Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 11:41 AM EST

PDB ID	:	8SID
EMDB ID	:	EMD-40506
Title	:	Human GABAA receptor alpha1-beta2-gamma2 subtype in complex with GABA plus dehydroepiandrosterone sulfate
Authors	:	Legesse, D.H.; Hibbs, R.E.
Deposited on	:	2023-04-14
Resolution	:	2.71 Å(reported)

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

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

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

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

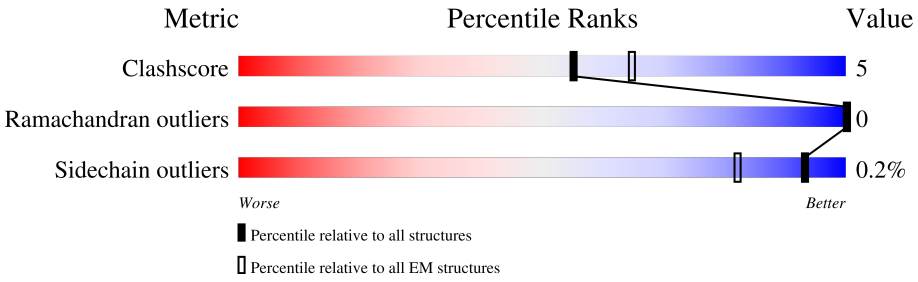
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.71 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	364	84% 8% 8%
1	C	364	85% 7% 8%
2	B	358	86% 9% 6%
2	D	358	83% 11% 6%
3	E	417	71% 8% 20%
4	I	213	45% 51%
4	L	213	43% 7% 50%
5	J	454	21% 5% 74%

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Mol	Chain	Length	Quality of chain
5	K	454	22% 74%
6	F	3	33% 33% 33%
6	H	3	100%
6	M	3	100%
7	G	10	30% 50% 20%
8	N	2	100%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 35011 atoms, of which 17238 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 beta-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0
			5473	1791	2741	440	485	16		
1	C	334	Total	C	H	N	O	S	0	0
			5473	1791	2741	440	485	16		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	SER	-	linker	UNP P47870
A	309	GLN	-	linker	UNP P47870
A	310	PRO	-	linker	UNP P47870
A	311	ALA	-	linker	UNP P47870
A	312	ARG	-	linker	UNP P47870
A	313	ALA	-	linker	UNP P47870
A	314	ALA	-	linker	UNP P47870
A	342	VAL	-	expression tag	UNP P47870
A	343	ASP	-	expression tag	UNP P47870
A	344	GLY	-	expression tag	UNP P47870
A	345	SER	-	expression tag	UNP P47870
A	346	GLY	-	expression tag	UNP P47870
A	347	ALA	-	expression tag	UNP P47870
A	348	THR	-	expression tag	UNP P47870
A	349	ASN	-	expression tag	UNP P47870
A	350	PHE	-	expression tag	UNP P47870
A	351	SER	-	expression tag	UNP P47870
A	352	LEU	-	expression tag	UNP P47870
A	353	LEU	-	expression tag	UNP P47870
A	354	LYS	-	expression tag	UNP P47870
A	355	GLN	-	expression tag	UNP P47870
A	356	ALA	-	expression tag	UNP P47870
A	357	GLY	-	expression tag	UNP P47870
A	358	ASP	-	expression tag	UNP P47870
A	359	VAL	-	expression tag	UNP P47870
A	360	GLU	-	expression tag	UNP P47870

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Chain	Residue	Modelled	Actual	Comment	Reference
A	361	GLU	-	expression tag	UNP P47870
A	362	ASN	-	expression tag	UNP P47870
A	363	PRO	-	expression tag	UNP P47870
A	364	GLY	-	expression tag	UNP P47870
C	308	SER	-	linker	UNP P47870
C	309	GLN	-	linker	UNP P47870
C	310	PRO	-	linker	UNP P47870
C	311	ALA	-	linker	UNP P47870
C	312	ARG	-	linker	UNP P47870
C	313	ALA	-	linker	UNP P47870
C	314	ALA	-	linker	UNP P47870
C	342	VAL	-	expression tag	UNP P47870
C	343	ASP	-	expression tag	UNP P47870
C	344	GLY	-	expression tag	UNP P47870
C	345	SER	-	expression tag	UNP P47870
C	346	GLY	-	expression tag	UNP P47870
C	347	ALA	-	expression tag	UNP P47870
C	348	THR	-	expression tag	UNP P47870
C	349	ASN	-	expression tag	UNP P47870
C	350	PHE	-	expression tag	UNP P47870
C	351	SER	-	expression tag	UNP P47870
C	352	LEU	-	expression tag	UNP P47870
C	353	LEU	-	expression tag	UNP P47870
C	354	LYS	-	expression tag	UNP P47870
C	355	GLN	-	expression tag	UNP P47870
C	356	ALA	-	expression tag	UNP P47870
C	357	GLY	-	expression tag	UNP P47870
C	358	ASP	-	expression tag	UNP P47870
C	359	VAL	-	expression tag	UNP P47870
C	360	GLU	-	expression tag	UNP P47870
C	361	GLU	-	expression tag	UNP P47870
C	362	ASN	-	expression tag	UNP P47870
C	363	PRO	-	expression tag	UNP P47870
C	364	GLY	-	expression tag	UNP P47870

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	338	Total	C	H	N	O	S	0	0
			5454	1763	2724	461	490	16		
2	D	338	Total	C	H	N	O	S	0	0
			5454	1763	2724	461	490	16		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	313	SER	-	linker	UNP P14867
B	314	GLN	-	linker	UNP P14867
B	315	PRO	-	linker	UNP P14867
B	316	ALA	-	linker	UNP P14867
B	317	ARG	-	linker	UNP P14867
B	318	ALA	-	linker	UNP P14867
B	319	ALA	-	linker	UNP P14867
D	313	SER	-	linker	UNP P14867
D	314	GLN	-	linker	UNP P14867
D	315	PRO	-	linker	UNP P14867
D	316	ALA	-	linker	UNP P14867
D	317	ARG	-	linker	UNP P14867
D	318	ALA	-	linker	UNP P14867
D	319	ALA	-	linker	UNP P14867

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	333	Total	C	H	N	O	S	0	0
			5443	1781	2714	448	485	15		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-36	TRP	-	expression tag	UNP P18507
E	-35	SER	-	expression tag	UNP P18507
E	-34	HIS	-	expression tag	UNP P18507
E	-33	PRO	-	expression tag	UNP P18507
E	-32	GLN	-	expression tag	UNP P18507
E	-31	PHE	-	expression tag	UNP P18507
E	-30	GLU	-	expression tag	UNP P18507
E	-29	LYS	-	expression tag	UNP P18507
E	-28	GLY	-	expression tag	UNP P18507
E	-27	GLY	-	expression tag	UNP P18507
E	-26	GLY	-	expression tag	UNP P18507
E	-25	SER	-	expression tag	UNP P18507
E	-24	GLY	-	expression tag	UNP P18507
E	-23	GLY	-	expression tag	UNP P18507
E	-22	GLY	-	expression tag	UNP P18507
E	-21	SER	-	expression tag	UNP P18507
E	-20	GLY	-	expression tag	UNP P18507

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	GLY	-	expression tag	UNP P18507
E	-18	SER	-	expression tag	UNP P18507
E	-17	SER	-	expression tag	UNP P18507
E	-16	ALA	-	expression tag	UNP P18507
E	-15	TRP	-	expression tag	UNP P18507
E	-14	SER	-	expression tag	UNP P18507
E	-13	HIS	-	expression tag	UNP P18507
E	-12	PRO	-	expression tag	UNP P18507
E	-11	GLN	-	expression tag	UNP P18507
E	-10	PHE	-	expression tag	UNP P18507
E	-9	GLU	-	expression tag	UNP P18507
E	-8	LYS	-	expression tag	UNP P18507
E	-7	LEU	-	expression tag	UNP P18507
E	-6	GLU	-	expression tag	UNP P18507
E	-5	VAL	-	expression tag	UNP P18507
E	-4	LEU	-	expression tag	UNP P18507
E	-3	PHE	-	expression tag	UNP P18507
E	-2	GLN	-	expression tag	UNP P18507
E	-1	GLY	-	expression tag	UNP P18507
E	0	PRO	-	expression tag	UNP P18507
E	323	SER	-	linker	UNP P18507
E	324	GLN	-	linker	UNP P18507
E	325	PRO	-	linker	UNP P18507
E	326	ALA	-	linker	UNP P18507
E	327	ARG	-	linker	UNP P18507
E	328	ALA	-	linker	UNP P18507
E	358	SER	-	expression tag	UNP P18507
E	359	ARG	-	expression tag	UNP P18507
E	360	GLY	-	expression tag	UNP P18507
E	361	SER	-	expression tag	UNP P18507
E	362	GLY	-	expression tag	UNP P18507
E	363	ALA	-	expression tag	UNP P18507
E	364	THR	-	expression tag	UNP P18507
E	365	ASN	-	expression tag	UNP P18507
E	366	PHE	-	expression tag	UNP P18507
E	367	SER	-	expression tag	UNP P18507
E	368	LEU	-	expression tag	UNP P18507
E	369	LEU	-	expression tag	UNP P18507
E	370	LYS	-	expression tag	UNP P18507
E	371	GLN	-	expression tag	UNP P18507
E	372	ALA	-	expression tag	UNP P18507
E	373	GLY	-	expression tag	UNP P18507

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Chain	Residue	Modelled	Actual	Comment	Reference
E	374	ASP	-	expression tag	UNP P18507
E	375	VAL	-	expression tag	UNP P18507
E	376	GLU	-	expression tag	UNP P18507
E	377	GLU	-	expression tag	UNP P18507
E	378	ASN	-	expression tag	UNP P18507
E	379	PRO	-	expression tag	UNP P18507
E	380	GLY	-	expression tag	UNP P18507

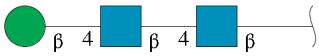
- Molecule 4 is a protein called Kappa Fab Light Chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	I	105	Total	C	H	N	O	S	0	0
			1573	504	771	130	163	5		
4	L	106	Total	C	H	N	O	S	0	0
			1595	510	784	132	164	5		

- Molecule 5 is a protein called IgG2b Fab Heavy Chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	J	116	Total	C	H	N	O	S	0	0
			1784	574	877	151	178	4		
5	K	117	Total	C	H	N	O	S	0	0
			1798	578	884	152	180	4		

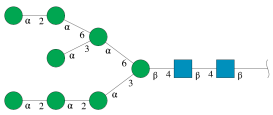
- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
6	H	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
6	M	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 7 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-mannopyra

nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

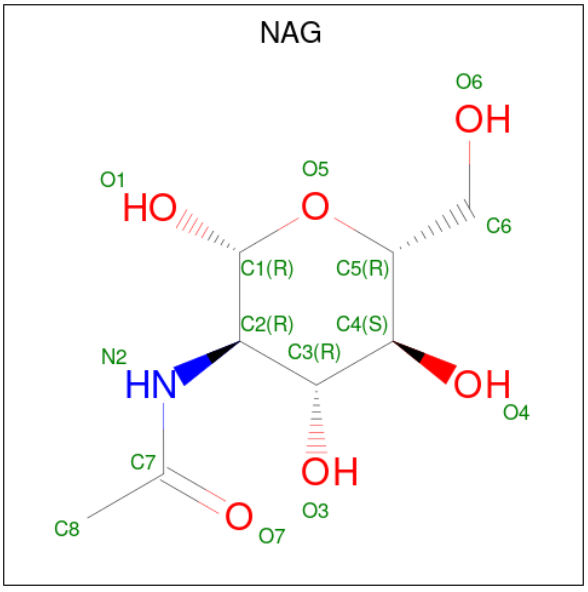


Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	10	Total	C	H	N	O	0	0
			213	64	97	2	50		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

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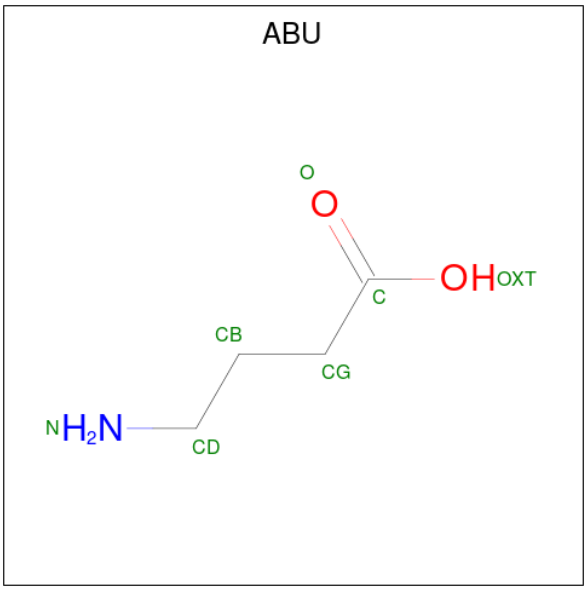
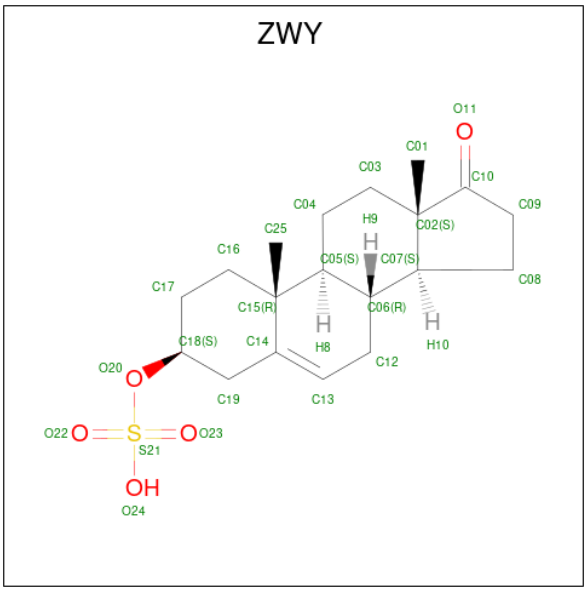
Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	H	N	O	0
			27	8	13	1	5	

- Molecule 10 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



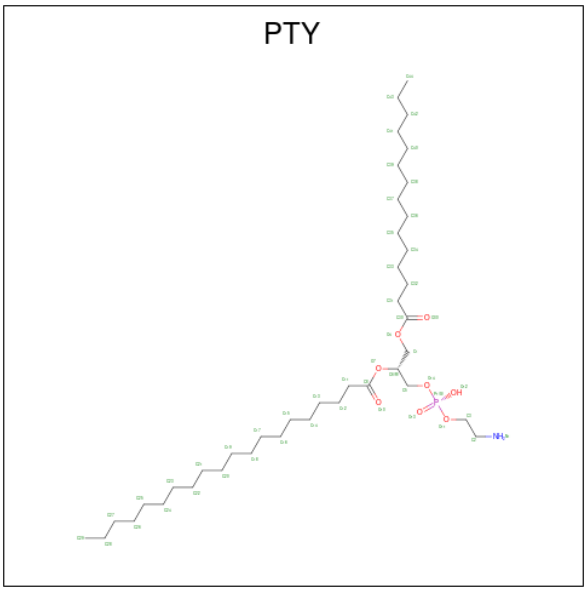
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			7	4	1	2	
10	C	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 11 is 17-oxoandrost-5-en-3beta-yl hydrogen sulfate (three-letter code: ZWY) (formula: $C_{19}H_{28}O_5S$).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	H	O	S	0
			53	19	28	5	1	

- Molecule 12 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	B	1	Total	C	N	O	P	0
			43	33	1	8	1	

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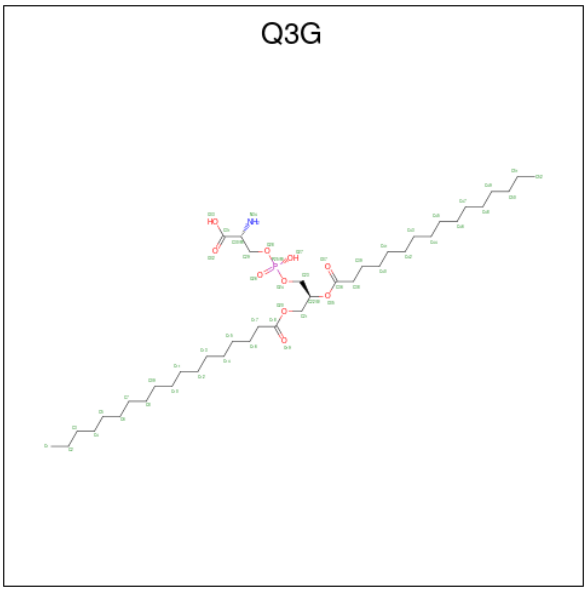
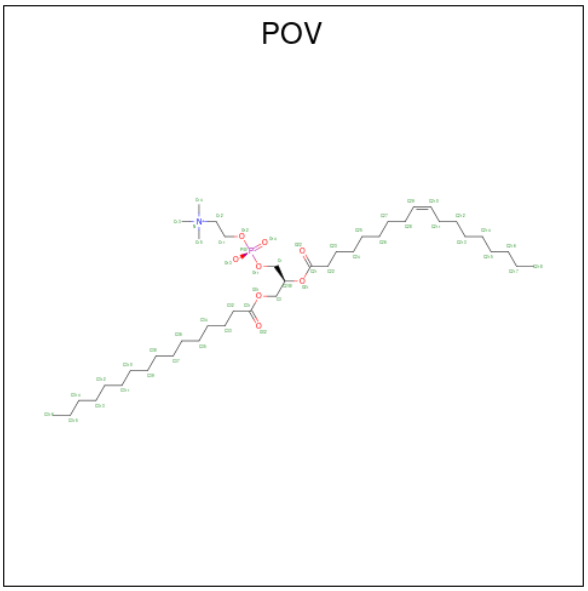
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
12	D	1	Total	C	N	O	P	0
			46	36	1	8	1	
12	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	D	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 13 is O-[(R)-[(2S)-2-(hexadecanoyloxy)-3-(octadecanoyloxy)propoxy](hydroxy)phosphoryl]-D-serine (three-letter code: Q3G) (formula: $C_{40}H_{78}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			41	29	1	10	1	

