Full wwPDB EM Validation Report ⓘ

Sep 14, 2024 – 10:01 am BST

PDB ID	:	9EQG
EMDB ID	:	EMD-19907
Title	:	CryoEM structure of human full-length alpha1beta3gamma2L GABA(A)R in complex with GABA and puerarin
Authors	:	Kasaragod, V.B.; Aricescu, A.R.
Deposited on	:	2024-03-21
Resolution	:	2.40 Å(reported)
Based on initial model	:	6HUP

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:

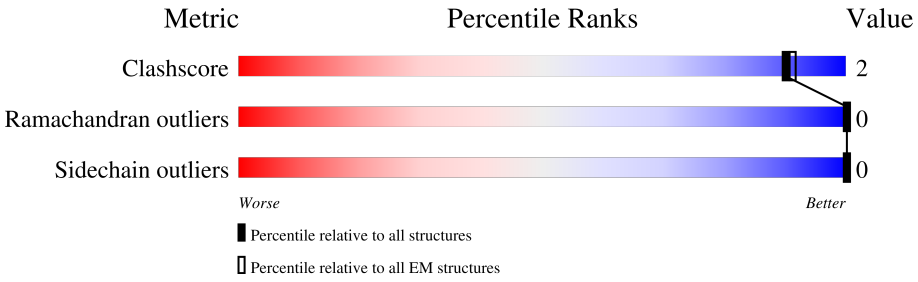
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.40 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	464	72% · 24%
1	D	464	73% · 24%
2	B	473	69% · 27%
2	E	473	70% · 27%
3	C	495	65% · 33%
4	F	10	30% 70%
5	G	6	50% 50%
5	I	6	33% 67%

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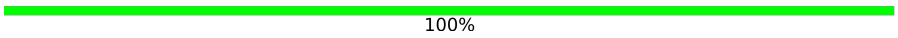
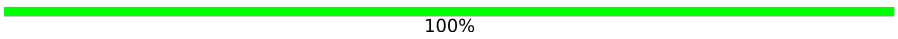
Mol	Chain	Length	Quality of chain
5	J	6	
6	H	3	
6	K	3	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 15459 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	352	Total	C	N	O	S	2	0
			2860	1850	480	514	16		
1	D	353	Total	C	N	O	S	1	0
			2863	1851	482	514	16		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P14867
A	-33	LYS	-	expression tag	UNP P14867
A	-32	LYS	-	expression tag	UNP P14867
A	-31	SER	-	expression tag	UNP P14867
A	-30	PRO	-	expression tag	UNP P14867
A	-29	GLY	-	expression tag	UNP P14867
A	-28	LEU	-	expression tag	UNP P14867
A	-27	SER	-	expression tag	UNP P14867
A	-26	ASP	-	expression tag	UNP P14867
A	-25	TYR	-	expression tag	UNP P14867
A	-24	LEU	-	expression tag	UNP P14867
A	-23	TRP	-	expression tag	UNP P14867
A	-22	ALA	-	expression tag	UNP P14867
A	-21	TRP	-	expression tag	UNP P14867
A	-20	THR	-	expression tag	UNP P14867
A	-19	LEU	-	expression tag	UNP P14867
A	-18	PHE	-	expression tag	UNP P14867
A	-17	LEU	-	expression tag	UNP P14867
A	-16	SER	-	expression tag	UNP P14867
A	-15	THR	-	expression tag	UNP P14867
A	-14	LEU	-	expression tag	UNP P14867
A	-13	THR	-	expression tag	UNP P14867
A	-12	GLY	-	expression tag	UNP P14867
A	-11	ARG	-	expression tag	UNP P14867
A	-10	SER	-	expression tag	UNP P14867
A	-9	TYR	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P14867
A	-7	ASP	-	expression tag	UNP P14867
A	-6	TYR	-	expression tag	UNP P14867
A	-5	LYS	-	expression tag	UNP P14867
A	-4	ASP	-	expression tag	UNP P14867
A	-3	ASP	-	expression tag	UNP P14867
A	-2	ASP	-	expression tag	UNP P14867
A	-1	ASP	-	expression tag	UNP P14867
A	0	LYS	-	expression tag	UNP P14867
D	-34	MET	-	initiating methionine	UNP P14867
D	-33	LYS	-	expression tag	UNP P14867
D	-32	LYS	-	expression tag	UNP P14867
D	-31	SER	-	expression tag	UNP P14867
D	-30	PRO	-	expression tag	UNP P14867
D	-29	GLY	-	expression tag	UNP P14867
D	-28	LEU	-	expression tag	UNP P14867
D	-27	SER	-	expression tag	UNP P14867
D	-26	ASP	-	expression tag	UNP P14867
D	-25	TYR	-	expression tag	UNP P14867
D	-24	LEU	-	expression tag	UNP P14867
D	-23	TRP	-	expression tag	UNP P14867
D	-22	ALA	-	expression tag	UNP P14867
D	-21	TRP	-	expression tag	UNP P14867
D	-20	THR	-	expression tag	UNP P14867
D	-19	LEU	-	expression tag	UNP P14867
D	-18	PHE	-	expression tag	UNP P14867
D	-17	LEU	-	expression tag	UNP P14867
D	-16	SER	-	expression tag	UNP P14867
D	-15	THR	-	expression tag	UNP P14867
D	-14	LEU	-	expression tag	UNP P14867
D	-13	THR	-	expression tag	UNP P14867
D	-12	GLY	-	expression tag	UNP P14867
D	-11	ARG	-	expression tag	UNP P14867
D	-10	SER	-	expression tag	UNP P14867
D	-9	TYR	-	expression tag	UNP P14867
D	-8	GLY	-	expression tag	UNP P14867
D	-7	ASP	-	expression tag	UNP P14867
D	-6	TYR	-	expression tag	UNP P14867
D	-5	LYS	-	expression tag	UNP P14867
D	-4	ASP	-	expression tag	UNP P14867
D	-3	ASP	-	expression tag	UNP P14867
D	-2	ASP	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	expression tag	UNP P14867
D	0	LYS	-	expression tag	UNP P14867

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	344	Total	C	N	O	S	1	0
			2833	1855	464	498	16		
2	E	345	Total	C	N	O	S	2	0
			2845	1862	468	499	16		

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

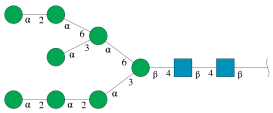
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	332	Total	C	N	O	S	2	0
			2749	1794	457	483	15		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	437	GLY	-	expression tag	UNP P18507
C	438	GLY	-	expression tag	UNP P18507
C	439	SER	-	expression tag	UNP P18507
C	440	GLY	-	expression tag	UNP P18507
C	441	GLY	-	expression tag	UNP P18507
C	442	SER	-	expression tag	UNP P18507
C	443	GLY	-	expression tag	UNP P18507
C	444	GLY	-	expression tag	UNP P18507
C	445	SER	-	expression tag	UNP P18507
C	446	GLY	-	expression tag	UNP P18507
C	447	LYS	-	expression tag	UNP P18507
C	448	THR	-	expression tag	UNP P18507
C	449	GLU	-	expression tag	UNP P18507
C	450	THR	-	expression tag	UNP P18507
C	451	SER	-	expression tag	UNP P18507
C	452	GLN	-	expression tag	UNP P18507
C	453	VAL	-	expression tag	UNP P18507
C	454	ALA	-	expression tag	UNP P18507
C	455	PRO	-	expression tag	UNP P18507
C	456	ALA	-	expression tag	UNP P18507

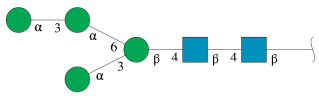
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



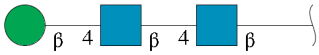
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

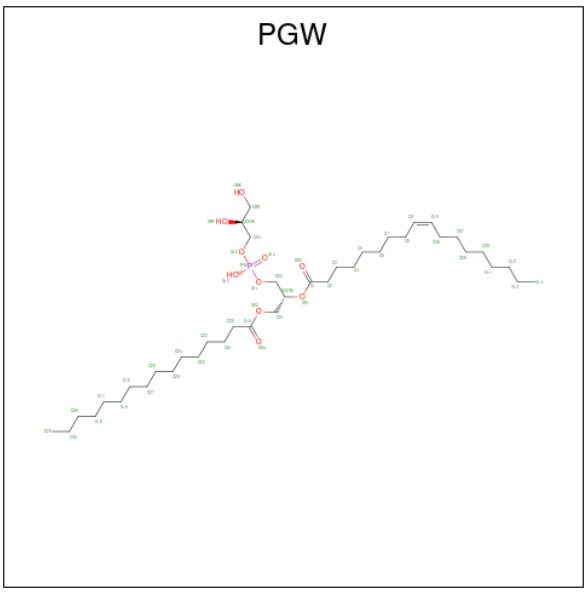
- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

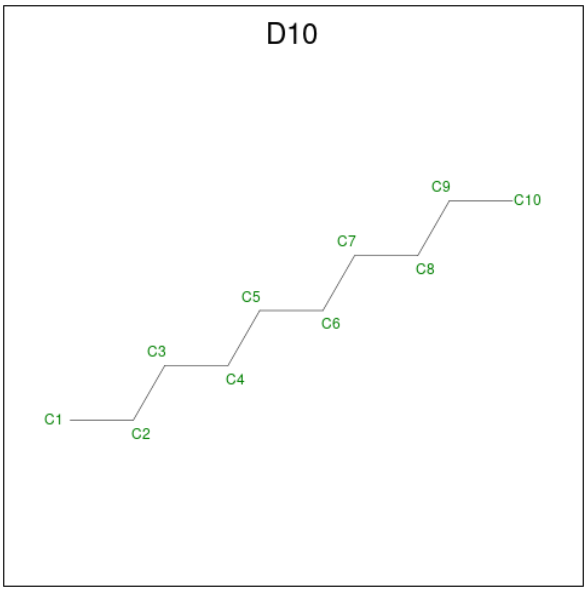
- Molecule 7 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula:

$C_{40}H_{77}O_{10}P$).



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

- Molecule 8 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	C	0
			10	10	

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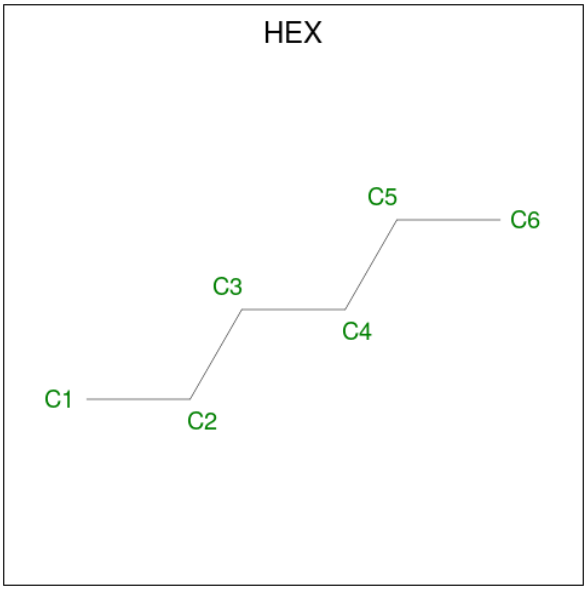
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C 10 10	0
8	A	1	Total C 10 10	0
8	B	1	Total C 10 10	0
8	C	1	Total C 10 10	0
8	C	1	Total C 10 10	0
8	C	1	Total C 10 10	0
8	D	1	Total C 10 10	0
8	D	1	Total C 10 10	0
8	E	1	Total C 10 10	0
8	E	1	Total C 10 10	0

- Molecule 9 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C 6 6	0

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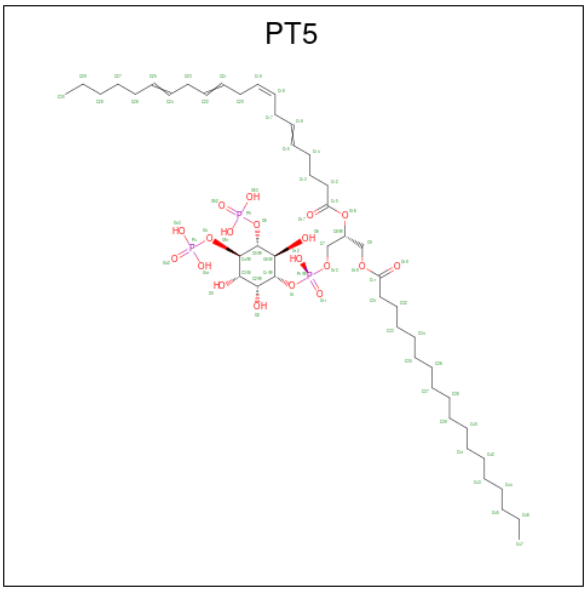
Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C 6 6	0
9	A	1	Total C 6 6	0
9	B	1	Total C 6 6	0
9	B	1	Total C 6 6	0
9	C	1	Total C 6 6	0
9	C	1	Total C 6 6	0
9	E	1	Total C 6 6	0
9	E	1	Total C 6 6	0
9	E	1	Total C 6 6	0

- Molecule 10 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O P 69 47 19 3	0

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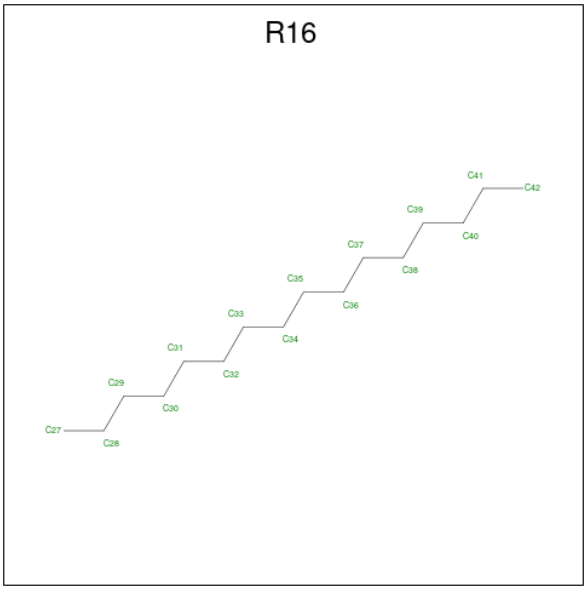
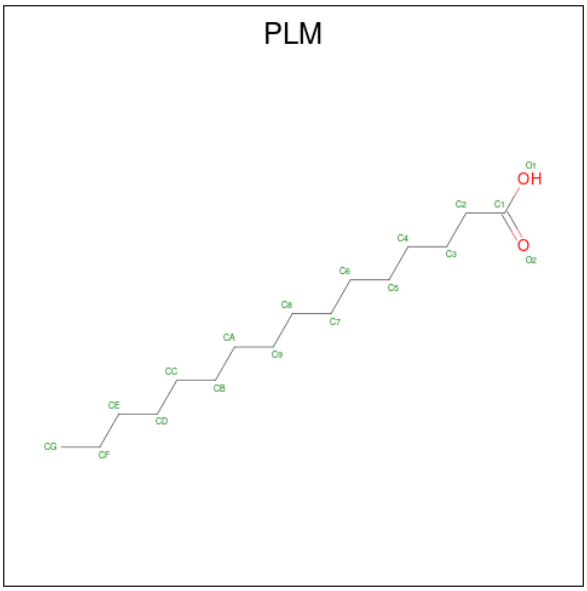
Mol	Chain	Residues	Atoms				AltConf
10	D	1	Total	C	O	P	0
			69	47	19	3	

- Molecule 11 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	C	0
			16	16	
11	B	1	Total	C	0
			16	16	
11	B	1	Total	C	0
			16	16	
11	C	1	Total	C	0
			16	16	
11	E	1	Total	C	0
			16	16	

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

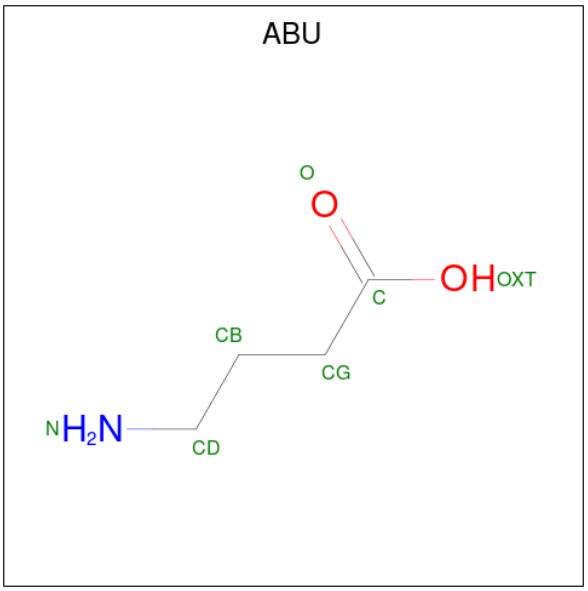


Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C O 18 16 2	0
12	C	1	Total C O 18 16 2	0
12	D	1	Total C O 18 16 2	0

