wwPDB EM Validation Summary Report (i)

Nov 4, 2023 – 10:15 AM EDT

PDB ID	:	6D6T
EMDB ID	:	EMD-7816
Title	:	Human GABA-A receptor alpha1-beta2-gamma2 subtype in complex with GABA and flumazenil, conformation B
Authors	:	Zhu, S.; Noviello, C.M.; Teng, J.; Walsh Jr, R.M.; Kim, J.J.; Hibbs, R.E.
Deposited on	:	2018-04-22
Resolution	:	3.86 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 (i) 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 (1)) were used in the production of this report:

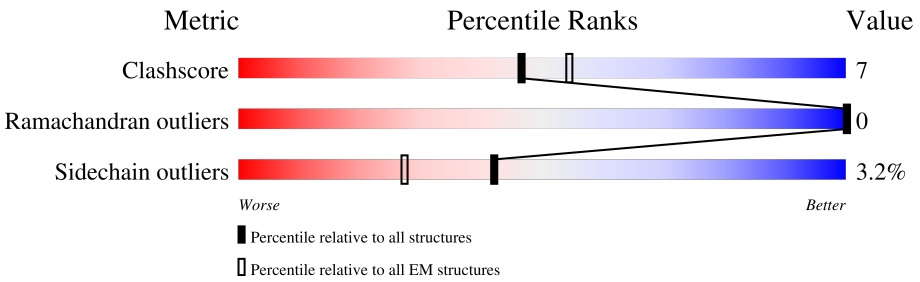
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	81% 16% • •
1	C	341	18% 76% 21% • •
2	B	358	• 73% 18% • 7%
2	D	358	• 76% 18% • 6%
3	E	366	5% 69% 13% • 17%
4	I	213	46% • 50%
4	L	213	46% • 50%
5	J	454	19% 6% 74%

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Mol	Chain	Length	Quality of chain
5	K	454	21% • 74%
6	F	3	67% 33%
6	H	3	33% 33% 33%
7	G	8	50% 50%
8	M	5	60% 40%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17197 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,Gamma-a minobutyric acid receptor subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	333	2726	1788	439	483	16	0	0
1	C	333	2726	1788	439	483	16	0	0

There are 14 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
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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	333	2688	1741	451	480	16	0	0
2	D	337	2722	1759	460	487	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 Human GABA-A receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	302	2336	1493	404	429	10	0	0

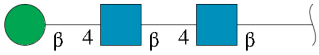
- Molecule 4 is a protein called Kappa Fab Light Chain.

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

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

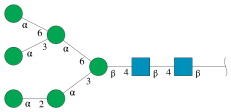
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	116	907	574	151	178	4	0	0
5	K	116	907	573	151	179	4	0	0

- 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.



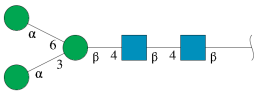
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	3	39	22	2	15	0	0
6	H	3	39	22	2	15	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



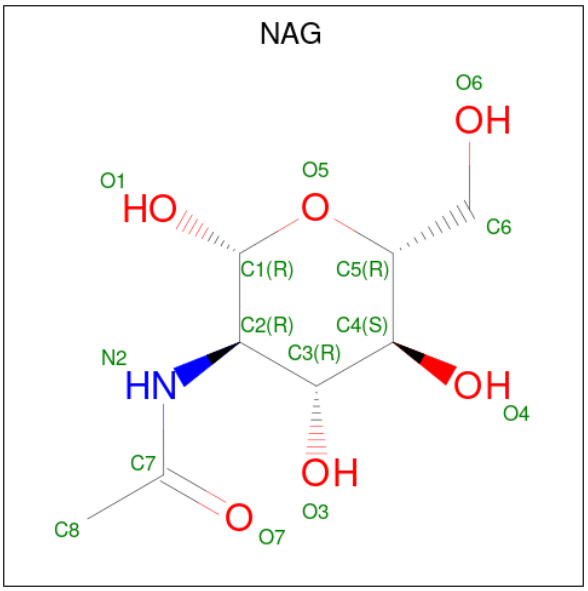
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	8	94	52	2	40	0	0

- Molecule 8 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.



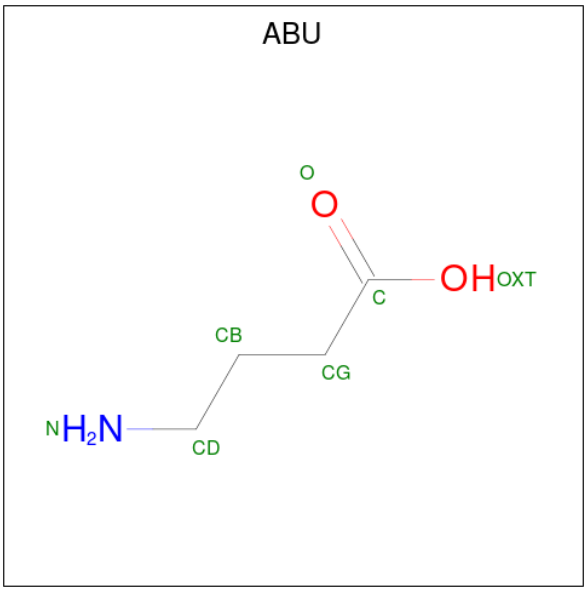
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	M	5	61	34	2	25	0	0

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



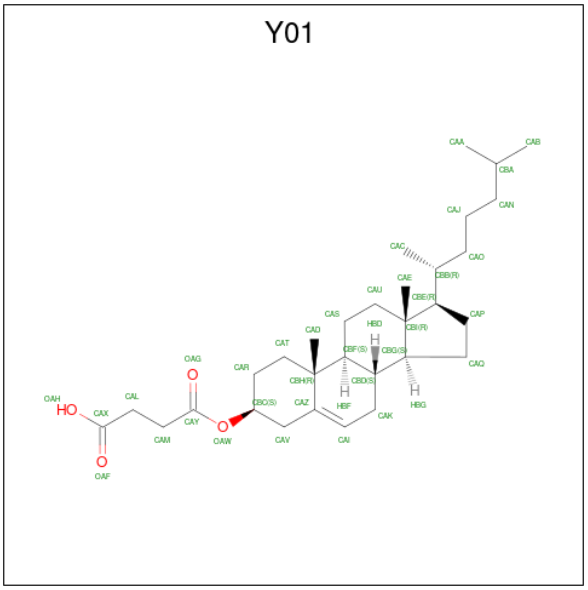
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	A	1	14	8	1	5	0
9	C	1	14	8	1	5	0
9	E	1	14	8	1	5	0

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



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

- Molecule 11 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
11	A	1	21	20	1		0
11	A	1	21	20	1		0
11	A	1	21	20	1		0
11	A	1	21	20	1		0
11	A	1	21	20	1		0
11	B	1	21	20	1		0
11	B	1	21	20	1		0
11	B	1	21	20	1		0
11	B	1	21	20	1		0

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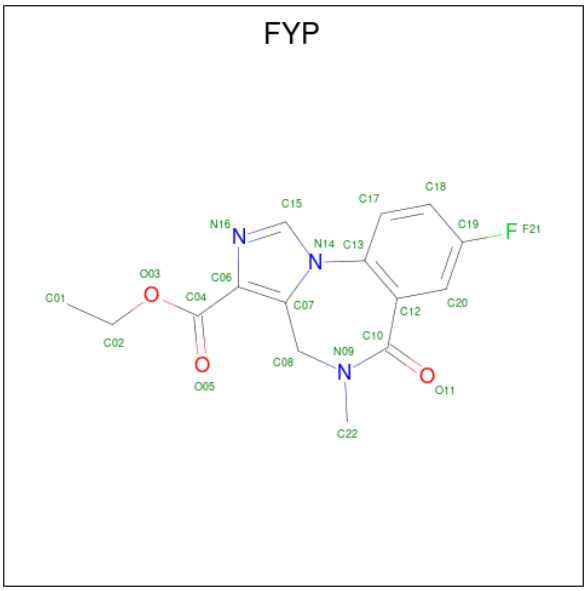
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	D	1	21	20	1	0
			Total	C	O	
11	D	1	21	20	1	0
			Total	C	O	
11	D	1	21	20	1	0

- Molecule 12 is ethyl 8-fluoro-5-methyl-6-oxo-5,6-dihydro-4H-imidazo[1,5-a][1,4]benzodiazepine-3-carboxylate (three-letter code: FYP) (formula: $C_{15}H_{14}FN_3O_3$).



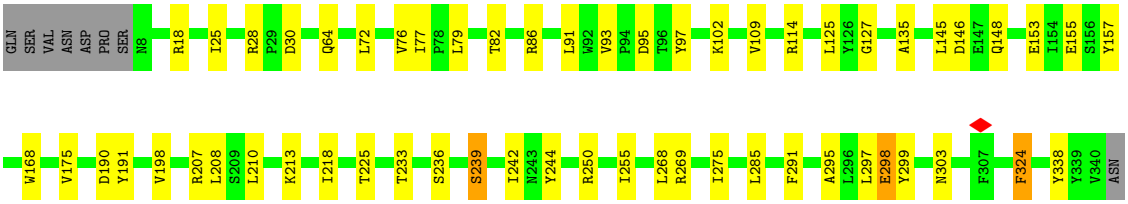
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
12	D	1	22	15	1	3	3	0

3 Residue-property plots (i)

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

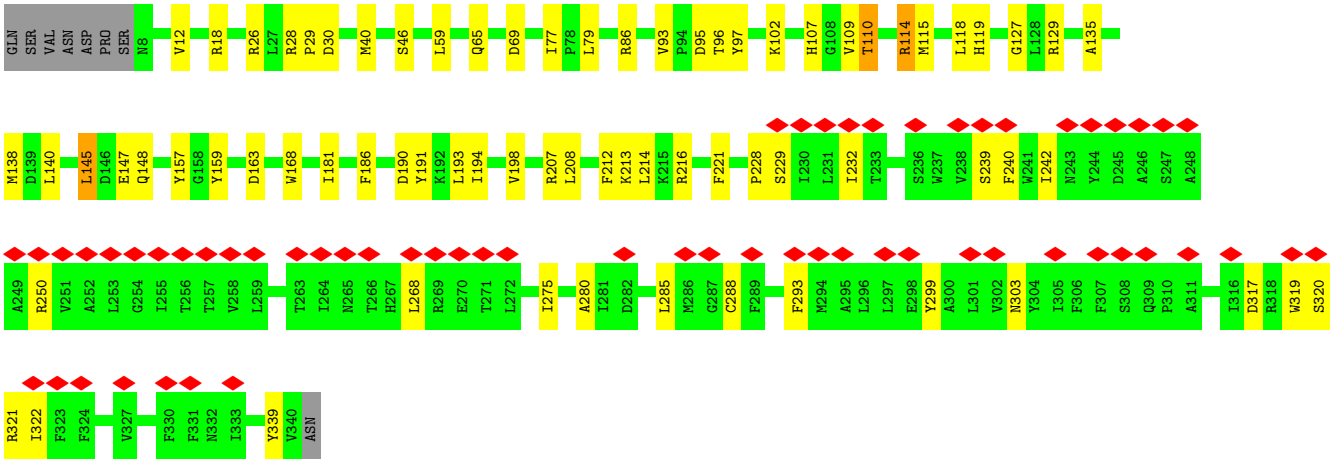
• Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2,Gamma-aminobutyric acid receptor subunit beta-2

Chain A:



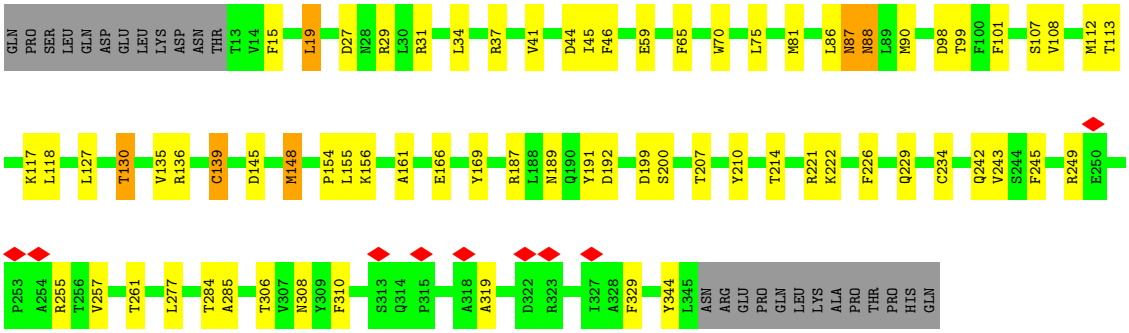
• Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2,Gamma-aminobutyric acid receptor subunit beta-2

Chain C:



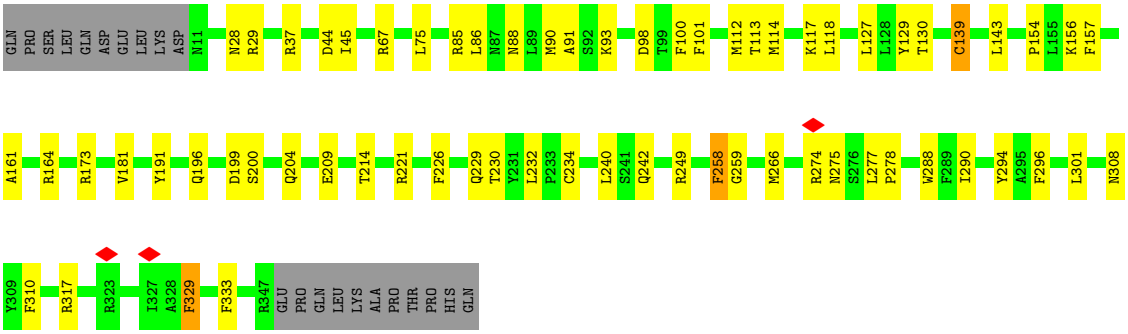
• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1,Gamma-aminobutyric acid receptor subunit alpha-1

Chain B:



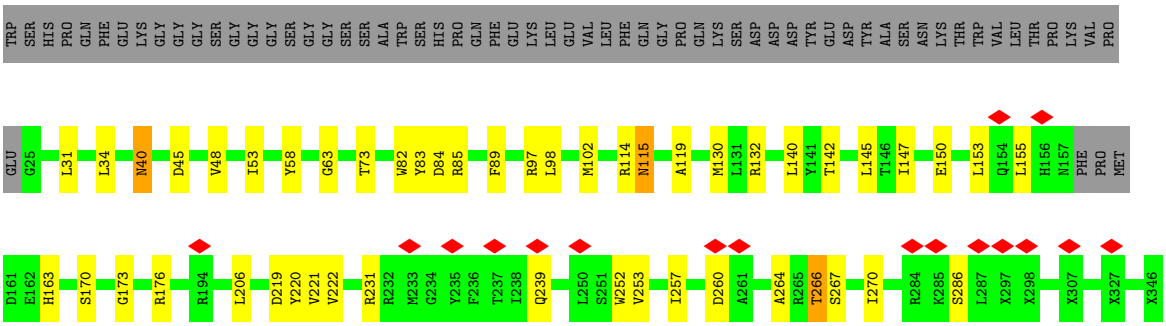
• Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1,Gamma-aminobutyric acid receptor subunit alpha-1

Chain D:



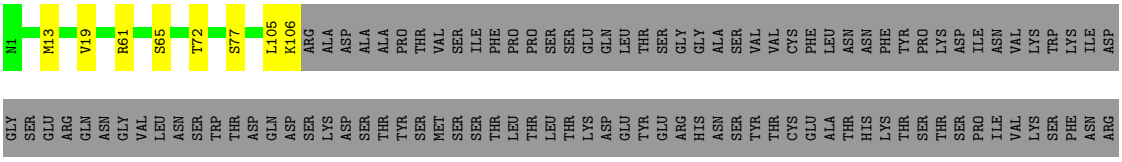
• Molecule 3: Human GABA-A receptor subunit gamma-2

Chain E:



• Molecule 4: Kappa Fab Light Chain

Chain I:



ASN GLU CYS

• Molecule 4: Kappa Fab Light Chain

Chain L: 46% • 50%

N1 S14 V29 L46 Y49 Y92 L105 K106 ARG ALA ASP ALA ALA PRO THR VAL SER ILE PHE PRO PRO SER SER GLU GLN LEU THR SER GLY GLY ALA SER VAL VAL CYS PHE LEU ASN ASN PHE TYR PRO LYS ASP ILE ASN VAL LYS TRP LYS ILE ASP GLY SER

GLU ARG GLN ASN GLY VAL LEU ASN SER TRP THR ASP GLN ASP SER LYS ASP SER THR TYR SER MET SER SER THR LEU THR LEU THR LYS ASP GLU TYR GLU ARG HIS ASN SER TYR THR CYS GLU ALA THR HIS LYS THR SER THR SER PRO ILE VAL LYS SER PHE ASN ARG ASN GLU

CYS

• Molecule 5: IgG2b Fab Heavy Chain

Chain J: 19% 6% 74%

GLU V2 Q5 Q6 K19 F27 N28 I29 K30 Y33 M34 V37 K38 Q39 L45 E46 W47 I48 G49 R50 I51 D52 P53 T58 K59 K63 F64 N77 T78 A79 Y80 C96 A97 R98 K99 Q110 S117 THR ALA LYS THR THR PRO PRO SER VAL TYR PRO

LEU ALA PRO GLY CYS GLY ASP THR THR GLY SER SER VAL THR LEU GLY CYS LEU VAL LYS GLY TYR PHE PRO GLU SER VAL THR VAL THR TRP ASN SER GLY SER LEU SER SER SER VAL HIS THR PHE PRO ALA LEU LEU GLN SER GLY LEU TYR THR MET SER SER SER VAL THR VAL

PRO SER SER THR TRP PRO SER GLN THR VAL THR CYS SER VAL ALA HIS PRO ALA SER SER THR THR VAL ASP LYS LYS LEU GLU PRO SER GLY PRO ILE SER THR ILE ASN PRO CYS PRO PRO CYS LYS GLU CYS HIS LYS CYS PRO ALA PRO ASN LEU GLU GLY GLY PRO SER VAL PHE

ILE PHE PRO PRO ASN ILE LYS ASP VAL LEU MET ILE SER LEU THR PRO LYS VAL THR CYS VAL VAL VAL ASP VAL SER GLU ASP ASP PRO ASP VAL GLN ILE SER TRP PHE VAL ASN ASN VAL GLU VAL HIS THR ALA GLN THR GLN THR HIS ARG GLU ASP TYR ASN SER THR ILE ARG

VAL VAL SER THR LEU PRO ILE GLN HIS GLN ASP TRP MET SER GLY LYS GLU PHE LYS CYS LYS VAL VAL ASN ASN LYS ASP LEU PRO SER PRO ILE GLU ARG THR ILE SER LYS ILE LYS GLY LEU VAL ARG ALA PRO GLN GLN VAL TYR ILE LEU PRO PRO PRO ALA GLU GLN LEU SER ARG LYS

ASP VAL SER LEU THR CYS LEU VAL VAL GLY PHE ASN PRO GLY ASP ILE SER VAL GLU TRP THR SER ASN GLY HIS THR GLU GLU ASN TYR LYS ASP THR ALA PRO VAL LEU ASP SER ASP GLY SER TYR PHE ILE TYR SER LYS LEU ASN MET LYS THR SER LYS TRP GLU LYS THR ASP

SER PHE SER CYS ASN VAL ARG HIS GLU GLY LEU LYS ASN TYR TYR LEU LYS LYS THR ILE SER ARG SER PRO GLY LYS

• Molecule 5: IgG2b Fab Heavy Chain

Chain K: 21% • 74%

GLU VAL Q3 Q6 F27 T32 K38 Q39 I48 K63 F64 T91 A92 R98 K99 M105 D106 Y107 W108 G109 Q110 G111 T112 T115 T118 ALA LYS THR THR PRO PRO SER VAL TYR PRO LEU ALA PRO GLY CYS GLY ASP THR THR GLY SER SER VAL THR

LEU GLY CYS LEU VAL LYS GLY TYR PHE PRO GLU SER VAL THR VAL THR TRP ASN SER GLY SER LEU SER SER SER VAL HIS THR PHE PRO ALA LEU LEU GLN SER GLY LEU TYR THR MET SER SER SER VAL THR VAL PRO SER SER THR TRP PRO SER GLN THR VAL THR CYS SER VAL

ALA HIS PRO ALA SER SER THR THR VAL ASP LYS LYS LEU GLU PRO SER GLY PRO ILE SER THR ILE ASN PRO CYS LYS GLU CYS HIS LYS CYS PRO ALA PRO ASN LEU GLU GLY GLY PRO SER VAL PHE ILE PHE PRO PRO ASN ILE LYS ASP VAL LEU MET ILE SER LEU

THR PRO LYS VAL THR CYS VAL VAL VAL ASP VAL SER GLU ASP ASP PRO ASP VAL GLN ILE SER TRP PHE VAL ASN ASN VAL GLU VAL HIS THR ALA GLN THR GLN THR HIS ARG GLU ASP TYR ASN SER THR ILE ARG VAL VAL SER THR LEU PRO ILE GLN HIS GLN ASP TRP MET SER

GLY LYS GLU PHE LYS CYS LYS VAL ASN ASN LYS ASP LEU PRO SER PRO ILE GLU ARG THR ILE SER LYS ILE LYS GLY LEU VAL ARG ALA PRO GLN VAL TYR ILE LEU PRO PRO PRO ALA GLU GLN LEU SER ARG LYS ASP VAL SER LEU THR CYS LEU VAL VAL GLY PHE ASN PRO GLY

ASP ILE SER VAL GLU TRP THR SER ASN GLY HIS THR GLU GLU ASN TYR LYS ASP THR ALA PRO VAL LEU ASP SER ASP GLY SER TYR PHE ILE TYR SER LYS LEU ASN MET LYS THR SER LYS TRP GLU LYS THR ASP SER PHE SER CYS ASN VAL ARG HIS GLU GLY LEU LYS ASN TYR

TYR LEU LYS LYS THR ILE SER ARG SER PRO GLY LYS

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

Chain F: 67% 33%

NAG1 NAG2 BMA3

• 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: 33% 33% 33%

NAG1 NAG2 BMA3

• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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: 50% 50%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8

• Molecule 8: 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: 60% 40%

NAG1 NAG2 BMA3 MAN4 MAN5

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200442	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 ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	278.2, 278.2, 278.2	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ABU, BMA, MAN, FYP, NAG, Y01

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	0.32	0/2798	0.44	0/3810
1	C	0.29	0/2798	0.42	0/3810
2	B	0.30	0/2757	0.43	0/3748
2	D	0.32	0/2791	0.44	0/3794
3	E	0.31	0/2177	0.45	0/2962
4	I	0.32	0/829	0.45	0/1123
4	L	0.31	0/829	0.46	0/1123
5	J	0.29	0/928	0.47	0/1260
5	K	0.29	0/928	0.44	0/1260
All	All	0.31	0/16835	0.44	0/22890

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 (i)

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	2726	0	2736	38	0
1	C	2726	0	2736	41	0
2	B	2688	0	2686	43	0
2	D	2722	0	2718	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2336	0	2163	34	0
4	I	811	0	784	4	0
4	L	811	0	784	4	0
5	J	907	0	877	22	0
5	K	907	0	875	10	0
6	F	39	0	34	1	0
6	H	39	0	34	3	0
7	G	94	0	79	0	0
8	M	61	0	52	0	0
9	A	14	0	13	0	0
9	C	14	0	13	0	0
9	E	14	0	13	0	0
10	A	7	0	0	0	0
10	C	7	0	0	1	0
11	A	105	0	140	5	0
11	B	84	0	112	2	0
11	D	63	0	84	1	0
12	D	22	0	0	0	0
All	All	17197	0	16933	223	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 223 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)
5:J:29:ILE:HG13	5:J:77:ASN:OD1	1.43	1.16
3:E:130:MET:HB3	3:E:142:THR:HG22	1.29	1.10
3:E:130:MET:HB3	3:E:142:THR:CG2	1.81	1.08
2:B:249:ARG:HH12	2:B:319:ALA:HA	1.53	0.73
1:A:146:ASP:OD2	1:A:148:GLN:NE2	2.21	0.73

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	331/341 (97%)	320 (97%)	11 (3%)	0	100	100
1	C	331/341 (97%)	325 (98%)	6 (2%)	0	100	100
2	B	331/358 (92%)	317 (96%)	14 (4%)	0	100	100
2	D	335/358 (94%)	322 (96%)	13 (4%)	0	100	100
3	E	256/366 (70%)	239 (93%)	17 (7%)	0	100	100
4	I	104/213 (49%)	100 (96%)	4 (4%)	0	100	100
4	L	104/213 (49%)	100 (96%)	4 (4%)	0	100	100
5	J	114/454 (25%)	112 (98%)	2 (2%)	0	100	100
5	K	114/454 (25%)	110 (96%)	4 (4%)	0	100	100
All	All	2020/3098 (65%)	1945 (96%)	75 (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	301/309 (97%)	291 (97%)	10 (3%)	38	63
1	C	301/309 (97%)	289 (96%)	12 (4%)	31	58
2	B	295/319 (92%)	281 (95%)	14 (5%)	26	54
2	D	299/319 (94%)	287 (96%)	12 (4%)	31	58
3	E	239/293 (82%)	233 (98%)	6 (2%)	47	68
4	I	90/188 (48%)	90 (100%)	0	100	100
4	L	90/188 (48%)	90 (100%)	0	100	100
5	J	97/407 (24%)	94 (97%)	3 (3%)	40	64
5	K	97/407 (24%)	96 (99%)	1 (1%)	76	85
All	All	1809/2739 (66%)	1751 (97%)	58 (3%)	42	63

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	93	VAL
5	J	96	CYS
1	C	303	ASN
5	J	78	THR
3	E	83	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	216	HIS
2	D	337	ASN
4	I	6	GLN
3	E	115	ASN
2	B	229	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

19 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	0.25	0	17,19,21	0.56	0
6	NAG	F	2	6	14,14,15	0.26	0	17,19,21	0.45	0
6	BMA	F	3	6	11,11,12	0.58	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	G	1	2,7	14,14,15	0.21	0	17,19,21	0.51	0
7	NAG	G	2	7	14,14,15	0.26	0	17,19,21	0.38	0
7	BMA	G	3	7	11,11,12	0.59	0	15,15,17	0.88	0
7	MAN	G	4	7	11,11,12	0.82	0	15,15,17	1.52	2 (13%)
7	MAN	G	5	7	11,11,12	0.73	0	15,15,17	0.83	0
7	MAN	G	6	7	11,11,12	0.88	1 (9%)	15,15,17	1.13	1 (6%)
7	MAN	G	7	7	11,11,12	0.68	1 (9%)	15,15,17	1.23	2 (13%)
7	MAN	G	8	7	11,11,12	0.93	1 (9%)	15,15,17	1.41	2 (13%)
6	NAG	H	1	6,1	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	H	2	6	14,14,15	0.40	0	17,19,21	1.25	1 (5%)
6	BMA	H	3	6	11,11,12	0.90	0	15,15,17	0.94	0
8	NAG	M	1	8,2	14,14,15	0.38	0	17,19,21	0.40	0
8	NAG	M	2	8	14,14,15	0.26	0	17,19,21	0.43	0
8	BMA	M	3	8	11,11,12	0.52	0	15,15,17	0.76	0
8	MAN	M	4	8	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
8	MAN	M	5	8	11,11,12	0.60	0	15,15,17	1.17	2 (13%)

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	-	3/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	1/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	MAN	G	4	7	-	2/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	0/1/1/1
7	MAN	G	6	7	-	1/2/19/22	0/1/1/1
7	MAN	G	7	7	-	2/2/19/22	0/1/1/1
7	MAN	G	8	7	-	2/2/19/22	1/1/1/1
6	NAG	H	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
8	NAG	M	1	8,2	-	1/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	M	3	8	-	2/2/19/22	0/1/1/1
8	MAN	M	4	8	-	2/2/19/22	0/1/1/1
8	MAN	M	5	8	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	8	MAN	C1-C2	2.52	1.58	1.52
7	G	6	MAN	O5-C1	-2.24	1.40	1.43
7	G	7	MAN	C1-C2	2.03	1.56	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	4	MAN	C1-O5-C5	4.58	118.40	112.19
6	H	2	NAG	C2-N2-C7	4.30	129.02	122.90
7	G	8	MAN	C1-O5-C5	3.63	117.11	112.19
7	G	7	MAN	C1-O5-C5	3.20	116.52	112.19
8	M	5	MAN	C1-O5-C5	2.98	116.23	112.19

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C4-C5-C6-O6
8	M	3	BMA	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6
7	G	8	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	8	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 4 short contacts:

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

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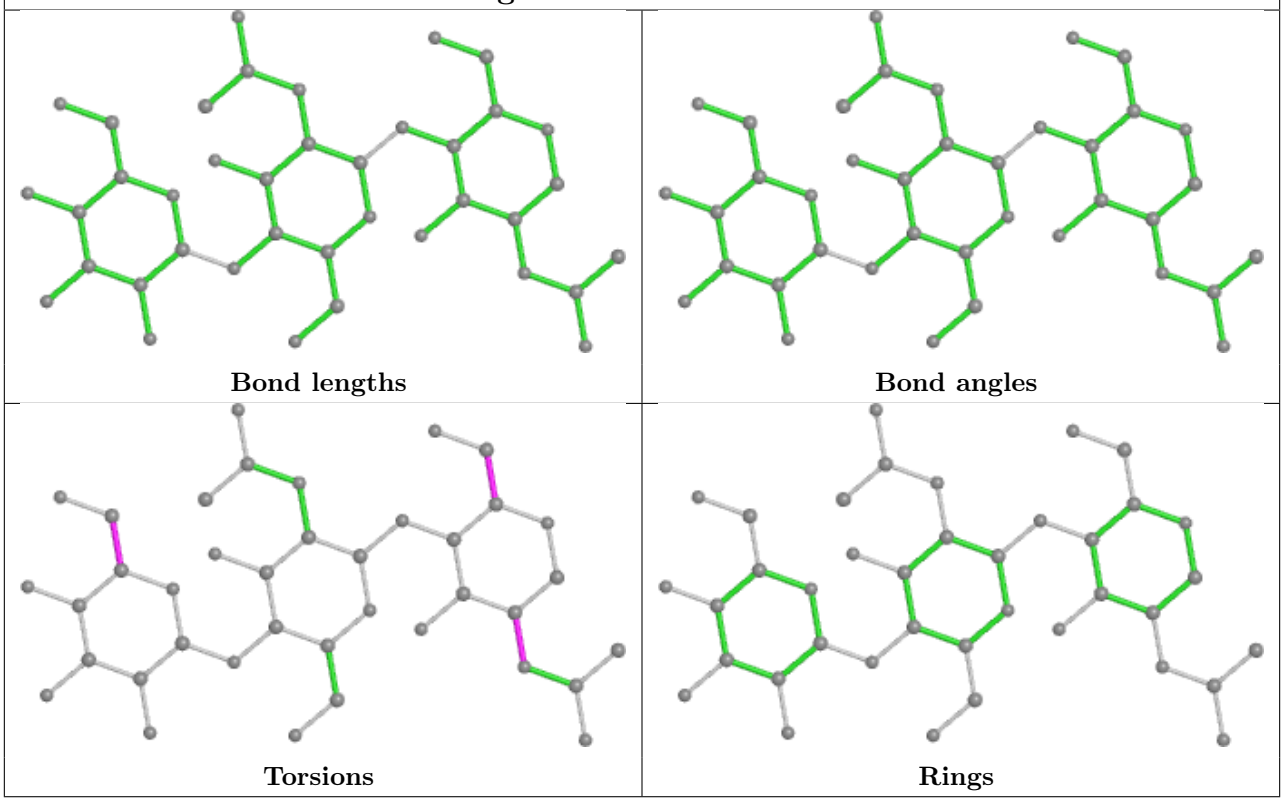
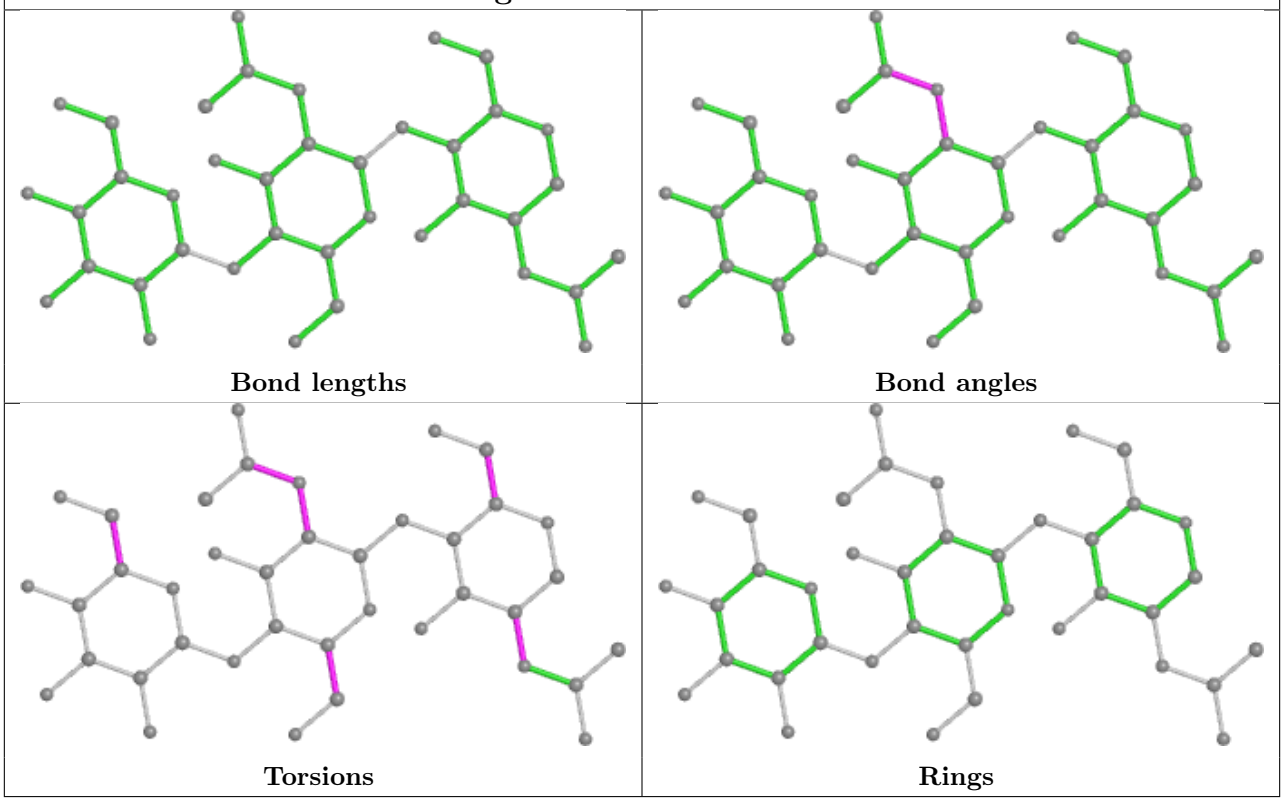
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	2	NAG	2	0

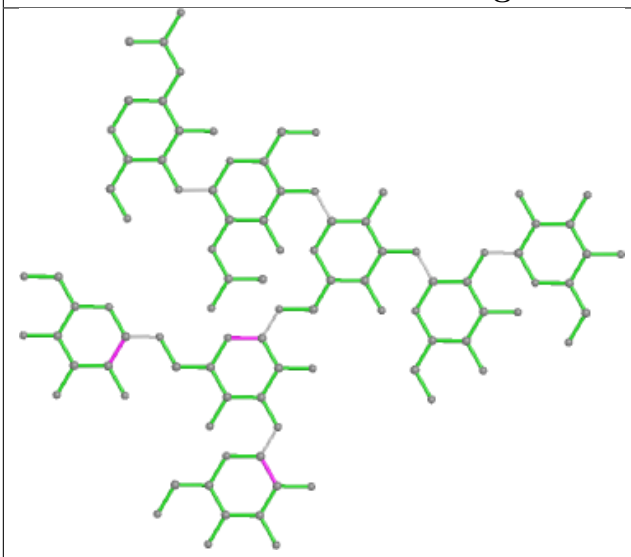
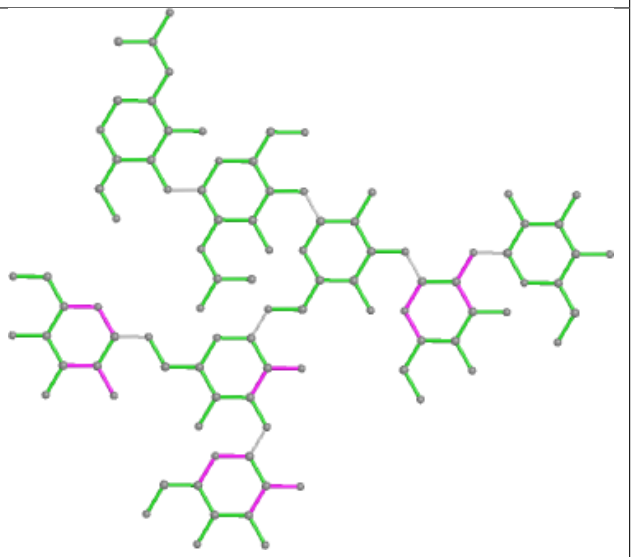
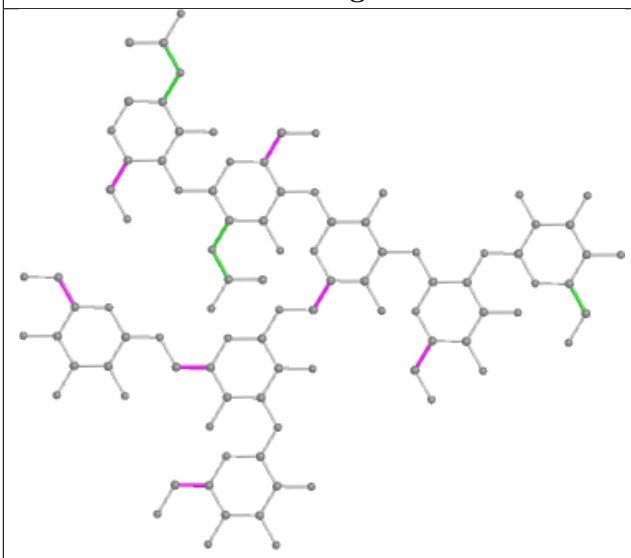
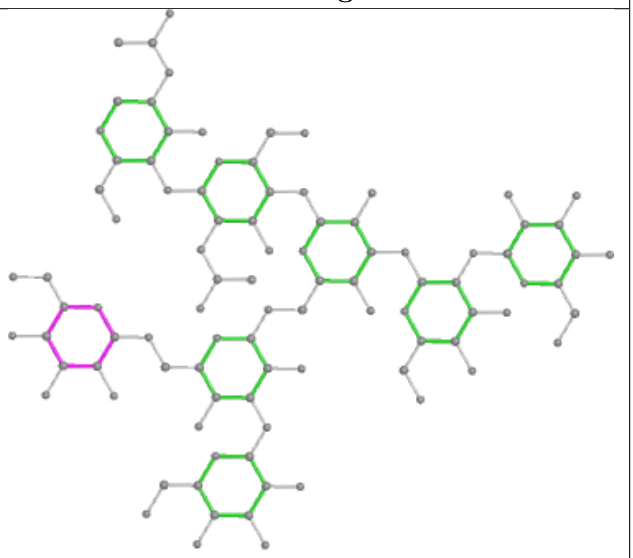
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain F

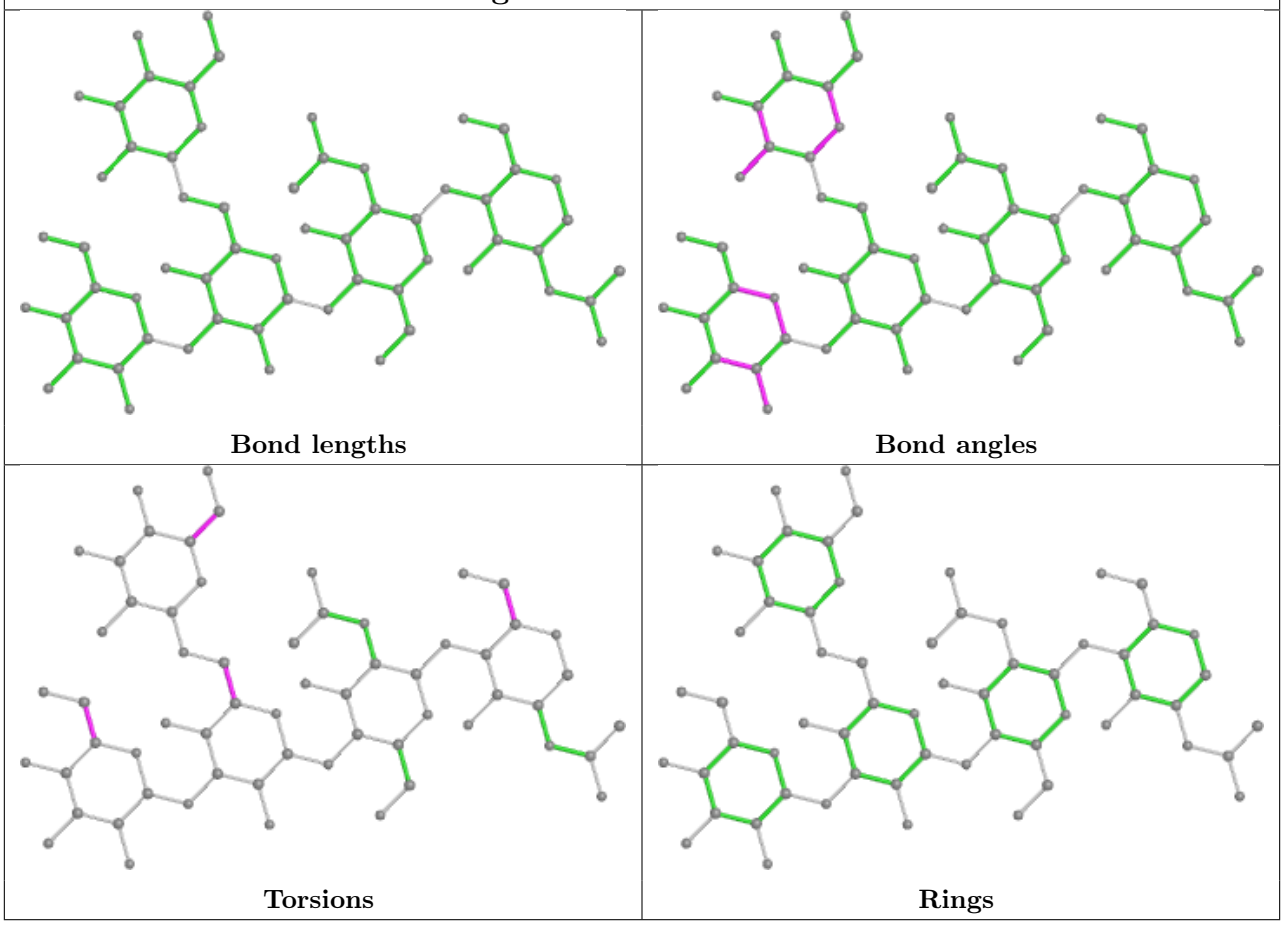


Oligosaccharide Chain H



Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M



5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
9	NAG	E	401	3	14,14,15	0.22	0	17,19,21	0.41	0
11	Y01	A	408	-	24,24,38	0.83	1 (4%)	37,39,57	1.71	9 (24%)
11	Y01	B	409	-	24,24,38	0.82	1 (4%)	37,39,57	1.70	9 (24%)
11	Y01	B	411	-	24,24,38	0.82	1 (4%)	37,39,57	1.69	9 (24%)
11	Y01	B	412	-	24,24,38	0.82	1 (4%)	37,39,57	1.69	9 (24%)
9	NAG	C	404	1	14,14,15	0.15	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ABU	C	405	-	6,6,6	0.85	0	6,6,6	1.17	1 (16%)
11	Y01	A	407	-	24,24,38	0.81	1 (4%)	37,39,57	1.71	8 (21%)
12	FYP	D	406	-	22,24,24	1.29	3 (13%)	26,35,35	1.20	3 (11%)
11	Y01	A	410	-	24,24,38	0.83	1 (4%)	37,39,57	1.70	9 (24%)
9	NAG	A	404	1	14,14,15	0.18	0	17,19,21	0.38	0
10	ABU	A	405	-	6,6,6	0.86	0	6,6,6	1.14	0
11	Y01	A	406	-	24,24,38	0.82	1 (4%)	37,39,57	1.71	9 (24%)
11	Y01	D	408	-	24,24,38	0.82	1 (4%)	37,39,57	1.71	9 (24%)
11	Y01	D	407	-	24,24,38	0.82	1 (4%)	37,39,57	1.70	9 (24%)
11	Y01	A	409	-	24,24,38	0.82	1 (4%)	37,39,57	1.73	9 (24%)
11	Y01	D	409	-	24,24,38	0.83	1 (4%)	37,39,57	1.71	9 (24%)
11	Y01	B	410	-	24,24,38	0.83	1 (4%)	37,39,57	1.70	9 (24%)

