wwPDB EM Validation Summary Report

May 19, 2025 – 01:07 AM EDT

PDB ID	:	8VRN / pdb_00008vrn
EMDB ID	:	EMD-43485
Title	:	Human GABAA receptor alpha1-beta2-gamma2 subtype in complex with GABA plus PPTQ
Authors	:	Chojnacka, W.; Teng, J.; Kim, J.J.; Jensen, A.A.; Hibbs, R.E.
Deposited on	:	2024-01-22
Resolution	:	2.57 Å(reported)

This is a wwPDB EM Validation Summary 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:

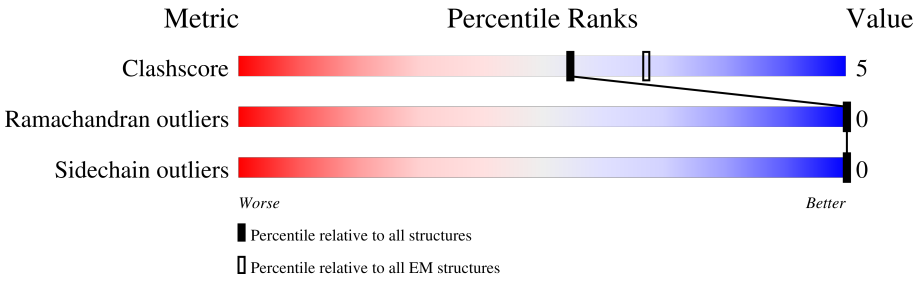
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 2.57 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	364	84% 8% 8%
1	C	364	81% 11% 8%
2	B	358	88% 6% 6%
2	D	358	86% 8% 6%
3	E	417	73% 6% 20%
4	I	213	44% 6% 51%
4	L	213	46% • 50%
5	J	454	24% • 74%

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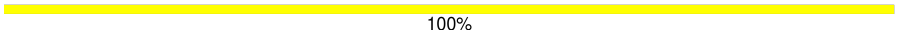
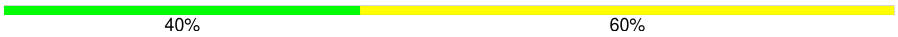
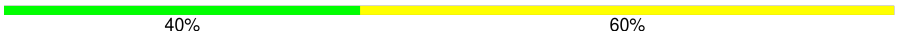
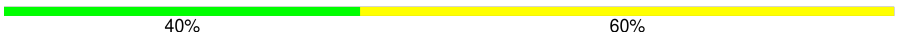
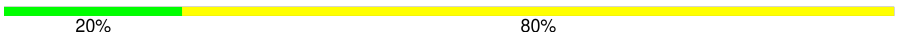
Mol	Chain	Length	Quality of chain
5	K	454	
6	F	2	
6	N	2	
6	O	2	
7	G	5	
7	M	5	
7	P	5	
8	H	10	

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
11	PTY	A	403	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 17865 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 beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total 2731	C 1790	N 440	O 485	S 16	0	0
1	C	334	Total 2731	C 1790	N 440	O 485	S 16	0	0

There are 16 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	315	ALA	-	linker	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	315	ALA	-	linker	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 2730	C 1763	N 461	O 490	S 16	0	0
2	D	338	Total 2730	C 1763	N 461	O 490	S 16	0	0

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	N	O	S	0	0
			2729	1781	448	485	15		

There are 44 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	329	ALA	-	linker	UNP P18507

- Molecule 4 is a protein called Kappa FAB light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	105	Total	C	N	O	S	0	0
			802	504	130	163	5		
4	L	106	Total	C	N	O	S	0	0
			811	510	132	164	5		

- Molecule 5 is a protein called IGG2B FAB heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	116	Total	C	N	O	S	0	0
			907	574	151	178	4		

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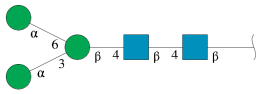
Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	117	Total	C	N	O	S	0	0
			914	578	152	180	4		

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

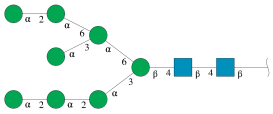
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called 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.



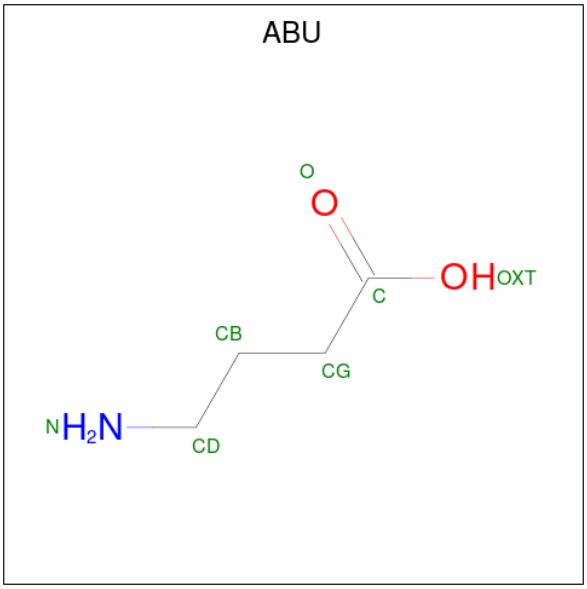
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	5	Total	C	N	O	0	0
			61	34	2	25		
7	M	5	Total	C	N	O	0	0
			61	34	2	25		
7	P	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 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.



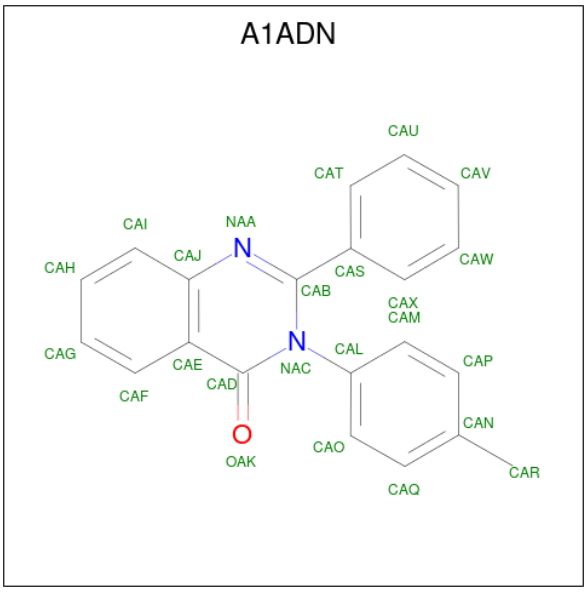
Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$).



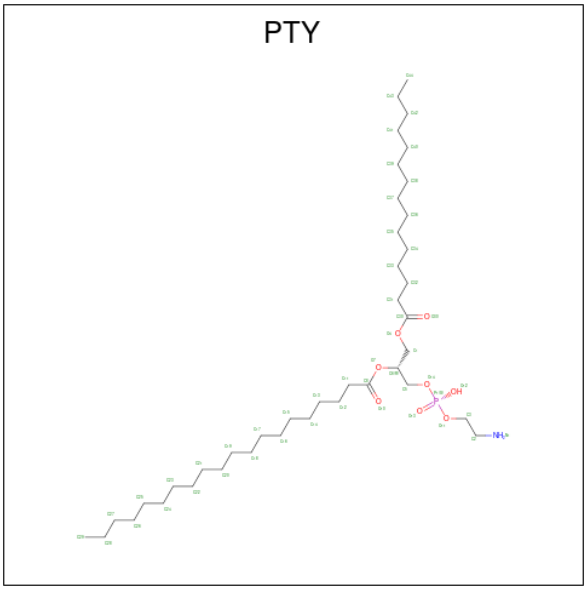
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			7	4	1	2	
9	C	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 10 is 3-(4-methylphenyl)-2-phenylquinazolin-4(3H)-one (CCD ID: A1ADN) (formula: $C_{21}H_{16}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			24	21	2	1	
10	C	1	Total	C	N	O	0
			24	21	2	1	

- Molecule 11 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
11	B	1	Total	C	N	O	P	0
			41	31	1	8	1	

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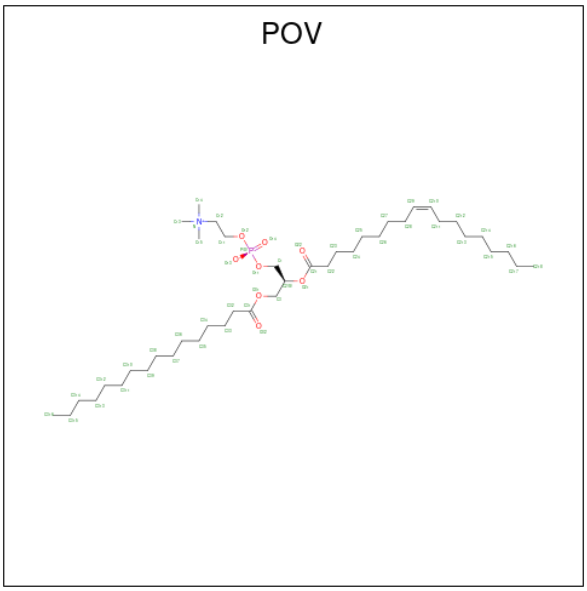
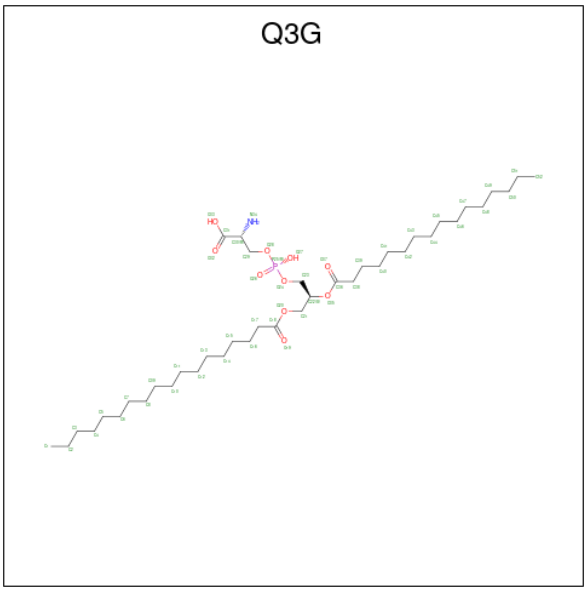
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
11	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
11	D	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 12 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	N	O	P	0
			34	24	1	8	1	

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



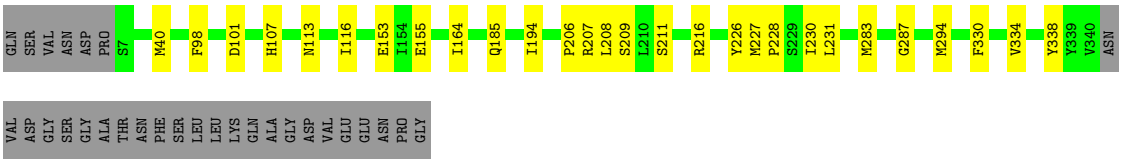
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			45	33	1	10	1	
13	D	1	Total	C	N	O	P	0
			52	40	1	10	1	

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.

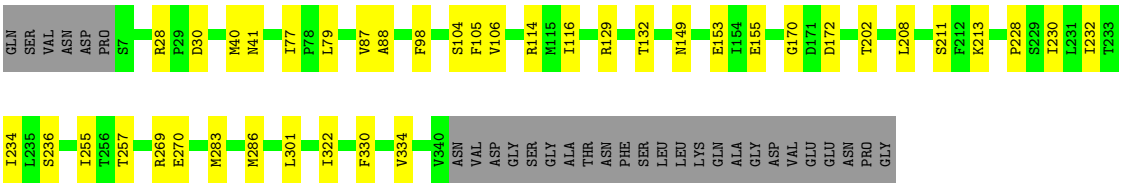
• Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2

Chain A:



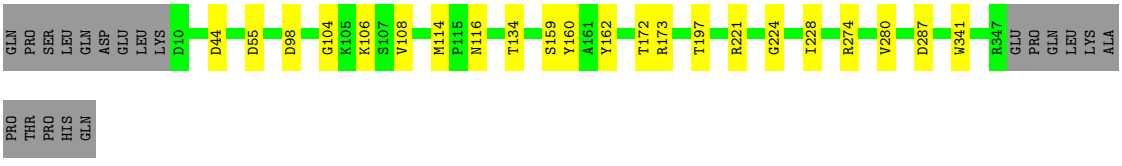
• Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2

Chain C:



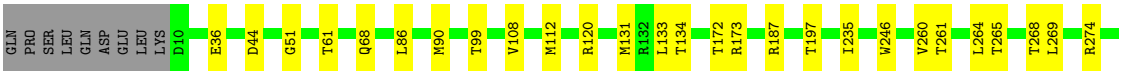
• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

Chain B:



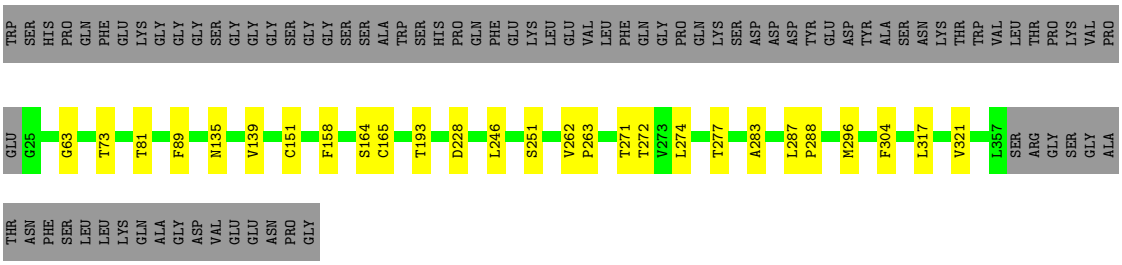
• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

Chain D:



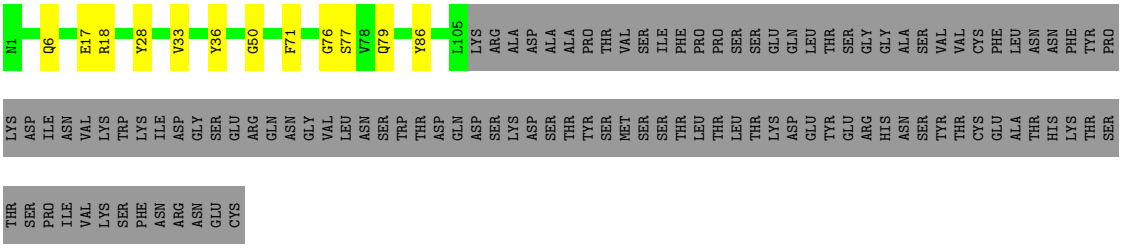
• Molecule 3: Gamma-aminobutyric acid receptor subunit gamma-2

Chain E:



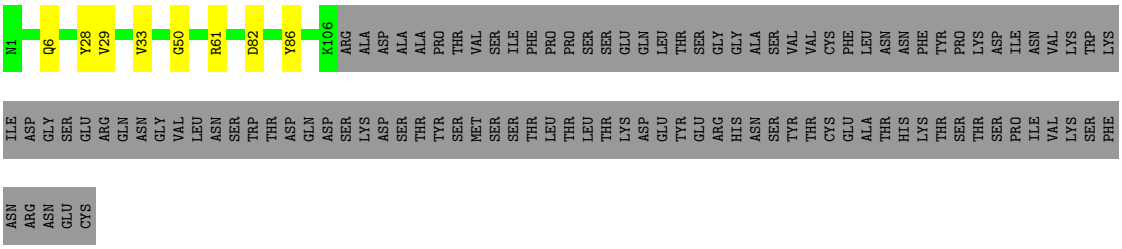
• Molecule 4: Kappa FAB light chain

Chain I:



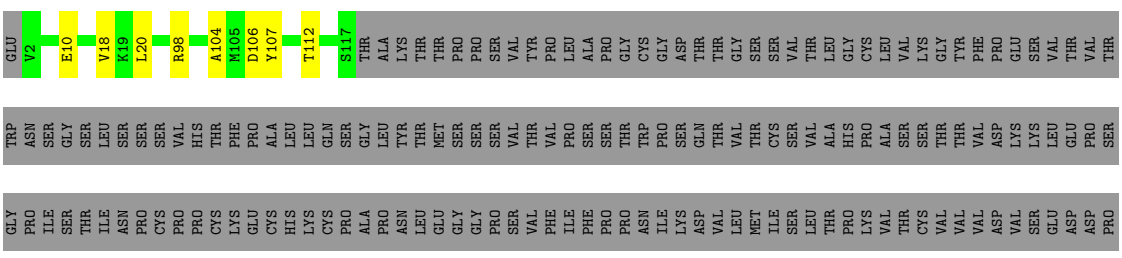
• Molecule 4: Kappa FAB light chain

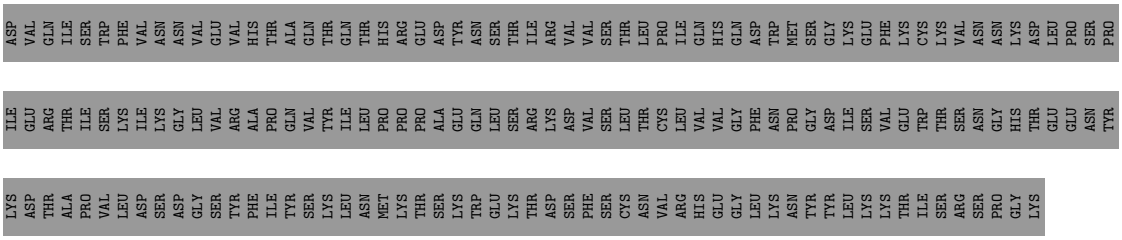
Chain L:



• Molecule 5: IGG2B FAB heavy chain

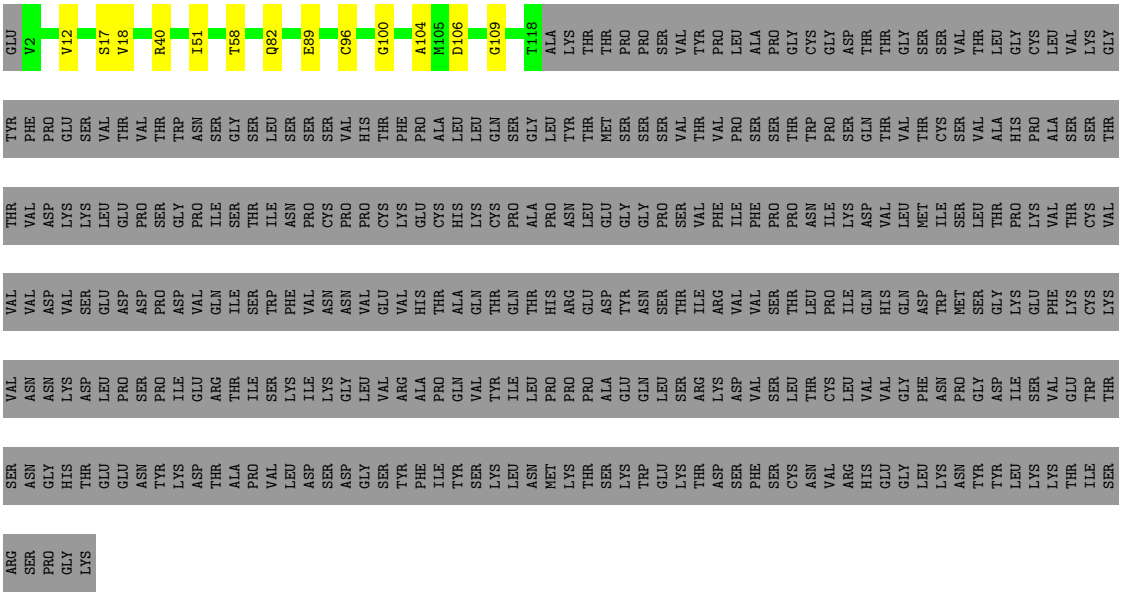
Chain J:





• Molecule 5: IGG2B FAB heavy chain

Chain K:



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

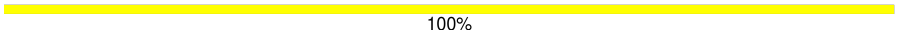
Chain F:

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

Chain N:

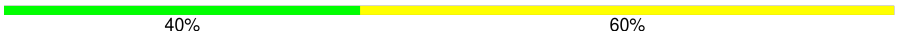
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



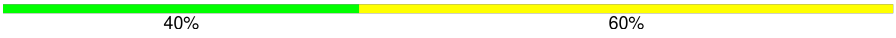
• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 7: 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 M:



• Molecule 7: 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 P:

• Molecule 8: 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 H:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	308.16, 308.16, 308.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, Q3G, MAN, ABU, A1ADN, POV, PTY

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	0.22	0/2803	0.34	0/3816
1	C	0.22	0/2803	0.36	0/3816
2	B	0.23	0/2799	0.34	0/3805
2	D	0.25	0/2799	0.37	0/3805
3	E	0.22	0/2805	0.36	0/3822
4	I	0.22	0/820	0.33	0/1112
4	L	0.21	0/829	0.33	0/1123
5	J	0.17	0/928	0.28	0/1260
5	K	0.18	0/935	0.28	0/1270
All	All	0.22	0/17521	0.35	0/23829

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	2731	0	2737	36	0
1	C	2731	0	2737	36	0
2	B	2730	0	2724	18	0
2	D	2730	0	2724	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2729	0	2714	24	0
4	I	802	0	771	9	0
4	L	811	0	784	5	0
5	J	907	0	877	5	0
5	K	914	0	884	7	0
6	F	28	0	25	0	0
6	N	28	0	25	0	0
6	O	28	0	25	0	0
7	G	61	0	52	2	0
7	M	61	0	52	3	0
7	P	61	0	52	0	0
8	H	116	0	97	0	0
9	A	7	0	0	0	0
9	C	7	0	0	1	0
10	A	24	0	0	0	0
10	C	24	0	0	0	0
11	A	41	0	55	25	0
11	B	41	0	58	11	0
11	C	82	0	113	24	0
11	D	40	0	56	11	0
12	B	34	0	40	2	0
13	C	45	0	0	1	0
13	D	52	0	0	1	0
All	All	17865	0	17602	174	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.

The worst 5 of 174 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:231:LEU:HD13	3:E:304:PHE:CE2	1.41	1.52
1:A:231:LEU:CD1	3:E:304:PHE:CE2	2.29	1.15
1:A:231:LEU:CD1	3:E:304:PHE:HE2	1.61	1.14
1:A:283:MET:HE1	11:A:403:PTY:C31	1.80	1.10
1:A:283:MET:HE1	11:A:403:PTY:H312	1.38	1.05

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%)	321 (97%)	11 (3%)	0	100	100
1	C	332/364 (91%)	320 (96%)	12 (4%)	0	100	100
2	B	336/358 (94%)	328 (98%)	8 (2%)	0	100	100
2	D	336/358 (94%)	328 (98%)	8 (2%)	0	100	100
3	E	331/417 (79%)	316 (96%)	15 (4%)	0	100	100
4	I	103/213 (48%)	94 (91%)	9 (9%)	0	100	100
4	L	104/213 (49%)	97 (93%)	7 (7%)	0	100	100
5	J	114/454 (25%)	110 (96%)	4 (4%)	0	100	100
5	K	115/454 (25%)	107 (93%)	8 (7%)	0	100	100
All	All	2103/3195 (66%)	2021 (96%)	82 (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%)	302 (100%)	0	100	100
1	C	302/326 (93%)	302 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	1883 (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. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	242	GLN
3	E	152	GLN
2	B	308	ASN
1	C	303	ASN
1	C	332	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)

31 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	6,1	14,14,15	0.32	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	F	2	6	14,14,15	0.61	1 (7%)	17,19,21	0.77	1 (5%)
7	NAG	G	1	1,7	14,14,15	0.30	0	17,19,21	0.69	0
7	NAG	G	2	7	14,14,15	0.26	0	17,19,21	0.52	0
7	BMA	G	3	7	11,11,12	0.70	0	15,15,17	0.76	0
7	MAN	G	4	7	11,11,12	0.65	0	15,15,17	0.83	1 (6%)
7	MAN	G	5	7	11,11,12	0.77	0	15,15,17	1.46	4 (26%)
8	NAG	H	1	8,2	14,14,15	0.31	0	17,19,21	0.58	0
8	MAN	H	10	8	11,11,12	0.45	0	15,15,17	1.01	2 (13%)
8	NAG	H	2	8	14,14,15	0.19	0	17,19,21	0.43	0
8	BMA	H	3	8	11,11,12	0.88	1 (9%)	15,15,17	0.99	1 (6%)
8	MAN	H	4	8	11,11,12	0.56	0	15,15,17	1.26	2 (13%)
8	MAN	H	5	8	11,11,12	0.57	0	15,15,17	0.90	1 (6%)
8	MAN	H	6	8	11,11,12	0.65	0	15,15,17	0.86	1 (6%)
8	MAN	H	7	8	11,11,12	1.01	1 (9%)	15,15,17	1.07	1 (6%)
8	MAN	H	8	8	11,11,12	0.58	0	15,15,17	1.20	2 (13%)
8	MAN	H	9	8	11,11,12	0.55	0	15,15,17	0.95	1 (6%)
7	NAG	M	1	1,7	14,14,15	0.26	0	17,19,21	0.54	0
7	NAG	M	2	7	14,14,15	0.25	0	17,19,21	0.53	0
7	BMA	M	3	7	11,11,12	0.58	0	15,15,17	0.84	0
7	MAN	M	4	7	11,11,12	0.70	0	15,15,17	0.87	0
7	MAN	M	5	7	11,11,12	0.51	0	15,15,17	0.85	0
6	NAG	N	1	6,3	14,14,15	0.59	1 (7%)	17,19,21	0.63	0
6	NAG	N	2	6	14,14,15	0.31	0	17,19,21	0.45	0
6	NAG	O	1	6	14,14,15	0.41	0	17,19,21	0.80	1 (5%)
6	NAG	O	2	6	14,14,15	0.39	0	17,19,21	0.89	1 (5%)
7	NAG	P	1	7,2	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	P	2	7	14,14,15	0.20	0	17,19,21	0.57	0
7	BMA	P	3	7	11,11,12	0.89	0	15,15,17	1.31	1 (6%)
7	MAN	P	4	7	11,11,12	1.05	2 (18%)	15,15,17	0.89	1 (6%)
7	MAN	P	5	7	11,11,12	0.73	0	15,15,17	1.65	4 (26%)

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	6,1	-	2/6/23/26	0/1/1/1

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	7	MAN	O5-C1	-2.65	1.39	1.43
8	H	3	BMA	O5-C1	-2.41	1.39	1.43
7	P	4	MAN	O5-C1	-2.21	1.40	1.43
6	F	2	NAG	O5-C1	-2.05	1.40	1.43
7	P	4	MAN	C4-C3	2.03	1.57	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	4	MAN	C1-O5-C5	3.81	117.30	112.19
7	P	5	MAN	C1-O5-C5	3.75	117.21	112.19
8	H	8	MAN	C1-O5-C5	3.41	116.75	112.19
7	G	5	MAN	C1-O5-C5	2.99	116.20	112.19
8	H	7	MAN	O2-C2-C3	-2.89	104.17	110.15

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	O	2	NAG	C1-C2-N2-C7
6	O	2	NAG	O7-C7-N2-C2
7	G	1	NAG	C3-C2-N2-C7
7	M	1	NAG	C1-C2-N2-C7
6	O	2	NAG	C8-C7-N2-C2

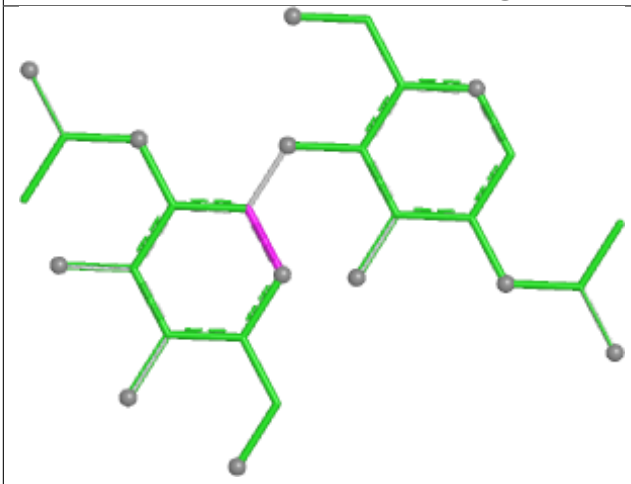
There are no ring outliers.

