



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:46 AM UTC

PDB ID : 6QEX / pdb_00006qex
EMDB ID : EMD-4539
Title : Nanodisc reconstituted human ABCB1 in complex with UIC2 fab and taxol
Authors : Alam, A.; Locher, K.P.
Deposited on : 2019-01-08
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

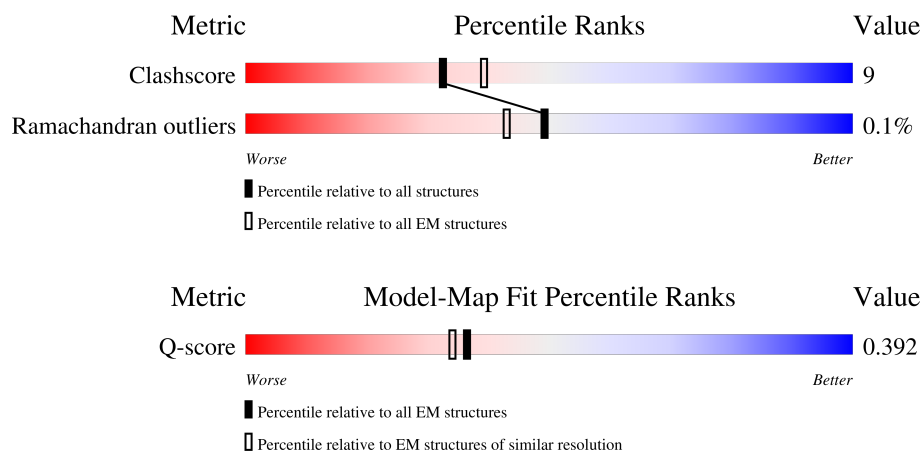
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1280	
2	B	220	
3	C	225	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13251 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 Multidrug resistance protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0
			9191	5918	1559	1677	37		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	893	ALA	SER	variant	UNP P08183

- Molecule 2 is a protein called UIC2 Fab lightchain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	220	Total	C	N	O	S	1	0
			1713	1071	292	342	8		

- Molecule 3 is a protein called UIC2 Fab heavy chain.

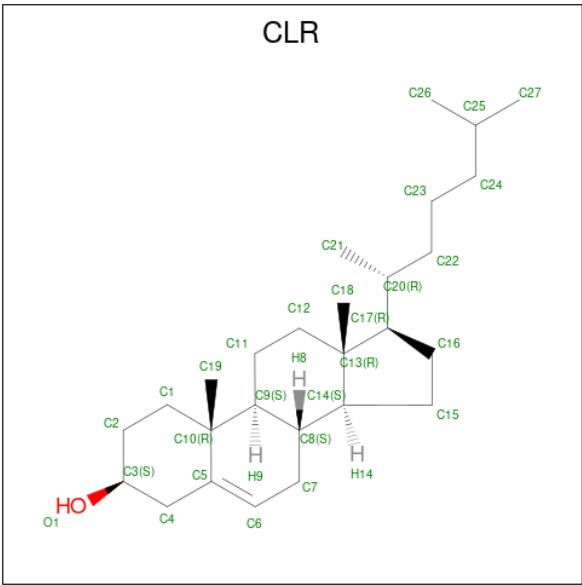
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	225	Total	C	N	O	S	0	0
			1717	1098	274	337	8		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



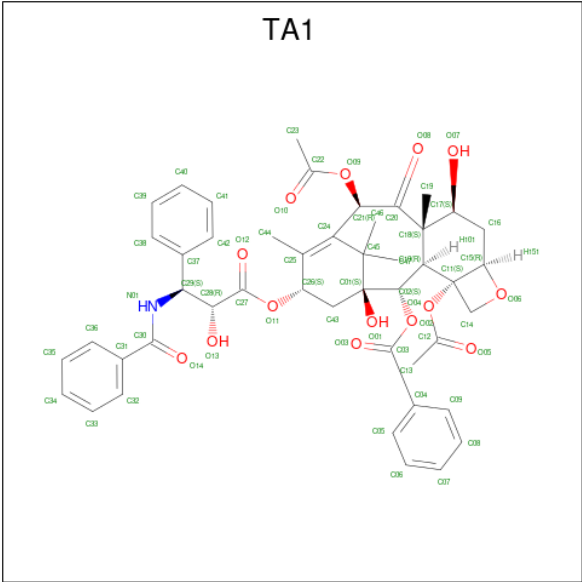
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	

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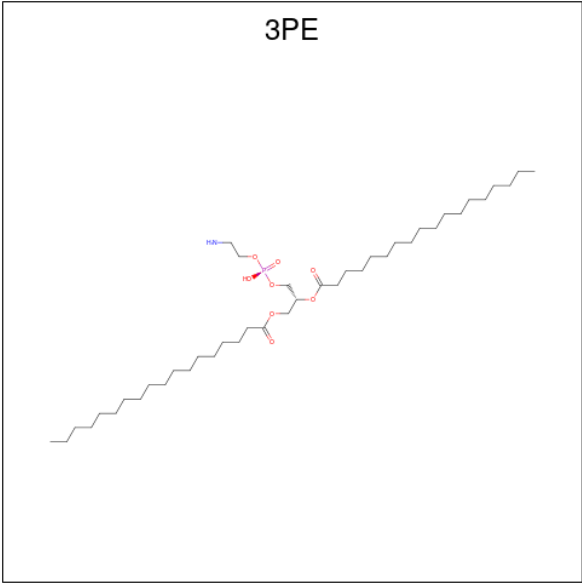
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	

- Molecule 6 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			62	47	1	14	

- Molecule 7 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).

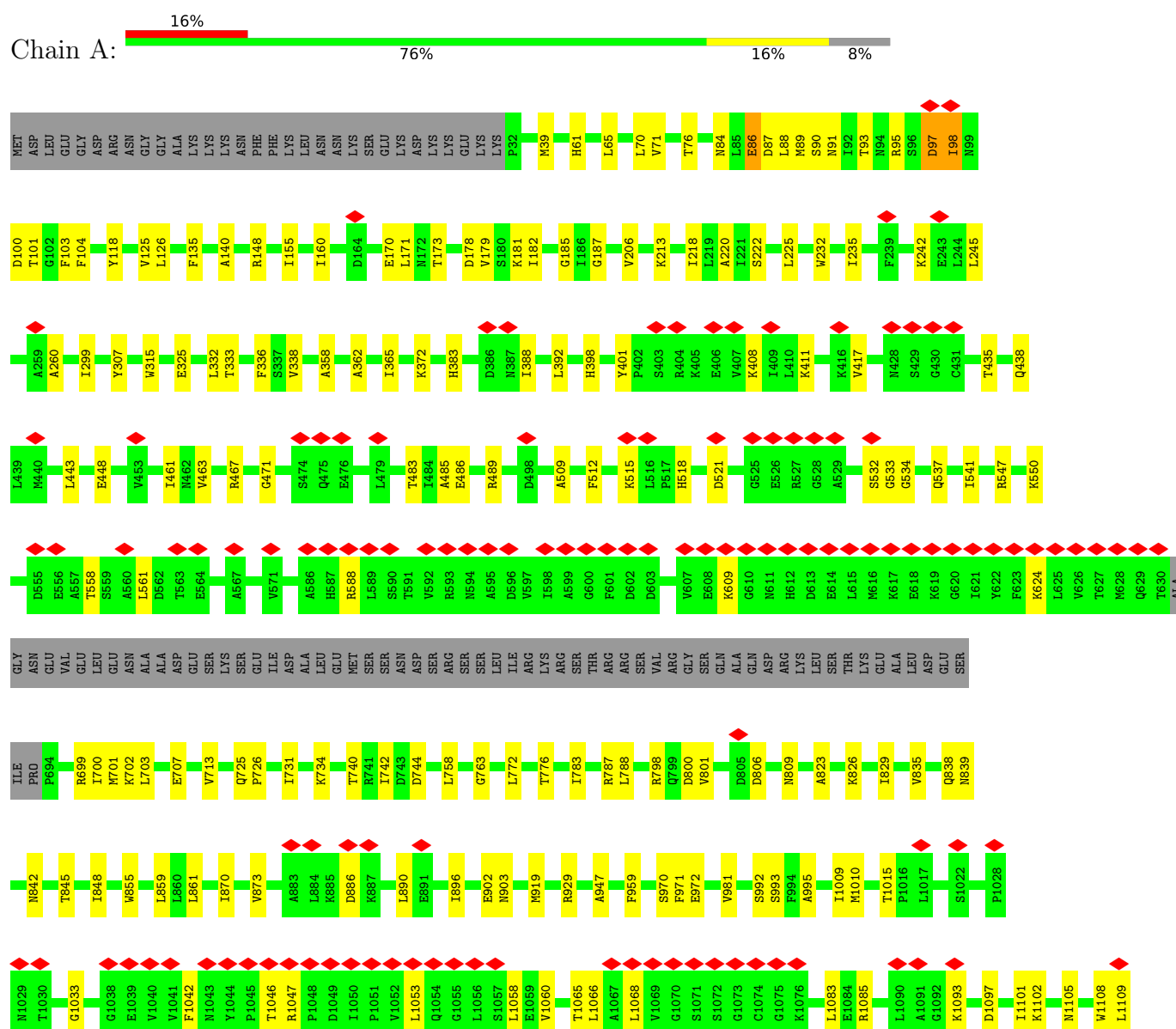


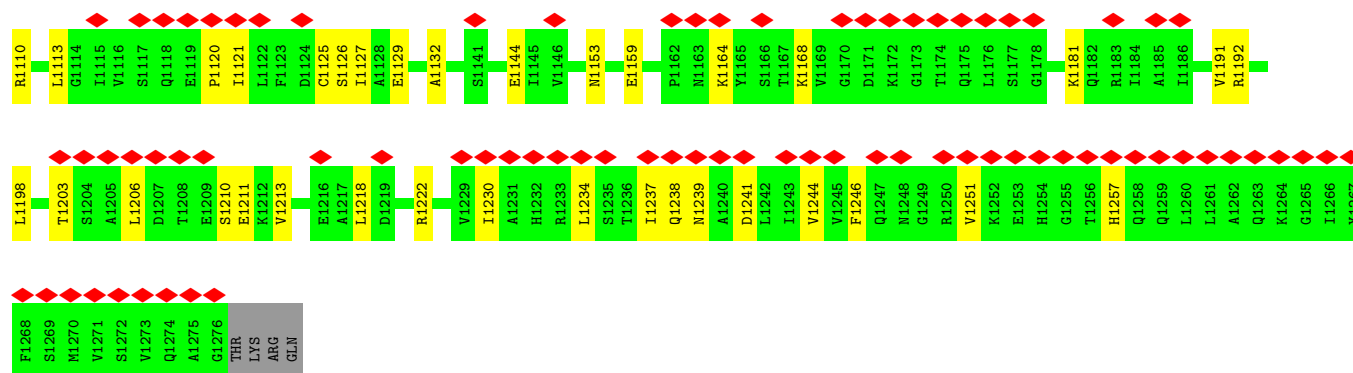
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
7	A	1	Total	C	N	O	P	0
			39	29	1	8	1	

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.

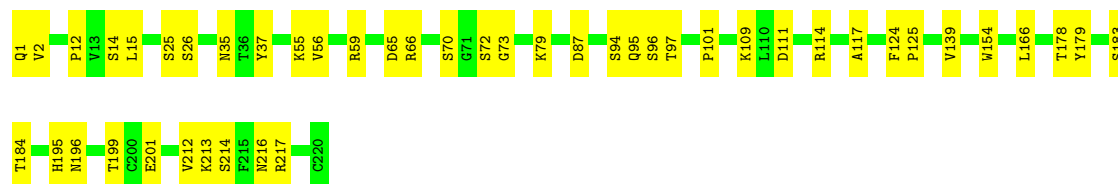
• Molecule 1: Multidrug resistance protein 1





