



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 03:36 am GMT

PDB ID : 6S7O
EMDB ID : EMD-10110
Title : Cryo-EM structure of human oligosaccharyltransferase complex OST-A
Authors : Ramirez, A.S.; Kowal, J.; Locher, K.P.
Deposited on : 2019-07-05
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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

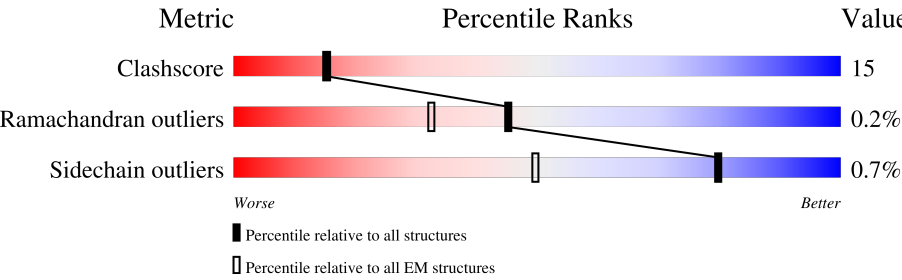
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	705	
2	B	37	
3	C	79	
4	D	113	
5	E	607	
6	F	631	
7	G	456	
8	H	149	

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Mol	Chain	Length	Quality of chain
9	I	3	<div><div></div><div>33%67%33%</div></div>
10	J	8	<div><div></div><div>12%25%75%</div></div>
11	K	8	<div><div></div><div>12%75%12%</div></div>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 18118 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 STT3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	656	Total	C	N	O	S	0	0
			5313	3484	856	937	36		

- Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	33	Total	C	N	O	S	0	0
			258	174	39	43	2		

- Molecule 3 is a protein called Transmembrane protein 258.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	78	Total	C	N	O	S	0	0
			634	435	91	105	3		

- Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	110	Total	C	N	O	S	0	0
			862	573	135	150	4		

- Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	560	Total	C	N	O	S	0	0
			4179	2671	712	789	7		

- Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	241	Total	C	N	O	S	0	0
			1919	1257	316	342	4		

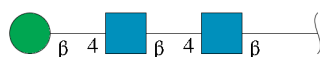
- Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	411	Total	C	N	O	S	0	0
			3238	2088	534	611	5		

- Molecule 8 is a protein called Oligosaccharyltransferase complex subunit OSTC.

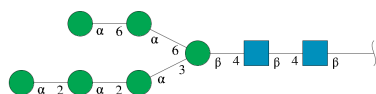
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	108	Total	C	N	O	S	0	0
			845	570	130	138	7		

- Molecule 9 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
9	I	3	Total	C	N	O	0	0
			39	22	2	15		

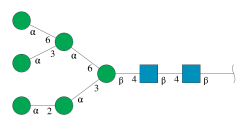
- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

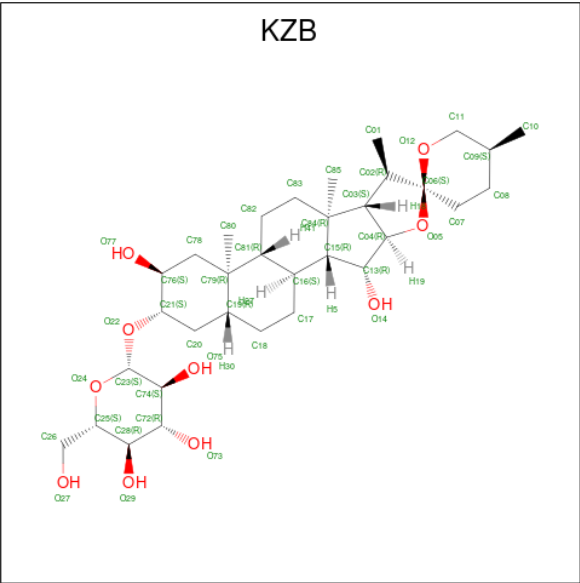
- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

ranose-(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	K	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 12 is (2 {S},3 {R},4 {R},5 {S},6 {S})-2-(hydroxymethyl)-6-[(1 {S},2 {R},3 {R},4 {R},5' {S},6 {S},7 {R},8 {S},9 {R},12 {R},13 {R},15 {S},16 {S},18 {R})-5',7,9,13-tetramethyl-3,15-bis(oxidanyl)spiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]icosane-6,2'-oxane]-16-yl]oxy-oxane-3,4,5-triol (three-letter code: KZB) (formula: C₃₃H₅₄O₁₀).



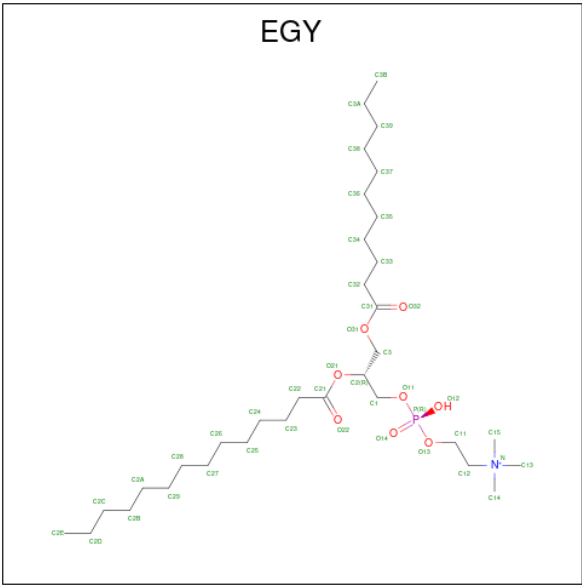
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			43	33	10	
12	A	1	Total	C	O	0
			43	33	10	
12	A	1	Total	C	O	0
			32	27	5	
12	E	1	Total	C	O	0
			32	27	5	
12	E	1	Total	C	O	0
			32	27	5	
12	F	1	Total	C	O	0
			32	27	5	

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Mol	Chain	Residues	Atoms			AltConf
12	F	1	Total	C	O	0
			32	27	5	
12	F	1	Total	C	O	0
			32	27	5	
12	G	1	Total	C	O	0
			32	27	5	

- Molecule 13 is (4R,7R)-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-7-[(undecanoyloxy)methyl]-3,5,8-trioxa-4lambda 5 -phosphadocosan-1-aminium (three-letter code: EGY) (formula: C₃₃H₆₇NO₈P).

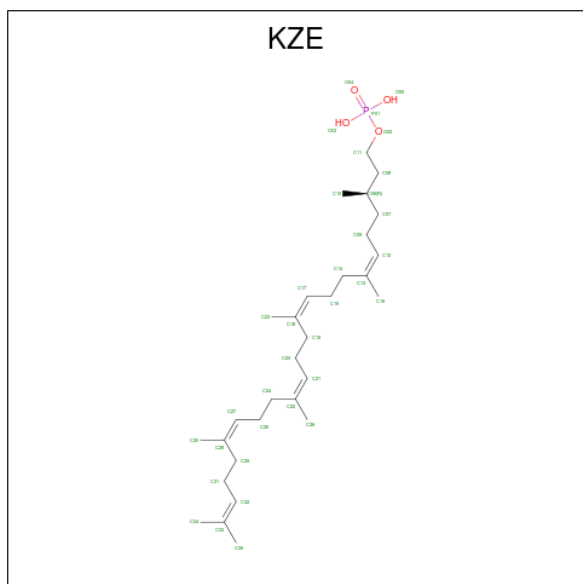


Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
13	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
13	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
13	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
13	D	1	Total	C	N	O	P	0
			43	33	1	8	1	
13	E	1	Total	C	N	O	P	0
			43	33	1	8	1	
13	F	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	
14	E	1	Total	Mg	0
			1	1	

- Molecule 15 is [(3 {R},6 {Z},10 {Z},14 {Z},18 {Z})-3,7,11,15,19,23-hexamethyltetraacosa-6,10,14,18,22-pentaenyl] dihydrogen phosphate (three-letter code: KZE) (formula: C₃₀H₅₃O₄P).

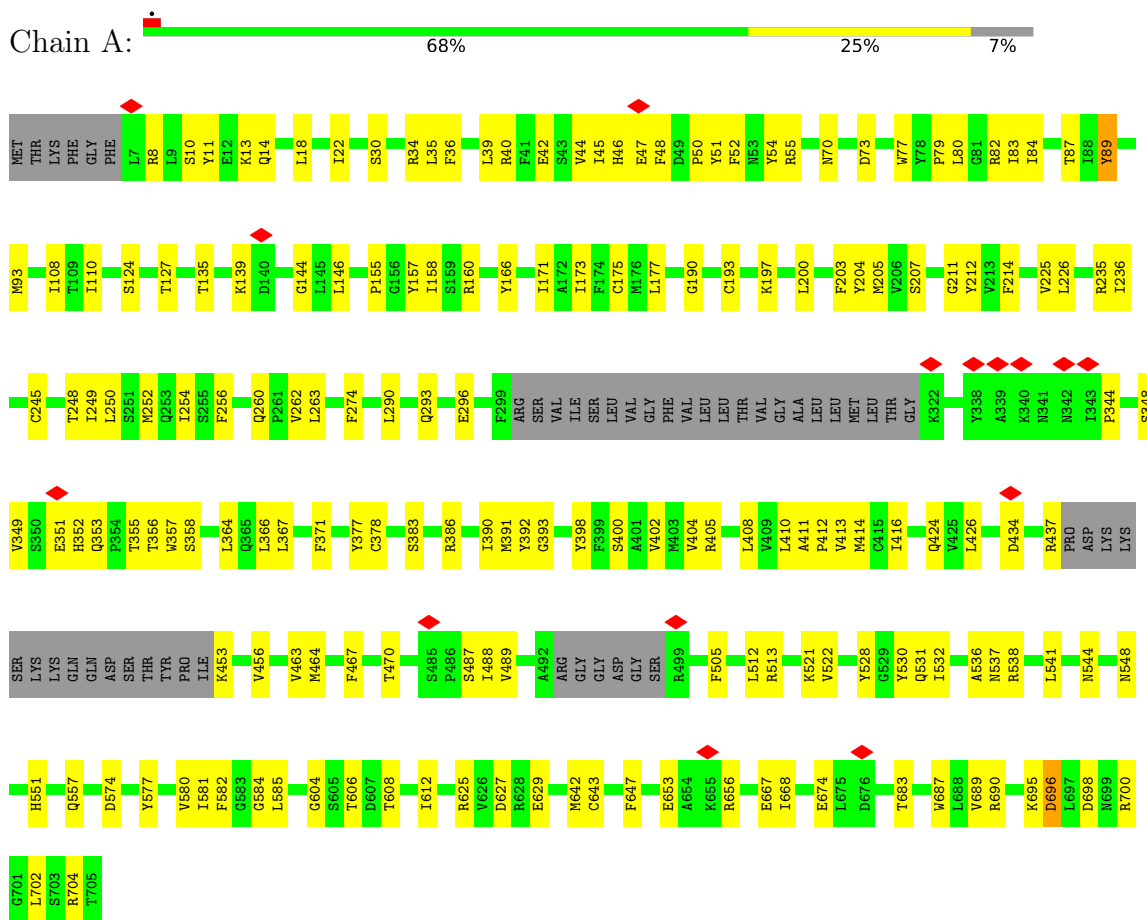


Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	O	P	0
			30	25	4	1	

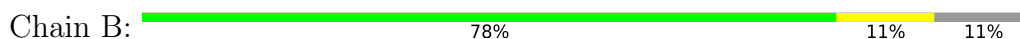
3 Residue-property plots

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

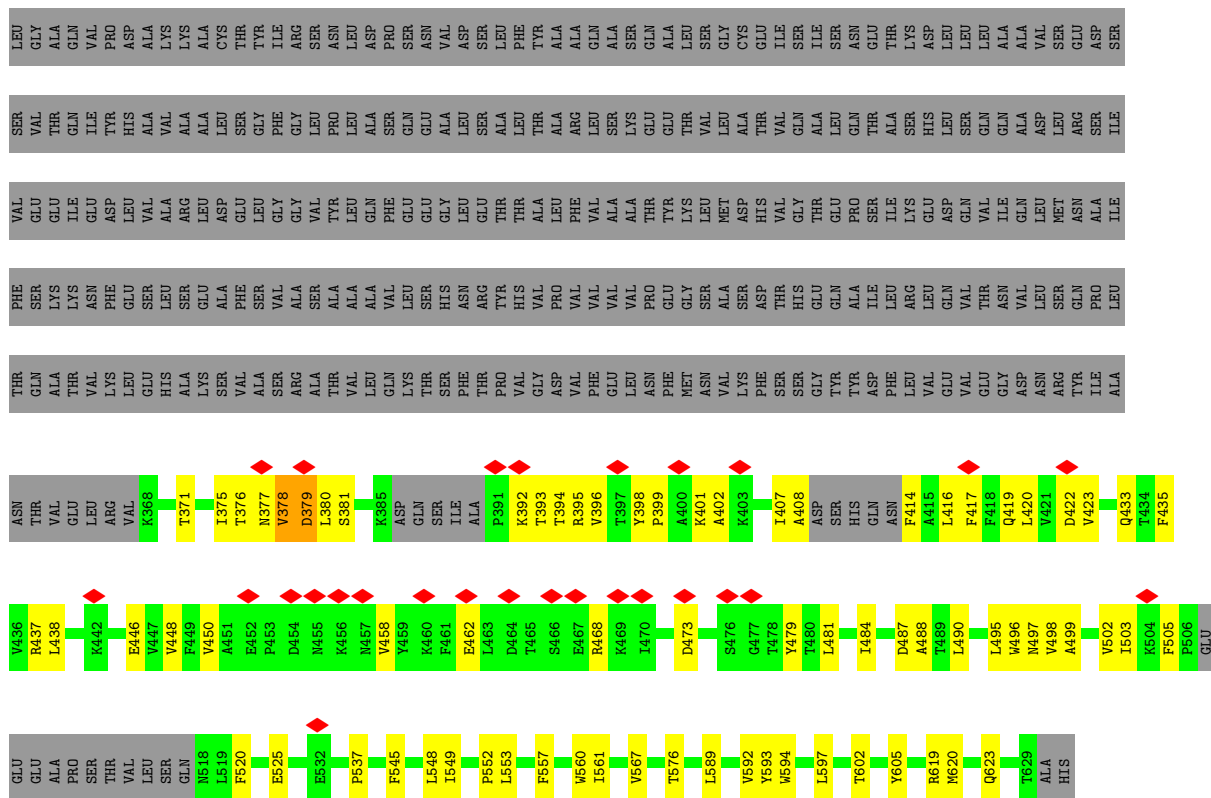
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A



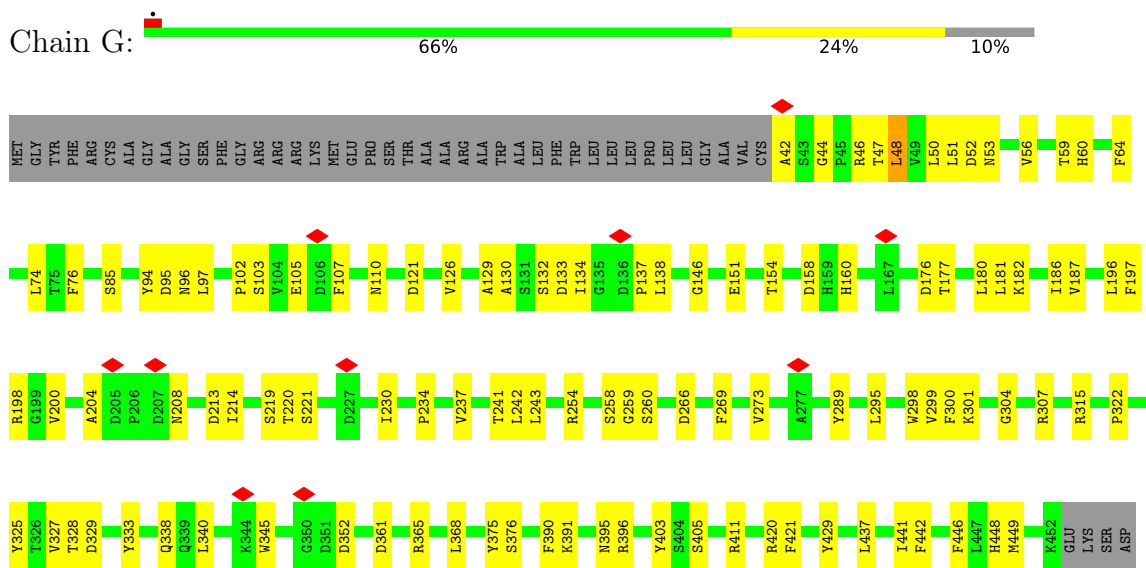
- Molecule 2: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4



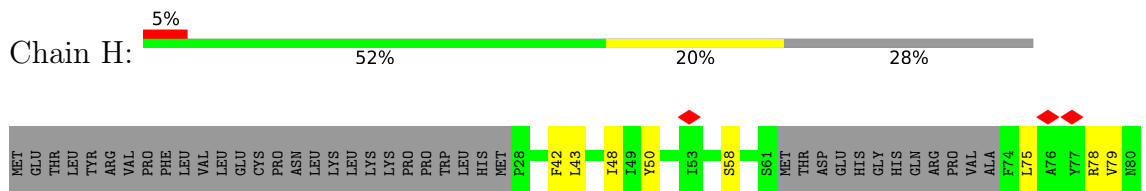
- Molecule 3: Transmembrane protein 258



• Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit



• Molecule 8: Oligosaccharyltransferase complex subunit OSTC

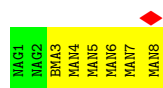




- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	156950	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 ($e^-/\text{\AA}^2$)	68	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	0.059	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0106	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: MAN, BMA, KZB, KZE, NAG, MG, 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	0.37	2/5461 (0.0%)	0.46	0/7416
2	B	0.39	0/263	0.42	0/360
3	C	0.29	0/654	0.41	0/893
4	D	0.33	0/882	0.43	0/1197
5	E	0.33	0/4268	0.47	0/5827
6	F	0.31	0/1963	0.49	0/2668
7	G	0.30	0/3320	0.47	0/4509
8	H	0.32	0/866	0.43	0/1171
All	All	0.34	2/17677 (0.0%)	0.46	0/24041

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	GLN	C-N	9.18	1.51	1.34
1	A	89	TYR	C-N	8.41	1.50	1.34

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	5313	0	5255	196	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	258	0	272	14	0
3	C	634	0	647	8	0
4	D	862	0	880	29	0
5	E	4179	0	3875	137	0
6	F	1919	0	1962	63	0
7	G	3238	0	3179	93	0
8	H	845	0	880	31	0
9	I	39	0	34	1	0
10	J	94	0	79	0	0
11	K	94	0	79	4	0
12	A	118	0	0	1	0
12	E	64	0	0	0	0
12	F	96	0	0	0	0
12	G	32	0	0	0	0
13	A	86	0	0	0	0
13	C	86	0	0	0	0
13	D	43	0	0	1	0
13	E	43	0	0	2	0
13	F	43	0	0	0	0
14	A	1	0	0	0	0
14	E	1	0	0	0	0
15	A	30	0	0	2	0
All	All	18118	0	17142	514	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 15.

