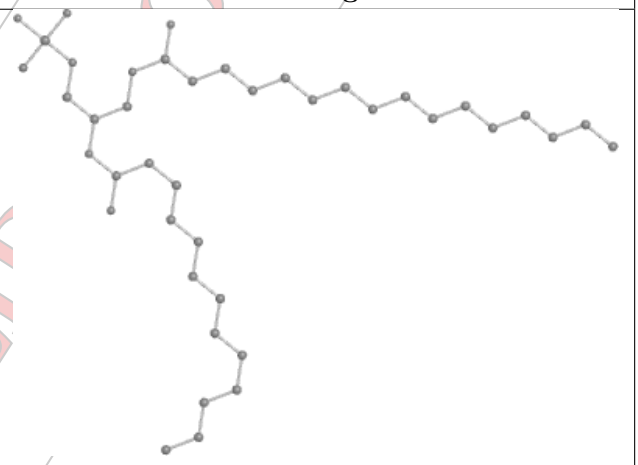
Bond lengths



Bond angles

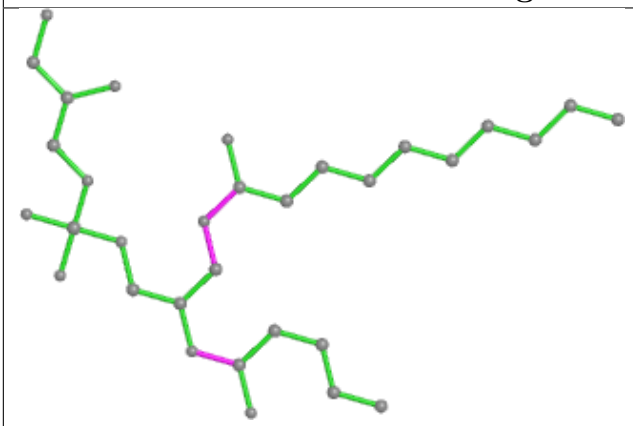


Torsions

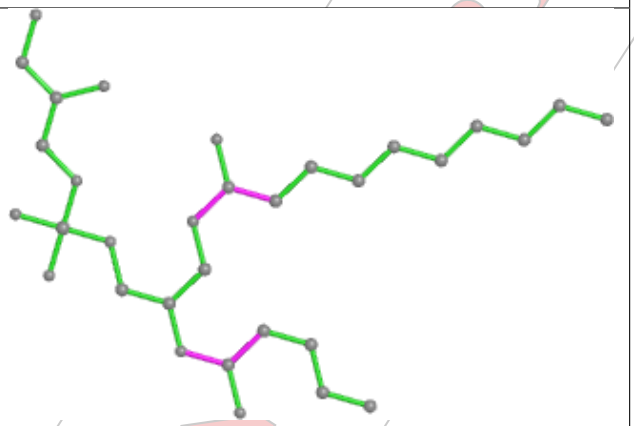


Rings

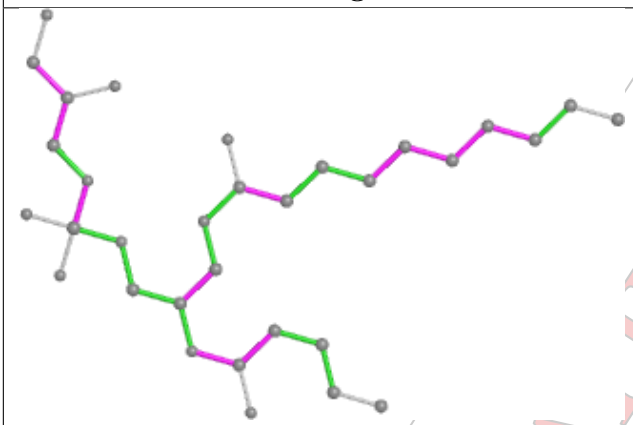
Ligand PGW A 905



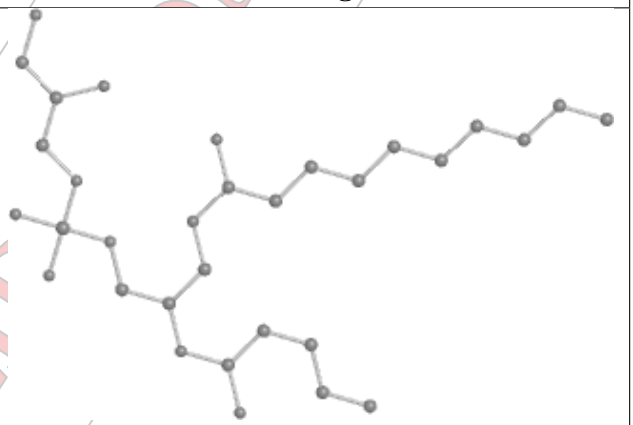
Bond lengths



Bond angles

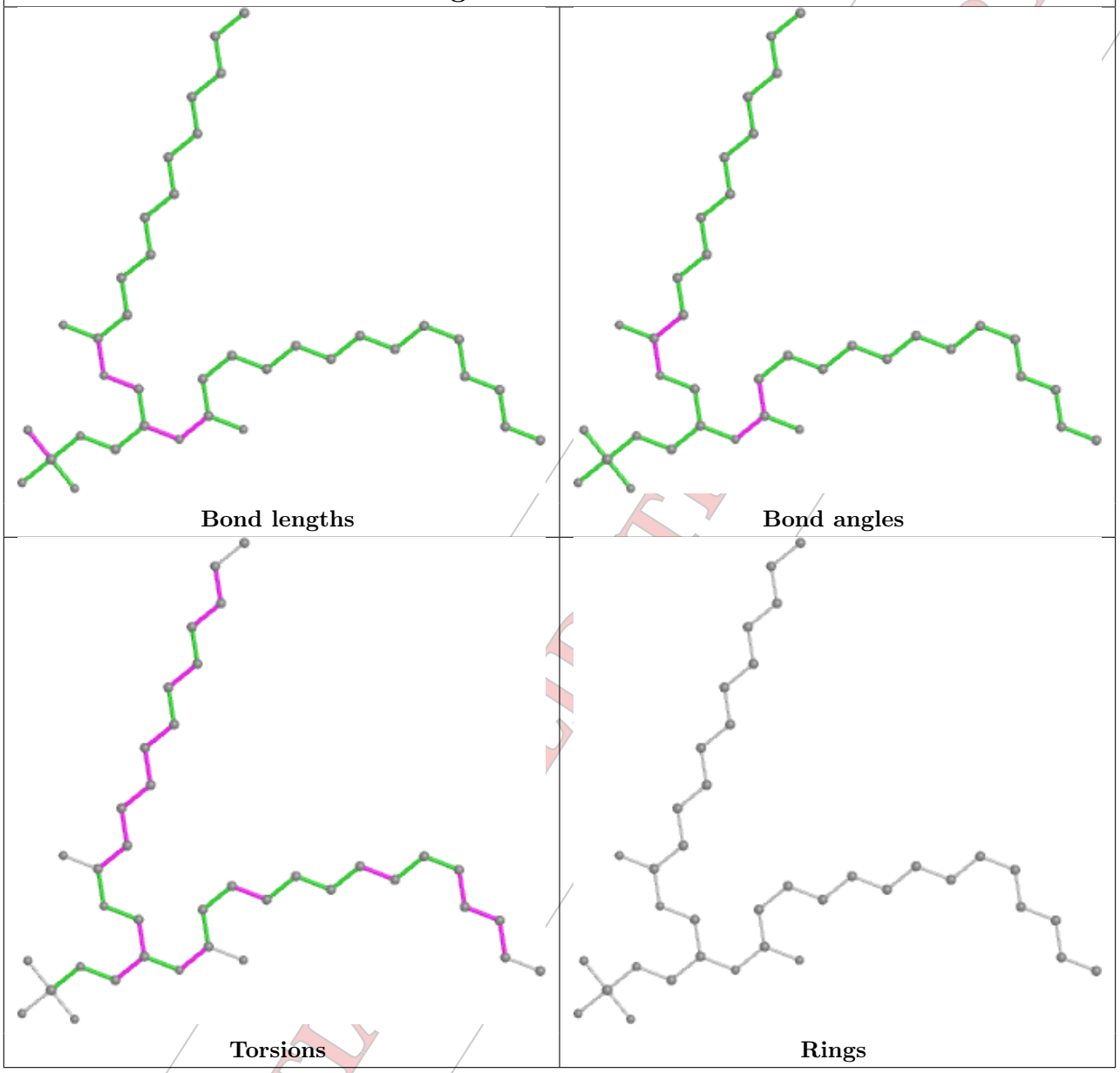


Torsions



Rings

Ligand PGW A 907



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

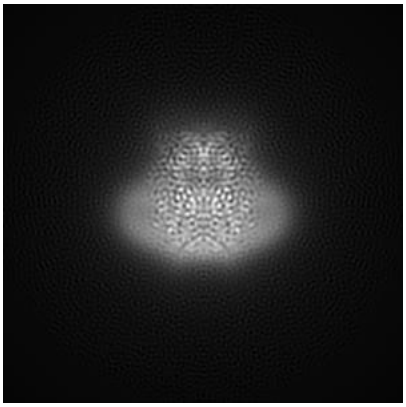
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24723. These allow visual inspection of the internal detail of the map and identification of artifacts.

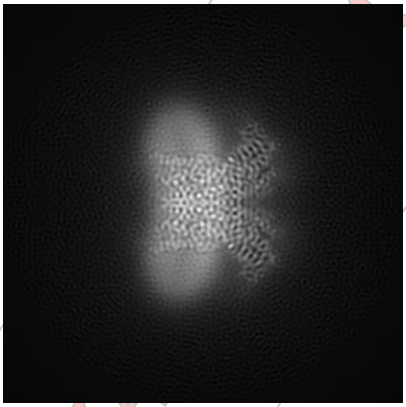
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

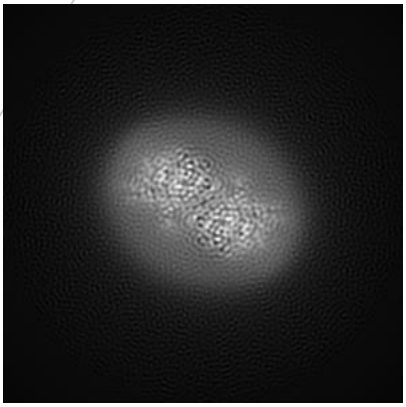
6.1.1 Primary map



X



Y

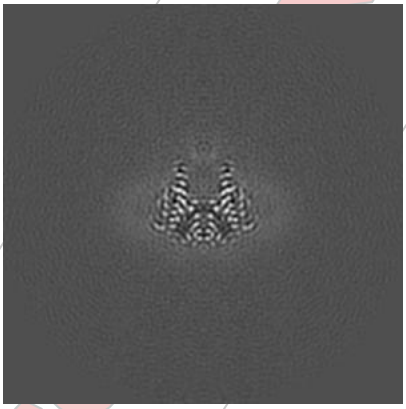


Z

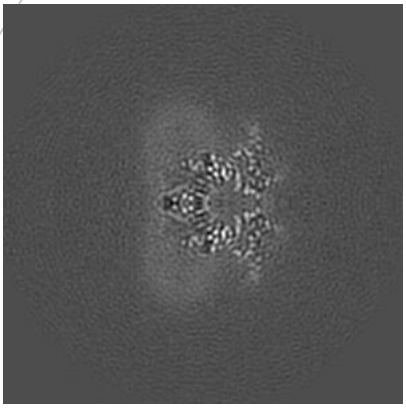
The images above show the map projected in three orthogonal directions.

6.2 Central slices

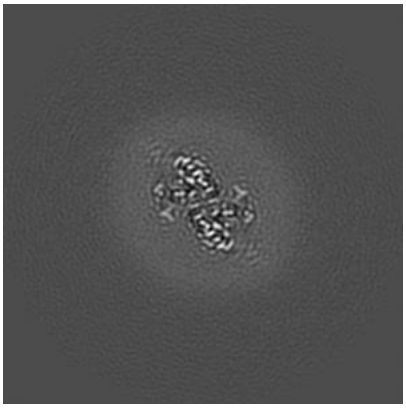
6.2.1 Primary map



X Index: 128



Y Index: 128

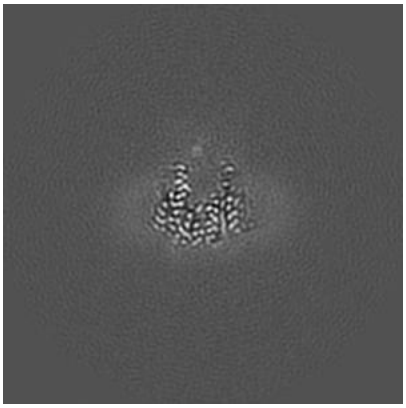


Z Index: 128

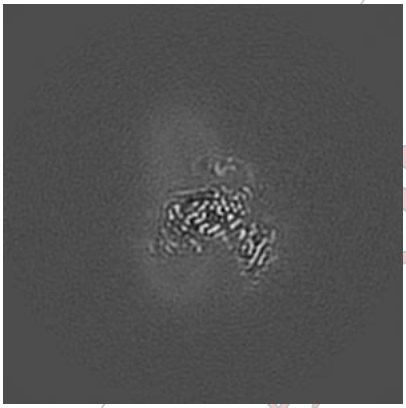
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

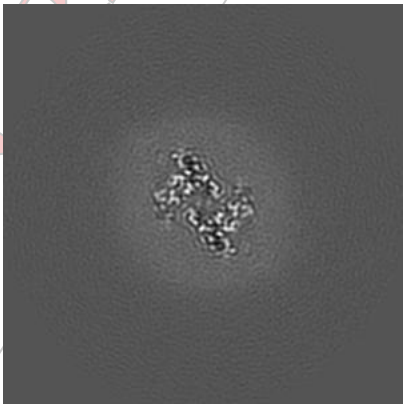
6.3.1 Primary map



X Index: 130



Y Index: 142

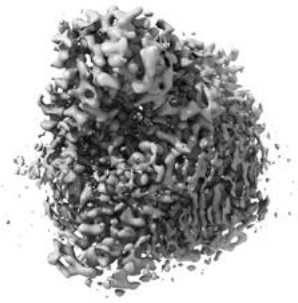


Z Index: 131

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

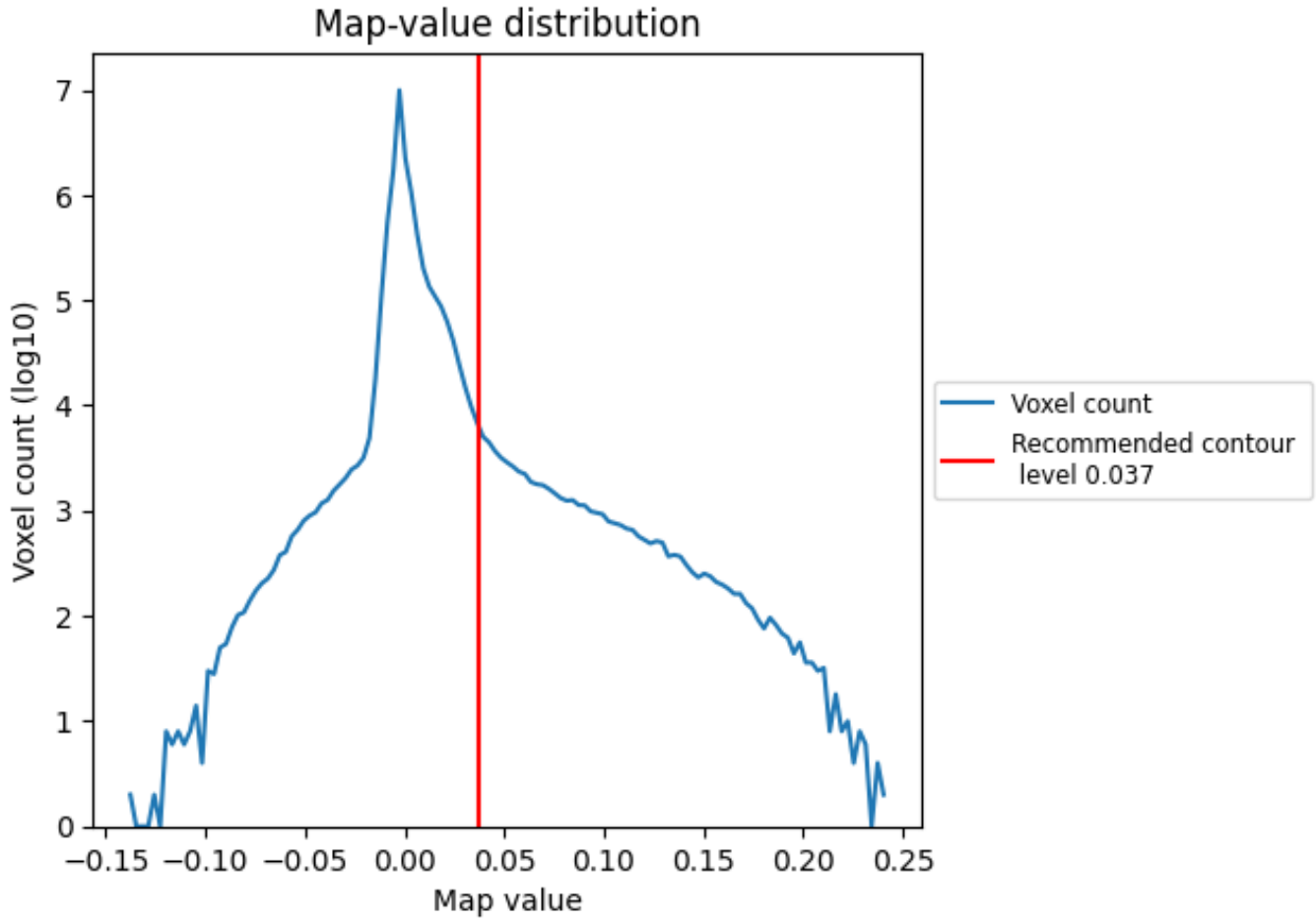
6.5 Mask visualisation (i)

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

7 Map analysis

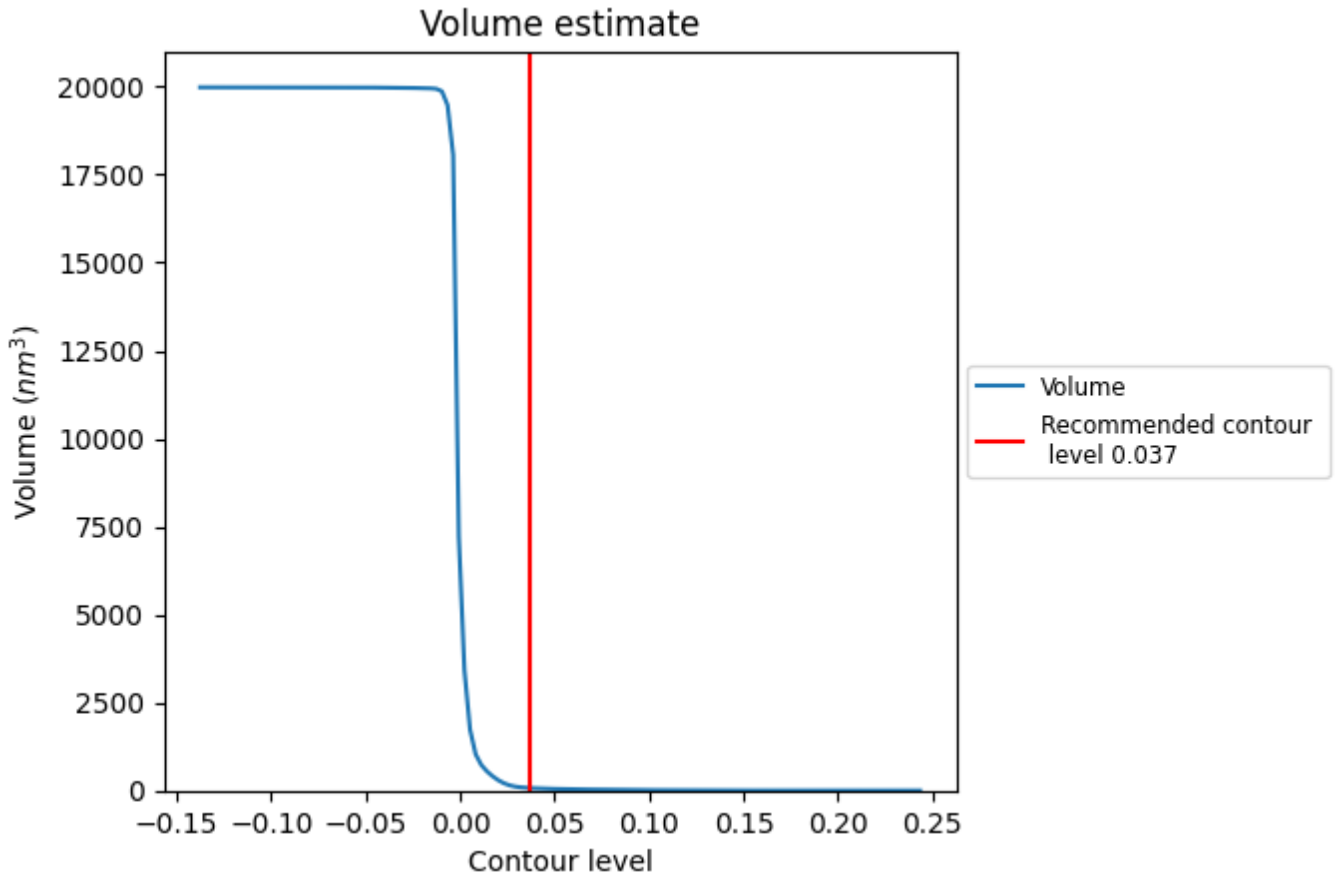
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

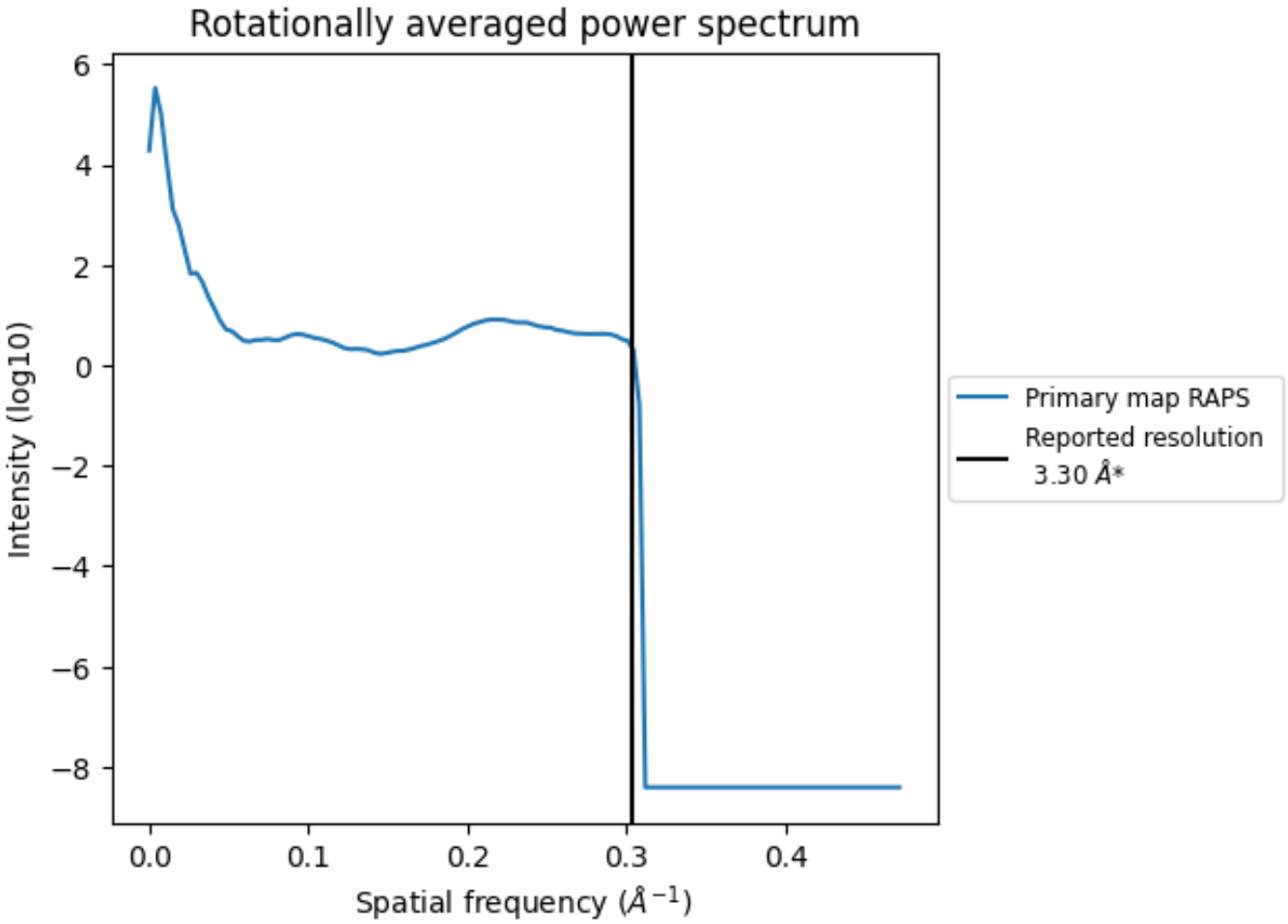
7.2 Volume estimate



The volume at the recommended contour level is 71 nm^3; this corresponds to an approximate mass of 65 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)

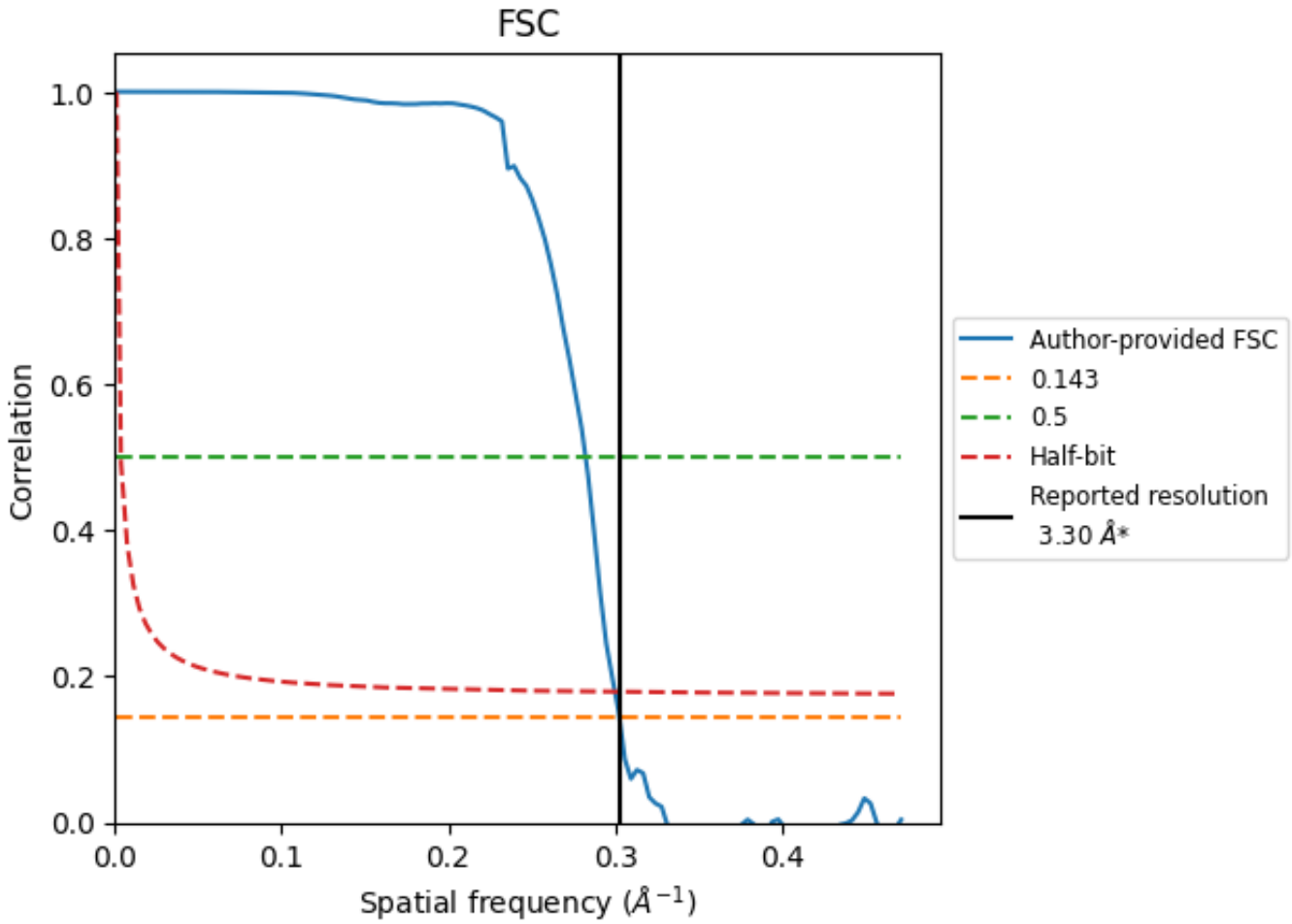


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

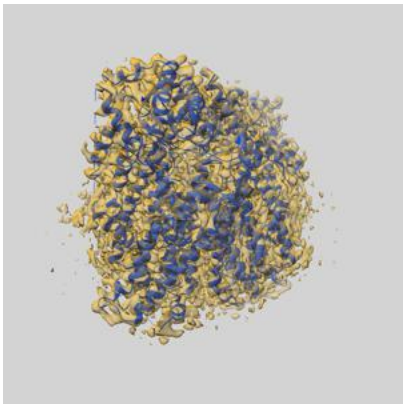
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.54	3.33
Unmasked-calculated*	-	-	-

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

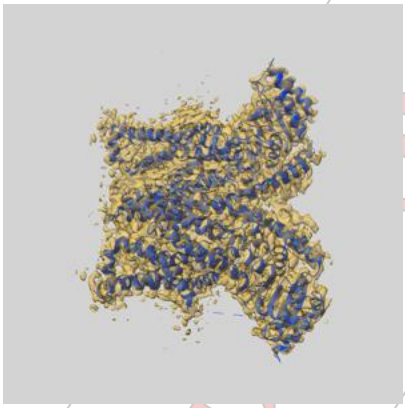
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24723 and PDB model 7RX3. Per-residue inclusion information can be found in section 3 on page 5.

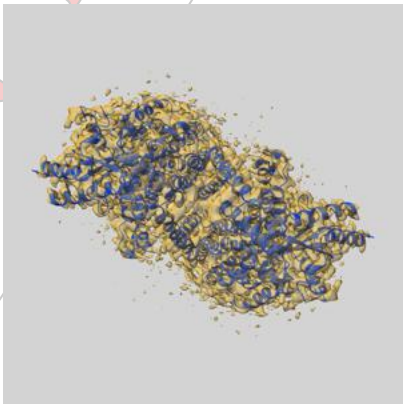
9.1 Map-model overlay



X



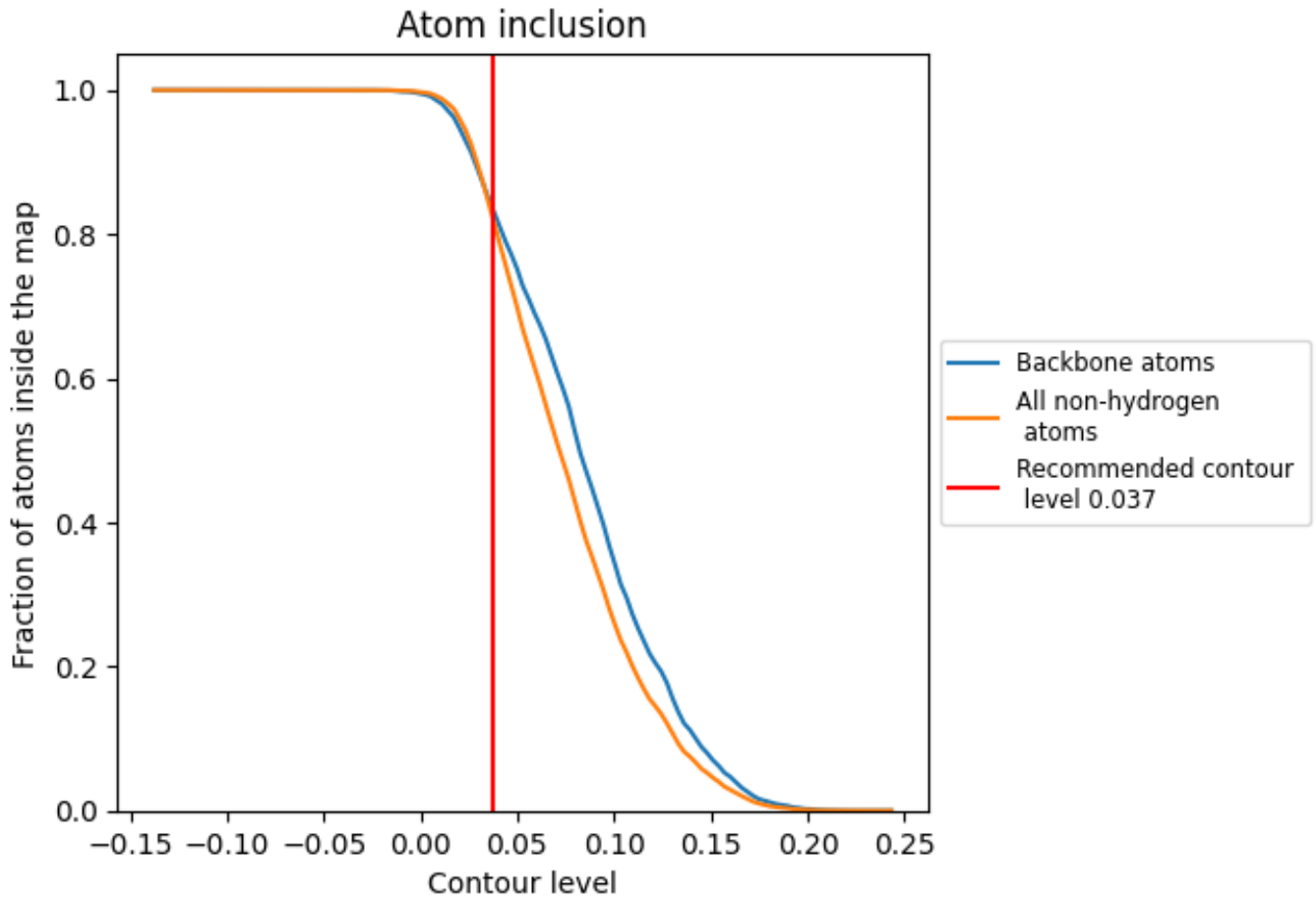
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.037 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 Atom inclusion



At the recommended contour level, 84% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

Full wwPDB EM Validation Report ⓘ

Aug 30, 2021 – 10:19 AM EDT

PDB ID	:	7RXH
EMDB ID	:	EMD-24731
Title	:	afTMEM16 in C18 lipid nanodiscs with MSP1E3 scaffold protein in the presence of Ca2+, monomer with extra lipids
Deposited on	:	2021-08-23
Resolution	:	2.30 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

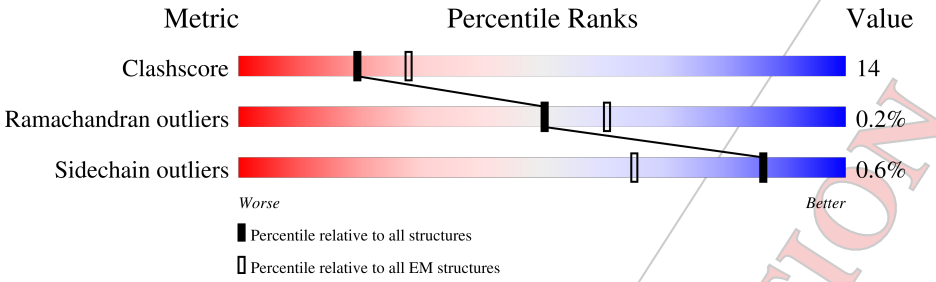
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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 <=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	735	63% 22% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5631 atoms, of which 48 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.

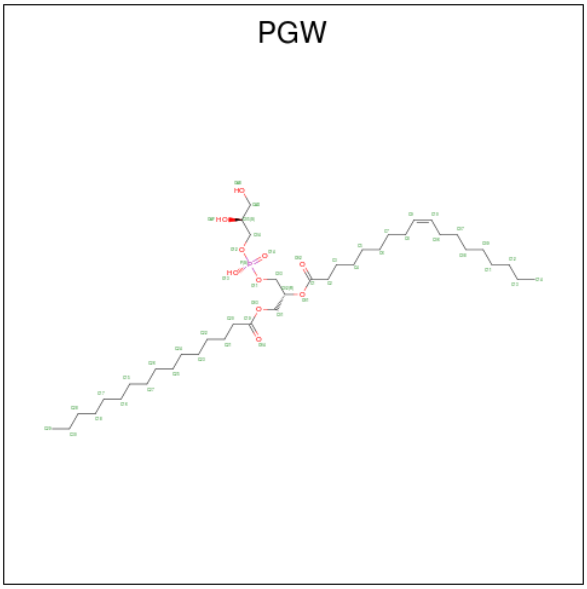
- Molecule 1 is a protein called afTMEM16 lipid scramblase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	626	5062	3303	849	892	18	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	2	2	2	0

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	A	1	495	350	130	15	0
3	A	1	Total 495	C 350	O 130	P 15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0
3	A	1	Total C O P 495 350 130 15	0

- Molecule 4 is water.