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	NAG	E	401	3	-	4/6/23/26	0/1/1/1
11	Y01	A	408	-	-	-	0/4/4/4
11	Y01	B	409	-	-	-	0/4/4/4
11	Y01	B	411	-	-	-	0/4/4/4
11	Y01	B	412	-	-	-	0/4/4/4
9	NAG	C	404	1	-	2/6/23/26	0/1/1/1
11	Y01	D	409	-	-	-	0/4/4/4
10	ABU	C	405	-	-	2/4/4/4	-
11	Y01	A	407	-	-	-	0/4/4/4
11	Y01	A	410	-	-	-	0/4/4/4
9	NAG	A	404	1	-	1/6/23/26	0/1/1/1
10	ABU	A	405	-	-	2/4/4/4	-
11	Y01	A	406	-	-	-	0/4/4/4
11	Y01	D	408	-	-	-	0/4/4/4
12	FYP	D	406	-	-	0/7/23/23	0/2/3/3
11	Y01	A	409	-	-	-	0/4/4/4
11	Y01	D	407	-	-	-	0/4/4/4
11	Y01	B	410	-	-	-	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	406	FYP	C08-C07	-2.97	1.47	1.51
12	D	406	FYP	C15-N16	-2.65	1.30	1.35
12	D	406	FYP	C10-N09	-2.43	1.33	1.35
11	B	410	Y01	CBH-CBF	-2.24	1.52	1.56
11	A	408	Y01	CBH-CBF	-2.24	1.52	1.56

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	409	Y01	CBI-CBG-CBD	-4.87	107.17	114.38
11	D	409	Y01	CBI-CBG-CBD	-4.80	107.27	114.38
11	A	406	Y01	CBI-CBG-CBD	-4.77	107.31	114.38
11	D	408	Y01	CBI-CBG-CBD	-4.75	107.34	114.38
11	A	408	Y01	CBI-CBG-CBD	-4.75	107.35	114.38

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	404	NAG	C4-C5-C6-O6
9	C	404	NAG	O5-C5-C6-O6
9	E	401	NAG	O5-C5-C6-O6
9	E	401	NAG	C8-C7-N2-C2
9	E	401	NAG	O7-C7-N2-C2

There are no ring outliers.

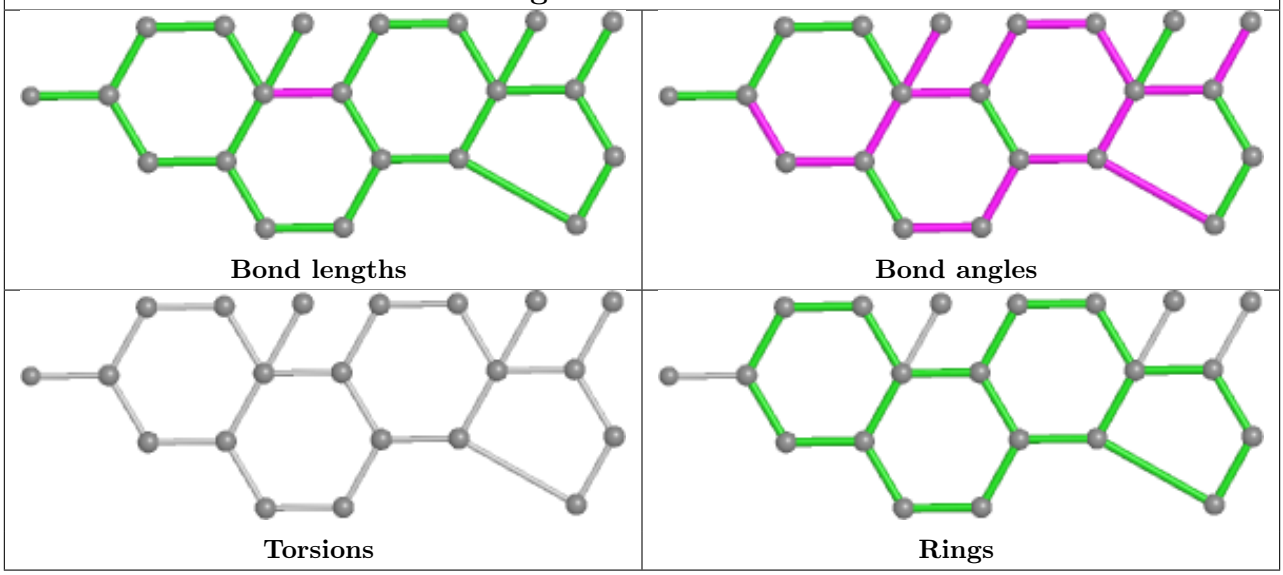
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	409	Y01	1	0
11	B	411	Y01	1	0
10	C	405	ABU	1	0
11	A	407	Y01	1	0
11	A	406	Y01	2	0
11	D	407	Y01	1	0
11	A	409	Y01	2	0

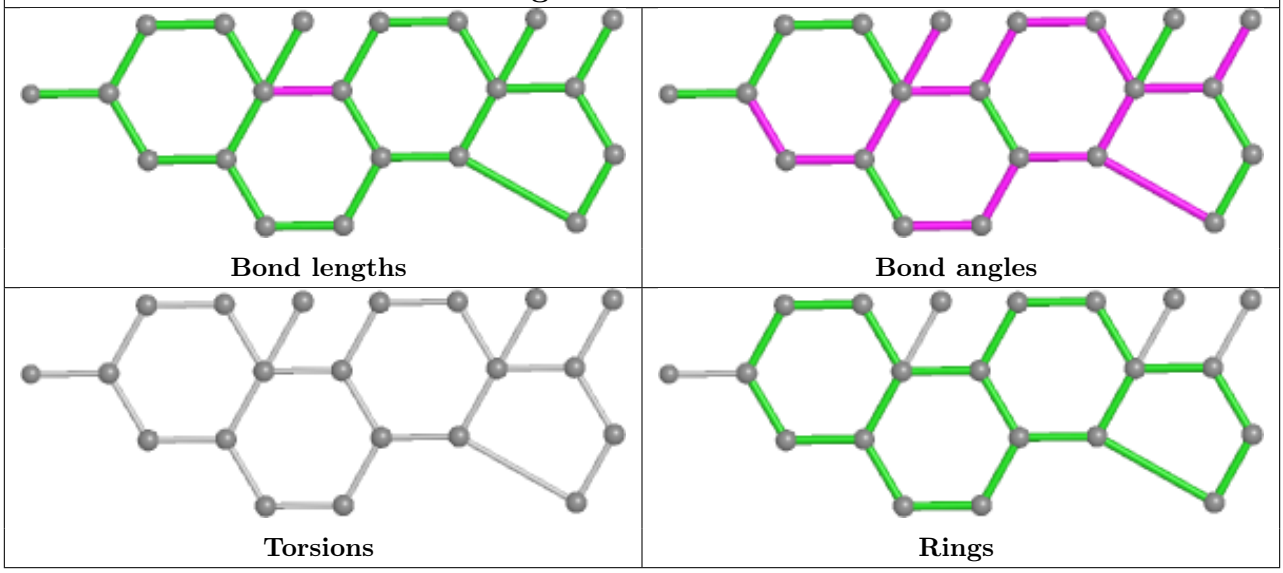
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

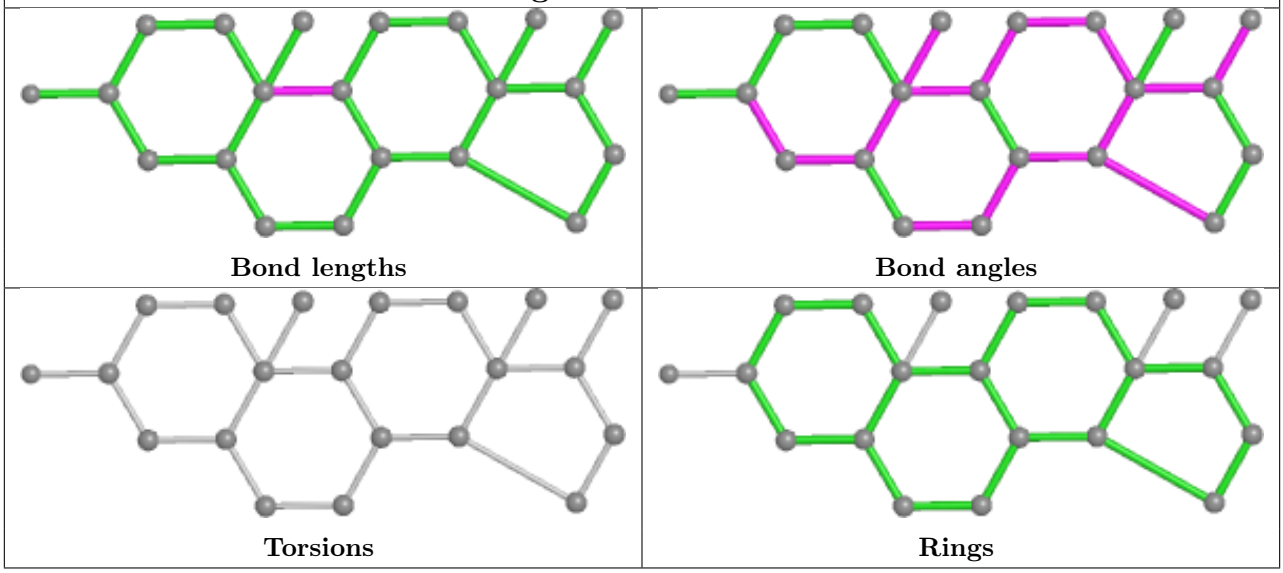
Ligand Y01 A 408



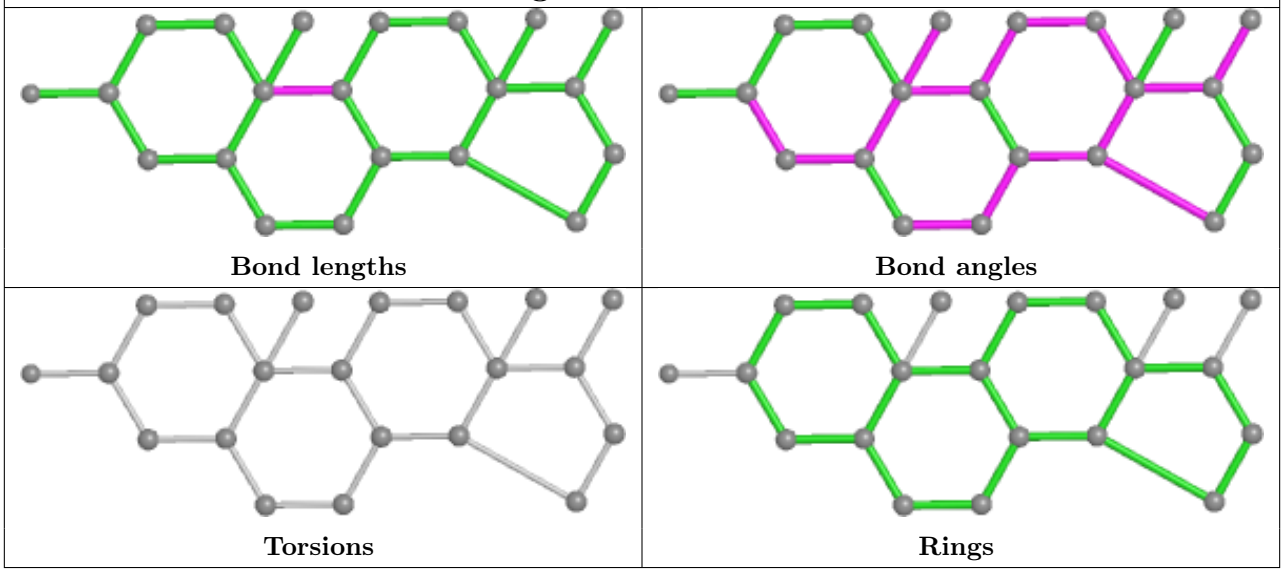
Ligand Y01 B 409

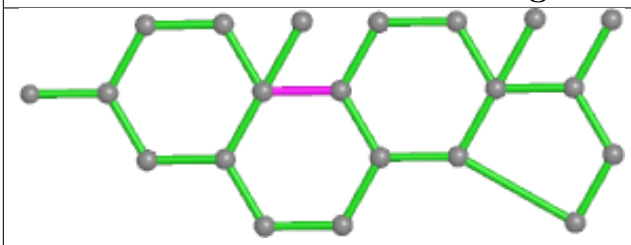
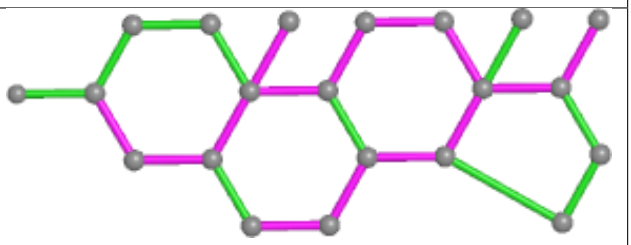
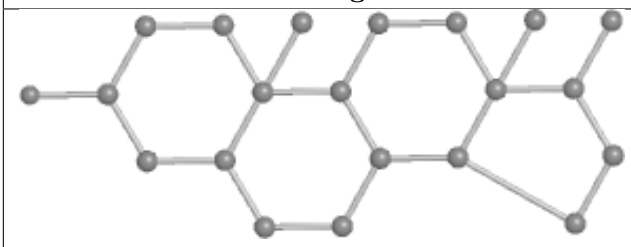
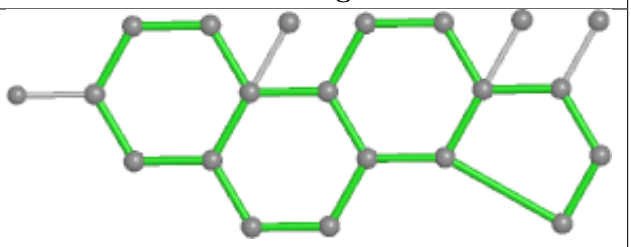