4 monomers are involved in 5 short contacts:

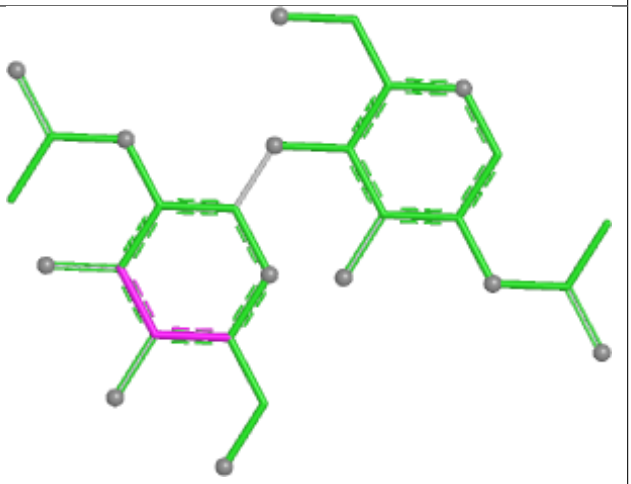
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1	NAG	2	0
7	M	4	MAN	1	0
7	M	3	BMA	1	0
7	G	1	NAG	2	0

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

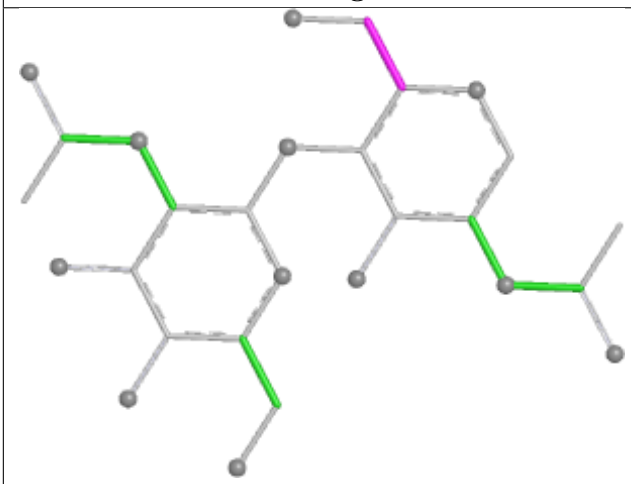
Oligosaccharide Chain F



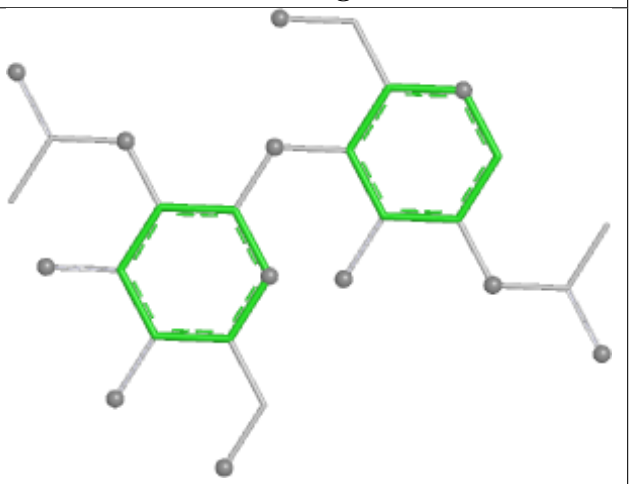
Bond lengths



Bond angles

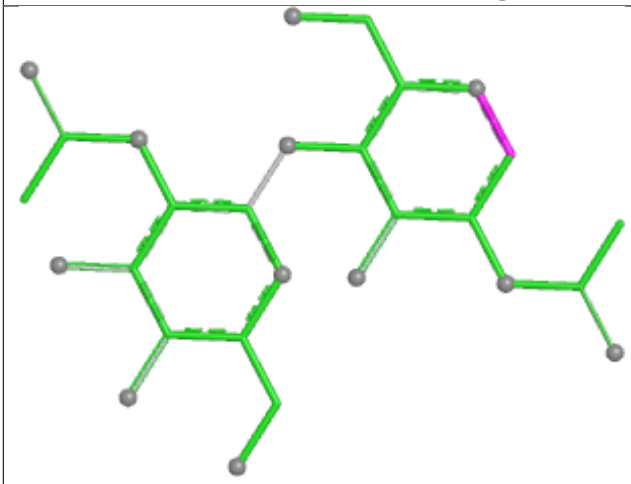


Torsions

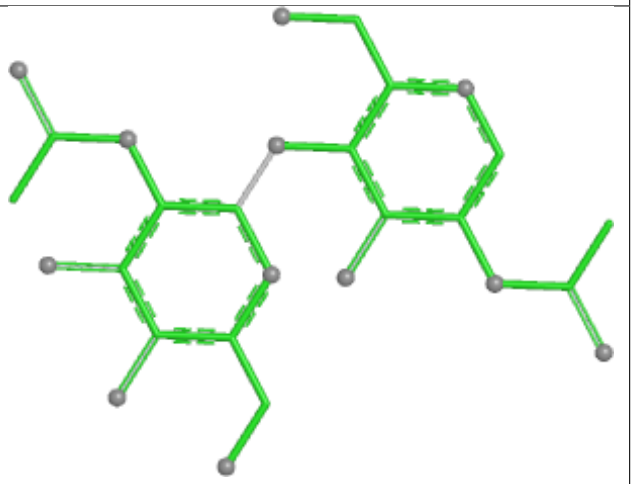


Rings

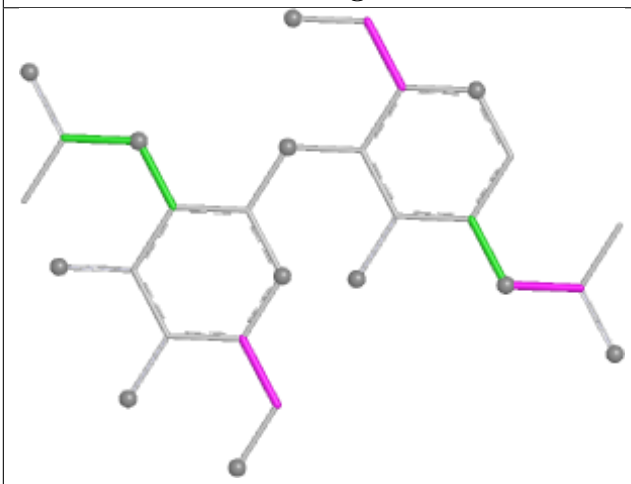
Oligosaccharide Chain N



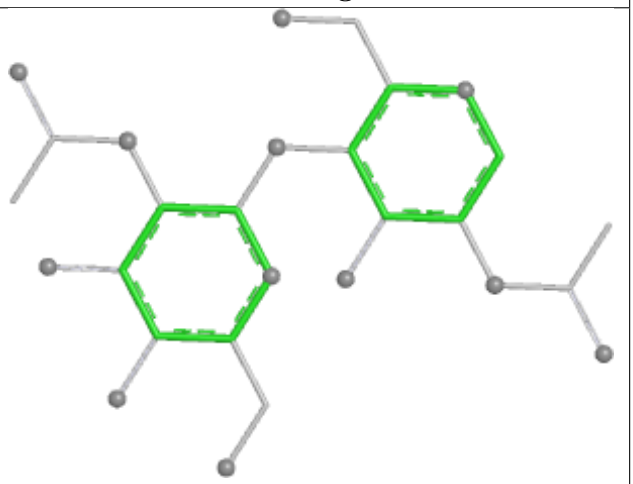
Bond lengths



Bond angles

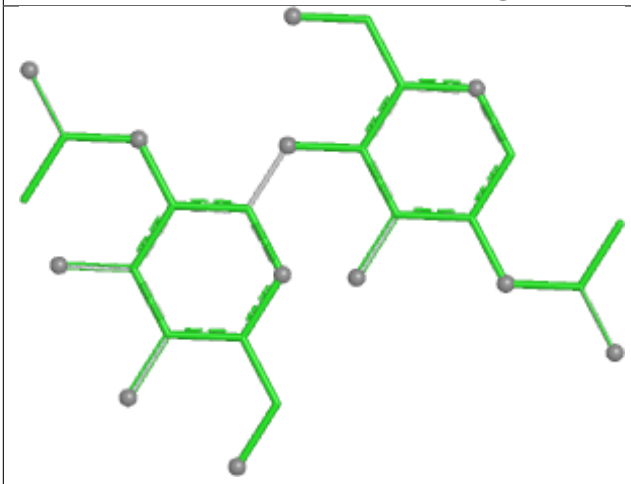


Torsions

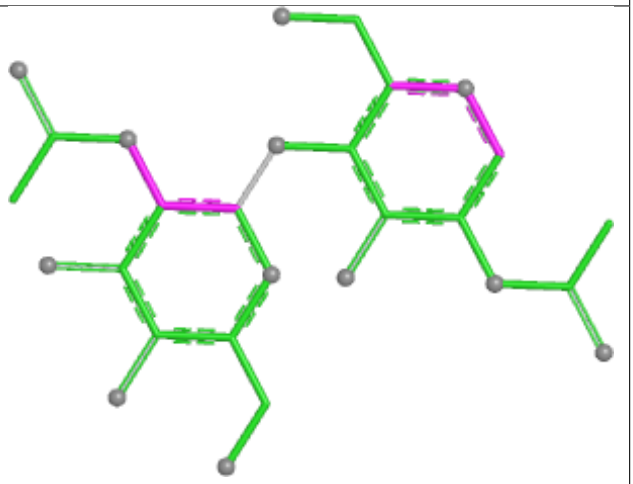


Rings

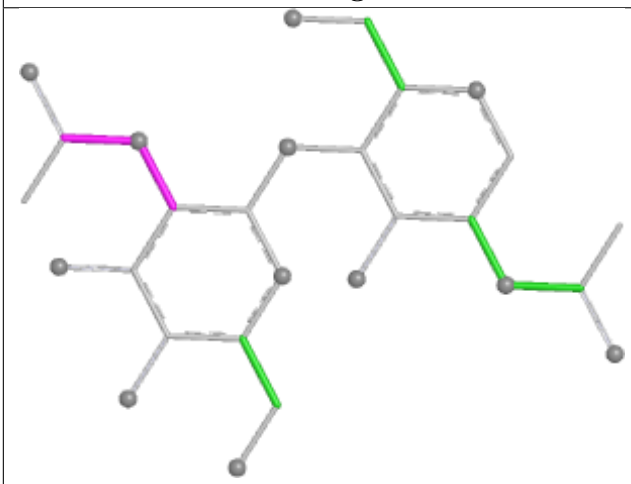
Oligosaccharide Chain O



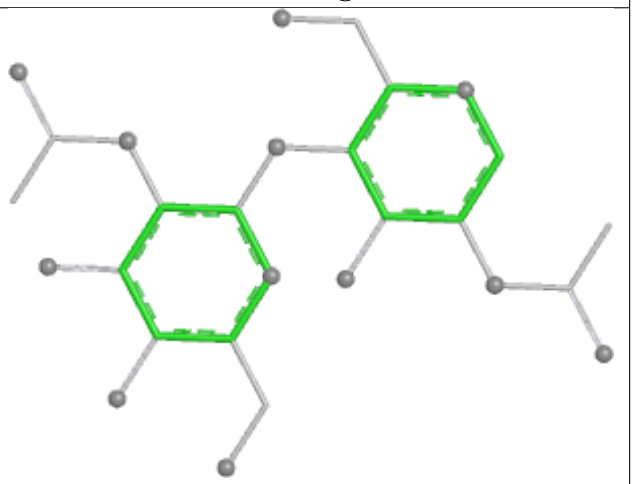
Bond lengths



Bond angles

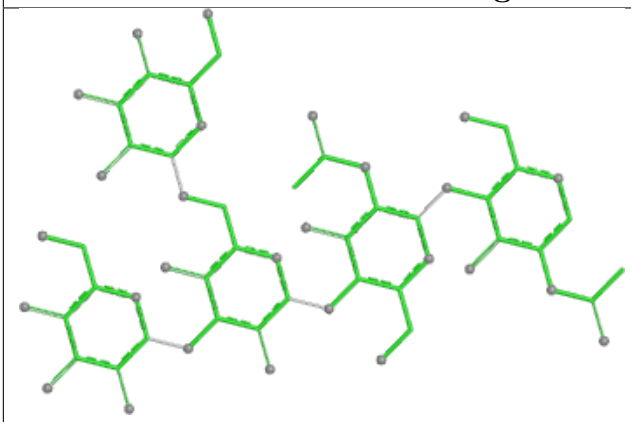


Torsions

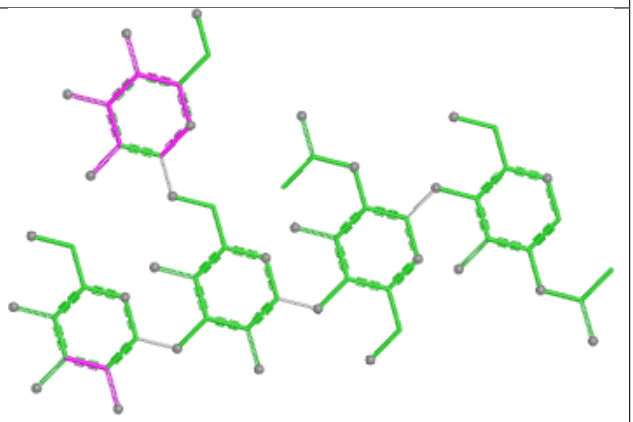


Rings

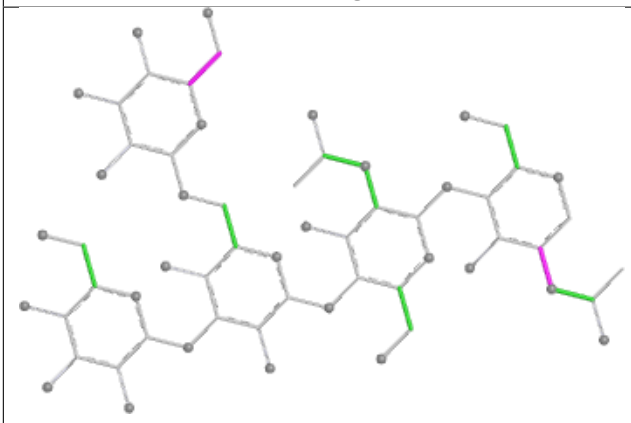
Oligosaccharide Chain G



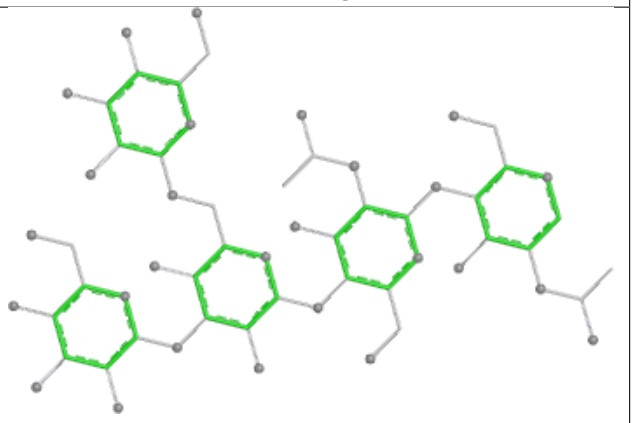
Bond lengths



Bond angles

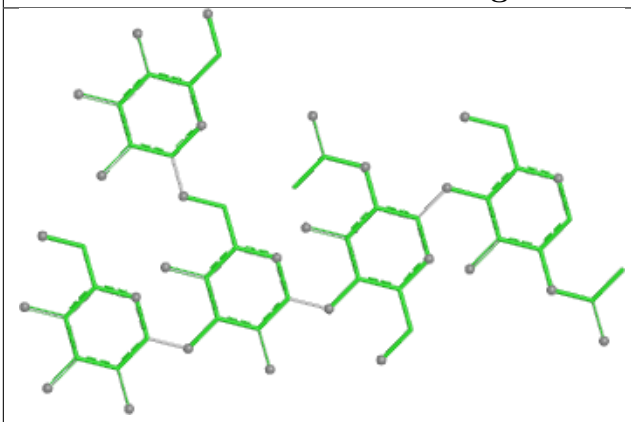


Torsions

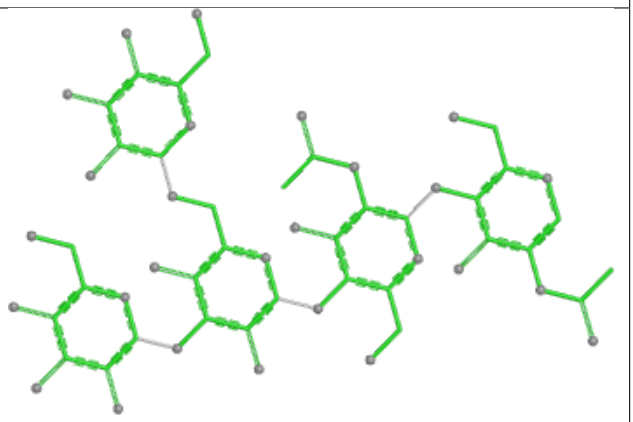


Rings

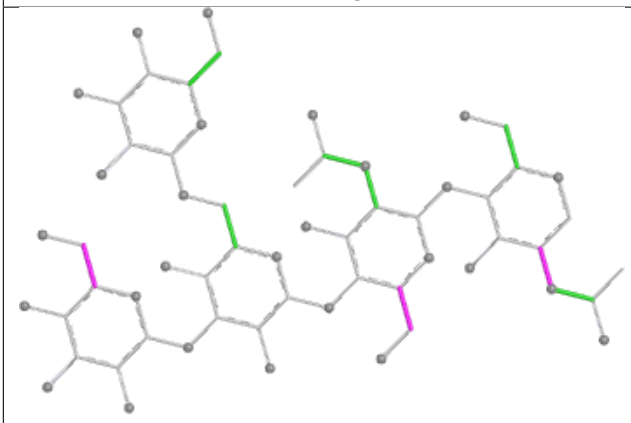
Oligosaccharide Chain M



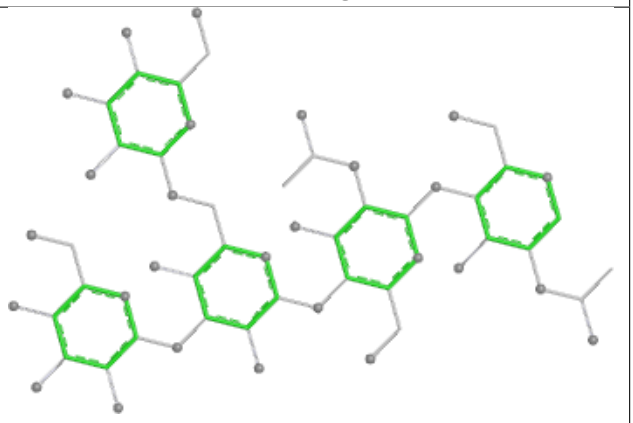
Bond lengths



Bond angles

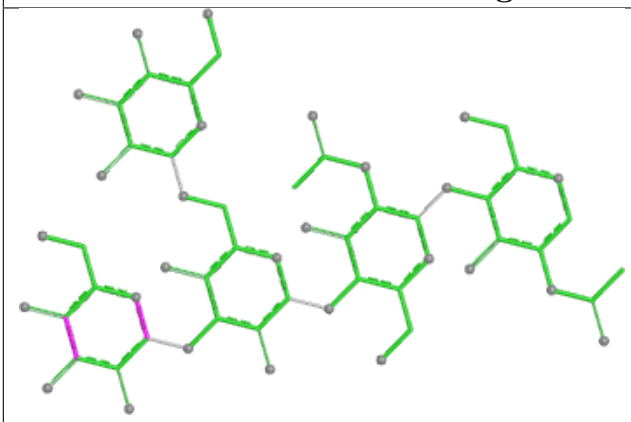


Torsions

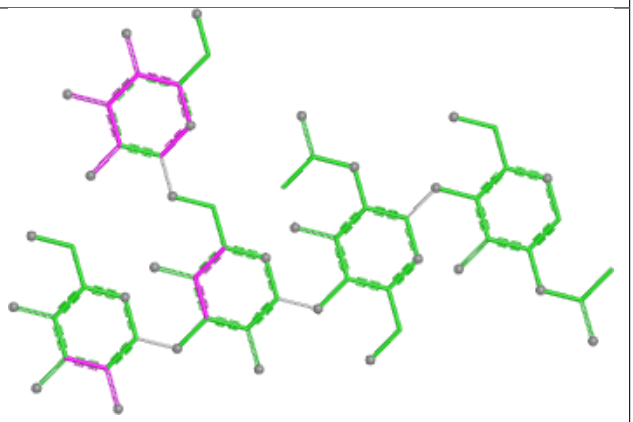


Rings

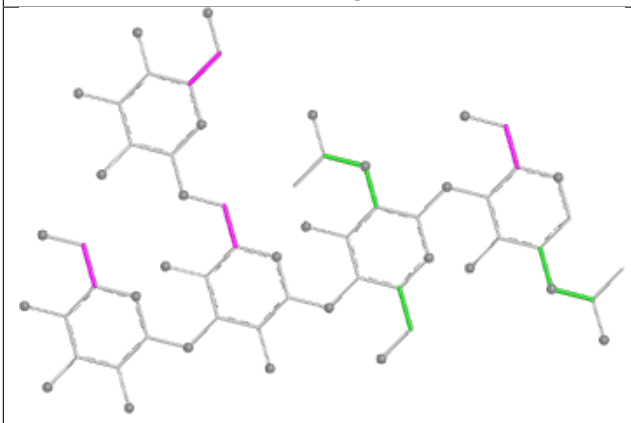
Oligosaccharide Chain P



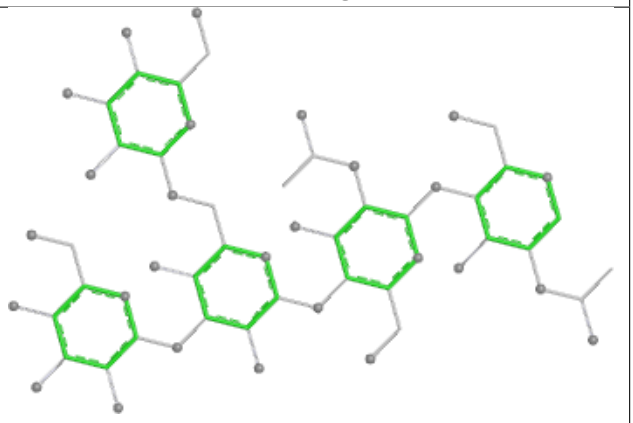
Bond lengths



Bond angles

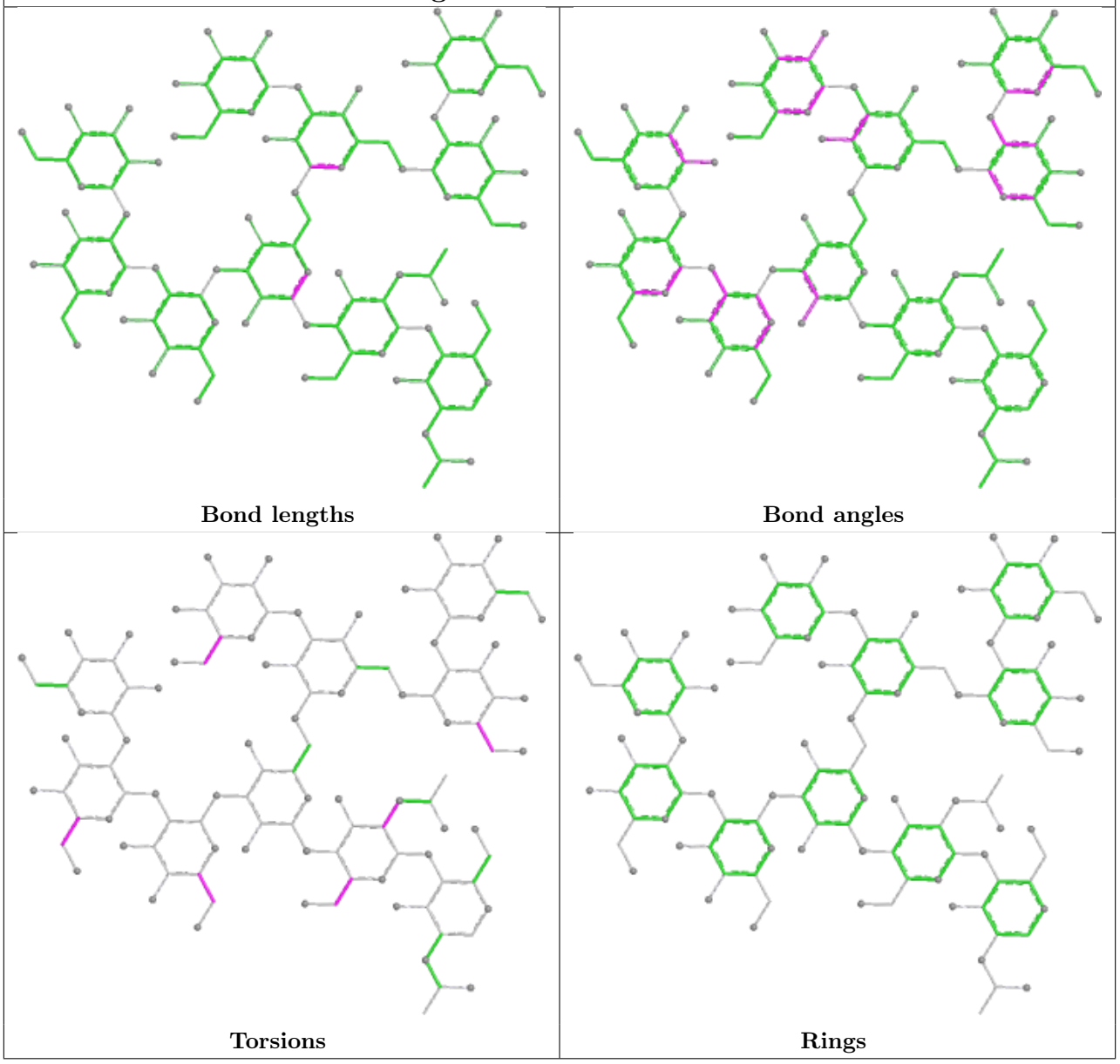


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	PTY	D	402	-	39,39,49	0.32	0	42,44,54	0.34	0
12	POV	B	402	-	33,33,51	0.97	1 (3%)	39,41,59	0.92	1 (2%)
13	Q3G	D	401	-	50,51,51	0.40	0	52,58,58	0.36	0
11	PTY	C	403	-	40,40,49	0.31	0	43,45,54	0.34	0
