



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:51 AM UTC

PDB ID : 6C26 / pdb_00006c26
EMDB ID : EMD-7336
Title : The Cryo-EM structure of a eukaryotic oligosaccharyl transferase complex
Authors : Bai, L.; Li, H.
Deposited on : 2018-01-06
Resolution : 3.50 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:

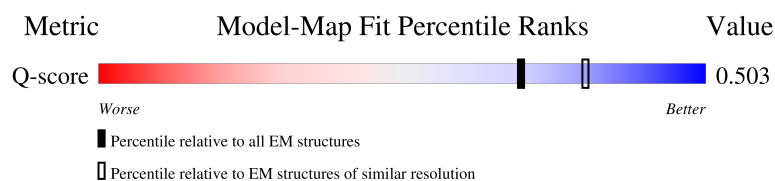
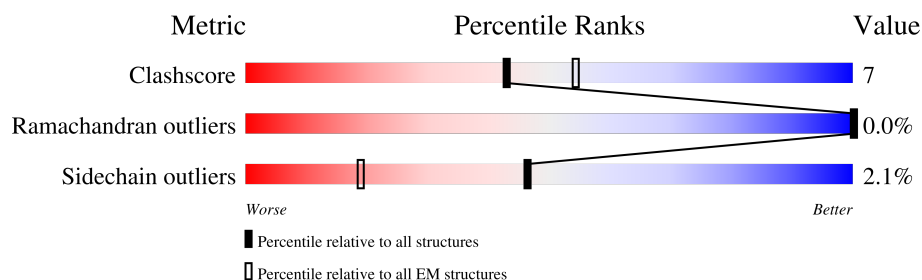
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	718	
2	1	476	
3	5	86	
4	4	36	

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Mol	Chain	Length	Quality of chain
5	2	130	5% 70% 12% 17%
6	3	350	5% 33% 64%
7	C	286	17% 74% 12% 13%
8	B	430	73% 18% 8%
9	D	7	29% 29% 57% 14%
10	E	3	67% 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17188 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 STT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	648	Total	C	N	O	S	0	0
			5225	3456	839	907	23		

- Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	432	Total	C	N	O	S	0	0
			3496	2267	560	662	7		

- Molecule 3 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	84	Total	C	N	O	S	0	0
			659	443	98	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	34	Total	C	N	O	S	0	0
			259	167	39	50	3		

- Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	108	Total	C	N	O	S	0	0
			883	598	139	140	6		

- Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	126	Total	C	N	O	S	0	0
			1028	700	154	167	7		

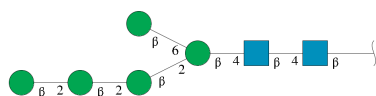
- Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	248	Total	C	N	O	S	0	0
			1940	1272	311	353	4		

- Molecule 8 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1.

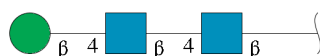
Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	397	Total	C	N	O	S	0	0
			3218	2063	531	620	4		

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-2)-[beta-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.



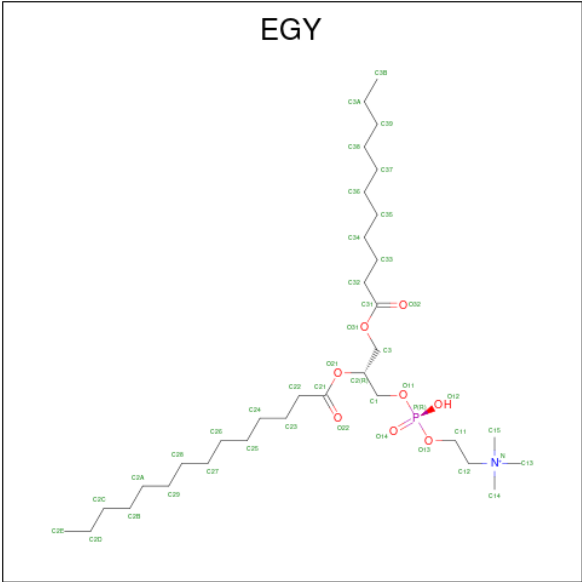
Mol	Chain	Residues	Atoms				AltConf	Trace
9	D	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 10 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.



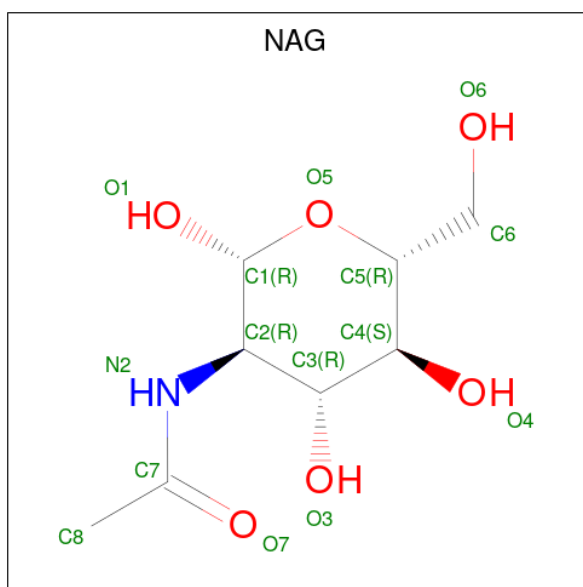
Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is (4R,7R)-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-7-[(undecanoyloxy)methyl]-3,5,8-trioxa-4lambda 5 -phosphadocosan-1-aminium (CCD ID: EGY) (formula: C₃₃H₆₇NO₈P).

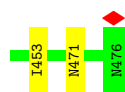


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	1	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	1	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	3	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	C	1	Total	C	N	O	P	0
			43	33	1	8	1	

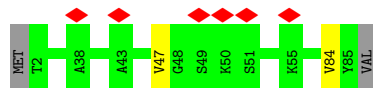
- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



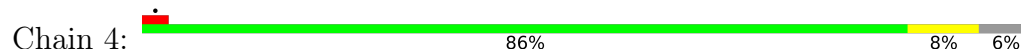
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	B	1	14	8	1	5	0



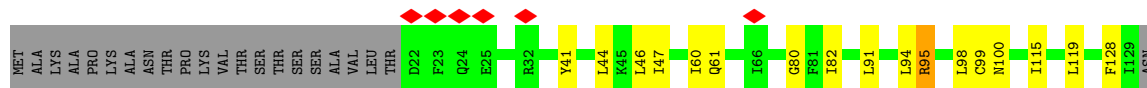
- Molecule 3: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5



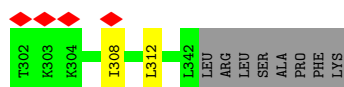
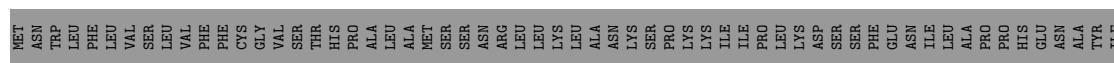
- Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4



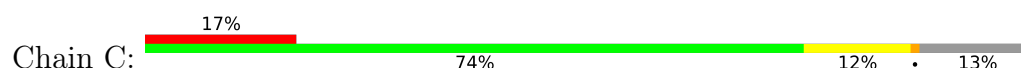
- Molecule 5: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2

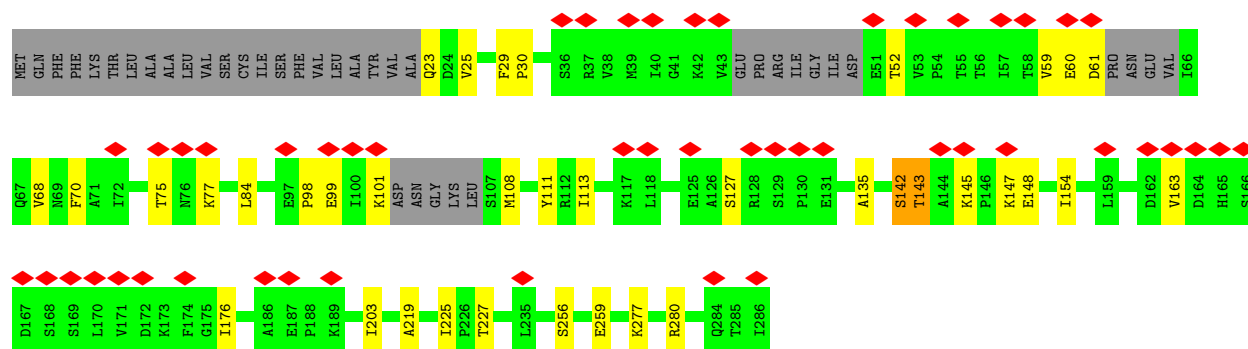


- Molecule 6: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 3



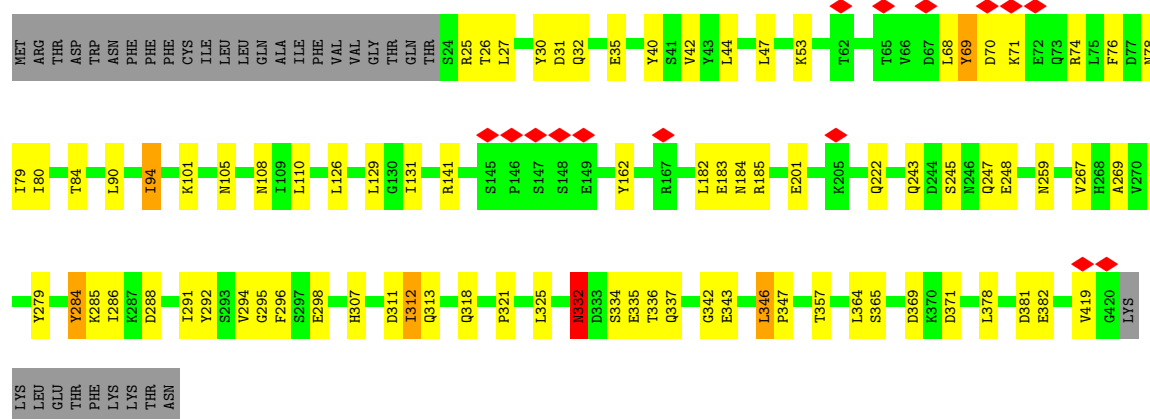
- Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1





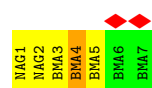
- Molecule 8: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1

Chain B: 73% 18% 8%



- Molecule 9: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-2)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 29% 29% 57% 14%



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

Chain E: 67% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	282202	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	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	0.290	Depositor
Minimum map value	-0.188	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	278.528, 278.528, 278.528	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.088, 1.088, 1.088	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, EGY

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	0.48	0/5377	0.76	8/7309 (0.1%)
2	1	0.44	0/3595	0.72	3/4891 (0.1%)
3	5	0.30	0/677	0.61	1/916 (0.1%)
4	4	0.36	0/262	0.57	0/355
5	2	0.39	0/906	0.63	0/1222
6	3	0.32	0/1057	0.65	0/1435
7	C	0.30	0/1981	0.68	1/2690 (0.0%)
8	B	0.43	0/3300	0.77	10/4482 (0.2%)
All	All	0.42	0/17155	0.72	23/23300 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	TYR	CA-C-N	-15.51	103.90	119.56
1	A	76	TYR	C-N-CA	-15.51	103.90	119.56
2	1	209	GLU	N-CA-C	8.78	120.85	111.28
8	B	346	LEU	CA-C-N	8.51	129.03	119.92
8	B	346	LEU	C-N-CA	8.51	129.03	119.92
1	A	278	ILE	N-CA-C	8.21	118.99	110.62
1	A	76	TYR	N-CA-C	7.51	123.89	113.45
8	B	311	ASP	N-CA-C	6.59	119.64	108.90
2	1	230	LEU	CA-CB-CG	6.54	139.20	116.30
8	B	334	SER	N-CA-C	6.27	118.11	111.28
8	B	284	TYR	N-CA-C	6.24	119.28	110.23
1	A	263	SER	N-CA-C	6.13	118.69	110.35
1	A	264	ASN	N-CA-C	6.00	117.83	111.28
1	A	601	GLU	N-CA-C	5.84	117.73	111.36
8	B	245	SER	N-CA-C	5.74	117.33	111.14
2	1	397	PRO	N-CA-C	5.68	124.16	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	47	VAL	N-CA-C	-5.54	107.08	112.29
8	B	312	ILE	CA-C-N	-5.31	113.53	122.29
8	B	312	ILE	C-N-CA	-5.31	113.53	122.29
8	B	332	ASN	N-CA-C	5.25	117.95	109.40
1	A	76	TYR	C-N-CD	5.22	146.41	125.00
7	C	142	SER	N-CA-C	5.20	118.72	112.38
8	B	248	GLU	N-CA-C	5.17	116.91	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5225	0	5201	61	0
2	1	3496	0	3376	37	0
3	5	659	0	668	0	0
4	4	259	0	268	6	0
5	2	883	0	914	16	0
6	3	1028	0	1062	5	0
7	C	1940	0	1991	25	0
8	B	3218	0	3120	93	0
9	D	83	0	70	2	0
10	E	39	0	34	0	0
11	1	86	0	0	0	0
11	3	43	0	0	0	0
11	4	43	0	0	0	0
11	A	129	0	0	1	0
11	C	43	0	0	0	0
12	B	14	0	13	0	0
All	All	17188	0	16717	225	0