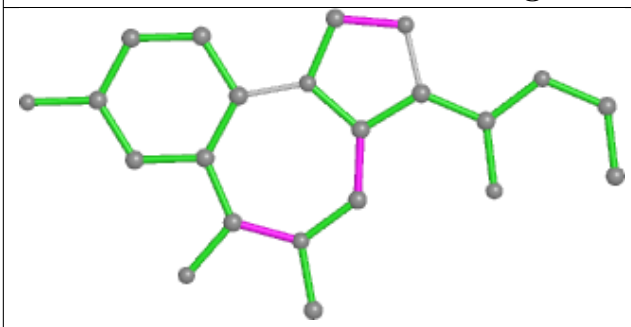
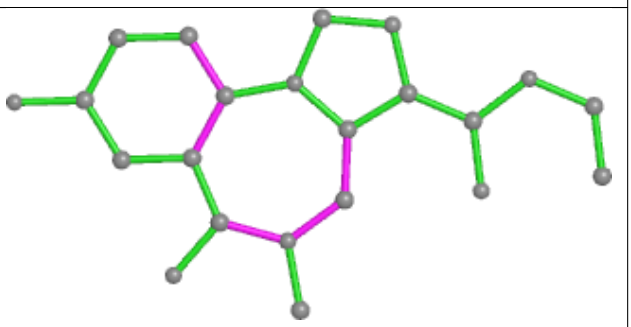
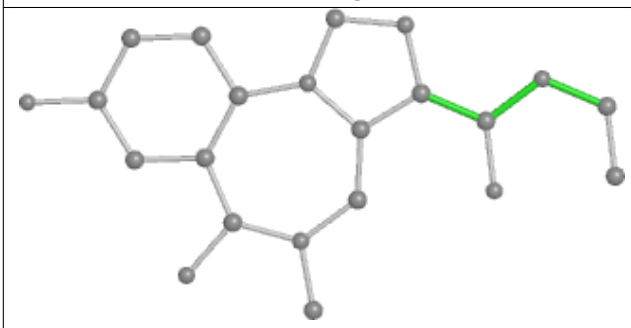
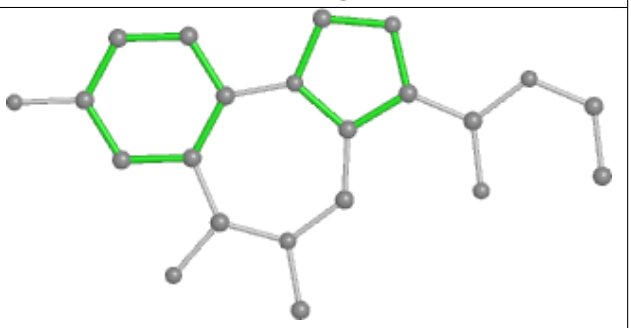
Ligand Y01 B 411



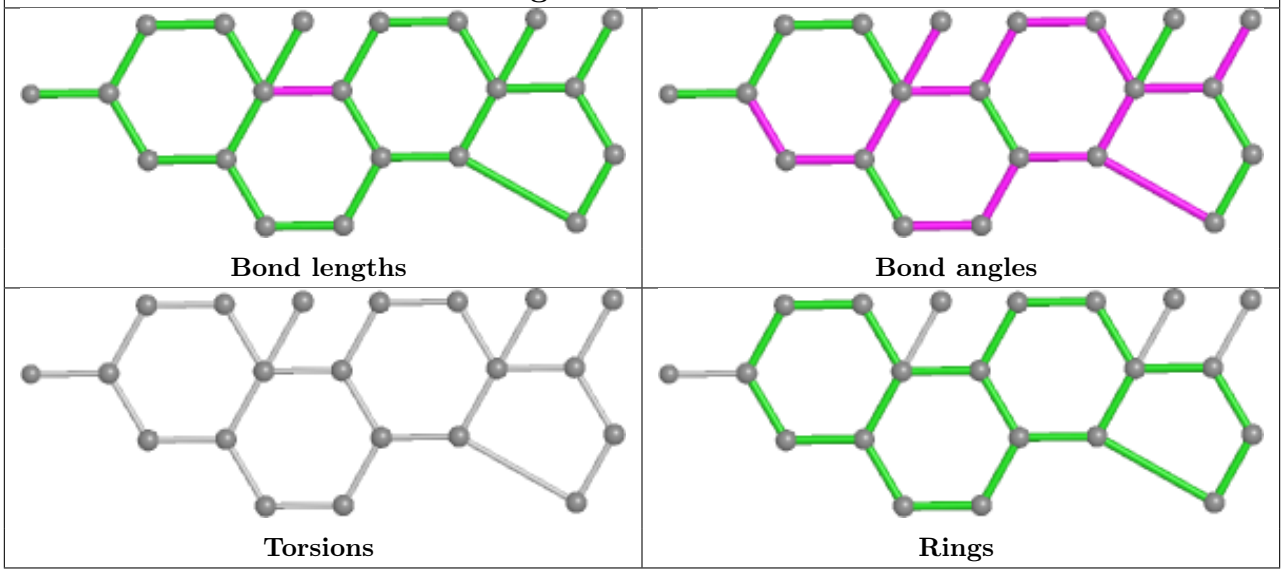
Ligand Y01 B 412



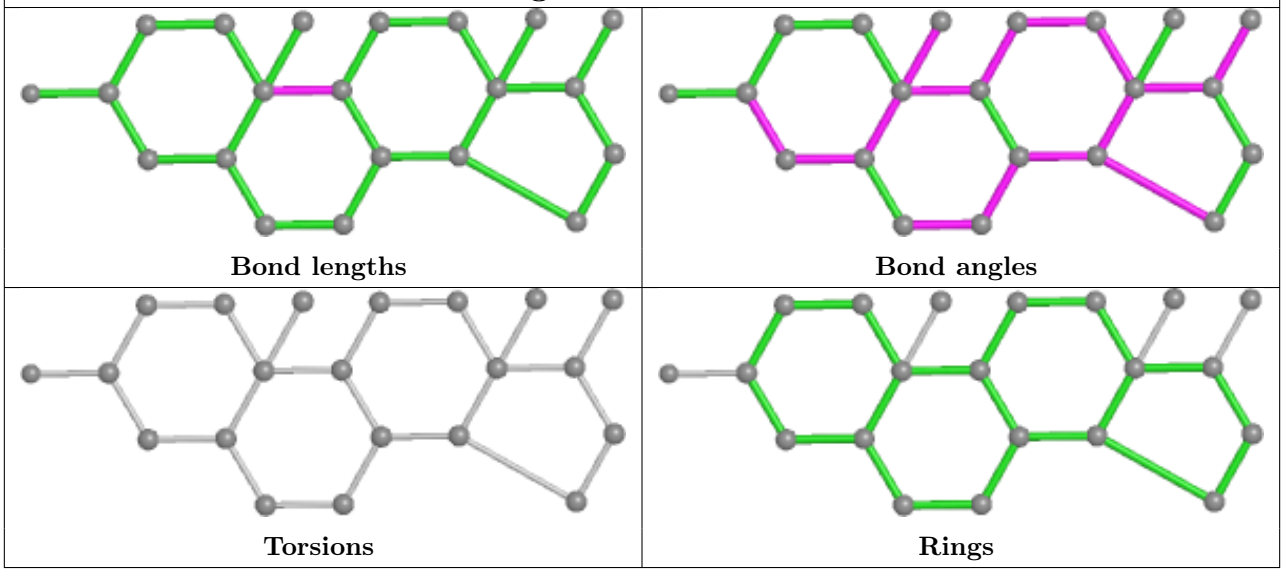
Ligand Y01 A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FYP D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