All (514) 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)
7:G:158:ASP:OD1	7:G:220:THR:HG22	1.46	1.15
1:A:39:LEU:HD12	2:B:7:LEU:HD22	1.31	1.12
1:A:39:LEU:HD11	2:B:7:LEU:HD13	1.18	1.11
5:E:88:VAL:HG12	5:E:92:ASP:HB3	1.33	1.08
1:A:392:TYR:CE2	1:A:413:VAL:HG22	1.91	1.06
8:H:106:ARG:NH2	8:H:120:LEU:HD11	1.74	1.03
5:E:336:LEU:HD12	5:E:341:TYR:CE2	1.93	1.03
6:F:495:LEU:HD22	7:G:160:HIS:HE2	1.29	0.97
5:E:70:LEU:HD21	5:E:101:ARG:NH1	1.78	0.97
7:G:333:TYR:O	7:G:376:SER:HA	1.65	0.97
5:E:40:VAL:HG12	5:E:49:VAL:HG12	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:75:LEU:HD12	8:H:81:GLY:HA3	1.50	0.93
1:A:392:TYR:CE2	1:A:413:VAL:CG2	2.50	0.93
1:A:39:LEU:CD1	2:B:7:LEU:HD13	2.00	0.92
1:A:400:SER:CB	1:A:410:LEU:HD12	1.99	0.92
6:F:495:LEU:HD22	7:G:160:HIS:NE2	1.85	0.91
5:E:88:VAL:HG12	5:E:92:ASP:CB	2.02	0.90
1:A:83:ILE:O	1:A:87:THR:HG23	1.72	0.87
5:E:387:TYR:CD1	5:E:413:LYS:HE2	2.10	0.87
1:A:226:LEU:HD13	1:A:236:ILE:HD13	1.56	0.86
1:A:698:ASP:OD2	1:A:702:LEU:HB2	1.74	0.86
8:H:99:LEU:O	8:H:103:ILE:HG13	1.76	0.86
7:G:158:ASP:OD1	7:G:220:THR:CG2	2.24	0.86
1:A:226:LEU:CD1	1:A:236:ILE:HD13	2.05	0.85
8:H:106:ARG:HH21	8:H:120:LEU:HD11	1.35	0.85
5:E:55:LEU:HD11	5:E:69:PHE:CE1	2.12	0.84
5:E:188:LEU:HD22	5:E:203:PHE:HE2	1.42	0.83
5:E:70:LEU:CD2	5:E:101:ARG:NH1	2.42	0.83
1:A:225:VAL:HG21	1:A:391:MET:SD	2.19	0.82
7:G:160:HIS:ND1	7:G:220:THR:HG21	1.94	0.82
5:E:241:ASN:HB2	5:E:336:LEU:O	1.80	0.81
5:E:383:ILE:HD11	5:E:424:ILE:HD11	1.62	0.81
5:E:387:TYR:CE1	5:E:413:LYS:HE2	2.15	0.81
1:A:392:TYR:CD2	1:A:413:VAL:HG22	2.16	0.81
5:E:40:VAL:HG12	5:E:49:VAL:CG1	2.11	0.81
6:F:589:LEU:HD11	6:F:605:TYR:HB3	1.61	0.79
1:A:392:TYR:CZ	1:A:413:VAL:CG2	2.64	0.79
5:E:371:LYS:HG2	5:E:410:VAL:HG12	1.64	0.79
5:E:40:VAL:CG1	5:E:49:VAL:HG12	2.13	0.78
1:A:357:TRP:HD1	8:H:82:GLN:HE22	1.29	0.78
5:E:70:LEU:HD21	5:E:101:ARG:HH11	1.49	0.77
1:A:48:PHE:HA	1:A:51:TYR:HD2	1.50	0.76
6:F:379:ASP:HA	6:F:395:ARG:HA	1.67	0.76
5:E:336:LEU:HD23	5:E:336:LEU:N	2.01	0.76
5:E:286:ALA:HB2	5:E:311:SER:HA	1.67	0.76
1:A:522:VAL:HG12	1:A:577:TYR:HB2	1.67	0.76
5:E:146:ILE:HG23	5:E:150:GLU:HB2	1.68	0.76
1:A:39:LEU:CD1	2:B:7:LEU:HD22	2.13	0.75
7:G:180:LEU:HD23	7:G:182:LYS:H	1.52	0.75
1:A:173:ILE:HD11	1:A:408:LEU:HG	1.69	0.74
1:A:39:LEU:HD11	2:B:7:LEU:CD1	2.11	0.74
7:G:204:ALA:HB2	7:G:242:LEU:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:GLN:HG2	1:A:612:ILE:HD11	1.70	0.73
1:A:87:THR:O	1:A:256:PHE:CE2	2.42	0.73
5:E:238:HIS:CE1	5:E:375:PRO:HG3	2.23	0.73
1:A:410:LEU:HD23	1:A:410:LEU:O	1.88	0.72
5:E:336:LEU:HD12	5:E:341:TYR:HE2	1.53	0.72
1:A:87:THR:C	1:A:256:PHE:HD2	1.93	0.71
7:G:160:HIS:ND1	7:G:220:THR:CG2	2.53	0.70
1:A:44:VAL:CG1	1:A:488:ILE:HD11	2.22	0.70
1:A:392:TYR:CZ	1:A:413:VAL:HG23	2.27	0.70
1:A:44:VAL:HG11	1:A:488:ILE:HD11	1.74	0.69
8:H:107:SER:HB2	8:H:120:LEU:HD22	1.75	0.69
5:E:344:ASN:HB2	5:E:349:TYR:CD2	2.27	0.69
4:D:109:MET:CE	6:F:594:TRP:HB2	2.23	0.69
7:G:180:LEU:HD21	7:G:187:VAL:HG21	1.75	0.68
5:E:336:LEU:HD23	5:E:336:LEU:H	1.57	0.68
1:A:34:ARG:HD3	1:A:158:ILE:HG13	1.74	0.68
5:E:308:LEU:HD22	5:E:313:GLU:HG3	1.76	0.68
1:A:400:SER:HB2	1:A:410:LEU:HD12	1.75	0.68
5:E:46:LEU:HD11	5:E:136:THR:HG22	1.76	0.67
6:F:495:LEU:HG	6:F:495:LEU:O	1.93	0.67
8:H:106:ARG:C	8:H:106:ARG:HD2	2.14	0.67
1:A:521:LYS:HD2	1:A:574:ASP:O	1.94	0.67
5:E:336:LEU:CD1	5:E:341:TYR:CE2	2.74	0.67
1:A:393:GLY:HA2	1:A:413:VAL:HG11	1.77	0.67
1:A:45:ILE:HD12	1:A:54:TYR:CG	2.30	0.67
6:F:487:ASP:OD1	6:F:488:ALA:N	2.28	0.67
1:A:364:LEU:HD23	1:A:414:MET:HG2	1.77	0.66
8:H:58:SER:HA	8:H:84:ILE:HG12	1.76	0.66
5:E:417:VAL:H	5:E:420:HIS:HD2	1.43	0.66
1:A:696:ASP:OD1	1:A:696:ASP:N	2.26	0.66
6:F:408:ALA:HB2	6:F:414:PHE:HB2	1.76	0.66
1:A:700:ARG:NH2	7:G:121:ASP:OD1	2.28	0.66
8:H:106:ARG:CZ	8:H:120:LEU:HD11	2.26	0.66
1:A:249:ILE:HG22	4:D:107:VAL:CG1	2.26	0.65
1:A:695:LYS:HD3	1:A:704:ARG:NH1	2.12	0.65
8:H:82:GLN:OE1	8:H:87:GLY:HA3	1.97	0.65
1:A:225:VAL:HG11	1:A:391:MET:CE	2.27	0.65
7:G:51:LEU:HD23	7:G:56:VAL:HB	1.79	0.64
1:A:364:LEU:HB3	1:A:367:LEU:HB2	1.78	0.64
1:A:226:LEU:HD11	1:A:236:ILE:CD1	2.27	0.64
5:E:286:ALA:HA	5:E:312:VAL:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:307:ILE:N	5:E:307:ILE:HD12	2.13	0.64
6:F:402:ALA:HB3	6:F:499:ALA:HB2	1.78	0.64
7:G:197:PHE:HD2	7:G:260:SER:HB3	1.61	0.64
1:A:366:LEU:O	1:A:366:LEU:HD23	1.98	0.64
7:G:315:ARG:NH1	7:G:329:ASP:OD2	2.31	0.64
4:D:109:MET:HE2	6:F:594:TRP:HB2	1.80	0.63
6:F:462:GLU:O	6:F:468:ARG:NH2	2.31	0.63
1:A:245:CYS:SG	4:D:68:ILE:HD12	2.39	0.63
1:A:530:TYR:CE2	1:A:544:ASN:HB3	2.33	0.63
1:A:34:ARG:NH2	1:A:124:SER:OG	2.31	0.63
1:A:87:THR:O	1:A:256:PHE:HE2	1.82	0.63
1:A:35:LEU:HD12	1:A:35:LEU:O	1.99	0.62
5:E:57:HIS:HB3	5:E:123:PRO:HA	1.79	0.62
1:A:383:SER:HB3	1:A:386:ARG:HD3	1.82	0.62
5:E:146:ILE:CG2	5:E:150:GLU:HB2	2.30	0.62
4:D:26:LEU:HD22	7:G:449:MET:HE3	1.80	0.62
1:A:226:LEU:CD1	1:A:236:ILE:CD1	2.78	0.62
5:E:168:THR:OG1	5:E:171:GLN:NE2	2.26	0.62
1:A:83:ILE:O	1:A:87:THR:CG2	2.47	0.62
1:A:456:VAL:HG11	8:H:121:LEU:HD11	1.81	0.62
6:F:437:ARG:NH2	6:F:446:GLU:OE2	2.33	0.62
5:E:156:PHE:O	5:E:215:LYS:HA	1.99	0.61
1:A:87:THR:C	1:A:256:PHE:CD2	2.73	0.61
6:F:553:LEU:HD11	7:G:437:LEU:HD22	1.81	0.61
5:E:38:ARG:NH2	5:E:162:PHE:HA	2.16	0.61
1:A:695:LYS:HD3	1:A:704:ARG:HH12	1.66	0.61
5:E:174:ARG:HE	5:E:197:LEU:HD12	1.66	0.61
6:F:375:ILE:HG12	6:F:420:LEU:CD2	2.31	0.61
6:F:435:PHE:HB2	6:F:484:ILE:HD11	1.82	0.61
5:E:71:LEU:CD2	5:E:84:LEU:HD21	2.31	0.60
1:A:87:THR:O	1:A:256:PHE:CD2	2.55	0.60
1:A:537:ASN:HD21	9:I:1:NAG:C1	2.15	0.60
1:A:225:VAL:HG11	1:A:391:MET:HE1	1.84	0.60
6:F:576:THR:HG22	6:F:620:MET:HG3	1.83	0.60
6:F:380:LEU:HD13	6:F:414:PHE:CE1	2.37	0.60
1:A:653:GLU:HB2	1:A:656:ARG:HB2	1.84	0.59
1:A:13:LYS:HG2	3:C:42:THR:HG21	1.84	0.59
5:E:38:ARG:HH22	5:E:162:PHE:HA	1.65	0.59
5:E:146:ILE:HD12	5:E:255:ALA:HB1	1.85	0.59
7:G:132:SER:H	7:G:200:VAL:HG13	1.67	0.59
1:A:45:ILE:CD1	1:A:54:TYR:HB2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD11	1:A:548:ASN:HD22	1.67	0.59
1:A:160:ARG:HG2	1:A:408:LEU:HD22	1.84	0.59
7:G:340:LEU:HD12	7:G:345:TRP:CZ2	2.38	0.59
1:A:357:TRP:CD1	8:H:87:GLY:HA2	2.38	0.59
1:A:39:LEU:HD12	2:B:7:LEU:CD2	2.20	0.58
5:E:264:TYR:CE1	5:E:268:ARG:HD3	2.38	0.58
1:A:48:PHE:HA	1:A:51:TYR:CD2	2.35	0.58
4:D:85:PHE:HD2	4:D:88:ILE:HD12	1.67	0.58
1:A:22:ILE:CG1	2:B:21:LEU:HD22	2.34	0.58
7:G:160:HIS:HB2	7:G:220:THR:HG21	1.85	0.58
1:A:36:PHE:CE1	2:B:7:LEU:HD23	2.38	0.58
1:A:226:LEU:HD11	1:A:236:ILE:HD13	1.83	0.58
1:A:203:PHE:CE1	1:A:254:ILE:HD11	2.39	0.58
1:A:225:VAL:HG21	1:A:391:MET:CE	2.32	0.58
1:A:367:LEU:HB3	1:A:414:MET:HG2	1.84	0.58
5:E:250:LEU:O	5:E:327:LYS:HA	2.03	0.58
5:E:348:GLN:HG2	5:E:429:THR:HG22	1.86	0.57
7:G:269:PHE:HD1	7:G:289:TYR:HB2	1.68	0.57
4:D:41:GLN:HE22	4:D:59:GLY:C	2.08	0.57
1:A:426:LEU:HD11	1:A:464:MET:HG2	1.87	0.56
1:A:528:TYR:CZ	1:A:581:ILE:HD12	2.39	0.56
5:E:392:ALA:HB1	5:E:393:PRO:HD2	1.87	0.56
5:E:392:ALA:HB2	5:E:412:TYR:HE2	1.70	0.56
1:A:203:PHE:HB2	1:A:250:LEU:HB3	1.87	0.56
6:F:375:ILE:HG12	6:F:420:LEU:HD23	1.87	0.56
1:A:254:ILE:HG22	1:A:254:ILE:O	2.04	0.56
7:G:325:TYR:O	7:G:411:ARG:N	2.39	0.56
5:E:188:LEU:HD22	5:E:203:PHE:CE2	2.31	0.56
6:F:419:GLN:HG2	6:F:458:VAL:HG23	1.87	0.56
6:F:481:LEU:O	6:F:497:ASN:HA	2.04	0.56
7:G:295:LEU:O	7:G:299:VAL:HG13	2.05	0.56
5:E:55:LEU:HD11	5:E:69:PHE:CD1	2.40	0.55
5:E:389:ILE:HG22	5:E:413:LYS:HD2	1.88	0.55
1:A:200:LEU:HD11	4:D:103:ILE:HD13	1.88	0.55
8:H:83:TYR:HB2	8:H:86:GLU:HG2	1.89	0.55
6:F:435:PHE:CD1	6:F:450:VAL:HG22	2.42	0.55
1:A:366:LEU:HD23	1:A:366:LEU:C	2.27	0.55
5:E:294:ARG:NH2	13:E:711:EGY:O12	2.35	0.55
1:A:80:LEU:CD1	1:A:548:ASN:HD22	2.19	0.54
1:A:505:PHE:HE1	1:A:581:ILE:HD13	1.72	0.54
6:F:371:THR:HB	6:F:490:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:CG2	4:D:107:VAL:HG12	2.36	0.54
5:E:287:ALA:HB1	5:E:337:PRO:HD2	1.89	0.54
6:F:379:ASP:HA	6:F:394:THR:O	2.08	0.54
7:G:220:THR:HG22	7:G:220:THR:O	2.07	0.54
1:A:585:LEU:HD23	1:A:687:TRP:HB2	1.90	0.54
6:F:520:PHE:HB3	7:G:395:ASN:ND2	2.23	0.54
7:G:269:PHE:HE1	7:G:289:TYR:HA	1.72	0.54
5:E:172:THR:HG22	5:E:202:PRO:HB3	1.88	0.54
7:G:213:ASP:HB3	7:G:242:LEU:HD22	1.90	0.53
4:D:21:PRO:HD2	4:D:24:LEU:HD22	1.90	0.53
5:E:38:ARG:NH2	5:E:161:TYR:O	2.41	0.53
5:E:221:ASN:HB2	5:E:274:ILE:HG22	1.90	0.53
5:E:390:SER:HB2	5:E:412:TYR:O	2.09	0.53
1:A:366:LEU:CD1	1:A:467:PHE:HB3	2.38	0.53
1:A:580:VAL:HG21	1:A:642:MET:HG2	1.89	0.53
8:H:106:ARG:HD2	8:H:106:ARG:O	2.09	0.53
6:F:593:TYR:HD1	6:F:602:THR:HG1	1.56	0.53
1:A:400:SER:OG	1:A:410:LEU:HB2	2.09	0.53
5:E:88:VAL:CG1	5:E:92:ASP:CB	2.82	0.53
6:F:473:ASP:N	6:F:473:ASP:OD1	2.42	0.52
7:G:390:PHE:O	7:G:405:SER:HA	2.09	0.52
1:A:290:LEU:HD21	4:D:12:PHE:HB2	1.91	0.52
1:A:344:PRO:O	1:A:348:SER:OG	2.27	0.52
6:F:378:VAL:HA	6:F:417:PHE:O	2.09	0.52
1:A:135:THR:HG22	1:A:416:ILE:HG23	1.91	0.52
7:G:395:ASN:O	7:G:396:ARG:HD2	2.09	0.52
1:A:250:LEU:HD21	4:D:107:VAL:HG21	1.92	0.52
5:E:381:ILE:HG21	5:E:409:ILE:HD11	1.92	0.52
5:E:382:GLU:HG2	5:E:427:HIS:HB2	1.90	0.52
6:F:549:ILE:O	6:F:552:PRO:HD2	2.10	0.52
7:G:234:PRO:HG2	7:G:237:VAL:HB	1.91	0.52
8:H:106:ARG:HH21	8:H:120:LEU:CD1	2.16	0.52
1:A:82:ARG:NH2	1:A:87:THR:OG1	2.43	0.52
7:G:146:GLY:HA3	7:G:208:ASN:HD21	1.73	0.52
7:G:196:LEU:HD13	7:G:273:VAL:HG12	1.90	0.52
1:A:10:SER:HB3	1:A:13:LYS:HG3	1.91	0.52
5:E:200:TYR:HH	5:E:214:PHE:HE1	1.57	0.52
8:H:106:ARG:NH2	8:H:120:LEU:CD1	2.62	0.52
5:E:336:LEU:HD12	5:E:341:TYR:CD2	2.44	0.51
1:A:357:TRP:HD1	8:H:82:GLN:NE2	2.04	0.51
3:C:69:LEU:HD13	5:E:439:PRO:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:392:ALA:CB	5:E:412:TYR:HE2	2.23	0.51
5:E:48:LYS:HG2	5:E:134:VAL:HG22	1.93	0.51
5:E:344:ASN:HB2	5:E:349:TYR:CE2	2.45	0.51
1:A:82:ARG:HH21	1:A:84:ILE:HG12	1.75	0.51
1:A:93:MET:SD	1:A:93:MET:N	2.83	0.51
6:F:401:LYS:HG3	6:F:497:ASN:O	2.11	0.51
5:E:69:PHE:HB2	5:E:117:LEU:HD11	1.93	0.51
5:E:256:VAL:HA	5:E:324:GLY:HA3	1.93	0.51
1:A:190:GLY:HA3	1:A:235:ARG:HG2	1.91	0.51
1:A:355:THR:HG22	1:A:404:VAL:HG22	1.93	0.51
1:A:34:ARG:NH2	1:A:157:TYR:CD2	2.79	0.50
1:A:193:CYS:O	1:A:197:LYS:HG2	2.11	0.50
1:A:225:VAL:HG11	1:A:391:MET:HE3	1.93	0.50
1:A:674:GLU:N	1:A:674:GLU:OE1	2.44	0.50
3:C:15:PRO:HA	3:C:18:PHE:CD2	2.46	0.50
8:H:50:TYR:CD2	8:H:82:GLN:HB3	2.46	0.50
1:A:274:PHE:CZ	4:D:68:ILE:HD11	2.46	0.50
2:B:21:LEU:O	2:B:21:LEU:HD23	2.10	0.50
7:G:48:LEU:HD22	7:G:50:LEU:HD12	1.93	0.50
1:A:627:ASP:HA	1:A:667:GLU:O	2.11	0.50
4:D:48:VAL:HG21	6:F:537:PRO:HG3	1.94	0.50
5:E:55:LEU:HD21	5:E:69:PHE:HE1	1.76	0.50
7:G:46:ARG:NH1	7:G:95:ASP:OD2	2.44	0.50
1:A:171:ILE:HD11	1:A:204:TYR:OH	2.11	0.50
1:A:30:SER:O	1:A:34:ARG:HG2	2.12	0.50
1:A:155:PRO:HA	1:A:158:ILE:HG22	1.93	0.50
1:A:249:ILE:CG2	4:D:107:VAL:CG1	2.90	0.50
1:A:400:SER:OG	1:A:410:LEU:HD12	2.11	0.50
7:G:269:PHE:CE1	7:G:289:TYR:HA	2.47	0.50
1:A:358:SER:OG	8:H:79:VAL:O	2.23	0.50
1:A:367:LEU:HB3	1:A:414:MET:CG	2.42	0.50
5:E:146:ILE:CD1	5:E:152:GLN:HA	2.42	0.50
7:G:322:PRO:HD2	7:G:325:TYR:HE1	1.76	0.50
1:A:351:GLU:OE1	1:A:351:GLU:N	2.40	0.50
5:E:40:VAL:HG12	5:E:49:VAL:CB	2.41	0.50
5:E:193:ARG:HG2	5:E:198:LEU:HG	1.93	0.50
5:E:392:ALA:HB2	5:E:412:TYR:CE2	2.47	0.50
7:G:105:GLU:HA	7:G:137:PRO:HG3	1.94	0.50
7:G:254:ARG:NH1	7:G:304:GLY:O	2.45	0.50
5:E:376:GLU:OE1	5:E:376:GLU:N	2.38	0.50
1:A:45:ILE:CD1	1:A:54:TYR:CG	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG23	1:A:177:LEU:HD12	1.93	0.49
1:A:83:ILE:HG13	1:A:87:THR:HG23	1.93	0.49
5:E:380:ASN:O	5:E:428:TYR:HA	2.12	0.49
1:A:377:TYR:HE2	1:A:424:GLN:NE2	2.09	0.49
7:G:160:HIS:CG	7:G:220:THR:HG21	2.47	0.49
7:G:197:PHE:HZ	7:G:243:LEU:HD22	1.76	0.49
7:G:368:LEU:HB3	7:G:375:TYR:HB3	1.94	0.49
5:E:121:LEU:H	5:E:121:LEU:HD23	1.78	0.49
6:F:433:GLN:HG3	6:F:435:PHE:CD2	2.47	0.49
1:A:356:THR:HB	8:H:82:GLN:HB2	1.94	0.49
7:G:391:LYS:NZ	7:G:403:TYR:OH	2.45	0.49
1:A:18:LEU:HD23	2:B:25:TYR:HD1	1.77	0.49
7:G:130:ALA:O	7:G:260:SER:N	2.45	0.49
1:A:52:PHE:HB2	1:A:530:TYR:CD1	2.47	0.49
5:E:413:LYS:HD3	5:E:416:LEU:HD11	1.94	0.49
6:F:437:ARG:HG3	6:F:448:VAL:HG22	1.95	0.49
6:F:619:ARG:NH1	6:F:623:GLN:OE1	2.45	0.49
1:A:225:VAL:HG21	1:A:391:MET:HE1	1.93	0.49
1:A:249:ILE:HG22	4:D:107:VAL:HG11	1.93	0.49
1:A:293:GLN:O	1:A:296:GLU:HG2	2.13	0.49
6:F:398:TYR:CG	6:F:399:PRO:HD3	2.48	0.49
7:G:221:SER:OG	7:G:241:THR:HG21	2.13	0.48
1:A:214:PHE:HB2	15:A:818:KZE:C14	2.43	0.48
5:E:387:TYR:CE1	5:E:413:LYS:CE	2.94	0.48
7:G:230:ILE:HD11	7:G:234:PRO:HD3	1.95	0.48
1:A:22:ILE:HD11	2:B:21:LEU:HD22	1.95	0.48
7:G:307:ARG:NH1	7:G:338:GLN:OE1	2.36	0.48
1:A:364:LEU:HG	1:A:367:LEU:HD22	1.96	0.48
4:D:21:PRO:HD2	4:D:24:LEU:HB2	1.95	0.48
5:E:291:VAL:HG21	5:E:305:LEU:HD13	1.95	0.48
8:H:78:ARG:O	8:H:142:LYS:HE2	2.13	0.48
7:G:361:ASP:N	7:G:361:ASP:OD1	2.46	0.48
1:A:89:TYR:HB3	1:A:207:SER:O	2.13	0.48
1:A:226:LEU:HD11	1:A:236:ILE:HD11	1.96	0.48
5:E:70:LEU:HD22	5:E:101:ARG:NH1	2.28	0.48
7:G:146:GLY:HA3	7:G:208:ASN:ND2	2.28	0.48
1:A:39:LEU:CD1	2:B:7:LEU:CD1	2.83	0.48
6:F:520:PHE:HB2	7:G:395:ASN:O	2.14	0.48
7:G:44:GLY:HA3	7:G:95:ASP:OD2	2.13	0.48
1:A:488:ILE:HG22	1:A:531:GLN:HE21	1.79	0.47
5:E:352:LYS:HB3	5:E:425:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PRO:HG2	1:A:551:HIS:CE1	2.48	0.47
5:E:315:GLU:OE1	11:K:7:MAN:O6	2.31	0.47
6:F:495:LEU:N	6:F:495:LEU:HD23	2.30	0.47
1:A:582:PHE:CZ	1:A:584:GLY:HA3	2.49	0.47
5:E:460:ASP:OD1	5:E:460:ASP:N	2.47	0.47
1:A:463:VAL:O	1:A:467:PHE:HD1	1.98	0.47
8:H:134:MET:O	8:H:138:PHE:HD1	1.97	0.47
1:A:364:LEU:HD23	1:A:367:LEU:HB3	1.96	0.47
5:E:291:VAL:HG23	11:K:2:NAG:H81	1.96	0.47
6:F:496:TRP:HZ3	6:F:498:VAL:HA	1.80	0.47
1:A:357:TRP:CD1	8:H:82:GLN:NE2	2.72	0.47
3:C:64:MET:HG2	5:E:446:PHE:CE1	2.50	0.47
5:E:224:PHE:O	5:E:252:HIS:ND1	2.48	0.47
5:E:336:LEU:N	5:E:336:LEU:CD2	2.73	0.47
5:E:436:LEU:O	5:E:439:PRO:HD2	2.14	0.47
5:E:71:LEU:HD23	5:E:84:LEU:HD21	1.96	0.47
5:E:236:VAL:HA	5:E:242:ILE:HG22	1.97	0.47
1:A:44:VAL:HG13	1:A:488:ILE:HD11	1.94	0.47
6:F:496:TRP:CZ3	6:F:498:VAL:HA	2.50	0.47
1:A:391:MET:HB2	1:A:391:MET:HE2	1.52	0.46
1:A:50:PRO:HB3	1:A:166:TYR:O	2.15	0.46
1:A:377:TYR:C	1:A:377:TYR:CD1	2.89	0.46
1:A:349:VAL:HB	1:A:352:HIS:ND1	2.30	0.46
1:A:392:TYR:CD2	1:A:413:VAL:CG2	2.88	0.46
7:G:52:ASP:O	7:G:53:ASN:ND2	2.48	0.46
1:A:211:GLY:O	1:A:214:PHE:HB3	2.15	0.46
6:F:495:LEU:HD22	7:G:160:HIS:CD2	2.49	0.46
1:A:11:TYR:HA	1:A:14:GLN:HE21	1.81	0.46
1:A:532:ILE:HG23	1:A:536:ALA:HB3	1.97	0.46
1:A:647:PHE:CD2	1:A:668:ILE:HD11	2.50	0.46
1:A:512:LEU:HD21	1:A:522:VAL:HG11	1.97	0.46
1:A:687:TRP:CZ2	5:E:264:TYR:HB2	2.50	0.46
3:C:35:TRP:HB3	3:C:56:ILE:HD11	1.98	0.46
5:E:279:SER:HB3	5:E:317:ARG:HG2	1.98	0.46
5:E:98:LEU:HD13	5:E:113:PHE:HE1	1.81	0.46
1:A:249:ILE:HG22	4:D:107:VAL:HG12	1.94	0.46
1:A:371:PHE:HB2	1:A:414:MET:SD	2.56	0.46
5:E:69:PHE:HB3	5:E:115:VAL:HB	1.97	0.46
5:E:320:PHE:CD1	5:E:326:TRP:HE3	2.34	0.46
6:F:435:PHE:HD1	6:F:450:VAL:HG22	1.81	0.46
7:G:64:PHE:HD1	7:G:74:LEU:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:327:VAL:HG12	7:G:328:THR:HG23	1.97	0.46
1:A:364:LEU:CD2	1:A:414:MET:HG2	2.44	0.46
4:D:44:TYR:HB2	6:F:545:PHE:CE1	2.51	0.46
7:G:103:SER:N	7:G:133:ASP:O	2.49	0.46
8:H:43:LEU:HB3	8:H:48:ILE:CD1	2.46	0.46
1:A:45:ILE:HD13	1:A:54:TYR:HB2	1.98	0.45
1:A:378:CYS:HB3	1:A:390:ILE:HD11	1.98	0.45
3:C:25:LEU:HD23	3:C:66:PHE:HB3	1.97	0.45
5:E:282:THR:HG22	5:E:359:VAL:O	2.15	0.45
5:E:370:VAL:O	5:E:410:VAL:HA	2.16	0.45
6:F:438:LEU:HD12	6:F:479:TYR:HB3	1.97	0.45
1:A:274:PHE:HZ	4:D:68:ILE:HD11	1.81	0.45
6:F:548:LEU:O	6:F:552:PRO:HD3	2.17	0.45
7:G:176:ASP:OD1	7:G:177:THR:N	2.48	0.45
7:G:197:PHE:CZ	7:G:243:LEU:HD13	2.51	0.45
5:E:352:LYS:CB	5:E:425:VAL:HG12	2.46	0.45
1:A:364:LEU:HD23	1:A:367:LEU:CB	2.47	0.45
1:A:411:ALA:HB3	1:A:412:PRO:HD3	1.97	0.45
5:E:55:LEU:HD11	5:E:69:PHE:HE1	1.74	0.45
5:E:207:PRO:HG2	5:E:210:SER:HA	1.97	0.45
5:E:354:ARG:HA	5:E:422:GLN:O	2.15	0.45
8:H:98:GLY:O	8:H:102:ILE:HG12	2.16	0.45
5:E:121:LEU:HB3	5:E:127:ILE:HD11	1.98	0.45
1:A:77:TRP:HA	1:A:541:LEU:O	2.17	0.45
4:D:27:LEU:HD13	7:G:442:PHE:CZ	2.52	0.45
5:E:231:THR:O	5:E:246:GLU:HA	2.16	0.45
5:E:476:ALA:O	5:E:480:GLU:HG2	2.17	0.45
7:G:102:PRO:HG3	7:G:130:ALA:HA	1.99	0.45
5:E:160:HIS:HE1	5:E:200:TYR:HE2	1.64	0.45
1:A:55:ARG:NH1	1:A:73:ASP:OD2	2.49	0.45
4:D:26:LEU:HD22	7:G:449:MET:CE	2.44	0.45
6:F:401:LYS:HG2	6:F:402:ALA:H	1.82	0.45
4:D:54:ASN:OD1	4:D:55:SER:N	2.49	0.45
5:E:218:TYR:CE2	5:E:220:ASN:HB2	2.52	0.45
6:F:376:THR:O	6:F:378:VAL:N	2.50	0.45
1:A:488:ILE:HG22	1:A:531:GLN:NE2	2.33	0.44
5:E:294:ARG:HH12	13:E:711:EGY:P	2.40	0.44
6:F:594:TRP:O	7:G:420:ARG:NH2	2.49	0.44
7:G:56:VAL:HA	7:G:59:THR:HG22	2.00	0.44
1:A:262:VAL:HG23	1:A:263:LEU:HD22	2.00	0.44
7:G:213:ASP:CB	7:G:242:LEU:HD22	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HG12	2:B:21:LEU:HD22	1.99	0.44
1:A:44:VAL:HG11	1:A:488:ILE:CD1	2.45	0.44
1:A:643:CYS:HA	1:A:690:ARG:HD3	1.99	0.44
5:E:336:LEU:HB2	5:E:337:PRO:HD2	2.00	0.44
5:E:478:ILE:HG21	5:E:531:ALA:HB2	2.00	0.44
1:A:205:MET:HE3	1:A:212:TYR:HA	2.00	0.44
6:F:381:SER:HB2	6:F:392:LYS:O	2.18	0.44
1:A:225:VAL:CG2	1:A:391:MET:SD	2.99	0.44
7:G:186:ILE:HG12	7:G:298:TRP:NE1	2.33	0.44
7:G:197:PHE:CE1	7:G:243:LEU:HD13	2.52	0.44
8:H:58:SER:HA	8:H:84:ILE:CG1	2.46	0.44
1:A:155:PRO:O	1:A:158:ILE:HG22	2.18	0.44
1:A:434:ASP:O	1:A:437:ARG:NH1	2.50	0.44
1:A:488:ILE:HG13	1:A:489:VAL:HG23	1.99	0.44
1:A:226:LEU:HD23	1:A:226:LEU:O	2.18	0.43
7:G:74:LEU:HD23	7:G:76:PHE:CZ	2.53	0.43
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.83	0.43
1:A:70:ASN:ND2	1:A:70:ASN:O	2.51	0.43
5:E:351:LEU:O	5:E:425:VAL:HA	2.18	0.43
6:F:497:ASN:OD1	6:F:497:ASN:N	2.44	0.43
6:F:560:TRP:HZ3	7:G:441:ILE:HG22	1.83	0.43
7:G:129:ALA:HA	7:G:258:SER:O	2.18	0.43
1:A:34:ARG:CZ	1:A:124:SER:OG	2.66	0.43
1:A:683:THR:O	5:E:263:ARG:HD3	2.19	0.43
5:E:41:ASP:OD1	5:E:48:LYS:HB2	2.18	0.43
7:G:266:ASP:HA	7:G:269:PHE:HD2	1.83	0.43
1:A:157:TYR:CD1	1:A:173:ILE:HD12	2.53	0.43
5:E:308:LEU:HD22	5:E:313:GLU:CG	2.47	0.43
5:E:148:GLN:O	5:E:148:GLN:HG2	2.19	0.43
5:E:187:LYS:HG3	5:E:191:PRO:HD2	2.00	0.43
7:G:181:LEU:HB2	7:G:214:ILE:HA	2.00	0.43
7:G:241:THR:O	7:G:243:LEU:HG	2.18	0.43
1:A:453:LYS:HZ3	1:A:453:LYS:HB2	1.83	0.43
5:E:308:LEU:HD21	5:E:313:GLU:CD	2.38	0.43
8:H:106:ARG:C	8:H:106:ARG:CD	2.87	0.43
1:A:683:THR:HB	5:E:263:ARG:HB2	2.01	0.43
5:E:234:ILE:HG12	5:E:244:VAL:HG12	1.99	0.43
6:F:433:GLN:HG3	6:F:435:PHE:HD2	1.84	0.43
7:G:48:LEU:HD12	7:G:94:TYR:CD2	2.54	0.43
7:G:51:LEU:HD11	7:G:76:PHE:HD2	1.83	0.43
7:G:198:ARG:O	7:G:198:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HD11	1:A:408:LEU:CG	2.45	0.43
1:A:398:TYR:O	1:A:402:VAL:HG23	2.18	0.43
5:E:371:LYS:HA	5:E:409:ILE:O	2.18	0.43
8:H:104:LEU:O	8:H:107:SER:HB3	2.19	0.43
1:A:248:THR:O	1:A:252:MET:HG2	2.18	0.43
1:A:513:ARG:O	1:A:538:ARG:NH2	2.51	0.43
1:A:604:GLY:CA	1:A:612:ILE:HD12	2.49	0.43
1:A:625:ARG:NH2	1:A:629:GLU:OE1	2.52	0.43
6:F:422:ASP:OD1	6:F:423:VAL:N	2.52	0.43
5:E:235:GLU:HA	5:E:373:ILE:HB	2.01	0.43
1:A:408:LEU:O	1:A:412:PRO:HD3	2.19	0.42
4:D:57:LEU:O	4:D:61:ILE:HG12	2.19	0.42
8:H:50:TYR:CE2	8:H:82:GLN:HB3	2.54	0.42
5:E:180:ARG:HB3	5:E:195:GLU:O	2.18	0.42
7:G:103:SER:HB3	7:G:133:ASP:HB3	2.01	0.42
7:G:107:PHE:HE2	7:G:137:PRO:HB2	1.84	0.42
5:E:69:PHE:HE2	5:E:71:LEU:HD13	1.83	0.42
5:E:307:ILE:N	5:E:307:ILE:CD1	2.81	0.42
6:F:503:ILE:HG22	6:F:505:PHE:HD1	1.84	0.42
7:G:151:GLU:HB3	7:G:154:THR:HG23	2.01	0.42
7:G:258:SER:OG	7:G:259:GLY:O	2.34	0.42
1:A:135:THR:OG1	1:A:144:GLY:HA2	2.20	0.42
13:D:701:EGY:O12	5:E:462:SER:HA	2.19	0.42
5:E:45:HIS:HE1	5:E:364:VAL:HG12	1.85	0.42
6:F:398:TYR:HA	6:F:496:TRP:CZ2	2.54	0.42
7:G:42:ALA:HA	7:G:301:LYS:HB3	2.00	0.42
1:A:42:GLU:H	1:A:42:GLU:HG3	1.70	0.42
1:A:467:PHE:O	1:A:470:THR:HG22	2.19	0.42
4:D:57:LEU:HD23	4:D:57:LEU:HA	1.85	0.42
5:E:36:VAL:O	5:E:171:GLN:HA	2.19	0.42
5:E:159:ASN:OD1	5:E:160:HIS:N	2.53	0.42
5:E:234:ILE:HG23	5:E:244:VAL:HG12	2.01	0.42
1:A:353:GLN:O	1:A:404:VAL:HG23	2.19	0.42
5:E:415:ASN:HD22	5:E:415:ASN:HA	1.61	0.42
7:G:85:SER:HB2	7:G:110:ASN:HD22	1.84	0.42
7:G:204:ALA:CB	7:G:242:LEU:HD11	2.44	0.42
7:G:97:LEU:HD23	7:G:126:VAL:HG22	2.01	0.42
6:F:380:LEU:HD13	6:F:414:PHE:HE1	1.84	0.42
1:A:35:LEU:H	1:A:35:LEU:HG	1.73	0.42
5:E:399:THR:N	5:E:402:ASP:OD2	2.53	0.42
7:G:97:LEU:HB3	7:G:126:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:30:TYR:CE2	4:D:34:ILE:HD11	2.55	0.41
4:D:85:PHE:CD2	4:D:88:ILE:HD12	2.51	0.41
5:E:57:HIS:CE1	5:E:63:THR:HG21	2.55	0.41
7:G:160:HIS:CB	7:G:220:THR:HG21	2.48	0.41
1:A:108:ILE:O	1:A:110:ILE:HG13	2.20	0.41
1:A:175:CYS:CB	1:A:205:MET:HG2	2.50	0.41
5:E:49:VAL:HG23	5:E:49:VAL:O	2.20	0.41
6:F:567:VAL:HA	7:G:448:HIS:O	2.19	0.41
1:A:47:GLU:HA	1:A:487:SER:HB2	2.02	0.41
1:A:249:ILE:HG23	1:A:249:ILE:HD12	1.80	0.41
12:A:812:KZB:O29	12:A:812:KZB:O27	2.39	0.41
6:F:407:ILE:HA	6:F:502:VAL:O	2.21	0.41
1:A:411:ALA:N	1:A:412:PRO:CD	2.84	0.41
1:A:522:VAL:HA	1:A:577:TYR:O	2.20	0.41
6:F:416:LEU:HD12	6:F:416:LEU:O	2.20	0.41
6:F:592:VAL:HG12	6:F:597:LEU:HD13	2.02	0.41
7:G:134:ILE:O	7:G:138:LEU:HD12	2.20	0.41
4:D:77:ILE:HD13	7:G:446:PHE:HZ	1.85	0.41
5:E:300:VAL:O	11:K:1:NAG:O6	2.27	0.41
7:G:47:THR:HG22	7:G:96:ASN:HB2	2.03	0.41
1:A:46:HIS:O	1:A:50:PRO:HD2	2.20	0.41
5:E:387:TYR:HE1	5:E:413:LYS:CD	2.33	0.41
7:G:352:ASP:N	7:G:352:ASP:OD1	2.51	0.41
7:G:421:PHE:HA	7:G:429:TYR:HE2	1.85	0.41
1:A:405:ARG:HH22	15:A:818:KZE:C11	2.33	0.41
3:C:79:VAL:HG11	5:E:401:LEU:HB2	2.02	0.41
5:E:225:LEU:HD12	5:E:225:LEU:HA	1.89	0.41
7:G:299:VAL:HG23	7:G:300:PHE:CD1	2.56	0.41
1:A:45:ILE:HD11	1:A:54:TYR:CD1	2.55	0.41
1:A:157:TYR:CE1	1:A:173:ILE:HD12	2.56	0.41
1:A:392:TYR:CE2	1:A:413:VAL:HG23	2.47	0.41
1:A:606:THR:O	1:A:608:THR:N	2.54	0.41
5:E:305:LEU:HD22	11:K:2:NAG:C7	2.51	0.41
5:E:365:ILE:HB	5:E:416:LEU:HB2	2.03	0.41
7:G:47:THR:OG1	7:G:74:LEU:HD12	2.21	0.41
7:G:60:HIS:O	7:G:64:PHE:HD2	2.04	0.41
6:F:525:GLU:HG3	7:G:365:ARG:O	2.21	0.41
3:C:52:LYS:O	3:C:56:ILE:HG22	2.20	0.40
5:E:383:ILE:CD1	5:E:424:ILE:HD11	2.41	0.40
6:F:396:VAL:HG11	6:F:402:ALA:HB2	2.02	0.40
1:A:146:LEU:HD13	2:B:22:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:CG2	1:A:50:PRO:HB2	2.51	0.40
6:F:381:SER:CB	6:F:393:THR:HG22	2.52	0.40
8:H:108:ASN:O	8:H:108:ASN:ND2	2.55	0.40
1:A:349:VAL:HB	1:A:352:HIS:CE1	2.57	0.40
1:A:581:ILE:HG12	1:A:689:VAL:HG22	2.03	0.40
5:E:70:LEU:CD1	5:E:114:THR:HG22	2.52	0.40
5:E:205:ASP:OD1	5:E:206:VAL:N	2.54	0.40
5:E:238:HIS:HE1	5:E:375:PRO:HG3	1.81	0.40
8:H:42:PHE:HB2	8:H:95:THR:OG1	2.21	0.40
4:D:44:TYR:HB2	6:F:545:PHE:CD1	2.56	0.40
6:F:557:PHE:O	6:F:561:ILE:HG23	2.21	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	648/705 (92%)	611 (94%)	36 (6%)	1 (0%)	44	75
2	B	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
3	C	76/79 (96%)	71 (93%)	5 (7%)	0	100	100
4	D	108/113 (96%)	104 (96%)	4 (4%)	0	100	100
5	E	556/607 (92%)	521 (94%)	35 (6%)	0	100	100
6	F	233/631 (37%)	221 (95%)	10 (4%)	2 (1%)	14	49
7	G	409/456 (90%)	379 (93%)	29 (7%)	1 (0%)	44	75
8	H	104/149 (70%)	101 (97%)	3 (3%)	0	100	100
All	All	2165/2777 (78%)	2038 (94%)	123 (6%)	4 (0%)	45	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	377	ASN
6	F	378	VAL
1	A	40	ARG
7	G	219	SER