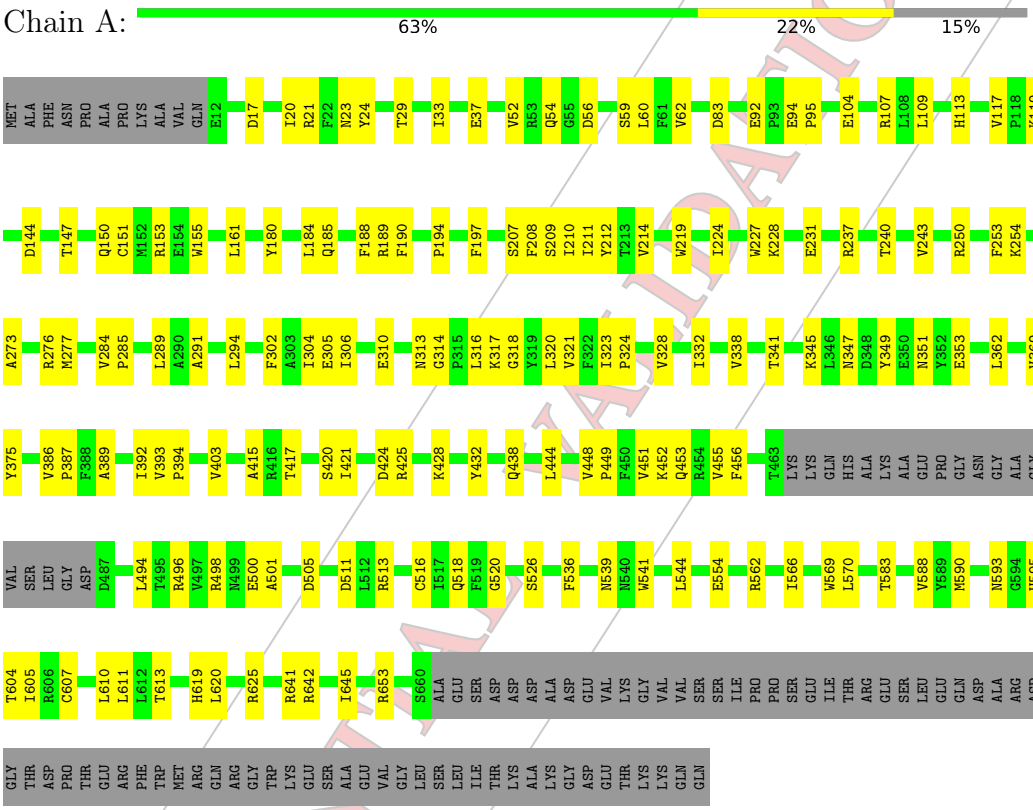
Mol	Chain	Residues	Atoms	AltConf
4	A	24	Total H O 72 48 24	0

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: afTMEM16 lipid scramblase

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1058829	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 ($e^-/Å^2$)	42.8227	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	0.040	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0049	Depositor
Map size (Å)	271.3728, 271.3728, 271.3728	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7067, 0.7067, 0.7067	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/5197	0.43	0/7070

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	5062	0	5018	134	0
2	A	2	0	0	0	0
3	A	495	0	558	51	0
4	A	24	48	0	4	0
All	All	5583	48	5576	156	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 14.

All (156) 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)
3:A:812:PGW:H23A	3:A:818:PGW:H2A	1.28	1.10
3:A:812:PGW:H23A	3:A:818:PGW:C2	1.84	1.06
1:A:604:THR:HG22	3:A:803:PGW:HAD	1.56	0.86
1:A:338:VAL:HG13	3:A:814:PGW:H2	1.59	0.85
1:A:349:TYR:OH	3:A:818:PGW:H03A	1.78	0.84
3:A:814:PGW:H20	3:A:814:PGW:H3A	1.57	0.83
1:A:109:LEU:HD21	1:A:562:ARG:HD2	1.60	0.83
3:A:814:PGW:H20	3:A:814:PGW:C3	2.12	0.79
1:A:304:ILE:HG22	1:A:324:PRO:HG3	1.65	0.78
1:A:393:VAL:HG23	1:A:394:PRO:HD3	1.65	0.77
1:A:452:LYS:HE2	1:A:456:PHE:CE2	2.20	0.77
1:A:389:ALA:HA	1:A:392:ILE:HB	1.70	0.74
3:A:812:PGW:H23A	3:A:818:PGW:H2	1.69	0.72
1:A:598:PRO:HG3	1:A:605:ILE:HD11	1.72	0.71
1:A:313:ASN:H	1:A:415:ALA:HB1	1.57	0.70
1:A:17:ASP:OD1	1:A:107:ARG:NH1	2.25	0.69
1:A:209:SER:HA	3:A:808:PGW:H04	1.75	0.69
1:A:452:LYS:HE2	1:A:456:PHE:HE2	1.56	0.69
1:A:184:LEU:HD23	1:A:544:LEU:HD23	1.75	0.68
1:A:291:ALA:HA	1:A:372:ILE:HD13	1.77	0.66
1:A:496:ARG:NH1	1:A:500:GLU:OE2	2.29	0.66
3:A:805:PGW:H02	3:A:806:PGW:H01A	1.78	0.66
3:A:814:PGW:H4A	3:A:814:PGW:H22	1.78	0.66
1:A:318:GLY:HA2	1:A:321:VAL:HG22	1.79	0.65
1:A:21:ARG:NH2	1:A:501:ALA:O	2.29	0.65
3:A:812:PGW:C23	3:A:818:PGW:H2A	2.19	0.64
1:A:189:ARG:HD3	3:A:810:PGW:H03A	1.79	0.63
1:A:294:LEU:HD11	1:A:369:VAL:HG13	1.80	0.63
1:A:228:LYS:HG2	1:A:570:LEU:HD21	1.79	0.63
1:A:452:LYS:CE	1:A:456:PHE:CE2	2.83	0.62
1:A:539:ASN:HB2	3:A:807:PGW:H09	1.81	0.62
1:A:310:GLU:OE2	1:A:425:ARG:NH2	2.31	0.62
1:A:52:VAL:CG1	1:A:60:LEU:HD23	2.30	0.62
1:A:109:LEU:CD2	1:A:562:ARG:HD2	2.28	0.62
1:A:313:ASN:N	1:A:415:ALA:O	2.34	0.60
1:A:338:VAL:CG1	3:A:814:PGW:H5	2.33	0.59
1:A:610:LEU:HD21	3:A:806:PGW:H25A	1.84	0.59
1:A:583:THR:HG22	3:A:806:PGW:H18A	1.84	0.58
1:A:119:LYS:HA	1:A:123:GLY:O	2.03	0.58
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.86	0.58
1:A:29:THR:O	1:A:33:ILE:HG12	2.04	0.58
1:A:273:ALA:O	1:A:277:MET:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:CG1	3:A:814:PGW:H2	2.33	0.56
1:A:305:GLU:OE1	1:A:425:ARG:NH1	2.36	0.55
1:A:253:PHE:CZ	1:A:353:GLU:HG2	2.41	0.55
1:A:151:CYS:HB3	1:A:155:TRP:CZ2	2.42	0.54
1:A:593:ASN:HD21	1:A:597:GLY:HA2	1.73	0.53
3:A:815:PGW:O02	3:A:815:PGW:H03	2.08	0.52
1:A:323:ILE:HB	1:A:324:PRO:HD3	1.92	0.52
1:A:386:VAL:HG12	1:A:598:PRO:HG2	1.91	0.52
1:A:607:CYS:O	1:A:611:LEU:HD23	2.10	0.52
1:A:188:PHE:CE1	1:A:541:TRP:HB2	2.44	0.51
1:A:494:LEU:O	1:A:498:ARG:HG3	2.10	0.51
1:A:21:ARG:NH1	1:A:137:ASP:OD2	2.42	0.51
3:A:812:PGW:O14	3:A:812:PGW:H01A	2.10	0.51
1:A:54:GLN:NE2	1:A:56:ASP:O	2.28	0.51
1:A:620:LEU:HG	3:A:803:PGW:H28	1.92	0.51
1:A:21:ARG:HD2	1:A:137:ASP:HB3	1.93	0.50
1:A:448:VAL:CG2	1:A:449:PRO:HD3	2.41	0.50
1:A:316:LEU:O	1:A:320:LEU:HG	2.11	0.50
1:A:180:TYR:CZ	1:A:511:ASP:HB3	2.46	0.50
1:A:607:CYS:SG	3:A:805:PGW:H2A	2.52	0.50
1:A:94:GLU:HB3	1:A:95:PRO:HD2	1.93	0.49
1:A:317:LYS:O	1:A:321:VAL:HG13	2.12	0.49
3:A:809:PGW:H24A	3:A:810:PGW:O04	2.13	0.49
1:A:161:LEU:N	1:A:185:GLN:OE1	2.43	0.49
1:A:227:TRP:CE2	1:A:231:GLU:HG3	2.48	0.49
1:A:24:TYR:CE2	1:A:60:LEU:HD12	2.47	0.49
1:A:52:VAL:HG11	1:A:60:LEU:HD23	1.93	0.49
1:A:444:LEU:HA	1:A:448:VAL:HG22	1.93	0.49
1:A:211:ILE:HD13	3:A:808:PGW:H6A	1.95	0.49
1:A:313:ASN:N	1:A:415:ALA:HB1	2.27	0.49
1:A:250:ARG:HD3	4:A:2701:HOH:O	2.12	0.49
1:A:393:VAL:CG2	1:A:394:PRO:HD3	2.40	0.48
1:A:613:THR:CG2	3:A:803:PGW:H22	2.43	0.48
1:A:516:CYS:SG	1:A:569:TRP:HB3	2.54	0.48
1:A:386:VAL:HB	1:A:387:PRO:HD3	1.95	0.48
1:A:104:GLU:HG3	1:A:107:ARG:NH2	2.29	0.48
1:A:208:PHE:O	3:A:808:PGW:HADA	2.14	0.48
1:A:151:CYS:HB3	1:A:155:TRP:CH2	2.48	0.48
1:A:375:TYR:OH	1:A:520:GLY:HA3	2.14	0.48
3:A:818:PGW:H25A	3:A:818:PGW:H15A	1.46	0.47
1:A:190:PHE:O	1:A:194:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HG22	1:A:228:LYS:HE2	1.97	0.46
1:A:276:ARG:HH11	1:A:351:ASN:HB3	1.79	0.46
1:A:387:PRO:HG3	1:A:590:MET:HE1	1.98	0.46
1:A:432:TYR:CE2	3:A:816:PGW:H23A	2.50	0.46
1:A:453:GLN:HE22	1:A:554:GLU:HA	1.81	0.46
1:A:320:LEU:HD22	1:A:323:ILE:HD11	1.97	0.46
1:A:611:LEU:HD21	3:A:805:PGW:H6A	1.98	0.45
3:A:814:PGW:H20	3:A:814:PGW:H3	1.95	0.45
1:A:641:ARG:O	1:A:645:ILE:HG12	2.16	0.45
3:A:812:PGW:C24	3:A:818:PGW:H4A	2.47	0.45
1:A:619:HIS:HB3	3:A:813:PGW:H06A	1.98	0.45
1:A:338:VAL:HG11	3:A:814:PGW:H5	1.98	0.45
1:A:320:LEU:HD13	1:A:403:VAL:HB	2.00	0.44
1:A:338:VAL:HG11	3:A:814:PGW:C5	2.47	0.44
1:A:254:LYS:O	1:A:351:ASN:ND2	2.48	0.44
1:A:289:LEU:HD22	3:A:814:PGW:C23	2.46	0.44
1:A:302:PHE:O	1:A:306:ILE:HG12	2.18	0.44
1:A:212:TYR:OH	1:A:526:SER:HB2	2.17	0.44
1:A:294:LEU:CD1	1:A:369:VAL:HG13	2.47	0.44
1:A:425:ARG:HD2	4:A:2722:HOH:O	2.17	0.44
1:A:613:THR:HG23	3:A:803:PGW:H22	2.00	0.44
1:A:197:PHE:HD1	3:A:809:PGW:H30A	1.81	0.44
1:A:240:THR:O	1:A:243:VAL:HB	2.18	0.44
1:A:438:GLN:HE22	1:A:518:GLN:HE21	1.66	0.44
1:A:593:ASN:ND2	1:A:597:GLY:HA2	2.32	0.44
1:A:604:THR:CG2	3:A:803:PGW:HAD	2.37	0.44
1:A:324:PRO:O	1:A:328:VAL:HG23	2.18	0.44
1:A:424:ASP:HB3	1:A:428:LYS:HE2	1.99	0.43
1:A:261:ASP:OD1	1:A:261:ASP:N	2.51	0.43
1:A:194:PRO:HD3	1:A:219:TRP:CD1	2.53	0.43
1:A:150:GLN:OE1	1:A:153:ARG:NH1	2.41	0.43
1:A:231:GLU:OE2	1:A:566:ILE:HG12	2.18	0.43
1:A:92:GLU:OE2	1:A:653:ARG:HD2	2.19	0.43
1:A:209:SER:CA	3:A:808:PGW:H04	2.45	0.43
1:A:318:GLY:HA2	1:A:321:VAL:CG2	2.48	0.43
1:A:625:ARG:NH2	4:A:2704:HOH:O	2.29	0.43
3:A:818:PGW:H06A	3:A:818:PGW:H8	1.74	0.43
1:A:237:ARG:HA	1:A:642:ARG:HH12	1.84	0.43
1:A:318:GLY:CA	1:A:321:VAL:HG22	2.49	0.42
1:A:23:ASN:HD22	1:A:59:SER:HB3	1.85	0.42
1:A:83:ASP:OD2	1:A:562:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:HIS:O	1:A:117:VAL:HG22	2.19	0.42
1:A:210:ILE:HG12	1:A:588:VAL:HG11	2.01	0.42
1:A:347:ASN:ND2	1:A:362:LEU:HB2	2.34	0.42
1:A:451:VAL:O	1:A:455:VAL:HG23	2.20	0.42
3:A:805:PGW:O04	3:A:805:PGW:H03	2.19	0.42
1:A:285:PRO:HD3	3:A:818:PGW:H06A	2.02	0.42
3:A:805:PGW:H01A	3:A:806:PGW:H02	2.01	0.42
1:A:291:ALA:HA	1:A:372:ILE:CD1	2.48	0.42
1:A:33:ILE:O	1:A:37:GLU:HG3	2.18	0.42
1:A:619:HIS:CB	3:A:813:PGW:H06A	2.49	0.42
1:A:619:HIS:CD2	3:A:813:PGW:H6	2.55	0.42
3:A:809:PGW:C2	3:A:809:PGW:H01	2.49	0.42
1:A:144:ASP:OD2	1:A:147:THR:OG1	2.31	0.41
1:A:314:GLY:N	1:A:415:ALA:HB1	2.35	0.41
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.86	0.41
3:A:816:PGW:H20A	3:A:816:PGW:H23	1.71	0.41
1:A:54:GLN:O	1:A:498:ARG:NH1	2.48	0.41
1:A:209:SER:OG	1:A:211:ILE:HG22	2.21	0.41
3:A:806:PGW:H26A	3:A:806:PGW:H16	1.83	0.41
1:A:341:THR:O	1:A:345:LYS:HD3	2.20	0.41
1:A:518:GLN:HG2	1:A:536:PHE:CE2	2.56	0.41
3:A:805:PGW:C01	3:A:806:PGW:H02	2.51	0.41
1:A:332:ILE:HD13	1:A:332:ILE:HA	1.88	0.41
1:A:370:ASN:HD21	1:A:513:ARG:HE	1.69	0.40
1:A:20:ILE:HB	1:A:62:VAL:HB	2.03	0.40
1:A:214:VAL:HG22	3:A:803:PGW:H15	2.03	0.40
1:A:444:LEU:HA	1:A:448:VAL:CG2	2.51	0.40
1:A:448:VAL:HG23	1:A:449:PRO:HD3	2.03	0.40
1:A:23:ASN:ND2	1:A:59:SER:HB3	2.37	0.40
1:A:207:SER:OG	1:A:595:HIS:NE2	2.51	0.40
1:A:425:ARG:HD3	4:A:2717:HOH:O	2.22	0.40
3:A:811:PGW:H20A	3:A:811:PGW:H01A	1.86	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	622/735 (85%)	604 (97%)	17 (3%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	SER

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	540/646 (84%)	537 (99%)	3 (1%)	86 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	THR
1	A	421	ILE
1	A	505	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	78	GLN
1	A	148	ASN
1	A	171	ASN
1	A	283	GLN
1	A	370	ASN
1	A	400	HIS
1	A	438	GLN

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Mol	Chain	Res	Type
1	A	453	GLN
1	A	593	ASN

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)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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	PGW	A	810	-	26,26,50	1.29	4 (15%)	30,31,56	1.28	2 (6%)
3	PGW	A	813	-	43,43,50	1.01	4 (9%)	46,49,56	1.09	2 (4%)
3	PGW	A	817	-	21,21,50	1.40	4 (19%)	25,26,56	1.29	2 (8%)
3	PGW	A	805	-	33,33,50	1.14	4 (12%)	37,38,56	1.18	2 (5%)
3	PGW	A	814	-	22,22,50	1.37	4 (18%)	26,27,56	1.26	2 (7%)
3	PGW	A	806	-	37,37,50	0.98	3 (8%)	39,39,56	1.20	2 (5%)
3	PGW	A	807	-	30,30,50	1.22	4 (13%)	34,35,56	1.20	2 (5%)
3	PGW	A	803	-	44,44,50	0.98	3 (6%)	46,50,56	1.12	2 (4%)
3	PGW	A	816	-	27,27,50	0.46	0	31,32,56	0.59	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PGW	A	818	-	35,35,50	1.13	4 (11%)	39,40,56	1.16	2 (5%)
3	PGW	A	812	-	28,28,50	1.25	5 (17%)	32,33,56	1.23	2 (6%)
3	PGW	A	815	-	27,27,50	0.46	0	31,32,56	0.59	1 (3%)
3	PGW	A	809	-	31,31,50	1.16	4 (12%)	35,36,56	1.20	2 (5%)
3	PGW	A	804	-	24,24,50	1.31	4 (16%)	28,29,56	1.30	3 (10%)
3	PGW	A	811	-	27,27,50	1.24	5 (18%)	31,32,56	1.23	2 (6%)
3	PGW	A	808	-	24,24,50	1.06	1 (4%)	26,29,56	1.03	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGW	A	810	-	-	16/28/28/55	-
3	PGW	A	813	-	-	23/48/48/55	-
3	PGW	A	817	-	-	11/23/23/55	-
3	PGW	A	805	-	-	16/35/35/55	-
3	PGW	A	814	-	-	10/24/24/55	-
3	PGW	A	807	-	-	10/32/32/55	-
3	PGW	A	816	-	-	12/29/29/55	-
3	PGW	A	818	-	-	17/37/37/55	-
3	PGW	A	812	-	-	18/30/30/55	-
3	PGW	A	815	-	-	17/29/29/55	-
3	PGW	A	809	-	-	17/33/33/55	-
3	PGW	A	804	-	-	11/26/26/55	-
3	PGW	A	811	-	-	17/29/29/55	-
3	PGW	A	808	-	-	12/28/28/55	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	810	PGW	O01-C1	3.11	1.43	1.34
3	A	807	PGW	O01-C1	2.96	1.42	1.34
3	A	809	PGW	O01-C1	2.95	1.42	1.34
3	A	817	PGW	O01-C1	2.91	1.42	1.34
3	A	814	PGW	O01-C1	2.88	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	818	PGW	O01-C1	2.87	1.42	1.34
3	A	806	PGW	O01-C1	2.87	1.42	1.34
3	A	805	PGW	O01-C1	2.84	1.42	1.34
3	A	811	PGW	O01-C1	2.80	1.42	1.34
3	A	804	PGW	O01-C1	2.79	1.42	1.34
3	A	803	PGW	O01-C1	2.79	1.42	1.34
3	A	808	PGW	O01-C1	2.78	1.42	1.34
3	A	812	PGW	O01-C1	2.74	1.42	1.34
3	A	813	PGW	O01-C1	2.69	1.41	1.34
3	A	813	PGW	O03-C19	2.58	1.40	1.33
3	A	818	PGW	O03-C19	2.47	1.40	1.33
3	A	809	PGW	O03-C19	2.46	1.40	1.33
3	A	810	PGW	O03-C19	2.46	1.40	1.33
3	A	814	PGW	O03-C19	2.45	1.40	1.33
3	A	817	PGW	O03-C19	2.44	1.40	1.33
3	A	807	PGW	O03-C19	2.43	1.40	1.33
3	A	804	PGW	O03-C01	-2.38	1.39	1.45
3	A	805	PGW	O03-C19	2.38	1.40	1.33
3	A	803	PGW	O03-C19	2.37	1.40	1.33
3	A	807	PGW	P-O12	2.37	1.64	1.54
3	A	804	PGW	O03-C19	2.37	1.40	1.33
3	A	812	PGW	O03-C19	2.36	1.40	1.33
3	A	804	PGW	P-O12	2.34	1.63	1.54
3	A	812	PGW	P-O12	2.34	1.63	1.54
3	A	814	PGW	P-O12	2.34	1.63	1.54
3	A	805	PGW	P-O12	2.34	1.63	1.54
3	A	817	PGW	P-O12	2.33	1.63	1.54
3	A	811	PGW	O03-C19	2.33	1.40	1.33
3	A	809	PGW	O03-C01	-2.32	1.39	1.45
3	A	818	PGW	P-O12	2.32	1.63	1.54
3	A	805	PGW	O03-C01	-2.32	1.39	1.45
3	A	810	PGW	P-O12	2.32	1.63	1.54
3	A	811	PGW	P-O12	2.31	1.63	1.54
3	A	809	PGW	P-O12	2.31	1.63	1.54
3	A	806	PGW	O03-C01	-2.31	1.39	1.45
3	A	806	PGW	O03-C19	2.29	1.40	1.33
3	A	811	PGW	O03-C01	-2.29	1.39	1.45
3	A	807	PGW	O03-C01	-2.27	1.40	1.45
3	A	812	PGW	O03-C01	-2.27	1.40	1.45
3	A	814	PGW	O03-C01	-2.27	1.40	1.45
3	A	818	PGW	O03-C01	-2.26	1.40	1.45
3	A	803	PGW	O03-C01	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	817	PGW	O03-C01	-2.25	1.40	1.45
3	A	810	PGW	O03-C01	-2.25	1.40	1.45
3	A	813	PGW	O03-C01	-2.21	1.40	1.45
3	A	813	PGW	O01-C02	-2.08	1.41	1.46
3	A	812	PGW	O01-C02	-2.06	1.41	1.46
3	A	811	PGW	O01-C02	-2.01	1.41	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	810	PGW	O01-C1-C2	4.17	120.49	111.50
3	A	804	PGW	O01-C1-C2	4.12	120.39	111.50
3	A	806	PGW	O01-C1-C2	4.12	120.37	111.50
3	A	805	PGW	O01-C1-C2	4.10	120.35	111.50
3	A	813	PGW	O01-C1-C2	4.06	120.25	111.50
3	A	807	PGW	O01-C1-C2	4.04	120.22	111.50
3	A	812	PGW	O01-C1-C2	4.04	120.22	111.50
3	A	803	PGW	O01-C1-C2	4.03	120.19	111.50
3	A	809	PGW	O01-C1-C2	3.99	120.09	111.50
3	A	818	PGW	O01-C1-C2	3.99	120.09	111.50
3	A	811	PGW	O01-C1-C2	3.98	120.07	111.50
3	A	817	PGW	O01-C1-C2	3.96	120.03	111.50
3	A	814	PGW	O01-C1-C2	3.88	119.85	111.50
3	A	808	PGW	O01-C1-C2	3.80	119.68	111.50
3	A	810	PGW	O03-C19-C20	2.83	120.79	111.91
3	A	807	PGW	O03-C19-C20	2.73	120.48	111.91
3	A	813	PGW	O03-C19-C20	2.72	120.44	111.91
3	A	803	PGW	O03-C19-C20	2.64	120.19	111.91
3	A	806	PGW	O03-C19-C20	2.62	120.12	111.91
3	A	811	PGW	O03-C19-C20	2.57	119.97	111.91
3	A	814	PGW	O03-C19-C20	2.57	119.97	111.91
3	A	804	PGW	O03-C19-C20	2.55	119.92	111.91
3	A	817	PGW	O03-C19-C20	2.54	119.87	111.91
3	A	805	PGW	O03-C19-C20	2.54	119.86	111.91
3	A	809	PGW	O03-C19-C20	2.53	119.84	111.91
3	A	818	PGW	O03-C19-C20	2.52	119.82	111.91
3	A	812	PGW	O03-C19-C20	2.45	119.60	111.91
3	A	816	PGW	O13-P-O14	2.37	119.98	110.68
3	A	815	PGW	O13-P-O14	2.37	119.94	110.68
3	A	804	PGW	C02-O01-C1	-2.12	112.58	117.79

There are no chirality outliers.

All (207) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	PGW	C03-O11-P-O12
3	A	804	PGW	C03-O11-P-O14
3	A	805	PGW	C03-O11-P-O12
3	A	805	PGW	C03-O11-P-O13
3	A	805	PGW	C03-O11-P-O14
3	A	805	PGW	C2-C1-O01-C02
3	A	809	PGW	C2-C1-O01-C02
3	A	810	PGW	C03-O11-P-O13
3	A	810	PGW	C03-O11-P-O14
3	A	810	PGW	C2-C1-O01-C02
3	A	811	PGW	C03-O11-P-O12
3	A	811	PGW	C03-O11-P-O13
3	A	811	PGW	C03-O11-P-O14
3	A	811	PGW	O04-C19-O03-C01
3	A	811	PGW	C20-C19-O03-C01
3	A	813	PGW	OAF-C05-CAD-OAE
3	A	813	PGW	C04-C05-CAD-OAE
3	A	813	PGW	O12-C04-C05-CAD
3	A	815	PGW	C03-O11-P-O12
3	A	815	PGW	C03-O11-P-O13
3	A	815	PGW	C03-O11-P-O14
3	A	815	PGW	C2-C1-O01-C02
3	A	816	PGW	C2-C1-O01-C02
3	A	817	PGW	C03-O11-P-O12
3	A	817	PGW	C03-O11-P-O13
3	A	817	PGW	C03-O11-P-O14
3	A	818	PGW	C03-O11-P-O12
3	A	818	PGW	C03-O11-P-O13
3	A	818	PGW	C10-C06-C07-C08
3	A	812	PGW	O04-C19-O03-C01
3	A	809	PGW	O02-C1-O01-C02
3	A	810	PGW	O02-C1-O01-C02
3	A	815	PGW	O02-C1-O01-C02
3	A	816	PGW	O02-C1-O01-C02
3	A	809	PGW	C20-C19-O03-C01
3	A	812	PGW	C20-C19-O03-C01
3	A	805	PGW	O02-C1-O01-C02
3	A	814	PGW	O04-C19-O03-C01
3	A	814	PGW	C20-C19-O03-C01
3	A	816	PGW	C3-C4-C5-C6
3	A	809	PGW	O04-C19-O03-C01
3	A	818	PGW	C25-C26-C27-C15

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Mol	Chain	Res	Type	Atoms
3	A	813	PGW	O12-C04-C05-OAF
3	A	813	PGW	C19-C20-C21-C22
3	A	804	PGW	C1-C2-C3-C4
3	A	816	PGW	C1-C2-C3-C4
3	A	808	PGW	C1-C2-C3-C4
3	A	815	PGW	C1-C2-C3-C4
3	A	816	PGW	C19-C20-C21-C22
3	A	817	PGW	C19-C20-C21-C22
3	A	818	PGW	C1-C2-C3-C4
3	A	809	PGW	C19-C20-C21-C22
3	A	811	PGW	C1-C2-C3-C4
3	A	813	PGW	C10-C06-C07-C08
3	A	804	PGW	C21-C22-C23-C24
3	A	811	PGW	C24-C25-C26-C27
3	A	805	PGW	C23-C24-C25-C26
3	A	810	PGW	C2-C3-C4-C5
3	A	818	PGW	C2-C3-C4-C5
3	A	805	PGW	C2-C3-C4-C5
3	A	813	PGW	C24-C25-C26-C27
3	A	816	PGW	C20-C21-C22-C23
3	A	813	PGW	C16-C15-C27-C26
3	A	811	PGW	C22-C23-C24-C25
3	A	805	PGW	C16-C15-C27-C26
3	A	810	PGW	C20-C21-C22-C23
3	A	814	PGW	C2-C1-O01-C02
3	A	805	PGW	C21-C22-C23-C24
3	A	809	PGW	C21-C22-C23-C24
3	A	818	PGW	C24-C25-C26-C27
3	A	816	PGW	C21-C22-C23-C24
3	A	813	PGW	C5-C6-C7-C8
3	A	813	PGW	C22-C23-C24-C25
3	A	813	PGW	C25-C26-C27-C15
3	A	816	PGW	C4-C5-C6-C7
3	A	811	PGW	C23-C24-C25-C26
3	A	810	PGW	C1-C2-C3-C4
3	A	808	PGW	C3-C4-C5-C6
3	A	817	PGW	C2-C1-O01-C02
3	A	814	PGW	O02-C1-O01-C02
3	A	817	PGW	O02-C1-O01-C02
3	A	815	PGW	C2-C3-C4-C5
3	A	815	PGW	C4-C5-C6-C7
3	A	810	PGW	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
3	A	812	PGW	C1-C2-C3-C4
3	A	817	PGW	C21-C22-C23-C24
3	A	811	PGW	C21-C22-C23-C24
3	A	818	PGW	C19-C20-C21-C22
3	A	808	PGW	C2-C1-O01-C02
3	A	812	PGW	C2-C1-O01-C02
3	A	812	PGW	C7-C8-C9-C10
3	A	812	PGW	O02-C1-O01-C02
3	A	808	PGW	C4-C5-C6-C7
3	A	811	PGW	O03-C01-C02-O01
3	A	809	PGW	C20-C21-C22-C23
3	A	807	PGW	C5-C6-C7-C8
3	A	808	PGW	O02-C1-O01-C02
3	A	807	PGW	C02-C03-O11-P
3	A	804	PGW	C01-C02-C03-O11
3	A	805	PGW	C01-C02-C03-O11
3	A	818	PGW	C22-C23-C24-C25
3	A	815	PGW	C5-C6-C7-C8
3	A	817	PGW	C20-C21-C22-C23
3	A	818	PGW	C5-C6-C7-C8
3	A	818	PGW	C23-C24-C25-C26
3	A	813	PGW	C23-C24-C25-C26
3	A	809	PGW	O03-C01-C02-C03
3	A	804	PGW	C20-C21-C22-C23
3	A	804	PGW	C22-C23-C24-C25
3	A	809	PGW	C15-C16-C17-C18
3	A	804	PGW	C3-C4-C5-C6
3	A	818	PGW	C03-O11-P-O14
3	A	809	PGW	C23-C24-C25-C26
3	A	810	PGW	C24-C25-C26-C27
3	A	814	PGW	C2-C3-C4-C5
3	A	809	PGW	C01-C02-C03-O11
3	A	814	PGW	C01-C02-C03-O11
3	A	810	PGW	O03-C01-C02-C03
3	A	811	PGW	O03-C01-C02-C03
3	A	805	PGW	O01-C02-C03-O11
3	A	809	PGW	O01-C02-C03-O11
3	A	810	PGW	O01-C02-C03-O11
3	A	815	PGW	O01-C02-C03-O11
3	A	816	PGW	O01-C02-C03-O11
3	A	815	PGW	C19-C20-C21-C22
3	A	811	PGW	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	809	PGW	C16-C17-C18-C28
3	A	810	PGW	C03-O11-P-O12
3	A	812	PGW	C19-C20-C21-C22
3	A	808	PGW	C2-C3-C4-C5
3	A	809	PGW	C03-C02-O01-C1
3	A	815	PGW	C03-C02-O01-C1
3	A	813	PGW	C21-C22-C23-C24
3	A	805	PGW	C6-C7-C8-C9
3	A	808	PGW	O03-C01-C02-C03
3	A	809	PGW	C02-C03-O11-P
3	A	813	PGW	O03-C01-C02-C03
3	A	814	PGW	O01-C02-C03-O11
3	A	808	PGW	O03-C01-C02-O01
3	A	810	PGW	O03-C01-C02-O01
3	A	815	PGW	C22-C23-C24-C25
3	A	807	PGW	C19-C20-C21-C22
3	A	816	PGW	C20-C19-O03-C01
3	A	810	PGW	C22-C23-C24-C25
3	A	817	PGW	C20-C19-O03-C01
3	A	807	PGW	C06-C07-C08-C09
3	A	813	PGW	C03-O11-P-O14
3	A	813	PGW	C1-C2-C3-C4
3	A	811	PGW	C01-C02-C03-O11
3	A	815	PGW	C01-C02-C03-O11
3	A	816	PGW	C01-C02-C03-O11
3	A	812	PGW	C2-C3-C4-C5
3	A	807	PGW	C10-C06-C07-C08
3	A	812	PGW	C6-C7-C8-C9
3	A	811	PGW	O01-C02-C03-O11
3	A	805	PGW	C22-C23-C24-C25
3	A	816	PGW	O04-C19-O03-C01
3	A	817	PGW	O04-C19-O03-C01
3	A	805	PGW	O03-C19-C20-C21
3	A	818	PGW	O03-C19-C20-C21
3	A	812	PGW	O03-C01-C02-C03
3	A	809	PGW	O03-C01-C02-O01
3	A	812	PGW	O03-C01-C02-O01
3	A	818	PGW	C20-C19-O03-C01
3	A	804	PGW	C19-C20-C21-C22
3	A	812	PGW	C20-C21-C22-C23
3	A	818	PGW	O04-C19-O03-C01
3	A	810	PGW	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
3	A	814	PGW	O01-C1-C2-C3
3	A	805	PGW	C3-C4-C5-C6
3	A	804	PGW	O01-C02-C03-O11
3	A	807	PGW	O01-C02-C03-O11
3	A	813	PGW	O03-C01-C02-O01
3	A	808	PGW	C04-O12-P-O11
3	A	818	PGW	C4-C5-C6-C7
3	A	807	PGW	C4-C5-C6-C7
3	A	815	PGW	C3-C4-C5-C6
3	A	812	PGW	C02-C03-O11-P
3	A	807	PGW	C2-C3-C4-C5
3	A	815	PGW	C21-C22-C23-C24
3	A	813	PGW	C15-C16-C17-C18
3	A	814	PGW	C20-C21-C22-C23
3	A	815	PGW	O03-C19-C20-C21
3	A	808	PGW	C02-C01-O03-C19
3	A	813	PGW	O01-C02-C03-O11
3	A	817	PGW	O03-C01-C02-O01
3	A	804	PGW	C03-O11-P-O13
3	A	809	PGW	C22-C23-C24-C25
3	A	818	PGW	O02-C1-O01-C02
3	A	812	PGW	O01-C1-C2-C3
3	A	807	PGW	C01-C02-C03-O11
3	A	814	PGW	O03-C01-C02-O01
3	A	813	PGW	C7-C8-C9-C10
3	A	811	PGW	O01-C1-C2-C3
3	A	805	PGW	C4-C5-C6-C7
3	A	812	PGW	C3-C4-C5-C6
3	A	812	PGW	O02-C1-C2-C3
3	A	813	PGW	C03-O11-P-O12
3	A	808	PGW	C03-O11-P-O14
3	A	808	PGW	C04-O12-P-O14
3	A	813	PGW	C04-O12-P-O14
3	A	807	PGW	C07-C06-C10-C9
3	A	812	PGW	O03-C19-C20-C21
3	A	813	PGW	O03-C19-C20-C21
3	A	811	PGW	O02-C1-C2-C3
3	A	812	PGW	O04-C19-C20-C21
3	A	810	PGW	O03-C19-C20-C21

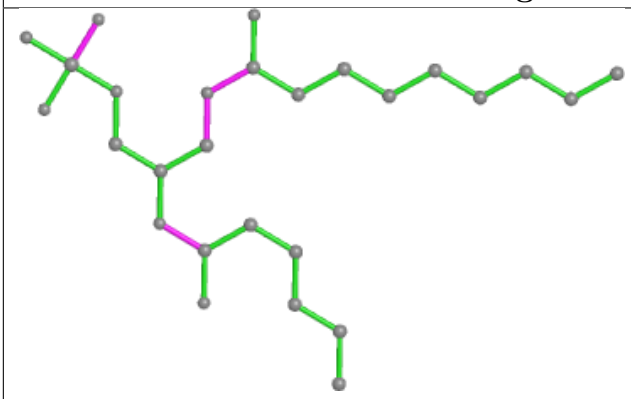
There are no ring outliers.

14 monomers are involved in 51 short contacts:

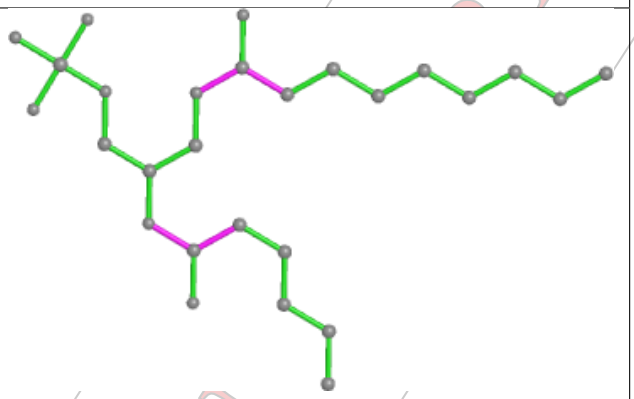
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	810	PGW	2	0
3	A	813	PGW	3	0
3	A	805	PGW	6	0
3	A	814	PGW	10	0
3	A	806	PGW	6	0
3	A	807	PGW	1	0
3	A	803	PGW	6	0
3	A	816	PGW	2	0
3	A	818	PGW	9	0
3	A	812	PGW	6	0
3	A	815	PGW	1	0
3	A	809	PGW	3	0
3	A	811	PGW	1	0
3	A	808	PGW	4	0

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 then 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.

