



Full wwPDB EM Validation Report ⓘ

Mar 30, 2023 – 12:15 PM JST

PDB ID : 8I2G
EMDB ID : EMD-35135
Title : FSHR-Follicle stimulating hormone-compound 716340-Gs complex
Authors : Duan, J.; Xu, P.; Yang, J.; Ji, Y.; Zhang, H.; Mao, C.; Luan, X.; Jiang, Y.;
Zhang, Y.; Zhang, S.; Xu, H.E.
Deposited on : 2023-01-14
Resolution : 2.80 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:

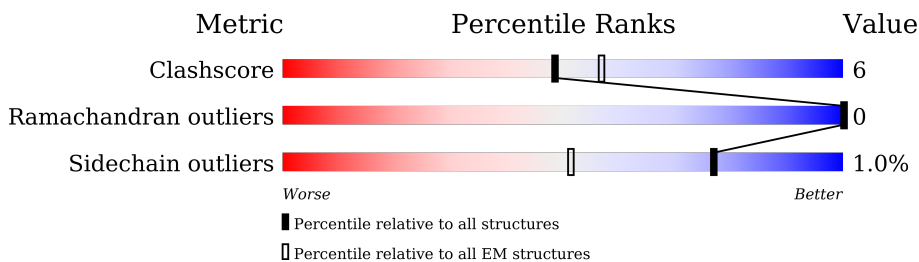
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	259	
2	B	345	
3	G	71	
4	N	128	
5	R	678	
6	X	92	
7	Y	109	
8	C	2	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 25551 atoms, of which 12857 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 chimera of Guanine nucleotide-binding protein G(s) subunit alpha and Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLas.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	227	3769	1193	1879	344	346	7	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	initiating methionine	UNP Q8R4A8
A	196	GLY	-	linker	UNP Q8R4A8
A	197	GLY	-	linker	UNP Q8R4A8
A	198	SER	-	linker	UNP Q8R4A8
A	199	GLY	-	linker	UNP Q8R4A8
A	200	GLY	-	linker	UNP Q8R4A8
A	201	SER	-	linker	UNP Q8R4A8
A	202	GLY	-	linker	UNP Q8R4A8
A	203	GLY	-	linker	UNP Q8R4A8
A	204	THR	-	linker	UNP Q8R4A8
A	205	THR	SER	engineered mutation	UNP Q5JWF2

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	338	5108	1604	2507	467	509	21	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	G	57	885	273	449	77	83	3	0	0

- Molecule 4 is a protein called Nb35.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	N	126	1889	599	928	168	188	6	0	0

- Molecule 5 is a protein called Follicle-stimulating hormone receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	R	595	9502	3057	4786	787	839	33	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	273	ILE	SER	engineered mutation	UNP P23945

- Molecule 6 is a protein called Glycoprotein hormones alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	X	88	1324	417	649	118	127	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	17	LEU	PHE	engineered mutation	UNP P01215

- Molecule 7 is a protein called Follitropin subunit beta.

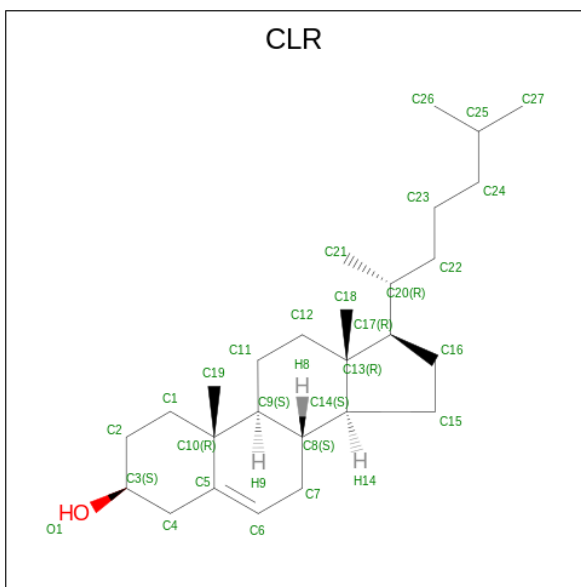
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	Y	109	1646	527	798	142	166	13	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	C	2	55	16	27	2	10		0	0

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



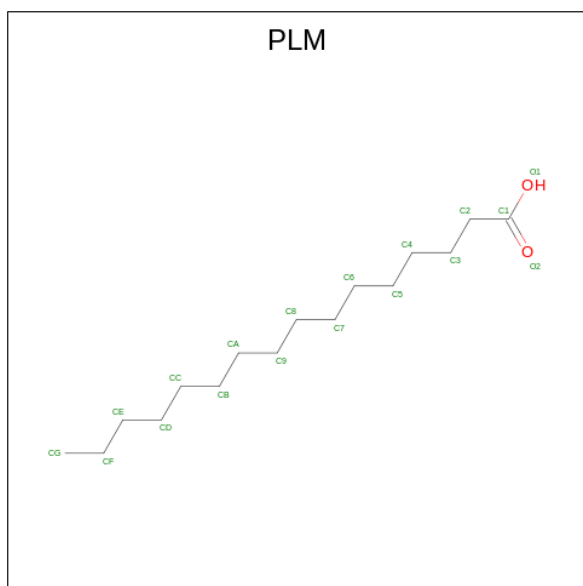
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	R	1	74	27	46	1	0
9	R	1	74	27	46	1	0
9	R	1	74	27	46	1	0
9	R	1	74	27	46	1	0
9	R	1	74	27	46	1	0

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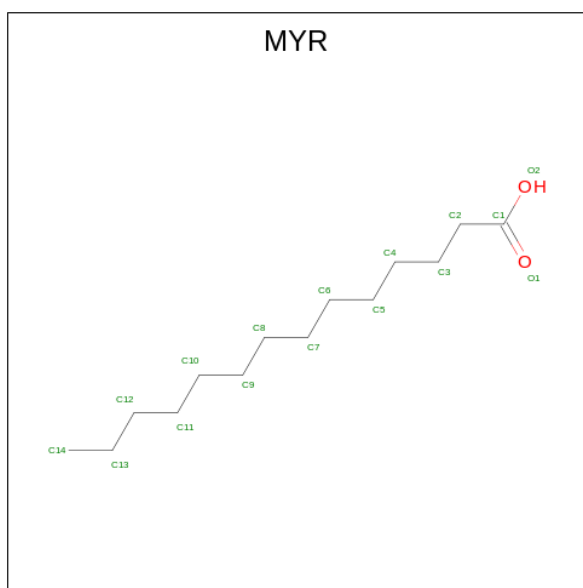
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	R	1	Total 74	C 27	H 46	O 1	0
9	R	1	Total 74	C 27	H 46	O 1	0
9	R	1	Total 74	C 27	H 46	O 1	0
9	R	1	Total 74	C 27	H 46	O 1	0
9	R	1	Total 74	C 27	H 46	O 1	0
9	R	1	Total 74	C 27	H 46	O 1	0
9	R	1	Total 74	C 27	H 46	O 1	0
9	R	1	Total 74	C 27	H 46	O 1	0

- Molecule 10 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



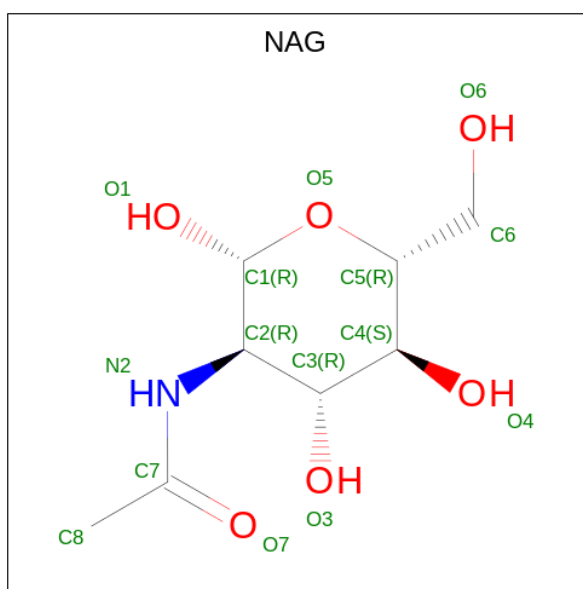
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
10	R	1	Total 49	C 16	H 31	O 2	0
10	R	1	Total 49	C 16	H 31	O 2	0
10	R	1	Total 49	C 16	H 31	O 2	0

- Molecule 11 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



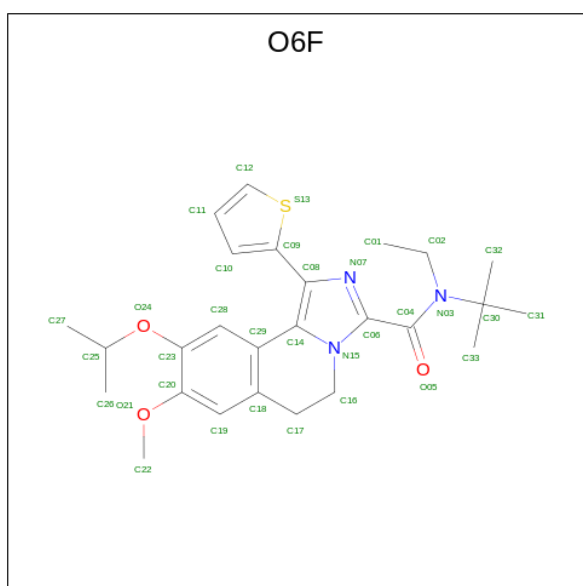
Mol	Chain	Residues	Atoms			AltConf	
11	R	1	Total	C	H	O	0
			43	14	27	2	
11	R	1	Total	C	H	O	0
			43	14	27	2	

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf	
12	R	1	Total	C	H	N	O	0
			28	8	14	1	5	
12	X	1	Total	C	H	N	O	0
			28	8	14	1	5	
12	Y	1	Total	C	H	N	O	0
			28	8	14	1	5	
12	Y	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 13 is N-tert-butyl-N-ethyl-8-methoxy-9-propan-2-yloxy-1-thiophen-2-yl-5,6-dihydroimidazo[5,1-a]isoquinoline-3-carboxamide (three-letter code: O6F) (formula: C₂₆H₃₃N₃O₃S) (labeled as "Ligand of Interest" by depositor).

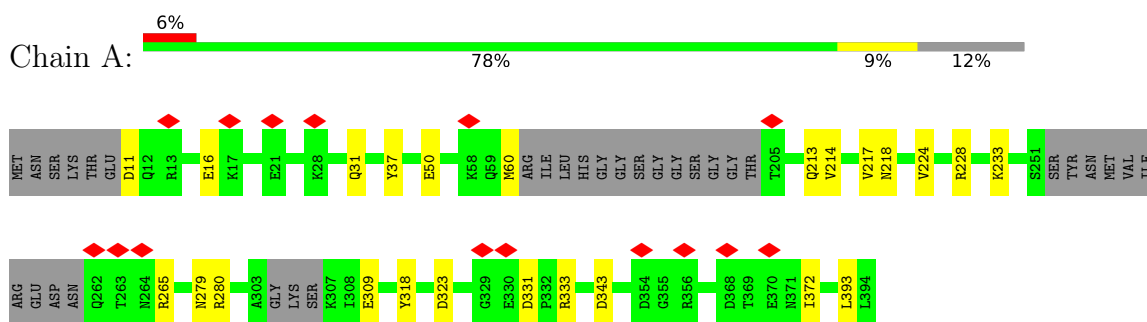


Mol	Chain	Residues	Atoms					AltConf	
13	R	1	Total	C	H	N	O	S	0
			66	26	33	3	3	1	

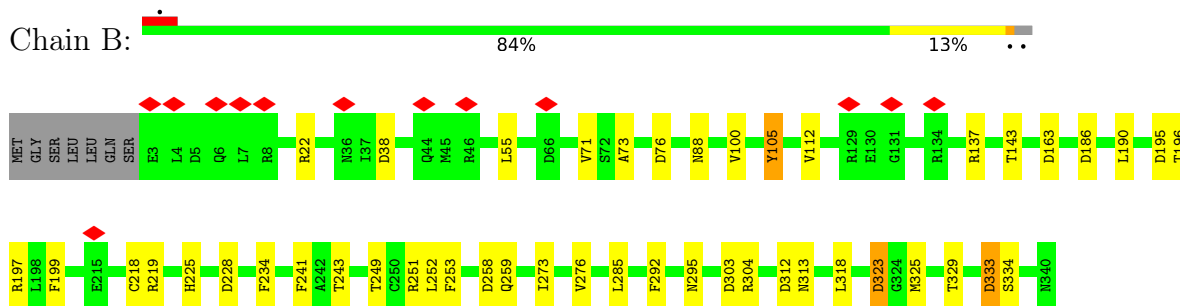
3 Residue-property plots [i](#)

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

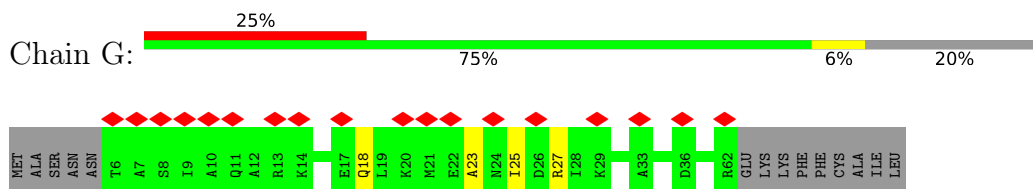
- Molecule 1: chimera of Guanine nucleotide-binding protein G(s) subunit alpha and Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLAs



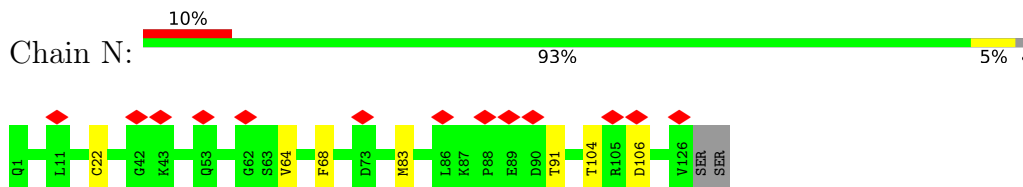
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: Nb35





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	477950	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.814	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	263.68, 263.68, 263.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.03, 1.03, 1.03	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: MYR, O6F, NAG, PLM, CLR