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

All (225) 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)
8:B:69:TYR:CE1	8:B:74:ARG:HB3	1.48	1.48
8:B:69:TYR:HE1	8:B:74:ARG:CB	1.39	1.33
8:B:279:TYR:HD1	8:B:284:TYR:CE2	1.48	1.31
8:B:291:ILE:HG22	8:B:342:GLY:O	1.17	1.31
8:B:279:TYR:CD1	8:B:284:TYR:CE2	2.32	1.16
2:1:229:PRO:O	2:1:230:LEU:HD13	1.48	1.13
7:C:77:LYS:NZ	7:C:143:THR:OG1	1.83	1.09
7:C:52:THR:HG21	7:C:147:LYS:O	1.55	1.04
8:B:267:VAL:HG11	8:B:295:GLY:HA3	1.36	1.04
8:B:243:GLN:NE2	8:B:247:GLN:CD	2.17	1.03
1:A:16:LEU:HD23	4:4:25:TYR:HD1	1.23	1.02
8:B:267:VAL:CG1	8:B:295:GLY:CA	2.41	0.98
8:B:69:TYR:CE1	8:B:74:ARG:CB	2.25	0.97
8:B:69:TYR:OH	8:B:105:ASN:ND2	1.95	0.97
8:B:267:VAL:HG12	8:B:295:GLY:CA	1.93	0.97
8:B:296:PHE:HE2	8:B:312:ILE:HD13	1.28	0.97
8:B:267:VAL:HG12	8:B:295:GLY:O	1.68	0.94
8:B:267:VAL:HG12	8:B:295:GLY:C	1.92	0.93
1:A:365:PHE:HB2	1:A:368:TRP:HE3	1.33	0.93
8:B:267:VAL:CG1	8:B:295:GLY:HA3	2.00	0.92
8:B:291:ILE:CG2	8:B:342:GLY:O	2.14	0.92
2:1:229:PRO:O	2:1:230:LEU:CD1	2.20	0.89
7:C:25:VAL:O	7:C:108:MET:HA	1.73	0.88
7:C:52:THR:CG2	7:C:147:LYS:O	2.21	0.87
2:1:220:LEU:HD13	2:1:222:ILE:HD11	1.55	0.87
8:B:279:TYR:CD1	8:B:284:TYR:HE2	1.93	0.87
8:B:419:VAL:HG12	8:B:419:VAL:O	1.75	0.87
1:A:78:LEU:HD12	1:A:78:LEU:O	1.76	0.86
8:B:296:PHE:HE2	8:B:312:ILE:CD1	1.90	0.84
8:B:69:TYR:HE1	8:B:74:ARG:HB3	0.66	0.81
8:B:243:GLN:HE22	8:B:247:GLN:CD	1.87	0.80
8:B:69:TYR:HD1	8:B:74:ARG:HA	1.47	0.79
8:B:243:GLN:NE2	8:B:247:GLN:OE1	2.16	0.79
2:1:171:LYS:O	2:1:209:GLU:O	2.00	0.78
5:2:95:ARG:HG3	5:2:95:ARG:HH11	1.49	0.78
8:B:286:ILE:CG2	8:B:378:LEU:HD22	2.14	0.77
8:B:44:LEU:O	8:B:47:LEU:HB3	1.84	0.77
8:B:286:ILE:HG22	8:B:378:LEU:HD22	1.64	0.77
8:B:69:TYR:CD1	8:B:74:ARG:HA	2.19	0.77
1:A:275:LEU:HD22	1:A:275:LEU:O	1.84	0.77
1:A:260:PRO:O	1:A:261:ILE:HD13	1.85	0.76
8:B:267:VAL:HG12	8:B:295:GLY:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:77:LYS:CE	7:C:143:THR:OG1	2.35	0.74
1:A:16:LEU:CD2	4:4:25:TYR:HD1	2.01	0.74
1:A:16:LEU:HD23	4:4:25:TYR:CD1	2.15	0.73
1:A:365:PHE:HB2	1:A:368:TRP:CE3	2.22	0.73
8:B:243:GLN:HE21	8:B:247:GLN:CD	1.97	0.73
8:B:279:TYR:CD1	8:B:284:TYR:CD2	2.76	0.71
1:A:373:GLY:O	1:A:377:LEU:HB2	1.91	0.71
1:A:262:ARG:HH21	1:A:262:ARG:HG3	1.56	0.70
2:1:220:LEU:HD13	2:1:222:ILE:CD1	2.19	0.70
2:1:220:LEU:CD1	2:1:222:ILE:HD11	2.22	0.70
8:B:267:VAL:CG1	8:B:295:GLY:N	2.54	0.70
8:B:296:PHE:CE2	8:B:312:ILE:HD13	2.19	0.70
2:1:33:ASN:HB3	2:1:55:ILE:HG22	1.74	0.69
2:1:230:LEU:CD2	2:1:260:LYS:O	2.41	0.69
8:B:286:ILE:CG2	8:B:378:LEU:CD2	2.70	0.69
8:B:286:ILE:HG21	8:B:378:LEU:CD2	2.23	0.68
5:2:44:LEU:HD12	5:2:95:ARG:CZ	2.25	0.68
8:B:69:TYR:HD2	8:B:101:LYS:NZ	1.91	0.67
5:2:95:ARG:HG3	5:2:95:ARG:NH1	2.08	0.67
8:B:321:PRO:O	9:D:4:BMA:O4	2.13	0.67
2:1:230:LEU:HD22	2:1:260:LYS:O	1.96	0.66
8:B:267:VAL:CG1	8:B:295:GLY:C	2.67	0.63
8:B:279:TYR:CE1	8:B:284:TYR:CD2	2.86	0.63
1:A:597:ILE:O	1:A:599:PRO:HD3	1.98	0.63
8:B:69:TYR:HD2	8:B:101:LYS:HZ2	1.44	0.62
8:B:267:VAL:HG11	8:B:295:GLY:CA	2.10	0.62
1:A:260:PRO:C	1:A:261:ILE:HD13	2.25	0.61
5:2:47:ILE:HG23	5:2:91:LEU:HD12	1.81	0.61
8:B:27:LEU:HD12	8:B:76:PHE:CZ	2.35	0.61
1:A:251:MET:HE1	1:A:261:ILE:HG12	1.82	0.61
8:B:129:LEU:O	8:B:185:ARG:NH1	2.34	0.61
8:B:296:PHE:CE2	8:B:312:ILE:CD1	2.79	0.60
1:A:374:VAL:O	1:A:378:PHE:HB2	2.02	0.59
1:A:262:ARG:HH21	1:A:262:ARG:CG	2.15	0.59
7:C:77:LYS:HE3	7:C:143:THR:OG1	2.02	0.59
2:1:220:LEU:CD1	2:1:222:ILE:CD1	2.81	0.59
1:A:251:MET:CE	1:A:261:ILE:HG12	2.32	0.59
5:2:99:CYS:SG	5:2:100:ASN:N	2.76	0.59
8:B:69:TYR:CD1	8:B:74:ARG:CA	2.85	0.58
8:B:80:ILE:HG22	8:B:110:LEU:HB3	1.86	0.58
8:B:357:THR:HG23	8:B:357:THR:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:29:PHE:HB3	7:C:68:VAL:HA	1.86	0.57
2:1:42:VAL:HG12	2:1:47:ILE:HG12	1.86	0.57
1:A:597:ILE:O	1:A:599:PRO:CD	2.53	0.57
1:A:506:ASN:HD21	2:1:334:ASN:H	1.50	0.57
1:A:119:ALA:HB1	1:A:160:SER:HB2	1.87	0.57
6:3:294:LEU:O	6:3:298:LEU:HB2	2.04	0.57
8:B:69:TYR:CE1	8:B:74:ARG:CA	2.88	0.57
7:C:256:SER:OG	7:C:259:GLU:OE1	2.23	0.56
1:A:275:LEU:HD22	1:A:275:LEU:C	2.30	0.56
1:A:673:GLU:OE1	2:1:270:ARG:NH1	2.38	0.56
7:C:60:GLU:HB3	7:C:70:PHE:HE1	1.71	0.56
8:B:295:GLY:HA2	8:B:337:GLN:O	2.06	0.56
1:A:413:ILE:O	1:A:417:ALA:HB3	2.06	0.55
8:B:267:VAL:HG12	8:B:295:GLY:H	1.70	0.55
2:1:230:LEU:HD21	2:1:260:LYS:O	2.06	0.55
7:C:59:VAL:HG12	7:C:61:ASP:H	1.71	0.55
2:1:471:ASN:HB3	7:C:280:ARG:HH12	1.71	0.54
8:B:69:TYR:CE1	8:B:74:ARG:HB2	2.38	0.54
2:1:65:GLU:N	2:1:117:ILE:O	2.40	0.54
8:B:419:VAL:O	8:B:419:VAL:CG1	2.48	0.54
2:1:229:PRO:C	2:1:230:LEU:CD1	2.81	0.54
5:2:60:ILE:HD11	7:C:203:ILE:HD11	1.89	0.54
1:A:530:THR:O	1:A:530:THR:OG1	2.25	0.54
8:B:31:ASP:HB2	8:B:84:THR:HG22	1.90	0.54
8:B:74:ARG:NH1	8:B:105:ASN:O	2.41	0.54
2:1:50:THR:HG22	2:1:134:LYS:HG2	1.89	0.53
2:1:293:MET:SD	2:1:293:MET:N	2.78	0.53
7:C:77:LYS:HZ1	7:C:143:THR:HG1	1.43	0.53
7:C:99:GLU:HG2	7:C:101:LYS:H	1.72	0.53
1:A:368:TRP:CD1	1:A:368:TRP:C	2.86	0.53
1:A:267:MET:CE	11:A:803:EGY:C29	2.87	0.53
8:B:35:GLU:HG3	8:B:40:TYR:HE2	1.74	0.53
8:B:69:TYR:CD2	8:B:101:LYS:NZ	2.73	0.53
1:A:77:PRO:O	8:B:318:GLN:NE2	2.39	0.52
2:1:180:SER:OG	2:1:181:SER:N	2.42	0.52
5:2:94:LEU:O	5:2:98:LEU:HB2	2.09	0.52
2:1:46:TYR:OH	2:1:429:GLN:NE2	2.42	0.52
8:B:69:TYR:CD1	8:B:74:ARG:CB	2.91	0.52
8:B:279:TYR:C	8:B:279:TYR:CD2	2.88	0.52
8:B:108:ASN:HD21	8:B:259:ASN:HD22	1.58	0.51
1:A:262:ARG:CG	1:A:262:ARG:NH2	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD23	1:A:270:LEU:O	2.11	0.51
8:B:42:VAL:HG11	8:B:243:GLN:HG3	1.92	0.50
8:B:25:ARG:HG2	8:B:53:LYS:HD2	1.93	0.50
2:1:156:LEU:O	2:1:223:VAL:HA	2.11	0.49
8:B:141:ARG:HH22	8:B:201:GLU:HB2	1.76	0.49
8:B:26:THR:HG22	8:B:78:ASN:HD22	1.76	0.49
6:3:308:ILE:O	6:3:312:LEU:HB2	2.13	0.49
8:B:279:TYR:CE1	8:B:284:TYR:CE2	2.96	0.49
5:2:41:TYR:HD1	8:B:419:VAL:CG2	2.26	0.48
1:A:78:LEU:HD22	9:D:1:NAG:H83	1.94	0.48
5:2:61:GLN:HE22	5:2:80:GLY:HA3	1.78	0.48
7:C:52:THR:HG23	7:C:147:LYS:O	2.12	0.48
1:A:413:ILE:O	1:A:417:ALA:CB	2.61	0.48
1:A:424:ILE:HD11	6:3:284:VAL:HG13	1.96	0.47
5:2:46:LEU:HD23	7:C:219:ALA:HB1	1.96	0.47
8:B:222:GLN:HE22	8:B:365:SER:HA	1.78	0.47
8:B:30:TYR:HE2	8:B:32:GLN:HE21	1.63	0.47
1:A:708:SER:OG	1:A:710:LYS:NZ	2.48	0.47
2:1:56:LYS:HA	2:1:128:GLU:HA	1.96	0.47
7:C:225:ILE:HG22	7:C:227:THR:HG23	1.97	0.47
1:A:141:SER:OG	4:4:29:ASP:OD2	2.33	0.47
7:C:30:PRO:HA	7:C:113:ILE:HG13	1.97	0.47
8:B:68:LEU:HD11	8:B:94:ILE:HG21	1.97	0.47
8:B:332:ASN:ND2	8:B:332:ASN:C	2.73	0.47
8:B:162:TYR:CD1	8:B:364:LEU:HD11	2.50	0.47
1:A:631:LYS:HE2	1:A:661:PRO:HG2	1.96	0.46
2:1:373:VAL:HG22	2:1:427:ILE:HG23	1.96	0.46
8:B:243:GLN:O	8:B:247:GLN:HB2	2.15	0.46
1:A:456:ILE:HD13	4:4:23:VAL:HG21	1.96	0.46
1:A:51:ASN:HD22	1:A:91:MET:HE3	1.80	0.46
1:A:72:ASP:OD1	1:A:72:ASP:N	2.41	0.46
8:B:291:ILE:HG23	8:B:343:GLU:HG2	1.98	0.46
2:1:209:GLU:N	2:1:209:GLU:OE1	2.49	0.45
8:B:269:ALA:HB2	8:B:294:VAL:HG23	1.97	0.45
5:2:41:TYR:CD1	8:B:419:VAL:CG2	2.99	0.45
1:A:185:ALA:HB2	1:A:193:HIS:HB2	1.97	0.45
2:1:300:THR:HB	2:1:342:THR:HG23	1.97	0.45
7:C:23:GLN:HA	7:C:75:THR:HG21	1.98	0.45
1:A:497:ARG:HH12	2:1:309:GLY:HA3	1.82	0.45
7:C:127:SER:HB3	7:C:163:VAL:HG22	1.99	0.45
8:B:26:THR:HG22	8:B:78:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:290:VAL:HG12	2:1:324:ARG:HG2	1.99	0.45
2:1:229:PRO:C	2:1:230:LEU:HD12	2.43	0.44
8:B:279:TYR:HE1	8:B:284:TYR:CD2	2.35	0.44
8:B:243:GLN:HE21	8:B:247:GLN:CG	2.31	0.44
1:A:508:ASP:OD1	1:A:508:ASP:N	2.49	0.44
8:B:381:ASP:OD1	8:B:381:ASP:O	2.36	0.44
1:A:176:MET:HE2	1:A:176:MET:HB2	1.89	0.44
1:A:248:VAL:HG21	5:2:82:ILE:HG21	1.98	0.44
1:A:382:LYS:HB2	1:A:385:HIS:CE1	2.52	0.44
1:A:672:SER:OG	1:A:673:GLU:N	2.49	0.44
2:1:239:ASP:OD1	2:1:239:ASP:N	2.49	0.44
1:A:368:TRP:CD1	1:A:368:TRP:O	2.70	0.44
8:B:298:GLU:HB2	8:B:307:HIS:HB2	2.00	0.44
1:A:159:ARG:HG3	1:A:407:LEU:HD22	1.98	0.44
2:1:317:GLU:HG3	2:1:318:ARG:H	1.83	0.44
5:2:115:ILE:O	5:2:119:LEU:HB2	2.18	0.43
8:B:279:TYR:HE1	8:B:284:TYR:HD2	1.65	0.43
8:B:286:ILE:HG22	8:B:378:LEU:CD2	2.35	0.43
7:C:84:LEU:O	7:C:135:ALA:HA	2.17	0.43
2:1:138:ASN:HD22	2:1:425:ASN:HD22	1.66	0.43
1:A:219:PRO:HB3	1:A:272:VAL:HG21	2.01	0.43
8:B:285:LYS:HD3	8:B:382:GLU:OE1	2.19	0.43
8:B:286:ILE:HG21	8:B:378:LEU:HD22	1.90	0.43
6:3:211:PHE:HA	6:3:214:ILE:HG22	2.00	0.43
1:A:16:LEU:CD2	4:4:25:TYR:CD1	2.91	0.43
7:C:277:LYS:HE2	7:C:277:LYS:HB3	1.87	0.43
1:A:262:ARG:CZ	1:A:262:ARG:CB	2.96	0.43
8:B:371:ASP:N	8:B:371:ASP:OD1	2.49	0.43
1:A:262:ARG:NH2	1:A:262:ARG:HB2	2.34	0.42
1:A:357:PRO:O	1:A:361:PHE:HB2	2.19	0.42
2:1:249:ILE:HD12	2:1:348:PHE:HD2	1.84	0.42
8:B:183:GLU:HG2	8:B:184:ASN:H	1.84	0.42
8:B:346:LEU:HA	8:B:347:PRO:HD3	1.83	0.42
1:A:273:PHE:CD2	1:A:273:PHE:C	2.98	0.42
8:B:369:ASP:OD1	8:B:369:ASP:N	2.51	0.42
8:B:312:ILE:HG22	8:B:313:GLN:N	2.35	0.42
1:A:176:MET:HE1	1:A:411:PRO:HB3	2.01	0.42
5:2:44:LEU:HD12	5:2:95:ARG:NH2	2.35	0.42
7:C:145:LYS:HB3	7:C:148:GLU:HB2	2.02	0.42
8:B:243:GLN:NE2	8:B:247:GLN:NE2	2.66	0.42
1:A:277:GLN:OE1	1:A:277:GLN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:PHE:HD1	1:A:389:ILE:HD13	1.84	0.42
1:A:572:ILE:HG22	1:A:677:VAL:HG12	2.02	0.42
6:3:237:PHE:CD2	6:3:237:PHE:C	2.98	0.42
8:B:271:HIS:HB3	8:B:292:TYR:HD1	1.85	0.42
2:1:391:ASP:OD1	2:1:391:ASP:N	2.53	0.41
2:1:366:LEU:HD11	2:1:374:TYR:CD2	2.56	0.41
2:1:408:SER:OG	2:1:409:TYR:N	2.49	0.41
8:B:126:LEU:HD13	8:B:131:ILE:HD11	2.01	0.41
1:A:252:GLN:HE22	5:2:128:PHE:HB2	1.85	0.41
5:2:95:ARG:NH1	5:2:95:ARG:CG	2.79	0.41
7:C:176:ILE:HD12	7:C:176:ILE:HA	1.98	0.41
1:A:75:TRP:NE1	1:A:534:ASP:OD1	2.54	0.41
1:A:548:LYS:HD2	1:A:598:TRP:CE3	2.56	0.41
8:B:335:GLU:HG3	8:B:336:THR:HG23	2.02	0.41
1:A:668:GLU:OE2	1:A:671:THR:OG1	2.23	0.40
1:A:78:LEU:O	1:A:78:LEU:CD1	2.59	0.40
2:1:84:TYR:HB2	2:1:132:VAL:HG22	2.02	0.40
7:C:98:PRO:HD2	7:C:111:TYR:CD1	2.56	0.40
8:B:288:ASP:N	8:B:288:ASP:OD1	2.54	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	640/718 (89%)	592 (92%)	47 (7%)	1 (0%)	43	74
2	1	426/476 (90%)	368 (86%)	58 (14%)	0	100	100
3	5	82/86 (95%)	82 (100%)	0	0	100	100
4	4	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
5	2	106/130 (82%)	100 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	3	122/350 (35%)	107 (88%)	15 (12%)	0	100	100
7	C	240/286 (84%)	201 (84%)	39 (16%)	0	100	100
8	B	395/430 (92%)	361 (91%)	34 (9%)	0	100	100
All	All	2043/2512 (81%)	1842 (90%)	200 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	TRP