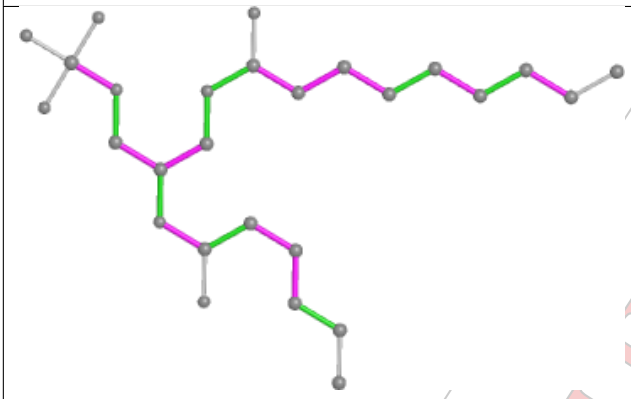
Ligand PGW A 810



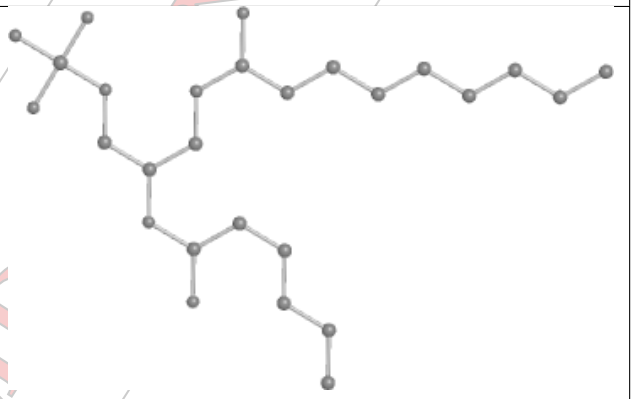
Bond lengths



Bond angles

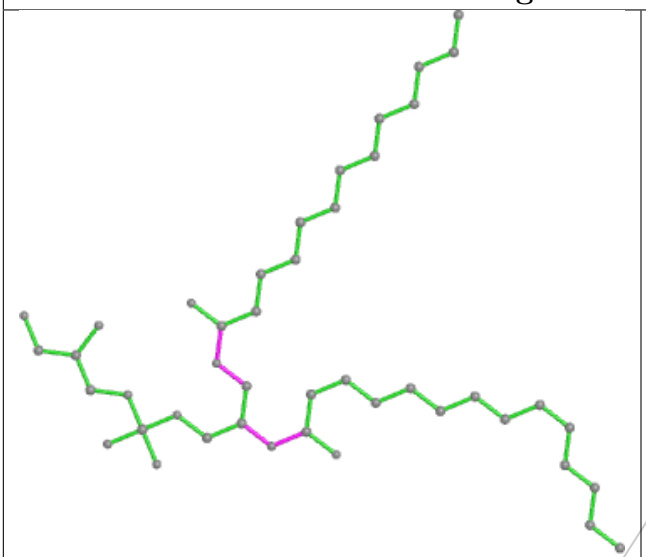


Torsions

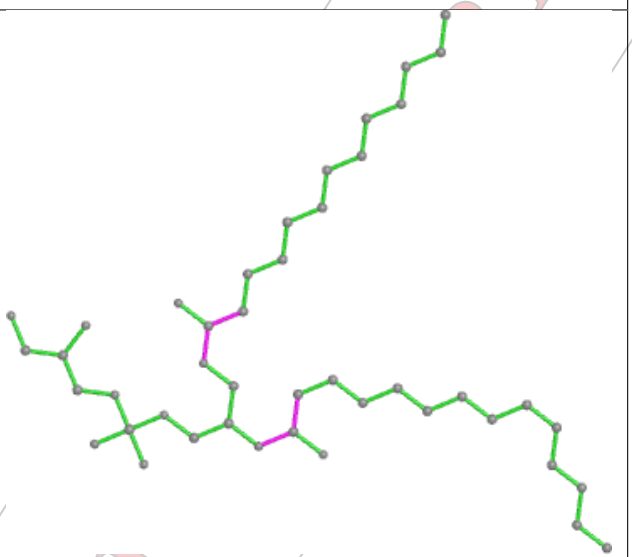


Rings

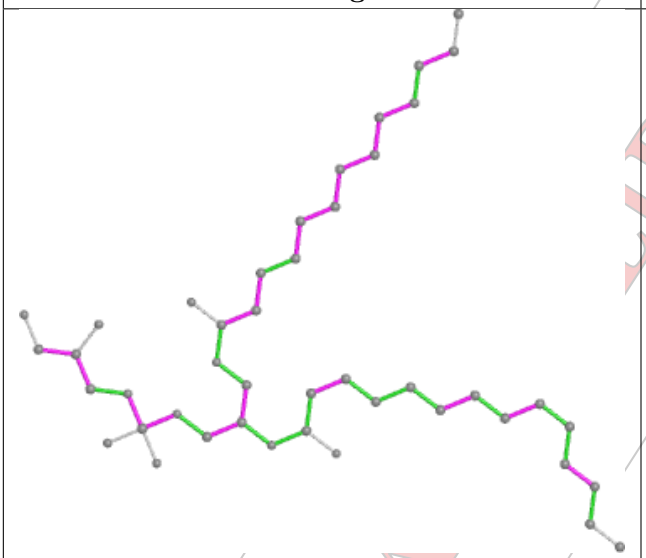
Ligand PGW A 813



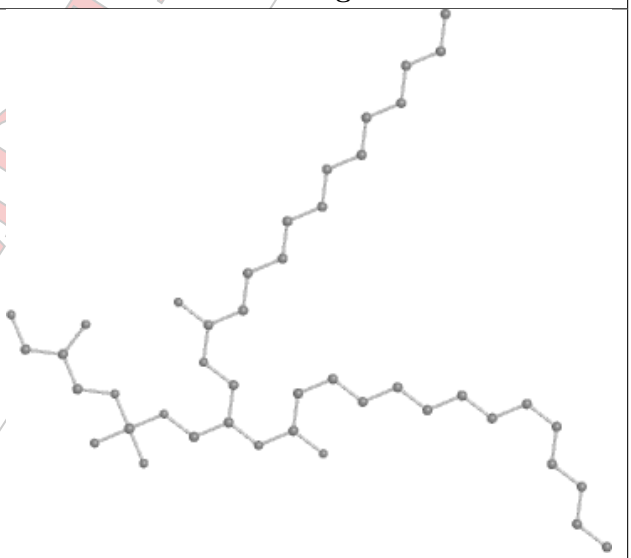
Bond lengths



Bond angles

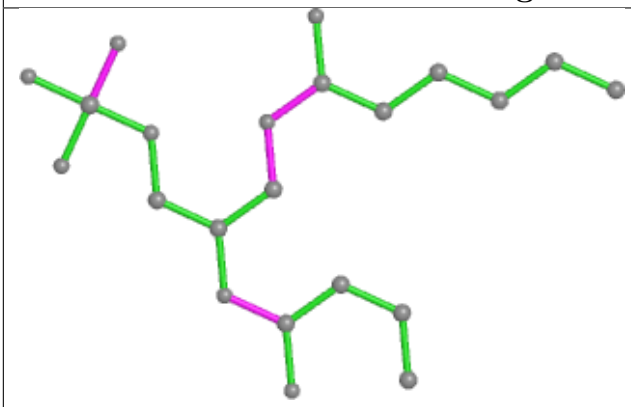


Torsions

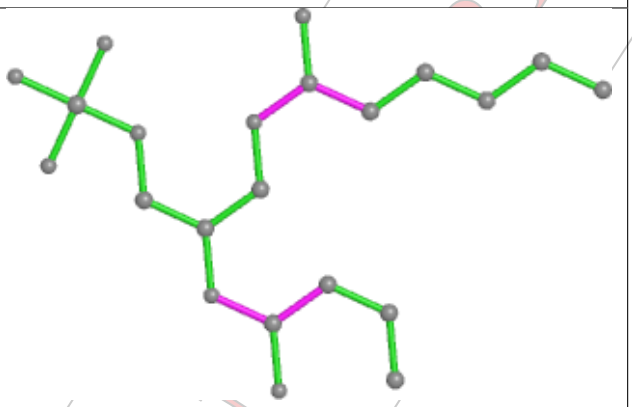


Rings

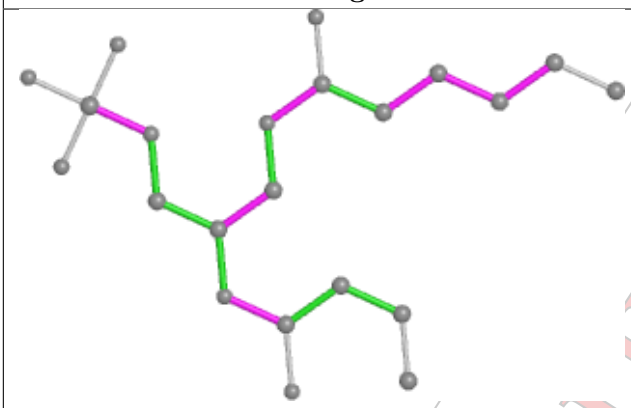
Ligand PGW A 817



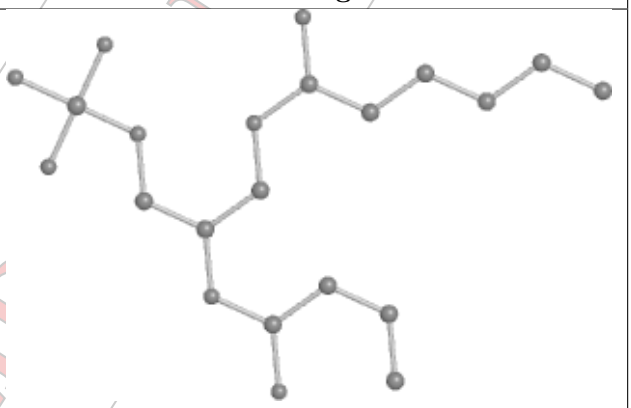
Bond lengths



Bond angles

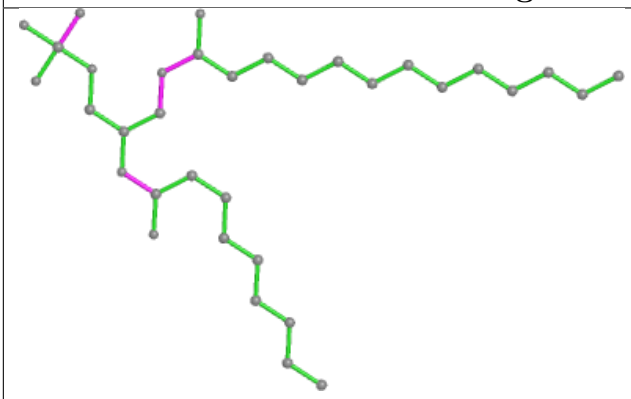


Torsions

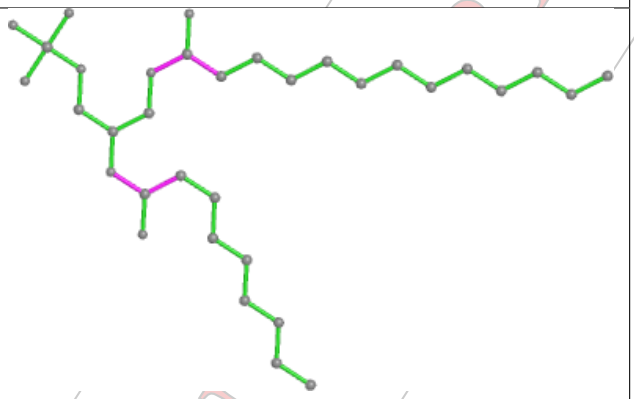


Rings

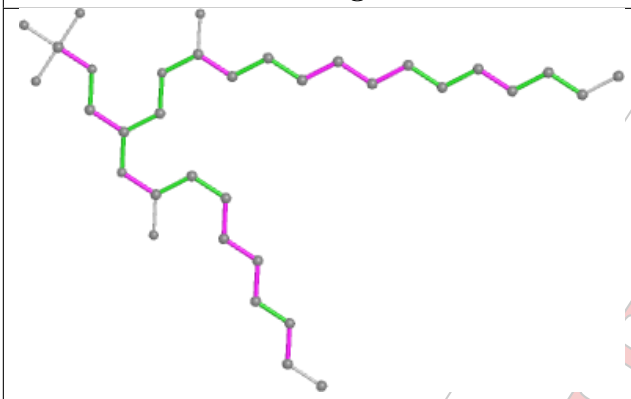
Ligand PGW A 805



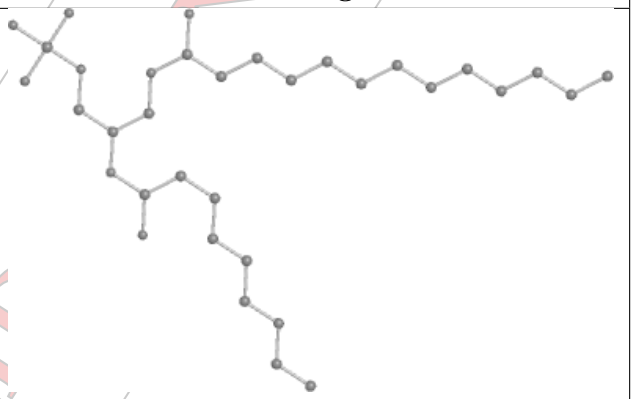
Bond lengths



Bond angles

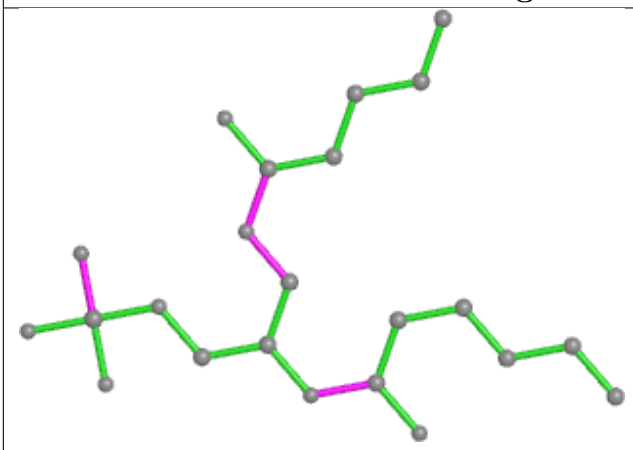


Torsions

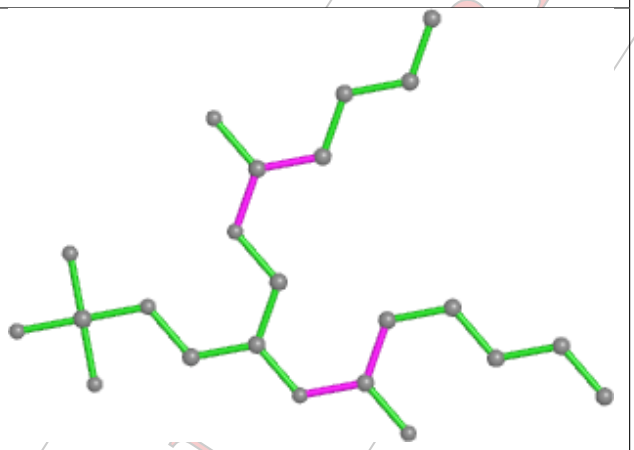


Rings

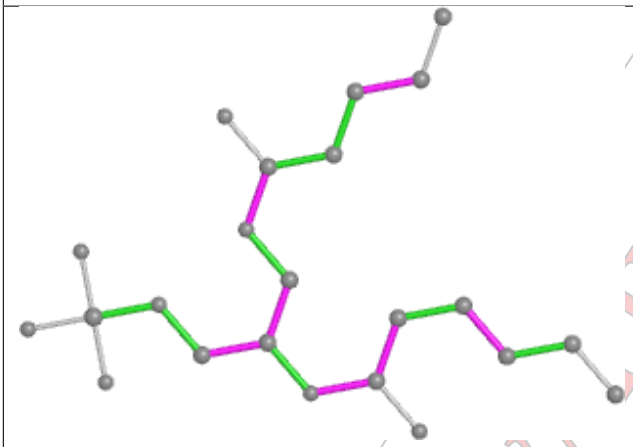
Ligand PGW A 814



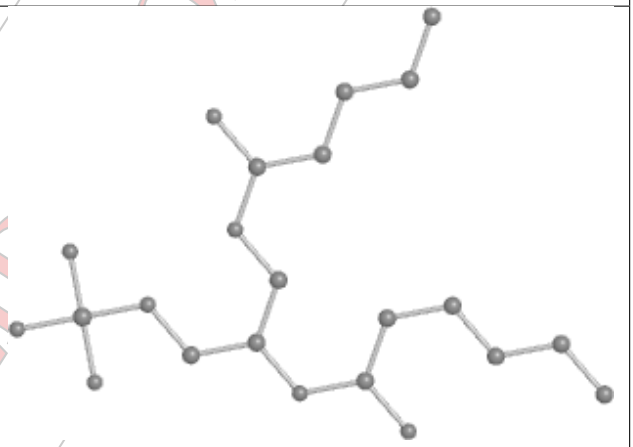
Bond lengths



Bond angles

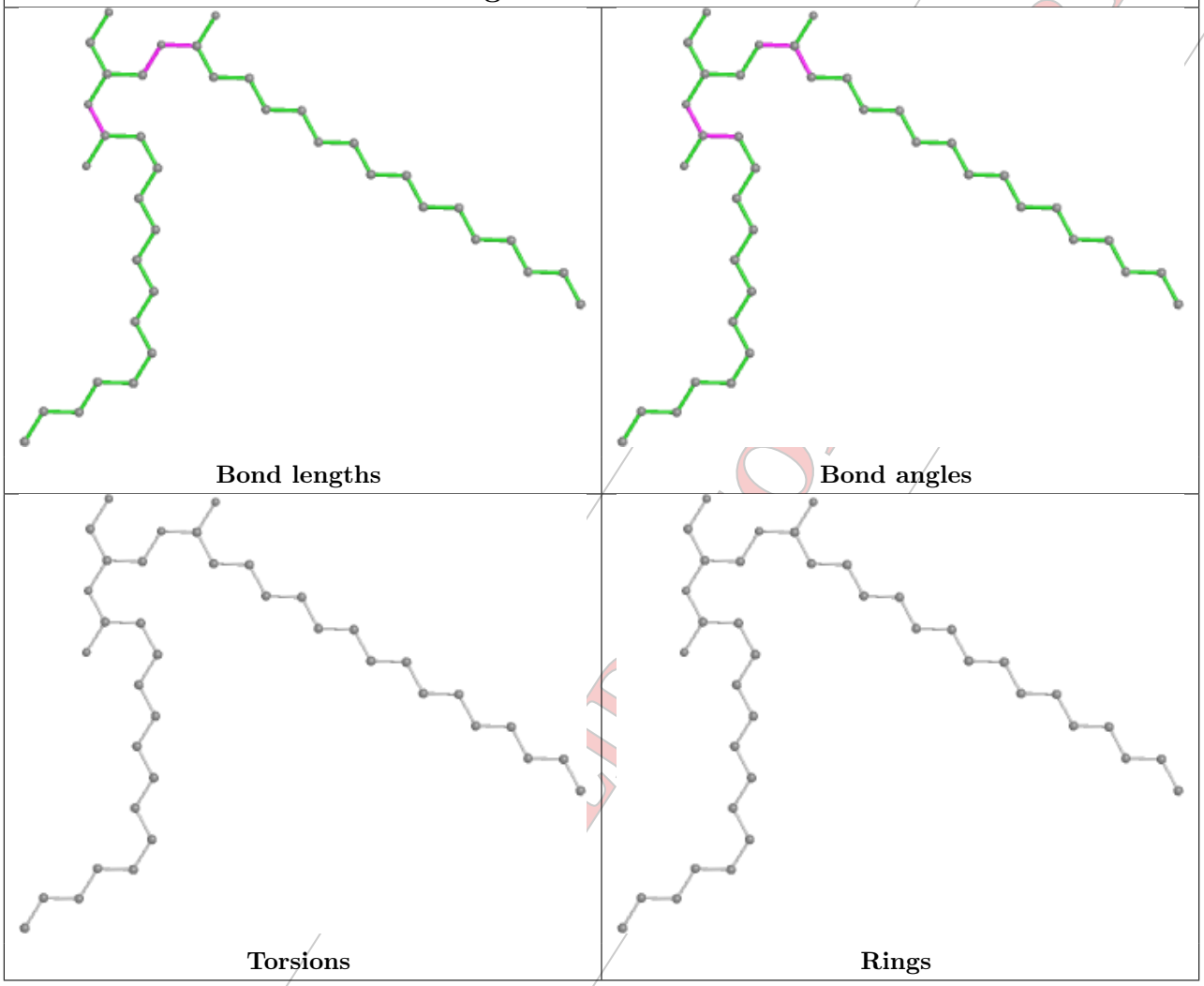


Torsions

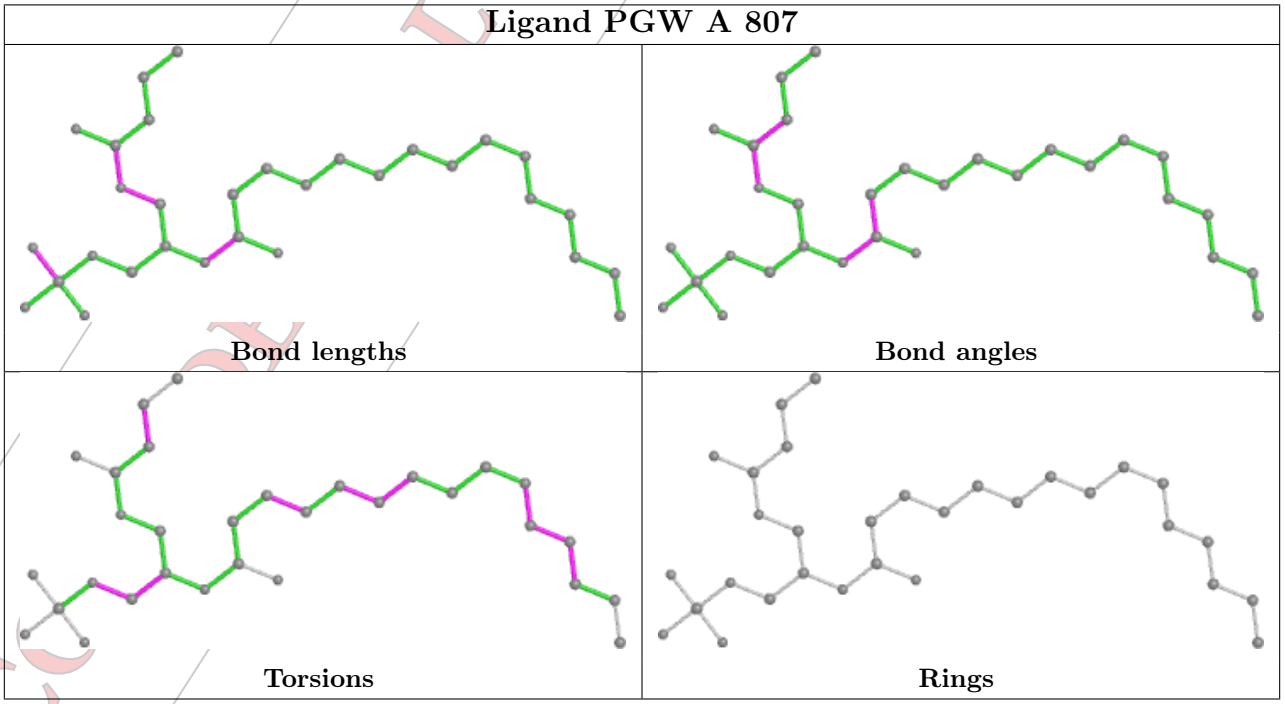


Rings

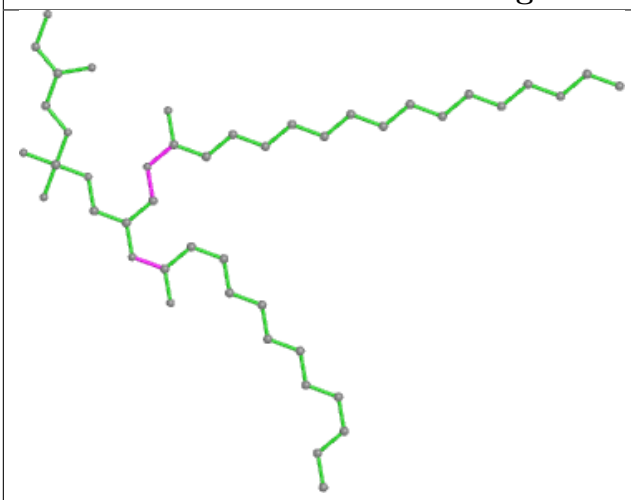
Ligand PGW A 806



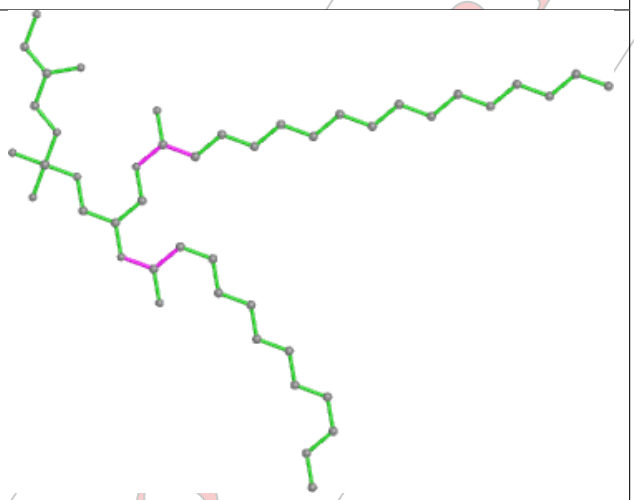
Ligand PGW A 807



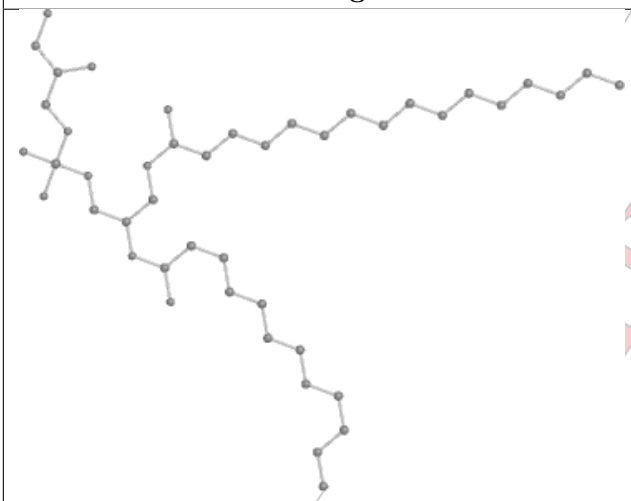
Ligand PGW A 803



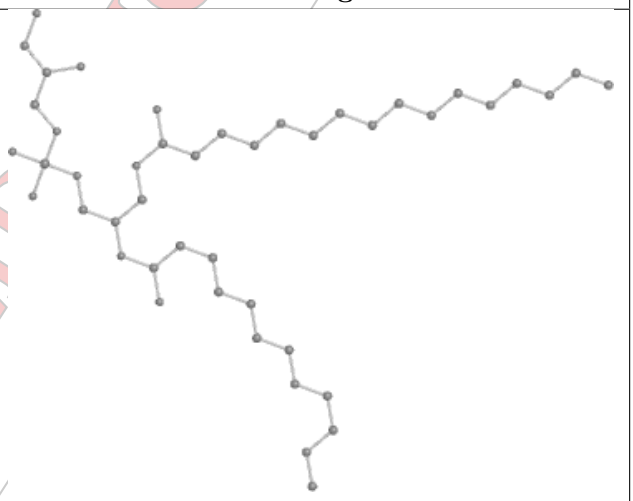
Bond lengths



Bond angles

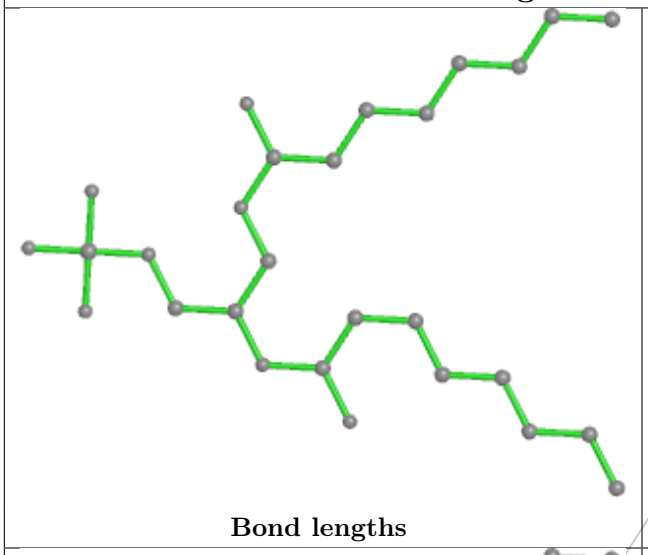


Torsions

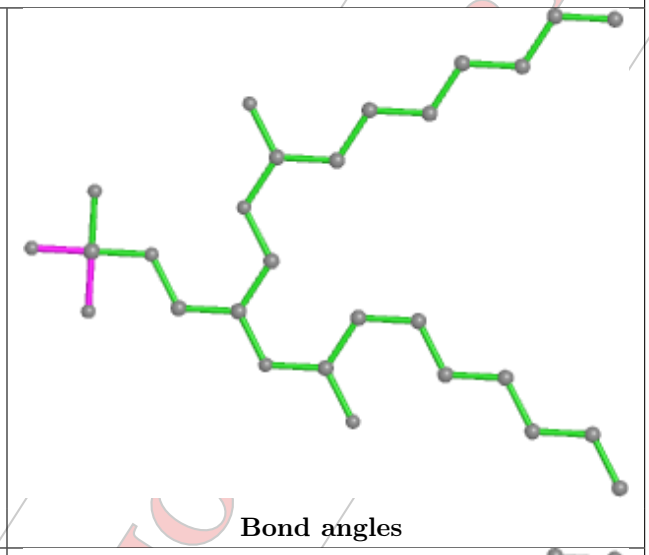


Rings

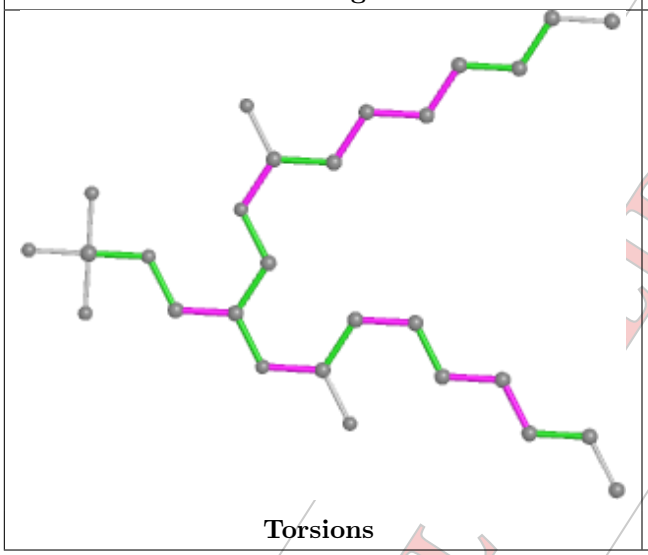
Ligand PGW A 816



Bond lengths



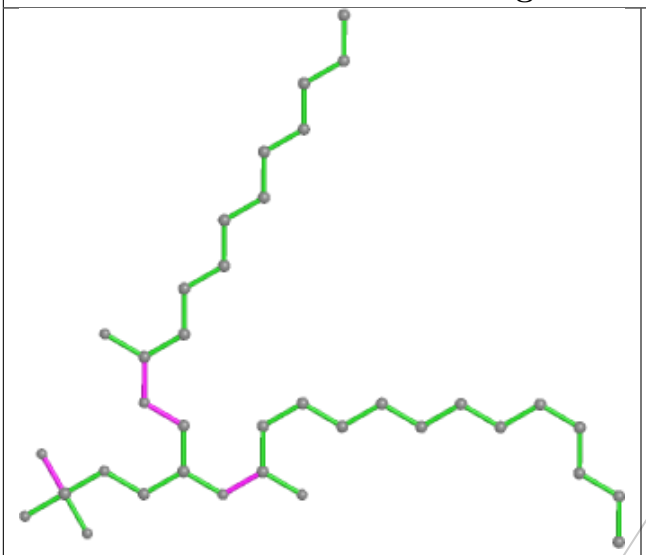
Bond angles



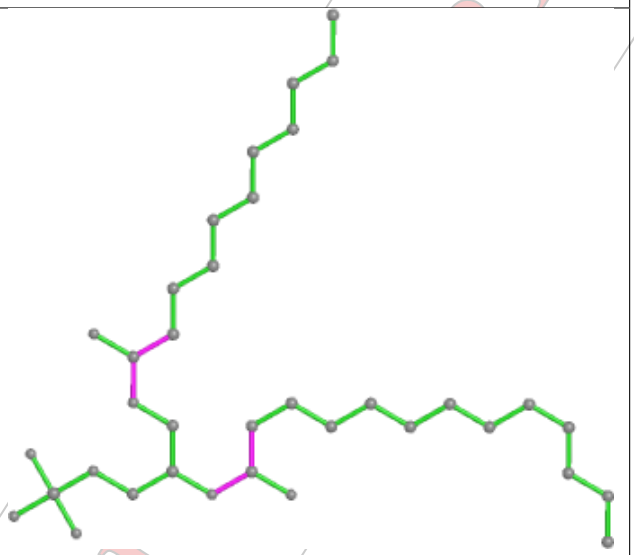
Torsions

Rings

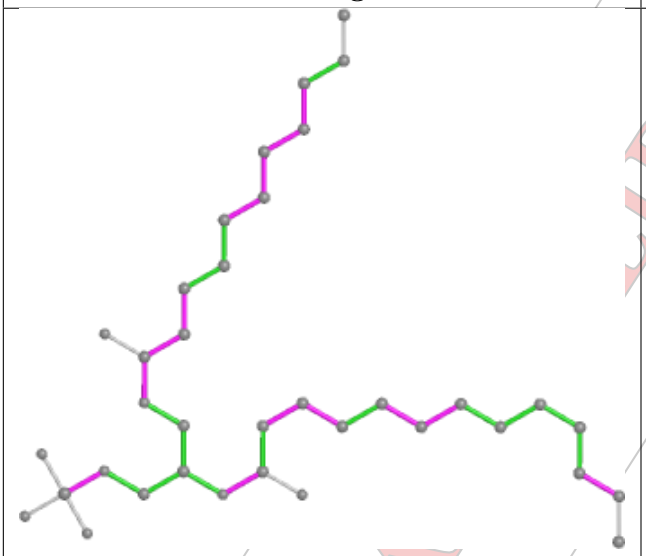
Ligand PGW A 818



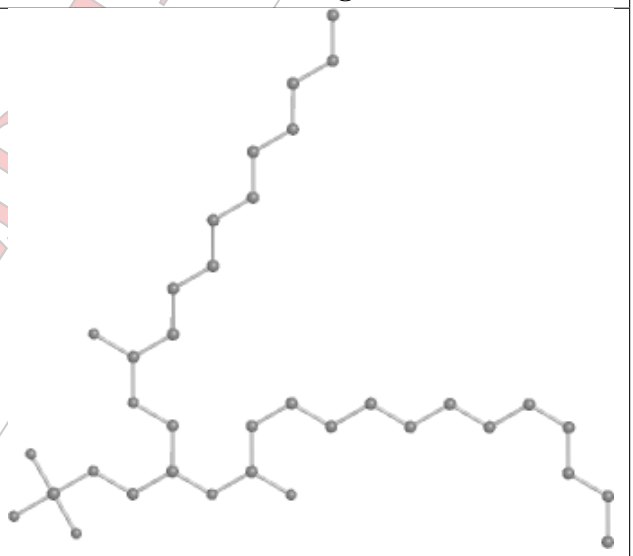
Bond lengths



Bond angles

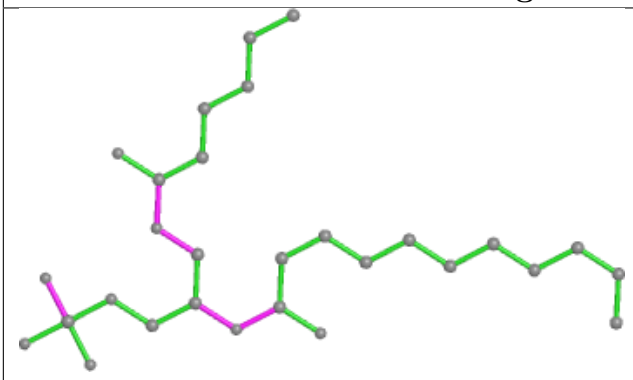


Torsions

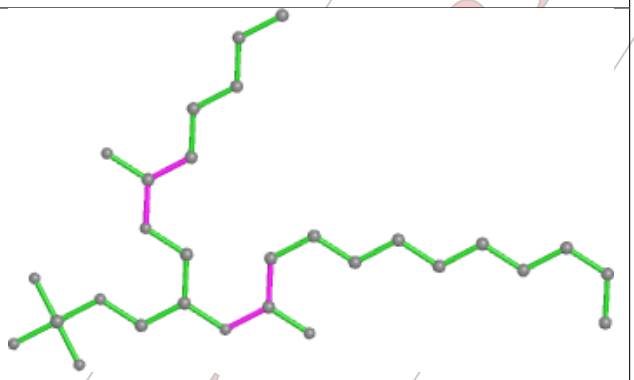


Rings

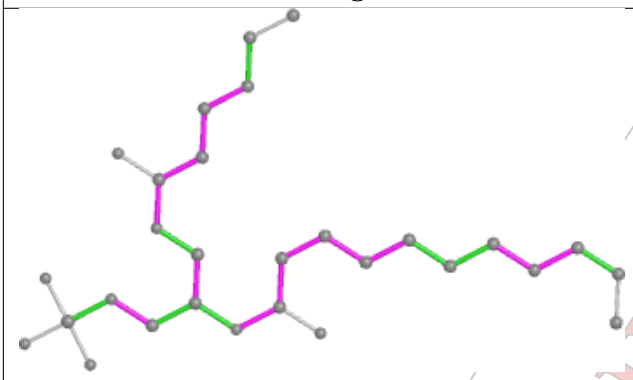
Ligand PGW A 812



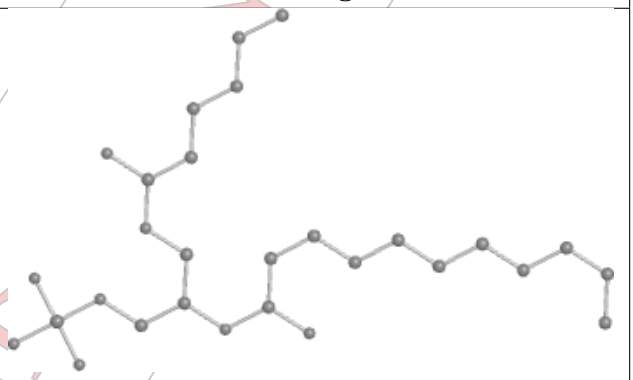
Bond lengths



Bond angles

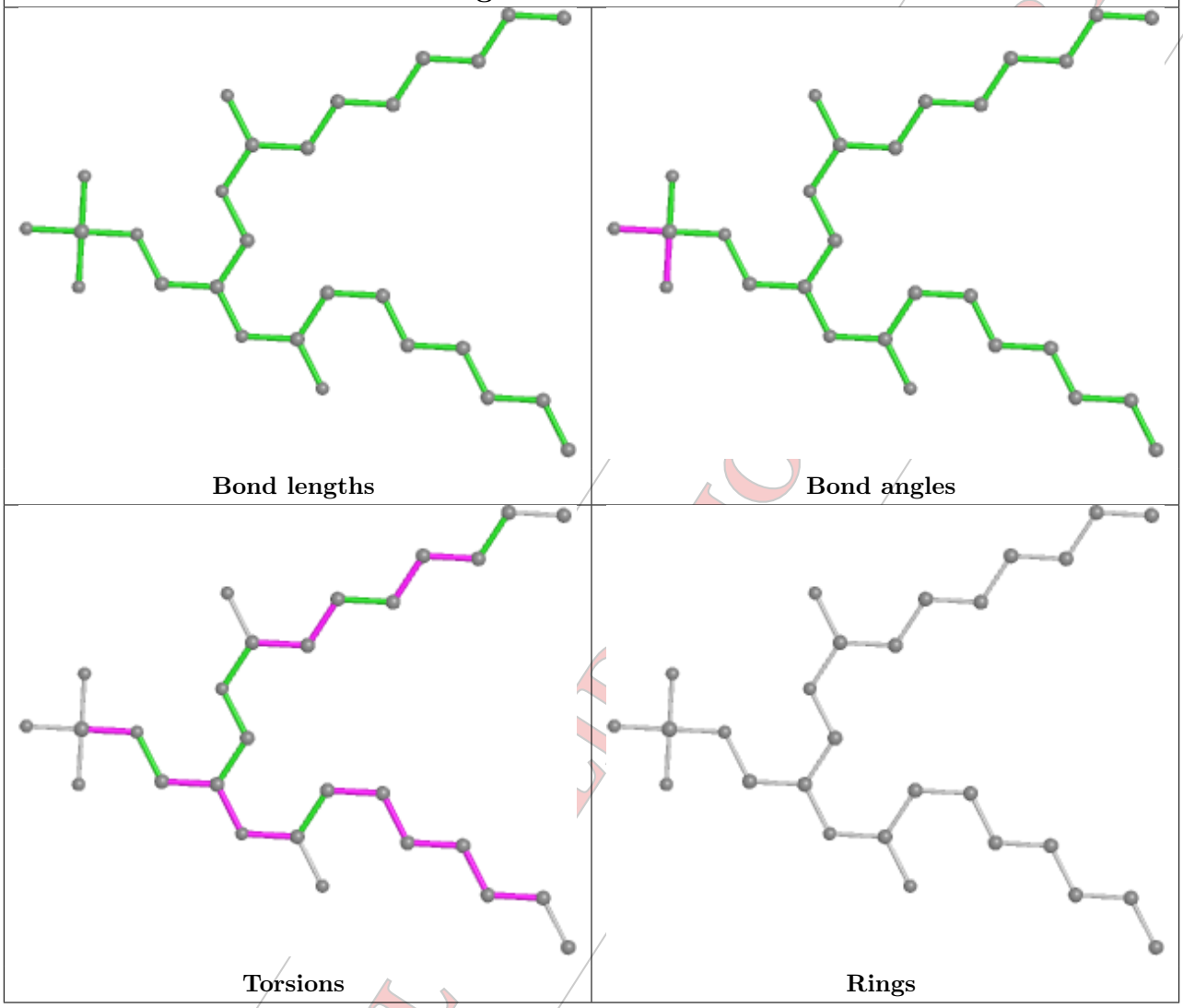


Torsions

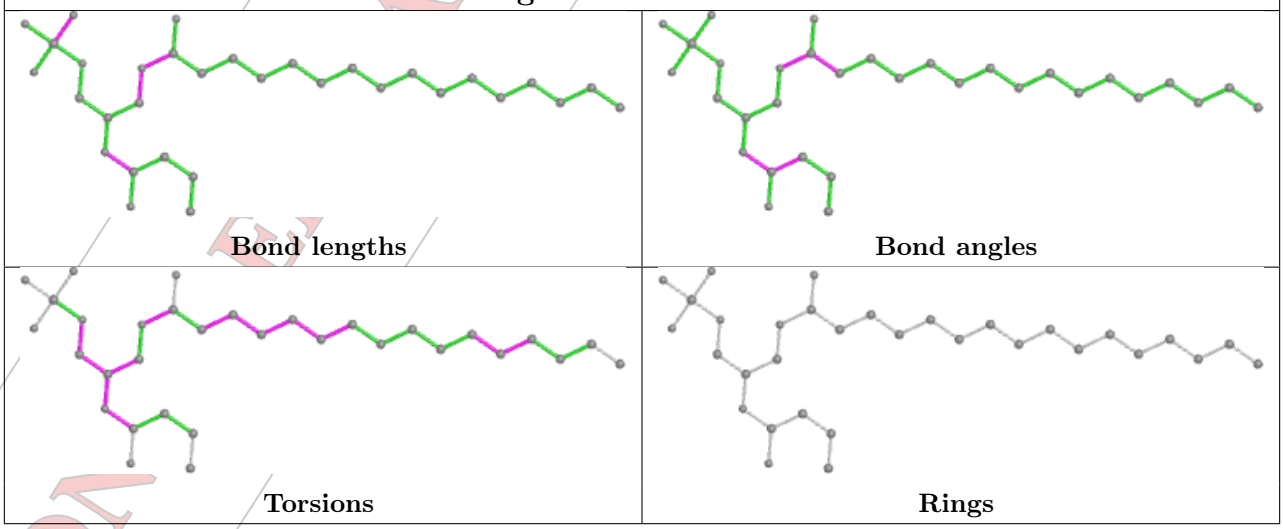


Rings

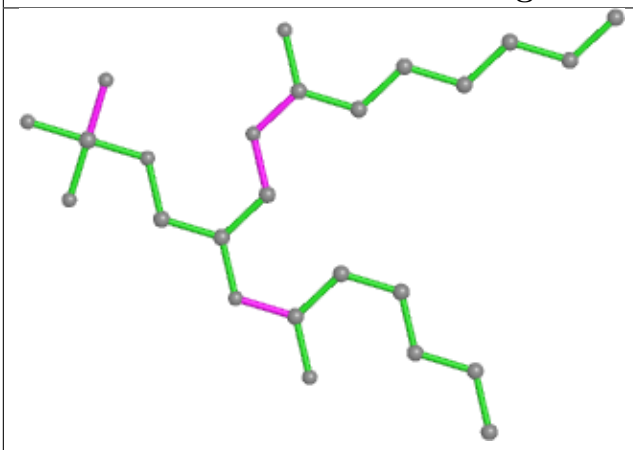
Ligand PGW A 815



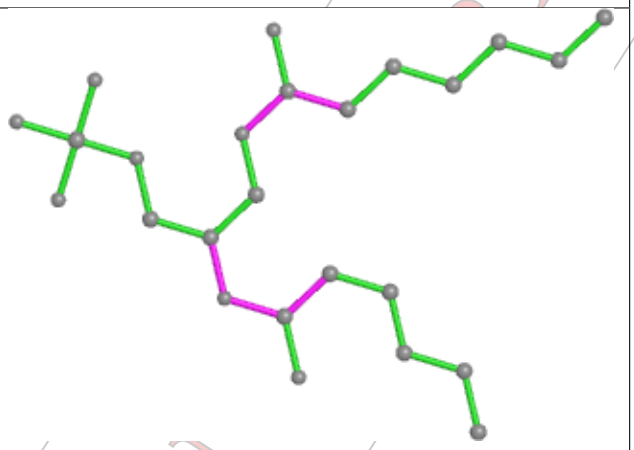
Ligand PGW A 809



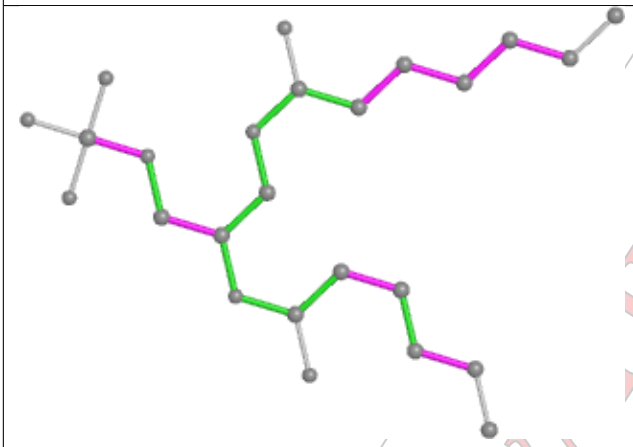
Ligand PGW A 804



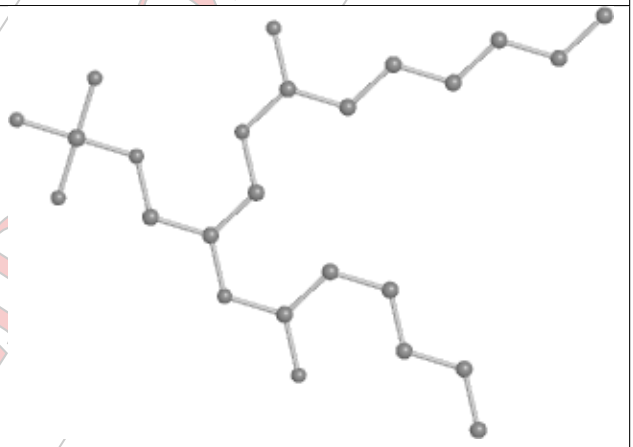
Bond lengths



Bond angles

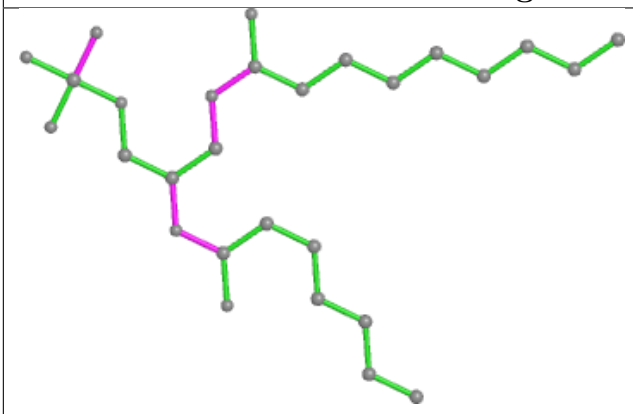


Torsions

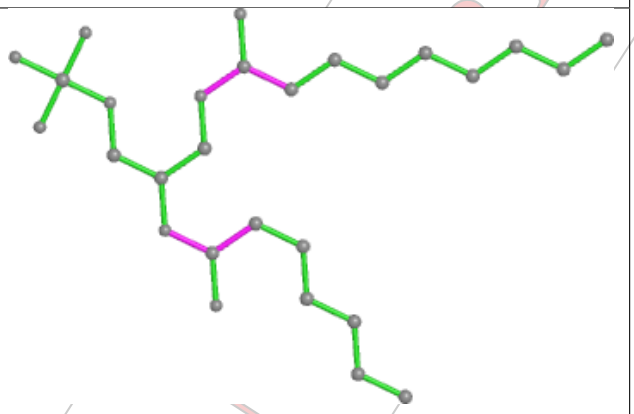


Rings

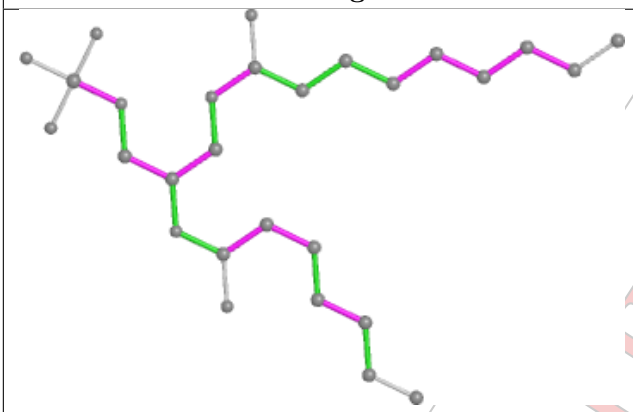
Ligand PGW A 811



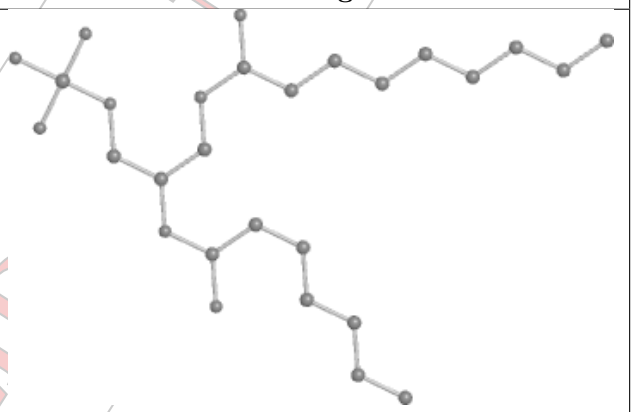