• Molecule 2: UIC2 Fab lightchain

Chain B: 79% 21%



• Molecule 3: UIC2 Fab heavy chain

Chain C: 87% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	262191	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 ($e^-/\text{\AA}^2$)	2.1	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	0.142	Depositor
Minimum map value	-0.088	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TA1, 3PE, NAG, 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	0.32	0/9361	0.59	5/12650 (0.0%)
2	B	0.44	0/1757	0.71	2/2384 (0.1%)
3	C	0.45	0/1767	0.57	0/2412
All	All	0.36	0/12885	0.60	7/17446 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	SER	N-CA-C	9.30	121.42	111.28
1	A	86	GLU	N-CA-C	8.62	120.68	111.28
2	B	94	SER	CA-C-N	6.51	133.42	121.70
2	B	94	SER	C-N-CA	6.51	133.42	121.70
1	A	100	ASP	N-CA-CB	5.60	118.13	110.01
1	A	98	ILE	N-CA-C	5.19	116.54	110.62
1	A	97	ASP	N-CA-C	5.14	120.03	113.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	55	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9191	0	9387	160	0
2	B	1713	0	1656	25	0
3	C	1717	0	1656	16	0
4	A	42	0	39	4	0
5	A	448	0	736	31	0
6	A	62	0	50	6	0
7	A	78	0	104	1	0
All	All	13251	0	13628	229	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 9.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:NH1	1:A:179:VAL:HG11	1.07	1.35
1:A:148:ARG:NH1	1:A:179:VAL:CG1	1.90	1.33
1:A:84:ASN:ND2	1:A:740:THR:O	1.62	1.30
1:A:700:ILE:O	1:A:829:ILE:HD11	1.39	1.18
1:A:700:ILE:C	1:A:829:ILE:HD11	1.87	0.98
1:A:93:THR:OG1	4:A:1301:NAG:H83	1.71	0.91
1:A:148:ARG:CZ	1:A:179:VAL:HG11	2.01	0.90
1:A:700:ILE:O	1:A:829:ILE:CD1	2.22	0.88
1:A:89:MET:HG3	1:A:103:PHE:HE2	1.38	0.86
1:A:88:LEU:HD23	1:A:88:LEU:N	2.01	0.75
5:A:1318:CLR:H71	5:A:1319:CLR:H71	1.67	0.75
1:A:148:ARG:HH12	1:A:179:VAL:CG1	1.98	0.73
1:A:148:ARG:HD3	1:A:179:VAL:HG21	1.69	0.73
1:A:89:MET:HG3	1:A:103:PHE:CE2	2.23	0.71
1:A:148:ARG:HH11	1:A:179:VAL:HG11	0.89	0.70
1:A:839:ASN:HD22	5:A:1306:CLR:H6	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1153:ASN:HD22	1:A:1213:VAL:HG11	1.62	0.64
4:A:1301:NAG:O7	4:A:1301:NAG:H3	1.98	0.63
1:A:534:GLY:HA2	1:A:537:GLN:HE21	1.62	0.63
1:A:1110:ARG:O	1:A:1192:ARG:NH2	2.32	0.63
1:A:98:ILE:HA	1:A:101:THR:OG1	2.00	0.61
1:A:873:VAL:HG23	1:A:993:SER:HB2	1.83	0.60
1:A:1046:THR:HG23	1:A:1047:ARG:HG3	1.84	0.59
1:A:798:ARG:HH12	1:A:1015:THR:HG23	1.66	0.59
2:B:195:HIS:O	2:B:217:ARG:NH1	2.35	0.59
1:A:870:ILE:HA	1:A:873:VAL:HG12	1.85	0.59
2:B:12:PRO:HA	2:B:111:ASP:HB2	1.85	0.58
6:A:1320:TA1:H472	6:A:1320:TA1:H193	1.85	0.58
2:B:95:GLN:NE2	2:B:96:SER:O	2.35	0.58
2:B:201:GLU:HG2	2:B:212:VAL:HG12	1.85	0.58
1:A:39:MET:HE1	1:A:182:ILE:HD12	1.85	0.58
1:A:160:ILE:HG13	1:A:443:LEU:HD23	1.85	0.58
1:A:148:ARG:NH1	1:A:179:VAL:HG12	2.11	0.57
1:A:315:TRP:HZ3	5:A:1313:CLR:H6	1.68	0.57
1:A:148:ARG:NH1	1:A:890:LEU:HD21	2.20	0.57
1:A:218:ILE:HG21	1:A:338:VAL:HG11	1.86	0.57
1:A:835:VAL:HG21	1:A:995:ALA:HB2	1.85	0.57
1:A:140:ALA:HB2	1:A:187:GLY:HA2	1.87	0.56
1:A:558:THR:OG1	1:A:588:ARG:NH1	2.39	0.55
3:C:110:ASP:OD1	3:C:110:ASP:N	2.39	0.55
1:A:148:ARG:HH11	1:A:179:VAL:CG1	1.80	0.55
2:B:70:SER:OG	2:B:79:LYS:NZ	2.40	0.54
1:A:213:LYS:NZ	1:A:325:GLU:OE2	2.39	0.54
1:A:70:LEU:HD23	1:A:333:THR:HG21	1.89	0.54
1:A:1083:LEU:HD23	1:A:1198:LEU:HD11	1.90	0.54
1:A:861:LEU:HB3	1:A:981:VAL:HG11	1.90	0.54
1:A:561:LEU:O	1:A:588:ARG:NH2	2.41	0.54
1:A:70:LEU:HD21	1:A:206:VAL:HG13	1.91	0.53
5:A:1318:CLR:H71	5:A:1319:CLR:C7	2.36	0.53
1:A:218:ILE:HG21	1:A:338:VAL:CG1	2.38	0.53
1:A:1085:ARG:HG2	1:A:1109:LEU:HD22	1.91	0.53
1:A:1065:THR:HB	1:A:1241:ASP:H	1.73	0.53
1:A:1058:LEU:HD11	1:A:1066:LEU:HD11	1.91	0.53
3:C:211:SER:HG	3:C:213:THR:HG1	1.50	0.53
1:A:336:PHE:CE2	6:A:1320:TA1:H061	2.44	0.53
1:A:88:LEU:HD23	1:A:88:LEU:H	1.74	0.52
1:A:87:ASP:OD2	1:A:742:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:ARG:NH2	1:A:1101:ILE:O	2.42	0.52
2:B:14:SER:OG	2:B:15:LEU:N	2.43	0.52
1:A:383:HIS:HB3	1:A:461:ILE:HG22	1.92	0.52
1:A:463:VAL:HG12	1:A:467:ARG:HD2	1.92	0.52
1:A:707:GLU:HG3	1:A:783:ILE:HD11	1.92	0.52
1:A:1125:CYS:SG	1:A:1126:SER:N	2.83	0.52
1:A:76:THR:HG21	1:A:332:LEU:HD22	1.92	0.52
1:A:91:ASN:ND2	1:A:91:ASN:O	2.43	0.51
1:A:93:THR:OG1	4:A:1301:NAG:C8	2.53	0.51
1:A:61:HIS:HD2	1:A:125:VAL:HG13	1.76	0.51
1:A:1238:GLN:OE1	1:A:1257:HIS:NE2	2.40	0.51
1:A:178:ASP:HB2	1:A:365:ILE:HD11	1.92	0.51
2:B:37:TYR:HB2	2:B:97:THR:HG22	1.93	0.51
1:A:98:ILE:C	1:A:101:THR:HG1	2.18	0.51
1:A:744:ASP:OD2	2:B:35:ASN:ND2	2.44	0.51
1:A:1060:VAL:HG22	1:A:1066:LEU:HD13	1.93	0.51
1:A:232:TRP:HD1	1:A:299:ILE:HD12	1.76	0.51
1:A:126:LEU:HB2	1:A:947:ALA:HB2	1.93	0.51
1:A:1234:LEU:HB3	1:A:1238:GLN:HE21	1.76	0.50
1:A:1042:PHE:HB3	1:A:1053:LEU:HD22	1.93	0.50
2:B:66:ARG:NH2	2:B:87:ASP:OD2	2.44	0.50
2:B:72:SER:OG	2:B:73:GLY:N	2.44	0.50
1:A:701:MET:HA	1:A:829:ILE:HD13	1.94	0.50
1:A:902:GLU:OE1	1:A:903:ASN:ND2	2.44	0.50
1:A:1126:SER:OG	1:A:1127:ILE:N	2.44	0.50
1:A:401:TYR:OH	1:A:438:GLN:NE2	2.44	0.50
2:B:25:SER:OG	2:B:26:SER:N	2.45	0.49
1:A:86:GLU:HG3	1:A:104:PHE:CZ	2.47	0.49
1:A:731:ILE:HD13	1:A:758:LEU:HB3	1.93	0.49
2:B:139:VAL:HG12	2:B:184:THR:HG22	1.95	0.49
2:B:199:THR:HG22	2:B:214:SER:HB2	1.94	0.49
1:A:260:ALA:HB2	1:A:1121:ILE:HD13	1.95	0.49
1:A:725:GLN:NE2	6:A:1320:TA1:O07	2.46	0.49
1:A:1120:PRO:HB2	1:A:1181:LYS:HD2	1.93	0.49
1:A:703:LEU:O	1:A:787:ARG:NH2	2.45	0.49
1:A:512:PHE:HA	1:A:515:LYS:HG2	1.94	0.48
1:A:823:ALA:O	1:A:826:LYS:NZ	2.40	0.48
1:A:170:GLU:HA	1:A:173:THR:HG22	1.95	0.48
1:A:185:GLY:HA3	1:A:358:ALA:HB2	1.96	0.48
1:A:1246:PHE:HE1	1:A:1251:VAL:HG22	1.78	0.48
1:A:896:ILE:HD13	1:A:919:MET:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1320:TA1:H431	6:A:1320:TA1:H421	1.95	0.48
3:C:73:ASP:OD2	3:C:76:SER:OG	2.32	0.47
1:A:148:ARG:CZ	1:A:890:LEU:HD21	2.45	0.47
1:A:135:PHE:CZ	5:A:1318:CLR:H72	2.50	0.47
1:A:1113:LEU:O	1:A:1192:ARG:NH2	2.44	0.47
2:B:59:ARG:NH1	2:B:65:ASP:OD1	2.47	0.47
1:A:518:HIS:HB3	1:A:521:ASP:HB3	1.97	0.47
1:A:1244:VAL:HG13	1:A:1251:VAL:HG13	1.97	0.47
2:B:124:PHE:HB2	2:B:139:VAL:HG23	1.97	0.47
1:A:148:ARG:CZ	1:A:179:VAL:CG1	2.78	0.47
1:A:383:HIS:HB3	1:A:461:ILE:HA	1.97	0.47
1:A:509:ALA:HB1	1:A:512:PHE:HE2	1.78	0.47
1:A:178:ASP:CB	1:A:365:ILE:HD11	2.45	0.47
2:B:166:LEU:HD11	3:C:180:GLN:HB3	1.96	0.47
1:A:970:SER:OG	1:A:971:PHE:N	2.48	0.46
5:A:1316:CLR:H183	5:A:1316:CLR:H20	1.83	0.46
1:A:97:ASP:O	1:A:101:THR:HG23	2.15	0.46
1:A:182:ILE:HD11	1:A:362:ALA:HB2	1.97	0.46
1:A:220:ALA:HB2	5:A:1317:CLR:H161	1.96	0.46
1:A:855:TRP:CE2	5:A:1316:CLR:H9	2.51	0.46
1:A:886:ASP:OD1	1:A:886:ASP:N	2.49	0.46
1:A:392:LEU:HB2	1:A:417:VAL:HB	1.98	0.46
5:A:1310:CLR:H222	5:A:1310:CLR:H162	1.71	0.46
5:A:1313:CLR:H162	5:A:1313:CLR:H221	1.72	0.46
1:A:485:ALA:O	1:A:489:ARG:HB2	2.16	0.45
1:A:408:LYS:HE2	1:A:408:LYS:HB3	1.81	0.45
1:A:61:HIS:CD2	1:A:125:VAL:HG13	2.52	0.45
1:A:515:LYS:HE3	1:A:515:LYS:HB3	1.74	0.45
2:B:2:VAL:HG22	2:B:96:SER:HB2	1.99	0.45
1:A:1105:ASN:HD22	1:A:1108:TRP:HB2	1.82	0.45
5:A:1319:CLR:H221	5:A:1319:CLR:H162	1.60	0.45
1:A:222:SER:HA	1:A:225:LEU:HB2	1.98	0.45
1:A:839:ASN:HB3	5:A:1306:CLR:H72	1.99	0.45
1:A:959:PHE:HE1	5:A:1311:CLR:H71	1.81	0.45
5:A:1316:CLR:H222	5:A:1316:CLR:H162	1.83	0.45
2:B:178:THR:OG1	2:B:179:TYR:N	2.50	0.45
1:A:609:LYS:HD2	1:A:609:LYS:HA	1.82	0.45
1:A:398:HIS:HD2	1:A:411:LYS:HD2	1.81	0.44
1:A:471:GLY:HA2	1:A:547:ARG:HH21	1.82	0.44
5:A:1315:CLR:H162	5:A:1315:CLR:H222	1.78	0.44
1:A:307:TYR:HD2	1:A:763:GLY:HA2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LYS:HA	1:A:181:LYS:HD2	1.81	0.44
1:A:800:ASP:OD1	1:A:801:VAL:N	2.50	0.44
5:A:1318:CLR:H211	5:A:1318:CLR:H232	1.78	0.44
1:A:788:LEU:HA	1:A:788:LEU:HD12	1.82	0.44
1:A:235:ILE:O	1:A:235:ILE:HG22	2.16	0.44
1:A:1168:LYS:HA	1:A:1168:LYS:HD3	1.81	0.44
1:A:1222:ARG:HH12	1:A:1239:ASN:HD22	1.66	0.44
1:A:98:ILE:O	1:A:101:THR:OG1	2.33	0.44
1:A:1093:LYS:HA	1:A:1093:LYS:HD3	1.92	0.43
1:A:95:ARG:H	1:A:95:ARG:CD	2.32	0.43
1:A:388:ILE:HD12	1:A:550:LYS:HG3	2.00	0.43
5:A:1304:CLR:H8	5:A:1304:CLR:H182	1.82	0.43
1:A:71:VAL:HG12	1:A:118:TYR:CZ	2.53	0.43
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.87	0.43
1:A:1159:GLU:HA	1:A:1164:LYS:HE3	1.99	0.43
5:A:1305:CLR:H122	5:A:1311:CLR:H152	2.01	0.43
2:B:109:LYS:HE3	2:B:109:LYS:HB3	1.87	0.43
1:A:483:THR:HG23	1:A:486:GLU:H	1.84	0.43
1:A:1129:GLU:HA	1:A:1132:ALA:HB3	2.00	0.43
5:A:1313:CLR:H213	5:A:1313:CLR:H231	1.81	0.43
5:A:1318:CLR:H151	5:A:1319:CLR:H151	2.00	0.43
1:A:1033:GLY:H	1:A:1097:ASP:CG	2.27	0.43
3:C:164:ASN:O	3:C:167:SER:OG	2.33	0.43
3:C:33:TYR:HD1	3:C:52:SER:HA	1.84	0.43
1:A:98:ILE:O	1:A:98:ILE:HG22	2.19	0.43
1:A:242:LYS:HA	1:A:245:LEU:HG	1.99	0.43
2:B:124:PHE:HA	2:B:125:PRO:HD3	1.90	0.43
6:A:1320:TA1:H193	6:A:1320:TA1:H021	1.61	0.42
1:A:95:ARG:CG	1:A:95:ARG:HH21	2.31	0.42
5:A:1316:CLR:H182	5:A:1316:CLR:H8	1.80	0.42
1:A:624:LYS:HE3	1:A:624:LYS:HB3	1.89	0.42
1:A:398:HIS:HB2	1:A:448:GLU:HB2	2.01	0.42
1:A:1144:GLU:HG3	1:A:1191:VAL:HG23	2.01	0.42
5:A:1308:CLR:H8	5:A:1308:CLR:H191	1.82	0.42
7:A:1321:3PE:H251	7:A:1321:3PE:H221	1.77	0.42
5:A:1306:CLR:H162	5:A:1306:CLR:H222	1.60	0.42
5:A:1313:CLR:H8	5:A:1313:CLR:H191	1.85	0.42
1:A:401:TYR:HE2	1:A:435:THR:HG23	1.85	0.42
1:A:726:PRO:HG2	1:A:845:THR:HG23	2.02	0.42
1:A:1068:LEU:HB2	1:A:1230:ILE:HG12	2.01	0.42
1:A:1203:THR:OG1	1:A:1211:GLU:OE2	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:HH12	1:A:179:VAL:HG12	1.76	0.41
1:A:532:SER:OG	1:A:533:GLY:N	2.53	0.41
1:A:1068:LEU:HD23	1:A:1244:VAL:HB	2.01	0.41
3:C:38:LYS:HB2	3:C:48:ILE:HD11	2.02	0.41
1:A:155:ILE:HD11	1:A:171:LEU:HD21	2.02	0.41
2:B:196:ASN:HB3	2:B:216:ASN:HD22	1.86	0.41
3:C:9:PRO:HB3	3:C:117:THR:HG23	2.02	0.41
3:C:91:SER:O	3:C:91:SER:OG	2.38	0.41
1:A:929:ARG:HA	1:A:929:ARG:HD3	1.86	0.41
1:A:218:ILE:CG2	1:A:338:VAL:HG11	2.49	0.41
1:A:713:VAL:HG13	1:A:776:THR:HG21	2.02	0.41
1:A:838:GLN:O	1:A:842:ASN:HB2	2.21	0.41
1:A:1234:LEU:HD13	1:A:1237:ILE:HD12	2.01	0.41
2:B:154:TRP:NE1	2:B:183:SER:OG	2.42	0.41
1:A:93:THR:HG1	4:A:1301:NAG:H83	1.79	0.41
5:A:1308:CLR:H162	5:A:1308:CLR:H221	1.74	0.41
1:A:839:ASN:HD21	1:A:992:SER:HB2	1.86	0.41
1:A:1210:SER:HA	1:A:1213:VAL:HG12	2.03	0.41
1:A:1101:ILE:HG13	1:A:1102:LYS:HD3	2.02	0.41
5:A:1310:CLR:H211	5:A:1310:CLR:H232	1.90	0.41
3:C:188:SER:OG	3:C:189:SER:N	2.54	0.41
1:A:699:ARG:HE	1:A:702:LYS:HE2	1.85	0.41
5:A:1315:CLR:H182	5:A:1315:CLR:H8	1.81	0.41
1:A:772:LEU:HD12	1:A:772:LEU:HA	1.93	0.41
6:A:1320:TA1:H162	6:A:1320:TA1:H192	1.86	0.41
2:B:1:GLN:HG3	2:B:101:PRO:HB3	2.03	0.41
3:C:133:LEU:HD11	3:C:150:LEU:HD23	2.02	0.41
1:A:1010:MET:HE3	1:A:1010:MET:HB3	1.90	0.41
5:A:1310:CLR:H193	5:A:1310:CLR:H111	1.89	0.41
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.90	0.40
5:A:1305:CLR:H14	5:A:1311:CLR:H151	2.01	0.40
2:B:114:ARG:HH12	2:B:117:ALA:HB2	1.86	0.40
1:A:332:LEU:O	1:A:336:PHE:HB2	2.21	0.40
1:A:806:ASP:HB2	1:A:809:ASN:HB2	2.04	0.40
1:A:1218:LEU:O	1:A:1222:ARG:N	2.55	0.40
1:A:1203:THR:HG23	1:A:1206:LEU:HB3	2.02	0.40
3:C:51:ILE:HD13	3:C:58:THR:HG22	2.02	0.40
3:C:204:CYS:O	3:C:216:ASP:HA	2.20	0.40
1:A:372:LYS:HA	1:A:372:LYS:HD2	1.94	0.40
1:A:734:LYS:NZ	1:A:972:GLU:OE2	2.53	0.40
5:A:1308:CLR:H213	5:A:1308:CLR:H231	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1315:CLR:H231	5:A:1315:CLR:H273	1.90	0.40
3:C:18:VAL:HG12	3:C:83:PHE:HB2	2.03	0.40
1:A:537:GLN:O	1:A:541:ILE:HG12	2.22	0.40
1:A:848:ILE:HD13	1:A:848:ILE:HA	1.90	0.40
1:A:1009:ILE:HD13	1:A:1009:ILE:HA	1.91	0.40
2:B:213:LYS:HA	2:B:213:LYS:HD3	1.86	0.40
3:C:179:LEU:HD12	3:C:184:TYR:HE1	1.87	0.40
3:C:196:THR:O	3:C:200:GLN:N	2.55	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	1178/1280 (92%)	1118 (95%)	60 (5%)	0	100	100
2	B	219/220 (100%)	200 (91%)	18 (8%)	1 (0%)	24	57
3	C	223/225 (99%)	204 (92%)	19 (8%)	0	100	100
All	All	1620/1725 (94%)	1522 (94%)	97 (6%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	VAL

5.3.2 Protein sidechains [i](#)

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

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 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$
5	CLR	A	1304	-	31,31,31	0.81	2 (6%)	48,48,48	1.43	8 (16%)
5	CLR	A	1312	-	31,31,31	0.71	1 (3%)	48,48,48	1.66	12 (25%)
5	CLR	A	1311	-	31,31,31	0.70	1 (3%)	48,48,48	1.54	9 (18%)
5	CLR	A	1319	-	31,31,31	0.70	1 (3%)	48,48,48	1.50	10 (20%)
5	CLR	A	1308	-	31,31,31	0.78	1 (3%)	48,48,48	1.56	8 (16%)
7	3PE	A	1322	-	38,38,50	1.03	4 (10%)	41,43,55	1.30	3 (7%)
5	CLR	A	1313	-	31,31,31	0.72	1 (3%)	48,48,48	1.58	7 (14%)
5	CLR	A	1314	-	31,31,31	0.71	1 (3%)	48,48,48	1.41	8 (16%)
5	CLR	A	1315	-	31,31,31	0.67	1 (3%)	48,48,48	1.38	5 (10%)
5	CLR	A	1316	-	31,31,31	0.64	1 (3%)	48,48,48	1.54	9 (18%)
5	CLR	A	1306	-	31,31,31	0.74	1 (3%)	48,48,48	1.56	9 (18%)
4	NAG	A	1301	1	14,14,15	2.28	4 (28%)	17,19,21	1.09	2 (11%)
5	CLR	A	1318	-	31,31,31	0.65	0	48,48,48	1.49	11 (22%)
4	NAG	A	1302	1	14,14,15	2.41	4 (28%)	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	3PE	A	1321	-	38,38,50	1.03	4 (10%)	41,43,55	1.20	3 (7%)
6	TA1	A	1320	-	68,68,68	1.58	10 (14%)	105,105,105	2.60	34 (32%)
5	CLR	A	1317	-	31,31,31	0.76	1 (3%)	48,48,48	1.37	4 (8%)
5	CLR	A	1307	-	31,31,31	0.74	1 (3%)	48,48,48	1.52	9 (18%)
5	CLR	A	1310	-	31,31,31	0.68	1 (3%)	48,48,48	1.50	9 (18%)
5	CLR	A	1309	-	31,31,31	0.70	1 (3%)	48,48,48	1.48	8 (16%)
5	CLR	A	1305	-	31,31,31	0.75	1 (3%)	48,48,48	1.57	9 (18%)
4	NAG	A	1303	1	14,14,15	2.36	4 (28%)	17,19,21	1.14	1 (5%)

