Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 04:38 pm BST

PDB ID	:	9FAS / pdb_00009fas
EMDB ID	:	EMD-50280
Title	:	CryoEM structure of human full-length alpha1beta3gamma2L GABA(A)R in complex with pregnenolone sulfate
Authors	:	Kasaragod, V.B.; Aricescu, A.R.
Deposited on	:	2024-05-10
Resolution	:	2.50 Å(reported)
Based on initial model	:	6HUK

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

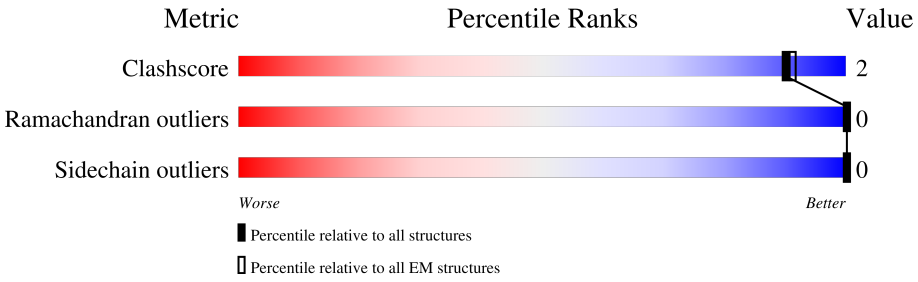
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	409	82% · 14%
1	D	409	85% · 14%
2	B	441	73% 5% 22%
2	E	441	74% · 22%
3	C	412	78% · 19%
4	F	10	10% 30% 70%
5	G	3	67% 100%
5	K	3	67% 67% 33%

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Mol	Chain	Length	Quality of chain
6	H	6	
6	J	6	
7	I	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	A8W	C	503	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 15501 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 Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	352	Total	C	N	O	S	1	0
			2857	1846	482	513	16		
1	D	353	Total	C	N	O	S	0	0
			2858	1847	481	514	16		

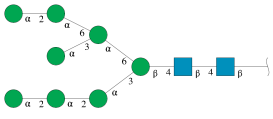
- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	344	Total	C	N	O	S	1	0
			2834	1855	464	499	16		
2	E	345	Total	C	N	O	S	0	0
			2829	1849	465	499	16		

- Molecule 3 is a protein called Isoform 1 of Gamma-aminobutyric acid receptor subunit gamma-2.

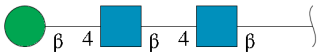
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	332	Total	C	N	O	S	2	0
			2750	1797	454	484	15		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



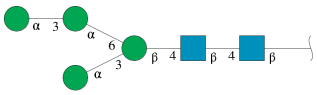
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



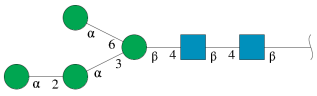
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



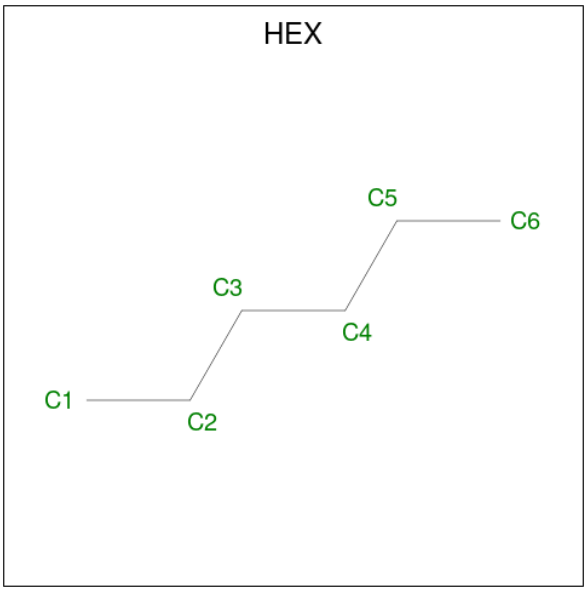
Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	6	Total	C	N	O	0	0
			72	40	2	30		
6	J	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



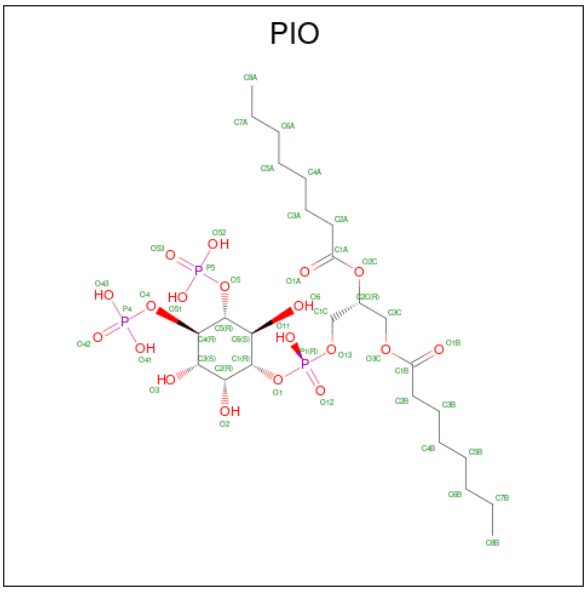
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 8 is HEXANE (CCD ID: HEX) (formula: C_6H_{14}).



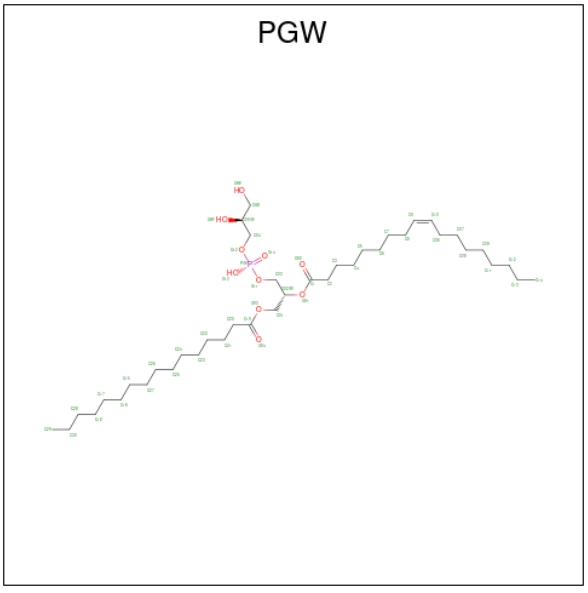
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C 6 6	0
8	B	1	Total C 6 6	0
8	B	1	Total C 6 6	0
8	C	1	Total C 6 6	0
8	D	1	Total C 6 6	0
8	D	1	Total C 6 6	0
8	E	1	Total C 6 6	0
8	E	1	Total C 6 6	0

- Molecule 9 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: $C_{25}H_{49}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			47	25	19	3	
9	D	1	Total	C	O	P	0
			47	25	19	3	

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



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

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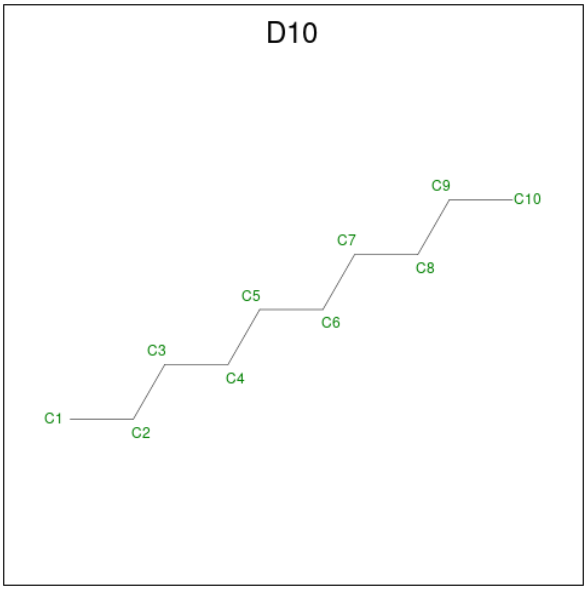
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O P 32 21 10 1	0
10	D	1	Total C O P 51 40 10 1	0

- Molecule 11 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C 10 10	0
11	A	1	Total C 10 10	0
11	A	1	Total C 10 10	0
11	A	1	Total C 10 10	0
11	B	1	Total C 10 10	0
11	B	1	Total C 10 10	0
11	B	1	Total C 10 10	0
11	B	1	Total C 10 10	0
11	C	1	Total C 10 10	0

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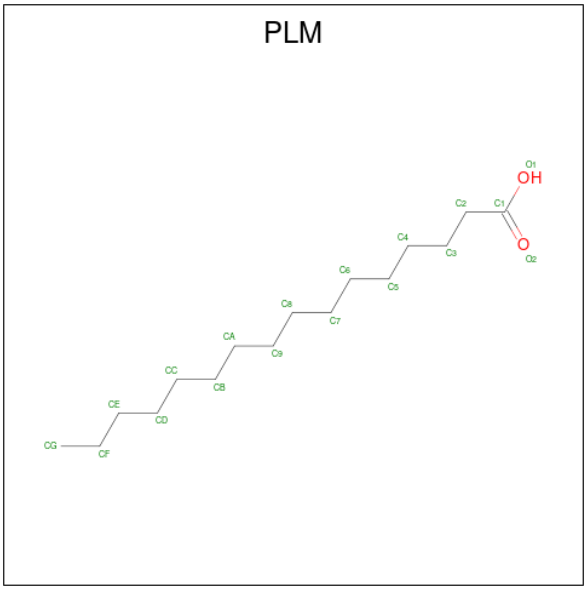
Mol	Chain	Residues	Atoms	AltConf
11	C	1	Total C 10 10	0
11	D	1	Total C 10 10	0
11	D	1	Total C 10 10	0
11	D	1	Total C 10 10	0
11	D	1	Total C 10 10	0
11	D	1	Total C 10 10	0
11	E	1	Total C 10 10	0
11	E	1	Total C 10 10	0

- Molecule 12 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).

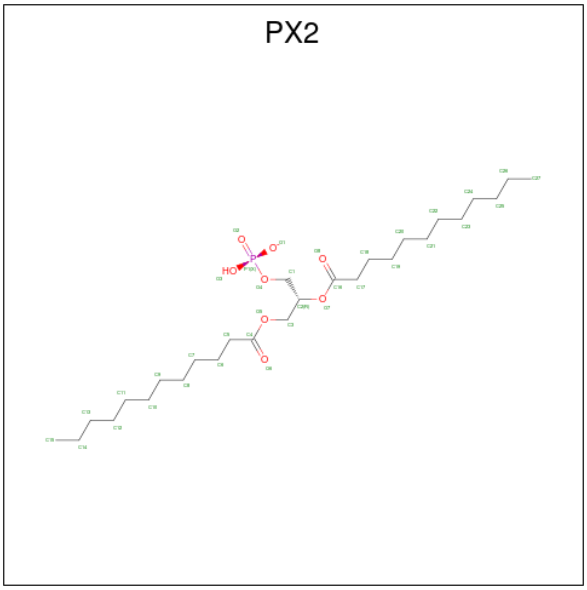


Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C O 18 16 2	0
12	C	1	Total C O 18 16 2	0
12	C	1	Total C O 18 16 2	0

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

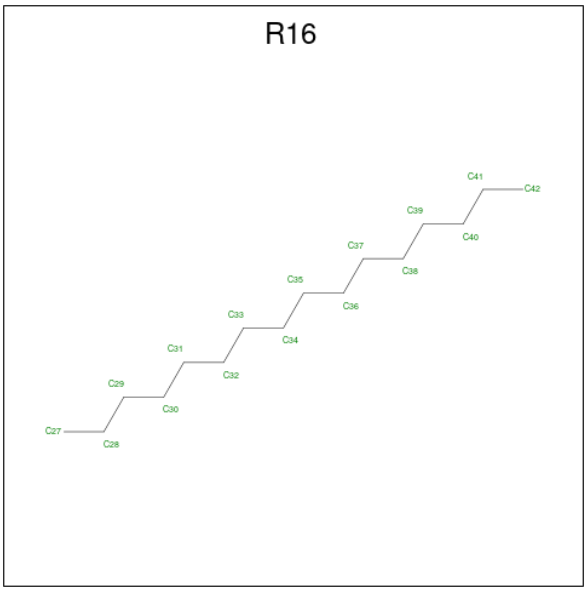
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Cl 1 1	0
13	C	1	Total Cl 1 1	0
13	D	1	Total Cl 1 1	0

- Molecule 14 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



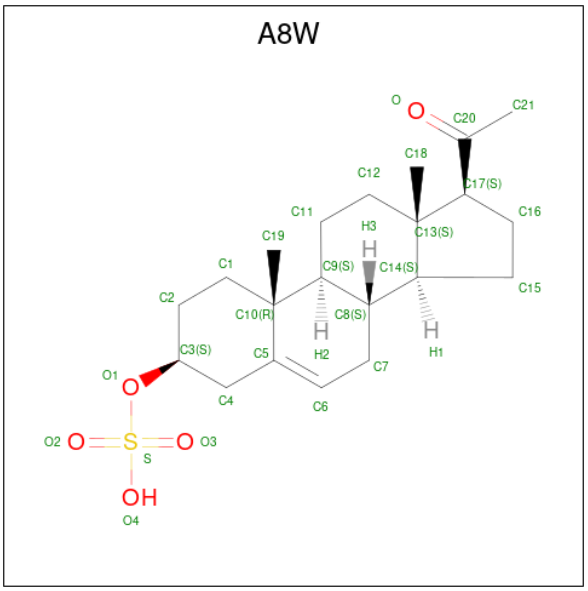
Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total C O P 36 27 8 1	0

- Molecule 15 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



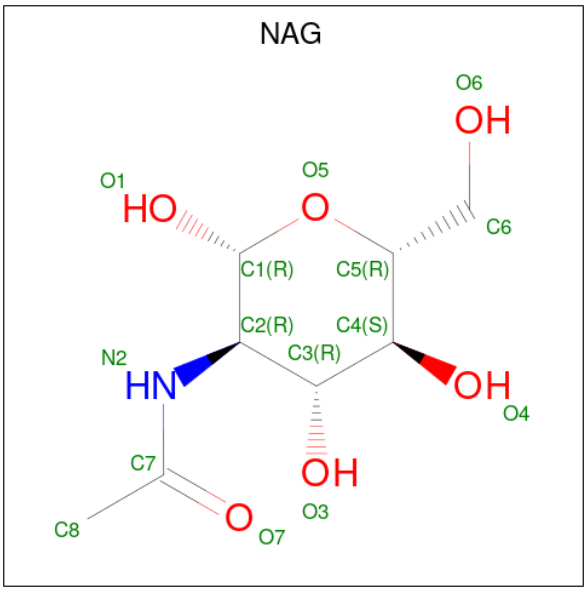
Mol	Chain	Residues	Atoms	AltConf
15	B	1	Total C 16 16	0
15	B	1	Total C 16 16	0
15	D	1	Total C 16 16	0
15	E	1	Total C 16 16	0
15	E	1	Total C 16 16	0

- Molecule 16 is Pregnenolone sulfate (CCD ID: A8W) (formula: $C_{21}H_{32}O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
16	C	1	27	21	5	1	0

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	C	1	14	8	1	5	0

- Molecule 18 is water.

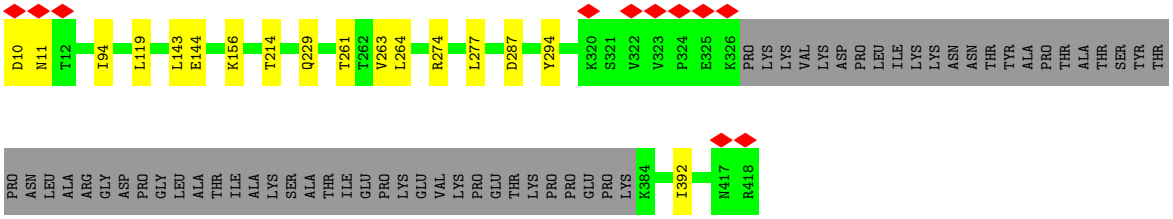
Mol	Chain	Residues	Atoms	AltConf
18	A	60	Total O 60 60	0
18	B	74	Total O 74 74	0
18	C	56	Total O 56 56	0
18	D	50	Total O 50 50	0
18	E	63	Total O 63 63	0

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.

