



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:10 PM UTC

PDB ID : 7OCI / pdb_00007oci
EMDB ID : EMD-12808
Title : Cryo-EM structure of yeast Ost6p containing oligosaccharyltransferase complex
Authors : Wild, R.; Neuhaus, J.D.; Eyring, J.; Irobalieva, R.N.; Kowal, J.; Lin, C.W.; Locher, K.P.; Aebi, M.
Deposited on : 2021-04-27
Resolution : 3.46 Å (reported)
Based on initial model : 6EZN

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:

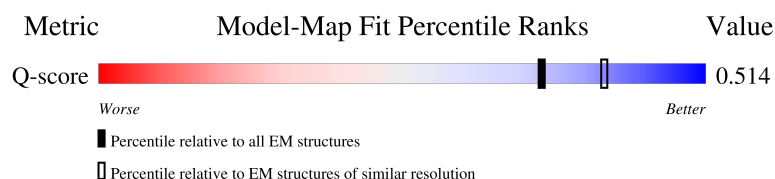
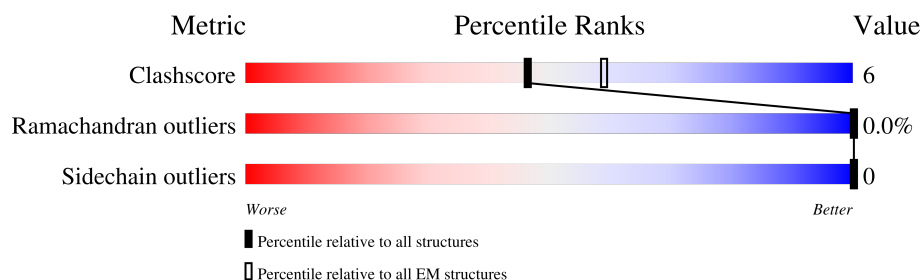
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.46 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.



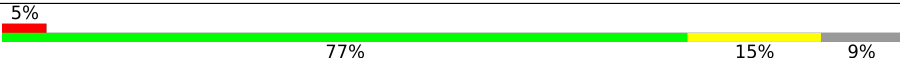
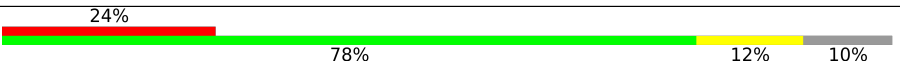
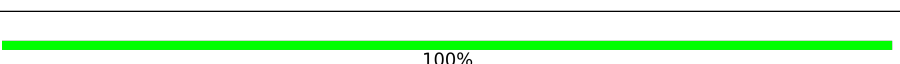
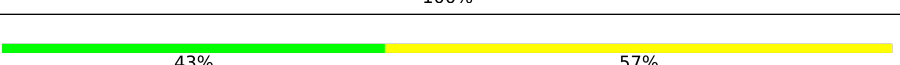
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13788 (2.96 - 3.96)

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	476	
2	B	130	
3	C	332	

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Mol	Chain	Length	Quality of chain
4	D	36	
5	E	86	
6	F	718	
7	G	430	
8	H	286	
9	I	24	
10	K	2	
11	J	7	

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
14	AJP	B	202	X	-	-	-
14	AJP	D	102	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 17077 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 Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	434	Total	C	N	O	S	0	0
			3503	2275	558	664	6		

- Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	108	Total	C	N	O	S	0	0
			869	588	139	136	6		

- Molecule 3 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	0	0
			933	638	138	148	9		

- Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	35	Total	C	N	O	S	0	0
			267	172	40	51	4		

- Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	85	Total	C	N	O	S	0	0
			666	448	99	118	1		

- Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	639	Total	C	N	O	S	0	0
			5130	3394	817	896	23		

- Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	393	Total	C	N	O	S	0	0
			3177	2041	524	609	3		

- Molecule 8 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	258	Total	C	N	O	S	0	0
			1873	1228	311	331	3		

- Molecule 9 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST6 - TM1.

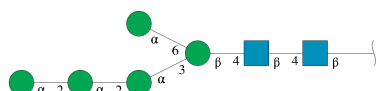
Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	24	Total	C	N	O		0	0
			120	72	24	24			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



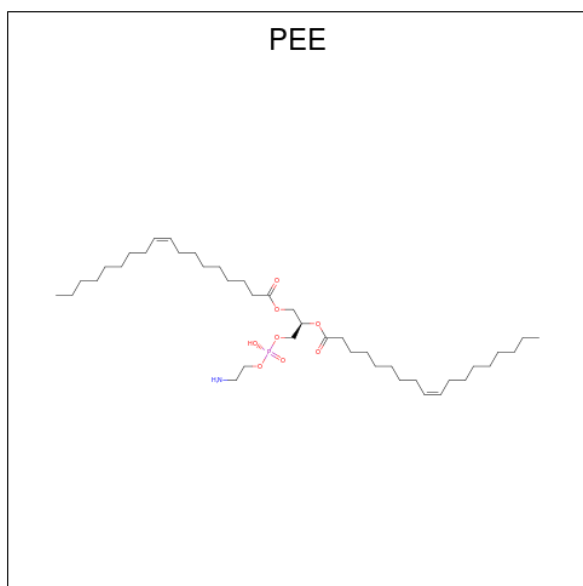
Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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
11	J	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 12 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	B	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
12	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	F	1	Total	C	N	O	P	0
			42	32	1	8	1	
12	H	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltCon
13	A	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0
13	G	1	Total 14	C 8	N 1	O 5	0

- Molecule 14 is Digitonin (CCD ID: AJP) (formula: $\text{C}_{56}\text{H}_{92}\text{O}_{29}$).



Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	C	O	0
			54	39	15	

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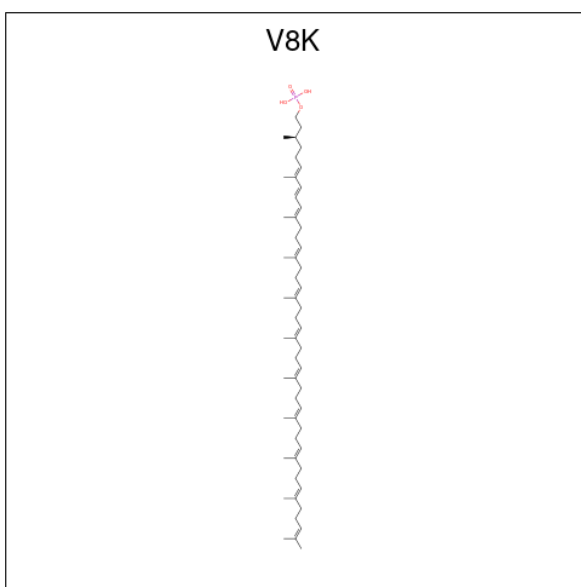
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Mol	Chain	Residues	Atoms			AltConf
14	D	1	Total	C	O	0
			43	33	10	

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

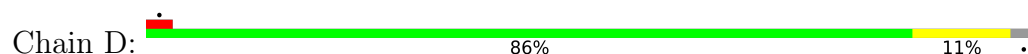
Mol	Chain	Residues	Atoms		AltConf
15	F	1	Total	Mg	0
			1	1	

- Molecule 16 is Dolichylphosphate (CCD ID: V8K) (formula: C₅₅H₉₁O₄P).

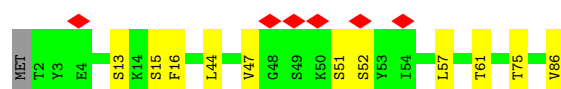
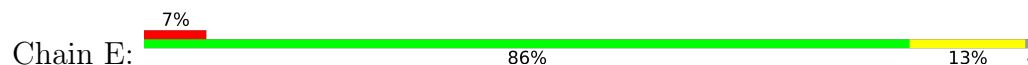


Mol	Chain	Residues	Atoms				AltConf
16	F	1	Total	C	O	P	0
			60	55	4	1	

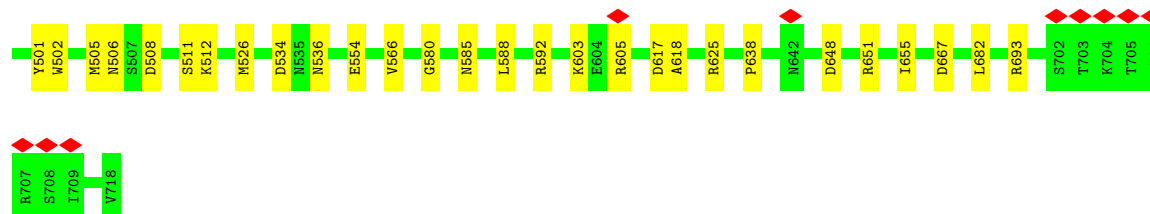
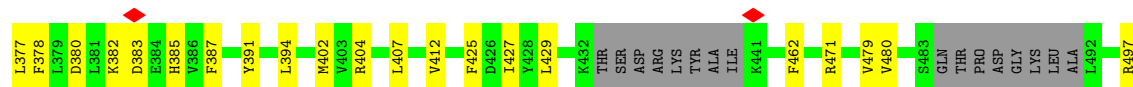
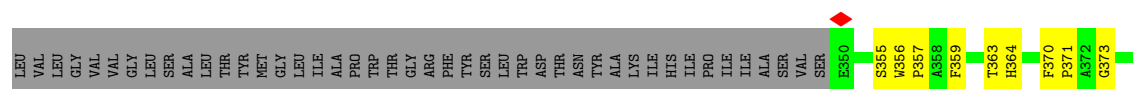
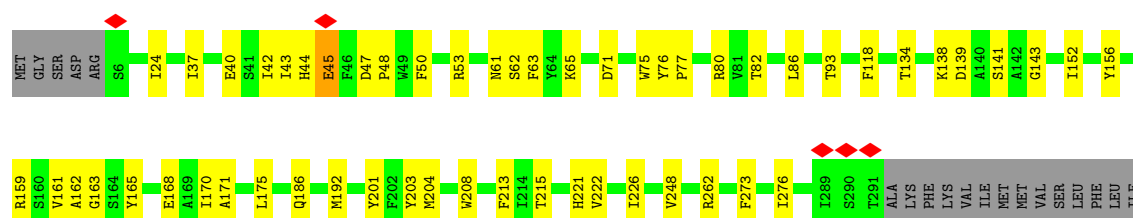
- Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4



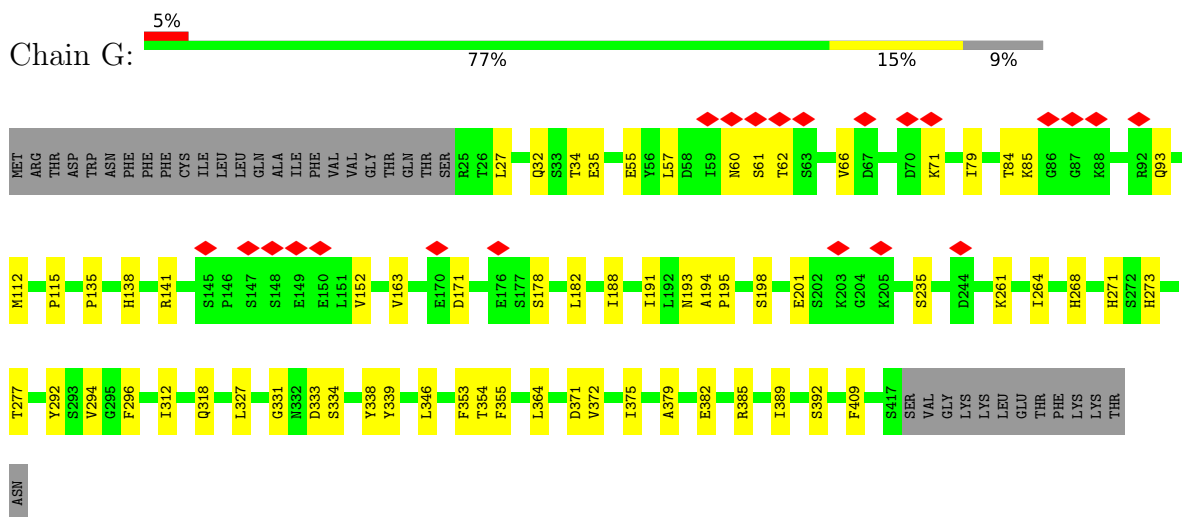
- Molecule 5: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5



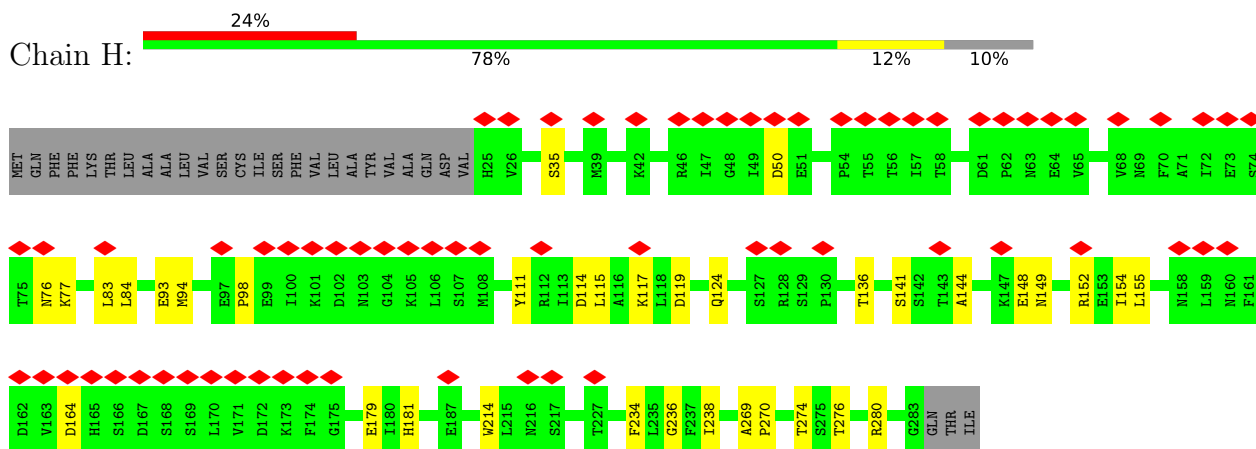
- Molecule 6: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