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

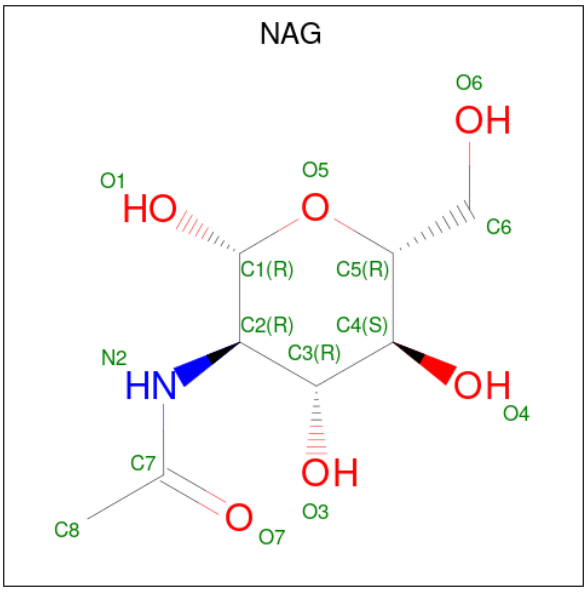
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Cl 1 1	0
13	C	1	Total Cl 1 1	0
13	D	1	Total Cl 1 1	0

- Molecule 14 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



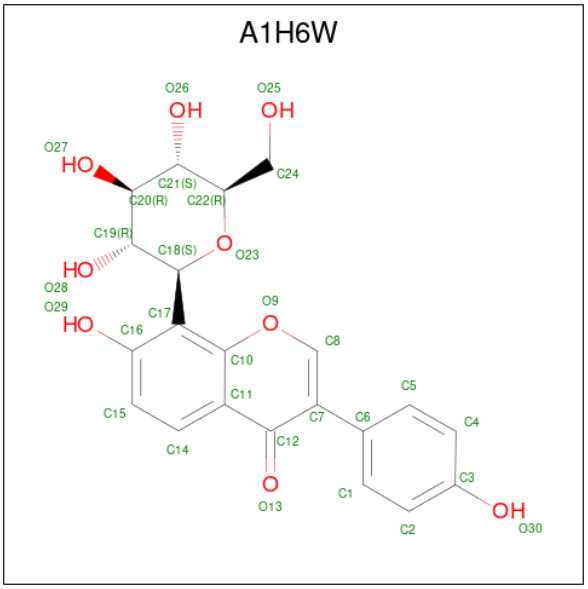
Mol	Chain	Residues	Atoms				AltConf
14	B	1	Total	C	N	O	0
			7	4	1	2	
14	E	1	Total	C	N	O	0
			7	4	1	2	

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



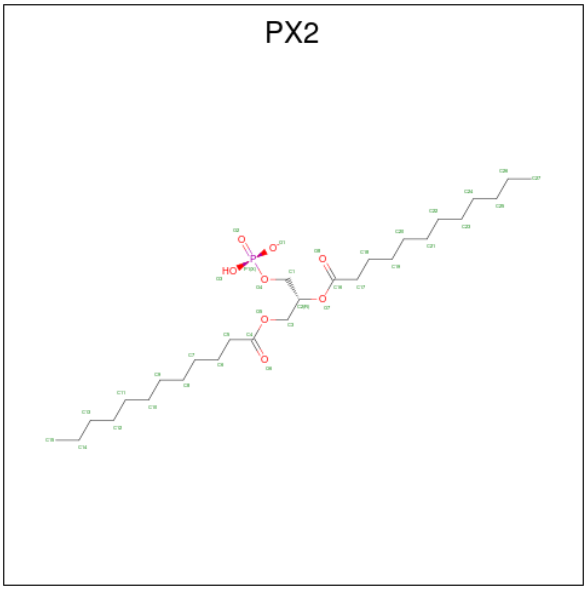
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 16 is Puerarin (three-letter code: A1H6W) (formula: $C_{21}H_{20}O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	D	1	30	21	9	0

- Molecule 17 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: $C_{27}H_{52}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	D	1	36	27	8	1	0

- Molecule 18 is water.

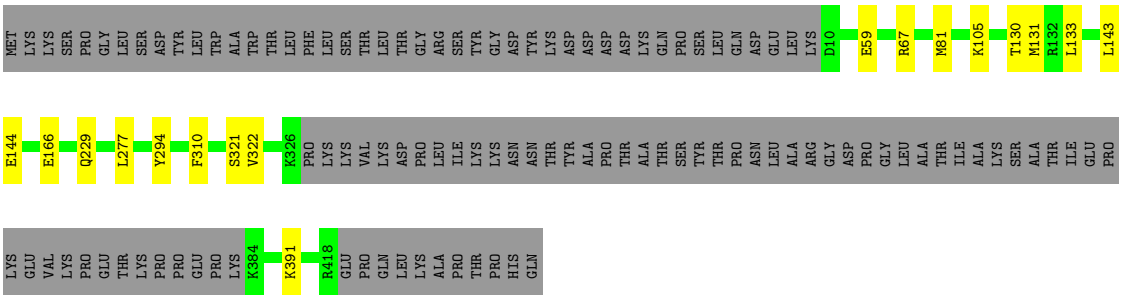
Mol	Chain	Residues	Atoms	AltConf
18	A	60	Total O 60 60	0
18	B	59	Total O 59 59	0
18	C	33	Total O 33 33	0
18	D	52	Total O 52 52	0
18	E	54	Total O 54 54	0

3 Residue-property plots (i)

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

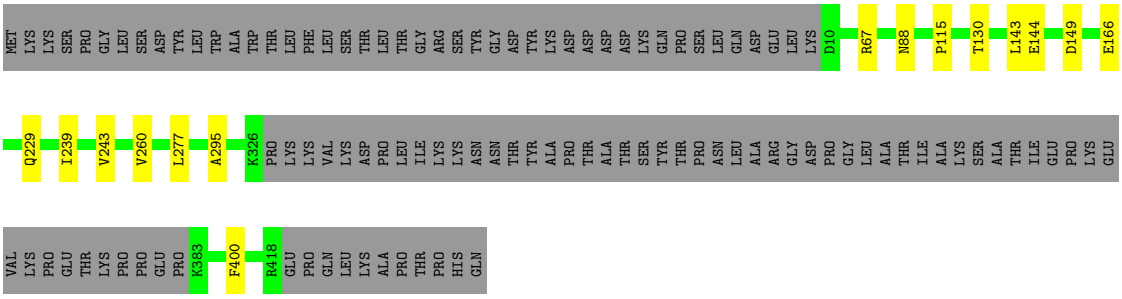
• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain A:



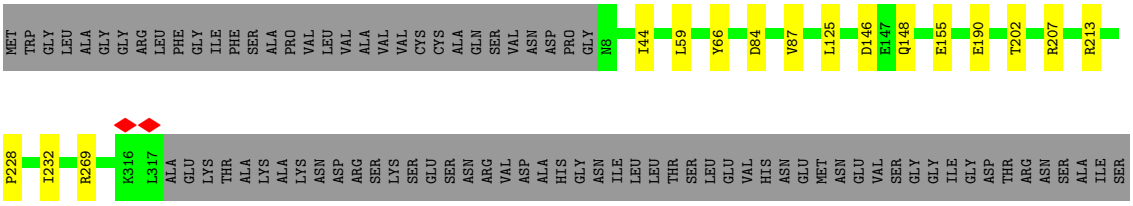
• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

Chain D:



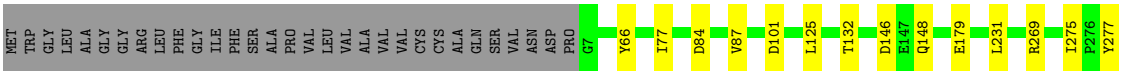
• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

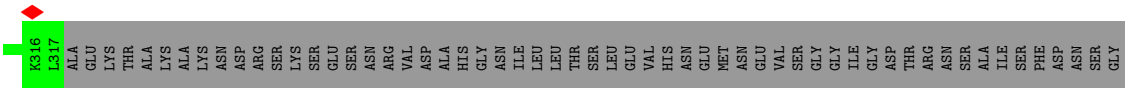
Chain B:

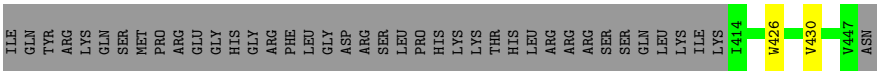


• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3

Chain E:







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

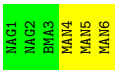
Chain C:

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

Chain F:

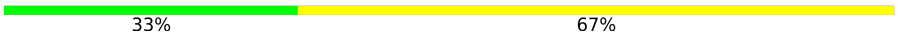
• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

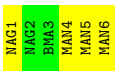
Chain G:



• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

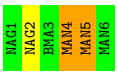
Chain I:





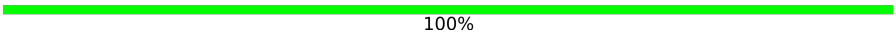
• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



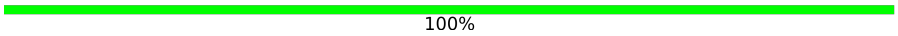
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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 K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122065	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	96000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.153	Depositor
Minimum map value	-0.437	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	421.888, 421.888, 421.888	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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, PLM, A1H6W, PX2, R16, CL, ABU, NAG, MAN, PT5, PGW, D10, HEX

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	0.27	0/2938	0.56	0/3989
1	D	0.26	0/2938	0.55	0/3989
2	B	0.26	0/2911	0.55	0/3959
2	E	0.26	0/2926	0.56	0/3978
3	C	0.26	0/2829	0.54	0/3848
All	All	0.26	0/14542	0.55	0/19763

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	2860	0	2857	12	0
1	D	2863	0	2859	12	0
2	B	2833	0	2836	9	0
2	E	2845	0	2852	10	0
3	C	2749	0	2752	7	0
4	F	116	0	97	0	0
5	G	72	0	61	0	0
5	I	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	72	0	61	2	0
6	H	39	0	34	0	0
6	K	39	0	34	0	0
7	A	51	0	76	0	0
7	D	51	0	76	1	0
8	A	30	0	66	0	0
8	B	10	0	22	0	0
8	C	30	0	66	0	0
8	D	20	0	44	0	0
8	E	20	0	44	0	0
9	A	18	0	42	0	0
9	B	12	0	28	0	0
9	C	12	0	28	0	0
9	E	18	0	42	0	0
10	A	69	0	80	2	0
10	D	69	0	80	2	0
11	A	16	0	34	0	0
11	B	32	0	68	0	0
11	C	16	0	34	0	0
11	E	16	0	34	0	0
12	A	18	0	31	0	0
12	C	18	0	31	0	0
12	D	18	0	31	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
14	B	7	0	0	1	0
14	E	7	0	0	1	0
15	C	14	0	13	0	0
16	D	30	0	0	0	0
17	D	36	0	52	0	0
18	A	60	0	0	2	0
18	B	59	0	0	0	0
18	C	33	0	0	0	0
18	D	52	0	0	3	0
18	E	54	0	0	0	0
All	All	15459	0	15526	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:MET:HE3	18:D:623:HOH:O	1.65	0.93
5:J:4:MAN:H3	5:J:5:MAN:H5	1.71	0.71
2:E:101:ASP:OD1	2:E:132:THR:OG1	2.08	0.70
3:C:45:ASP:OD1	3:C:85:ARG:NH1	2.25	0.70
1:D:143:LEU:HD13	1:D:277:LEU:HD22	1.73	0.68
1:D:166:GLU:OE1	18:D:601:HOH:O	2.16	0.62
3:C:209:THR:OG1	3:C:224:SER:OG	2.19	0.60
2:B:190:GLU:OE1	2:B:213:ARG:NH1	2.34	0.60
3:C:158:PHE:CE2	3:C:287:LEU:HD11	2.38	0.59
1:D:88:ASN:ND2	1:D:115:PRO:O	2.37	0.58
2:E:426:TRP:CE2	2:E:430:VAL:HG21	2.39	0.58
2:B:84:ASP:O	2:B:87:VAL:HG12	2.07	0.55
1:A:294:TYR:CE1	2:E:231:LEU:HD13	2.43	0.54
2:B:146:ASP:OD2	2:B:148:GLN:NE2	2.40	0.53
7:D:501:PGW:O12	7:D:501:PGW:OAE	2.21	0.52
1:A:310:PHE:CE2	10:A:505:PT5:H18	2.45	0.51
1:D:229:GLN:OE1	2:E:269:ARG:NH1	2.43	0.51
5:J:4:MAN:H3	5:J:5:MAN:C5	2.40	0.51
2:E:66[A]:TYR:CZ	2:E:125:LEU:HD13	2.46	0.51
1:A:229:GLN:OE1	2:B:269:ARG:NH1	2.41	0.50
1:A:166:GLU:OE2	18:A:601:HOH:O	2.19	0.49
1:A:81:MET:HE1	18:A:633:HOH:O	2.13	0.49
2:B:44:ILE:HD12	2:B:59:LEU:HD11	1.95	0.48
1:A:131:MET:CE	1:A:133:LEU:HD21	2.44	0.48
1:D:67:ARG:HB3	1:D:130:THR:HG23	1.97	0.47
1:A:144:GLU:N	1:A:144:GLU:OE1	2.48	0.47
3:C:268:LEU:HD23	1:D:260:VAL:CG2	2.45	0.47
2:E:275:ILE:HD12	2:E:277:TYR:CE1	2.49	0.47
1:A:143:LEU:HD13	1:A:277:LEU:HD22	1.96	0.47
2:B:228:PRO:O	2:B:232:ILE:HD12	2.15	0.47
1:A:321:SER:OG	1:A:322:VAL:N	2.49	0.46
3:C:130:MET:CE	18:D:623:HOH:O	2.42	0.46
1:D:400:PHE:CE1	10:D:506:PT5:H35	2.50	0.46
2:B:66[A]:TYR:CZ	2:B:125:LEU:HD13	2.50	0.46
1:A:391:LYS:HB2	10:A:505:PT5:H20	1.99	0.45
1:D:144:GLU:N	1:D:144:GLU:OE1	2.49	0.45
2:B:202:THR:OG1	14:B:3505:ABU:OXT	2.11	0.44
1:D:239:ILE:O	1:D:243:VAL:HG23	2.18	0.44
1:A:67:ARG:HB3	1:A:130:THR:HG23	1.99	0.44
3:C:34:LEU:HD22	3:C:87:LEU:HA	1.99	0.43
1:A:59:GLU:OE1	1:A:105:LYS:NZ	2.39	0.43
2:E:84:ASP:O	2:E:87:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:GLU:OE1	2:B:207:ARG:NH2	2.53	0.41
1:D:130:THR:HG21	14:E:3205:ABU:OXT	2.20	0.41
2:E:179:GLU:OE1	2:E:179:GLU:N	2.53	0.41
1:D:295:ALA:HB1	10:D:506:PT5:H50	2.03	0.41
2:E:146:ASP:OD2	2:E:148:GLN:NE2	2.49	0.41
2:E:77:ILE:HD12	2:E:77:ILE:H	1.86	0.40
1:D:149:ASP:OD1	1:D:149:ASP:N	2.55	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	350/464 (75%)	346 (99%)	4 (1%)	0	100	100
1	D	350/464 (75%)	346 (99%)	4 (1%)	0	100	100
2	B	341/473 (72%)	334 (98%)	7 (2%)	0	100	100
2	E	343/473 (72%)	330 (96%)	13 (4%)	0	100	100
3	C	330/495 (67%)	323 (98%)	7 (2%)	0	100	100
All	All	1714/2369 (72%)	1679 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/413 (76%)	316 (100%)	0	100	100
1	D	316/413 (76%)	316 (100%)	0	100	100
2	B	311/417 (75%)	311 (100%)	0	100	100
2	E	312/417 (75%)	312 (100%)	0	100	100
3	C	308/448 (69%)	308 (100%)	0	100	100
All	All	1563/2108 (74%)	1563 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