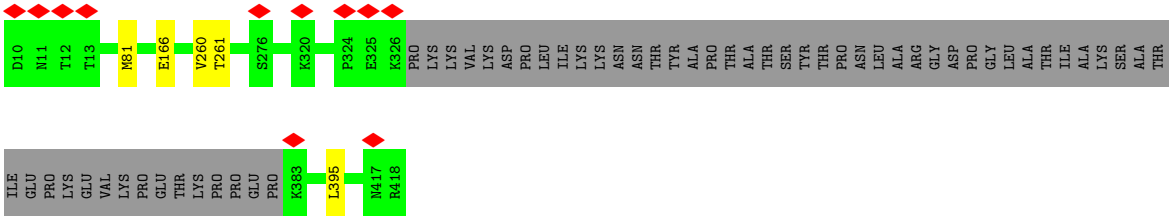
• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain A:



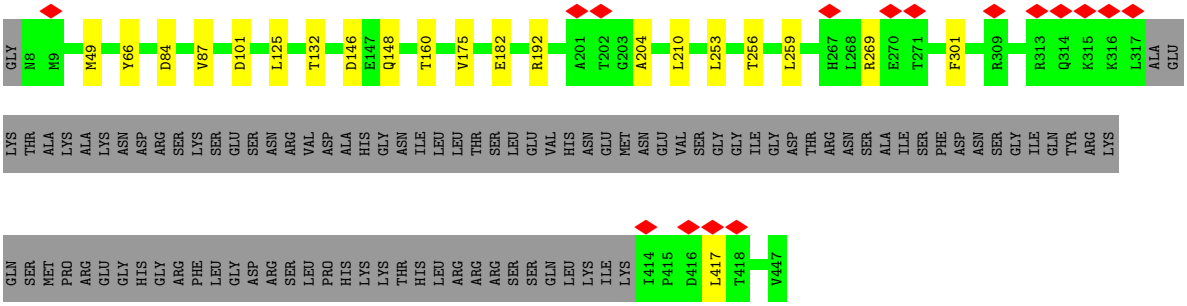
• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain D:



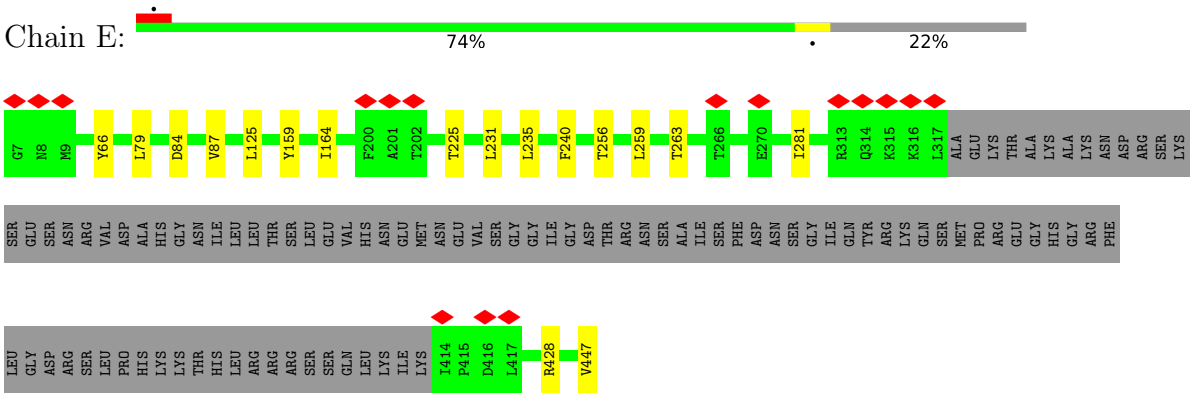
• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain B:



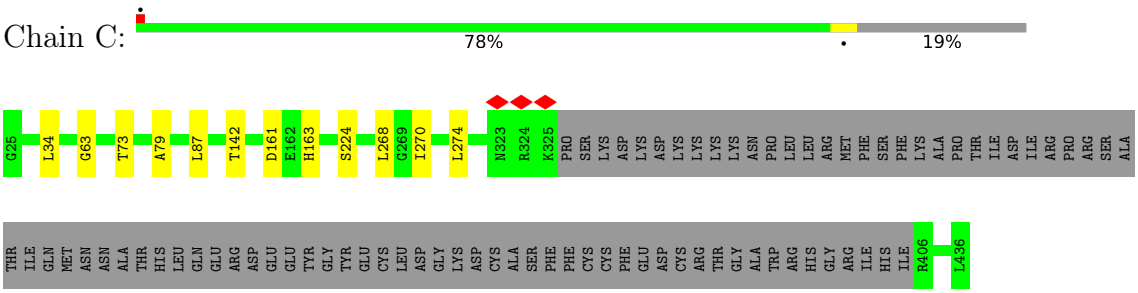
• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain E:



• Molecule 3: Isoform 1 of Gamma-aminobutyric acid receptor subunit gamma-2

Chain C:

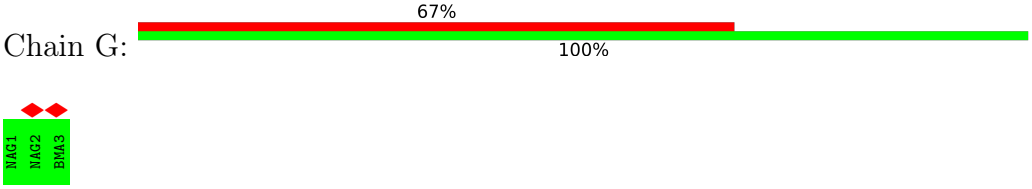


• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

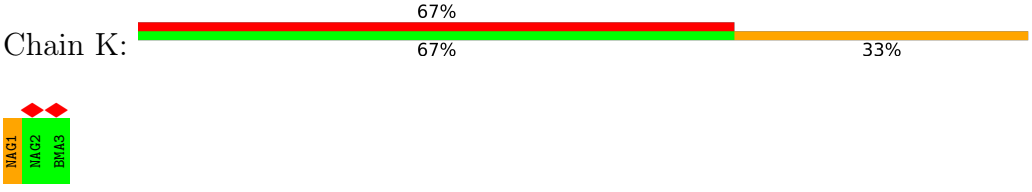
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



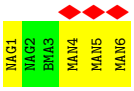
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



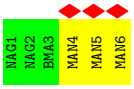
• Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



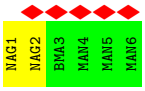
• Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86252	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.086	Depositor
Minimum map value	-0.991	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	360.912, 360.912, 360.912	wwPDB
Map dimensions	438, 438, 438	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82399994, 0.82399994, 0.82399994	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D10, PLM, MAN, R16, PGW, NAG, PIO, HEX, PX2, CL, A8W, BMA

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	0.15	0/2932	0.33	0/3980
1	D	0.14	0/2930	0.32	0/3977
2	B	0.14	0/2912	0.33	0/3959
2	E	0.14	0/2903	0.33	0/3946
3	C	0.15	0/2831	0.32	0/3850
All	All	0.14	0/14508	0.33	0/19712

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	2857	0	2851	14	0
1	D	2858	0	2851	6	0
2	B	2834	0	2837	16	0
2	E	2829	0	2830	14	0
3	C	2750	0	2748	10	0
4	F	116	0	97	0	0
5	G	39	0	34	0	0
5	K	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	72	0	61	1	0
6	J	72	0	61	0	0
7	I	72	0	61	0	0
8	A	6	0	14	0	0
8	B	12	0	28	0	0
8	C	6	0	14	0	0
8	D	12	0	28	0	0
8	E	12	0	28	0	0
9	A	47	0	44	2	0
9	D	47	0	44	1	0
10	A	83	0	110	0	0
10	D	51	0	76	1	0
11	A	40	0	88	0	0
11	B	40	0	88	0	0
11	C	20	0	44	0	0
11	D	50	0	110	0	0
11	E	20	0	44	0	0
12	A	18	0	31	0	0
12	C	36	0	62	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
14	B	36	0	52	0	0
15	B	32	0	68	0	0
15	D	16	0	34	0	0
15	E	32	0	68	0	0
16	C	27	0	0	0	0
17	C	14	0	13	0	0
18	A	60	0	0	0	0
18	B	74	0	0	0	0
18	C	56	0	0	1	0
18	D	50	0	0	1	0
18	E	63	0	0	0	0
All	All	15501	0	15553	49	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 2.

All (49) 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:264:LEU:HD11	2:E:256:THR:HG23	1.71	0.72
2:B:256:THR:HG23	3:C:274:LEU:HD11	1.72	0.70
1:A:274:ARG:NH2	1:A:287:ASP:OD2	2.25	0.69
2:E:225:THR:HG21	2:E:281:ILE:HD11	1.74	0.68
1:A:94:ILE:HD11	1:A:119:LEU:HD21	1.75	0.68
1:A:294:TYR:CE1	2:E:231:LEU:HD13	2.29	0.68
1:D:166:GLU:OE1	18:D:4001:HOH:O	2.13	0.66
2:B:101:ASP:OD1	2:B:132:THR:OG1	2.15	0.64
1:A:392:ILE:HD11	9:A:3702:PIO:H2AA	1.80	0.63
2:B:146:ASP:OD2	2:B:148:GLN:NE2	2.36	0.57
3:C:224:SER:OG	18:C:601:HOH:O	2.18	0.57
1:A:263:VAL:HG11	2:E:235:LEU:HD22	1.87	0.56
2:B:256:THR:CG2	3:C:274:LEU:HD11	2.34	0.56
2:E:447:VAL:HG12	2:E:447:VAL:OXT	2.08	0.54
2:B:182:GLU:N	2:B:182:GLU:OE1	2.42	0.53
10:D:3903:PGW:O12	10:D:3903:PGW:OAE	2.17	0.53
2:E:240:PHE:O	2:E:428:ARG:NH1	2.42	0.52
2:B:160:THR:OG1	2:B:204:ALA:O	2.23	0.52
2:E:66:TYR:CZ	2:E:125:LEU:HD13	2.44	0.52
1:A:294:TYR:HE1	2:E:231:LEU:HD13	1.73	0.51
2:E:225:THR:CG2	2:E:281:ILE:HD11	2.39	0.51
3:C:268:LEU:HD23	1:D:260:VAL:CG1	2.41	0.50
2:E:79:LEU:HA	5:K:1:NAG:H82	1.95	0.49
3:C:34:LEU:HD22	3:C:87:LEU:HA	1.95	0.49
3:C:79:ALA:CB	3:C:142:THR:HG22	2.42	0.49
2:B:301:PHE:HZ	2:B:417:LEU:HD12	1.78	0.48
1:D:395:LEU:HD23	9:D:3901:PIO:H7A	1.95	0.48
2:B:49:MET:SD	2:B:49:MET:N	2.87	0.47
1:A:144:GLU:N	1:A:144:GLU:OE1	2.46	0.47
2:E:259:LEU:O	2:E:263:THR:HG23	2.14	0.47
2:B:66[A]:TYR:CZ	2:B:125:LEU:HD13	2.51	0.46
1:A:156:LYS:HG2	1:A:214:THR:HG22	1.98	0.46
1:D:261:THR:HB	2:E:259:LEU:HD11	1.97	0.46
1:A:261:THR:HB	2:B:259:LEU:HD11	1.97	0.45
1:D:81:MET:SD	1:D:81:MET:N	2.90	0.44
2:E:84:ASP:O	2:E:87:VAL:HG12	2.18	0.44
2:E:159:TYR:CD2	2:E:164:ILE:HD12	2.53	0.44
2:B:253:LEU:HD23	3:C:270:ILE:HG21	2.00	0.44
1:A:392:ILE:HD11	9:A:3702:PIO:H2C	2.00	0.43
3:C:161:ASP:OD2	3:C:163:HIS:NE2	2.50	0.43
1:A:143:LEU:HD13	1:A:277:LEU:HD11	2.00	0.43
3:C:63:GLY:N	3:C:73:THR:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:ARG:NH1	6:H:1:NAG:O3	2.53	0.42
3:C:268:LEU:HD23	1:D:260:VAL:HG11	2.01	0.41
2:B:175:VAL:HG21	2:B:210:LEU:HD13	2.02	0.41
2:B:301:PHE:CZ	2:B:417:LEU:HD12	2.54	0.41
1:A:229:GLN:OE1	2:B:269:ARG:NE	2.54	0.41
2:B:84:ASP:O	2:B:87:VAL:HG12	2.20	0.40
1:A:10:ASP:OD1	1:A:11:ASN:N	2.53	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	349/409 (85%)	344 (99%)	5 (1%)	0	100	100
1	D	349/409 (85%)	341 (98%)	8 (2%)	0	100	100
2	B	341/441 (77%)	333 (98%)	8 (2%)	0	100	100
2	E	341/441 (77%)	334 (98%)	7 (2%)	0	100	100
3	C	330/412 (80%)	323 (98%)	7 (2%)	0	100	100
All	All	1710/2112 (81%)	1675 (98%)	35 (2%)	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	315/363 (87%)	315 (100%)	0	100	100
1	D	315/363 (87%)	315 (100%)	0	100	100
2	B	311/393 (79%)	311 (100%)	0	100	100
2	E	310/393 (79%)	310 (100%)	0	100	100
3	C	308/377 (82%)	308 (100%)	0	100	100
All	All	1559/1889 (82%)	1559 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	64	GLN
2	B	185	GLN
2	B	265	ASN
3	C	54	HIS
3	C	80	GLN
3	C	154	GLN
3	C	318	HIS
1	D	151	HIS
2	E	65	GLN
2	E	185	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)

34 monosaccharides 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	$\#\|Z\| > 2$
4	NAG	F	1	4,1	14,14,15	0.24	0	17,19,21	0.39	0
4	MAN	F	10	4	11,11,12	0.68	0	15,15,17	1.07	2 (13%)
4	NAG	F	2	4	14,14,15	0.18	0	17,19,21	0.51	0
4	BMA	F	3	4	11,11,12	0.60	0	15,15,17	0.73	0
4	MAN	F	4	4	11,11,12	0.71	0	15,15,17	1.02	2 (13%)
4	MAN	F	5	4	11,11,12	0.69	0	15,15,17	1.11	2 (13%)
4	MAN	F	6	4	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
4	MAN	F	7	4	11,11,12	0.72	1 (9%)	15,15,17	1.03	2 (13%)
4	MAN	F	8	4	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
4	MAN	F	9	4	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
5	NAG	G	1	5	14,14,15	0.40	0	17,19,21	0.64	0
5	NAG	G	2	5	14,14,15	0.39	0	17,19,21	0.50	0
5	BMA	G	3	5	11,11,12	0.31	0	15,15,17	0.62	0
6	NAG	H	1	6,2	14,14,15	0.25	0	17,19,21	0.40	0
6	NAG	H	2	6	14,14,15	0.20	0	17,19,21	0.45	0
6	BMA	H	3	6	11,11,12	0.56	0	15,15,17	0.80	0
6	MAN	H	4	6	11,11,12	0.69	0	15,15,17	1.06	2 (13%)
6	MAN	H	5	6	11,11,12	1.01	1 (9%)	15,15,17	1.26	2 (13%)
6	MAN	H	6	6	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
7	NAG	I	1	7,1	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
7	NAG	I	2	7	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
7	BMA	I	3	7	11,11,12	0.26	0	15,15,17	0.39	0
7	MAN	I	4	7	11,11,12	0.43	0	15,15,17	0.63	0
7	MAN	I	5	7	11,11,12	0.33	0	15,15,17	0.54	0
7	MAN	I	6	7	11,11,12	0.20	0	15,15,17	0.59	0
6	NAG	J	1	6,2	14,14,15	0.24	0	17,19,21	0.38	0
6	NAG	J	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	BMA	J	3	6	11,11,12	0.57	0	15,15,17	0.77	0
6	MAN	J	4	6	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
6	MAN	J	5	6	11,11,12	0.70	0	15,15,17	1.28	3 (20%)
6	MAN	J	6	6	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
5	NAG	K	1	2,5	14,14,15	0.43	0	17,19,21	1.10	1 (5%)
5	NAG	K	2	5	14,14,15	0.40	0	17,19,21	0.48	0
5	BMA	K	3	5	11,11,12	0.31	0	15,15,17	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	MAN	F	10	4	-	2/2/19/22	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	1/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
4	MAN	F	8	4	-	0/2/19/22	0/1/1/1
4	MAN	F	9	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
6	NAG	H	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	0/2/19/22	0/1/1/1
6	MAN	H	6	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	1/2/19/22	0/1/1/1
6	NAG	J	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	1/2/19/22	0/1/1/1
5	NAG	K	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	5	MAN	O5-C1	-2.48	1.39	1.43
4	F	7	MAN	O5-C1	-2.07	1.40	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	5	MAN	C1-O5-C5	3.12	116.42	112.19
6	J	5	MAN	C1-O5-C5	3.05	116.32	112.19
5	K	1	NAG	C1-C2-N2	3.03	115.66	110.49
4	F	8	MAN	C1-O5-C5	2.50	115.57	112.19
7	I	2	NAG	C2-N2-C7	2.46	126.41	122.90
4	F	10	MAN	O2-C2-C3	-2.36	105.41	110.14
4	F	7	MAN	O2-C2-C3	-2.34	105.45	110.14
6	J	5	MAN	O2-C2-C3	-2.32	105.49	110.14
4	F	6	MAN	O2-C2-C3	-2.31	105.50	110.14
6	H	6	MAN	O2-C2-C3	-2.31	105.51	110.14
6	H	6	MAN	C1-O5-C5	2.30	115.31	112.19
4	F	9	MAN	O2-C2-C3	-2.28	105.57	110.14
4	F	5	MAN	C1-O5-C5	2.28	115.28	112.19
6	H	4	MAN	O2-C2-C3	-2.28	105.58	110.14
6	H	5	MAN	O2-C2-C3	-2.28	105.58	110.14
6	J	5	MAN	O5-C1-C2	2.26	114.25	110.77
4	F	8	MAN	O2-C2-C3	-2.25	105.62	110.14
6	J	4	MAN	O2-C2-C3	-2.25	105.63	110.14
4	F	10	MAN	C1-O5-C5	2.22	115.20	112.19
6	J	6	MAN	O2-C2-C3	-2.21	105.70	110.14
6	H	4	MAN	C1-O5-C5	2.21	115.19	112.19
4	F	4	MAN	O2-C2-C3	-2.21	105.71	110.14
4	F	6	MAN	C1-O5-C5	2.20	115.17	112.19
6	J	4	MAN	C1-O5-C5	2.20	115.17	112.19
4	F	5	MAN	O2-C2-C3	-2.18	105.78	110.14
4	F	4	MAN	C1-O5-C5	2.17	115.13	112.19
6	J	6	MAN	C1-O5-C5	2.15	115.11	112.19
7	I	1	NAG	C1-C2-N2	2.14	114.14	110.49
4	F	9	MAN	C1-O5-C5	2.09	115.03	112.19
4	F	7	MAN	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	G	1	NAG	O7-C7-N2-C2
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
6	H	1	NAG	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
7	I	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
6	J	6	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7
7	I	1	NAG	C4-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7
4	F	10	MAN	C4-C5-C6-O6
4	F	10	MAN	O5-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7

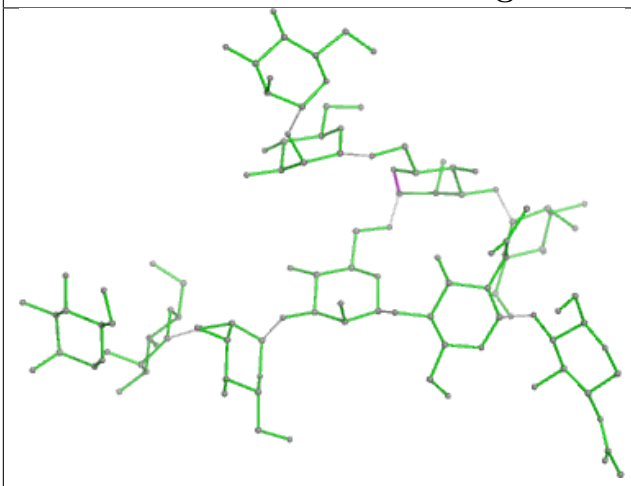
There are no ring outliers.