Bond lengths



Bond angles

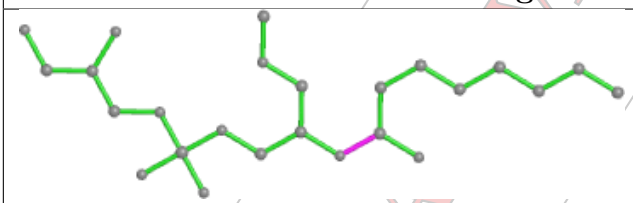


Torsions

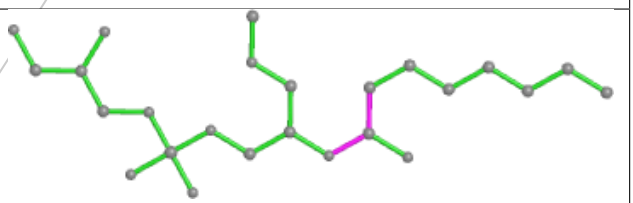


Rings

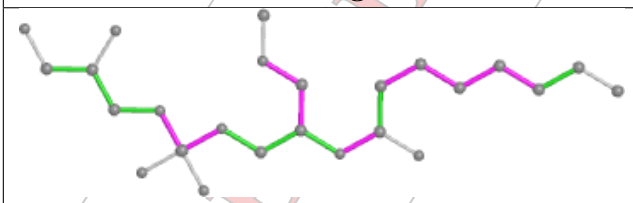
Ligand PGW A 808



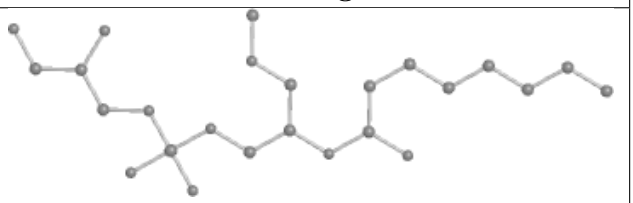
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

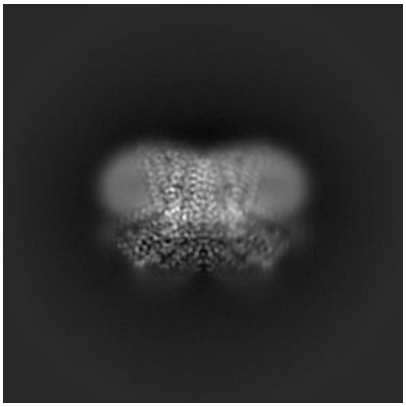
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24731. These allow visual inspection of the internal detail of the map and identification of artifacts.

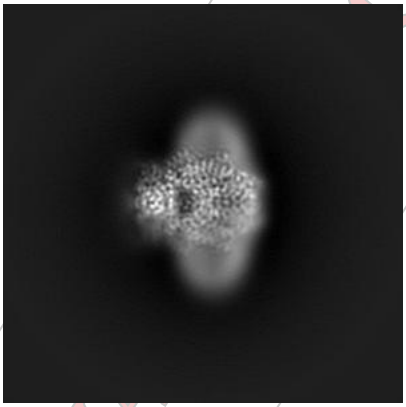
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

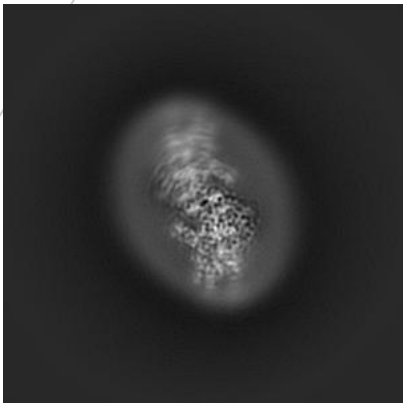
6.1.1 Primary map



X



Y

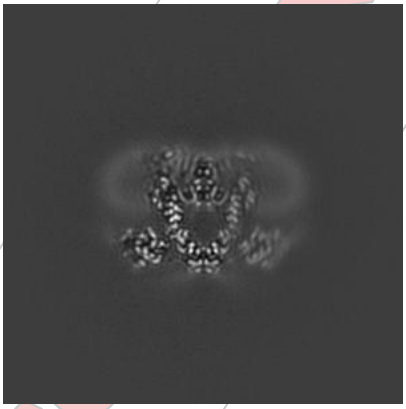


Z

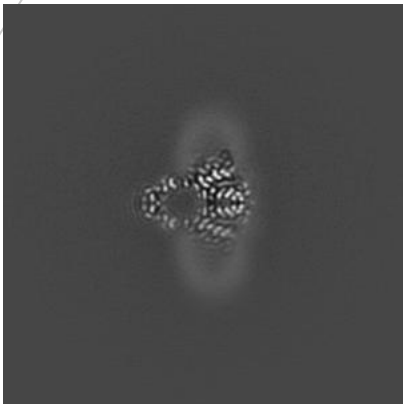
The images above show the map projected in three orthogonal directions.

6.2 Central slices

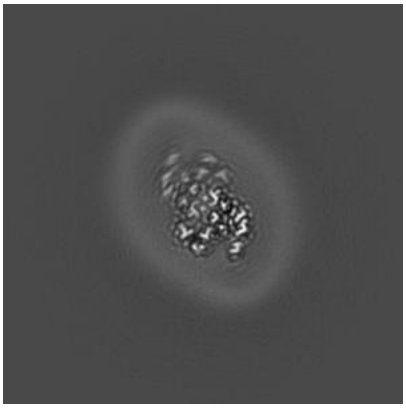
6.2.1 Primary map



X Index: 192



Y Index: 192

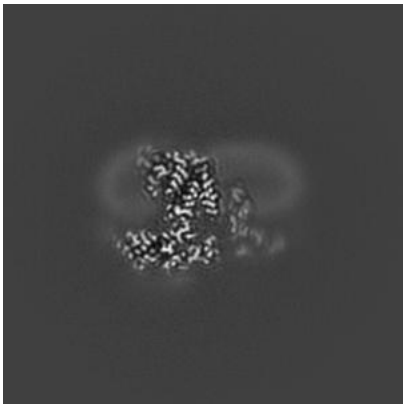


Z Index: 192

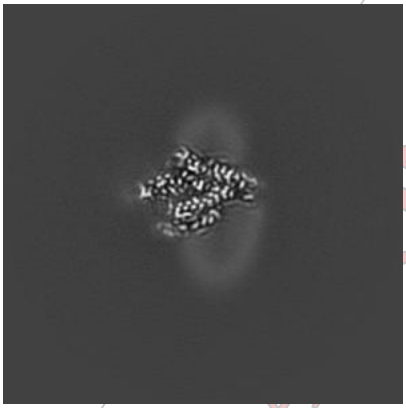
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

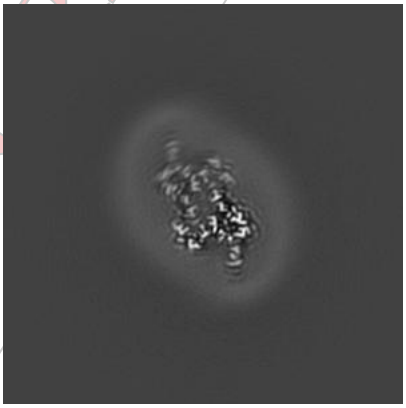
6.3.1 Primary map



X Index: 203



Y Index: 163

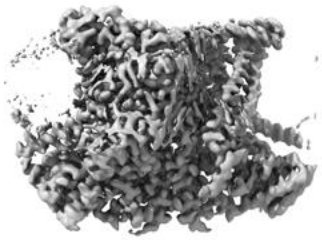


Z Index: 185

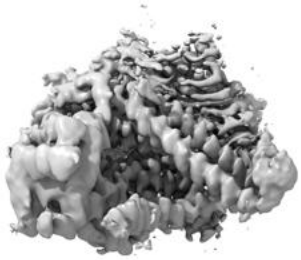
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0049. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

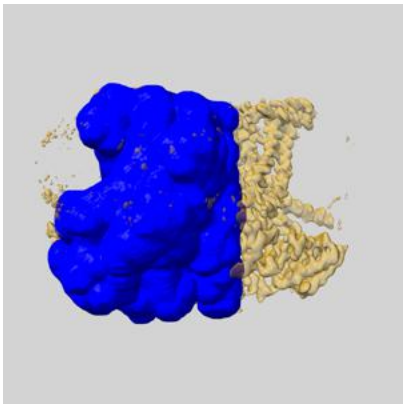
6.5 Mask visualisation (i)

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

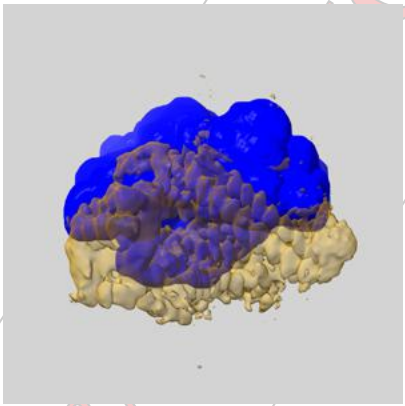
A mask typically either:

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

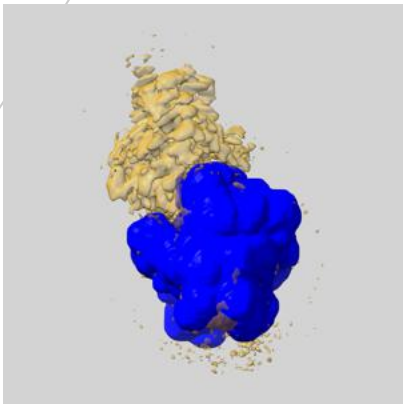
6.5.1 D_1000259171_em-mask-volume_P1.map.V2 (i)



X



Y

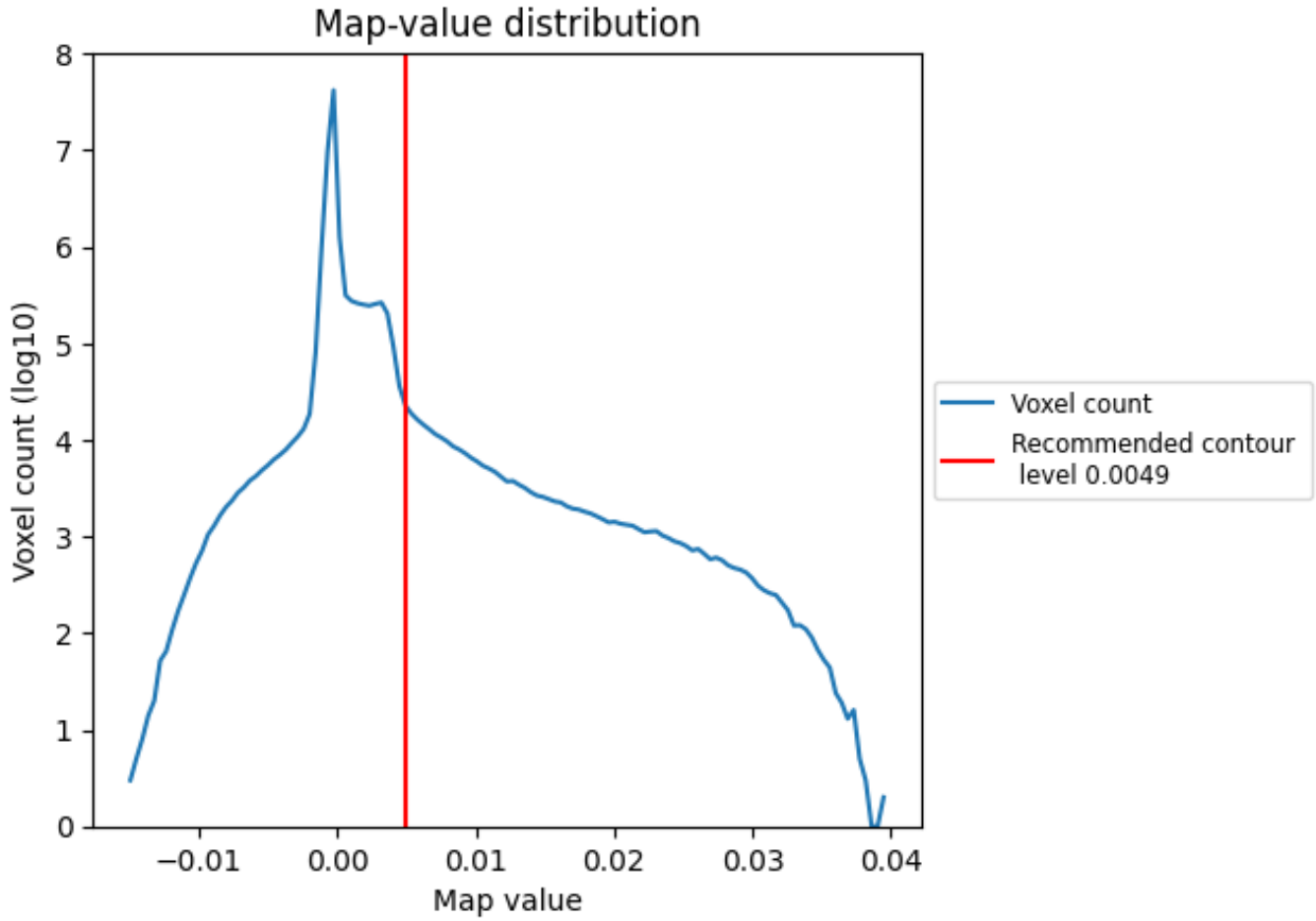


Z

7 Map analysis

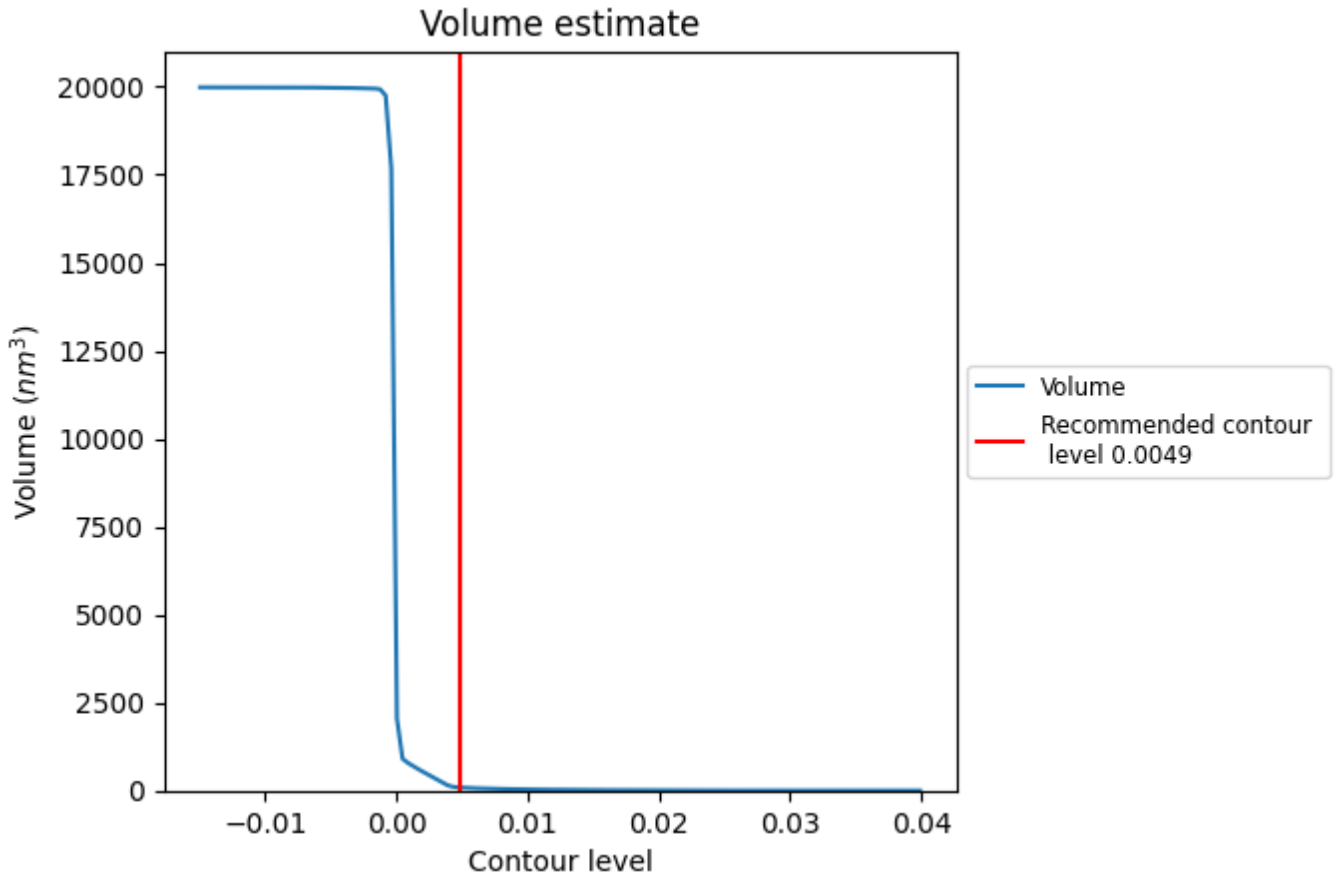
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

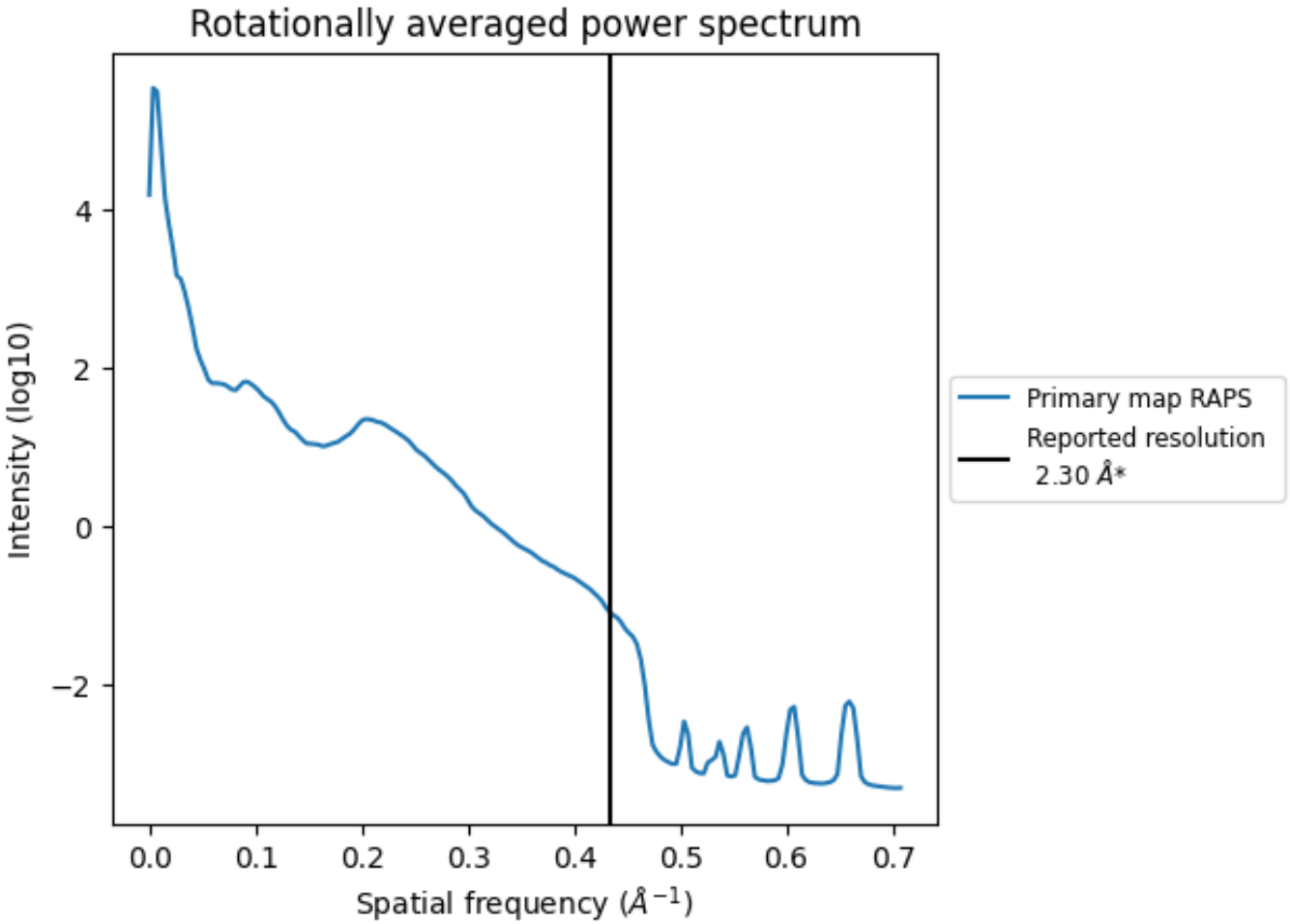
7.2 Volume estimate



The volume at the recommended contour level is 85 nm^3; this corresponds to an approximate mass of 77 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)

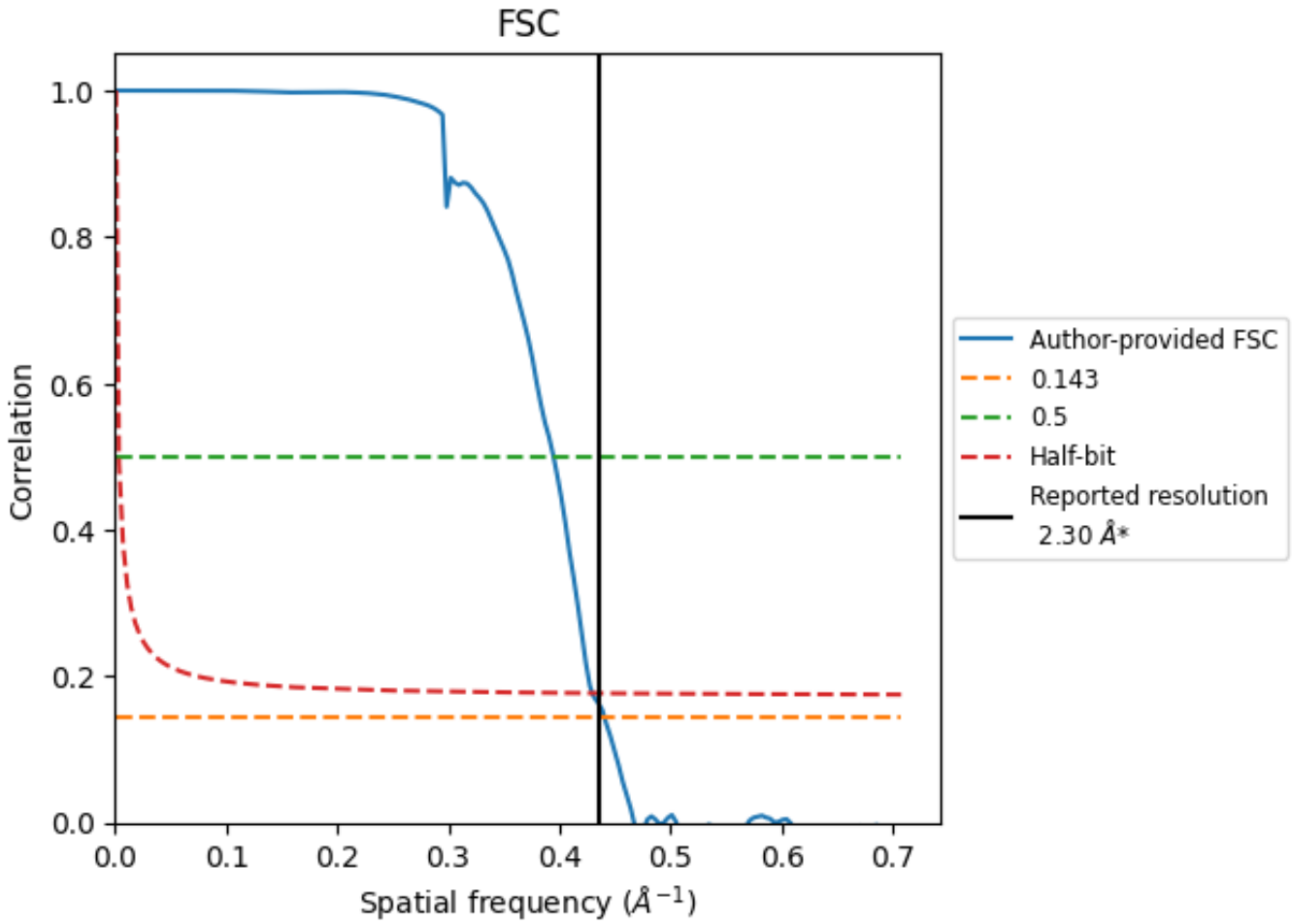


*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

8.2 Resolution estimates (i)

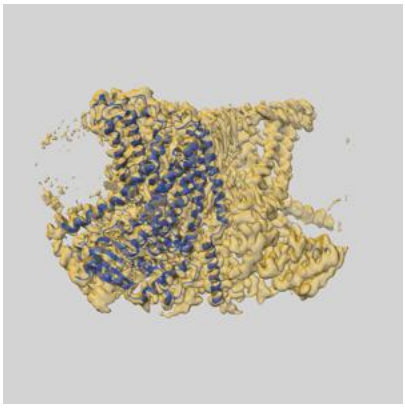
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.27	2.53	2.33
Unmasked-calculated*	-	-	-

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

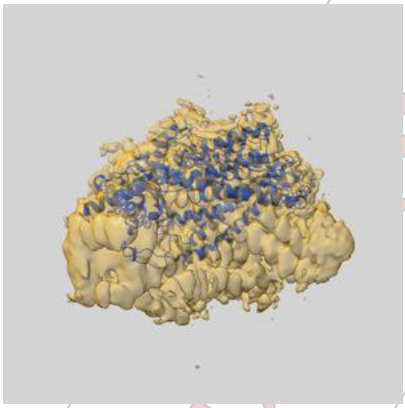
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24731 and PDB model 7RXH. Per-residue inclusion information can be found in section 3 on page 5.

