



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:38 PM UTC

PDB ID : 9CRS / pdb_00009crs
EMDB ID : EMD-45878
Title : Native human GABAA receptor of beta2-alpha1-beta2-alpha1-gamma2 assembly
Authors : Zhou, J.; Hibbs, R.E.; Noviello, C.M.
Deposited on : 2024-07-22
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

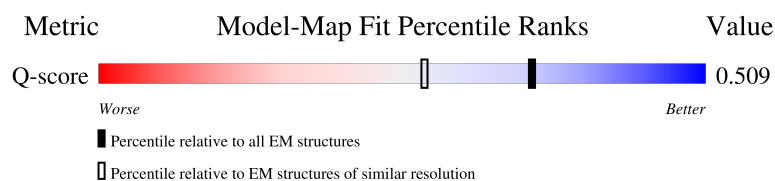
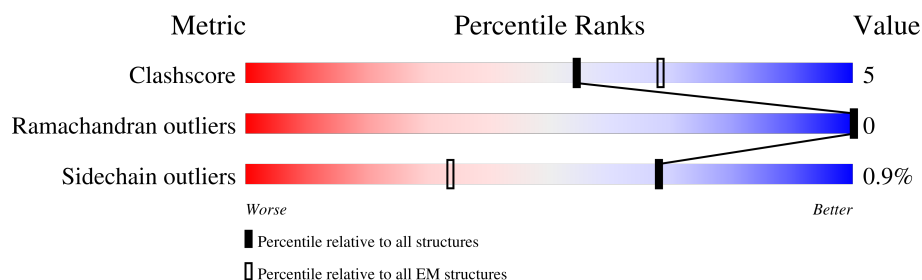
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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 $\leq 5\%$. 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	488	
1	C	488	
2	B	429	
2	D	429	

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Mol	Chain	Length	Quality of chain
3	E	436	
4	I	213	
4	L	213	
5	J	454	
5	K	454	
6	F	3	
6	M	3	
6	O	3	
7	G	2	
7	N	2	
8	H	8	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ABU	A	501	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17623 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	331	Total	C	N	O	S	0	0
			2716	1781	437	482	16		
1	C	332	Total	C	N	O	S	0	0
			2722	1784	438	484	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	346	Total	C	N	O	S	0	0
			2803	1812	472	503	16		
2	D	345	Total	C	N	O	S	0	0
			2794	1806	470	502	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	324	Total	C	N	O	S	0	0
			2661	1737	434	475	15		

- Molecule 4 is a protein called Kappa Fab_1F4 Light Chain.

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

- Molecule 5 is a protein called IgG2b Fab_1F4 Heavy Chain.

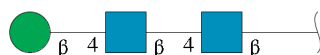
Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	116	Total	C	N	O	S	0	0
			907	574	151	178	4		

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

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



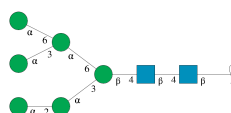
Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	3	Total	C	N	O		0	0
			39	22	2	15			
6	M	3	Total	C	N	O		0	0
			39	22	2	15			
6	O	3	Total	C	N	O		0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



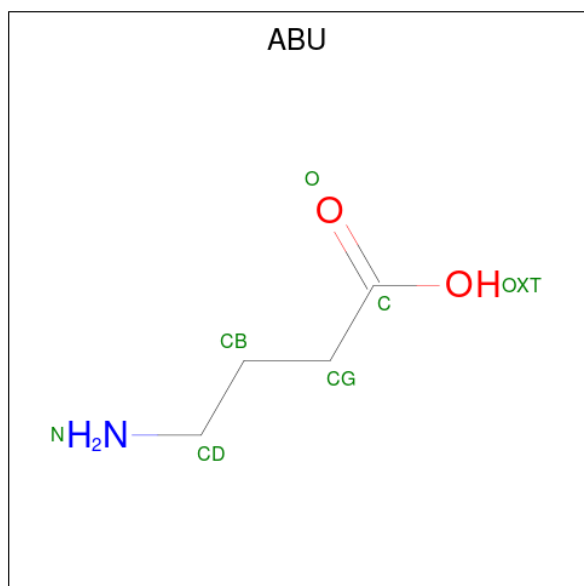
Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	2	Total	C	N	O		0	0
			28	16	2	10			
7	N	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 8 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.



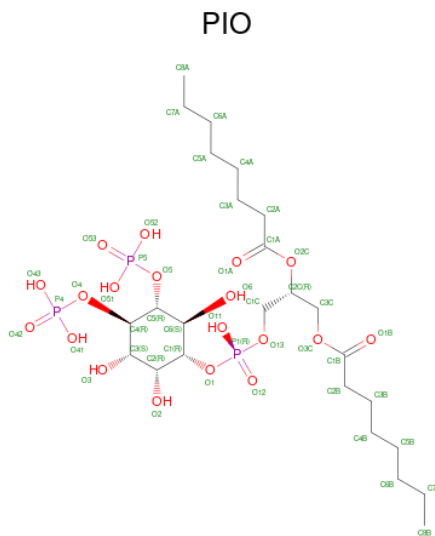
Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



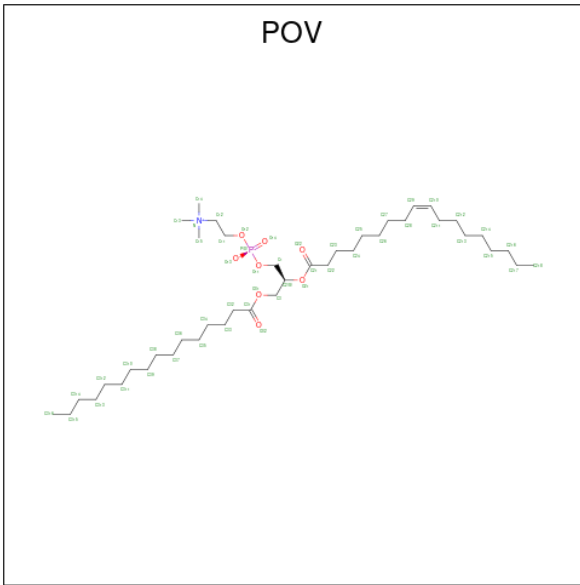
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			7	4	1	2	
9	C	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 10 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: $C_{25}H_{49}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethyl ammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total 52	C 42	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

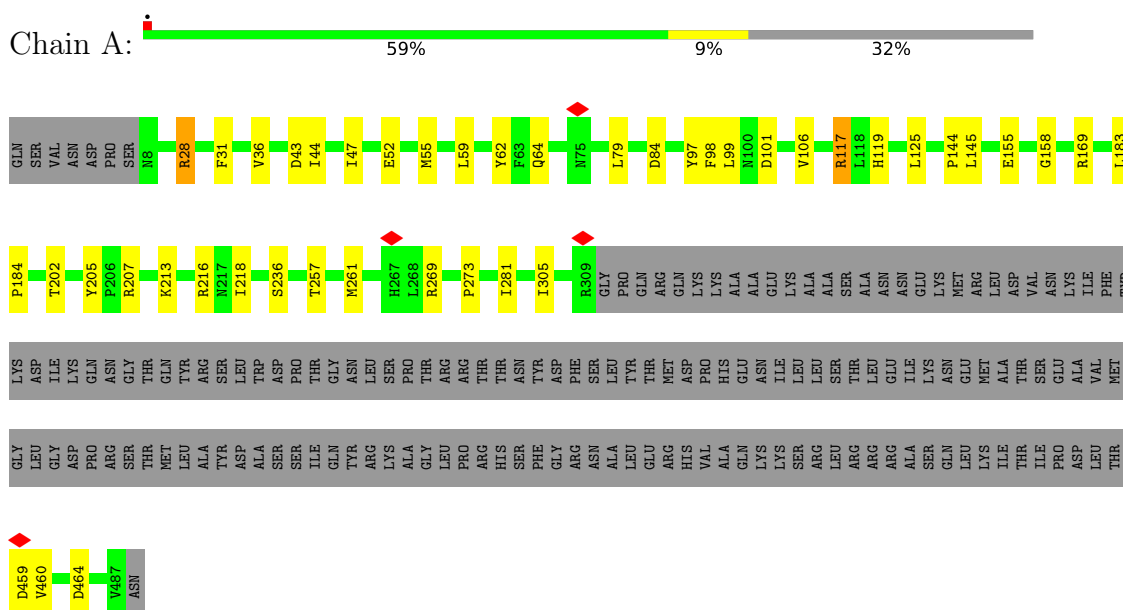


Mol	Chain	Residues	Atoms					AltConf
12	E	1	Total	C	N	O		0
			14	8	1	5		

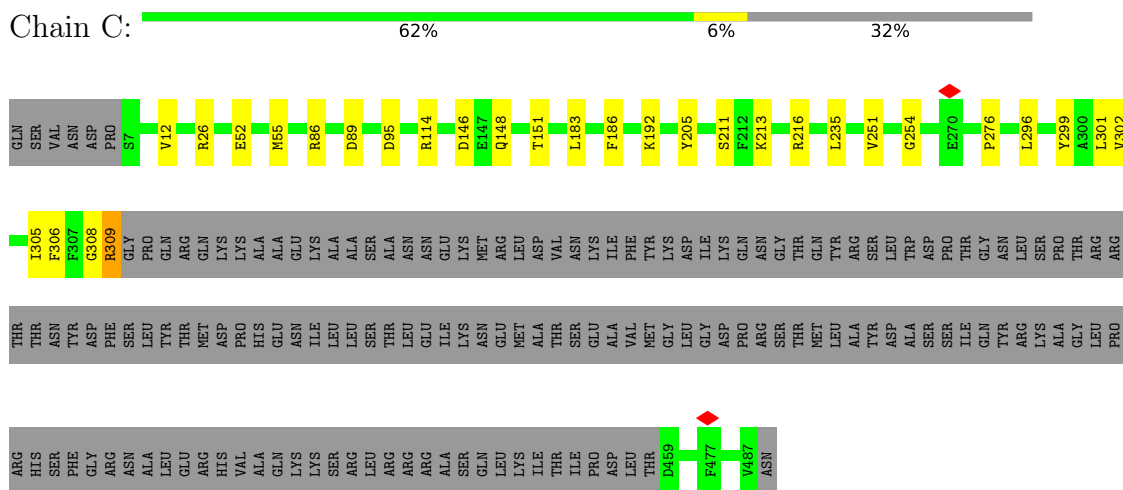
3 Residue-property plots [i](#)

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.

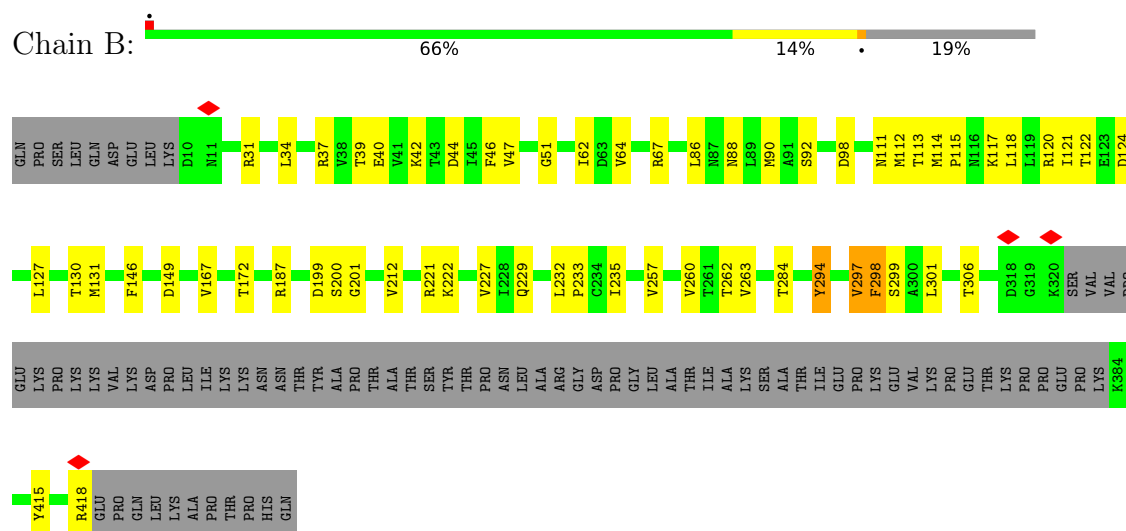
- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2



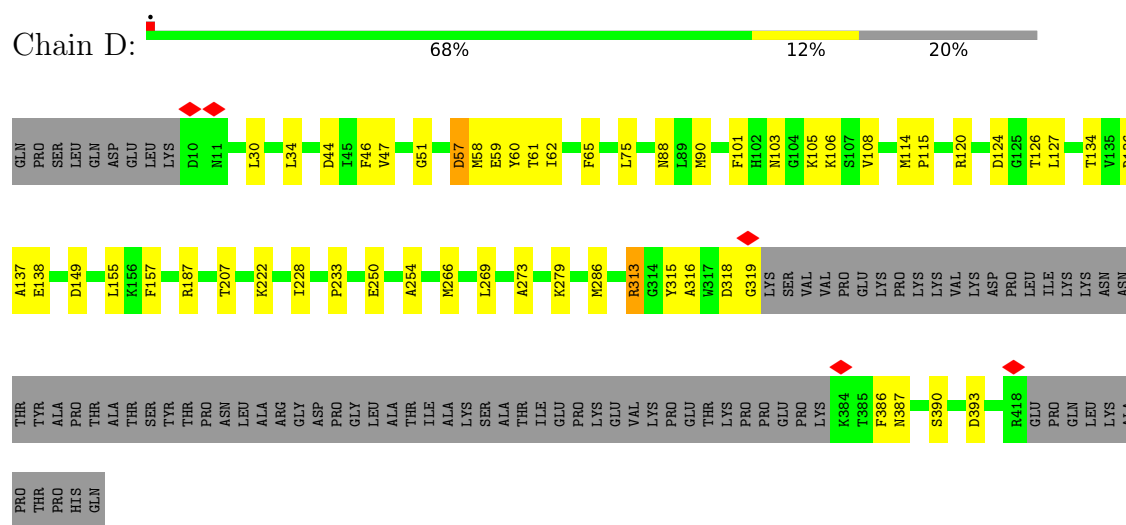
- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-2



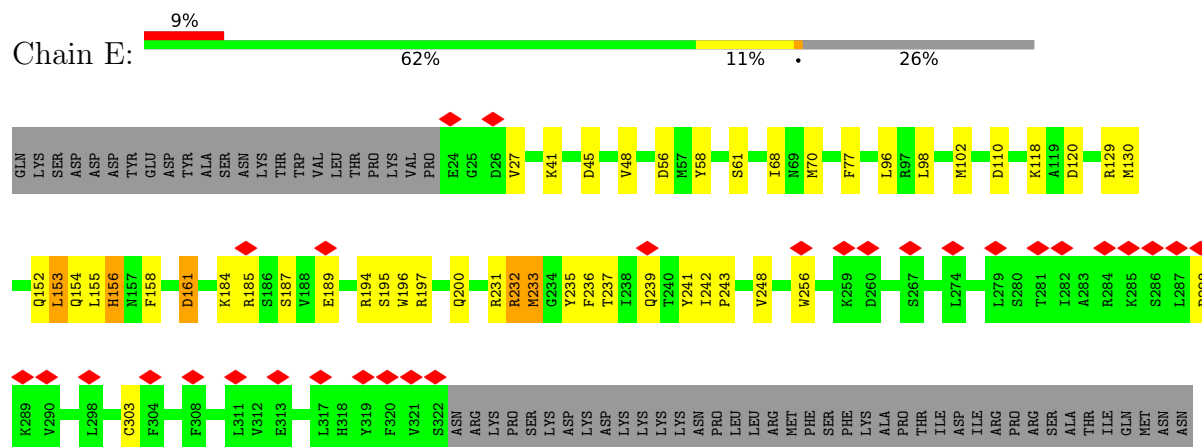
- Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

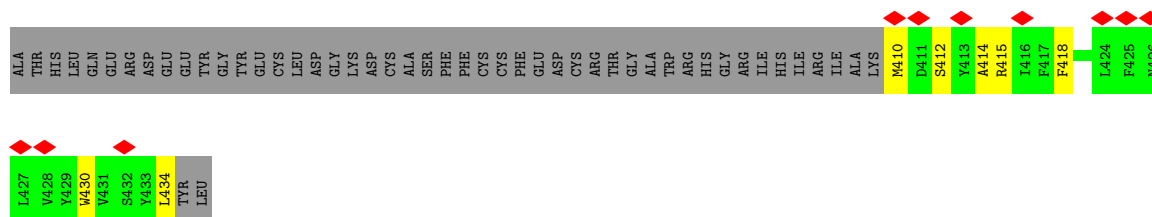


- Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-1

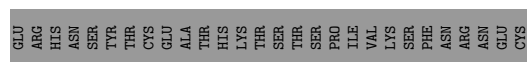
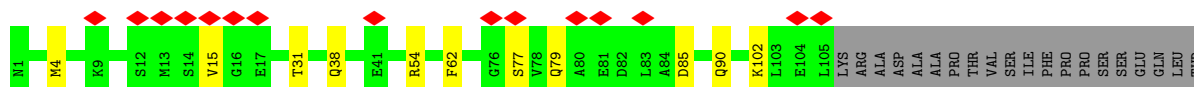
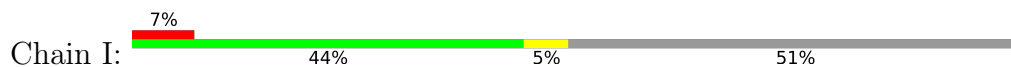