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	0.25	0/1924	0.52	0/2584
2	B	0.25	0/2648	0.55	0/3589
3	G	0.25	0/442	0.45	0/597
4	N	0.26	0/981	0.52	0/1329
5	R	0.25	0/4822	0.47	0/6555
6	X	0.26	0/690	0.53	0/933
7	Y	0.26	0/867	0.55	0/1177
All	All	0.25	0/12374	0.51	0/16764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1890	1879	1875	20	0
2	B	2601	2507	2505	37	0
3	G	436	449	448	3	0
4	N	961	928	928	5	0
5	R	4716	4786	4780	59	0
6	X	675	649	648	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Y	848	798	799	18	0
8	C	28	27	25	0	0
9	R	364	598	598	11	0
10	R	54	93	93	1	0
11	R	32	54	54	1	0
12	R	14	14	13	0	0
12	X	14	14	13	0	0
12	Y	28	28	26	1	0
13	R	33	33	0	0	0
All	All	12694	12857	12805	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (159) 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)
6:X:87:CYS:HB2	6:X:90:HIS:CD2	2.12	0.84
1:A:37:TYR:CD1	2:B:76:ASP:OD1	2.30	0.84
4:N:104:THR:OG1	4:N:106:ASP:OD1	1.97	0.83
6:X:87:CYS:CB	6:X:90:HIS:HD2	1.91	0.83
2:B:55:LEU:HD13	2:B:76:ASP:OD2	1.83	0.79
1:A:228:ARG:NH2	2:B:186:ASP:OD1	2.16	0.78
5:R:510:SER:OG	5:R:521:ASP:OD2	2.02	0.77
6:X:87:CYS:O	6:X:90:HIS:CD2	2.39	0.76
6:X:87:CYS:CB	6:X:90:HIS:CD2	2.69	0.75
1:A:318:TYR:OH	1:A:343:ASP:OD2	2.05	0.74
2:B:143:THR:OG1	2:B:163:ASP:OD1	2.05	0.73
7:Y:57:VAL:O	7:Y:78:VAL:N	2.20	0.73
1:A:213:GLN:NE2	1:A:218:ASN:OD1	2.22	0.72
5:R:168:LEU:HD23	5:R:173:VAL:HG11	1.71	0.71
5:R:362:TYR:CE1	5:R:609:ILE:HD11	2.29	0.68
5:R:149:LEU:HD11	5:R:165:PHE:HE1	1.57	0.68
6:X:87:CYS:HB2	6:X:90:HIS:HD2	1.52	0.68
2:B:22:ARG:NH1	2:B:258:ASP:O	2.29	0.66
7:Y:8:ILE:HD11	7:Y:25:THR:HG23	1.76	0.66
7:Y:8:ILE:CD1	7:Y:25:THR:HG23	2.28	0.64
5:R:599:VAL:HG12	5:R:599:VAL:O	1.98	0.63
7:Y:8:ILE:HD12	7:Y:8:ILE:O	2.00	0.62
7:Y:96:VAL:O	7:Y:97:ARG:HG3	2.00	0.61
6:X:87:CYS:O	6:X:90:HIS:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:102:ILE:HD12	5:R:127:ILE:HG13	1.83	0.61
1:A:331:ASP:OD1	1:A:333:ARG:N	2.34	0.60
5:R:149:LEU:CD1	5:R:165:PHE:CE1	2.84	0.60
7:Y:37:LEU:HD22	7:Y:44:ARG:HD2	1.84	0.60
2:B:333:ASP:O	2:B:334:SER:OG	2.11	0.59
5:R:373:SER:O	5:R:377:ILE:HG22	2.02	0.59
6:X:27:GLN:HG2	6:X:29:MET:SD	2.42	0.59
9:R:717:CLR:H72	9:R:718:CLR:H112	1.86	0.58
5:R:149:LEU:HD11	5:R:165:PHE:CE1	2.39	0.57
2:B:225:HIS:HE2	2:B:243:THR:HG1	1.48	0.57
2:B:225:HIS:CD2	2:B:243:THR:HG1	2.22	0.57
2:B:292:PHE:CD1	2:B:313:ASN:C	2.78	0.57
7:Y:17:CYS:SG	7:Y:66:CYS:N	2.79	0.56
1:A:60:MET:HG3	1:A:372:ILE:CG2	2.36	0.56
5:R:52:ARG:HG2	5:R:76:GLU:OE1	2.06	0.55
2:B:273:ILE:N	2:B:273:ILE:HD12	2.21	0.54
1:A:37:TYR:CE1	2:B:76:ASP:OD1	2.61	0.53
9:R:717:CLR:C7	9:R:718:CLR:H112	2.39	0.53
5:R:148:LEU:HD12	5:R:174:ILE:HG21	1.89	0.53
9:R:718:CLR:H212	9:R:718:CLR:H121	1.89	0.53
5:R:25:CYS:SG	5:R:26:SER:N	2.82	0.52
5:R:377:ILE:HD11	9:R:717:CLR:C26	2.39	0.52
9:R:702:CLR:H212	9:R:702:CLR:H183	1.92	0.52
5:R:149:LEU:HD13	5:R:165:PHE:CE1	2.45	0.52
6:X:87:CYS:HB3	6:X:90:HIS:CD2	2.44	0.51
1:A:214:VAL:HG22	1:A:372:ILE:HD13	1.92	0.51
2:B:323:ASP:OD1	2:B:325:MET:N	2.42	0.51
1:A:224:VAL:HG13	1:A:224:VAL:O	2.08	0.51
2:B:71:VAL:HG23	2:B:105:TYR:CE2	2.46	0.51
2:B:295:ASN:OD1	2:B:304:ARG:NH1	2.43	0.51
5:R:578:ILE:HD12	9:R:715:CLR:H261	1.92	0.51
2:B:22:ARG:HG2	2:B:259:GLN:OE1	2.10	0.51
5:R:127:ILE:O	5:R:127:ILE:HG22	2.10	0.51
6:X:61:VAL:HG22	6:X:62:ALA:H	1.76	0.51
5:R:149:LEU:CD1	5:R:165:PHE:HE1	2.19	0.50
2:B:323:ASP:OD1	2:B:323:ASP:C	2.50	0.50
5:R:481:VAL:HG13	5:R:481:VAL:O	2.11	0.50
2:B:276:VAL:HG13	2:B:285:LEU:HD11	1.92	0.50
7:Y:51:CYS:HA	7:Y:84:CYS:HA	1.94	0.50
5:R:114:GLU:O	5:R:117:GLN:NE2	2.41	0.50
3:G:23:ALA:O	3:G:27:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:ASP:C	2:B:334:SER:HG	2.10	0.49
1:A:31:GLN:HA	1:A:31:GLN:OE1	2.13	0.49
5:R:235:SER:C	5:R:260:LYS:HZ1	2.15	0.49
5:R:420:SER:HB2	9:R:717:CLR:H193	1.94	0.49
2:B:292:PHE:CD1	2:B:292:PHE:N	2.79	0.49
2:B:88:ASN:N	2:B:88:ASN:OD1	2.45	0.49
5:R:628:ILE:HG22	5:R:629:PHE:CD2	2.48	0.49
6:X:87:CYS:HB3	6:X:90:HIS:HD2	1.74	0.49
7:Y:96:VAL:O	7:Y:97:ARG:CG	2.60	0.49
5:R:127:ILE:HD12	5:R:127:ILE:N	2.28	0.48
1:A:233:LYS:NZ	2:B:228:ASP:OD2	2.42	0.48
11:R:709:MYR:H143	11:R:709:MYR:H102	1.96	0.48
2:B:303:ASP:OD1	2:B:304:ARG:N	2.46	0.48
5:R:29:VAL:HG13	5:R:50:GLU:HB3	1.95	0.48
5:R:565:SER:O	5:R:569:ARG:HG3	2.13	0.48
7:Y:62:ARG:NH2	7:Y:71:ASP:OD2	2.40	0.48
6:X:61:VAL:HG22	6:X:62:ALA:N	2.28	0.48
1:A:50:GLU:OE2	1:A:265:ARG:NH1	2.47	0.48
7:Y:25:THR:OG1	7:Y:26:THR:N	2.47	0.48
7:Y:1:ASN:ND2	7:Y:84:CYS:SG	2.87	0.48
1:A:16:GLU:C	1:A:16:GLU:OE2	2.51	0.47
5:R:121:ASN:O	5:R:123:GLN:OE1	2.32	0.47
5:R:425:THR:HG22	5:R:432:TYR:CD1	2.49	0.47
2:B:143:THR:N	2:B:163:ASP:OD2	2.45	0.47
2:B:228:ASP:N	2:B:228:ASP:OD1	2.45	0.47
5:R:126:LEU:O	5:R:126:LEU:HD23	2.15	0.47
5:R:101:ARG:NH1	5:R:126:LEU:HD13	2.30	0.47
2:B:195:ASP:O	2:B:197:ARG:HG3	2.15	0.47
5:R:98:HIS:HB2	5:R:123:GLN:OE1	2.15	0.46
1:A:279:ASN:OD1	1:A:280:ARG:N	2.48	0.46
2:B:218:CYS:O	3:G:18:GLN:NE2	2.43	0.46
4:N:64:VAL:HG13	4:N:68:PHE:CG	2.51	0.46
5:R:561:ILE:CD1	5:R:562:VAL:HG23	2.45	0.46
3:G:25:ILE:O	3:G:27:ARG:NH2	2.48	0.46
9:R:711:CLR:H213	9:R:711:CLR:C18	2.46	0.46
2:B:249:THR:OG1	2:B:251:ARG:NH1	2.48	0.46
5:R:376:ALA:O	5:R:380:ASN:ND2	2.44	0.46
5:R:122:LEU:HD23	5:R:141:ILE:HG21	1.98	0.46
5:R:393:LYS:NZ	5:R:394:LEU:O	2.49	0.46
5:R:528:GLN:NE2	5:R:596:SER:O	2.48	0.46
1:A:331:ASP:OD1	1:A:331:ASP:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:OD1	1:A:323:ASP:C	2.54	0.45
5:R:383:VAL:HG11	5:R:401:MET:HE1	1.98	0.45
9:R:711:CLR:H213	9:R:711:CLR:H183	1.98	0.45
5:R:291:ILE:HD13	6:X:71:MET:HG3	1.99	0.45
2:B:195:ASP:O	2:B:196:THR:HG22	2.17	0.45
1:A:11:ASP:N	1:A:11:ASP:OD1	2.50	0.45
5:R:331:THR:O	5:R:331:THR:HG22	2.17	0.45
5:R:149:LEU:CD2	5:R:177:LEU:HD11	2.47	0.44
6:X:28:CYS:SG	6:X:60:CYS:SG	3.15	0.44
6:X:90:HIS:CE1	7:Y:94:CYS:HB3	2.53	0.44
2:B:73:ALA:HB1	2:B:100:VAL:HG11	2.00	0.44
2:B:252:LEU:HD23	2:B:253:PHE:N	2.33	0.44
5:R:149:LEU:HD21	5:R:177:LEU:HD11	1.98	0.44
1:A:393:LEU:HD22	5:R:574:MET:HG2	2.00	0.43
5:R:514:VAL:HG13	5:R:517:CYS:H	1.83	0.43
2:B:219:ARG:HG2	2:B:219:ARG:HH11	1.83	0.43
6:X:60:CYS:HA	6:X:84:CYS:HA	2.00	0.43
6:X:71:MET:SD	6:X:71:MET:N	2.91	0.43
5:R:377:ILE:O	5:R:381:ILE:HG22	2.19	0.43
2:B:312:ASP:OD2	5:R:635:ARG:NH1	2.51	0.43
5:R:282:ARG:O	5:R:282:ARG:HG2	2.19	0.43
6:X:62:ALA:HB2	6:X:79:HIS:CD2	2.54	0.42
2:B:105:TYR:CD1	2:B:112:VAL:HG22	2.54	0.42
9:R:717:CLR:H6	9:R:718:CLR:H11	2.01	0.42
1:A:214:VAL:O	1:A:217:VAL:HG12	2.20	0.42
2:B:234:PHE:CD1	2:B:241:PHE:HB3	2.55	0.42
5:R:174:ILE:HD12	5:R:196:ASP:HB2	2.01	0.42
6:X:53:VAL:O	7:Y:93:ASP:N	2.48	0.42
2:B:71:VAL:HG23	2:B:105:TYR:CD2	2.55	0.42
2:B:137:ARG:HB2	2:B:137:ARG:NH1	2.34	0.42
7:Y:37:LEU:HD12	7:Y:37:LEU:N	2.34	0.42
5:R:424:HIS:ND1	10:R:708:PLM:O1	2.53	0.42
5:R:522:ILE:O	5:R:522:ILE:HG22	2.18	0.42
4:N:68:PHE:CD1	4:N:68:PHE:N	2.88	0.42
5:R:377:ILE:HG23	5:R:378:THR:N	2.35	0.42
5:R:151:ILE:HG22	5:R:180:ASN:HD21	1.85	0.41
5:R:285:ILE:HD12	5:R:285:ILE:N	2.35	0.41
4:N:91:THR:HG23	4:N:91:THR:O	2.21	0.41
5:R:569:ARG:O	5:R:573:ARG:HG2	2.20	0.41
5:R:576:MET:CE	9:R:716:CLR:H262	2.50	0.41
5:R:330:TYR:CG	5:R:331:THR:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:522:ILE:O	5:R:522:ILE:CG2	2.68	0.41
5:R:155:ILE:HD12	5:R:155:ILE:O	2.20	0.41
7:Y:24:ASN:ND2	12:Y:202:NAG:O7	2.54	0.41
7:Y:39:TYR:O	7:Y:44:ARG:NH1	2.54	0.41
5:R:126:LEU:HD23	5:R:126:LEU:C	2.41	0.41
4:N:68:PHE:CE2	4:N:83:MET:HE2	2.56	0.40
5:R:382:ILE:HA	5:R:385:VAL:HG12	2.02	0.40
6:X:90:HIS:HE1	7:Y:94:CYS:HB2	1.87	0.40
5:R:516:ILE:HD12	5:R:611:LEU:HD22	2.03	0.40
2:B:190:LEU:HD11	2:B:199:PHE:CE1	2.57	0.40
1:A:331:ASP:OD2	1:A:333:ARG:NH2	2.55	0.40
6:X:88:TYR:HB2	6:X:89:TYR:CD1	2.56	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	219/259 (85%)	217 (99%)	2 (1%)	0	100	100
2	B	336/345 (97%)	332 (99%)	4 (1%)	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	N	124/128 (97%)	123 (99%)	1 (1%)	0	100	100
5	R	591/678 (87%)	568 (96%)	23 (4%)	0	100	100
6	X	86/92 (94%)	80 (93%)	6 (7%)	0	100	100
7	Y	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
All	All	1518/1682 (90%)	1475 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/229 (89%)	203 (100%)	1 (0%)	88	96
2	B	281/287 (98%)	275 (98%)	6 (2%)	53	84
3	G	46/58 (79%)	46 (100%)	0	100	100
4	N	104/106 (98%)	103 (99%)	1 (1%)	76	93
5	R	533/610 (87%)	529 (99%)	4 (1%)	81	94
6	X	80/83 (96%)	80 (100%)	0	100	100
7	Y	97/97 (100%)	95 (98%)	2 (2%)	53	84
All	All	1345/1470 (92%)	1331 (99%)	14 (1%)	77	93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	GLU
2	B	38	ASP
2	B	105	TYR
2	B	318	LEU
2	B	323	ASP
2	B	329	THR
2	B	333	ASP
4	N	22	CYS
5	R	99	GLU
5	R	125	LEU
5	R	208	GLU
5	R	275	CYS
7	Y	46	LYS
7	Y	104	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	R	178	ASN