34 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1	4,1	14,14,15	0.23	0	17,19,21	0.42	0
4	MAN	F	10	4	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
4	NAG	F	2	4	14,14,15	0.18	0	17,19,21	0.49	0
4	BMA	F	3	4	11,11,12	0.58	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	F	4	4	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
4	MAN	F	5	4	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
4	MAN	F	6	4	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
4	MAN	F	7	4	11,11,12	0.78	1 (9%)	15,15,17	1.02	1 (6%)
4	MAN	F	8	4	11,11,12	0.72	1 (9%)	15,15,17	1.06	2 (13%)
4	MAN	F	9	4	11,11,12	0.71	0	15,15,17	1.04	1 (6%)
5	NAG	G	1	2,5	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	BMA	G	3	5	11,11,12	0.65	0	15,15,17	0.75	0
5	MAN	G	4	5	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
5	MAN	G	5	5	11,11,12	0.95	1 (9%)	15,15,17	1.33	2 (13%)
5	MAN	G	6	5	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
6	NAG	H	1	6,2	14,14,15	0.22	0	17,19,21	0.47	0
6	NAG	H	2	6	14,14,15	0.21	0	17,19,21	0.43	0
6	BMA	H	3	6	11,11,12	0.59	0	15,15,17	0.80	0
5	NAG	I	1	1,5	14,14,15	0.21	0	17,19,21	0.77	1 (5%)
5	NAG	I	2	5	14,14,15	0.19	0	17,19,21	0.42	0
5	BMA	I	3	5	11,11,12	0.60	0	15,15,17	0.80	0
5	MAN	I	4	5	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
5	MAN	I	5	5	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
5	MAN	I	6	5	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
5	NAG	J	1	2,5	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	J	2	5	14,14,15	0.86	0	17,19,21	1.53	3 (17%)
5	BMA	J	3	5	11,11,12	0.59	0	15,15,17	0.82	0
5	MAN	J	4	5	11,11,12	0.31	0	15,15,17	0.99	1 (6%)
5	MAN	J	5	5	11,11,12	0.27	0	15,15,17	1.29	2 (13%)
5	MAN	J	6	5	11,11,12	0.37	0	15,15,17	0.83	0
6	NAG	K	1	6,2	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.46	0
6	BMA	K	3	6	11,11,12	0.59	0	15,15,17	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	MAN	F	10	4	-	0/2/19/22	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	7	MAN	O5-C1	-2.32	1.40	1.43
5	G	5	MAN	O5-C1	-2.25	1.40	1.43
4	F	8	MAN	O5-C1	-2.05	1.40	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	2	NAG	O5-C1-C2	-4.19	104.67	111.29
5	G	5	MAN	C1-O5-C5	3.45	116.86	112.19
4	F	8	MAN	C1-O5-C5	2.72	115.87	112.19
5	J	5	MAN	C1-O5-C5	2.71	115.87	112.19
5	J	5	MAN	O5-C1-C2	2.62	114.82	110.77
5	I	1	NAG	C2-N2-C7	2.53	126.51	122.90
5	G	4	MAN	C1-O5-C5	2.39	115.43	112.19
4	F	7	MAN	O2-C2-C3	-2.34	105.44	110.14
5	I	6	MAN	C1-O5-C5	2.31	115.33	112.19
4	F	10	MAN	C1-O5-C5	2.31	115.32	112.19
5	I	5	MAN	C1-O5-C5	2.31	115.32	112.19
4	F	6	MAN	O2-C2-C3	-2.31	105.52	110.14
4	F	5	MAN	O2-C2-C3	-2.30	105.53	110.14
5	G	5	MAN	O2-C2-C3	-2.29	105.54	110.14
4	F	5	MAN	C1-O5-C5	2.27	115.27	112.19
4	F	4	MAN	O2-C2-C3	-2.27	105.59	110.14
5	G	6	MAN	O2-C2-C3	-2.26	105.60	110.14
4	F	10	MAN	O2-C2-C3	-2.26	105.62	110.14
5	I	4	MAN	O2-C2-C3	-2.25	105.64	110.14
5	I	6	MAN	O2-C2-C3	-2.24	105.65	110.14
5	G	6	MAN	C1-O5-C5	2.24	115.22	112.19
5	I	4	MAN	C1-O5-C5	2.24	115.22	112.19
4	F	6	MAN	C1-O5-C5	2.23	115.22	112.19
4	F	9	MAN	O2-C2-C3	-2.23	105.67	110.14
4	F	4	MAN	C1-O5-C5	2.23	115.21	112.19
5	I	5	MAN	O2-C2-C3	-2.21	105.71	110.14
5	G	4	MAN	O2-C2-C3	-2.20	105.73	110.14
5	J	2	NAG	O4-C4-C3	-2.18	105.30	110.35
4	F	8	MAN	O2-C2-C3	-2.18	105.77	110.14
5	J	2	NAG	C6-C5-C4	-2.07	108.15	113.00
5	J	4	MAN	C2-C3-C4	-2.05	107.36	110.89

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
4	F	9	MAN	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	9	MAN	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O7-C7-N2-C2
6	K	2	NAG	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
5	J	6	MAN	O5-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
6	H	1	NAG	C3-C2-N2-C7
6	K	2	NAG	C3-C2-N2-C7
6	H	1	NAG	C1-C2-N2-C7
6	K	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7

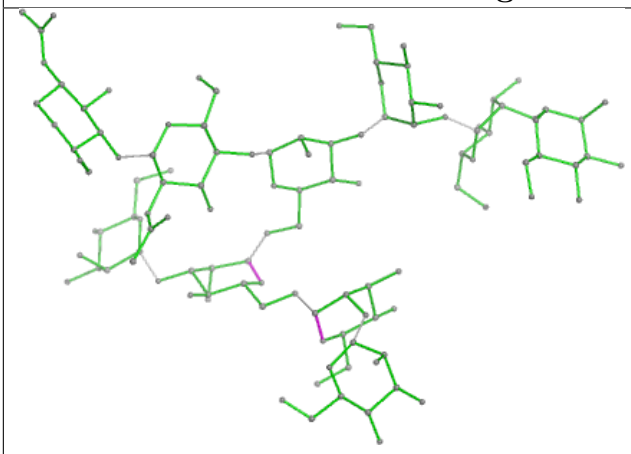
There are no ring outliers.

2 monomers are involved in 2 short contacts:

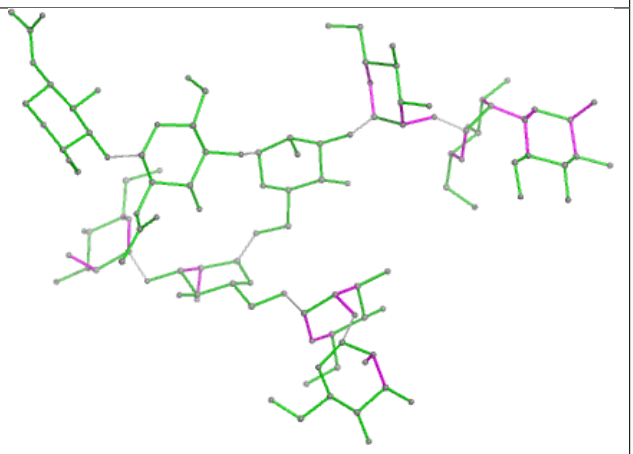
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	4	MAN	2	0
5	J	5	MAN	2	0