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	552/613 (90%)	539 (98%)	13 (2%)	43	64
2	1	391/426 (92%)	381 (97%)	10 (3%)	40	62
3	5	73/75 (97%)	72 (99%)	1 (1%)	59	71
4	4	31/33 (94%)	31 (100%)	0	100	100
5	2	97/115 (84%)	96 (99%)	1 (1%)	68	75
6	3	112/316 (35%)	111 (99%)	1 (1%)	70	76
7	C	216/249 (87%)	213 (99%)	3 (1%)	59	71
8	B	361/392 (92%)	352 (98%)	9 (2%)	42	63
All	All	1833/2219 (83%)	1795 (98%)	38 (2%)	46	66

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	81	VAL
1	A	145	LEU
1	A	261	ILE
1	A	262	ARG

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Mol	Chain	Res	Type
1	A	264	ASN
1	A	267	MET
1	A	275	LEU
1	A	276	ILE
1	A	576	LEU
1	A	588	LEU
1	A	629	LEU
1	A	660	VAL
2	1	40	ILE
2	1	194	LEU
2	1	195	LEU
2	1	203	PHE
2	1	209	GLU
2	1	230	LEU
2	1	377	VAL
2	1	396	VAL
2	1	427	ILE
2	1	453	ILE
3	5	84	VAL
5	2	95	ARG
6	3	236	MET
7	C	142	SER
7	C	143	THR
7	C	154	ILE
8	B	69	TYR
8	B	70	ASP
8	B	71	LYS
8	B	79	ILE
8	B	90	LEU
8	B	94	ILE
8	B	182	LEU
8	B	325	LEU
8	B	332	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	103	ASN
1	A	186	GLN
1	A	193	HIS
1	A	266	HIS

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Mol	Chain	Res	Type
1	A	364	HIS
1	A	506	ASN
1	A	688	GLN
2	1	118	GLN
2	1	278	GLN
2	1	302	HIS
2	1	425	ASN
2	1	434	GLN
5	2	61	GLN
7	C	181	HIS
8	B	78	ASN
8	B	93	GLN
8	B	105	ASN
8	B	108	ASN
8	B	138	HIS
8	B	157	HIS
8	B	222	GLN
8	B	240	ASN
8	B	243	GLN
8	B	307	HIS
8	B	332	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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
9	NAG	D	1	1,9	14,14,15	0.33	0	17,19,21	0.75	0
9	NAG	D	2	9	14,14,15	0.52	0	17,19,21	0.78	1 (5%)
9	BMA	D	3	9	11,11,12	1.64	1 (9%)	15,15,17	1.84	3 (20%)
9	BMA	D	4	9	11,11,12	2.94	5 (45%)	15,15,17	2.29	6 (40%)
9	BMA	D	5	9	11,11,12	2.07	3 (27%)	15,15,17	1.57	3 (20%)
9	BMA	D	6	9	11,11,12	0.90	0	15,15,17	0.77	0
9	BMA	D	7	9	11,11,12	0.81	0	15,15,17	1.01	0
10	NAG	E	1	10,2	14,14,15	0.62	0	17,19,21	2.44	4 (23%)
10	NAG	E	2	10	14,14,15	1.34	2 (14%)	17,19,21	2.70	4 (23%)
10	BMA	E	3	10	11,11,12	1.00	1 (9%)	15,15,17	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	D	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	D	2	9	-	2/6/23/26	0/1/1/1
9	BMA	D	3	9	-	2/2/19/22	0/1/1/1
9	BMA	D	4	9	-	1/2/19/22	0/1/1/1
9	BMA	D	5	9	-	2/2/19/22	0/1/1/1
9	BMA	D	6	9	-	2/2/19/22	0/1/1/1
9	BMA	D	7	9	-	0/2/19/22	0/1/1/1
10	NAG	E	1	10,2	-	6/6/23/26	0/1/1/1
10	NAG	E	2	10	-	4/6/23/26	0/1/1/1
10	BMA	E	3	10	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	4	BMA	O2-C2	6.53	1.57	1.43
9	D	4	BMA	C1-C2	4.86	1.63	1.52
9	D	3	BMA	C1-C2	4.79	1.63	1.52
9	D	5	BMA	O2-C2	3.82	1.51	1.43
9	D	5	BMA	C2-C3	3.70	1.58	1.52
10	E	2	NAG	C1-C2	3.46	1.57	1.52
9	D	4	BMA	C4-C5	3.35	1.60	1.53
9	D	5	BMA	C1-C2	3.24	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	2	NAG	O5-C1	3.11	1.48	1.43
10	E	3	BMA	C1-C2	2.32	1.57	1.52
9	D	4	BMA	C2-C3	2.27	1.56	1.52
9	D	4	BMA	C4-C3	2.24	1.58	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	2	NAG	C2-N2-C7	8.32	134.05	122.90
10	E	1	NAG	C2-N2-C7	8.26	133.97	122.90
10	E	2	NAG	C1-O5-C5	5.53	119.59	112.19
9	D	4	BMA	O2-C2-C1	5.39	121.56	109.22
9	D	3	BMA	O2-C2-C3	-5.03	99.74	110.15
10	E	1	NAG	C1-C2-N2	4.05	116.82	110.43
10	E	2	NAG	C1-C2-N2	3.84	116.48	110.43
9	D	4	BMA	C1-C2-C3	-3.61	104.38	109.64
9	D	3	BMA	C1-C2-C3	-3.37	104.73	109.64
9	D	5	BMA	O2-C2-C1	3.31	116.81	109.22
9	D	5	BMA	O2-C2-C3	2.91	116.18	110.15
9	D	4	BMA	C3-C4-C5	2.81	115.32	110.23
9	D	5	BMA	C2-C3-C4	2.76	115.72	110.86
9	D	2	NAG	C1-O5-C5	2.66	115.76	112.19
9	D	4	BMA	O5-C1-C2	-2.59	104.62	110.79
9	D	4	BMA	C2-C3-C4	2.53	115.31	110.86
9	D	3	BMA	O2-C2-C1	2.48	114.90	109.22
10	E	1	NAG	C1-O5-C5	2.22	115.16	112.19
10	E	1	NAG	C8-C7-N2	2.18	119.73	116.12
10	E	2	NAG	C8-C7-N2	2.17	119.72	116.12
9	D	4	BMA	O2-C2-C3	2.16	114.62	110.15