- Molecule 3: Gamma-aminobutyric acid receptor subunit gamma-2

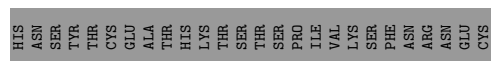
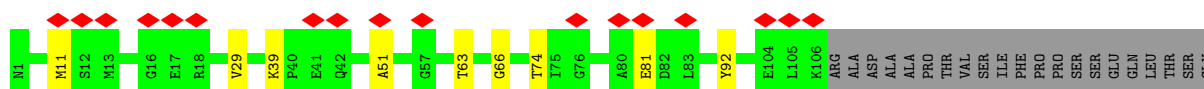




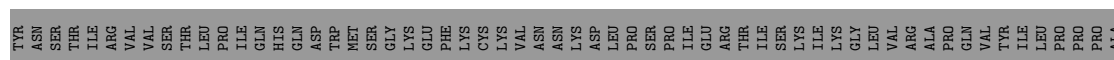
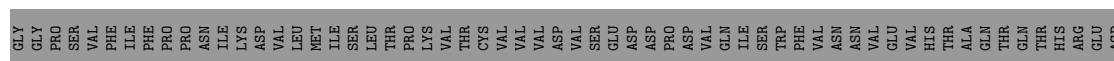
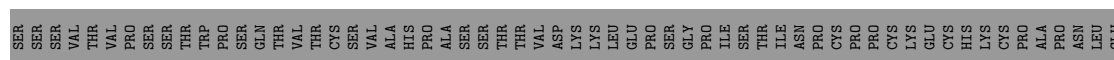
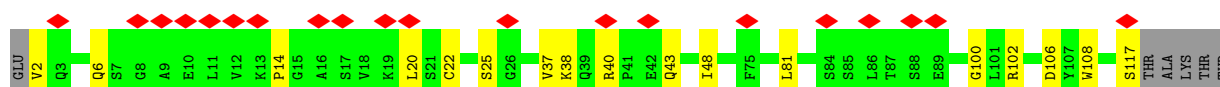
• Molecule 4: Kappa Fab_1F4 Light Chain



• Molecule 4: Kappa Fab_1F4 Light Chain

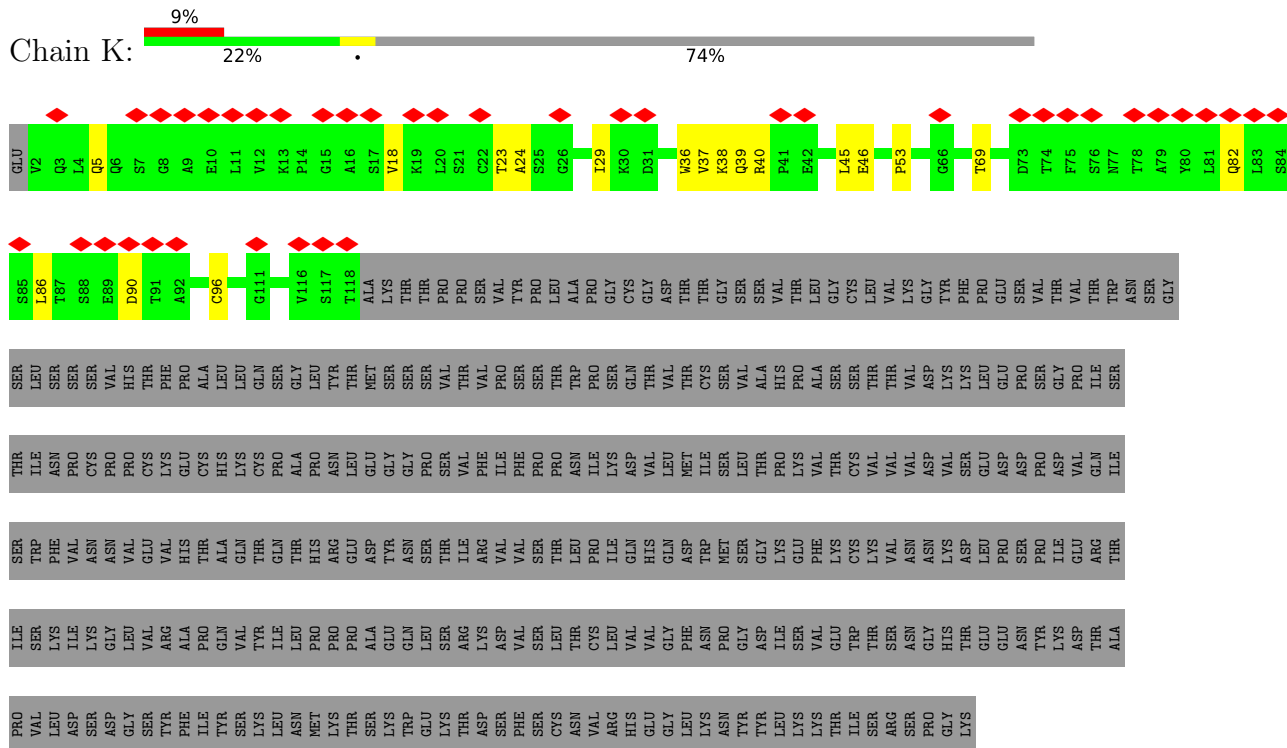


• Molecule 5: IgG2b Fab_1F4 Heavy Chain

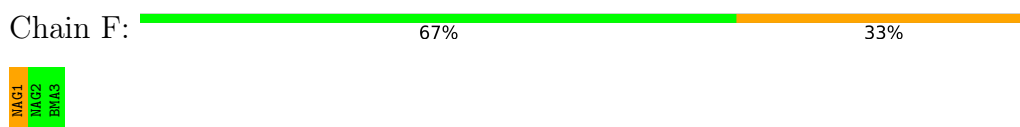


[illegible]

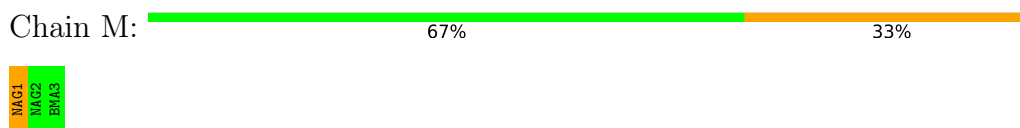
- Molecule 5: IgG2b Fab 1F4 Heavy Chain



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



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



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





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101120	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.674	Depositor
Minimum map value	-1.123	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	239.36, 239.36, 239.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.35	0/2786	0.62	1/3791 (0.0%)
1	C	0.27	0/2792	0.52	2/3799 (0.1%)
2	B	0.40	0/2874	0.64	1/3903 (0.0%)
2	D	0.36	0/2865	0.63	0/3892
3	E	0.46	0/2734	0.69	2/3724 (0.1%)
4	I	0.19	0/820	0.49	0/1112
4	L	0.19	0/829	0.50	0/1123
5	J	0.19	0/928	0.43	0/1260
5	K	0.17	0/935	0.44	0/1270
All	All	0.34	0/17563	0.59	6/23874 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
2	D	0	1
3	E	0	3
5	J	0	1
All	All	0	10

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	ARG	N-CA-C	-8.09	88.36	111.00
1	C	309	ARG	CB-CA-C	6.98	123.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	TYR	CB-CA-C	-6.37	100.88	110.88
1	A	184	PRO	CB-CA-C	-5.64	104.09	113.06
3	E	156	HIS	N-CA-C	-5.29	103.55	110.53
3	E	195	SER	N-CA-C	-5.17	106.93	113.18

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	28	ARG	Sidechain
2	B	221	ARG	Sidechain
2	B	31	ARG	Sidechain
2	B	37	ARG	Sidechain
2	D	313	ARG	Sidechain
3	E	194	ARG	Sidechain
3	E	197	ARG	Sidechain
3	E	232	ARG	Sidechain
5	J	102	ARG	Sidechain