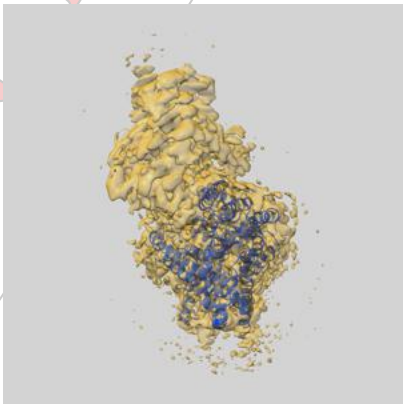
9.1 Map-model overlay



X



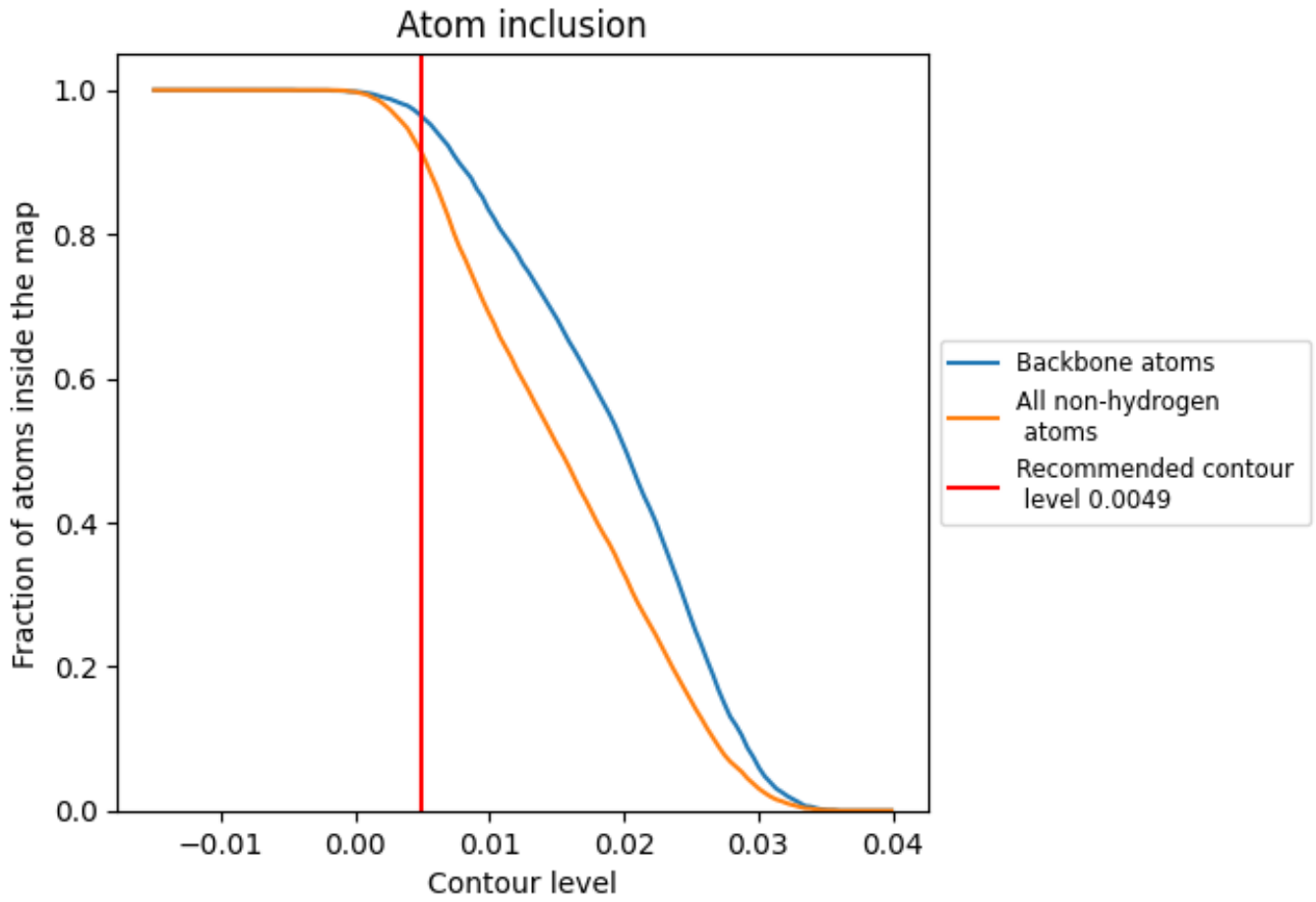
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0049 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 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

Full wwPDB EM Validation Report ⓘ

Aug 26, 2021 – 02:24 PM EDT

PDB ID	:	7RXA
EMDB ID	:	EMD-24726
Title	:	afTMEM16 DE/AA mutant in C14 lipid nanodiscs in the presence of Ca2+
Deposited on	:	2021-08-22
Resolution	:	3.08 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

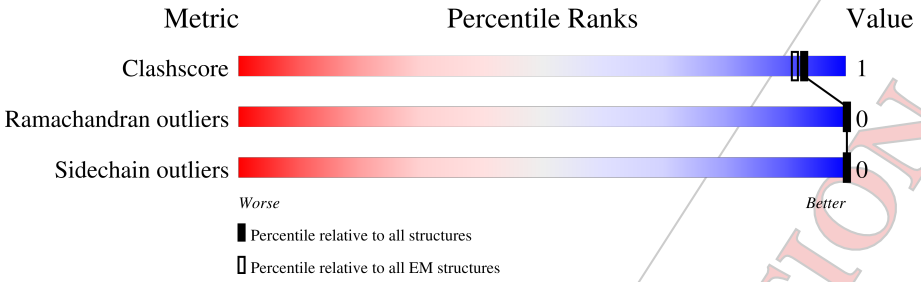
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.08 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 <=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	735	77% · 21%
1	B	735	76% · 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8694 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.

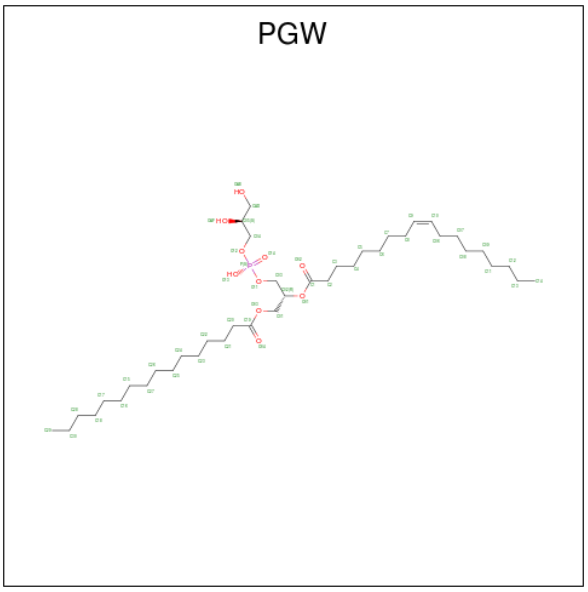
- Molecule 1 is a protein called afTMEM16 lipid scramblase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	578	Total 4221	C 2796	N 709	O 701	S 15	0	0
1	B	578	Total 4221	C 2796	N 709	O 701	S 15	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	511	ALA	ASP	engineered mutation	UNP Q4WA18
A	514	ALA	GLU	engineered mutation	UNP Q4WA18
B	511	ALA	ASP	engineered mutation	UNP Q4WA18
B	514	ALA	GLU	engineered mutation	UNP Q4WA18

- Molecule 2 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



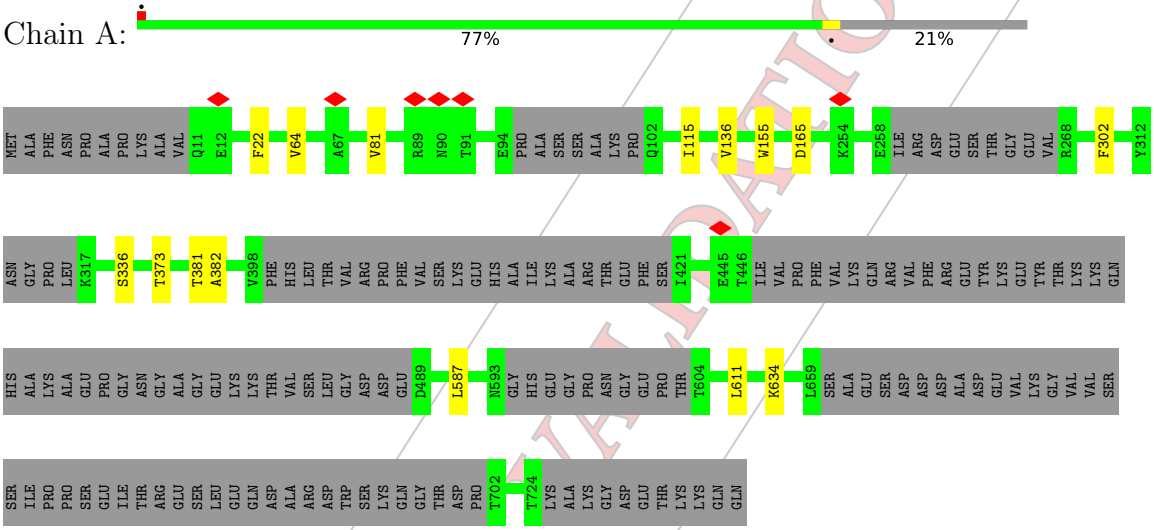
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			126	89	33	4	
2	A	1	Total	C	O	P	0
			126	89	33	4	
2	A	1	Total	C	O	P	0
			126	89	33	4	
2	A	1	Total	C	O	P	0
			126	89	33	4	
2	B	1	Total	C	O	P	0
			126	89	33	4	
2	B	1	Total	C	O	P	0
			126	89	33	4	
2	B	1	Total	C	O	P	0
			126	89	33	4	
2	B	1	Total	C	O	P	0
			126	89	33	4	

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.

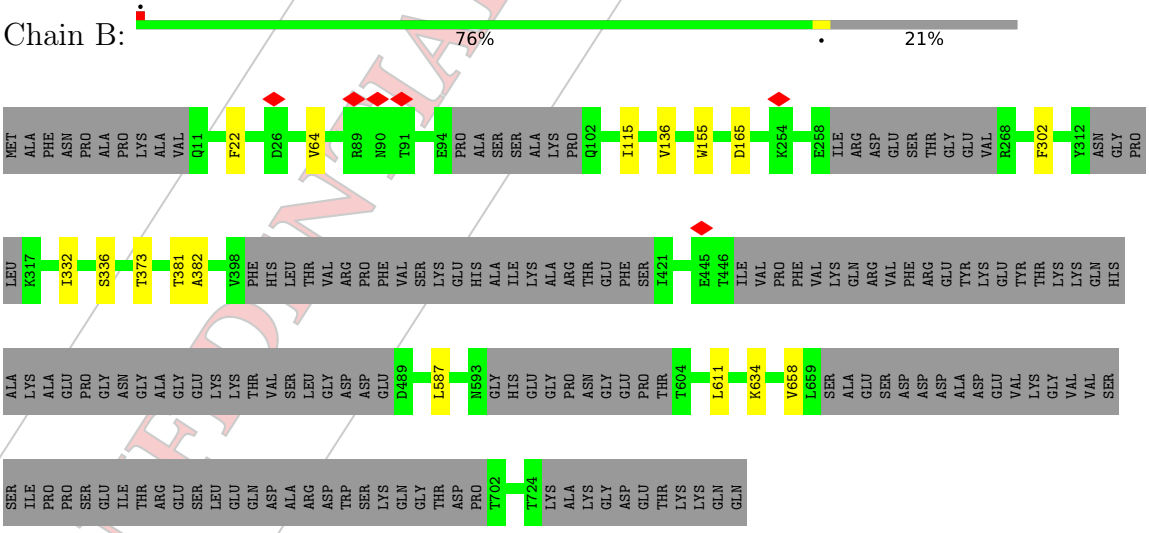
- Molecule 1: afTMEM16 lipid scramblase

Chain A:



- Molecule 1: afTMEM16 lipid scramblase

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155902	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 ($e^-/Å^2$)	42.18	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	0.177	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/4330	0.49	0/5936
1	B	0.30	0/4330	0.49	0/5936
All	All	0.30	0/8660	0.49	0/11872

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	4221	0	3861	10	0
1	B	4221	0	3861	11	0
2	A	126	0	141	4	0
2	B	126	0	141	3	0
All	All	8694	0	8004	22	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 1.

All (22) 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:155:TRP:NE1	1:A:165:ASP:OD1	2.42	0.53
1:B:155:TRP:NE1	1:B:165:ASP:OD1	2.42	0.51
1:A:611:LEU:HB3	1:B:611:LEU:HB3	1.92	0.51
1:A:336:SER:HB3	1:A:373:THR:HG21	1.93	0.51
1:B:336:SER:HB3	1:B:373:THR:HG21	1.93	0.51
1:B:634:LYS:CE	2:B:902:PGW:O14	2.60	0.50
1:A:634:LYS:HE2	2:A:803:PGW:O14	2.12	0.49
1:A:634:LYS:CE	2:A:803:PGW:O14	2.60	0.49
1:B:634:LYS:HE2	2:B:902:PGW:O14	2.12	0.48
1:A:382:ALA:HB1	1:A:587:LEU:HD21	1.96	0.48
1:B:382:ALA:HB1	1:B:587:LEU:HD21	1.96	0.48
1:A:64:VAL:HG11	1:A:115:ILE:HD11	1.98	0.46
1:B:64:VAL:HG11	1:B:115:ILE:HD11	1.98	0.44
1:B:22:PHE:HA	1:B:136:VAL:HA	2.00	0.44
2:A:804:PGW:H3	2:A:804:PGW:H6A	1.85	0.43
1:A:22:PHE:HA	1:A:136:VAL:HA	2.00	0.43
1:B:302:PHE:HZ	1:B:381:THR:HB	1.84	0.42
1:A:81:VAL:HG11	1:B:658:VAL:HG21	2.02	0.42
2:A:801:PGW:H5	2:A:801:PGW:H20A	2.01	0.42
1:A:302:PHE:HZ	1:A:381:THR:HB	1.84	0.41
2:B:904:PGW:H5	2:B:904:PGW:H20A	2.01	0.41
1:B:332:ILE:HD13	1:B:332:ILE:HA	1.94	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	562/735 (76%)	531 (94%)	31 (6%)	0	100	100
1	B	562/735 (76%)	532 (95%)	30 (5%)	0	100	100
All	All	1124/1470 (76%)	1063 (95%)	61 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/644 (58%)	370 (100%)	0	100	100
1	B	370/644 (58%)	370 (100%)	0	100	100
All	All	740/1288 (58%)	740 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	499	ASN
1	A	518	GLN
1	B	518	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 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	$\#\|Z\| > 2$
2	PGW	A	803	-	22,22,50	1.04	2 (9%)	24,27,56	0.86	1 (4%)
2	PGW	A	801	-	38,38,50	1.09	4 (10%)	41,43,56	1.13	2 (4%)
2	PGW	A	804	-	30,30,50	1.21	4 (13%)	33,35,56	1.17	2 (6%)
2	PGW	B	901	-	32,32,50	1.17	4 (12%)	36,37,56	1.14	2 (5%)
2	PGW	A	802	-	32,32,50	1.17	4 (12%)	36,37,56	1.14	2 (5%)
2	PGW	B	902	-	22,22,50	1.04	2 (9%)	24,27,56	0.86	1 (4%)
2	PGW	B	903	-	30,30,50	1.21	4 (13%)	33,35,56	1.17	2 (6%)
2	PGW	B	904	-	38,38,50	1.09	4 (10%)	41,43,56	1.13	2 (4%)

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
2	PGW	A	803	-	-	17/25/25/55	-
2	PGW	A	801	-	-	21/40/40/55	-
2	PGW	A	804	-	-	10/32/32/55	-
2	PGW	B	901	-	-	14/34/34/55	-
2	PGW	A	802	-	-	14/34/34/55	-
2	PGW	B	902	-	-	17/25/25/55	-
2	PGW	B	903	-	-	10/32/32/55	-
2	PGW	B	904	-	-	21/40/40/55	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PGW	O01-C1	2.95	1.42	1.34
2	B	904	PGW	O01-C1	2.94	1.42	1.34
2	A	804	PGW	O01-C1	2.89	1.42	1.34
2	B	903	PGW	O01-C1	2.88	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	PGW	O01-C1	2.86	1.42	1.34
2	A	802	PGW	O01-C1	2.84	1.42	1.34
2	A	801	PGW	O03-C19	2.49	1.40	1.33
2	B	904	PGW	O03-C19	2.49	1.40	1.33
2	B	902	PGW	O03-C19	2.47	1.40	1.33
2	A	804	PGW	O03-C19	2.47	1.40	1.33
2	B	903	PGW	O03-C19	2.47	1.40	1.33
2	A	803	PGW	O03-C19	2.46	1.40	1.33
2	A	802	PGW	O03-C19	2.43	1.40	1.33
2	B	901	PGW	O03-C19	2.42	1.40	1.33
2	B	901	PGW	P-O12	2.31	1.63	1.54
2	A	802	PGW	P-O12	2.30	1.63	1.54
2	B	902	PGW	O03-C01	-2.29	1.39	1.45
2	A	801	PGW	P-O12	2.29	1.63	1.54
2	A	804	PGW	O03-C01	-2.28	1.39	1.45
2	A	804	PGW	P-O12	2.28	1.63	1.54
2	B	903	PGW	P-O12	2.28	1.63	1.54
2	B	904	PGW	O03-C01	-2.27	1.40	1.45
2	B	903	PGW	O03-C01	-2.27	1.40	1.45
2	B	904	PGW	P-O12	2.27	1.63	1.54
2	A	803	PGW	O03-C01	-2.25	1.40	1.45
2	A	801	PGW	O03-C01	-2.24	1.40	1.45
2	A	802	PGW	O03-C01	-2.21	1.40	1.45
2	B	901	PGW	O03-C01	-2.19	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	904	PGW	O01-C1-C2	4.01	120.14	111.50
2	A	801	PGW	O01-C1-C2	4.00	120.12	111.50
2	B	903	PGW	O01-C1-C2	4.00	120.11	111.50
2	A	804	PGW	O01-C1-C2	3.98	120.08	111.50
2	B	901	PGW	O01-C1-C2	3.65	119.37	111.50
2	A	802	PGW	O01-C1-C2	3.62	119.31	111.50
2	A	803	PGW	O03-C19-C20	2.57	119.97	111.91
2	B	902	PGW	O03-C19-C20	2.56	119.95	111.91
2	B	901	PGW	O03-C19-C20	2.54	119.89	111.91
2	A	802	PGW	O03-C19-C20	2.53	119.86	111.91
2	B	904	PGW	O03-C19-C20	2.48	119.68	111.91
2	A	801	PGW	O03-C19-C20	2.47	119.66	111.91
2	B	903	PGW	O03-C19-C20	2.42	119.51	111.91
2	A	804	PGW	O03-C19-C20	2.41	119.47	111.91

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PGW	C03-O11-P-O12
2	A	801	PGW	C07-C06-C10-C9
2	A	803	PGW	C04-C05-CAD-OAE
2	A	803	PGW	C03-O11-P-O12
2	A	803	PGW	C03-O11-P-O13
2	A	803	PGW	C03-O11-P-O14
2	A	803	PGW	O01-C02-C03-O11
2	A	803	PGW	O12-C04-C05-OAF
2	A	804	PGW	C03-O11-P-O12
2	A	804	PGW	C07-C06-C10-C9
2	B	902	PGW	C04-C05-CAD-OAE
2	B	902	PGW	C03-O11-P-O12
2	B	902	PGW	C03-O11-P-O13
2	B	902	PGW	C03-O11-P-O14
2	B	902	PGW	O01-C02-C03-O11
2	B	902	PGW	O12-C04-C05-OAF
2	B	903	PGW	C03-O11-P-O12
2	B	903	PGW	C07-C06-C10-C9
2	B	904	PGW	C03-O11-P-O12
2	B	904	PGW	C07-C06-C10-C9
2	A	803	PGW	C01-C02-C03-O11
2	B	902	PGW	C01-C02-C03-O11
2	A	801	PGW	O03-C01-C02-O01
2	B	904	PGW	O03-C01-C02-O01
2	A	803	PGW	C04-O12-P-O11
2	B	902	PGW	C04-O12-P-O11
2	A	801	PGW	C21-C22-C23-C24
2	B	904	PGW	C21-C22-C23-C24
2	A	802	PGW	C4-C5-C6-C7
2	B	901	PGW	C4-C5-C6-C7
2	A	801	PGW	C4-C5-C6-C7
2	B	904	PGW	C4-C5-C6-C7
2	B	904	PGW	C25-C26-C27-C15
2	A	801	PGW	C25-C26-C27-C15
2	A	803	PGW	C21-C22-C23-C24
2	B	902	PGW	C21-C22-C23-C24
2	A	801	PGW	C5-C6-C7-C8
2	B	904	PGW	C5-C6-C7-C8
2	A	801	PGW	C24-C25-C26-C27
2	B	904	PGW	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	A	801	PGW	C20-C21-C22-C23
2	B	904	PGW	C20-C21-C22-C23
2	A	802	PGW	C22-C23-C24-C25
2	B	901	PGW	C22-C23-C24-C25
2	A	803	PGW	OAF-C05-CAD-OAE
2	B	902	PGW	OAF-C05-CAD-OAE
2	A	803	PGW	O12-C04-C05-CAD
2	B	901	PGW	C21-C22-C23-C24
2	A	802	PGW	C21-C22-C23-C24
2	A	802	PGW	C5-C6-C7-C8
2	B	901	PGW	C5-C6-C7-C8
2	A	804	PGW	C21-C22-C23-C24
2	B	903	PGW	C21-C22-C23-C24
2	A	804	PGW	C6-C7-C8-C9
2	B	903	PGW	C6-C7-C8-C9
2	B	902	PGW	O12-C04-C05-CAD
2	A	801	PGW	O03-C01-C02-C03
2	B	904	PGW	O03-C01-C02-C03
2	A	802	PGW	C24-C25-C26-C27
2	B	901	PGW	C24-C25-C26-C27
2	B	901	PGW	C19-C20-C21-C22
2	A	802	PGW	C19-C20-C21-C22
2	A	801	PGW	C27-C15-C16-C17
2	B	904	PGW	C27-C15-C16-C17
2	A	802	PGW	C6-C7-C8-C9
2	B	901	PGW	C6-C7-C8-C9
2	A	804	PGW	C22-C23-C24-C25
2	B	903	PGW	C22-C23-C24-C25
2	B	904	PGW	C22-C23-C24-C25
2	A	802	PGW	O03-C01-C02-O01
2	B	901	PGW	O03-C01-C02-O01
2	A	802	PGW	C20-C19-O03-C01
2	B	901	PGW	C20-C19-O03-C01
2	A	801	PGW	C22-C23-C24-C25
2	A	801	PGW	C03-O11-P-O13
2	A	804	PGW	C03-O11-P-O13
2	B	903	PGW	C03-O11-P-O13
2	B	904	PGW	C03-O11-P-O13
2	B	904	PGW	C17-C18-C28-C30
2	A	801	PGW	C17-C18-C28-C30
2	A	802	PGW	O03-C01-C02-C03
2	A	803	PGW	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
2	B	901	PGW	O03-C01-C02-C03
2	B	902	PGW	O03-C01-C02-O01
2	A	804	PGW	O01-C02-C03-O11
2	B	903	PGW	O01-C02-C03-O11
2	A	802	PGW	C23-C24-C25-C26
2	B	901	PGW	C23-C24-C25-C26
2	A	801	PGW	C1-C2-C3-C4
2	B	904	PGW	C1-C2-C3-C4
2	A	802	PGW	O04-C19-O03-C01
2	B	901	PGW	O04-C19-O03-C01
2	A	803	PGW	C04-O12-P-O13
2	A	803	PGW	C04-O12-P-O14
2	B	902	PGW	C04-O12-P-O13
2	B	902	PGW	C04-O12-P-O14
2	A	804	PGW	C01-C02-C03-O11
2	B	903	PGW	C01-C02-C03-O11
2	A	801	PGW	C19-C20-C21-C22
2	B	904	PGW	C19-C20-C21-C22
2	B	904	PGW	O02-C1-O01-C02
2	A	801	PGW	C2-C1-O01-C02
2	B	904	PGW	C2-C1-O01-C02
2	A	801	PGW	O02-C1-O01-C02
2	A	801	PGW	C03-O11-P-O14
2	A	804	PGW	C03-O11-P-O14
2	B	903	PGW	C03-O11-P-O14
2	B	904	PGW	C03-O11-P-O14
2	B	902	PGW	C20-C21-C22-C23
2	A	803	PGW	C20-C21-C22-C23
2	A	802	PGW	C7-C8-C9-C10
2	B	901	PGW	C7-C8-C9-C10
2	A	802	PGW	O01-C1-C2-C3
2	B	901	PGW	O01-C1-C2-C3
2	B	903	PGW	O03-C19-C20-C21
2	A	804	PGW	O03-C19-C20-C21
2	A	801	PGW	C7-C8-C9-C10
2	B	904	PGW	C7-C8-C9-C10
2	A	801	PGW	C15-C16-C17-C18
2	B	904	PGW	C15-C16-C17-C18
2	A	803	PGW	C22-C23-C24-C25
2	B	902	PGW	C22-C23-C24-C25
2	A	803	PGW	C05-C04-O12-P
2	B	902	PGW	C05-C04-O12-P

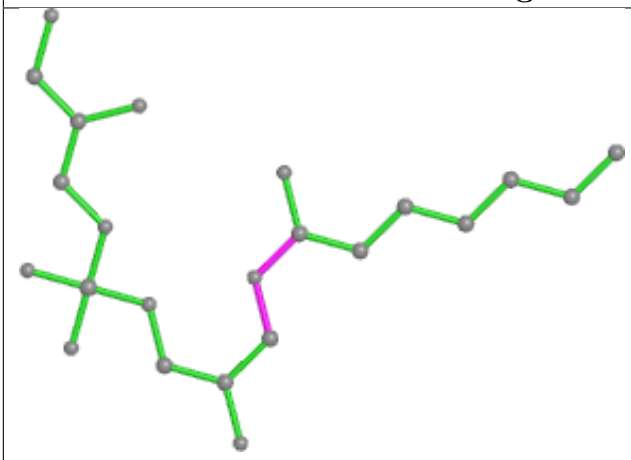
There are no ring outliers.

5 monomers are involved in 7 short contacts:

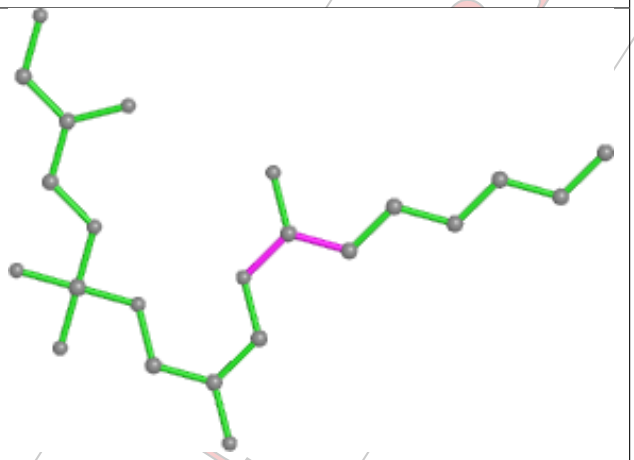
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	PGW	2	0
2	A	801	PGW	1	0
2	A	804	PGW	1	0
2	B	902	PGW	2	0
2	B	904	PGW	1	0