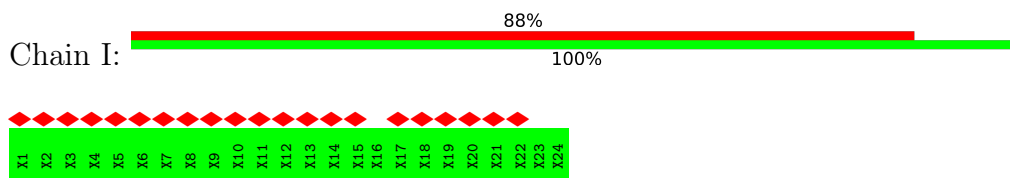
- Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1



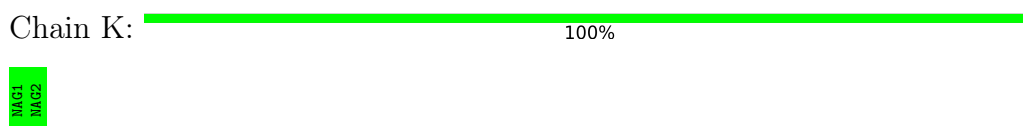
- Molecule 8: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1



- Molecule 9: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST6 - TM1



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAN1
MAN2
BOL3
MAN4
MAN5
MAN6
MAN7

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	220536	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 ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	322.56, 322.56, 322.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: MG, V8K, PEE, MAN, NAG, AJP, BMA

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	0.13	0/3605	0.34	0/4908
2	B	0.14	0/891	0.31	0/1203
3	C	0.13	0/961	0.27	0/1301
4	D	0.12	0/270	0.22	0/365
5	E	0.12	0/684	0.29	0/926
6	F	0.16	0/5281	0.35	0/7186
7	G	0.12	0/3259	0.32	0/4431
8	H	0.11	0/1912	0.31	0/2606
All	All	0.14	0/16863	0.32	0/22926

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	3503	0	3378	47	0
2	B	869	0	899	16	0
3	C	933	0	956	8	0
4	D	267	0	280	4	0
5	E	666	0	677	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	5130	0	5053	77	0
7	G	3177	0	3058	39	0
8	H	1873	0	1787	21	0
9	I	120	0	26	0	0
10	K	28	0	25	0	0
11	J	83	0	70	0	0
12	A	35	0	44	2	0
12	B	33	0	40	0	0
12	C	36	0	46	0	0
12	D	38	0	50	0	0
12	F	42	0	58	1	0
12	H	44	0	62	2	0
13	A	14	0	13	0	0
13	G	28	0	26	1	0
14	B	54	0	0	1	0
14	D	43	0	0	1	0
15	F	1	0	0	0	0
16	F	60	0	0	0	0
All	All	17077	0	16548	205	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 6.

All (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASP:HB3	1:A:415:GLY:HA2	1.70	0.72
6:F:42:ILE:HG13	6:F:43:ILE:H	1.57	0.69
6:F:77:PRO:O	7:G:318:GLN:NE2	2.27	0.67
6:F:588:LEU:O	6:F:592:ARG:HG2	1.96	0.65
6:F:580:GLY:O	6:F:585:ASN:ND2	2.23	0.65
7:G:354:THR:HG22	7:G:372:VAL:HG22	1.77	0.65
6:F:168:GLU:HA	6:F:171:ALA:HB3	1.80	0.64
6:F:40:GLU:OE2	6:F:497:ARG:NH1	2.29	0.64
7:G:163:VAL:HG11	7:G:191:ILE:HD13	1.79	0.64
4:D:29:ASP:OD2	6:F:141:SER:OG	2.16	0.64
1:A:232:GLN:NE2	1:A:375:ASP:OD2	2.28	0.64
6:F:364:HIS:HB3	6:F:462:PHE:HD1	1.64	0.62
1:A:31:TRP:HB3	1:A:55:ILE:HD11	1.81	0.62
6:F:391:TYR:CE2	6:F:412:VAL:HB	2.35	0.61
7:G:60:ASN:OD1	7:G:61:SER:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:617:ASP:OD1	6:F:618:ALA:N	2.31	0.61
7:G:57:LEU:HD11	7:G:62:THR:HG21	1.83	0.60
1:A:378:GLU:OE2	1:A:420:THR:OG1	2.19	0.60
6:F:554:GLU:OE2	6:F:693:ARG:NH2	2.35	0.60
3:C:220:MET:HE2	6:F:378:PHE:HB3	1.84	0.59
8:H:276:THR:O	8:H:280:ARG:HG2	2.03	0.59
1:A:33:ASN:HD22	1:A:170:THR:HG22	1.69	0.58
7:G:27:LEU:HB3	7:G:79:ILE:HD13	1.84	0.58
1:A:124:SER:HB3	1:A:127:GLU:HB2	1.84	0.58
3:C:284:LEU:O	3:C:288:VAL:HG23	2.04	0.58
1:A:377:VAL:HG21	1:A:426:LEU:HD12	1.86	0.57
6:F:603:LYS:HZ2	6:F:605:ARG:HE	1.52	0.57
1:A:64:THR:HG23	1:A:119:PHE:HB2	1.87	0.57
6:F:159:ARG:NH1	6:F:168:GLU:OE2	2.38	0.56
1:A:36:TYR:O	1:A:173:ALA:HA	2.05	0.56
1:A:199:ASN:OD1	1:A:200:GLY:N	2.38	0.56
1:A:144:TYR:HB3	1:A:145:PRO:HD3	1.87	0.56
7:G:193:ASN:OD1	7:G:194:ALA:N	2.39	0.55
6:F:222:VAL:O	6:F:226:ILE:HG12	2.07	0.55
7:G:264:ILE:HG13	7:G:364:LEU:HD21	1.88	0.55
6:F:479:VAL:HG13	6:F:480:VAL:HG23	1.88	0.55
14:B:202:AJP:C83	14:B:202:AJP:C81	2.85	0.54
2:B:113:GLU:HG2	6:F:192:MET:HB2	1.90	0.54
8:H:154:ILE:HG12	8:H:155:LEU:HD12	1.89	0.54
7:G:115:PRO:HD3	7:G:178:SER:HB3	1.88	0.53
6:F:213:PHE:HE2	6:F:391:TYR:HE1	1.55	0.53
8:H:50:ASP:O	8:H:152:ARG:NH1	2.42	0.53
2:B:79:ALA:HB2	2:B:128:PHE:HD2	1.73	0.53
6:F:425:PHE:HB3	6:F:429:LEU:HD12	1.90	0.53
4:D:7:LEU:HD22	6:F:37:ILE:HG13	1.91	0.53
1:A:408:SER:OG	1:A:409:TYR:N	2.41	0.53
6:F:62:SER:OG	6:F:63:PHE:N	2.42	0.53
2:B:62:CYS:O	2:B:65:ILE:HG22	2.10	0.52
1:A:40:ILE:HB	1:A:177:LEU:HD23	1.91	0.51
1:A:156:LEU:HD21	1:A:230:LEU:HD11	1.92	0.51
6:F:45:GLU:O	6:F:48:PRO:HD2	2.10	0.51
6:F:425:PHE:O	6:F:429:LEU:N	2.42	0.51
1:A:97:LEU:HG	1:A:98:ALA:H	1.75	0.51
1:A:298:GLY:O	1:A:343:ASN:ND2	2.43	0.51
6:F:356:TRP:CD1	6:F:357:PRO:HD3	2.46	0.51
1:A:306:ASP:OD1	1:A:307:LEU:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:201:TYR:HH	6:F:215:THR:HG1	1.59	0.50
1:A:453:ILE:HG21	5:E:75:THR:HG21	1.94	0.50
7:G:84:THR:HG22	7:G:85:LYS:H	1.77	0.50
12:A:1301:PEE:H8	12:F:902:PEE:H1	1.94	0.50
7:G:55:GLU:N	7:G:55:GLU:OE1	2.45	0.50
8:H:76:ASN:ND2	8:H:149:ASN:OD1	2.45	0.50
8:H:77:LYS:O	8:H:141:SER:OG	2.19	0.50
6:F:80:ARG:NH1	6:F:536:ASN:HD21	2.10	0.49
8:H:76:ASN:HD22	8:H:149:ASN:HA	1.77	0.49
5:E:15:SER:OG	5:E:16:PHE:N	2.45	0.49
6:F:80:ARG:CZ	6:F:536:ASN:HD21	2.25	0.49
7:G:327:LEU:HB3	7:G:339:TYR:HB3	1.93	0.49
6:F:50:PHE:HE2	6:F:86:LEU:HD13	1.78	0.49
1:A:42:VAL:HG12	1:A:47:ILE:HD12	1.95	0.49
1:A:449:LYS:HB3	1:A:450:PRO:HD3	1.94	0.49
14:D:102:AJP:C81	14:D:102:AJP:C83	2.91	0.49
1:A:184:GLU:O	1:A:222:ILE:HG13	2.13	0.49
1:A:249:ILE:HB	1:A:345:LEU:HD13	1.94	0.48
1:A:156:LEU:O	1:A:223:VAL:HA	2.13	0.48
7:G:333:ASP:OD1	7:G:334:SER:N	2.38	0.48
2:B:50:PHE:HB2	8:H:214:TRP:HZ2	1.78	0.48
3:C:289:PRO:HG2	6:F:427:ILE:HG21	1.95	0.48
6:F:221:HIS:CE1	6:F:387:PHE:HB2	2.48	0.48
7:G:379:ALA:HB3	7:G:382:GLU:OE1	2.13	0.48
3:C:273:LEU:O	3:C:277:VAL:HG23	2.13	0.48
6:F:44:HIS:ND1	6:F:163:GLY:HA3	2.29	0.48
7:G:271:HIS:HB3	7:G:292:TYR:HD1	1.79	0.48
8:H:84:LEU:HB3	8:H:93:GLU:OE1	2.13	0.47
6:F:566:VAL:O	6:F:682:LEU:HD12	2.15	0.47
5:E:44:LEU:HA	5:E:47:VAL:HG12	1.96	0.47
6:F:359:PHE:O	6:F:363:THR:OG1	2.28	0.47
6:F:382:LYS:HB2	6:F:385:HIS:ND1	2.29	0.47
12:H:1101:PEE:H27	12:H:1101:PEE:H33	1.68	0.47
1:A:38:ARG:HB2	1:A:51:ILE:HG22	1.96	0.47
6:F:648:ASP:OD2	6:F:651:ARG:NH2	2.48	0.47
7:G:32:GLN:HB2	13:G:502:NAG:H62	1.95	0.47
6:F:82:THR:HG22	6:F:86:LEU:HD22	1.96	0.47
2:B:65:ILE:HD11	2:B:71:ASN:HB3	1.97	0.46
6:F:175:LEU:HD13	6:F:204:MET:HE1	1.97	0.46
1:A:97:LEU:HD13	1:A:116:ILE:HD11	1.96	0.46
7:G:182:LEU:HD22	7:G:188:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:179:GLU:OE2	8:H:181:HIS:NE2	2.48	0.46
1:A:144:TYR:CE2	7:G:71:LYS:HG3	2.50	0.46
6:F:402:MET:HE2	6:F:404:ARG:HB3	1.97	0.46
1:A:85:PHE:HB2	1:A:88:GLU:HG2	1.97	0.46
1:A:237:ARG:O	1:A:237:ARG:HG3	2.14	0.46
6:F:152:ILE:O	6:F:152:ILE:HG13	2.15	0.46
7:G:331:GLY:HA3	7:G:338:TYR:HB2	1.98	0.46
7:G:34:THR:HG22	7:G:35:GLU:HG2	1.97	0.46
1:A:245:TRP:HB2	5:E:86:VAL:HG12	1.98	0.45
6:F:138:LYS:HG2	6:F:139:ASP:H	1.81	0.45
2:B:86:GLY:HA2	2:B:89:VAL:HG22	1.98	0.45
12:H:1101:PEE:H14	12:H:1101:PEE:H20	1.72	0.45
6:F:118:PHE:HZ	6:F:170:ILE:HD12	1.81	0.45
6:F:213:PHE:CE2	6:F:391:TYR:HE1	2.34	0.45
8:H:236:GLY:HA3	8:H:274:THR:HG21	1.98	0.45
7:G:201:GLU:HG3	7:G:201:GLU:O	2.16	0.45
7:G:355:PHE:HB2	7:G:371:ASP:OD1	2.17	0.45
1:A:351:VAL:O	5:E:13:SER:HB2	2.17	0.45
6:F:356:TRP:CG	6:F:357:PRO:HD3	2.52	0.45
2:B:38:ILE:HD11	2:B:45:LYS:HG3	1.98	0.44
7:G:409:PHE:HB2	8:H:214:TRP:CH2	2.52	0.44
6:F:501:TYR:CZ	6:F:505:MET:HE3	2.52	0.44
7:G:84:THR:HG22	7:G:85:LYS:N	2.31	0.44
8:H:35:SER:HA	8:H:115:LEU:HB2	1.99	0.44
3:C:237:VAL:HG23	3:C:242:ILE:HB	1.99	0.44
6:F:471:ARG:HH11	6:F:471:ARG:HG3	1.82	0.44
1:A:372:THR:H	1:A:428:SER:HB3	1.82	0.44
8:H:94:MET:HE1	8:H:119:ASP:H	1.83	0.44
6:F:625:ARG:HH11	6:F:625:ARG:HG3	1.83	0.44
3:C:284:LEU:HD12	3:C:284:LEU:HA	1.87	0.44
5:E:57:LEU:O	5:E:61:THR:HG23	2.18	0.44
2:B:72:PHE:HE2	7:G:389:ILE:HD13	1.83	0.44
4:D:27:ALA:HB2	6:F:429:LEU:HD13	2.00	0.44
2:B:34:TYR:OH	2:B:48:ASP:OD2	2.35	0.43
7:G:66:VAL:HG12	7:G:93:GLN:OE1	2.18	0.43
7:G:152:VAL:HG13	7:G:171:ASP:HB3	2.00	0.43
7:G:195:PRO:HG2	7:G:198:SER:HB3	1.99	0.43
1:A:196:GLY:HA3	1:A:203:PHE:CZ	2.54	0.43
2:B:109:ARG:NH2	2:B:113:GLU:OE2	2.40	0.43
6:F:48:PRO:HB3	6:F:165:TYR:HB3	2.00	0.43
6:F:262:ARG:HG2	6:F:262:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:TRP:HB2	1:A:211:ILE:HD11	1.99	0.43
6:F:273:PHE:O	6:F:276:ILE:HG22	2.18	0.43
1:A:36:TYR:CE2	1:A:164:PRO:HB3	2.53	0.43
1:A:395:PRO:HG3	1:A:434:GLN:H	1.84	0.43
6:F:47:ASP:HB3	6:F:48:PRO:HD3	2.01	0.43
2:B:124:VAL:HG11	6:F:248:VAL:HG13	1.99	0.43
6:F:134:THR:HB	6:F:143:GLY:HA2	2.01	0.43
2:B:35:PHE:HA	2:B:38:ILE:HG22	2.00	0.43
6:F:171:ALA:HB1	6:F:208:TRP:CE3	2.54	0.42
6:F:638:PRO:HG3	6:F:655:ILE:HG22	2.01	0.42
7:G:268:HIS:O	7:G:294:VAL:HA	2.19	0.42
7:G:296:PHE:CE2	7:G:312:ILE:HD13	2.54	0.42
8:H:114:ASP:OD1	8:H:117:LYS:N	2.52	0.42
6:F:168:GLU:OE1	6:F:168:GLU:N	2.49	0.42
8:H:269:ALA:HB3	8:H:270:PRO:HD3	2.01	0.42
1:A:75:PHE:HE1	1:A:96:LEU:HD22	1.84	0.42
2:B:73:PRO:HG3	7:G:392:SER:HB3	2.00	0.42
6:F:61:ASN:HB3	6:F:65:LYS:HE2	2.00	0.42
1:A:80:PHE:HB3	1:A:136:PHE:HB2	2.01	0.42
6:F:76:TYR:CE1	6:F:512:LYS:HE2	2.54	0.42
6:F:508:ASP:OD1	6:F:511:SER:HB3	2.20	0.42
6:F:156:TYR:HD1	6:F:407:LEU:HD11	1.84	0.42
6:F:394:LEU:HD23	6:F:394:LEU:HA	1.85	0.42
8:H:234:PHE:CZ	8:H:238:ILE:HD11	2.53	0.42
5:E:51:SER:OG	5:E:52:SER:N	2.53	0.42
6:F:53:ARG:NH2	6:F:71:ASP:OD1	2.46	0.42
6:F:93:THR:OG1	6:F:203:TYR:OH	2.28	0.42
7:G:112:MET:HE2	7:G:235:SER:HA	2.00	0.42
1:A:409:TYR:CE1	12:A:1301:PEE:H14	2.54	0.42
6:F:373:GLY:O	6:F:377:LEU:HG	2.20	0.42
4:D:18:MET:SD	6:F:24:ILE:HG12	2.60	0.42
8:H:124:GLN:NE2	8:H:164:ASP:O	2.50	0.42
6:F:161:VAL:HG12	6:F:162:ALA:H	1.85	0.42
1:A:351:VAL:HG12	1:A:359:PHE:CE2	2.55	0.41
6:F:186:GLN:HE22	6:F:383:ASP:HB3	1.85	0.41
7:G:273:HIS:HB2	7:G:277:THR:O	2.20	0.41
8:H:98:PRO:HB3	8:H:111:TYR:CZ	2.55	0.41
1:A:264:LEU:HD23	1:A:264:LEU:H	1.85	0.41
2:B:45:LYS:O	2:B:49:THR:HG22	2.20	0.41
6:F:75:TRP:NE1	6:F:534:ASP:OD1	2.53	0.41
6:F:355:SER:OG	6:F:357:PRO:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:370:PHE:HB3	6:F:371:PRO:HD3	2.02	0.41
1:A:32:GLU:O	1:A:55:ILE:HD12	2.20	0.41
6:F:380:ASP:N	6:F:380:ASP:OD1	2.52	0.41
7:G:141:ARG:NH1	7:G:201:GLU:OE2	2.54	0.41
1:A:398:PHE:HB3	1:A:423:TYR:CE2	2.56	0.41
1:A:72:SER:HB2	1:A:111:GLU:O	2.20	0.41
6:F:502:TRP:CD1	6:F:506:ASN:HD22	2.39	0.41
6:F:603:LYS:HG2	6:F:605:ARG:HH21	1.85	0.41
7:G:163:VAL:O	7:G:261:LYS:HE2	2.21	0.41
3:C:318:ILE:HD12	3:C:332:PHE:CE1	2.56	0.41
1:A:66:TYR:C	1:A:67:PHE:HD1	2.29	0.41
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.95	0.41
6:F:497:ARG:HG2	6:F:526:MET:SD	2.61	0.41
7:G:135:PRO:HG2	7:G:138:HIS:ND1	2.36	0.41
1:A:449:LYS:NZ	5:E:86:VAL:HB	2.36	0.41
2:B:48:ASP:OD1	2:B:49:THR:N	2.54	0.41
2:B:49:THR:HG23	8:H:214:TRP:HE1	1.85	0.41
6:F:377:LEU:HD22	6:F:385:HIS:CD2	2.55	0.41
7:G:318:GLN:HB2	7:G:353:PHE:CE1	2.56	0.41
7:G:346:LEU:HD13	7:G:375:ILE:HD13	2.03	0.41
3:C:232:THR:HG22	3:C:232:THR:O	2.20	0.40
8:H:83:LEU:HD12	8:H:136:THR:O	2.21	0.40
6:F:667:ASP:OD1	6:F:667:ASP:N	2.54	0.40
1:A:307:LEU:HB2	6:F:501:TYR:CE1	2.57	0.40
8:H:144:ALA:HB1	8:H:148:GLU:OE2	2.22	0.40
7:G:385:ARG:HA	7:G:385:ARG:HD2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/476 (90%)	414 (96%)	16 (4%)	0	100	100
2	B	106/130 (82%)	103 (97%)	3 (3%)	0	100	100
3	C	117/332 (35%)	116 (99%)	1 (1%)	0	100	100
4	D	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
5	E	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
6	F	631/718 (88%)	618 (98%)	12 (2%)	1 (0%)	43	74
7	G	391/430 (91%)	381 (97%)	10 (3%)	0	100	100
8	H	256/286 (90%)	244 (95%)	12 (5%)	0	100	100
All	All	2047/2494 (82%)	1989 (97%)	57 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	45	GLU