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	2716	0	2722	30	0
1	C	2722	0	2727	23	0
2	B	2803	0	2789	41	0
2	D	2794	0	2776	36	0
3	E	2661	0	2638	36	0
4	I	802	0	771	7	0
4	L	811	0	784	5	0
5	J	907	0	877	8	0
5	K	914	0	884	11	0
6	F	39	0	34	1	0
6	M	39	0	34	1	0
6	O	39	0	34	0	0
7	G	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	28	0	25	0	0
8	H	94	0	79	1	0
9	A	7	0	0	4	0
9	C	7	0	0	0	0
10	B	47	0	44	1	0
10	D	47	0	44	0	0
11	B	52	0	82	5	0
11	D	52	0	82	1	0
12	E	14	0	13	1	0
All	All	17623	0	17464	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (180) 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)
9:A:501:ABU:O	2:B:130:THR:HG21	1.75	0.85
1:A:155:GLU:OE2	9:A:501:ABU:N	2.10	0.84
3:E:236:PHE:HA	3:E:239:GLN:HB2	1.68	0.75
1:A:47:ILE:HG22	1:A:183:LEU:HD21	1.71	0.72
1:A:64:GLN:HE21	1:A:169:ARG:HH22	1.40	0.70
3:E:61:SER:HA	3:E:196:TRP:CD1	2.28	0.69
2:B:62:ILE:HG12	2:B:64:VAL:HG13	1.75	0.68
2:B:67:ARG:HG2	2:B:130:THR:HG23	1.76	0.68
2:B:227:VAL:HG21	11:B:602:POV:H34A	1.80	0.64
1:A:213:LYS:HB2	6:F:1:NAG:H83	1.80	0.64
2:D:105:LYS:HD2	2:D:138:GLU:HG2	1.82	0.61
2:B:306:THR:HG21	10:B:601:PIO:H4B	1.81	0.61
2:B:222:LYS:HE3	11:B:602:POV:H15A	1.82	0.61
1:A:236:SER:HB3	1:A:257:THR:HG21	1.83	0.61
3:E:242:ILE:HB	3:E:243:PRO:HD3	1.82	0.61
1:A:99:LEU:HD22	1:A:207:ARG:HH22	1.65	0.60
3:E:185:ARG:HA	12:E:501:NAG:H62	1.83	0.60
1:C:52:GLU:OE2	1:C:216:ARG:NH1	2.35	0.60
2:B:415:TYR:HA	2:B:418:ARG:HG2	1.83	0.60
2:D:318:ASP:O	2:D:319:GLY:C	2.45	0.59
3:E:161:ASP:OD1	3:E:161:ASP:N	2.33	0.59
1:A:106:VAL:HG23	2:B:112:MET:HE1	1.85	0.59
3:E:233:MET:SD	3:E:233:MET:N	2.67	0.59
1:A:97:TYR:HH	9:A:501:ABU:N	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:45:ASP:HB3	3:E:48:VAL:HB	1.85	0.58
2:D:103:ASN:ND2	2:D:137:ALA:HB1	2.19	0.57
3:E:412:SER:HA	3:E:415:ARG:HD2	1.86	0.57
1:A:155:GLU:OE1	1:A:207:ARG:NH2	2.38	0.57
2:B:34:LEU:HD23	1:C:12:VAL:HG11	1.87	0.56
5:J:20:LEU:HD22	5:J:81:LEU:HD12	1.87	0.56
4:L:51:ALA:HB1	4:L:66:GLY:HA3	1.88	0.56
2:B:88:ASN:ND2	2:B:115:PRO:O	2.38	0.56
3:E:58:TYR:HD2	3:E:77:PHE:HD2	1.54	0.56
2:D:390:SER:HB3	2:D:393:ASP:HB2	1.87	0.55
3:E:430:TRP:O	3:E:434:LEU:HB2	2.07	0.55
2:B:47:VAL:HG22	2:B:64:VAL:HG12	1.89	0.55
1:C:308:GLY:O	1:C:309:ARG:C	2.46	0.55
1:C:254:GLY:HA3	1:C:296:LEU:HD13	1.89	0.55
1:A:43:ASP:HB2	1:A:62:TYR:HB2	1.89	0.54
2:B:298:PHE:O	2:B:301:LEU:N	2.41	0.54
1:C:301:LEU:O	1:C:305:ILE:HG12	2.09	0.53
3:E:200:GLN:O	3:E:232:ARG:N	2.41	0.53
3:E:98:LEU:HD13	3:E:102:MET:HG3	1.89	0.53
2:B:39:THR:HB	2:B:167:VAL:HG22	1.91	0.52
5:K:38:LYS:NZ	5:K:90:ASP:OD1	2.38	0.52
2:B:34:LEU:CD2	1:C:12:VAL:HG11	2.39	0.51
1:C:306:PHE:O	1:C:309:ARG:O	2.29	0.51
2:B:86:LEU:HD13	2:B:90:MET:HG2	1.92	0.51
3:E:184:LYS:HB2	3:E:187:SER:HB3	1.93	0.51
2:B:298:PHE:O	2:B:299:SER:C	2.54	0.50
3:E:430:TRP:HE3	3:E:434:LEU:HD13	1.76	0.50
5:K:29:ILE:HG22	5:K:53:PRO:HG2	1.92	0.50
1:C:205:TYR:OH	2:D:120:ARG:NH2	2.45	0.50
2:B:233:PRO:HG3	11:B:602:POV:H21J	1.94	0.50
5:K:69:THR:HB	5:K:82:GLN:HB2	1.94	0.50
1:A:144:PRO:HD3	1:A:281:ILE:HB	1.94	0.50
2:D:75:LEU:HD22	2:D:127:LEU:HD11	1.93	0.49
2:D:250:GLU:HG3	2:D:316:ALA:HB2	1.93	0.49
4:I:4:MET:HE3	4:I:90:GLN:HG2	1.94	0.49
2:D:51:GLY:HA2	2:D:187:ARG:HB2	1.95	0.49
2:D:279:LYS:HD3	3:E:235:TYR:CE2	2.48	0.49
5:J:37:VAL:HG11	5:J:108:TRP:HZ3	1.78	0.49
5:K:24:ALA:HB3	5:K:29:ILE:HD11	1.94	0.49
1:C:146:ASP:OD2	1:C:148:GLN:NE2	2.46	0.49
3:E:56:ASP:HA	3:E:187:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:ASP:N	2:D:318:ASP:OD1	2.46	0.48
2:B:42:LYS:HB3	2:B:172:THR:HB	1.94	0.48
5:K:39:GLN:NE2	5:K:40:ARG:O	2.38	0.48
3:E:58:TYR:HA	3:E:189:GLU:O	2.14	0.48
3:E:412:SER:O	3:E:415:ARG:HB2	2.14	0.48
2:D:60:TYR:CE1	2:D:137:ALA:HB3	2.48	0.48
2:D:108:VAL:HB	2:D:134:THR:CG2	2.43	0.48
3:E:154:GLN:H	3:E:154:GLN:CD	2.22	0.47
3:E:231:ARG:HG2	3:E:232:ARG:N	2.28	0.47
3:E:256:TRP:HA	3:E:415:ARG:HH21	1.79	0.47
2:D:47:VAL:HG22	2:D:62:ILE:HD11	1.97	0.47
2:B:232:LEU:HD21	11:B:602:POV:H21D	1.96	0.46
3:E:110:ASP:OD1	3:E:110:ASP:N	2.40	0.46
1:A:117:ARG:HB3	1:A:125:LEU:HB3	1.97	0.46
2:B:114:MET:HE3	2:B:115:PRO:HD2	1.98	0.46
2:D:30:LEU:HB3	2:D:34:LEU:HD22	1.97	0.46
2:D:273:ALA:HB1	2:D:286:MET:HE3	1.98	0.46
4:L:39:LYS:NZ	4:L:81:GLU:O	2.49	0.46
2:D:57:ASP:O	2:D:58:MET:C	2.57	0.46
1:C:95:ASP:OD1	1:C:95:ASP:N	2.48	0.46
4:I:15:VAL:HG13	4:I:79:GLN:HA	1.98	0.46
2:D:44:ASP:N	2:D:44:ASP:OD1	2.49	0.46
5:J:100:GLY:HA3	5:J:106:ASP:HB2	1.98	0.46
1:A:52:GLU:OE2	1:A:216:ARG:NH1	2.40	0.46
4:I:54:ARG:NH1	4:I:62:PHE:O	2.49	0.46
2:B:149:ASP:OD1	2:B:149:ASP:N	2.47	0.46
3:E:412:SER:HA	3:E:415:ARG:HB2	1.98	0.46
2:D:46:PHE:HB3	2:D:65:PHE:HB2	1.98	0.45
2:B:257:VAL:HA	2:B:260:VAL:HG22	1.97	0.45
1:C:213:LYS:HB2	6:M:1:NAG:H83	1.97	0.45
1:C:89:ASP:OD2	1:C:114:ARG:NH2	2.47	0.45
1:C:151:THR:HG22	1:C:211:SER:HB3	1.98	0.45
2:D:106:LYS:HD2	2:D:106:LYS:HA	1.82	0.45
4:L:29:VAL:HG12	4:L:92:TYR:HB3	1.97	0.45
1:A:98:PHE:HB2	1:A:101:ASP:HB2	1.98	0.45
5:K:5:GLN:O	5:K:23:THR:N	2.45	0.45
2:B:200:SER:OG	2:B:201:GLY:N	2.50	0.44
1:C:276:PRO:HG3	2:D:222:LYS:HE3	1.99	0.44
3:E:68:ILE:HA	3:E:288:PRO:HB3	1.99	0.44
2:B:146:PHE:HB3	2:B:284:THR:HB	1.98	0.44
2:D:313:ARG:HH21	2:D:387:ASN:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HA	7:G:1:NAG:H82	2.00	0.44
2:D:228:ILE:HD11	11:D:602:POV:H24	2.00	0.44
3:E:120:ASP:N	3:E:120:ASP:OD1	2.51	0.44
5:J:40:ARG:HB3	5:J:43:GLN:HB2	2.00	0.44
5:K:37:VAL:HG11	5:K:45:LEU:HD23	1.99	0.44
2:B:51:GLY:HA2	2:B:187:ARG:HB2	1.99	0.44
1:C:192:LYS:HE3	1:C:192:LYS:HB2	1.80	0.43
1:A:55:MET:HE2	1:A:273:PRO:HG3	1.99	0.43
3:E:239:GLN:O	3:E:243:PRO:HG2	2.18	0.43
1:A:459:ASP:OD1	1:A:459:ASP:N	2.51	0.43
4:I:38:GLN:N	4:I:85:ASP:O	2.50	0.43
1:A:44:ILE:HD12	1:A:59:LEU:HD11	2.01	0.43
2:D:47:VAL:CG2	2:D:62:ILE:HD11	2.49	0.43
5:K:18:VAL:HG12	5:K:86:LEU:HD11	2.01	0.43
3:E:70:MET:HE1	3:E:153:LEU:O	2.19	0.43
1:A:145:LEU:HG	1:A:218:ILE:HD12	2.00	0.43
2:B:117:LYS:HG2	2:B:131:MET:HG2	2.00	0.43
5:K:36:TRP:HD1	5:K:96:CYS:HA	1.83	0.43
1:A:269:ARG:HH11	2:B:229:GLN:HG2	1.84	0.42
2:B:121:ILE:HG12	2:B:127:LEU:HD22	2.00	0.42
4:L:11:MET:SD	4:L:11:MET:N	2.92	0.42
1:A:158:GLY:HA2	2:B:118:LEU:HD12	2.01	0.42
1:A:464:ASP:OD1	1:A:464:ASP:N	2.49	0.42
2:D:149:ASP:OD1	2:D:149:ASP:N	2.50	0.42
2:D:233:PRO:HB2	2:D:269:LEU:HD21	2.01	0.42
3:E:129:ARG:NH1	8:H:5:MAN:O6	2.53	0.42
2:B:46:PHE:CB	2:B:67:ARG:HH12	2.33	0.42
2:B:98:ASP:OD1	2:B:98:ASP:N	2.44	0.42
3:E:154:GLN:O	3:E:154:GLN:HG2	2.20	0.42
3:E:248:VAL:HG11	3:E:303:CYS:HB3	2.00	0.42
1:A:84:ASP:HB2	3:E:41:LYS:HA	2.01	0.42
1:A:119:HIS:HE1	1:A:125:LEU:HB2	1.84	0.42
2:D:61:THR:HG23	2:D:136:ARG:HG2	2.00	0.42
1:A:47:ILE:CG2	1:A:183:LEU:HD21	2.46	0.42
2:B:92:SER:O	1:C:86:ARG:NH1	2.51	0.42
2:B:111:ASN:HA	2:B:115:PRO:HA	2.00	0.42
1:A:305:ILE:HG23	1:A:460:VAL:HG12	2.02	0.42
2:B:122:THR:OG1	2:B:124:ASP:OD1	2.31	0.41
2:D:313:ARG:HE	2:D:386:PHE:C	2.27	0.41
1:A:205:TYR:OH	2:B:120:ARG:NH2	2.53	0.41
2:D:207:THR:HG21	3:E:130:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:102:LYS:HE3	4:I:102:LYS:HB3	1.91	0.41
5:J:14:PRO:HD3	5:J:117:SER:H	1.84	0.41
4:L:63:THR:OG1	4:L:74:THR:OG1	2.37	0.41
2:B:44:ASP:OD1	2:B:44:ASP:N	2.53	0.41
3:E:27:VAL:HG13	3:E:96:LEU:HD22	2.02	0.41
5:K:36:TRP:NE1	5:K:96:CYS:SG	2.80	0.41
1:C:299:TYR:HA	1:C:302:VAL:HG12	2.02	0.41
1:C:251:VAL:HG21	2:D:254:ALA:HA	2.02	0.41
3:E:158:PHE:C	3:E:158:PHE:CD1	2.99	0.41
5:J:38:LYS:HB2	5:J:48:ILE:HD11	2.02	0.41
2:B:235:ILE:HD13	11:B:602:POV:H311	2.01	0.41
1:C:55:MET:HE3	1:C:55:MET:HB3	1.96	0.41
1:C:183:LEU:HD22	1:C:186:PHE:HB2	2.02	0.41
2:D:88:ASN:ND2	2:D:115:PRO:O	2.54	0.41
2:D:124:ASP:OD1	2:D:126:THR:OG1	2.32	0.41
2:D:266:MET:HE3	2:D:266:MET:HB3	1.95	0.41
3:E:237:THR:HA	3:E:241:TYR:HB2	2.03	0.41
2:D:60:TYR:OH	2:D:155:LEU:HB2	2.21	0.41
3:E:414:ALA:HB1	3:E:418:PHE:CD2	2.56	0.41
1:A:28:ARG:HG2	1:A:31:PHE:HA	2.03	0.40
1:A:202:THR:OG1	9:A:501:ABU:OXT	2.36	0.40
1:A:261:MET:HE2	1:A:261:MET:HB2	1.98	0.40
2:B:263:VAL:HG11	1:C:235:LEU:HD22	2.03	0.40
1:C:95:ASP:HA	2:D:114:MET:HB2	2.03	0.40
2:D:101:PHE:CD1	2:D:157:PHE:HB3	2.56	0.40
5:J:2:VAL:N	5:J:25:SER:O	2.55	0.40
2:B:112:MET:HA	2:B:113:THR:HA	1.91	0.40
1:C:26:ARG:HD2	2:D:90:MET:HE3	2.02	0.40
2:B:262:THR:HB	2:B:297:VAL:CG2	2.51	0.40
4:I:77:SER:O	4:I:79:GLN:NE2	2.54	0.40
5:J:6:GLN:HA	5:J:22:CYS:HA	2.03	0.40
2:B:199:ASP:OD1	4:I:31:THR:OG1	2.39	0.40
5:K:38:LYS:N	5:K:46:GLU:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	327/488 (67%)	315 (96%)	12 (4%)	0	100	100
1	C	328/488 (67%)	315 (96%)	13 (4%)	0	100	100
2	B	342/429 (80%)	326 (95%)	16 (5%)	0	100	100
2	D	341/429 (80%)	327 (96%)	14 (4%)	0	100	100
3	E	320/436 (73%)	309 (97%)	11 (3%)	0	100	100
4	I	103/213 (48%)	94 (91%)	9 (9%)	0	100	100
4	L	104/213 (49%)	100 (96%)	4 (4%)	0	100	100
5	J	114/454 (25%)	108 (95%)	6 (5%)	0	100	100
5	K	115/454 (25%)	113 (98%)	2 (2%)	0	100	100
All	All	2094/3604 (58%)	2007 (96%)	87 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	301/438 (69%)	300 (100%)	1 (0%)	86	96
1	C	302/438 (69%)	302 (100%)	0	100	100
2	B	308/382 (81%)	303 (98%)	5 (2%)	55	83
2	D	307/382 (80%)	304 (99%)	3 (1%)	68	89
3	E	299/400 (75%)	291 (97%)	8 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	89/188 (47%)	89 (100%)	0	100	100
4	L	90/188 (48%)	90 (100%)	0	100	100
5	J	97/407 (24%)	97 (100%)	0	100	100
5	K	98/407 (24%)	98 (100%)	0	100	100
All	All	1891/3230 (58%)	1874 (99%)	17 (1%)	68	90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
2	B	40	GLU
2	B	212	VAL
2	B	294	TYR
2	B	297	VAL
2	B	298	PHE
2	D	57	ASP
2	D	59	GLU
2	D	315	TYR
3	E	118	LYS
3	E	152	GLN
3	E	153	LEU
3	E	155	LEU
3	E	156	HIS
3	E	161	ASP
3	E	233	MET
3	E	410	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	148	GLN
1	A	185	GLN
2	B	151	HIS
2	B	204	GLN
2	B	408	ASN
1	C	148	GLN
1	C	185	GLN
1	C	217	ASN
2	D	116	ASN

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Mol	Chain	Res	Type
2	D	142	HIS
2	D	229	GLN
3	E	239	GLN
3	E	426	ASN
5	K	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

21 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	F	1	1,6	14,14,15	0.33	0	17,19,21	1.14	2 (11%)
6	NAG	F	2	6	14,14,15	0.25	0	17,19,21	0.56	0
6	BMA	F	3	6	11,11,12	0.73	0	15,15,17	0.81	0
7	NAG	G	1	1,7	14,14,15	0.42	0	17,19,21	1.18	1 (5%)
7	NAG	G	2	7	14,14,15	0.40	0	17,19,21	0.45	0
8	NAG	H	1	8,2	14,14,15	0.39	0	17,19,21	0.70	1 (5%)
8	NAG	H	2	8	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
8	BMA	H	3	8	11,11,12	0.54	0	15,15,17	0.55	0
8	MAN	H	4	8	11,11,12	0.49	0	15,15,17	0.61	0
8	MAN	H	5	8	11,11,12	0.36	0	15,15,17	0.53	0
8	MAN	H	6	8	11,11,12	0.38	0	15,15,17	0.44	0
8	MAN	H	7	8	11,11,12	0.31	0	15,15,17	0.46	0
8	MAN	H	8	8	11,11,12	0.31	0	15,15,17	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	M	1	1,6	14,14,15	0.39	0	17,19,21	1.12	2 (11%)
6	NAG	M	2	6	14,14,15	0.33	0	17,19,21	0.55	0
6	BMA	M	3	6	11,11,12	0.73	0	15,15,17	0.70	0
7	NAG	N	1	1,7	14,14,15	0.42	0	17,19,21	0.61	0
7	NAG	N	2	7	14,14,15	0.40	0	17,19,21	0.75	0
6	NAG	O	1	6,2	14,14,15	0.33	0	17,19,21	0.54	0
6	NAG	O	2	6	14,14,15	0.33	0	17,19,21	0.64	1 (5%)
6	BMA	O	3	6	11,11,12	0.74	0	15,15,17	0.77	0

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1	NAG	O5-C1-C2	-3.97	105.15	111.29
6	M	1	NAG	C2-N2-C7	3.22	127.21	122.90
6	F	1	NAG	C2-N2-C7	3.20	127.18	122.90
8	H	2	NAG	C1-C2-N2	2.58	114.49	110.43
6	F	1	NAG	C1-C2-N2	2.15	113.82	110.43
6	M	1	NAG	C1-C2-N2	2.12	113.77	110.43
8	H	1	NAG	C1-O5-C5	2.09	114.99	112.19
6	O	2	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	2	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
8	H	5	MAN	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
8	H	7	MAN	O5-C5-C6-O6
8	H	8	MAN	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	C3-C2-N2-C7
6	M	1	NAG	O5-C5-C6-O6
8	H	5	MAN	C4-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
7	N	2	NAG	O7-C7-N2-C2
6	F	1	NAG	C1-C2-N2-C7
6	M	1	NAG	C1-C2-N2-C7
6	F	1	NAG	C3-C2-N2-C7
6	M	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

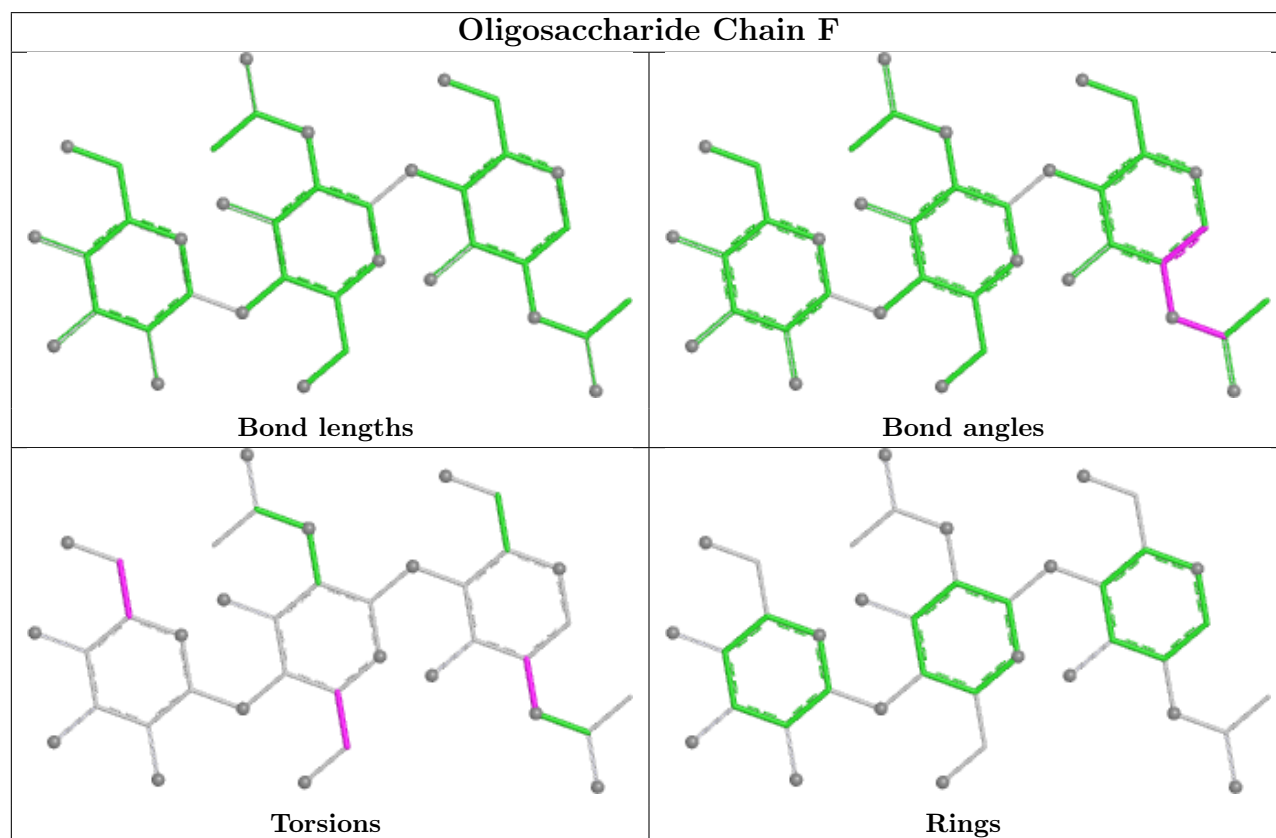
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1	NAG	1	0