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Mol	Chain	Res	Type
6	X	83	HIS
6	X	90	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 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
8	NAG	C	1	8,6	14,14,15	0.24	0	17,19,21	0.42	0
8	NAG	C	2	8	14,14,15	0.21	0	17,19,21	0.41	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
8	NAG	C	1	8,6	-	1/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

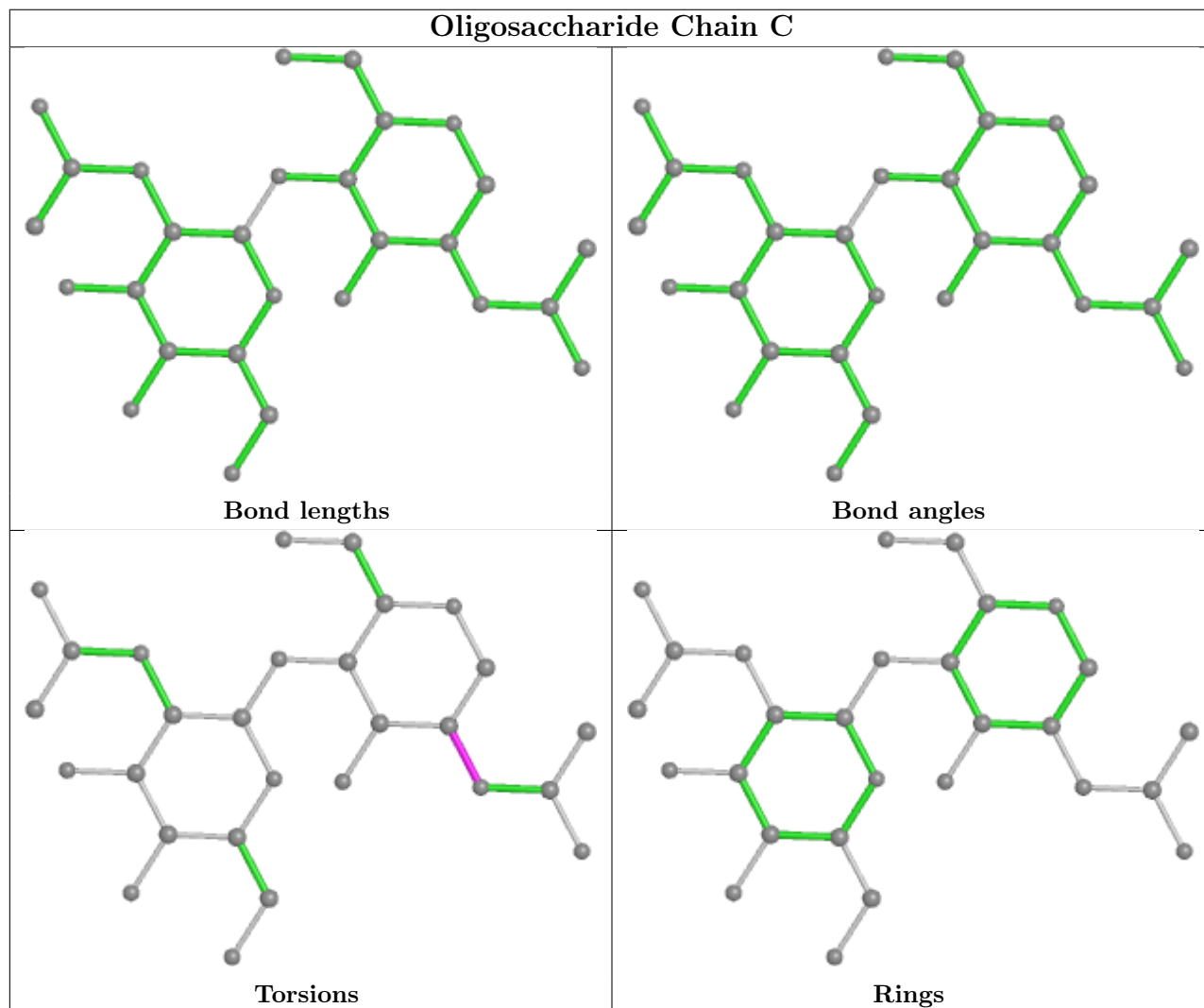
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLR	R	719	-	31,31,31	0.36	0	48,48,48	0.60	0
9	CLR	R	714	-	31,31,31	0.39	0	48,48,48	1.01	4 (8%)
10	PLM	R	707	-	17,17,17	0.92	1 (5%)	17,17,17	0.74	2 (11%)
9	CLR	R	716	-	31,31,31	0.36	0	48,48,48	0.64	0
11	MYR	R	709	-	15,15,15	0.54	0	15,15,15	1.00	0
9	CLR	R	702	-	31,31,31	0.38	0	48,48,48	0.76	0
9	CLR	R	717	-	31,31,31	0.37	0	48,48,48	0.80	1 (2%)
12	NAG	Y	202	-	14,14,15	0.20	0	17,19,21	0.41	0
9	CLR	R	711	-	31,31,31	0.37	0	48,48,48	0.59	1 (2%)
10	PLM	R	706	-	17,17,17	0.92	1 (5%)	17,17,17	0.75	2 (11%)
9	CLR	R	718	-	31,31,31	0.78	0	48,48,48	1.49	8 (16%)
9	CLR	R	704	-	31,31,31	0.35	0	48,48,48	0.48	0
12	NAG	X	101	-	14,14,15	0.21	0	17,19,21	0.41	0
9	CLR	R	701	-	31,31,31	0.37	0	48,48,48	0.53	0
11	MYR	R	710	-	15,15,15	0.52	0	15,15,15	1.02	1 (6%)
9	CLR	R	703	-	31,31,31	0.37	0	48,48,48	0.67	0
9	CLR	R	713	-	31,31,31	0.39	0	48,48,48	0.65	0
10	PLM	R	708	-	17,17,17	0.92	1 (5%)	17,17,17	0.74	2 (11%)
12	NAG	Y	201	7	14,14,15	0.30	0	17,19,21	0.53	0
9	CLR	R	705	-	31,31,31	0.35	0	48,48,48	0.56	0
13	O6F	R	720	-	34,36,36	6.45	21 (61%)	35,54,54	4.97	18 (51%)
9	CLR	R	715	-	31,31,31	0.34	0	48,48,48	1.34	7 (14%)
12	NAG	R	712	5	14,14,15	0.21	0	17,19,21	0.41	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	CLR	R	719	-	-	3/10/68/68	0/4/4/4
9	CLR	R	714	-	-	4/10/68/68	0/4/4/4
10	PLM	R	707	-	-	6/15/15/15	-
9	CLR	R	716	-	-	1/10/68/68	0/4/4/4
11	MYR	R	709	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLR	R	702	-	-	6/10/68/68	0/4/4/4
9	CLR	R	717	-	-	2/10/68/68	0/4/4/4
12	NAG	Y	202	-	-	2/6/23/26	0/1/1/1
9	CLR	R	711	-	-	5/10/68/68	0/4/4/4
10	PLM	R	706	-	-	6/15/15/15	-
9	CLR	R	718	-	-	3/10/68/68	0/4/4/4
9	CLR	R	704	-	-	3/10/68/68	0/4/4/4
12	NAG	X	101	-	-	0/6/23/26	0/1/1/1
9	CLR	R	701	-	-	3/10/68/68	0/4/4/4
11	MYR	R	710	-	-	4/13/13/13	-
9	CLR	R	703	-	-	4/10/68/68	0/4/4/4
9	CLR	R	713	-	-	4/10/68/68	0/4/4/4
10	PLM	R	708	-	-	7/15/15/15	-
12	NAG	Y	201	7	-	0/6/23/26	0/1/1/1
9	CLR	R	705	-	-	3/10/68/68	0/4/4/4
13	O6F	R	720	-	-	5/18/35/35	0/4/4/4
9	CLR	R	715	-	-	6/10/68/68	0/4/4/4
12	NAG	R	712	5	-	0/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	720	O6F	C29-C18	18.22	1.66	1.40
13	R	720	O6F	C23-C20	-14.22	1.10	1.40
13	R	720	O6F	C16-C17	-11.93	1.35	1.51
13	R	720	O6F	C17-C18	-10.24	1.33	1.51
13	R	720	O6F	C04-N03	9.93	1.50	1.35
13	R	720	O6F	C29-C14	8.98	1.60	1.46
13	R	720	O6F	C28-C23	-8.94	1.22	1.38
13	R	720	O6F	C19-C18	7.60	1.52	1.39
13	R	720	O6F	C19-C20	-6.83	1.26	1.38
13	R	720	O6F	C11-C10	6.42	1.60	1.39
13	R	720	O6F	C09-S13	-5.95	1.66	1.72
13	R	720	O6F	C06-N07	5.84	1.43	1.34
13	R	720	O6F	C06-C04	5.32	1.57	1.53
13	R	720	O6F	C28-C29	5.13	1.48	1.39
13	R	720	O6F	C16-N15	-5.02	1.43	1.49
13	R	720	O6F	C08-N07	4.56	1.48	1.37
13	R	720	O6F	C11-C12	3.92	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	720	O6F	O24-C23	3.56	1.43	1.37
10	R	707	PLM	C2-C1	2.94	1.57	1.50
13	R	720	O6F	O21-C20	2.93	1.41	1.37
10	R	706	PLM	C2-C1	2.93	1.57	1.50
10	R	708	PLM	C2-C1	2.91	1.57	1.50
13	R	720	O6F	C14-C08	-2.69	1.37	1.43
13	R	720	O6F	C08-C09	2.10	1.53	1.49

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	720	O6F	C16-C17-C18	13.87	125.64	109.79
13	R	720	O6F	C17-C18-C19	12.24	144.45	119.91
13	R	720	O6F	C17-C16-N15	11.63	124.70	109.55
13	R	720	O6F	C19-C18-C29	-11.57	104.72	119.39
13	R	720	O6F	C28-C29-C18	-6.98	109.90	119.14
13	R	720	O6F	C17-C18-C29	-6.41	110.82	118.64
13	R	720	O6F	C16-N15-C06	5.19	138.14	125.05
13	R	720	O6F	C19-C20-C23	4.68	126.06	119.84
13	R	720	O6F	C11-C12-S13	-4.51	109.32	112.98
13	R	720	O6F	C28-C23-C20	4.24	125.47	119.84
9	R	718	CLR	C14-C8-C9	-3.67	104.18	109.09
13	R	720	O6F	C20-C19-C18	3.62	126.89	121.09
13	R	720	O6F	O21-C20-C19	-3.62	117.89	124.12
9	R	715	CLR	C16-C17-C20	3.46	117.50	112.15
9	R	718	CLR	C2-C3-C4	-3.38	105.67	110.31
9	R	718	CLR	C7-C8-C9	3.17	113.56	109.71
9	R	718	CLR	C11-C9-C8	-3.00	107.44	111.75
9	R	718	CLR	C3-C4-C5	-2.93	107.05	112.03
13	R	720	O6F	C29-C28-C23	2.88	126.93	120.68
13	R	720	O6F	C01-C02-N03	-2.82	109.00	113.39
9	R	715	CLR	C4-C5-C10	2.72	120.04	116.42
13	R	720	O6F	C32-C30-N03	2.69	113.08	109.63
9	R	715	CLR	C16-C17-C13	-2.56	100.75	103.84
13	R	720	O6F	C30-N03-C04	-2.55	117.87	119.72
9	R	718	CLR	C16-C15-C14	-2.46	100.26	105.13
9	R	717	CLR	C15-C14-C13	2.45	106.79	103.84
9	R	715	CLR	C9-C10-C5	-2.44	105.82	109.65
9	R	714	CLR	C10-C9-C8	-2.38	109.17	112.73
9	R	714	CLR	C14-C8-C9	2.23	112.07	109.09
10	R	708	PLM	O1-C1-O2	2.21	128.82	123.30
10	R	707	PLM	O1-C1-O2	2.20	128.78	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	R	706	PLM	O1-C1-O2	2.20	128.78	123.30
13	R	720	O6F	C06-C04-N03	2.17	121.51	118.24
9	R	715	CLR	C17-C13-C14	-2.17	97.50	100.07
9	R	711	CLR	C21-C20-C17	2.15	116.22	112.92
9	R	715	CLR	C1-C10-C5	2.11	112.62	108.75
9	R	714	CLR	C12-C13-C14	-2.11	104.00	107.27
9	R	714	CLR	C17-C13-C14	2.10	102.56	100.07
9	R	715	CLR	C11-C9-C10	2.07	115.80	113.08
13	R	720	O6F	O24-C23-C28	-2.05	119.15	123.79
9	R	718	CLR	C4-C5-C6	-2.04	117.66	120.61
9	R	718	CLR	C11-C12-C13	-2.02	109.32	112.78
10	R	707	PLM	O2-C1-C2	-2.01	116.61	123.08
11	R	710	MYR	O2-C1-C2	2.01	120.48	114.03
10	R	706	PLM	O2-C1-C2	-2.01	116.64	123.08
10	R	708	PLM	O2-C1-C2	-2.00	116.65	123.08