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	574/615 (93%)	571 (100%)	3 (0%)	86	93
2	B	29/33 (88%)	29 (100%)	0	100	100
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	96/98 (98%)	96 (100%)	0	100	100
5	E	407/537 (76%)	402 (99%)	5 (1%)	67	82
6	F	211/541 (39%)	210 (100%)	1 (0%)	86	93
7	G	357/390 (92%)	356 (100%)	1 (0%)	91	96
8	H	92/130 (71%)	90 (98%)	2 (2%)	47	70
All	All	1835/2414 (76%)	1823 (99%)	12 (1%)	80	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	139	LYS
1	A	696	ASP
5	E	32	ILE
5	E	336	LEU
5	E	354	ARG
5	E	415	ASN
5	E	425	VAL
6	F	379	ASP
7	G	48	LEU
8	H	116	ASN
8	H	146	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	70	ASN
1	A	114	ASN
1	A	291	ASN
1	A	424	GLN
1	A	514	HIS
1	A	515	ASN
1	A	531	GLN
1	A	537	ASN
1	A	545	ASN
1	A	594	ASN
1	A	665	ASN
4	D	81	ASN
5	E	45	HIS
5	E	57	HIS
5	E	171	GLN
5	E	238	HIS
5	E	267	GLN
5	E	415	ASN
6	F	377	ASN
6	F	457	ASN
6	F	618	ASN
7	G	53	ASN
7	G	110	ASN
7	G	159	HIS
7	G	208	ASN
7	G	285	GLN
7	G	342	ASN
7	G	415	HIS
8	H	108	ASN
8	H	111	ASN
8	H	116	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	I	1	9	14,14,15	0.76	1 (7%)	17,19,21	0.53	0
9	NAG	I	2	9	14,14,15	0.35	0	17,19,21	0.36	0
9	BMA	I	3	9	11,11,12	0.56	0	15,15,17	0.77	0
10	NAG	J	1	10,1	14,14,15	0.26	0	17,19,21	0.39	0
10	NAG	J	2	10	14,14,15	0.26	0	17,19,21	0.41	0
10	BMA	J	3	10	11,11,12	0.80	1 (9%)	15,15,17	0.71	0
10	MAN	J	4	10	11,11,12	0.70	1 (9%)	15,15,17	1.07	2 (13%)
10	MAN	J	5	10	11,11,12	0.73	1 (9%)	15,15,17	1.00	2 (13%)
10	MAN	J	6	10	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
10	MAN	J	7	10	11,11,12	0.73	0	15,15,17	1.32	2 (13%)
10	MAN	J	8	10	11,11,12	0.75	0	15,15,17	1.20	2 (13%)
11	NAG	K	1	11,5	14,14,15	0.24	0	17,19,21	0.45	0
11	NAG	K	2	11	14,14,15	0.27	0	17,19,21	0.42	0
11	BMA	K	3	11	11,11,12	0.54	0	15,15,17	0.80	0
11	MAN	K	4	11	11,11,12	0.71	1 (9%)	15,15,17	1.00	2 (13%)
11	MAN	K	5	11	11,11,12	0.71	0	15,15,17	0.98	2 (13%)
11	MAN	K	6	11	11,11,12	0.78	1 (9%)	15,15,17	1.09	2 (13%)
11	MAN	K	7	11	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
11	MAN	K	8	11	11,11,12	0.65	0	15,15,17	1.02	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	I	1	9	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	I	3	9	-	2/2/19/22	0/1/1/1
10	NAG	J	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	J	2	10	-	0/6/23/26	0/1/1/1
10	BMA	J	3	10	-	0/2/19/22	0/1/1/1
10	MAN	J	4	10	-	2/2/19/22	0/1/1/1
10	MAN	J	5	10	-	2/2/19/22	0/1/1/1
10	MAN	J	6	10	-	0/2/19/22	0/1/1/1
10	MAN	J	7	10	-	2/2/19/22	1/1/1/1
10	MAN	J	8	10	-	1/2/19/22	1/1/1/1
11	NAG	K	1	11,5	-	2/6/23/26	0/1/1/1
11	NAG	K	2	11	-	2/6/23/26	0/1/1/1
11	BMA	K	3	11	-	1/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
11	MAN	K	5	11	-	0/2/19/22	0/1/1/1
11	MAN	K	6	11	-	2/2/19/22	0/1/1/1
11	MAN	K	7	11	-	2/2/19/22	0/1/1/1
11	MAN	K	8	11	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	NAG	O5-C1	-2.59	1.39	1.43
10	J	3	BMA	O5-C1	-2.25	1.40	1.43
11	K	6	MAN	O5-C1	-2.25	1.40	1.43
10	J	5	MAN	O5-C1	-2.15	1.40	1.43
11	K	4	MAN	O5-C1	-2.10	1.40	1.43
10	J	4	MAN	O5-C1	-2.09	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	7	MAN	C1-O5-C5	3.59	117.05	112.19
10	J	8	MAN	C1-O5-C5	3.34	116.71	112.19
11	K	6	MAN	C1-O5-C5	2.76	115.93	112.19
11	K	6	MAN	O2-C2-C3	-2.64	104.84	110.14
10	J	4	MAN	C1-O5-C5	2.55	115.65	112.19
10	J	7	MAN	O2-C2-C3	-2.50	105.12	110.14
11	K	4	MAN	O2-C2-C3	-2.41	105.30	110.14
11	K	8	MAN	O2-C2-C3	-2.37	105.38	110.14
10	J	6	MAN	C1-O5-C5	2.36	115.39	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	8	MAN	C1-O5-C5	2.36	115.39	112.19
10	J	6	MAN	O2-C2-C3	-2.36	105.41	110.14
11	K	7	MAN	O2-C2-C3	-2.35	105.43	110.14
10	J	4	MAN	O2-C2-C3	-2.30	105.53	110.14
10	J	8	MAN	O2-C2-C3	-2.28	105.58	110.14
11	K	5	MAN	O2-C2-C3	-2.27	105.60	110.14
10	J	5	MAN	O2-C2-C3	-2.26	105.60	110.14
10	J	5	MAN	C1-O5-C5	2.25	115.23	112.19
11	K	5	MAN	C1-O5-C5	2.23	115.22	112.19
11	K	4	MAN	C1-O5-C5	2.18	115.15	112.19
11	K	7	MAN	C1-O5-C5	2.13	115.08	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	5	MAN	O5-C5-C6-O6
11	K	2	NAG	O5-C5-C6-O6
11	K	6	MAN	O5-C5-C6-O6
10	J	7	MAN	C4-C5-C6-O6
10	J	5	MAN	C4-C5-C6-O6
11	K	2	NAG	C4-C5-C6-O6
11	K	6	MAN	C4-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
9	I	3	BMA	O5-C5-C6-O6
9	I	1	NAG	C8-C7-N2-C2
9	I	1	NAG	O7-C7-N2-C2
11	K	1	NAG	C8-C7-N2-C2
11	K	1	NAG	O7-C7-N2-C2
10	J	7	MAN	O5-C5-C6-O6
10	J	1	NAG	C4-C5-C6-O6
10	J	4	MAN	O5-C5-C6-O6
10	J	4	MAN	C4-C5-C6-O6
10	J	8	MAN	O5-C5-C6-O6
11	K	7	MAN	C4-C5-C6-O6
11	K	7	MAN	O5-C5-C6-O6
9	I	3	BMA	C4-C5-C6-O6
11	K	3	BMA	C4-C5-C6-O6