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
5	CLR	A	1304	-	-	3/10/68/68	0/4/4/4
5	CLR	A	1312	-	-	9/10/68/68	0/4/4/4
5	CLR	A	1311	-	-	5/10/68/68	0/4/4/4
5	CLR	A	1319	-	-	6/10/68/68	0/4/4/4
5	CLR	A	1308	-	-	9/10/68/68	0/4/4/4
7	3PE	A	1322	-	-	22/42/42/54	-
5	CLR	A	1313	-	-	6/10/68/68	0/4/4/4
5	CLR	A	1314	-	-	5/10/68/68	0/4/4/4
5	CLR	A	1315	-	-	1/10/68/68	0/4/4/4
5	CLR	A	1316	-	-	5/10/68/68	0/4/4/4
5	CLR	A	1306	-	-	5/10/68/68	0/4/4/4
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	CLR	A	1318	-	-	7/10/68/68	0/4/4/4
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
7	3PE	A	1321	-	-	22/42/42/54	-
6	TA1	A	1320	-	-	22/41/127/127	0/7/7/7
5	CLR	A	1317	-	-	9/10/68/68	0/4/4/4
5	CLR	A	1307	-	-	3/10/68/68	0/4/4/4
5	CLR	A	1310	-	-	7/10/68/68	0/4/4/4
5	CLR	A	1309	-	-	5/10/68/68	0/4/4/4
5	CLR	A	1305	-	-	7/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	NAG	O5-C1	5.30	1.52	1.43
4	A	1303	NAG	O5-C1	5.17	1.52	1.43
4	A	1301	NAG	O5-C1	4.99	1.52	1.43
4	A	1302	NAG	C7-N2	4.74	1.49	1.34
4	A	1303	NAG	C7-N2	4.73	1.49	1.34
6	A	1320	TA1	O02-C03	-4.69	1.25	1.34
6	A	1320	TA1	O04-C12	-4.58	1.26	1.35
6	A	1320	TA1	O02-C02	4.48	1.52	1.45
4	A	1301	NAG	C7-N2	4.44	1.48	1.34
6	A	1320	TA1	O09-C22	-4.05	1.26	1.35
4	A	1302	NAG	C2-N2	3.58	1.52	1.46
4	A	1303	NAG	C2-N2	3.56	1.52	1.46
6	A	1320	TA1	O11-C27	-3.54	1.26	1.34
6	A	1320	TA1	O11-C26	3.39	1.52	1.45
6	A	1320	TA1	C18-C10	-3.38	1.49	1.57
4	A	1301	NAG	C2-N2	2.92	1.51	1.46
6	A	1320	TA1	O04-C11	2.87	1.51	1.46
5	A	1308	CLR	C10-C9	-2.72	1.51	1.56
5	A	1304	CLR	C10-C9	-2.62	1.51	1.56
6	A	1320	TA1	O09-C21	2.61	1.50	1.44
5	A	1317	CLR	C10-C9	-2.58	1.51	1.56
5	A	1309	CLR	C10-C9	-2.56	1.52	1.56
4	A	1301	NAG	O7-C7	-2.55	1.17	1.23
4	A	1302	NAG	O7-C7	-2.54	1.17	1.23
5	A	1306	CLR	C10-C9	-2.53	1.52	1.56
4	A	1303	NAG	O7-C7	-2.50	1.17	1.23
5	A	1313	CLR	C10-C9	-2.44	1.52	1.56
5	A	1310	CLR	C10-C9	-2.42	1.52	1.56
5	A	1311	CLR	C10-C9	-2.42	1.52	1.56
5	A	1319	CLR	C10-C9	-2.41	1.52	1.56
7	A	1322	3PE	O31-C31	2.40	1.40	1.33
7	A	1321	3PE	O21-C21	2.40	1.41	1.34
5	A	1307	CLR	C10-C9	-2.33	1.52	1.56
5	A	1314	CLR	C10-C9	-2.31	1.52	1.56
5	A	1312	CLR	C10-C9	-2.30	1.52	1.56
7	A	1321	3PE	O31-C3	-2.27	1.40	1.45
5	A	1315	CLR	C10-C9	-2.26	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1321	3PE	O31-C31	2.25	1.39	1.33
7	A	1322	3PE	O21-C21	2.25	1.40	1.34
7	A	1321	3PE	O21-C2	-2.16	1.41	1.46
7	A	1322	3PE	O21-C2	-2.12	1.41	1.46
7	A	1322	3PE	O31-C3	-2.11	1.40	1.45
5	A	1304	CLR	C10-C5	-2.08	1.48	1.52
5	A	1305	CLR	C10-C9	-2.06	1.52	1.56
5	A	1316	CLR	C10-C9	-2.06	1.52	1.56
6	A	1320	TA1	O06-C15	-2.04	1.42	1.46

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1320	TA1	O09-C21-C24	9.90	126.44	110.02
6	A	1320	TA1	O02-C02-C10	7.87	122.44	108.17
6	A	1320	TA1	O11-C27-C28	6.45	121.36	111.13
6	A	1320	TA1	C19-C18-C17	-6.07	97.94	109.61
6	A	1320	TA1	C21-C24-C25	-5.76	112.12	120.29
6	A	1320	TA1	C11-C10-C02	5.50	122.30	111.70
6	A	1320	TA1	O02-C03-C04	5.44	120.65	111.90
6	A	1320	TA1	O04-C12-C13	5.28	119.62	110.67
6	A	1320	TA1	C10-C18-C17	5.12	116.28	106.55
6	A	1320	TA1	C47-C45-C46	-4.84	92.56	106.29
6	A	1320	TA1	O09-C22-C23	4.77	119.60	111.09
5	A	1316	CLR	C13-C17-C20	-4.57	112.44	119.50
6	A	1320	TA1	C11-C10-C18	4.49	117.19	110.78
7	A	1322	3PE	O21-C21-C22	4.38	120.95	111.48
5	A	1312	CLR	C19-C10-C9	-4.22	106.92	111.66
5	A	1308	CLR	C19-C10-C9	-4.18	106.97	111.66
5	A	1317	CLR	C19-C10-C9	-4.12	107.03	111.66
5	A	1313	CLR	C10-C9-C8	-4.05	106.79	112.71
5	A	1313	CLR	C19-C10-C9	-4.05	107.12	111.66
5	A	1306	CLR	C19-C10-C9	-3.94	107.24	111.66
6	A	1320	TA1	C44-C25-C24	-3.90	120.67	125.32
7	A	1321	3PE	O21-C21-C22	3.86	119.84	111.48
6	A	1320	TA1	O08-C20-C21	-3.86	114.65	119.28
5	A	1314	CLR	C19-C10-C9	-3.85	107.33	111.66
5	A	1305	CLR	C21-C20-C22	-3.84	104.39	110.34
5	A	1307	CLR	C19-C10-C9	-3.81	107.39	111.66
5	A	1307	CLR	C21-C20-C22	-3.80	104.46	110.34
5	A	1308	CLR	C10-C9-C8	-3.79	107.17	112.71
5	A	1304	CLR	C19-C10-C9	-3.79	107.41	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1310	CLR	C19-C10-C9	-3.68	107.53	111.66
5	A	1311	CLR	C19-C10-C9	-3.65	107.57	111.66
5	A	1317	CLR	C13-C17-C20	-3.62	113.90	119.50
5	A	1311	CLR	C21-C20-C22	-3.62	104.73	110.34
5	A	1308	CLR	C13-C17-C20	-3.56	114.00	119.50
5	A	1309	CLR	C10-C9-C8	-3.46	107.66	112.71
5	A	1309	CLR	C19-C10-C9	-3.45	107.79	111.66
5	A	1316	CLR	C13-C14-C8	-3.44	109.53	114.41
5	A	1312	CLR	C13-C17-C20	-3.41	114.24	119.50
5	A	1318	CLR	C13-C17-C20	-3.38	114.28	119.50
5	A	1306	CLR	C13-C17-C20	-3.27	114.45	119.50
5	A	1304	CLR	C14-C8-C9	-3.27	104.82	109.09
6	A	1320	TA1	C18-C20-C21	3.26	128.36	121.38
5	A	1305	CLR	C13-C17-C20	-3.25	114.48	119.50
5	A	1319	CLR	C13-C17-C20	-3.22	114.52	119.50
5	A	1315	CLR	C13-C14-C8	-3.21	109.86	114.41
5	A	1308	CLR	C15-C14-C8	-3.21	113.98	119.10
5	A	1315	CLR	C19-C10-C9	-3.14	108.13	111.66
5	A	1305	CLR	C7-C8-C14	-3.11	106.53	110.93
5	A	1306	CLR	C7-C8-C14	-3.09	106.55	110.93
5	A	1318	CLR	C13-C14-C8	-3.05	110.08	114.41
5	A	1316	CLR	C19-C10-C9	-3.05	108.24	111.66
5	A	1319	CLR	C19-C10-C9	-3.05	108.24	111.66
5	A	1305	CLR	C3-C4-C5	-3.03	107.22	112.05
5	A	1314	CLR	C4-C5-C6	-2.94	116.58	120.57
5	A	1311	CLR	C16-C17-C20	-2.93	107.74	112.18
5	A	1319	CLR	C13-C14-C8	-2.93	110.25	114.41
6	A	1320	TA1	O06-C15-C11	2.93	93.78	90.58
6	A	1320	TA1	C26-O11-C27	2.91	121.82	116.58
6	A	1320	TA1	C14-C11-C15	-2.91	82.38	85.38
5	A	1313	CLR	C4-C5-C6	-2.90	116.64	120.57
5	A	1311	CLR	C4-C5-C6	-2.89	116.64	120.57
6	A	1320	TA1	O11-C27-O12	-2.89	118.73	123.95
5	A	1312	CLR	C10-C9-C8	-2.89	108.50	112.71
5	A	1304	CLR	C13-C14-C8	-2.86	110.36	114.41
5	A	1313	CLR	C13-C14-C8	-2.85	110.36	114.41
7	A	1322	3PE	O31-C31-C32	2.85	120.53	111.83
5	A	1318	CLR	C19-C10-C9	-2.84	108.47	111.66
5	A	1313	CLR	C13-C17-C20	-2.83	115.12	119.50
5	A	1306	CLR	C4-C5-C6	-2.83	116.73	120.57
6	A	1320	TA1	C11-O04-C12	2.83	126.34	119.17
5	A	1310	CLR	C13-C17-C20	-2.82	115.14	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1320	TA1	C01-C43-C26	2.81	120.17	114.98
6	A	1320	TA1	O04-C11-C10	2.81	113.59	109.24
5	A	1318	CLR	C4-C5-C6	-2.81	116.76	120.57
5	A	1314	CLR	C15-C14-C8	-2.81	114.62	119.10
6	A	1320	TA1	C37-C29-N01	-2.81	106.67	112.07
5	A	1309	CLR	C21-C20-C22	-2.80	106.01	110.34
4	A	1302	NAG	C2-N2-C7	2.79	126.64	122.90
5	A	1312	CLR	C4-C5-C6	-2.78	116.80	120.57
4	A	1303	NAG	C2-N2-C7	2.78	126.62	122.90
5	A	1318	CLR	C3-C4-C5	-2.75	107.67	112.05
6	A	1320	TA1	C16-C15-C11	-2.74	115.91	119.63
5	A	1312	CLR	C13-C14-C8	-2.73	110.53	114.41
5	A	1312	CLR	C21-C20-C17	-2.73	108.79	112.88
5	A	1319	CLR	C3-C4-C5	-2.73	107.71	112.05
5	A	1307	CLR	C4-C5-C6	-2.71	116.89	120.57
5	A	1313	CLR	C15-C14-C8	-2.71	114.77	119.10
7	A	1321	3PE	O31-C31-C32	2.69	120.03	111.83
6	A	1320	TA1	C26-C25-C24	2.68	122.15	117.73
5	A	1317	CLR	C4-C5-C6	-2.67	116.95	120.57
5	A	1306	CLR	C15-C14-C8	-2.67	114.84	119.10
5	A	1312	CLR	C3-C4-C5	-2.67	107.81	112.05
5	A	1318	CLR	C21-C20-C17	-2.65	108.91	112.88
5	A	1310	CLR	C4-C5-C6	-2.64	116.99	120.57
5	A	1310	CLR	C10-C9-C8	-2.63	108.87	112.71
7	A	1322	3PE	O12-P-O14	-2.62	100.24	112.44
5	A	1318	CLR	C7-C8-C14	-2.62	107.22	110.93
5	A	1306	CLR	C10-C9-C8	-2.62	108.89	112.71
5	A	1319	CLR	C4-C5-C6	-2.62	117.02	120.57
6	A	1320	TA1	C19-C18-C20	2.61	113.30	106.56
5	A	1308	CLR	C4-C5-C6	-2.59	117.05	120.57
5	A	1311	CLR	C15-C14-C8	-2.59	114.97	119.10
5	A	1312	CLR	C15-C14-C8	-2.58	114.98	119.10
5	A	1311	CLR	C7-C8-C14	-2.58	107.28	110.93
5	A	1319	CLR	C2-C3-C4	-2.56	106.70	110.29
5	A	1315	CLR	C4-C5-C6	-2.55	117.11	120.57
5	A	1309	CLR	C15-C14-C8	-2.54	115.04	119.10
5	A	1306	CLR	C21-C20-C17	-2.54	109.07	112.88
5	A	1305	CLR	C15-C14-C8	-2.54	115.05	119.10
5	A	1304	CLR	C4-C5-C6	-2.54	117.12	120.57
5	A	1307	CLR	C15-C14-C8	-2.52	115.08	119.10
5	A	1310	CLR	C15-C14-C8	-2.50	115.10	119.10
5	A	1316	CLR	C21-C20-C17	-2.49	109.14	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1316	CLR	C4-C5-C6	-2.48	117.21	120.57
5	A	1313	CLR	C8-C7-C6	-2.47	109.34	112.76
5	A	1315	CLR	C21-C20-C22	-2.47	106.52	110.34
7	A	1321	3PE	O12-P-O14	-2.46	100.99	112.44
5	A	1314	CLR	C10-C9-C8	-2.45	109.13	112.71
5	A	1319	CLR	C10-C9-C8	-2.44	109.14	112.71
5	A	1305	CLR	C19-C10-C9	-2.43	108.94	111.66
5	A	1319	CLR	C4-C5-C10	2.41	119.51	116.42
5	A	1309	CLR	C4-C5-C6	-2.39	117.33	120.57
5	A	1315	CLR	C14-C8-C9	-2.39	105.96	109.09
5	A	1306	CLR	C4-C5-C10	2.38	119.47	116.42
4	A	1301	NAG	C8-C7-N2	2.38	120.06	116.12
5	A	1311	CLR	C3-C4-C5	-2.37	108.27	112.05
5	A	1307	CLR	C7-C8-C14	-2.37	107.58	110.93
6	A	1320	TA1	C45-C24-C21	2.36	126.51	119.08
5	A	1310	CLR	C3-C4-C5	-2.34	108.32	112.05
5	A	1312	CLR	C7-C8-C14	-2.34	107.62	110.93
5	A	1316	CLR	C14-C8-C9	-2.33	106.04	109.09
5	A	1311	CLR	C14-C8-C9	-2.33	106.04	109.09
5	A	1318	CLR	C4-C5-C10	2.33	119.40	116.42
5	A	1308	CLR	C3-C4-C5	-2.32	108.36	112.05
5	A	1314	CLR	C7-C8-C14	-2.31	107.66	110.93
5	A	1310	CLR	C13-C14-C8	-2.31	111.14	114.41
5	A	1308	CLR	C13-C14-C8	-2.30	111.14	114.41
5	A	1312	CLR	C2-C3-C4	-2.30	107.05	110.29
6	A	1320	TA1	C45-C01-C02	2.30	114.46	111.93
5	A	1305	CLR	C2-C3-C4	-2.30	107.06	110.29
5	A	1307	CLR	C3-C4-C5	-2.29	108.40	112.05
6	A	1320	TA1	C24-C21-C20	-2.29	108.33	113.31
6	A	1320	TA1	C29-C28-C27	2.28	117.04	111.01
5	A	1316	CLR	C9-C10-C5	2.26	112.96	109.65
5	A	1316	CLR	C17-C13-C14	2.26	102.69	100.10
5	A	1305	CLR	C4-C5-C6	-2.23	117.55	120.57
5	A	1316	CLR	C22-C20-C17	2.23	114.95	110.33
5	A	1304	CLR	C15-C14-C8	-2.23	115.55	119.10
5	A	1314	CLR	C16-C15-C14	-2.22	100.80	105.14
5	A	1307	CLR	C13-C14-C8	-2.21	111.28	114.41
5	A	1309	CLR	C13-C14-C8	-2.20	111.29	114.41
5	A	1304	CLR	C3-C4-C5	-2.20	108.55	112.05
6	A	1320	TA1	C15-C16-C17	-2.19	107.34	113.52
5	A	1304	CLR	C7-C8-C14	-2.18	107.84	110.93
5	A	1312	CLR	C21-C20-C22	-2.18	106.96	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1305	CLR	C13-C14-C8	-2.18	111.32	114.41
5	A	1318	CLR	C9-C10-C5	2.17	112.83	109.65
5	A	1310	CLR	C21-C20-C22	-2.16	106.99	110.34
6	A	1320	TA1	C43-C01-C45	2.16	115.38	111.48
5	A	1318	CLR	C15-C14-C8	-2.13	115.70	119.10
5	A	1306	CLR	C16-C15-C14	-2.13	100.98	105.14
5	A	1319	CLR	C16-C15-C14	-2.12	100.99	105.14
5	A	1311	CLR	C13-C14-C8	-2.12	111.40	114.41
5	A	1317	CLR	C7-C8-C14	-2.12	107.93	110.93
4	A	1301	NAG	C2-N2-C7	-2.12	120.06	122.90
5	A	1307	CLR	C14-C8-C9	-2.12	106.32	109.09
5	A	1309	CLR	C16-C15-C14	-2.10	101.03	105.14
5	A	1307	CLR	C16-C15-C14	-2.10	101.04	105.14
6	A	1320	TA1	O04-C11-C15	-2.10	107.43	112.26
5	A	1304	CLR	C18-C13-C14	-2.08	107.90	111.68
5	A	1314	CLR	C4-C5-C10	2.05	119.05	116.42
5	A	1318	CLR	C2-C3-C4	-2.04	107.42	110.29
5	A	1319	CLR	C7-C8-C14	-2.04	108.05	110.93
5	A	1308	CLR	C12-C13-C17	2.03	119.59	116.60
5	A	1310	CLR	C16-C15-C14	-2.02	101.18	105.14
5	A	1314	CLR	C12-C13-C17	2.02	119.58	116.60
5	A	1309	CLR	C13-C17-C20	-2.02	116.38	119.50
6	A	1320	TA1	O11-C26-C25	2.02	114.64	109.85
5	A	1312	CLR	C9-C10-C5	2.01	112.59	109.65
4	A	1302	NAG	O7-C7-C8	-2.00	118.48	122.05