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	R	714	CLR	C21-C20-C22-C23
9	R	719	CLR	C21-C20-C22-C23
9	R	715	CLR	C13-C17-C20-C22
9	R	703	CLR	C17-C20-C22-C23
9	R	705	CLR	C17-C20-C22-C23
9	R	719	CLR	C17-C20-C22-C23
13	R	720	O6F	C26-C25-O24-C23
9	R	703	CLR	C21-C20-C22-C23
13	R	720	O6F	C23-C20-O21-C22
9	R	711	CLR	C13-C17-C20-C22
9	R	717	CLR	C17-C20-C22-C23
9	R	717	CLR	C21-C20-C22-C23
9	R	718	CLR	C22-C23-C24-C25
13	R	720	O6F	C27-C25-O24-C23
9	R	711	CLR	C16-C17-C20-C22
10	R	708	PLM	C1-C2-C3-C4
9	R	705	CLR	C21-C20-C22-C23
9	R	703	CLR	C20-C22-C23-C24
13	R	720	O6F	C19-C20-O21-C22
9	R	715	CLR	C13-C17-C20-C21
9	R	713	CLR	C20-C22-C23-C24
10	R	706	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
9	R	714	CLR	C22-C23-C24-C25
10	R	707	PLM	C6-C7-C8-C9
11	R	710	MYR	C3-C4-C5-C6
9	R	711	CLR	C16-C17-C20-C21
9	R	702	CLR	C23-C24-C25-C27
9	R	716	CLR	C20-C22-C23-C24
9	R	702	CLR	C23-C24-C25-C26
10	R	707	PLM	C8-C9-CA-CB
9	R	715	CLR	C16-C17-C20-C21
9	R	701	CLR	C23-C24-C25-C26
9	R	713	CLR	C23-C24-C25-C26
9	R	702	CLR	C20-C22-C23-C24
11	R	709	MYR	C1-C2-C3-C4
10	R	708	PLM	CC-CD-CE-CF
9	R	704	CLR	C23-C24-C25-C27
9	R	718	CLR	C23-C24-C25-C27
9	R	715	CLR	C16-C17-C20-C22
9	R	715	CLR	C20-C22-C23-C24
9	R	701	CLR	C20-C22-C23-C24
11	R	709	MYR	C11-C10-C9-C8
9	R	719	CLR	C20-C22-C23-C24
9	R	701	CLR	C23-C24-C25-C27
9	R	711	CLR	C20-C22-C23-C24
9	R	703	CLR	C22-C23-C24-C25
9	R	704	CLR	C23-C24-C25-C26
9	R	718	CLR	C23-C24-C25-C26
10	R	707	PLM	C1-C2-C3-C4
10	R	706	PLM	C7-C8-C9-CA
9	R	714	CLR	C23-C24-C25-C26
11	R	709	MYR	C11-C12-C13-C14
12	Y	202	NAG	C4-C5-C6-O6
11	R	709	MYR	C3-C4-C5-C6
9	R	704	CLR	C20-C22-C23-C24
9	R	713	CLR	C23-C24-C25-C27
11	R	710	MYR	C6-C7-C8-C9
9	R	714	CLR	C23-C24-C25-C27
9	R	702	CLR	C17-C20-C22-C23
10	R	708	PLM	C4-C5-C6-C7
10	R	706	PLM	C6-C7-C8-C9
10	R	706	PLM	C1-C2-C3-C4
9	R	711	CLR	C23-C24-C25-C27
10	R	706	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	R	709	MYR	O1-C1-C2-C3
9	R	702	CLR	C21-C20-C22-C23
10	R	707	PLM	O2-C1-C2-C3
11	R	710	MYR	O1-C1-C2-C3
10	R	708	PLM	C7-C8-C9-CA
10	R	707	PLM	O1-C1-C2-C3
9	R	715	CLR	C22-C23-C24-C25
13	R	720	O6F	C20-C23-O24-C25
10	R	706	PLM	O1-C1-C2-C3
11	R	709	MYR	O2-C1-C2-C3
11	R	710	MYR	O2-C1-C2-C3
9	R	702	CLR	C22-C23-C24-C25
12	Y	202	NAG	O5-C5-C6-O6
10	R	708	PLM	C6-C7-C8-C9
10	R	708	PLM	O1-C1-C2-C3
10	R	708	PLM	O2-C1-C2-C3
9	R	713	CLR	C17-C20-C22-C23
9	R	705	CLR	C23-C24-C25-C26
10	R	707	PLM	C3-C4-C5-C6

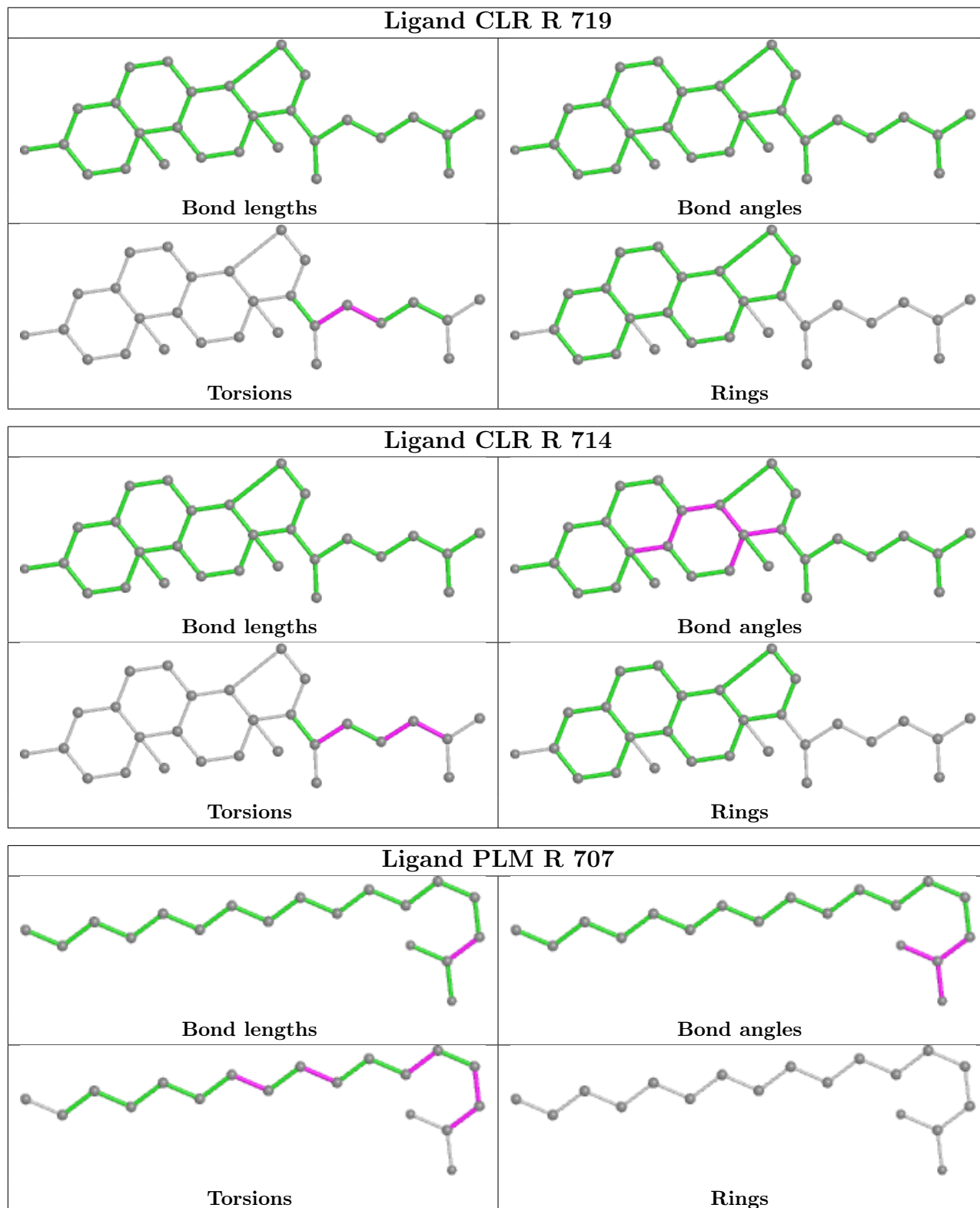
There are no ring outliers.

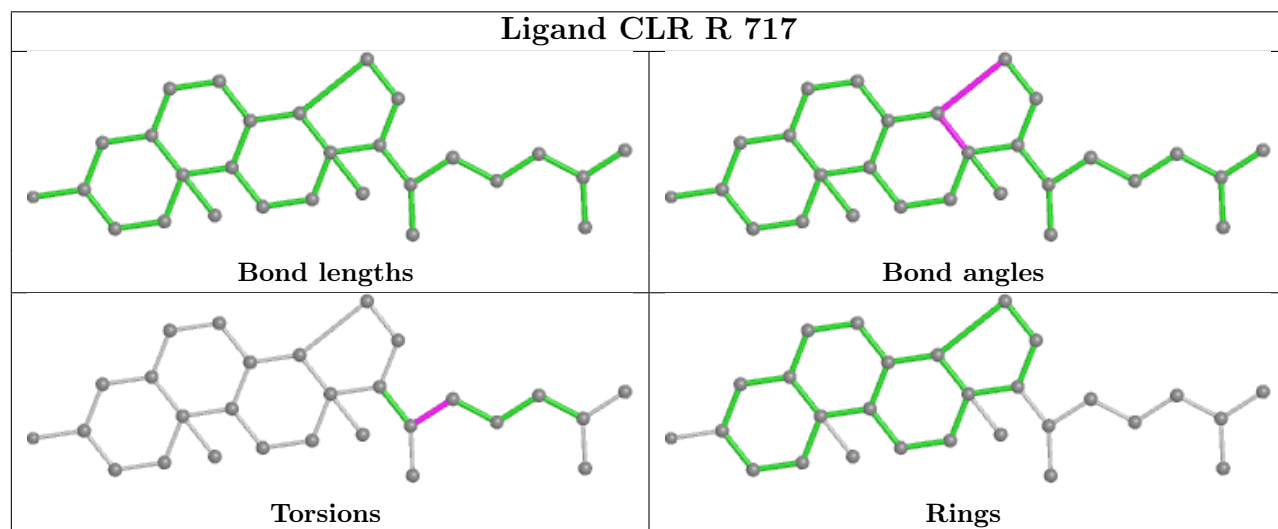
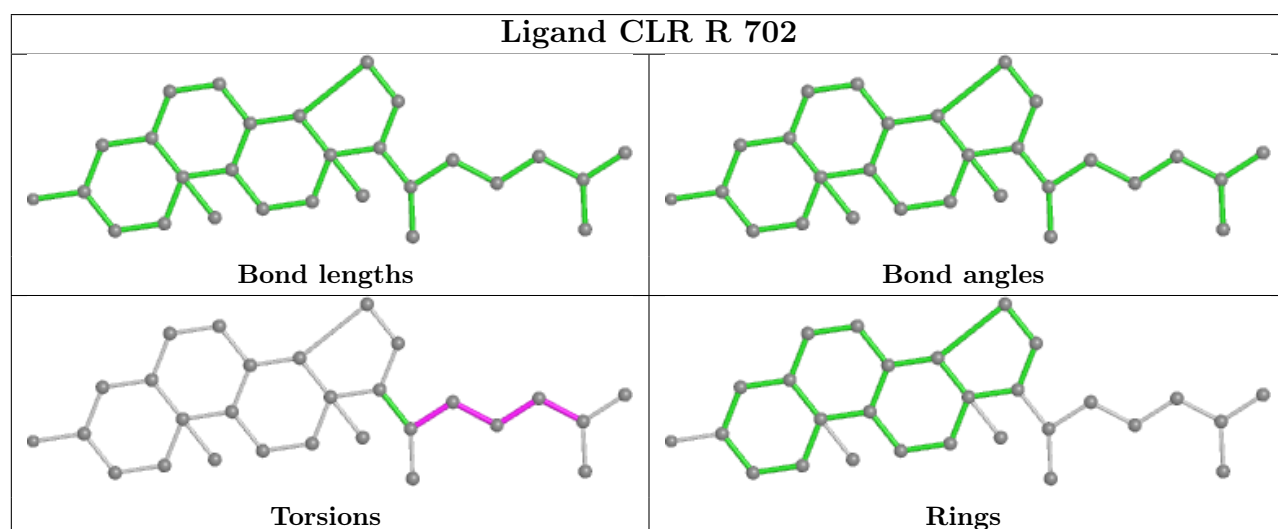
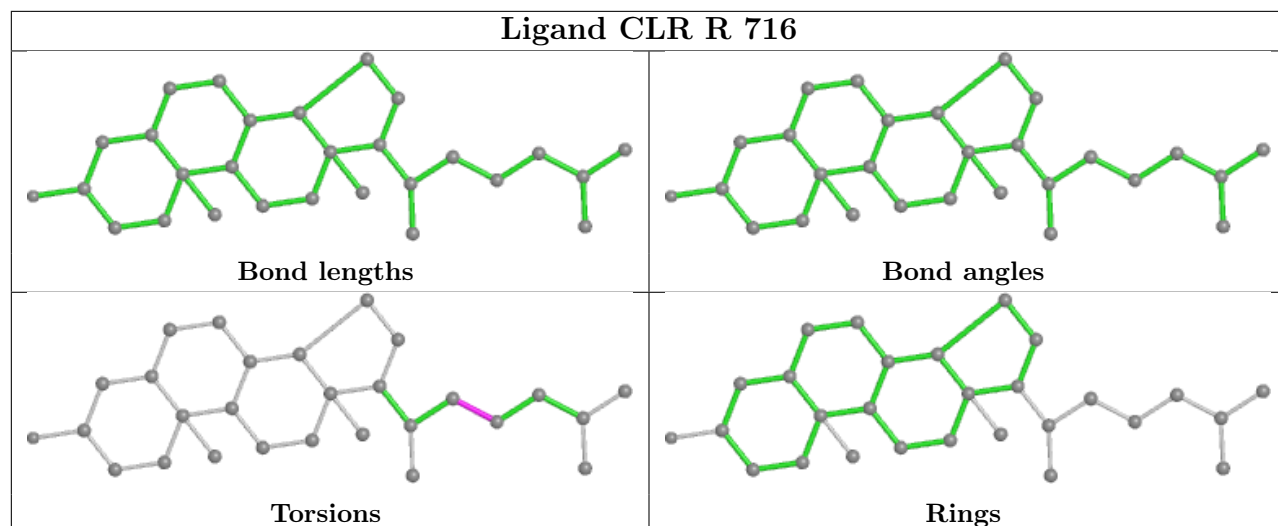
9 monomers are involved in 14 short contacts:

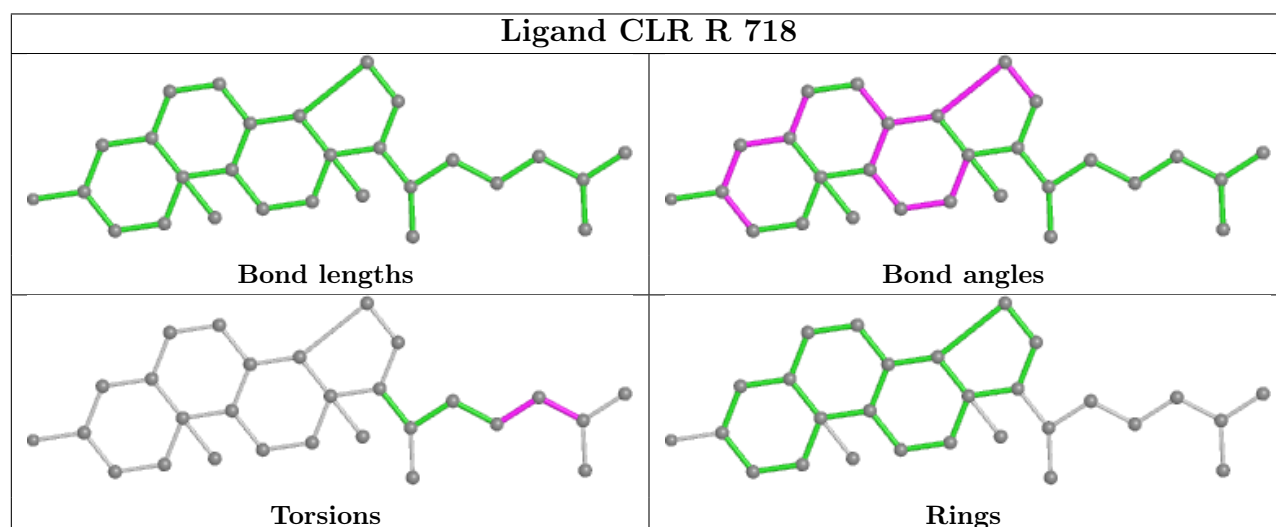
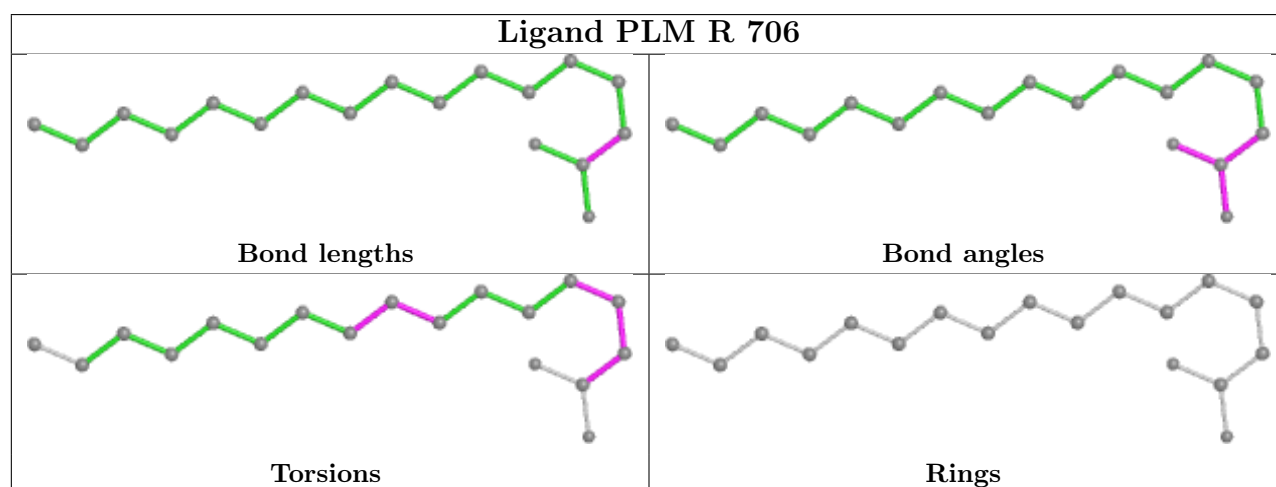
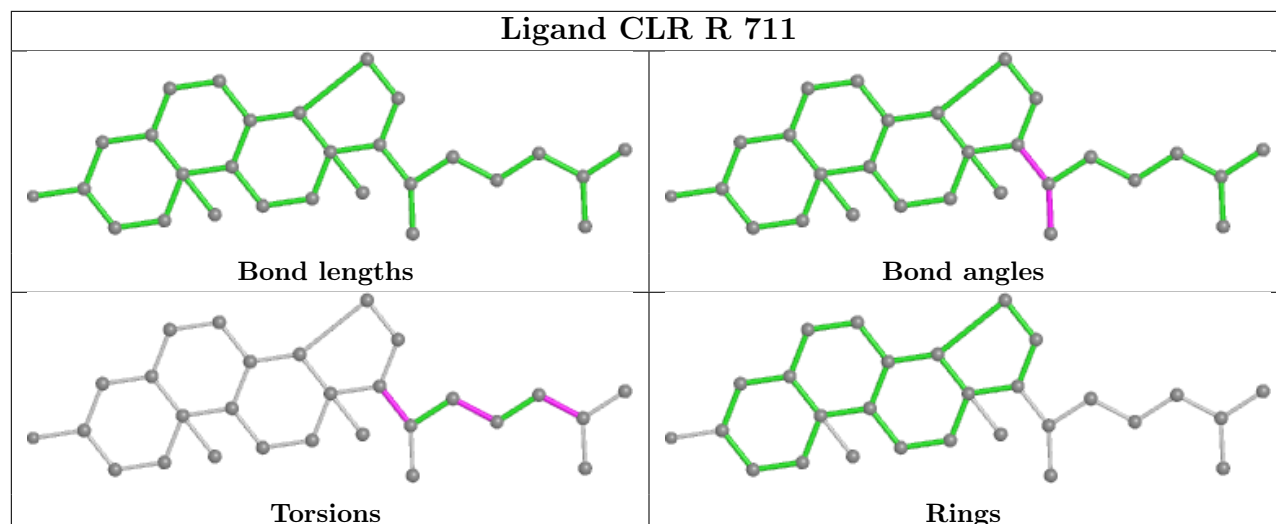
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	716	CLR	1	0
11	R	709	MYR	1	0
9	R	702	CLR	1	0
9	R	717	CLR	5	0
12	Y	202	NAG	1	0
9	R	711	CLR	2	0
9	R	718	CLR	4	0
10	R	708	PLM	1	0
9	R	715	CLR	1	0

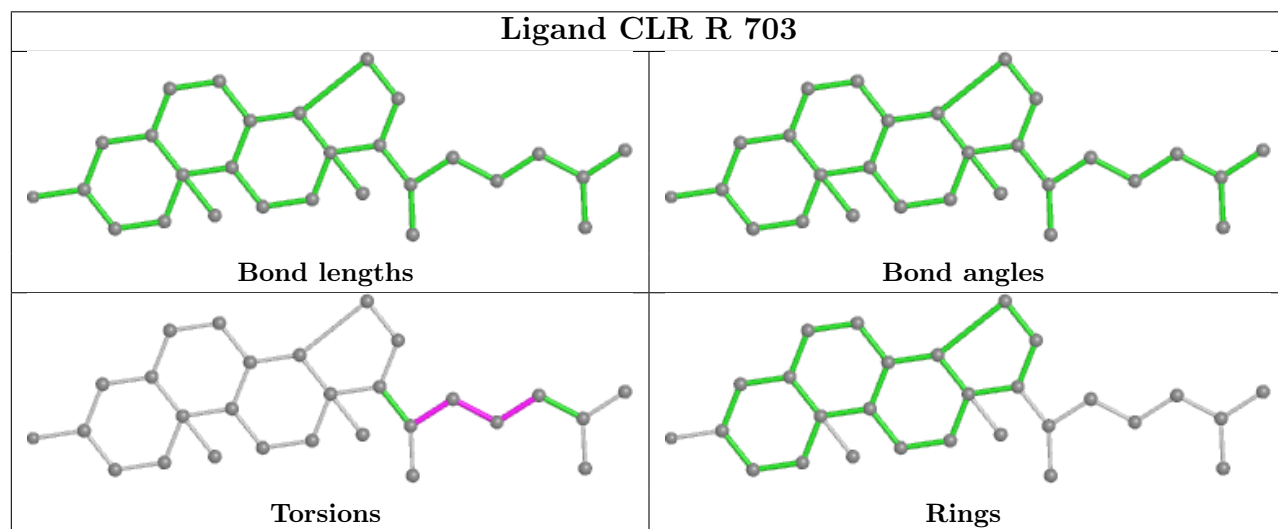
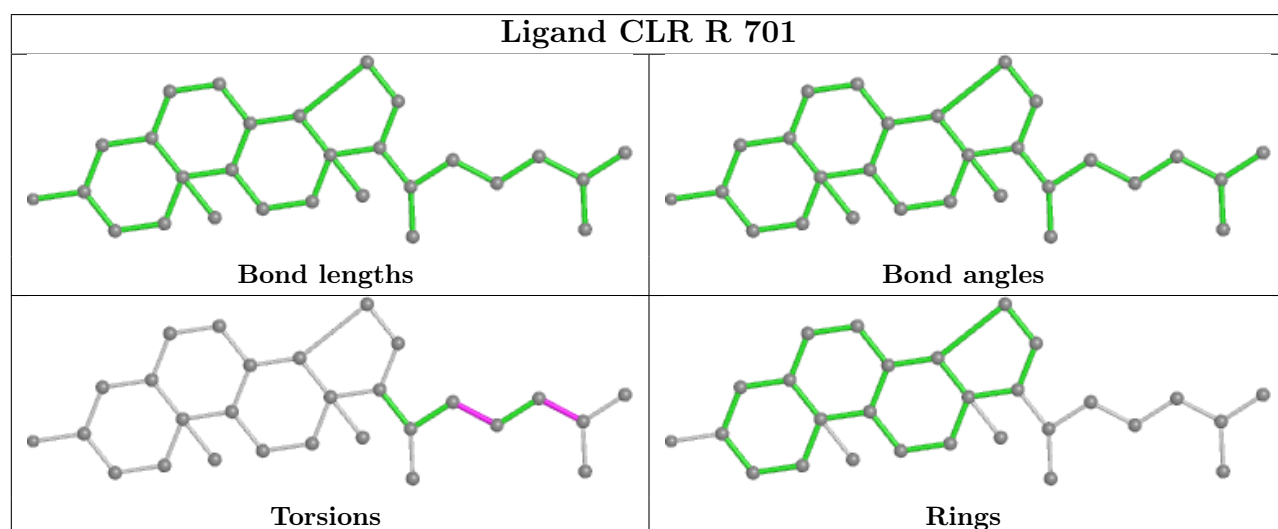
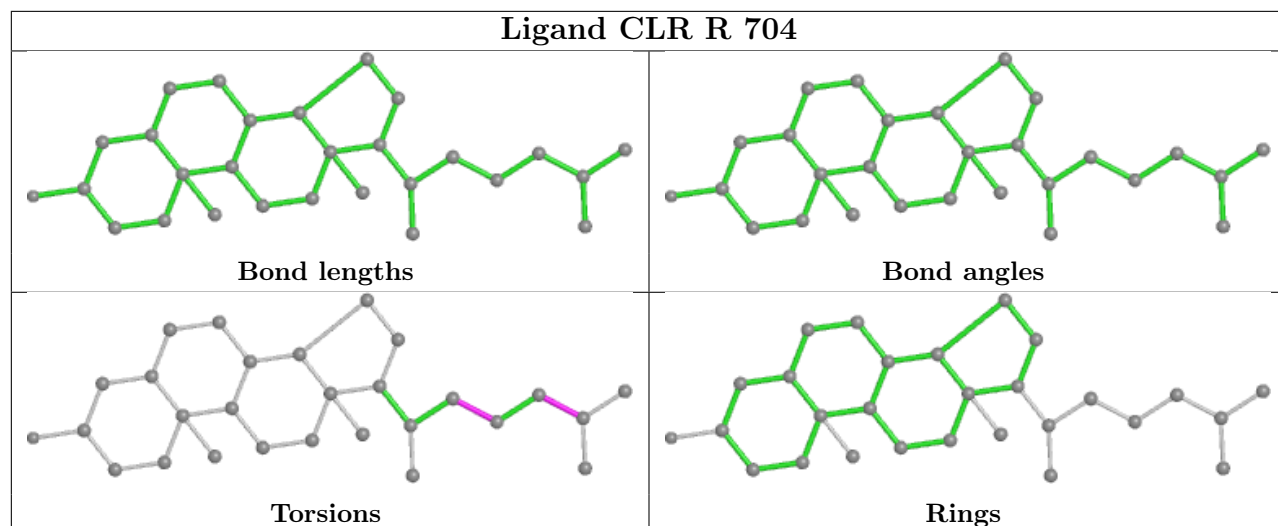
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

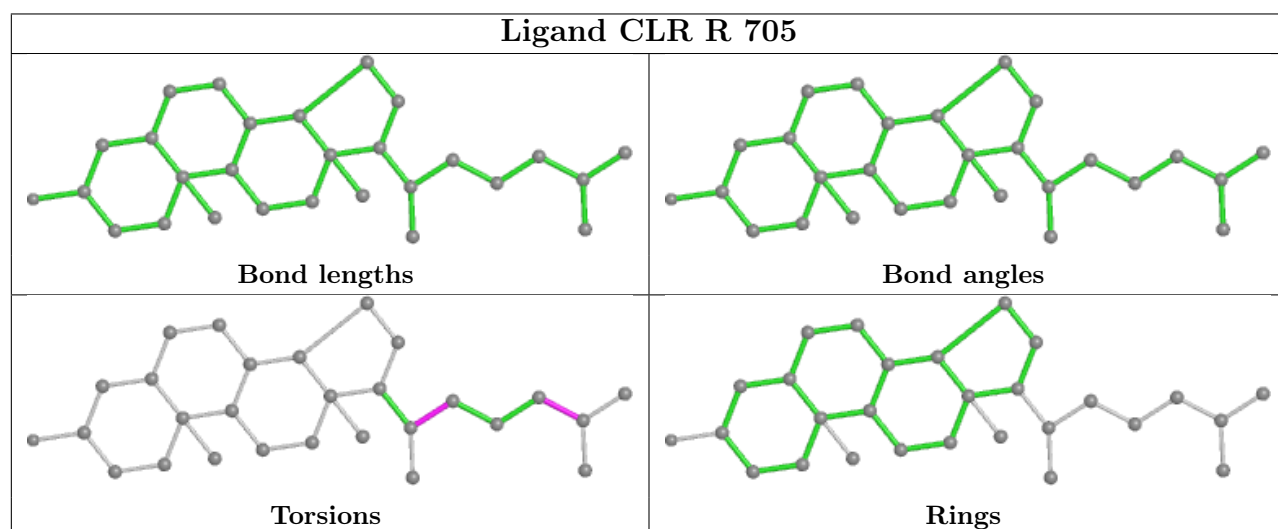
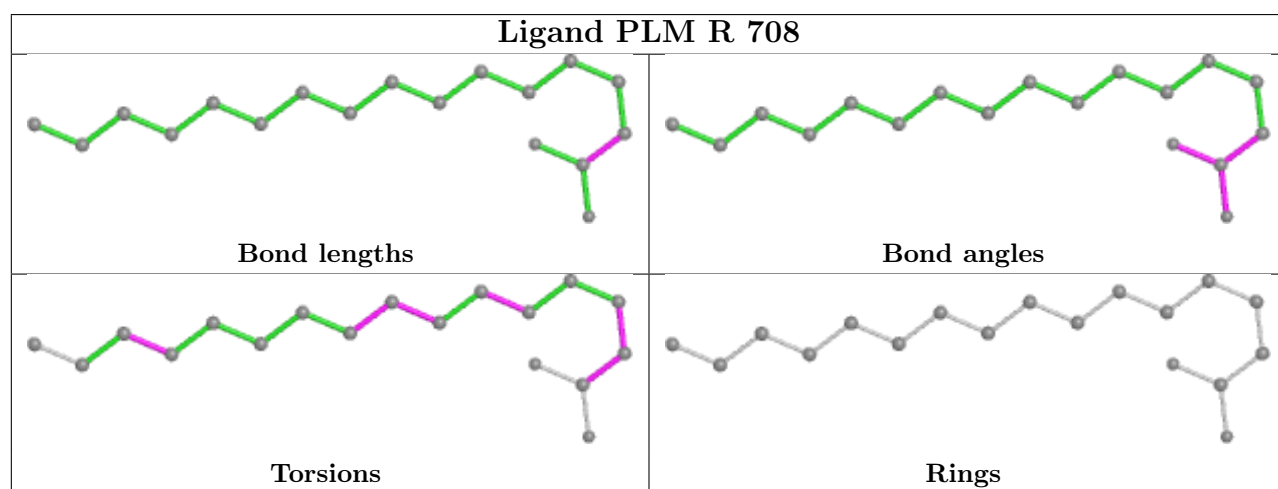
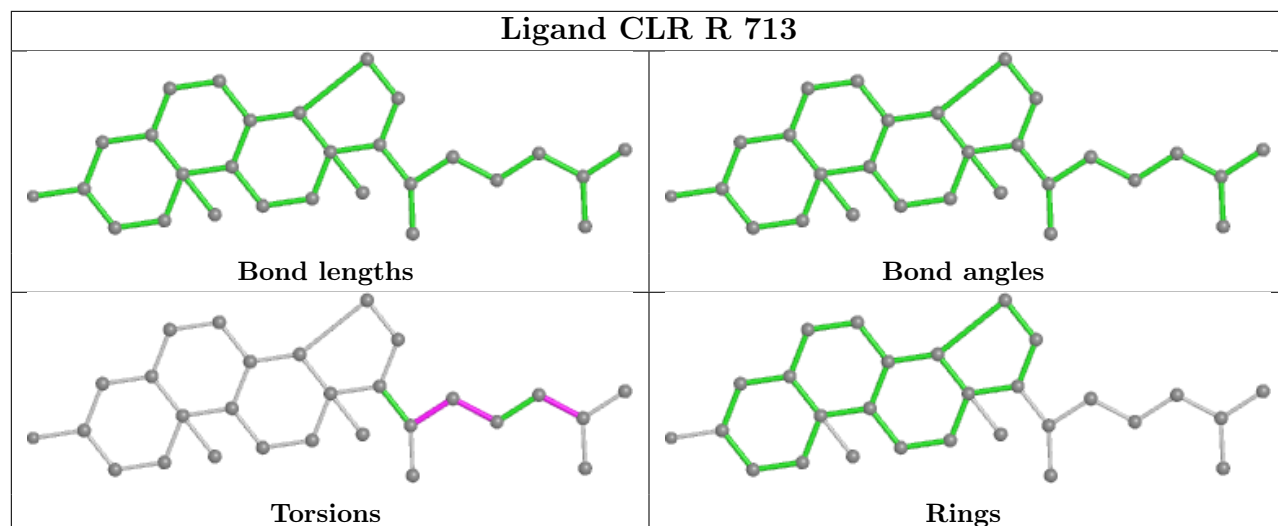
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