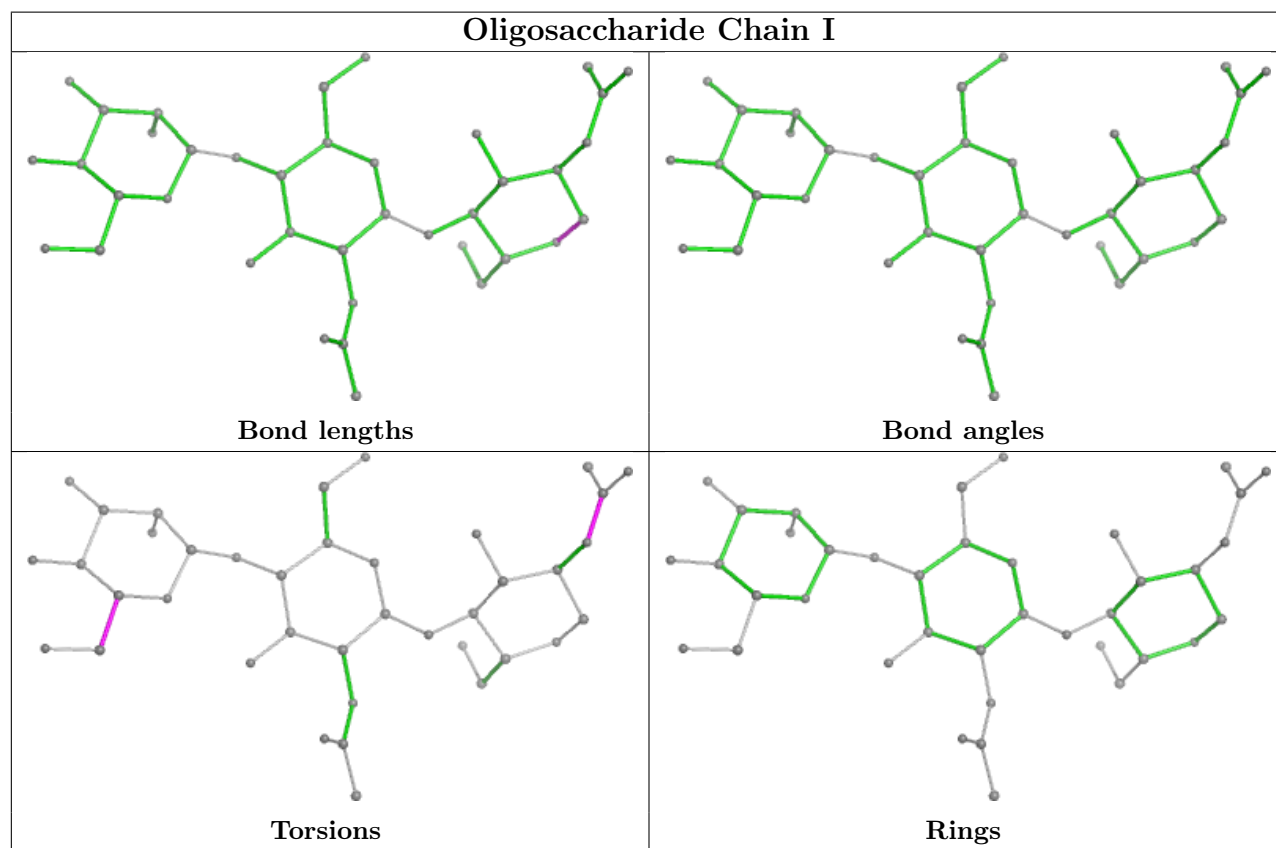
All (2) ring outliers are listed below:

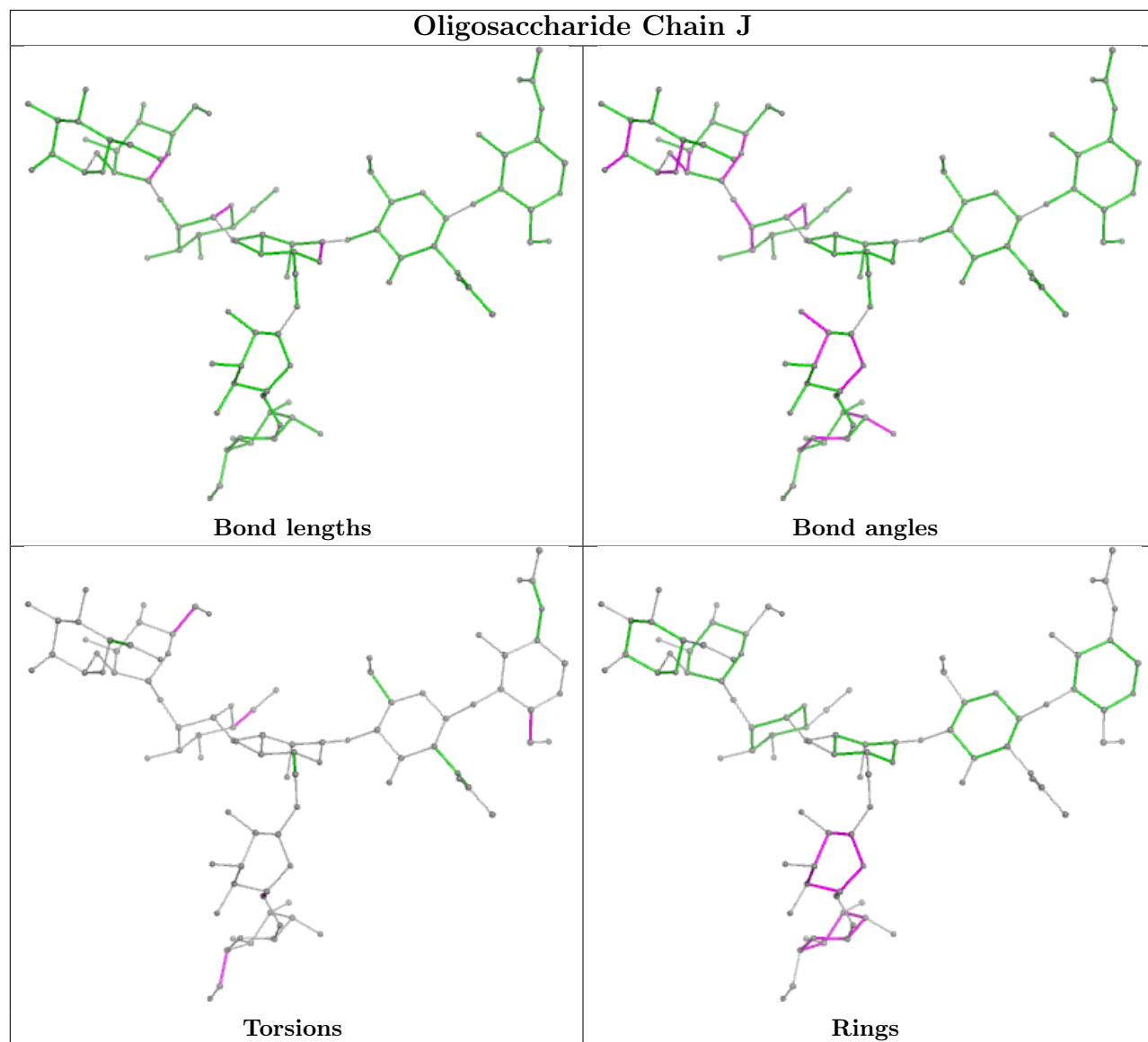
Mol	Chain	Res	Type	Atoms
10	J	8	MAN	C1-C2-C3-C4-C5-O5
10	J	7	MAN	C1-C2-C3-C4-C5-O5

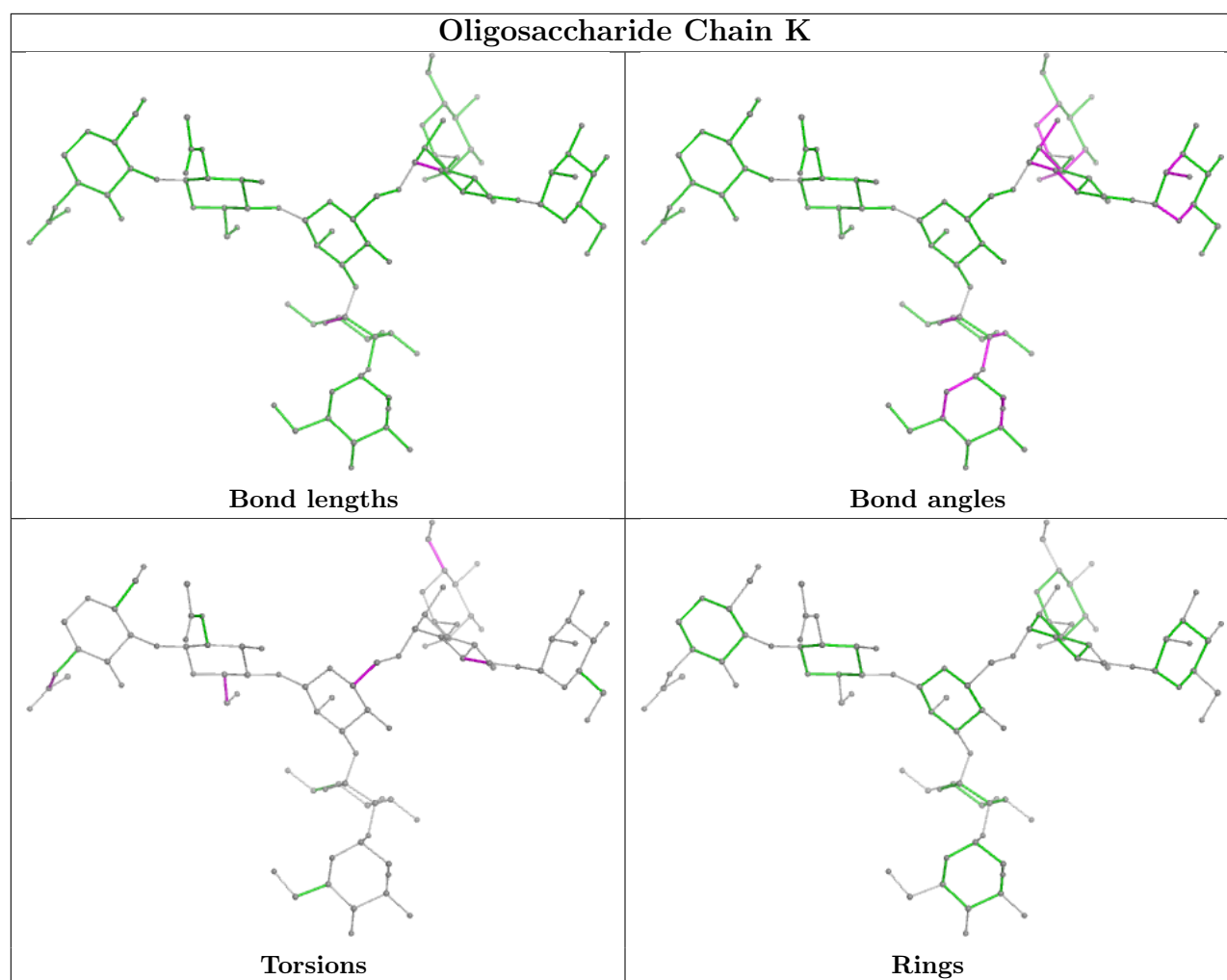
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1	NAG	1	0
11	K	7	MAN	1	0
11	K	1	NAG	1	0
11	K	2	NAG	2	0

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







5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	KZB	A	813	-	49,49,49	0.61	0	74,80,80	1.89	11 (14%)
13	EGY	D	701	-	42,42,42	1.35	5 (11%)	48,50,50	1.31	4 (8%)
12	KZB	F	701	-	37,37,49	0.68	1 (2%)	58,62,80	2.08	13 (22%)
15	KZE	A	818	-	29,29,34	1.56	5 (17%)	35,36,42	1.51	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	KZB	A	814	-	37,37,49	0.73	1 (2%)	58,62,80	2.09	13 (22%)
12	KZB	E	709	-	37,37,49	0.70	1 (2%)	58,62,80	2.03	14 (24%)
12	KZB	F	702	-	37,37,49	0.61	0	58,62,80	1.94	11 (18%)
12	KZB	F	703	-	37,37,49	0.70	0	58,62,80	2.00	12 (20%)
13	EGY	C	102	-	42,42,42	1.36	6 (14%)	48,50,50	1.08	2 (4%)
13	EGY	E	711	-	42,42,42	1.33	6 (14%)	48,50,50	1.09	2 (4%)
13	EGY	A	816	-	42,42,42	1.34	6 (14%)	48,50,50	1.10	2 (4%)
13	EGY	F	704	-	42,42,42	1.36	6 (14%)	48,50,50	1.18	2 (4%)
12	KZB	A	812	-	49,49,49	0.69	1 (2%)	74,80,80	2.00	16 (21%)
13	EGY	C	101	13	42,42,42	1.36	6 (14%)	48,50,50	1.12	2 (4%)
12	KZB	E	710	-	37,37,49	0.76	1 (2%)	58,62,80	2.09	15 (25%)
13	EGY	A	815	13	42,42,42	1.35	6 (14%)	48,50,50	1.10	2 (4%)
12	KZB	G	501	-	37,37,49	0.69	0	58,62,80	2.04	12 (20%)

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	KZB	A	813	-	-	3/6/121/121	0/7/7/7
13	EGY	D	701	-	-	16/46/46/46	-
12	KZB	F	701	-	-	-	0/6/6/7
15	KZE	A	818	-	-	10/31/31/37	-
13	EGY	C	102	-	-	26/46/46/46	-
13	EGY	F	704	-	-	20/46/46/46	-
12	KZB	A	814	-	-	-	0/6/6/7
12	KZB	E	709	-	-	-	0/6/6/7
13	EGY	E	711	-	-	17/46/46/46	-
12	KZB	F	702	-	-	-	0/6/6/7
13	EGY	A	816	-	-	19/46/46/46	-
12	KZB	F	703	-	-	-	0/6/6/7
12	KZB	A	812	-	-	5/6/121/121	0/7/7/7
13	EGY	C	101	13	-	25/46/46/46	-
12	KZB	E	710	-	-	-	0/6/6/7
13	EGY	A	815	13	-	24/46/46/46	-
12	KZB	G	501	-	-	-	0/6/6/7

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	818	KZE	P01-O04	4.48	1.65	1.50
13	F	704	EGY	O21-C21	3.57	1.44	1.34
13	C	102	EGY	O21-C21	3.55	1.44	1.34
13	E	711	EGY	O21-C21	3.50	1.44	1.34
13	A	815	EGY	O21-C21	3.47	1.44	1.34
13	C	101	EGY	O21-C21	3.46	1.44	1.34
13	D	701	EGY	O31-C31	3.40	1.43	1.33
13	D	701	EGY	O21-C21	3.39	1.43	1.34
13	F	704	EGY	O31-C31	3.37	1.43	1.33
13	A	816	EGY	O21-C21	3.37	1.43	1.34
13	A	816	EGY	O31-C31	3.34	1.43	1.33
13	A	815	EGY	O31-C31	3.33	1.43	1.33
13	C	102	EGY	O31-C31	3.33	1.43	1.33
13	C	101	EGY	O31-C31	3.33	1.43	1.33
13	E	711	EGY	O31-C31	3.26	1.42	1.33
13	A	816	EGY	O21-C2	-2.64	1.40	1.46
13	E	711	EGY	O21-C2	-2.57	1.40	1.46
13	C	101	EGY	O21-C2	-2.55	1.40	1.46
13	A	815	EGY	O21-C2	-2.53	1.40	1.46
13	C	102	EGY	O21-C2	-2.47	1.40	1.46
13	D	701	EGY	O21-C2	-2.43	1.40	1.46
13	F	704	EGY	O21-C2	-2.38	1.40	1.46
15	A	818	KZE	C14-C13	2.33	1.56	1.51
15	A	818	KZE	P01-O05	-2.25	1.46	1.54
13	C	102	EGY	P-O13	2.19	1.68	1.59
12	E	709	KZB	C84-C03	-2.14	1.51	1.56
13	D	701	EGY	P-O13	2.13	1.67	1.59
13	A	816	EGY	P-O13	2.13	1.67	1.59
13	A	815	EGY	P-O13	2.12	1.67	1.59
13	C	101	EGY	P-O11	2.12	1.67	1.59
13	E	711	EGY	P-O13	2.12	1.67	1.59
13	C	101	EGY	P-O13	2.12	1.67	1.59
13	C	102	EGY	P-O11	2.12	1.67	1.59
15	A	818	KZE	C29-C28	2.11	1.56	1.50
13	D	701	EGY	P-O11	2.10	1.67	1.59
12	A	812	KZB	C84-C03	-2.10	1.51	1.56
13	C	102	EGY	C22-C21	2.09	1.56	1.50
15	A	818	KZE	P01-O03	-2.08	1.46	1.54
13	C	101	EGY	C22-C21	2.08	1.56	1.50
13	A	815	EGY	P-O11	2.08	1.67	1.59
12	E	710	KZB	C84-C03	-2.08	1.51	1.56
13	F	704	EGY	P-O11	2.07	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	815	EGY	C22-C21	2.06	1.56	1.50
13	A	816	EGY	P-O11	2.05	1.67	1.59
13	A	816	EGY	C22-C21	2.05	1.56	1.50
13	F	704	EGY	P-O13	2.04	1.67	1.59
13	F	704	EGY	C13-N	-2.03	1.44	1.50
12	F	701	KZB	C84-C03	-2.02	1.52	1.56
12	A	814	KZB	C84-C03	-2.02	1.52	1.56
13	E	711	EGY	C22-C21	2.01	1.56	1.50
13	E	711	EGY	P-O11	2.01	1.67	1.59