2 monomers are involved in 2 short contacts:

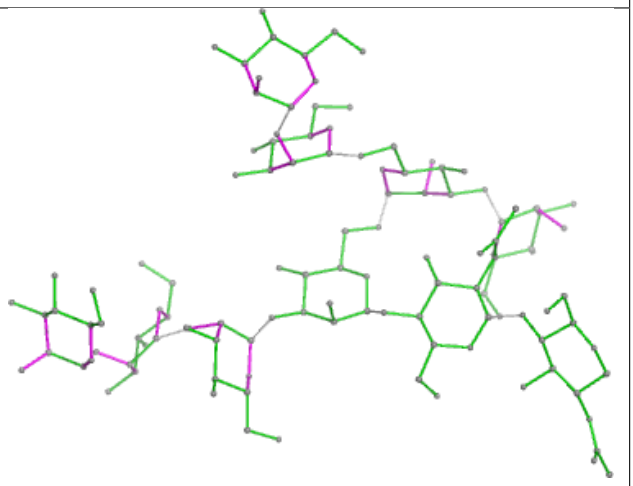
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1	NAG	1	0
5	K	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

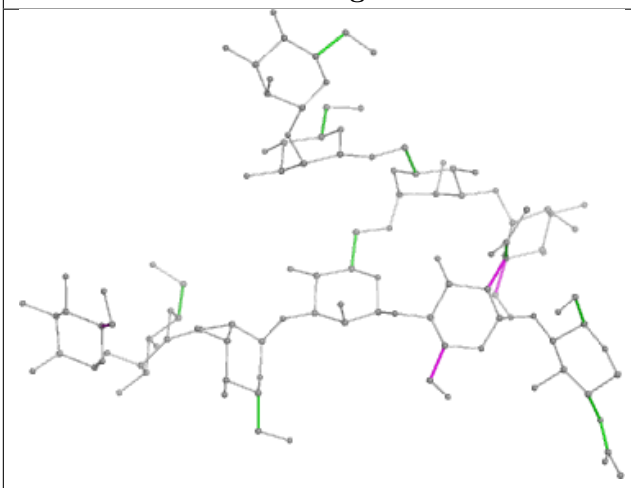
Oligosaccharide Chain F



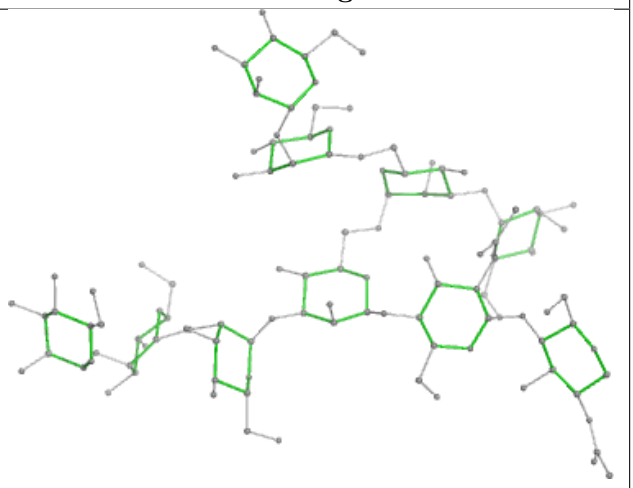
Bond lengths



Bond angles

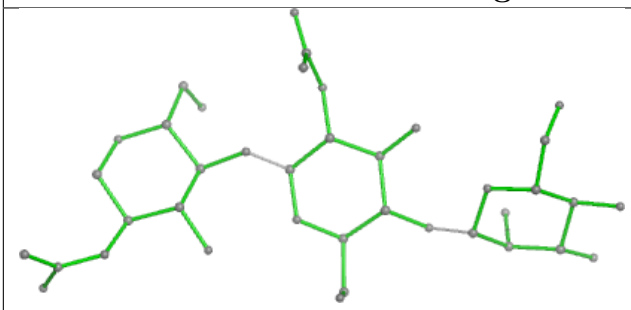


Torsions

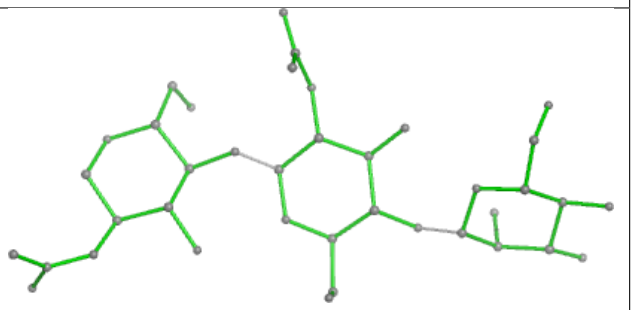


Rings

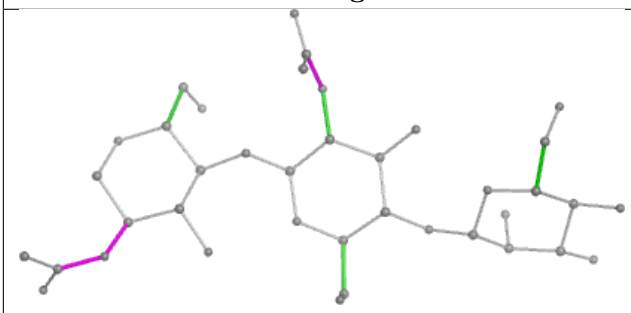
Oligosaccharide Chain G



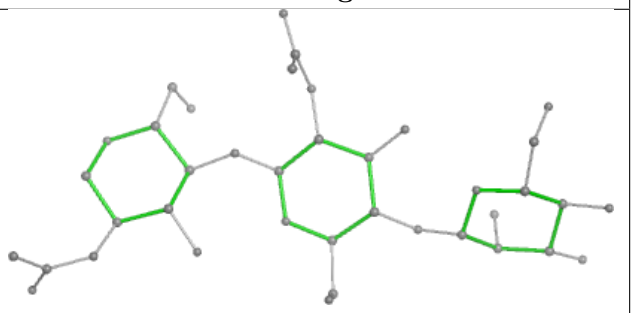
Bond lengths



Bond angles

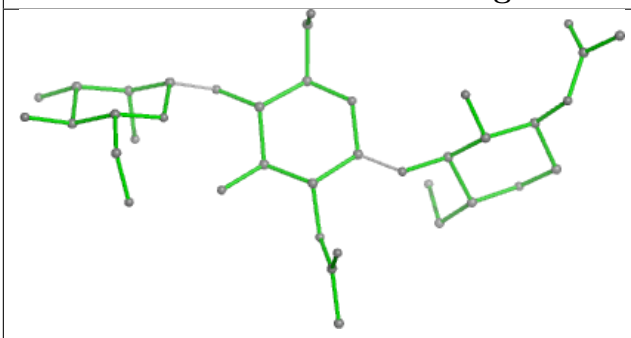


Torsions

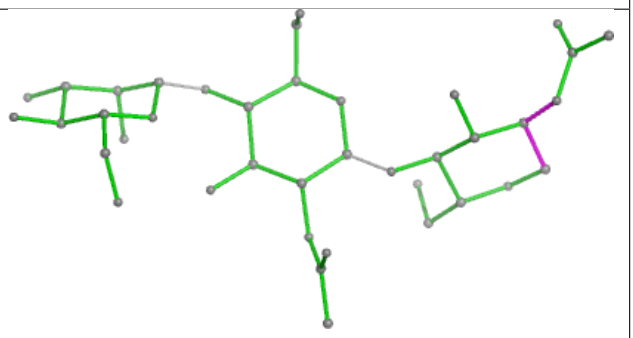


Rings

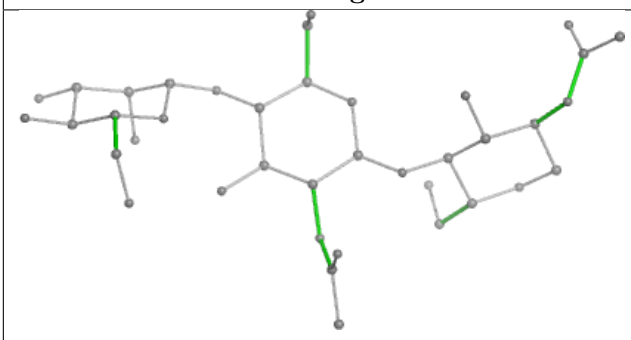
Oligosaccharide Chain K



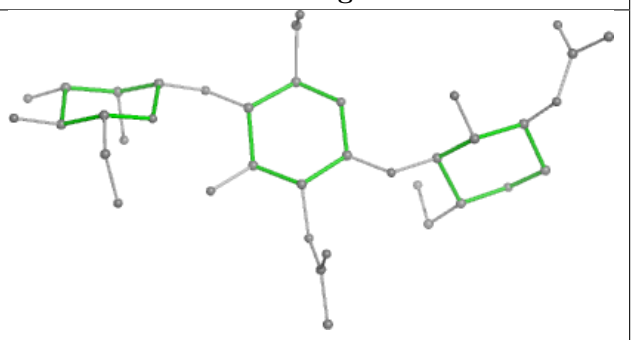
Bond lengths



Bond angles

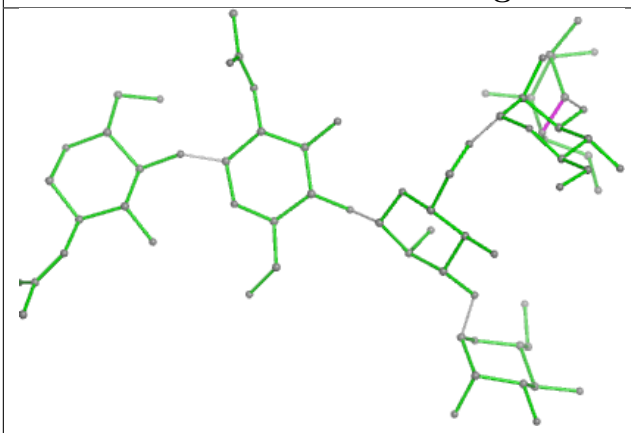


Torsions

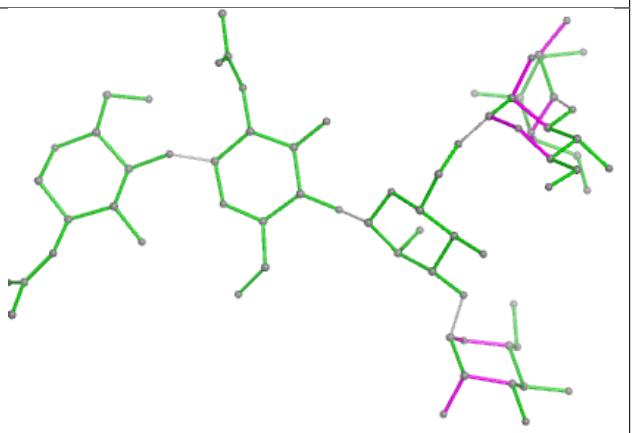


Rings

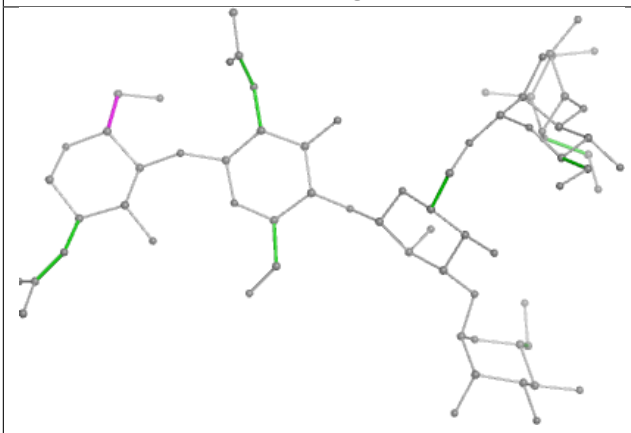
Oligosaccharide Chain H



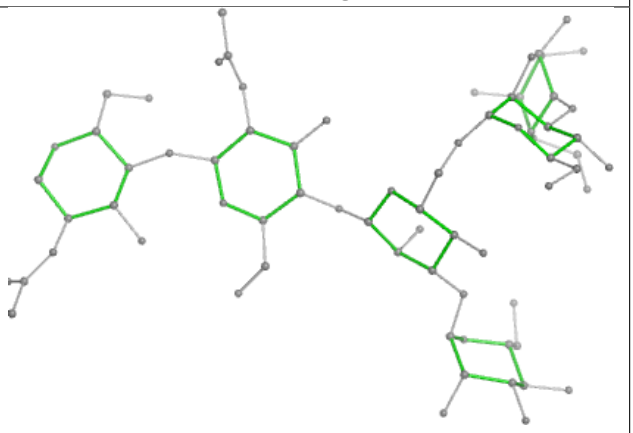
Bond lengths



Bond angles

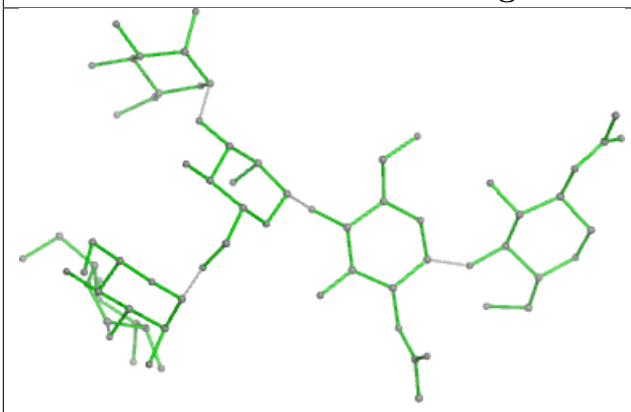


Torsions

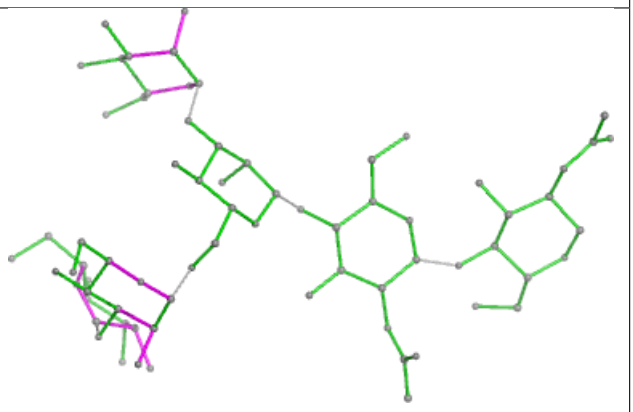


Rings

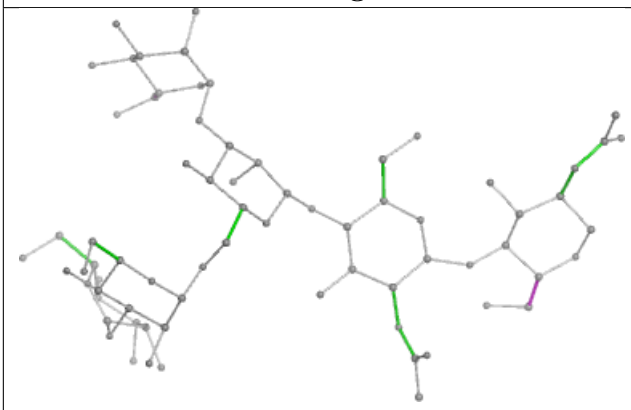
Oligosaccharide Chain J



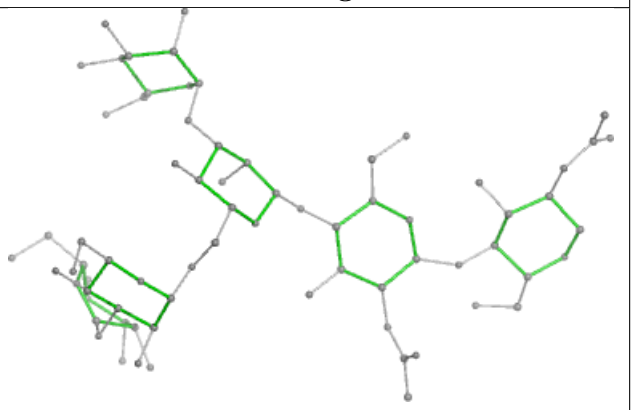
Bond lengths



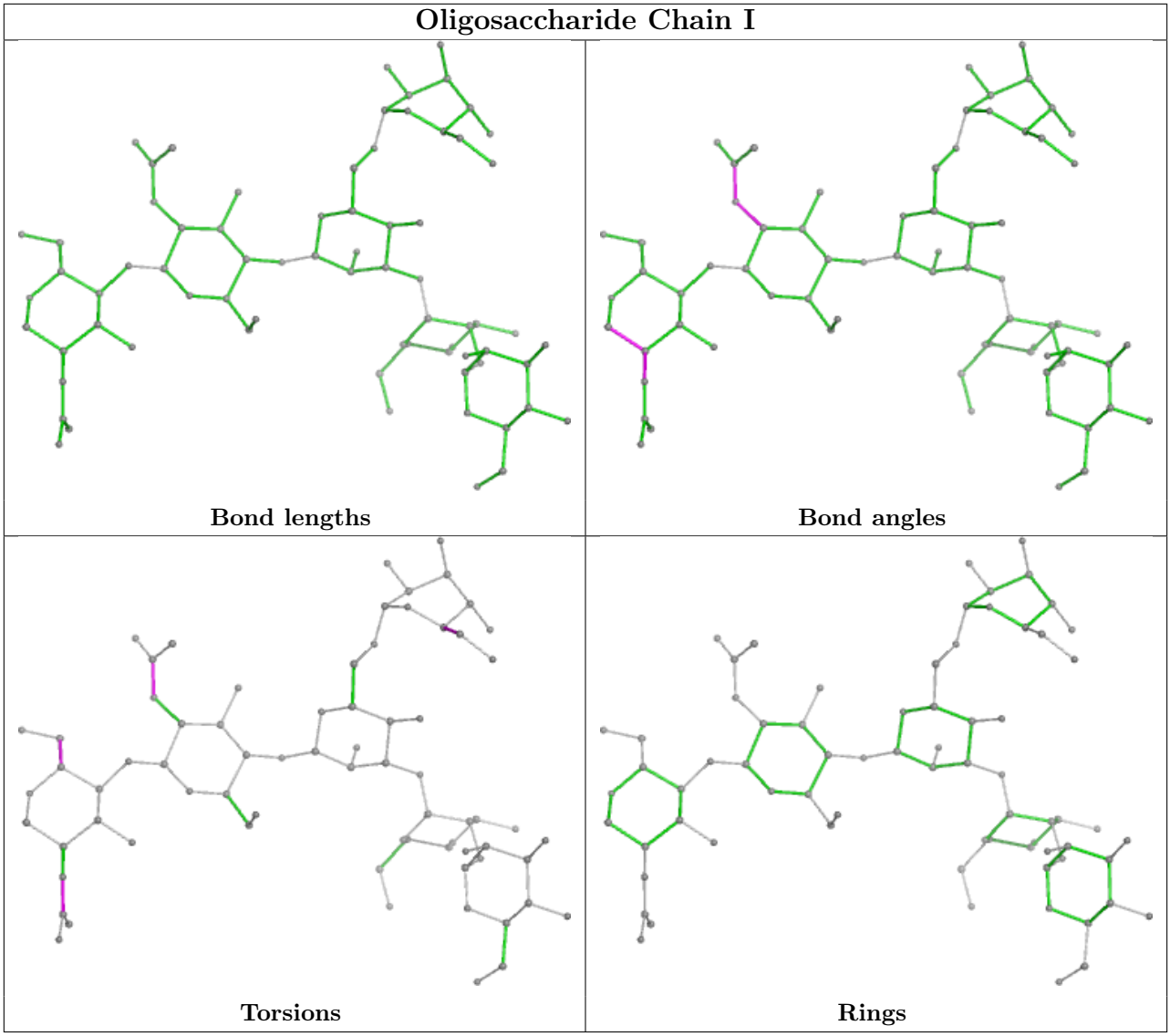
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 3 are monoatomic - leaving 41 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	$\#\|Z\| > 2$
12	PLM	A	3708	-	17,17,17	0.58	0	17,17,17	1.05	1 (5%)
11	D10	C	506	-	9,9,9	0.32	0	8,8,8	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	HEX	C	505	-	5,5,5	0.30	0	4,4,4	0.57	0
12	PLM	C	501	-	17,17,17	0.59	0	17,17,17	1.00	0
16	A8W	C	503	-	30,30,30	0.37	0	45,49,49	0.97	4 (8%)
8	HEX	E	3206	-	5,5,5	0.31	0	4,4,4	0.55	0
15	R16	D	3908	-	15,15,15	0.30	0	14,14,14	0.74	0
15	R16	B	505	-	15,15,15	0.32	0	14,14,14	0.67	0
11	D10	D	3909	-	9,9,9	0.35	0	8,8,8	0.62	0
15	R16	E	3201	-	15,15,15	0.29	0	14,14,14	0.83	0
9	PIO	D	3901	-	47,47,47	0.50	0	61,65,65	0.51	0
10	PGW	D	3903	-	50,50,50	0.96	3 (6%)	53,56,56	0.97	2 (3%)
14	PX2	B	501	-	35,35,35	1.02	4 (11%)	39,40,40	1.10	2 (5%)
11	D10	A	3705	-	9,9,9	0.29	0	8,8,8	0.78	0
8	HEX	A	3701	-	5,5,5	0.30	0	4,4,4	0.58	0
11	D10	A	3709	-	9,9,9	0.32	0	8,8,8	0.69	0
11	D10	B	503	-	9,9,9	0.30	0	8,8,8	0.76	0
11	D10	E	3205	-	9,9,9	0.30	0	8,8,8	0.79	0
8	HEX	E	3203	-	5,5,5	0.30	0	4,4,4	0.58	0
11	D10	B	509	-	9,9,9	0.33	0	8,8,8	0.65	0
11	D10	C	502	-	9,9,9	0.29	0	8,8,8	0.78	0
8	HEX	D	3902	-	5,5,5	0.31	0	4,4,4	0.56	0
11	D10	E	3202	-	9,9,9	0.32	0	8,8,8	0.72	0
11	D10	D	3906	-	9,9,9	0.30	0	8,8,8	0.76	0
9	PIO	A	3702	-	47,47,47	0.48	0	61,65,65	0.61	1 (1%)
11	D10	A	3704	-	9,9,9	0.31	0	8,8,8	0.70	0
11	D10	A	3706	-	9,9,9	0.31	0	8,8,8	0.70	0
11	D10	B	507	-	9,9,9	0.29	0	8,8,8	0.78	0
11	D10	D	3910	-	9,9,9	0.31	0	8,8,8	0.71	0
17	NAG	C	504	-	14,14,15	0.36	0	17,19,21	0.37	0
15	R16	E	3204	-	15,15,15	0.31	0	14,14,14	0.74	0
11	D10	D	3907	-	9,9,9	0.32	0	8,8,8	0.69	0
8	HEX	B	504	-	5,5,5	0.33	0	4,4,4	0.48	0
8	HEX	B	506	-	5,5,5	0.31	0	4,4,4	0.57	0
15	R16	B	502	-	15,15,15	0.29	0	14,14,14	0.84	0
10	PGW	A	3707	-	31,31,50	1.16	2 (6%)	34,37,56	1.03	2 (5%)
11	D10	B	508	-	9,9,9	0.32	0	8,8,8	0.70	0
10	PGW	A	3703	-	50,50,50	0.97	2 (4%)	53,56,56	0.97	2 (3%)
8	HEX	D	3904	-	5,5,5	0.32	0	4,4,4	0.49	0
12	PLM	C	507	-	17,17,17	0.58	0	17,17,17	1.07	1 (5%)
11	D10	D	3905	-	9,9,9	0.32	0	8,8,8	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PLM	A	3708	-	-	1/15/15/15	-
11	D10	C	506	-	-	2/7/7/7	-
8	HEX	C	505	-	-	0/3/3/3	-
12	PLM	C	501	-	-	1/15/15/15	-
16	A8W	C	503	-	1/1/10/11	2/9/67/67	0/4/4/4
8	HEX	E	3206	-	-	0/3/3/3	-
15	R16	D	3908	-	-	3/13/13/13	-
15	R16	B	505	-	-	1/13/13/13	-
11	D10	D	3909	-	-	1/7/7/7	-
15	R16	E	3201	-	-	1/13/13/13	-
9	PIO	D	3901	-	-	2/44/68/68	0/1/1/1
10	PGW	D	3903	-	-	18/55/55/55	-
14	PX2	B	501	-	-	19/37/37/37	-
11	D10	A	3705	-	-	0/7/7/7	-
8	HEX	A	3701	-	-	0/3/3/3	-
11	D10	A	3709	-	-	1/7/7/7	-
11	D10	B	503	-	-	0/7/7/7	-
11	D10	E	3205	-	-	0/7/7/7	-
8	HEX	E	3203	-	-	0/3/3/3	-
11	D10	B	509	-	-	3/7/7/7	-
11	D10	C	502	-	-	0/7/7/7	-
8	HEX	D	3902	-	-	0/3/3/3	-
11	D10	E	3202	-	-	0/7/7/7	-
11	D10	D	3906	-	-	0/7/7/7	-
9	PIO	A	3702	-	-	13/44/68/68	0/1/1/1
11	D10	A	3704	-	-	0/7/7/7	-
11	D10	A	3706	-	-	0/7/7/7	-
11	D10	B	507	-	-	0/7/7/7	-
11	D10	D	3910	-	-	0/7/7/7	-
17	NAG	C	504	-	-	1/6/23/26	0/1/1/1
15	R16	E	3204	-	-	4/13/13/13	-
11	D10	D	3907	-	-	0/7/7/7	-
8	HEX	B	504	-	-	0/3/3/3	-
8	HEX	B	506	-	-	0/3/3/3	-
15	R16	B	502	-	-	1/13/13/13	-
10	PGW	A	3707	-	-	9/36/36/55	-
11	D10	B	508	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PGW	A	3703	-	-	25/55/55/55	-