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	2	NAG	O5-C5-C6-O6
9	D	6	BMA	O5-C5-C6-O6
9	D	3	BMA	C4-C5-C6-O6
10	E	3	BMA	O5-C5-C6-O6
9	D	2	NAG	C4-C5-C6-O6
9	D	5	BMA	O5-C5-C6-O6
9	D	3	BMA	O5-C5-C6-O6
9	D	6	BMA	C4-C5-C6-O6

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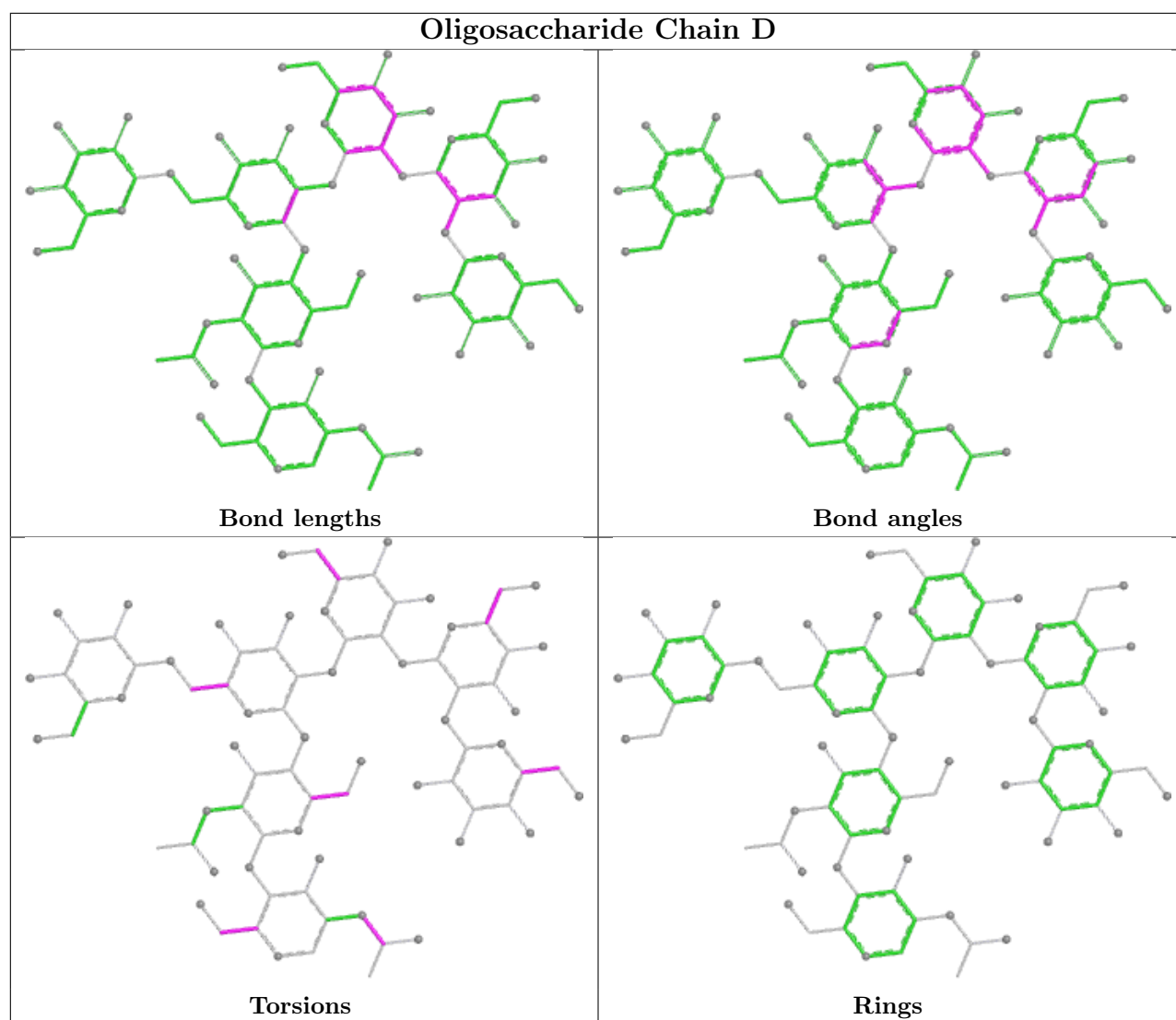
Mol	Chain	Res	Type	Atoms
9	D	1	NAG	C8-C7-N2-C2
9	D	1	NAG	O7-C7-N2-C2
10	E	1	NAG	C8-C7-N2-C2
10	E	1	NAG	O7-C7-N2-C2
10	E	2	NAG	C8-C7-N2-C2
10	E	2	NAG	O7-C7-N2-C2
10	E	3	BMA	C4-C5-C6-O6
9	D	4	BMA	O5-C5-C6-O6
9	D	5	BMA	C4-C5-C6-O6
10	E	1	NAG	C4-C5-C6-O6
10	E	1	NAG	C3-C2-N2-C7
10	E	1	NAG	O5-C5-C6-O6
9	D	1	NAG	C4-C5-C6-O6
10	E	1	NAG	C1-C2-N2-C7
10	E	2	NAG	C1-C2-N2-C7
10	E	2	NAG	C3-C2-N2-C7

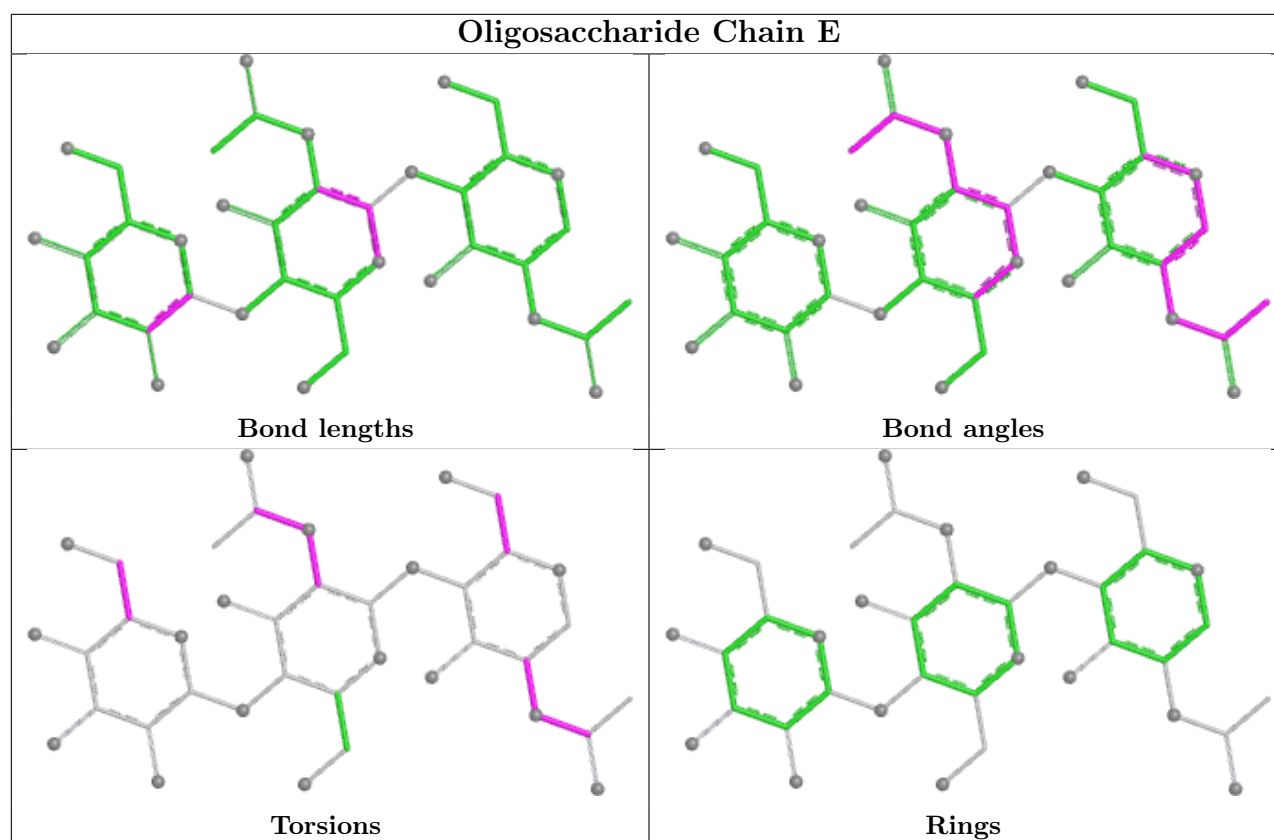
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	4	BMA	1	0
9	D	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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	EGY	A	802	-	42,42,42	1.28	6 (14%)	48,50,50	1.14	3 (6%)
11	EGY	C	301	-	42,42,42	1.32	5 (11%)	48,50,50	1.14	2 (4%)
11	EGY	3	401	-	42,42,42	1.28	4 (9%)	48,50,50	1.10	2 (4%)
11	EGY	A	803	-	42,42,42	1.29	5 (11%)	48,50,50	1.06	3 (6%)
11	EGY	1	502	-	42,42,42	1.28	4 (9%)	48,50,50	1.10	2 (4%)
12	NAG	B	601	8	14,14,15	0.64	0	17,19,21	1.06	2 (11%)
11	EGY	4	101	-	42,42,42	1.28	4 (9%)	48,50,50	1.07	2 (4%)
11	EGY	A	801	-	42,42,42	1.26	3 (7%)	48,50,50	1.11	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	EGY	1	501	-	42,42,42	1.27	4 (9%)	48,50,50	1.13	2 (4%)

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	EGY	A	802	-	-	18/46/46/46	-
11	EGY	C	301	-	-	20/46/46/46	-
11	EGY	3	401	-	-	26/46/46/46	-
11	EGY	A	803	-	-	18/46/46/46	-
11	EGY	1	502	-	-	23/46/46/46	-
12	NAG	B	601	8	-	4/6/23/26	0/1/1/1
11	EGY	4	101	-	-	17/46/46/46	-
11	EGY	A	801	-	-	24/46/46/46	-
11	EGY	1	501	-	-	19/46/46/46	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	301	EGY	O21-C21	3.25	1.43	1.34
11	4	101	EGY	O31-C31	3.18	1.42	1.33
11	A	803	EGY	O31-C31	3.14	1.42	1.33
11	C	301	EGY	O31-C31	3.14	1.42	1.33
11	3	401	EGY	O31-C31	3.09	1.42	1.33
11	A	801	EGY	O31-C31	3.08	1.42	1.33
11	4	101	EGY	O21-C21	3.07	1.42	1.34
11	1	502	EGY	O31-C31	3.07	1.42	1.33
11	1	501	EGY	O31-C31	3.05	1.42	1.33
11	A	802	EGY	O21-C21	3.05	1.42	1.34
11	1	502	EGY	O21-C21	3.01	1.42	1.34
11	3	401	EGY	O21-C21	2.94	1.42	1.34
11	1	501	EGY	O21-C21	2.93	1.42	1.34
11	A	801	EGY	O21-C21	2.93	1.42	1.34
11	A	803	EGY	O21-C21	2.87	1.42	1.34
11	A	802	EGY	O31-C31	2.70	1.41	1.33
11	A	803	EGY	O21-C2	-2.58	1.40	1.46
11	3	401	EGY	O21-C2	-2.54	1.40	1.46
11	1	501	EGY	O21-C2	-2.46	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	801	EGY	O21-C2	-2.45	1.40	1.46
11	A	802	EGY	O21-C2	-2.42	1.40	1.46
11	1	502	EGY	O21-C2	-2.42	1.40	1.46
11	4	101	EGY	O21-C2	-2.35	1.41	1.46
11	C	301	EGY	O21-C2	-2.26	1.41	1.46
11	A	802	EGY	P-O13	2.20	1.68	1.59
11	C	301	EGY	C22-C21	2.13	1.56	1.50
11	A	803	EGY	P-O13	2.13	1.67	1.59
11	1	501	EGY	P-O13	2.11	1.67	1.59
11	1	502	EGY	P-O13	2.10	1.67	1.59
11	A	802	EGY	C22-C21	2.10	1.56	1.50
11	3	401	EGY	P-O13	2.09	1.67	1.59
11	4	101	EGY	P-O13	2.05	1.67	1.59
11	C	301	EGY	P-O11	2.02	1.67	1.59
11	A	802	EGY	P-O11	2.00	1.67	1.59
11	A	803	EGY	P-O11	2.00	1.67	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	301	EGY	O21-C21-C22	4.56	121.35	111.48
11	1	501	EGY	O21-C21-C22	4.25	120.67	111.48
11	A	802	EGY	O21-C21-C22	4.13	120.42	111.48
11	A	801	EGY	O21-C21-C22	4.05	120.23	111.48
11	1	502	EGY	O21-C21-C22	4.05	120.23	111.48
11	3	401	EGY	O21-C21-C22	4.01	120.16	111.48
11	A	803	EGY	O21-C21-C22	3.65	119.37	111.48
11	4	101	EGY	O21-C21-C22	3.59	119.24	111.48
12	B	601	NAG	C2-N2-C7	3.22	127.22	122.90
11	C	301	EGY	O31-C31-C32	2.99	120.97	111.83
11	A	803	EGY	O31-C31-C32	2.82	120.43	111.83
11	1	502	EGY	O31-C31-C32	2.73	120.17	111.83
11	4	101	EGY	O31-C31-C32	2.64	119.88	111.83
11	3	401	EGY	O31-C31-C32	2.61	119.78	111.83
11	A	801	EGY	O31-C31-C32	2.58	119.71	111.83
11	A	802	EGY	O31-C31-C32	2.44	119.27	111.83
11	1	501	EGY	O31-C31-C32	2.40	119.17	111.83
11	A	802	EGY	C3-C2-C1	-2.18	106.71	111.78
12	B	601	NAG	C1-O5-C5	2.06	114.95	112.19
11	A	803	EGY	C23-C22-C21	-2.02	106.28	113.69