10	A1ADN	A	402	-	27,27,27	2.26	8 (29%)	37,38,38	1.35	5 (13%)
13	Q3G	C	404	-	43,44,51	0.43	0	45,51,58	0.36	0
9	ABU	C	401	-	6,6,6	0.89	0	6,6,6	1.33	0
11	PTY	B	401	-	40,40,49	0.33	0	43,45,54	0.35	0
11	PTY	C	405	-	40,40,49	0.31	0	43,45,54	0.32	0
9	ABU	A	401	-	6,6,6	0.87	0	6,6,6	1.44	0
11	PTY	A	403	-	40,40,49	0.32	0	43,45,54	0.32	0
10	A1ADN	C	402	-	27,27,27	2.29	8 (29%)	37,38,38	1.26	4 (10%)

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
11	PTY	D	402	-	-	24/43/43/53	-
12	POV	B	402	-	-	19/37/37/55	-
13	Q3G	D	401	-	-	33/57/57/57	-
11	PTY	C	403	-	-	27/44/44/53	-
10	A1ADN	A	402	-	-	0/8/8/8	0/4/4/4
13	Q3G	C	404	-	-	29/50/50/57	-
9	ABU	C	401	-	-	2/4/4/4	-
11	PTY	B	401	-	-	21/44/44/53	-
11	PTY	C	405	-	-	22/44/44/53	-
9	ABU	A	401	-	-	2/4/4/4	-
11	PTY	A	403	-	-	22/44/44/53	-
10	A1ADN	C	402	-	-	0/8/8/8	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	402	A1ADN	CAL-NAC	-6.53	1.34	1.44
10	A	402	A1ADN	CAL-NAC	-6.42	1.34	1.44
10	C	402	A1ADN	CAS-CAB	-5.08	1.39	1.47
10	A	402	A1ADN	CAS-CAB	-5.03	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	402	A1ADN	CAE-CAD	-4.42	1.38	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	402	A1ADN	NAC-CAB-NAA	-3.96	120.41	123.60
10	A	402	A1ADN	NAC-CAB-NAA	-3.89	120.47	123.60
10	A	402	A1ADN	CAE-CAD-NAC	3.74	119.81	114.69
10	C	402	A1ADN	CAE-CAD-NAC	3.68	119.73	114.69
10	A	402	A1ADN	CAE-CAJ-NAA	-3.06	119.34	122.41

There are no chirality outliers.

5 of 201 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	403	PTY	C2-C3-O11-P1
11	A	403	PTY	C5-O14-P1-O11
11	A	403	PTY	C5-O14-P1-O12
11	A	403	PTY	C5-O14-P1-O13
11	B	401	PTY	N1-C2-C3-O11

There are no ring outliers.

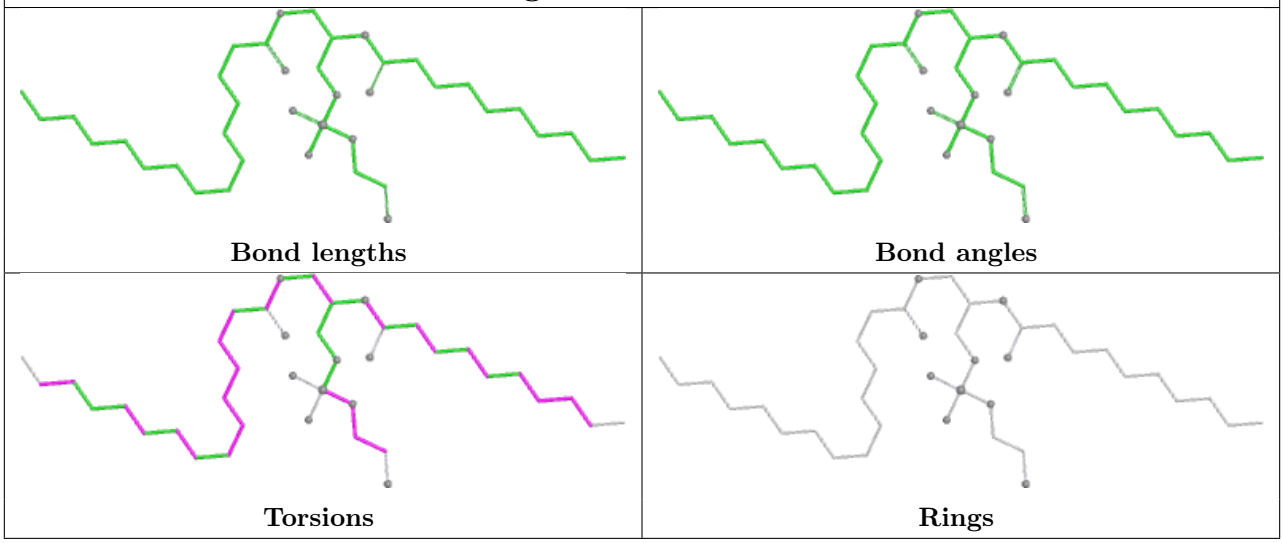
9 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	402	PTY	11	0
12	B	402	POV	2	0
13	D	401	Q3G	1	0
11	C	403	PTY	4	0
13	C	404	Q3G	1	0
9	C	401	ABU	1	0
11	B	401	PTY	11	0
11	C	405	PTY	20	0
11	A	403	PTY	25	0