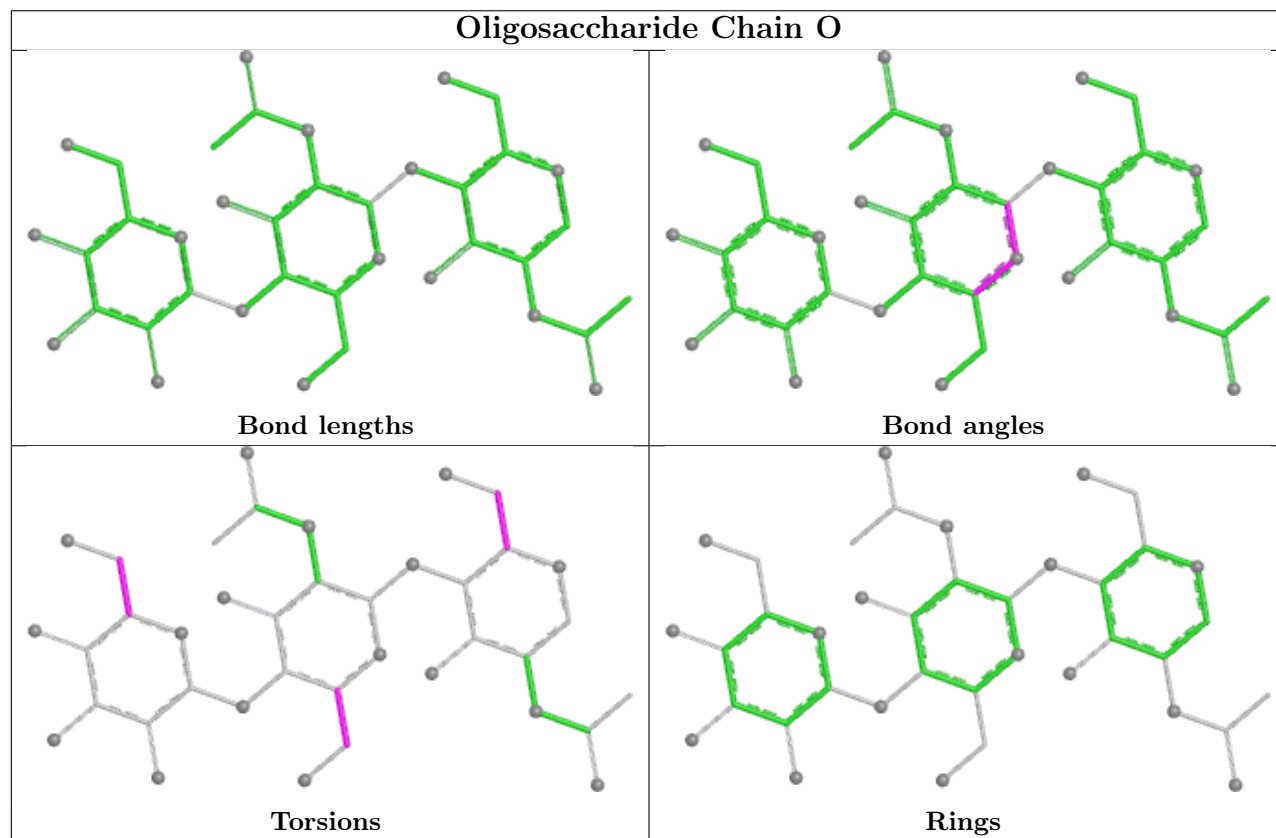
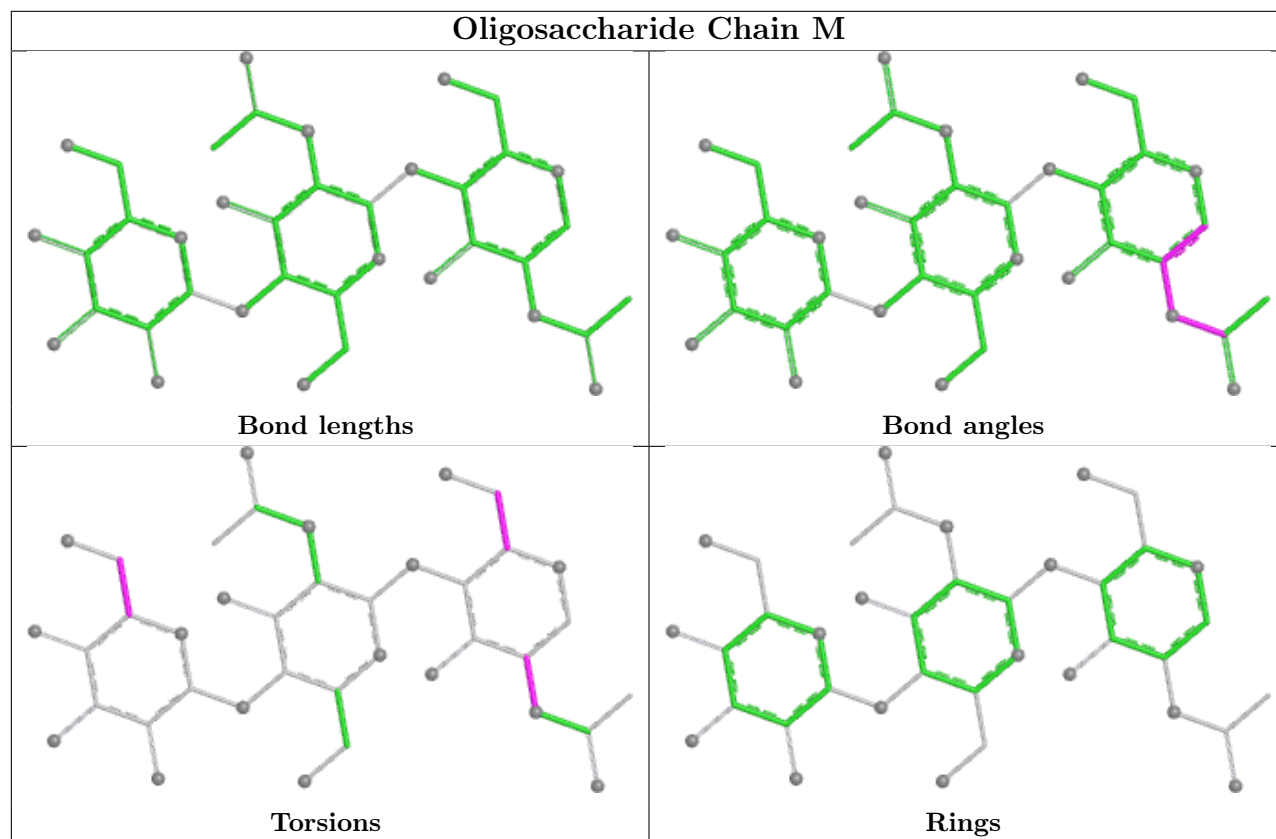
Continued on next page...

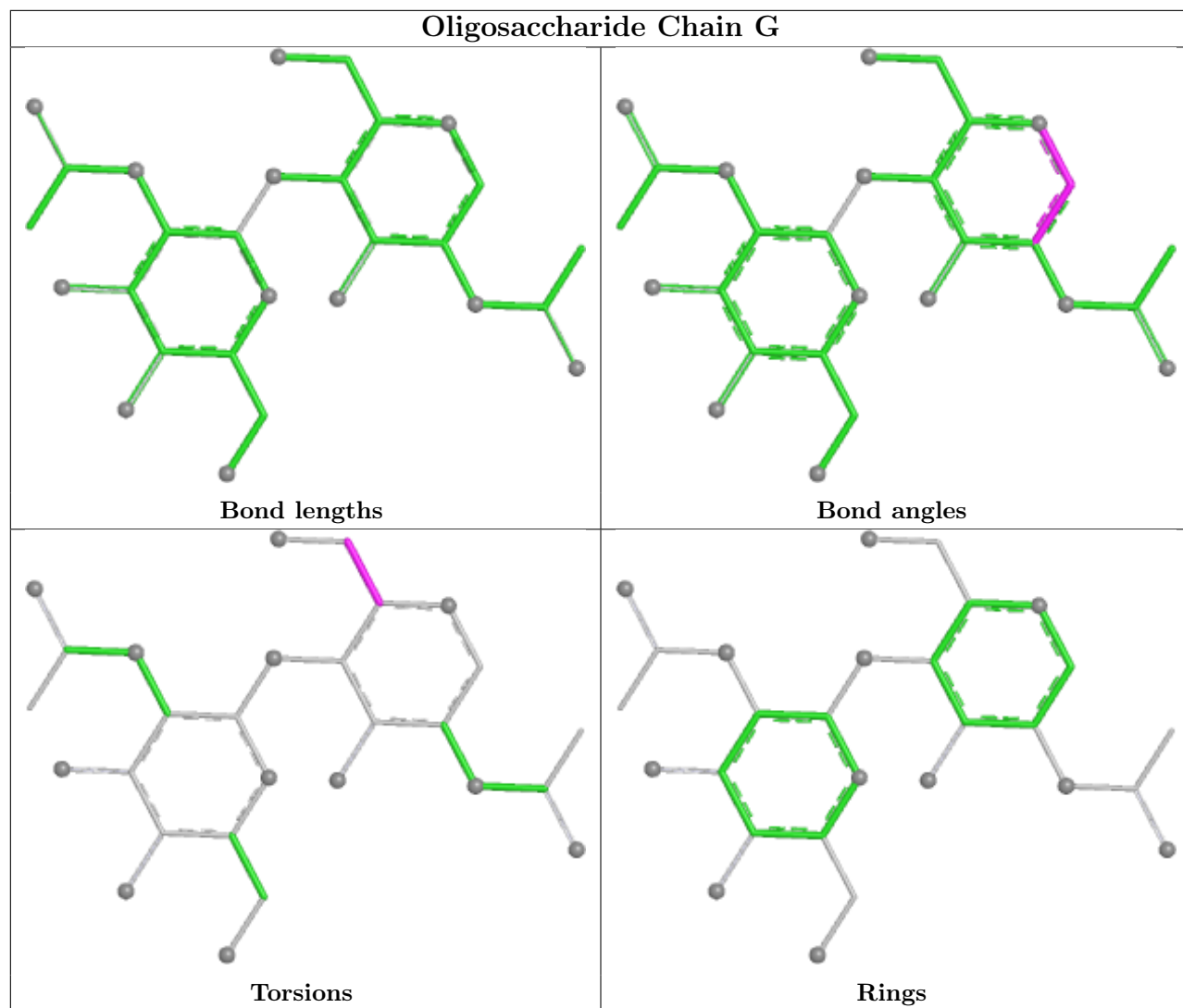
Continued from previous page...

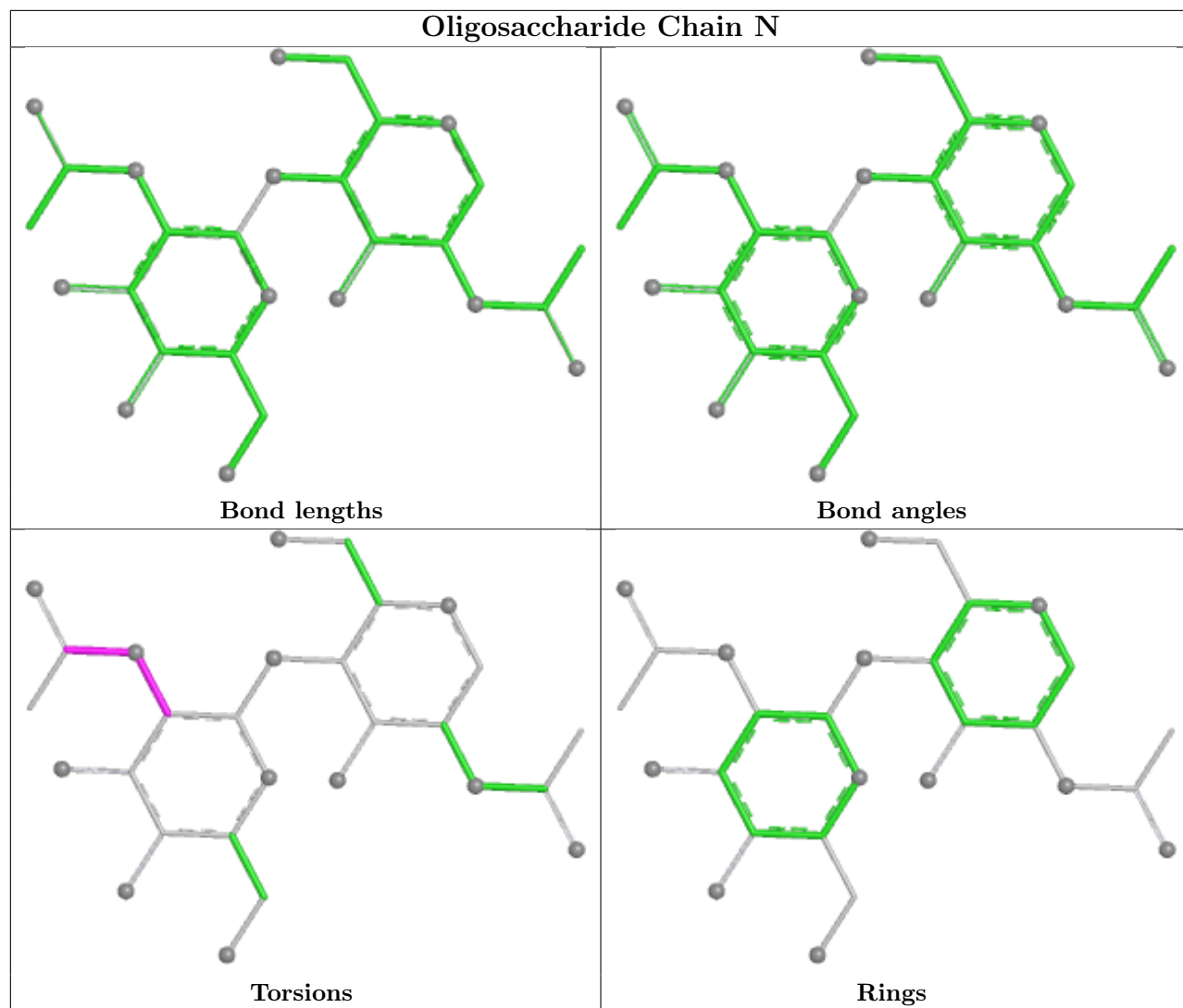
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	1	0
8	H	5	MAN	1	0
7	G	1	NAG	1	0

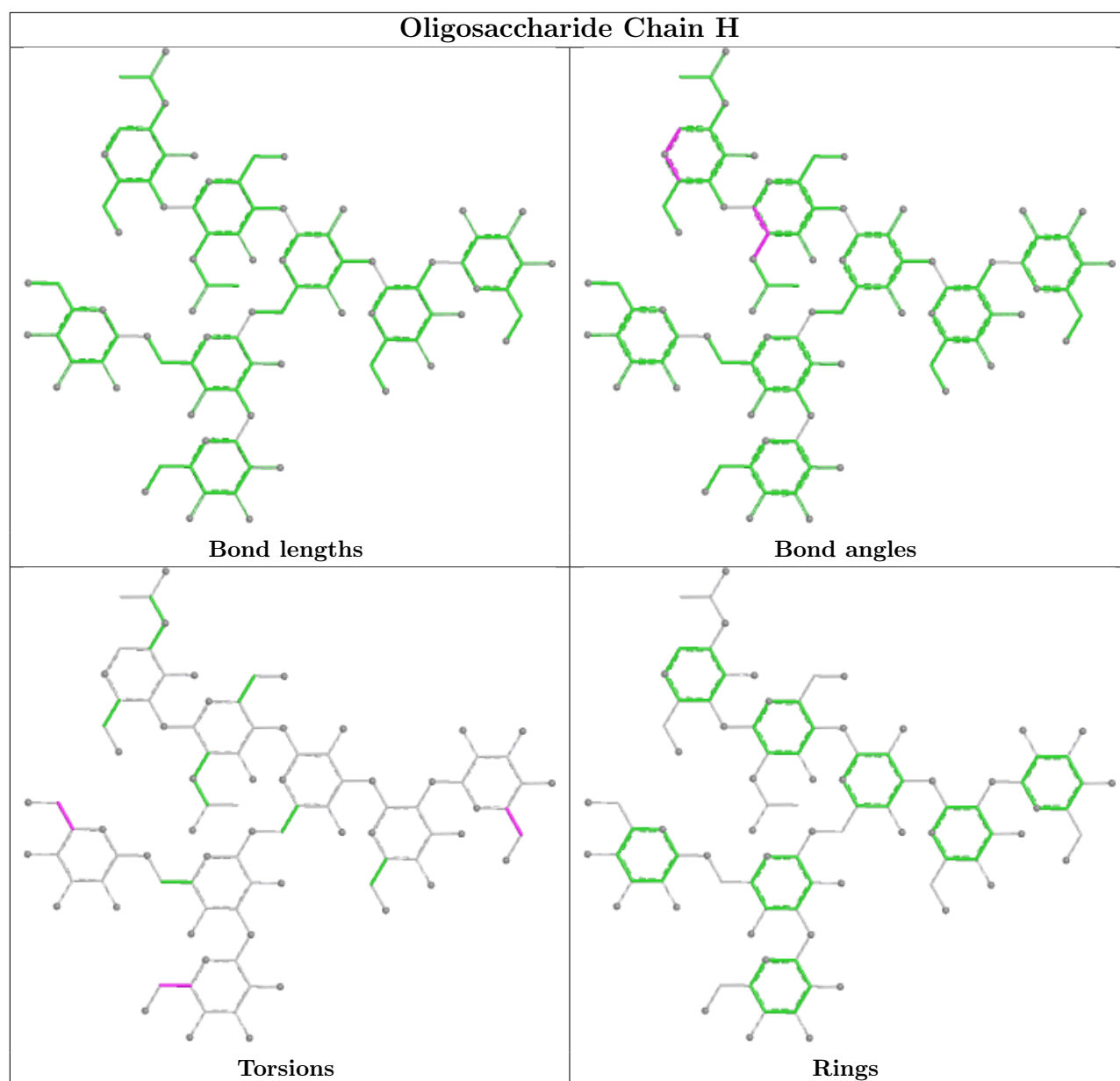
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PIO	D	601	-	47,47,47	0.59	2 (4%)	62,65,65	0.43	0
9	ABU	C	501	-	6,6,6	0.78	0	6,6,6	0.80	0
9	ABU	A	501	-	6,6,6	1.93	2 (33%)	6,6,6	1.60	1 (16%)
12	NAG	E	501	3	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
10	PIO	B	601	-	47,47,47	0.58	0	62,65,65	0.45	0
11	POV	B	602	-	51,51,51	0.31	0	57,59,59	0.35	0
11	POV	D	602	-	51,51,51	0.35	0	57,59,59	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PIO	D	601	-	-	3/44/68/68	0/1/1/1
9	ABU	C	501	-	-	0/4/4/4	-
9	ABU	A	501	-	-	0/4/4/4	-
12	NAG	E	501	3	-	4/6/23/26	0/1/1/1
10	PIO	B	601	-	-	2/44/68/68	0/1/1/1
11	POV	B	602	-	-	13/55/55/55	-
11	POV	D	602	-	-	17/55/55/55	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	501	ABU	O-C	3.64	1.34	1.22
9	A	501	ABU	OXT-C	-2.99	1.20	1.30
10	D	601	PIO	P4-O4	2.03	1.63	1.59
10	D	601	PIO	P5-O5	2.02	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	501	ABU	CB-CG-C	-2.73	107.39	114.51
12	E	501	NAG	C2-N2-C7	2.16	125.79	122.90

There are no chirality outliers.