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	389/426 (91%)	389 (100%)	0	100	100
2	B	94/115 (82%)	94 (100%)	0	100	100
3	C	100/301 (33%)	100 (100%)	0	100	100
4	D	32/33 (97%)	32 (100%)	0	100	100
5	E	74/75 (99%)	74 (100%)	0	100	100
6	F	538/613 (88%)	538 (100%)	0	100	100
7	G	351/392 (90%)	351 (100%)	0	100	100
8	H	174/249 (70%)	174 (100%)	0	100	100
All	All	1752/2204 (80%)	1752 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	406	GLN
2	B	61	GLN
2	B	87	GLN
6	F	61	ASN
6	F	68	ASN
6	F	186	GLN
6	F	536	ASN
6	F	681	GLN
7	G	78	ASN
7	G	242	ASN
7	G	268	HIS
7	G	307	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 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	$\# Z > 2$
11	NAG	J	1	6,11	14,14,15	0.32	0	17,19,21	0.50	0
11	NAG	J	2	11	14,14,15	0.21	0	17,19,21	0.52	0
11	BMA	J	3	11	11,11,12	0.45	0	15,15,17	0.83	0
11	MAN	J	4	11	11,11,12	0.62	0	15,15,17	1.16	1 (6%)
11	MAN	J	5	11	11,11,12	0.68	0	15,15,17	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	J	6	11	11,11,12	0.61	0	15,15,17	0.89	1 (6%)
11	MAN	J	7	11	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
10	NAG	K	1	10,1	14,14,15	0.34	0	17,19,21	0.68	0
10	NAG	K	2	10	14,14,15	0.23	0	17,19,21	0.54	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
11	NAG	J	1	6,11	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
11	BMA	J	3	11	-	1/2/19/22	0/1/1/1
11	MAN	J	4	11	-	0/2/19/22	0/1/1/1
11	MAN	J	5	11	-	1/2/19/22	0/1/1/1
11	MAN	J	6	11	-	0/2/19/22	0/1/1/1
11	MAN	J	7	11	-	0/2/19/22	0/1/1/1
10	NAG	K	1	10,1	-	4/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	4	MAN	O2-C2-C3	-3.11	103.72	110.15
11	J	5	MAN	O2-C2-C3	-2.66	104.64	110.15
11	J	7	MAN	O2-C2-C3	-2.17	105.66	110.15
11	J	6	MAN	O2-C2-C3	-2.13	105.74	110.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	K	2	NAG	O5-C5-C6-O6
11	J	3	BMA	O5-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
11	J	5	MAN	O5-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6

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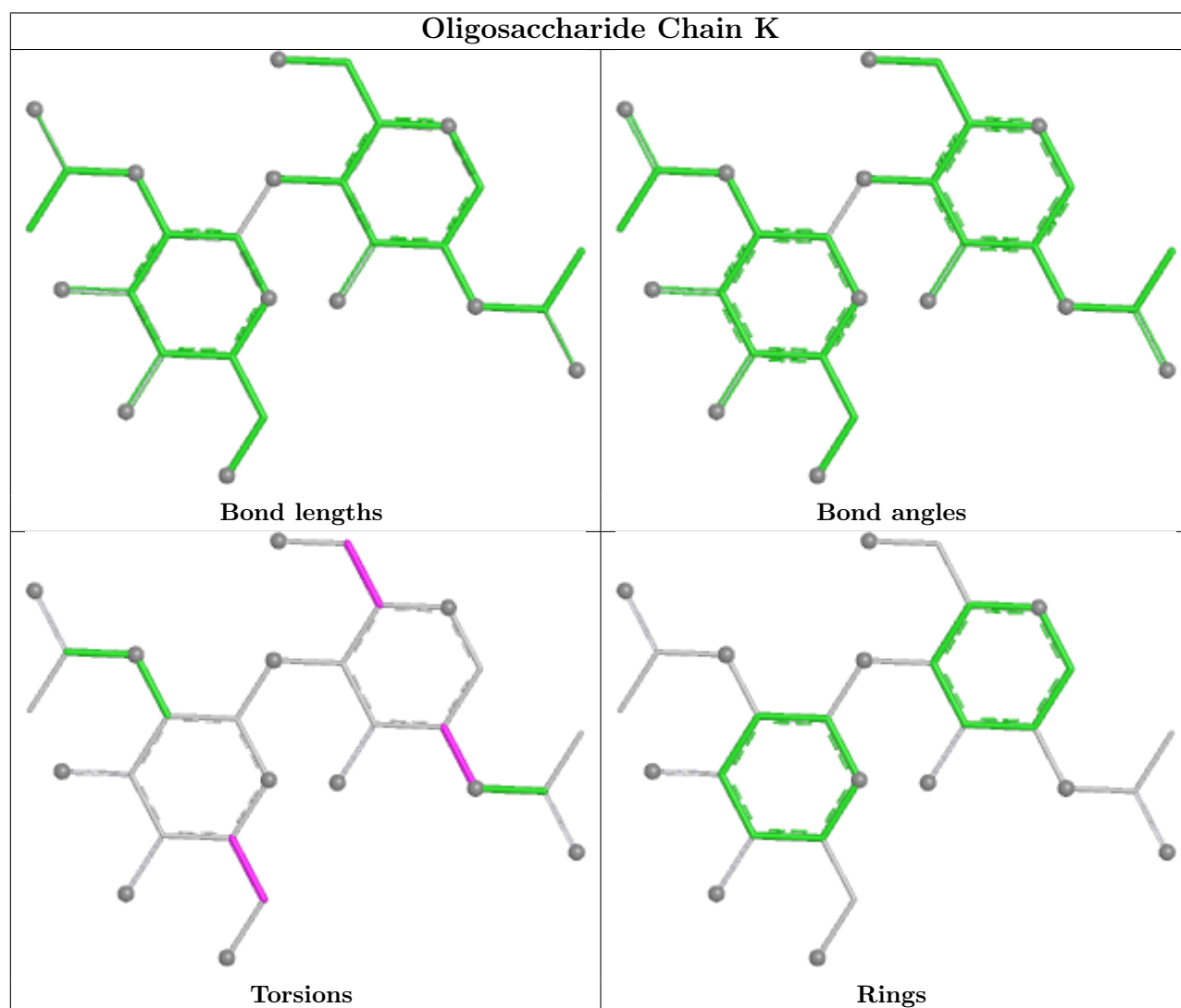
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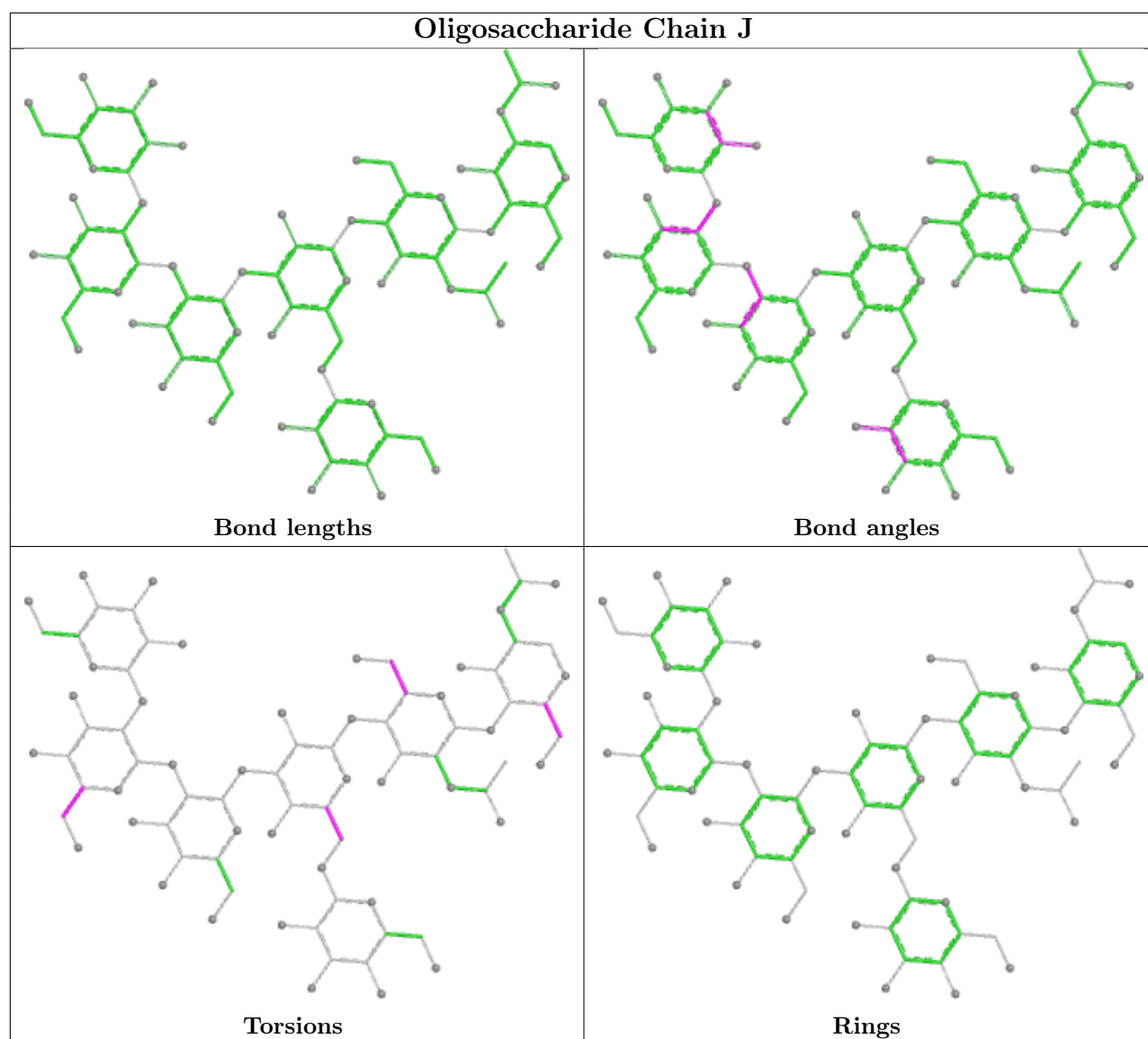
Mol	Chain	Res	Type	Atoms
11	J	1	NAG	C4-C5-C6-O6
10	K	1	NAG	C3-C2-N2-C7
11	J	1	NAG	O5-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
10	K	1	NAG	C1-C2-N2-C7
10	K	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	PEE	A	1301	-	34,34,50	1.70	5 (14%)	37,39,55	1.29	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PEE	B	201	-	32,32,50	1.58	4 (12%)	35,37,55	1.13	4 (11%)
12	PEE	H	1101	-	43,43,50	1.55	5 (11%)	46,48,55	1.24	6 (13%)
12	PEE	D	101	-	37,37,50	1.49	4 (10%)	40,42,55	1.18	4 (10%)
13	NAG	G	501	7	14,14,15	0.24	0	17,19,21	0.38	0
14	AJP	B	202	-	61,61,95	0.45	0	93,98,149	1.22	9 (9%)
13	NAG	A	1302	1	14,14,15	0.25	0	17,19,21	0.47	0
12	PEE	F	902	-	41,41,50	1.61	5 (12%)	44,46,55	1.29	6 (13%)
12	PEE	C	1801	-	35,35,50	1.67	5 (14%)	38,40,55	1.28	5 (13%)
13	NAG	G	502	7	14,14,15	0.53	0	17,19,21	0.46	0
16	V8K	F	903	15	59,59,59	1.87	8 (13%)	70,72,72	1.60	16 (22%)
14	AJP	D	102	-	49,49,95	0.55	1 (2%)	75,80,149	1.29	9 (12%)