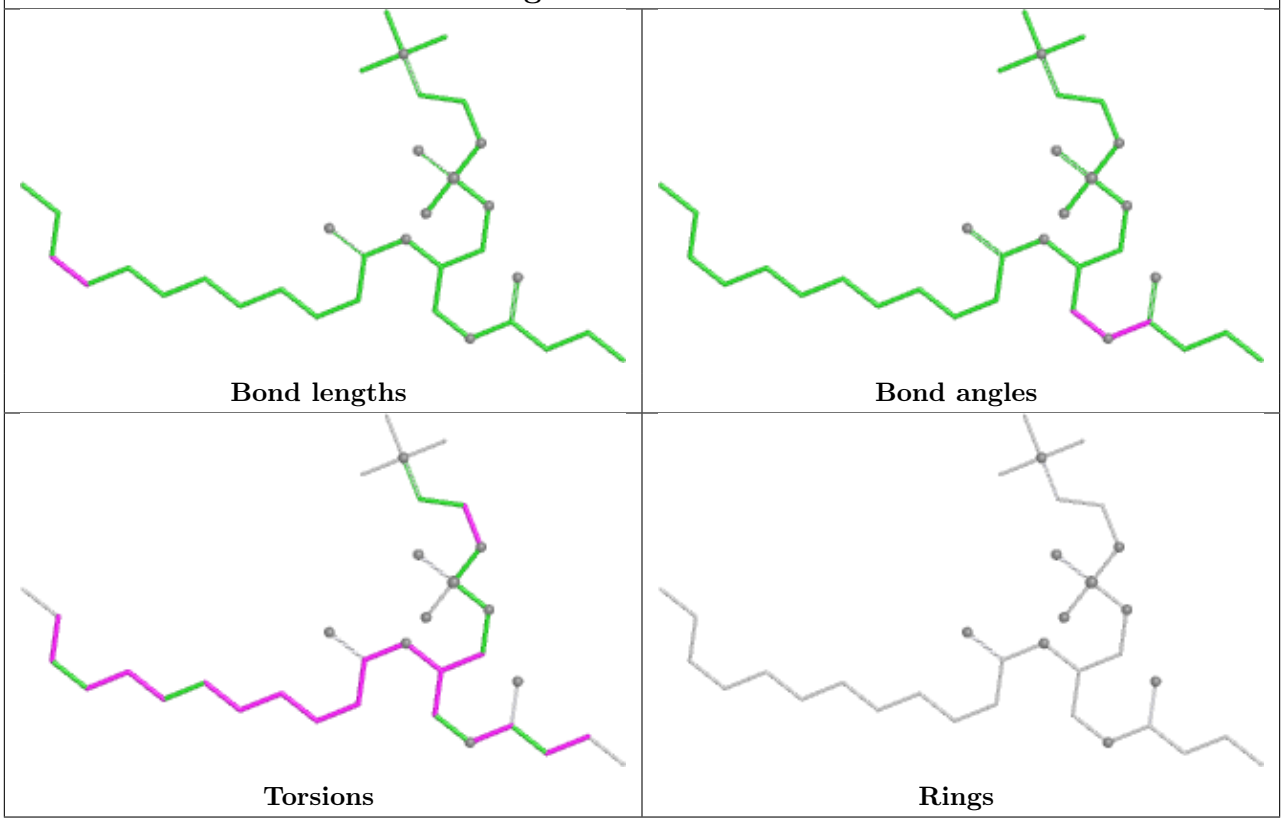
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

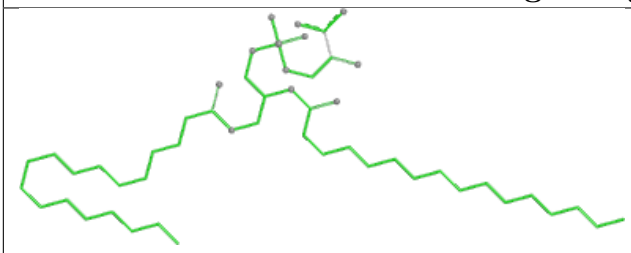
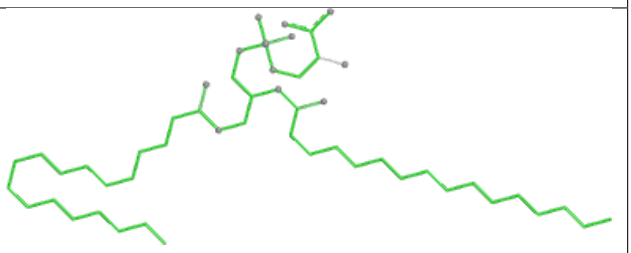
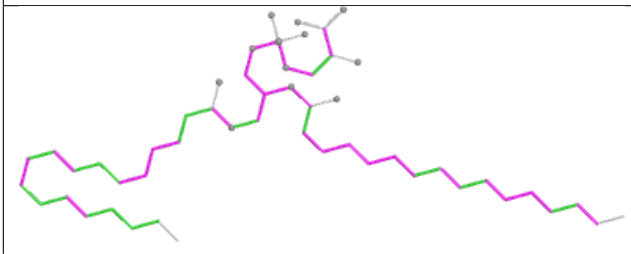
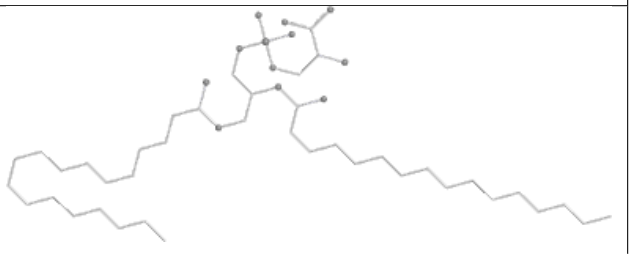
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

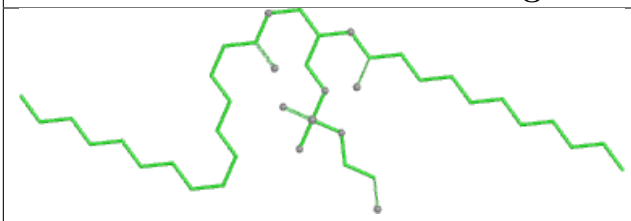
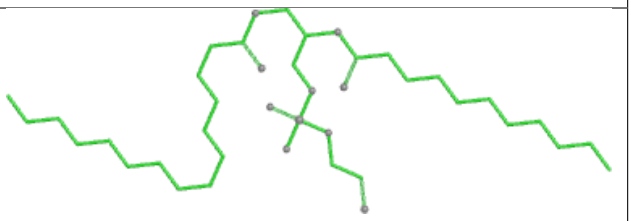
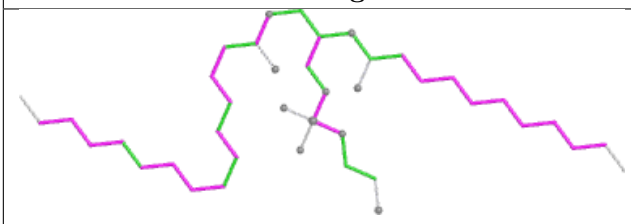
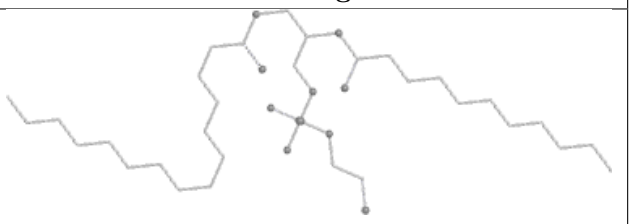
Ligand PTY D 402



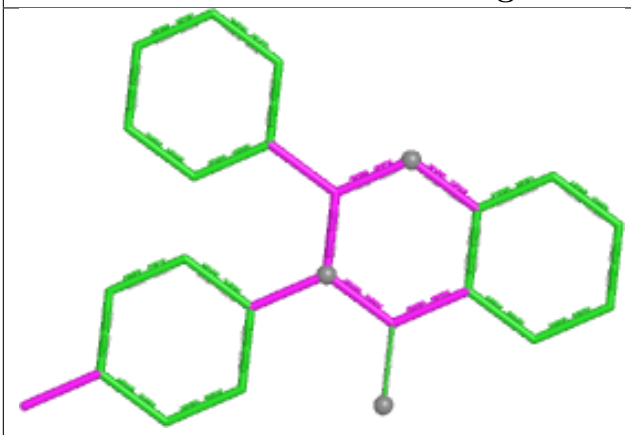
Ligand POV B 402



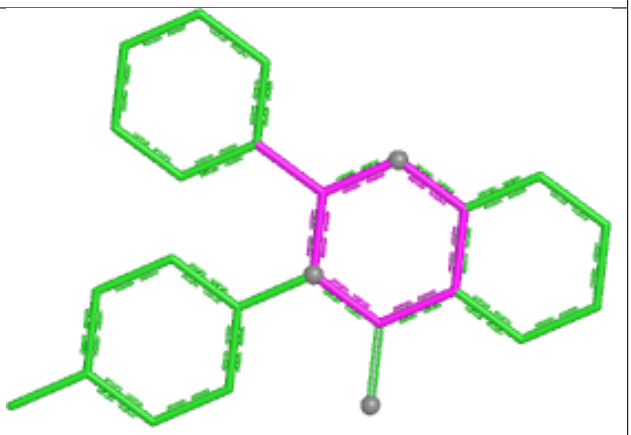
Ligand Q3G D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY C 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