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	801	EGY	C11-O13-P-O12
11	A	801	EGY	C11-O13-P-O14
11	A	801	EGY	C11-O13-P-O11
11	A	801	EGY	C1-O11-P-O12
11	A	801	EGY	C1-O11-P-O14
11	A	801	EGY	C1-O11-P-O13
11	A	801	EGY	C22-C21-O21-C2
11	A	803	EGY	C11-O13-P-O11
11	A	803	EGY	C1-O11-P-O12
11	A	803	EGY	C1-O11-P-O14
11	A	803	EGY	C1-O11-P-O13
11	1	501	EGY	C11-O13-P-O14
11	1	501	EGY	C11-O13-P-O11
11	1	501	EGY	C1-O11-P-O14
11	1	501	EGY	C1-O11-P-O13
11	1	501	EGY	C12-C11-O13-P
11	1	502	EGY	C11-O13-P-O14
11	1	502	EGY	C1-O11-P-O14
11	1	502	EGY	C1-O11-P-O13
11	1	502	EGY	C12-C11-O13-P
11	4	101	EGY	C11-O13-P-O12
11	4	101	EGY	C11-O13-P-O14
11	4	101	EGY	C11-O13-P-O11
11	4	101	EGY	O13-C11-C12-N
11	3	401	EGY	C11-O13-P-O12
11	3	401	EGY	C11-O13-P-O11
11	3	401	EGY	C1-O11-P-O12
11	3	401	EGY	C1-O11-P-O13
11	3	401	EGY	C12-C11-O13-P
11	3	401	EGY	O13-C11-C12-N
11	3	401	EGY	O11-C1-C2-O21
11	3	401	EGY	C22-C21-O21-C2
11	C	301	EGY	C11-O13-P-O12
11	C	301	EGY	C11-O13-P-O14
11	C	301	EGY	C11-O13-P-O11
11	C	301	EGY	C1-O11-P-O13
11	C	301	EGY	O13-C11-C12-N
11	C	301	EGY	O22-C21-O21-C2
11	C	301	EGY	C22-C21-O21-C2
11	A	801	EGY	O32-C31-O31-C3
11	A	803	EGY	O32-C31-O31-C3
11	A	801	EGY	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
11	1	502	EGY	O32-C31-O31-C3
11	C	301	EGY	O32-C31-O31-C3
11	A	801	EGY	O22-C21-O21-C2
11	3	401	EGY	O22-C21-O21-C2
11	A	803	EGY	C32-C31-O31-C3
11	1	502	EGY	C32-C31-O31-C3
11	C	301	EGY	C32-C31-O31-C3
11	A	802	EGY	C32-C31-O31-C3
11	1	501	EGY	C32-C31-O31-C3
11	4	101	EGY	C32-C31-O31-C3
11	A	802	EGY	O32-C31-O31-C3
11	1	501	EGY	O32-C31-O31-C3
11	A	801	EGY	C21-C22-C23-C24
11	4	101	EGY	O32-C31-O31-C3
11	1	502	EGY	C21-C22-C23-C24
11	3	401	EGY	C11-C12-N-C13
11	3	401	EGY	C11-C12-N-C14
11	3	401	EGY	C11-C12-N-C15
11	4	101	EGY	C22-C23-C24-C25
11	3	401	EGY	C36-C37-C38-C39
11	C	301	EGY	C36-C37-C38-C39
11	A	801	EGY	C37-C38-C39-C3A
11	1	502	EGY	C22-C21-O21-C2
11	A	803	EGY	C33-C34-C35-C36
11	A	802	EGY	C31-C32-C33-C34
11	1	502	EGY	C35-C36-C37-C38
11	1	502	EGY	C34-C35-C36-C37
11	4	101	EGY	C34-C35-C36-C37
11	3	401	EGY	C23-C24-C25-C26
11	C	301	EGY	C37-C38-C39-C3A
11	1	502	EGY	C36-C37-C38-C39
11	C	301	EGY	C25-C26-C27-C28
11	4	101	EGY	C23-C24-C25-C26
11	1	501	EGY	C25-C26-C27-C28
11	A	803	EGY	C21-C22-C23-C24
11	1	502	EGY	C31-C32-C33-C34
11	A	801	EGY	C25-C26-C27-C28
11	A	802	EGY	C26-C27-C28-C29
11	4	101	EGY	C21-C22-C23-C24
11	1	502	EGY	O22-C21-O21-C2
11	1	501	EGY	C29-C2A-C2B-C2C
11	1	501	EGY	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
11	1	501	EGY	C28-C29-C2A-C2B
11	C	301	EGY	C24-C25-C26-C27
11	1	501	EGY	O11-C1-C2-C3
11	1	502	EGY	O11-C1-C2-C3
11	3	401	EGY	C31-C32-C33-C34
11	C	301	EGY	C1-C2-C3-O31
11	1	502	EGY	C37-C38-C39-C3A
11	A	801	EGY	C32-C33-C34-C35
11	A	801	EGY	C27-C28-C29-C2A
11	A	802	EGY	C22-C21-O21-C2
11	1	501	EGY	C27-C28-C29-C2A
11	A	801	EGY	C26-C27-C28-C29
11	3	401	EGY	O11-C1-C2-C3
11	3	401	EGY	C28-C29-C2A-C2B
11	3	401	EGY	C29-C2A-C2B-C2C
11	A	803	EGY	C28-C29-C2A-C2B
11	3	401	EGY	C1-C2-C3-O31
11	3	401	EGY	C26-C27-C28-C29
11	1	501	EGY	O11-C1-C2-O21
11	A	803	EGY	O21-C2-C3-O31
11	C	301	EGY	O21-C2-C3-O31
11	A	802	EGY	C33-C34-C35-C36
11	A	802	EGY	O22-C21-O21-C2
11	A	803	EGY	C36-C37-C38-C39
11	4	101	EGY	C38-C39-C3A-C3B
11	A	801	EGY	C24-C25-C26-C27
11	1	502	EGY	O11-C1-C2-O21
11	3	401	EGY	C32-C33-C34-C35
11	3	401	EGY	C33-C34-C35-C36
11	A	803	EGY	C32-C33-C34-C35
11	A	801	EGY	O13-C11-C12-N
11	A	803	EGY	O13-C11-C12-N
11	C	301	EGY	C34-C35-C36-C37
11	1	501	EGY	C38-C39-C3A-C3B
11	C	301	EGY	O11-C1-C2-C3
11	C	301	EGY	O11-C1-C2-O21
12	B	601	NAG	C4-C5-C6-O6
11	A	802	EGY	C34-C35-C36-C37
11	3	401	EGY	O21-C2-C3-O31
11	A	803	EGY	C1-C2-C3-O31
11	A	802	EGY	C11-O13-P-O12
11	A	802	EGY	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
11	A	802	EGY	C11-O13-P-O11
11	A	802	EGY	C11-C12-N-C14
11	3	401	EGY	C1-O11-P-O14
11	C	301	EGY	C1-O11-P-O12
11	1	502	EGY	C2B-C2C-C2D-C2E
11	4	101	EGY	C37-C38-C39-C3A
11	4	101	EGY	C31-C32-C33-C34
11	1	501	EGY	C2B-C2C-C2D-C2E
11	1	502	EGY	C33-C34-C35-C36
11	A	802	EGY	C11-C12-N-C13
11	A	802	EGY	C11-C12-N-C15
11	A	803	EGY	C27-C28-C29-C2A
11	A	801	EGY	C23-C24-C25-C26
11	1	502	EGY	C23-C24-C25-C26
11	3	401	EGY	O31-C31-C32-C33
11	1	502	EGY	C22-C23-C24-C25
11	A	801	EGY	C38-C39-C3A-C3B
11	C	301	EGY	C2B-C2C-C2D-C2E
11	1	502	EGY	C38-C39-C3A-C3B
12	B	601	NAG	C1-C2-N2-C7
11	A	801	EGY	C22-C23-C24-C25
11	A	802	EGY	O11-C1-C2-O21
12	B	601	NAG	C3-C2-N2-C7
11	A	803	EGY	C23-C24-C25-C26
11	A	803	EGY	O31-C31-C32-C33
11	A	801	EGY	C33-C34-C35-C36
11	4	101	EGY	O21-C21-C22-C23
11	1	501	EGY	O13-C11-C12-N
11	3	401	EGY	C2A-C2B-C2C-C2D
11	1	502	EGY	O21-C21-C22-C23
11	1	501	EGY	O22-C21-O21-C2
11	A	802	EGY	C38-C39-C3A-C3B
11	4	101	EGY	O31-C31-C32-C33
11	A	801	EGY	O21-C2-C3-O31
11	1	501	EGY	C22-C21-O21-C2
11	A	802	EGY	O21-C21-C22-C23
11	1	502	EGY	O22-C21-C22-C23
11	4	101	EGY	O32-C31-C32-C33
11	A	803	EGY	O32-C31-C32-C33
11	A	801	EGY	O31-C31-C32-C33
11	4	101	EGY	O22-C21-C22-C23
12	B	601	NAG	O5-C5-C6-O6

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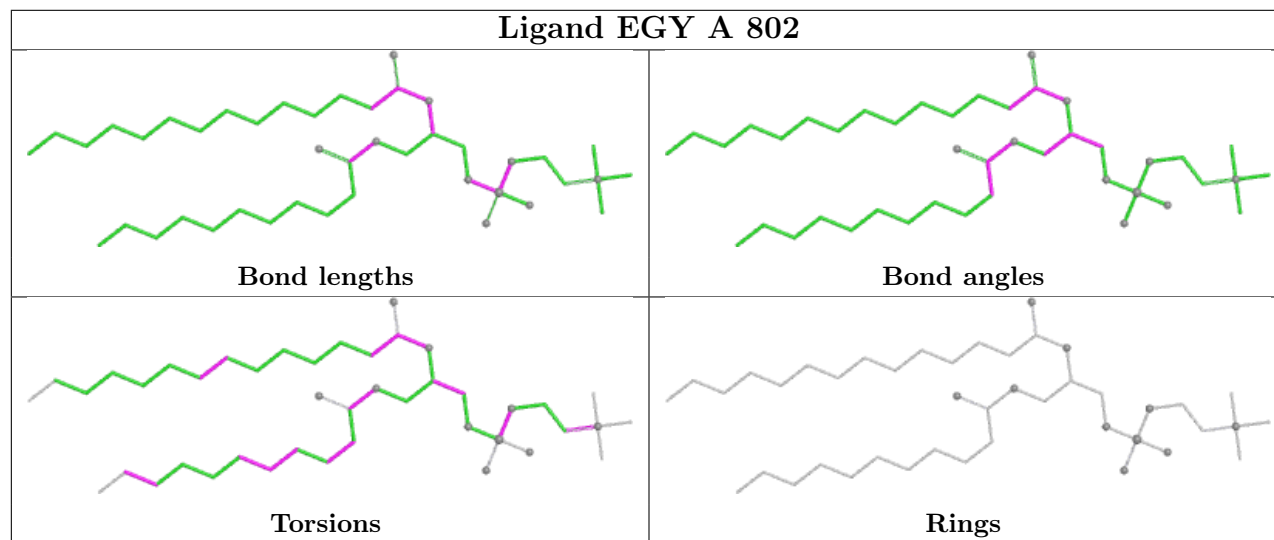
Mol	Chain	Res	Type	Atoms
11	A	802	EGY	O22-C21-C22-C23