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
12	PEE	A	1301	-	-	19/38/38/54	-
12	PEE	B	201	-	-	12/36/36/54	-
12	PEE	H	1101	-	-	24/47/47/54	-
12	PEE	D	101	-	-	19/41/41/54	-
14	AJP	B	202	-	21/21/24/38	3/12/147/220	0/8/8/11
13	NAG	G	501	7	-	1/6/23/26	0/1/1/1
13	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
12	PEE	F	902	-	-	24/45/45/54	-
12	PEE	C	1801	-	-	15/39/39/54	-
13	NAG	G	502	7	-	3/6/23/26	0/1/1/1
16	V8K	F	903	15	-	27/67/67/67	-
14	AJP	D	102	-	16/16/19/38	3/6/121/220	0/7/7/11

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	903	V8K	P57-O56	7.99	1.85	1.60
16	F	903	V8K	C45-C46	7.66	1.54	1.34
12	F	902	PEE	C39-C38	4.45	1.57	1.31
12	H	1101	PEE	C39-C38	4.44	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1301	PEE	C39-C38	4.33	1.57	1.29
12	C	1801	PEE	C39-C38	4.31	1.57	1.29
12	F	902	PEE	C18-C19	4.25	1.55	1.31
12	D	101	PEE	C18-C19	4.21	1.55	1.31
12	H	1101	PEE	C18-C19	4.18	1.55	1.31
12	B	201	PEE	C19-C18	4.11	1.55	1.29
12	A	1301	PEE	C19-C18	4.09	1.55	1.29
12	D	101	PEE	O3-C30	3.66	1.44	1.33
12	C	1801	PEE	O3-C30	3.62	1.43	1.33
12	B	201	PEE	O3-C30	3.60	1.43	1.33
12	C	1801	PEE	C18-C19	3.58	1.55	1.29
12	H	1101	PEE	O3-C30	3.57	1.43	1.33
12	F	902	PEE	O3-C30	3.56	1.43	1.33
12	A	1301	PEE	O3-C30	3.55	1.43	1.33
12	C	1801	PEE	O2-C10	3.53	1.44	1.34
12	F	902	PEE	O2-C10	3.52	1.44	1.34
12	B	201	PEE	O2-C10	3.40	1.43	1.34
12	H	1101	PEE	O2-C10	3.39	1.43	1.34
12	D	101	PEE	O2-C10	3.39	1.43	1.34
12	A	1301	PEE	O2-C10	3.27	1.43	1.34
16	F	903	V8K	C46-C47	2.85	1.52	1.46
16	F	903	V8K	C54-C55	2.67	1.60	1.50
16	F	903	V8K	C45-C44	2.56	1.51	1.43
12	B	201	PEE	C11-C10	2.50	1.58	1.50
16	F	903	V8K	O56-C55	-2.47	1.34	1.44
12	F	902	PEE	C11-C10	2.40	1.57	1.50
12	A	1301	PEE	C11-C10	2.35	1.57	1.50
12	D	101	PEE	C11-C10	2.34	1.57	1.50
16	F	903	V8K	C11-C12	2.33	1.56	1.51
12	C	1801	PEE	C11-C10	2.29	1.57	1.50
12	H	1101	PEE	C11-C10	2.27	1.57	1.50
14	D	102	AJP	C16-C11	-2.18	1.51	1.54
16	F	903	V8K	C16-C17	2.02	1.55	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	903	V8K	C46-C47-C49	4.54	124.82	118.49
14	B	202	AJP	C06-C07-C08	-4.32	97.34	104.28
12	A	1301	PEE	O2-C10-C11	4.09	120.33	111.48
12	C	1801	PEE	O2-C10-C11	3.95	120.02	111.48
12	H	1101	PEE	O2-C10-C11	3.94	120.01	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	101	PEE	O2-C10-C11	3.92	119.95	111.48
12	F	902	PEE	O2-C10-C11	3.88	119.88	111.48
12	B	201	PEE	O2-C10-C11	3.53	119.12	111.48
14	D	102	AJP	C06-C07-C08	-3.43	98.77	104.28
14	B	202	AJP	O09-C08-C10	3.40	117.08	110.20
14	B	202	AJP	O25-C23-C24	3.27	116.00	109.64
16	F	903	V8K	C48-C47-C49	-3.13	118.31	123.73
14	D	102	AJP	O09-C08-C10	3.09	116.45	110.20
12	F	902	PEE	O3-C30-C31	3.09	121.25	111.83
14	D	102	AJP	C21-C20-C15	2.97	114.09	110.10
14	B	202	AJP	C05-C06-C07	-2.97	98.99	103.37
14	D	102	AJP	C20-C21-C22	-2.94	109.33	114.17
14	B	202	AJP	C11-C16-C15	-2.89	104.06	109.17
16	F	903	V8K	C45-C46-C47	-2.89	118.44	126.36
14	D	102	AJP	C13-C12-C07	2.89	119.47	115.36
12	H	1101	PEE	O3-C30-C31	2.82	120.44	111.83
12	F	902	PEE	C20-C19-C18	-2.78	109.70	126.42
12	C	1801	PEE	C17-C18-C19	-2.75	109.64	130.48
14	D	102	AJP	O09-C08-C07	-2.72	97.82	104.08
14	B	202	AJP	C11-C12-C07	-2.71	96.07	100.16
14	D	102	AJP	C20-C15-C16	-2.70	109.69	112.43
12	A	1301	PEE	O3-C30-C31	2.69	120.03	111.83
16	F	903	V8K	C40-C39-C37	2.66	133.72	127.62
16	F	903	V8K	C13-C12-C14	-2.64	116.84	123.63
16	F	903	V8K	C16-C17-C19	2.64	127.09	121.17
12	D	101	PEE	O3-C30-C31	2.63	119.84	111.83
12	C	1801	PEE	O3-C30-C31	2.55	119.60	111.83
16	F	903	V8K	C40-C41-C42	2.47	121.36	113.19
16	F	903	V8K	O60-P57-O56	-2.41	100.37	106.67
14	B	202	AJP	O09-C08-C07	-2.39	98.58	104.08
16	F	903	V8K	C44-C45-C46	-2.36	116.35	123.20
12	B	201	PEE	C17-C18-C19	-2.36	109.47	126.65
12	A	1301	PEE	C17-C18-C19	-2.35	109.48	126.65
12	C	1801	PEE	C37-C38-C39	-2.35	109.48	126.65
12	B	201	PEE	O3-C30-C31	2.35	119.00	111.83
16	F	903	V8K	C11-C12-C14	2.33	126.40	121.17
14	B	202	AJP	O34-C29-C30	2.28	115.47	109.48
14	D	102	AJP	C11-C12-C07	-2.28	96.72	100.16
12	A	1301	PEE	C37-C38-C39	-2.27	110.07	126.65
16	F	903	V8K	C18-C17-C19	-2.24	117.88	123.63
16	F	903	V8K	C25-C26-C27	2.21	120.51	113.19
12	C	1801	PEE	C20-C19-C18	-2.18	109.39	126.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	102	AJP	C12-C07-C06	2.18	126.93	120.50
16	F	903	V8K	C16-C15-C14	2.16	122.72	112.02
12	F	902	PEE	C37-C38-C39	-2.12	108.95	124.83
12	H	1101	PEE	C17-C18-C19	-2.12	108.98	124.83
12	B	201	PEE	O2-C10-O4	-2.09	118.82	123.70
12	D	101	PEE	C20-C19-C18	-2.07	109.33	124.83
16	F	903	V8K	C10-C11-C12	2.07	120.03	113.19
16	F	903	V8K	O60-P57-O58	2.07	115.55	107.80
12	H	1101	PEE	C20-C19-C18	-2.07	109.35	124.83
14	B	202	AJP	C20-C21-C22	-2.06	110.78	114.17
12	H	1101	PEE	C37-C38-C39	-2.04	109.52	124.83
12	H	1101	PEE	C40-C39-C38	-2.04	109.54	124.83
12	F	902	PEE	C17-C18-C19	-2.03	109.66	124.83
12	F	902	PEE	C40-C39-C38	-2.02	109.66	124.83
12	D	101	PEE	C17-C18-C19	-2.01	109.81	124.83
16	F	903	V8K	C36-C35-C34	2.00	121.92	112.02

All (37) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	B	202	AJP	C38
14	B	202	AJP	C10
14	B	202	AJP	C39
14	B	202	AJP	C02
14	B	202	AJP	C15
14	B	202	AJP	C07
14	B	202	AJP	C27
14	B	202	AJP	C11
14	B	202	AJP	C20
14	B	202	AJP	C23
14	B	202	AJP	C26
14	B	202	AJP	C28
14	B	202	AJP	C16
14	B	202	AJP	C22
14	B	202	AJP	C30
14	B	202	AJP	C05
14	B	202	AJP	C12
14	B	202	AJP	C36
14	B	202	AJP	C35
14	B	202	AJP	C19
14	B	202	AJP	C37
14	D	102	AJP	C15

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Mol	Chain	Res	Type	Atom
14	D	102	AJP	C16
14	D	102	AJP	C22
14	D	102	AJP	C30
14	D	102	AJP	C11
14	D	102	AJP	C07
14	D	102	AJP	C27
14	D	102	AJP	C05
14	D	102	AJP	C12
14	D	102	AJP	C20
14	D	102	AJP	C23
14	D	102	AJP	C26
14	D	102	AJP	C28
14	D	102	AJP	C10
14	D	102	AJP	C19
14	D	102	AJP	C02

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1301	PEE	C1-O3P-P-O2P
12	A	1301	PEE	C1-O3P-P-O1P
12	A	1301	PEE	C1-O3P-P-O4P
12	A	1301	PEE	O4P-C4-C5-N
12	C	1801	PEE	C17-C18-C19-C20
12	C	1801	PEE	C4-O4P-P-O3P
12	C	1801	PEE	O4P-C4-C5-N
12	D	101	PEE	C17-C18-C19-C20
12	D	101	PEE	C11-C10-O2-C2
12	D	101	PEE	C4-O4P-P-O3P
12	D	101	PEE	C4-O4P-P-O1P
12	D	101	PEE	O4P-C4-C5-N
12	F	902	PEE	C1-O3P-P-O1P
12	F	902	PEE	C1-O3P-P-O4P
12	F	902	PEE	C4-O4P-P-O3P
12	F	902	PEE	C4-O4P-P-O1P
12	H	1101	PEE	O4-C10-O2-C2
16	F	903	V8K	C32-C34-C35-C36
16	F	903	V8K	C37-C39-C40-C41
16	F	903	V8K	C55-O56-P57-O58
16	F	903	V8K	C55-O56-P57-O59
16	F	903	V8K	C55-O56-P57-O60
14	B	202	AJP	O40-C35-O34-C29