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1320	TA1	O10-C22-O09-C21
6	A	1320	TA1	C23-C22-O09-C21
6	A	1320	TA1	O12-C27-O11-C26
6	A	1320	TA1	C27-C28-C29-N01
6	A	1320	TA1	O13-C28-C29-N01
6	A	1320	TA1	O13-C28-C29-C37
7	A	1321	3PE	C1-O11-P-O13
7	A	1321	3PE	C1-O11-P-O14
7	A	1321	3PE	C11-O13-P-O14
7	A	1321	3PE	O13-C11-C12-N
7	A	1322	3PE	C11-O13-P-O11
7	A	1322	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
7	A	1322	3PE	C11-O13-P-O14
7	A	1322	3PE	C22-C21-O21-C2
6	A	1320	TA1	O14-C30-N01-C29
6	A	1320	TA1	C31-C30-N01-C29
5	A	1318	CLR	C21-C20-C22-C23
7	A	1321	3PE	O32-C31-O31-C3
7	A	1322	3PE	O32-C31-O31-C3
5	A	1305	CLR	C13-C17-C20-C21
5	A	1316	CLR	C13-C17-C20-C21
5	A	1317	CLR	C13-C17-C20-C21
5	A	1318	CLR	C13-C17-C20-C22
7	A	1321	3PE	O22-C21-O21-C2
7	A	1322	3PE	O22-C21-O21-C2
7	A	1322	3PE	C32-C31-O31-C3
7	A	1321	3PE	C22-C21-O21-C2
5	A	1317	CLR	C21-C20-C22-C23
5	A	1312	CLR	C16-C17-C20-C21
5	A	1316	CLR	C16-C17-C20-C21
5	A	1317	CLR	C16-C17-C20-C21
5	A	1312	CLR	C13-C17-C20-C21
5	A	1318	CLR	C13-C17-C20-C21
5	A	1308	CLR	C13-C17-C20-C22
5	A	1316	CLR	C13-C17-C20-C22
5	A	1317	CLR	C13-C17-C20-C22
4	A	1302	NAG	O5-C5-C6-O6
7	A	1321	3PE	C32-C31-O31-C3
5	A	1306	CLR	C13-C17-C20-C21
5	A	1316	CLR	C16-C17-C20-C22
4	A	1302	NAG	C4-C5-C6-O6
5	A	1305	CLR	C21-C20-C22-C23
5	A	1307	CLR	C21-C20-C22-C23
5	A	1314	CLR	C21-C20-C22-C23
5	A	1312	CLR	C13-C17-C20-C22
5	A	1305	CLR	C17-C20-C22-C23
5	A	1307	CLR	C17-C20-C22-C23
5	A	1312	CLR	C17-C20-C22-C23
5	A	1317	CLR	C17-C20-C22-C23
6	A	1320	TA1	C28-C27-O11-C26
5	A	1318	CLR	C16-C17-C20-C21
5	A	1305	CLR	C13-C17-C20-C22
5	A	1308	CLR	C17-C20-C22-C23
5	A	1319	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
6	A	1320	TA1	C13-C12-O04-C11
5	A	1308	CLR	C13-C17-C20-C21
5	A	1306	CLR	C13-C17-C20-C22
7	A	1321	3PE	O11-C1-C2-O21
5	A	1311	CLR	C21-C20-C22-C23
5	A	1312	CLR	C21-C20-C22-C23
5	A	1311	CLR	C22-C23-C24-C25
5	A	1305	CLR	C16-C17-C20-C21
5	A	1317	CLR	C16-C17-C20-C22
6	A	1320	TA1	O05-C12-O04-C11
7	A	1321	3PE	C31-C32-C33-C34
5	A	1306	CLR	C20-C22-C23-C24
5	A	1308	CLR	C20-C22-C23-C24
5	A	1316	CLR	C20-C22-C23-C24
5	A	1318	CLR	C20-C22-C23-C24
5	A	1306	CLR	C16-C17-C20-C21
6	A	1320	TA1	C37-C29-N01-C30
7	A	1322	3PE	C21-C22-C23-C24
5	A	1318	CLR	C16-C17-C20-C22
6	A	1320	TA1	O14-C30-C31-C36
5	A	1311	CLR	C17-C20-C22-C23
6	A	1320	TA1	N01-C30-C31-C36
5	A	1305	CLR	C20-C22-C23-C24
5	A	1304	CLR	C20-C22-C23-C24
5	A	1319	CLR	C13-C17-C20-C22
5	A	1310	CLR	C23-C24-C25-C27
5	A	1312	CLR	C23-C24-C25-C26
7	A	1321	3PE	C36-C37-C38-C39
5	A	1310	CLR	C23-C24-C25-C26
5	A	1312	CLR	C23-C24-C25-C27
5	A	1309	CLR	C22-C23-C24-C25
6	A	1320	TA1	O14-C30-C31-C32
6	A	1320	TA1	N01-C30-C31-C32
4	A	1301	NAG	O5-C5-C6-O6
7	A	1322	3PE	C23-C24-C25-C26
7	A	1321	3PE	C25-C26-C27-C28
5	A	1317	CLR	C23-C24-C25-C27
5	A	1310	CLR	C13-C17-C20-C21
7	A	1322	3PE	O11-C1-C2-O21
7	A	1322	3PE	C33-C34-C35-C36
7	A	1321	3PE	C33-C34-C35-C36
7	A	1322	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	A	1313	CLR	C17-C20-C22-C23
7	A	1321	3PE	O11-C1-C2-C3
7	A	1322	3PE	O11-C1-C2-C3
5	A	1318	CLR	C17-C20-C22-C23
5	A	1312	CLR	C16-C17-C20-C22
4	A	1301	NAG	C3-C2-N2-C7
5	A	1308	CLR	C16-C17-C20-C21
5	A	1319	CLR	C13-C17-C20-C21
5	A	1313	CLR	C22-C23-C24-C25
5	A	1304	CLR	C21-C20-C22-C23
7	A	1322	3PE	C3-C2-O21-C21
5	A	1306	CLR	C16-C17-C20-C22
5	A	1308	CLR	C16-C17-C20-C22
5	A	1310	CLR	C16-C17-C20-C21
5	A	1319	CLR	C16-C17-C20-C21
7	A	1321	3PE	C2-C1-O11-P
5	A	1317	CLR	C22-C23-C24-C25
5	A	1319	CLR	C16-C17-C20-C22
5	A	1310	CLR	C13-C17-C20-C22
5	A	1305	CLR	C16-C17-C20-C22
5	A	1313	CLR	C13-C17-C20-C22
4	A	1302	NAG	C1-C2-N2-C7
7	A	1321	3PE	C23-C24-C25-C26
6	A	1320	TA1	C27-C28-C29-C37
5	A	1319	CLR	C21-C20-C22-C23
5	A	1314	CLR	C20-C22-C23-C24
5	A	1308	CLR	C23-C24-C25-C26
5	A	1313	CLR	C20-C22-C23-C24
7	A	1322	3PE	C31-C32-C33-C34
7	A	1321	3PE	C28-C29-C2A-C2B
7	A	1322	3PE	C39-C3A-C3B-C3C
5	A	1317	CLR	C23-C24-C25-C26
5	A	1313	CLR	C13-C17-C20-C21
5	A	1310	CLR	C20-C22-C23-C24
5	A	1308	CLR	C21-C20-C22-C23
7	A	1321	3PE	C3-C2-O21-C21
7	A	1321	3PE	C1-C2-C3-O31
7	A	1321	3PE	O21-C2-C3-O31
5	A	1309	CLR	C13-C17-C20-C21
5	A	1308	CLR	C23-C24-C25-C27
5	A	1314	CLR	C13-C17-C20-C21
5	A	1309	CLR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	A	1309	CLR	C23-C24-C25-C27
6	A	1320	TA1	C28-C29-N01-C30
5	A	1315	CLR	C13-C17-C20-C21
4	A	1303	NAG	C3-C2-N2-C7
7	A	1322	3PE	C1-O11-P-O14
7	A	1322	3PE	C2-C3-O31-C31
5	A	1312	CLR	C20-C22-C23-C24
5	A	1310	CLR	C16-C17-C20-C22
7	A	1322	3PE	C2-C1-O11-P
5	A	1314	CLR	C13-C17-C20-C22
5	A	1311	CLR	C23-C24-C25-C27
5	A	1309	CLR	C21-C20-C22-C23
5	A	1304	CLR	C13-C17-C20-C21
5	A	1311	CLR	C23-C24-C25-C26
5	A	1313	CLR	C16-C17-C20-C22
6	A	1320	TA1	O11-C27-C28-O13
4	A	1303	NAG	C1-C2-N2-C7
4	A	1302	NAG	C3-C2-N2-C7
5	A	1307	CLR	C13-C17-C20-C21
5	A	1314	CLR	C16-C17-C20-C22
7	A	1321	3PE	O31-C31-C32-C33
6	A	1320	TA1	O12-C27-C28-O13
6	A	1320	TA1	C20-C21-O09-C22
7	A	1322	3PE	O31-C31-C32-C33
7	A	1321	3PE	O32-C31-C32-C33
7	A	1322	3PE	C22-C23-C24-C25
7	A	1322	3PE	O32-C31-C32-C33
6	A	1320	TA1	O11-C27-C28-C29

There are no ring outliers.

15 monomers are involved in 42 short contacts:

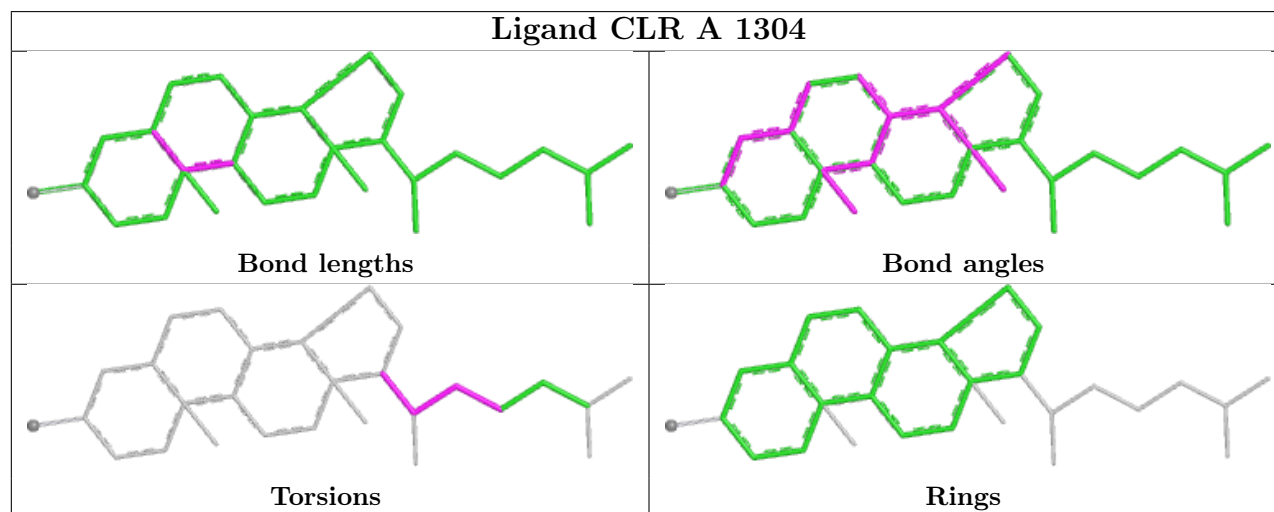
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1304	CLR	1	0
5	A	1311	CLR	3	0
5	A	1319	CLR	4	0
5	A	1308	CLR	3	0
5	A	1313	CLR	4	0
5	A	1315	CLR	3	0
5	A	1316	CLR	4	0
5	A	1306	CLR	3	0
4	A	1301	NAG	4	0

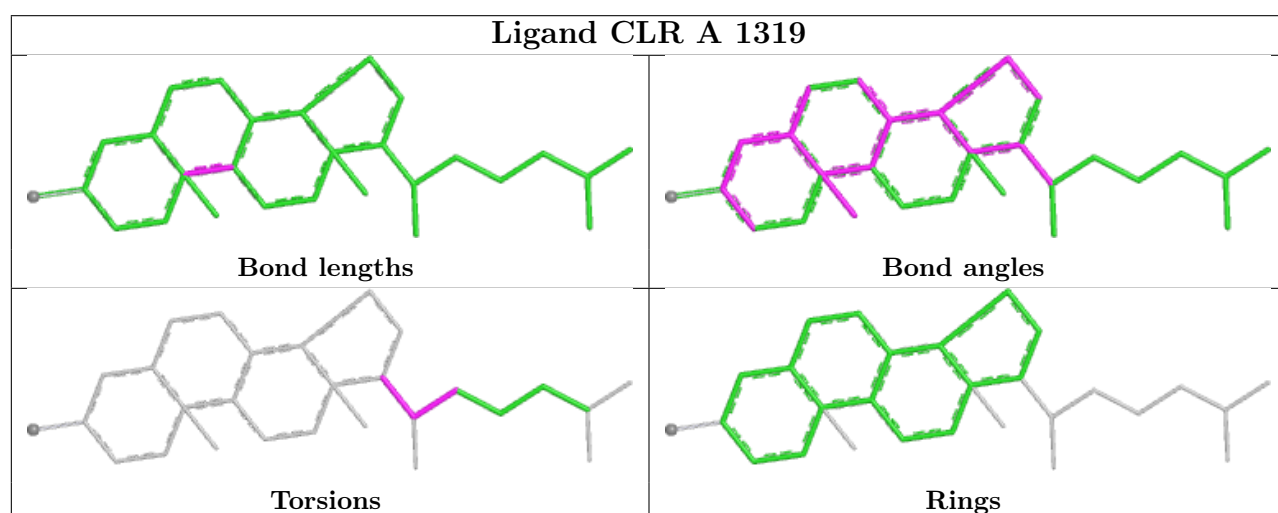
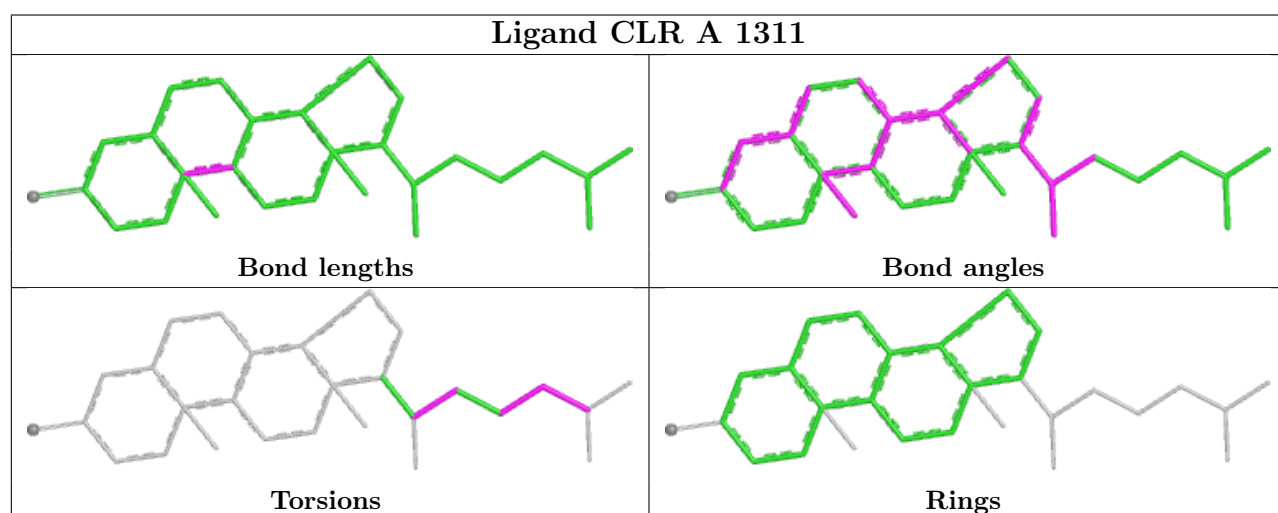
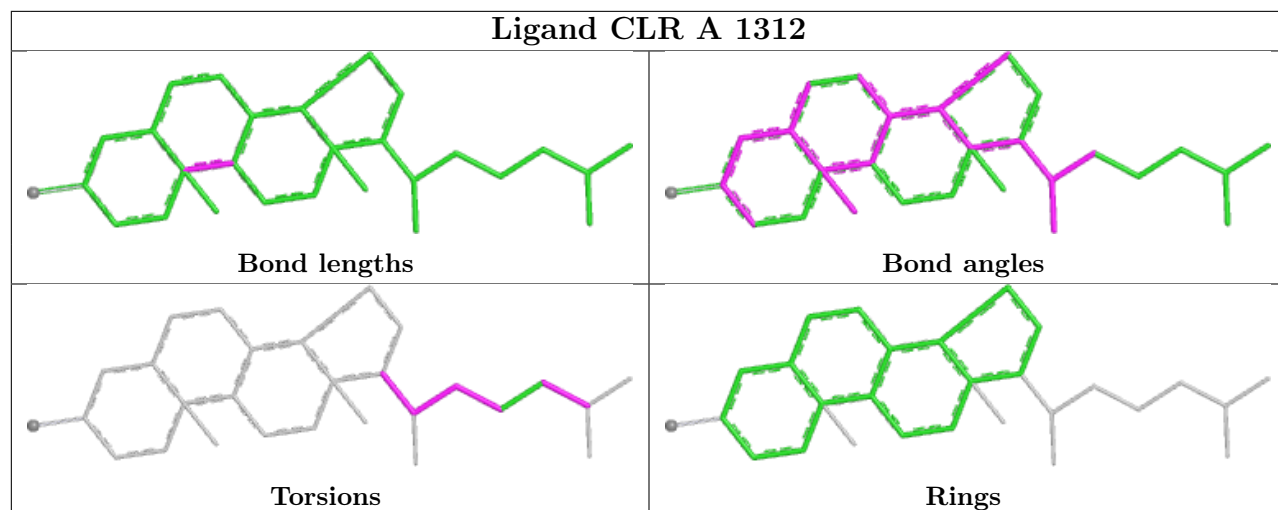
Continued on next page...