- Molecule 14 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



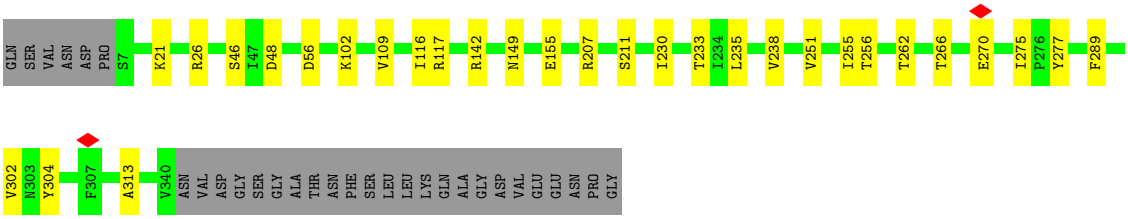
Mol	Chain	Residues	Atoms					AltConf
14	D	1	Total	C	N	O	P	0
			37	27	1	8	1	

3 Residue-property plots (i)

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

• Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2

Chain A:

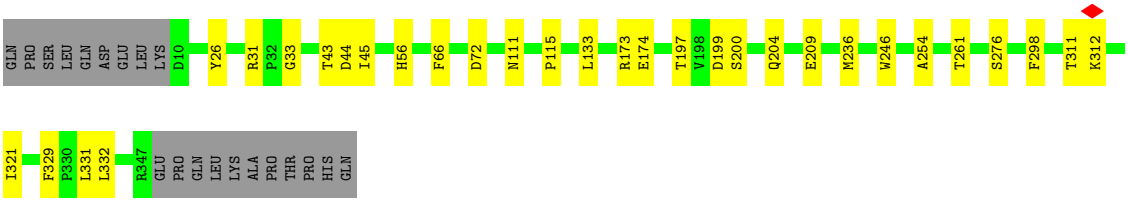


• Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2

Chain C:

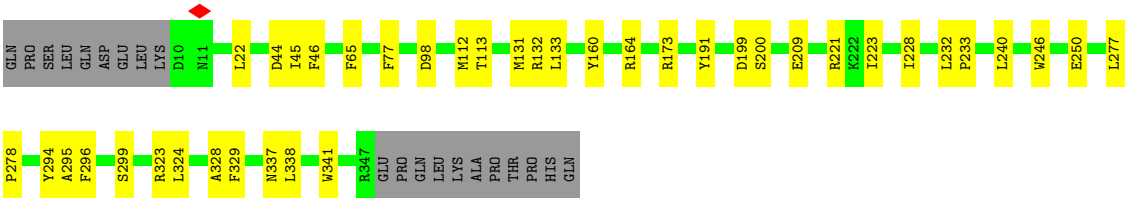
• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

Chain B:



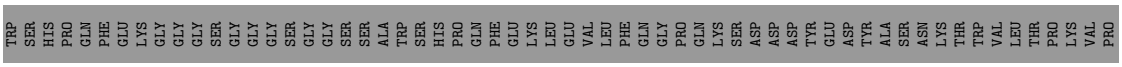
• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

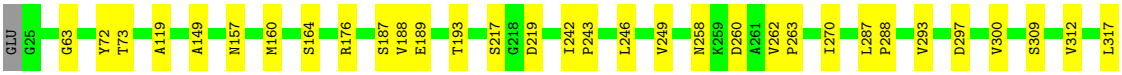
Chain D:



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

Chain E:



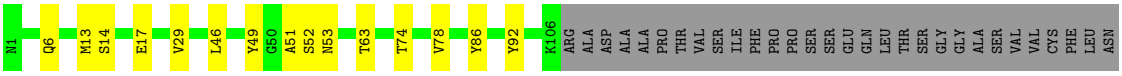


• Molecule 4: Kappa Fab Light Chain

Chain I:

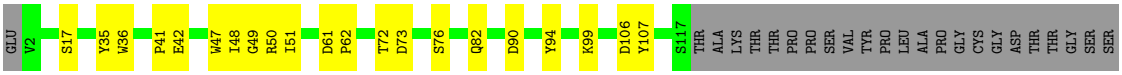
• Molecule 4: Kappa Fab Light Chain

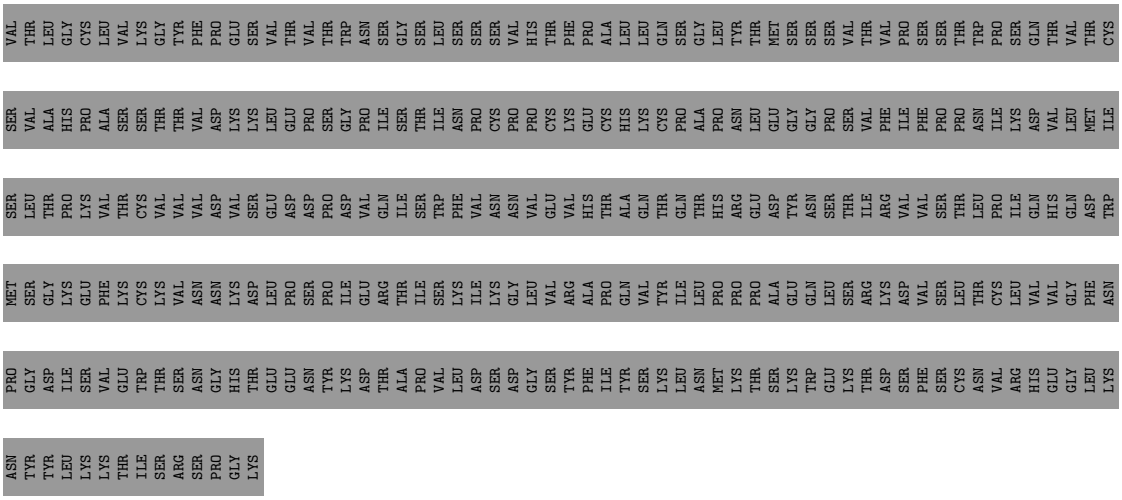
Chain L:



• Molecule 5: IgG2b Fab Heavy Chain

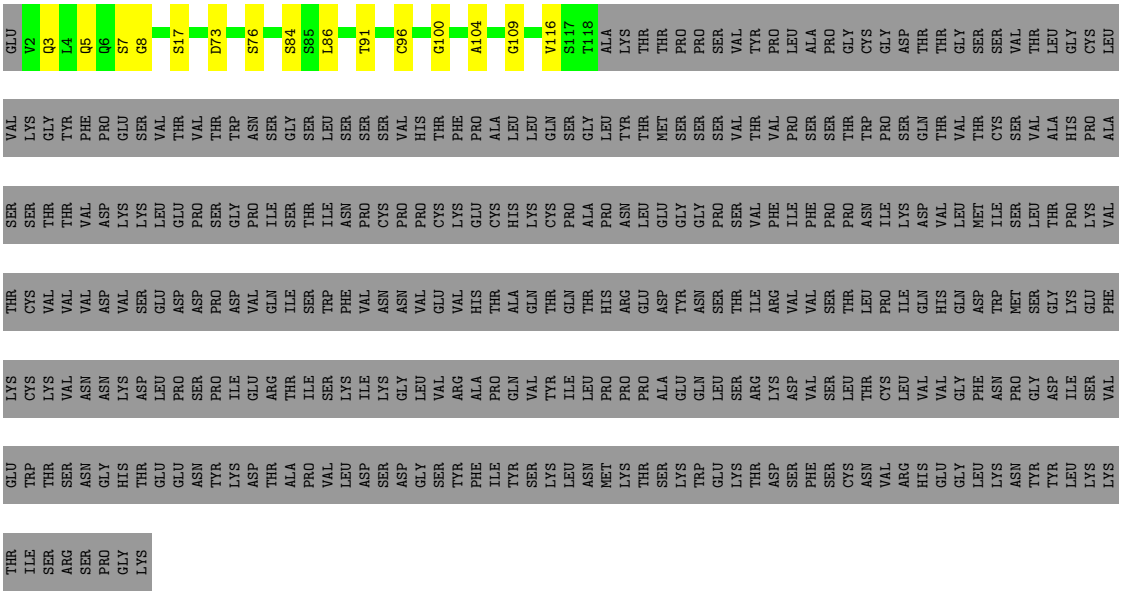
Chain J:





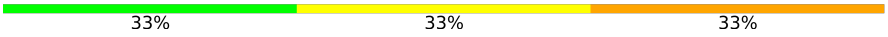
• Molecule 5: IgG2b Fab Heavy Chain

Chain K:



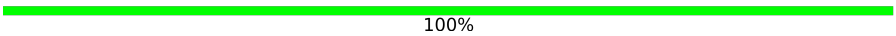
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



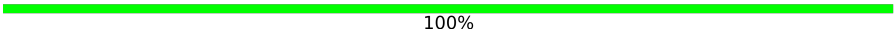
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



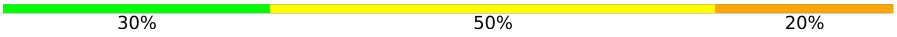
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• Molecule 7: 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 G:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188416	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.00	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	307.98718, 307.98718, 307.98718	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0694, 1.0694, 1.0694	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZWY, POV, PTY, MAN, NAG, BMA, ABU, Q3G

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	0.33	0/2804	0.52	0/3818
1	C	0.33	0/2804	0.51	0/3818
2	B	0.32	0/2799	0.53	0/3805
2	D	0.33	0/2799	0.53	0/3805
3	E	0.31	0/2805	0.52	0/3822
4	I	0.36	0/820	0.51	0/1112
4	L	0.35	0/829	0.49	0/1123
5	J	0.32	0/928	0.51	0/1260
5	K	0.32	0/935	0.49	0/1270
All	All	0.33	0/17523	0.52	0/23833