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Mol	Chain	Res	Type	Atoms
12	D	101	PEE	O4-C10-O2-C2
12	H	1101	PEE	C11-C10-O2-C2
16	F	903	V8K	C20-C21-C22-C23
16	F	903	V8K	C10-C11-C12-C13
16	F	903	V8K	C40-C41-C42-C43
16	F	903	V8K	C20-C21-C22-C24
16	F	903	V8K	C40-C41-C42-C44
12	H	1101	PEE	C31-C30-O3-C3
16	F	903	V8K	C15-C16-C17-C18
16	F	903	V8K	C35-C36-C37-C38
16	F	903	V8K	C15-C16-C17-C19
16	F	903	V8K	C35-C36-C37-C39
12	H	1101	PEE	O5-C30-O3-C3
16	F	903	V8K	C14-C15-C16-C17
16	F	903	V8K	C19-C20-C21-C22
16	F	903	V8K	C24-C25-C26-C27
16	F	903	V8K	C39-C40-C41-C42
12	A	1301	PEE	C31-C30-O3-C3
12	H	1101	PEE	C11-C12-C13-C14
16	F	903	V8K	C30-C31-C32-C33
16	F	903	V8K	C10-C11-C12-C14
16	F	903	V8K	C30-C31-C32-C34
16	F	903	V8K	C45-C46-C47-C48
16	F	903	V8K	C45-C46-C47-C49
13	A	1302	NAG	C4-C5-C6-O6
13	G	502	NAG	C8-C7-N2-C2
13	G	502	NAG	O7-C7-N2-C2
14	B	202	AJP	C36-C35-O34-C29
12	A	1301	PEE	C16-C17-C18-C19
12	A	1301	PEE	C36-C37-C38-C39
12	A	1301	PEE	O5-C30-O3-C3
12	A	1301	PEE	C10-C11-C12-C13
12	F	902	PEE	C11-C10-O2-C2
12	C	1801	PEE	C30-C31-C32-C33
12	F	902	PEE	O4-C10-O2-C2
12	C	1801	PEE	C11-C10-O2-C2
14	D	102	AJP	O31-C30-C32-O33
12	C	1801	PEE	O4-C10-O2-C2
13	A	1302	NAG	O5-C5-C6-O6
14	B	202	AJP	O31-C30-C32-O33
12	D	101	PEE	C31-C30-O3-C3
12	C	1801	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
12	H	1101	PEE	C14-C15-C16-C17
12	H	1101	PEE	C31-C32-C33-C34
12	F	902	PEE	C10-C11-C12-C13
12	A	1301	PEE	C12-C13-C14-C15
12	C	1801	PEE	C31-C32-C33-C34
12	D	101	PEE	C12-C13-C14-C15
12	B	201	PEE	C32-C33-C34-C35
12	D	101	PEE	C31-C32-C33-C34
12	B	201	PEE	C14-C15-C16-C17
12	D	101	PEE	C10-C11-C12-C13
12	C	1801	PEE	C12-C13-C14-C15
12	H	1101	PEE	C37-C38-C39-C40
12	D	101	PEE	O5-C30-O3-C3
12	D	101	PEE	C20-C21-C22-C23
12	A	1301	PEE	C32-C33-C34-C35
12	F	902	PEE	C12-C13-C14-C15
12	H	1101	PEE	C34-C35-C36-C37
12	A	1301	PEE	C11-C12-C13-C14
12	F	902	PEE	C15-C16-C17-C18
12	H	1101	PEE	C19-C20-C21-C22
12	H	1101	PEE	C35-C36-C37-C38
12	F	902	PEE	C34-C35-C36-C37
13	G	502	NAG	O5-C5-C6-O6
12	F	902	PEE	C1-C2-C3-O3
12	H	1101	PEE	C1-C2-C3-O3
12	D	101	PEE	C19-C20-C21-C22
12	F	902	PEE	C35-C36-C37-C38
12	H	1101	PEE	C15-C16-C17-C18
12	H	1101	PEE	C12-C13-C14-C15
12	F	902	PEE	C3-C2-O2-C10
12	C	1801	PEE	C32-C33-C34-C35
12	A	1301	PEE	C30-C31-C32-C33
12	H	1101	PEE	C18-C19-C20-C21
12	C	1801	PEE	C31-C30-O3-C3
12	A	1301	PEE	O2-C2-C3-O3
12	D	101	PEE	C21-C22-C23-C24
12	D	101	PEE	C13-C14-C15-C16
16	F	903	V8K	C05-C06-C07-C08
12	A	1301	PEE	C33-C34-C35-C36
12	H	1101	PEE	C32-C33-C34-C35
14	D	102	AJP	C27-C26-O25-C23
16	F	903	V8K	C05-C06-C07-C09

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Mol	Chain	Res	Type	Atoms
12	F	902	PEE	O2-C2-C3-O3
12	A	1301	PEE	C13-C14-C15-C16
12	H	1101	PEE	C16-C17-C18-C19
12	C	1801	PEE	O5-C30-O3-C3
12	C	1801	PEE	C3-C2-O2-C10
12	B	201	PEE	C34-C35-C36-C37
12	B	201	PEE	O3P-C1-C2-O2
12	H	1101	PEE	O2-C2-C3-O3
12	H	1101	PEE	C20-C21-C22-C23
12	F	902	PEE	O3P-C1-C2-O2
12	B	201	PEE	C16-C17-C18-C19
12	A	1301	PEE	C1-C2-C3-O3
12	D	101	PEE	C18-C19-C20-C21
12	B	201	PEE	C1-O3P-P-O1P
12	B	201	PEE	C1-O3P-P-O4P
12	B	201	PEE	C4-O4P-P-O1P
12	B	201	PEE	O4P-C4-C5-N
12	D	101	PEE	C4-O4P-P-O2P
12	F	902	PEE	C1-O3P-P-O2P
12	F	902	PEE	C4-O4P-P-O2P
12	H	1101	PEE	C1-O3P-P-O4P
16	F	903	V8K	C42-C44-C45-C46
12	A	1301	PEE	C14-C15-C16-C17
12	F	902	PEE	C31-C30-O3-C3
14	D	102	AJP	O31-C26-O25-C23
12	F	902	PEE	O5-C30-O3-C3
12	F	902	PEE	C40-C41-C42-C43
12	H	1101	PEE	C39-C40-C41-C42
12	H	1101	PEE	C22-C23-C24-C25
12	H	1101	PEE	C13-C14-C15-C16
12	D	101	PEE	C34-C35-C36-C37
12	B	201	PEE	O2-C2-C3-O3
12	C	1801	PEE	C15-C16-C17-C18
13	A	1302	NAG	C1-C2-N2-C7
13	G	501	NAG	C1-C2-N2-C7
12	F	902	PEE	O3P-C1-C2-C3
12	F	902	PEE	C38-C39-C40-C41
12	D	101	PEE	C16-C17-C18-C19
12	F	902	PEE	C36-C37-C38-C39
12	B	201	PEE	O3P-C1-C2-C3
12	H	1101	PEE	O3P-C1-C2-O2
12	C	1801	PEE	O3-C30-C31-C32

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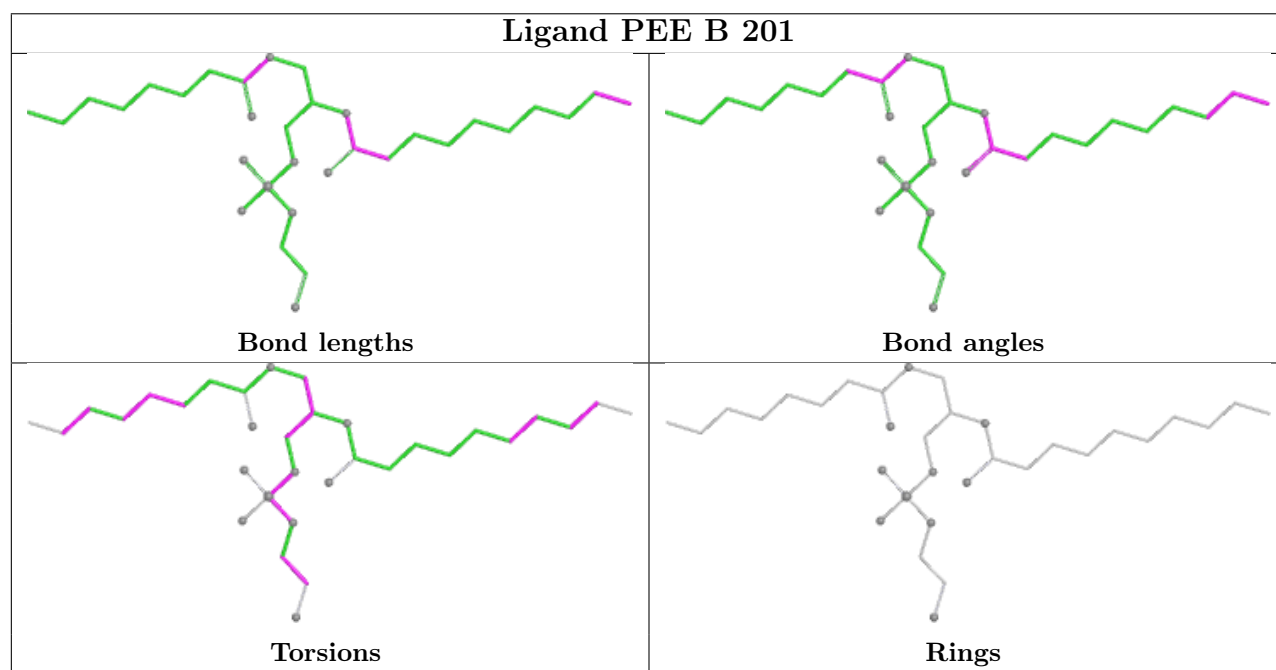
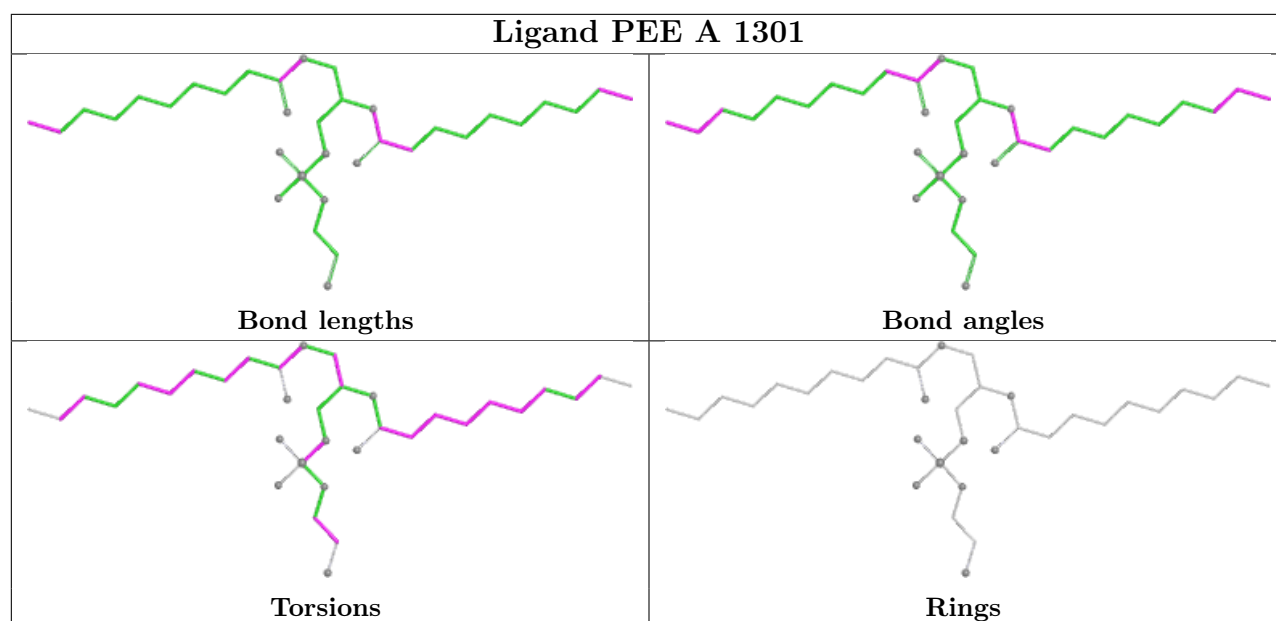
Mol	Chain	Res	Type	Atoms
12	A	1301	PEE	O2-C10-C11-C12
16	F	903	V8K	C34-C35-C36-C37
12	B	201	PEE	C31-C32-C33-C34
12	F	902	PEE	C33-C34-C35-C36

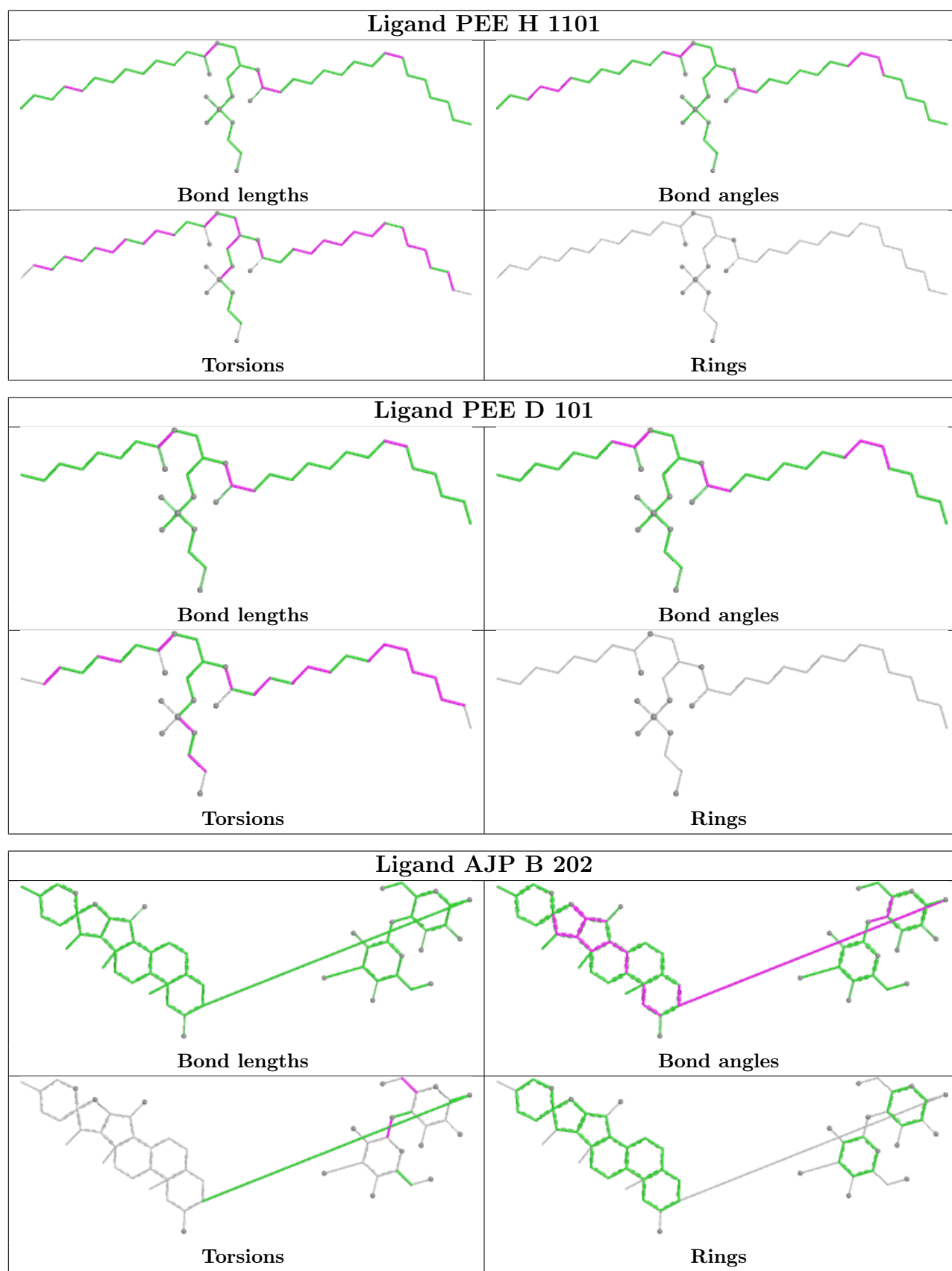
There are no ring outliers.