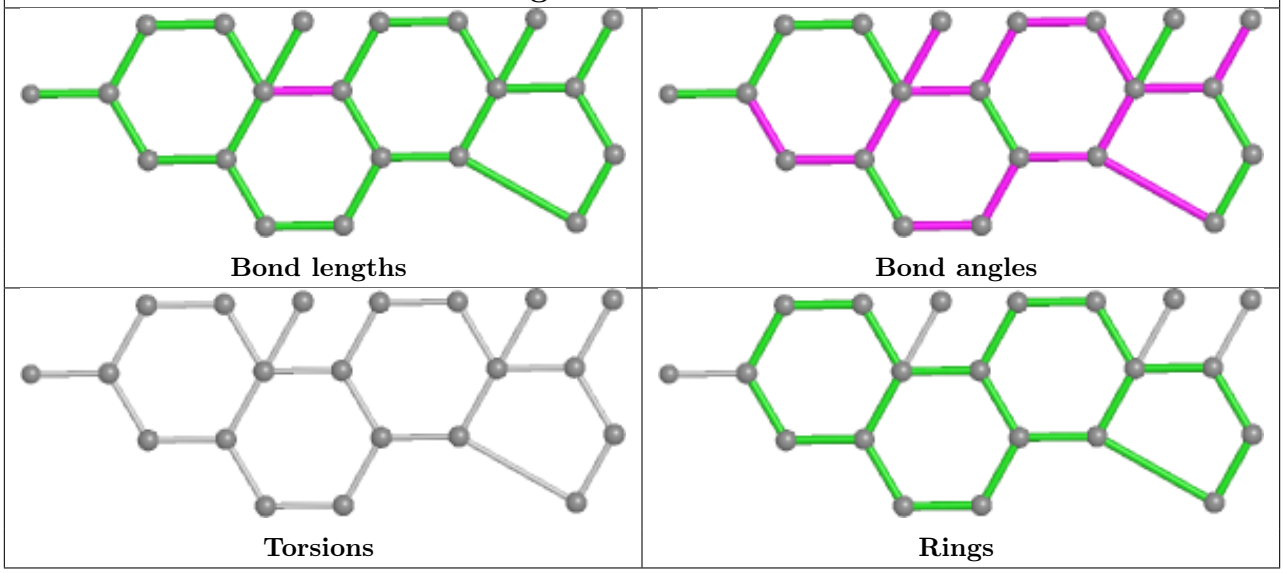
Ligand Y01 A 410



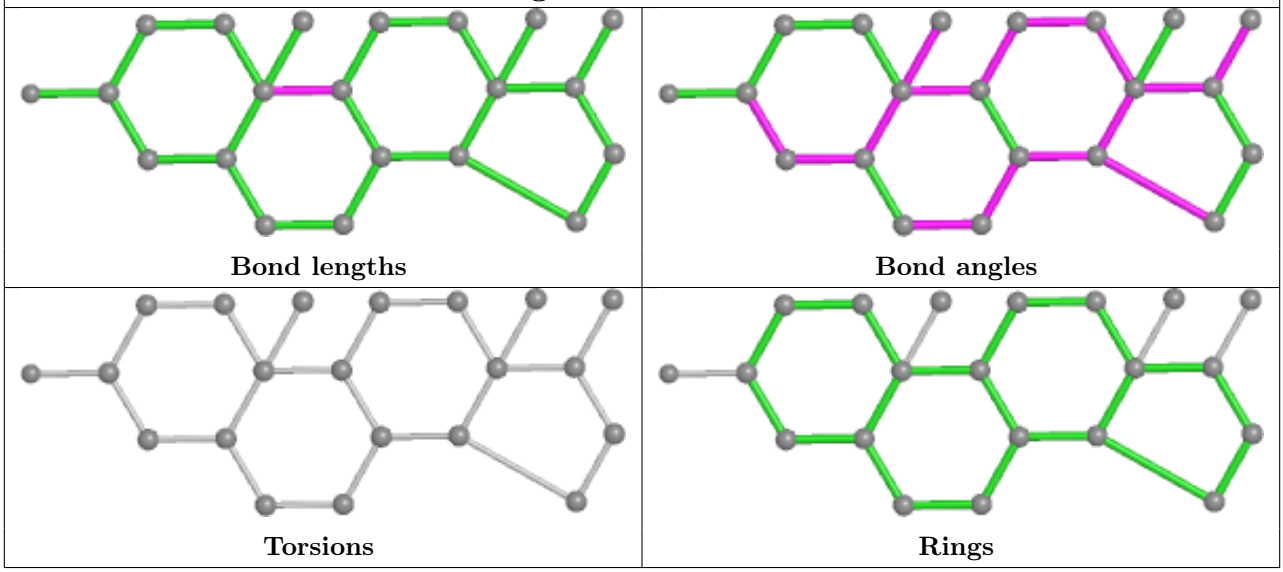
Ligand Y01 A 406



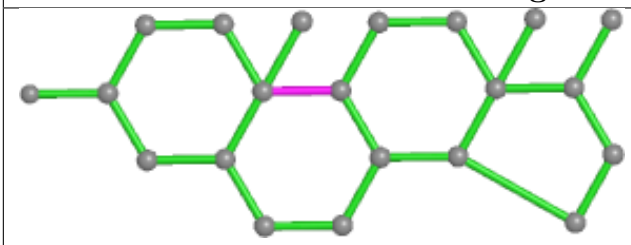
Ligand Y01 D 408



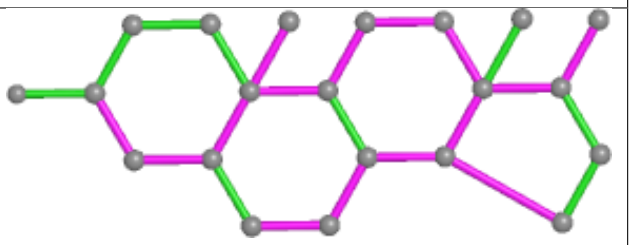
Ligand Y01 D 407



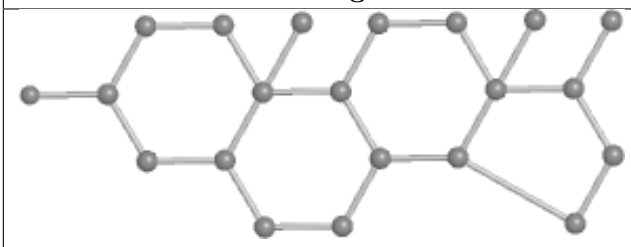
Ligand Y01 A 409



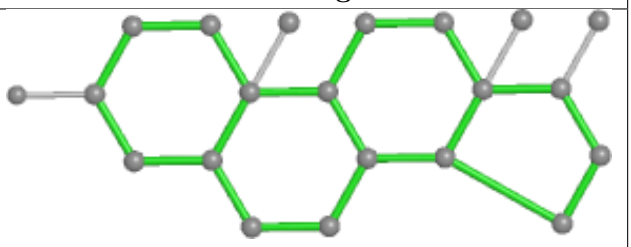
Bond lengths



Bond angles

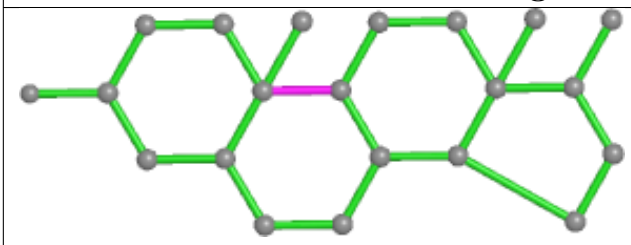


Torsions

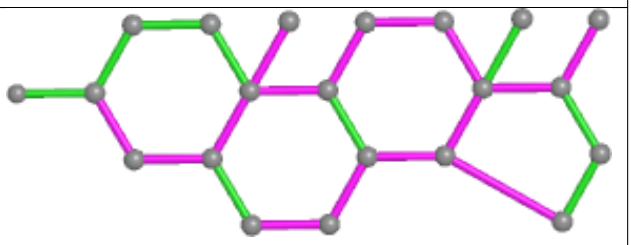


Rings

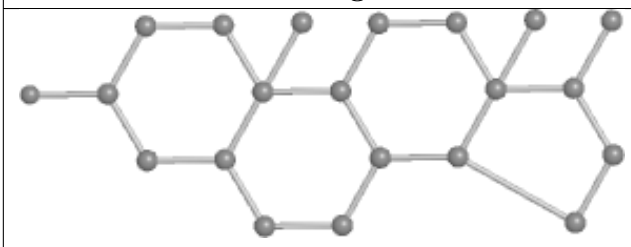
Ligand Y01 D 409



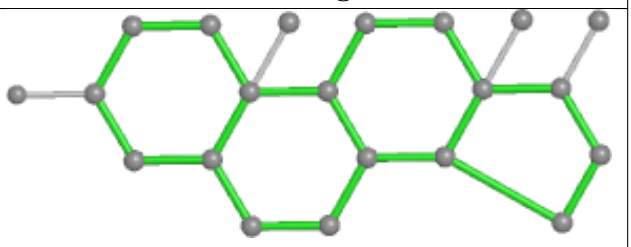
Bond lengths



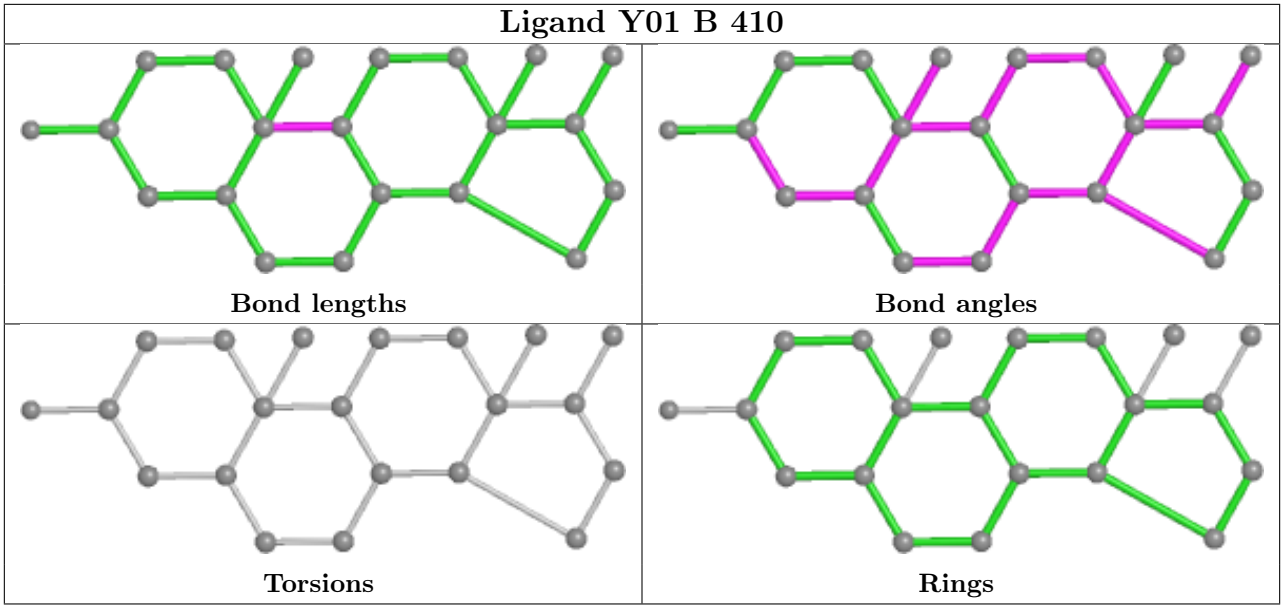
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	318:UNK	C	327:UNK	N	16.64
1	E	287:LEU	C	297:UNK	N	10.85

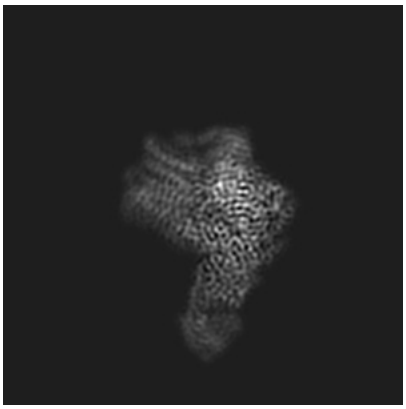
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7816. These allow visual inspection of the internal detail of the map and identification of artifacts.

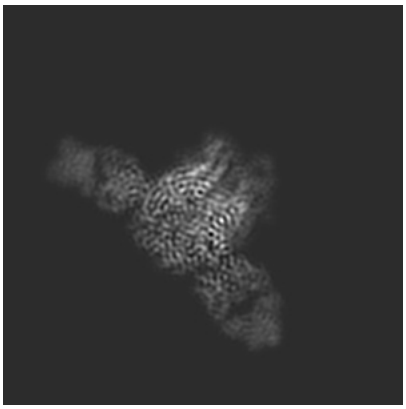
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

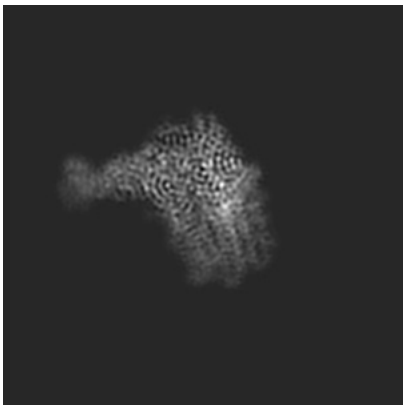
6.1.1 Primary map



X

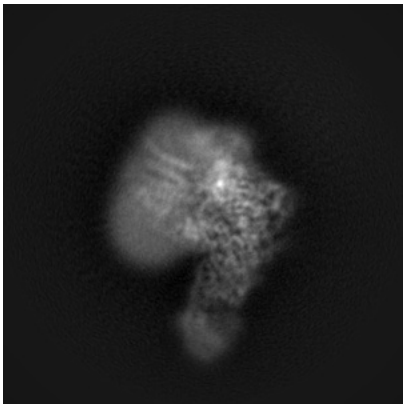


Y

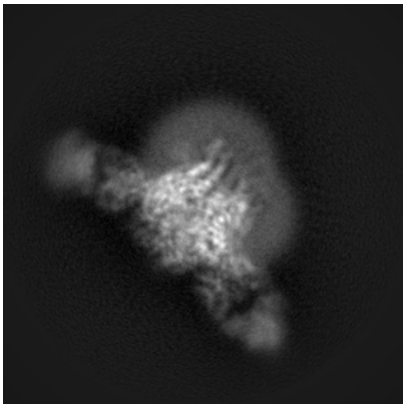


Z

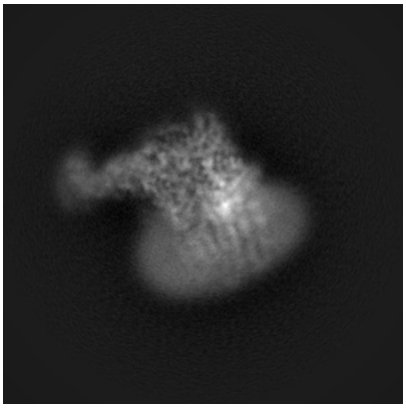
6.1.2 Raw map



X



Y



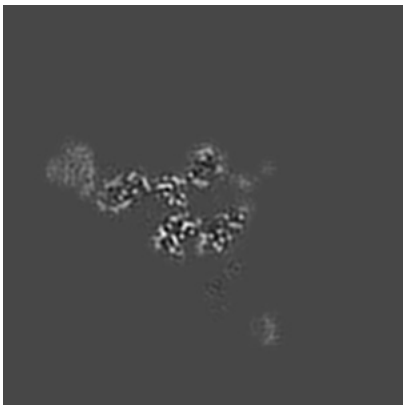
Z

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

6.2 Central slices (i)

6.2.1 Primary map

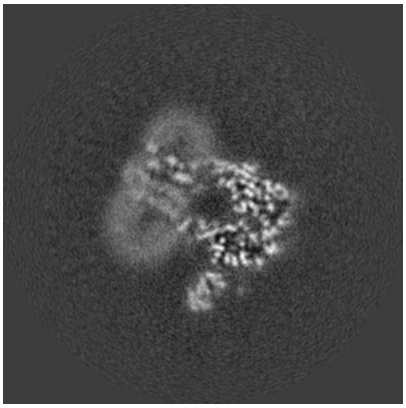
X Index: 130



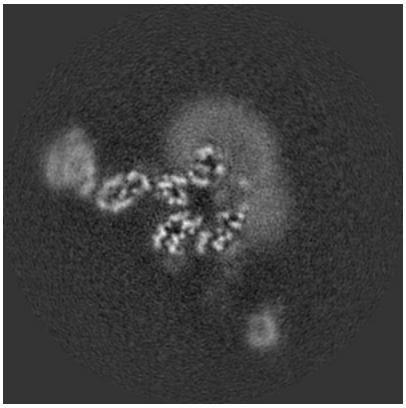
Y Index: 130

Z Index: 130

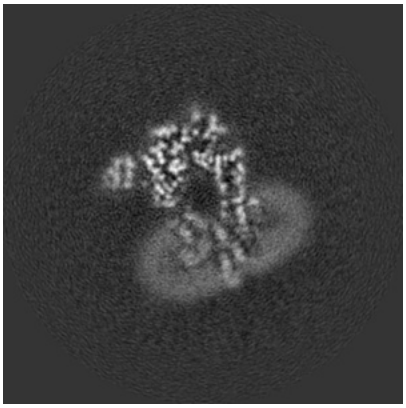
6.2.2 Raw map



X Index: 130



Y Index: 130



Z Index: 130

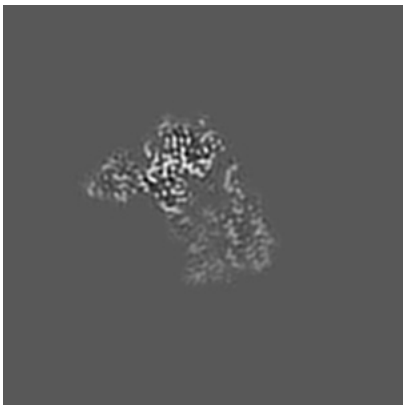
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

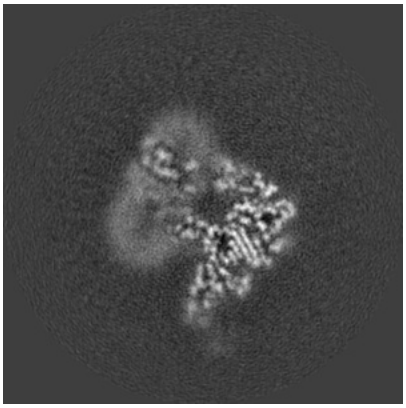
X Index: 134

Y Index: 146

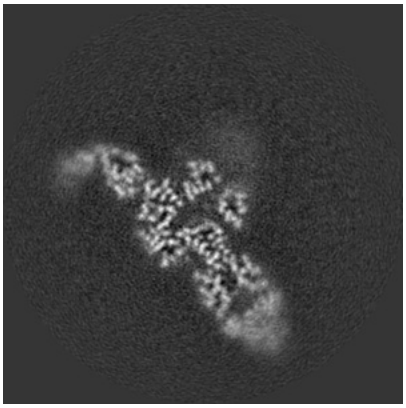


Z Index: 138

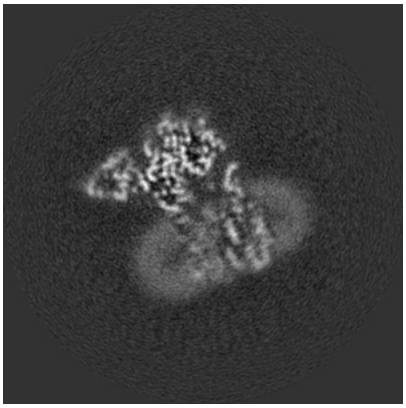
6.3.2 Raw map



X Index: 135



Y Index: 147

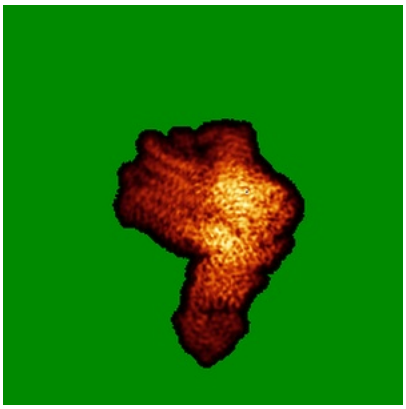


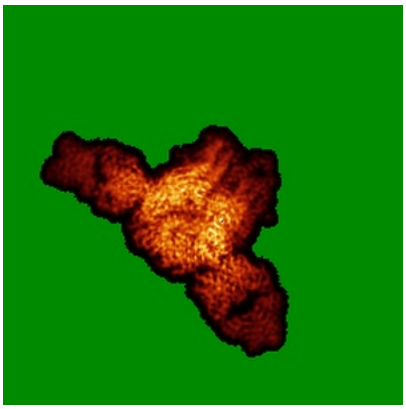
Z Index: 138

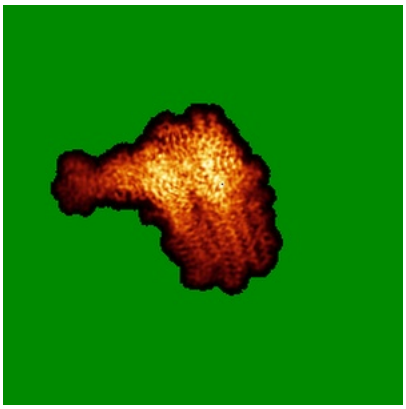
The images above show the largest variance slices of the map in three orthogonal directions.