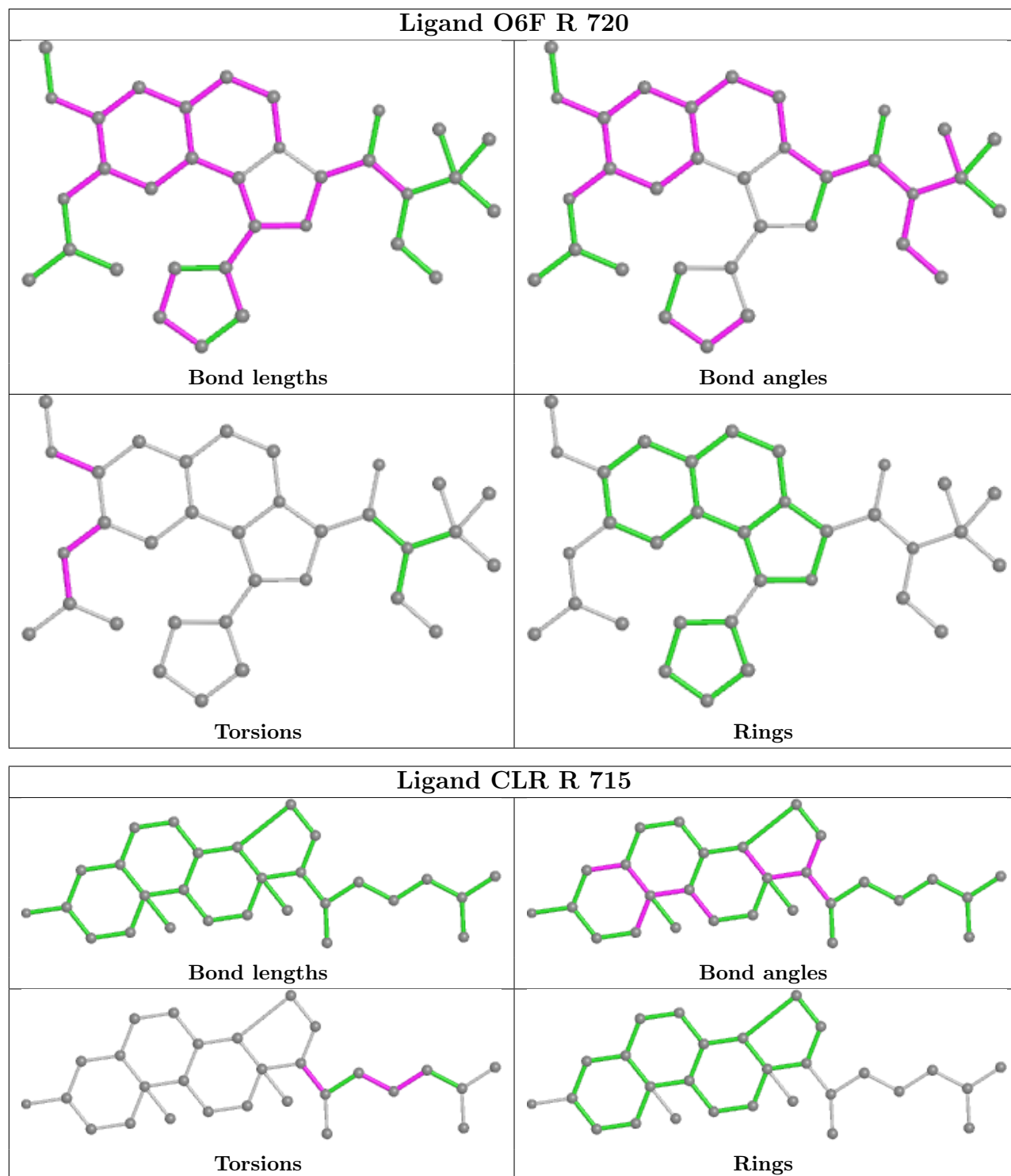












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

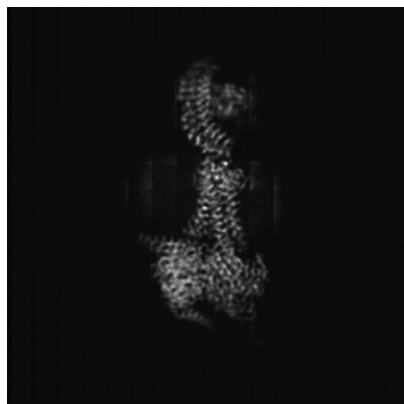
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35135. These allow visual inspection of the internal detail of the map and identification of artifacts.

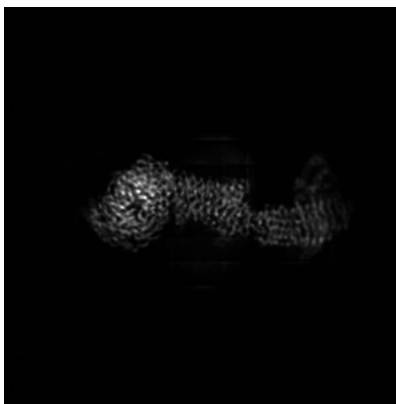
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

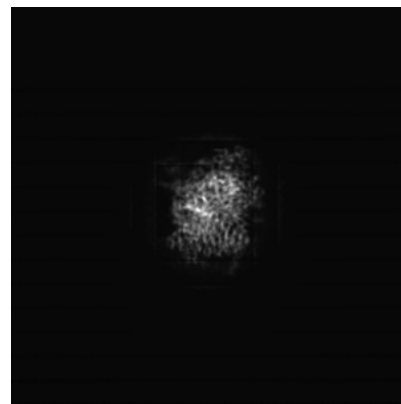
6.1.1 Primary map



X

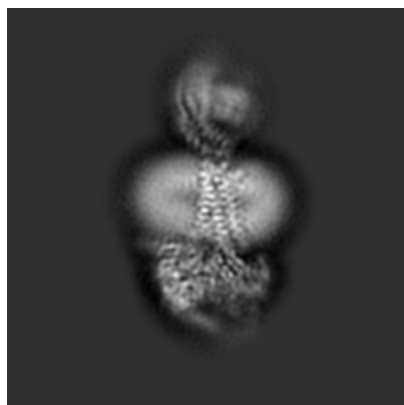


Y

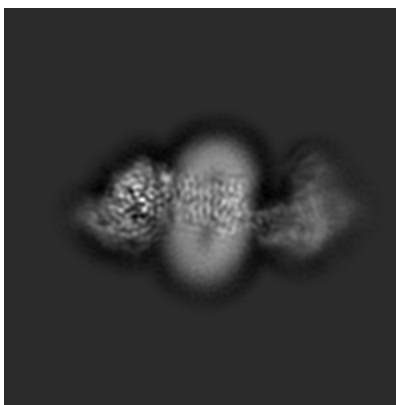


Z

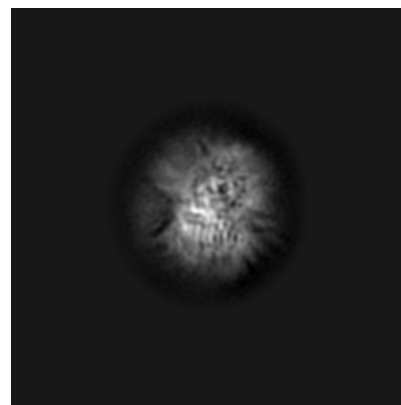
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128

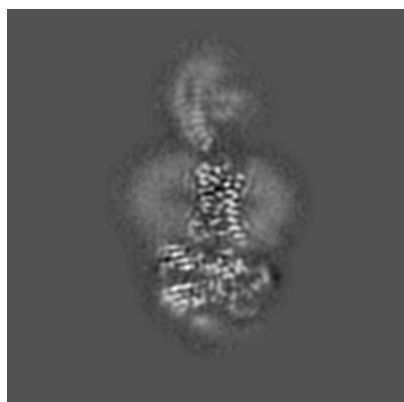


Y Index: 128

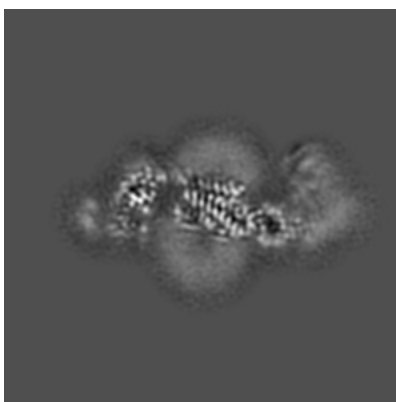


Z Index: 128

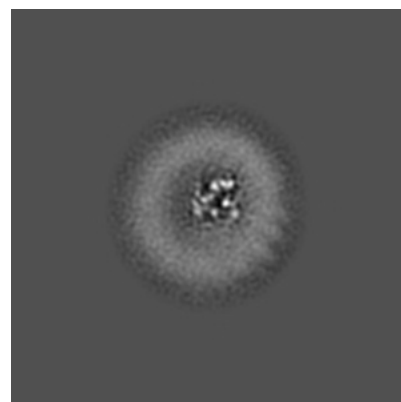
6.2.2 Raw map



X Index: 110



Y Index: 110

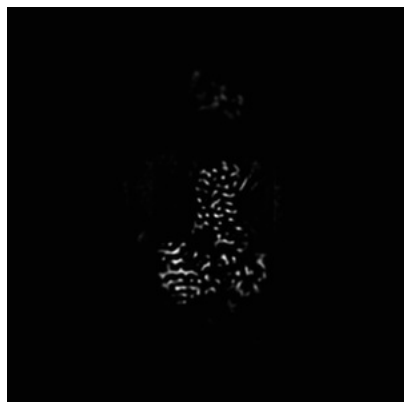


Z Index: 110

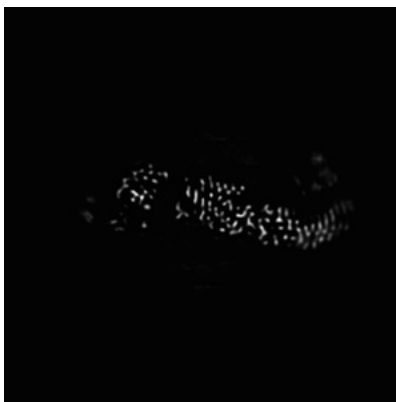
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 137

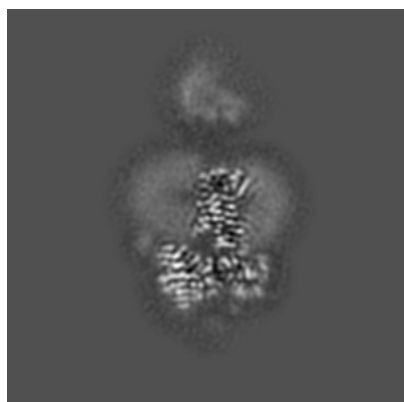


Y Index: 127

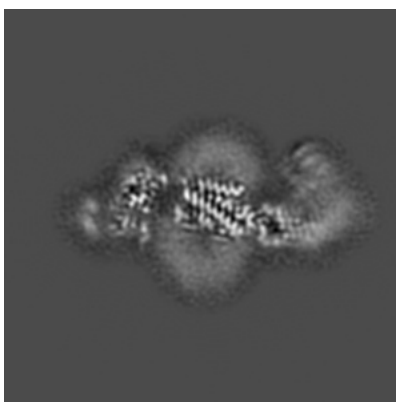


Z Index: 90

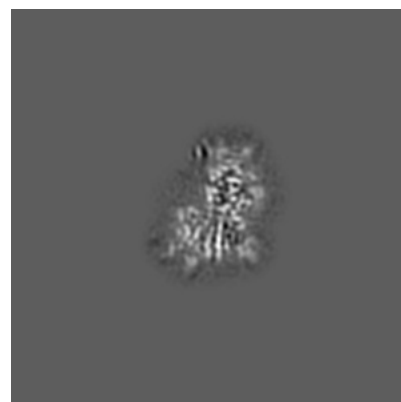
6.3.2 Raw map



X Index: 117



Y Index: 109

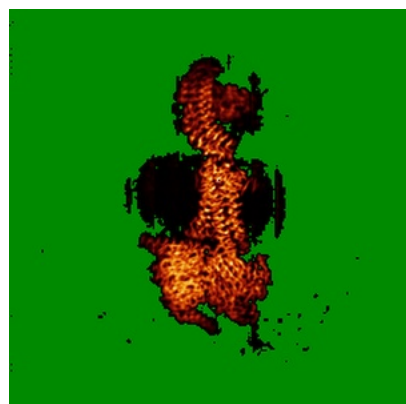


Z Index: 76

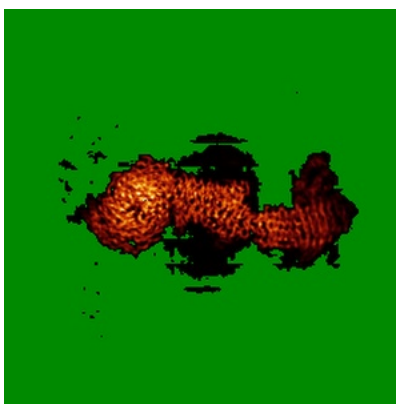
The images above show the largest variance slices of the map in three orthogonal directions.