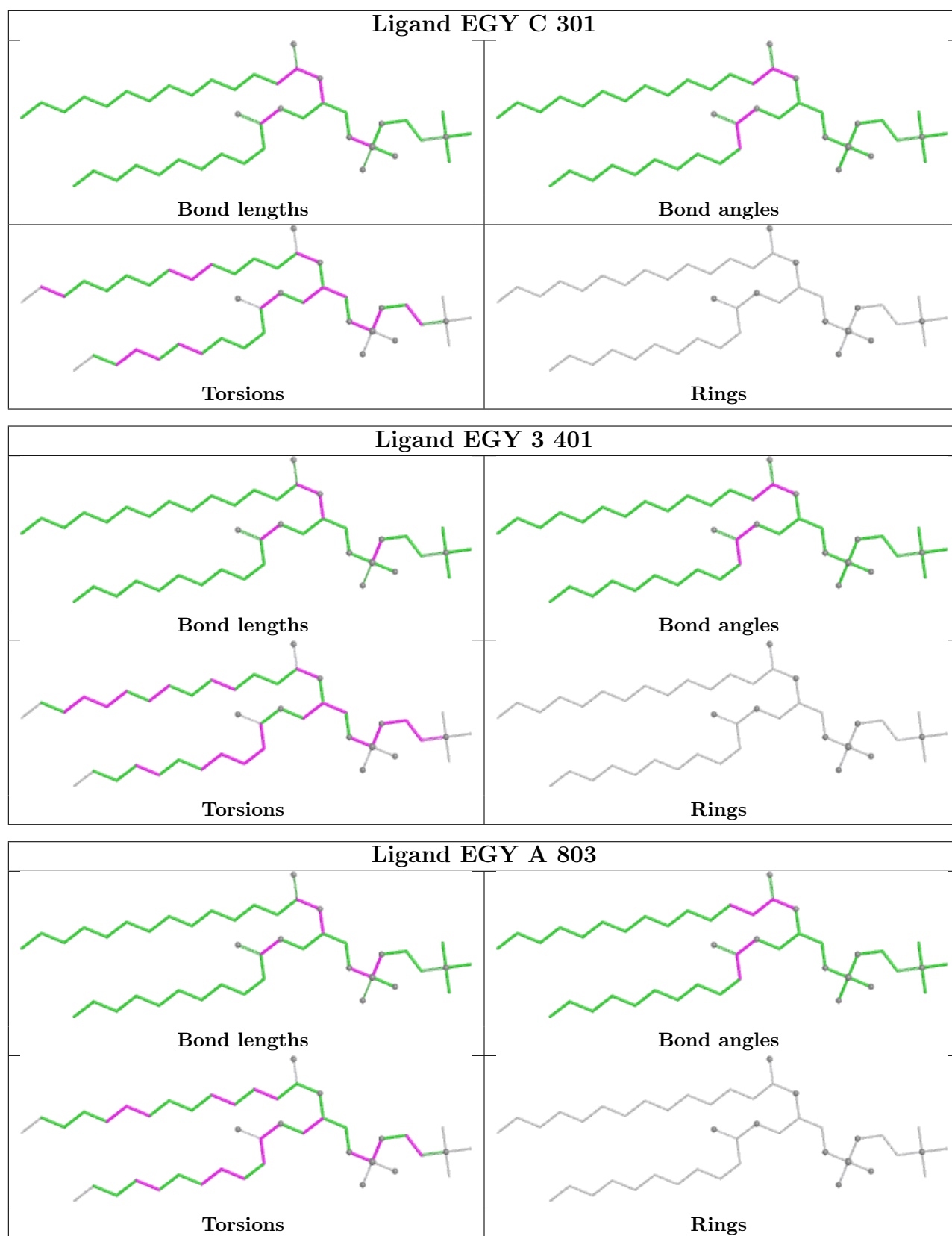
There are no ring outliers.

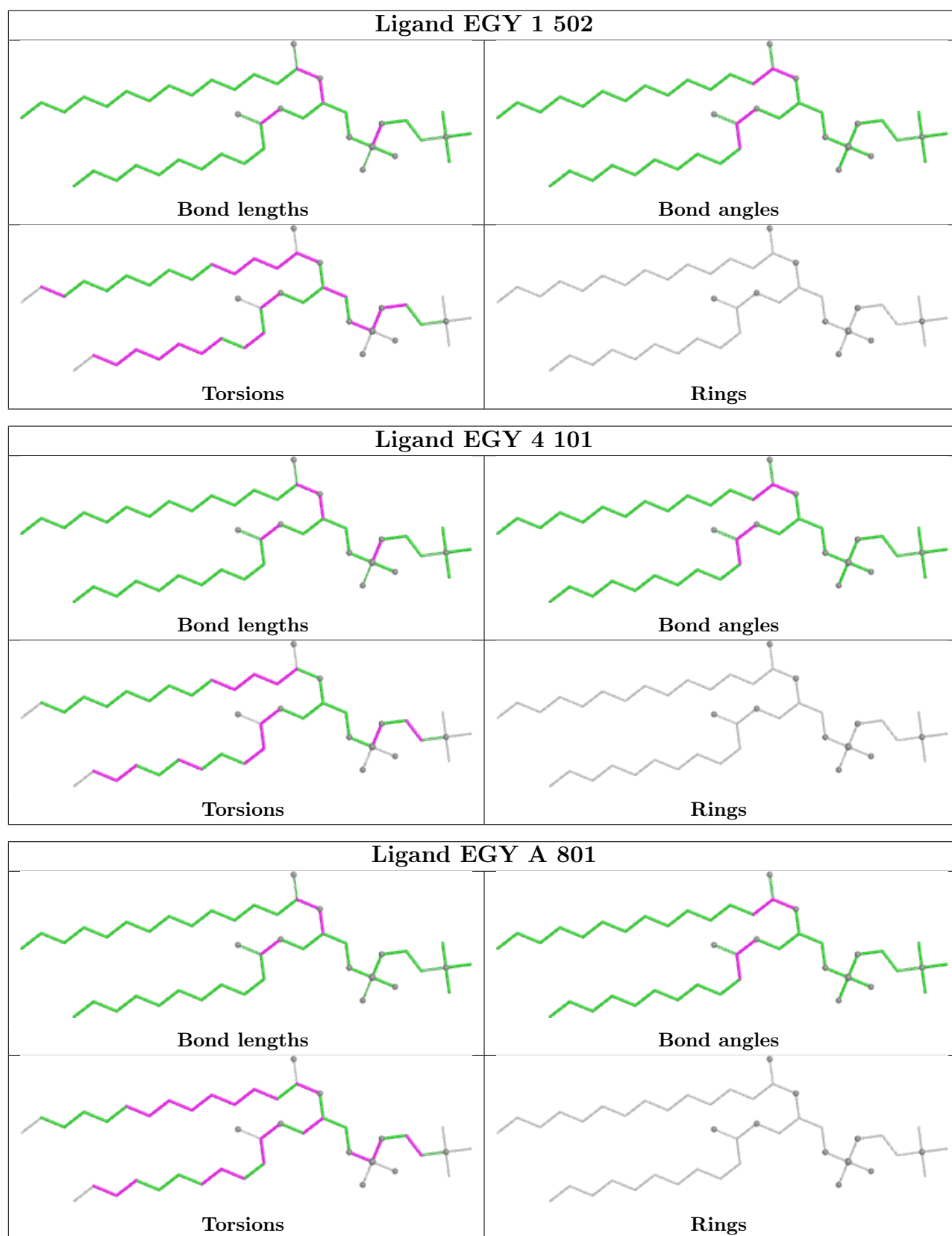
1 monomer is involved in 1 short contact:

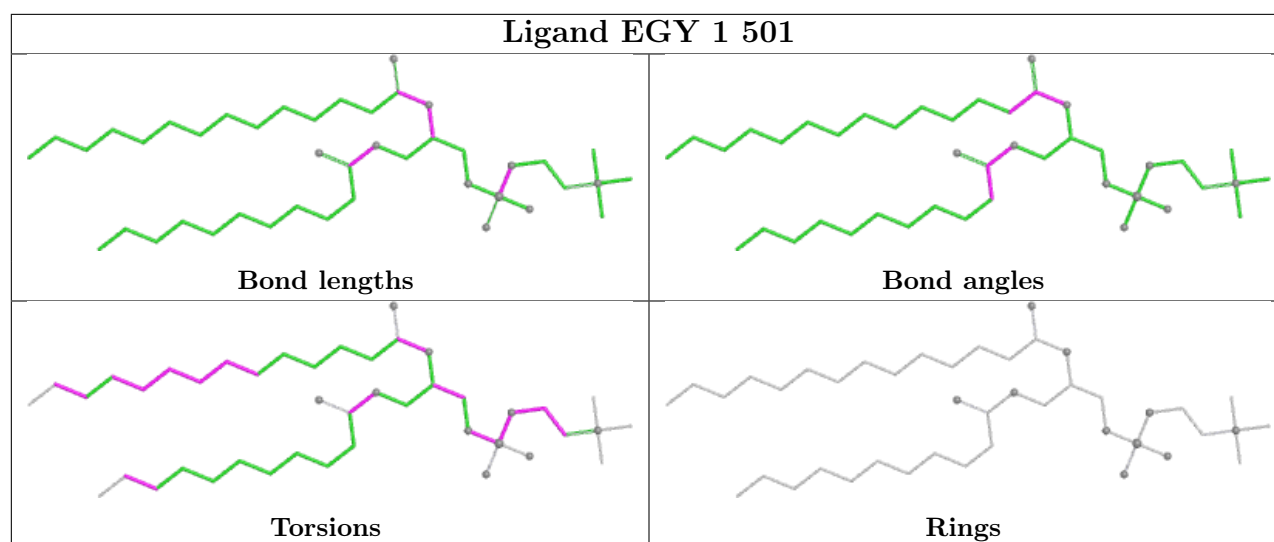
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	803	EGY	1	0

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.

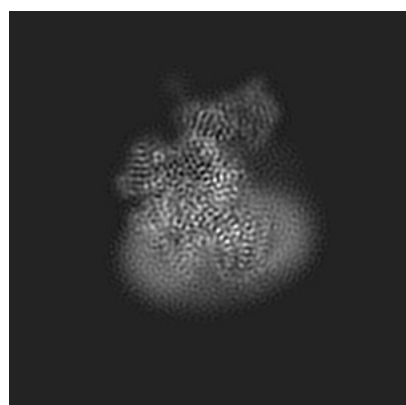
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7336. These allow visual inspection of the internal detail of the map and identification of artifacts.