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

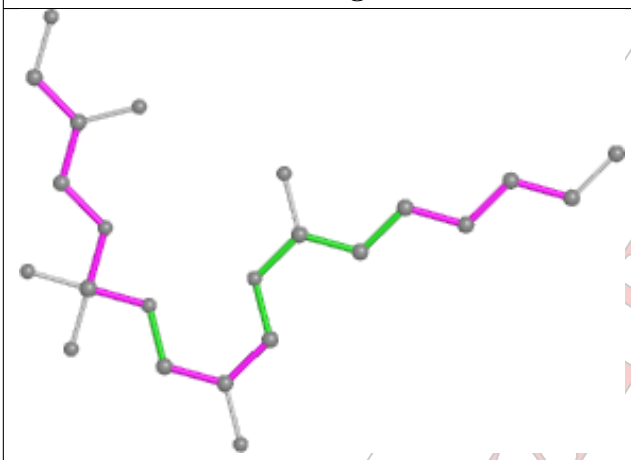
Ligand PGW A 803



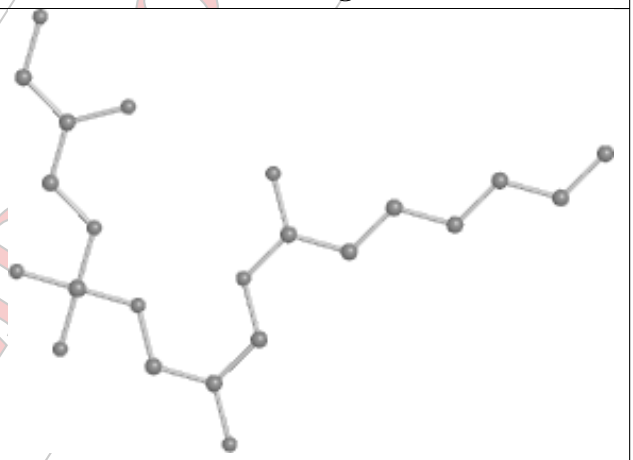
Bond lengths



Bond angles

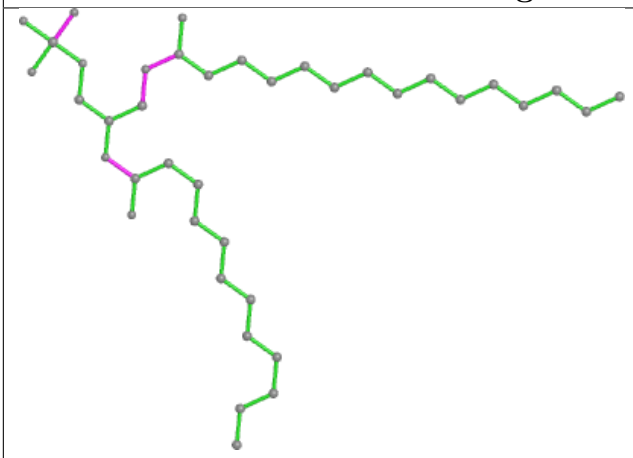


Torsions

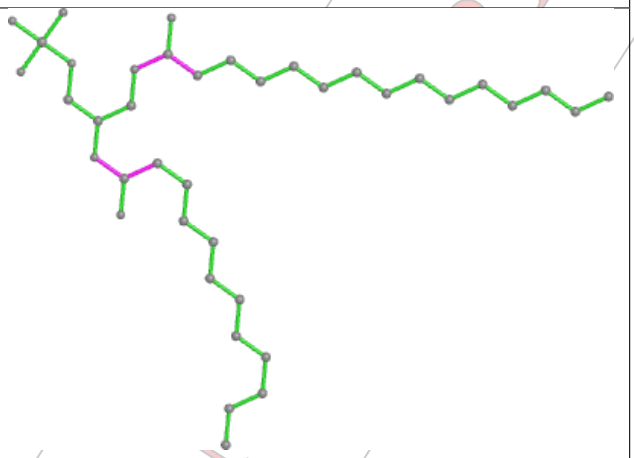


Rings

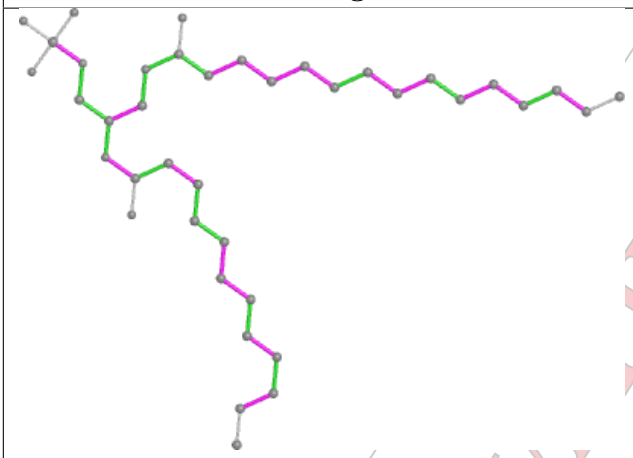
Ligand PGW A 801



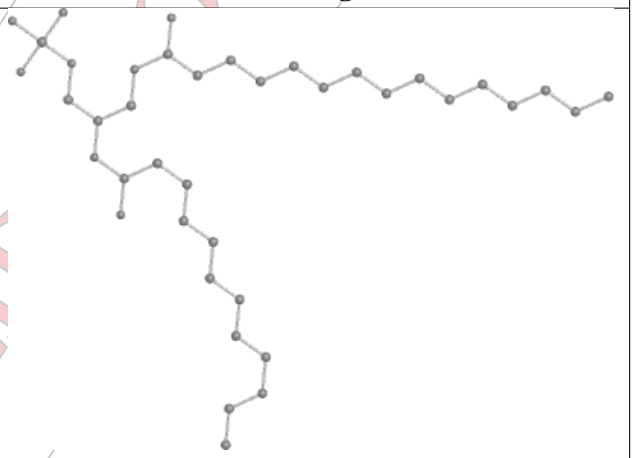
Bond lengths



Bond angles

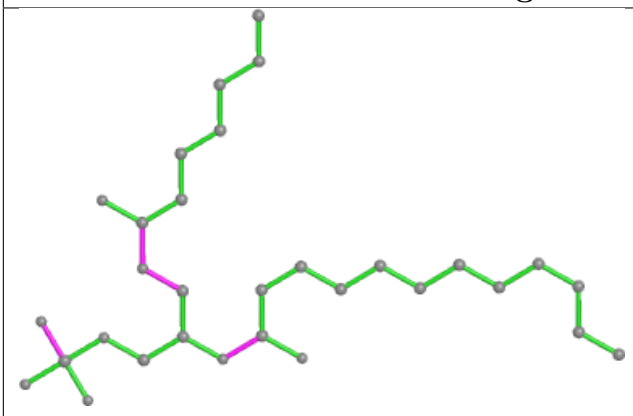


Torsions

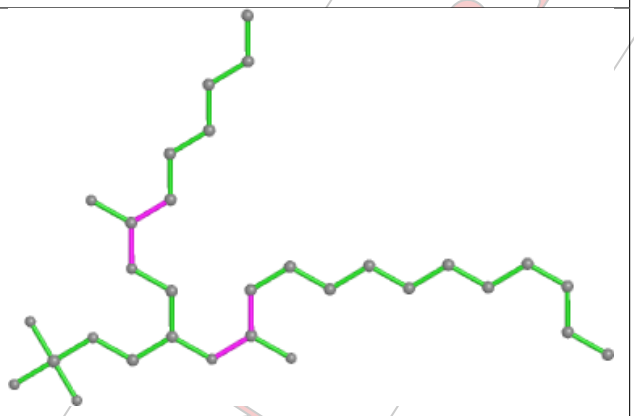


Rings

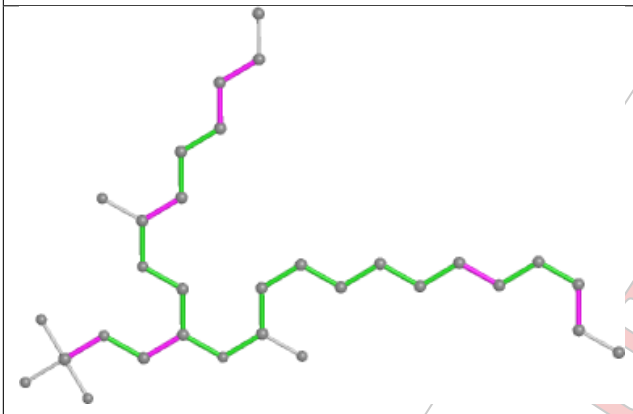
Ligand PGW A 804



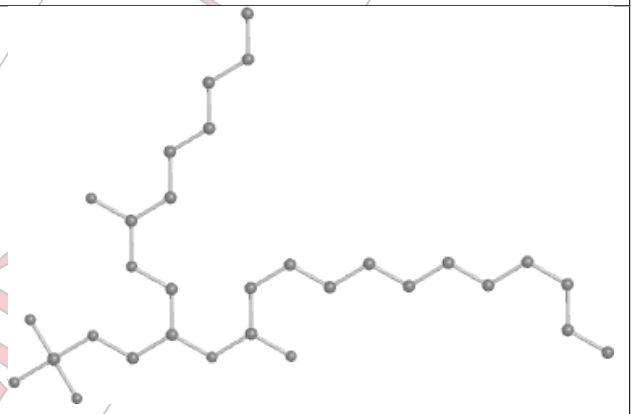
Bond lengths



Bond angles

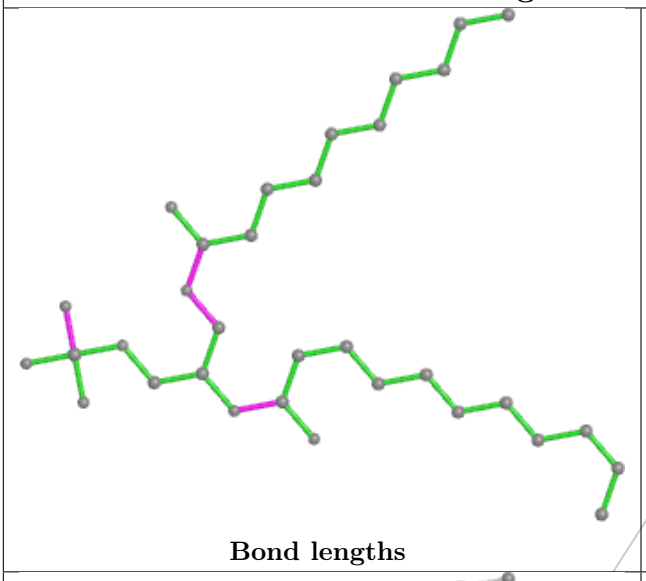


Torsions

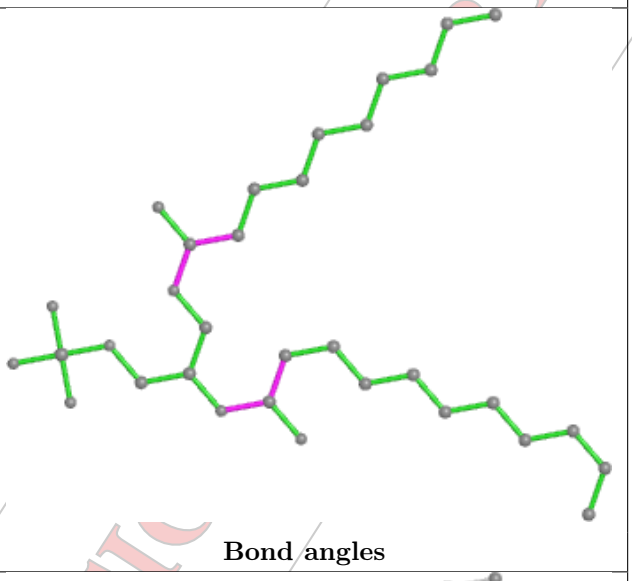


Rings

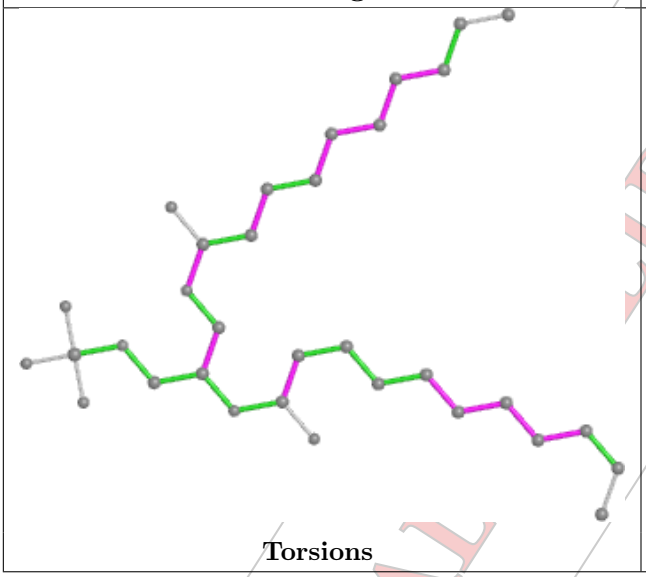
Ligand PGW B 901



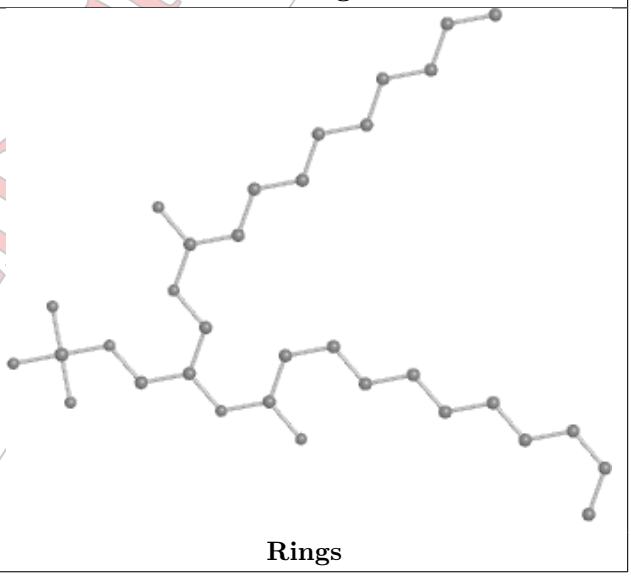
Bond lengths



Bond angles

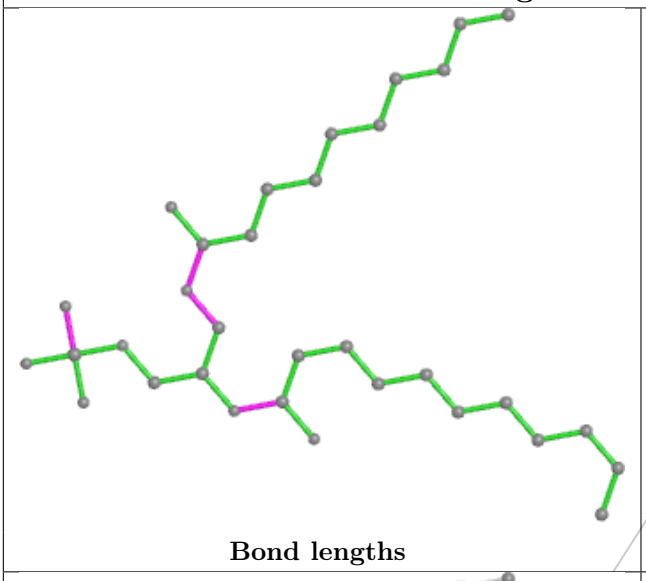


Torsions

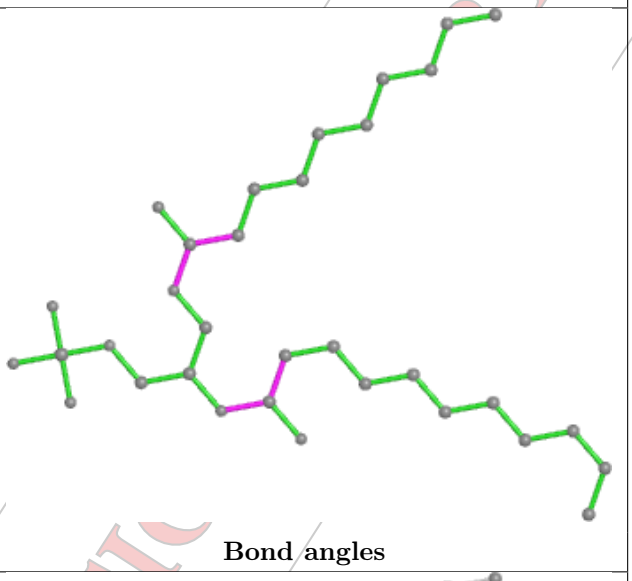


Rings

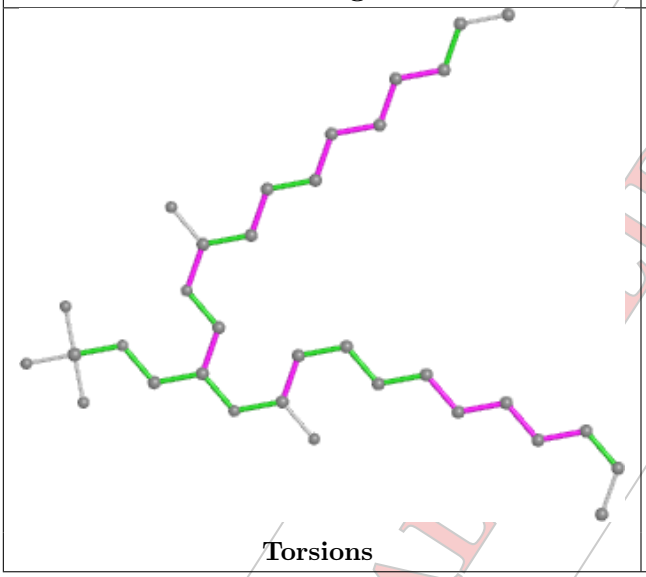
Ligand PGW A 802



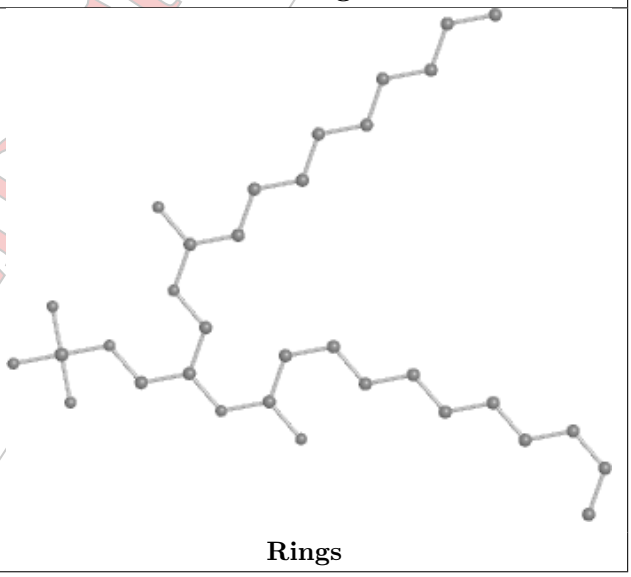
Bond lengths



Bond angles

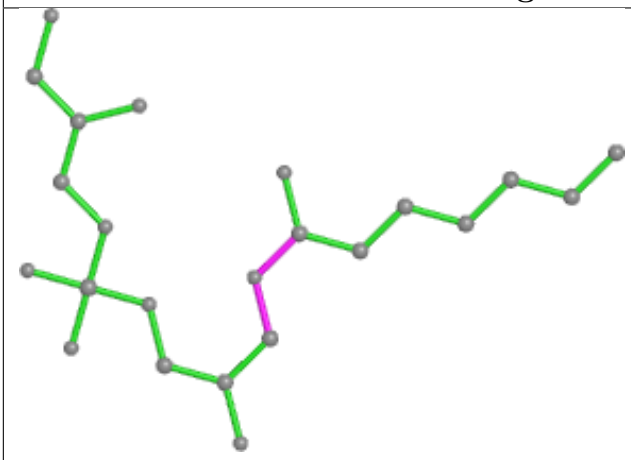


Torsions

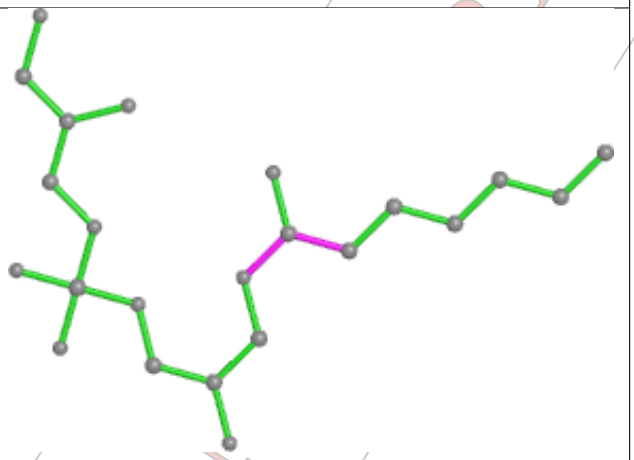


Rings

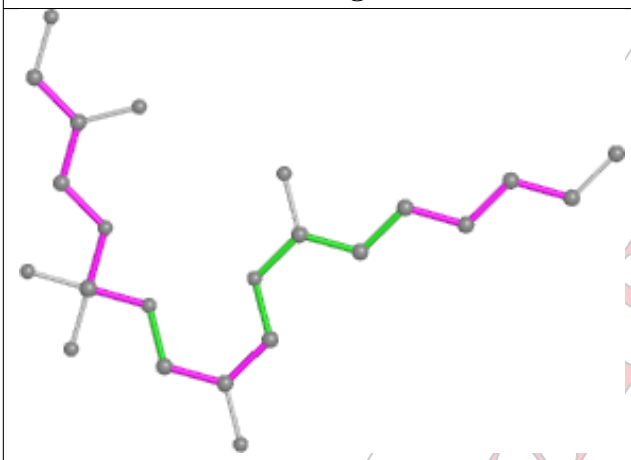
Ligand PGW B 902



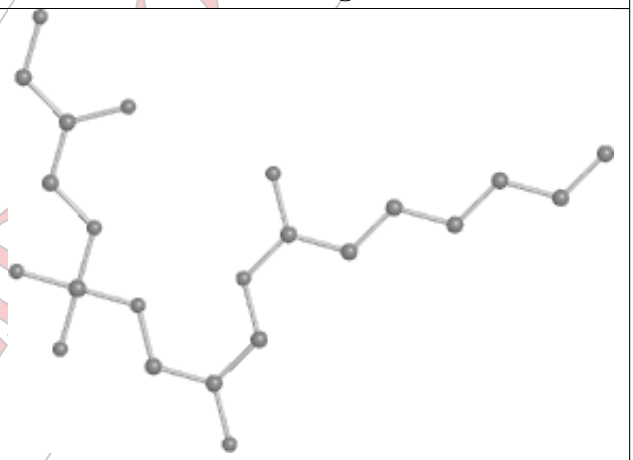
Bond lengths



Bond angles

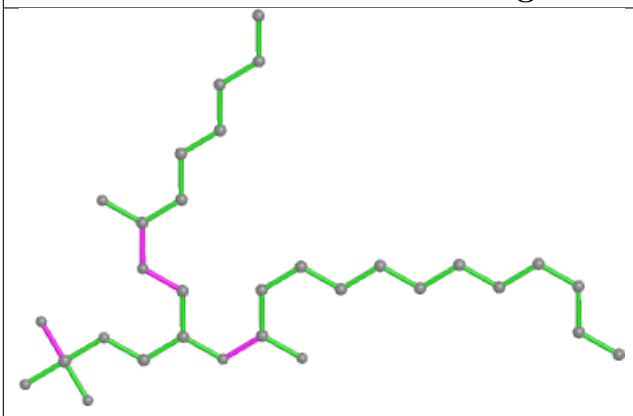


Torsions

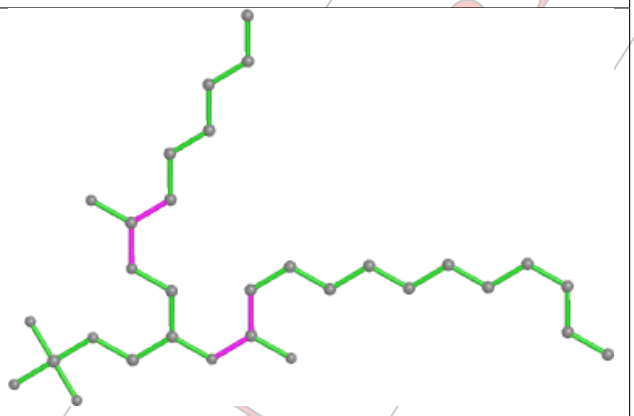


Rings

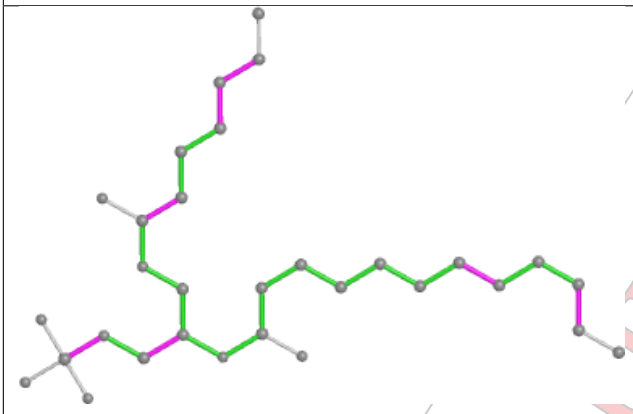
Ligand PGW B 903



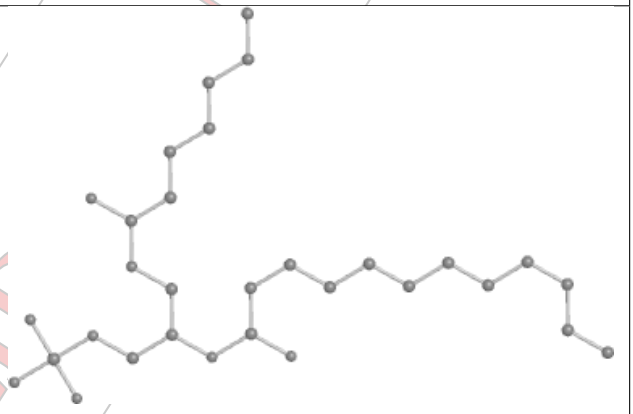
Bond lengths



Bond angles

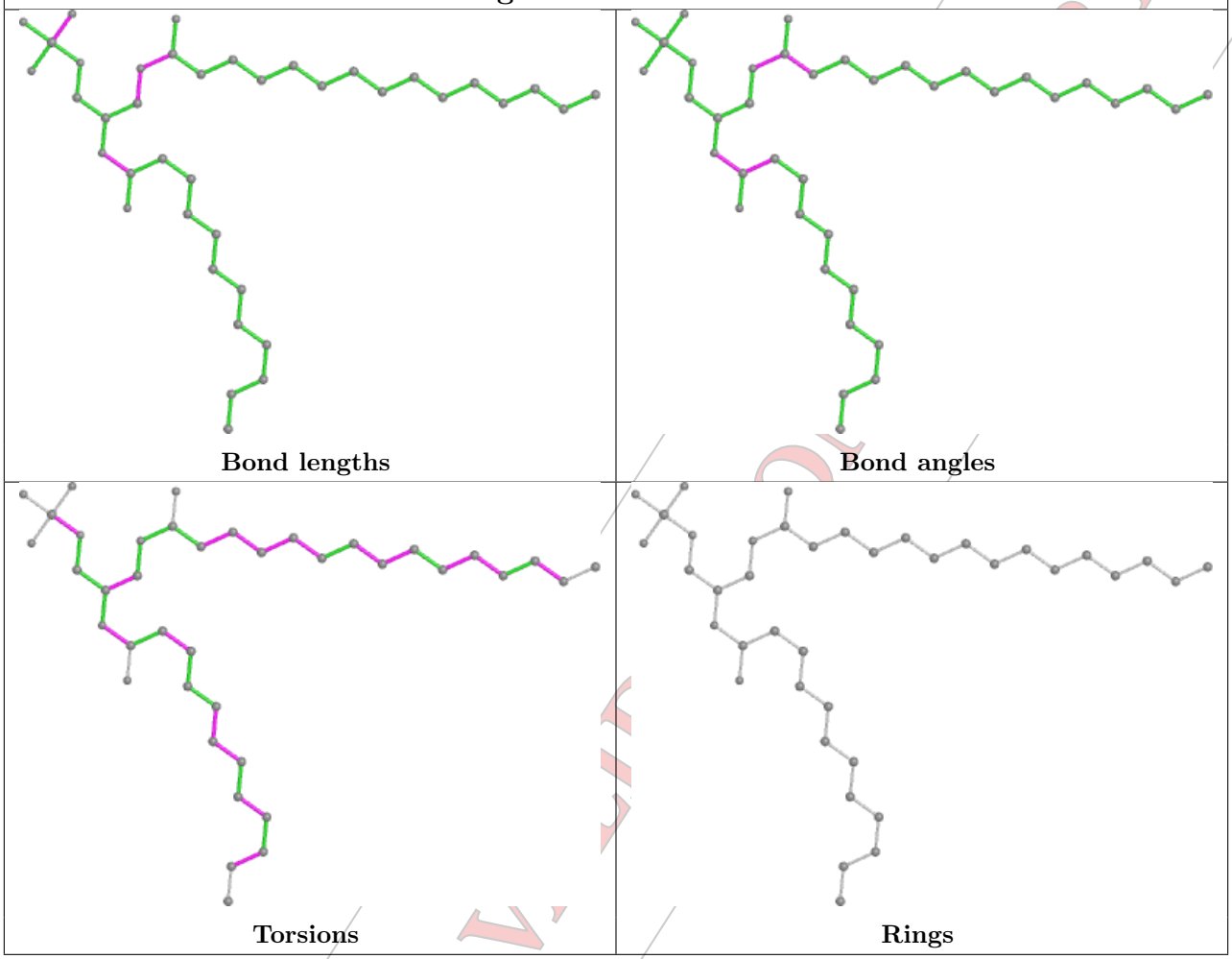


Torsions



Rings

Ligand PGW B 904



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

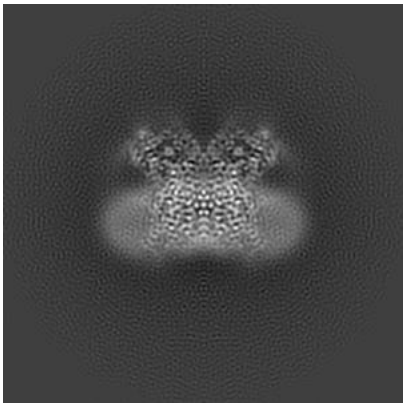
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24726. These allow visual inspection of the internal detail of the map and identification of artifacts.

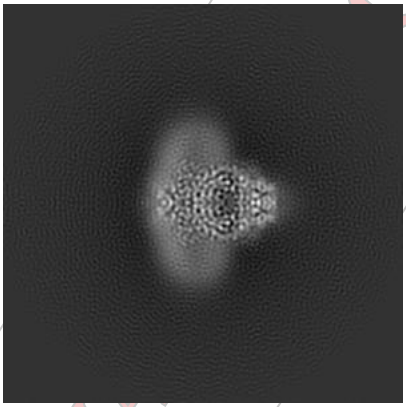
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

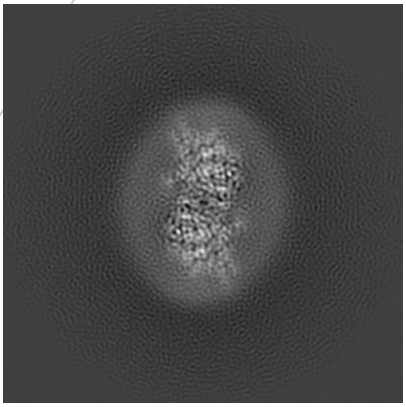
6.1.1 Primary map



X



Y

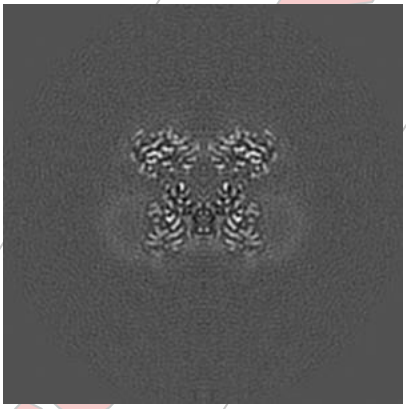


Z

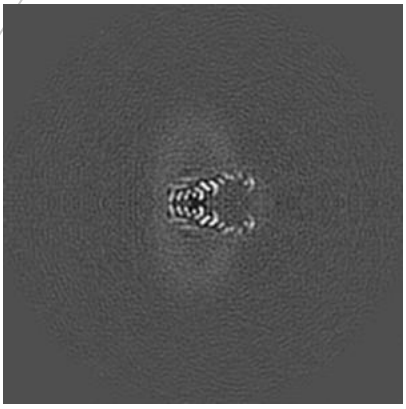
The images above show the map projected in three orthogonal directions.

6.2 Central slices

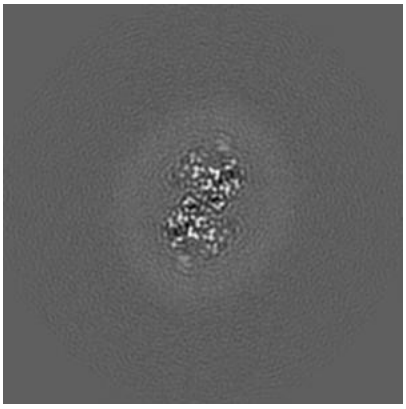
6.2.1 Primary map



X Index: 128



Y Index: 128

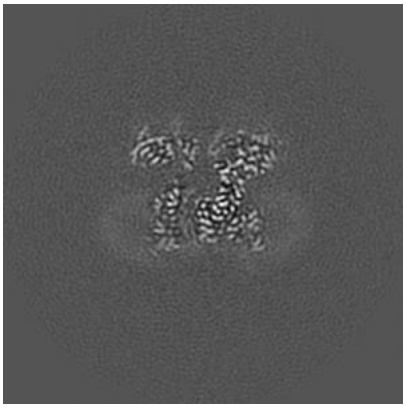


Z Index: 128

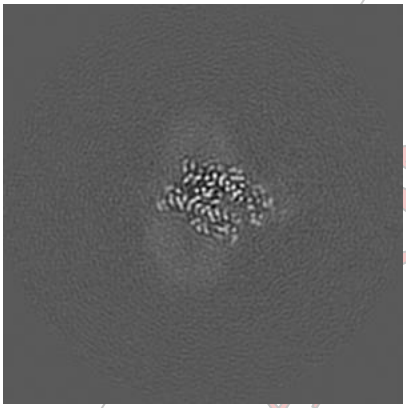
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

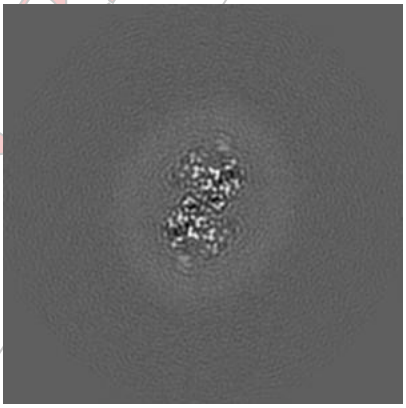
6.3.1 Primary map



X Index: 132



Y Index: 147

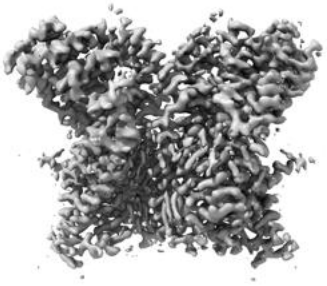


Z Index: 128

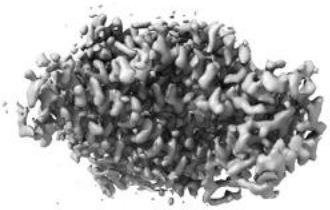
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

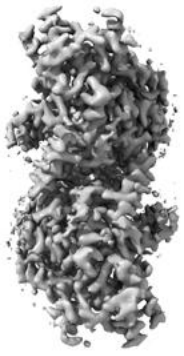
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

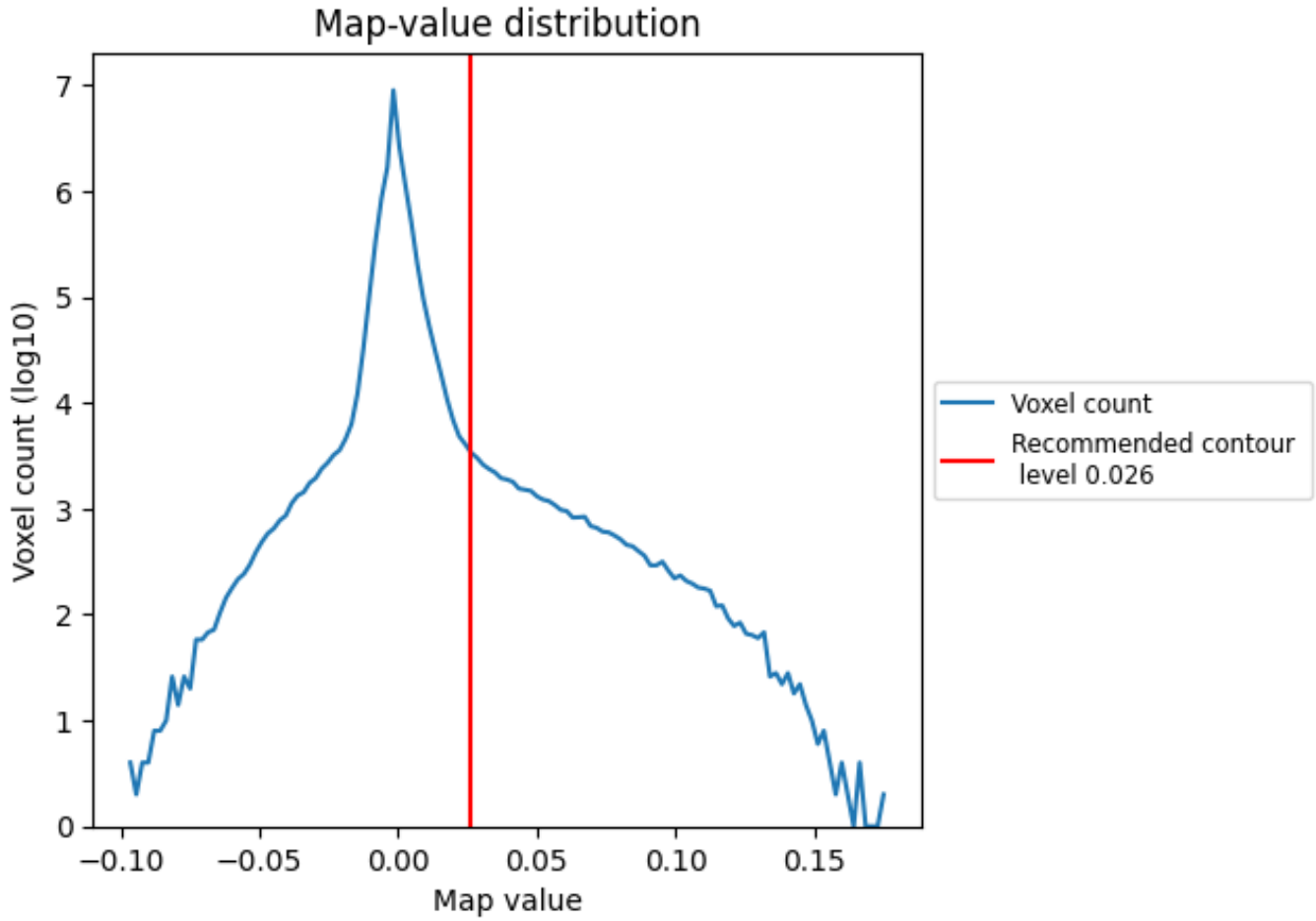
6.5 Mask visualisation (i)

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

7 Map analysis

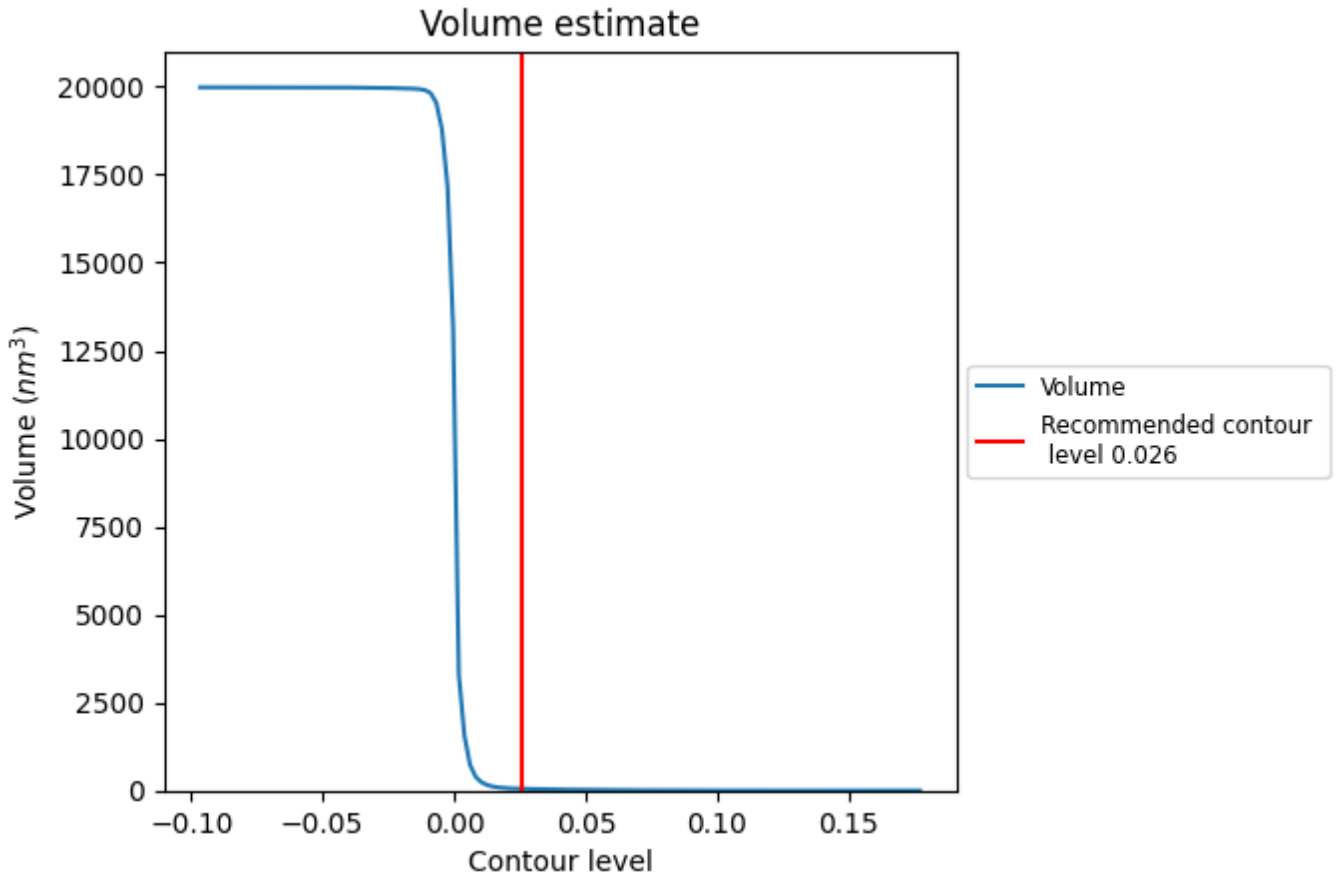
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

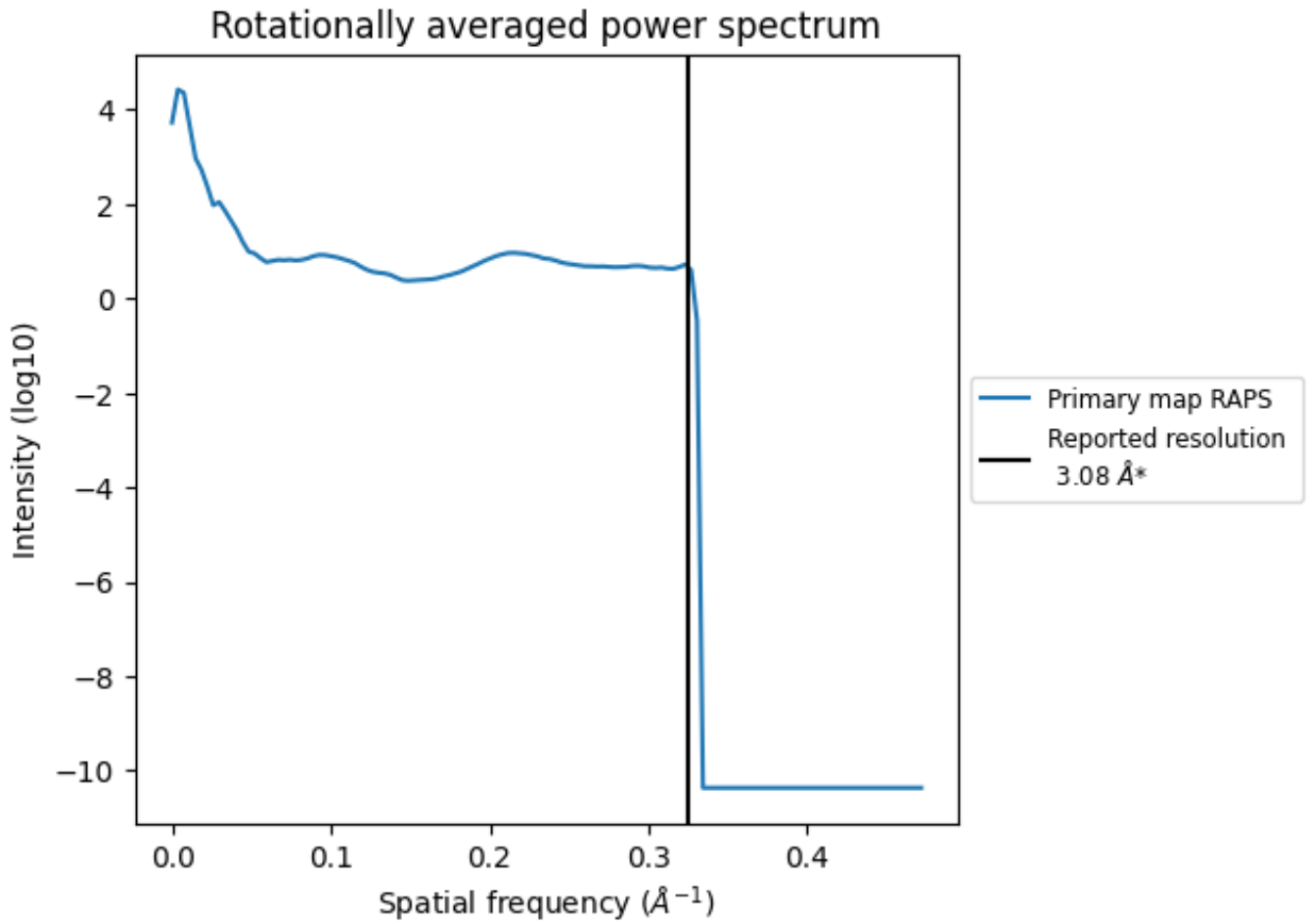
7.2 Volume estimate (i)



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 46 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)

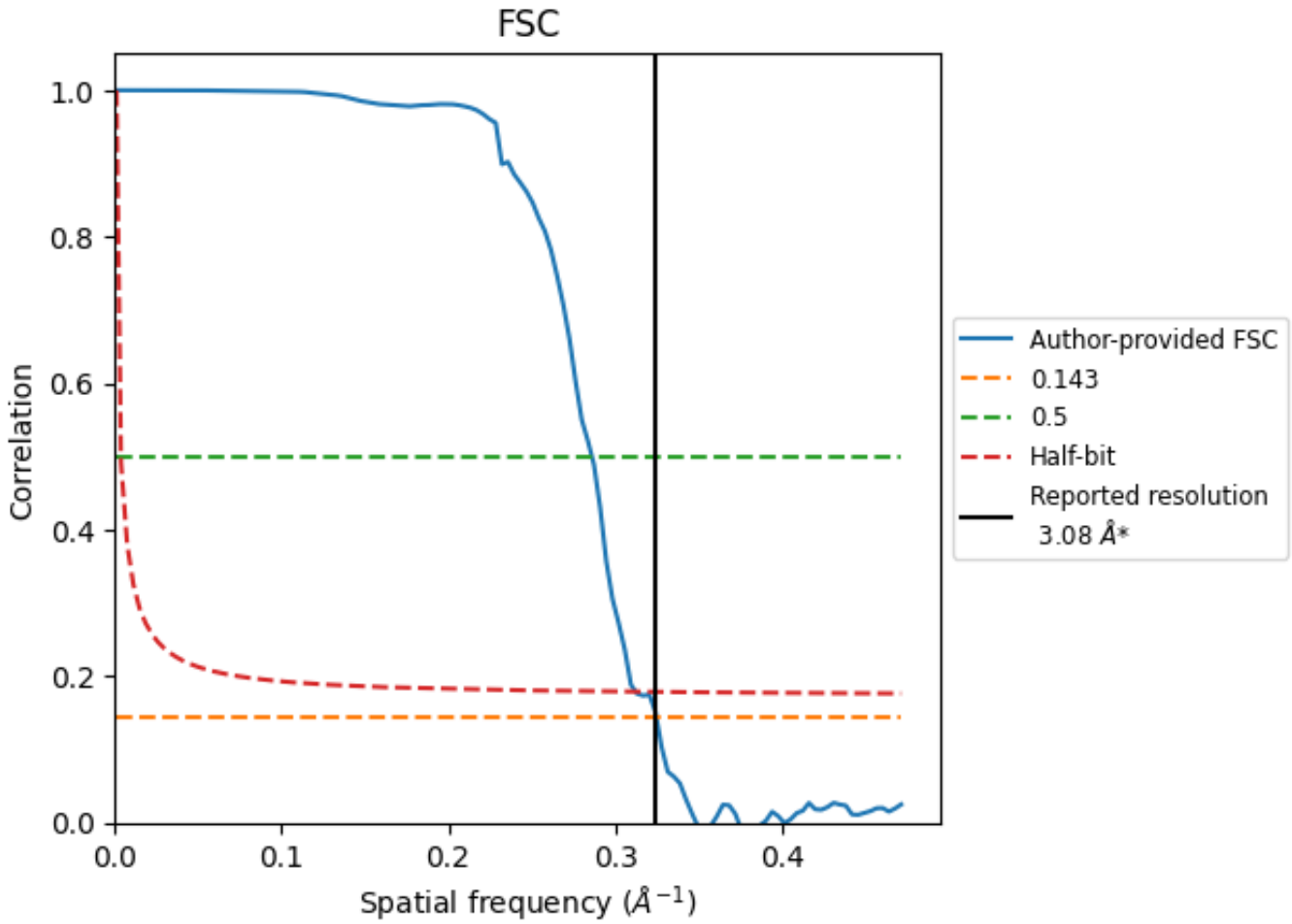


*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8.2 Resolution estimates (i)

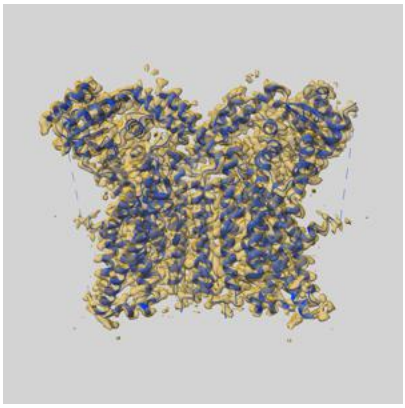
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.50	3.20
Unmasked-calculated*	-	-	-

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

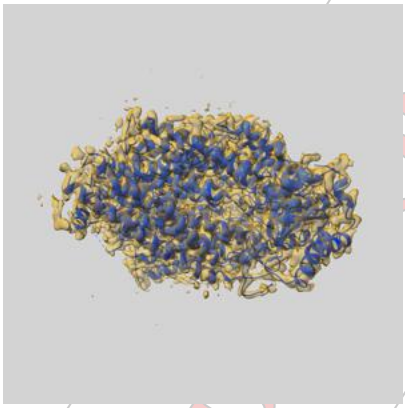
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24726 and PDB model 7RXA. Per-residue inclusion information can be found in section 3 on page 5.