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	2732	2741	2742	23	0
1	C	2732	2741	2741	18	0
2	B	2730	2724	2724	24	0
2	D	2730	2724	2724	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2729	2714	2714	24	0
4	I	802	771	771	6	0
4	L	811	784	784	8	0
5	J	907	877	877	11	0
5	K	914	884	884	8	0
6	F	39	34	34	5	0
6	H	39	34	34	0	0
6	M	39	34	34	0	0
7	G	116	97	97	1	0
8	N	28	25	25	0	0
9	A	14	13	13	0	0
9	C	14	13	13	0	0
10	A	7	0	0	1	0
10	C	7	0	0	1	0
11	A	25	28	0	3	0
12	B	142	0	215	25	0
12	D	138	0	207	43	0
13	C	41	0	0	5	0
14	D	37	0	46	3	0
All	All	17773	17238	17679	186	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 5.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:TRP:CH2	12:B:403:PTY:H111	2.16	0.81
2:D:324:LEU:HD23	12:D:403:PTY:H121	1.68	0.75
2:D:338:LEU:HD11	14:D:401:POV:H28A	1.70	0.73
12:B:403:PTY:HC11	12:B:403:PTY:H122	1.70	0.72
12:D:404:PTY:H162	12:D:404:PTY:H121	1.72	0.72
12:D:402:PTY:HC52	12:D:402:PTY:N1	2.07	0.69
1:A:155:GLU:OE1	1:A:207:ARG:NH2	2.25	0.69
12:B:401:PTY:HC32	12:B:401:PTY:HC51	1.72	0.69
3:E:258:ASN:ND2	3:E:260:ASP:OD1	2.26	0.69
12:D:404:PTY:H132	12:D:404:PTY:HC11	1.76	0.68
11:A:403:ZWY:C09	3:E:263:PRO:HB2	2.25	0.67
12:D:404:PTY:HC11	12:D:404:PTY:C13	2.24	0.66
12:D:404:PTY:C20	12:D:404:PTY:H161	2.26	0.66
12:D:404:PTY:H132	12:D:404:PTY:C1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:SER:HB2	1:C:257:THR:HG21	1.80	0.63
1:C:28:ARG:NH1	1:C:30:ASP:O	2.32	0.62
1:C:155:GLU:OE2	10:C:402:ABU:N	2.33	0.62
12:D:404:PTY:H131	12:D:404:PTY:C17	2.29	0.62
2:B:44:ASP:OD2	2:B:173:ARG:NH2	2.34	0.61
1:A:235:LEU:O	1:A:238:VAL:HG12	2.00	0.60
2:B:31:ARG:NH1	2:B:33:GLY:O	2.34	0.60
1:A:262:THR:HG23	12:B:401:PTY:H272	1.83	0.60
2:D:246:TRP:HZ2	12:D:404:PTY:H141	1.66	0.60
2:B:56:HIS:NE2	2:B:276:SER:O	2.35	0.59
5:J:47:TRP:NE1	5:J:49:GLY:O	2.35	0.59
2:D:191:TYR:OH	2:D:221:ARG:NH2	2.34	0.59
1:A:251:VAL:HG21	2:B:254:ALA:HB1	1.85	0.59
1:A:149:ASN:ND2	6:F:1:NAG:C1	2.67	0.58
2:D:223:ILE:CG2	12:D:402:PTY:HC51	2.33	0.57
13:C:403:Q3G:C23	12:D:402:PTY:H122	2.34	0.57
4:L:63:THR:OG1	4:L:74:THR:OG1	2.23	0.57
12:D:404:PTY:HC11	12:D:404:PTY:H122	1.86	0.57
12:D:404:PTY:H351	12:D:404:PTY:H181	1.88	0.56
2:B:174:GLU:OE2	5:J:50:ARG:NH1	2.39	0.56
13:C:403:Q3G:O28	12:D:402:PTY:H111	2.06	0.56
3:E:63:GLY:N	3:E:73:THR:O	2.39	0.55
5:K:100:GLY:N	5:K:104:ALA:O	2.35	0.55
11:A:403:ZWY:O11	1:C:248:ALA:HB1	2.07	0.54
12:D:404:PTY:HC11	12:D:404:PTY:C12	2.37	0.54
2:D:328:ALA:HB1	12:D:403:PTY:H162	1.88	0.54
1:A:289:PHE:CE1	12:B:401:PTY:H262	2.43	0.53
2:D:232:LEU:HD11	12:D:402:PTY:H162	1.91	0.53
2:D:337:ASN:ND2	12:D:402:PTY:H402	2.24	0.53
6:F:1:NAG:O3	6:F:2:NAG:O5	2.22	0.53
14:D:401:POV:H25A	12:D:402:PTY:H381	1.91	0.53
2:D:223:ILE:HG23	12:D:402:PTY:HC51	1.90	0.53
4:I:6:GLN:NE2	4:I:86:TYR:O	2.41	0.52
1:A:109:VAL:HG11	3:E:119:ALA:HB3	1.92	0.52
2:B:44:ASP:OD1	2:B:45:ILE:N	2.42	0.52
1:A:155:GLU:OE2	10:A:402:ABU:N	2.43	0.52
1:A:46:SER:OG	1:A:48:ASP:OD1	2.26	0.52
1:A:230:ILE:O	1:A:233:THR:HG22	2.10	0.52
5:J:61:ASP:OD1	5:J:62:PRO:HD2	2.10	0.52
2:D:44:ASP:OD1	2:D:45:ILE:N	2.42	0.52
12:D:404:PTY:H322	12:D:404:PTY:HC12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4:MAN:O3	7:G:6:MAN:O6	2.17	0.51
2:D:131:MET:HE2	2:D:133:LEU:HD21	1.92	0.51
2:B:246:TRP:HH2	12:B:403:PTY:H111	1.69	0.51
1:A:56:ASP:OD2	1:A:102:LYS:NZ	2.43	0.51
2:B:298:PHE:HB3	12:B:402:PTY:H382	1.93	0.50
12:B:403:PTY:H443	12:B:403:PTY:H372	1.92	0.50
3:E:157:ASN:O	3:E:160:MET:N	2.44	0.50
5:K:7:SER:OG	5:K:8:GLY:N	2.45	0.50
12:D:402:PTY:HC52	12:D:402:PTY:HN11	1.74	0.50
1:C:232:ILE:CG2	1:C:257:THR:HG23	2.42	0.50
4:L:6:GLN:NE2	4:L:86:TYR:O	2.36	0.50
2:B:26:TYR:OH	2:B:72:ASP:OD2	2.28	0.50
5:J:106:ASP:OD1	5:J:107:TYR:N	2.45	0.50
2:B:331:LEU:HD12	12:B:403:PTY:H212	1.94	0.50
1:A:275:ILE:HD12	1:A:277:TYR:CE1	2.47	0.49
2:D:323:ARG:HD3	12:D:404:PTY:HN12	1.77	0.49
1:C:232:ILE:HG23	1:C:257:THR:HG23	1.94	0.49
2:B:298:PHE:CG	12:B:402:PTY:H401	2.48	0.49
4:L:14:SER:N	4:L:17:GLU:OE2	2.45	0.49
5:J:73:ASP:OD1	5:J:76:SER:OG	2.27	0.48
3:E:187:SER:OG	3:E:188:VAL:N	2.46	0.48
2:B:204:GLN:NE2	2:B:209:GLU:OE2	2.46	0.48
12:B:403:PTY:H192	12:B:403:PTY:H161	1.71	0.48
4:I:14:SER:N	4:I:17:GLU:OE2	2.46	0.48
5:J:41:PRO:HB2	5:J:42:GLU:OE1	2.13	0.48
13:C:403:Q3G:N34	12:D:402:PTY:C3	2.76	0.48
12:D:402:PTY:H332	12:D:402:PTY:H361	1.60	0.48
5:K:96:CYS:O	5:K:109:GLY:N	2.47	0.48
13:C:403:Q3G:O24	12:D:402:PTY:H112	2.13	0.47
2:D:329:PHE:CZ	12:D:403:PTY:H181	2.50	0.47
5:K:3:GLN:NE2	5:K:5:GLN:OE1	2.47	0.47
12:D:404:PTY:H351	12:D:404:PTY:H171	1.96	0.47
3:E:287:LEU:HB2	3:E:288:PRO:HD2	1.96	0.47
5:J:90:ASP:OD1	5:J:94:TYR:OH	2.33	0.47
1:C:301:LEU:HD11	12:D:404:PTY:H442	1.96	0.47
1:A:255:ILE:HG23	2:B:261:THR:HG21	1.96	0.47
1:A:117:ARG:NH2	3:E:217:SER:OG	2.48	0.46
1:A:256:THR:HG21	3:E:270:ILE:HG13	1.97	0.46
2:D:232:LEU:HD13	12:D:402:PTY:H182	1.95	0.46
5:K:73:ASP:OD2	5:K:76:SER:OG	2.30	0.46
1:A:142:ARG:HG2	1:A:142:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:TRP:CZ2	12:D:404:PTY:H141	2.47	0.46
12:B:403:PTY:H391	12:B:403:PTY:H362	1.47	0.46
2:D:44:ASP:OD2	2:D:173:ARG:NH2	2.49	0.46
3:E:164:SER:O	3:E:164:SER:OG	2.32	0.46
2:B:311:THR:HG22	2:B:312:LYS:HG3	1.97	0.46
2:D:299:SER:HA	12:D:403:PTY:H351	1.98	0.46
2:B:66:PHE:HB2	2:B:133:LEU:HD21	1.97	0.45
1:C:265:ASN:OD1	1:C:269:ARG:NE	2.49	0.45
4:L:13:MET:HE3	4:L:78:VAL:HG21	1.99	0.45
12:B:402:PTY:H392	12:B:402:PTY:H422	1.67	0.45
4:L:51:ALA:O	4:L:52:SER:OG	2.31	0.45
1:A:211:SER:HB2	6:F:1:NAG:O7	2.17	0.45
1:A:304:TYR:CE1	12:B:403:PTY:HC22	2.52	0.45
2:D:228:ILE:HD11	12:D:402:PTY:H121	1.99	0.45
1:A:302:VAL:HG13	1:A:313:ALA:HB1	1.98	0.45
2:B:321:ILE:HG21	12:B:402:PTY:HC52	1.98	0.45
3:E:309:SER:HA	3:E:312:VAL:HG12	1.98	0.45
3:E:189:GLU:O	3:E:189:GLU:HG3	2.17	0.44
1:C:222:ILE:O	1:C:227:MET:HG2	2.16	0.44
3:E:176:ARG:N	3:E:219:ASP:O	2.42	0.44
12:B:403:PTY:H142	12:B:403:PTY:H172	1.34	0.44
1:C:43:ASP:HB3	1:C:62:TYR:HB2	1.98	0.44
1:C:265:ASN:O	1:C:269:ARG:NE	2.50	0.44
2:B:329:PHE:CE2	12:B:402:PTY:H191	2.52	0.44
1:C:230:ILE:O	1:C:234:ILE:HG12	2.18	0.44
2:D:250:GLU:N	2:D:250:GLU:OE1	2.50	0.44
1:A:149:ASN:HD21	6:F:1:NAG:C7	2.31	0.44
12:B:401:PTY:H252	12:B:401:PTY:H222	1.86	0.44
3:E:246:LEU:HA	3:E:249:VAL:HG22	1.98	0.44
2:D:232:LEU:HB2	2:D:233:PRO:HD3	2.00	0.44
2:D:294:TYR:CE2	3:E:246:LEU:HD13	2.53	0.44
3:E:262:VAL:N	3:E:263:PRO:HD2	2.32	0.44
3:E:297:ASP:HA	3:E:300:VAL:HG22	1.99	0.44
3:E:72:TYR:CE1	3:E:149:ALA:HB3	2.53	0.43
2:B:197:THR:HG23	4:I:28:TYR:CE1	2.54	0.43
1:C:332:ASN:OD1	1:C:336:TRP:CD1	2.72	0.43
2:D:199:ASP:OD1	2:D:200:SER:N	2.50	0.43
3:E:193:THR:HG22	3:E:193:THR:O	2.18	0.43
2:B:111:ASN:HA	2:B:115:PRO:HA	2.00	0.43
12:B:403:PTY:H342	12:B:403:PTY:H371	1.59	0.43
1:C:146:ASP:OD2	1:C:148:GLN:NE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:PHE:HB3	2:D:65:PHE:HB2	2.00	0.43
2:D:164:ARG:N	2:D:209:GLU:O	2.50	0.43
3:E:317:LEU:O	3:E:321:VAL:HG23	2.19	0.43
2:B:236:MET:HG3	12:B:401:PTY:H241	2.00	0.43
4:L:29:VAL:HG12	4:L:92:TYR:HB3	2.01	0.43
12:B:403:PTY:H322	12:B:403:PTY:H351	1.74	0.42
11:A:403:ZWY:C09	3:E:263:PRO:CB	2.95	0.42
1:C:258:VAL:HG11	2:D:240:LEU:CD1	2.49	0.42
3:E:323:SER:OG	3:E:324:GLN:N	2.52	0.42
2:B:199:ASP:OD1	2:B:200:SER:N	2.51	0.42
2:D:338:LEU:HD11	14:D:401:POV:C28	2.42	0.42
12:B:402:PTY:H442	1:C:231:LEU:HD11	2.01	0.42
4:I:11:MET:HE1	4:I:19:VAL:HG23	2.00	0.42
1:A:116:ILE:O	1:A:116:ILE:HG23	2.19	0.42
12:D:403:PTY:O13	12:D:403:PTY:HC6	2.19	0.42
5:K:86:LEU:HD13	5:K:116:VAL:HG11	2.01	0.42
1:A:149:ASN:HD21	6:F:1:NAG:C1	2.33	0.42
12:D:403:PTY:H232	12:D:403:PTY:H262	1.55	0.42
4:I:33:VAL:HG21	4:I:71:PHE:CG	2.55	0.42
1:A:266:THR:O	1:A:270:GLU:HG2	2.20	0.42
5:J:17:SER:OG	5:J:82:GLN:OE1	2.38	0.42
4:L:49:TYR:O	4:L:53:ASN:HB2	2.19	0.42
1:C:40:MET:HG3	1:C:208:LEU:HD12	2.02	0.41
2:D:22:LEU:HD11	2:D:77:PHE:HB3	2.02	0.41
2:D:341:TRP:CZ3	12:D:402:PTY:H322	2.55	0.41
2:D:329:PHE:CE1	12:D:403:PTY:H172	2.55	0.41
5:J:51:ILE:HD13	5:J:72:THR:HG23	2.03	0.41
2:D:98:ASP:OD2	2:D:160:TYR:O	2.38	0.41
2:D:223:ILE:HG22	12:D:402:PTY:HC51	2.01	0.41
2:D:296:PHE:CE2	12:D:403:PTY:H211	2.55	0.41
12:B:401:PTY:HC51	12:B:401:PTY:C3	2.44	0.41
2:D:112:MET:HA	2:D:113:THR:HA	1.84	0.41
12:D:404:PTY:H161	12:D:404:PTY:H201	1.99	0.41
5:J:36:TRP:O	5:J:48:ILE:HB	2.21	0.41
4:L:46:LEU:HD21	4:L:49:TYR:HB3	2.03	0.41
2:D:295:ALA:HA	12:D:403:PTY:H432	2.03	0.41
2:B:332:LEU:HD12	12:B:402:PTY:H181	2.03	0.41
1:C:101:ASP:OD1	2:D:132:ARG:NH2	2.40	0.41
5:K:17:SER:OG	5:K:84:SER:O	2.36	0.41
12:B:402:PTY:O7	12:B:402:PTY:HC21	2.20	0.41
5:J:35:TYR:HE1	5:J:99:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:242:ILE:HB	3:E:243:PRO:HD3	2.02	0.40
4:I:33:VAL:O	4:I:33:VAL:HG23	2.21	0.40
2:D:296:PHE:CD2	12:D:403:PTY:H211	2.56	0.40
2:B:43:THR:HG22	2:B:44:ASP:N	2.36	0.40
3:E:293:VAL:HG23	3:E:297:ASP:OD1	2.21	0.40
5:K:91:THR:HB	5:K:116:VAL:HG22	2.04	0.40
13:C:403:Q3G:N34	12:D:402:PTY:HC31	2.37	0.40
2:D:277:LEU:HG	2:D:278:PRO:HD2	2.02	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	332/364 (91%)	320 (96%)	12 (4%)	0	100	100
1	C	332/364 (91%)	320 (96%)	12 (4%)	0	100	100
2	B	336/358 (94%)	324 (96%)	12 (4%)	0	100	100
2	D	336/358 (94%)	327 (97%)	9 (3%)	0	100	100
3	E	331/417 (79%)	309 (93%)	22 (7%)	0	100	100
4	I	103/213 (48%)	96 (93%)	7 (7%)	0	100	100
4	L	104/213 (49%)	95 (91%)	9 (9%)	0	100	100
5	J	114/454 (25%)	107 (94%)	7 (6%)	0	100	100
5	K	115/454 (25%)	110 (96%)	5 (4%)	0	100	100
All	All	2103/3195 (66%)	2008 (96%)	95 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	302/326 (93%)	300 (99%)	2 (1%)	84 93
1	C	302/326 (93%)	301 (100%)	1 (0%)	92 97
2	B	300/319 (94%)	300 (100%)	0	100 100
2	D	300/319 (94%)	300 (100%)	0	100 100
3	E	305/372 (82%)	305 (100%)	0	100 100
4	I	89/188 (47%)	89 (100%)	0	100 100
4	L	90/188 (48%)	90 (100%)	0	100 100
5	J	97/407 (24%)	97 (100%)	0	100 100
5	K	98/407 (24%)	98 (100%)	0	100 100
All	All	1883/2852 (66%)	1880 (100%)	3 (0%)	93 98

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

Mol	Chain	Res	Type
1	A	21	LYS
1	A	26	ARG
1	C	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	267	HIS
2	B	102	HIS
2	D	56	HIS
2	D	337	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)

21 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	$\#\|Z\| > 2$
6	NAG	F	1	6	14,14,15	0.58	1 (7%)	17,19,21	0.51	0
6	NAG	F	2	6	14,14,15	0.21	0	17,19,21	0.47	0
6	BMA	F	3	6	11,11,12	0.56	0	15,15,17	0.68	0
7	NAG	G	1	2,7	14,14,15	0.30	0	17,19,21	0.52	0
7	MAN	G	10	7	11,11,12	0.56	0	15,15,17	1.11	2 (13%)
7	NAG	G	2	7	14,14,15	0.26	0	17,19,21	0.37	0
7	BMA	G	3	7	11,11,12	0.55	0	15,15,17	0.73	0
7	MAN	G	4	7	11,11,12	0.49	0	15,15,17	1.37	2 (13%)
7	MAN	G	5	7	11,11,12	0.60	0	15,15,17	0.95	1 (6%)
7	MAN	G	6	7	11,11,12	0.57	0	15,15,17	0.89	1 (6%)
7	MAN	G	7	7	11,11,12	0.96	1 (9%)	15,15,17	1.03	1 (6%)
7	MAN	G	8	7	11,11,12	0.52	0	15,15,17	1.15	2 (13%)
7	MAN	G	9	7	11,11,12	0.54	0	15,15,17	0.94	1 (6%)
6	NAG	H	1	6,1	14,14,15	0.25	0	17,19,21	0.55	0
6	NAG	H	2	6	14,14,15	0.27	0	17,19,21	0.53	0
6	BMA	H	3	6	11,11,12	0.58	0	15,15,17	0.71	0
6	NAG	M	1	6,2	14,14,15	0.35	0	17,19,21	0.39	0
6	NAG	M	2	6	14,14,15	0.23	0	17,19,21	0.53	0
6	BMA	M	3	6	11,11,12	0.55	0	15,15,17	0.74	0
8	NAG	N	1	3,8	14,14,15	0.42	0	17,19,21	0.56	0
8	NAG	N	2	8	14,14,15	0.26	0	17,19,21	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	7	MAN	O5-C1	-2.63	1.39	1.43
6	F	1	NAG	O5-C1	-2.05	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	4	MAN	C1-O5-C5	3.72	117.24	112.19
7	G	8	MAN	C1-O5-C5	3.14	116.44	112.19
7	G	10	MAN	C1-O5-C5	2.80	115.99	112.19
7	G	4	MAN	O2-C2-C3	-2.63	104.87	110.14
7	G	7	MAN	O2-C2-C3	-2.59	104.94	110.14
7	G	8	MAN	O2-C2-C3	-2.35	105.42	110.14
7	G	10	MAN	O2-C2-C3	-2.30	105.54	110.14
7	G	9	MAN	C1-O5-C5	2.29	115.29	112.19
7	G	6	MAN	O2-C2-C3	-2.25	105.64	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	5	MAN	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	2	NAG	O5-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6
7	G	3	BMA	C4-C5-C6-O6
8	N	1	NAG	C8-C7-N2-C2
8	N	1	NAG	O7-C7-N2-C2
8	N	2	NAG	C4-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
7	G	5	MAN	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
6	H	1	NAG	C1-C2-N2-C7
7	G	2	NAG	C4-C5-C6-O6
7	G	10	MAN	O5-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	F	1	NAG	C1-C2-N2-C7
6	F	1	NAG	C4-C5-C6-O6
7	G	5	MAN	C4-C5-C6-O6
6	M	3	BMA	C4-C5-C6-O6

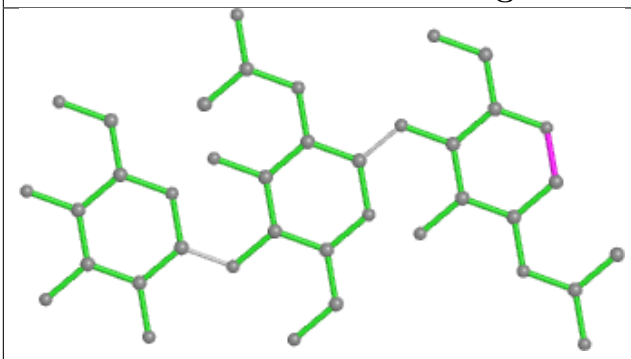
There are no ring outliers.