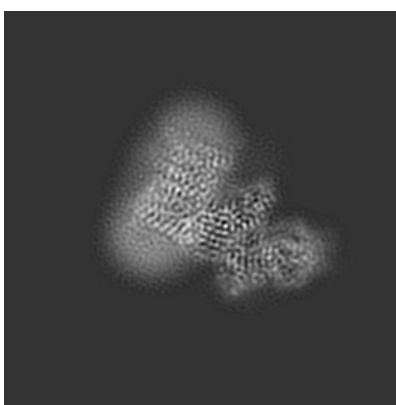
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

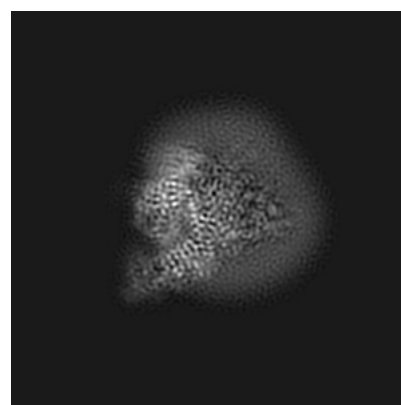
6.1.1 Primary map



X



Y

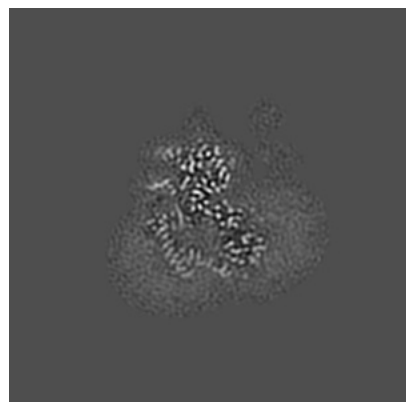


Z

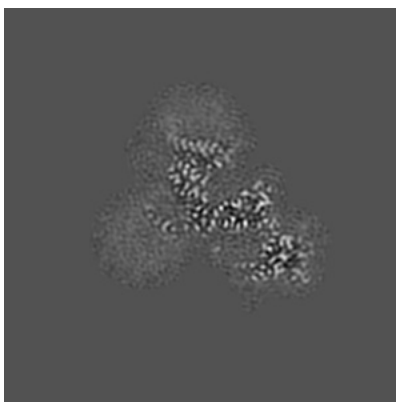
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

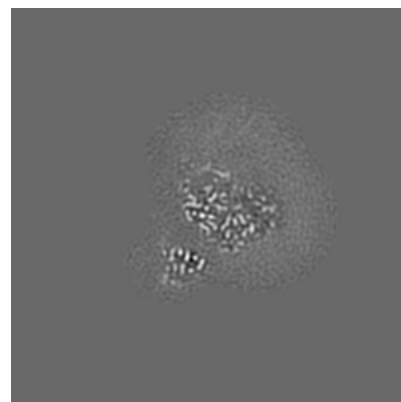
6.2.1 Primary map



X Index: 128



Y Index: 128

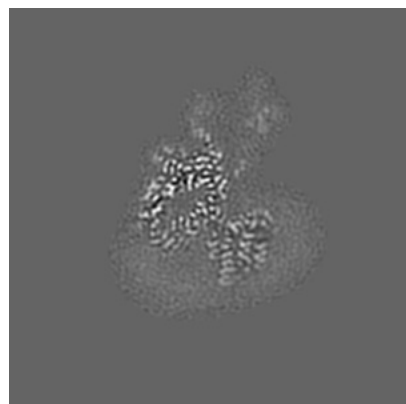


Z Index: 128

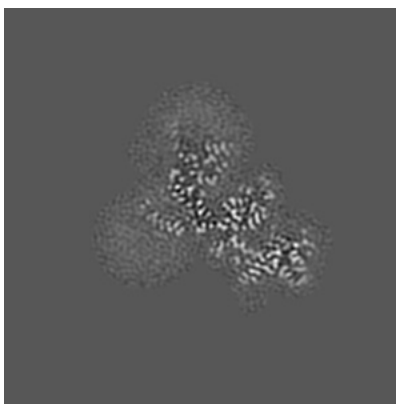
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

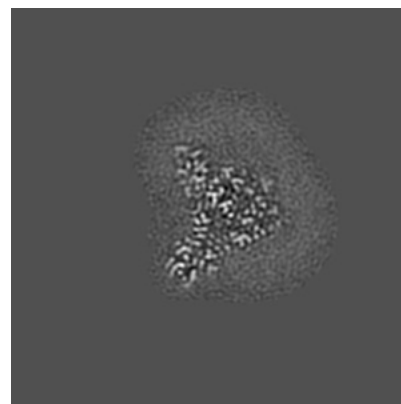
6.3.1 Primary map



X Index: 118



Y Index: 131

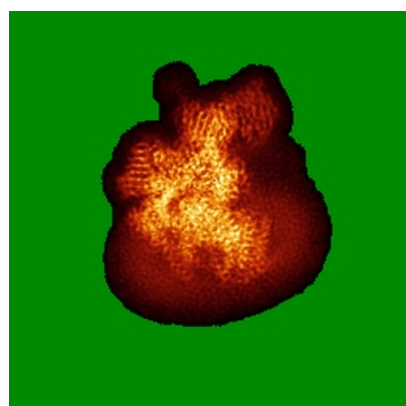


Z Index: 118

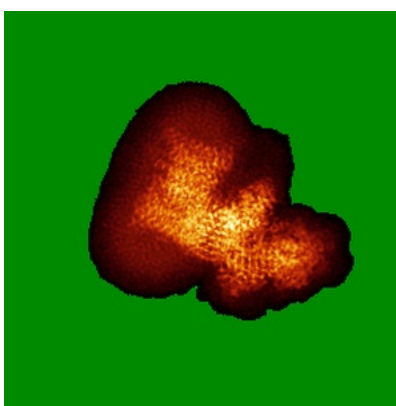
The images above show the largest variance slices of the map in three orthogonal directions.

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

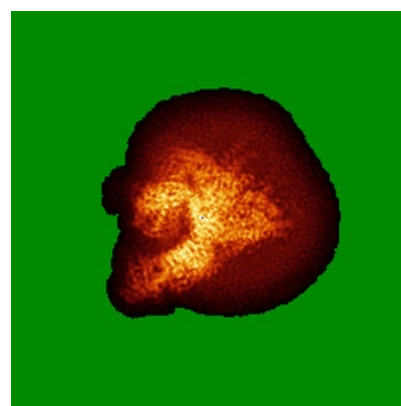
6.4.1 Primary map



X



Y

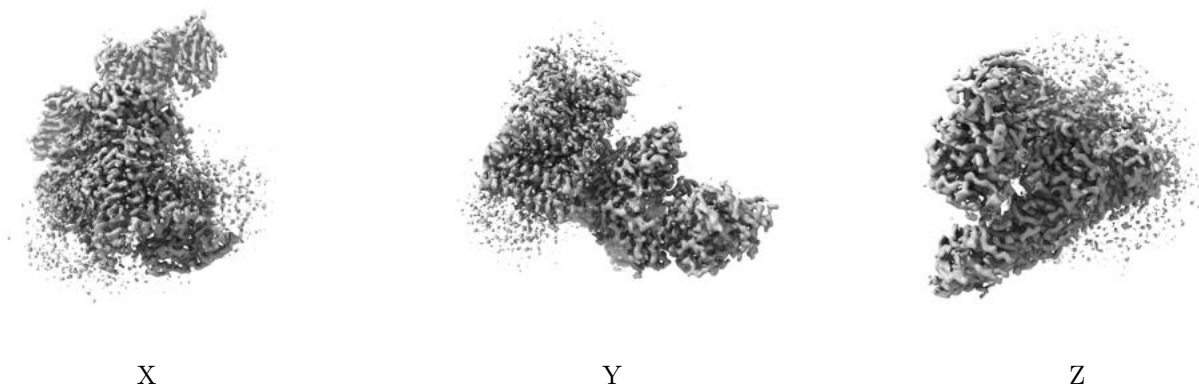


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

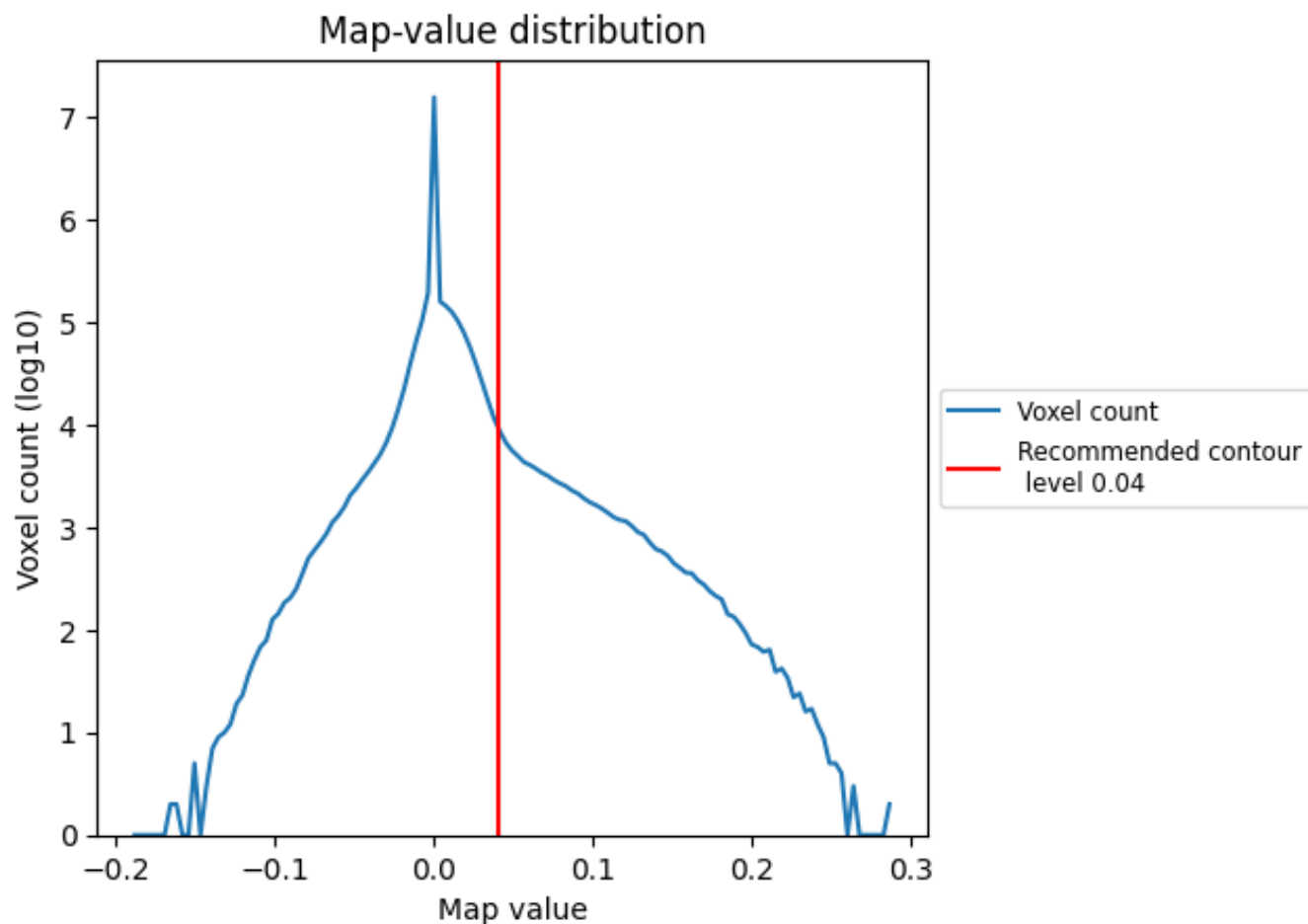
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

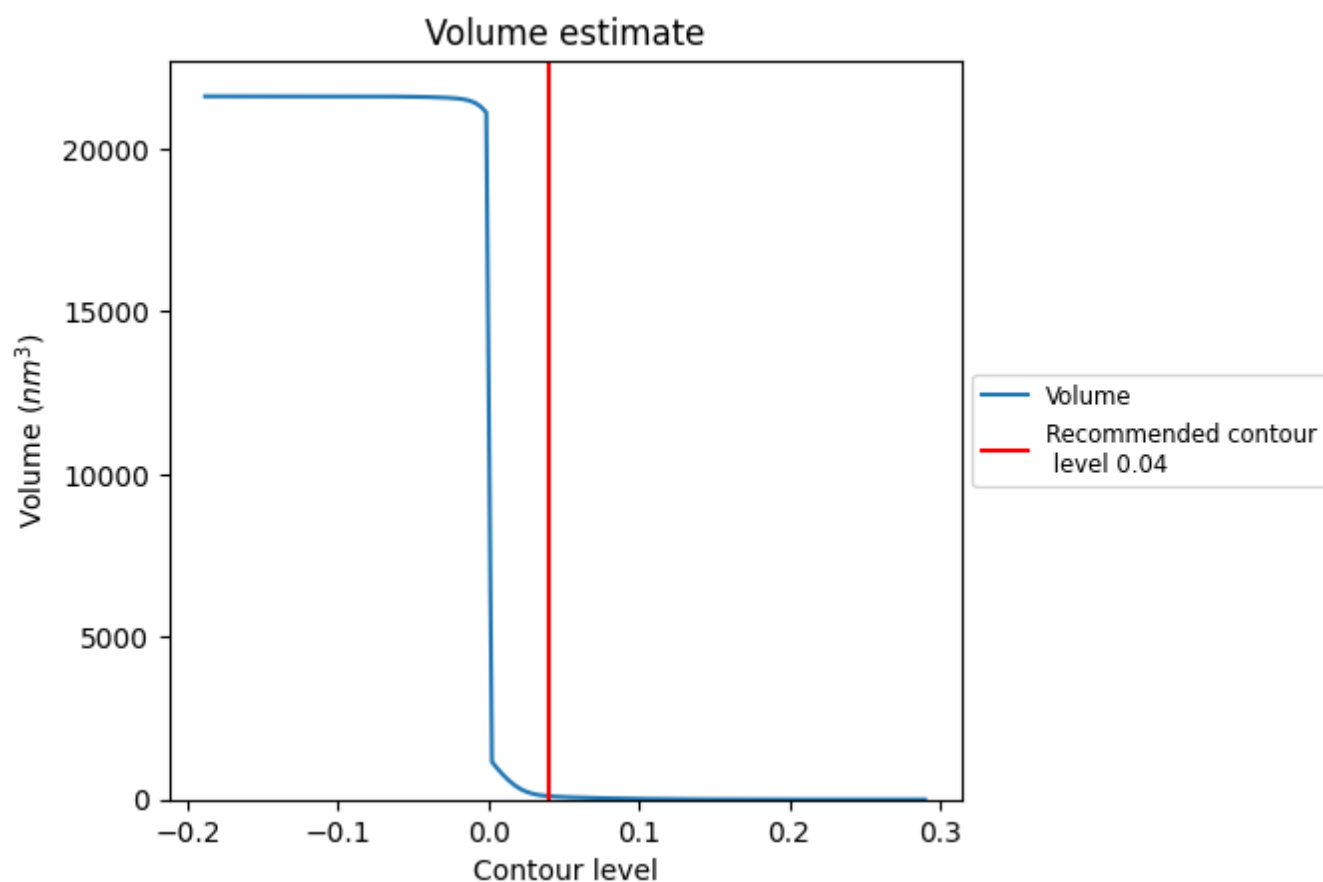
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