8	HEX	D	3904	-	-	0/3/3/3	-
12	PLM	C	507	-	-	3/15/15/15	-
11	D10	D	3905	-	-	1/7/7/7	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	3703	PGW	O03-C19	3.03	1.42	1.33
10	D	3903	PGW	O03-C19	2.91	1.41	1.33
10	A	3707	PGW	O03-C19	2.89	1.41	1.33
10	A	3703	PGW	O01-C1	2.82	1.42	1.34
10	A	3707	PGW	O01-C1	2.77	1.42	1.34
14	B	501	PX2	O5-C4	2.69	1.41	1.33
10	D	3903	PGW	O01-C1	2.62	1.41	1.34
14	B	501	PX2	O7-C2	-2.38	1.40	1.46
14	B	501	PX2	O7-C16	2.32	1.40	1.34
10	D	3903	PGW	O01-C02	-2.04	1.41	1.46
14	B	501	PX2	O5-C3	-2.01	1.40	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	3703	PGW	O01-C1-C2	3.90	119.91	111.50
10	A	3707	PGW	O01-C1-C2	3.86	119.83	111.50
14	B	501	PX2	O7-C16-C17	3.77	119.62	111.50
10	D	3903	PGW	O01-C1-C2	3.57	119.19	111.50
16	C	503	A8W	O3-S-O2	3.04	124.41	112.22
10	A	3703	PGW	O03-C19-C20	2.63	120.17	111.91
10	D	3903	PGW	O03-C19-C20	2.59	120.02	111.91
14	B	501	PX2	O5-C4-C5	2.55	119.91	111.91
16	C	503	A8W	C2-C1-C10	2.55	118.26	112.74
9	A	3702	PIO	O2C-C1A-C2A	2.40	116.67	111.50
10	A	3707	PGW	O03-C19-C20	2.40	119.42	111.91
16	C	503	A8W	C16-C15-C14	-2.31	100.55	105.13
16	C	503	A8W	C3-O1-S	2.15	120.03	117.64
12	C	507	PLM	C3-C2-C1	-2.13	109.11	114.47
12	A	3708	PLM	C3-C2-C1	-2.06	109.28	114.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	503	A8W	C3

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	3702	PIO	O1A-C1A-O2C-C2C
9	A	3702	PIO	C2A-C1A-O2C-C2C
10	A	3703	PGW	C04-C05-CAD-OAE
10	A	3703	PGW	C04-O12-P-O11
10	A	3703	PGW	C04-O12-P-O13
10	A	3703	PGW	C04-O12-P-O14
10	A	3703	PGW	C2-C1-O01-C02
10	A	3707	PGW	C04-O12-P-O14
10	A	3707	PGW	O12-C04-C05-CAD
10	D	3903	PGW	C03-O11-P-O13
10	D	3903	PGW	C03-O11-P-O14
14	B	501	PX2	C1-O4-P1-O1
14	B	501	PX2	C1-O4-P1-O2
14	B	501	PX2	C1-O4-P1-O3
14	B	501	PX2	C17-C16-O7-C2
16	C	503	A8W	C2-C3-O1-S
16	C	503	A8W	C4-C3-O1-S
10	A	3703	PGW	O02-C1-O01-C02
14	B	501	PX2	O8-C16-O7-C2
10	D	3903	PGW	O02-C1-O01-C02
14	B	501	PX2	O6-C4-O5-C3
10	A	3707	PGW	O12-C04-C05-OAF
10	D	3903	PGW	O12-C04-C05-OAF
10	D	3903	PGW	C2-C1-O01-C02
14	B	501	PX2	C5-C4-O5-C3
10	D	3903	PGW	O12-C04-C05-CAD
14	B	501	PX2	C16-C17-C18-C19
10	A	3707	PGW	C04-O12-P-O11
10	D	3903	PGW	C03-O11-P-O12
9	A	3702	PIO	C2B-C3B-C4B-C5B
10	A	3703	PGW	C24-C25-C26-C27
10	A	3707	PGW	C2-C3-C4-C5
14	B	501	PX2	C19-C20-C21-C22
10	D	3903	PGW	C23-C24-C25-C26
15	E	3204	R16	C34-C35-C36-C37
10	D	3903	PGW	C06-C07-C08-C09
10	D	3903	PGW	C27-C15-C16-C17
10	A	3703	PGW	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
10	A	3703	PGW	C27-C15-C16-C17
15	D	3908	R16	C32-C33-C34-C35
10	A	3703	PGW	OAF-C05-CAD-OAE
15	D	3908	R16	C30-C31-C32-C33
11	C	506	D10	C5-C6-C7-C8
11	B	509	D10	C3-C4-C5-C6
10	D	3903	PGW	C17-C18-C28-C30
10	D	3903	PGW	C20-C21-C22-C23
10	A	3703	PGW	C08-C09-C11-C12
12	A	3708	PLM	C3-C4-C5-C6
10	A	3703	PGW	C20-C21-C22-C23
10	A	3703	PGW	C03-O11-P-O12
10	A	3703	PGW	C6-C7-C8-C9
15	E	3201	R16	C33-C34-C35-C36
10	D	3903	PGW	C08-C09-C11-C12
14	B	501	PX2	C5-C6-C7-C8
11	B	509	D10	C1-C2-C3-C4
15	B	505	R16	C35-C36-C37-C38
10	A	3703	PGW	O01-C02-C03-O11
14	B	501	PX2	O7-C2-C3-O5
15	B	502	R16	C34-C35-C36-C37
9	A	3702	PIO	C1C-C2C-C3C-O3C
9	A	3702	PIO	C2A-C3A-C4A-C5A
14	B	501	PX2	C22-C23-C24-C25
15	E	3204	R16	C28-C29-C30-C31
14	B	501	PX2	C6-C7-C8-C9
9	A	3702	PIO	C4A-C5A-C6A-C7A
14	B	501	PX2	C11-C10-C9-C8
9	D	3901	PIO	C2A-C3A-C4A-C5A
9	A	3702	PIO	O2C-C2C-C3C-O3C
10	D	3903	PGW	C6-C7-C8-C9
12	C	507	PLM	C5-C6-C7-C8
10	A	3703	PGW	C03-O11-P-O13
10	A	3703	PGW	C17-C18-C28-C30
11	A	3709	D10	C2-C3-C4-C5
10	A	3703	PGW	C07-C06-C10-C9
14	B	501	PX2	C1-C2-C3-O5
9	A	3702	PIO	O1B-C1B-O3C-C3C
10	A	3703	PGW	C09-C11-C12-C13
10	A	3707	PGW	C03-O11-P-O12
12	C	501	PLM	C7-C8-C9-CA
9	A	3702	PIO	C4B-C5B-C6B-C7B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	3702	PIO	C2B-C1B-O3C-C3C
15	D	3908	R16	C29-C30-C31-C32
10	A	3707	PGW	C05-C04-O12-P
10	D	3903	PGW	C5-C6-C7-C8
10	A	3703	PGW	C02-C03-O11-P
14	B	501	PX2	C23-C24-C25-C26
10	A	3707	PGW	C02-C01-O03-C19
11	C	506	D10	C4-C5-C6-C7
9	A	3702	PIO	C3A-C4A-C5A-C6A
10	D	3903	PGW	C2-C3-C4-C5
11	D	3905	D10	C3-C4-C5-C6
10	A	3703	PGW	C01-C02-C03-O11
14	B	501	PX2	C10-C11-C12-C13
10	A	3703	PGW	C01-C02-O01-C1
10	A	3703	PGW	C03-C02-O01-C1
10	A	3703	PGW	C7-C8-C9-C10
12	C	507	PLM	O1-C1-C2-C3
15	E	3204	R16	C30-C31-C32-C33
12	C	507	PLM	O2-C1-C2-C3
11	D	3909	D10	C2-C3-C4-C5
17	C	504	NAG	C1-C2-N2-C7
9	A	3702	PIO	O3C-C1B-C2B-C3B
14	B	501	PX2	O5-C4-C5-C6
15	E	3204	R16	C29-C30-C31-C32
9	A	3702	PIO	O1B-C1B-C2B-C3B
10	D	3903	PGW	C3-C4-C5-C6
10	D	3903	PGW	C24-C25-C26-C27
10	A	3703	PGW	C03-O11-P-O14
10	A	3707	PGW	C03-O11-P-O14
9	D	3901	PIO	O2C-C1A-C2A-C3A
14	B	501	PX2	O6-C4-C5-C6
11	B	509	D10	C2-C3-C4-C5

There are no ring outliers.