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

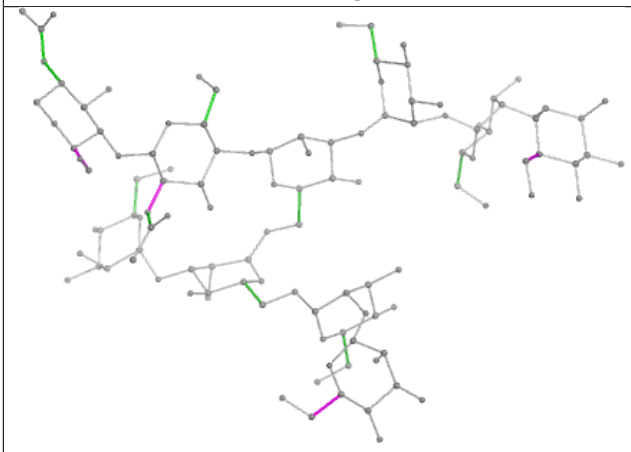
Oligosaccharide Chain F



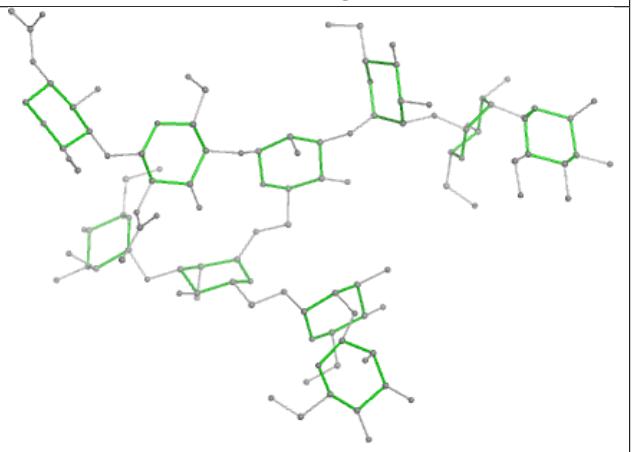
Bond lengths



Bond angles

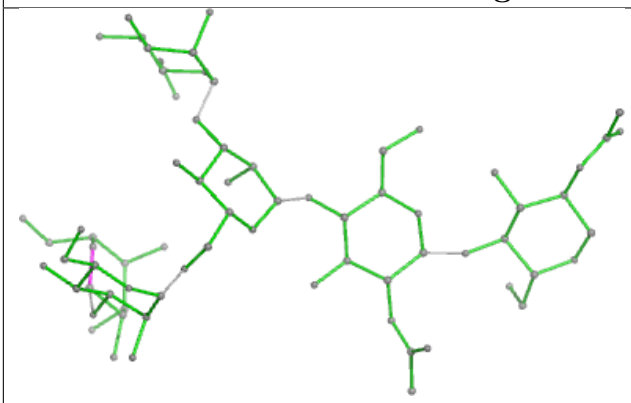


Torsions

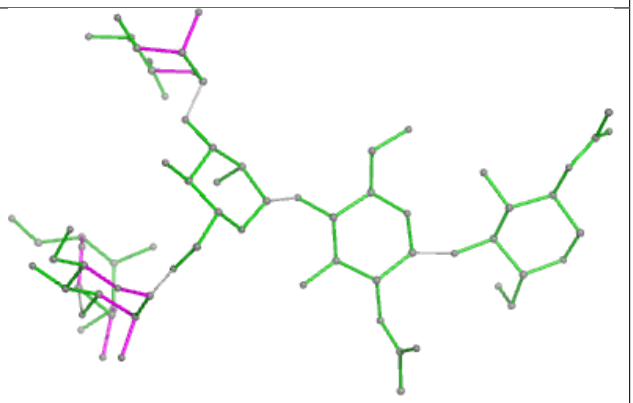


Rings

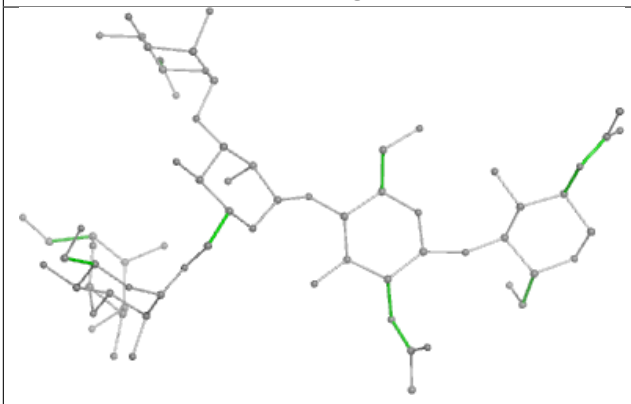
Oligosaccharide Chain G



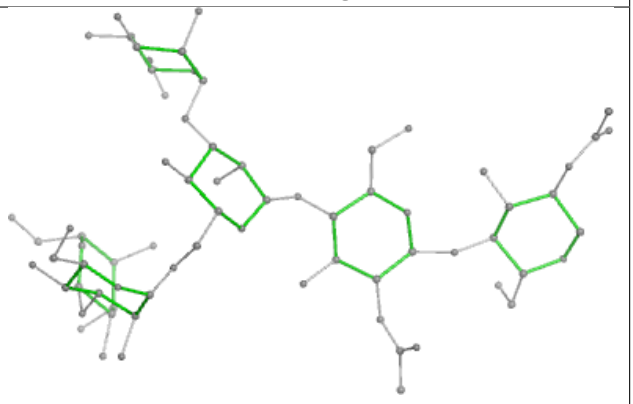
Bond lengths



Bond angles

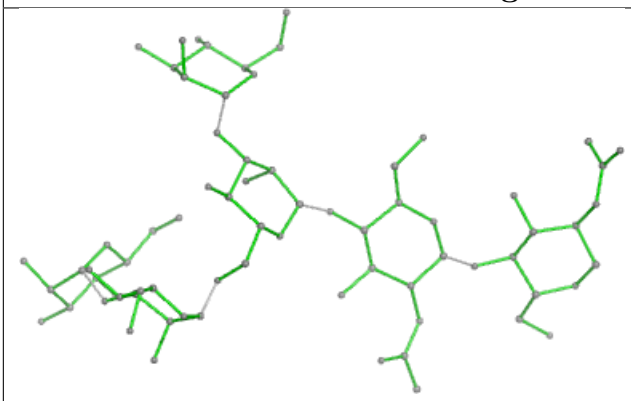


Torsions

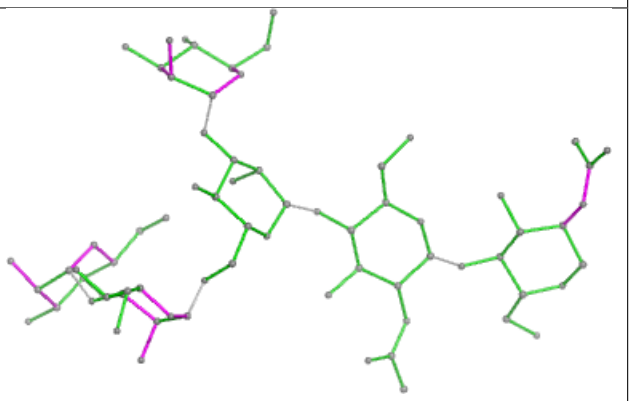


Rings

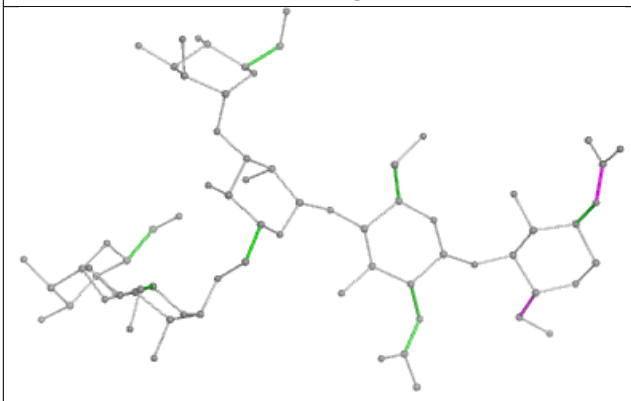
Oligosaccharide Chain I



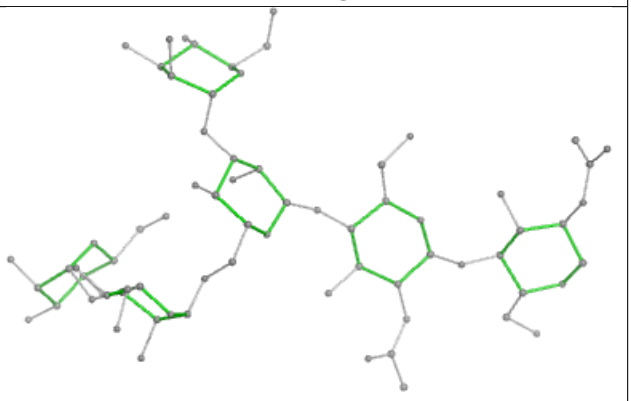
Bond lengths



Bond angles

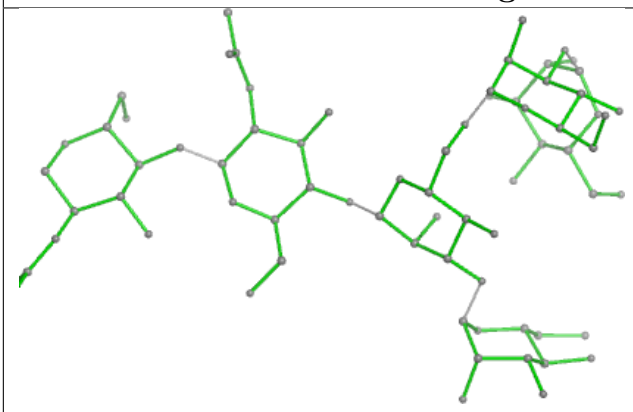


Torsions

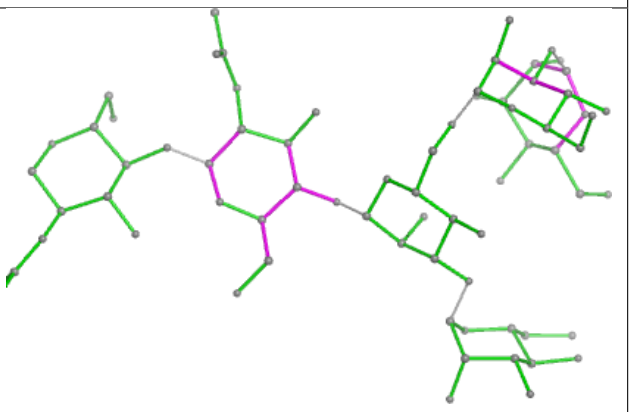


Rings

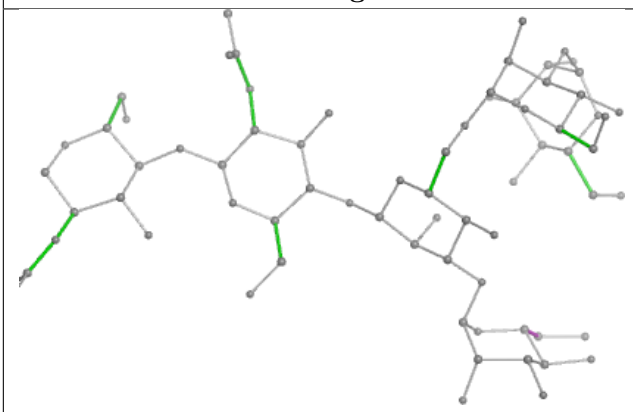
Oligosaccharide Chain J



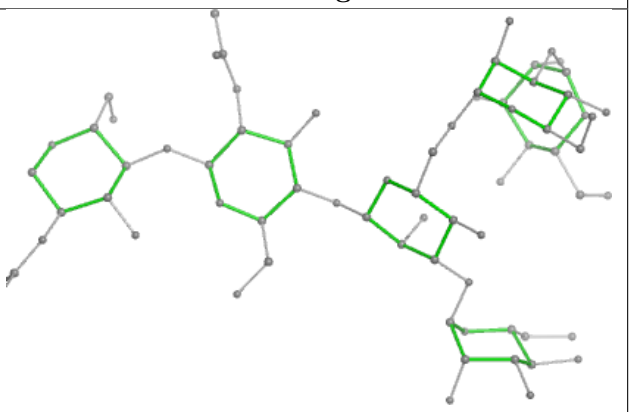
Bond lengths



Bond angles

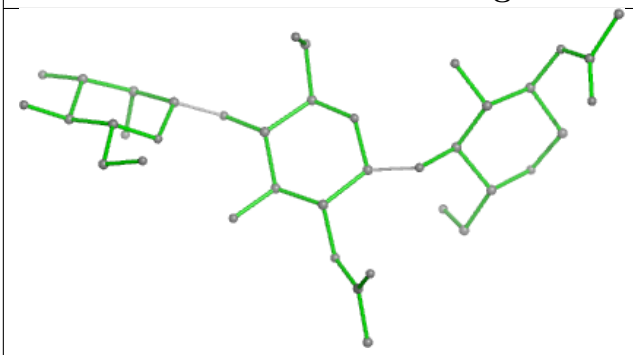


Torsions

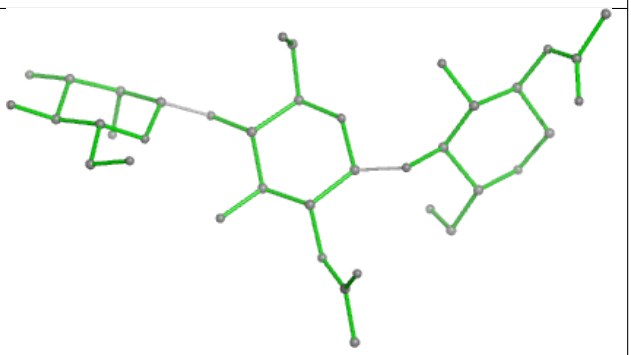


Rings

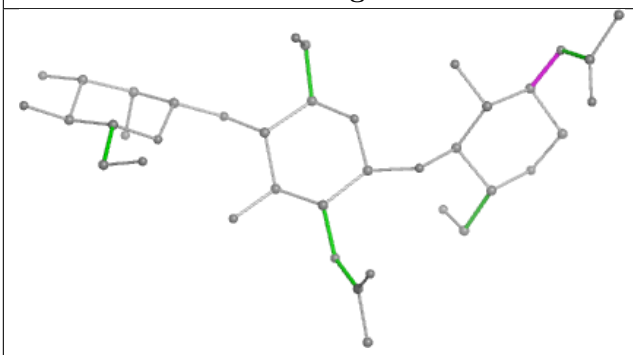
Oligosaccharide Chain H



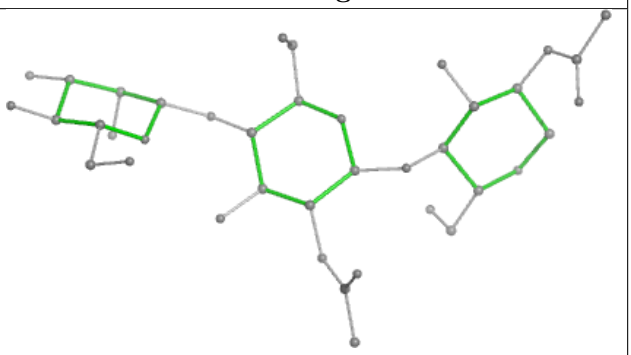
Bond lengths



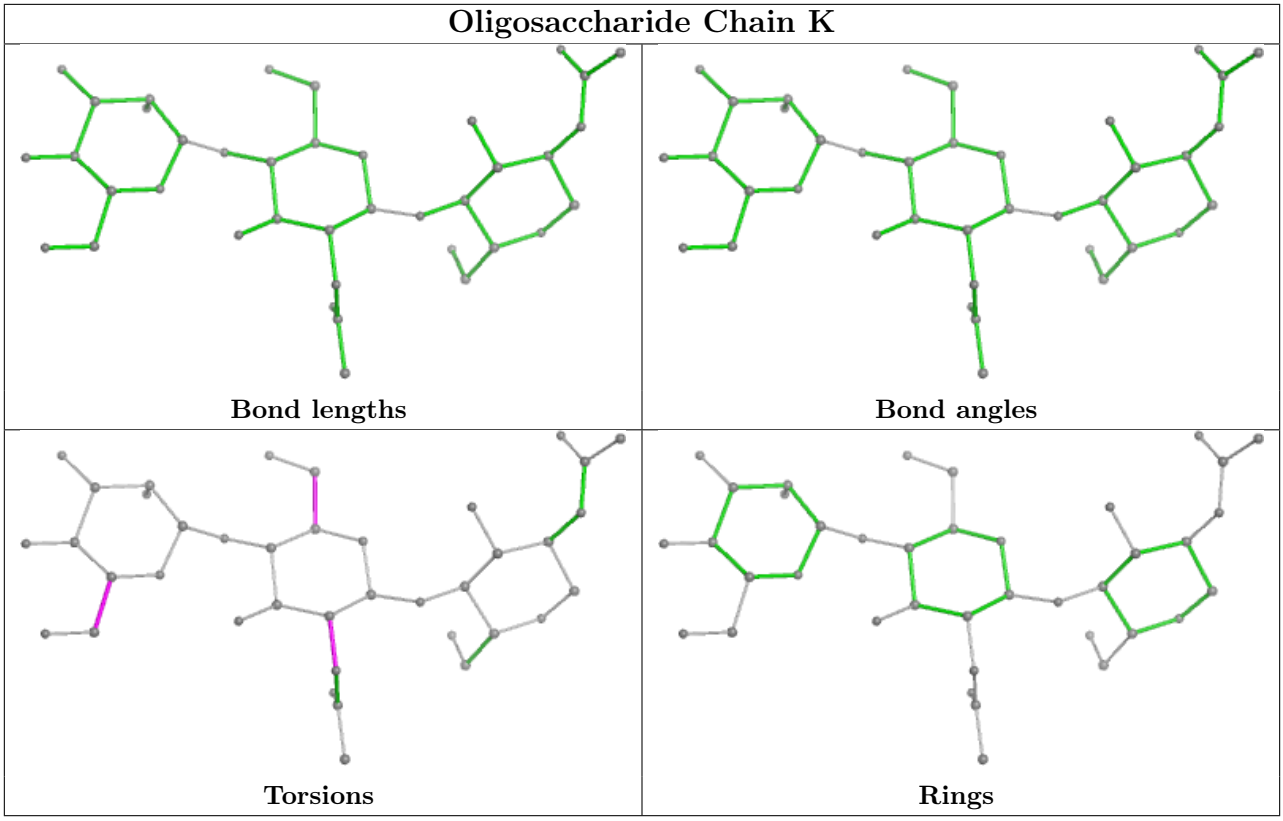
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 3 are monoatomic - leaving 38 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	HEX	A	508	-	5,5,5	0.31	0	4,4,4	0.56	0
14	ABU	E	3205	-	6,6,6	0.89	0	6,6,6	1.41	1 (16%)
8	D10	D	504	-	9,9,9	0.34	0	8,8,8	0.64	0
9	HEX	B	3506	-	5,5,5	0.31	0	4,4,4	0.57	0
9	HEX	E	3203	-	5,5,5	0.30	0	4,4,4	0.56	0
9	HEX	E	3207	-	5,5,5	0.31	0	4,4,4	0.56	0
10	PT5	D	506	-	69,69,69	0.43	0	83,87,87	0.49	0
8	D10	E	3204	-	9,9,9	0.32	0	8,8,8	0.67	0
11	R16	C	508	-	15,15,15	0.30	0	14,14,14	0.82	0
14	ABU	B	3505	-	6,6,6	0.86	0	6,6,6	1.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	R16	A	506	-	15,15,15	0.27	0	14,14,14	0.89	0
9	HEX	E	3206	-	5,5,5	0.31	0	4,4,4	0.56	0
8	D10	D	503	-	9,9,9	0.30	0	8,8,8	0.75	0
12	PLM	D	502	-	17,17,17	0.59	0	17,17,17	1.05	0
9	HEX	A	504	-	5,5,5	0.31	0	4,4,4	0.56	0
8	D10	E	3202	-	9,9,9	0.29	0	8,8,8	0.80	0
7	PGW	A	501	-	50,50,50	0.98	2 (4%)	53,56,56	0.93	2 (3%)
17	PX2	D	507	-	35,35,35	1.03	3 (8%)	39,40,40	1.11	2 (5%)
9	HEX	B	3504	-	5,5,5	0.31	0	4,4,4	0.56	0
8	D10	A	502	-	9,9,9	0.28	0	8,8,8	0.80	0
9	HEX	C	504	-	5,5,5	0.30	0	4,4,4	0.57	0
15	NAG	C	506	3	14,14,15	0.22	0	17,19,21	0.46	0
16	A1H6W	D	505	-	33,33,33	0.21	0	45,49,49	0.67	1 (2%)
12	PLM	A	510	-	17,17,17	0.58	0	17,17,17	1.03	0
11	R16	E	3201	-	15,15,15	0.30	0	14,14,14	0.82	0
8	D10	A	503	-	9,9,9	0.31	0	8,8,8	0.69	0
11	R16	B	3501	-	15,15,15	0.30	0	14,14,14	0.82	0
8	D10	C	503	-	9,9,9	0.30	0	8,8,8	0.77	0
8	D10	B	3502	-	9,9,9	0.30	0	8,8,8	0.76	0
8	D10	C	501	-	9,9,9	0.29	0	8,8,8	0.80	0
12	PLM	C	502	-	17,17,17	0.59	0	17,17,17	1.01	0
10	PT5	A	505	-	69,69,69	0.43	0	83,87,87	0.48	0
7	PGW	D	501	-	50,50,50	0.96	3 (6%)	53,56,56	1.05	2 (3%)
8	D10	A	509	-	9,9,9	0.31	0	8,8,8	0.68	0
11	R16	B	3503	-	15,15,15	0.31	0	14,14,14	0.75	0
9	HEX	A	507	-	5,5,5	0.31	0	4,4,4	0.56	0
9	HEX	C	507	-	5,5,5	0.33	0	4,4,4	0.48	0
8	D10	C	505	-	9,9,9	0.31	0	8,8,8	0.74	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
9	HEX	A	508	-	-	0/3/3/3	-
14	ABU	E	3205	-	-	0/4/4/4	-
8	D10	D	504	-	-	1/7/7/7	-
9	HEX	B	3506	-	-	0/3/3/3	-
9	HEX	E	3203	-	-	0/3/3/3	-
9	HEX	E	3207	-	-	0/3/3/3	-
10	PT5	D	506	-	-	12/66/90/90	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D10	E	3204	-	-	3/7/7/7	-
11	R16	C	508	-	-	3/13/13/13	-
14	ABU	B	3505	-	-	2/4/4/4	-
11	R16	A	506	-	-	1/13/13/13	-
9	HEX	E	3206	-	-	0/3/3/3	-
8	D10	D	503	-	-	1/7/7/7	-
12	PLM	D	502	-	-	7/15/15/15	-
9	HEX	A	504	-	-	0/3/3/3	-
8	D10	E	3202	-	-	0/7/7/7	-
7	PGW	A	501	-	-	23/55/55/55	-
17	PX2	D	507	-	-	15/37/37/37	-
9	HEX	B	3504	-	-	0/3/3/3	-
8	D10	A	502	-	-	0/7/7/7	-
9	HEX	C	504	-	-	0/3/3/3	-
15	NAG	C	506	3	-	0/6/23/26	0/1/1/1
16	A1H6W	D	505	-	-	2/10/30/30	0/4/4/4
12	PLM	A	510	-	-	3/15/15/15	-
11	R16	E	3201	-	-	2/13/13/13	-
8	D10	A	503	-	-	0/7/7/7	-
11	R16	B	3501	-	-	1/13/13/13	-
8	D10	C	503	-	-	1/7/7/7	-
8	D10	B	3502	-	-	0/7/7/7	-
8	D10	C	501	-	-	0/7/7/7	-
12	PLM	C	502	-	-	1/15/15/15	-
10	PT5	A	505	-	-	21/66/90/90	0/1/1/1
7	PGW	D	501	-	-	20/55/55/55	-
8	D10	A	509	-	-	2/7/7/7	-
11	R16	B	3503	-	-	4/13/13/13	-
9	HEX	A	507	-	-	0/3/3/3	-
9	HEX	C	507	-	-	0/3/3/3	-
8	D10	C	505	-	-	1/7/7/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	501	PGW	O03-C19	2.97	1.42	1.33
7	D	501	PGW	O03-C19	2.85	1.41	1.33
7	D	501	PGW	O01-C1	2.72	1.42	1.34
17	D	507	PX2	O5-C4	2.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	501	PGW	O01-C1	2.60	1.41	1.34
17	D	507	PX2	O7-C16	2.40	1.41	1.34
17	D	507	PX2	O7-C2	-2.32	1.40	1.46
7	D	501	PGW	O01-C02	-2.06	1.41	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	501	PGW	O01-C1-C2	3.90	119.90	111.50
17	D	507	PX2	O7-C16-C17	3.72	119.51	111.50
7	A	501	PGW	O01-C1-C2	3.67	119.41	111.50
17	D	507	PX2	O5-C4-C5	2.92	121.07	111.91
16	D	505	A1H6W	C17-C18-C19	2.75	119.57	112.94
7	D	501	PGW	O03-C19-C20	2.60	120.06	111.91
7	A	501	PGW	O03-C19-C20	2.46	119.64	111.91
14	E	3205	ABU	CB-CG-C	-2.07	109.24	114.47

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	501	PGW	C03-O11-P-O12
7	D	501	PGW	O12-C04-C05-CAD
17	D	507	PX2	C1-O4-P1-O1
17	D	507	PX2	C1-O4-P1-O2
17	D	507	PX2	C1-O4-P1-O3
17	D	507	PX2	C5-C4-O5-C3
17	D	507	PX2	O6-C4-O5-C3
10	A	505	PT5	C31-C11-O18-C9
10	A	505	PT5	O19-C11-O18-C9
10	A	505	PT5	C12-C10-O16-C8
16	D	505	A1H6W	C21-C22-C24-O25
7	A	501	PGW	C1-C2-C3-C4
7	D	501	PGW	O12-C04-C05-OAF
10	A	505	PT5	O16-C8-C9-O18
10	D	506	PT5	C14-C15-C16-C17
10	A	505	PT5	O17-C10-O16-C8
16	D	505	A1H6W	O23-C22-C24-O25
7	A	501	PGW	C2-C1-O01-C02
10	D	506	PT5	C12-C10-O16-C8
7	A	501	PGW	C04-O12-P-O11
7	A	501	PGW	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
10	D	506	PT5	O17-C10-O16-C8
7	D	501	PGW	C27-C15-C16-C17
17	D	507	PX2	C11-C10-C9-C8
17	D	507	PX2	C5-C6-C7-C8
7	A	501	PGW	C08-C09-C11-C12
8	D	504	D10	C5-C6-C7-C8
7	D	501	PGW	C06-C07-C08-C09
11	B	3503	R16	C35-C36-C37-C38
7	A	501	PGW	C04-C05-CAD-OAE
7	A	501	PGW	C27-C15-C16-C17
11	C	508	R16	C30-C31-C32-C33
7	D	501	PGW	C2-C3-C4-C5
11	B	3503	R16	C29-C30-C31-C32
17	D	507	PX2	C19-C20-C21-C22
17	D	507	PX2	C21-C22-C23-C24
8	C	503	D10	C3-C4-C5-C6
10	A	505	PT5	C39-C40-C41-C42
12	D	502	PLM	C3-C4-C5-C6
7	D	501	PGW	C4-C5-C6-C7
11	E	3201	R16	C33-C34-C35-C36
7	D	501	PGW	C2-C1-O01-C02
10	A	505	PT5	C11-C31-C32-C33
7	A	501	PGW	C16-C15-C27-C26
17	D	507	PX2	C10-C11-C12-C13
11	B	3503	R16	C31-C32-C33-C34
12	C	502	PLM	C7-C8-C9-CA
7	D	501	PGW	O02-C1-O01-C02
8	A	509	D10	C4-C5-C6-C7
8	A	509	D10	C5-C6-C7-C8
10	D	506	PT5	C32-C33-C34-C35
12	A	510	PLM	C4-C5-C6-C7
10	A	505	PT5	C7-C8-C9-O18
8	E	3204	D10	C2-C3-C4-C5
8	C	505	D10	C5-C6-C7-C8
7	A	501	PGW	C23-C24-C25-C26
11	C	508	R16	C33-C34-C35-C36
7	A	501	PGW	O03-C19-C20-C21
7	D	501	PGW	C20-C21-C22-C23
7	A	501	PGW	C05-C04-O12-P
10	D	506	PT5	C24-C25-C26-C27
10	A	505	PT5	C18-C19-C20-C21
10	A	505	PT5	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
7	A	501	PGW	OAF-C05-CAD-OAE
17	D	507	PX2	C23-C24-C25-C26
10	D	506	PT5	O16-C8-C9-O18
10	A	505	PT5	C37-C38-C39-C40
7	D	501	PGW	C23-C24-C25-C26
8	E	3204	D10	C4-C5-C6-C7
10	A	505	PT5	C5-O5-P5-O51
10	D	506	PT5	C4-O4-P4-O43
10	D	506	PT5	C5-O5-P5-O51
10	D	506	PT5	C5-O5-P5-O53
8	D	503	D10	C1-C2-C3-C4
10	A	505	PT5	C10-C12-C13-C14
11	B	3501	R16	C28-C29-C30-C31
7	A	501	PGW	C04-O12-P-O13
7	A	501	PGW	C04-O12-P-O14
7	D	501	PGW	C03-O11-P-O14
10	A	505	PT5	C31-C32-C33-C34
10	A	505	PT5	C35-C36-C37-C38
7	D	501	PGW	C08-C09-C11-C12
12	D	502	PLM	C5-C6-C7-C8
7	D	501	PGW	C22-C23-C24-C25
10	A	505	PT5	C43-C44-C45-C46
8	E	3204	D10	C5-C6-C7-C8
14	B	3505	ABU	OXT-C-CG-CB
14	B	3505	ABU	O-C-CG-CB
10	A	505	PT5	C19-C20-C21-C22
11	C	508	R16	C32-C33-C34-C35
7	A	501	PGW	C09-C11-C12-C13
12	D	502	PLM	C7-C8-C9-CA
7	A	501	PGW	C7-C8-C9-C10
12	A	510	PLM	O1-C1-C2-C3
12	D	502	PLM	O1-C1-C2-C3
7	A	501	PGW	O04-C19-C20-C21
17	D	507	PX2	O5-C4-C5-C6
12	A	510	PLM	O2-C1-C2-C3
12	D	502	PLM	O2-C1-C2-C3
12	D	502	PLM	C9-CA-CB-CC
7	D	501	PGW	C17-C18-C28-C30
17	D	507	PX2	O7-C16-C17-C18
7	A	501	PGW	C02-C03-O11-P
7	D	501	PGW	O03-C01-C02-O01
10	D	506	PT5	C4-O4-P4-O42