4 monomers are involved in 6 short contacts:

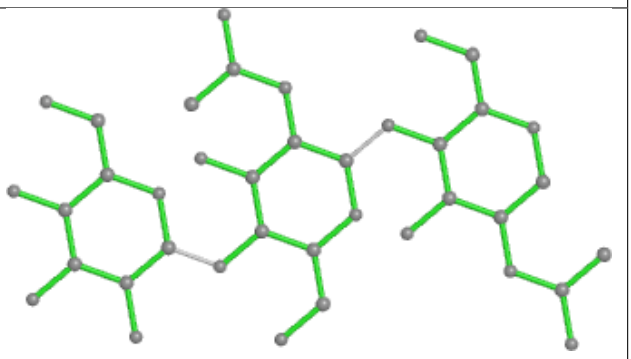
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	5	0
7	G	6	MAN	1	0
7	G	4	MAN	1	0
6	F	2	NAG	1	0

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

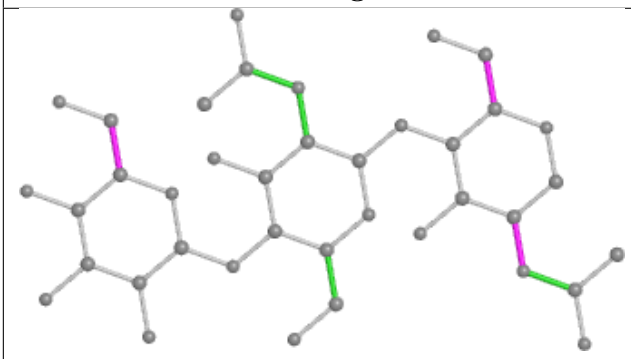
Oligosaccharide Chain F



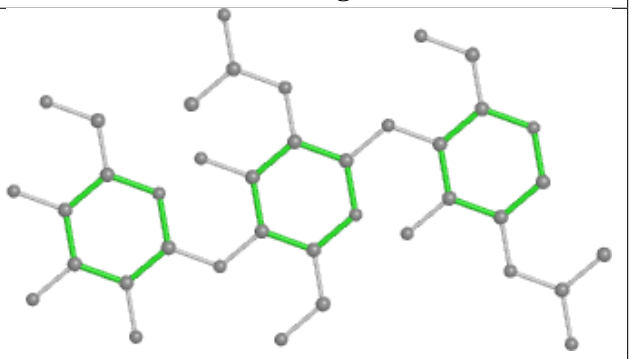
Bond lengths



Bond angles

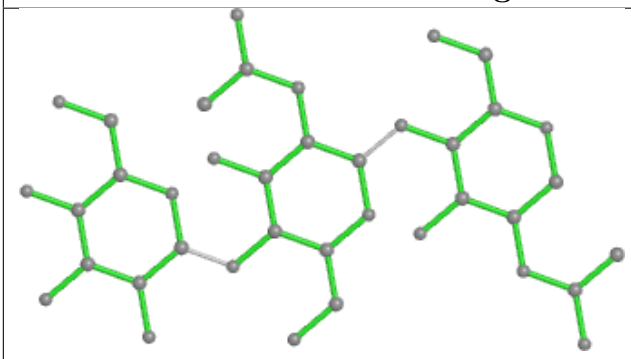


Torsions

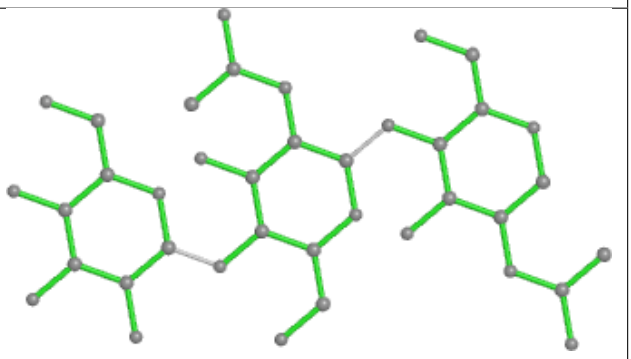


Rings

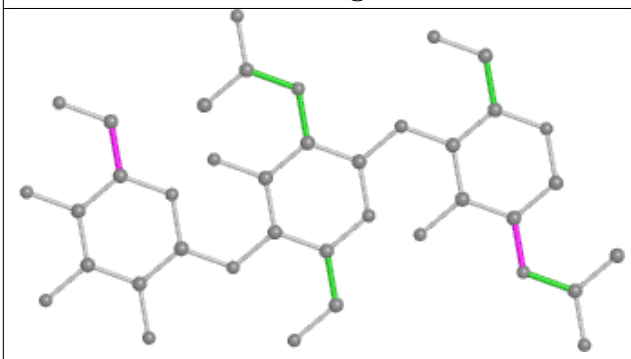
Oligosaccharide Chain H



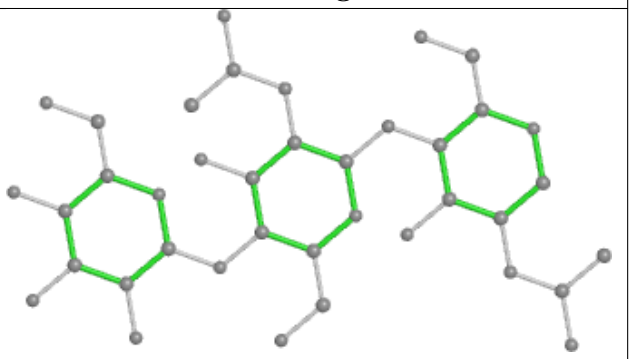
Bond lengths



Bond angles

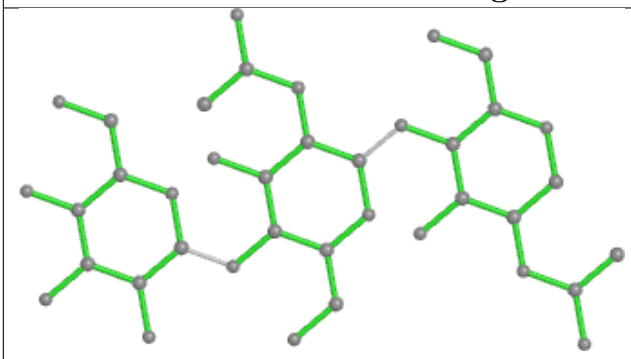


Torsions

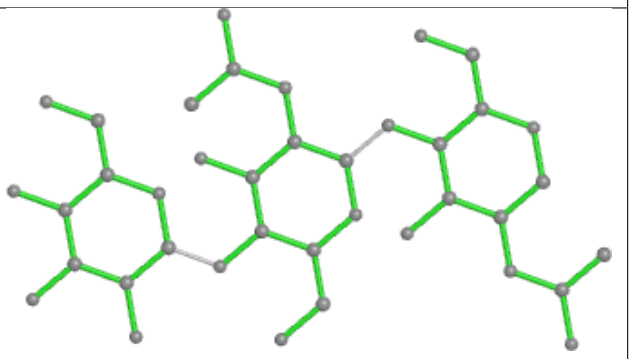


Rings

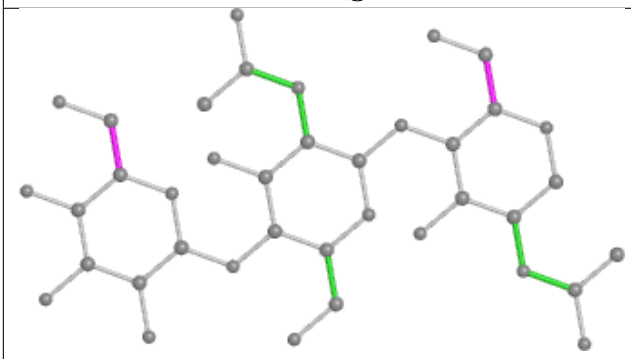
Oligosaccharide Chain M



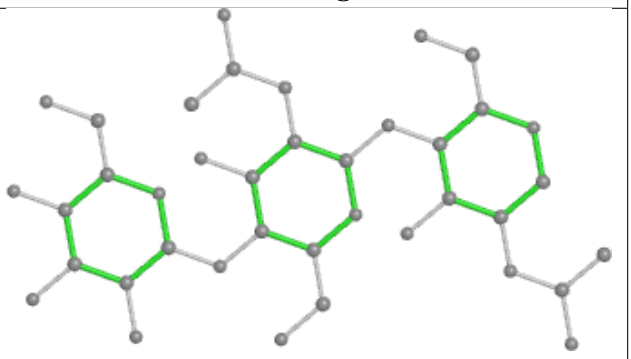
Bond lengths



Bond angles

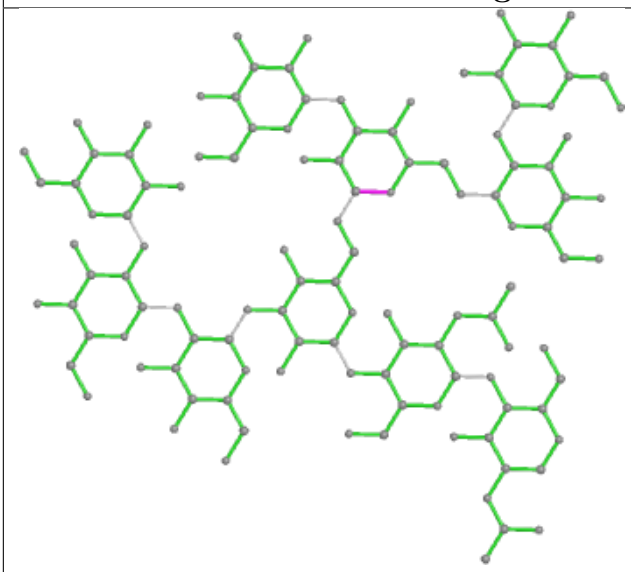


Torsions

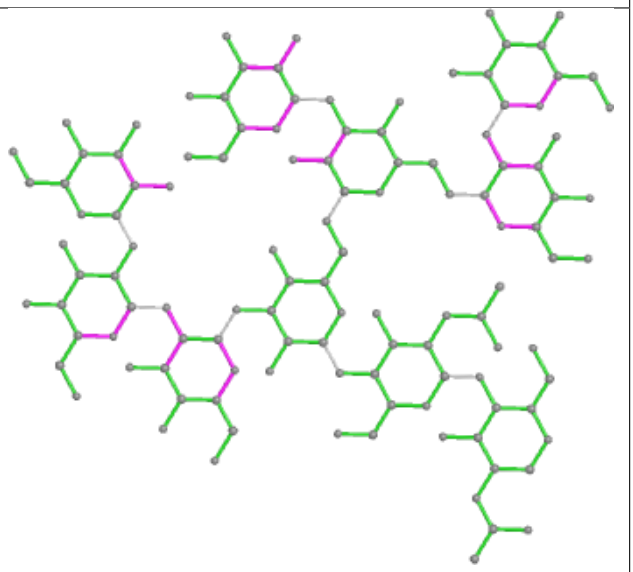


Rings

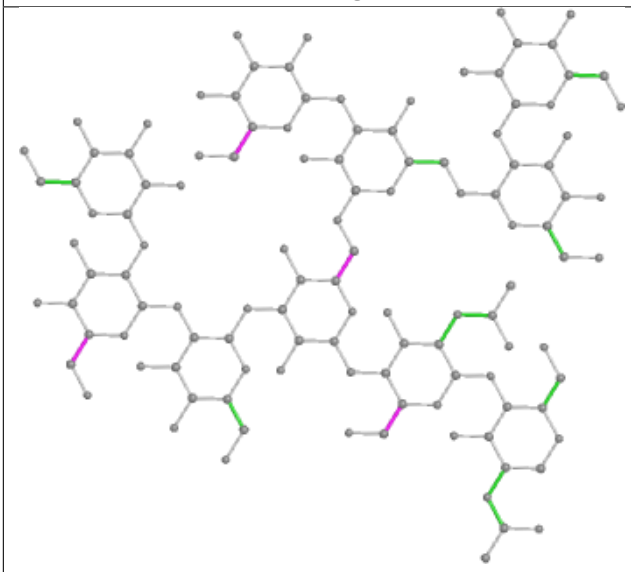
Oligosaccharide Chain G



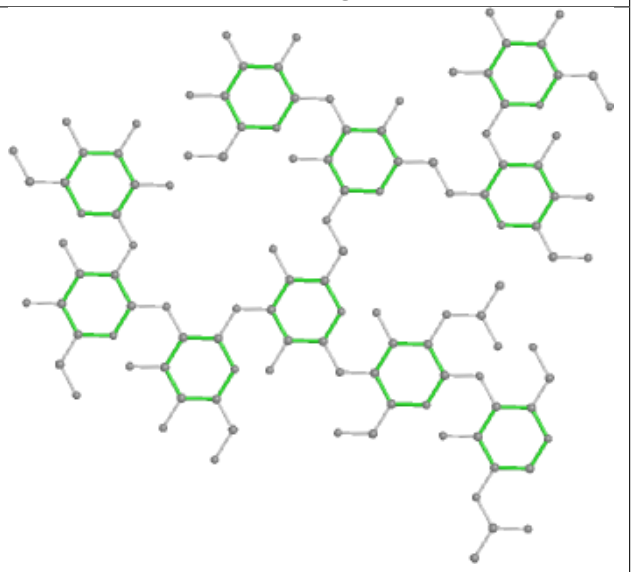
Bond lengths



Bond angles

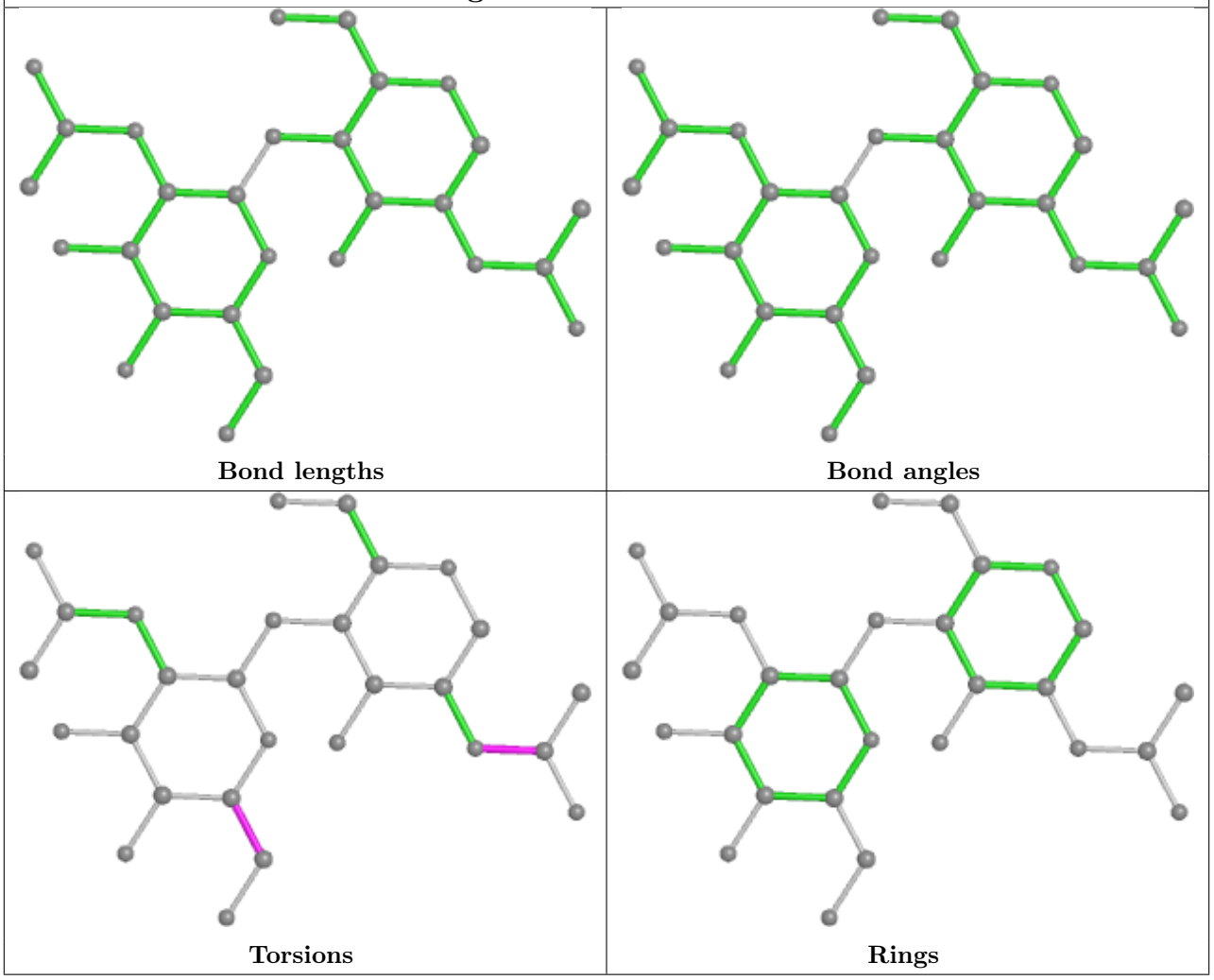


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
10	ABU	C	402	-	6,6,6	0.86	0	6,6,6	1.48	1 (16%)
12	PTY	D	403	-	49,49,49	0.27	0	52,54,54	0.32	0
12	PTY	B	403	-	48,48,49	0.29	0	51,53,54	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	POV	D	401	-	36,36,51	0.94	1 (2%)	41,44,59	0.81	1 (2%)
10	ABU	A	402	-	6,6,6	0.85	0	6,6,6	1.49	1 (16%)
12	PTY	D	404	-	41,41,49	0.30	0	44,46,54	0.33	0
12	PTY	D	402	-	45,45,49	0.28	0	48,50,54	0.34	0
9	NAG	C	401	1	14,14,15	0.22	0	17,19,21	0.42	0
12	PTY	B	402	-	42,42,49	0.29	0	45,47,54	0.34	0
11	ZWY	A	403	-	28,28,28	0.26	0	42,46,46	0.64	1 (2%)
12	PTY	B	401	-	49,49,49	0.27	0	52,54,54	0.31	0
13	Q3G	C	403	-	39,40,51	0.68	0	43,47,58	0.99	1 (2%)
9	NAG	A	401	1	14,14,15	0.18	0	17,19,21	0.48	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
10	ABU	C	402	-	-	2/4/4/4	-
12	PTY	D	403	-	-	34/53/53/53	-
12	PTY	B	403	-	-	38/52/52/53	-
14	POV	D	401	-	-	13/40/40/55	-
10	ABU	A	402	-	-	0/4/4/4	-
12	PTY	D	404	-	-	29/45/45/53	-
12	PTY	D	402	-	-	25/49/49/53	-
9	NAG	C	401	1	-	2/6/23/26	0/1/1/1
12	PTY	B	402	-	-	31/46/46/53	-
11	ZWY	A	403	-	-	0/5/63/63	0/4/4/4
12	PTY	B	401	-	-	28/53/53/53	-
13	Q3G	C	403	-	-	17/46/46/57	-
9	NAG	A	401	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	401	POV	C29-C210	3.74	1.53	1.31

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	403	Q3G	C21-O20-C18	-2.98	106.10	117.12
11	A	403	ZWY	O23-S21-O22	2.62	122.73	112.22
10	A	402	ABU	CB-CG-C	-2.18	108.98	114.47
10	C	402	ABU	CB-CG-C	-2.06	109.28	114.47
14	D	401	POV	C3-O31-C31	-2.05	109.52	117.12

There are no chirality outliers.