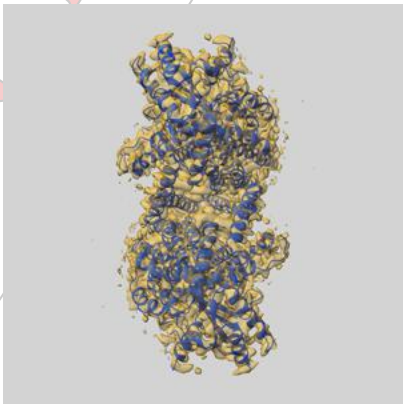
9.1 Map-model overlay



X



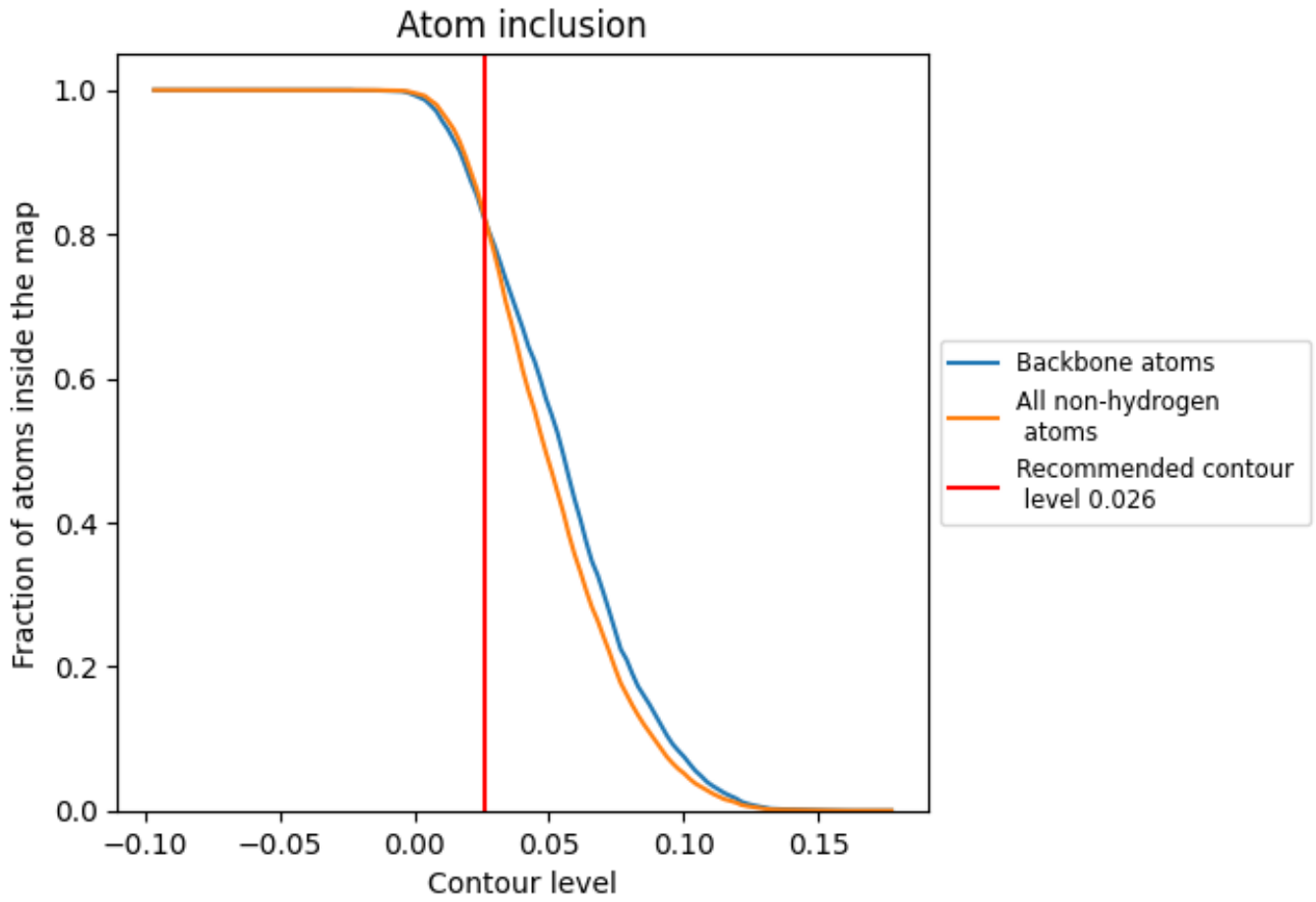
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

Full wwPDB EM Validation Report ⓘ

Aug 27, 2021 – 09:09 AM EDT

PDB ID	:	7RXB
EMDB ID	:	EMD-24727
Title	:	afTMEM16 lipid scramblase in C18 lipid nanodiscs in the absence of Ca2+
Deposited on	:	2021-08-22
Resolution	:	3.07 Å(reported)

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

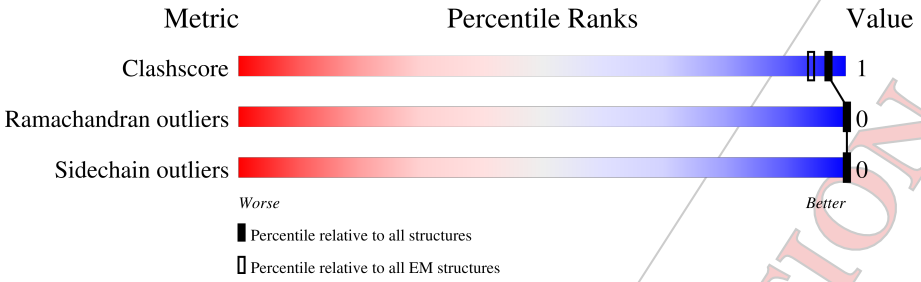
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.07 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 <=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	735	73% · 25%
1	B	735	73% · 25%

2 Entry composition

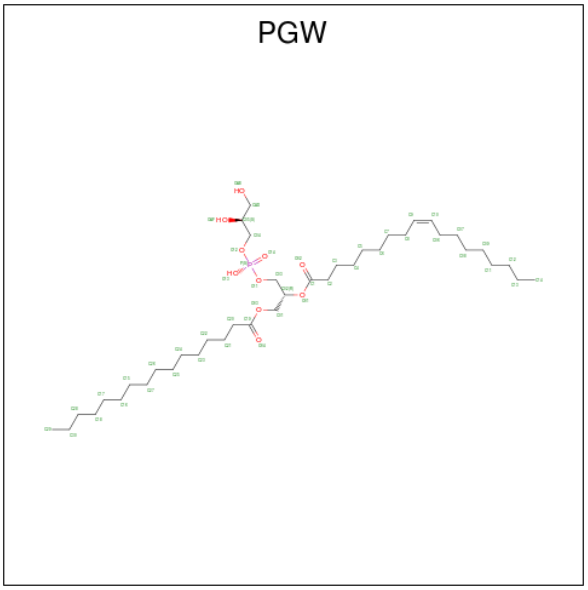
There are 2 unique types of molecules in this entry. The entry contains 8506 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 afTMEM16 lipid scramblase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	548	Total	C	N	O	S	0	0
			4153	2760	691	686	16		
1	B	548	Total	C	N	O	S	0	0
			4153	2760	691	686	16		

- Molecule 2 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			100	70	27	3	
2	A	1	Total	C	O	P	0
			100	70	27	3	
2	A	1	Total	C	O	P	0
			100	70	27	3	
2	A	1	Total	C	O	P	0
			100	70	27	3	

Continued on next page...

Continued from previous page...

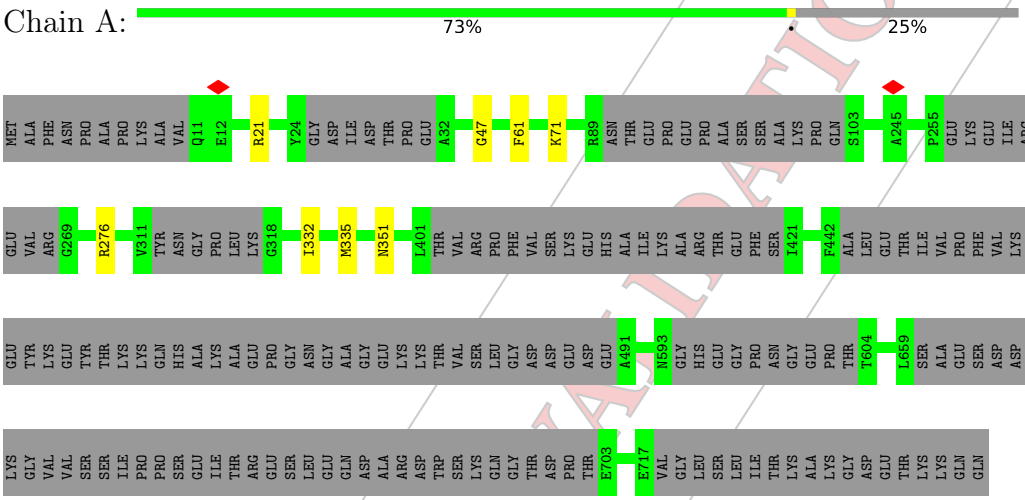
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	O	P	0
			100	70	27	3	
2	B	1	Total	C	O	P	0
			100	70	27	3	
2	B	1	Total	C	O	P	0
			100	70	27	3	
2	B	1	Total	C	O	P	0
			100	70	27	3	

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.

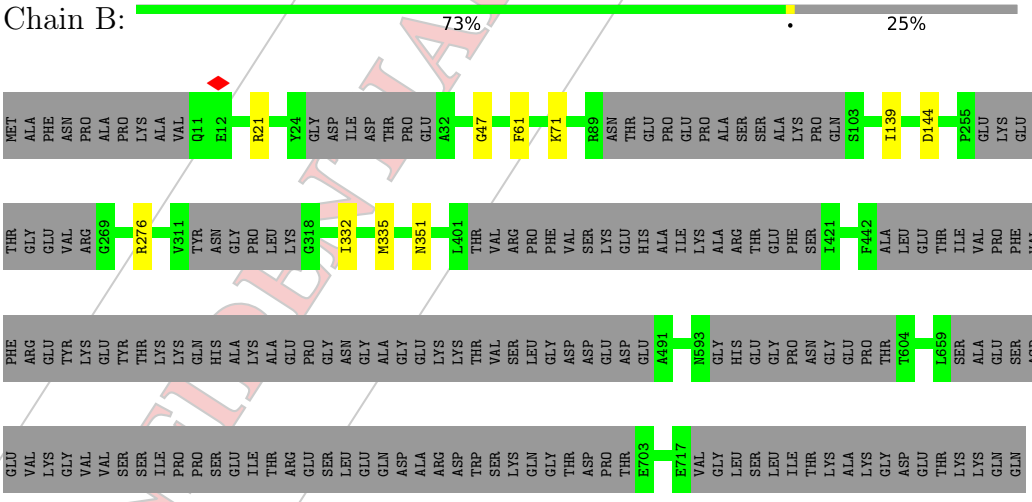
• Molecule 1: afTMEM16 lipid scramblase

Chain A:



• Molecule 1: afTMEM16 lipid scramblase

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151197	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 ($e^-/Å^2$)	59.13	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	0.141	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	218.112, 218.112, 218.112	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.852, 0.852, 0.852	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.42	0/4263	0.55	0/5833
1	B	0.42	0/4263	0.55	0/5833
All	All	0.42	0/8526	0.55	0/11666

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	4153	0	3963	4	0
1	B	4153	0	3963	6	0
2	A	100	0	109	0	0
2	B	100	0	109	0	0
All	All	8506	0	8144	10	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 1.

All (10) 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:47:GLY:HA3	1:B:71:LYS:HD3	1.94	0.49
1:A:47:GLY:HA3	1:A:71:LYS:HD3	1.94	0.48
1:A:332:ILE:HA	1:A:335:MET:HG2	1.96	0.48
1:B:332:ILE:HA	1:B:335:MET:HG2	1.96	0.47
1:A:276:ARG:NH1	1:A:351:ASN:O	2.47	0.47
1:B:276:ARG:NH1	1:B:351:ASN:O	2.47	0.47
1:B:21:ARG:HD3	1:B:61:PHE:HE1	1.82	0.45
1:B:144:ASP:OD2	1:B:144:ASP:N	2.47	0.45
1:A:21:ARG:HD3	1:A:61:PHE:HE1	1.82	0.43
1:B:139:ILE:HD13	1:B:139:ILE:HG21	1.93	0.41

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	530/735 (72%)	498 (94%)	32 (6%)	0	100	100
1	B	530/735 (72%)	498 (94%)	32 (6%)	0	100	100
All	All	1060/1470 (72%)	996 (94%)	64 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/646 (62%)	397 (100%)	0	100	100
1	B	397/646 (62%)	397 (100%)	0	100	100
All	All	794/1292 (62%)	794 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	518	GLN
1	B	280	GLN
1	B	518	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\|>2$
2	PGW	B	1003	-	19,19,50	1.42	4 (21%)	21,21,56	1.49	3 (14%)
2	PGW	A	802	-	19,19,50	1.42	4 (21%)	21,21,56	1.49	3 (14%)
2	PGW	B	1004	-	31,31,50	1.18	5 (16%)	35,36,56	1.29	2 (5%)
2	PGW	B	1002	-	26,26,50	0.96	3 (11%)	29,30,56	0.95	1 (3%)
2	PGW	A	803	-	31,31,50	1.17	5 (16%)	35,36,56	1.29	2 (5%)
2	PGW	B	1001	-	20,20,50	1.37	4 (20%)	24,25,56	1.25	1 (4%)
2	PGW	A	801	-	26,26,50	0.97	3 (11%)	29,30,56	0.95	1 (3%)
2	PGW	A	804	-	20,20,50	1.37	4 (20%)	24,25,56	1.25	1 (4%)

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
2	PGW	B	1003	-	-	9/20/20/55	-
2	PGW	A	802	-	-	9/20/20/55	-
2	PGW	B	1004	-	-	19/33/33/55	-
2	PGW	B	1002	-	-	11/26/26/55	-
2	PGW	A	803	-	-	19/33/33/55	-
2	PGW	B	1001	-	-	8/21/21/55	-
2	PGW	A	801	-	-	11/26/26/55	-
2	PGW	A	804	-	-	8/21/21/55	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	PGW	O01-C02	-3.19	1.41	1.47
2	B	1003	PGW	O01-C02	-3.15	1.41	1.47
2	B	1003	PGW	O01-C1	2.86	1.42	1.34
2	A	802	PGW	O01-C1	2.85	1.42	1.34
2	A	803	PGW	O01-C1	2.79	1.42	1.34
2	B	1004	PGW	O01-C1	2.78	1.42	1.34
2	B	1001	PGW	O01-C1	2.73	1.42	1.34
2	A	804	PGW	O01-C1	2.73	1.42	1.34
2	A	804	PGW	O03-C01	-2.56	1.39	1.45
2	A	801	PGW	O03-C19	2.56	1.40	1.33
2	B	1001	PGW	O03-C01	-2.55	1.39	1.45
2	B	1002	PGW	O03-C19	2.54	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1004	PGW	O03-C01	-2.50	1.39	1.45
2	A	803	PGW	O03-C01	-2.49	1.39	1.45
2	A	802	PGW	O03-C19	2.42	1.40	1.33
2	B	1003	PGW	O03-C19	2.41	1.40	1.33
2	A	802	PGW	O03-C01	-2.39	1.39	1.45
2	B	1003	PGW	O03-C01	-2.39	1.39	1.45
2	B	1004	PGW	P-O12	2.33	1.63	1.54
2	A	803	PGW	P-O12	2.33	1.63	1.54
2	B	1001	PGW	O01-C02	-2.27	1.40	1.46
2	A	804	PGW	P-O12	2.26	1.63	1.54
2	B	1001	PGW	P-O12	2.26	1.63	1.54
2	B	1004	PGW	O03-C19	2.25	1.39	1.33
2	A	804	PGW	O01-C02	-2.24	1.41	1.46
2	A	803	PGW	O03-C19	2.24	1.39	1.33
2	A	801	PGW	O03-C01	-2.21	1.40	1.45
2	B	1004	PGW	O01-C02	-2.20	1.41	1.46
2	A	803	PGW	O01-C02	-2.20	1.41	1.46
2	B	1002	PGW	O03-C01	-2.15	1.40	1.45
2	A	801	PGW	P-O12	2.15	1.63	1.54
2	B	1002	PGW	P-O12	2.14	1.63	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1004	PGW	O01-C1-C2	4.36	120.90	111.50
2	A	803	PGW	O01-C1-C2	4.32	120.82	111.50
2	B	1003	PGW	O01-C1-C2	3.93	119.96	111.50
2	A	802	PGW	O01-C1-C2	3.92	119.96	111.50
2	A	804	PGW	O01-C1-C2	3.87	119.84	111.50
2	B	1001	PGW	O01-C1-C2	3.84	119.79	111.50
2	B	1004	PGW	O03-C19-C20	2.71	120.40	111.91
2	A	803	PGW	O03-C19-C20	2.70	120.38	111.91
2	A	802	PGW	C02-O01-C1	-2.69	114.41	117.88
2	B	1003	PGW	C02-O01-C1	-2.67	114.44	117.88
2	A	801	PGW	O03-C19-C20	2.46	119.62	111.91
2	B	1002	PGW	O03-C19-C20	2.45	119.59	111.91
2	A	802	PGW	O03-C19-C20	2.45	119.59	111.91
2	B	1003	PGW	O03-C19-C20	2.44	119.58	111.91

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PGW	C01-C02-C03-O11
2	A	802	PGW	O03-C01-C02-C03
2	A	802	PGW	O02-C1-O01-C02
2	A	803	PGW	C03-O11-P-O12
2	A	803	PGW	C03-O11-P-O13
2	A	803	PGW	C2-C1-O01-C02
2	A	804	PGW	C03-O11-P-O12
2	A	804	PGW	C03-O11-P-O13
2	A	804	PGW	C03-O11-P-O14
2	B	1001	PGW	C03-O11-P-O12
2	B	1001	PGW	C03-O11-P-O13
2	B	1001	PGW	C03-O11-P-O14
2	B	1002	PGW	C01-C02-C03-O11
2	B	1003	PGW	O03-C01-C02-C03
2	B	1003	PGW	O02-C1-O01-C02
2	B	1004	PGW	C03-O11-P-O12
2	B	1004	PGW	C03-O11-P-O13
2	B	1004	PGW	C2-C1-O01-C02
2	A	802	PGW	C2-C1-O01-C02
2	B	1003	PGW	C2-C1-O01-C02
2	A	803	PGW	O02-C1-O01-C02
2	B	1004	PGW	O02-C1-O01-C02
2	A	801	PGW	O01-C02-C03-O11
2	B	1002	PGW	O01-C02-C03-O11
2	A	804	PGW	C1-C2-C3-C4
2	B	1001	PGW	C1-C2-C3-C4
2	A	804	PGW	O03-C01-C02-O01
2	B	1001	PGW	O03-C01-C02-O01
2	A	801	PGW	C23-C24-C25-C26
2	A	803	PGW	C16-C15-C27-C26
2	B	1002	PGW	C23-C24-C25-C26
2	B	1004	PGW	C16-C15-C27-C26
2	A	802	PGW	C19-C20-C21-C22
2	B	1003	PGW	C19-C20-C21-C22
2	A	804	PGW	C2-C3-C4-C5
2	B	1001	PGW	C2-C3-C4-C5
2	B	1004	PGW	C24-C25-C26-C27
2	A	803	PGW	C24-C25-C26-C27
2	A	801	PGW	C20-C21-C22-C23
2	B	1002	PGW	C20-C21-C22-C23
2	A	801	PGW	C22-C23-C24-C25
2	A	801	PGW	C24-C25-C26-C27
2	B	1002	PGW	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	B	1002	PGW	C24-C25-C26-C27
2	B	1004	PGW	C20-C21-C22-C23
2	A	803	PGW	C20-C21-C22-C23
2	A	803	PGW	C2-C3-C4-C5
2	B	1004	PGW	C2-C3-C4-C5
2	A	803	PGW	C1-C2-C3-C4
2	A	803	PGW	C19-C20-C21-C22
2	B	1004	PGW	C1-C2-C3-C4
2	B	1004	PGW	C19-C20-C21-C22
2	A	803	PGW	C20-C19-O03-C01
2	B	1004	PGW	C20-C19-O03-C01
2	A	803	PGW	O03-C01-C02-O01
2	B	1004	PGW	O03-C01-C02-O01
2	B	1002	PGW	C21-C22-C23-C24
2	A	801	PGW	C21-C22-C23-C24
2	A	802	PGW	C22-C23-C24-C25
2	B	1003	PGW	C22-C23-C24-C25
2	A	803	PGW	O04-C19-O03-C01
2	B	1004	PGW	O04-C19-O03-C01
2	B	1002	PGW	C16-C17-C18-C28
2	A	801	PGW	C16-C17-C18-C28
2	A	803	PGW	C03-O11-P-O14
2	B	1004	PGW	C03-O11-P-O14
2	A	803	PGW	C01-C02-C03-O11
2	B	1004	PGW	C01-C02-C03-O11
2	A	803	PGW	O03-C01-C02-C03
2	A	804	PGW	O03-C01-C02-C03
2	B	1001	PGW	O03-C01-C02-C03
2	B	1004	PGW	O03-C01-C02-C03
2	A	803	PGW	O01-C02-C03-O11
2	B	1004	PGW	O01-C02-C03-O11
2	A	802	PGW	O03-C01-C02-O01
2	B	1003	PGW	O03-C01-C02-O01
2	A	804	PGW	C3-C4-C5-C6
2	B	1001	PGW	C3-C4-C5-C6
2	A	801	PGW	C02-C03-O11-P
2	B	1002	PGW	C02-C03-O11-P
2	A	801	PGW	C18-C28-C30-C29
2	B	1002	PGW	C18-C28-C30-C29
2	A	801	PGW	C27-C15-C16-C17
2	B	1002	PGW	C27-C15-C16-C17
2	A	803	PGW	C25-C26-C27-C15

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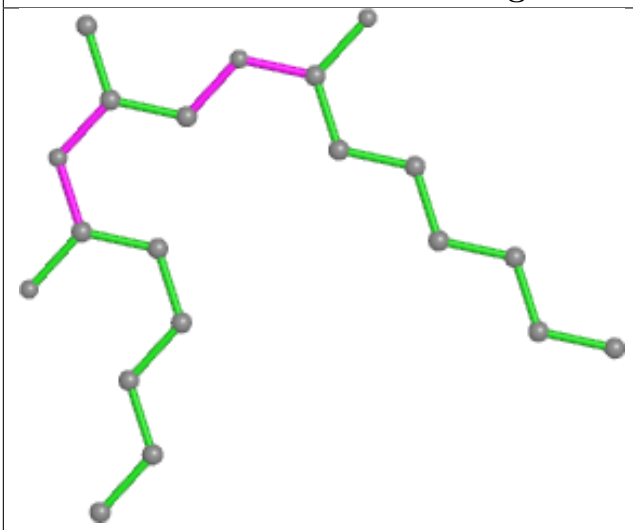
Mol	Chain	Res	Type	Atoms
2	B	1004	PGW	C25-C26-C27-C15
2	A	803	PGW	C22-C23-C24-C25
2	B	1004	PGW	C22-C23-C24-C25
2	B	1003	PGW	C21-C22-C23-C24
2	A	802	PGW	C21-C22-C23-C24
2	A	802	PGW	O01-C1-C2-C3
2	B	1003	PGW	O01-C1-C2-C3
2	A	802	PGW	O02-C1-C2-C3
2	B	1003	PGW	O02-C1-C2-C3

There are no ring outliers.

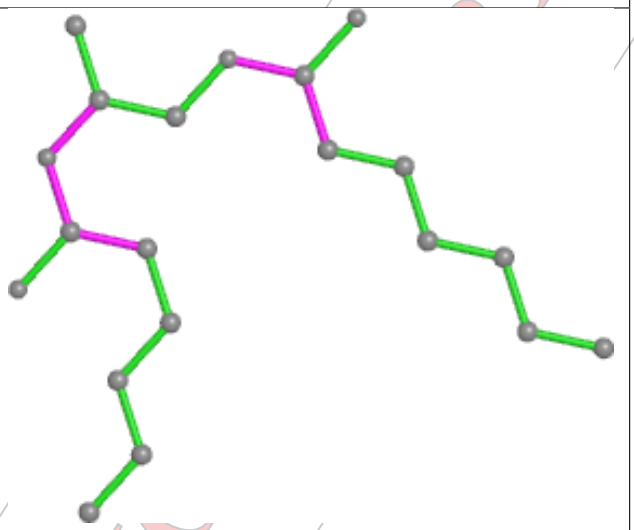
No monomer is involved in short contacts.

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 then 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.

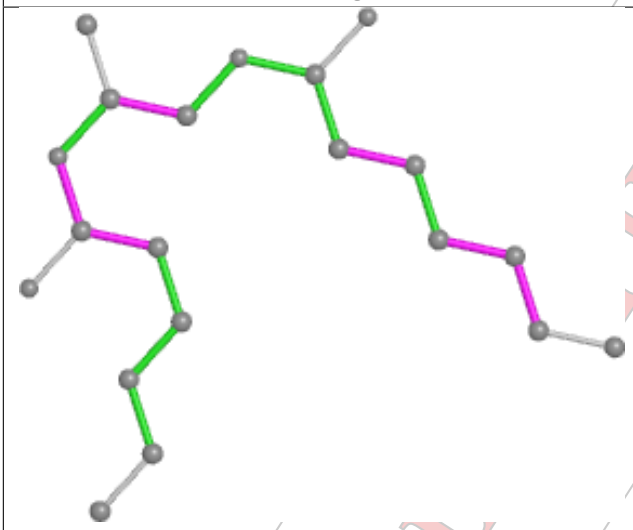
Ligand PGW B 1003



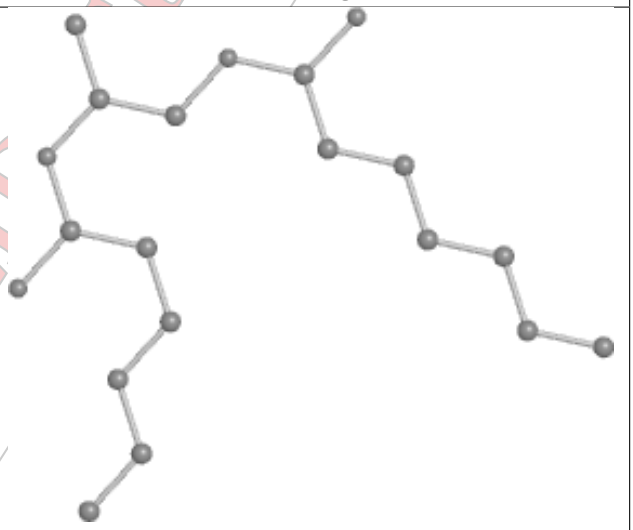
Bond lengths



Bond angles

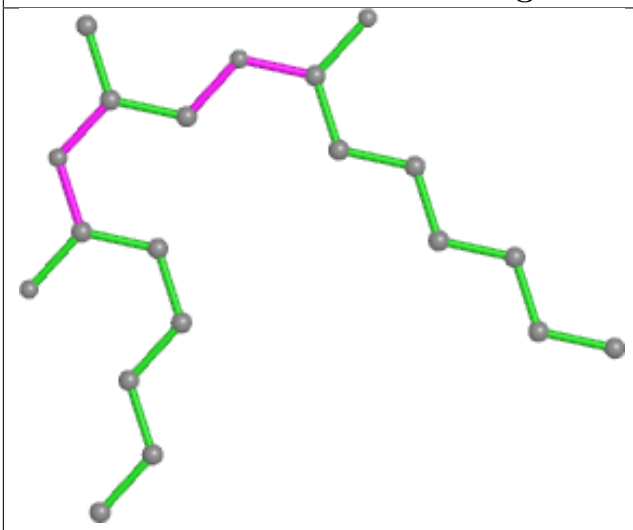


Torsions



Rings

Ligand PGW A 802



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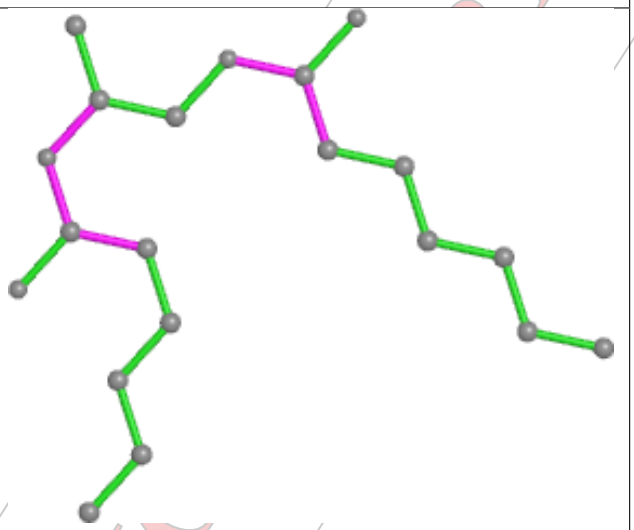
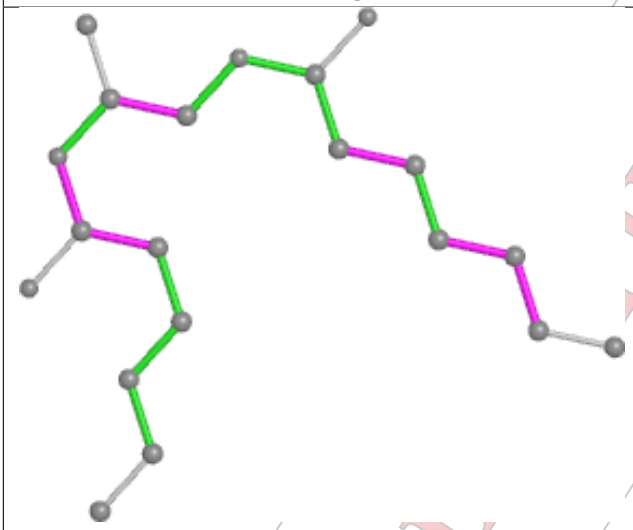
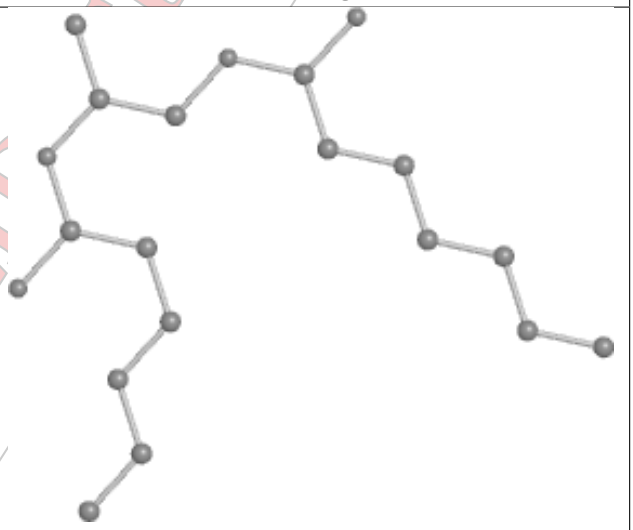