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Mol	Chain	Res	Type	Atoms
11	A	506	R16	C38-C39-C40-C41
7	D	501	PGW	C7-C8-C9-C10
7	A	501	PGW	C18-C28-C30-C29
10	A	505	PT5	C20-C21-C22-C23
11	B	3503	R16	C38-C39-C40-C41
7	A	501	PGW	C07-C08-C09-C11
7	D	501	PGW	O01-C1-C2-C3
7	D	501	PGW	C09-C11-C12-C13
17	D	507	PX2	O8-C16-C17-C18
10	D	506	PT5	C7-C8-C9-O18
7	D	501	PGW	C03-O11-P-O12
10	A	505	PT5	C38-C39-C40-C41
11	E	3201	R16	C34-C35-C36-C37
7	D	501	PGW	O02-C1-C2-C3
7	A	501	PGW	O01-C1-C2-C3
17	D	507	PX2	C17-C18-C19-C20
12	D	502	PLM	C4-C5-C6-C7
10	A	505	PT5	C14-C15-C16-C17
10	A	505	PT5	O18-C11-C31-C32
7	A	501	PGW	O02-C1-C2-C3
10	D	506	PT5	O16-C10-C12-C13

There are no ring outliers.

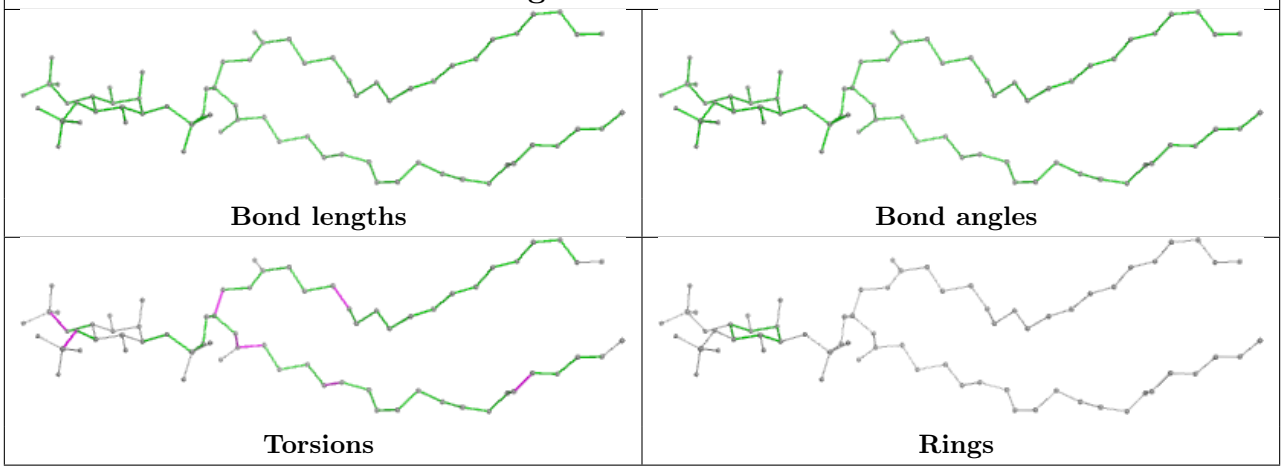
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	3205	ABU	1	0
10	D	506	PT5	2	0
14	B	3505	ABU	1	0
10	A	505	PT5	2	0
7	D	501	PGW	1	0

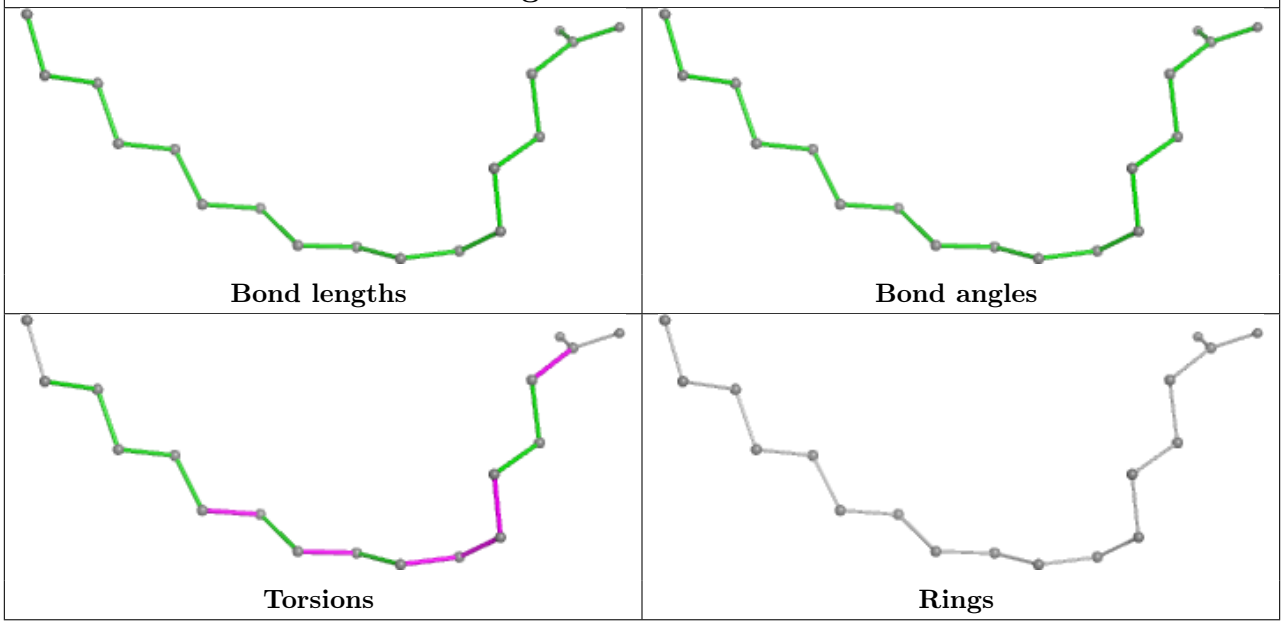
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