All (221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	401	PTY	N1-C2-C3-O11
12	B	402	PTY	N1-C2-C3-O11
12	B	402	PTY	C3-O11-P1-O13
12	B	402	PTY	C5-O14-P1-O12
12	B	402	PTY	C5-O14-P1-O13
12	B	403	PTY	C31-C30-O4-C1
12	B	403	PTY	O30-C30-O4-C1
12	B	403	PTY	C11-C8-O7-C6
12	B	403	PTY	C3-O11-P1-O12
12	B	403	PTY	C3-O11-P1-O13
12	B	403	PTY	C3-O11-P1-O14
12	B	403	PTY	C5-O14-P1-O12
12	B	403	PTY	C5-O14-P1-O13
12	D	402	PTY	N1-C2-C3-O11
12	D	402	PTY	C3-O11-P1-O13
12	D	402	PTY	C5-O14-P1-O13
12	D	403	PTY	C6-C5-O14-P1
12	D	403	PTY	C11-C8-O7-C6
12	D	403	PTY	C5-O14-P1-O13
12	D	404	PTY	C6-C5-O14-P1
12	D	404	PTY	C3-O11-P1-O12
12	D	404	PTY	C5-O14-P1-O11
12	D	404	PTY	C5-O14-P1-O13
13	C	403	Q3G	N34-C30-C31-O32
14	D	401	POV	C11-O12-P-O14
12	D	403	PTY	O30-C30-O4-C1
12	B	401	PTY	O30-C30-O4-C1
12	D	404	PTY	O30-C30-O4-C1
12	B	403	PTY	O10-C8-O7-C6
12	D	403	PTY	O10-C8-O7-C6
9	A	401	NAG	C4-C5-C6-O6
12	B	401	PTY	C31-C30-O4-C1
12	D	403	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
12	D	404	PTY	C31-C30-O4-C1
9	A	401	NAG	O5-C5-C6-O6
12	D	403	PTY	C23-C24-C25-C26
12	D	403	PTY	C32-C33-C34-C35
12	D	402	PTY	C33-C34-C35-C36
13	C	403	Q3G	C17-C18-O20-C21
12	D	404	PTY	C11-C8-O7-C6
12	D	404	PTY	C13-C14-C15-C16
12	B	401	PTY	C24-C25-C26-C27
12	B	403	PTY	C14-C15-C16-C17
12	B	403	PTY	C34-C35-C36-C37
12	D	403	PTY	C17-C18-C19-C20
12	D	403	PTY	C40-C41-C42-C43
12	B	403	PTY	C11-C12-C13-C14
12	B	403	PTY	C36-C37-C38-C39
12	D	404	PTY	C33-C34-C35-C36
13	C	403	Q3G	O19-C18-O20-C21
12	B	403	PTY	C16-C17-C18-C19
12	D	402	PTY	C30-C31-C32-C33
14	D	401	POV	C32-C31-O31-C3
12	B	403	PTY	C32-C33-C34-C35
12	B	401	PTY	C30-C31-C32-C33
12	B	402	PTY	C30-C31-C32-C33
12	D	403	PTY	C8-C11-C12-C13
13	C	403	Q3G	N34-C30-C31-O33
12	B	401	PTY	C13-C14-C15-C16
12	D	404	PTY	O10-C8-O7-C6
12	D	404	PTY	C16-C17-C18-C19
12	B	402	PTY	C39-C40-C41-C42
14	D	401	POV	O32-C31-O31-C3
12	B	402	PTY	C3-O11-P1-O14
12	B	402	PTY	C5-O14-P1-O11
12	B	403	PTY	C5-O14-P1-O11
13	C	403	Q3G	C23-O24-P25-O28
14	D	401	POV	O22-C21-O21-C2
12	B	401	PTY	C22-C23-C24-C25
12	B	402	PTY	C8-C11-C12-C13
12	B	402	PTY	C31-C32-C33-C34
12	D	402	PTY	C13-C14-C15-C16
12	B	401	PTY	C11-C8-O7-C6
14	D	401	POV	C22-C21-O21-C2
12	B	402	PTY	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
12	B	403	PTY	C15-C16-C17-C18
12	D	404	PTY	C15-C16-C17-C18
12	D	402	PTY	C32-C33-C34-C35
12	D	403	PTY	C5-C6-O7-C8
12	B	401	PTY	O10-C8-O7-C6
12	B	401	PTY	C25-C26-C27-C28
12	B	401	PTY	C21-C22-C23-C24
12	B	402	PTY	C17-C18-C19-C20
12	B	402	PTY	C33-C34-C35-C36
13	C	403	Q3G	C45-C46-C47-C48
12	B	402	PTY	C37-C38-C39-C40
12	B	402	PTY	C13-C14-C15-C16
12	D	402	PTY	C12-C13-C14-C15
12	D	403	PTY	C34-C35-C36-C37
12	D	402	PTY	C18-C19-C20-C21
12	D	403	PTY	C11-C12-C13-C14
12	D	403	PTY	C13-C14-C15-C16
12	B	403	PTY	C35-C36-C37-C38
12	B	401	PTY	C35-C36-C37-C38
12	B	402	PTY	C35-C36-C37-C38
12	B	403	PTY	C19-C20-C21-C22
12	B	403	PTY	C37-C38-C39-C40
12	D	403	PTY	C31-C32-C33-C34
12	B	401	PTY	C16-C17-C18-C19
12	D	402	PTY	C19-C20-C21-C22
12	D	403	PTY	C12-C13-C14-C15
12	B	403	PTY	C12-C13-C14-C15
12	B	402	PTY	C11-C8-O7-C6
12	D	404	PTY	C31-C32-C33-C34
12	B	403	PTY	C41-C42-C43-C44
12	D	402	PTY	C20-C21-C22-C23
12	B	403	PTY	C23-C24-C25-C26
12	B	402	PTY	O10-C8-O7-C6
12	D	402	PTY	C22-C23-C24-C25
14	D	401	POV	C29-C210-C211-C212
12	B	401	PTY	C11-C12-C13-C14
12	B	402	PTY	C12-C13-C14-C15
12	B	402	PTY	C32-C33-C34-C35
12	D	403	PTY	C39-C40-C41-C42
12	D	402	PTY	C40-C41-C42-C43
12	B	403	PTY	C40-C41-C42-C43
12	D	403	PTY	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	D	404	PTY	C34-C35-C36-C37
12	B	403	PTY	C18-C19-C20-C21
12	B	403	PTY	C38-C39-C40-C41
12	D	402	PTY	C36-C37-C38-C39
12	D	402	PTY	C39-C40-C41-C42
12	B	403	PTY	C21-C22-C23-C24
12	D	402	PTY	C3-O11-P1-O14
12	D	403	PTY	C5-O14-P1-O11
12	D	404	PTY	C3-O11-P1-O14
14	D	401	POV	C11-O12-P-O11
12	B	403	PTY	C13-C14-C15-C16
12	D	403	PTY	C21-C22-C23-C24
12	D	403	PTY	C24-C25-C26-C27
12	D	404	PTY	C18-C19-C20-C21
12	D	402	PTY	C15-C16-C17-C18
12	B	402	PTY	C19-C20-C21-C22
12	B	402	PTY	C41-C42-C43-C44
12	D	402	PTY	C14-C15-C16-C17
12	B	402	PTY	C15-C16-C17-C18
13	C	403	Q3G	C12-C13-C14-C15
13	C	403	Q3G	C22-C23-O24-P25
12	D	402	PTY	O14-C5-C6-O7
12	D	404	PTY	O14-C5-C6-O7
12	B	401	PTY	C20-C21-C22-C23
12	D	403	PTY	C36-C37-C38-C39
12	B	401	PTY	C19-C20-C21-C22
12	B	402	PTY	O14-C5-C6-C1
12	D	402	PTY	O14-C5-C6-C1
12	D	403	PTY	O14-C5-C6-C1
12	D	404	PTY	O14-C5-C6-C1
12	D	404	PTY	C36-C37-C38-C39
12	B	401	PTY	C31-C32-C33-C34
12	D	404	PTY	C40-C41-C42-C43
12	B	402	PTY	O14-C5-C6-O7
12	D	403	PTY	C18-C19-C20-C21
12	D	404	PTY	O4-C1-C6-O7
12	B	403	PTY	C25-C26-C27-C28
12	B	402	PTY	C14-C15-C16-C17
12	B	401	PTY	C39-C40-C41-C42
12	B	401	PTY	C17-C18-C19-C20
12	D	404	PTY	C17-C18-C19-C20
13	C	403	Q3G	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
12	B	403	PTY	C22-C23-C24-C25
12	D	402	PTY	C41-C42-C43-C44
12	D	403	PTY	C15-C16-C17-C18
12	B	403	PTY	O4-C1-C6-C5
12	B	403	PTY	O4-C1-C6-O7
12	D	404	PTY	C35-C36-C37-C38
13	C	403	Q3G	C29-C30-C31-O32
13	C	403	Q3G	C29-C30-C31-O33
12	D	403	PTY	C26-C27-C28-C29
12	B	402	PTY	C3-O11-P1-O12
12	D	403	PTY	C5-O14-P1-O12
12	D	404	PTY	C3-O11-P1-O13
13	C	403	Q3G	C23-O24-P25-O26
12	D	403	PTY	C14-C15-C16-C17
12	B	402	PTY	C2-C3-O11-P1
12	D	402	PTY	C2-C3-O11-P1
12	D	404	PTY	C2-C3-O11-P1
14	D	401	POV	C12-C11-O12-P
12	D	404	PTY	O4-C1-C6-C5
14	D	401	POV	O12-C11-C12-N
12	B	401	PTY	O4-C1-C6-O7
12	D	403	PTY	C25-C26-C27-C28
12	B	401	PTY	C34-C35-C36-C37
14	D	401	POV	C1-C2-O21-C21
12	B	403	PTY	O14-C5-C6-O7
12	D	403	PTY	O14-C5-C6-O7
12	B	402	PTY	C18-C19-C20-C21
12	D	403	PTY	O4-C1-C6-O7
12	D	403	PTY	C3-O11-P1-O14
13	C	403	Q3G	C29-O28-P25-O24
9	C	401	NAG	C4-C5-C6-O6
12	B	401	PTY	C18-C19-C20-C21
12	D	404	PTY	C39-C40-C41-C42
12	D	402	PTY	C37-C38-C39-C40
13	C	403	Q3G	C14-C15-C16-C17
9	C	401	NAG	O5-C5-C6-O6
12	B	401	PTY	O4-C1-C6-C5
12	B	401	PTY	C15-C16-C17-C18
12	B	401	PTY	C26-C27-C28-C29
10	C	402	ABU	O-C-CG-CB
12	B	401	PTY	C37-C38-C39-C40
12	B	403	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
10	C	402	ABU	OXT-C-CG-CB
12	B	403	PTY	O14-C5-C6-C1
12	B	401	PTY	C38-C39-C40-C41
14	D	401	POV	O31-C31-C32-C33
13	C	403	Q3G	O35-C36-C38-C39
12	D	404	PTY	O4-C30-C31-C32
13	C	403	Q3G	C30-C29-O28-P25
12	D	402	PTY	C17-C18-C19-C20
14	D	401	POV	O32-C31-C32-C33
12	D	403	PTY	C3-O11-P1-O13
14	D	401	POV	C11-O12-P-O13
12	D	404	PTY	O30-C30-C31-C32
13	C	403	Q3G	O37-C36-C38-C39
12	B	402	PTY	C36-C37-C38-C39
12	B	401	PTY	C14-C15-C16-C17
12	B	402	PTY	O4-C30-C31-C32
12	B	403	PTY	O4-C30-C31-C32
12	D	402	PTY	O4-C30-C31-C32
12	B	403	PTY	C33-C34-C35-C36
12	B	403	PTY	O30-C30-C31-C32

There are no ring outliers.

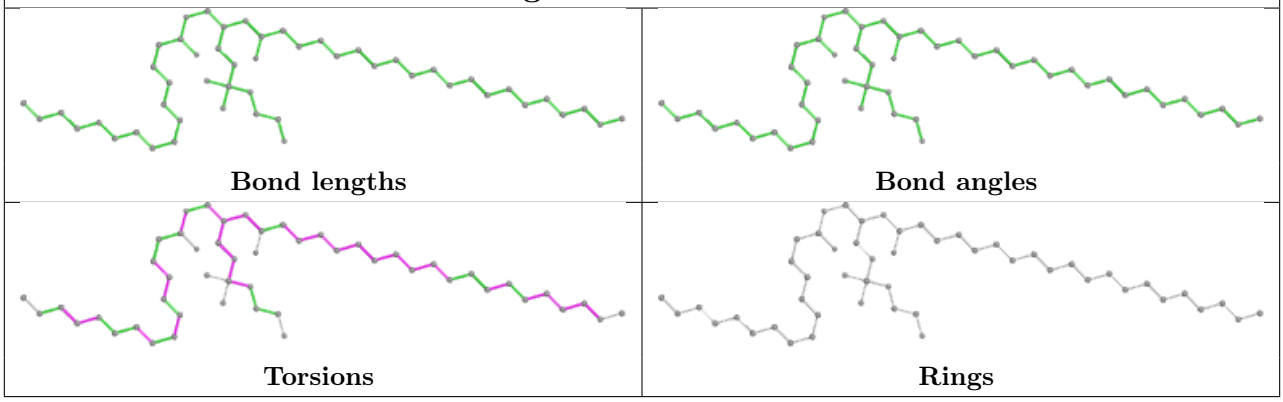
11 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	402	ABU	1	0
12	D	403	PTY	10	0
12	B	403	PTY	11	0
14	D	401	POV	3	0
10	A	402	ABU	1	0
12	D	404	PTY	16	0
12	D	402	PTY	17	0
12	B	402	PTY	8	0
11	A	403	ZWY	3	0
12	B	401	PTY	6	0
13	C	403	Q3G	5	0

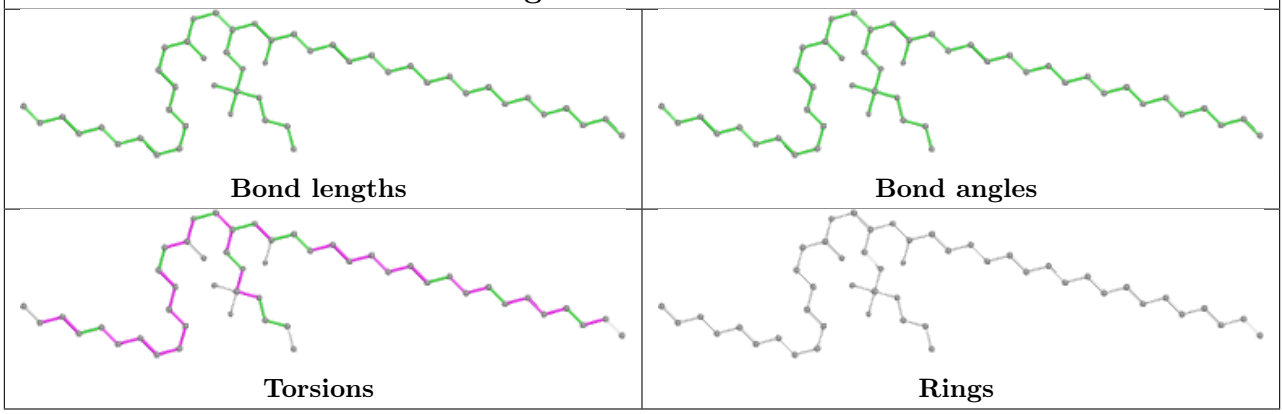
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