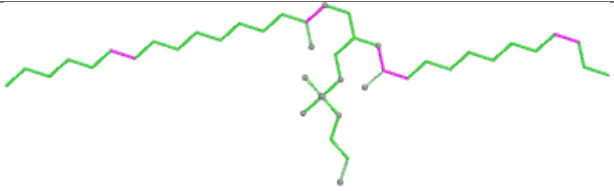
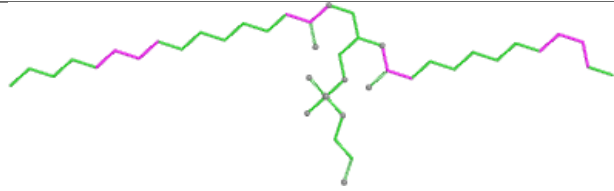
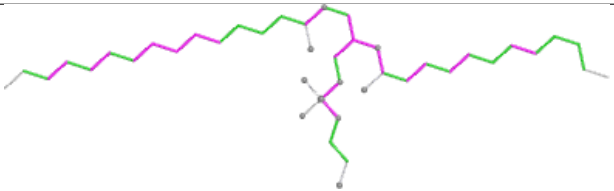
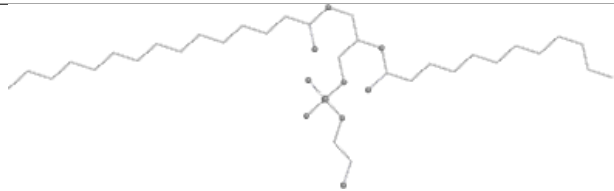
6 monomers are involved in 7 short contacts:

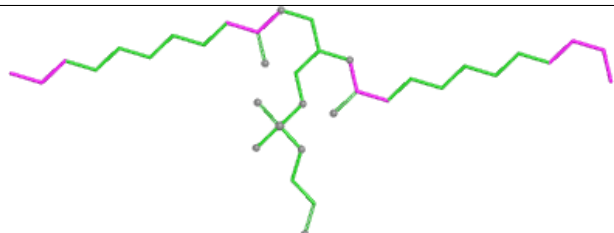
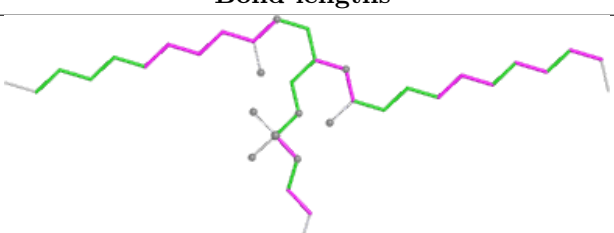
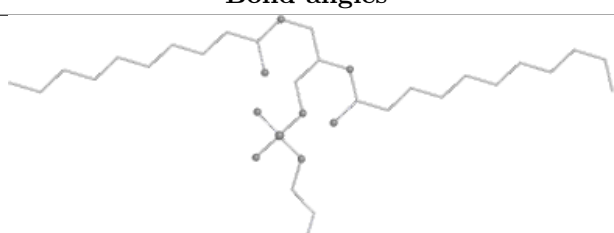
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1301	PEE	2	0
12	H	1101	PEE	2	0
14	B	202	AJP	1	0
12	F	902	PEE	1	0
13	G	502	NAG	1	0
14	D	102	AJP	1	0

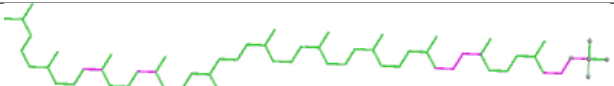
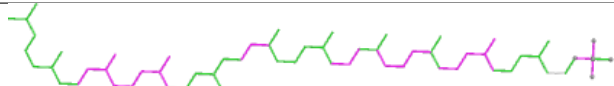
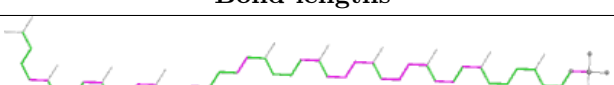
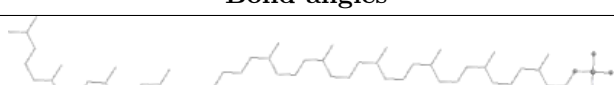
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

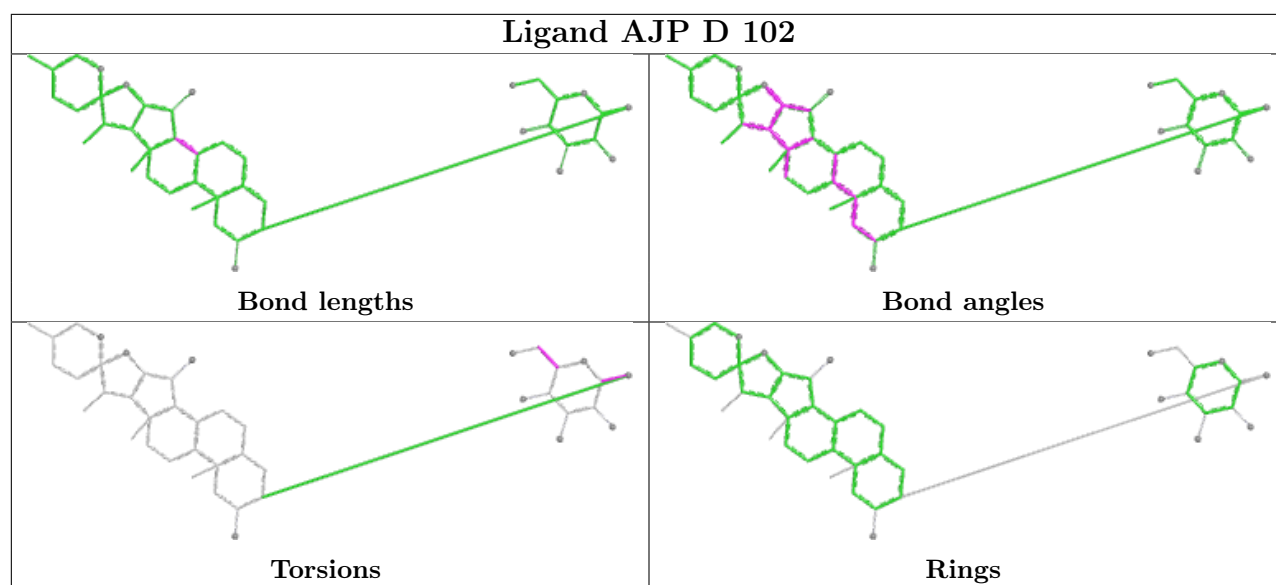




Ligand PEE F 902	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE C 1801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand V8K F 903	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

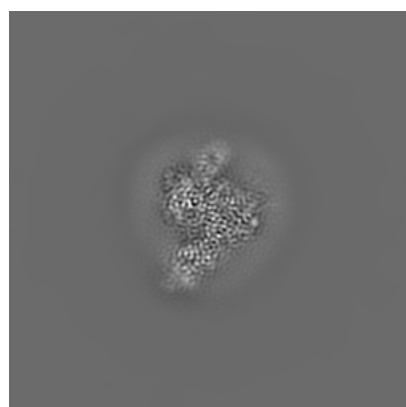
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12808. These allow visual inspection of the internal detail of the map and identification of artifacts.

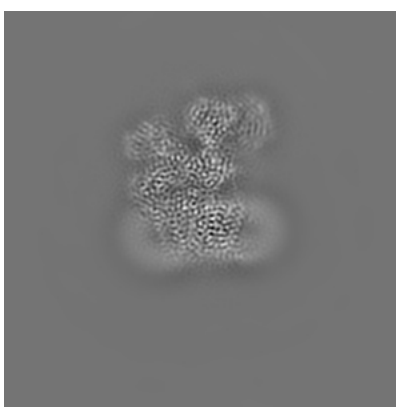
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

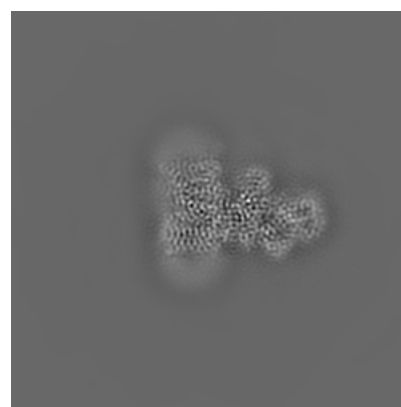
6.1.1 Primary map



X



Y

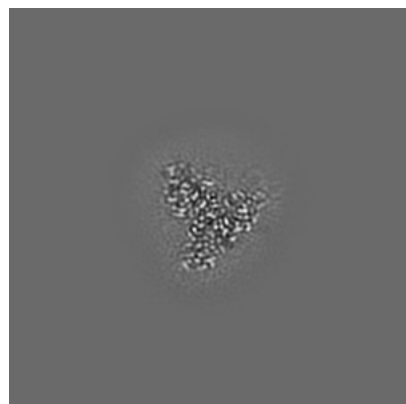


Z

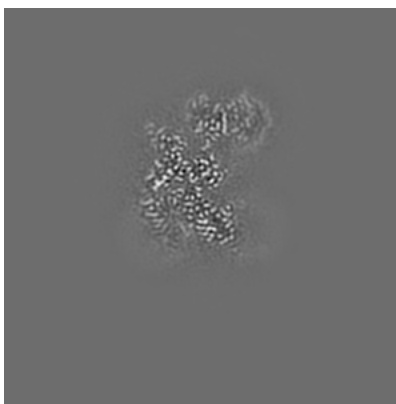
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

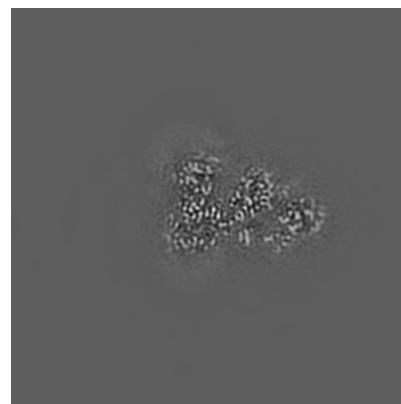
6.2.1 Primary map



X Index: 192



Y Index: 192

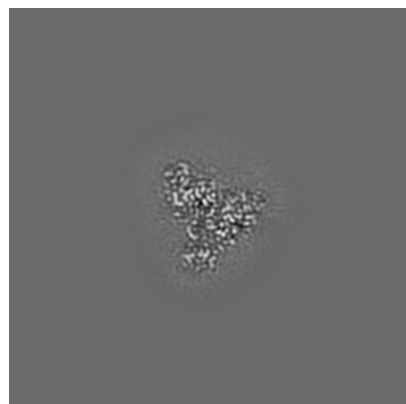


Z Index: 192

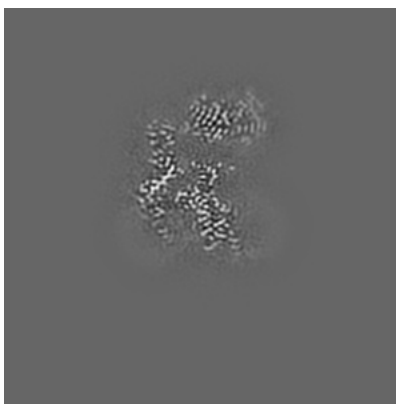
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

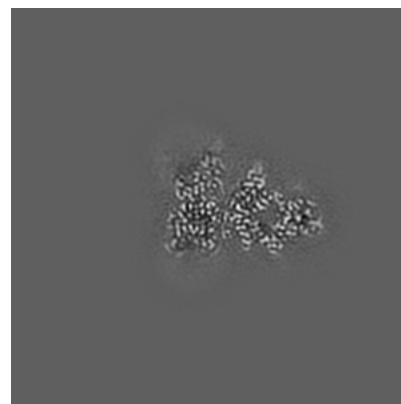
6.3.1 Primary map



X Index: 190



Y Index: 185

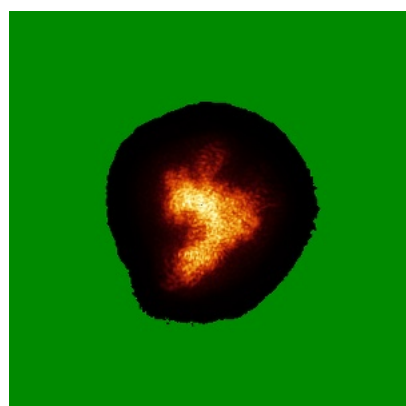


Z Index: 199

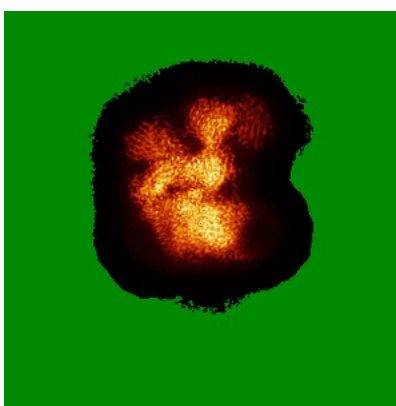
The images above show the largest variance slices of the map in three orthogonal directions.