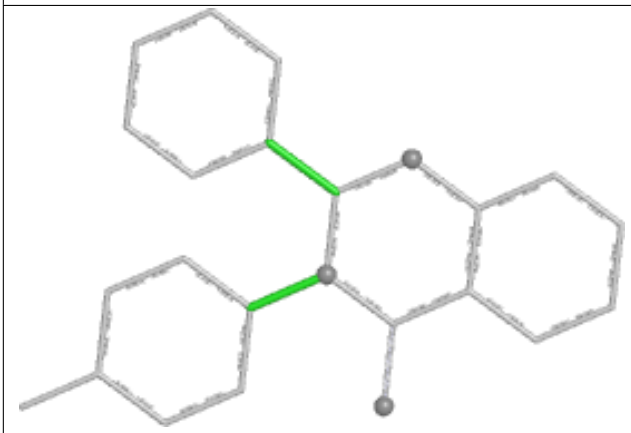
Ligand A1ADN A 402



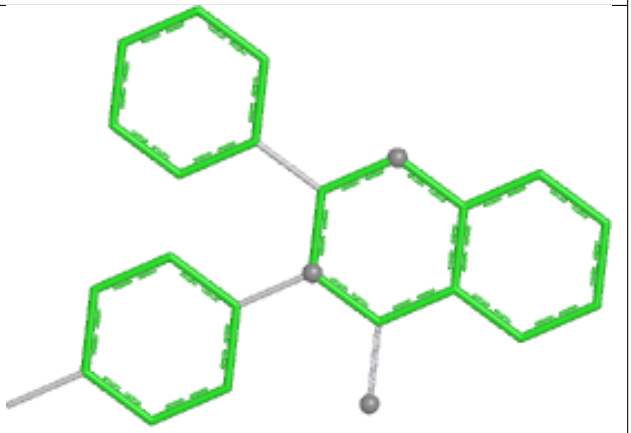
Bond lengths



Bond angles

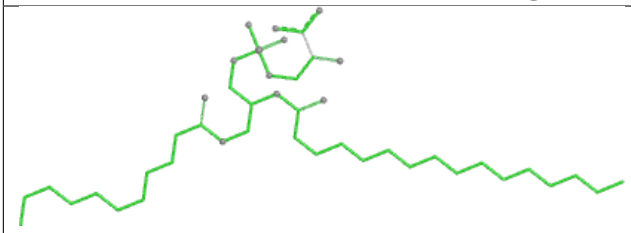


Torsions

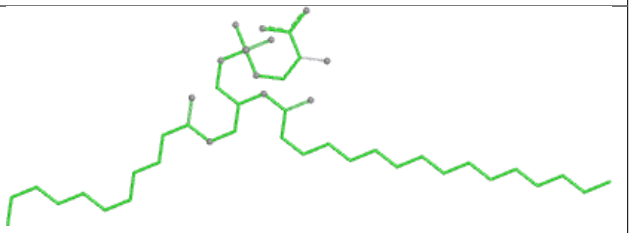


Rings

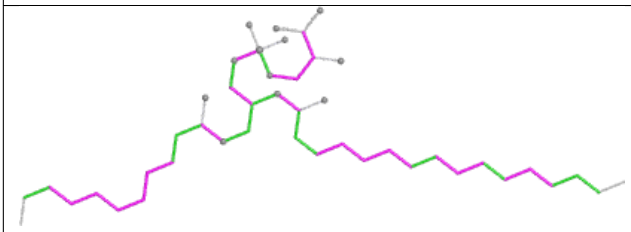
Ligand Q3G C 404



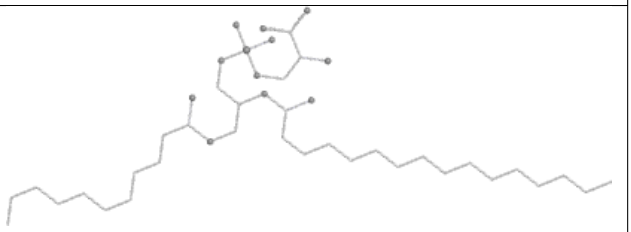
Bond lengths



Bond angles

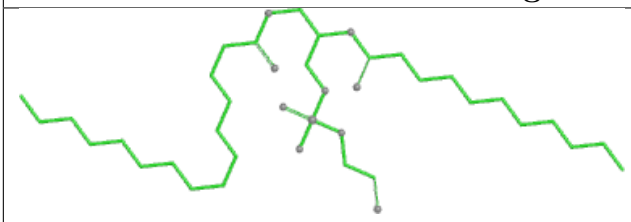


Torsions

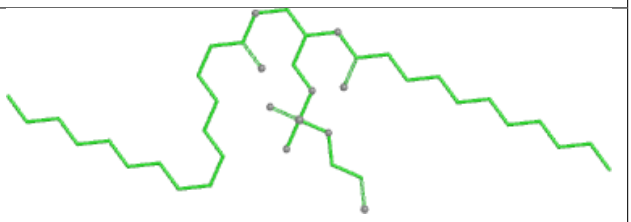


Rings

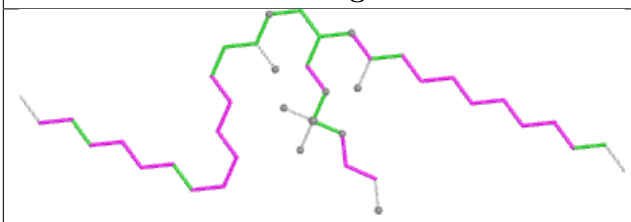
Ligand PTY B 401



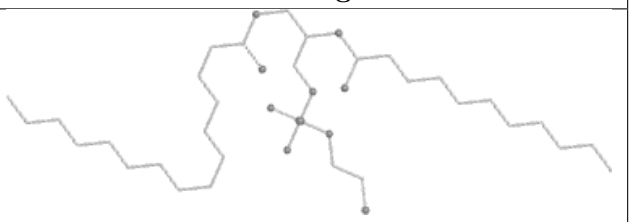
Bond lengths



Bond angles

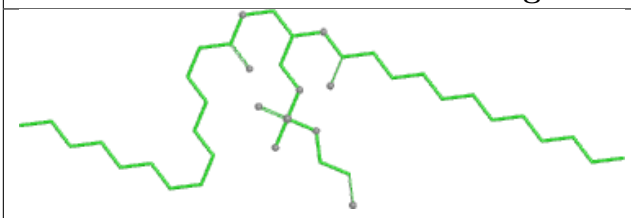


Torsions

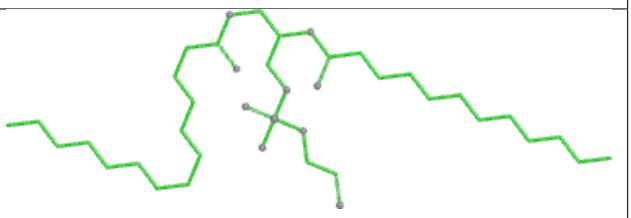


Rings

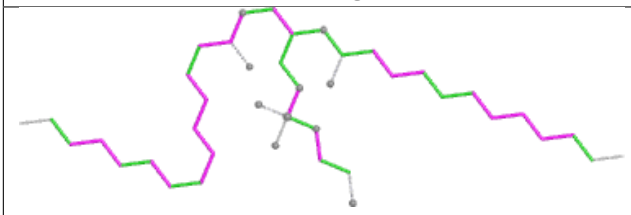
Ligand PTY C 405



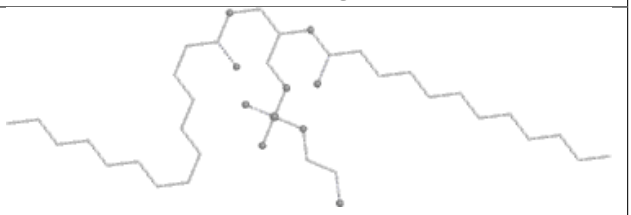
Bond lengths



Bond angles

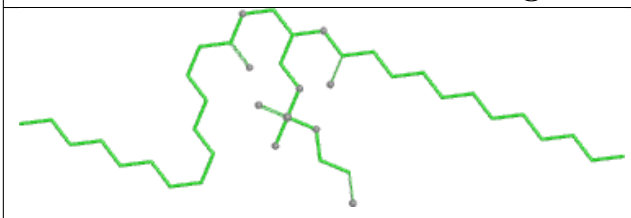


Torsions

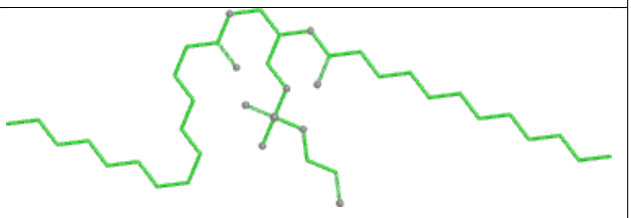


Rings

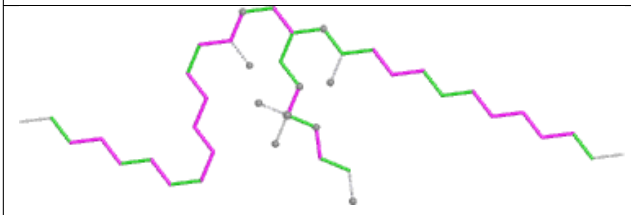
Ligand PTY A 403



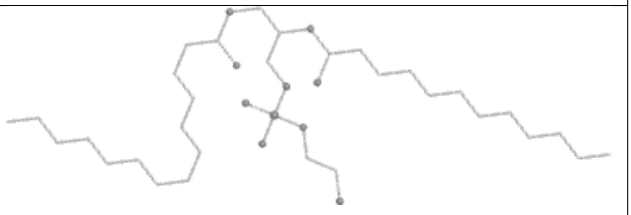
Bond lengths



Bond angles

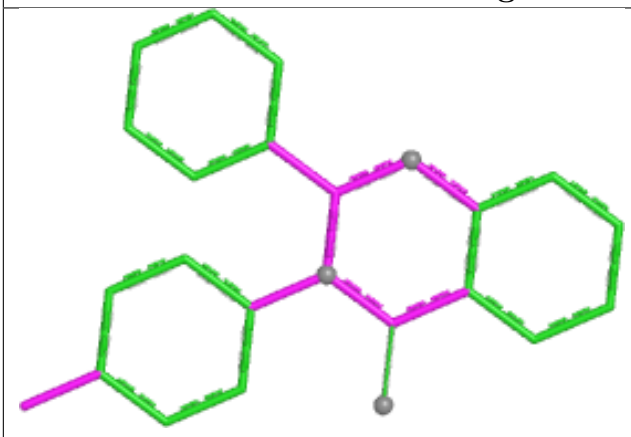


Torsions

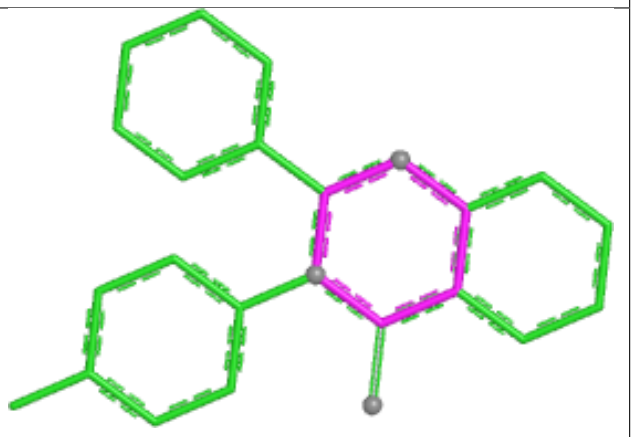


Rings

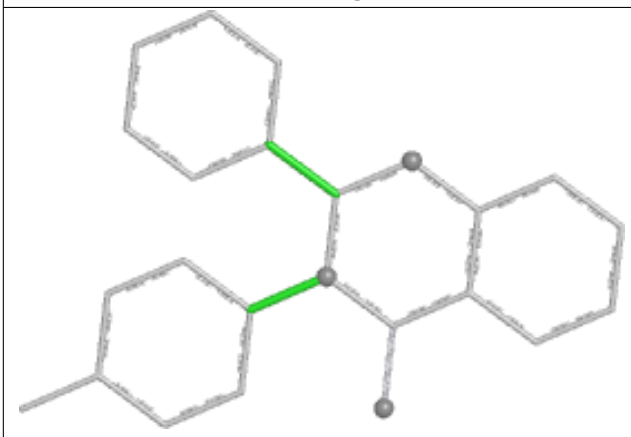
Ligand A1ADN C 402



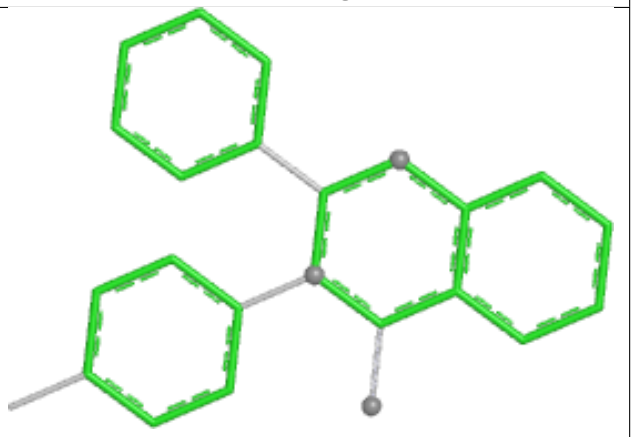
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

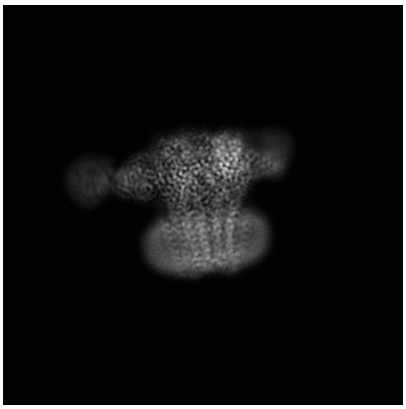
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43485. These allow visual inspection of the internal detail of the map and identification of artifacts.

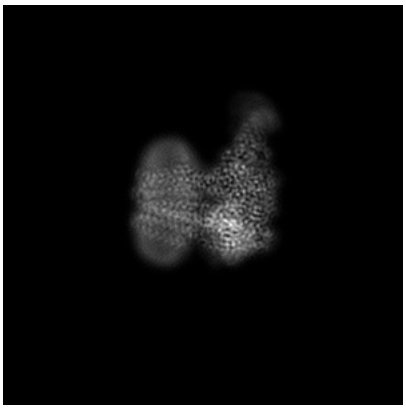
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

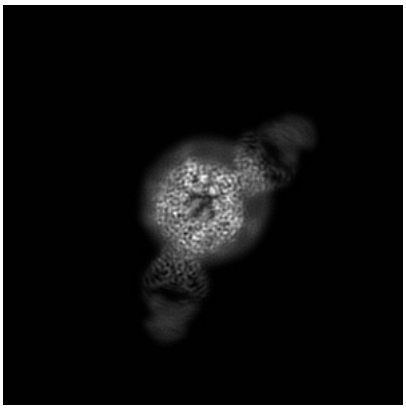
6.1.1 Primary map



X

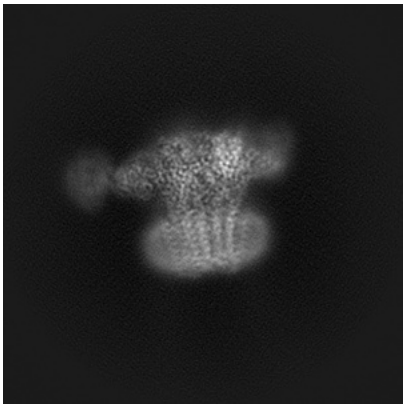


Y

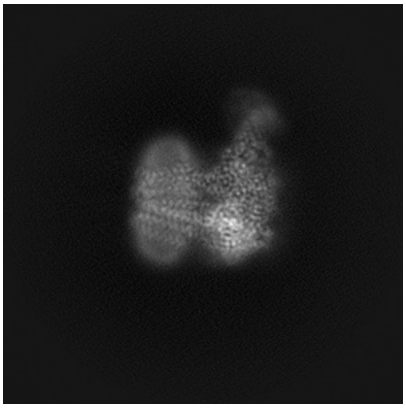


Z

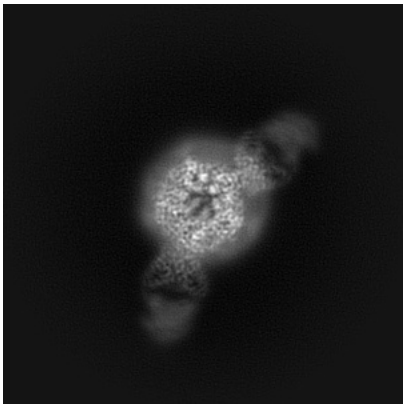
6.1.2 Raw map



X



Y



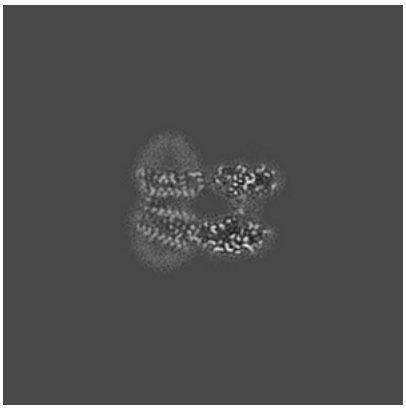
Z

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

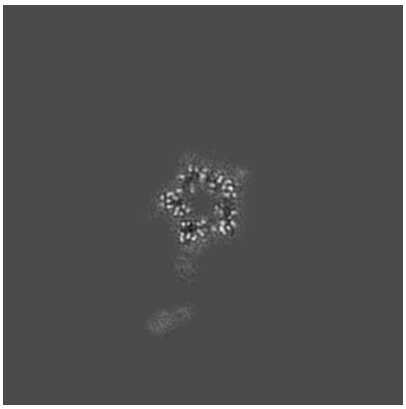
6.2 Central slices (i)

6.2.1 Primary map

X Index: 144

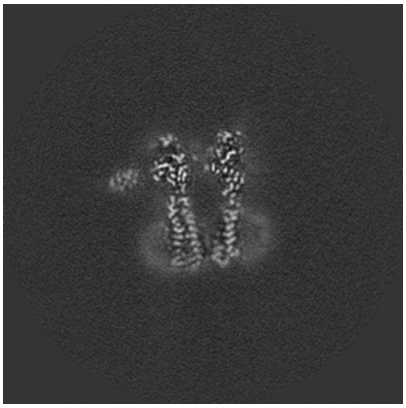


Y Index: 144

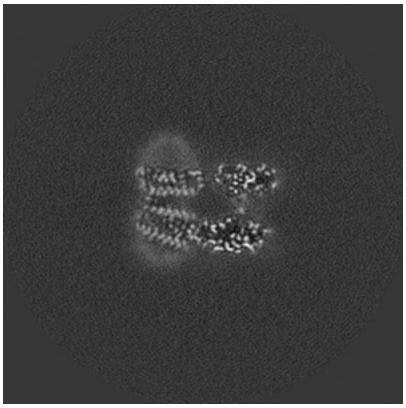


Z Index: 144

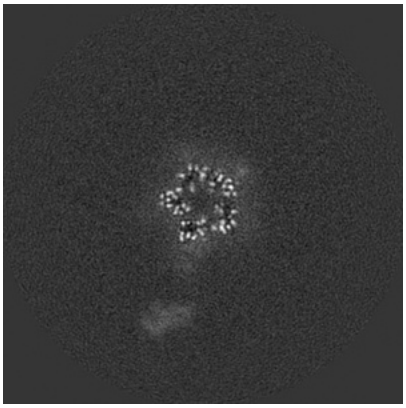
6.2.2 Raw map



X Index: 144



Y Index: 144

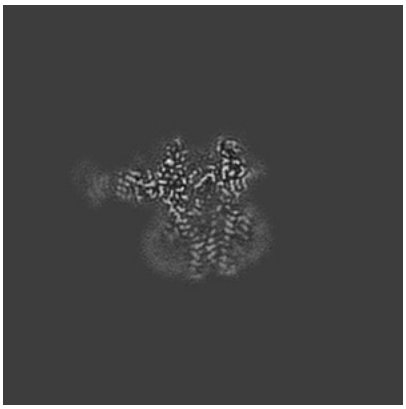


Z Index: 144

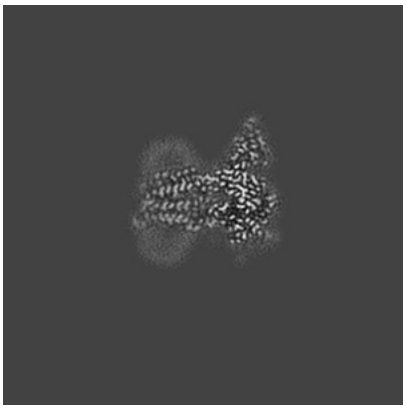
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