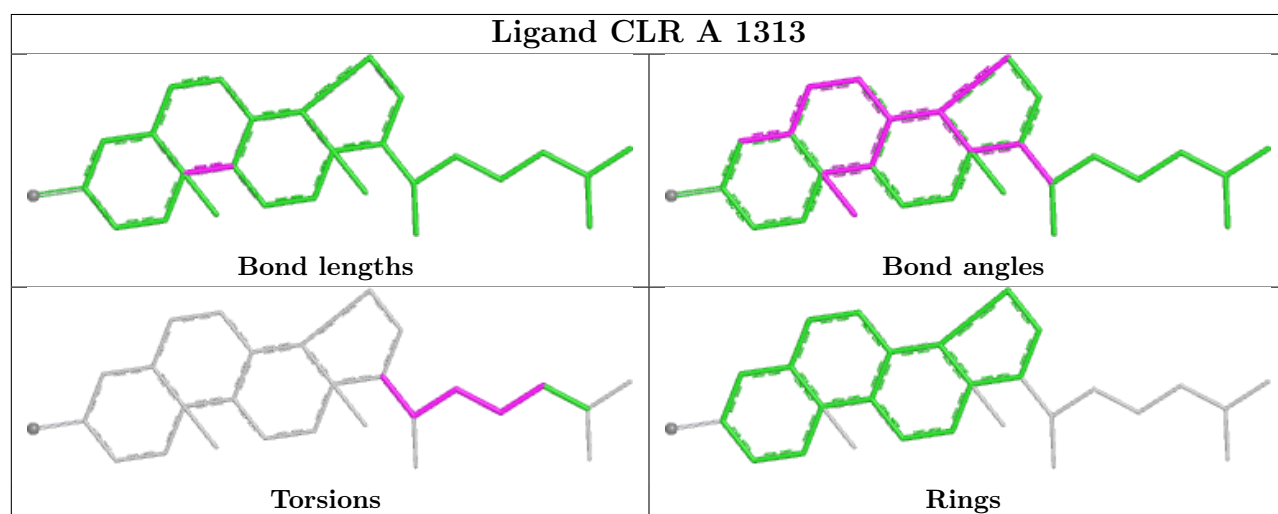
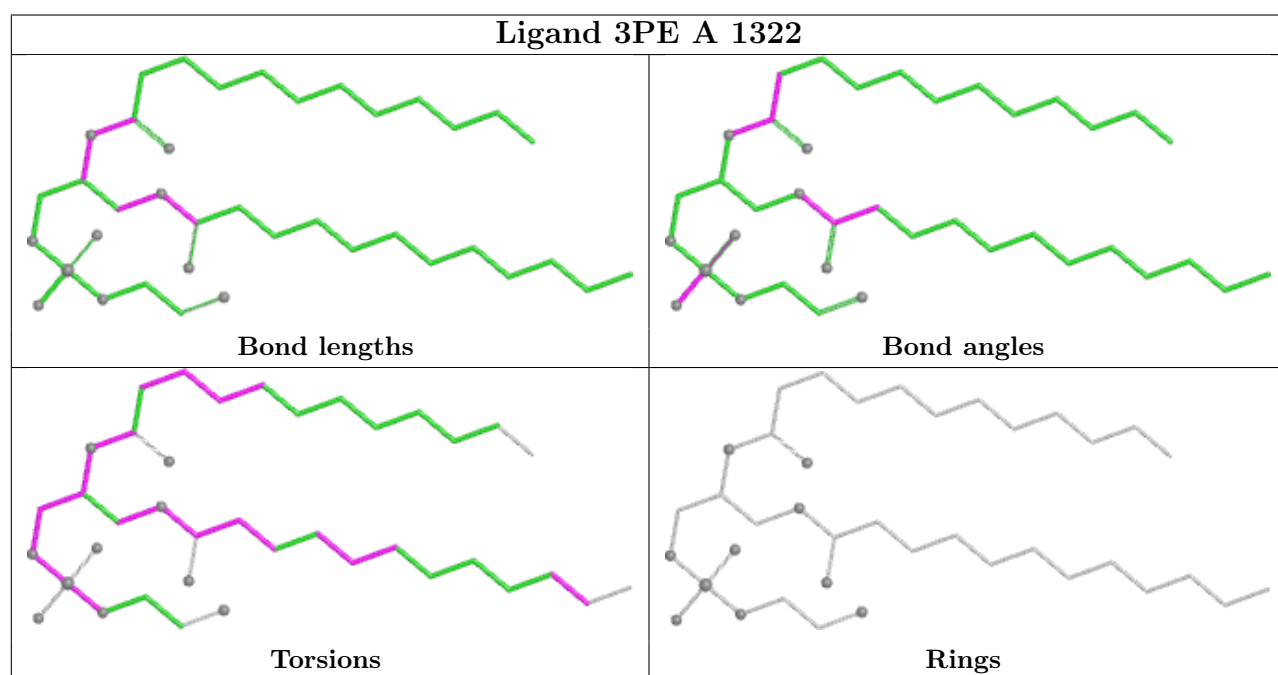
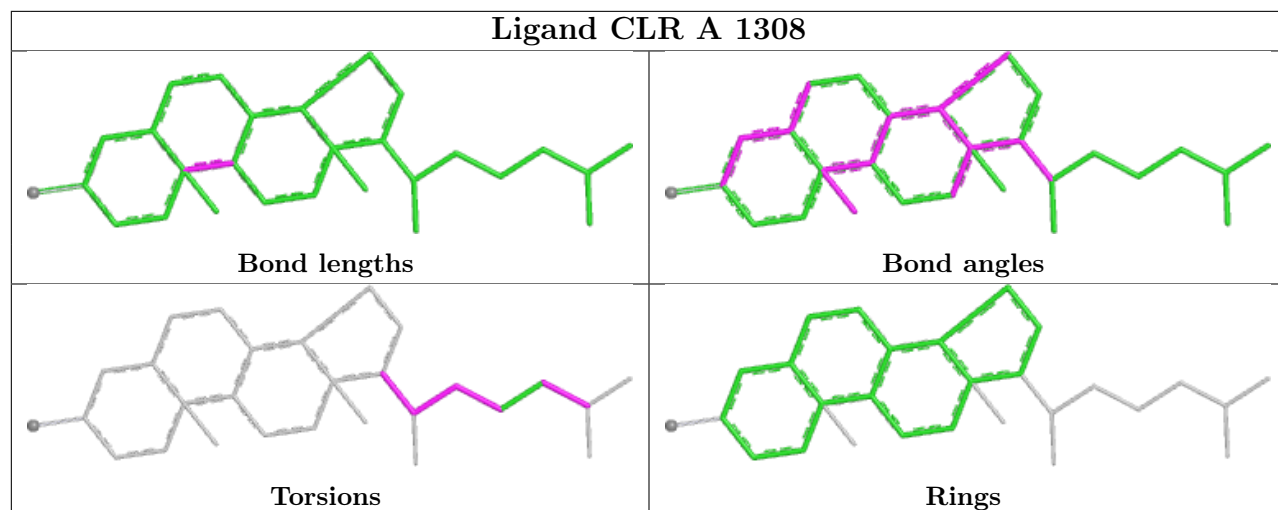
Continued from previous page...

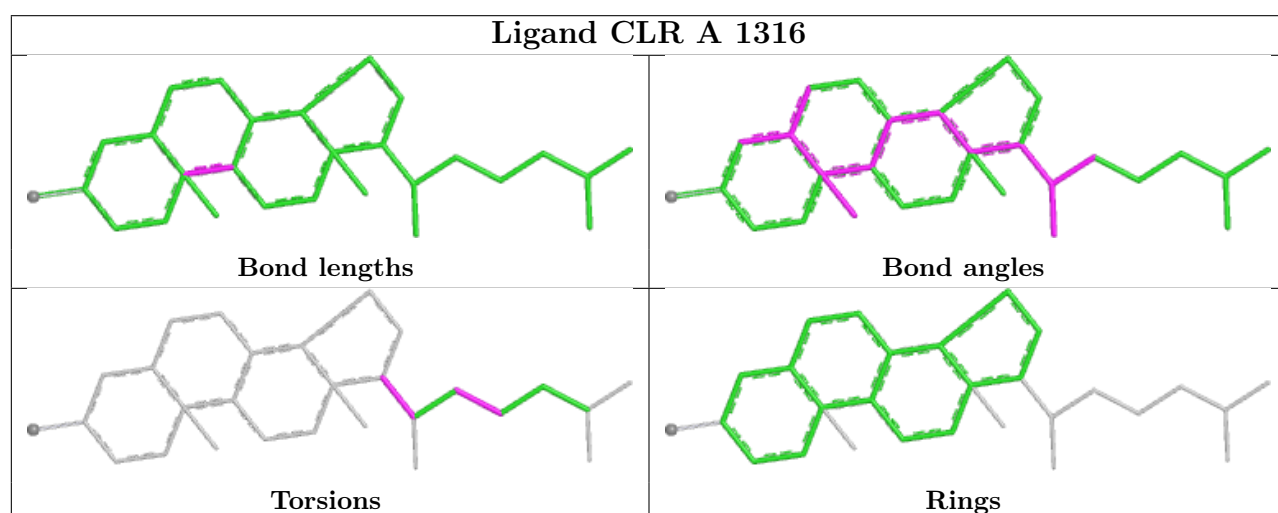
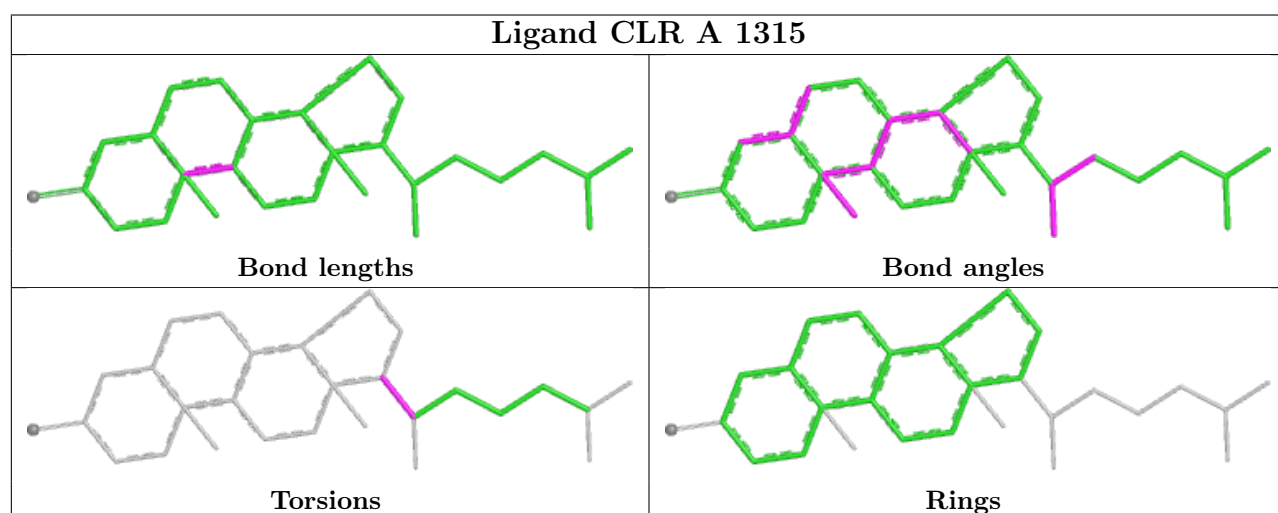
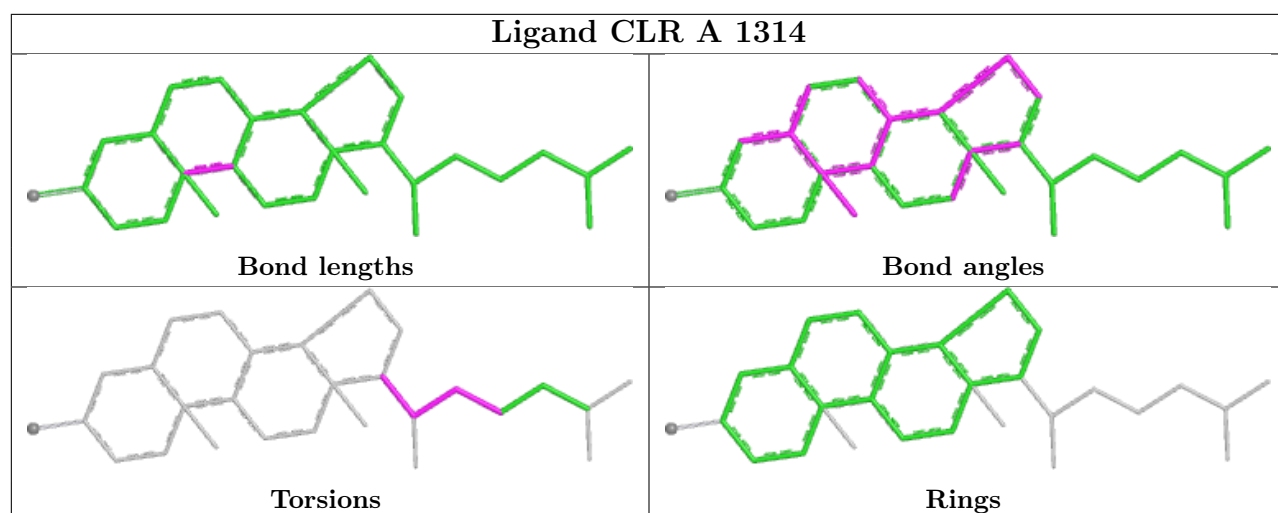
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1318	CLR	5	0
7	A	1321	3PE	1	0
6	A	1320	TA1	6	0
5	A	1317	CLR	1	0
5	A	1310	CLR	3	0
5	A	1305	CLR	2	0