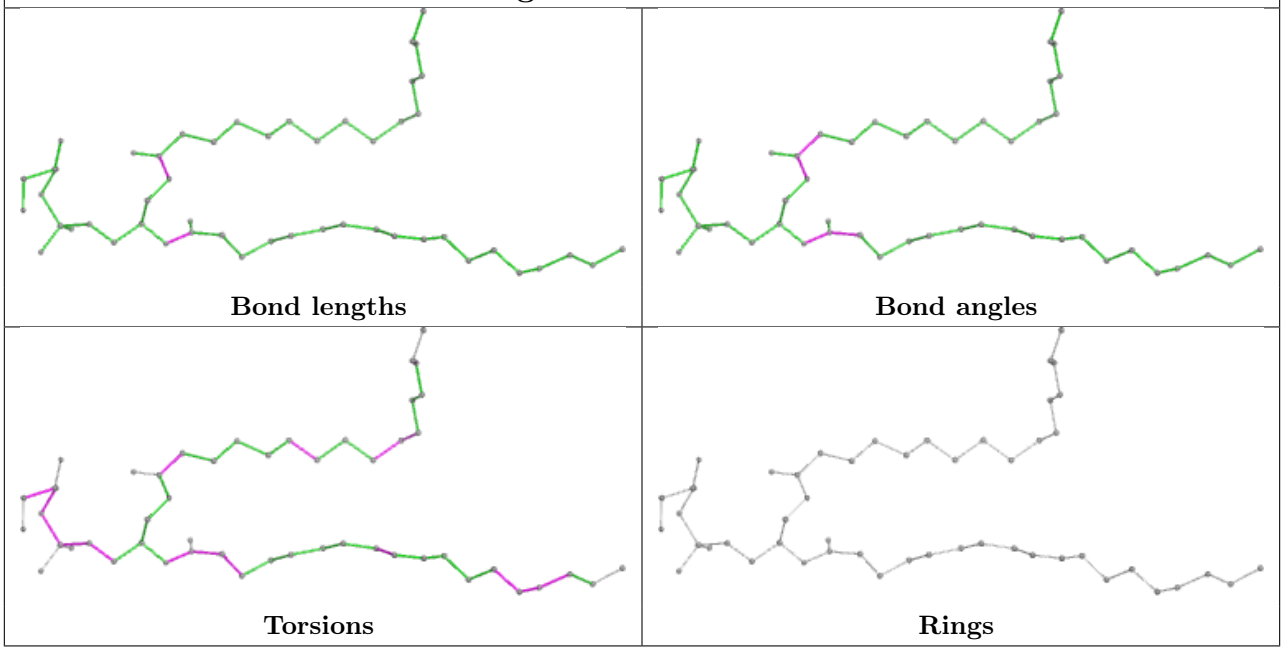
Ligand PT5 D 506



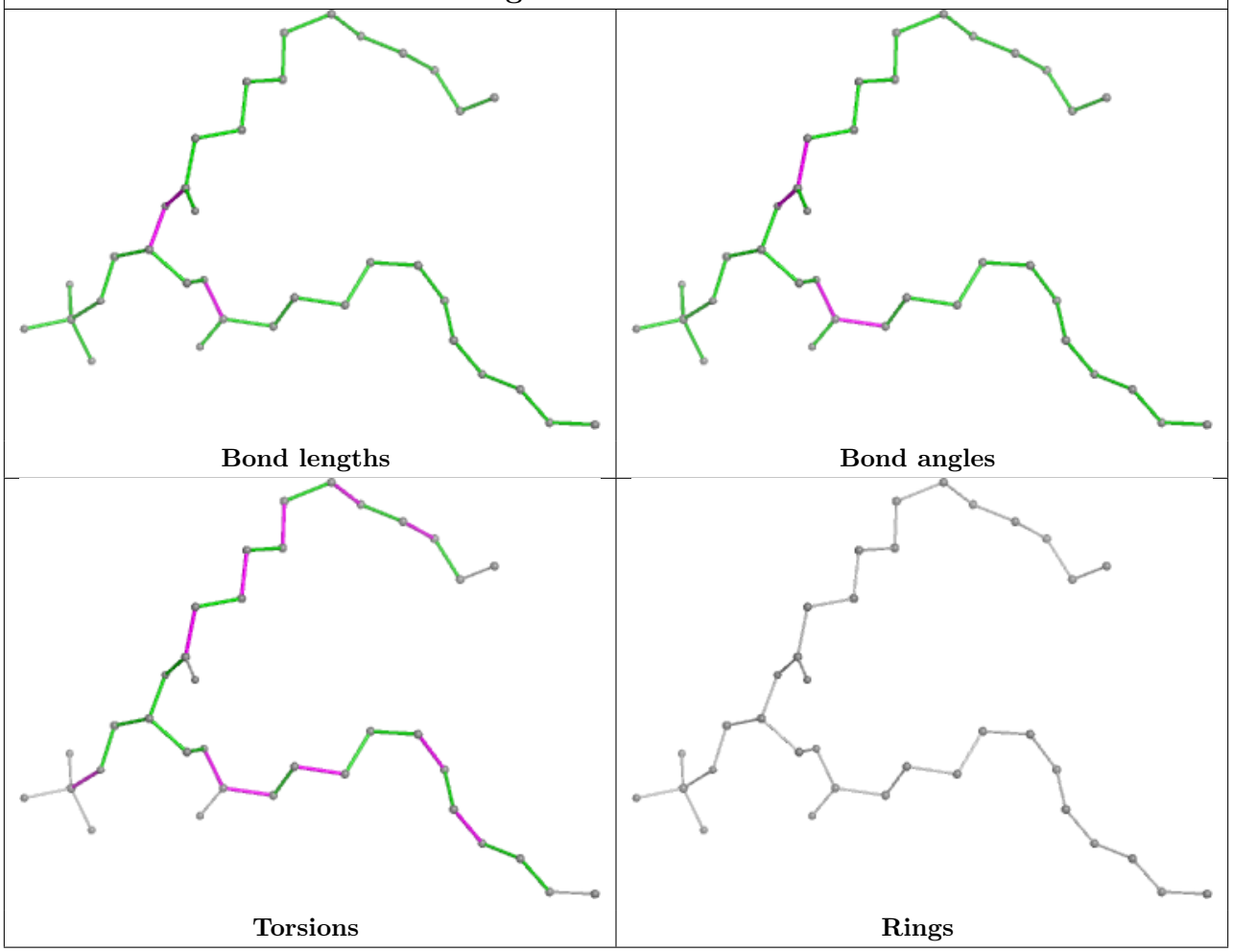
Ligand PLM D 502



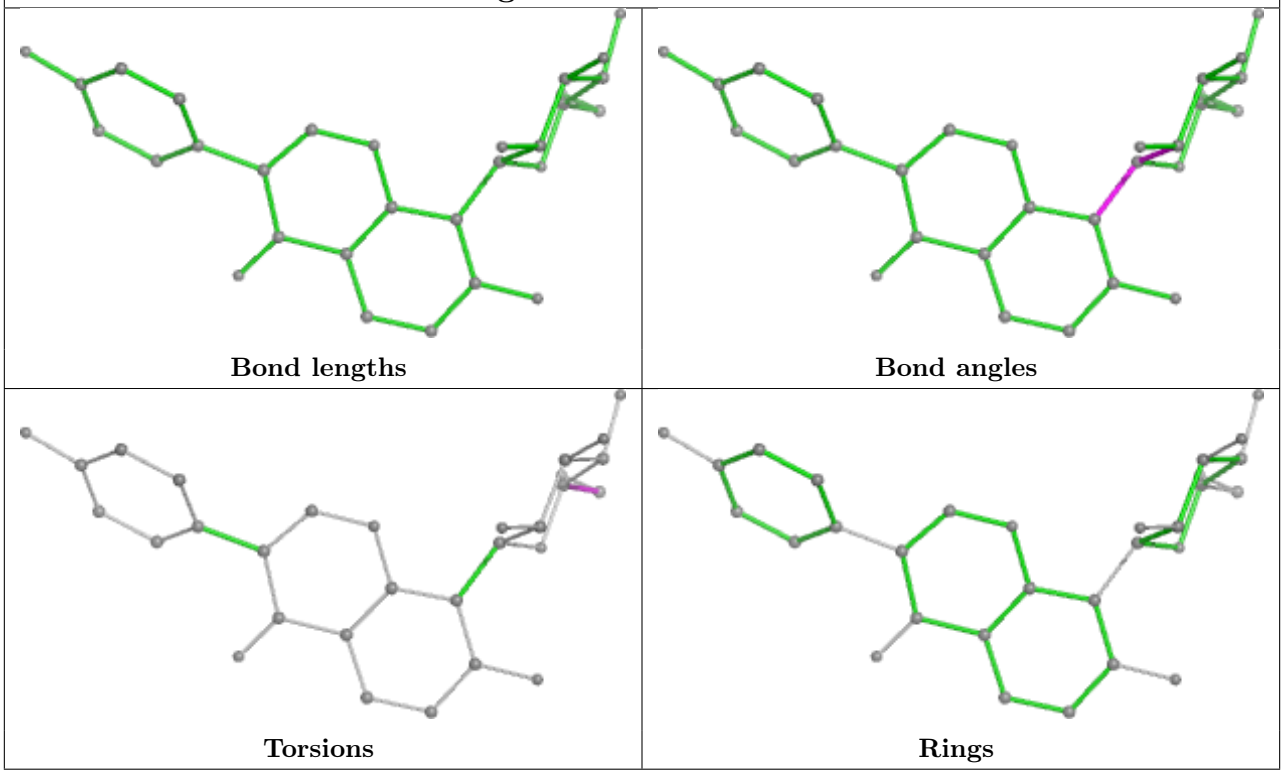
Ligand PGW A 501



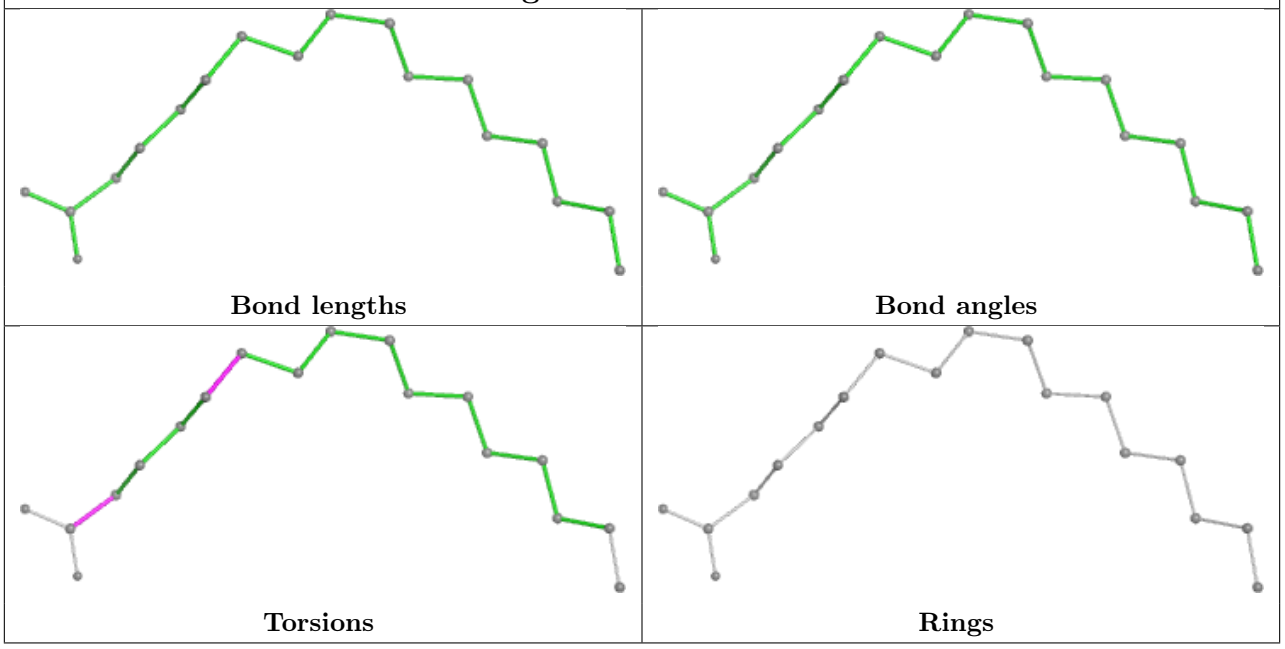
Ligand PX2 D 507



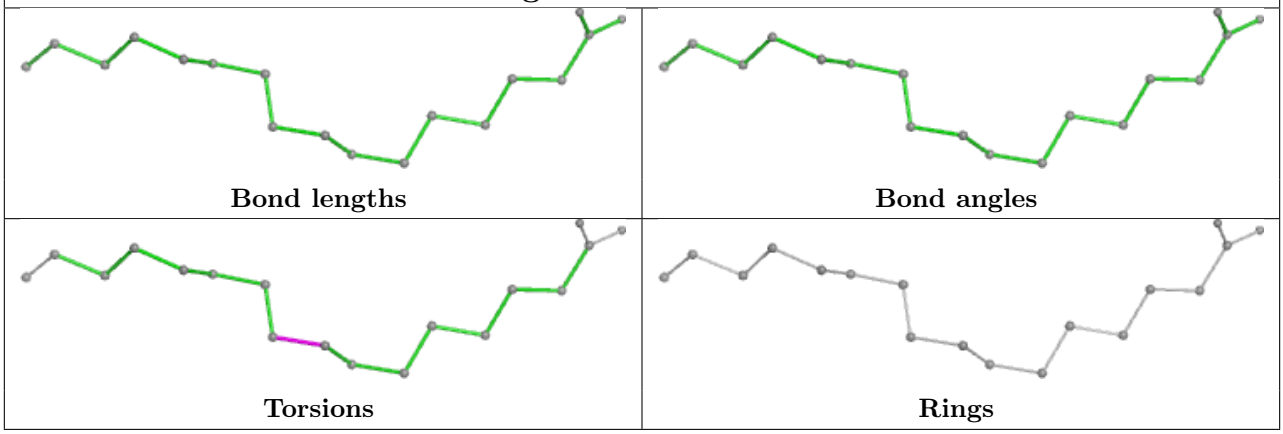
Ligand A1H6W D 505



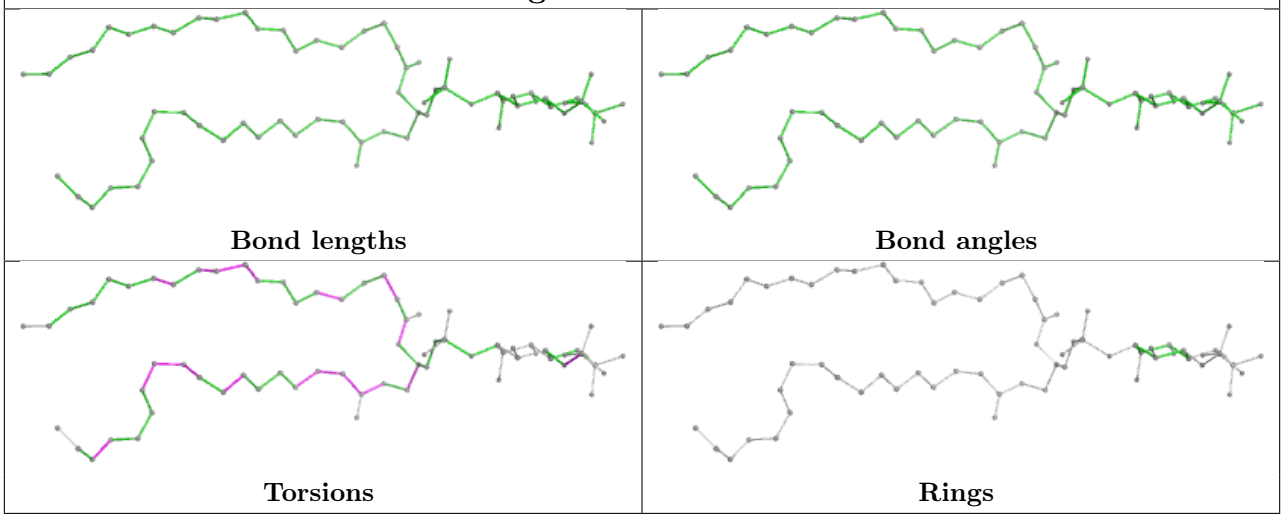
Ligand PLM A 510



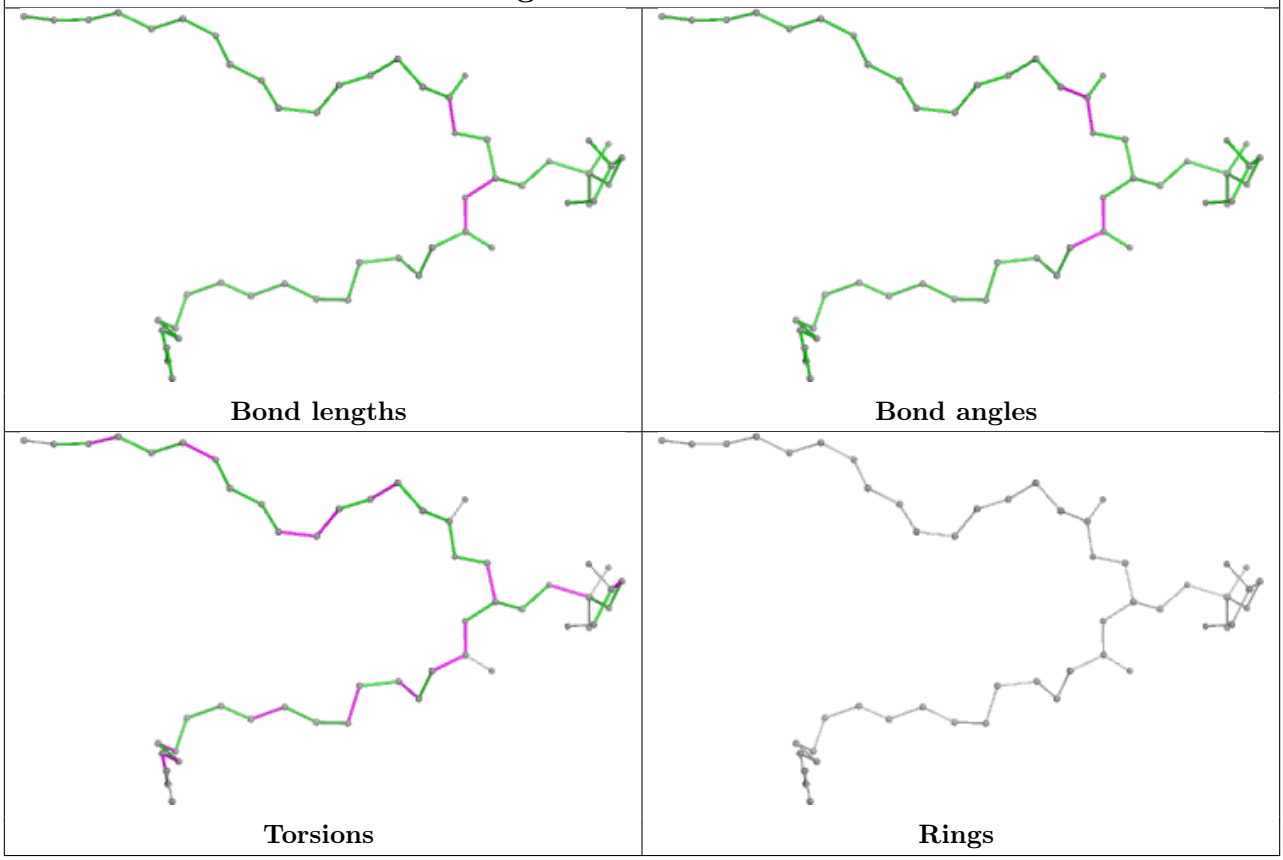
Ligand PLM C 502



Ligand PT5 A 505



Ligand PGW D 501



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.

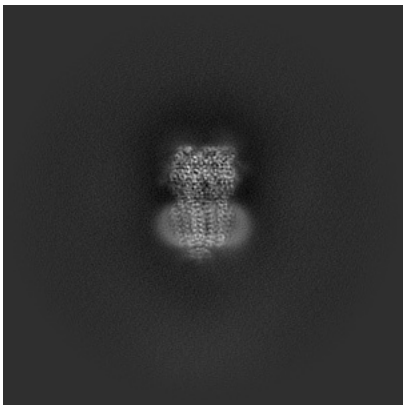
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19907. These allow visual inspection of the internal detail of the map and identification of artifacts.

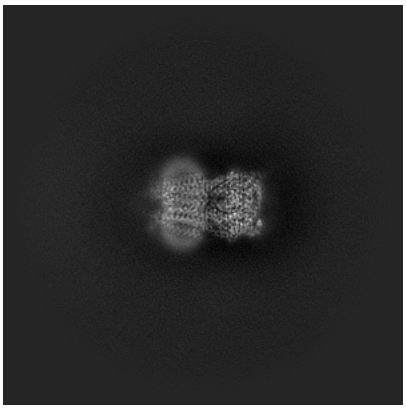
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

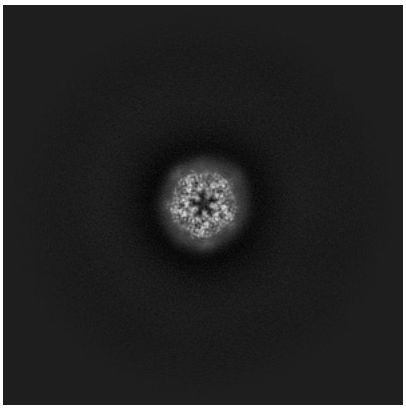
6.1.1 Primary map



X

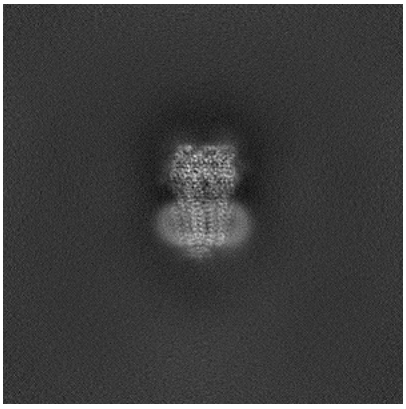


Y

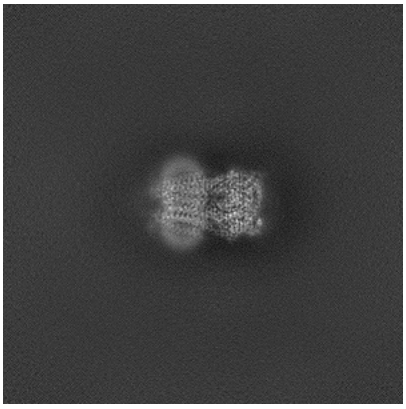


Z

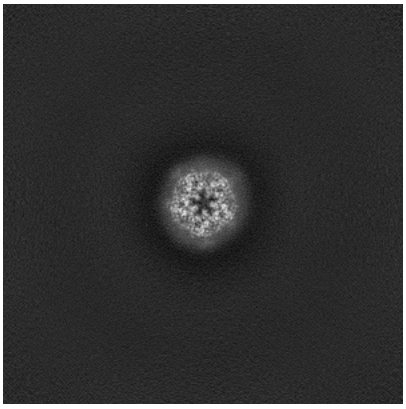
6.1.2 Raw map



X



Y

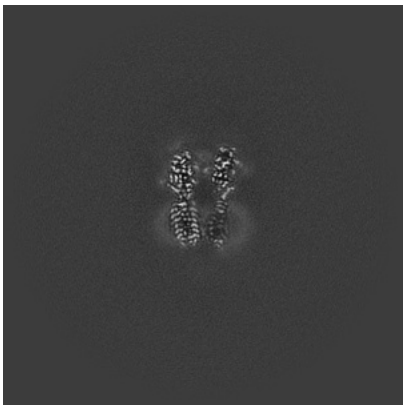


Z

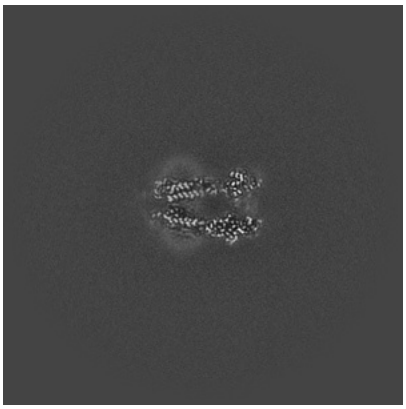
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

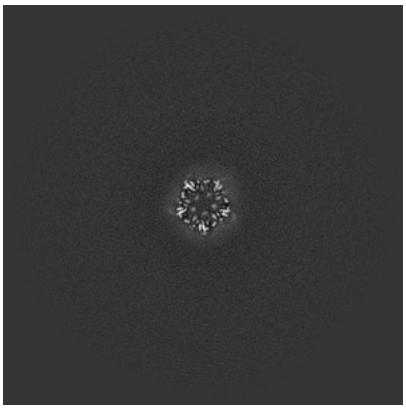
6.2.1 Primary map



X Index: 256

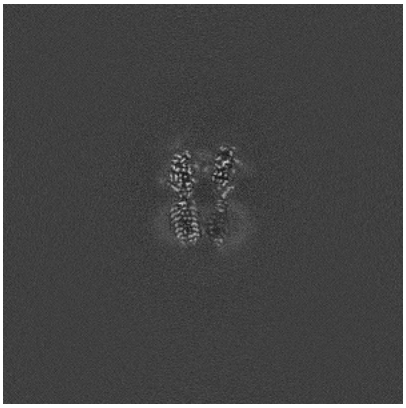


Y Index: 256

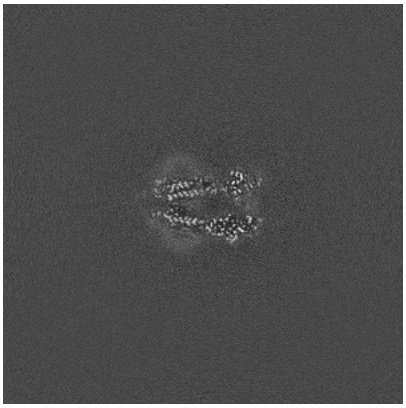


Z Index: 256

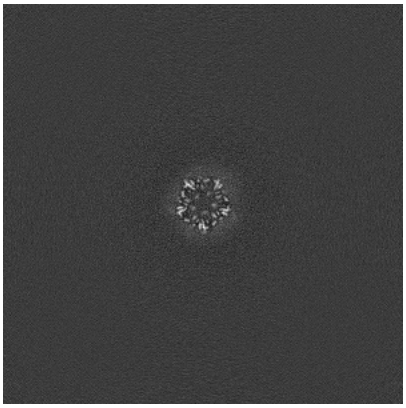
6.2.2 Raw map



X Index: 256



Y Index: 256

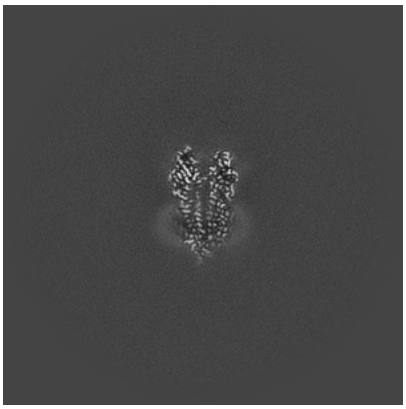


Z Index: 256

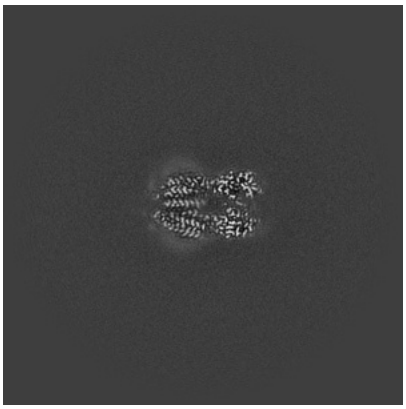
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