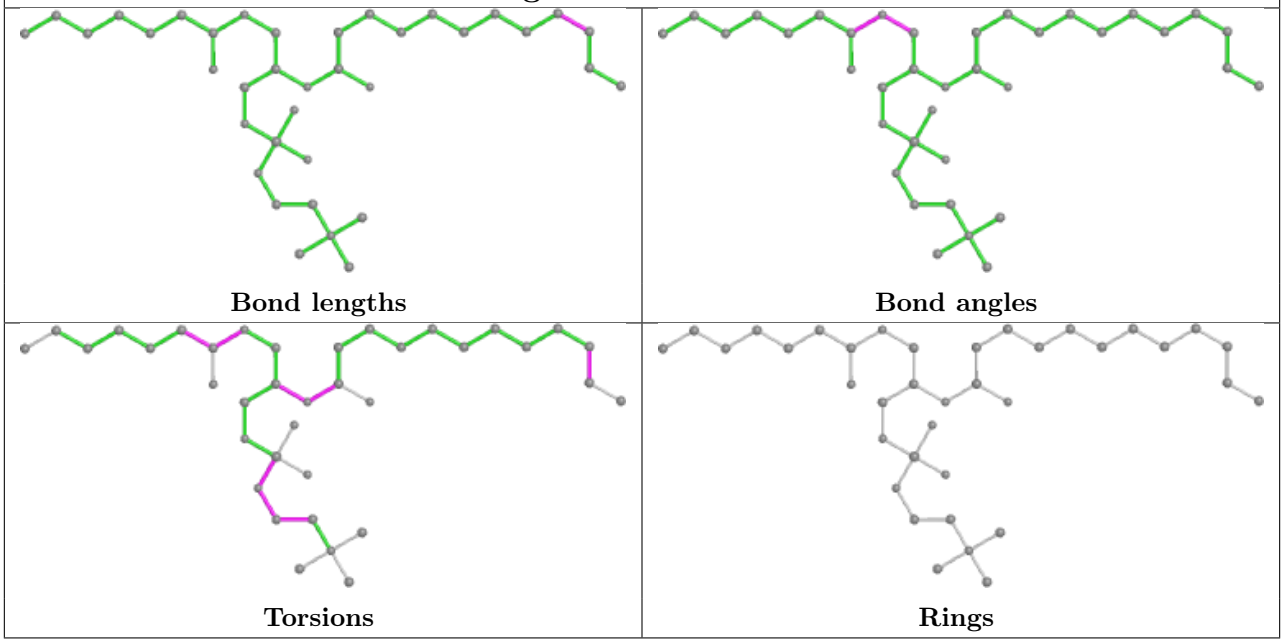
Ligand PTY D 403



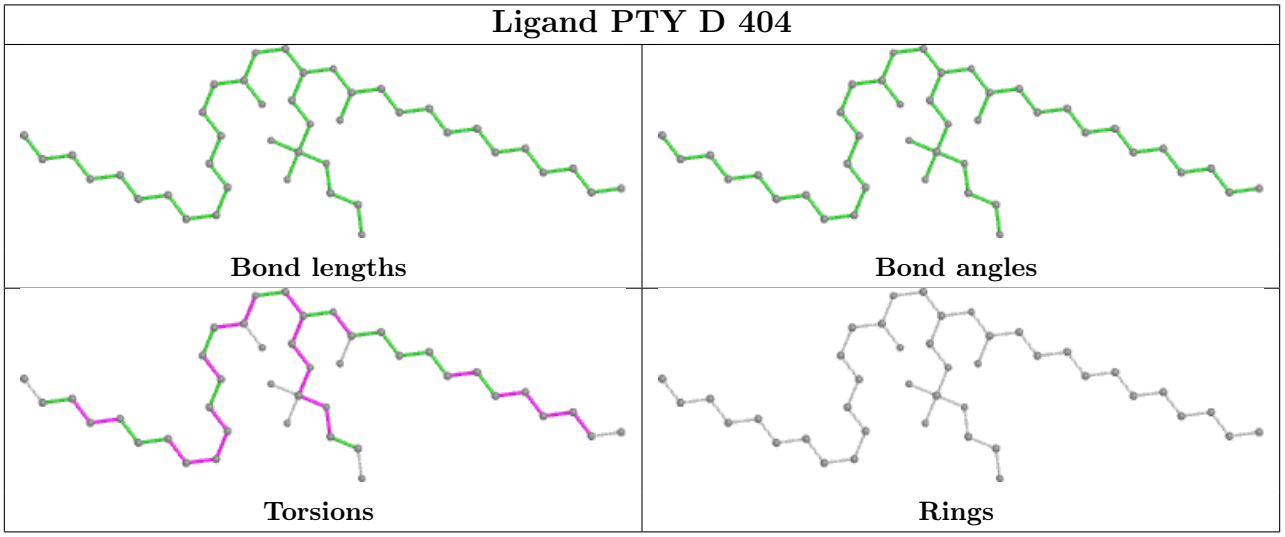
Ligand PTY B 403



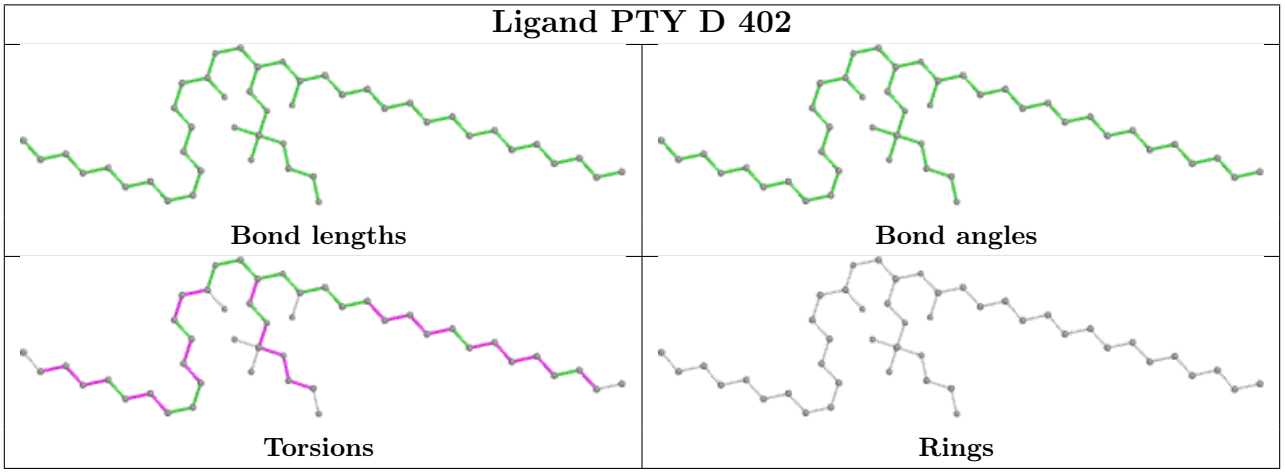
Ligand POV D 401



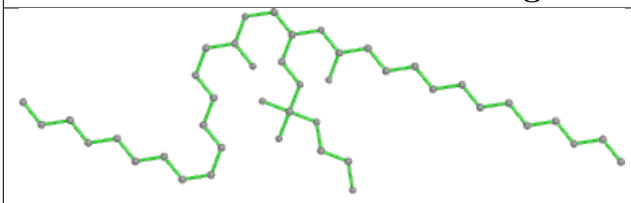
Ligand PTY D 404



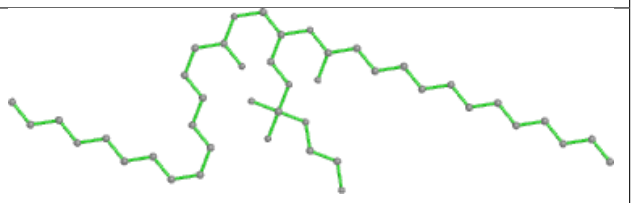
Ligand PTY D 402



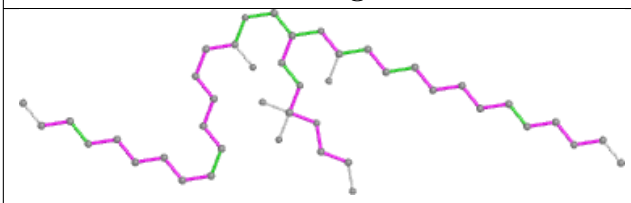
Ligand PTY B 402



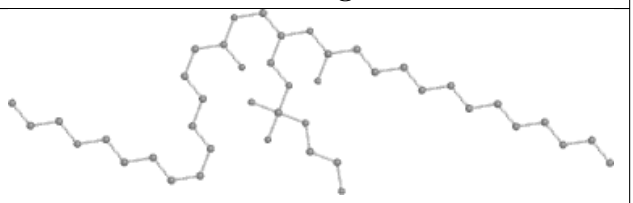
Bond lengths



Bond angles

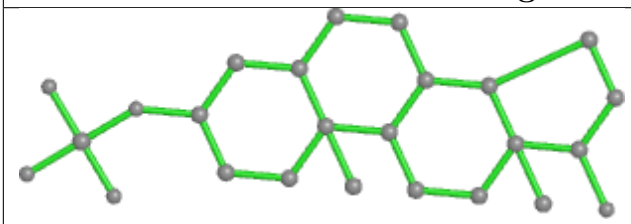


Torsions

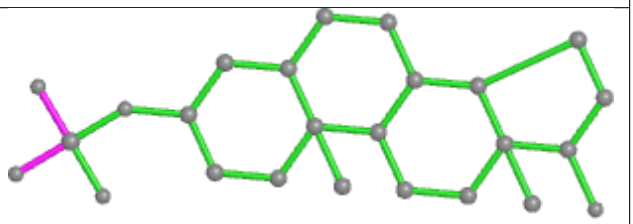


Rings

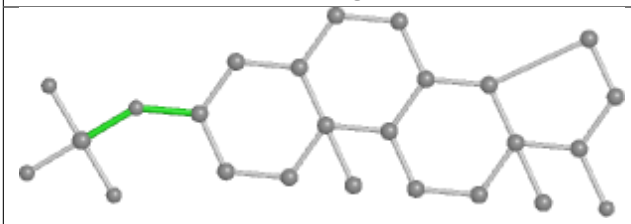
Ligand ZWY A 403



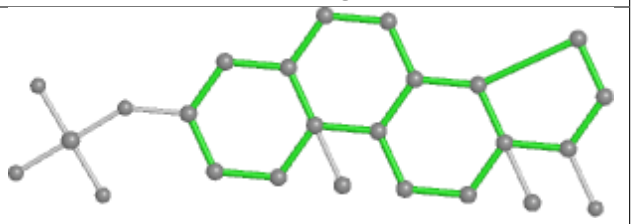
Bond lengths



Bond angles

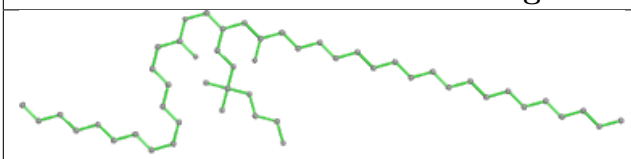


Torsions

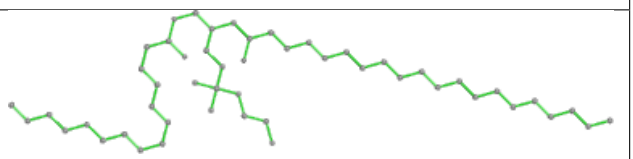


Rings

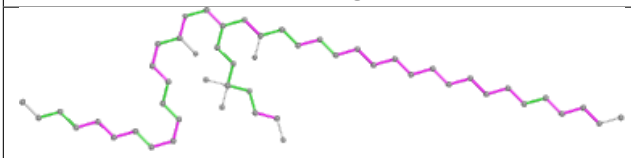
Ligand PTY B 401



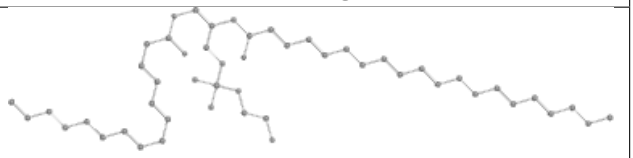
Bond lengths



Bond angles

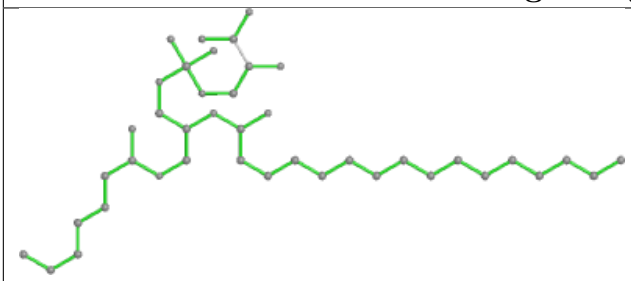


Torsions

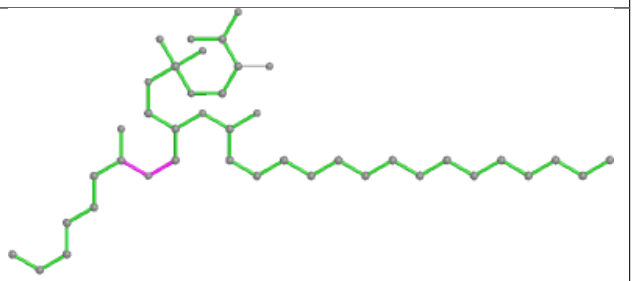


Rings

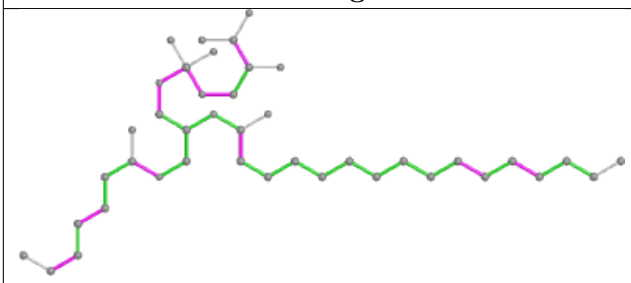
Ligand Q3G C 403



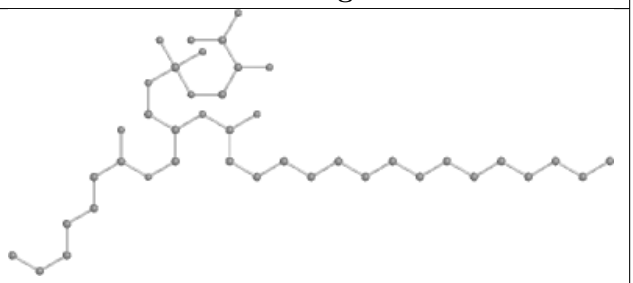
Bond lengths



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.

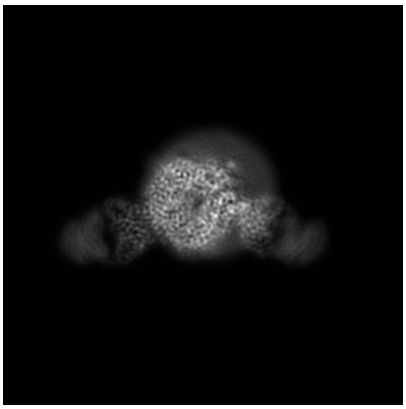
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40506. These allow visual inspection of the internal detail of the map and identification of artifacts.

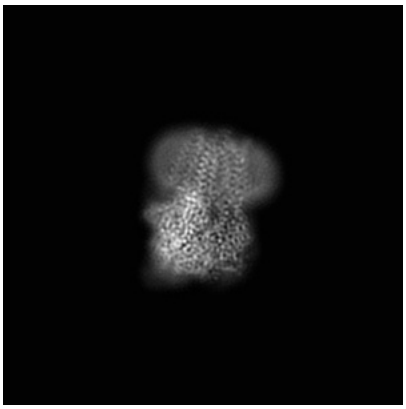
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

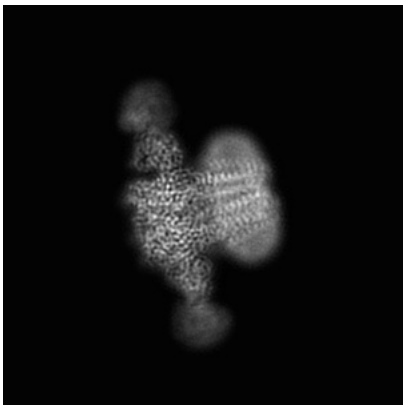
6.1.1 Primary map



X

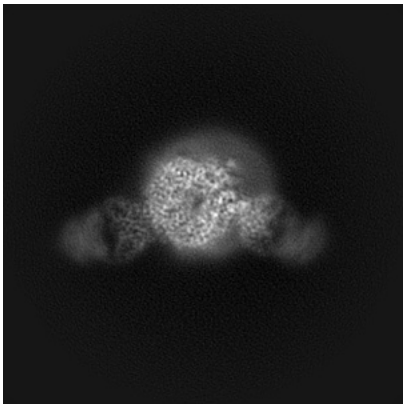


Y

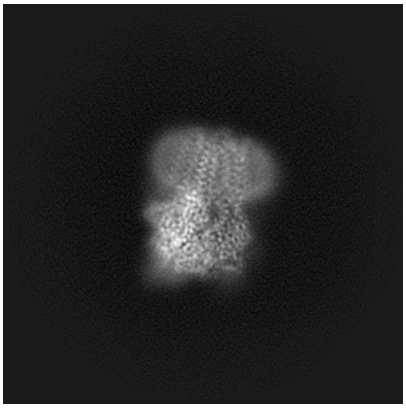


Z

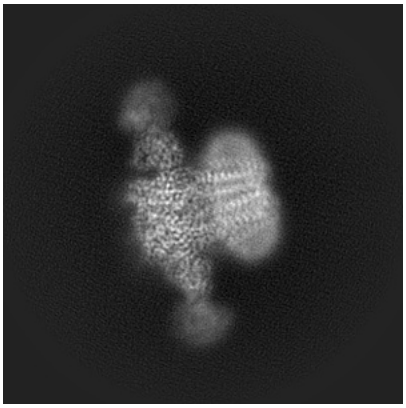
6.1.2 Raw map



X



Y

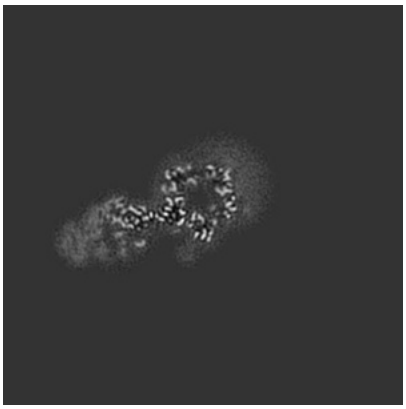


Z

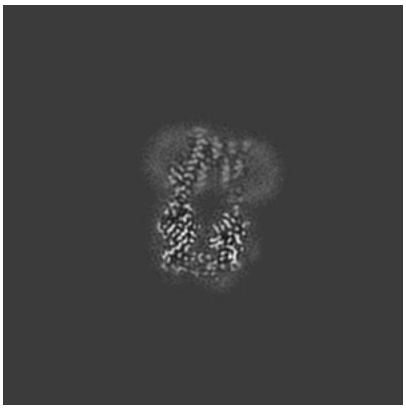
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