Bond angles

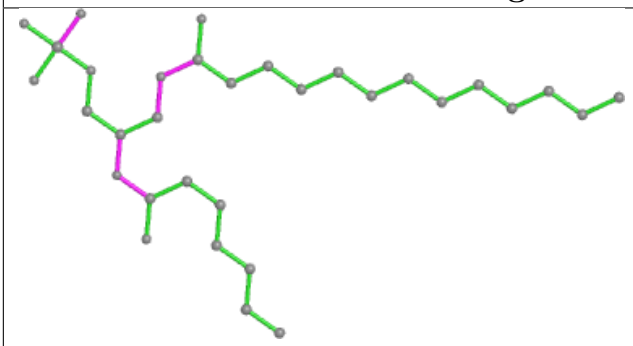


Torsions

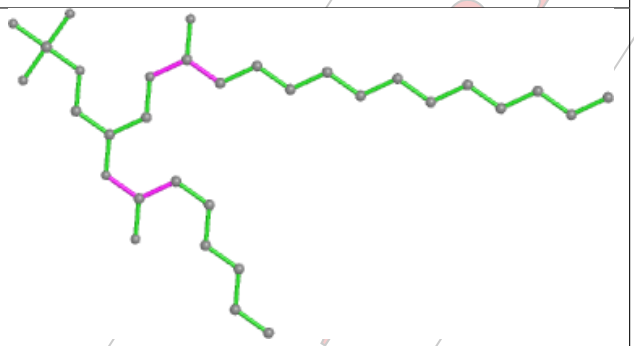


Rings

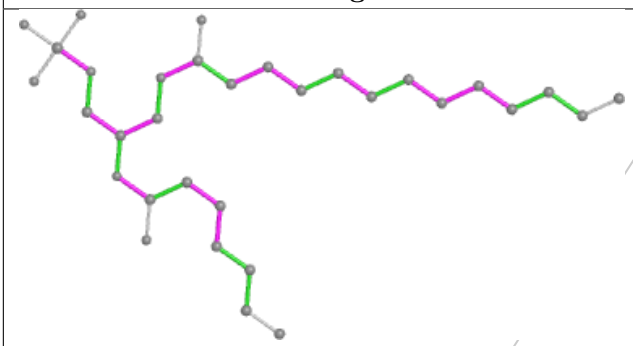
Ligand PGW B 1004



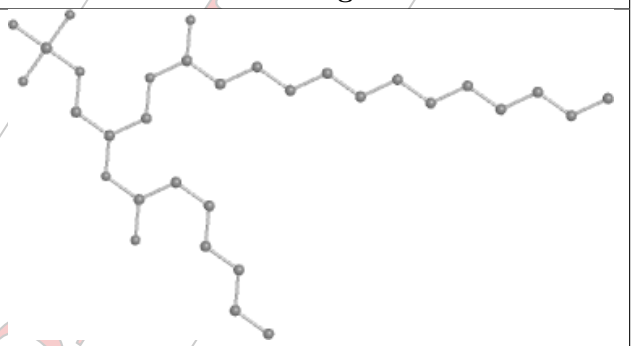
Bond lengths



Bond angles

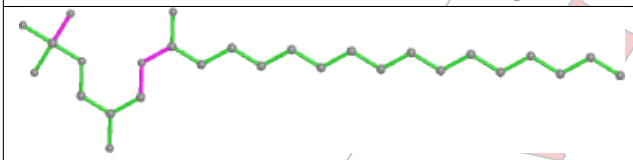


Torsions

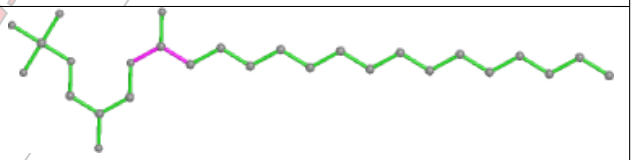


Rings

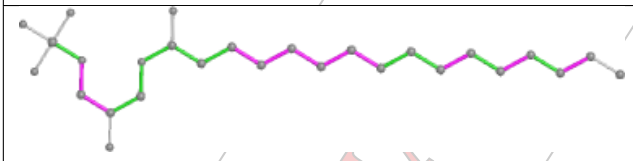
Ligand PGW B 1002



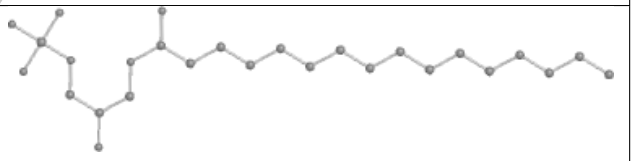
Bond lengths



Bond angles

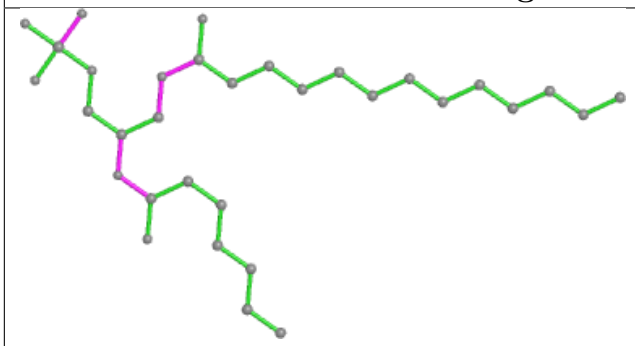


Torsions

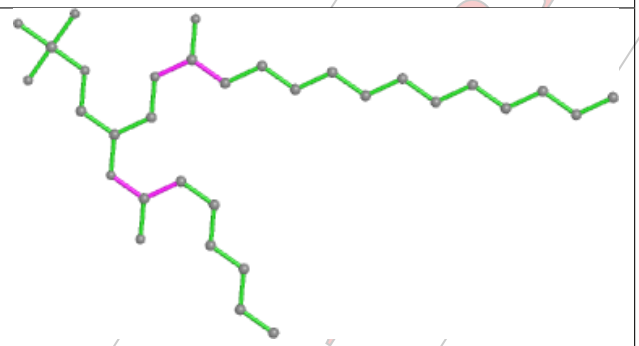


Rings

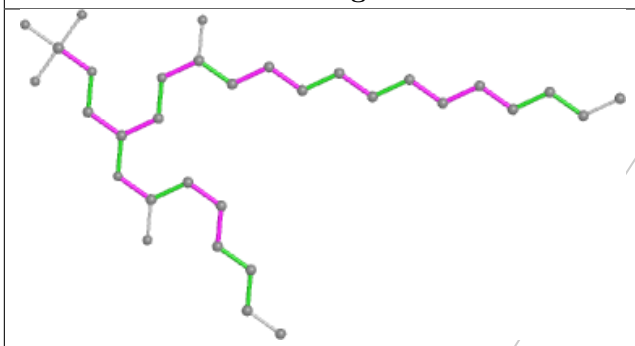
Ligand PGW A 803



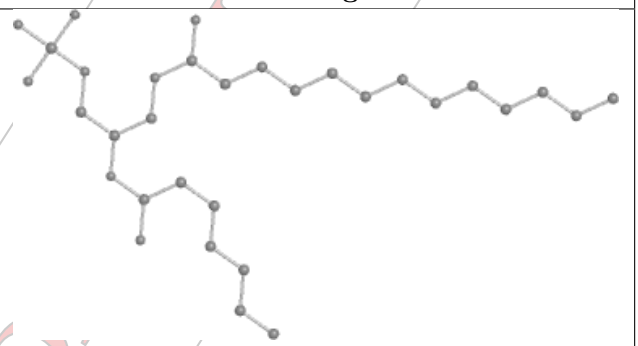
Bond lengths



Bond angles

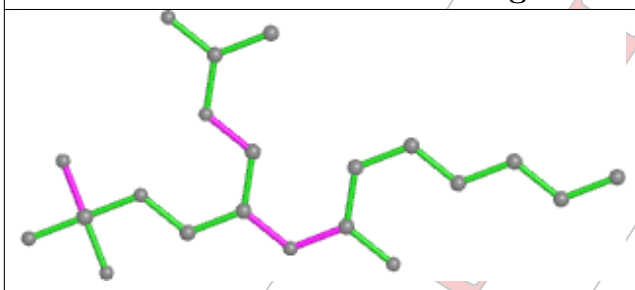


Torsions

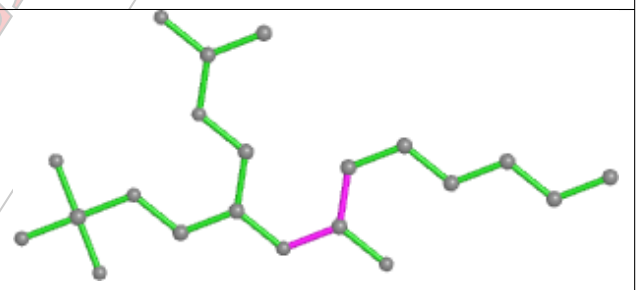


Rings

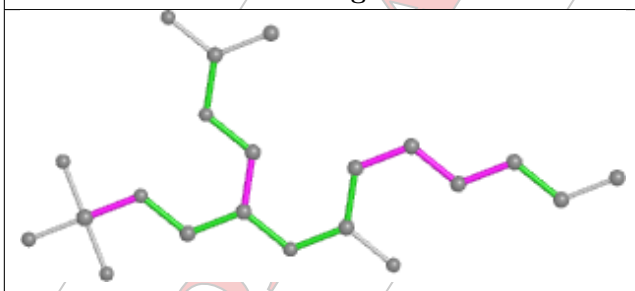
Ligand PGW B 1001



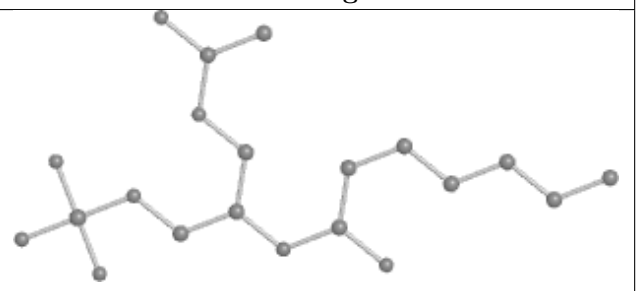
Bond lengths



Bond angles

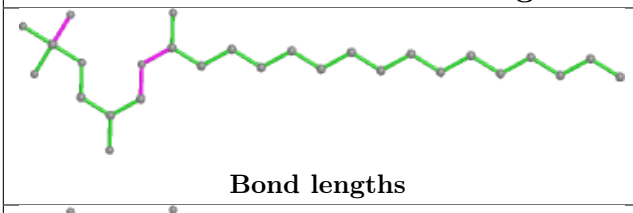


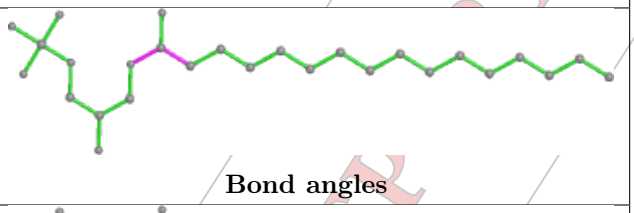
Torsions

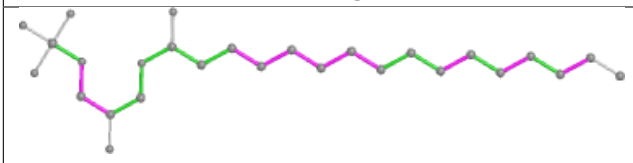


Rings

Ligand PGW A 801

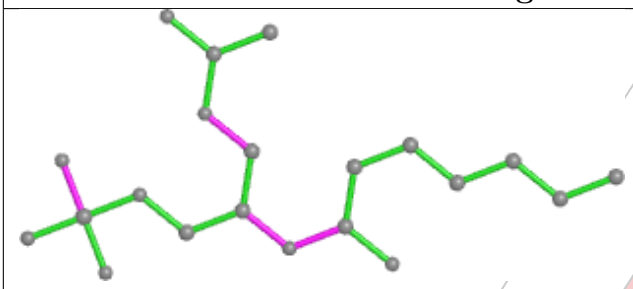

Bond lengths

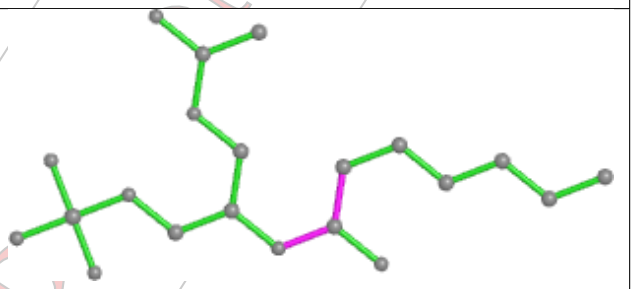

Bond angles


Torsions


Rings

Ligand PGW A 804


Bond lengths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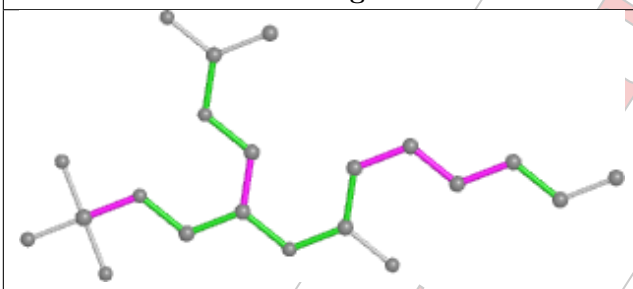
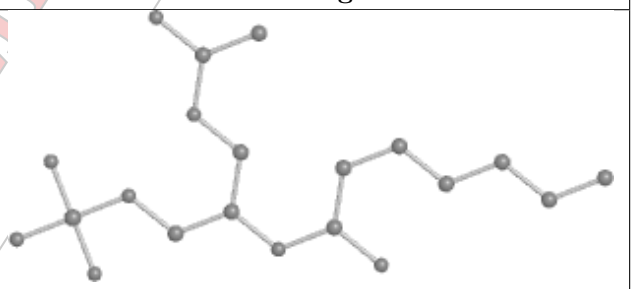

Torsions


Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

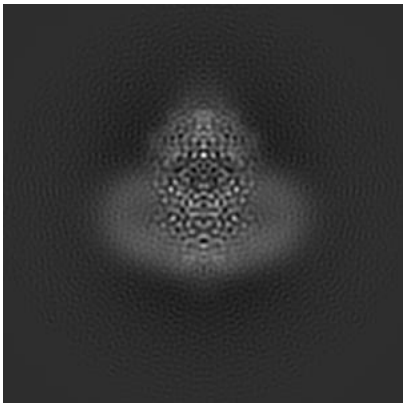
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24727. These allow visual inspection of the internal detail of the map and identification of artifacts.

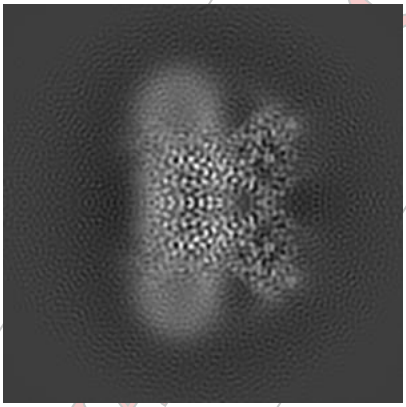
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

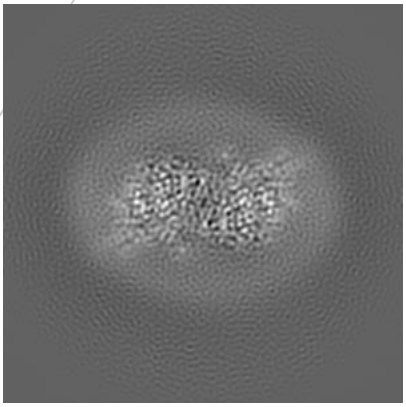
6.1.1 Primary map



X



Y

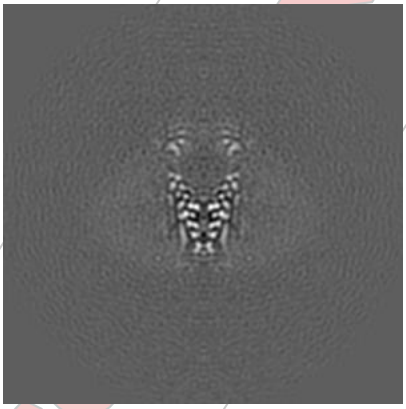


Z

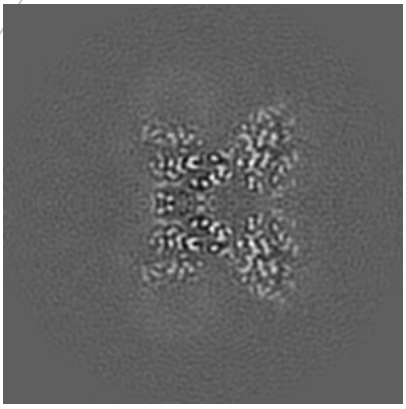
The images above show the map projected in three orthogonal directions.

6.2 Central slices

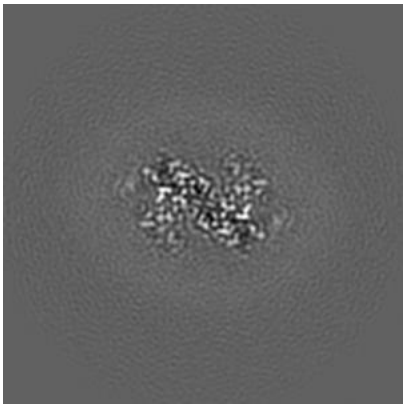
6.2.1 Primary map



X Index: 128



Y Index: 128

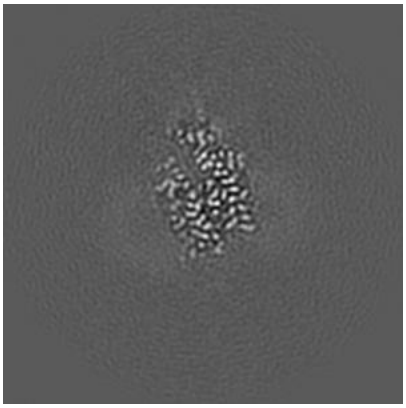


Z Index: 128

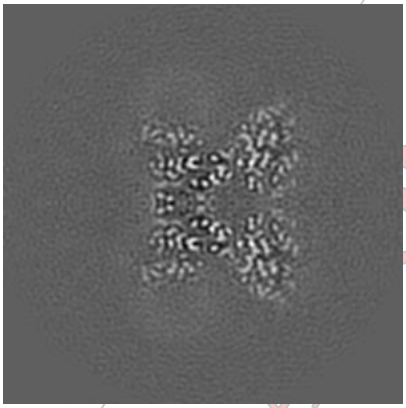
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

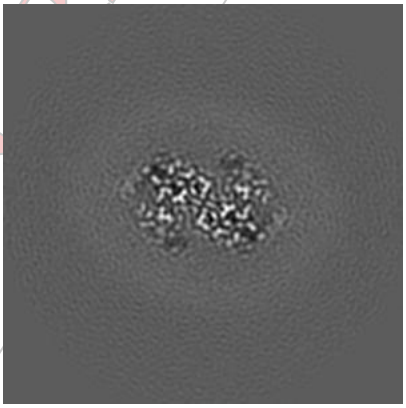
6.3.1 Primary map



X Index: 102



Y Index: 128

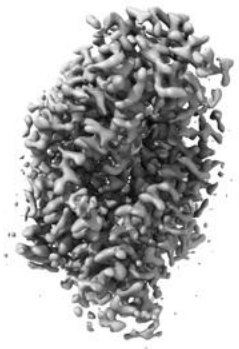


Z Index: 127

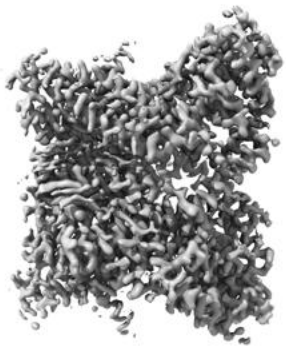
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

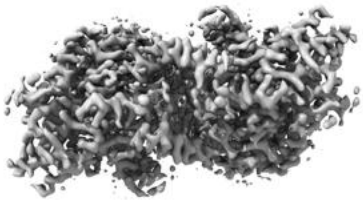
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

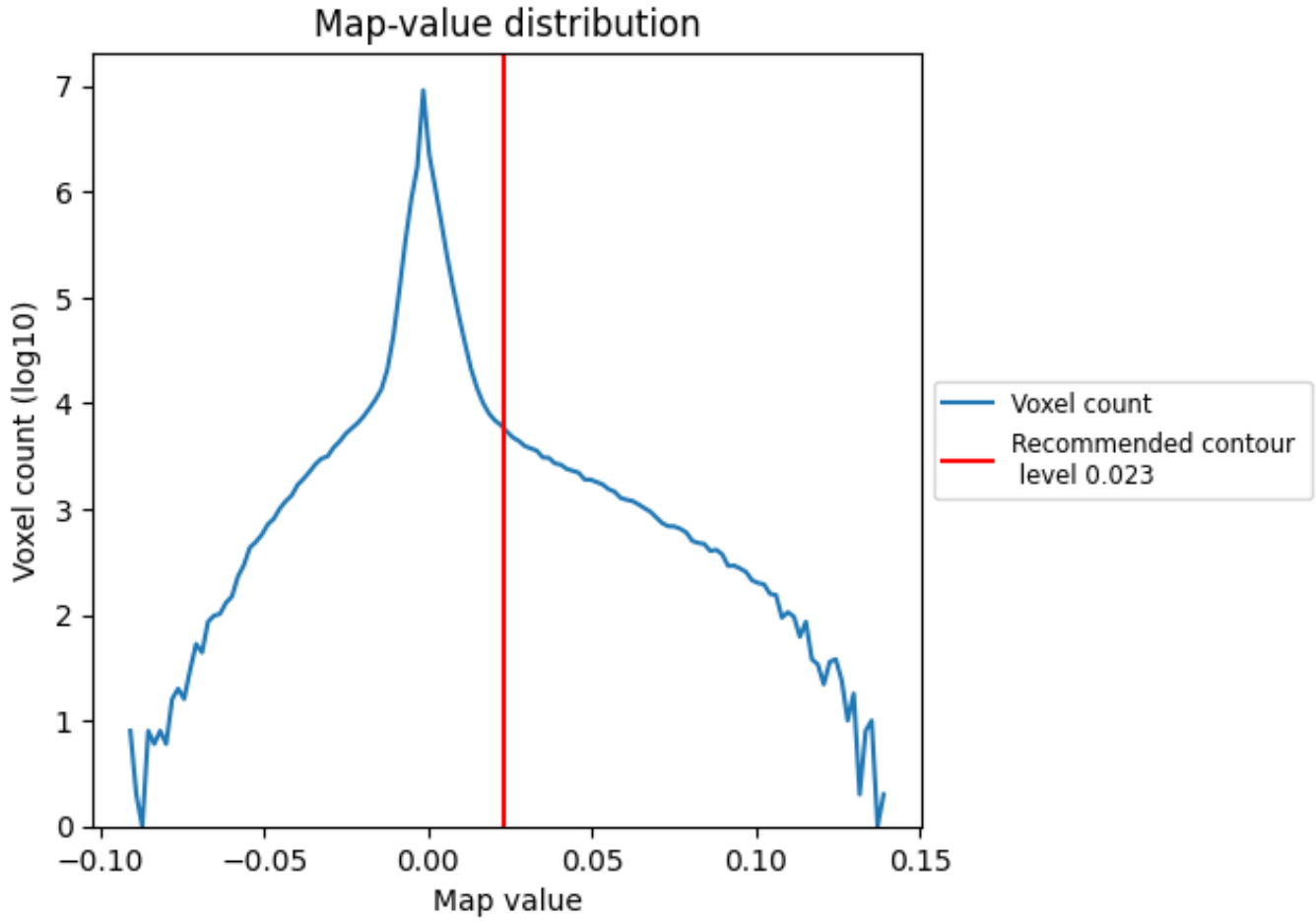
6.5 Mask visualisation (i)

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

7 Map analysis

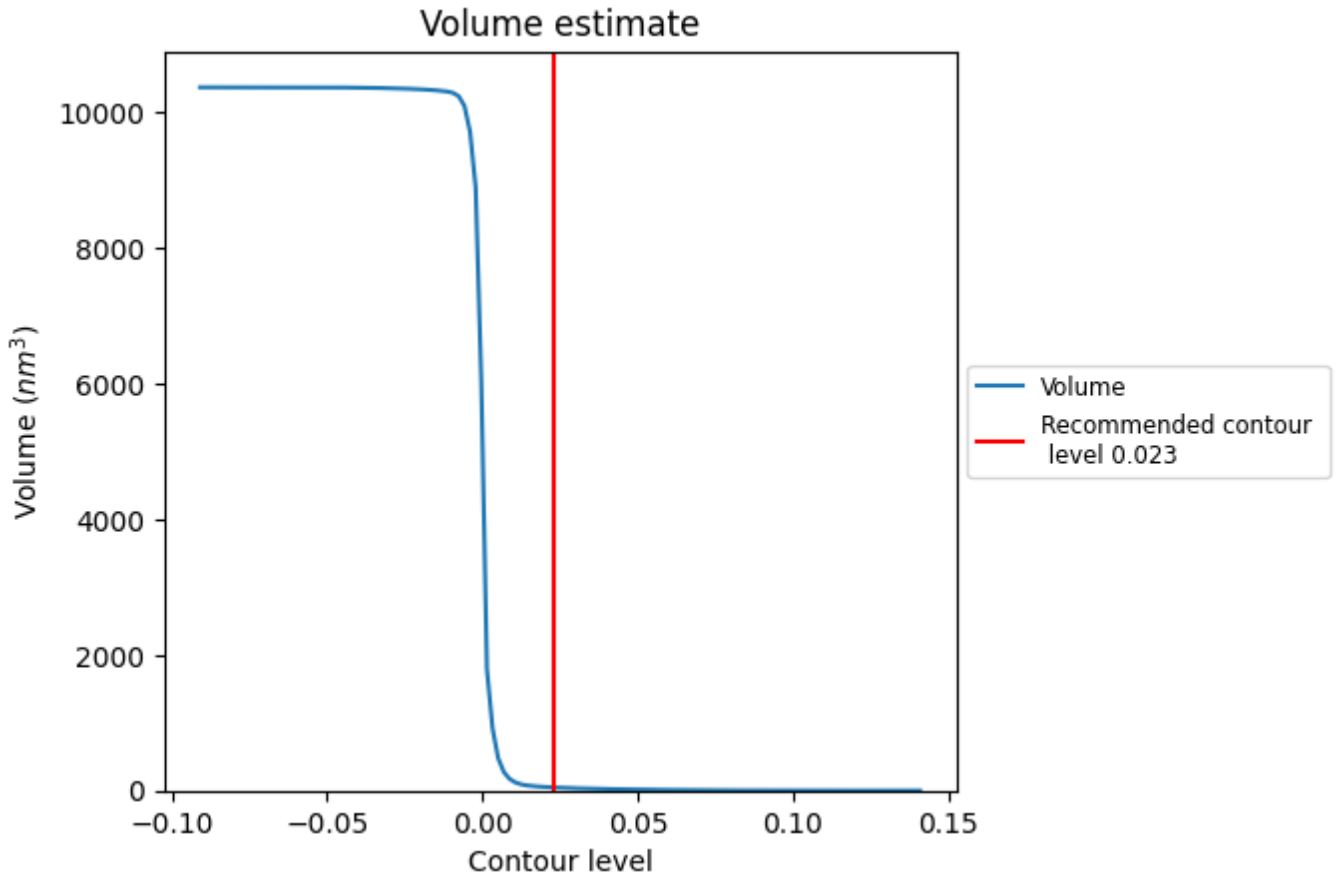
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

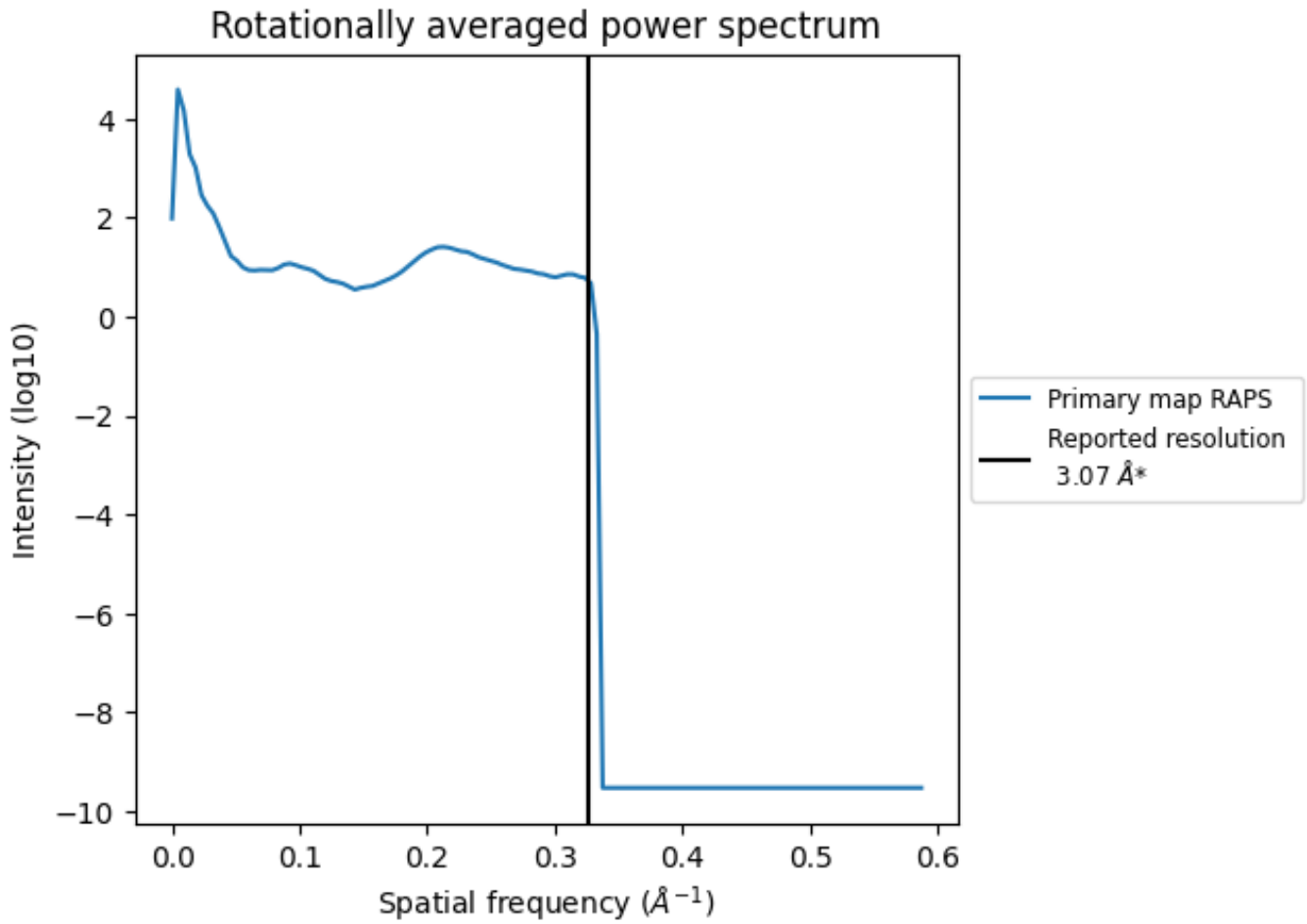
7.2 Volume estimate



The volume at the recommended contour level is 46 nm^3; this corresponds to an approximate mass of 42 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)

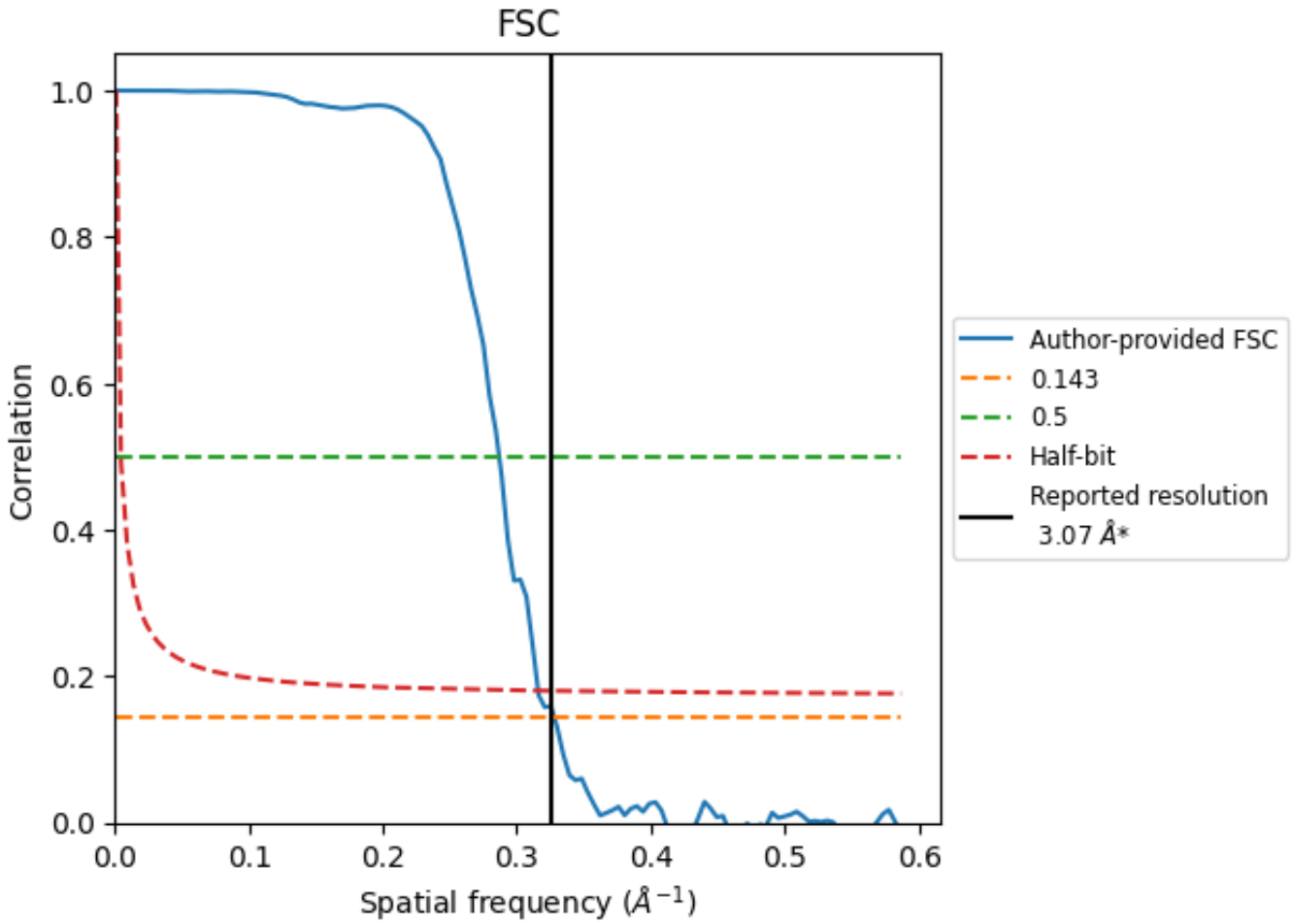


*Reported resolution corresponds to spatial frequency of 0.326 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.326 Å^{-1}

8.2 Resolution estimates (i)

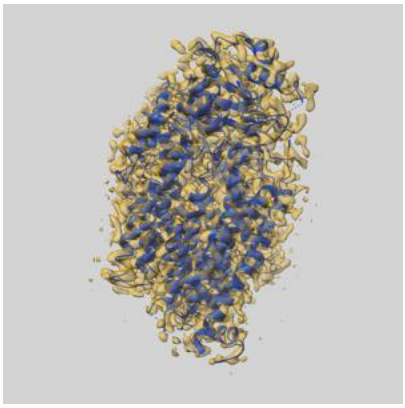
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.05	3.49	3.17
Unmasked-calculated*	-	-	-

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

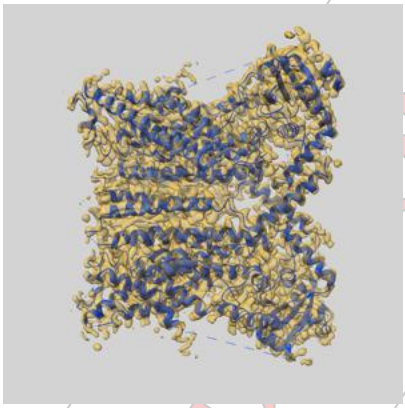
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24727 and PDB model 7RXB. Per-residue inclusion information can be found in section 3 on page 5.

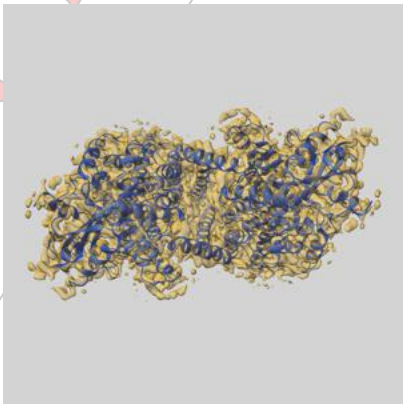
9.1 Map-model overlay



X



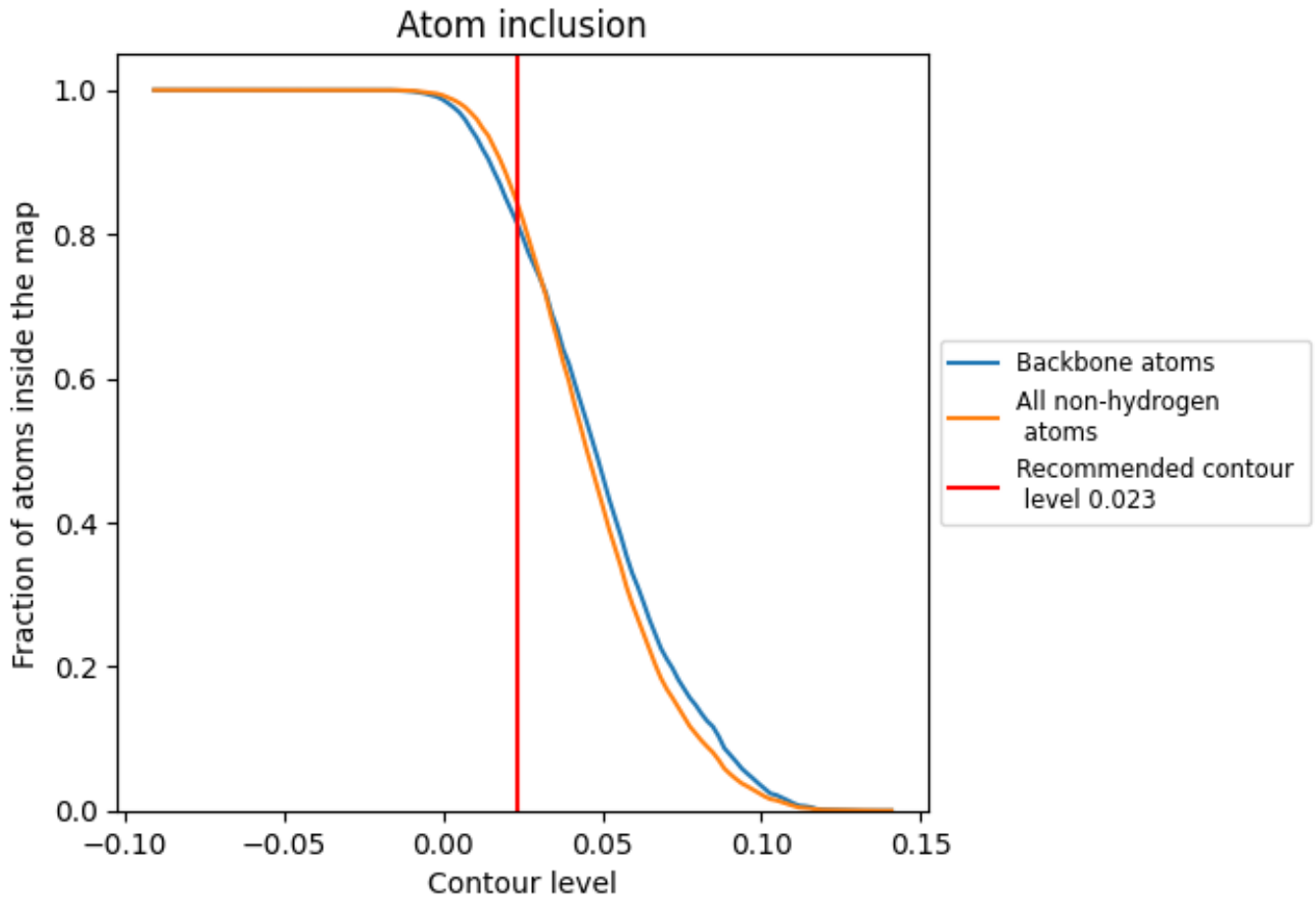
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 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 Atom inclusion



At the recommended contour level, 82% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.