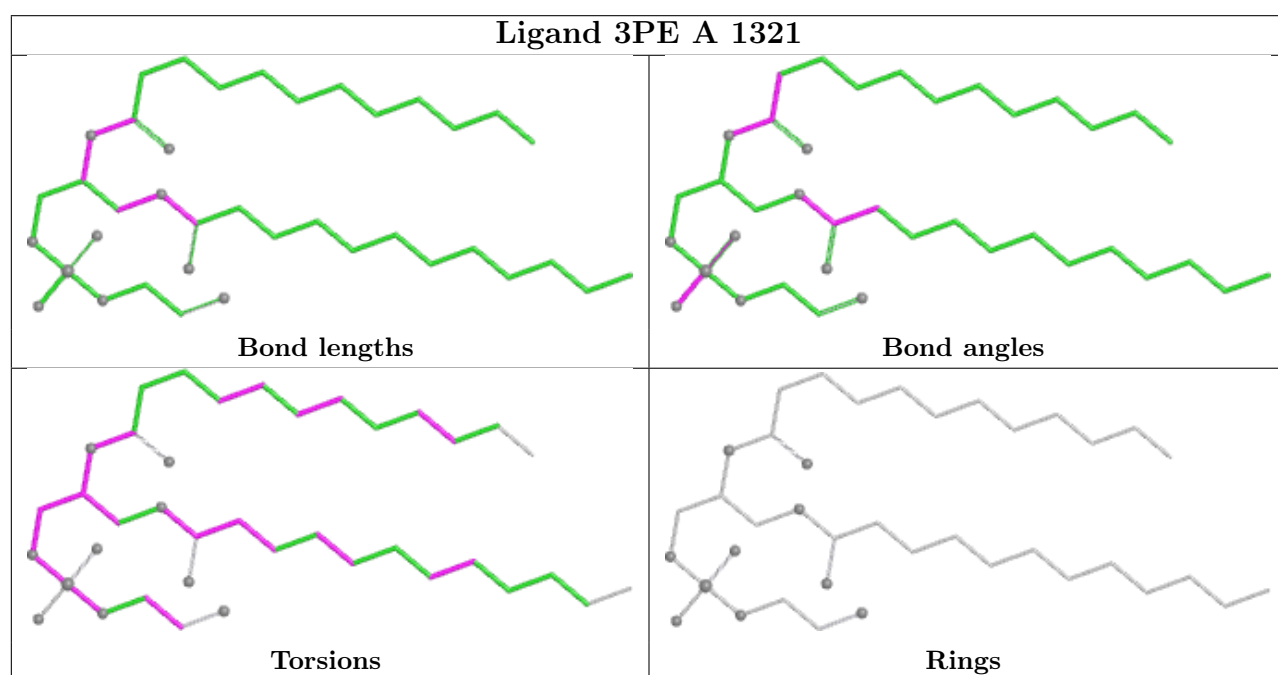
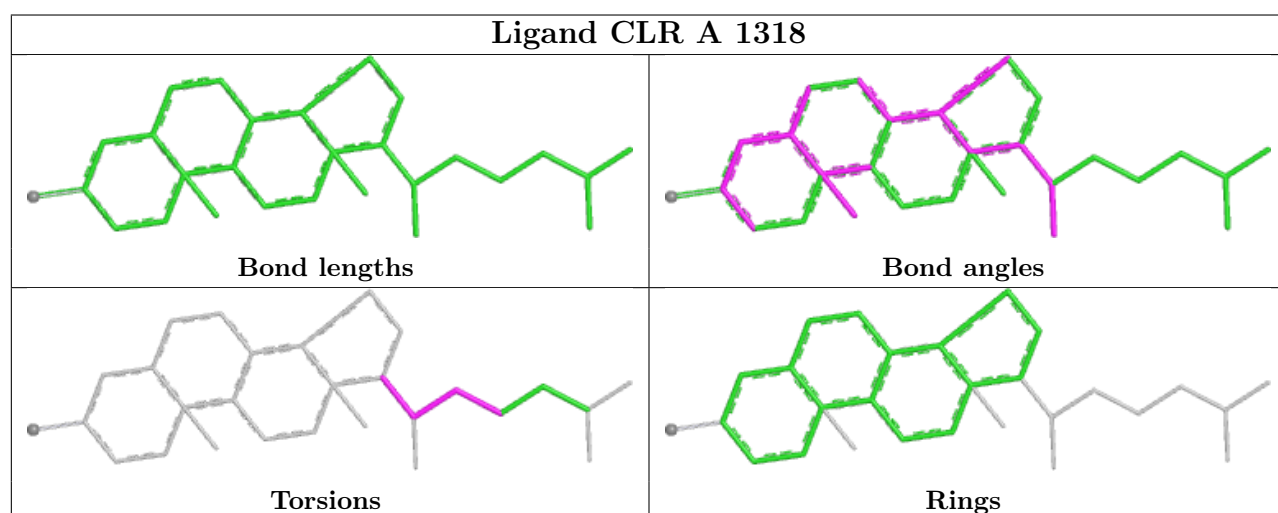
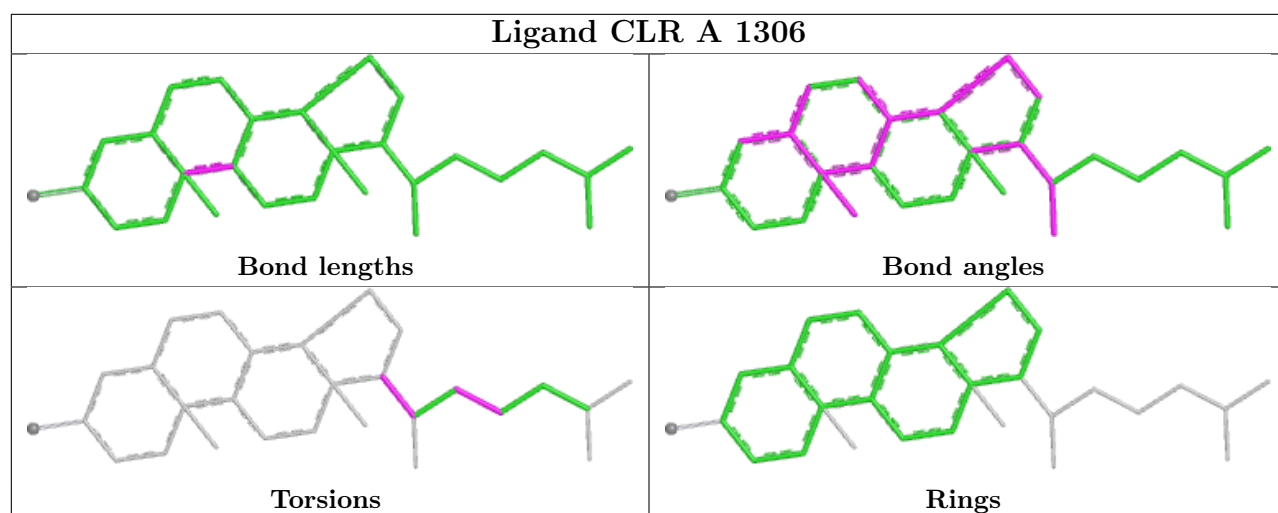
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

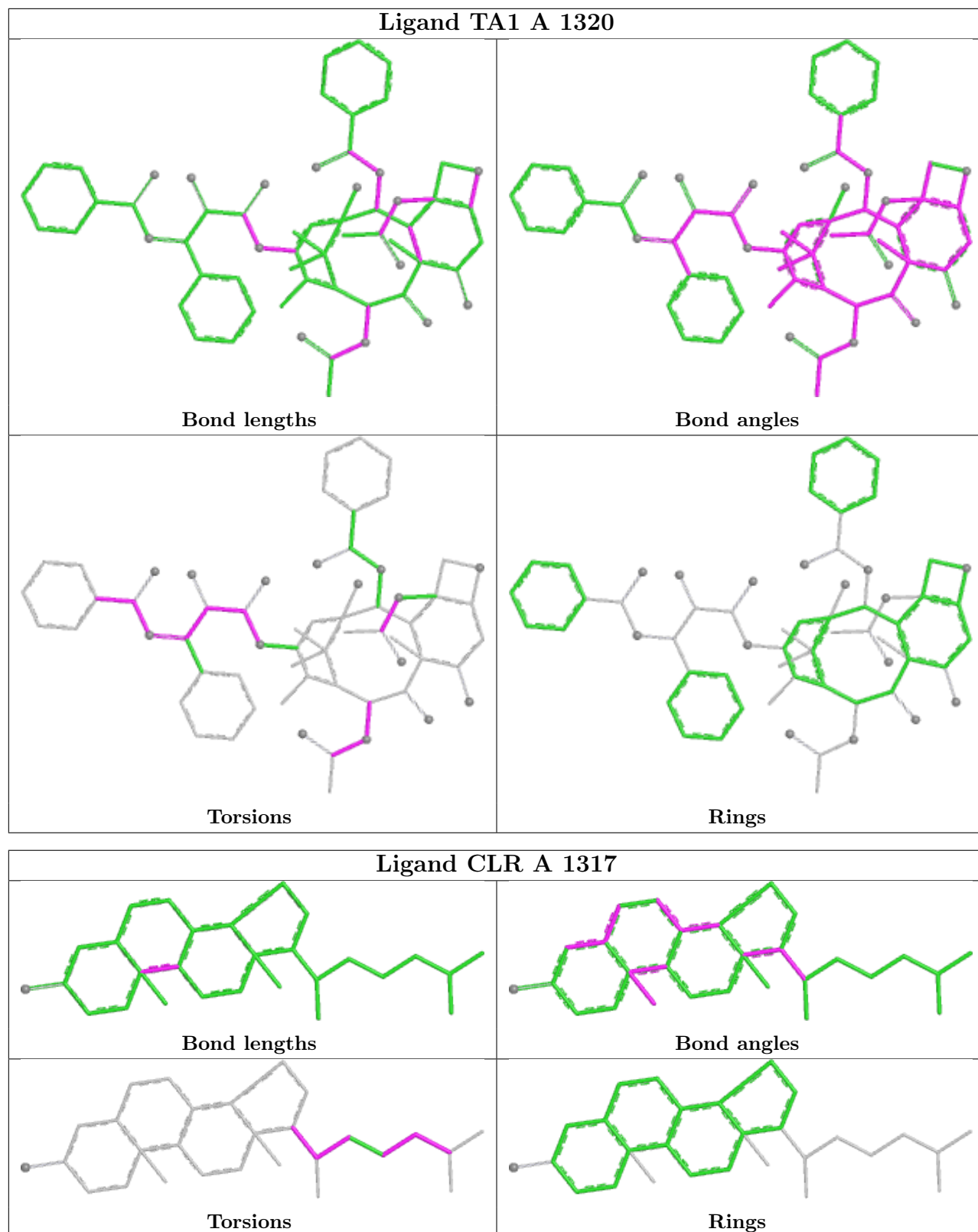


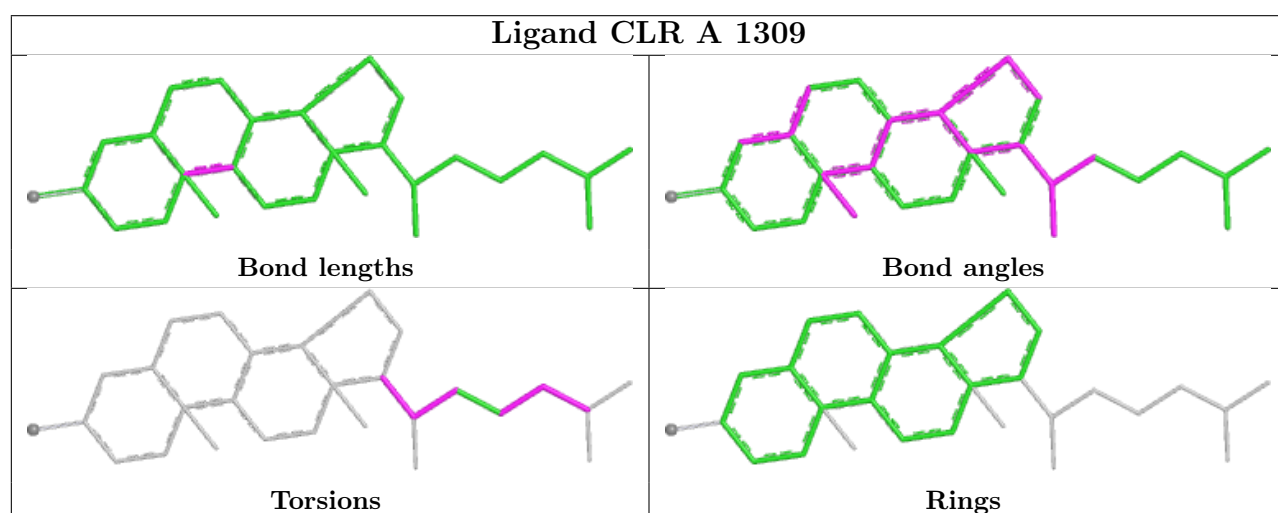
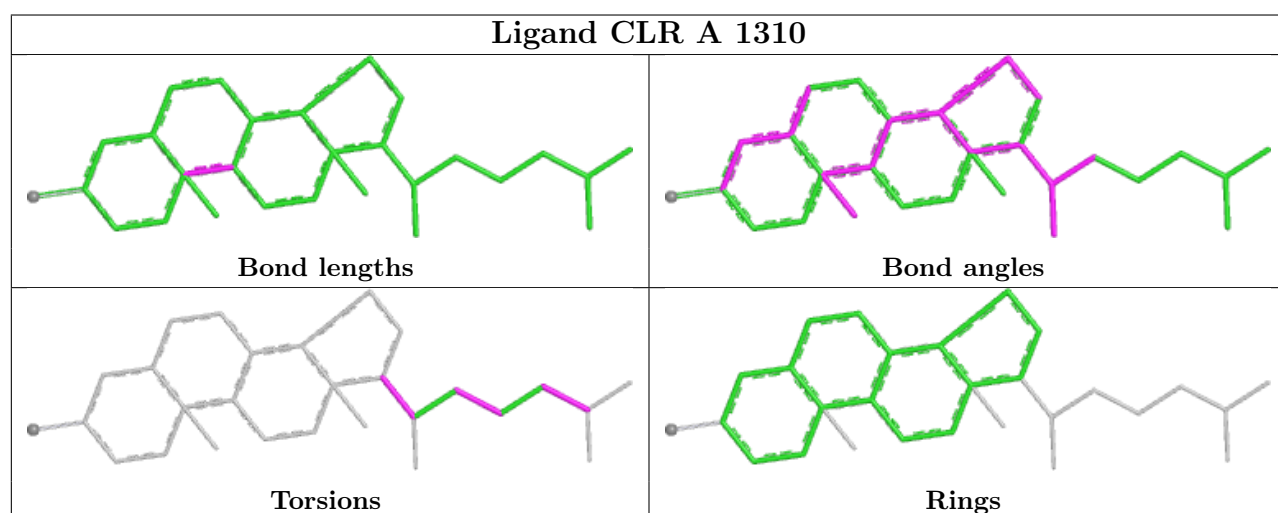
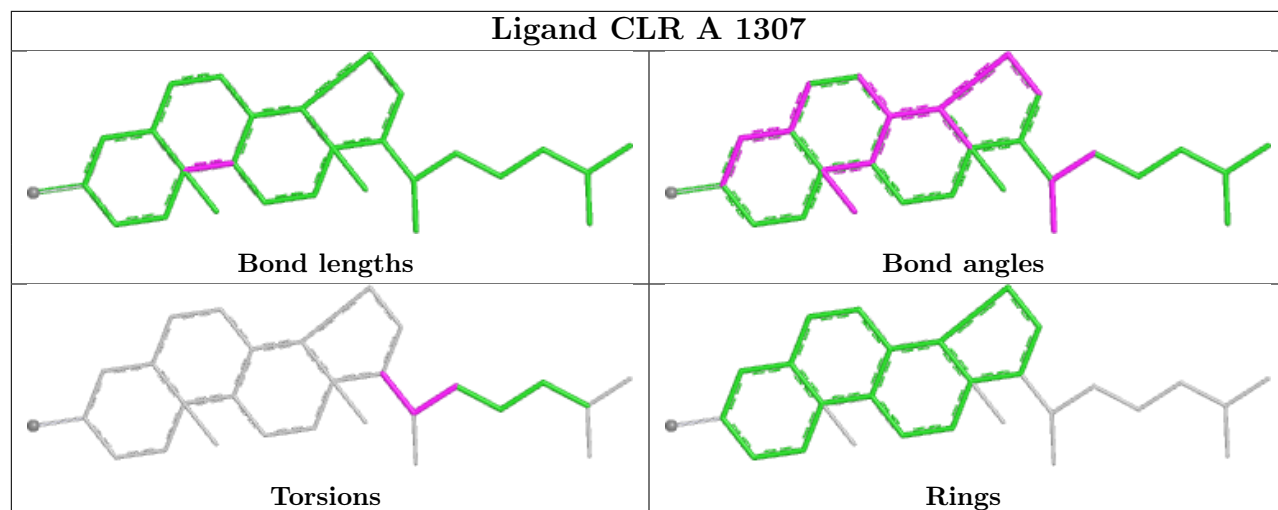


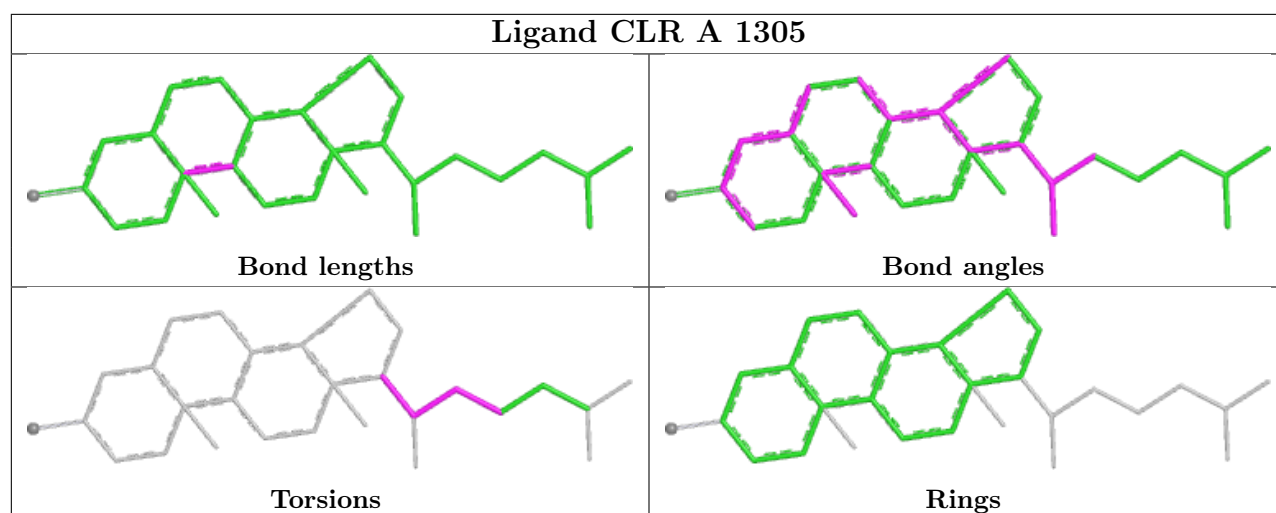












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

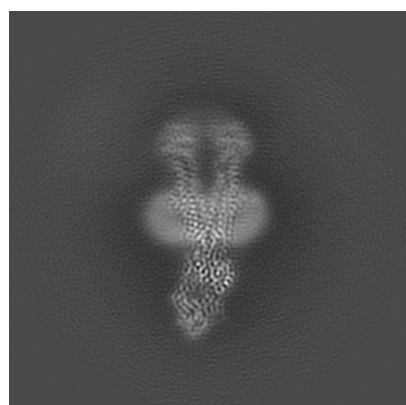
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4539. These allow visual inspection of the internal detail of the map and identification of artifacts.