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

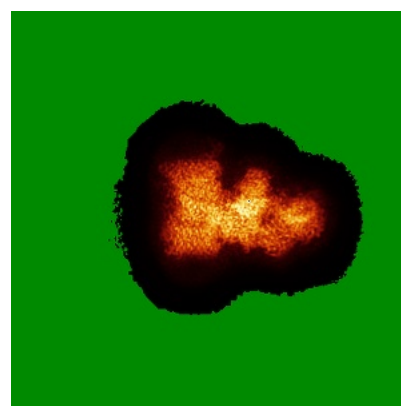
6.4.1 Primary map



X



Y



Z

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](#)

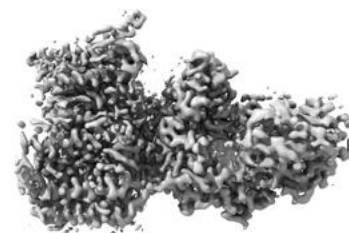
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

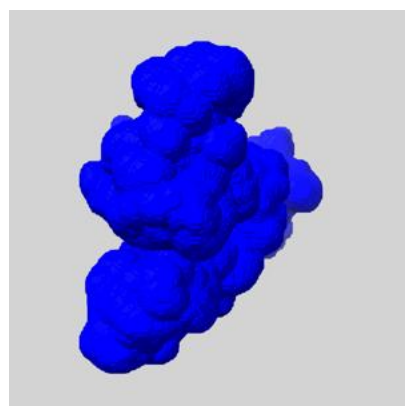
6.6 Mask visualisation [i](#)

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

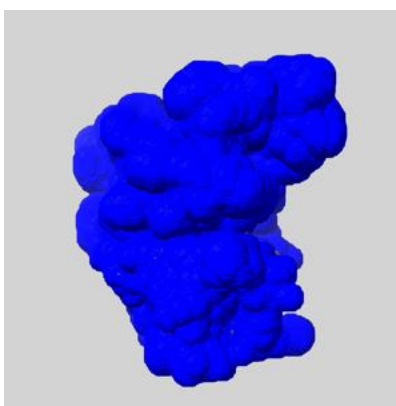
A mask typically either:

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

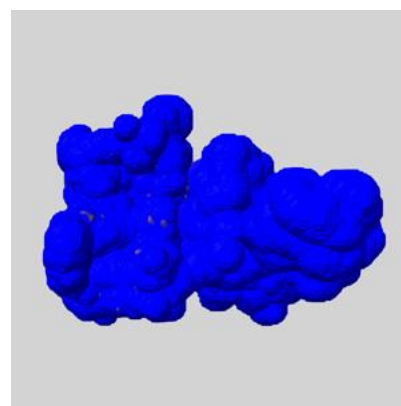
6.6.1 emd_12808_msk_1.map [i](#)



X



Y

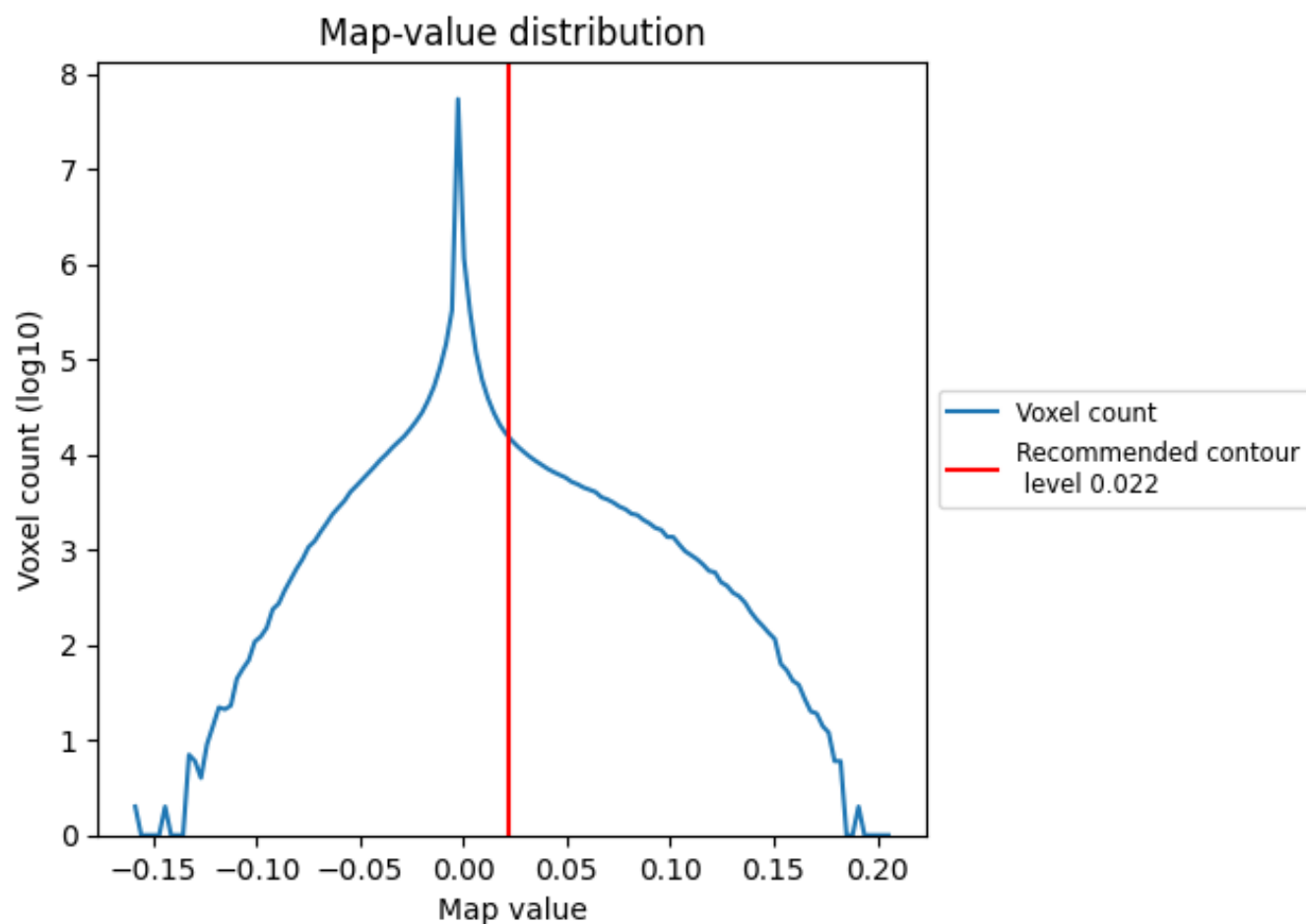


Z

7 Map analysis [i](#)

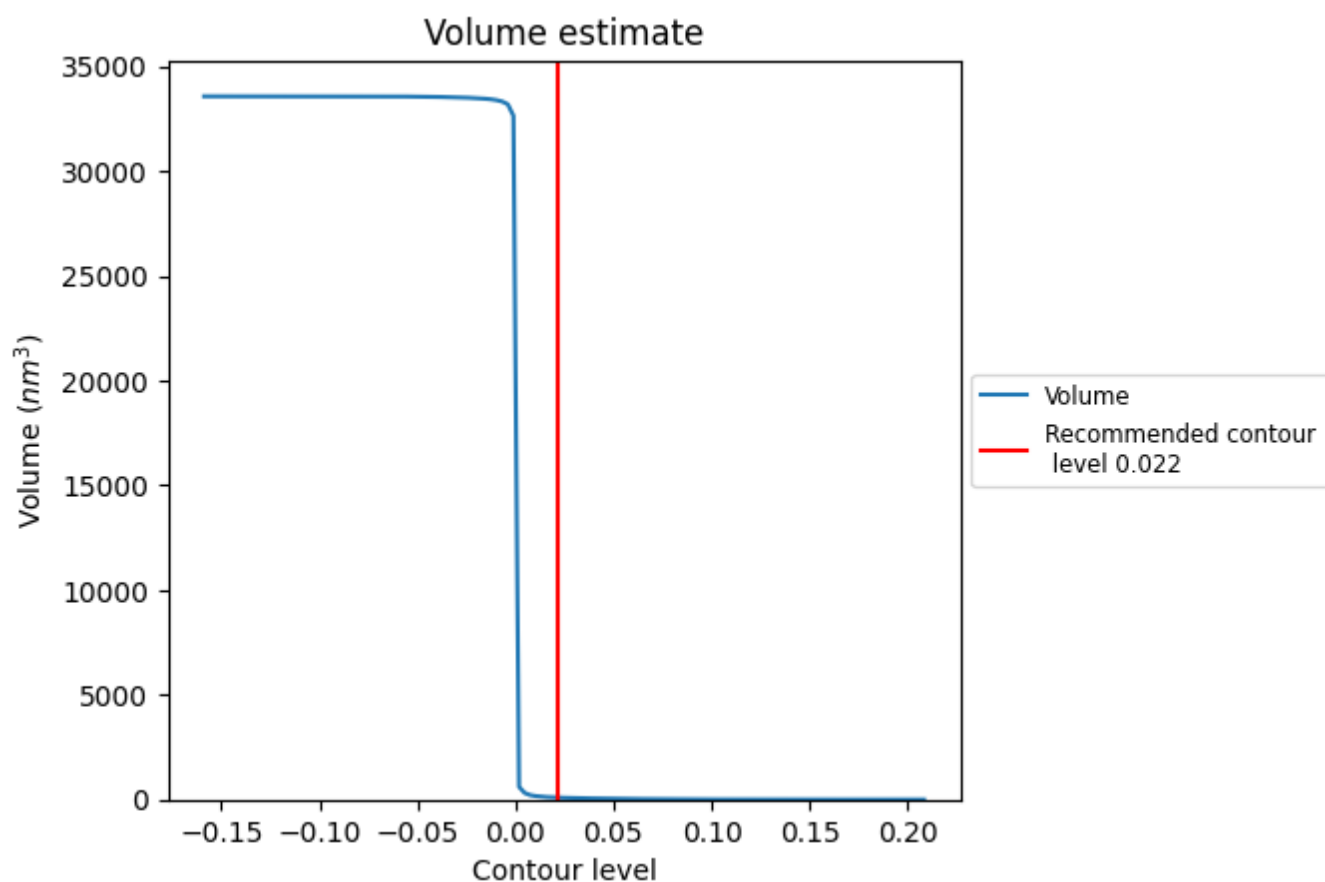
This section contains the results of statistical analysis of the map.

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.

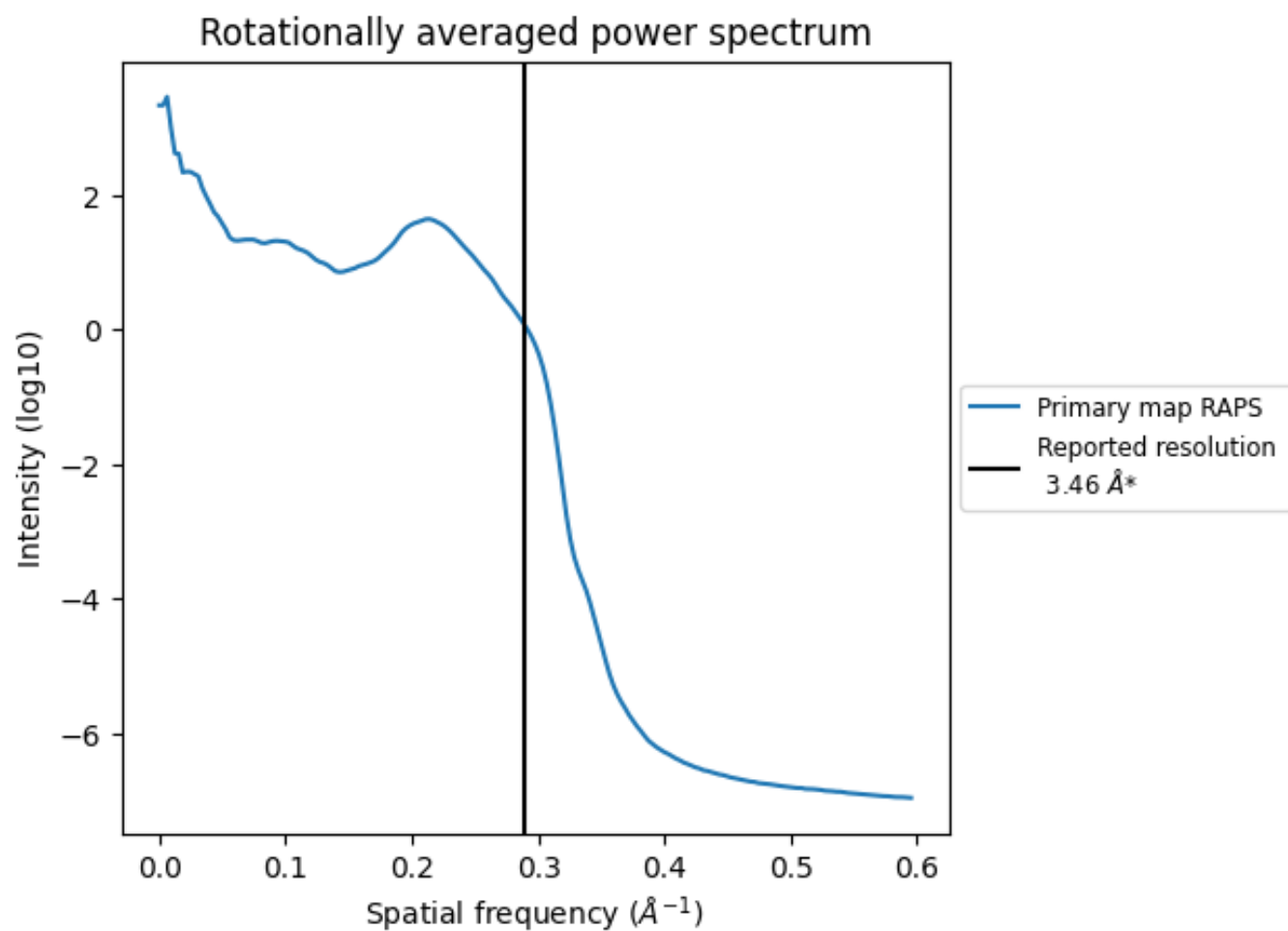
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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 ⓘ