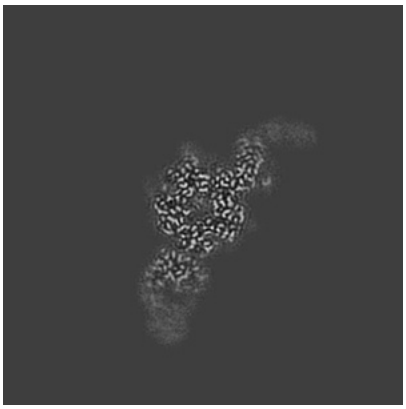
6.3.1 Primary map



X Index: 132

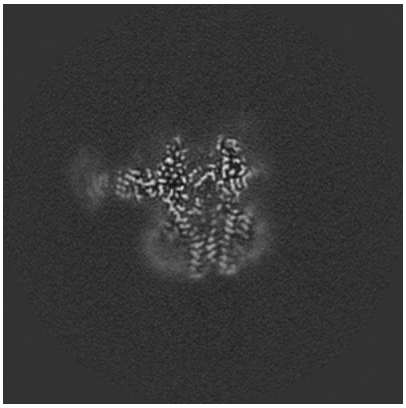


Y Index: 161

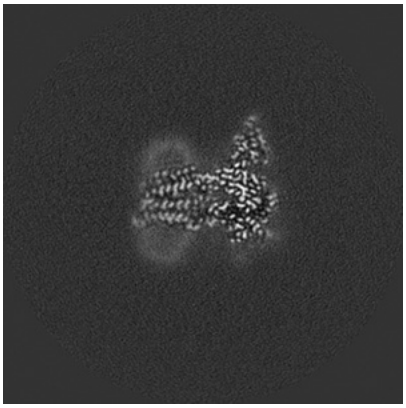


Z Index: 167

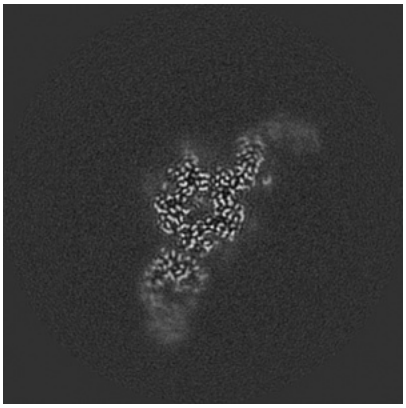
6.3.2 Raw map



X Index: 132



Y Index: 161

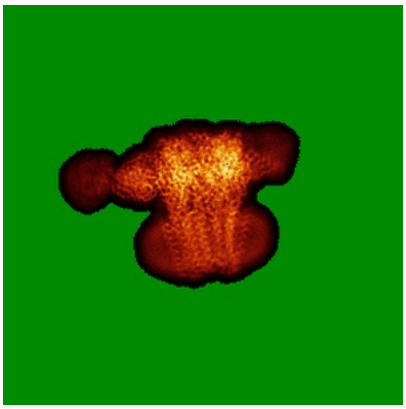


Z Index: 167

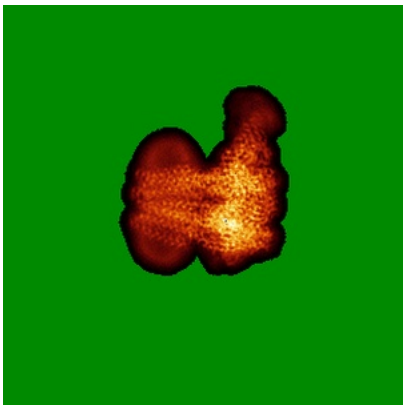
The images above show the largest variance slices of the map in three orthogonal directions.

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

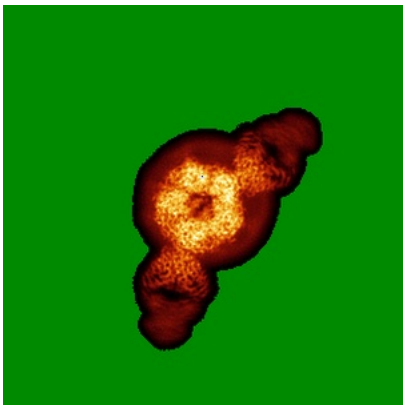
6.4.1 Primary map



X

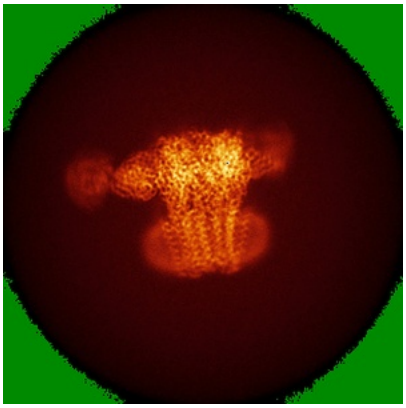


Y

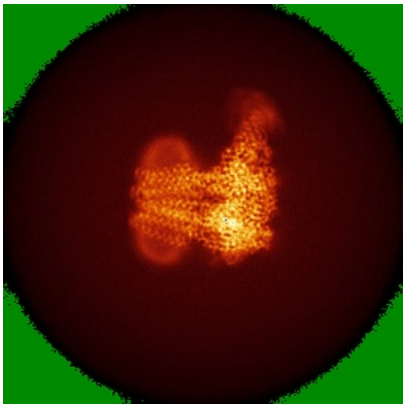


Z

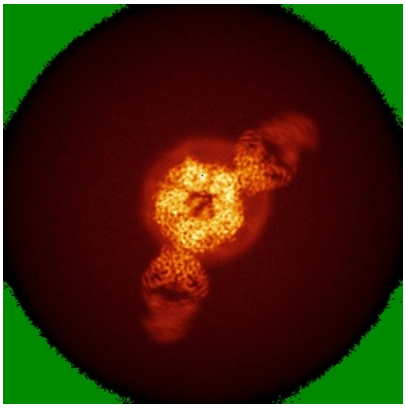
6.4.2 Raw map



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 0.014. 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.

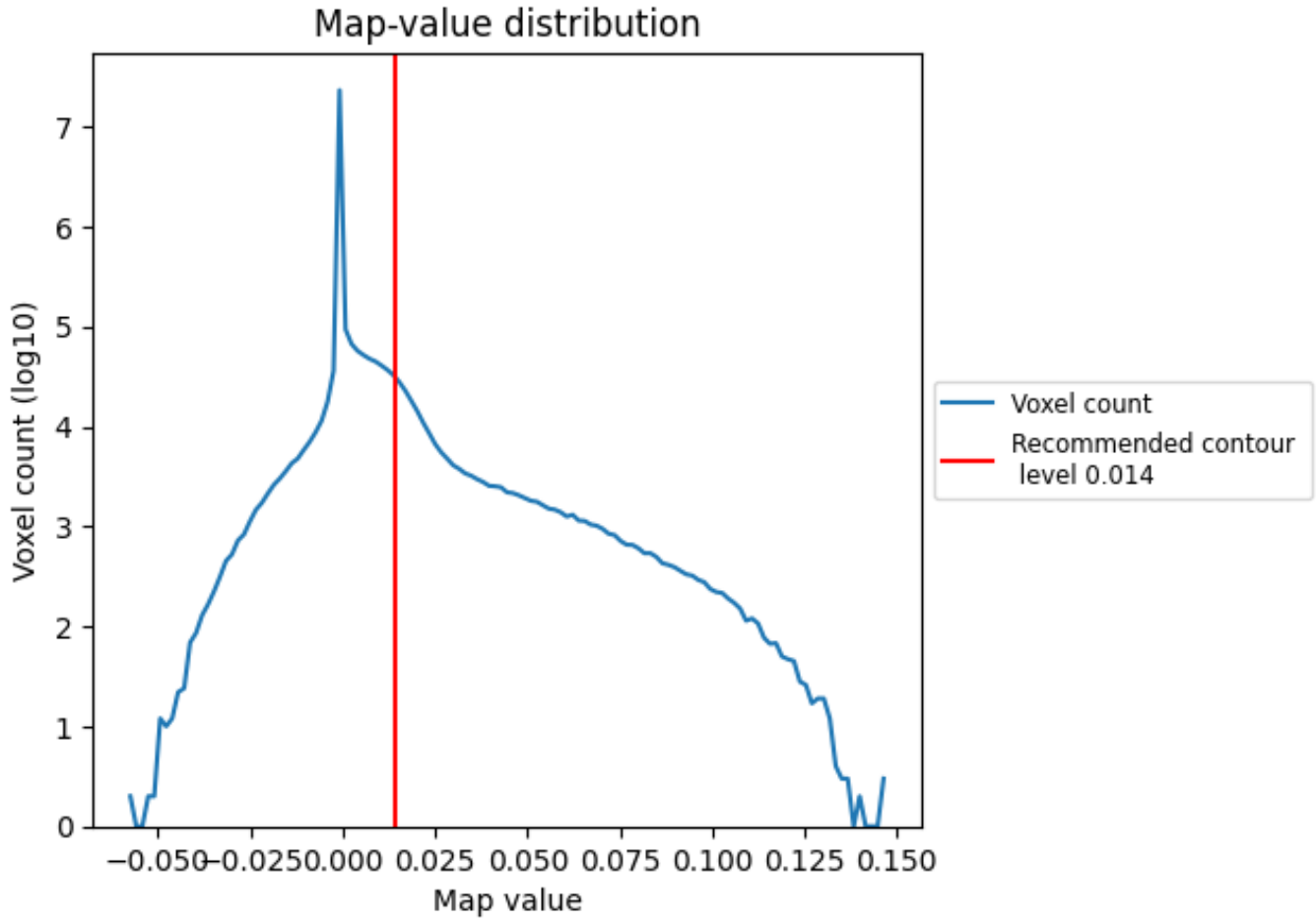
6.6 Mask visualisation (i)

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

7 Map analysis

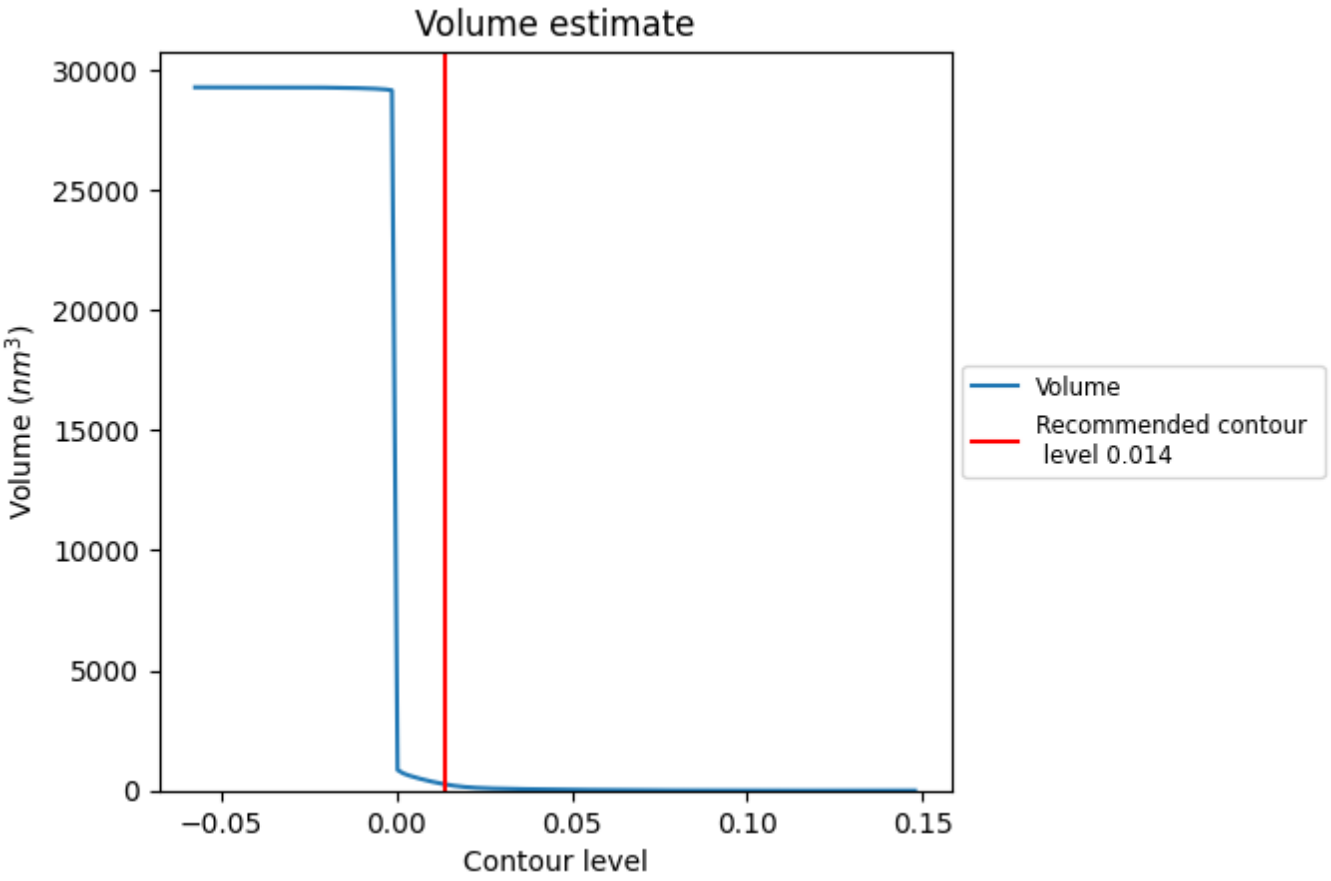
This section contains the results of statistical analysis of the map.

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.