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

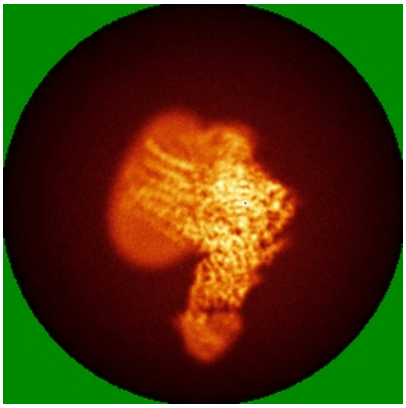
6.4.1 Primary map

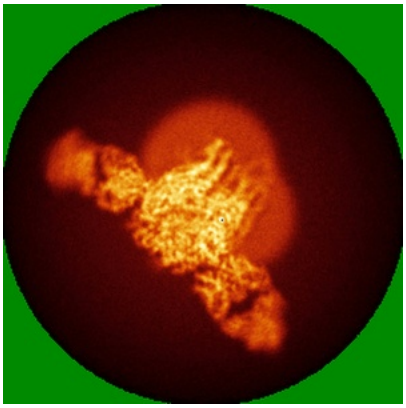

X

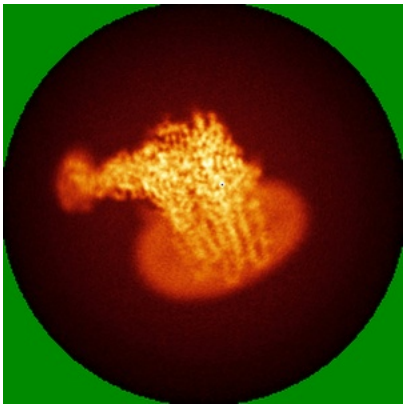

Y


Z

6.4.2 Raw map


X

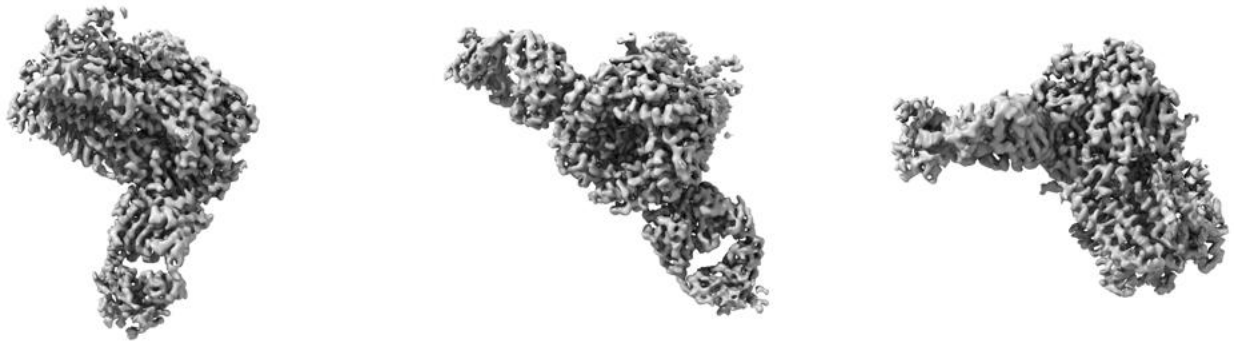

Y


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)

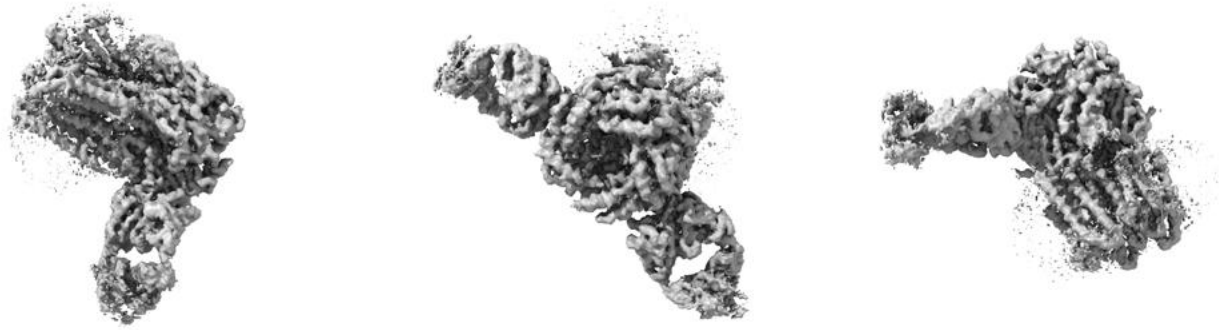
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. 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.

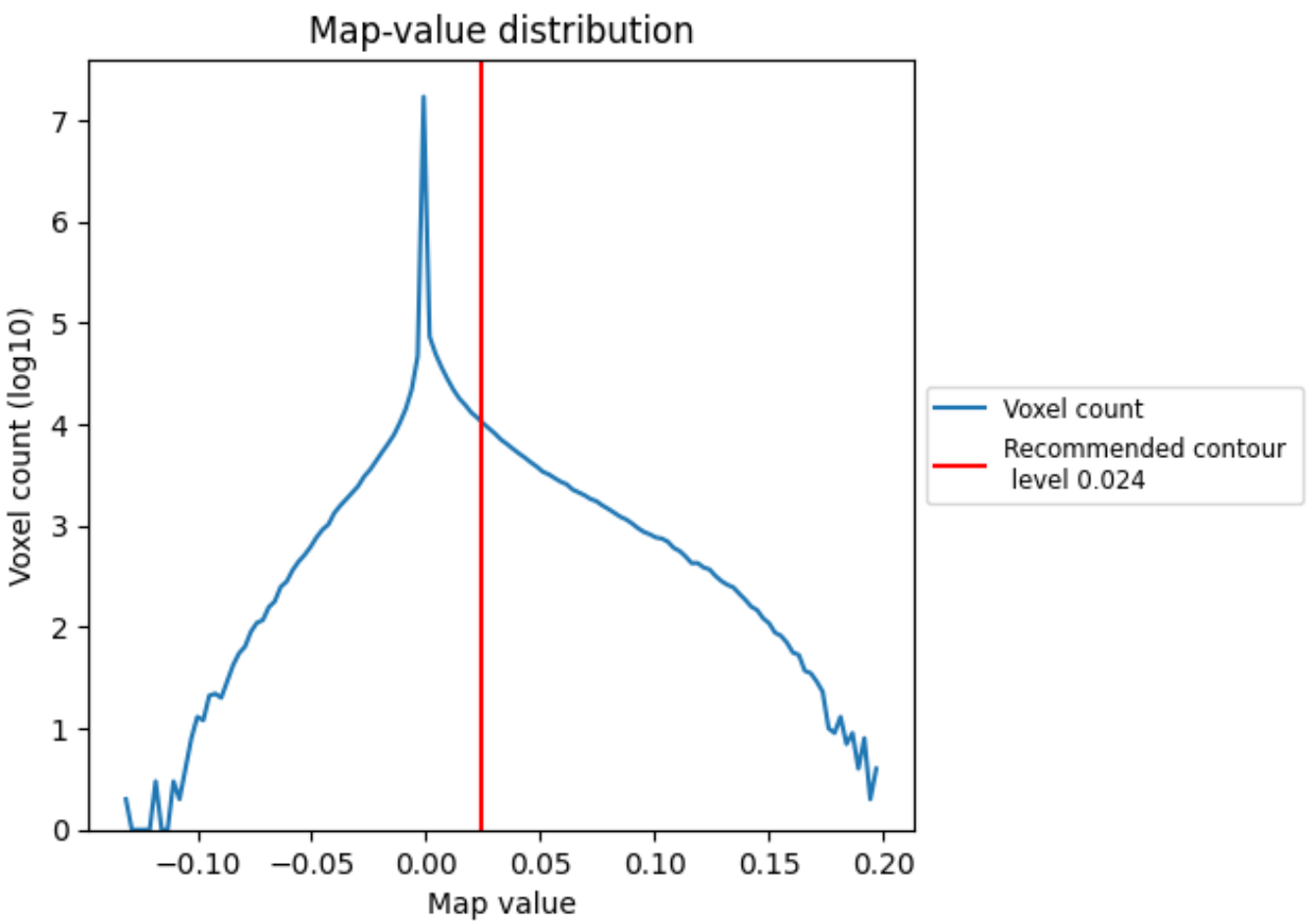
6.6 Mask visualisation (i)

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

7 Map analysis (i)

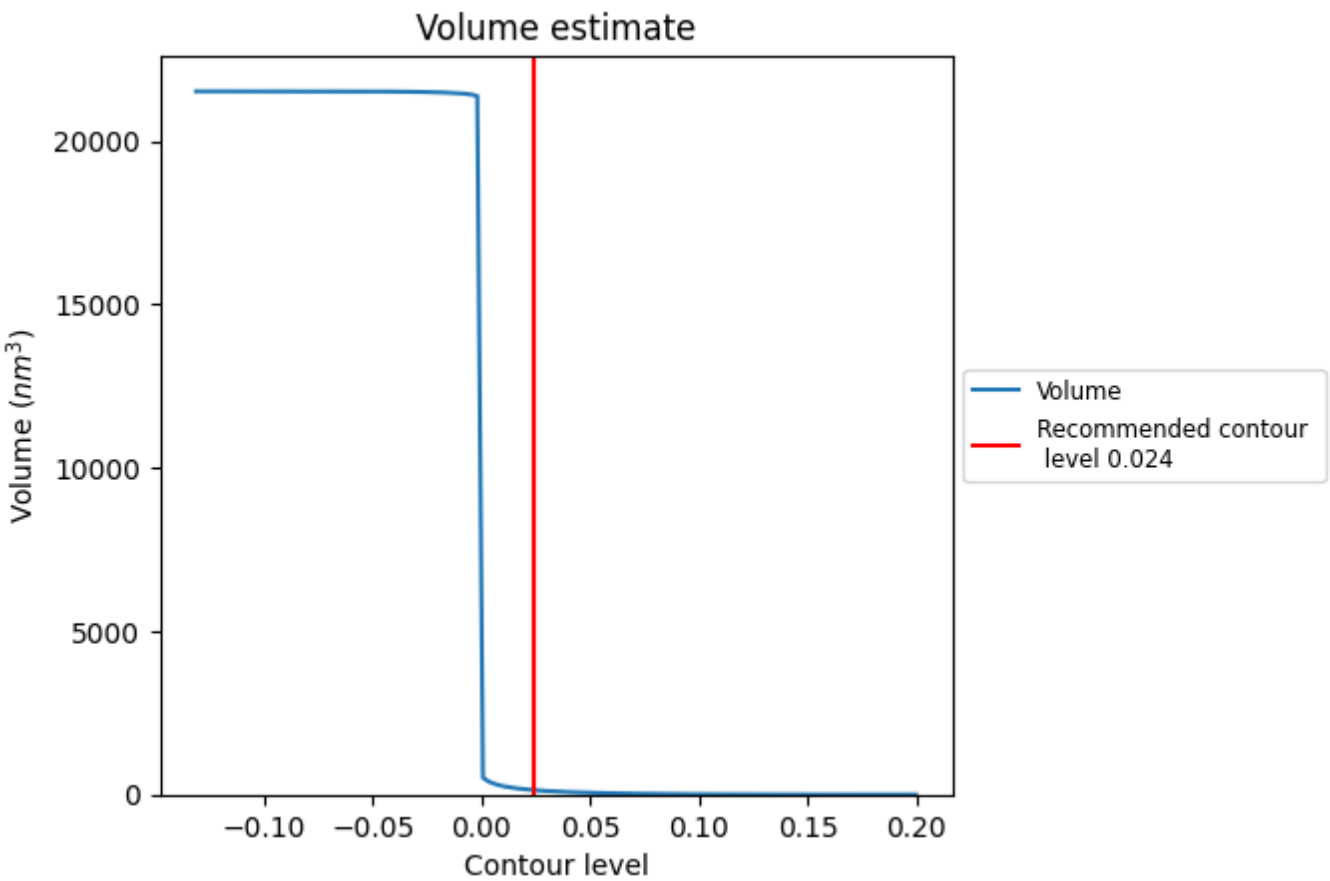
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