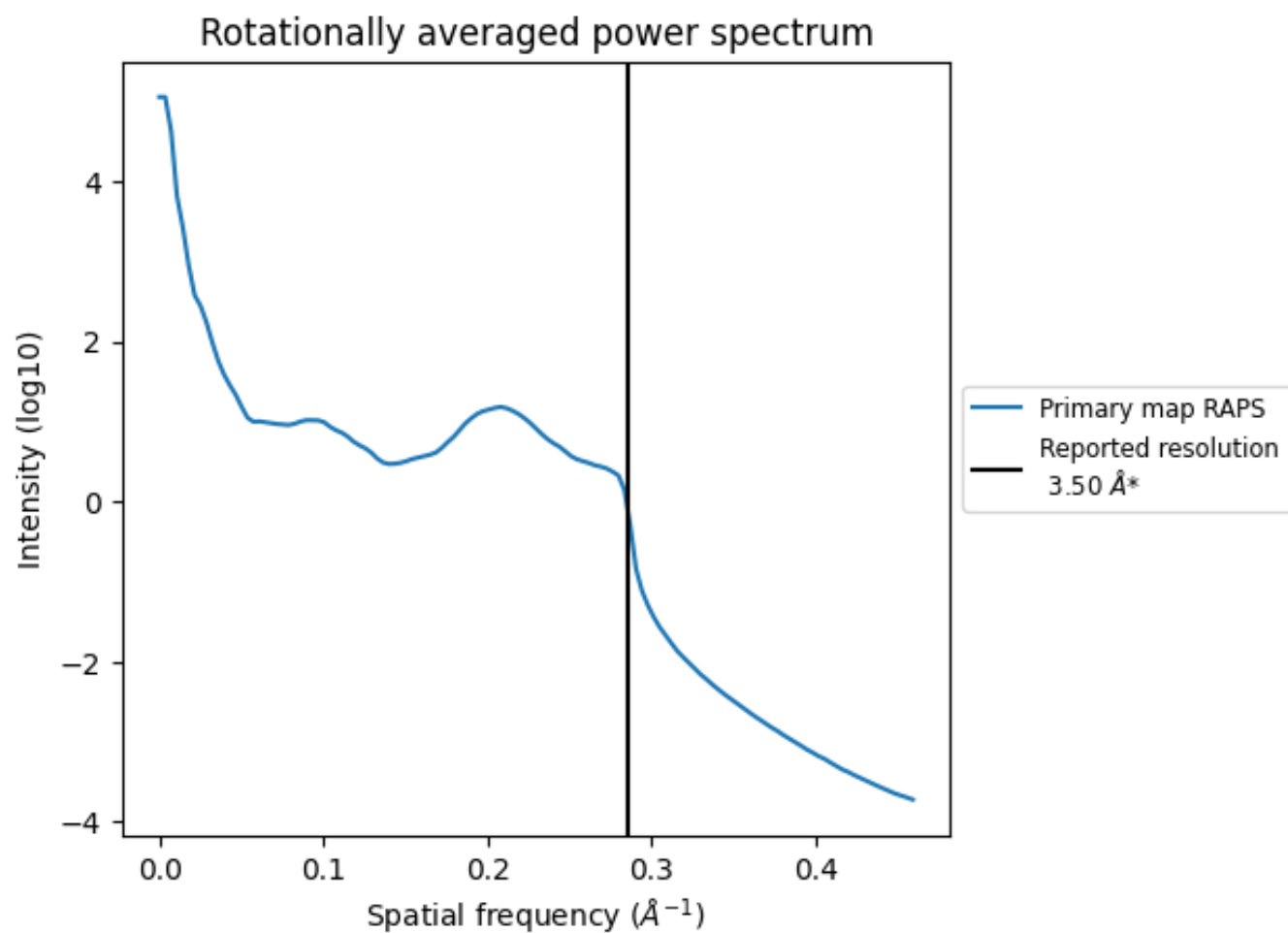
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

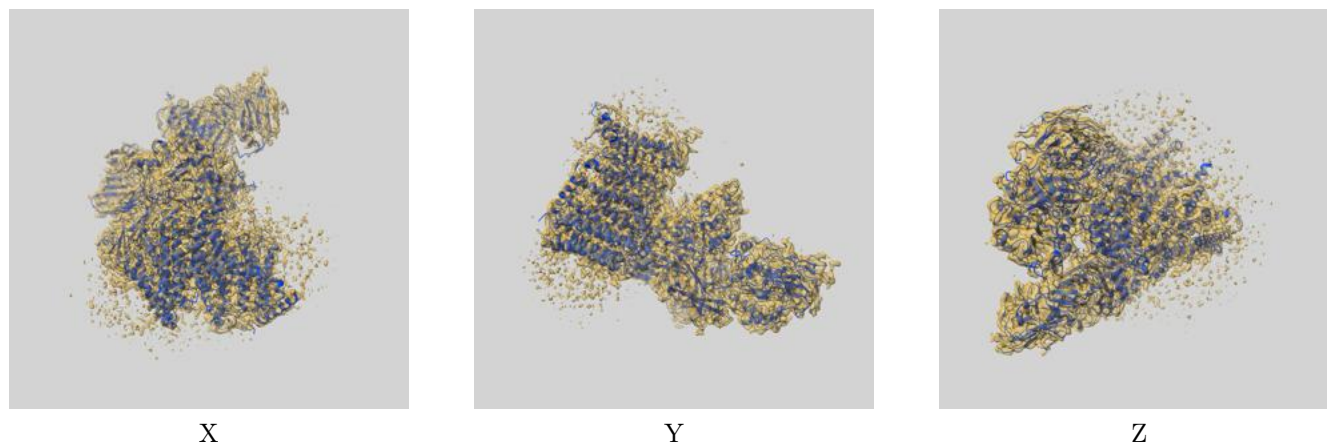
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

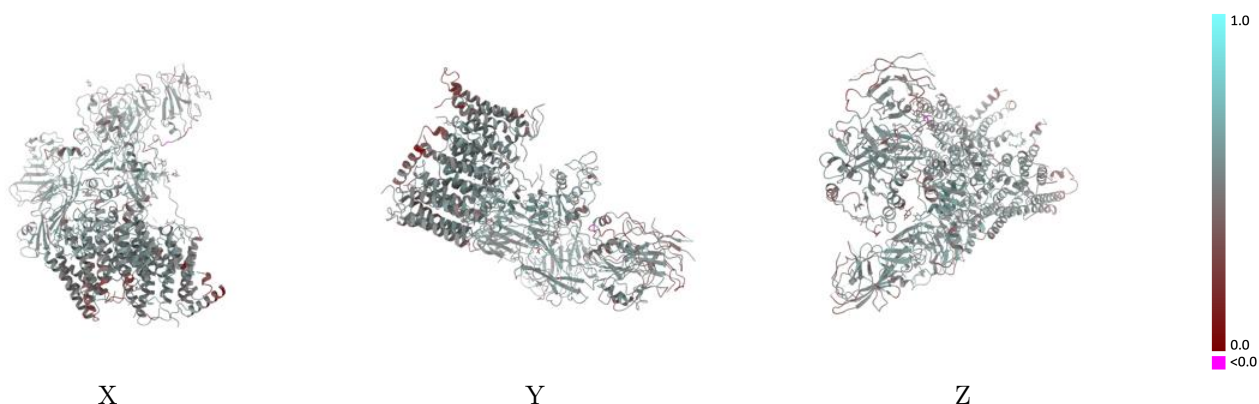
This section contains information regarding the fit between EMDB map EMD-7336 and PDB model 6C26. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)

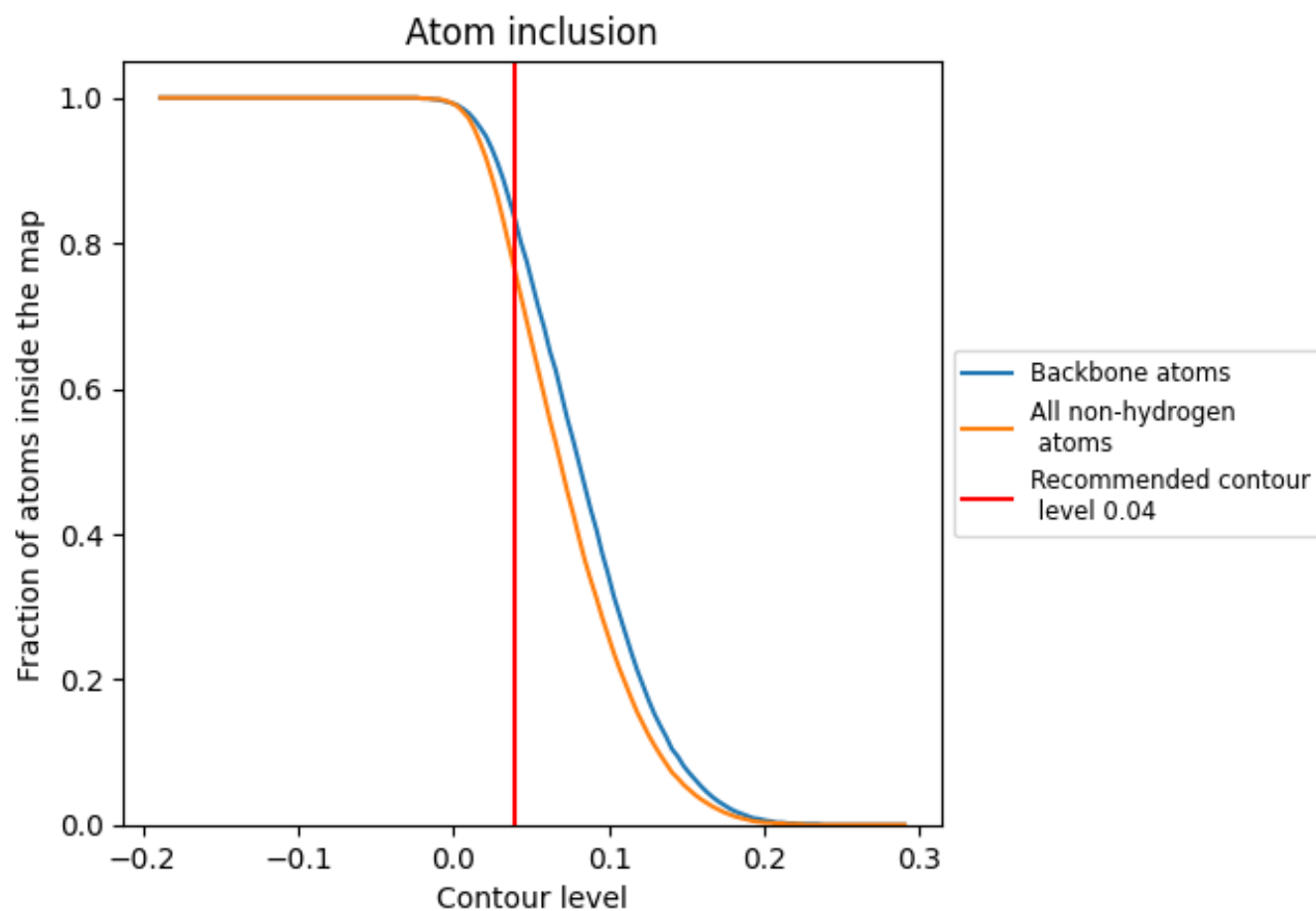


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.5030
1	0.7770	0.5110
2	0.7550	0.4790
3	0.6460	0.4520
4	0.8040	0.5200
5	0.6880	0.4810
A	0.8130	0.5270
B	0.7840	0.5090
C	0.6230	0.4580
D	0.6870	0.4880
E	0.4870	0.3960