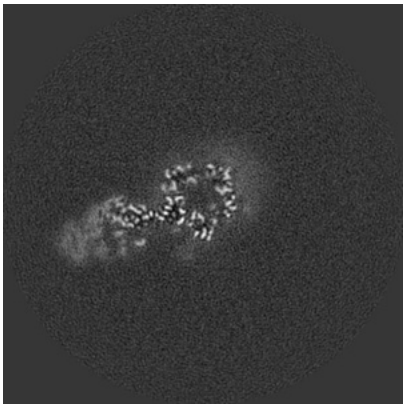
X Index: 144



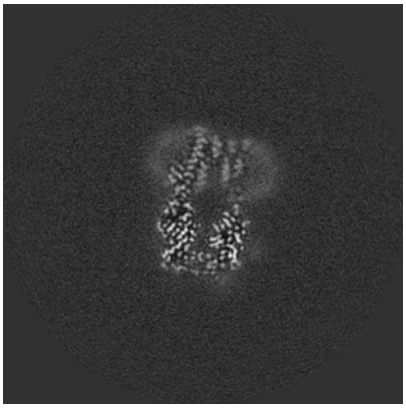
Y Index: 144

Z Index: 144

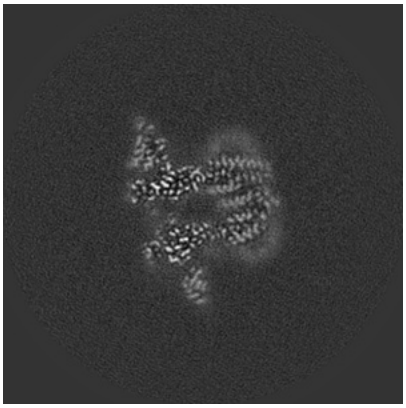
6.2.2 Raw map



X Index: 144



Y Index: 144

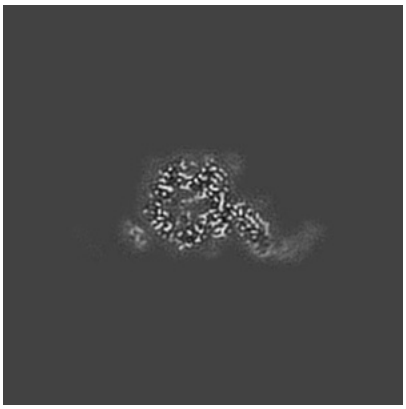


Z Index: 144

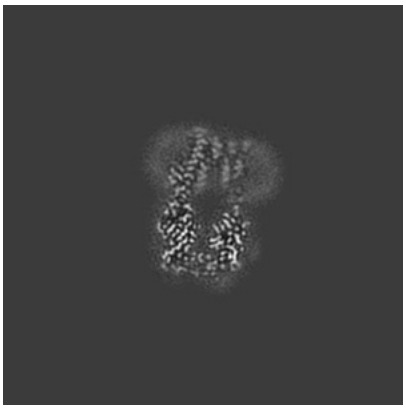
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

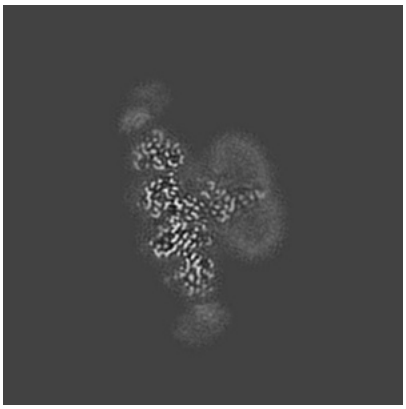
6.3.1 Primary map



X Index: 118

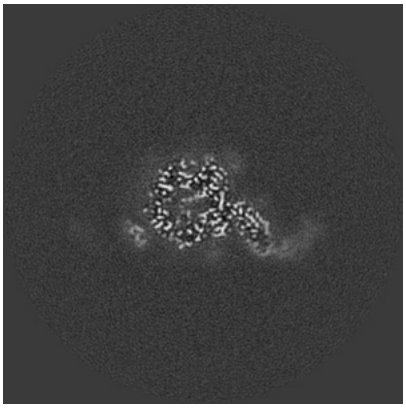


Y Index: 144

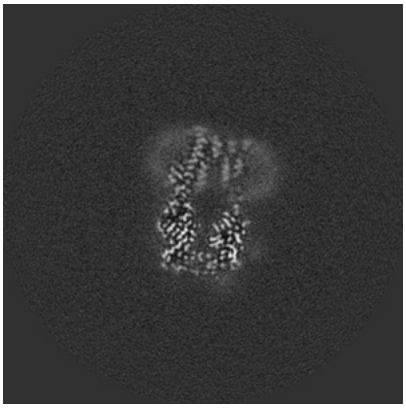


Z Index: 131

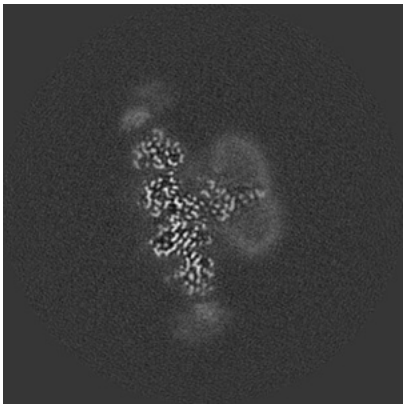
6.3.2 Raw map



X Index: 118



Y Index: 144

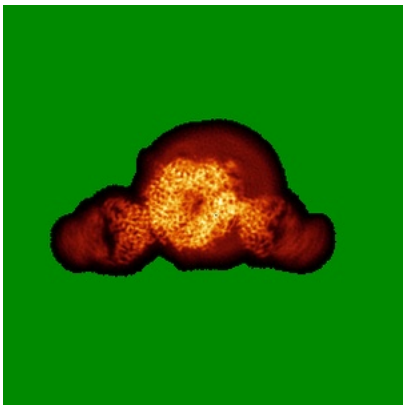


Z Index: 131

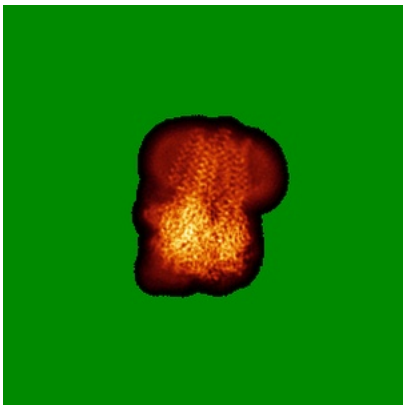
The images above show the largest variance slices of the map in three orthogonal directions.

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

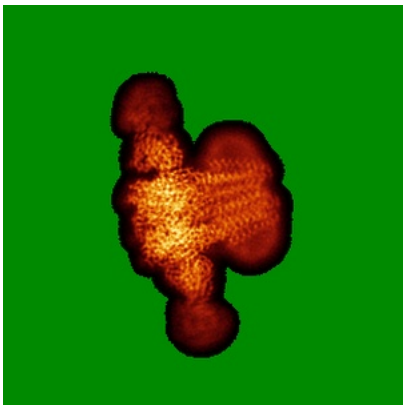
6.4.1 Primary map



X

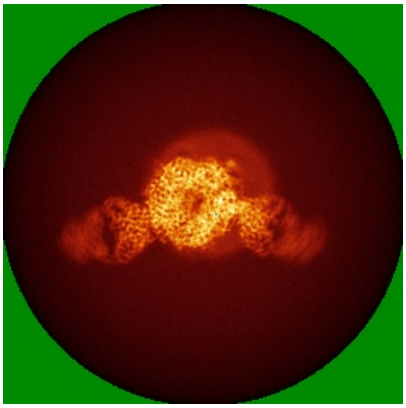


Y

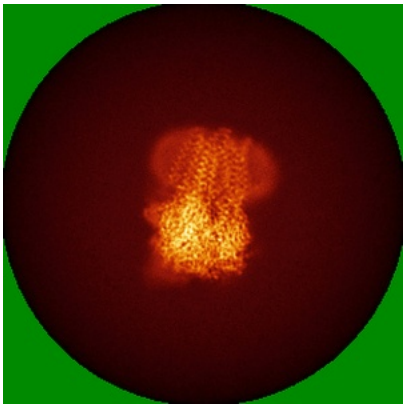


Z

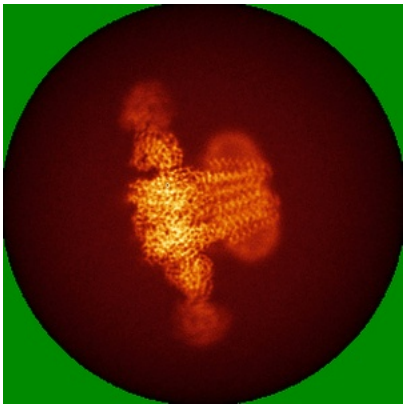
6.4.2 Raw map



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 0.015. 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.

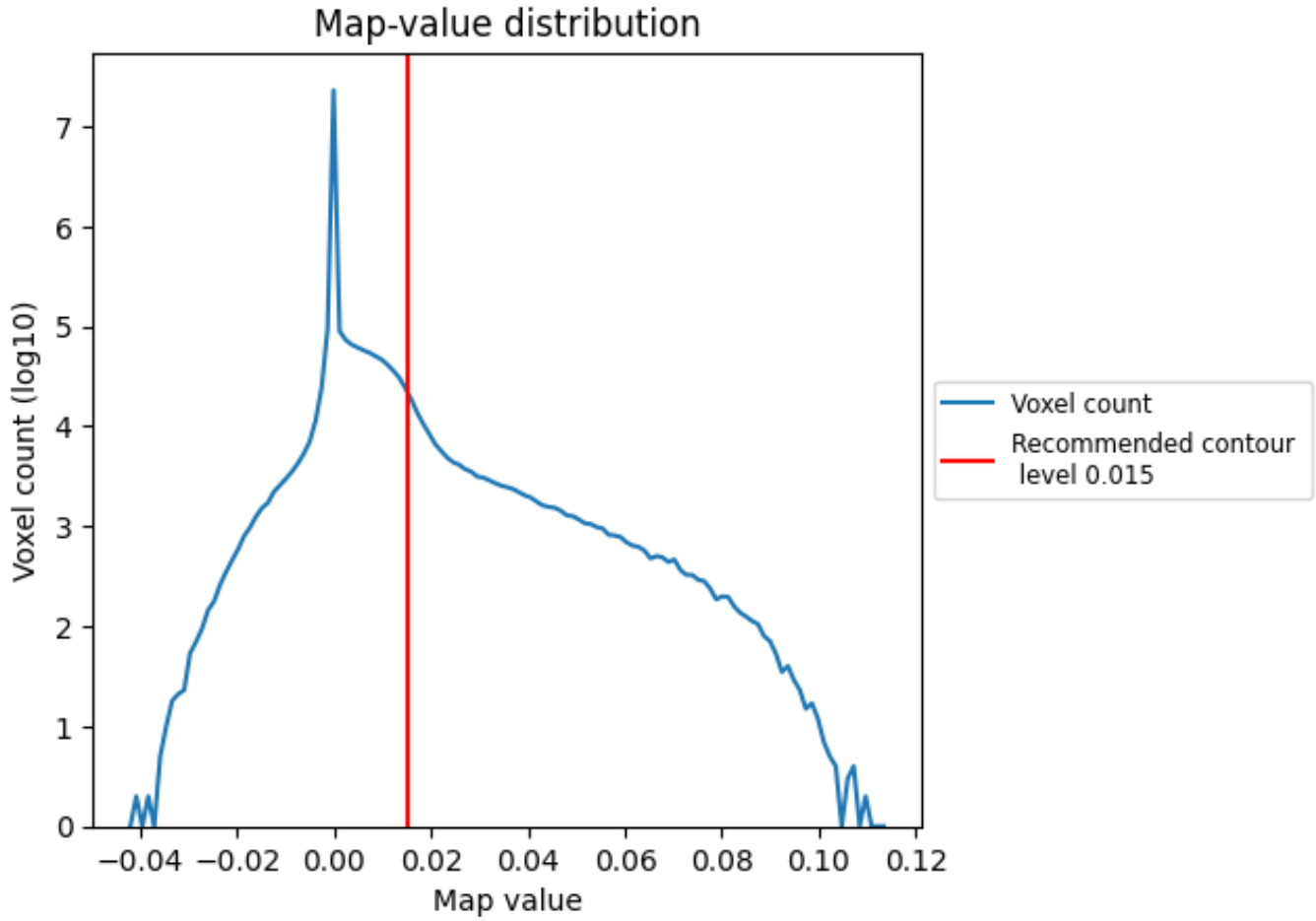
6.6 Mask visualisation (i)

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

7 Map analysis

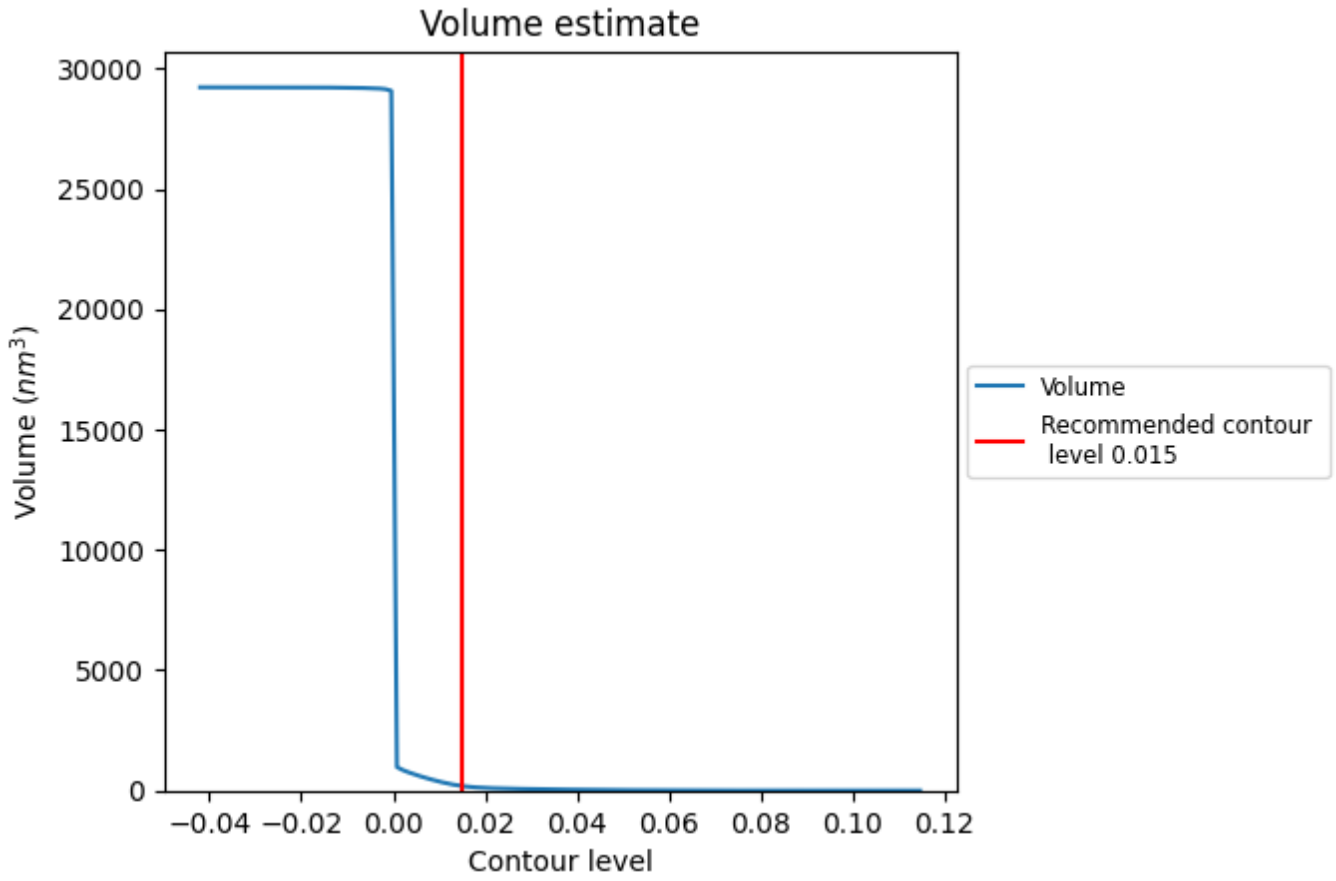
This section contains the results of statistical analysis of the map.