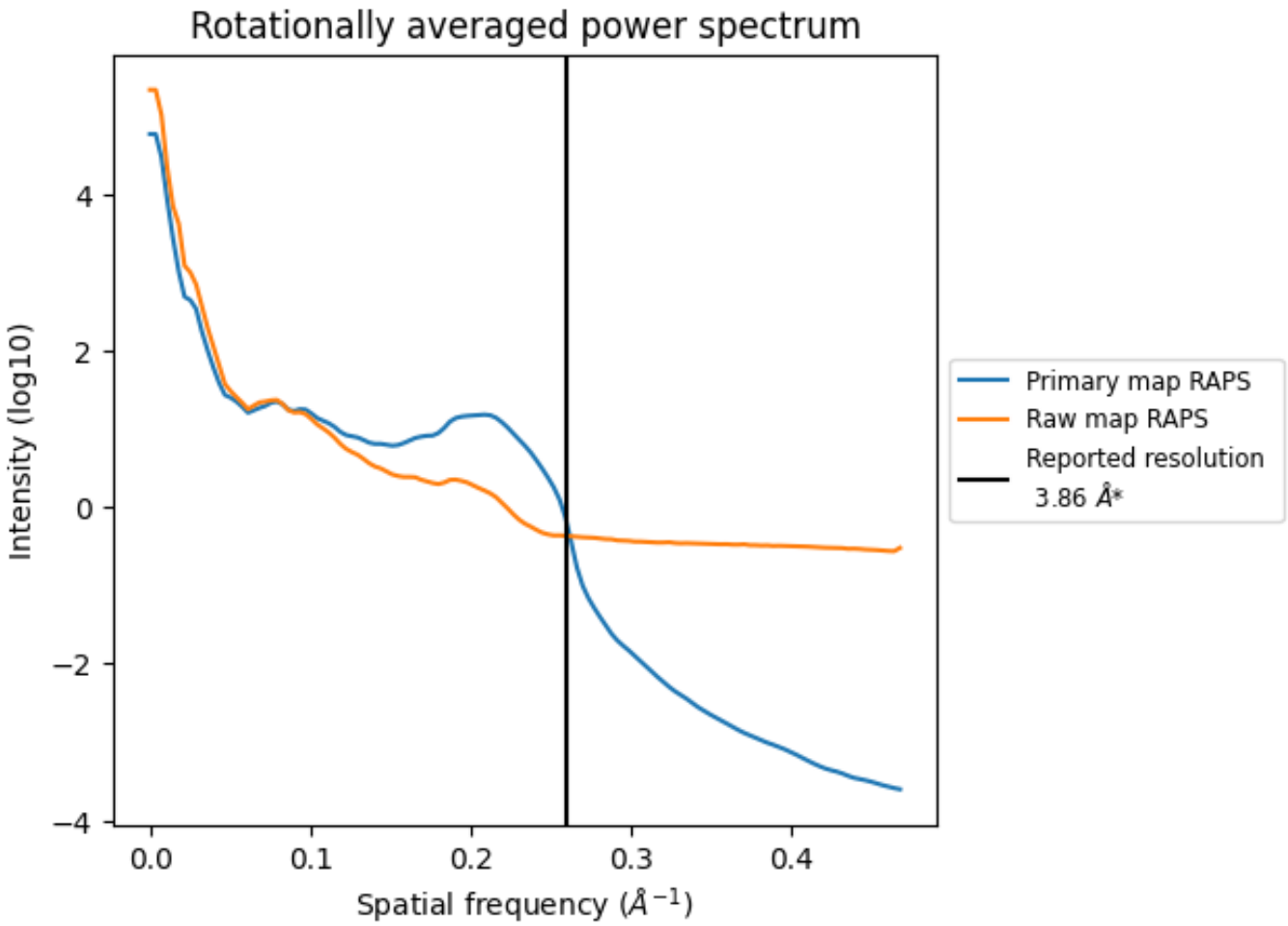
7.2 Volume estimate (i)



The volume at the recommended contour level is 138 nm^3; this corresponds to an approximate mass of 125 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)

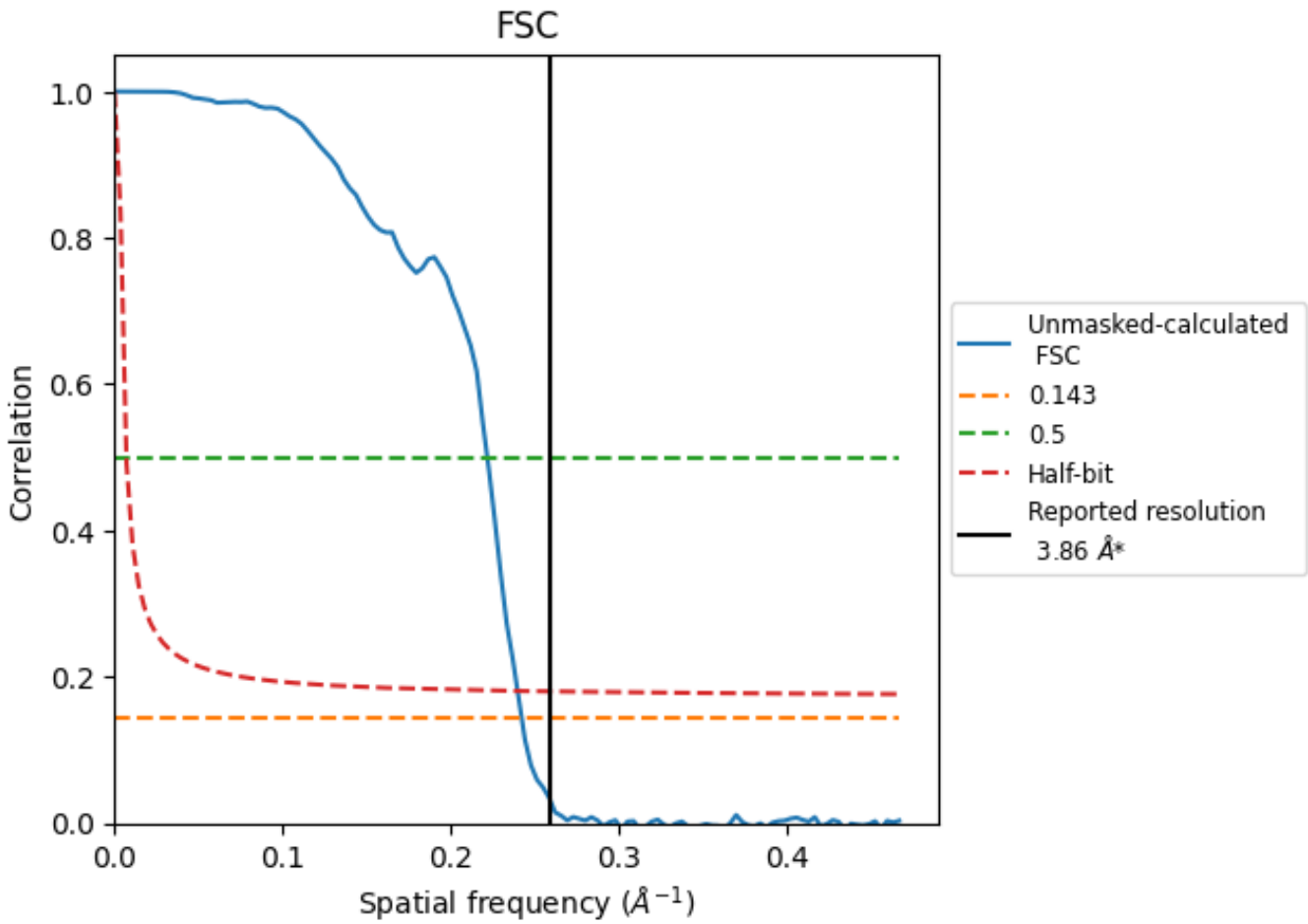


*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

8.2 Resolution estimates (i)

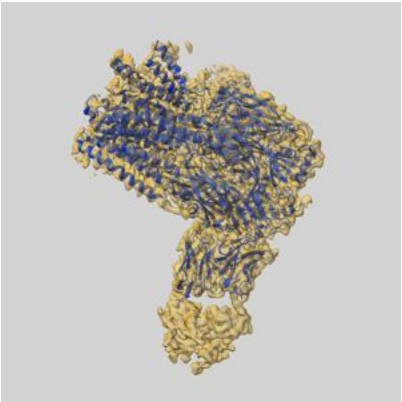
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.12	4.50	4.17

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

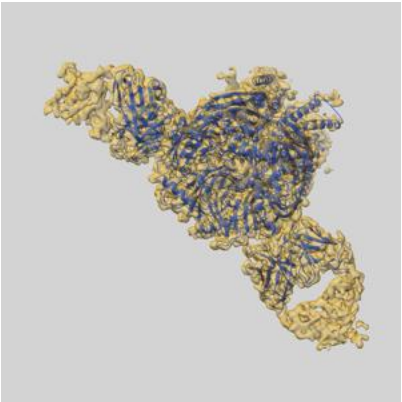
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7816 and PDB model 6D6T. Per-residue inclusion information can be found in section 3 on page 10.

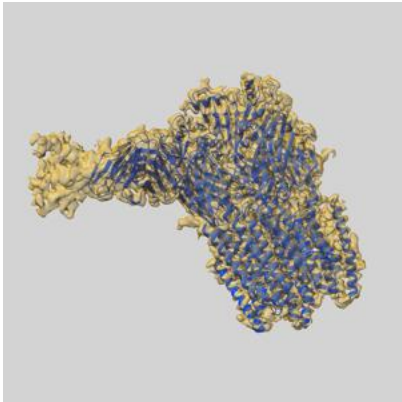
9.1 Map-model overlay (i)



X



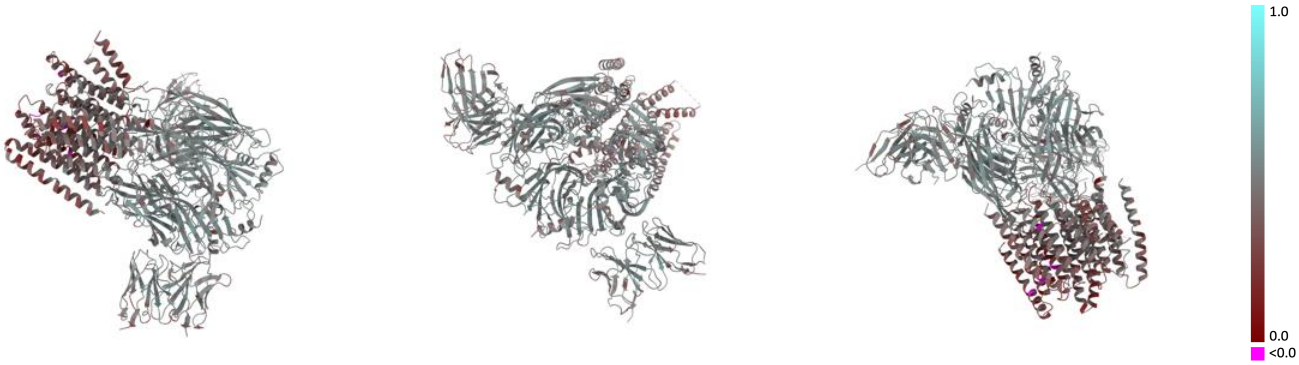
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 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

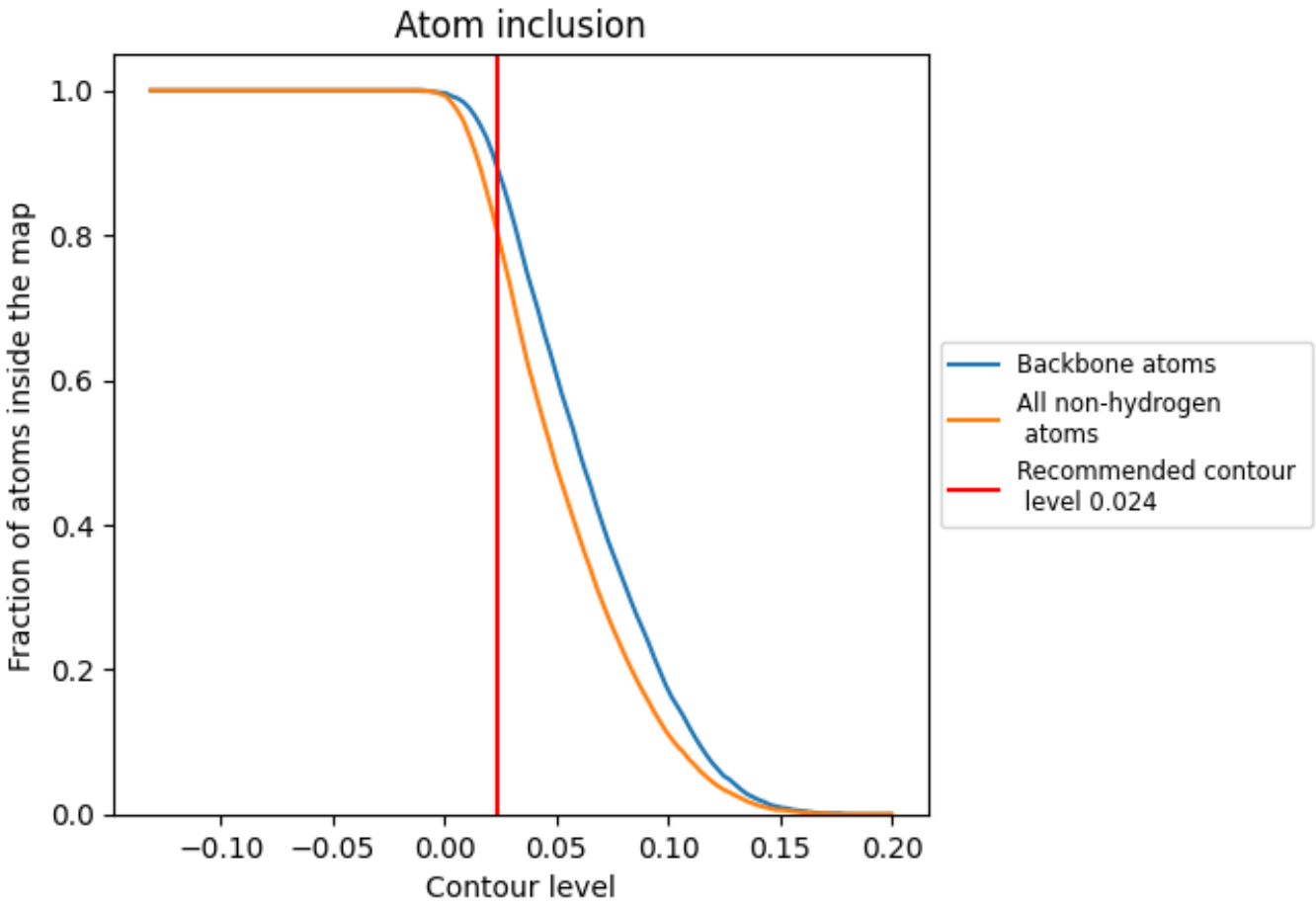
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.4600
A	0.8170	0.4700
B	0.7960	0.4610
C	0.6980	0.4100
D	0.8220	0.4660
E	0.7910	0.4680
F	0.8720	0.4860
G	0.9040	0.4850
H	0.7950	0.4570
I	0.8390	0.4770
J	0.8440	0.4790
K	0.8450	0.4800
L	0.8620	0.4820
M	0.7870	0.5150