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

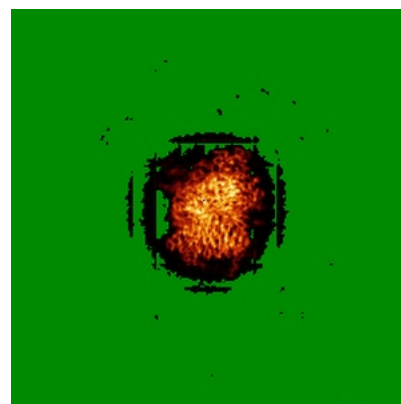
6.4.1 Primary map



X

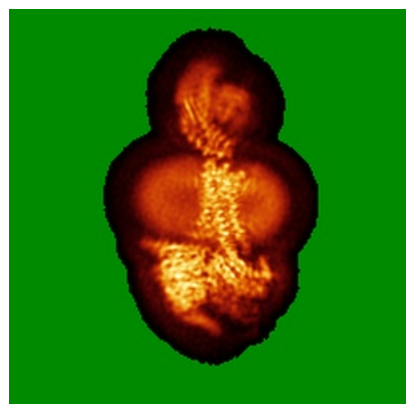


Y

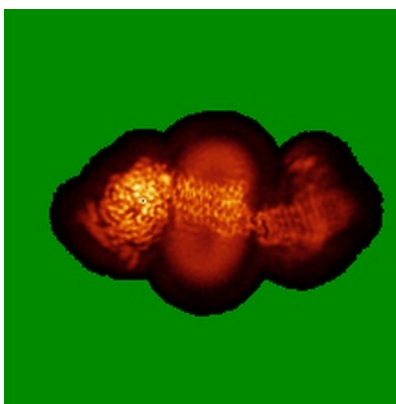


Z

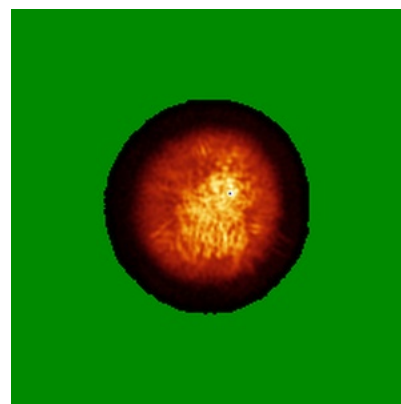
6.4.2 Raw map



X



Y

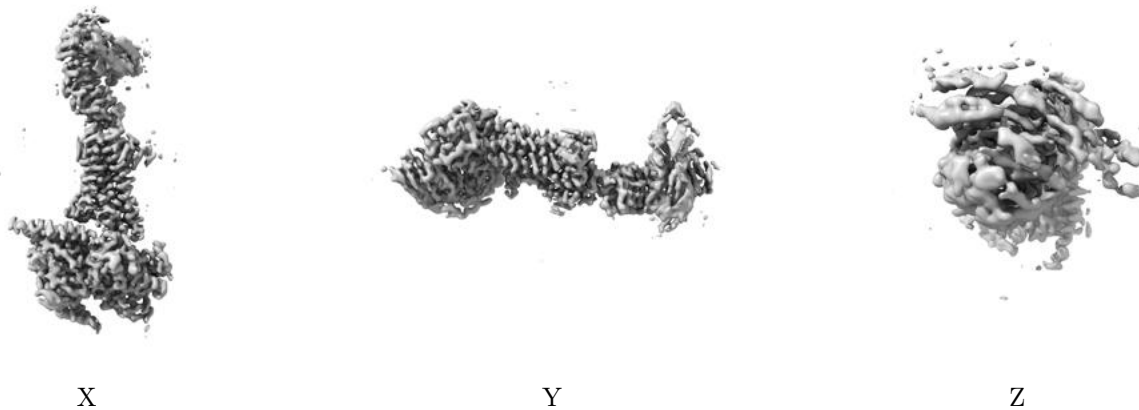


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

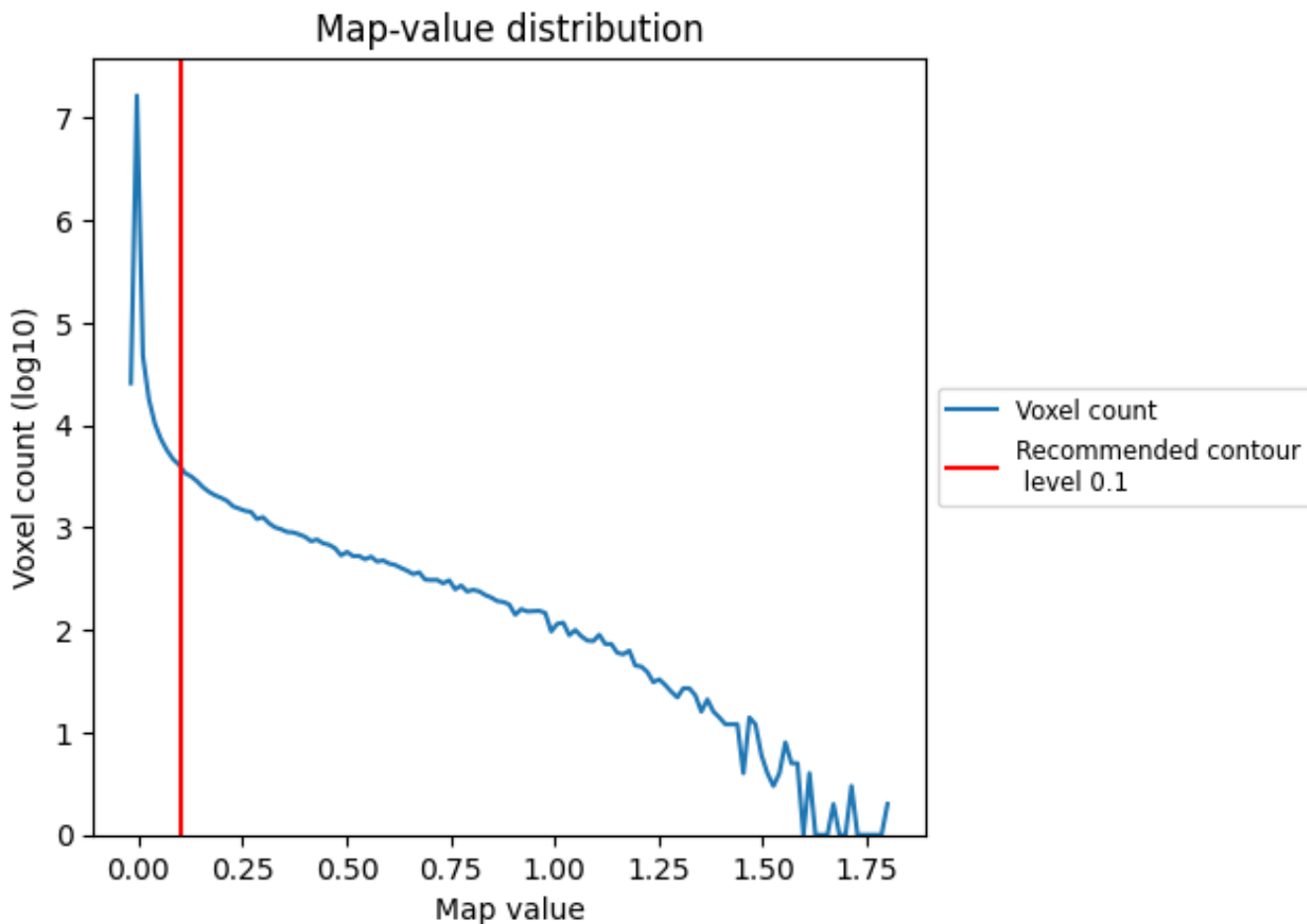
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

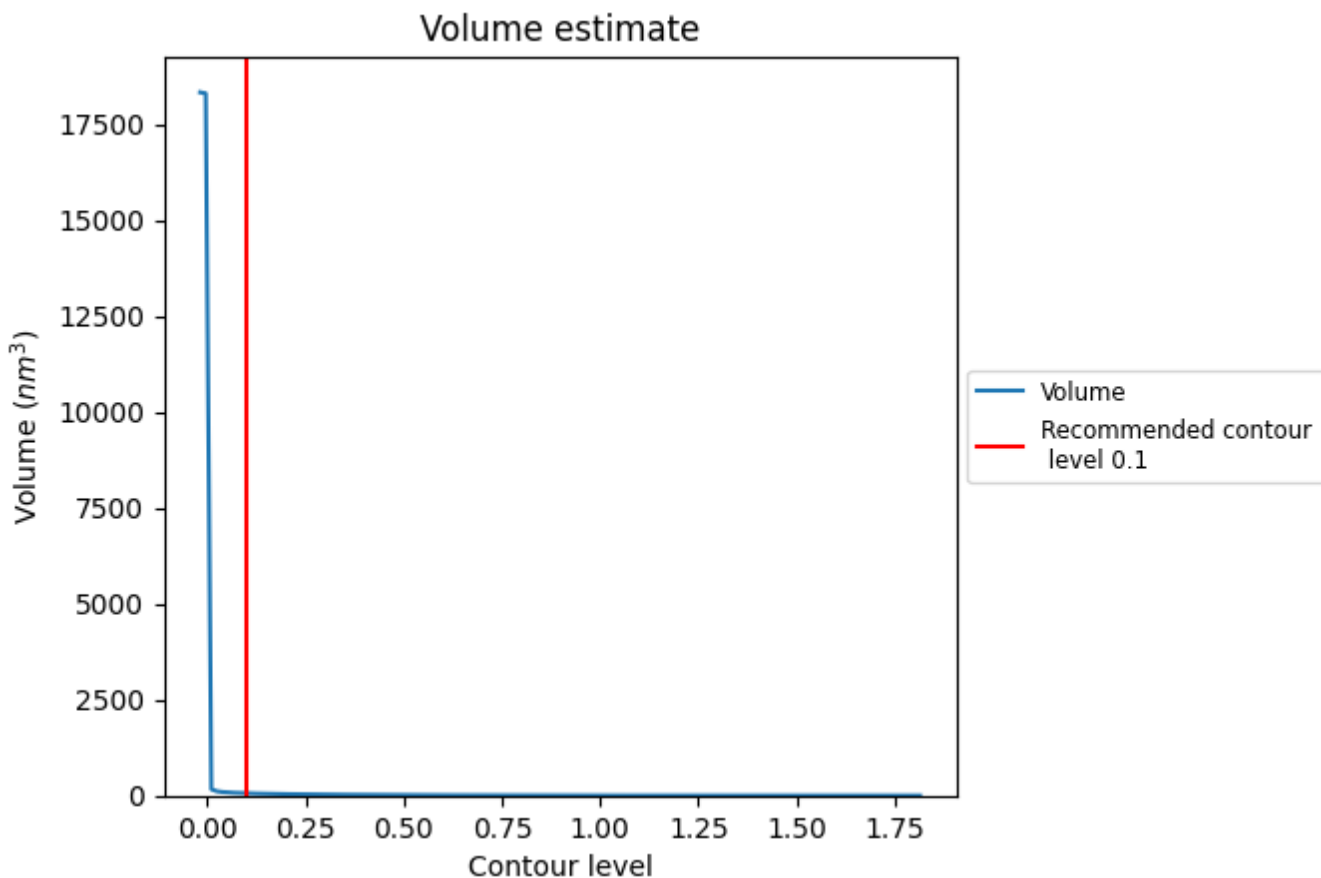
This section contains the results of statistical analysis of the map.

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.

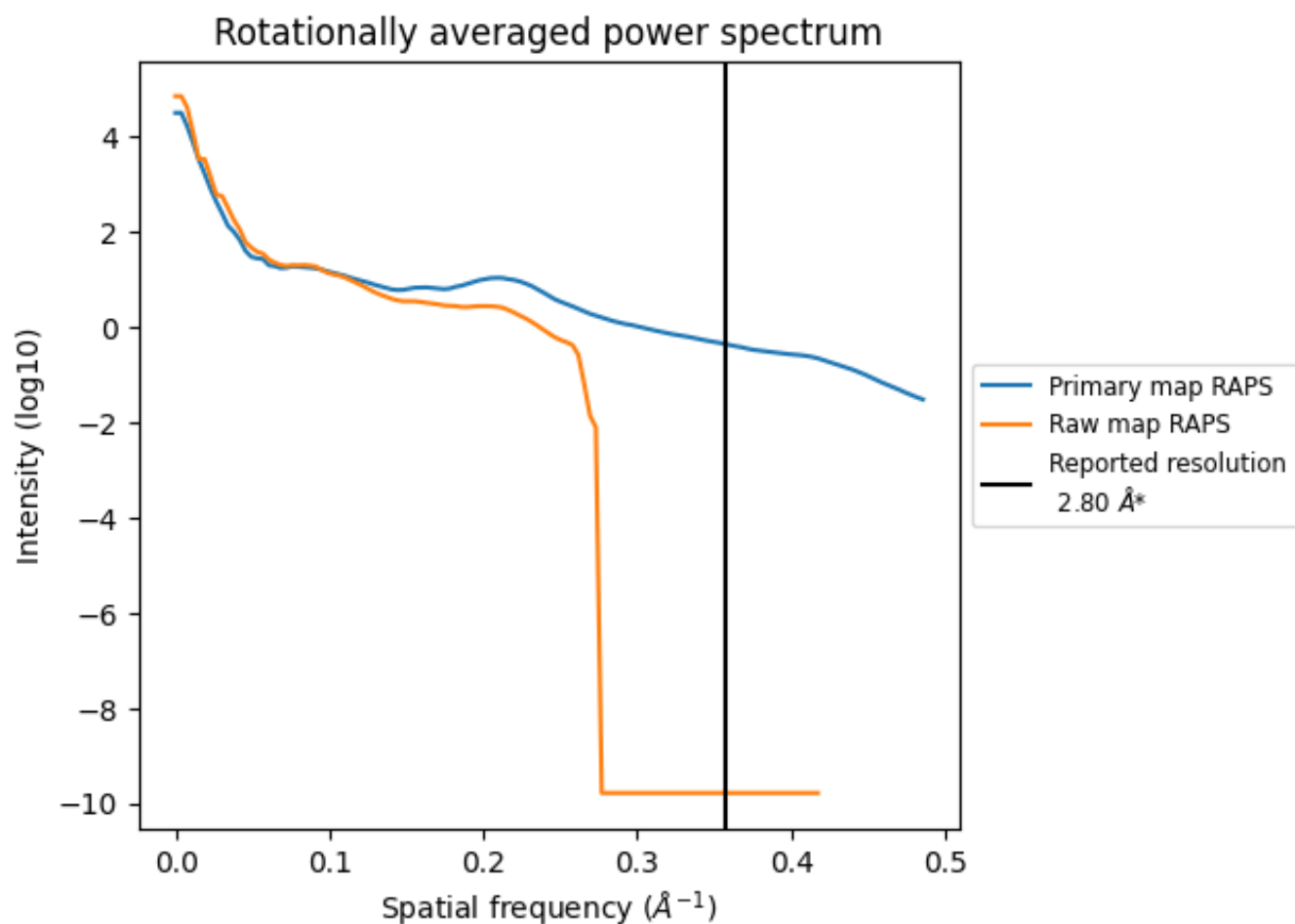
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm^3 ; this corresponds to an approximate mass of 54 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](#)