All (39) torsion outliers are listed below:

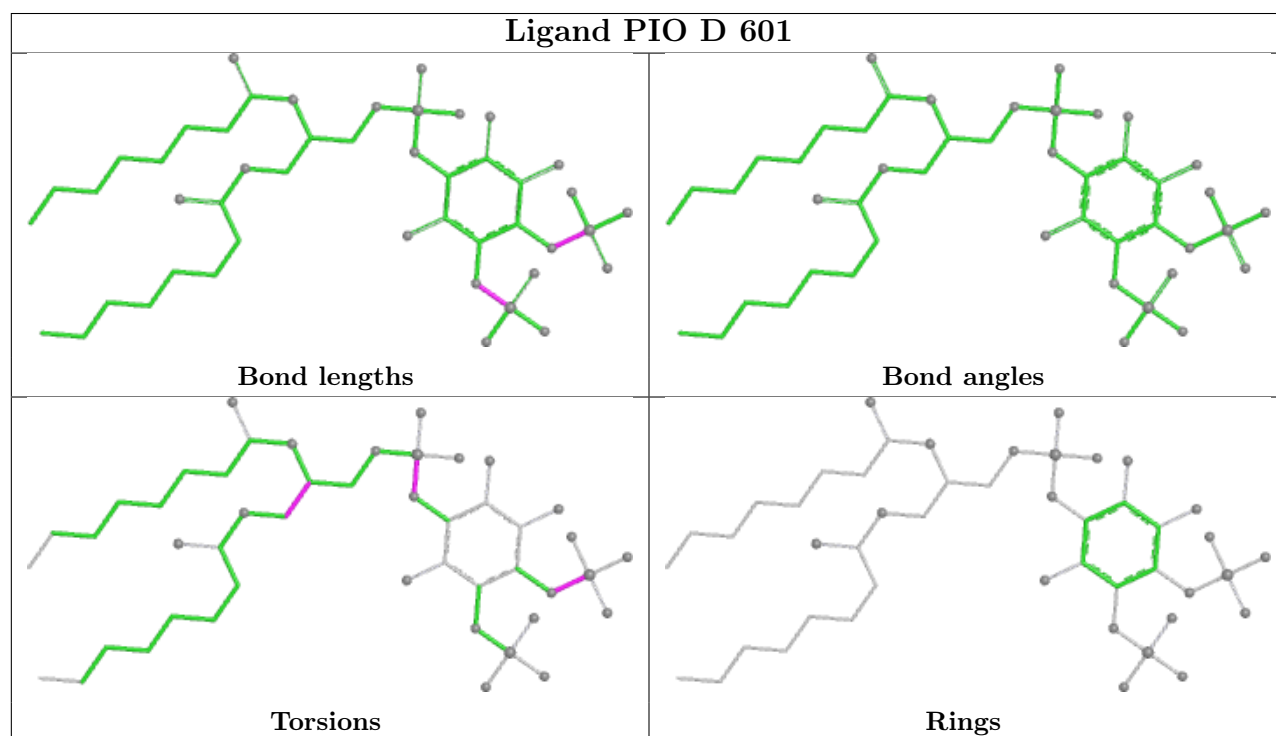
Mol	Chain	Res	Type	Atoms
11	B	602	POV	C1-O11-P-O13
11	B	602	POV	C32-C31-O31-C3
11	B	602	POV	O32-C31-O31-C3
11	D	602	POV	C1-O11-P-O12
11	D	602	POV	C1-O11-P-O13
11	D	602	POV	C1-O11-P-O14
11	D	602	POV	C11-O12-P-O14
11	D	602	POV	C32-C31-O31-C3
11	D	602	POV	O32-C31-O31-C3
12	E	501	NAG	C3-C2-N2-C7
12	E	501	NAG	C8-C7-N2-C2
12	E	501	NAG	O7-C7-N2-C2
11	B	602	POV	C211-C210-C29-C28
11	D	602	POV	C37-C38-C39-C310
11	D	602	POV	C22-C23-C24-C25
11	B	602	POV	C37-C38-C39-C310
11	B	602	POV	C22-C21-O21-C2
11	B	602	POV	O22-C21-O21-C2
12	E	501	NAG	O5-C5-C6-O6
11	D	602	POV	C26-C27-C28-C29
11	B	602	POV	C25-C26-C27-C28
11	D	602	POV	O11-C1-C2-O21
11	D	602	POV	C12-C11-O12-P
11	D	602	POV	O11-C1-C2-C3
11	D	602	POV	C29-C210-C211-C212
11	D	602	POV	C11-O12-P-O11
11	D	602	POV	C11-O12-P-O13
11	B	602	POV	C211-C212-C213-C214
10	B	601	PIO	C4-O4-P4-O43
10	D	601	PIO	C4-O4-P4-O41
11	B	602	POV	C21-C22-C23-C24
11	B	602	POV	C1-C2-O21-C21
11	B	602	POV	C12-C11-O12-P
10	D	601	PIO	C1-O1-P1-O12
11	D	602	POV	C25-C26-C27-C28
10	D	601	PIO	O2C-C2C-C3C-O3C
11	B	602	POV	C22-C23-C24-C25
10	B	601	PIO	C4-O4-P4-O42
11	D	602	POV	O21-C21-C22-C23

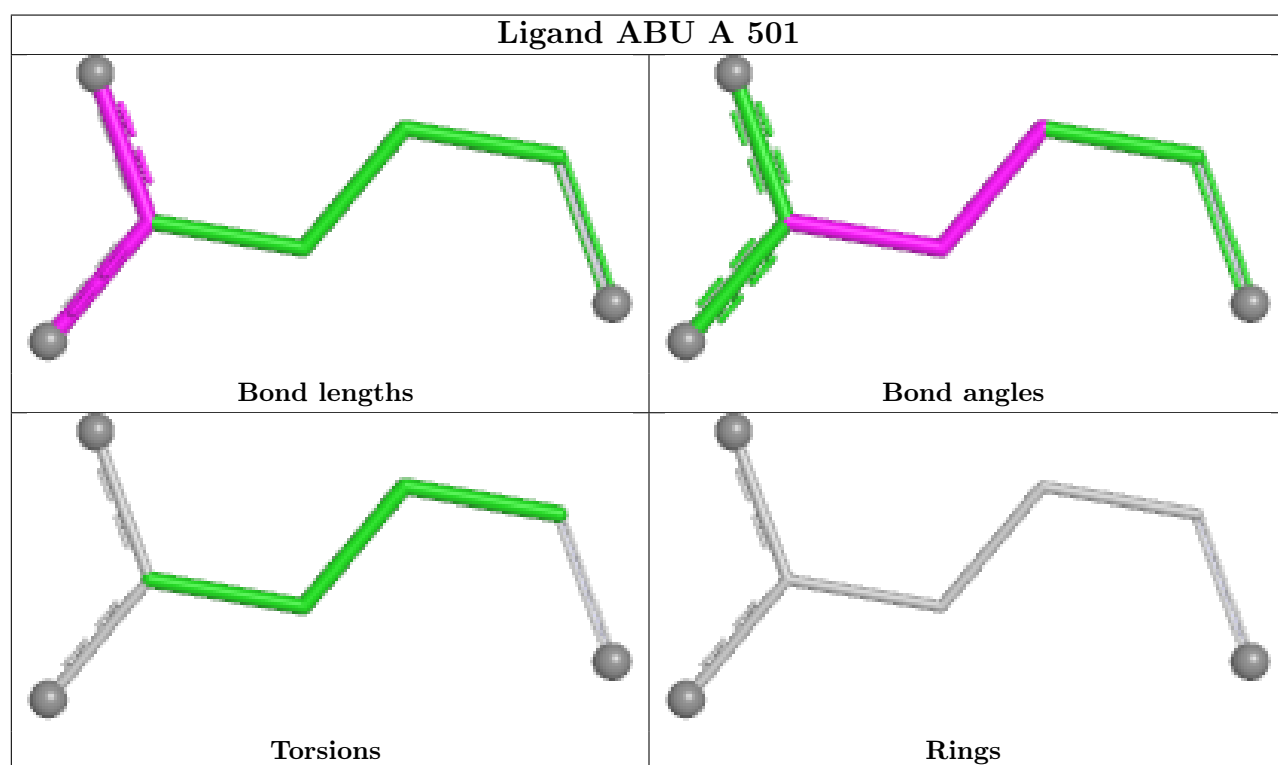
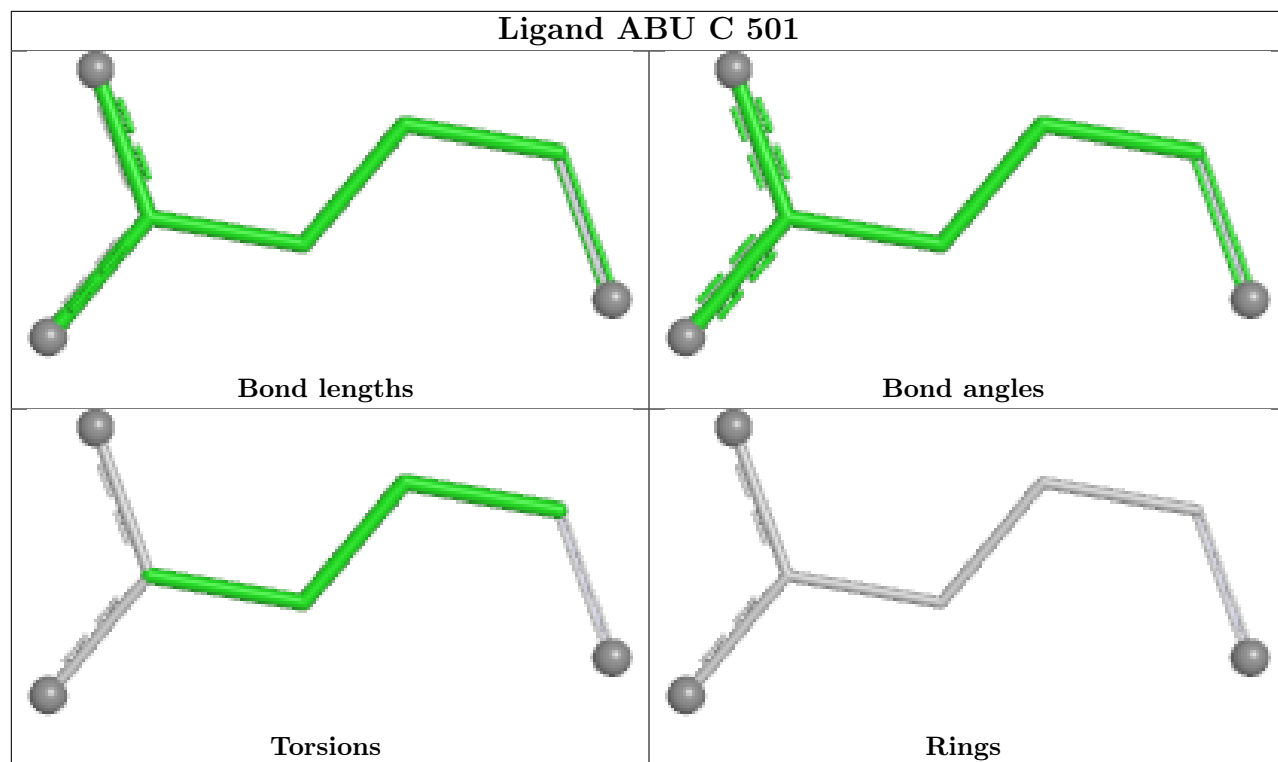
There are no ring outliers.

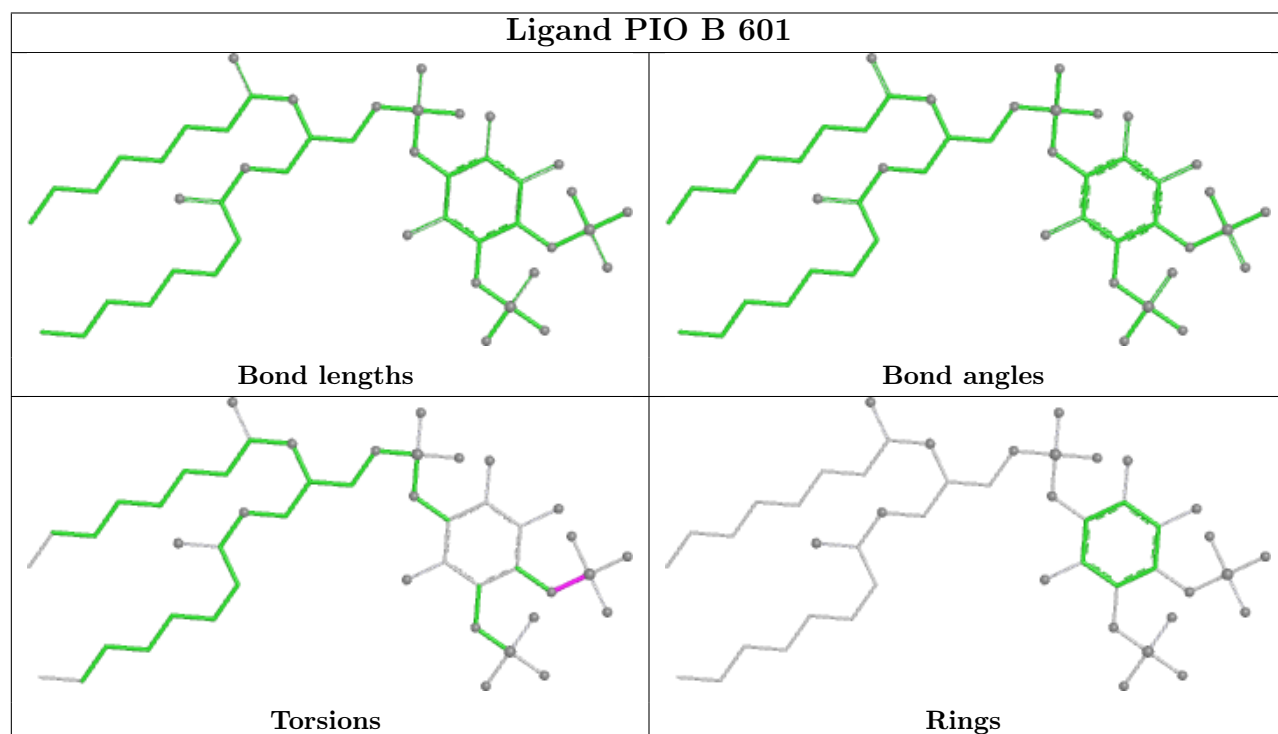
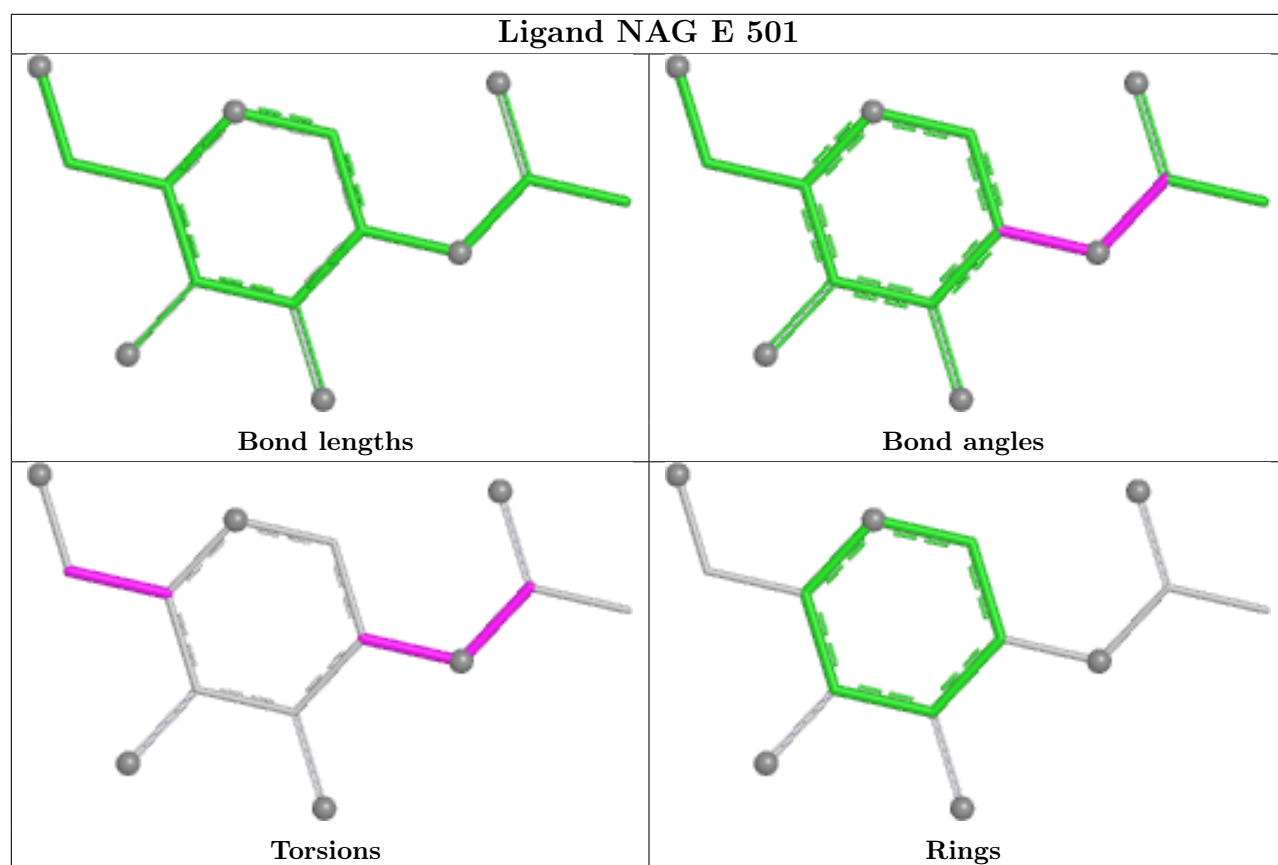
5 monomers are involved in 12 short contacts:

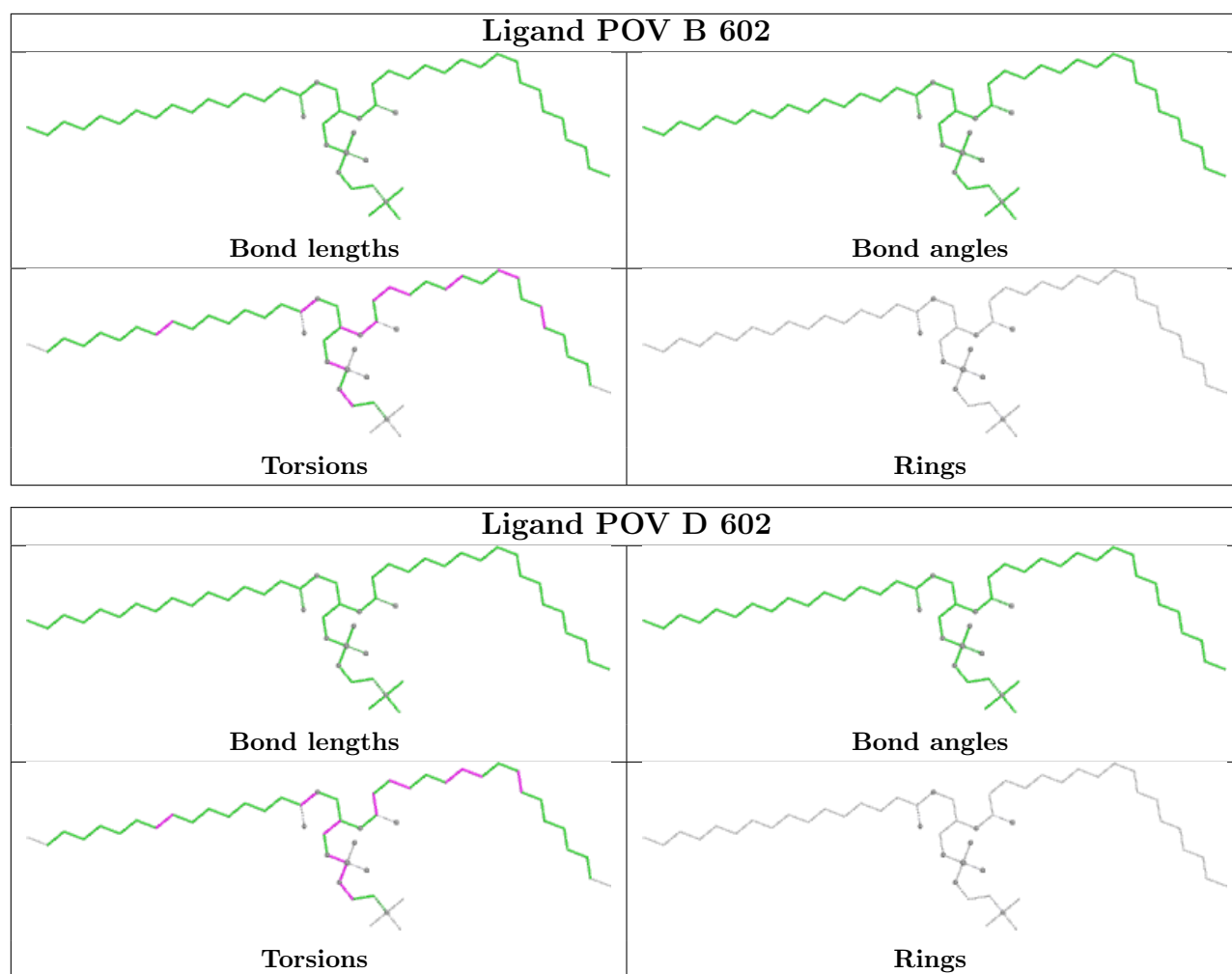
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	501	ABU	4	0
12	E	501	NAG	1	0
10	B	601	PIO	1	0
11	B	602	POV	5	0
11	D	602	POV	1	0

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 than 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.









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.

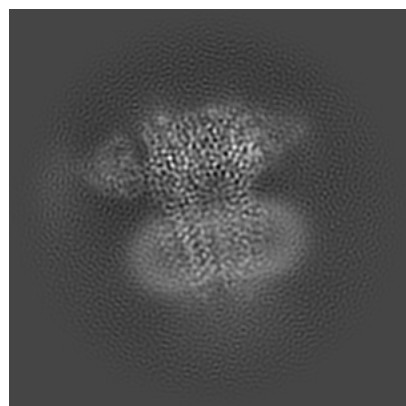
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45878. These allow visual inspection of the internal detail of the map and identification of artifacts.

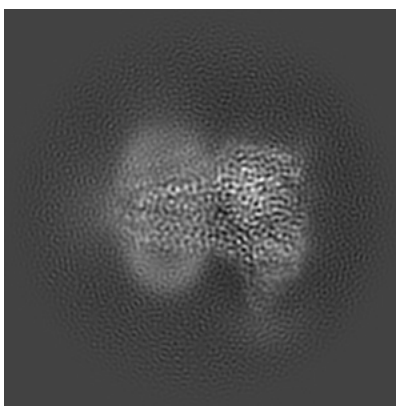
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

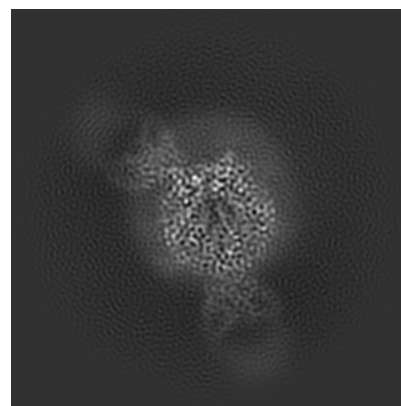
6.1.1 Primary map



X

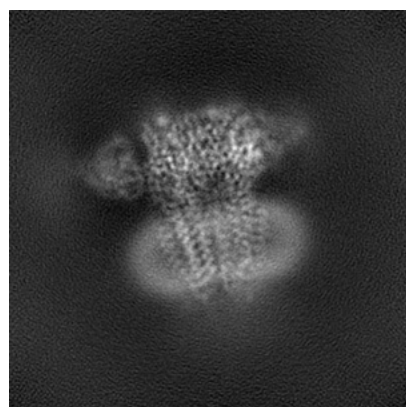


Y

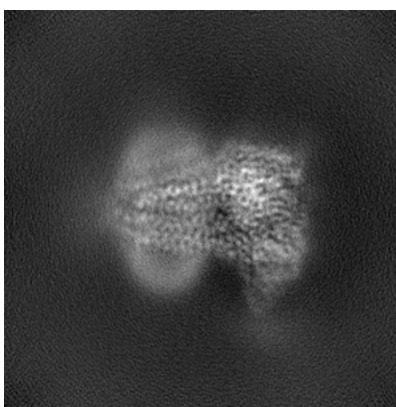


Z

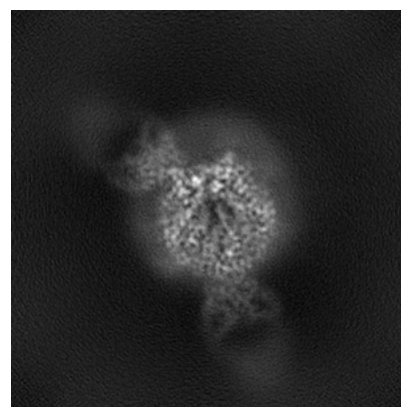
6.1.2 Raw map



X



Y

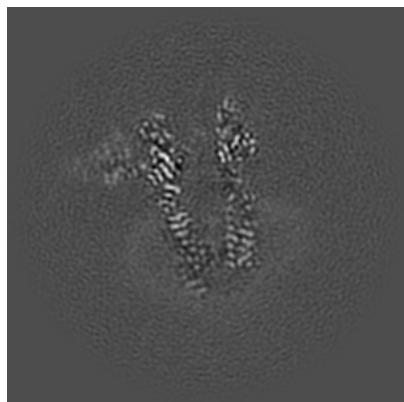


Z

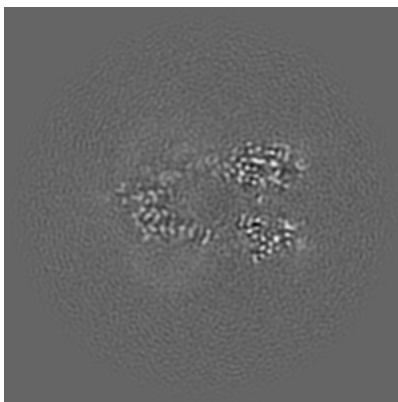
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

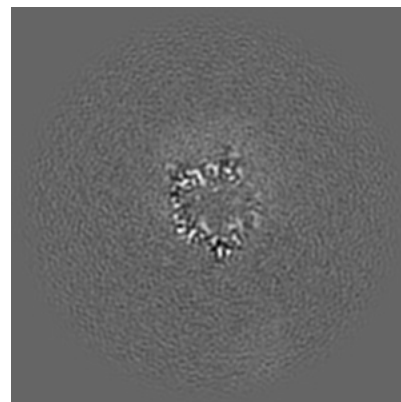
6.2.1 Primary map



X Index: 128

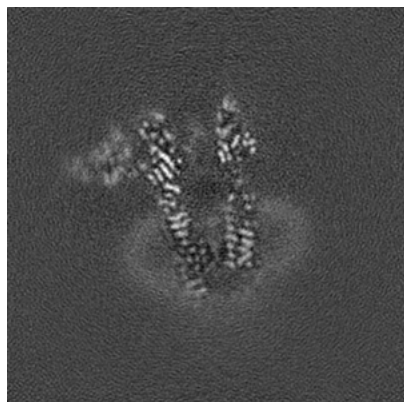


Y Index: 128

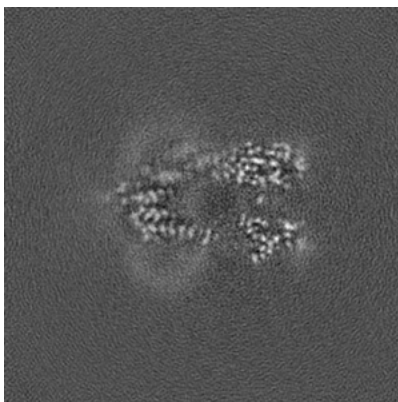


Z Index: 128

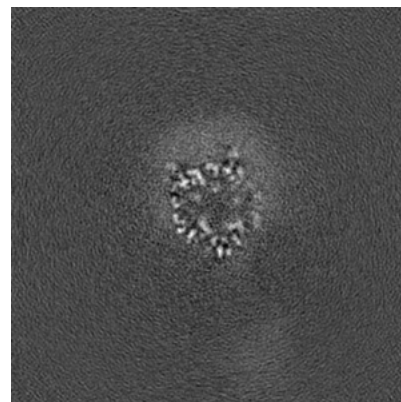
6.2.2 Raw map



X Index: 128



Y Index: 128

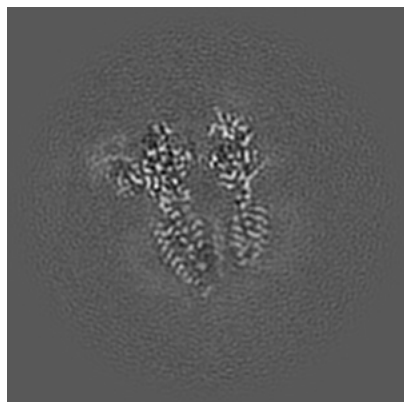


Z Index: 128

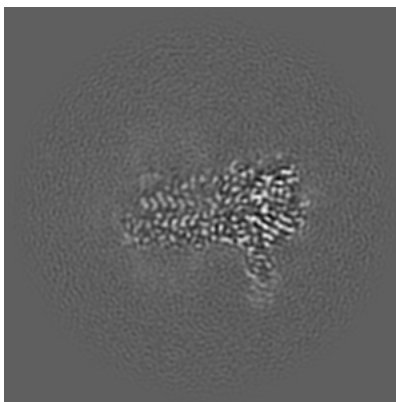
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

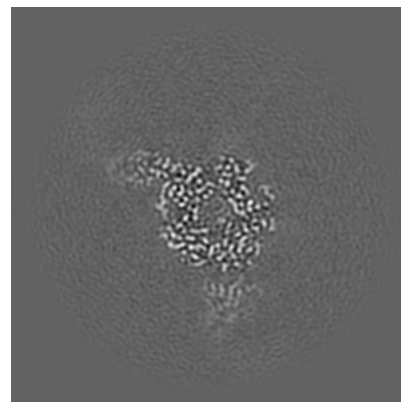
6.3.1 Primary map



X Index: 139

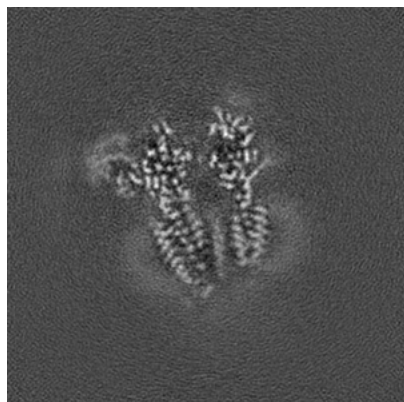


Y Index: 144

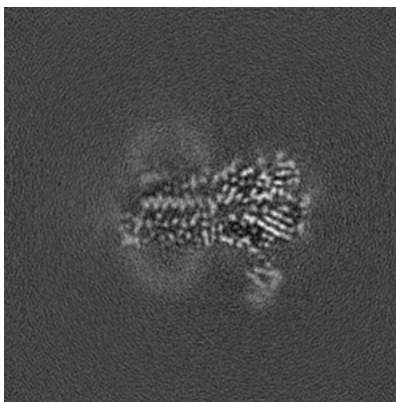


Z Index: 160

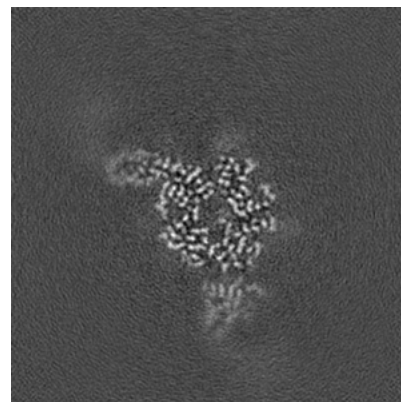
6.3.2 Raw map



X Index: 139



Y Index: 143

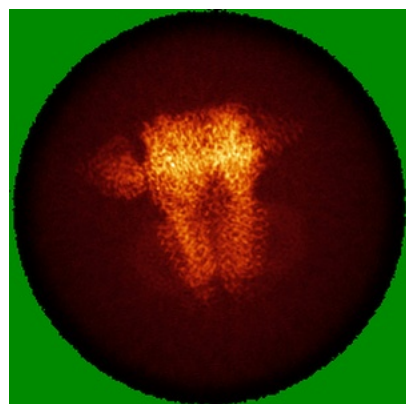


Z Index: 160

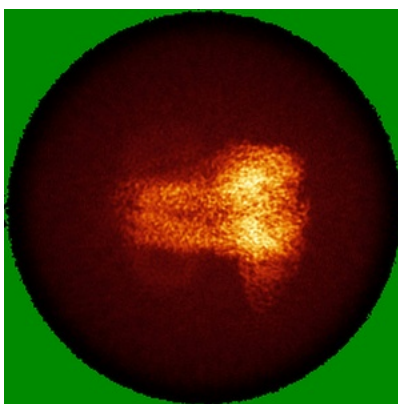
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