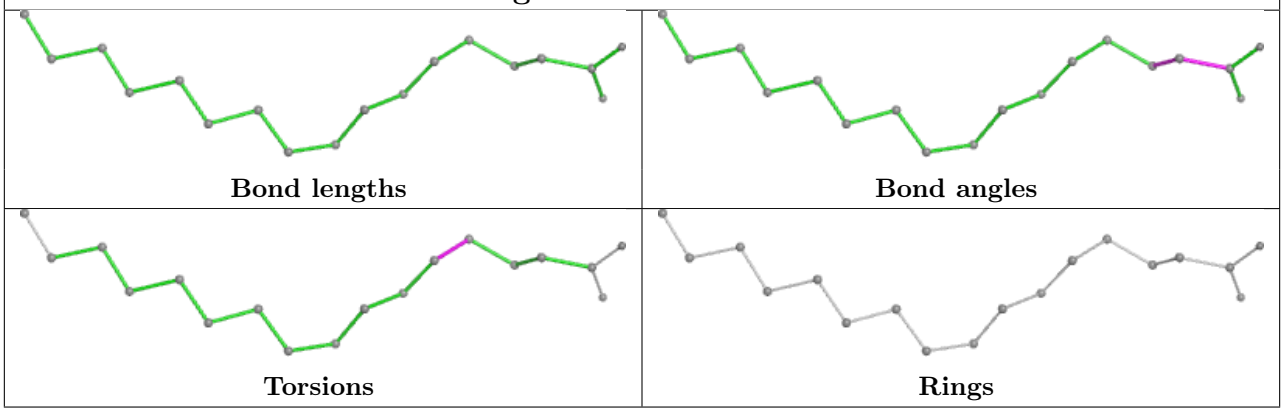
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	3901	PIO	1	0
10	D	3903	PGW	1	0
9	A	3702	PIO	2	0

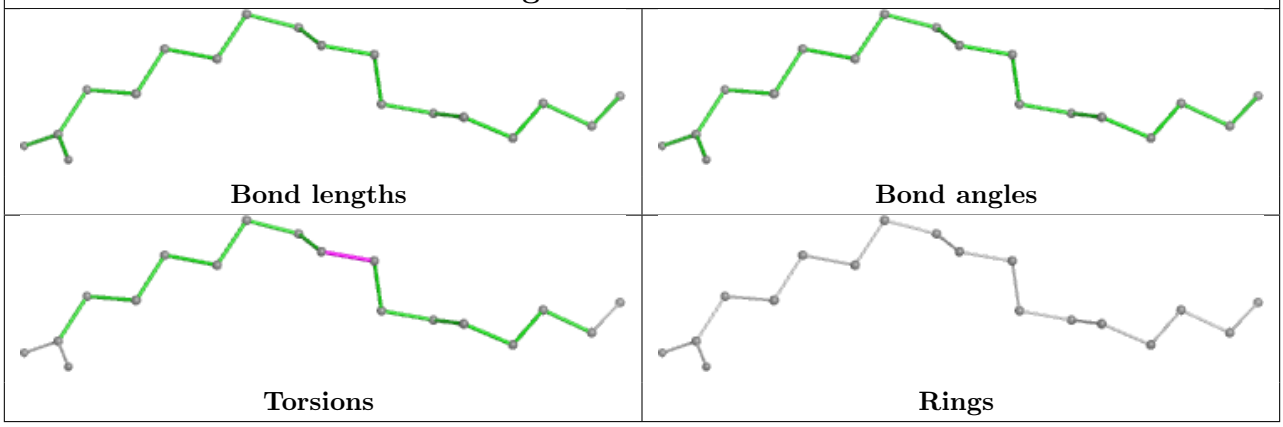
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