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	813	KZB	O05-C04-C13	9.01	128.71	110.17
12	F	701	KZB	O05-C04-C13	8.61	127.90	110.17
12	A	812	KZB	O05-C04-C13	8.59	127.86	110.17
12	E	710	KZB	O05-C04-C13	8.57	127.81	110.17
12	E	709	KZB	O05-C04-C13	8.55	127.76	110.17
12	G	501	KZB	O05-C04-C13	8.53	127.73	110.17
12	A	814	KZB	O05-C04-C13	8.47	127.59	110.17
12	F	702	KZB	O05-C04-C13	8.34	127.33	110.17
12	F	703	KZB	O05-C04-C13	8.33	127.31	110.17
12	A	813	KZB	C84-C03-C04	-7.03	97.28	104.88
12	G	501	KZB	C84-C03-C04	-6.54	97.82	104.88
12	F	701	KZB	C84-C03-C04	-6.47	97.89	104.88
12	A	812	KZB	C84-C03-C04	-6.17	98.21	104.88
13	D	701	EGY	O21-C21-C22	5.62	123.62	111.50
12	F	702	KZB	C84-C03-C04	-5.48	98.96	104.88
12	A	814	KZB	C84-C03-C04	-5.41	99.04	104.88
12	A	812	KZB	O12-C06-C07	5.37	115.76	110.77
12	F	703	KZB	C84-C03-C04	-5.33	99.12	104.88
12	E	709	KZB	C84-C03-C04	-5.25	99.21	104.88
12	E	709	KZB	C19-C20-C21	-5.18	108.75	114.46
12	F	701	KZB	C19-C20-C21	-4.89	109.06	114.46
12	G	501	KZB	C19-C20-C21	-4.80	109.17	114.46
12	A	813	KZB	C79-C81-C16	-4.65	107.54	112.42
12	F	702	KZB	C19-C20-C21	-4.61	109.38	114.46
12	A	813	KZB	C17-C16-C81	-4.55	104.85	110.49
12	A	814	KZB	C11-O12-C06	4.51	122.27	113.72
12	A	814	KZB	C19-C20-C21	-4.43	109.57	114.46
12	E	710	KZB	C19-C20-C21	-4.36	109.64	114.46
13	F	704	EGY	O21-C21-C22	4.35	120.88	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	710	KZB	C11-O12-C06	4.35	121.95	113.72
12	F	703	KZB	C79-C81-C16	-4.33	107.87	112.42
13	A	815	EGY	O21-C21-C22	4.29	120.75	111.50
12	F	703	KZB	C17-C16-C81	-4.18	105.31	110.49
13	C	101	EGY	O21-C21-C22	4.13	120.40	111.50
13	C	102	EGY	O21-C21-C22	4.05	120.23	111.50
13	E	711	EGY	O21-C21-C22	4.02	120.16	111.50
12	G	501	KZB	C82-C81-C79	-3.90	109.42	113.91
12	A	812	KZB	C79-C81-C16	-3.89	108.33	112.42
13	A	816	EGY	O21-C21-C22	3.77	119.63	111.50
12	E	710	KZB	C84-C03-C04	-3.69	100.89	104.88
12	F	703	KZB	C19-C20-C21	-3.67	110.41	114.46
12	A	812	KZB	C17-C16-C81	-3.59	106.04	110.49
12	A	814	KZB	C17-C16-C81	-3.58	106.05	110.49
12	E	710	KZB	C02-C03-C04	-3.55	97.88	104.34
12	F	702	KZB	C17-C16-C81	-3.48	106.17	110.49
12	A	814	KZB	C84-C15-C16	-3.48	108.83	113.82
12	F	701	KZB	C17-C16-C81	-3.45	106.22	110.49
12	A	812	KZB	C07-C06-C02	-3.32	108.86	115.69
12	E	710	KZB	C84-C15-C16	-3.31	109.07	113.82
13	F	704	EGY	O31-C31-C32	3.29	122.22	111.91
12	A	814	KZB	C82-C81-C79	-3.28	110.13	113.91
12	G	501	KZB	C17-C16-C81	-3.28	106.43	110.49
12	F	701	KZB	C82-C81-C79	-3.22	110.20	113.91
12	E	709	KZB	C17-C16-C81	-3.16	106.58	110.49
12	G	501	KZB	C84-C15-C16	-3.11	109.35	113.82
12	A	814	KZB	O12-C06-C07	3.11	113.66	110.77
12	F	701	KZB	C79-C81-C16	-3.09	109.17	112.42
12	E	710	KZB	C08-C09-C11	3.07	112.83	108.56
12	F	703	KZB	C02-C03-C04	-2.96	98.95	104.34
15	A	818	KZE	C20-C21-C22	-2.94	120.58	127.66
12	A	812	KZB	C82-C81-C79	-2.93	110.54	113.91
12	A	812	KZB	O12-C11-C09	-2.92	107.98	112.18
12	A	812	KZB	C79-C78-C76	-2.90	109.33	114.09
12	E	710	KZB	C17-C16-C81	-2.87	106.93	110.49
13	D	701	EGY	O31-C31-C32	2.87	120.91	111.91
12	E	710	KZB	C01-C02-C06	2.85	120.12	114.92
12	A	814	KZB	C79-C81-C16	-2.85	109.43	112.42
13	A	816	EGY	O31-C31-C32	2.84	120.81	111.91
12	F	701	KZB	C07-C06-C02	-2.83	109.86	115.69
12	F	702	KZB	C79-C81-C16	-2.81	109.46	112.42
12	E	710	KZB	C82-C81-C79	-2.79	110.69	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	703	KZB	C84-C03-C02	2.79	130.06	120.56
12	E	710	KZB	O12-C06-C07	2.79	113.36	110.77
15	A	818	KZE	C15-C17-C18	-2.78	120.96	127.66
12	A	812	KZB	C84-C03-C02	2.78	130.01	120.56
12	A	813	KZB	C84-C03-C02	2.76	129.95	120.56
12	G	501	KZB	C84-C03-C02	2.75	129.91	120.56
12	F	702	KZB	C84-C03-C02	2.73	129.85	120.56
12	E	709	KZB	O12-C11-C09	-2.72	108.26	112.18
15	A	818	KZE	C16-C13-C14	2.71	119.83	115.27
12	A	812	KZB	C82-C83-C84	-2.68	108.19	112.78
12	A	813	KZB	C18-C17-C16	-2.68	107.73	112.14
12	F	702	KZB	C84-C15-C16	-2.67	109.98	113.82
12	F	701	KZB	C84-C03-C02	2.67	129.65	120.56
13	C	102	EGY	O31-C31-C32	2.67	120.29	111.91
12	A	812	KZB	C11-O12-C06	2.65	118.75	113.72
12	A	812	KZB	C08-C09-C11	-2.64	104.89	108.56
12	E	709	KZB	C84-C03-C02	2.63	129.50	120.56
12	E	709	KZB	C82-C81-C79	-2.62	110.89	113.91
13	C	101	EGY	O31-C31-C32	2.60	120.06	111.91
12	A	814	KZB	C84-C03-C02	2.59	129.36	120.56
12	F	703	KZB	C82-C81-C79	-2.56	110.96	113.91
15	A	818	KZE	C09-C12-C13	-2.55	121.51	127.66
12	E	710	KZB	C06-C02-C03	-2.54	99.23	103.37
12	A	813	KZB	C82-C81-C79	-2.54	110.98	113.91
12	F	702	KZB	C82-C81-C79	-2.54	110.99	113.91
12	E	710	KZB	C84-C03-C02	2.53	129.16	120.56
12	F	701	KZB	C20-C19-C79	-2.52	109.98	112.66
15	A	818	KZE	C23-C18-C19	2.52	119.51	115.27
13	E	711	EGY	O31-C31-C32	2.47	119.66	111.91
15	A	818	KZE	C26-C22-C24	2.46	119.42	115.27
12	F	703	KZB	C20-C19-C79	-2.46	110.04	112.66
12	F	701	KZB	C18-C17-C16	-2.46	108.09	112.14
12	G	501	KZB	C18-C17-C16	-2.46	108.09	112.14
13	A	815	EGY	O31-C31-C32	2.46	119.61	111.91
12	E	709	KZB	C07-C06-C02	-2.45	110.66	115.69
12	A	813	KZB	C79-C78-C76	-2.44	110.08	114.09
12	E	709	KZB	C78-C79-C19	2.44	109.89	107.14
12	F	703	KZB	O12-C11-C09	-2.44	108.67	112.18
12	E	709	KZB	C82-C83-C84	-2.41	108.65	112.78
12	F	703	KZB	C79-C78-C76	-2.41	110.14	114.09
12	E	710	KZB	C79-C81-C16	-2.40	109.90	112.42
12	A	814	KZB	C20-C19-C79	-2.39	110.12	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	701	EGY	C2-O21-C21	-2.37	111.96	117.79
12	A	814	KZB	C18-C17-C16	-2.37	108.24	112.14
12	E	709	KZB	C07-C08-C09	-2.37	106.81	111.81
12	F	701	KZB	C84-C15-C16	-2.34	110.46	113.82
12	A	813	KZB	C84-C15-C16	-2.33	110.48	113.82
12	F	701	KZB	O12-C11-C09	-2.29	108.89	112.18
12	A	812	KZB	C07-C08-C09	-2.25	107.07	111.81
15	A	818	KZE	C30-C28-C29	2.24	119.54	114.60
12	A	813	KZB	C82-C83-C84	-2.22	108.98	112.78
12	E	710	KZB	C79-C78-C76	-2.21	110.46	114.09
12	E	709	KZB	O12-C06-C07	2.20	112.82	110.77
12	F	701	KZB	C07-C08-C09	-2.18	107.20	111.81
13	D	701	EGY	O21-C21-O22	-2.18	118.43	123.70
12	F	703	KZB	C18-C17-C16	-2.17	108.56	112.14
12	G	501	KZB	C83-C84-C15	-2.15	103.89	108.19
12	F	702	KZB	C18-C17-C16	-2.15	108.60	112.14
12	F	702	KZB	C79-C78-C76	-2.15	110.57	114.09
12	A	812	KZB	C84-C15-C16	-2.11	110.78	113.82
15	A	818	KZE	C25-C27-C28	-2.11	120.53	127.75
12	G	501	KZB	C07-C06-C02	-2.11	111.35	115.69
12	F	702	KZB	C02-C03-C04	-2.09	100.55	104.34
12	A	813	KZB	C07-C06-C02	-2.07	111.43	115.69
12	G	501	KZB	O12-C11-C09	-2.03	109.26	112.18
12	A	814	KZB	C79-C78-C76	-2.03	110.77	114.09
12	E	709	KZB	C79-C78-C76	-2.01	110.79	114.09
12	E	709	KZB	C02-C03-C04	-2.01	100.68	104.34
12	A	812	KZB	C78-C79-C19	2.00	109.40	107.14
12	G	501	KZB	C79-C81-C16	-2.00	110.32	112.42

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	816	EGY	O13-C11-C12-N
13	C	101	EGY	C11-O13-P-O12
13	C	101	EGY	C1-O11-P-O12
13	C	101	EGY	C1-O11-P-O14
13	C	101	EGY	O13-C11-C12-N
13	C	102	EGY	C11-O13-P-O14
13	E	711	EGY	C11-O13-P-O12
13	E	711	EGY	C11-O13-P-O11
13	E	711	EGY	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
13	E	711	EGY	C1-O11-P-O14
13	E	711	EGY	C1-O11-P-O13
13	E	711	EGY	O13-C11-C12-N
13	F	704	EGY	C11-O13-P-O12
13	F	704	EGY	C11-O13-P-O14
13	F	704	EGY	C11-O13-P-O11
13	F	704	EGY	C1-O11-P-O14
13	F	704	EGY	O13-C11-C12-N
13	F	704	EGY	C22-C21-O21-C2
15	A	818	KZE	C06-C07-C09-C12
15	A	818	KZE	C06-C08-C11-O02
15	A	818	KZE	C12-C13-C14-C15
15	A	818	KZE	C16-C13-C14-C15
15	A	818	KZE	C11-O02-P01-O03
15	A	818	KZE	C11-O02-P01-O04
15	A	818	KZE	C11-O02-P01-O05
13	A	815	EGY	O32-C31-O31-C3
13	C	101	EGY	O32-C31-O31-C3
13	E	711	EGY	O32-C31-O31-C3
13	C	101	EGY	C32-C31-O31-C3
13	E	711	EGY	C32-C31-O31-C3
13	A	815	EGY	C32-C31-O31-C3
13	F	704	EGY	O22-C21-O21-C2
13	E	711	EGY	C32-C33-C34-C35
13	A	815	EGY	C34-C35-C36-C37
15	A	818	KZE	C13-C14-C15-C17
15	A	818	KZE	C22-C24-C25-C27
12	A	812	KZB	O24-C25-C26-O27
13	A	816	EGY	C32-C31-O31-C3
13	C	102	EGY	C32-C31-O31-C3
13	F	704	EGY	C32-C31-O31-C3
13	C	102	EGY	C31-C32-C33-C34
13	C	102	EGY	C21-C22-C23-C24
13	D	701	EGY	C31-C32-C33-C34
13	E	711	EGY	C31-C32-C33-C34
13	F	704	EGY	C21-C22-C23-C24
13	F	704	EGY	C31-C32-C33-C34
13	A	816	EGY	O32-C31-O31-C3
13	C	102	EGY	O32-C31-O31-C3
15	A	818	KZE	C18-C19-C20-C21
13	F	704	EGY	O32-C31-O31-C3
13	C	101	EGY	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	C	101	EGY	C11-O13-P-O11
13	C	101	EGY	C1-O11-P-O13
13	C	102	EGY	C11-O13-P-O11
13	D	701	EGY	C11-O13-P-O11
13	F	704	EGY	C1-O11-P-O13
12	A	812	KZB	C74-C23-O22-C21
12	A	812	KZB	O24-C23-O22-C21
12	A	813	KZB	O24-C23-O22-C21
13	D	701	EGY	C35-C36-C37-C38
13	D	701	EGY	C25-C26-C27-C28
13	A	816	EGY	C33-C34-C35-C36
13	F	704	EGY	C33-C34-C35-C36
13	C	101	EGY	C27-C28-C29-C2A
13	A	815	EGY	C22-C23-C24-C25
13	A	816	EGY	C25-C26-C27-C28
13	D	701	EGY	C33-C34-C35-C36
13	E	711	EGY	C24-C25-C26-C27
13	C	102	EGY	C35-C36-C37-C38
13	A	815	EGY	C27-C28-C29-C2A
13	E	711	EGY	C33-C34-C35-C36
13	A	815	EGY	C25-C26-C27-C28
13	C	101	EGY	C25-C26-C27-C28
12	A	813	KZB	C74-C23-O22-C21
13	C	102	EGY	C22-C23-C24-C25
13	C	102	EGY	C22-C21-O21-C2
13	C	102	EGY	O22-C21-O21-C2
13	A	816	EGY	C31-C32-C33-C34
13	F	704	EGY	C23-C24-C25-C26
13	C	101	EGY	C29-C2A-C2B-C2C
13	F	704	EGY	C28-C29-C2A-C2B
13	A	815	EGY	C1-C2-C3-O31
13	E	711	EGY	C22-C23-C24-C25
13	A	816	EGY	C28-C29-C2A-C2B
13	D	701	EGY	C21-C22-C23-C24
13	A	815	EGY	C35-C36-C37-C38
13	A	816	EGY	C35-C36-C37-C38
13	D	701	EGY	C23-C24-C25-C26
13	E	711	EGY	C36-C37-C38-C39
13	C	101	EGY	C36-C37-C38-C39
13	A	815	EGY	O11-C1-C2-C3
13	A	816	EGY	C22-C23-C24-C25
13	A	815	EGY	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
13	C	101	EGY	C1-C2-C3-O31
13	C	102	EGY	C1-C2-C3-O31
13	F	704	EGY	C1-C2-C3-O31
13	A	816	EGY	C23-C24-C25-C26
13	C	101	EGY	C32-C33-C34-C35
13	D	701	EGY	C28-C29-C2A-C2B
13	C	101	EGY	O21-C2-C3-O31
13	C	102	EGY	O21-C2-C3-O31
13	F	704	EGY	O21-C2-C3-O31
13	C	102	EGY	C33-C34-C35-C36
13	C	101	EGY	C23-C24-C25-C26
13	D	701	EGY	C26-C27-C28-C29
13	A	816	EGY	C32-C33-C34-C35
13	A	815	EGY	O11-C1-C2-O21
13	D	701	EGY	O11-C1-C2-O21
13	C	102	EGY	C25-C26-C27-C28
13	C	102	EGY	C28-C29-C2A-C2B
12	A	812	KZB	C20-C21-O22-C23
13	A	816	EGY	O22-C21-O21-C2
13	C	101	EGY	C11-O13-P-O14
13	D	701	EGY	C11-O13-P-O14
13	E	711	EGY	C11-O13-P-O14
13	C	102	EGY	C23-C24-C25-C26
13	C	101	EGY	O11-C1-C2-O21
12	A	813	KZB	C28-C25-C26-O27
13	A	816	EGY	C22-C21-O21-C2
13	A	815	EGY	O13-C11-C12-N
13	A	815	EGY	C29-C2A-C2B-C2C
13	C	102	EGY	O13-C11-C12-N
13	D	701	EGY	O13-C11-C12-N
13	E	711	EGY	C35-C36-C37-C38
13	D	701	EGY	O31-C31-C32-C33
13	F	704	EGY	C3-C2-O21-C21
13	A	815	EGY	C24-C25-C26-C27
13	D	701	EGY	C22-C23-C24-C25
13	A	816	EGY	O11-C1-C2-O21
13	A	815	EGY	O21-C2-C3-O31
13	A	815	EGY	C11-O13-P-O11
13	A	815	EGY	C1-O11-P-O13
13	C	102	EGY	C1-O11-P-O13
13	F	704	EGY	C34-C35-C36-C37
13	C	102	EGY	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
13	C	102	EGY	O11-C1-C2-O21
12	A	812	KZB	C28-C25-C26-O27
13	D	701	EGY	C2A-C2B-C2C-C2D
13	A	816	EGY	C26-C27-C28-C29
13	C	101	EGY	O11-C1-C2-C3
13	C	102	EGY	O11-C1-C2-C3
13	A	815	EGY	C21-C22-C23-C24
13	A	815	EGY	C37-C38-C39-C3A
13	A	815	EGY	C31-C32-C33-C34
13	C	101	EGY	C34-C35-C36-C37
13	F	704	EGY	C26-C27-C28-C29
13	A	815	EGY	O21-C21-C22-C23
13	C	101	EGY	O31-C31-C32-C33
13	C	102	EGY	C2A-C2B-C2C-C2D
13	A	816	EGY	O11-C1-C2-C3
13	D	701	EGY	O11-C1-C2-C3
13	C	101	EGY	C24-C25-C26-C27
13	A	816	EGY	C36-C37-C38-C39
13	C	102	EGY	C26-C27-C28-C29
13	C	101	EGY	O32-C31-C32-C33
13	A	815	EGY	C32-C33-C34-C35
13	A	816	EGY	C2A-C2B-C2C-C2D
13	E	711	EGY	C28-C29-C2A-C2B
13	A	815	EGY	O22-C21-C22-C23
13	A	815	EGY	C12-C11-O13-P
13	A	816	EGY	C12-C11-O13-P
13	C	101	EGY	C12-C11-O13-P
13	C	102	EGY	C36-C37-C38-C39
13	C	102	EGY	C24-C25-C26-C27
13	C	102	EGY	C34-C35-C36-C37

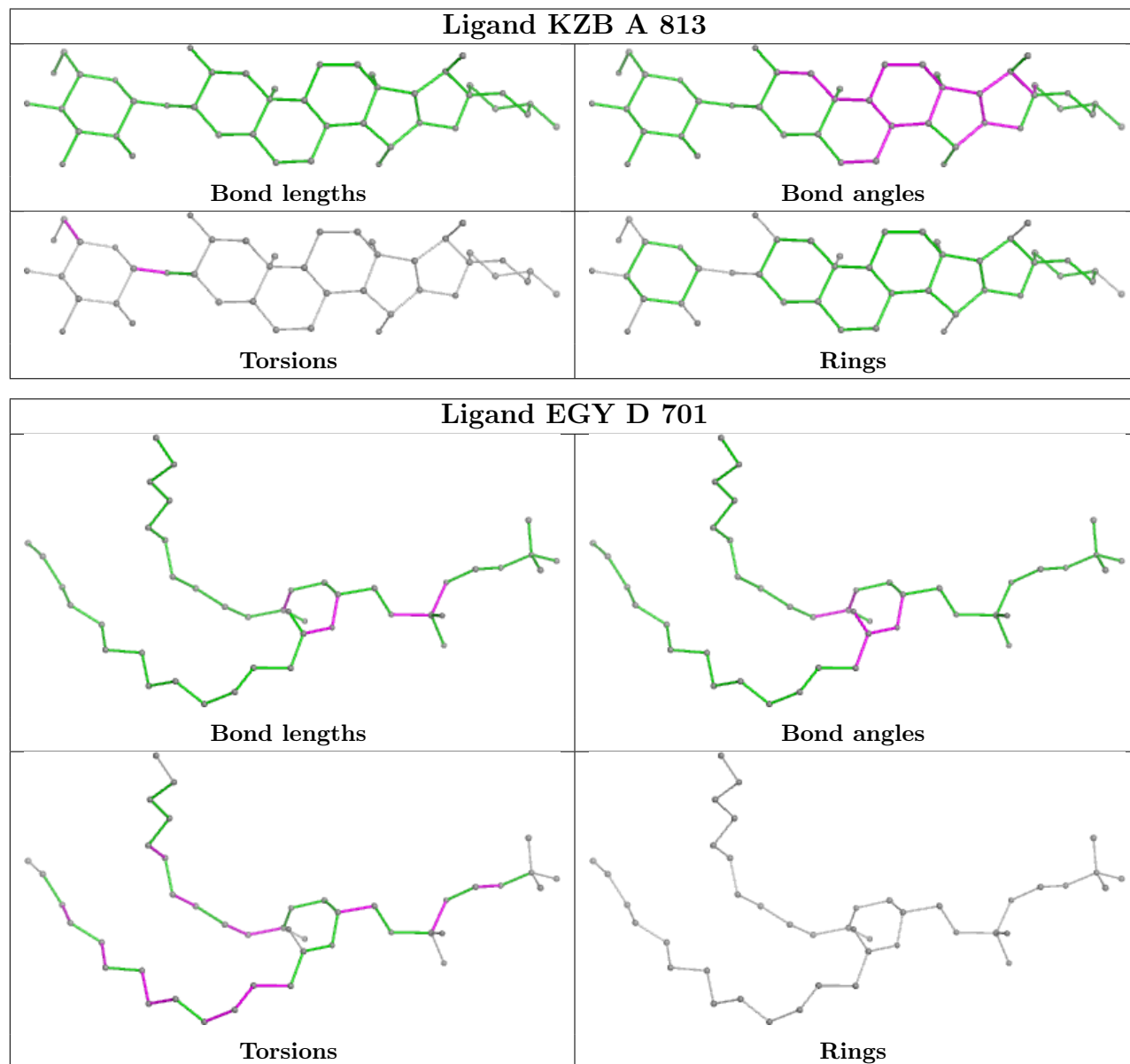
There are no ring outliers.