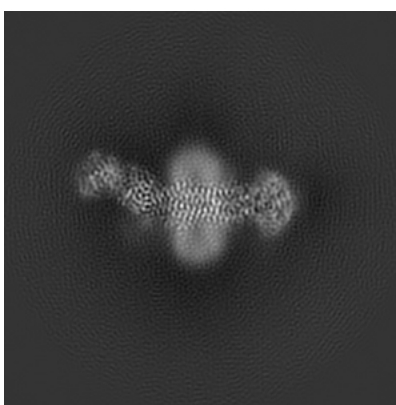
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

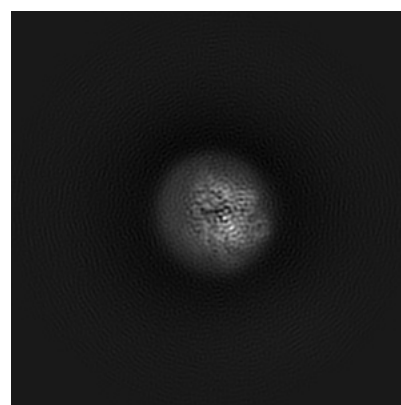
6.1.1 Primary map



X



Y

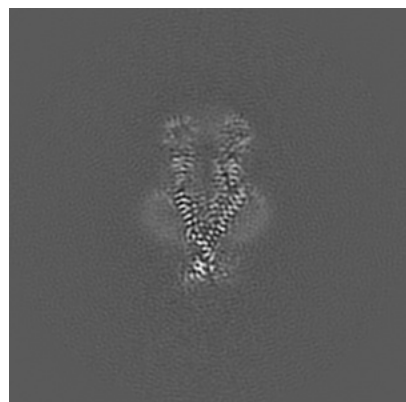


Z

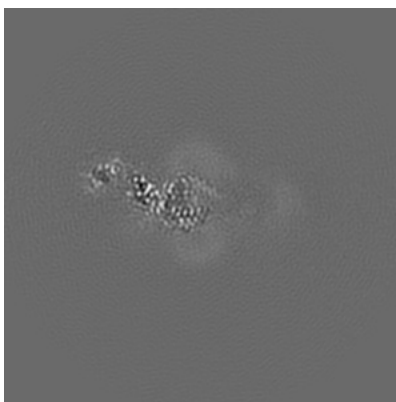
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

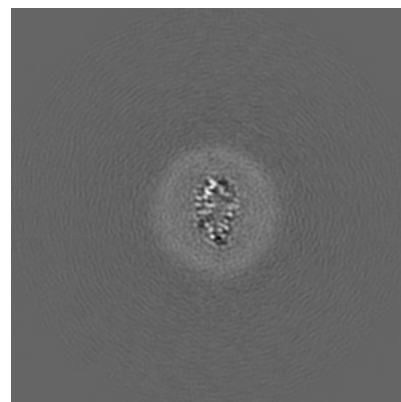
6.2.1 Primary map



X Index: 200



Y Index: 200

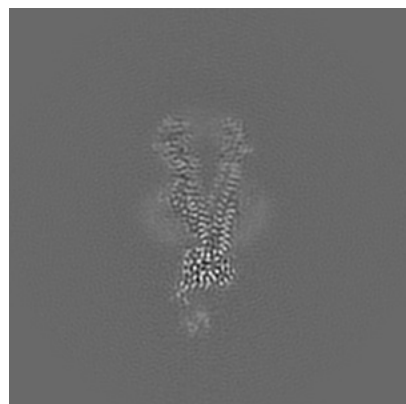


Z Index: 200

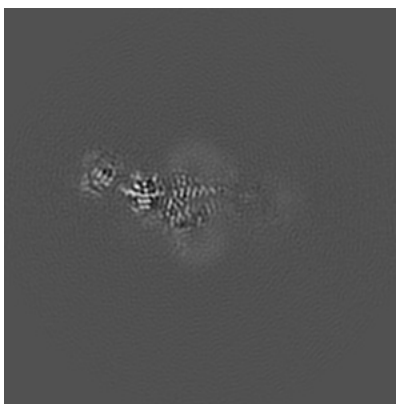
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

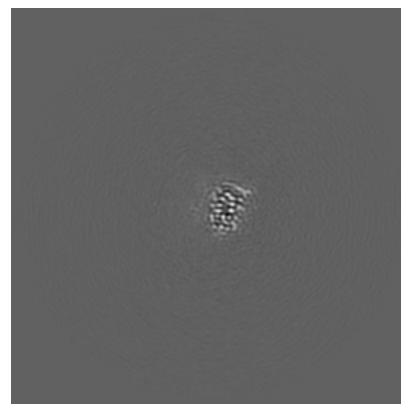
6.3.1 Primary map



X Index: 214



Y Index: 192

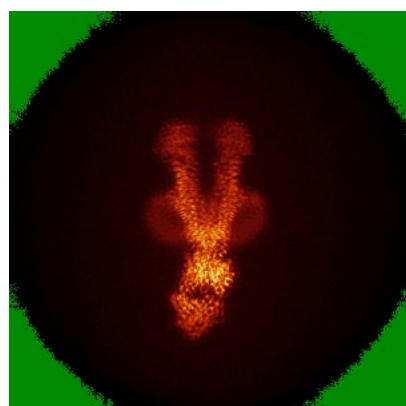


Z Index: 138

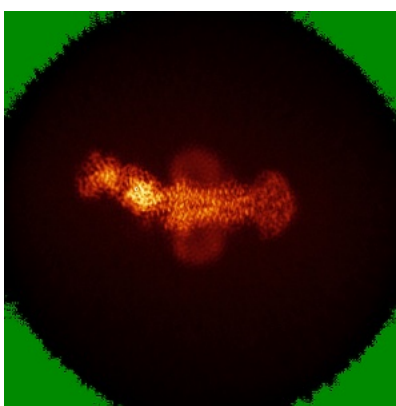
The images above show the largest variance slices of the map in three orthogonal directions.

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

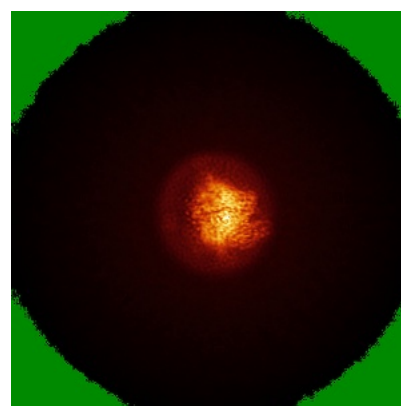
6.4.1 Primary map



X



Y

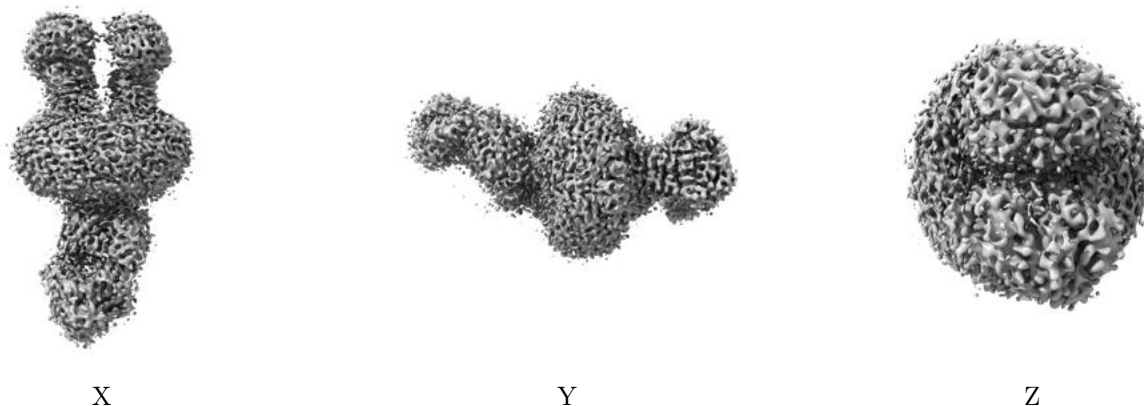


Z

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

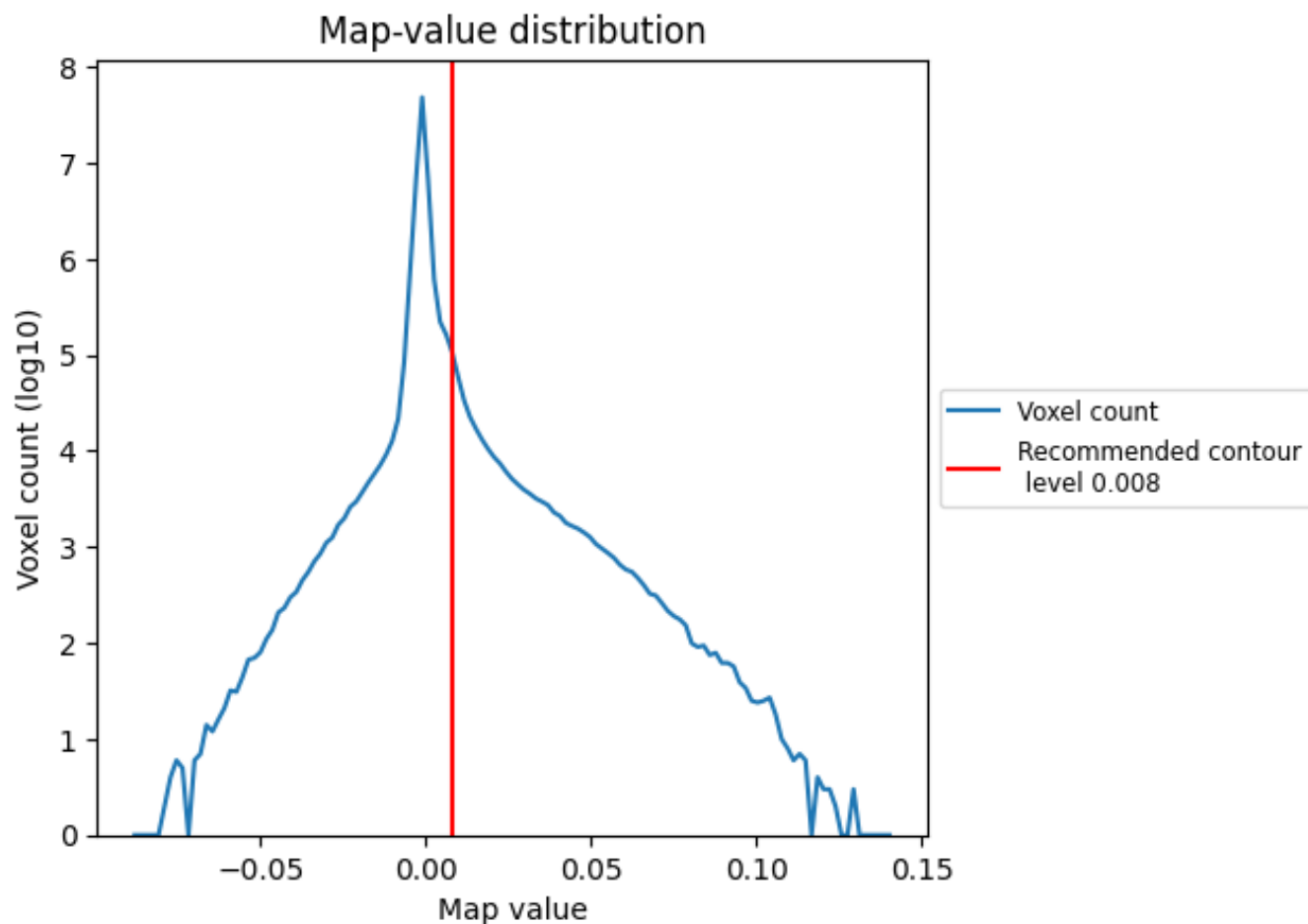
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

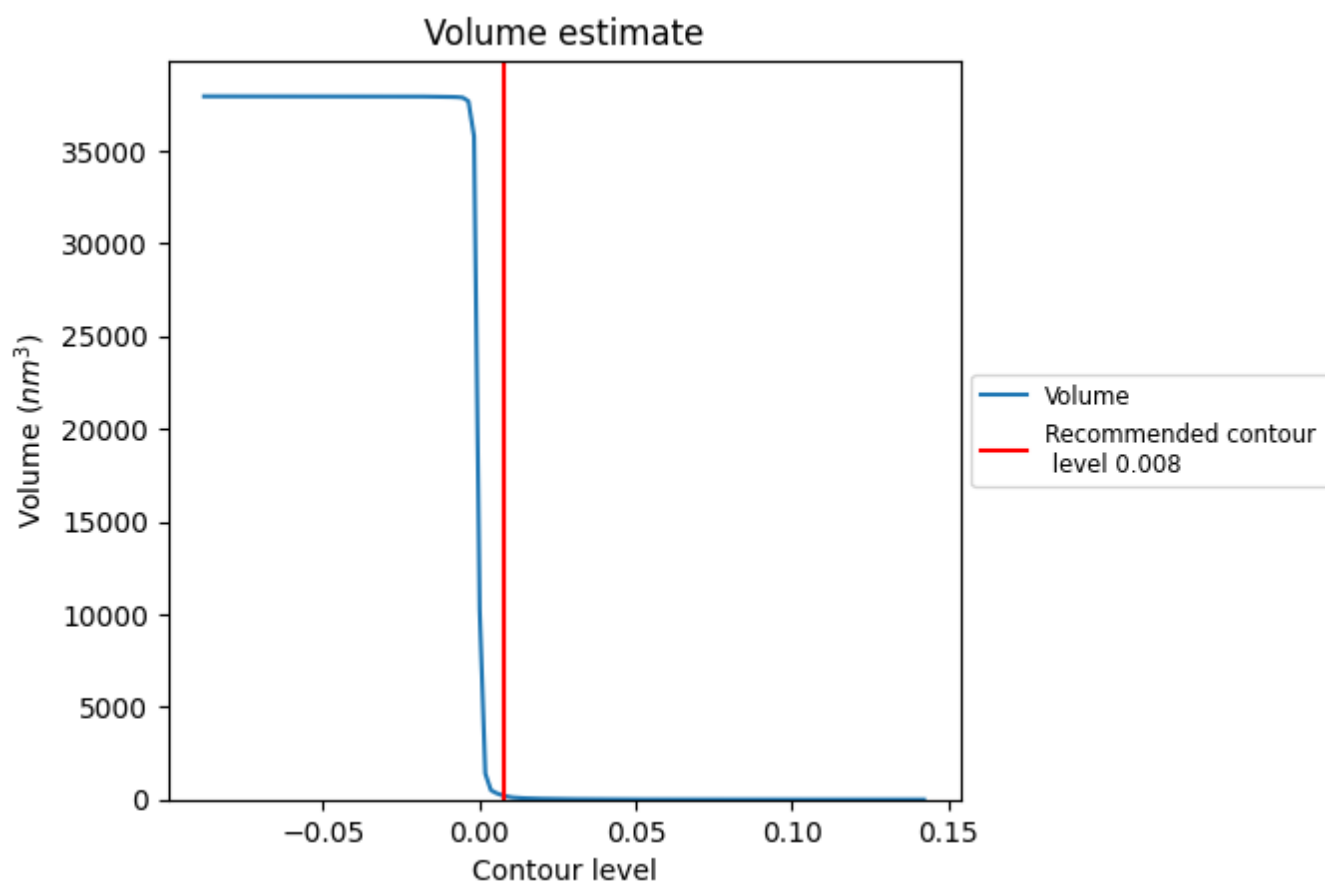
This section contains the results of statistical analysis of the map.