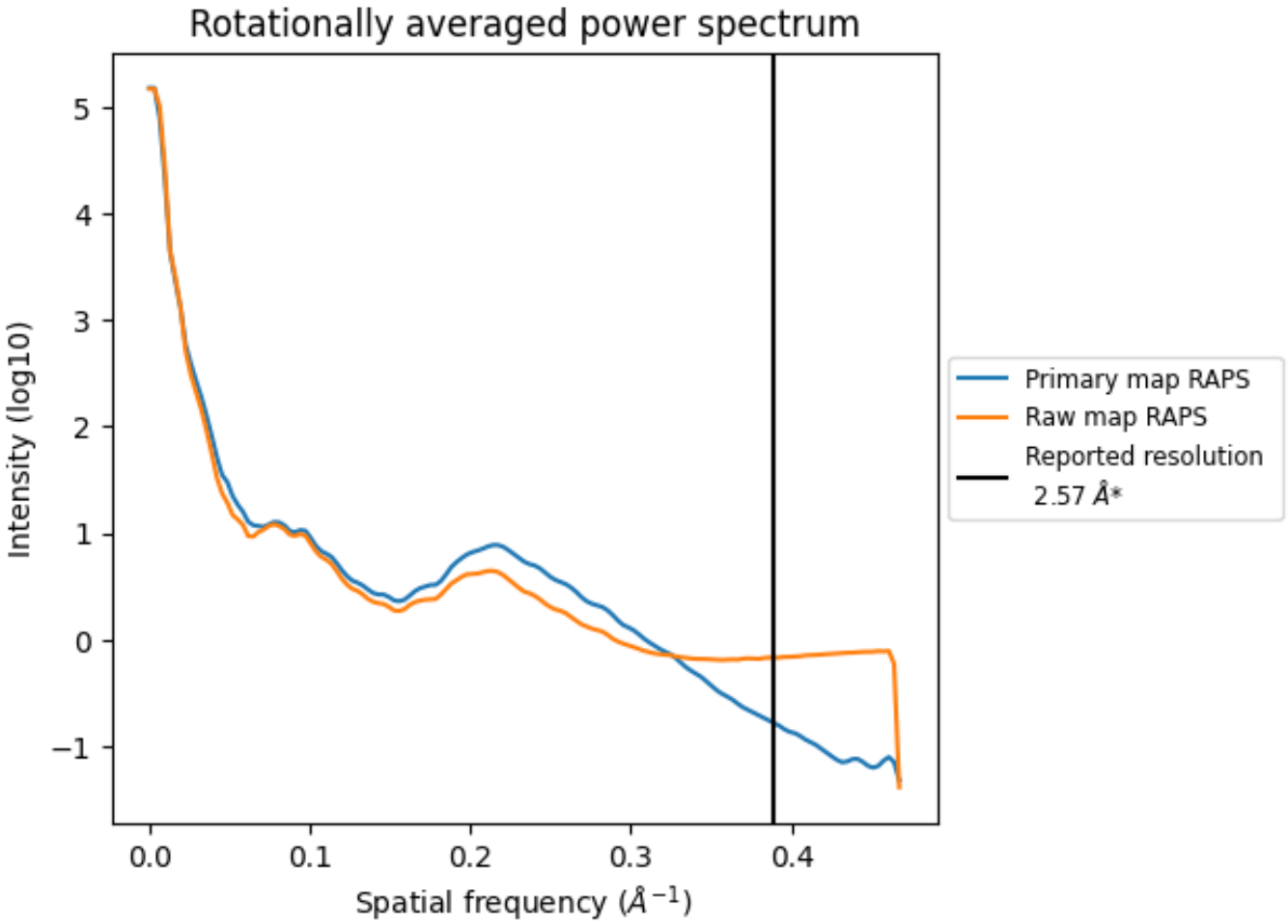
7.2 Volume estimate (i)



The volume at the recommended contour level is 257 nm^3; this corresponds to an approximate mass of 232 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)

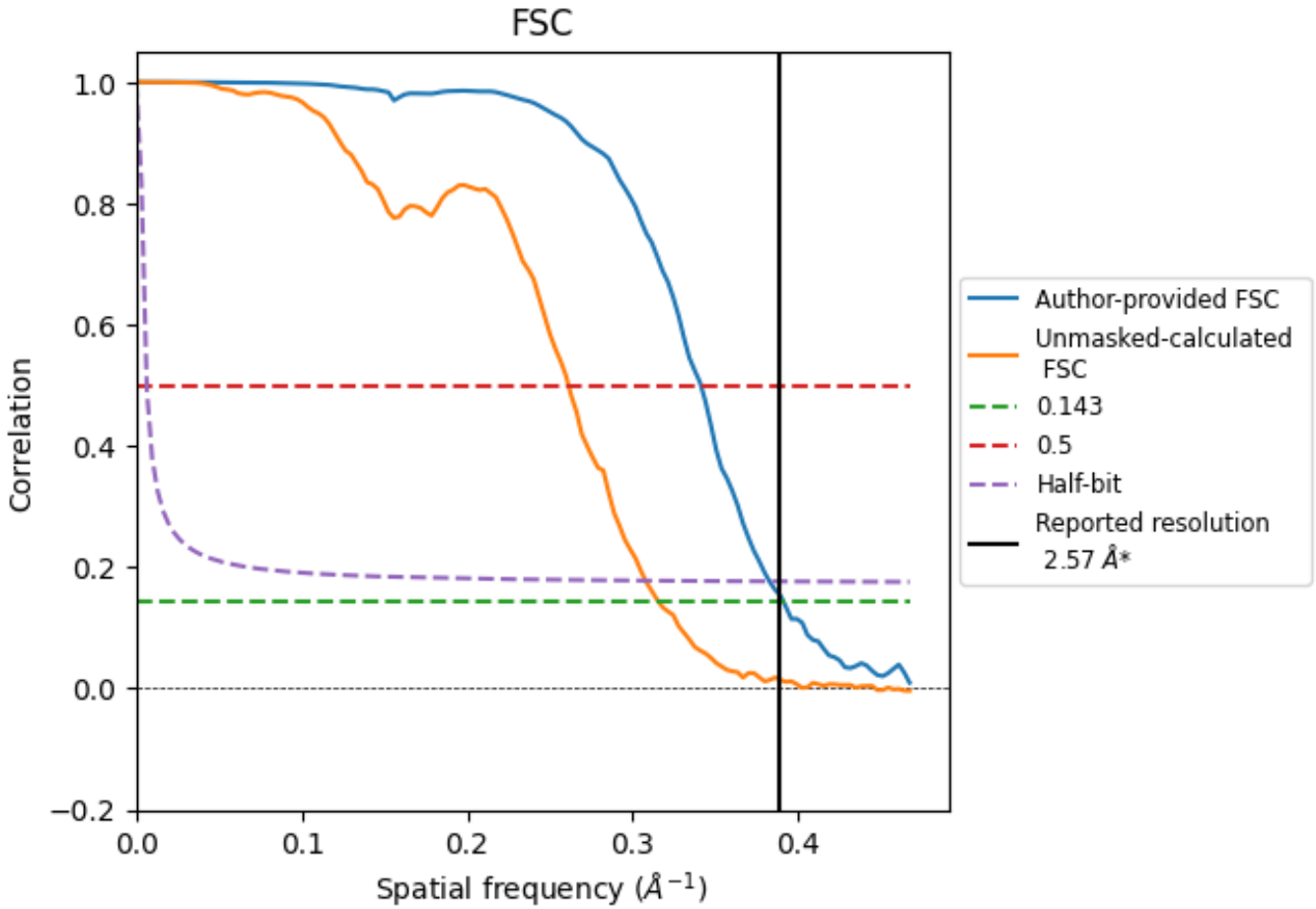


*Reported resolution corresponds to spatial frequency of 0.389 $Å^{-1}$

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 0.389 Å^{-1}

8.2 Resolution estimates (i)

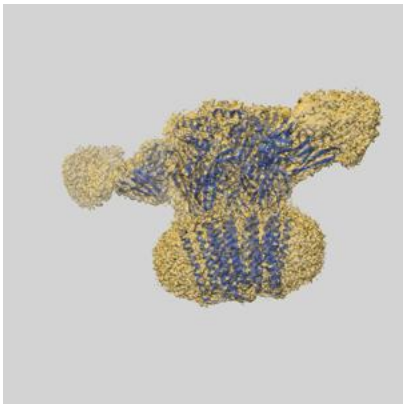
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.56	2.93	2.61
Unmasked-calculated*	3.17	3.83	3.25

*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 3.17 differs from the reported value 2.57 by more than 10 %

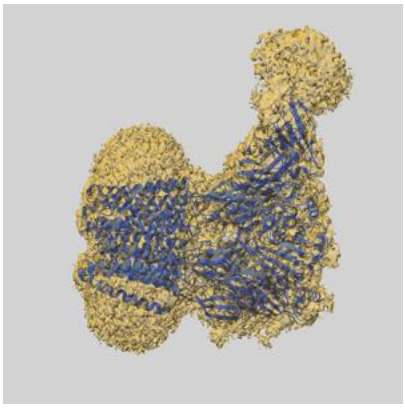
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43485 and PDB model 8VRN. Per-residue inclusion information can be found in section 3 on page 12.

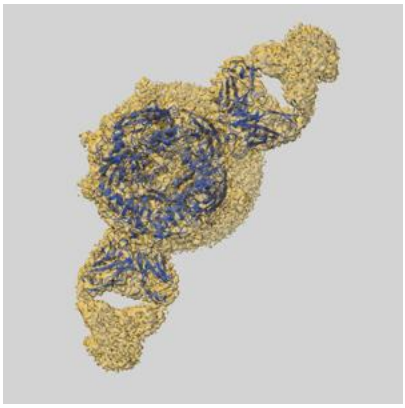
9.1 Map-model overlay



X



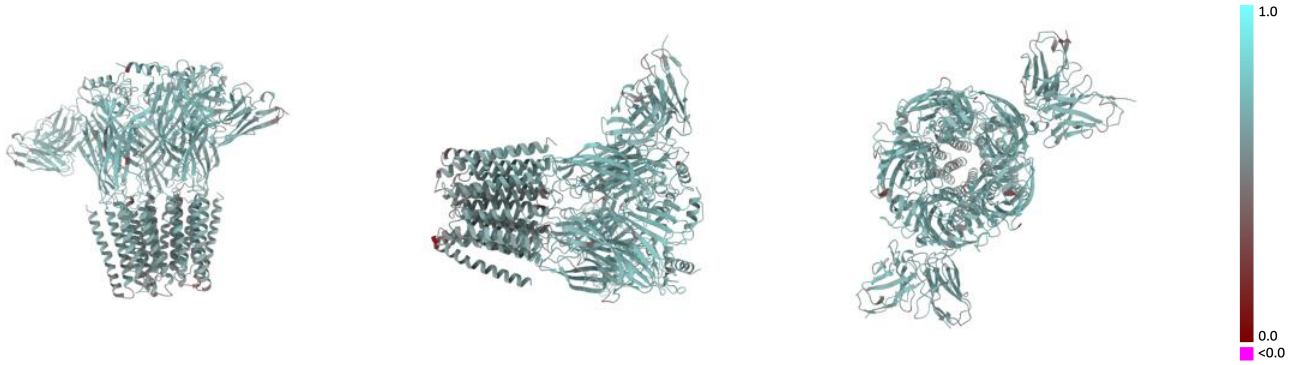
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

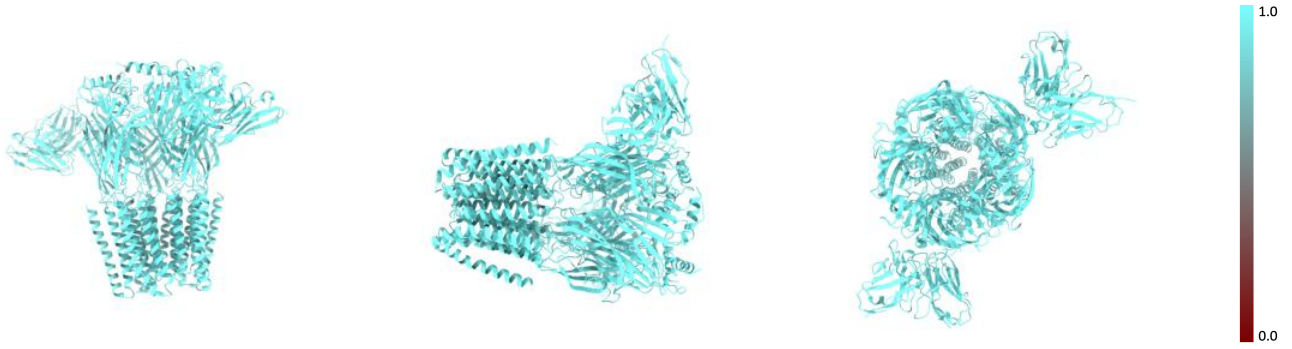
9.2 Q-score mapped to coordinate model (i)



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.

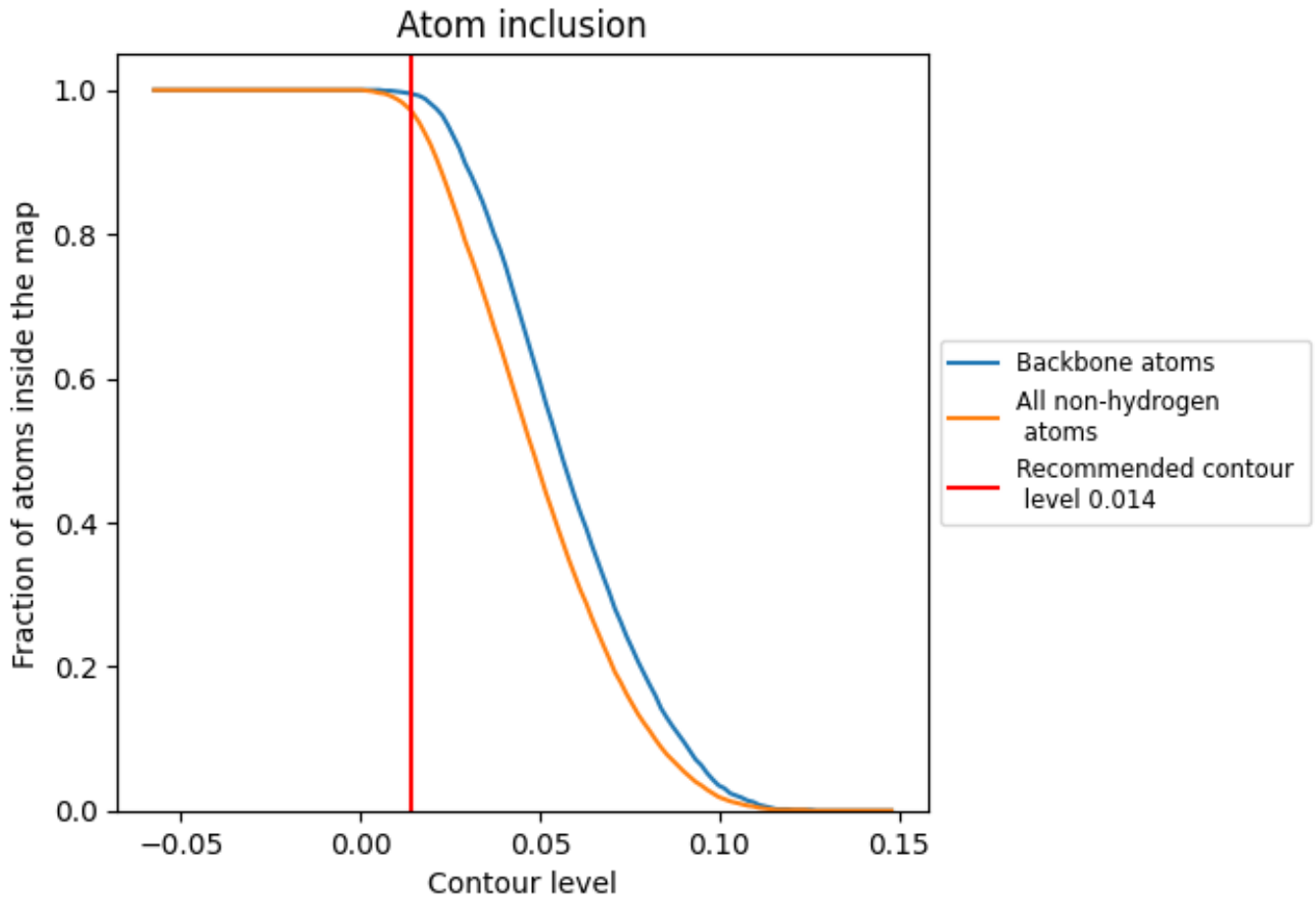
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.6180
A	0.9700	0.6170
B	0.9750	0.6290
C	0.9770	0.6230
D	0.9790	0.6290
E	0.9740	0.6140
F	0.7140	0.3880
G	0.8850	0.5180
H	0.9740	0.5980
I	0.9580	0.6080
J	0.9630	0.6040
K	0.9690	0.6060
L	0.9570	0.6050
M	0.9670	0.5660
N	0.9640	0.5530
O	0.8570	0.5250
P	0.9840	0.5600