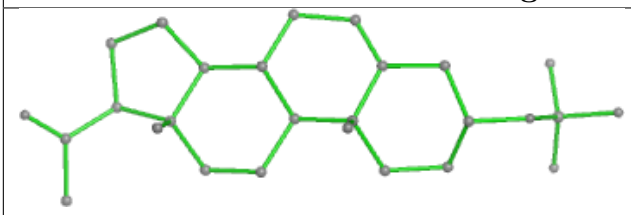
Ligand PLM A 3708



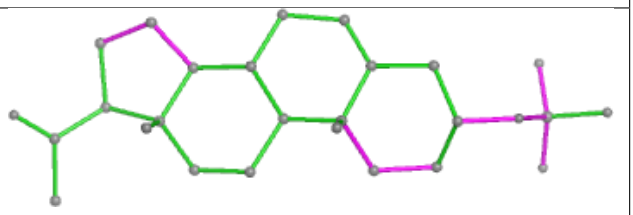
Ligand PLM C 501



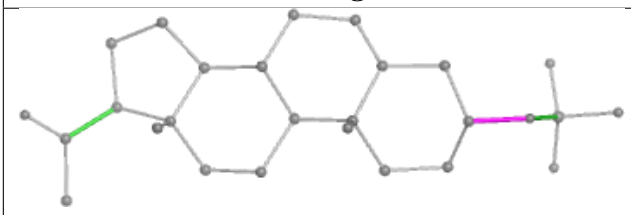
Ligand A8W C 503



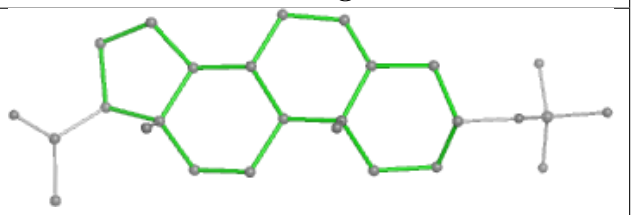
Bond lengths



Bond angles

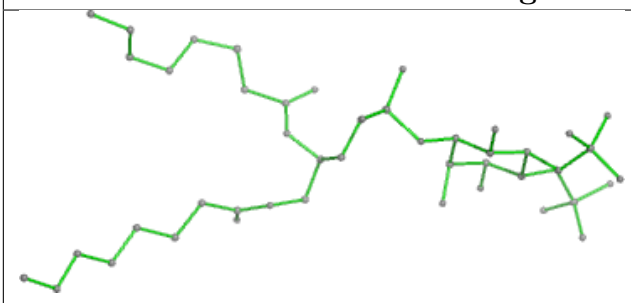


Torsions

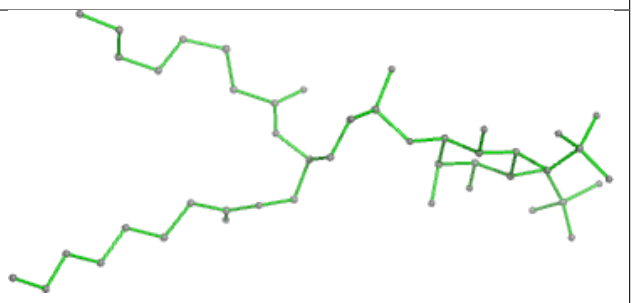


Rings

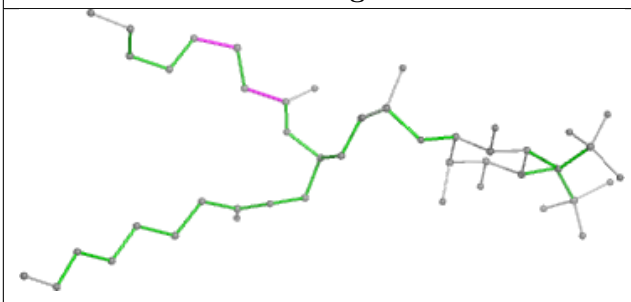
Ligand PIO D 3901



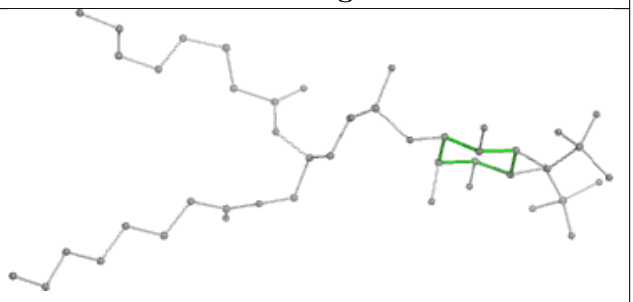
Bond lengths



Bond angles

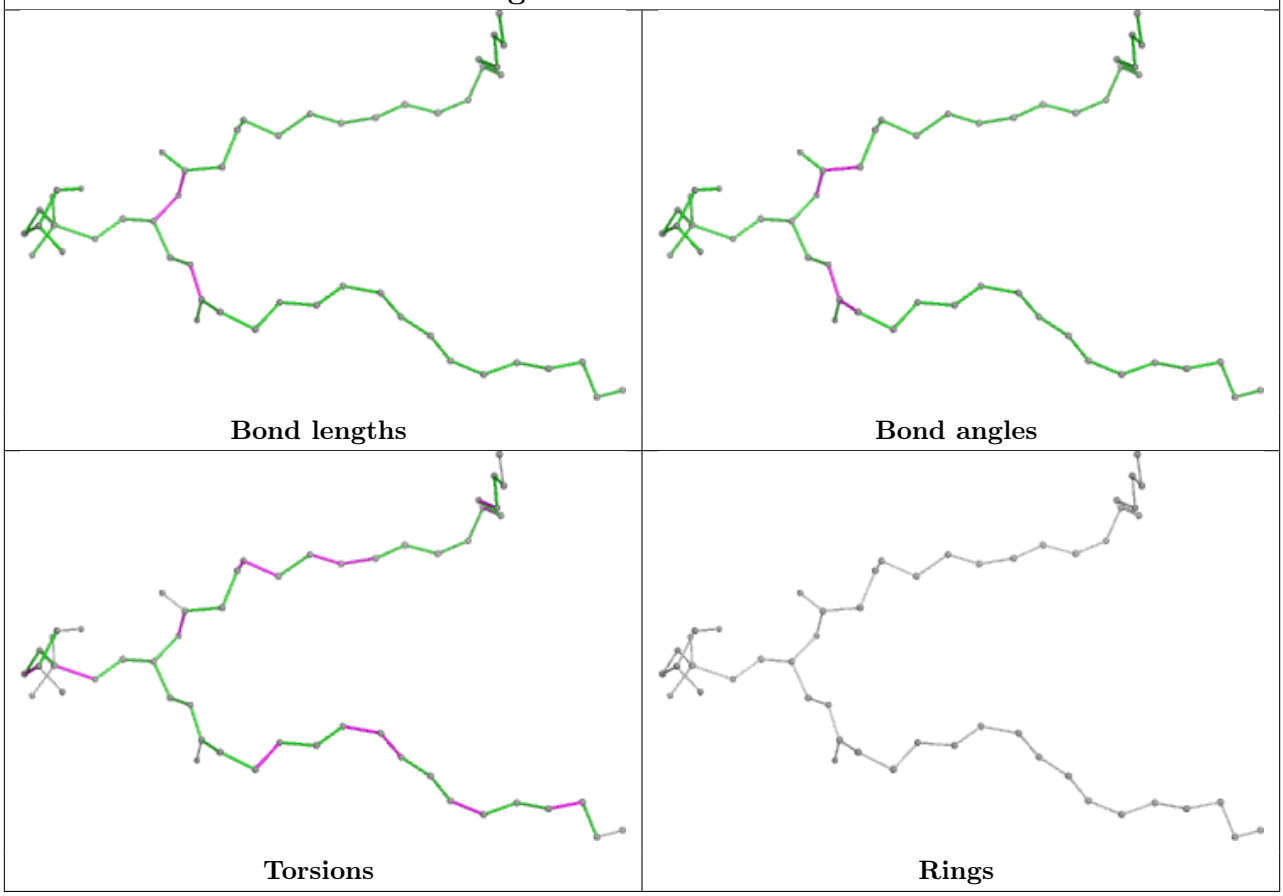


Torsions

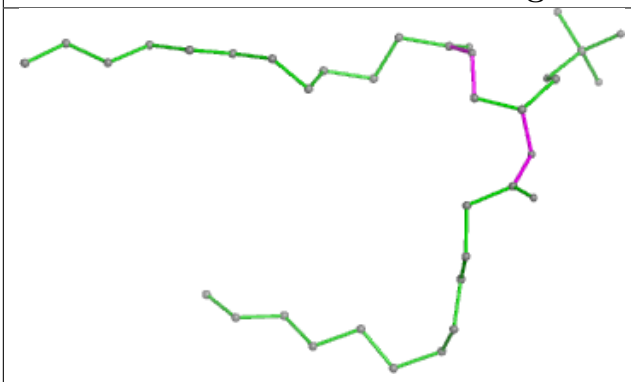


Rings

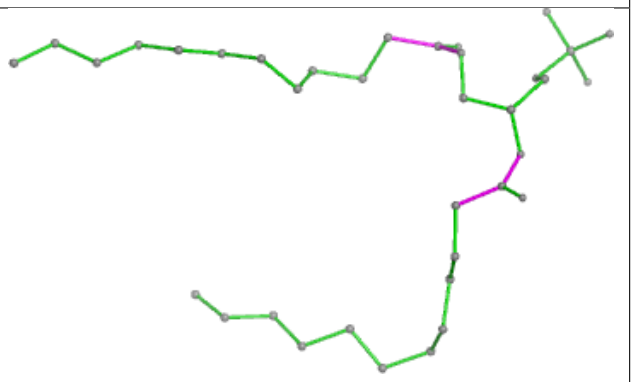
Ligand PGW D 3903



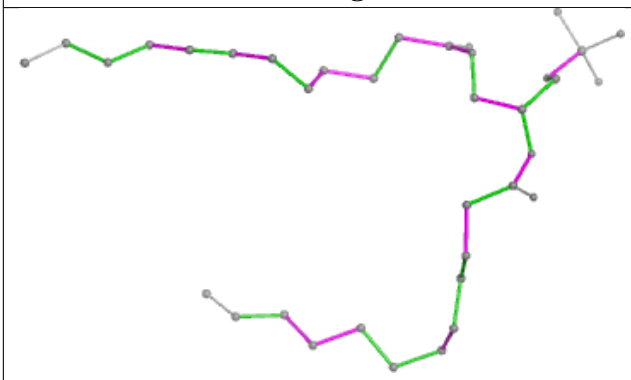
Ligand PX2 B 501



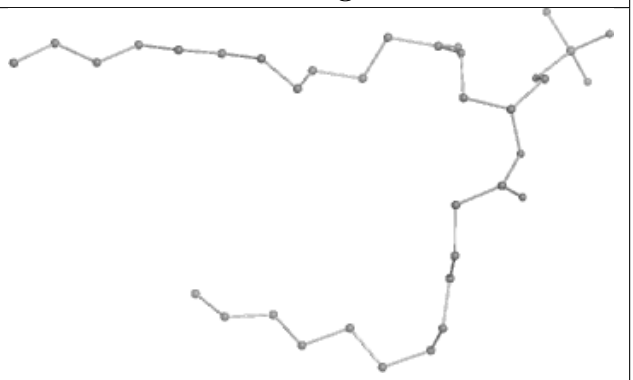
Bond lengths



Bond angles

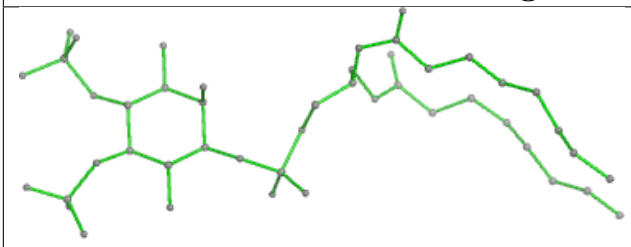


Torsions

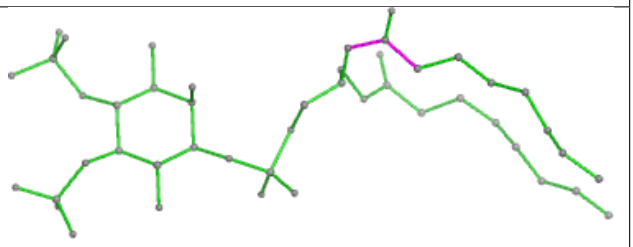


Rings

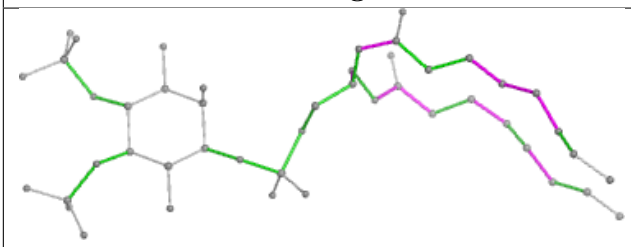
Ligand PIO A 3702



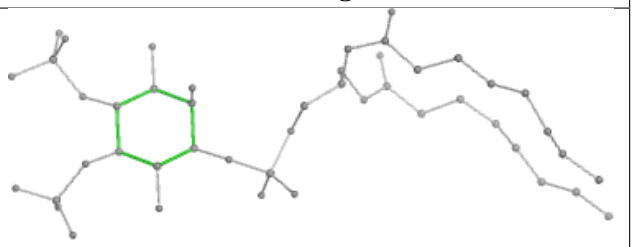
Bond lengths



Bond angles

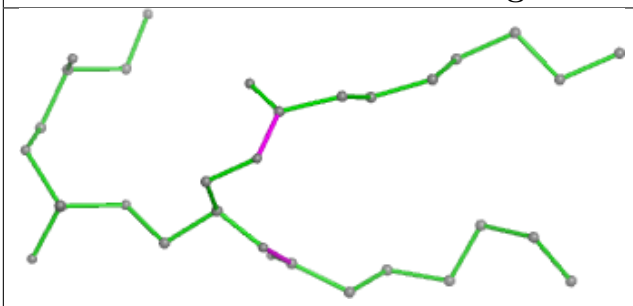


Torsions

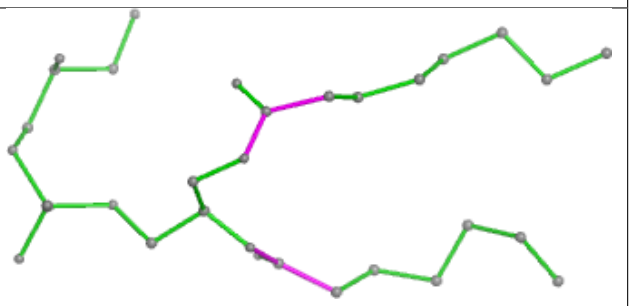


Rings

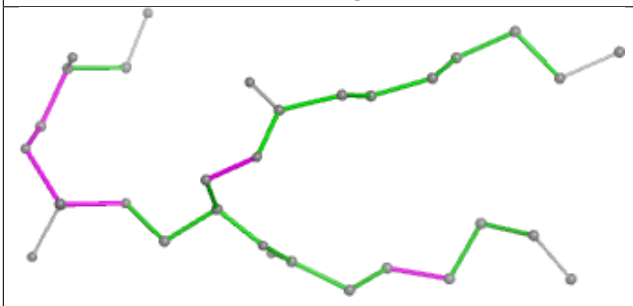
Ligand PGW A 3707



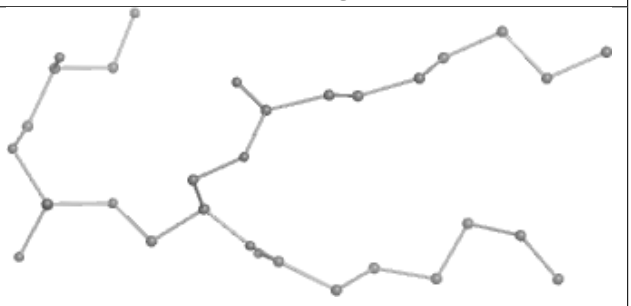
Bond lengths



Bond angles

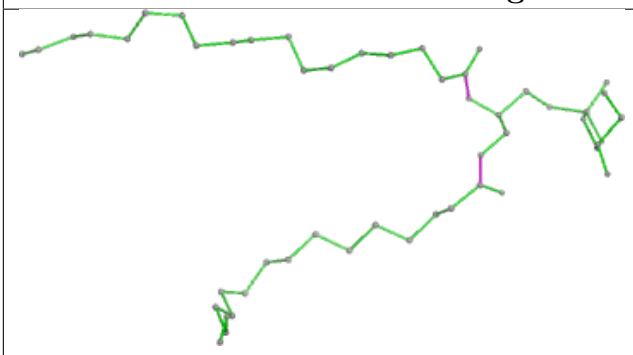


Torsions

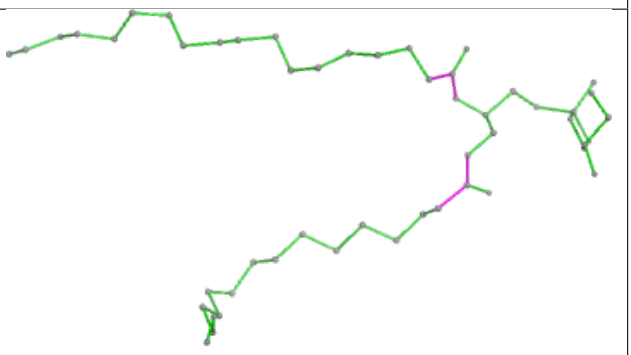


Rings

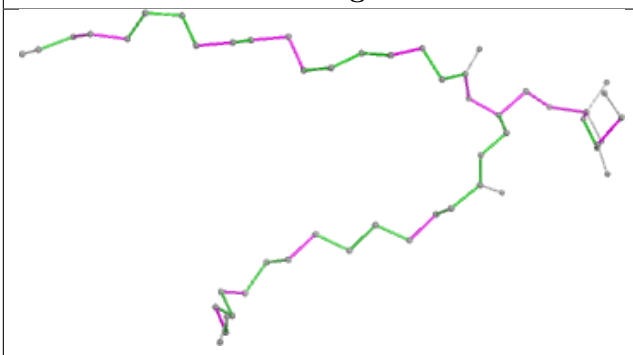
Ligand PGW A 3703



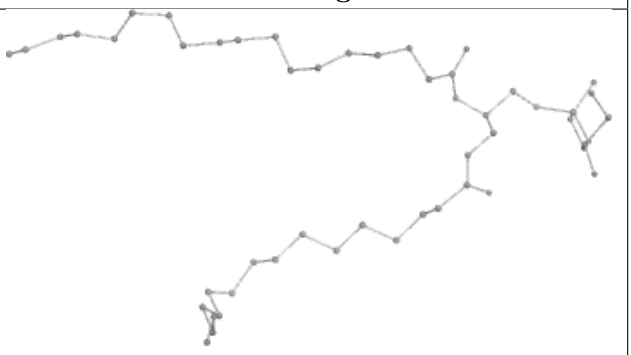
Bond lengths



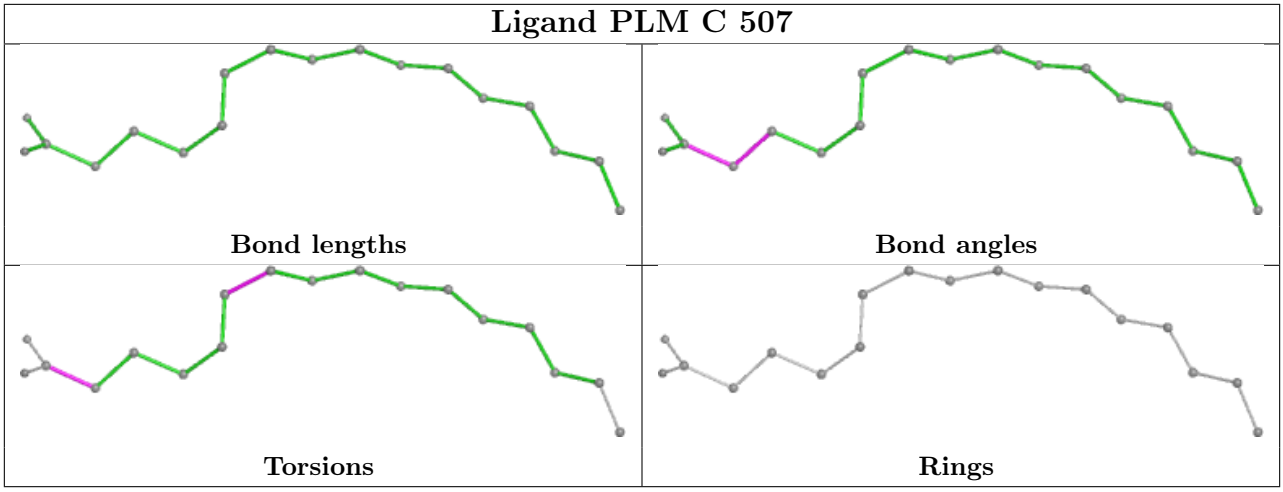
Bond angles



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.

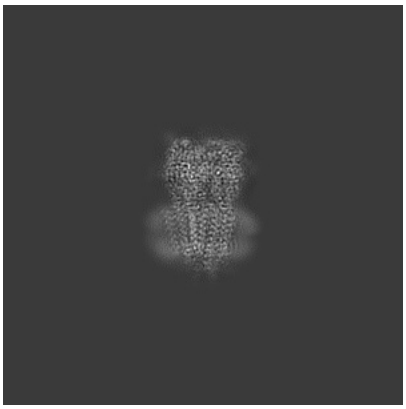
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50280. These allow visual inspection of the internal detail of the map and identification of artifacts.

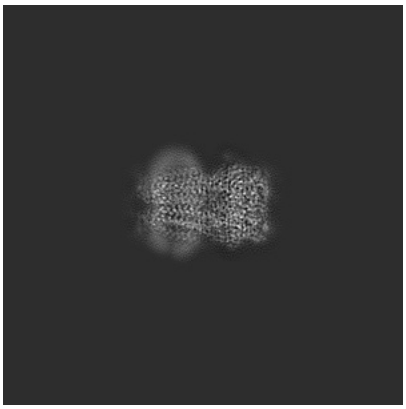
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

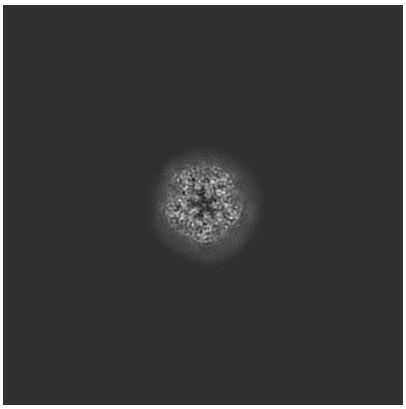
6.1.1 Primary map



X

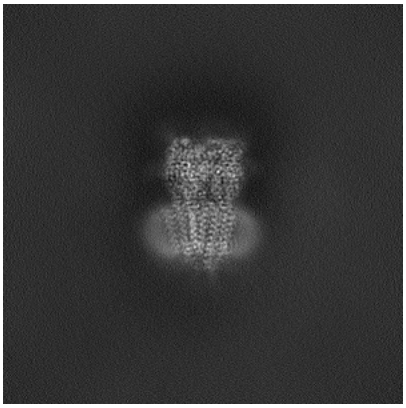


Y

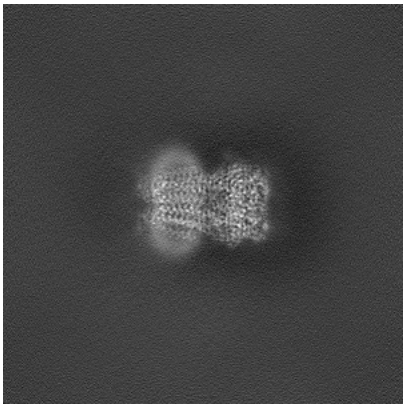


Z

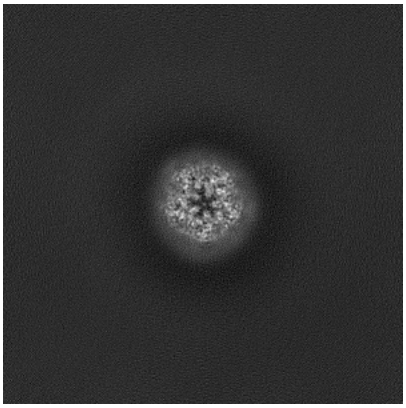
6.1.2 Raw map



X



Y

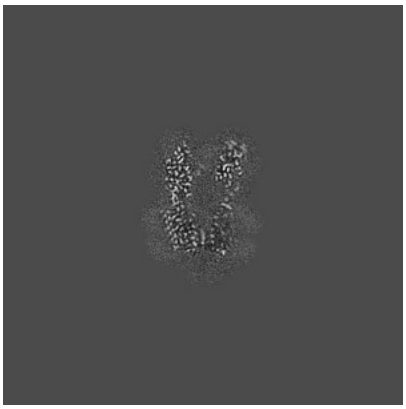


Z

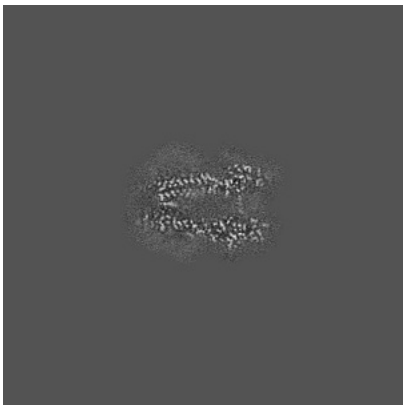
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

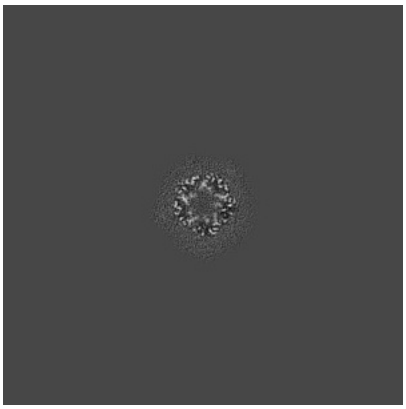
6.2.1 Primary map



X Index: 219

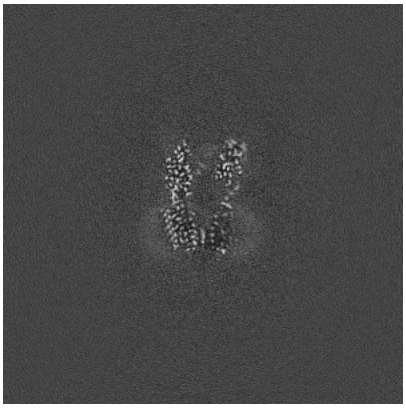


Y Index: 219

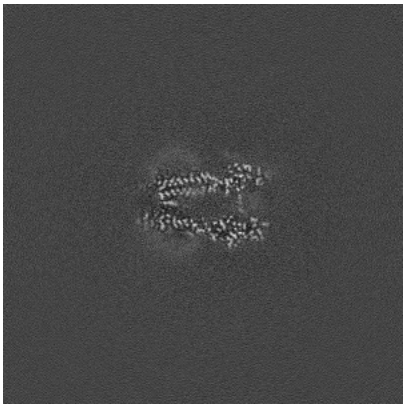


Z Index: 219

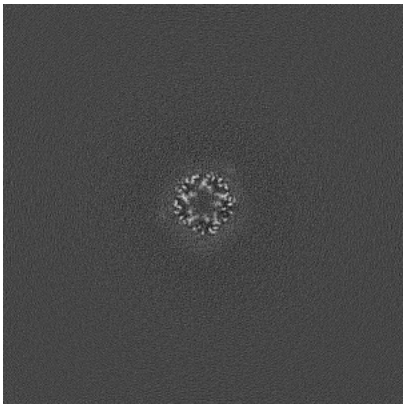
6.2.2 Raw map



X Index: 219



Y Index: 219

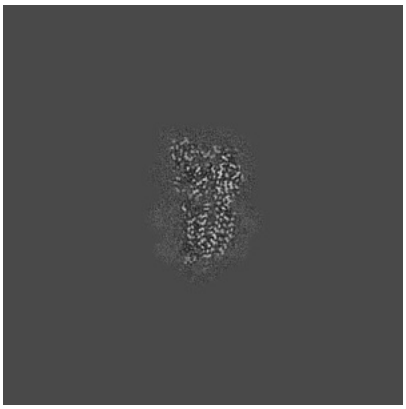


Z Index: 219

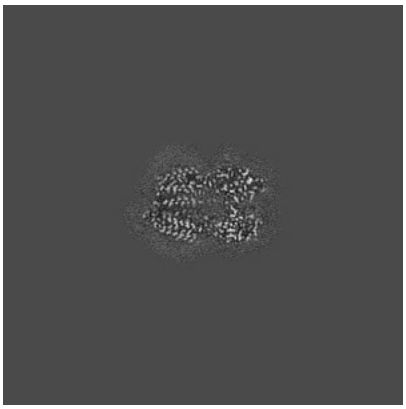
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