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.

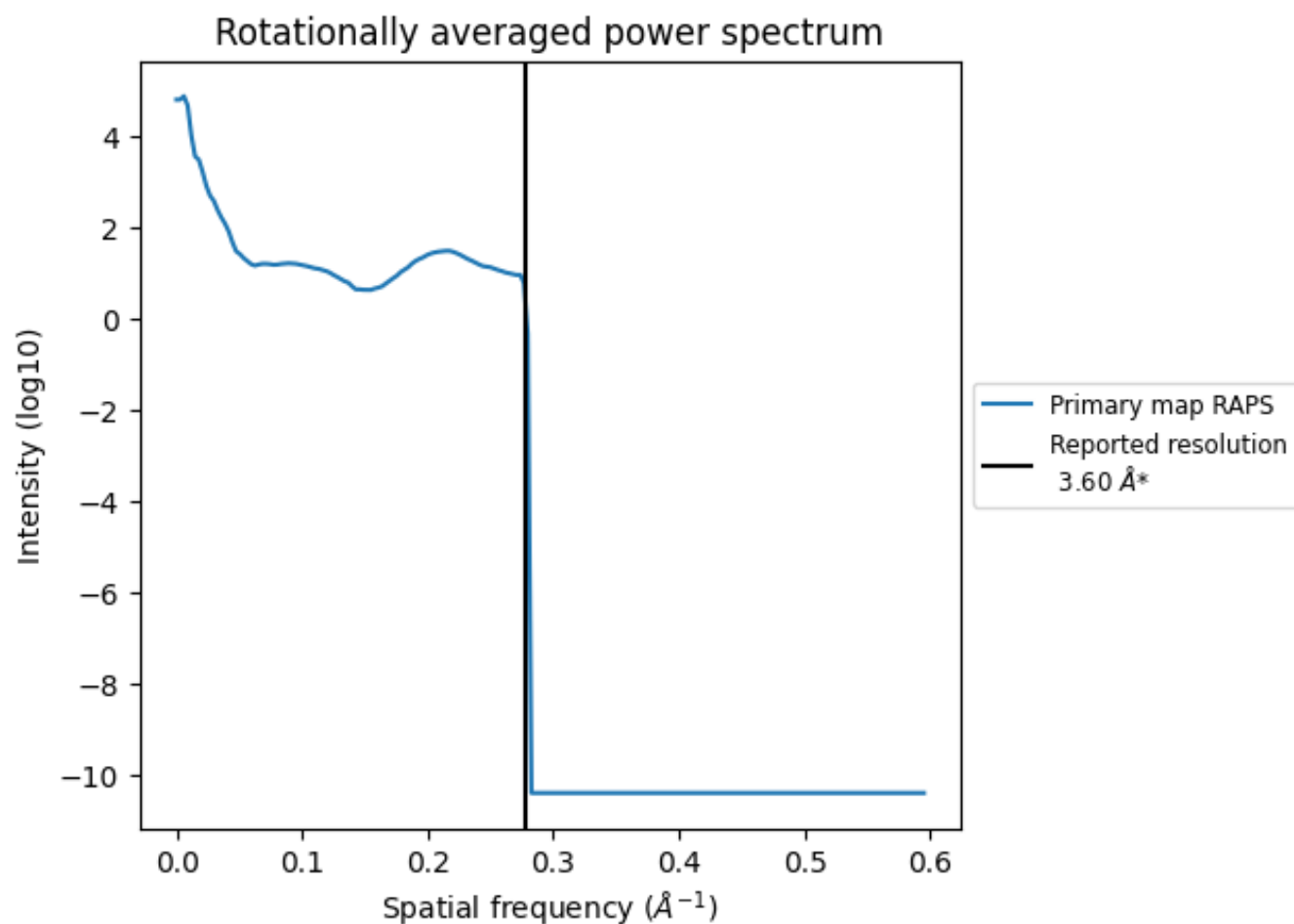
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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 ⓘ

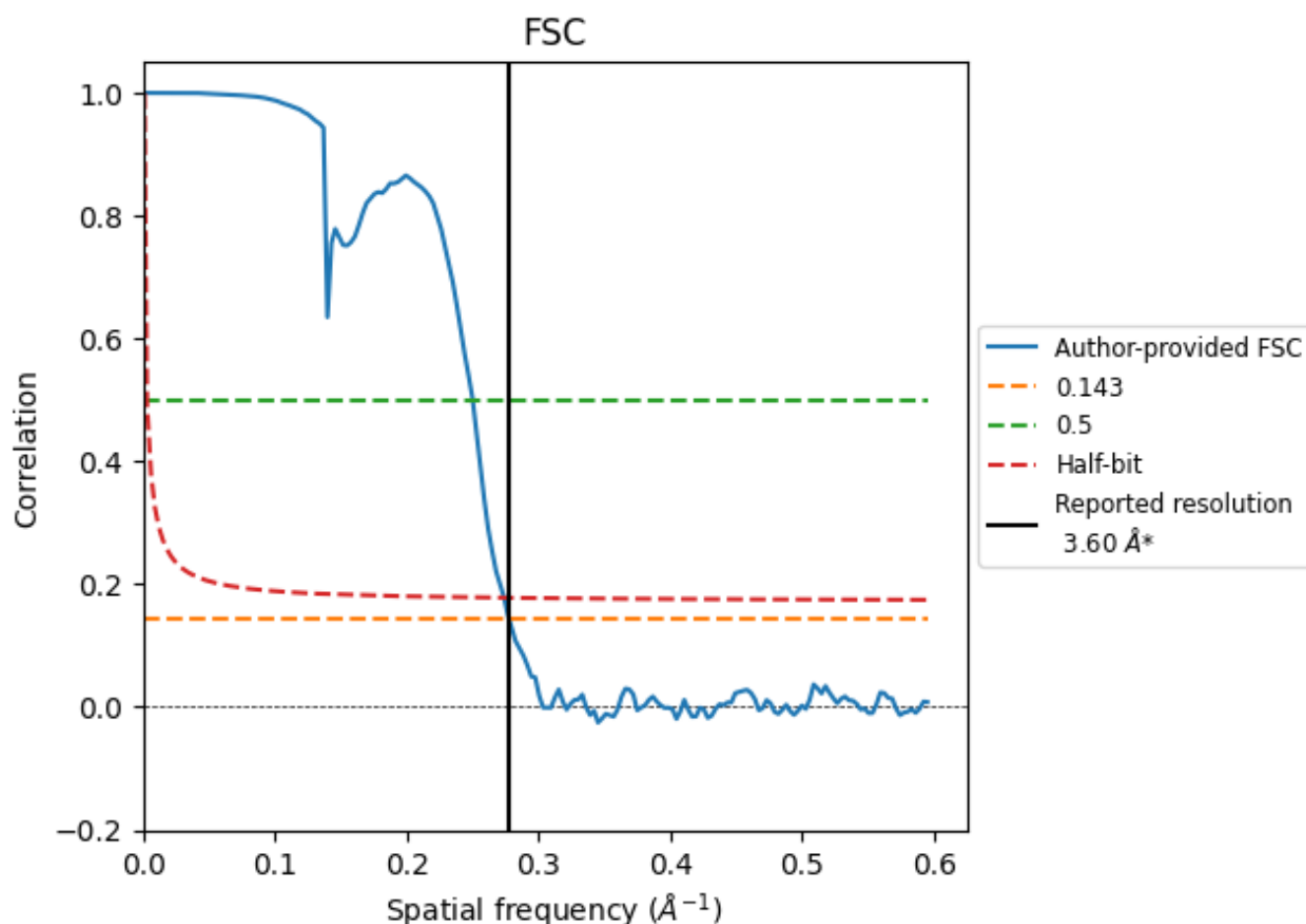


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

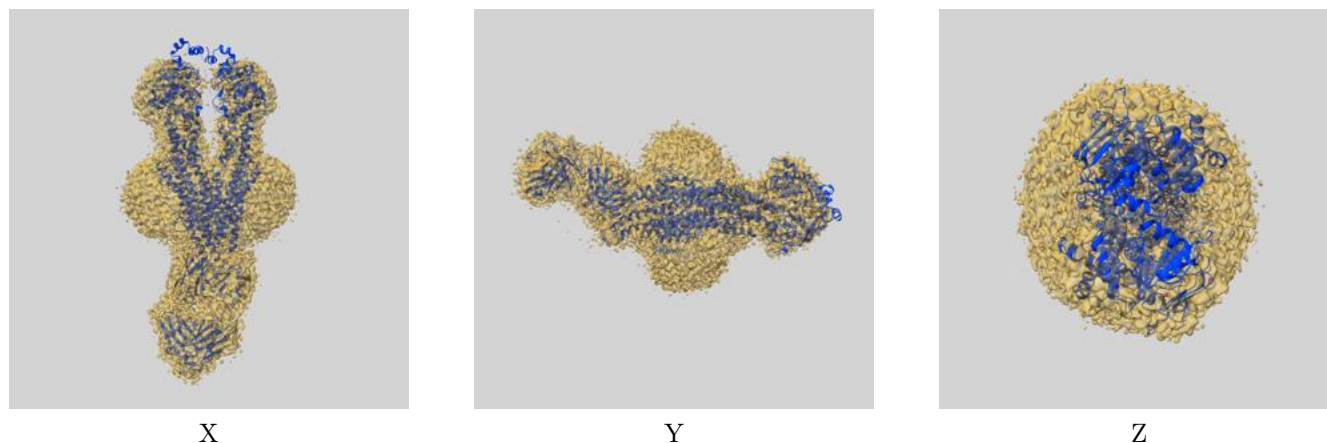
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.00	3.65
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

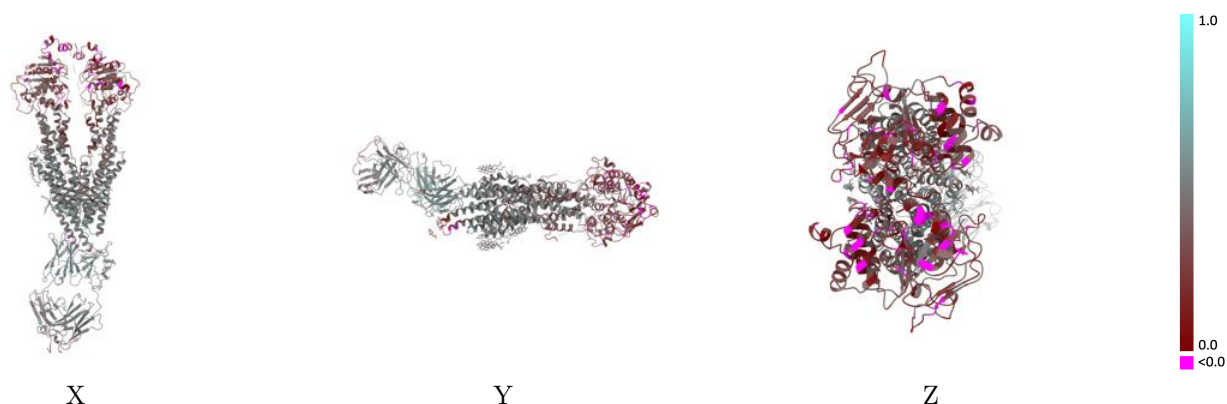
This section contains information regarding the fit between EMDB map EMD-4539 and PDB model 6QEX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



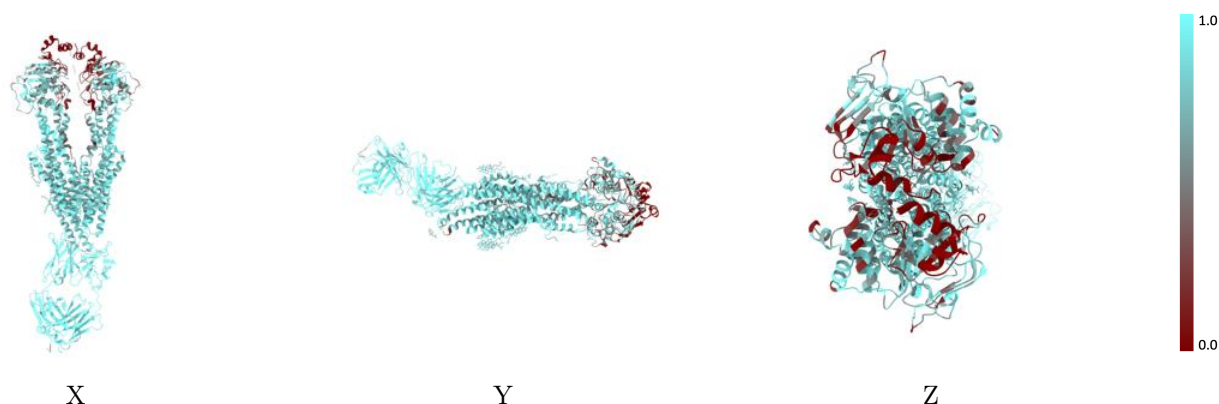
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



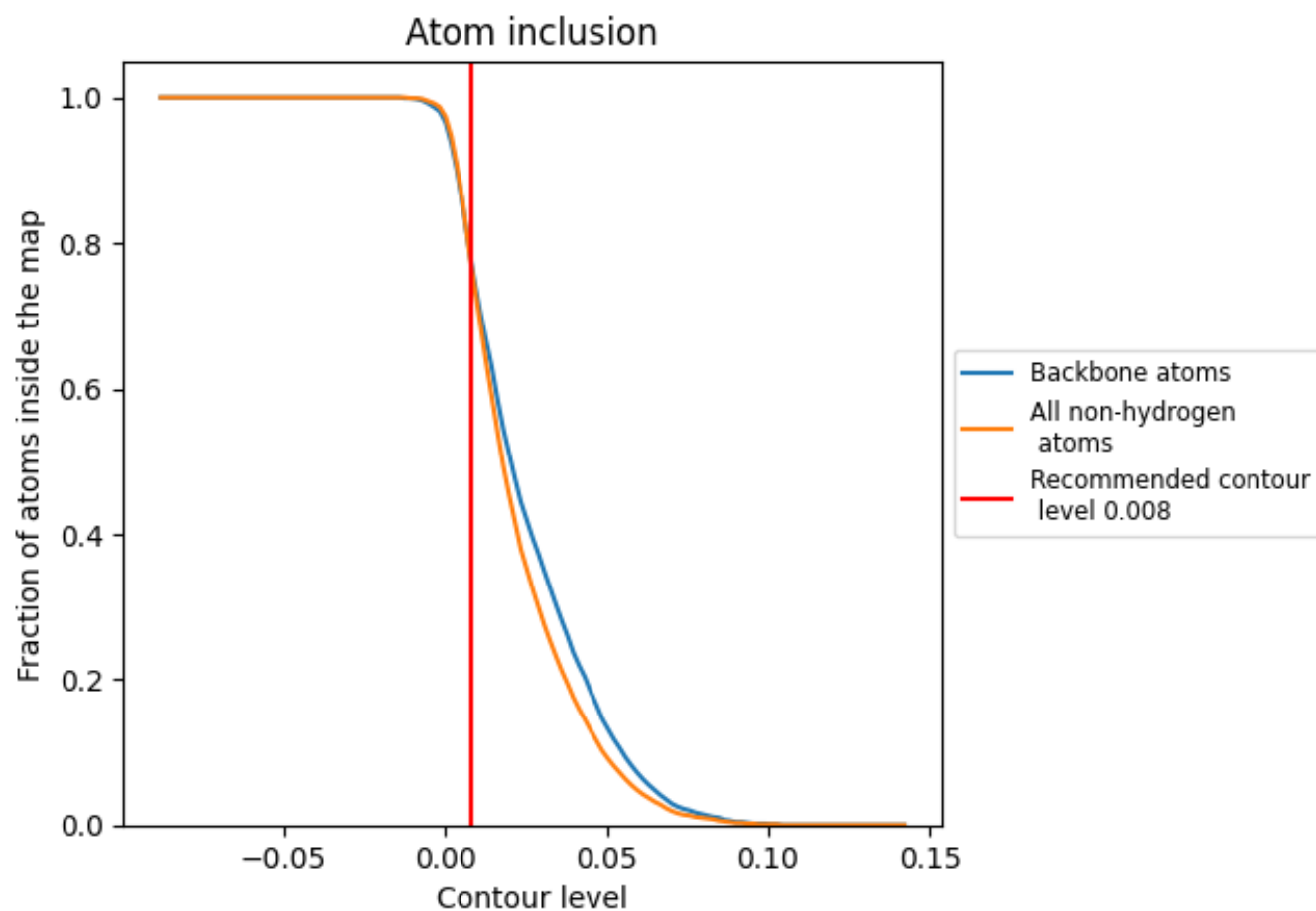
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.3920
A	0.7140	0.3560
B	0.9500	0.4860
C	0.9490	0.5090