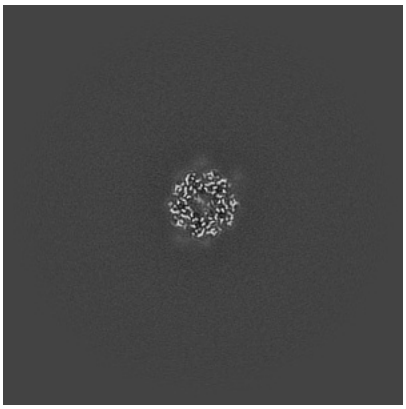
6.3.1 Primary map



X Index: 243

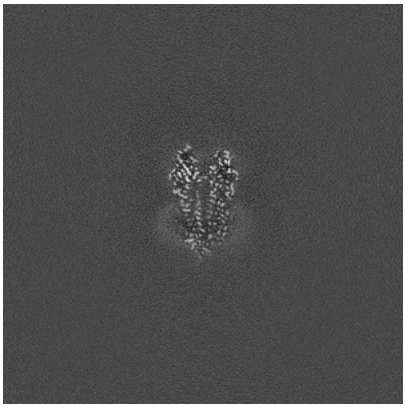


Y Index: 246

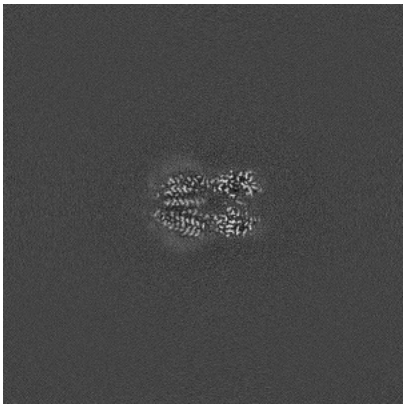


Z Index: 299

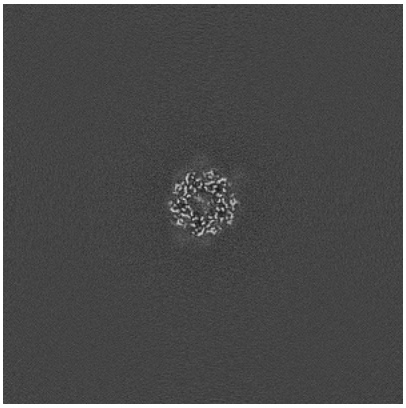
6.3.2 Raw map



X Index: 243



Y Index: 246

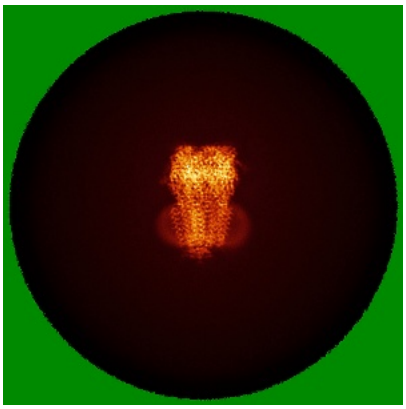


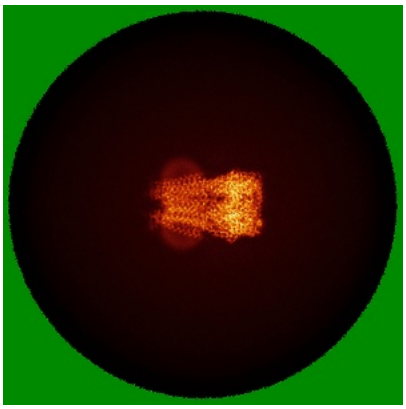
Z Index: 299

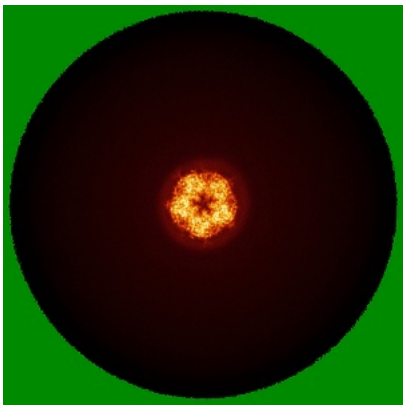
The images above show the largest variance slices of the map in three orthogonal directions.

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

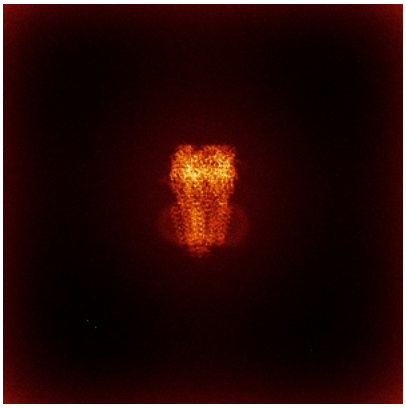
6.4.1 Primary map

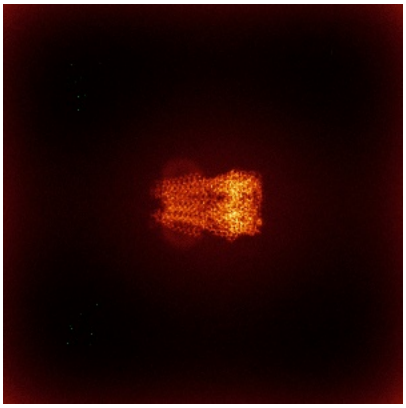

X

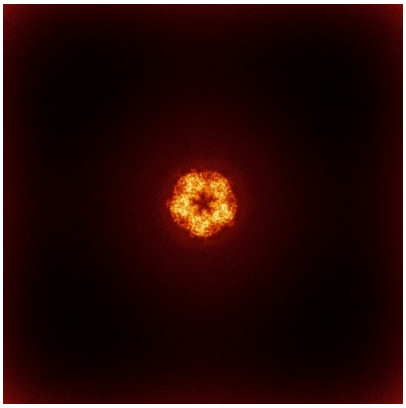

Y


Z

6.4.2 Raw map


X

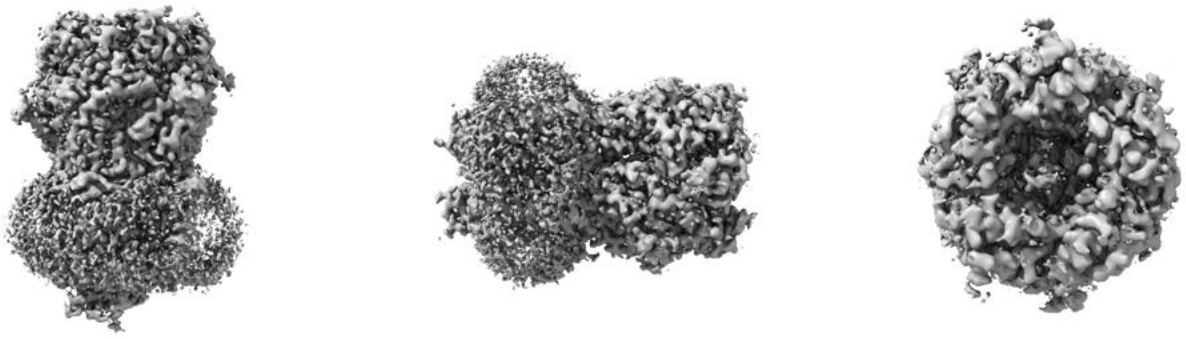

Y


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 0.12. 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.

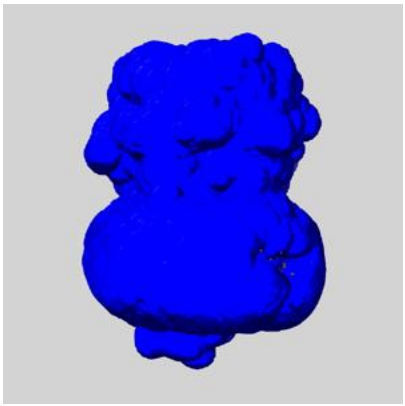
6.6 Mask visualisation (i)

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

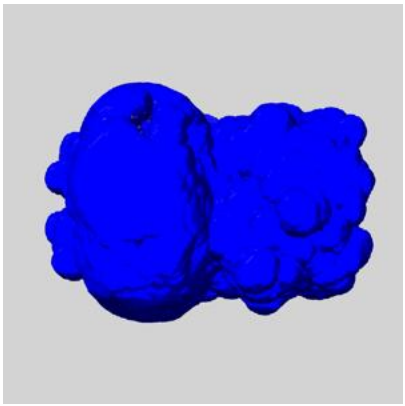
A mask typically either:

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

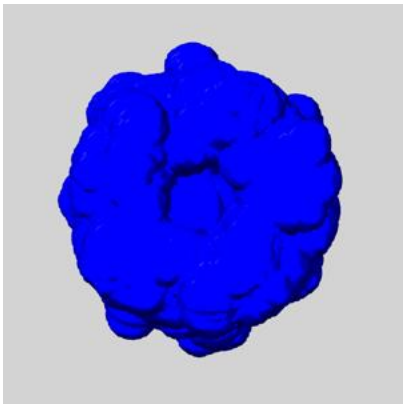
6.6.1 emd_19907_msk_1.map (i)



X



Y

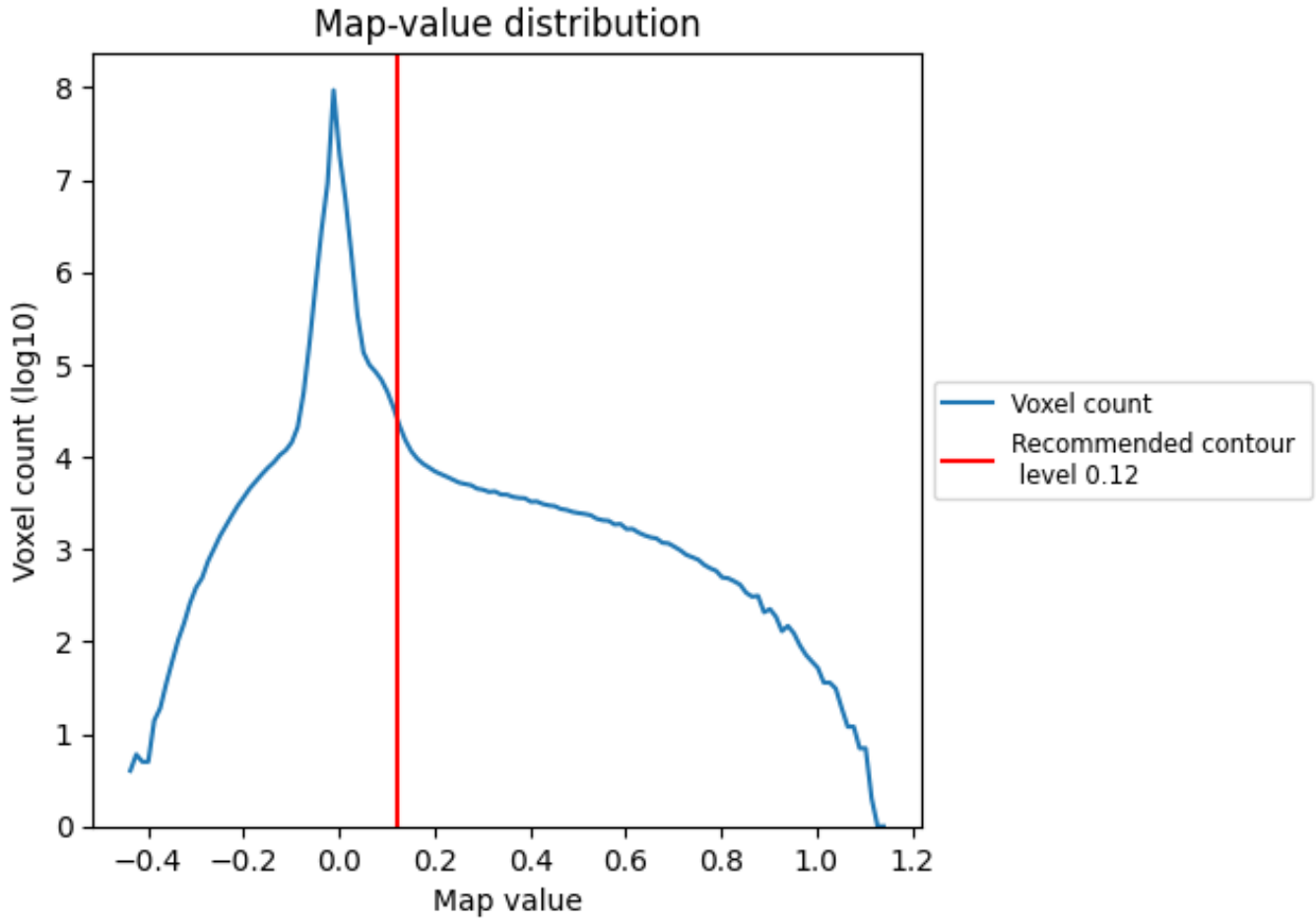


Z

7 Map analysis

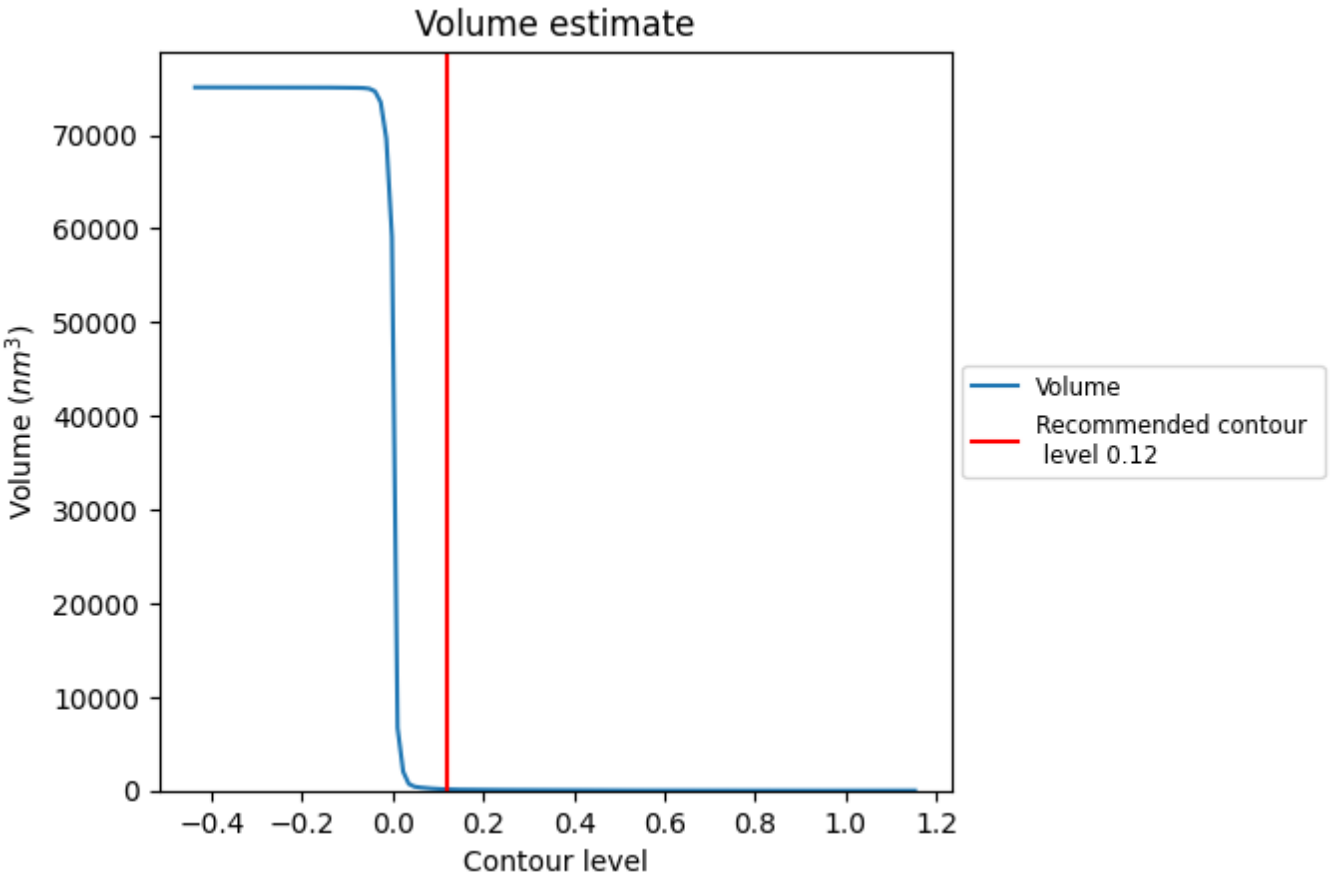
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