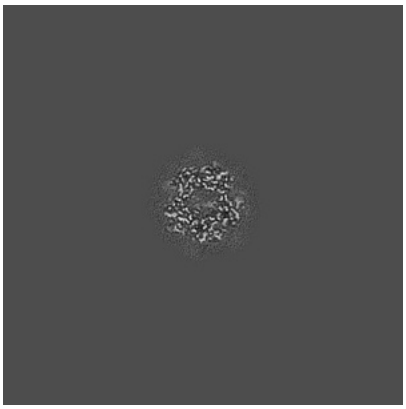
6.3.1 Primary map



X Index: 200

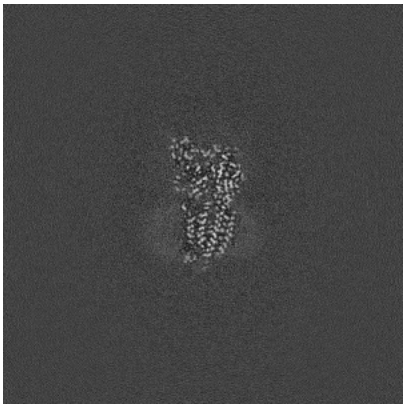


Y Index: 207

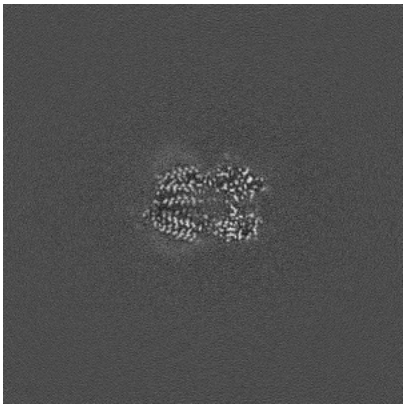


Z Index: 259

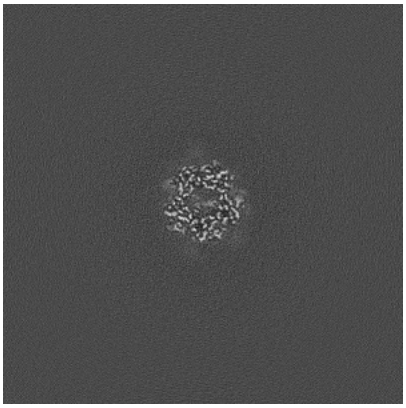
6.3.2 Raw map



X Index: 200



Y Index: 207

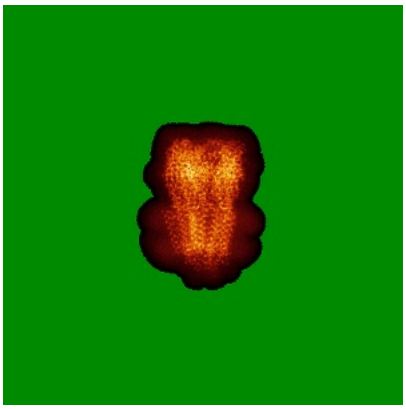


Z Index: 259

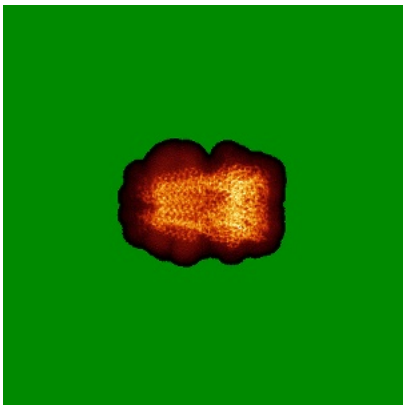
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

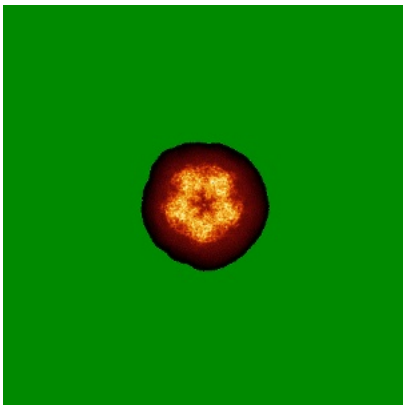
6.4.1 Primary map



X

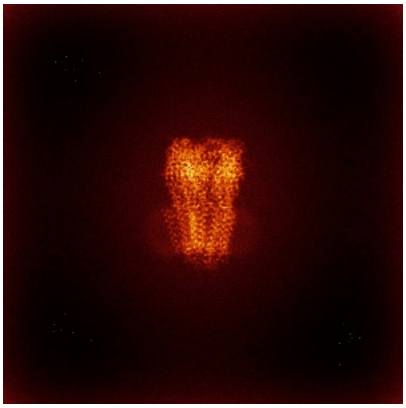


Y

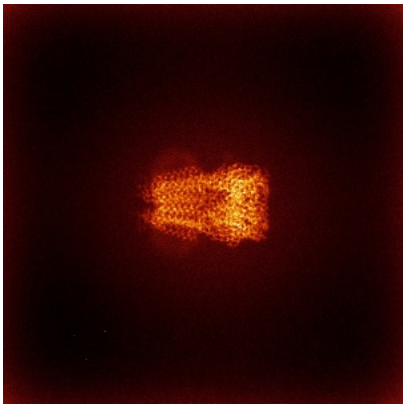


Z

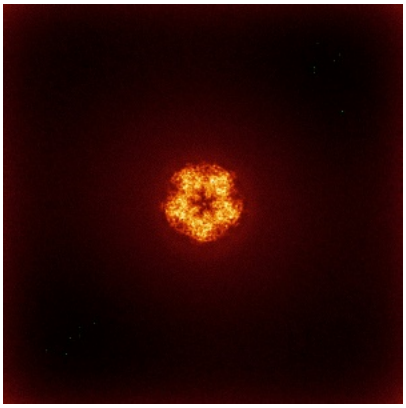
6.4.2 Raw map



X



Y

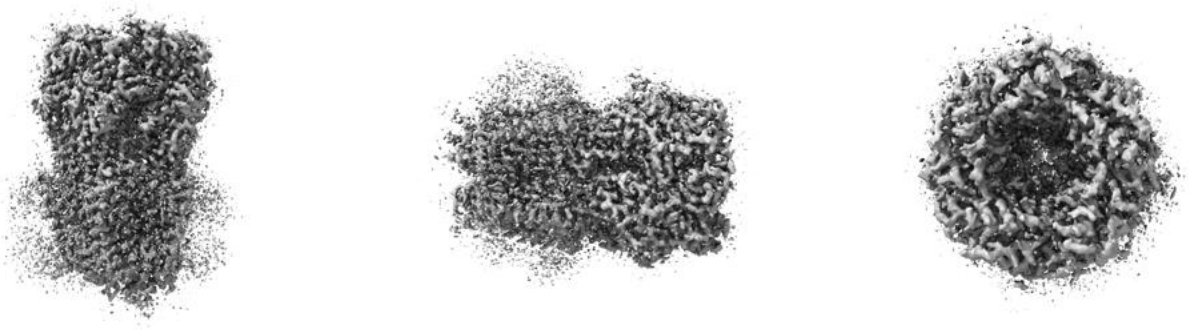


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

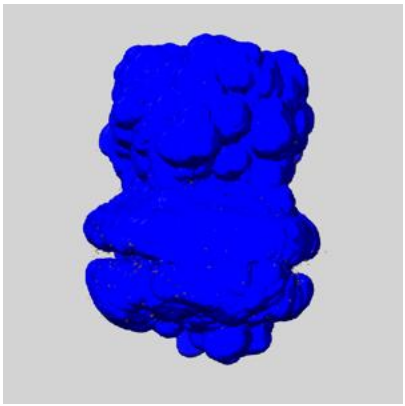
6.6 Mask visualisation

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

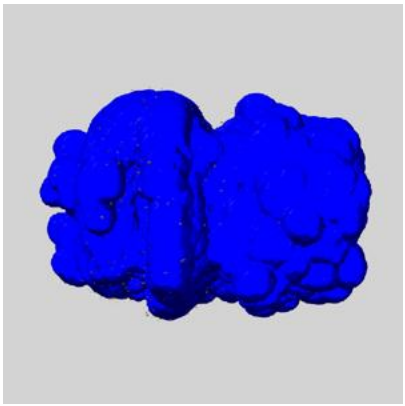
A mask typically either:

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

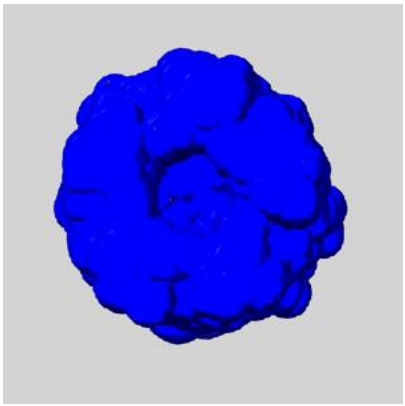
6.6.1 emd_50280_msk_1.map



X



Y

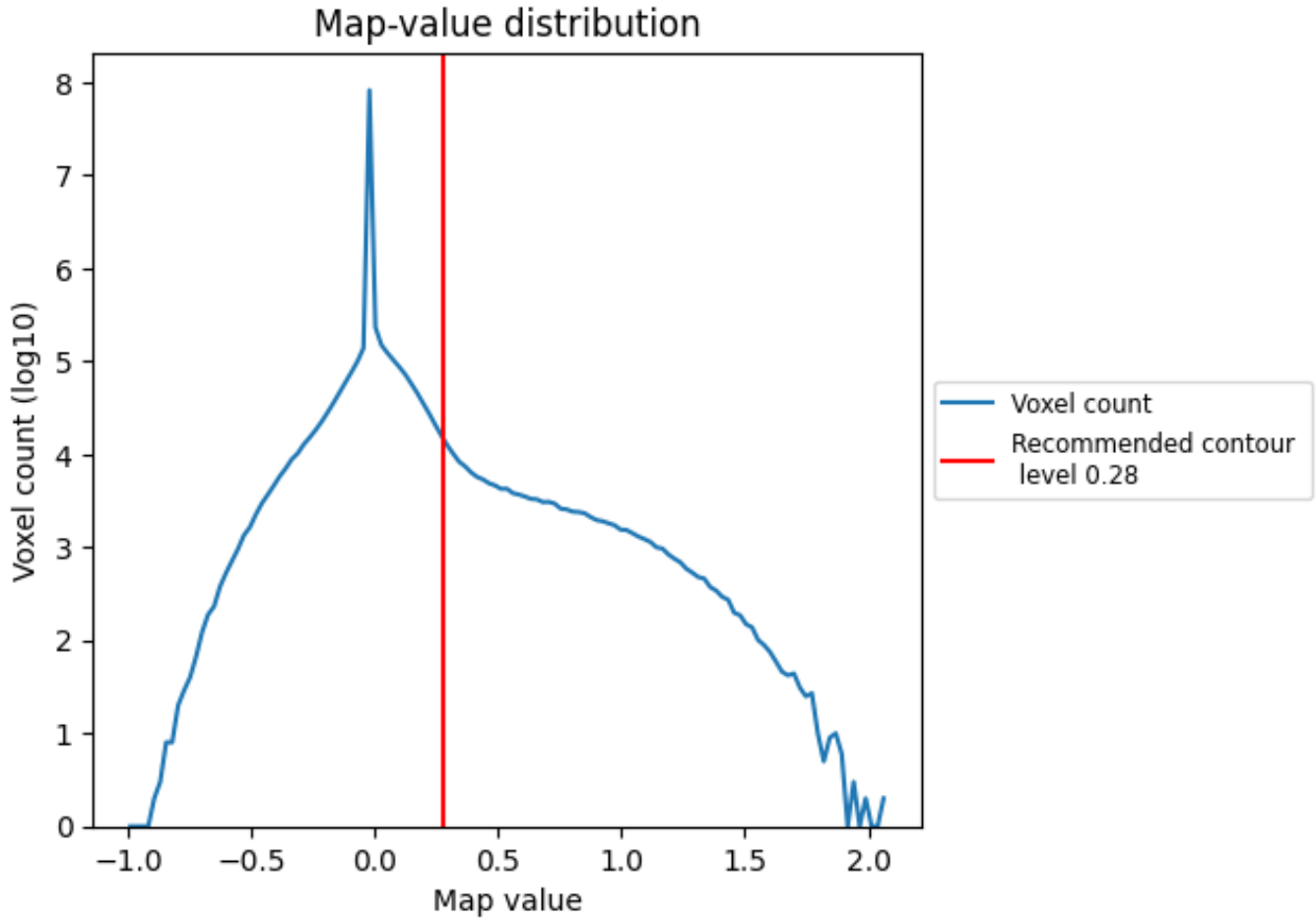


Z

7 Map analysis

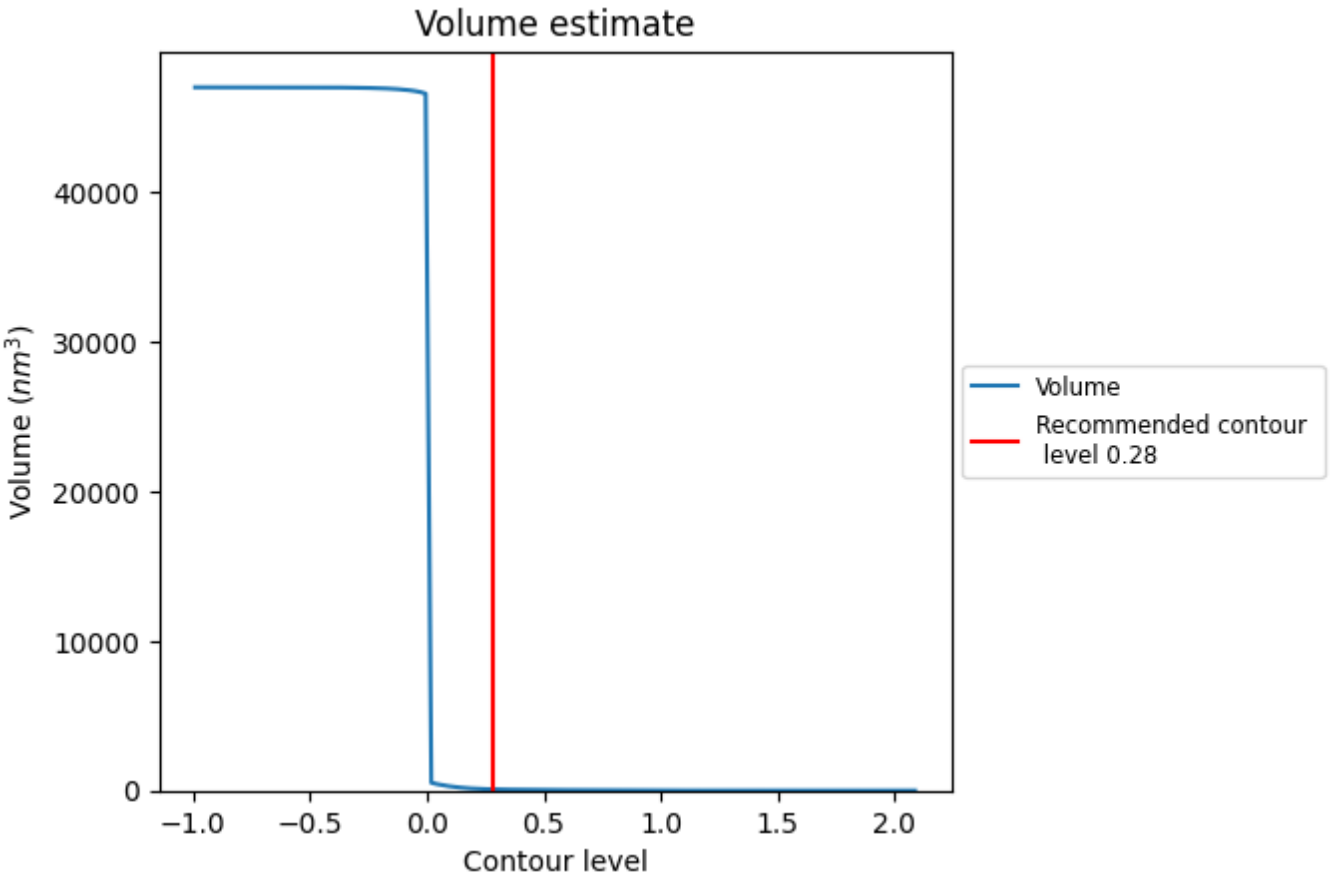
This section contains the results of statistical analysis of the map.