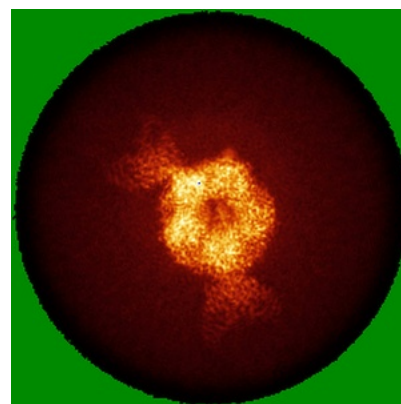
6.4.1 Primary map



X

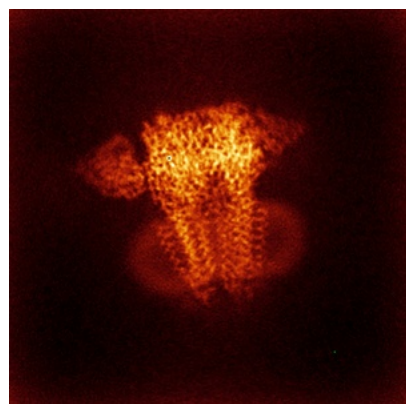


Y

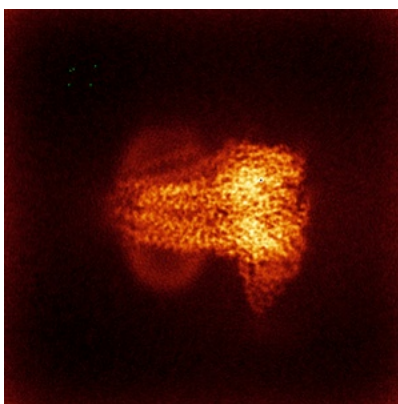


Z

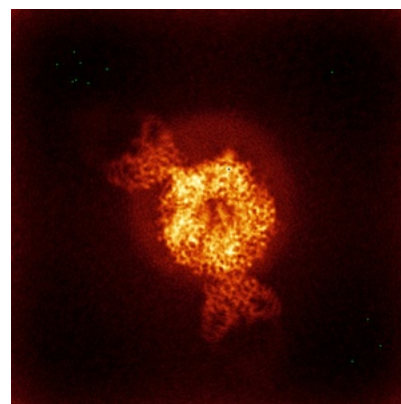
6.4.2 Raw map



X



Y

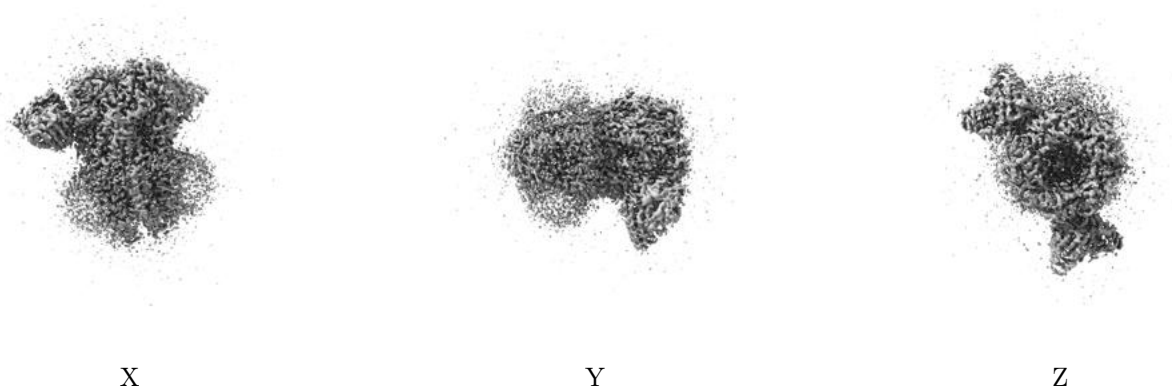


Z

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.

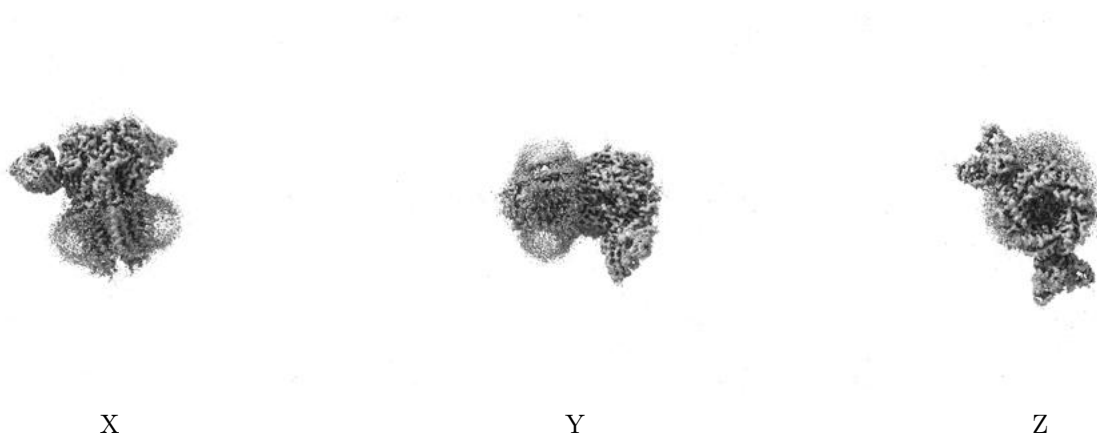
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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



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.

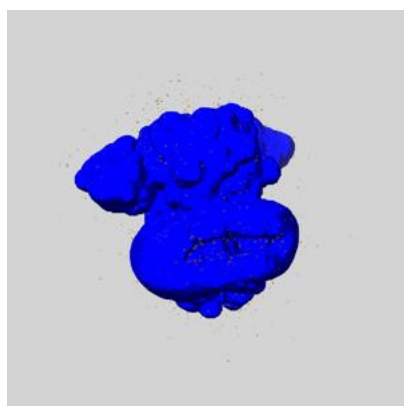
6.6 Mask visualisation [i](#)

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

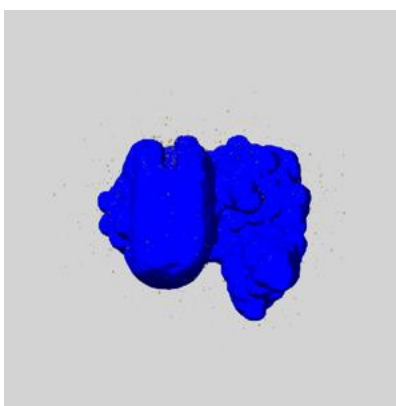
A mask typically either:

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

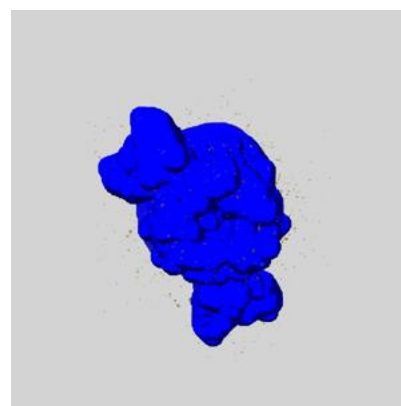
6.6.1 emd_45878_msk_1.map [i](#)



X



Y

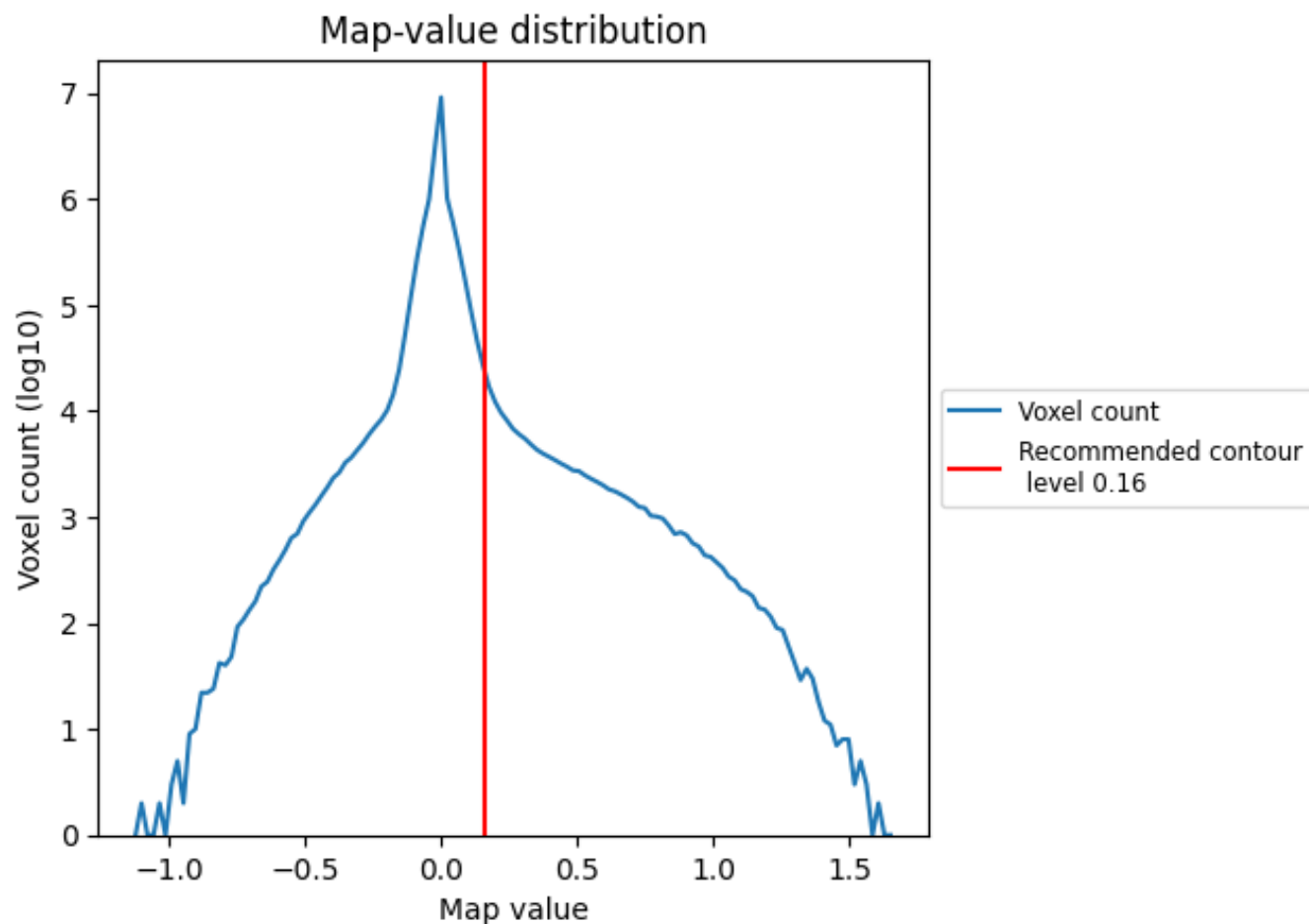


Z

7 Map analysis [i](#)

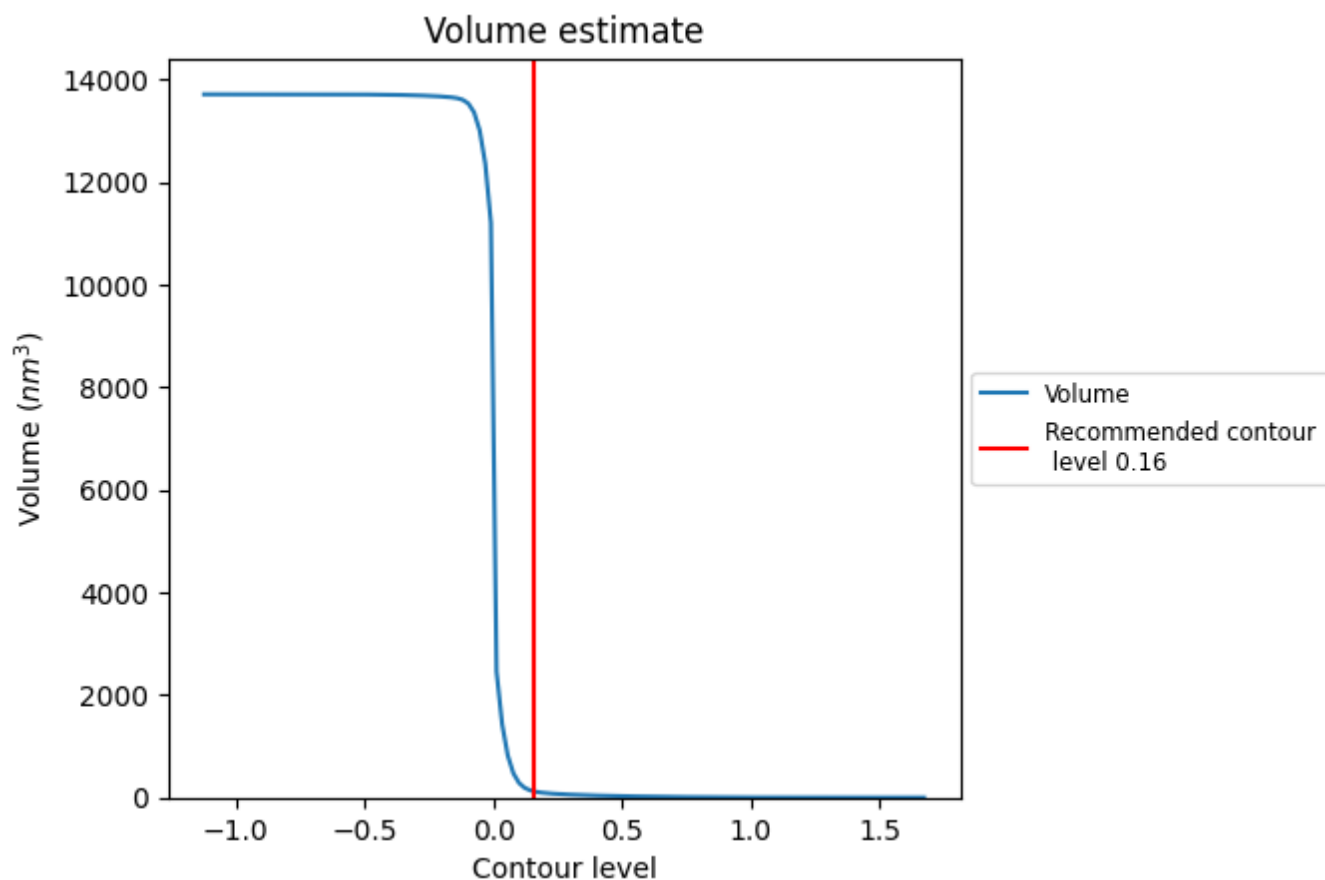
This section contains the results of statistical analysis of the map.

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.