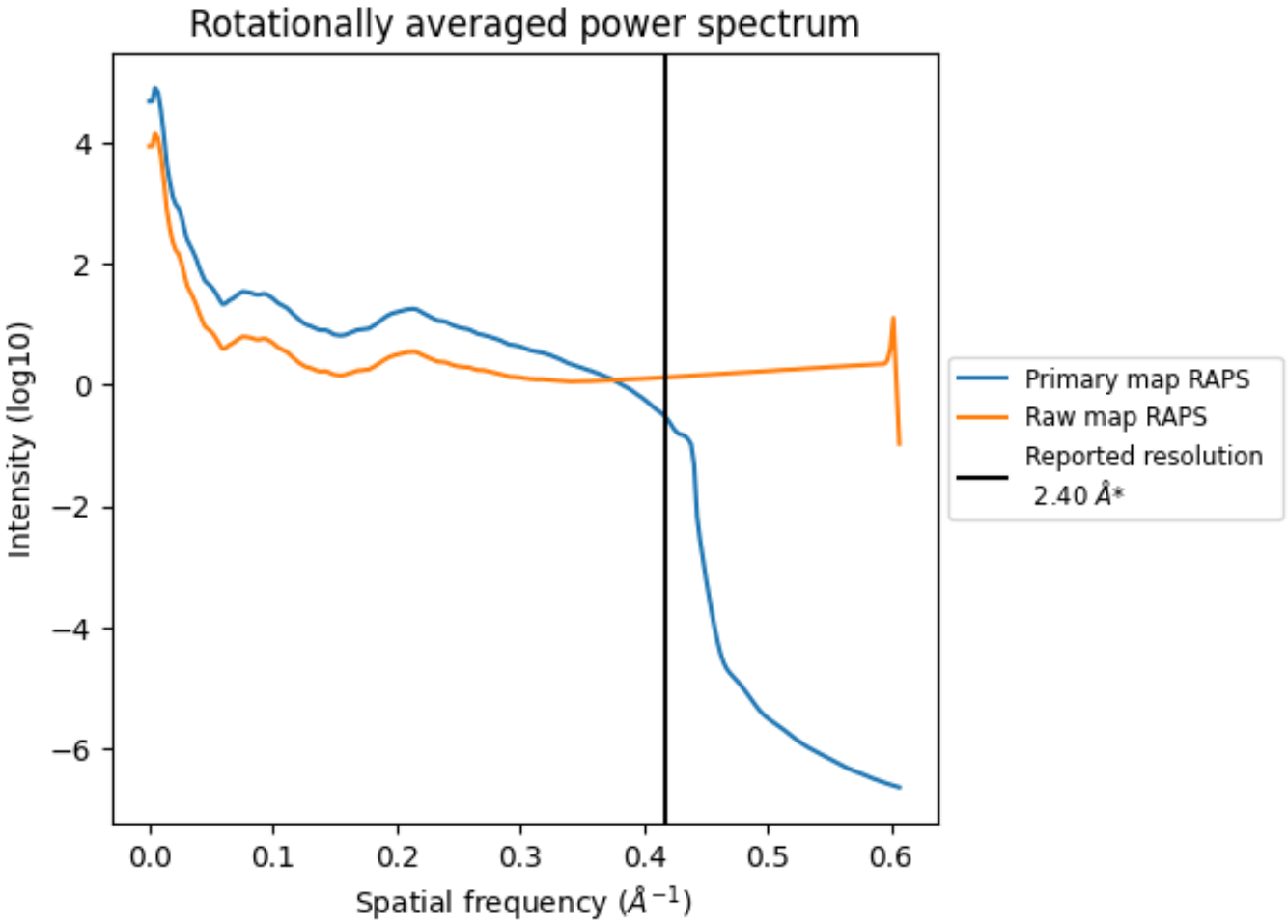
7.2 Volume estimate



The volume at the recommended contour level is 129 nm^3; this corresponds to an approximate mass of 117 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)

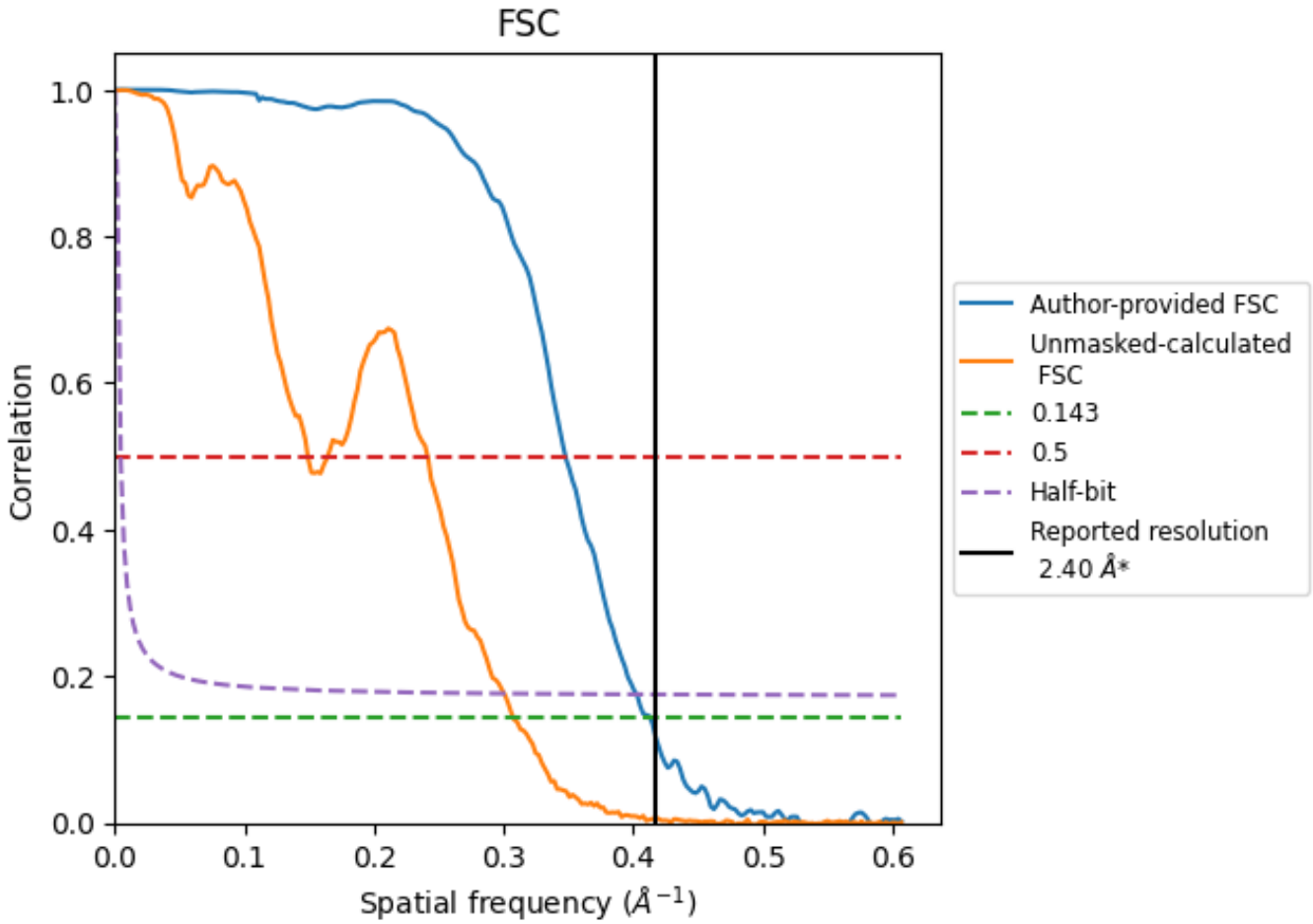


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

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 0.417 $Å^{-1}$

8.2 Resolution estimates (i)

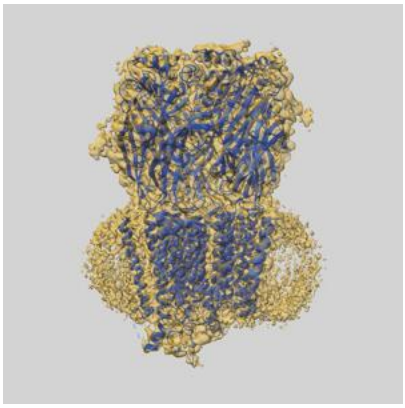
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.42	2.88	2.48
Unmasked-calculated*	3.25	6.71	3.33

*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 3.25 differs from the reported value 2.4 by more than 10 %

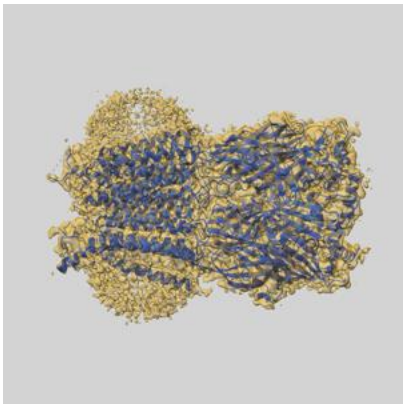
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19907 and PDB model 9EQG. Per-residue inclusion information can be found in section 3 on page 16.

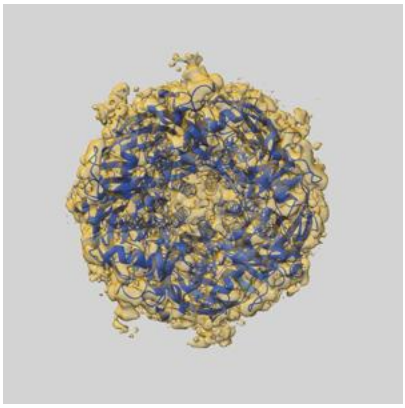
9.1 Map-model overlay



X



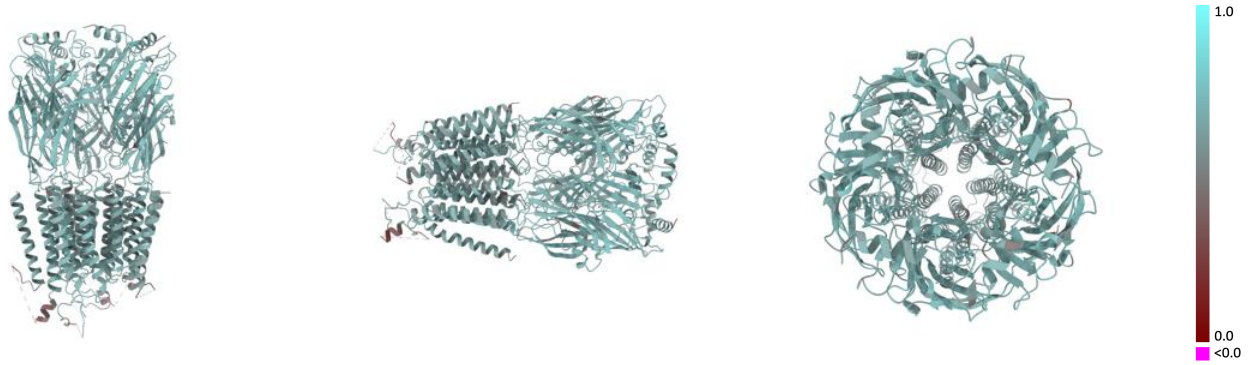
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

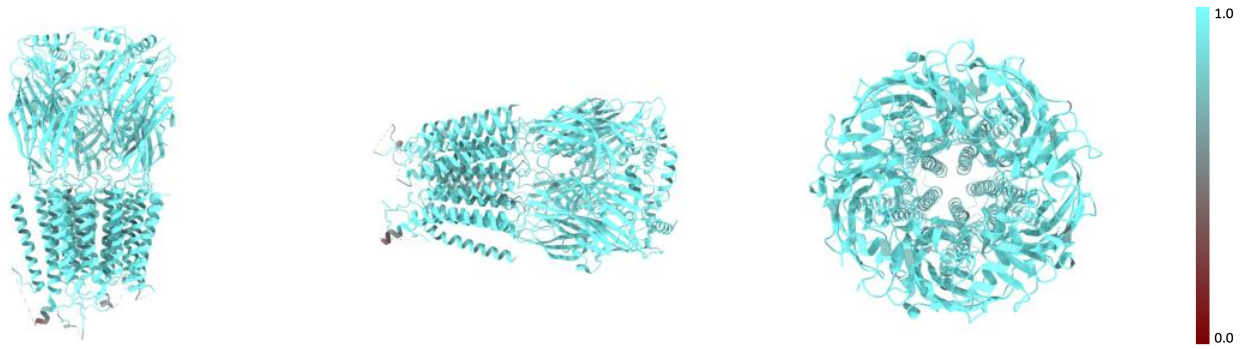
9.2 Q-score mapped to coordinate model (i)



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.

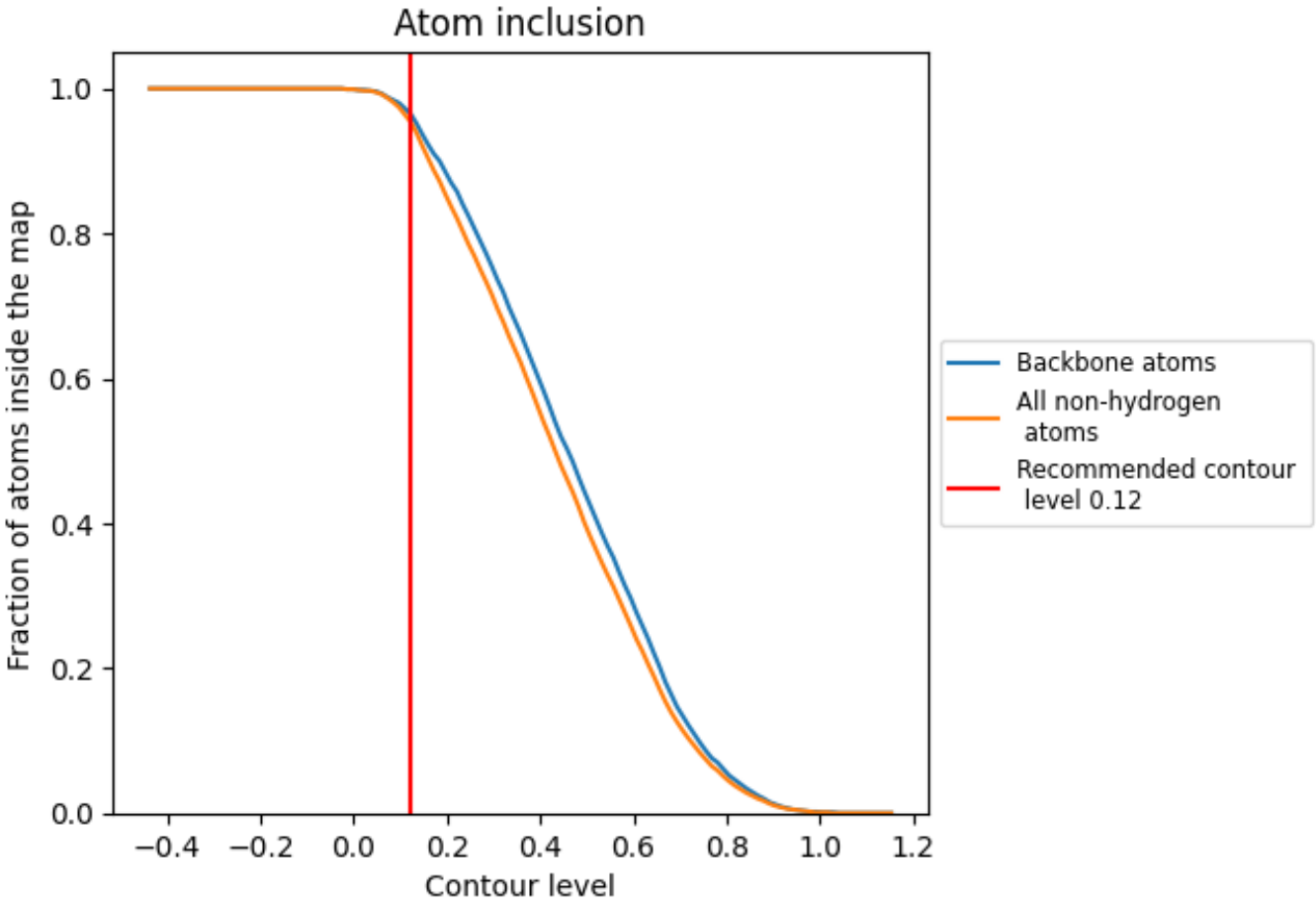
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.6270
A	0.9630	0.6350
B	0.9570	0.6250
C	0.9540	0.6240
D	0.9550	0.6300
E	0.9610	0.6280
F	0.9050	0.5640
G	0.9580	0.5920
H	0.9490	0.5470
I	0.8890	0.5610
J	0.9440	0.5870
K	0.7690	0.4940