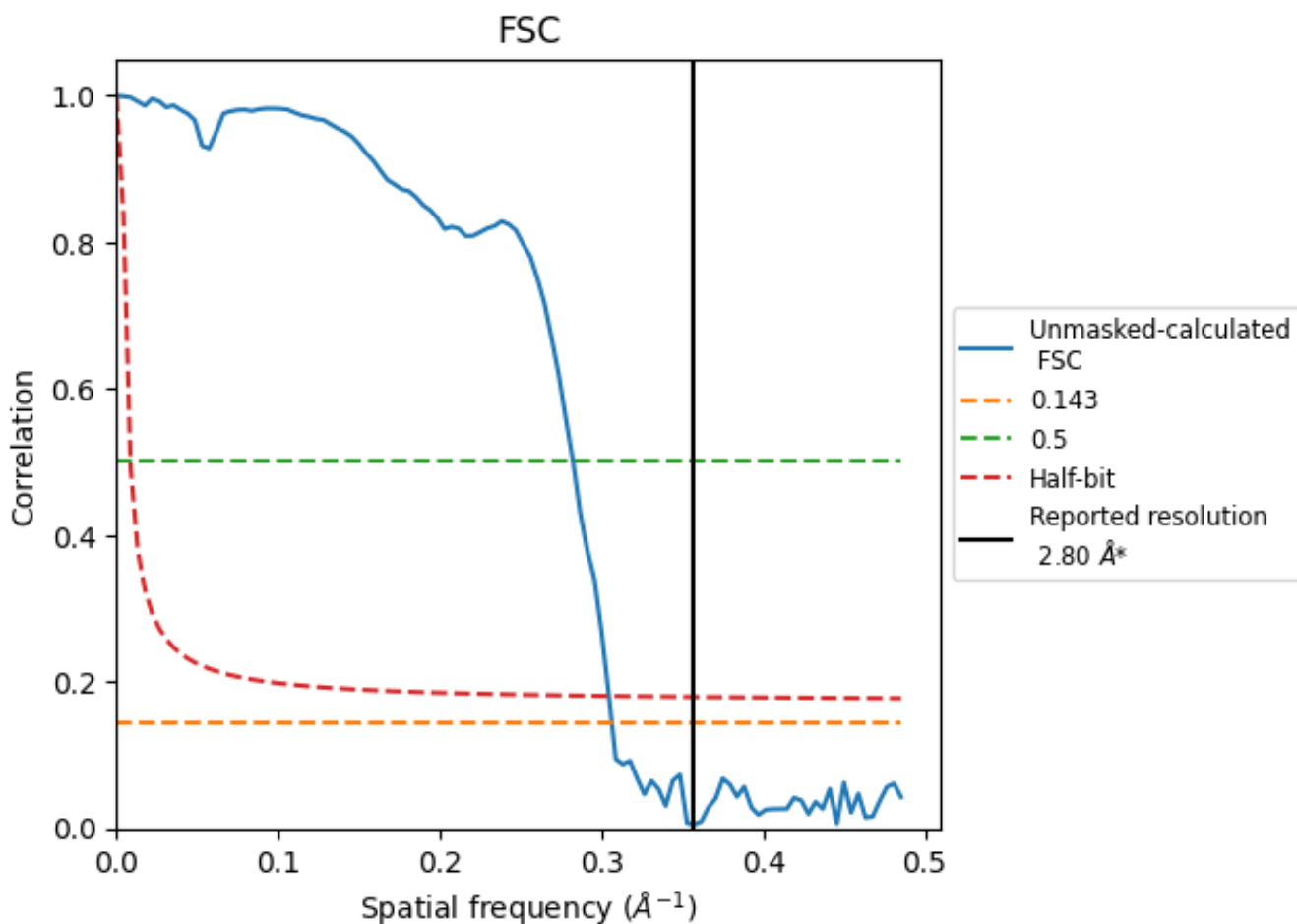


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357\AA^{-1}

8.2 Resolution estimates [i](#)

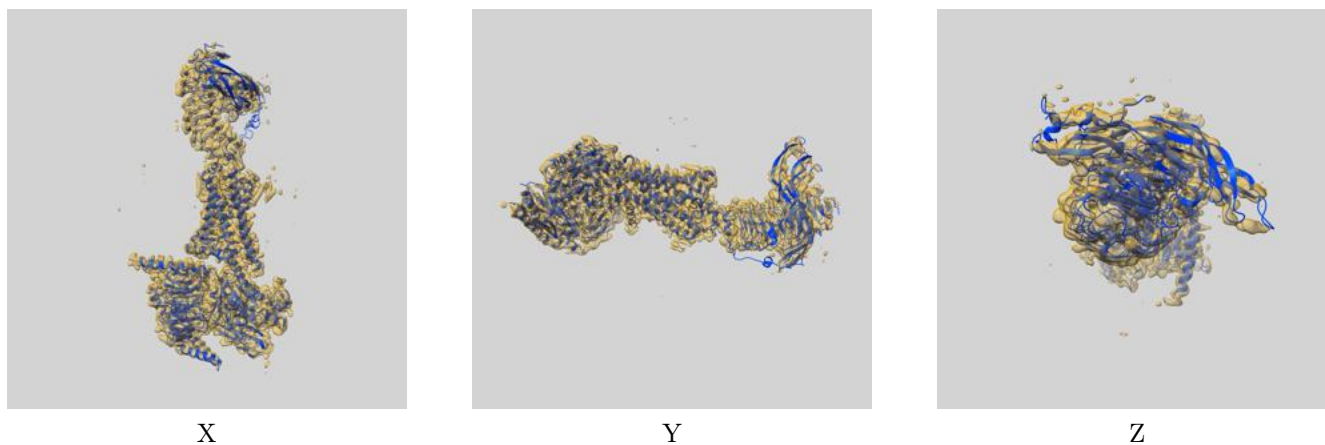
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.54	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

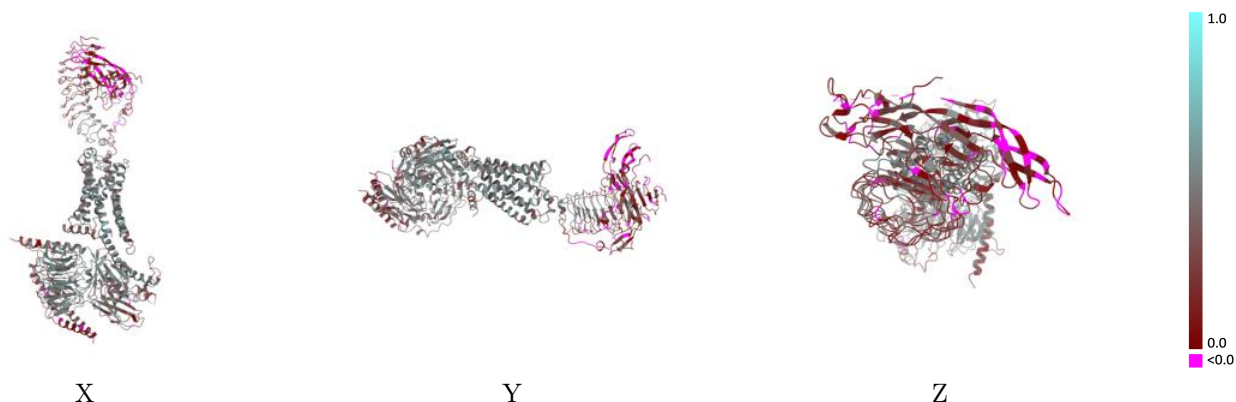
This section contains information regarding the fit between EMDB map EMD-35135 and PDB model 8I2G. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



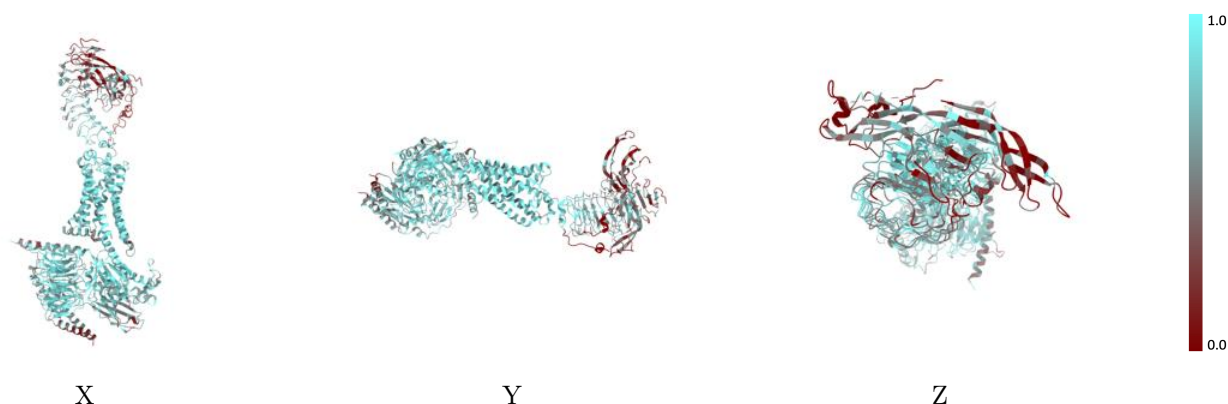
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



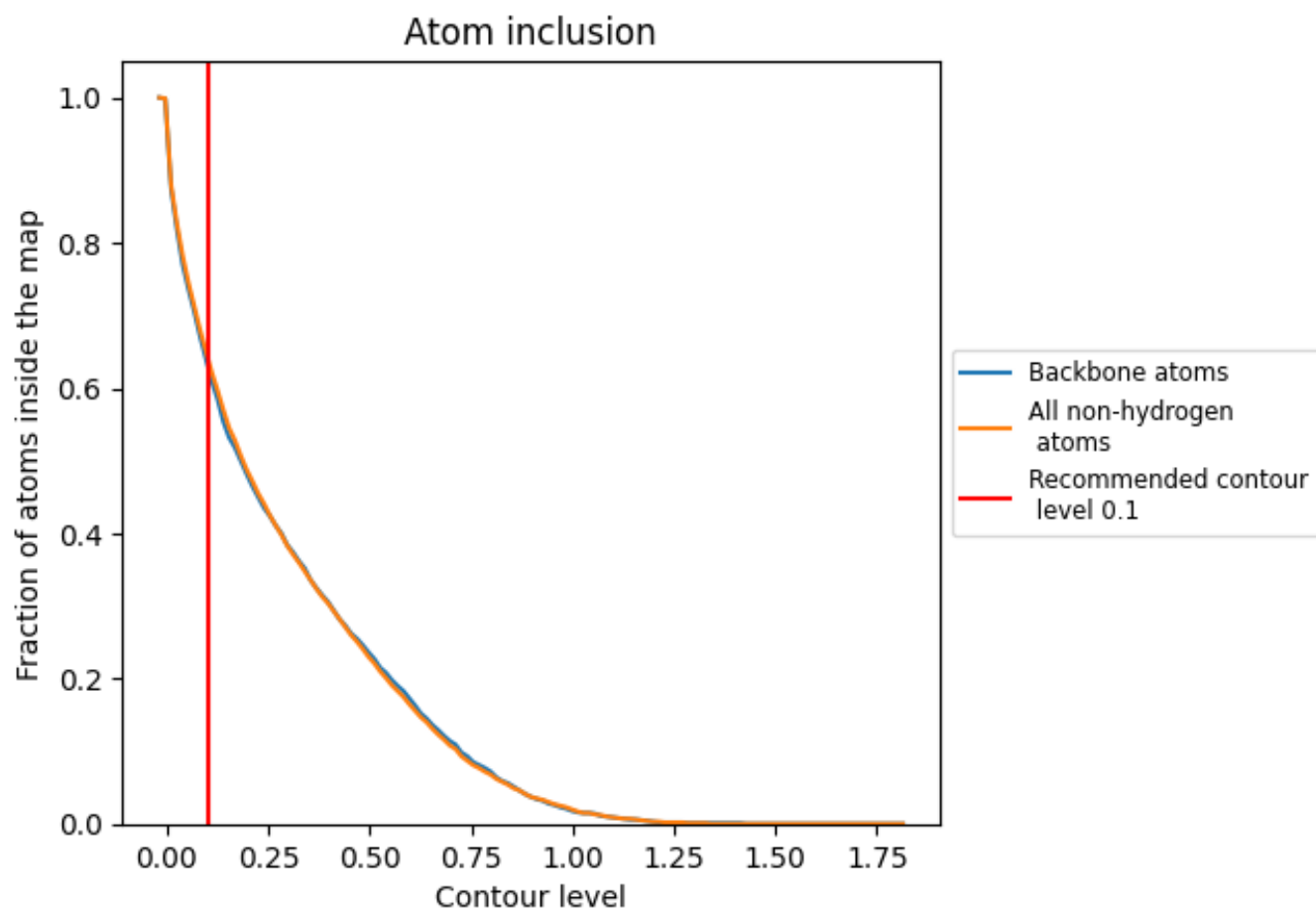
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 64% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6430	 0.3630
A	 0.7700	 0.4500
B	 0.7790	 0.4460
C	 0.2140	 0.0840
G	 0.5340	 0.2220
N	 0.6720	 0.3880
R	 0.6320	 0.3650
X	 0.3890	 0.1960
Y	 0.3170	 0.1000