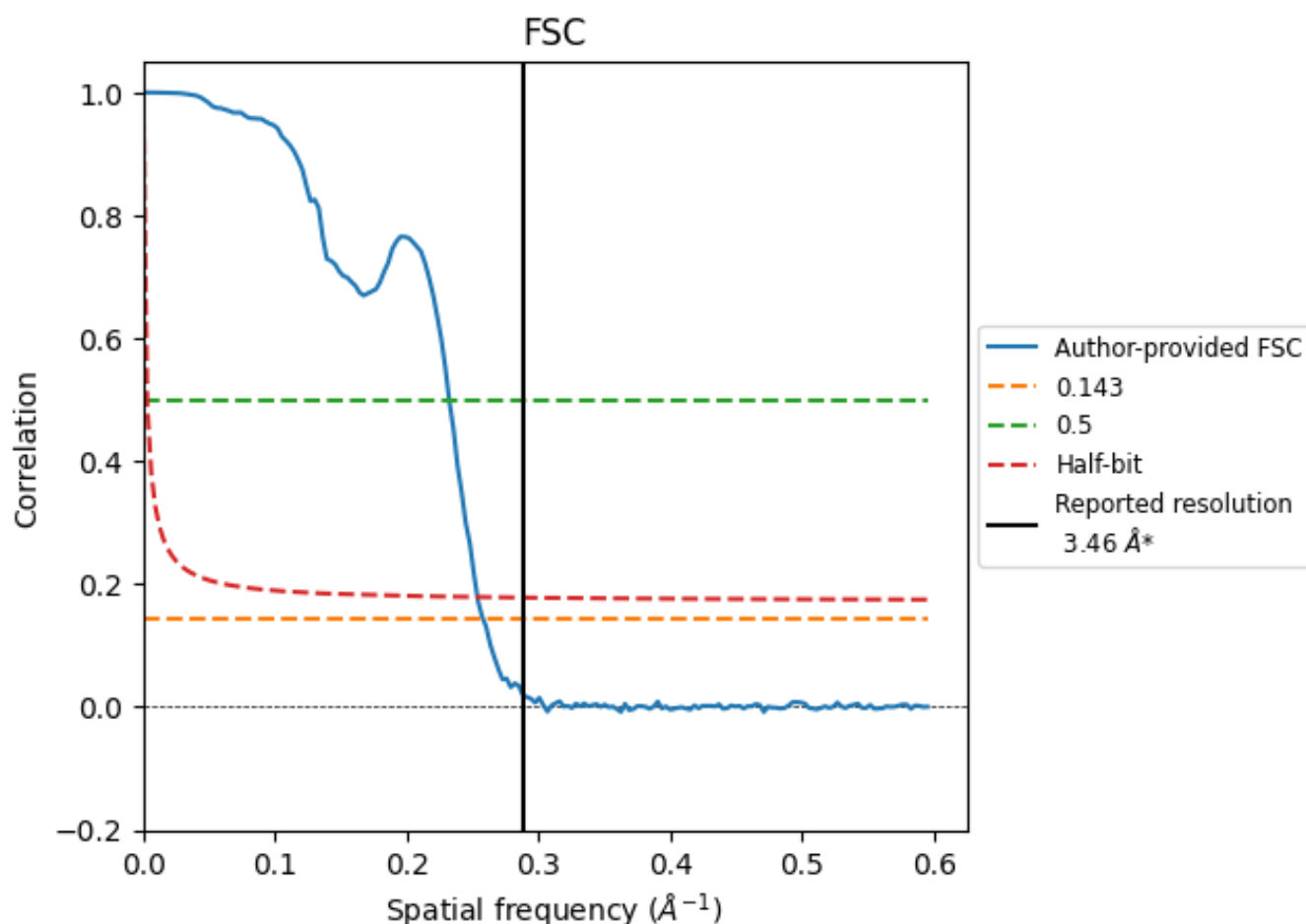


*Reported resolution corresponds to spatial frequency of 0.289 $\text{\AA}^{-1}$

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 0.289 Å⁻¹

8.2 Resolution estimates [i](#)

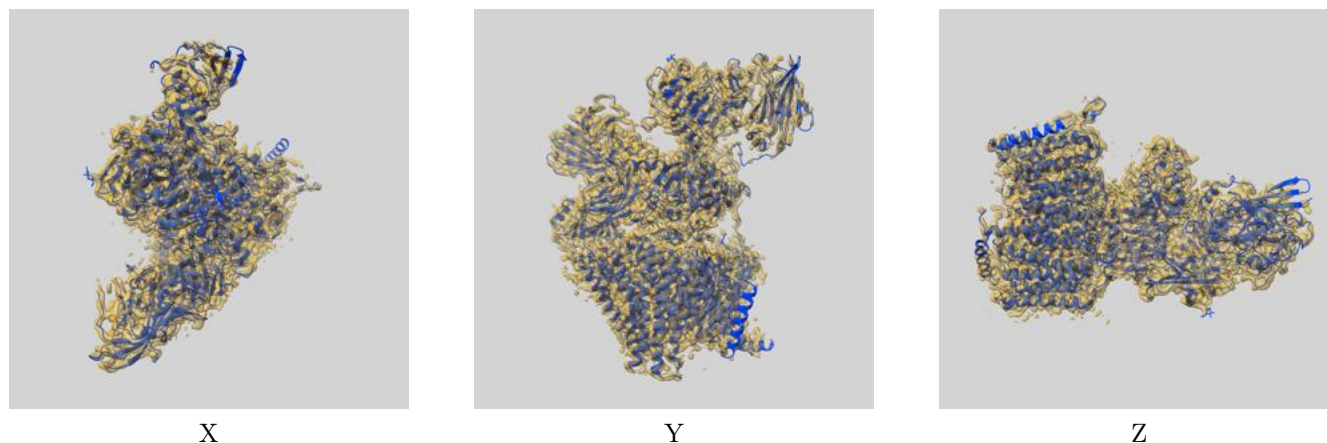
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.88	4.30	3.94
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.46 by more than 10 %

9 Map-model fit [i](#)

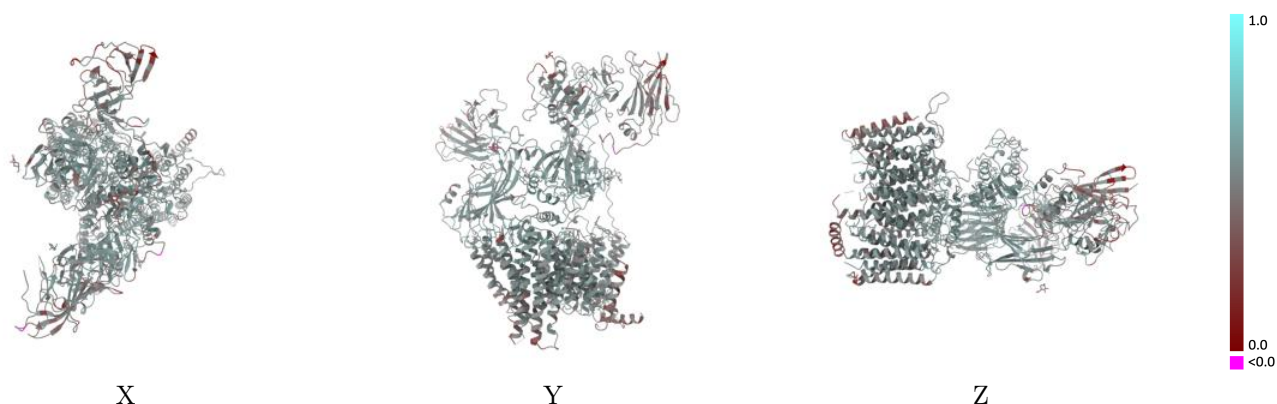
This section contains information regarding the fit between EMDB map EMD-12808 and PDB model 7OCI. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



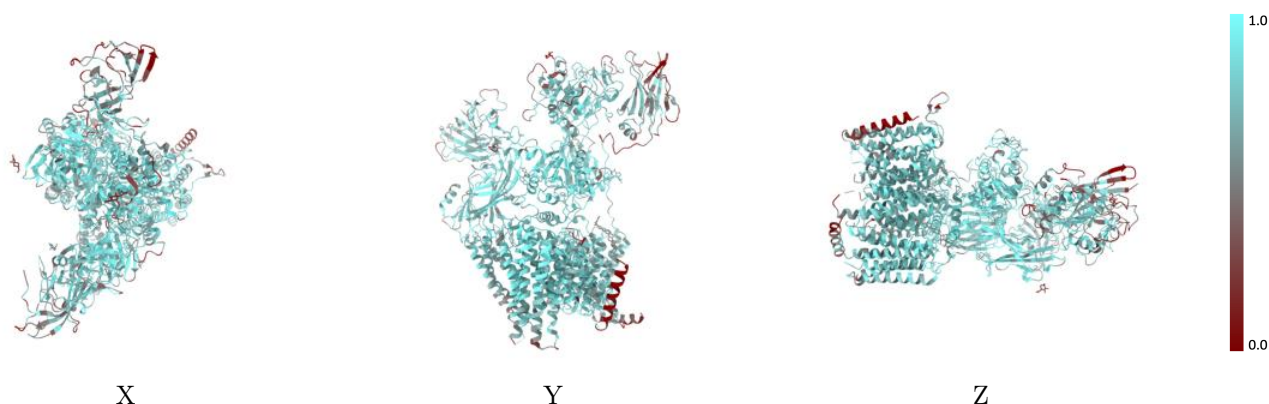
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



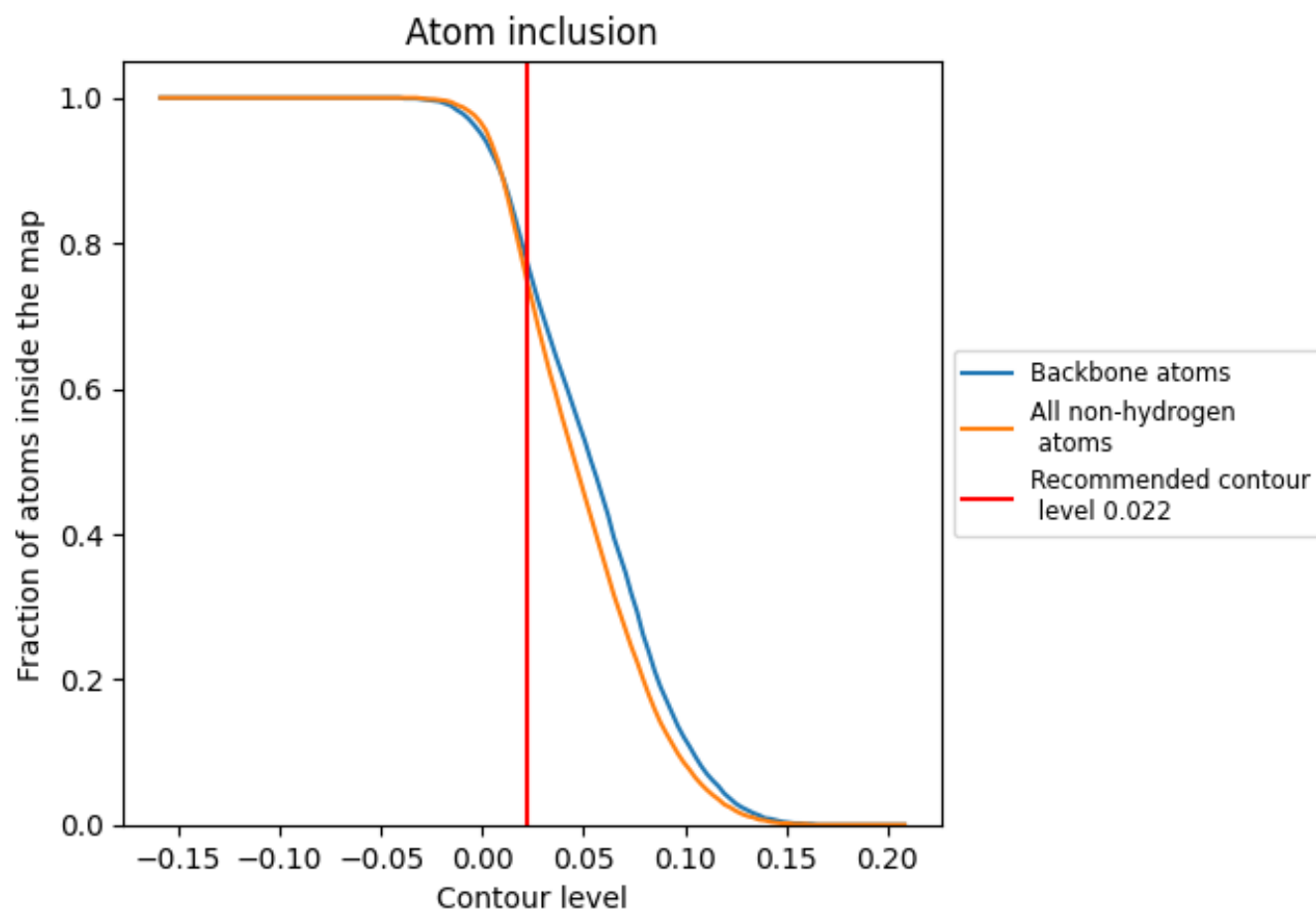
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 75% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.5140
A	0.7400	0.5150
B	0.7390	0.4990
C	0.7190	0.4960
D	0.7550	0.5210
E	0.6930	0.4830
F	0.8280	0.5410
G	0.7690	0.5230
H	0.5970	0.4590
I	0.1250	0.3940
J	0.8430	0.5380
K	0.7500	0.5020

1.0

0.0

<0.0