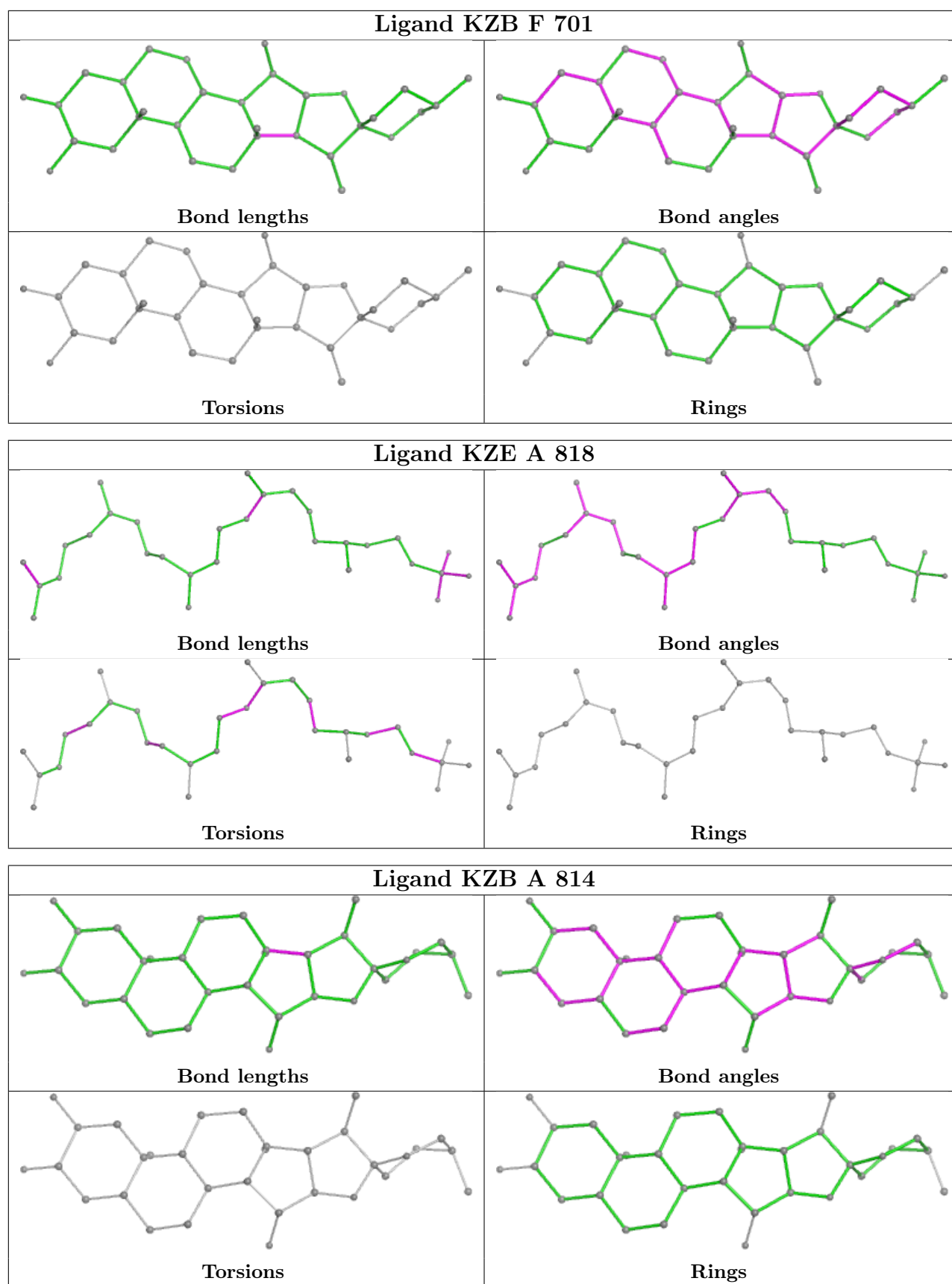
4 monomers are involved in 6 short contacts:

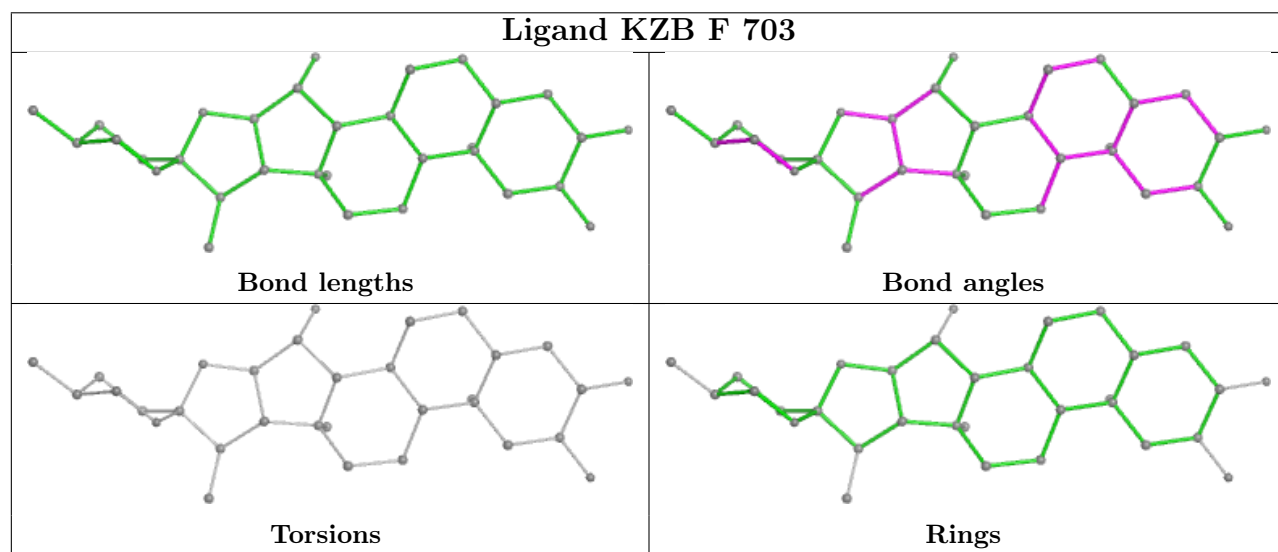
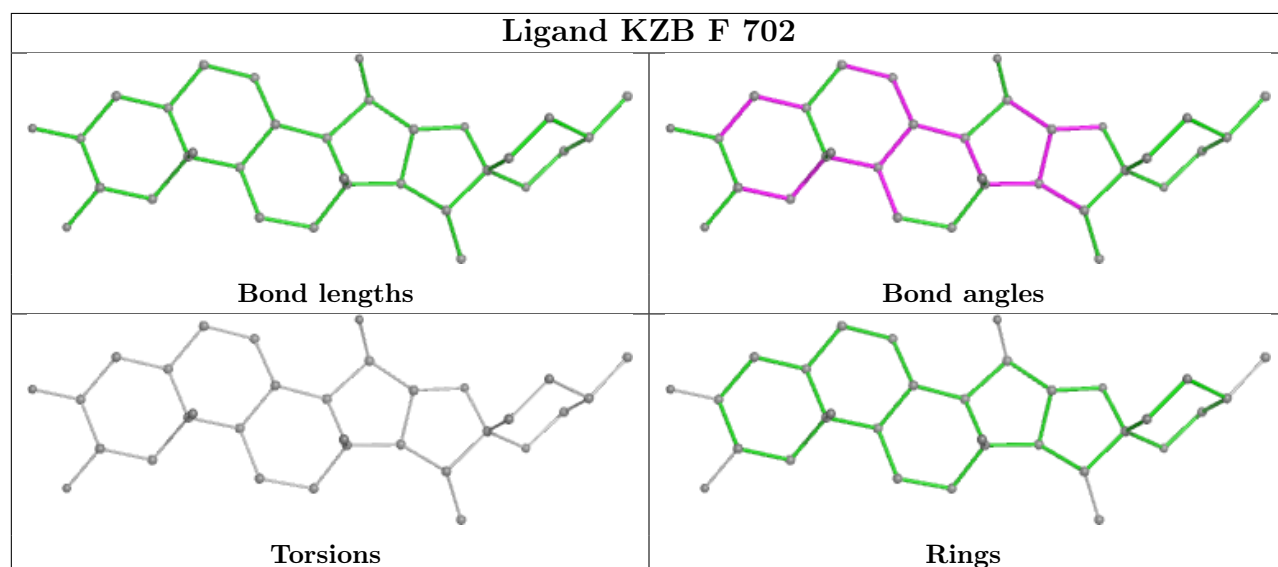
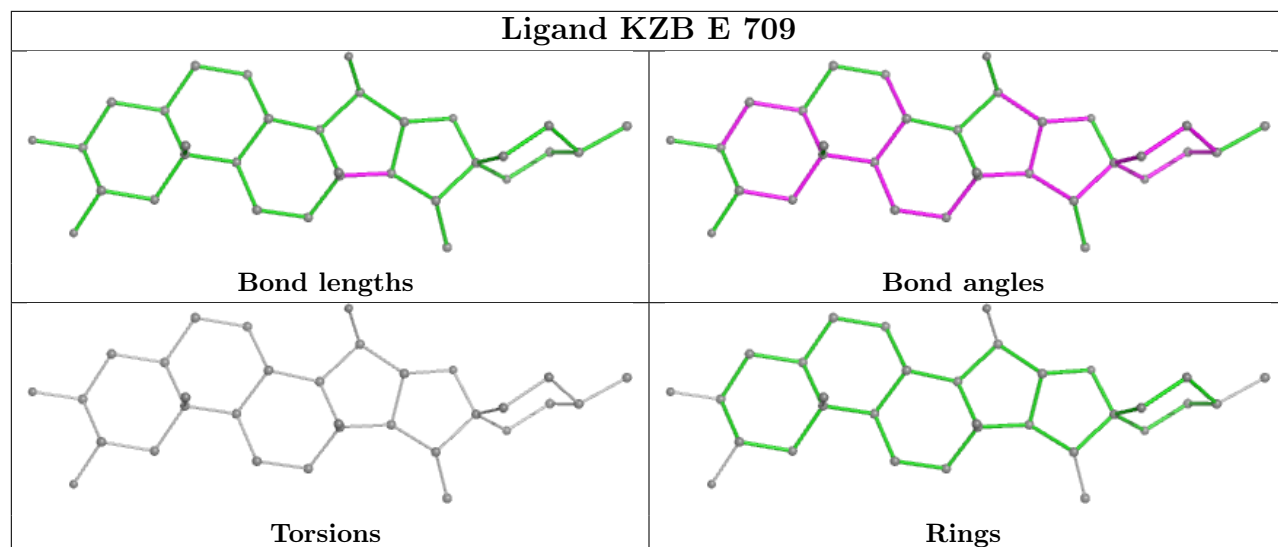
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	701	EGY	1	0
15	A	818	KZE	2	0
13	E	711	EGY	2	0
12	A	812	KZB	1	0

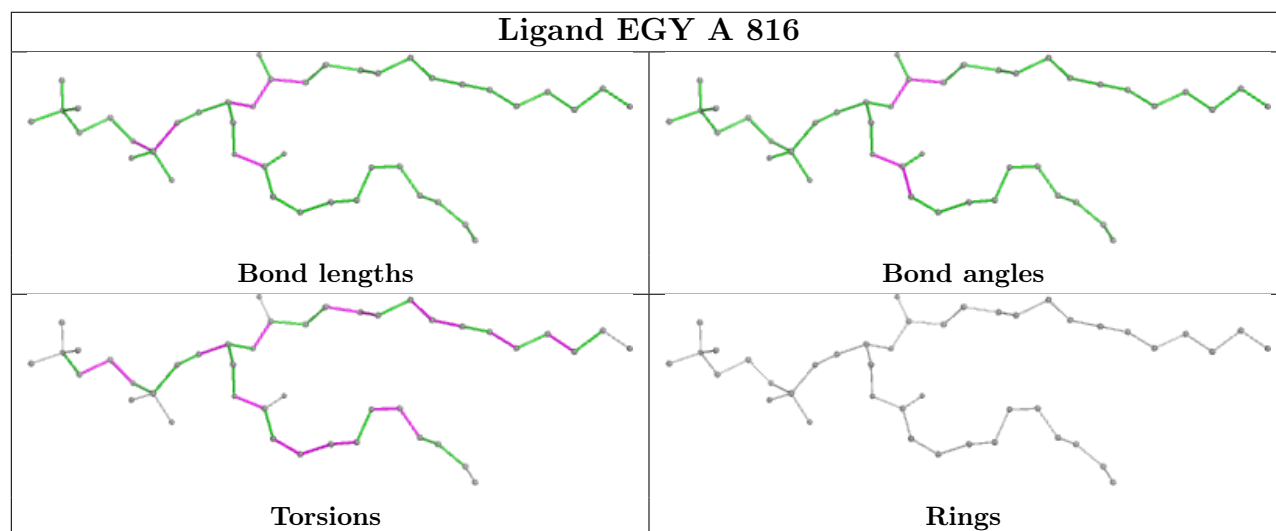
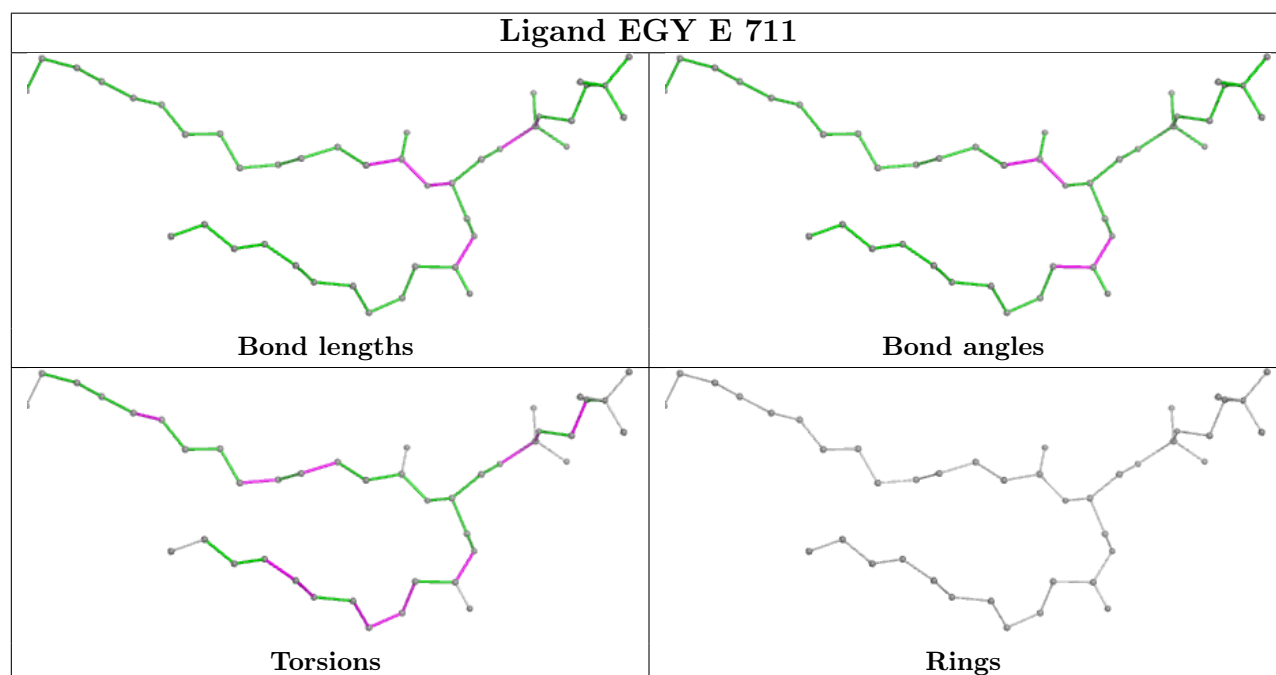
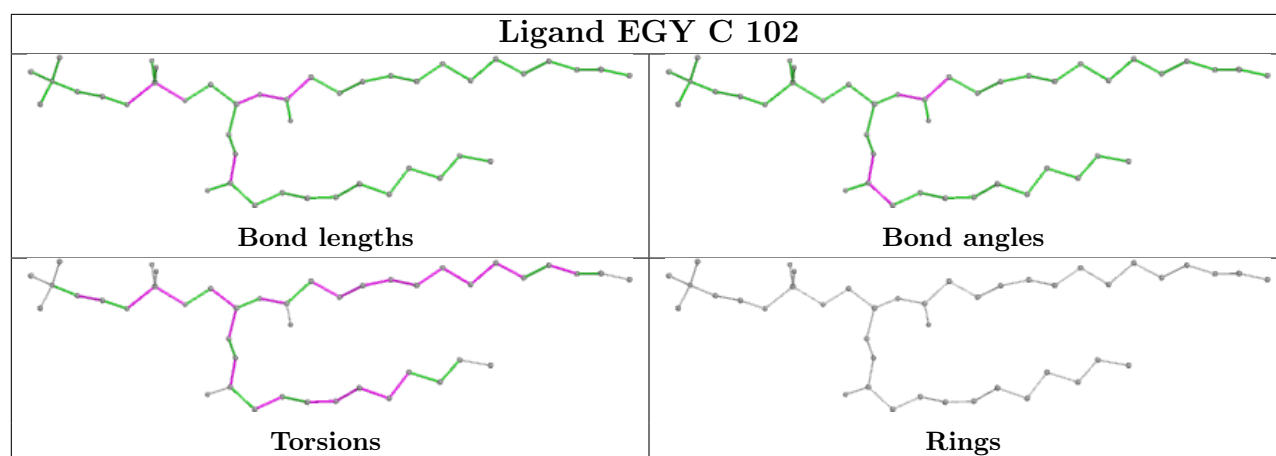
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