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.

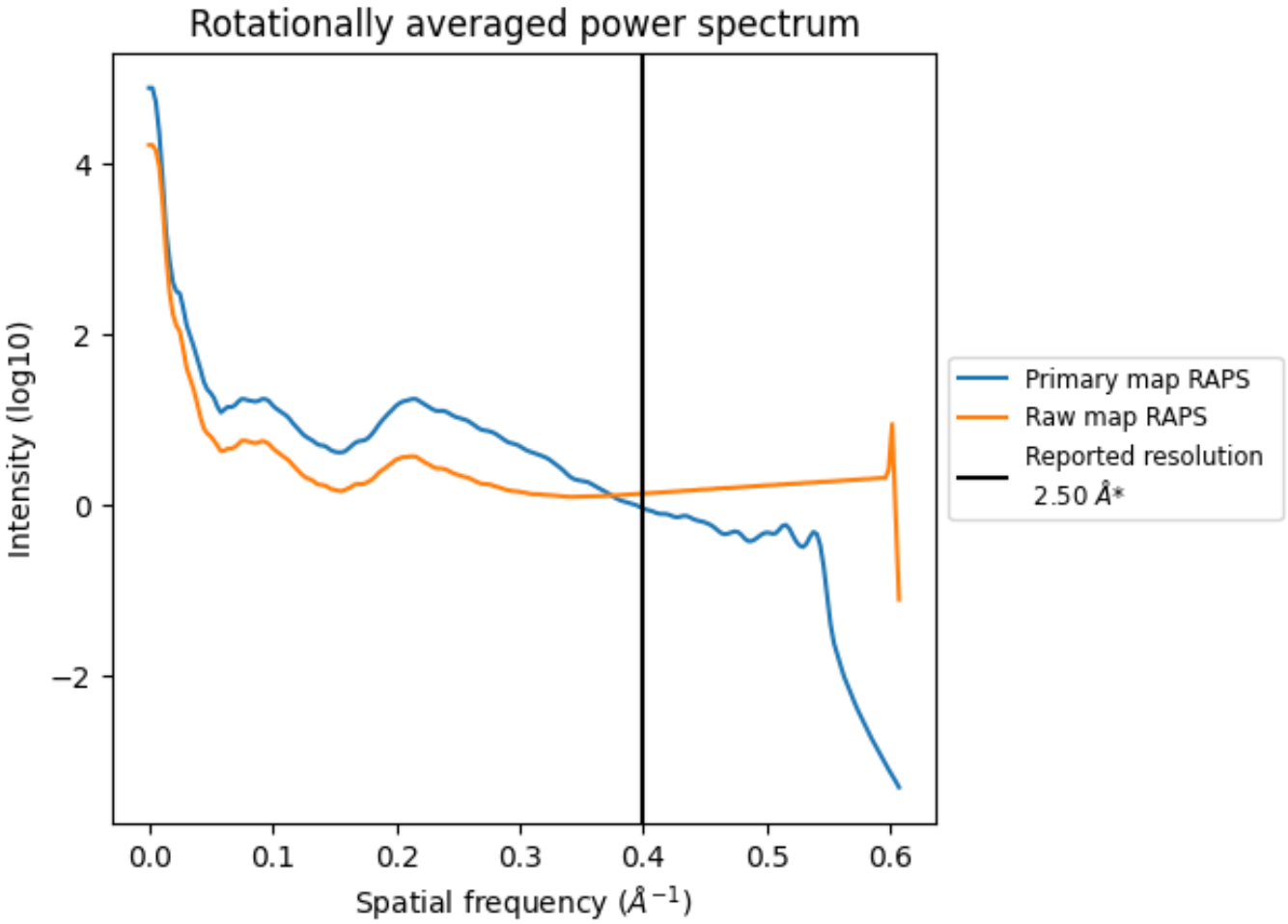
7.2 Volume estimate



The volume at the recommended contour level is 83 nm^3; this corresponds to an approximate mass of 75 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)

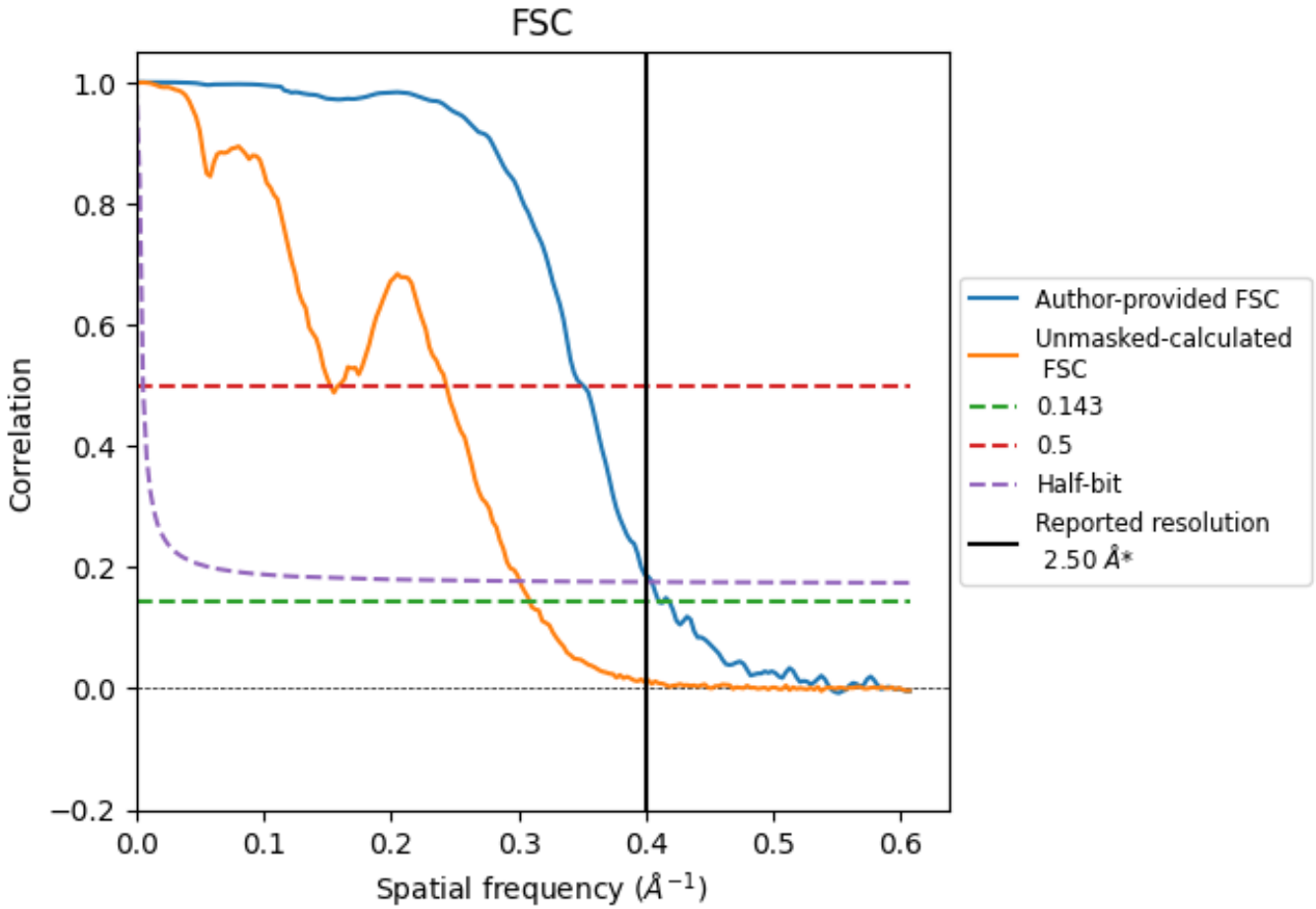


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

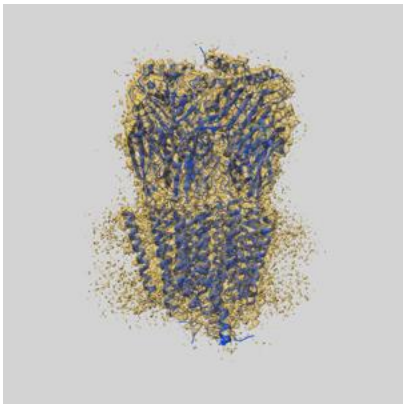
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.44	2.85	2.47
Unmasked-calculated*	3.24	6.57	3.32

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.24 differs from the reported value 2.5 by more than 10 %

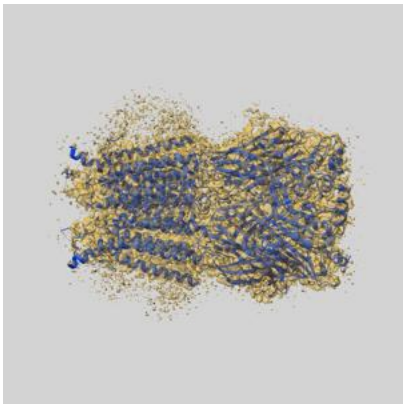
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50280 and PDB model 9FAS. Per-residue inclusion information can be found in section 3 on page 14.

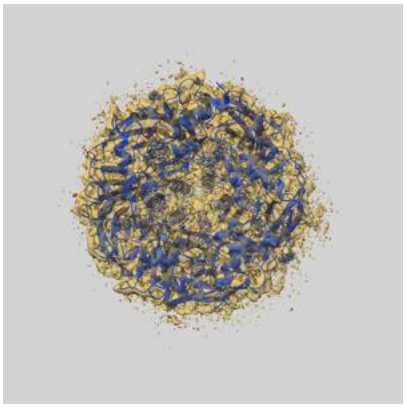
9.1 Map-model overlay



X



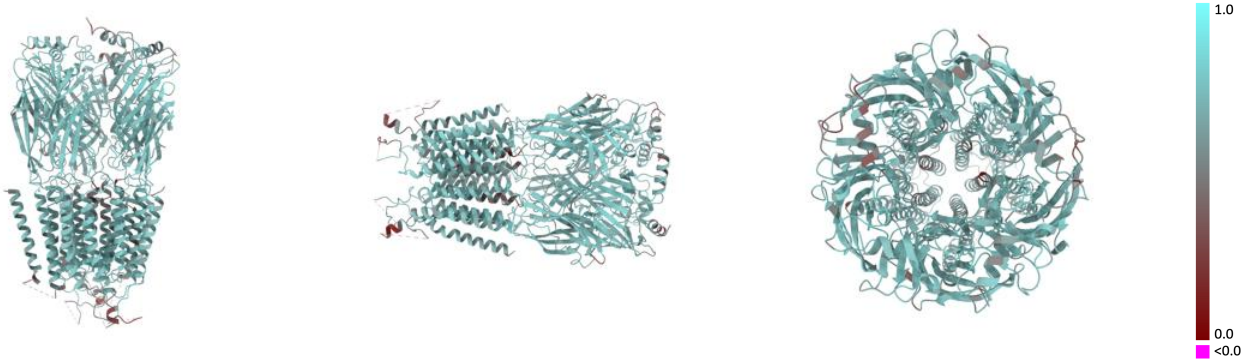
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

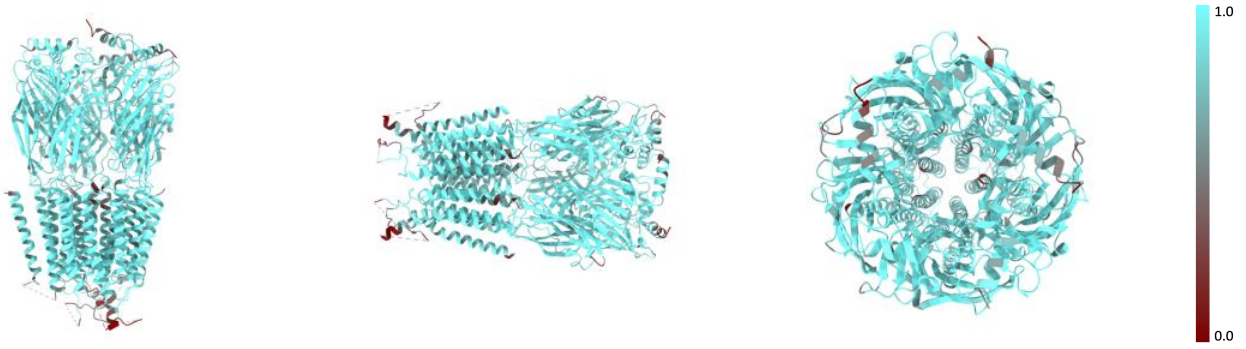
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

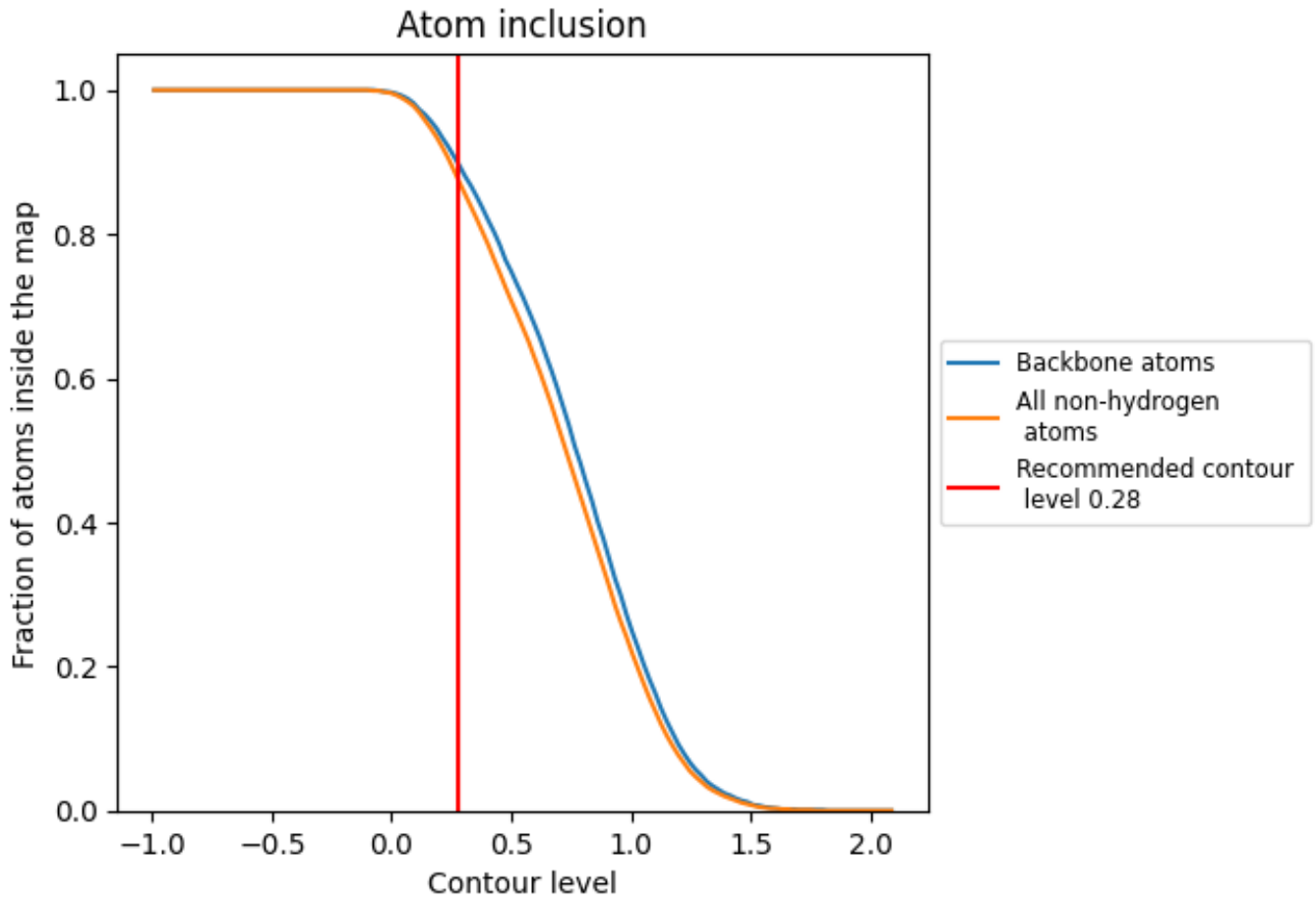
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.6540
A	0.8740	0.6580
B	0.8850	0.6520
C	0.9100	0.6650
D	0.8890	0.6640
E	0.8870	0.6540
F	0.6720	0.5640
G	0.3590	0.4010
H	0.5830	0.5360
I	0.1940	0.3510
J	0.5280	0.5350
K	0.2820	0.4200