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.

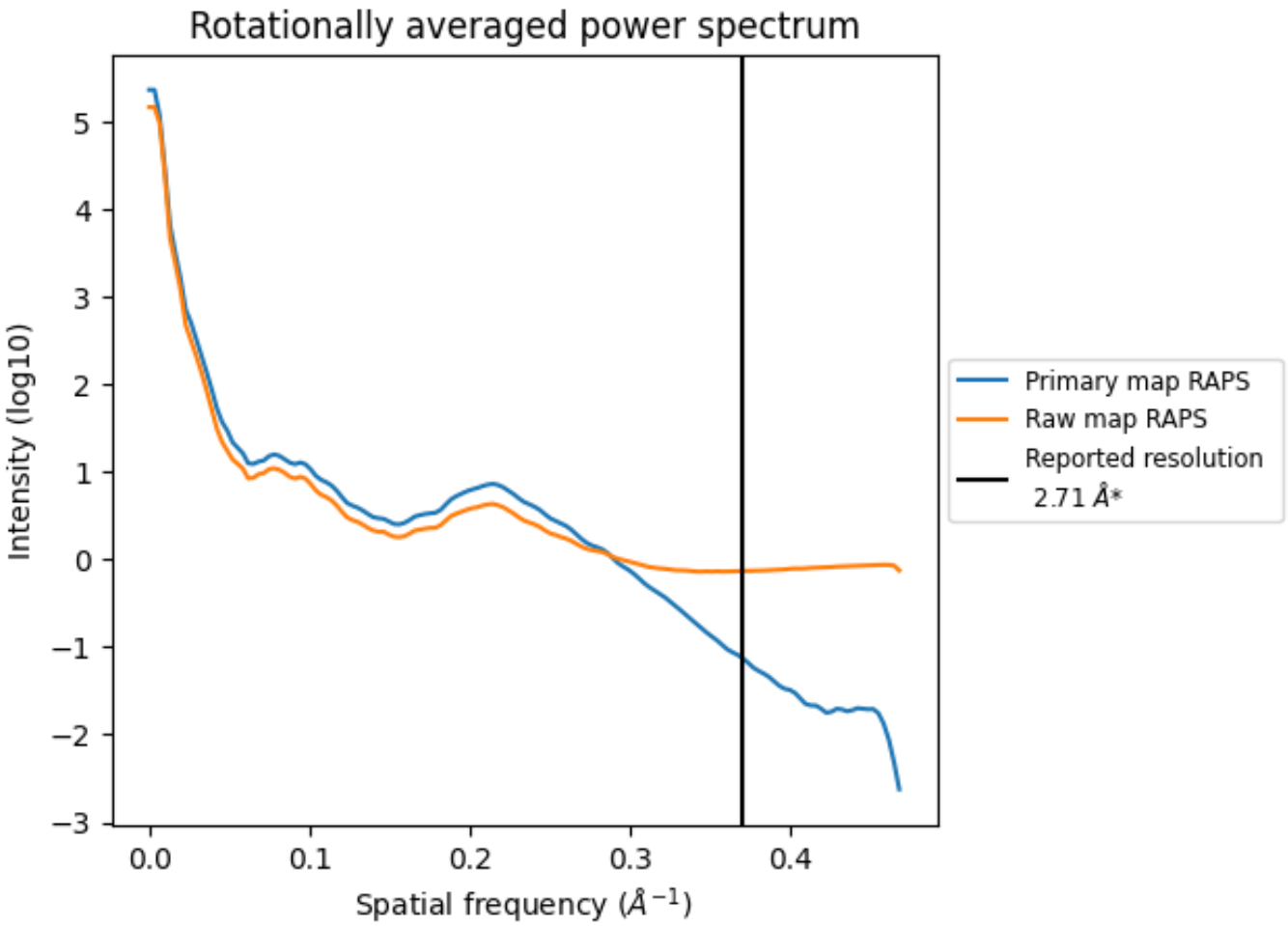
7.2 Volume estimate (i)



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 171 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)

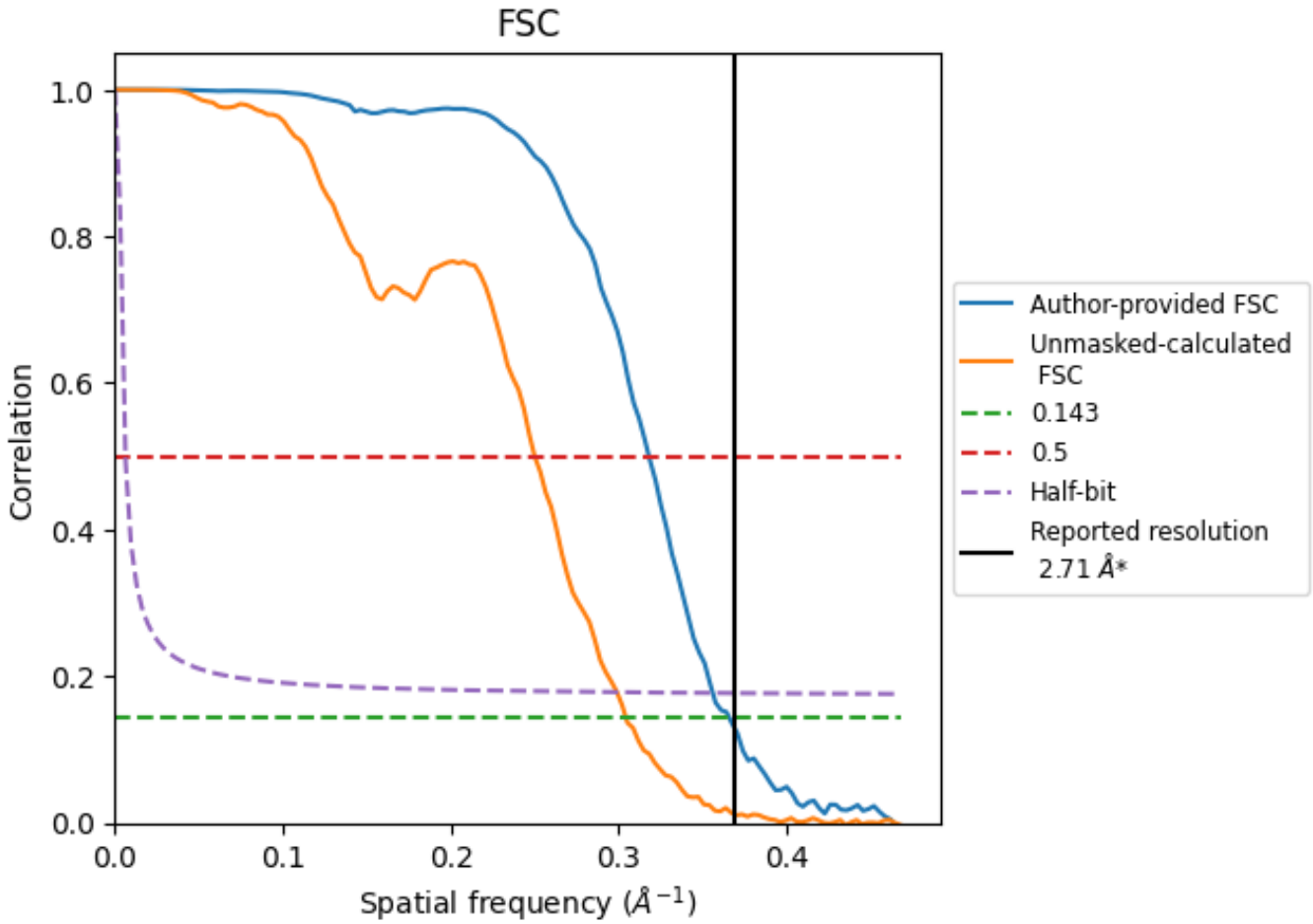


*Reported resolution corresponds to spatial frequency of 0.369 Å^{-1}

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 0.369 Å^{-1}

8.2 Resolution estimates (i)

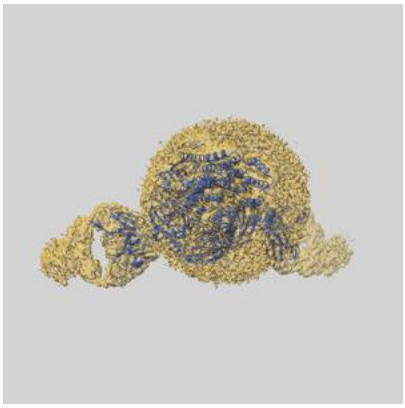
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.73	3.14	2.81
Unmasked-calculated*	3.29	4.00	3.35

*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 3.29 differs from the reported value 2.71 by more than 10 %

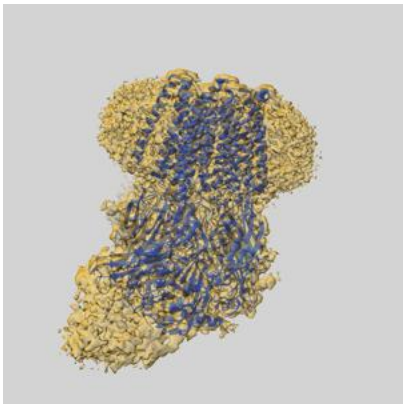
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40506 and PDB model 8SID. Per-residue inclusion information can be found in section 3 on page 14.

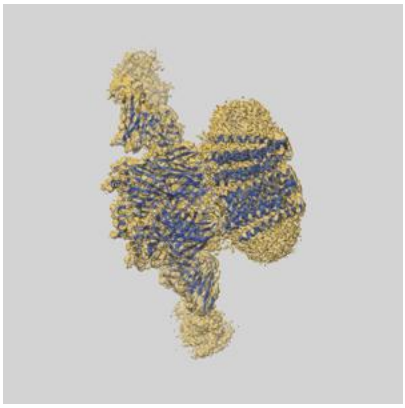
9.1 Map-model overlay



X



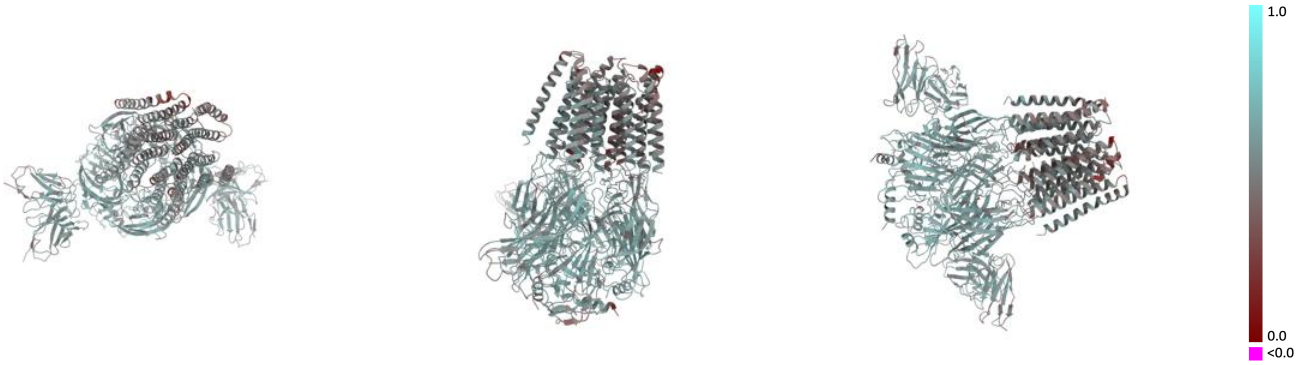
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

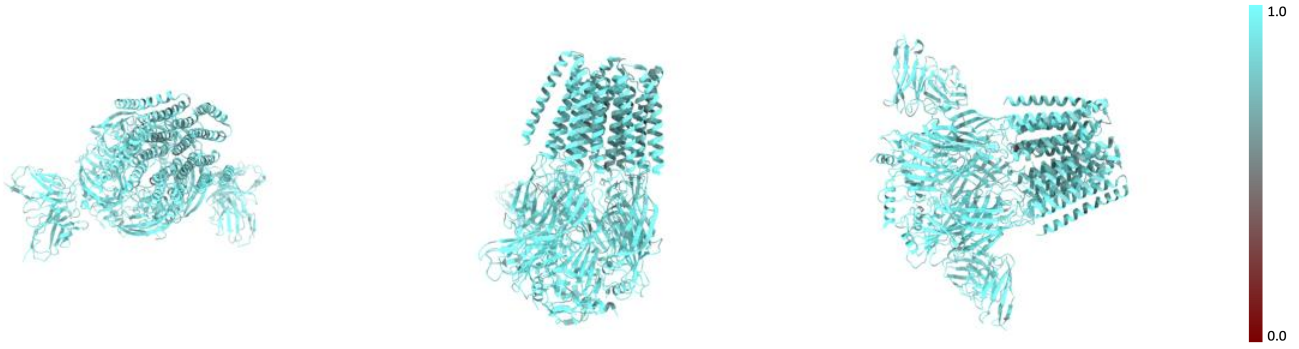
9.2 Q-score mapped to coordinate model (i)



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.

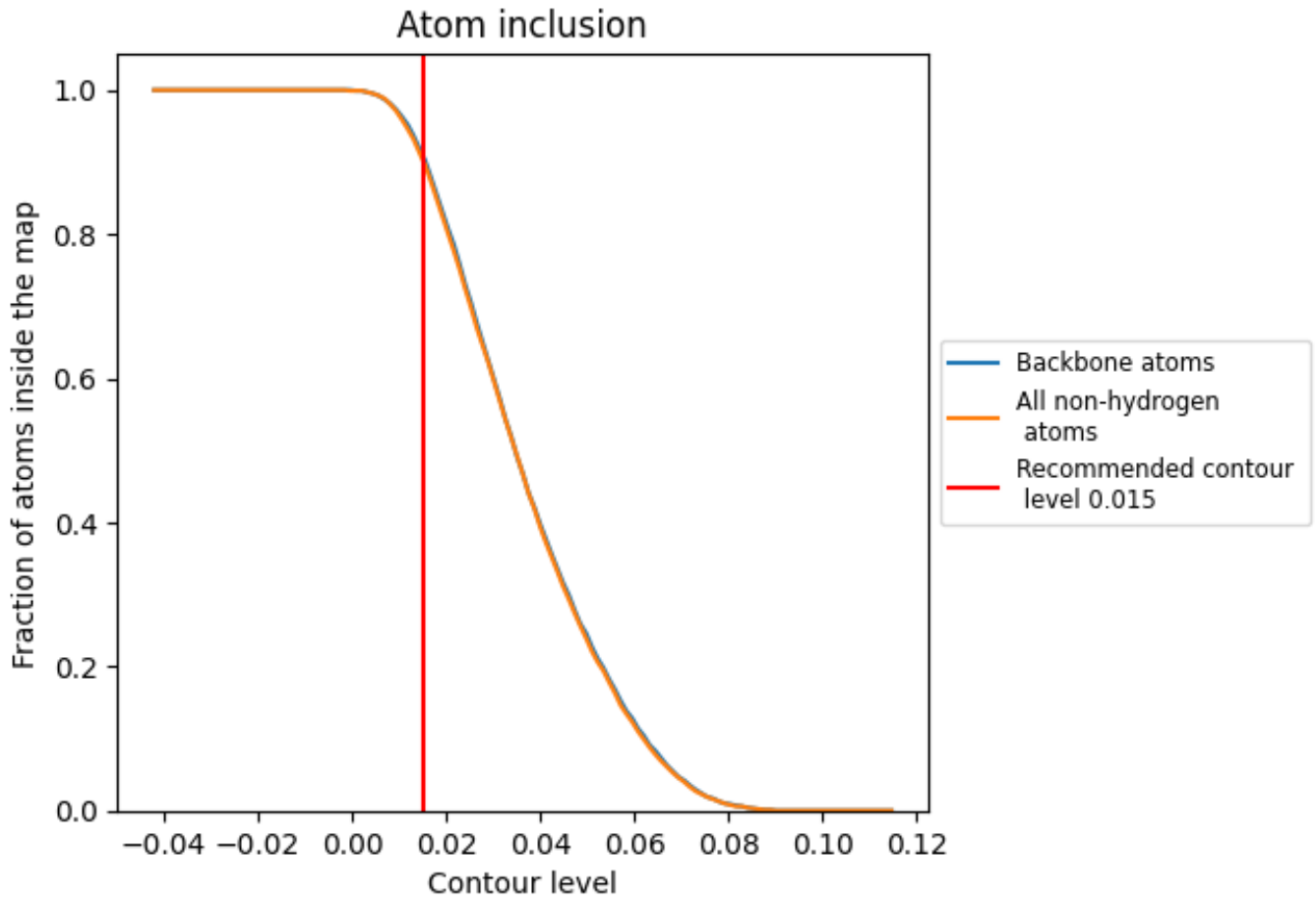
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9030	0.5390
A	0.9080	0.5320
B	0.8980	0.5440
C	0.9150	0.5510
D	0.9070	0.5500
E	0.9010	0.5230
F	0.8720	0.4850
G	0.9140	0.5500
H	0.9740	0.5400
I	0.9020	0.5420
J	0.9020	0.5270
K	0.9070	0.5400
L	0.9070	0.5320
M	0.9740	0.5760
N	0.8570	0.4150