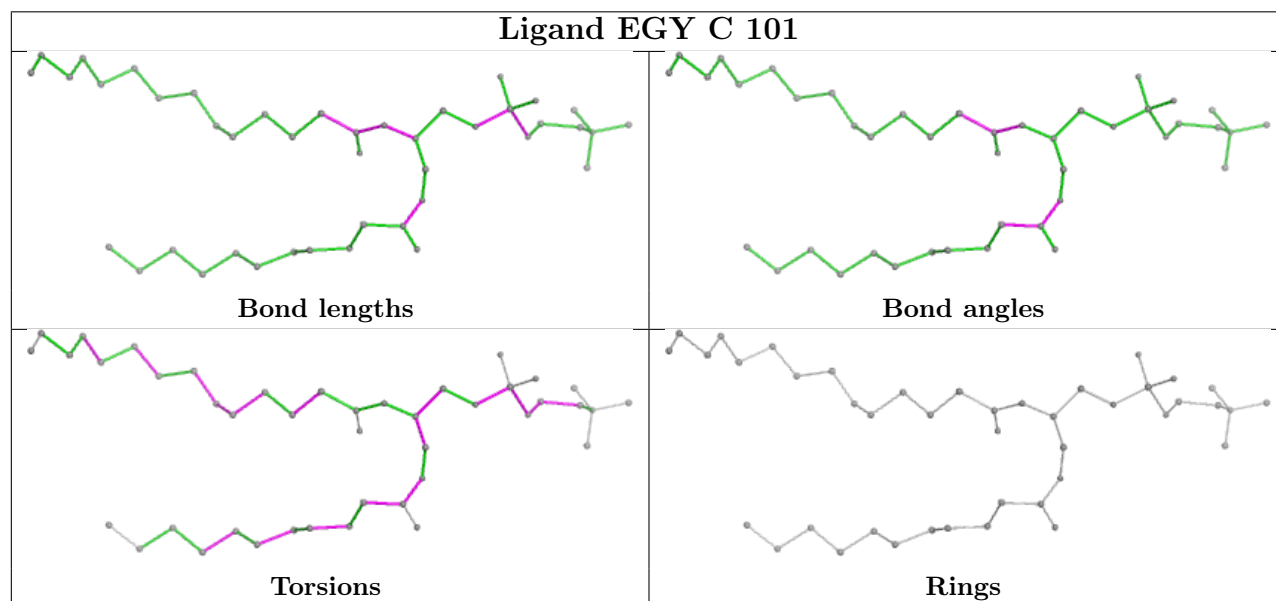
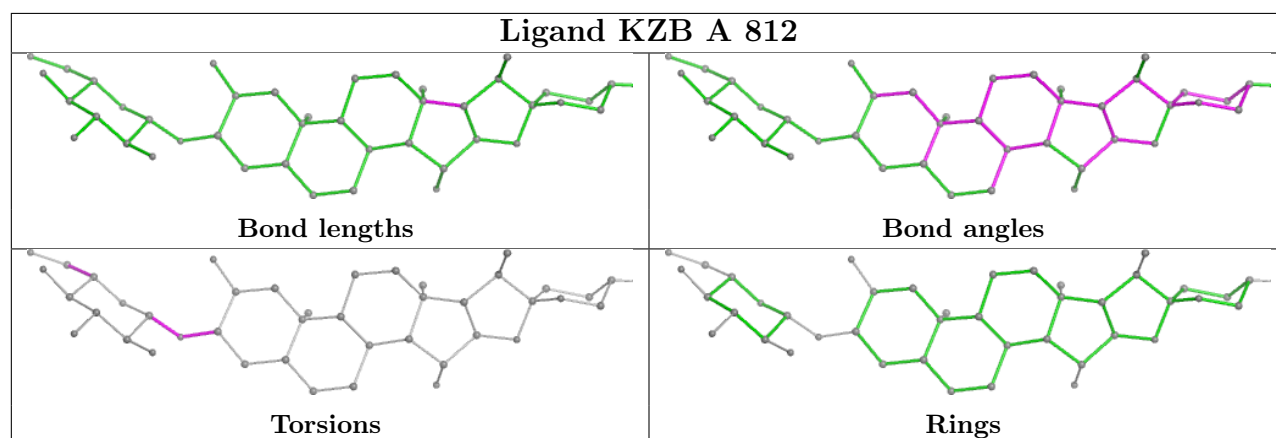
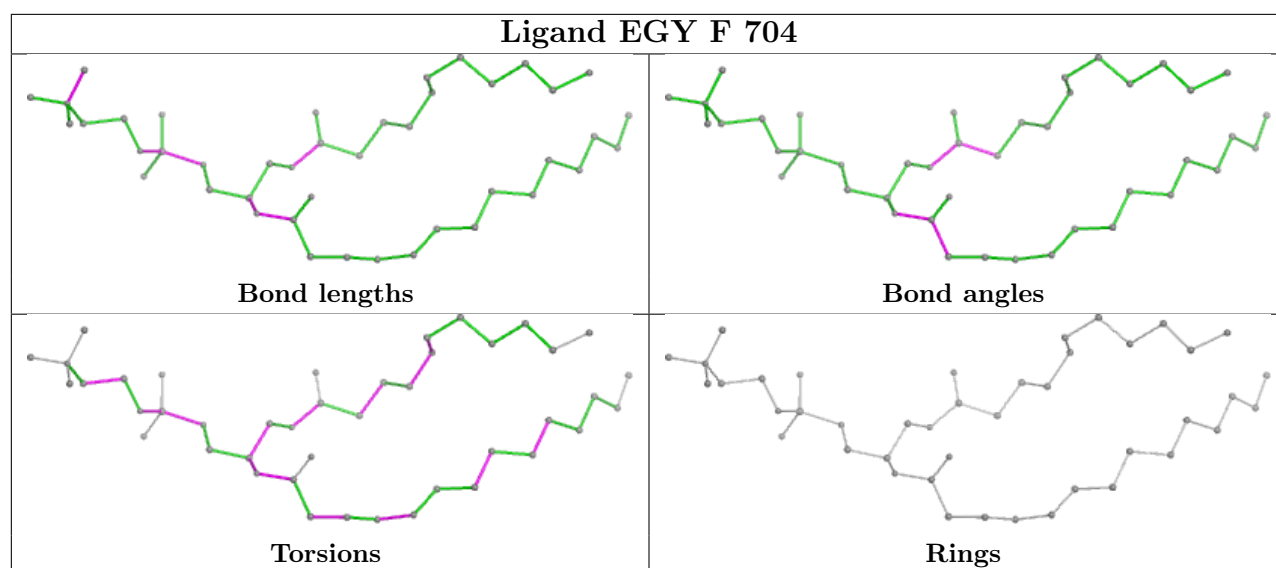
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

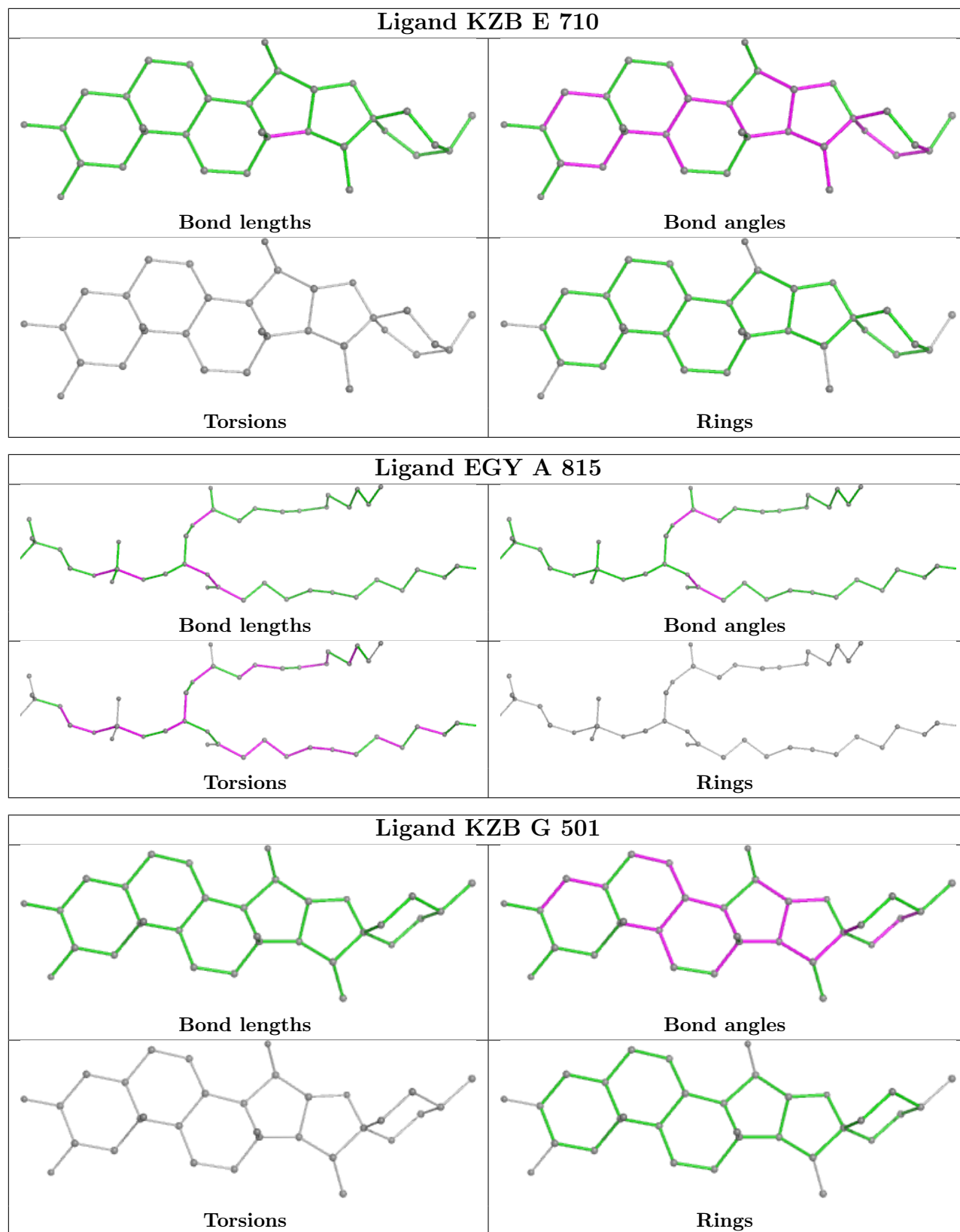












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

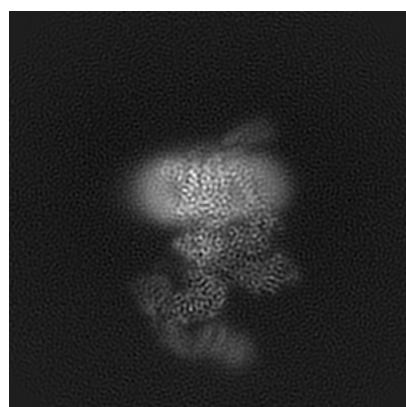
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10110. These allow visual inspection of the internal detail of the map and identification of artifacts.

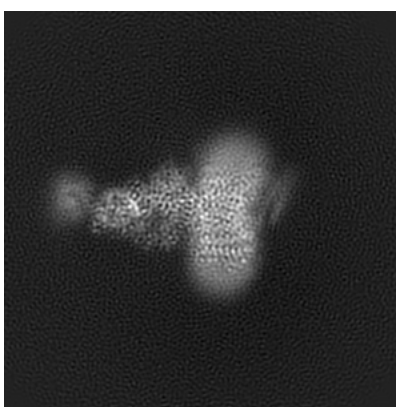
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

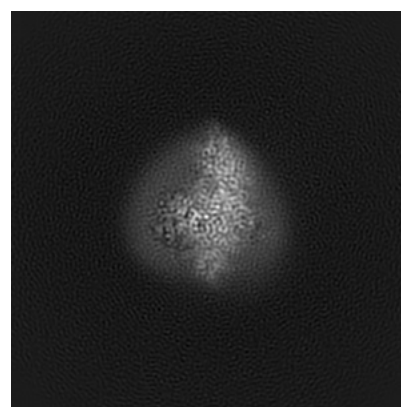
6.1.1 Primary map



X



Y

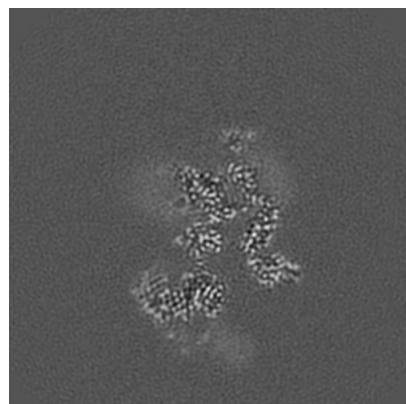


Z

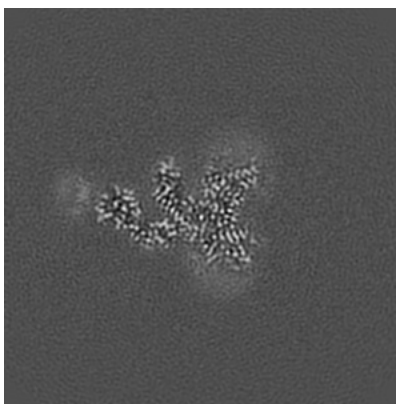
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

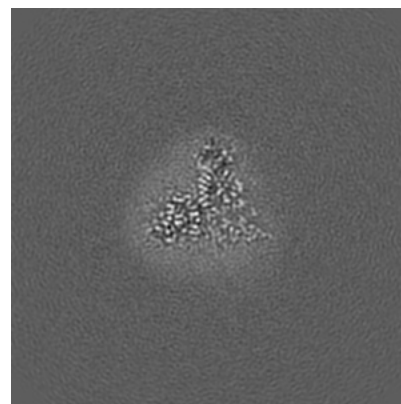
6.2.1 Primary map



X Index: 192



Y Index: 192

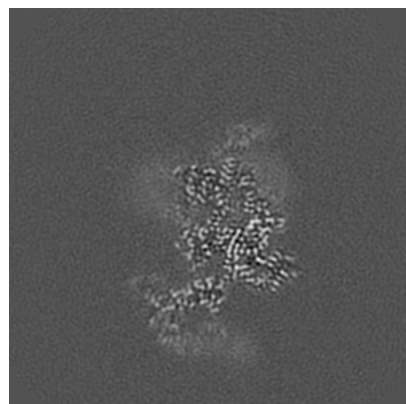


Z Index: 192

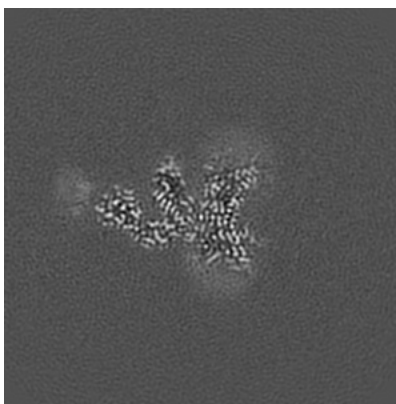
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

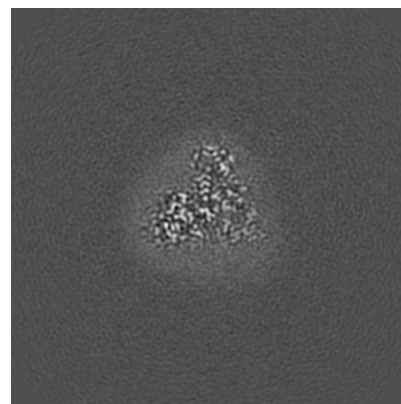
6.3.1 Primary map



X Index: 201



Y Index: 191

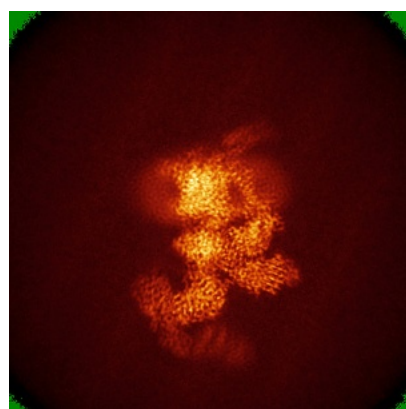


Z Index: 194

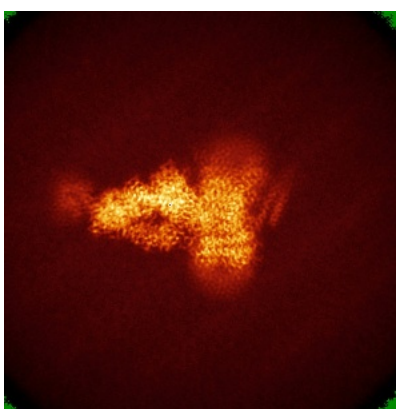
The images above show the largest variance slices of the map in three orthogonal directions.

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

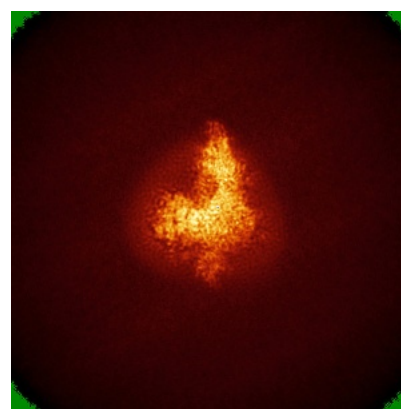
6.4.1 Primary map



X



Y

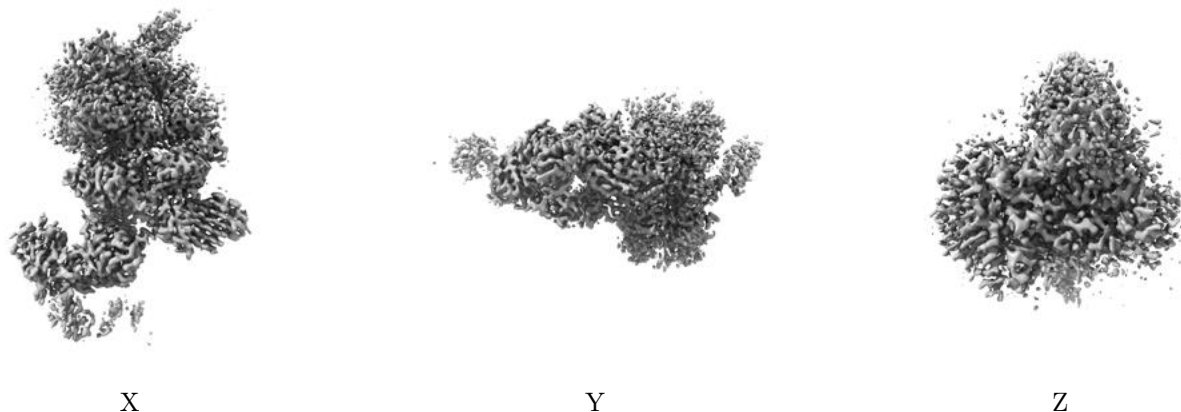


Z

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 0.0106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

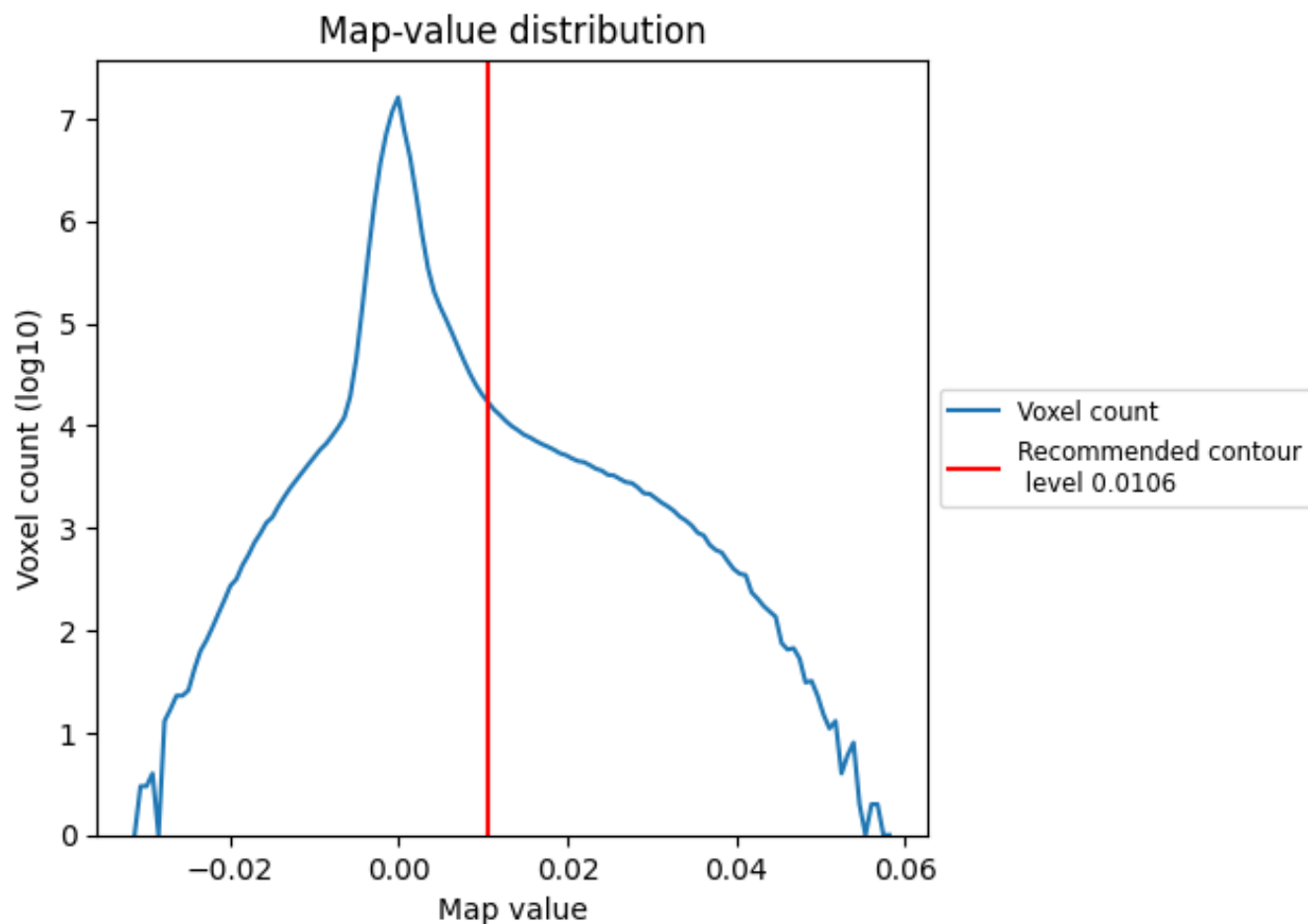
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