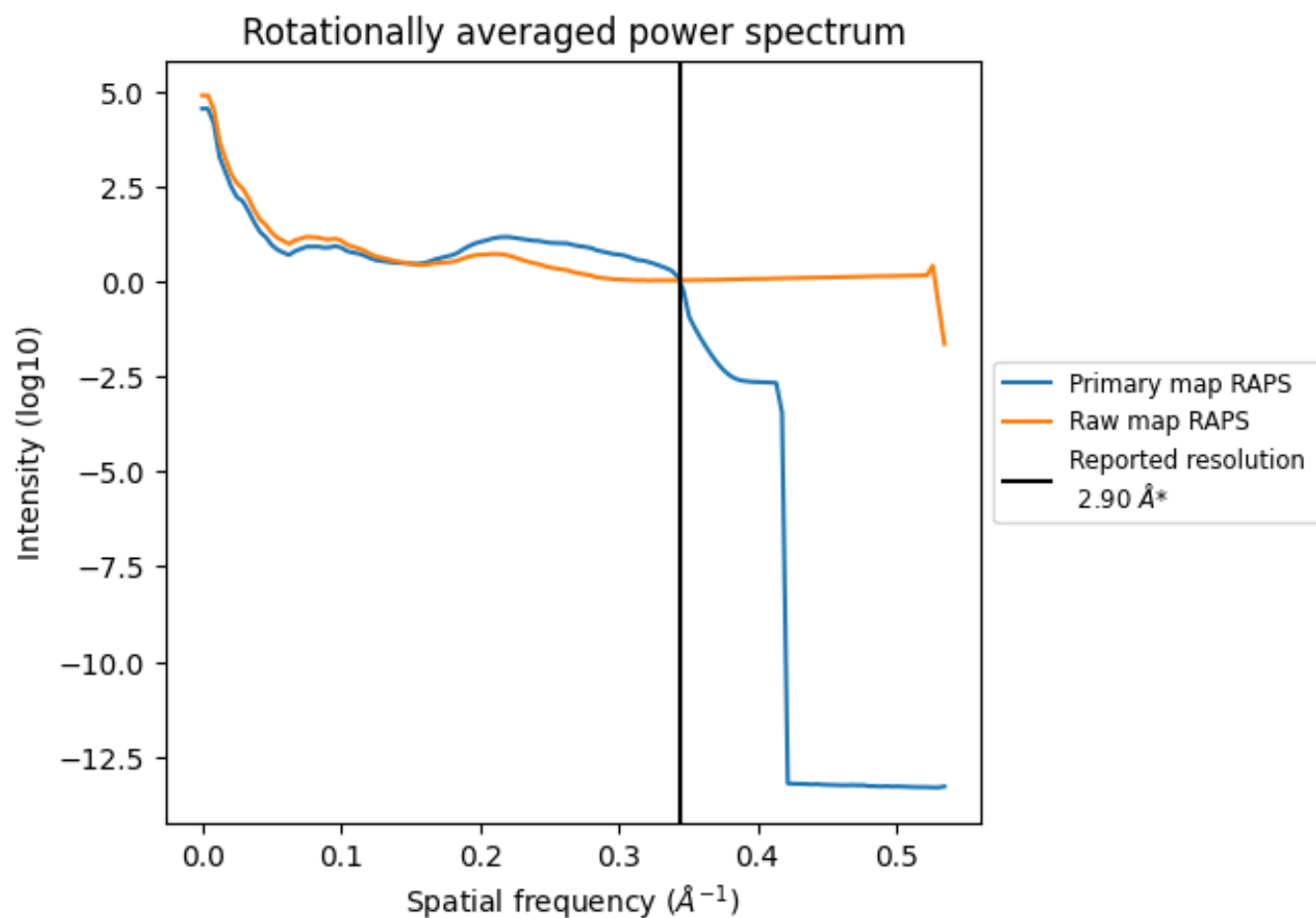
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 108 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 ⓘ

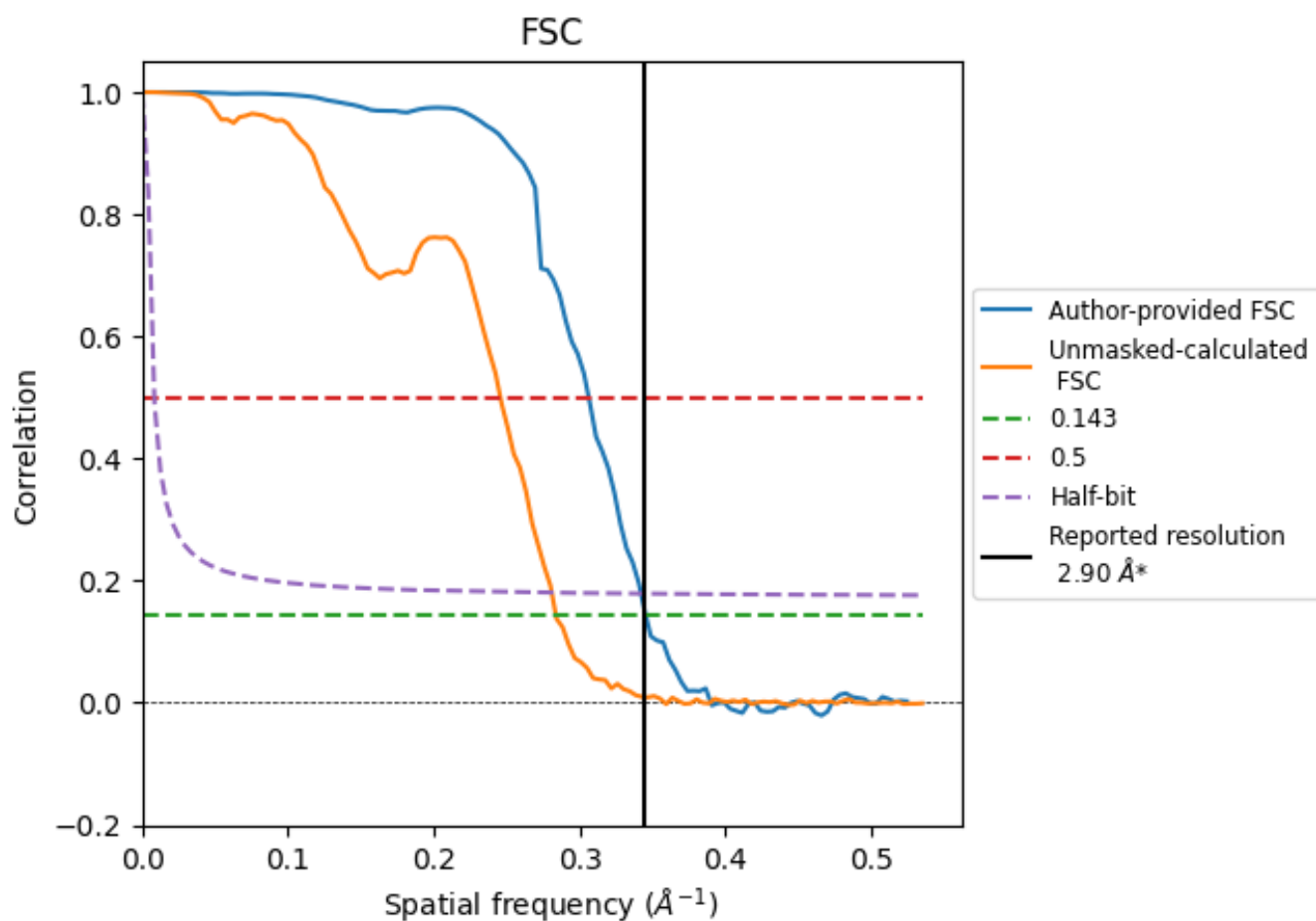


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

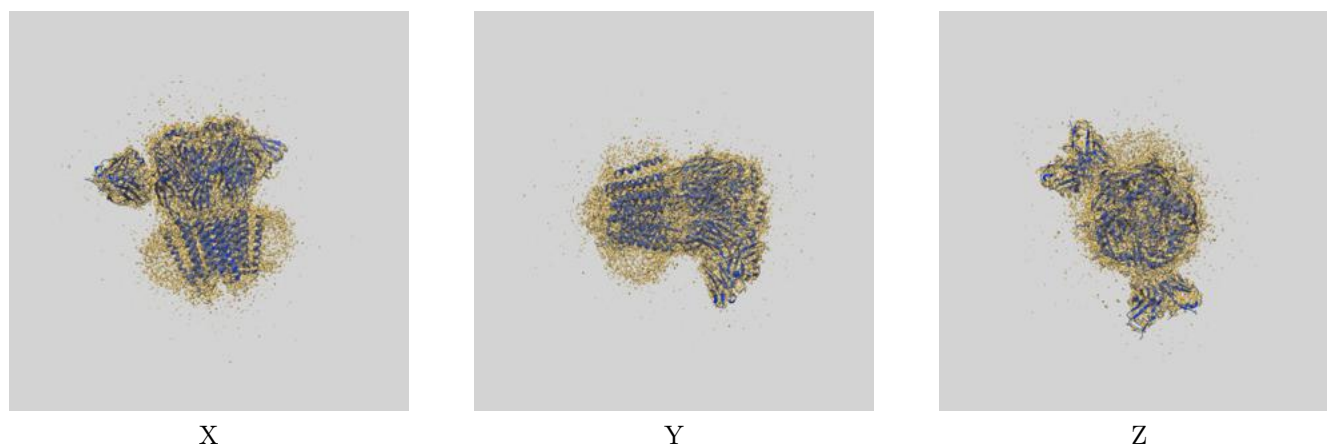
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.27	2.92
Unmasked-calculated*	3.52	4.07	3.56

*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 3.52 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

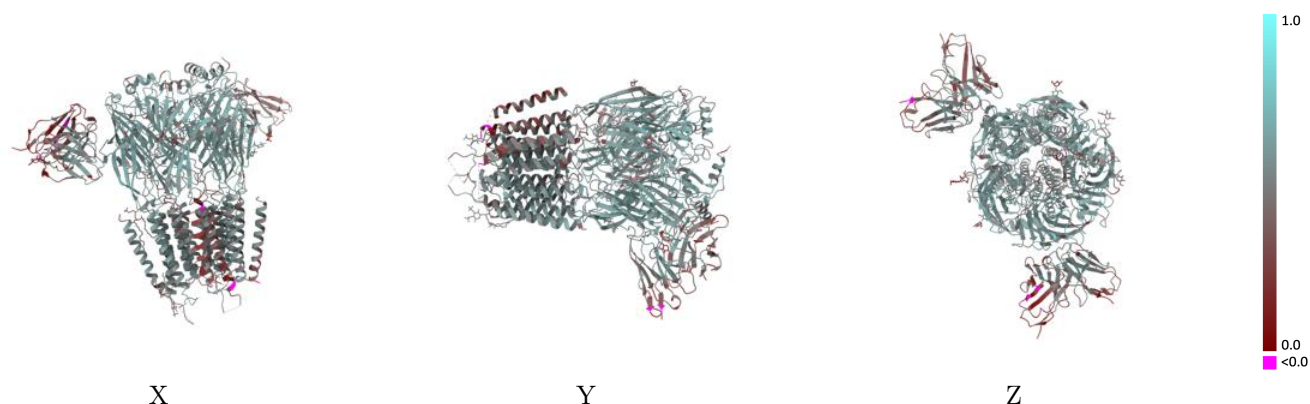
This section contains information regarding the fit between EMDB map EMD-45878 and PDB model 9CRS. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



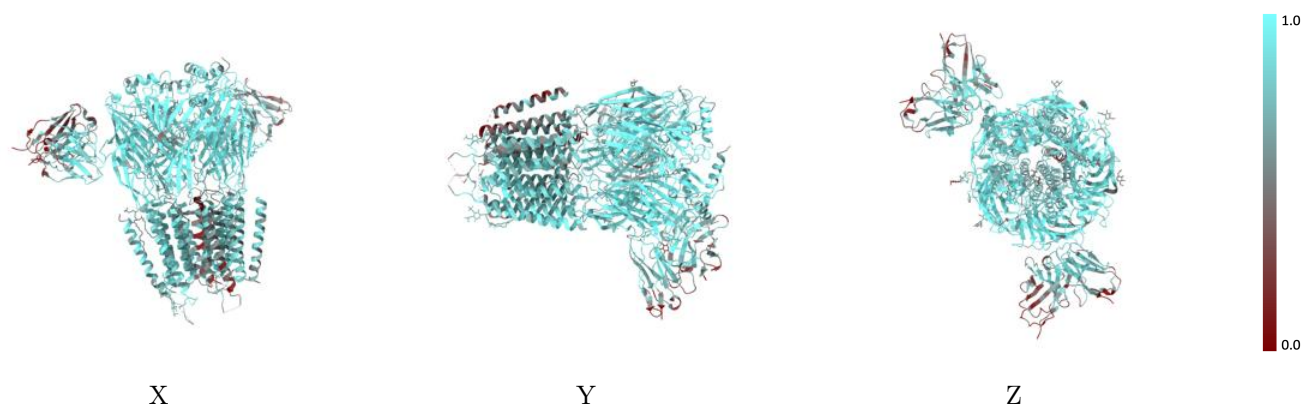
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



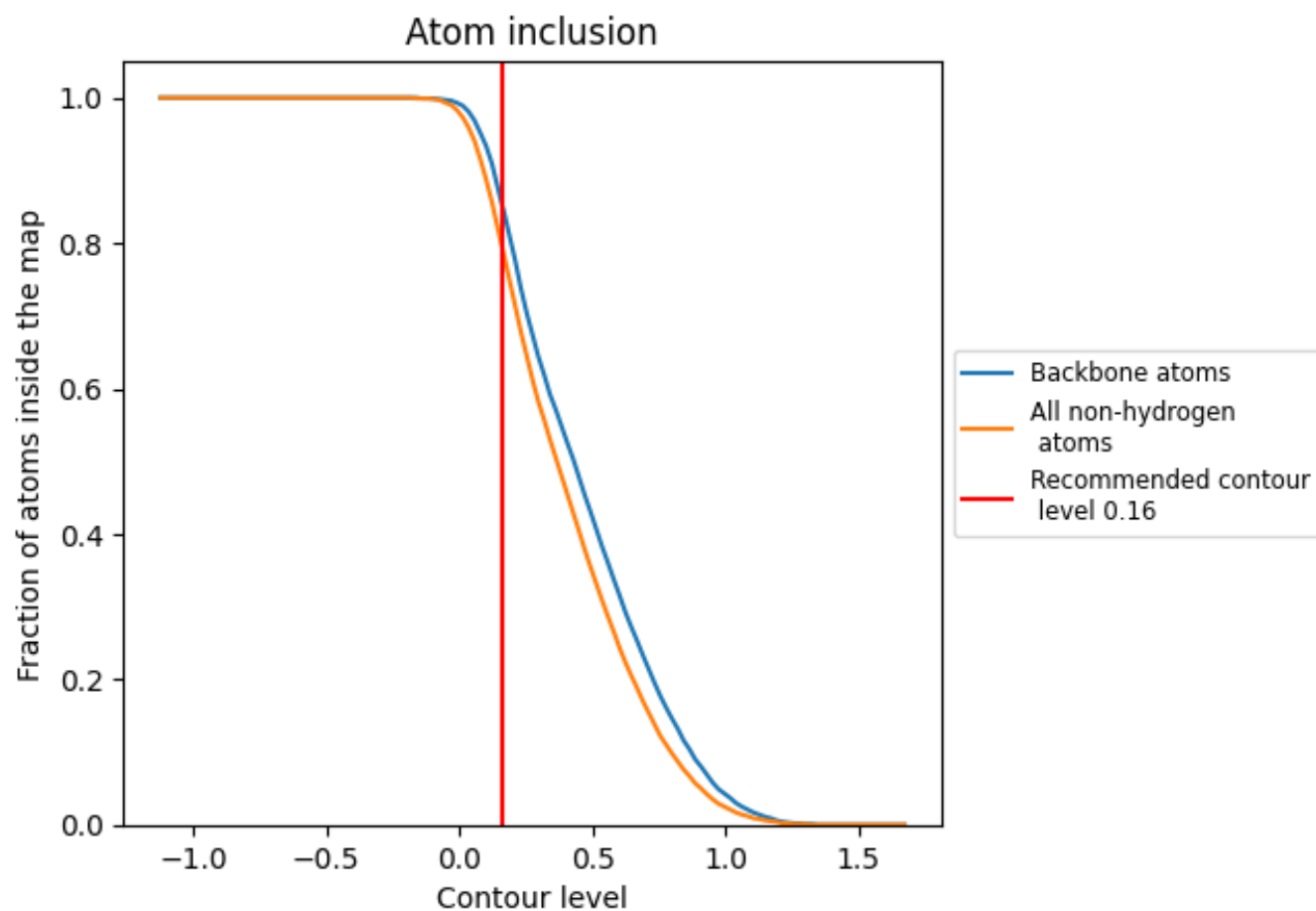
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7950	<div></div> 0.5090
A	<div></div> 0.8460	<div></div> 0.5400
B	<div></div> 0.8690	<div></div> 0.5570
C	<div></div> 0.8660	<div></div> 0.5490
D	<div></div> 0.8600	<div></div> 0.5500
E	<div></div> 0.7370	<div></div> 0.4800
F	<div></div> 0.8210	<div></div> 0.4420
G	<div></div> 0.6430	<div></div> 0.4320
H	<div></div> 0.7340	<div></div> 0.4910
I	<div></div> 0.6800	<div></div> 0.4300
J	<div></div> 0.6450	<div></div> 0.4200
K	<div></div> 0.5350	<div></div> 0.3390
L	<div></div> 0.7010	<div></div> 0.4420
M	<div></div> 0.7180	<div></div> 0.4400
N	<div></div> 0.5000	<div></div> 0.2000
O	<div></div> 0.6150	<div></div> 0.4830