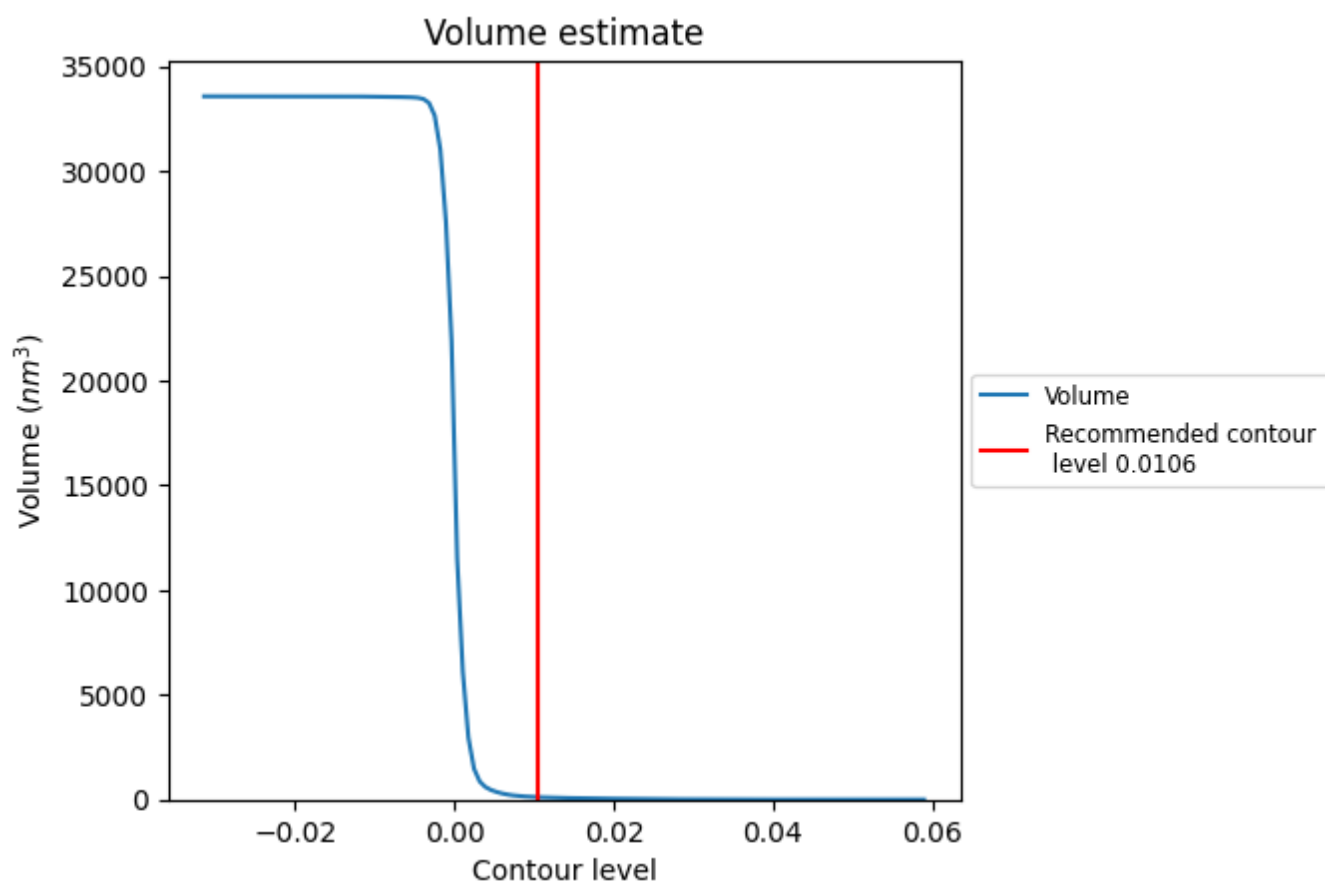
This section contains the results of statistical analysis of the map.

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.

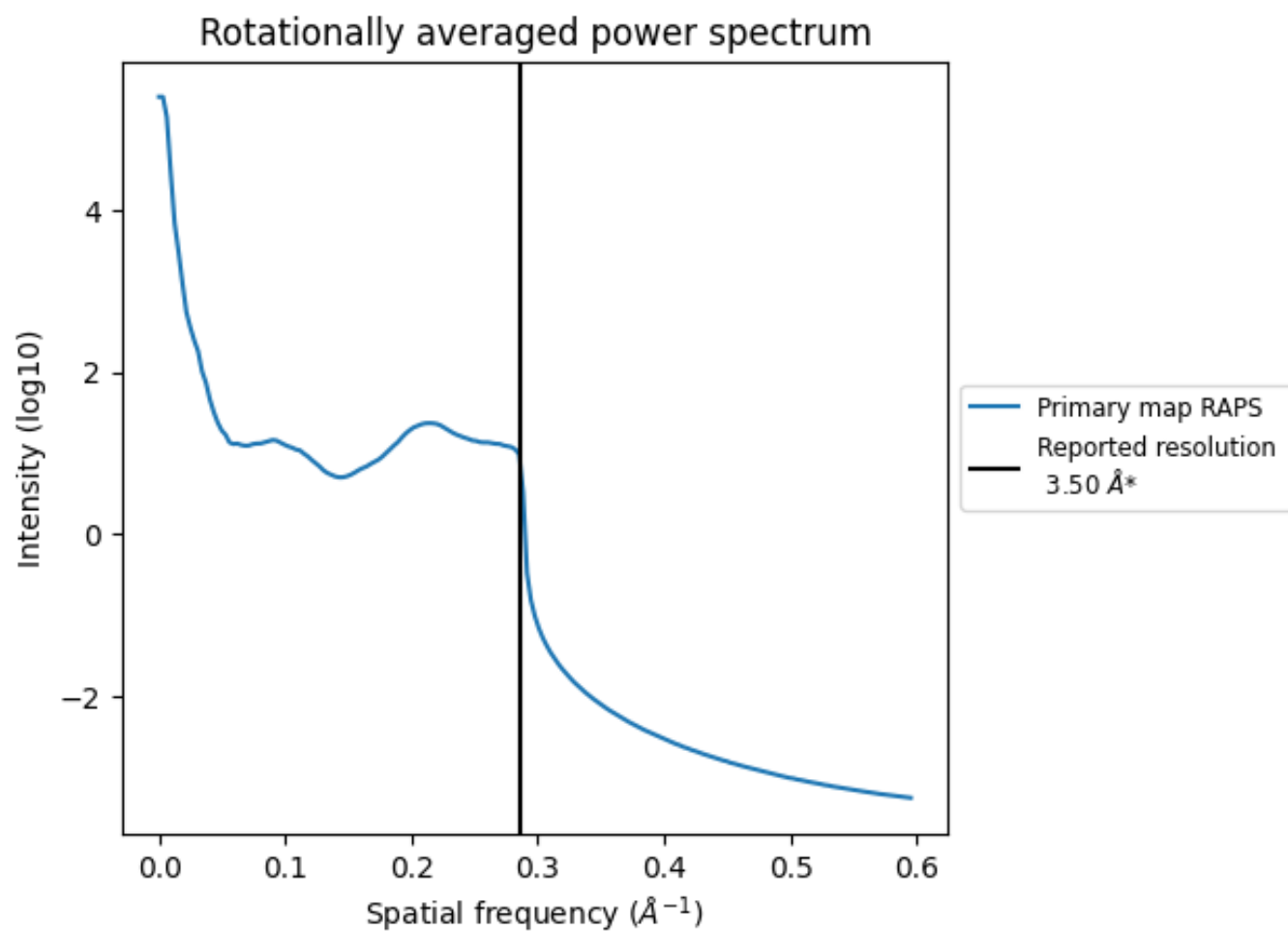
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

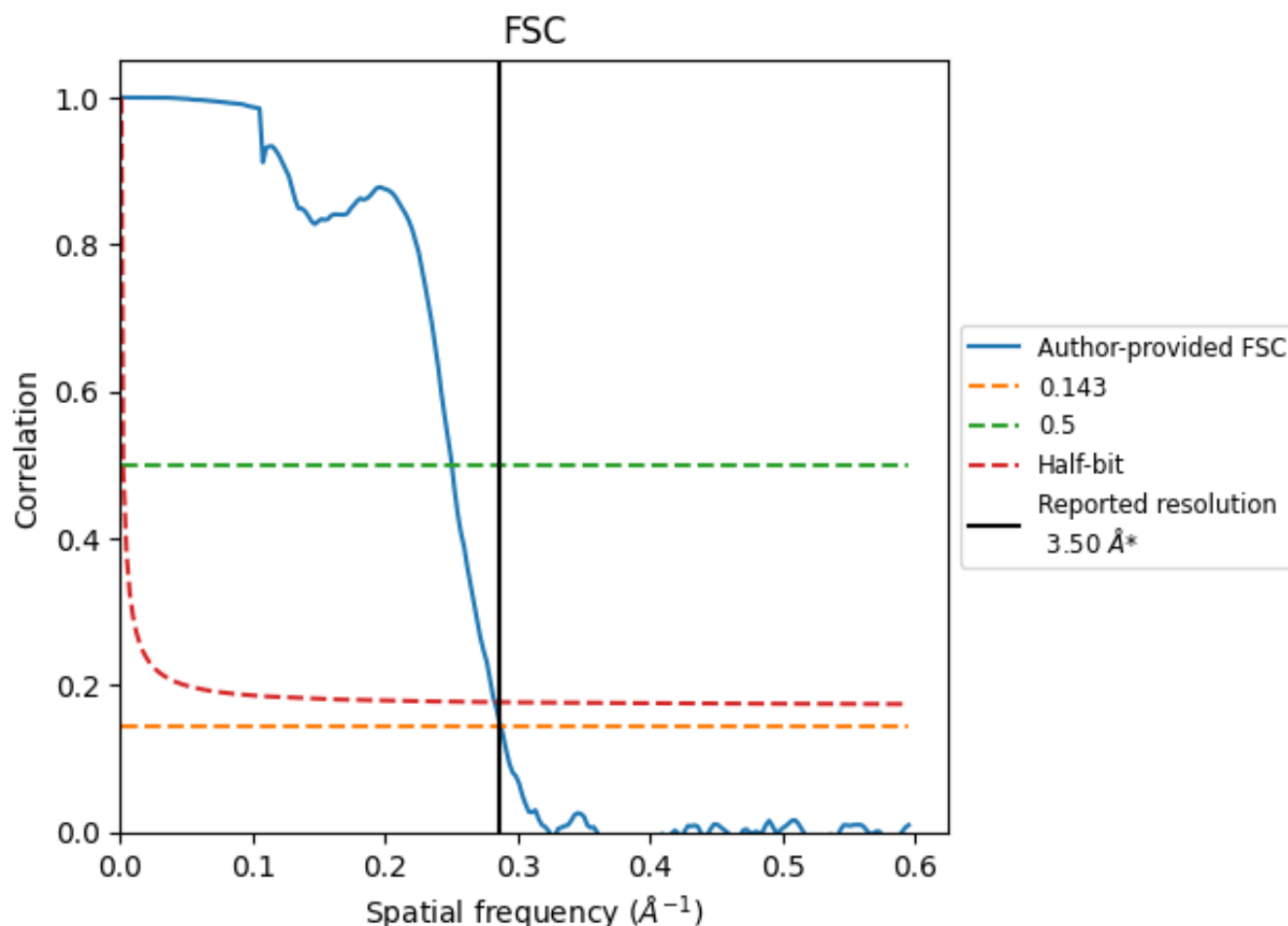


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

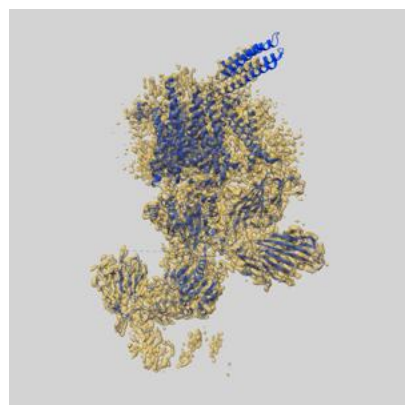
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.00	3.54
Unmasked-calculated*	-	-	-

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

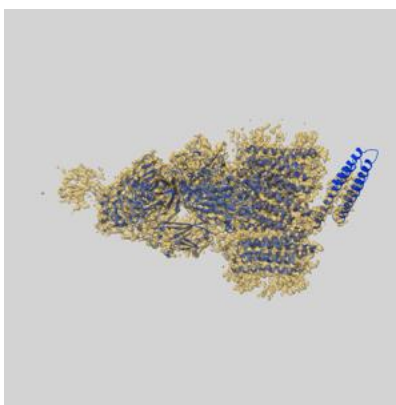
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10110 and PDB model 6S7O. Per-residue inclusion information can be found in section [3](#) on page [9](#).

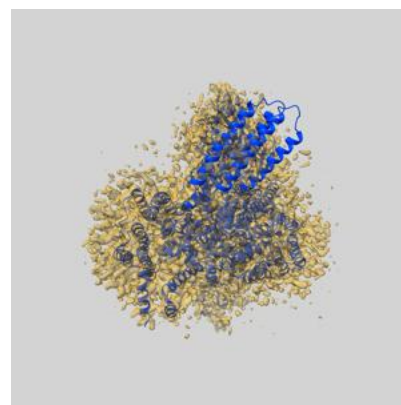
9.1 Map-model overlay [i](#)



X



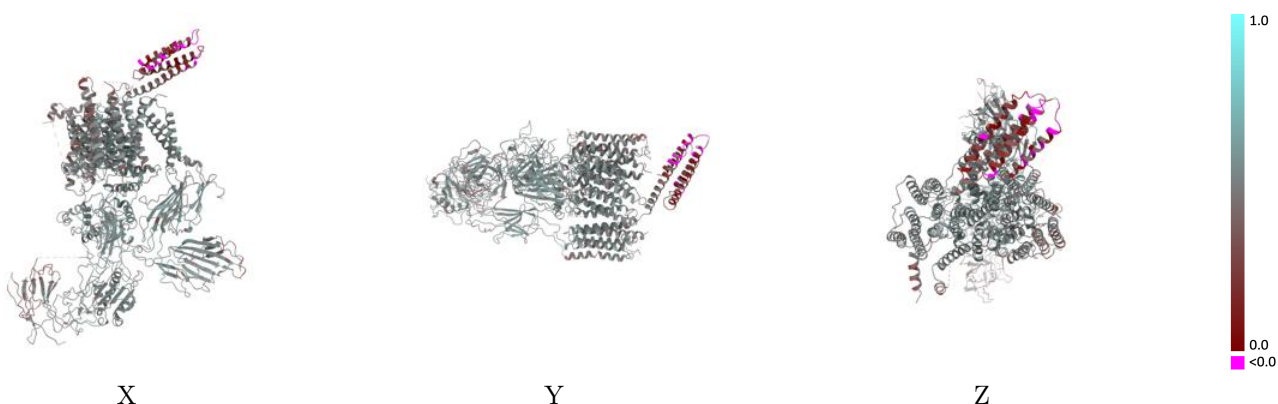
Y



Z

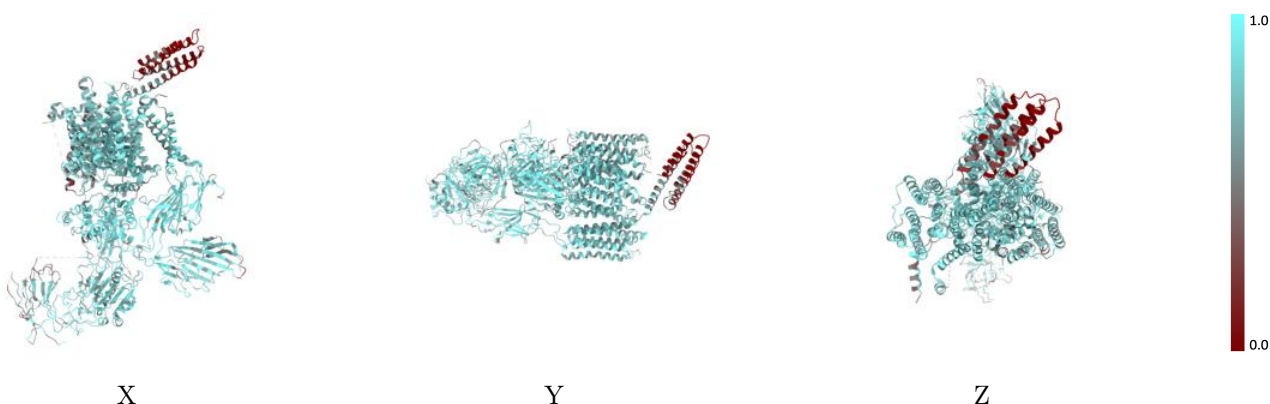
The images above show the 3D surface view of the map at the recommended contour level 0.0106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



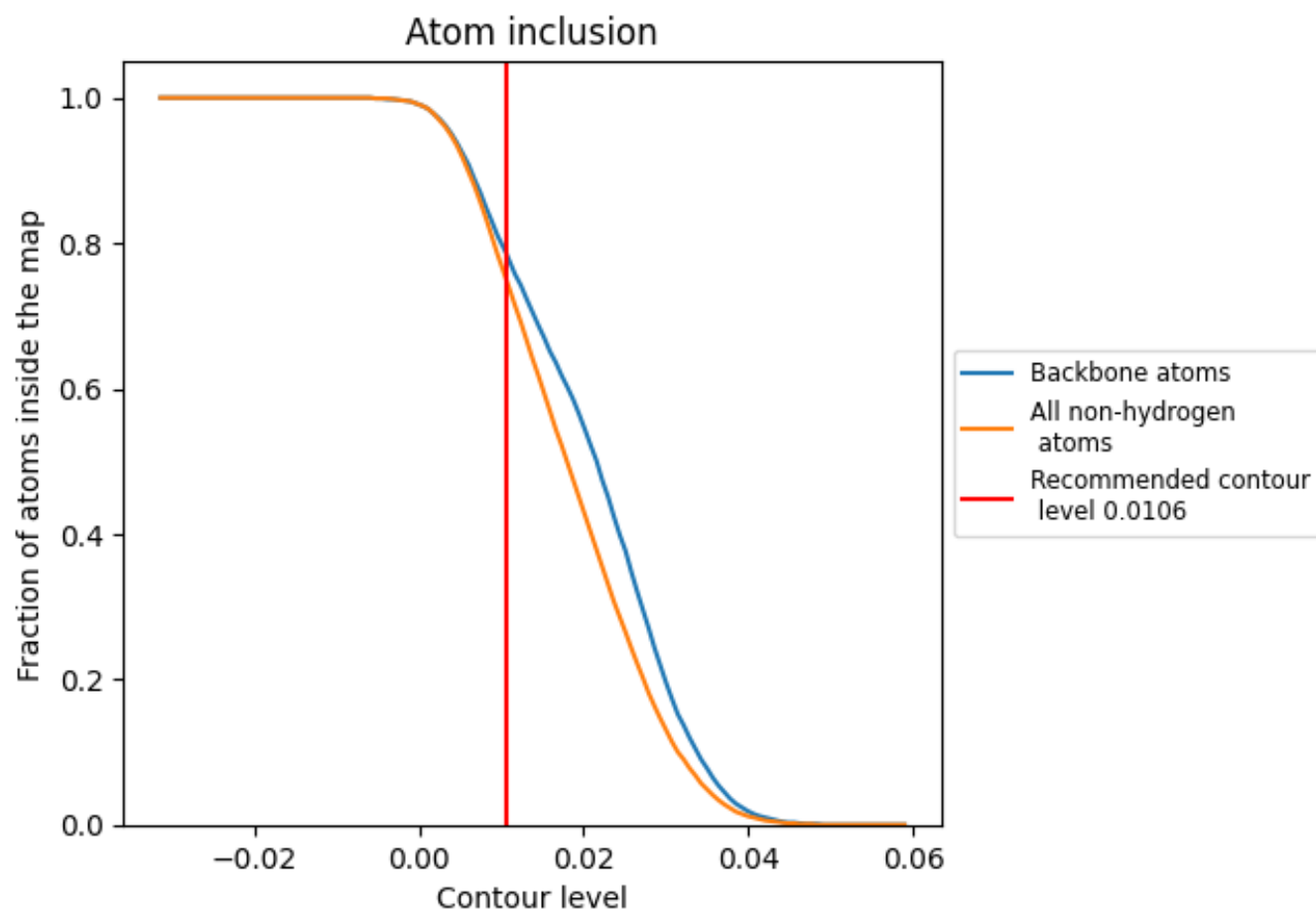
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0106).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (0.0106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7500	<div></div> 0.4850
A	<div></div> 0.7930	<div></div> 0.5100
B	<div></div> 0.7580	<div></div> 0.4730
C	<div></div> 0.7530	<div></div> 0.5020
D	<div></div> 0.7770	<div></div> 0.4890
E	<div></div> 0.6960	<div></div> 0.4580
F	<div></div> 0.6940	<div></div> 0.4500
G	<div></div> 0.7970	<div></div> 0.5100
H	<div></div> 0.6910	<div></div> 0.4390
I	<div></div> 0.4100	<div></div> 0.2920
J	<div></div> 0.7020	<div></div> 0.5050
K	<div></div> 0.7230	<div></div> 0.5310

1.0

0.0

<0.0