



Full wwPDB EM Validation Report ⓘ

Nov 10, 2025 – 01:18 PM EST

PDB ID : 9NQ9 / pdb_00009nq9
EMDB ID : EMD-49646
Title : Magnesium ions-bound closed-state cryo-EM structure of human TRPV6 in cNW11 nanodiscs
Authors : Neuberger, A.; Sobolevsky, A.I.
Deposited on : 2025-03-12
Resolution : 2.97 Å(reported)
Based on initial model : 7S8B

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.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

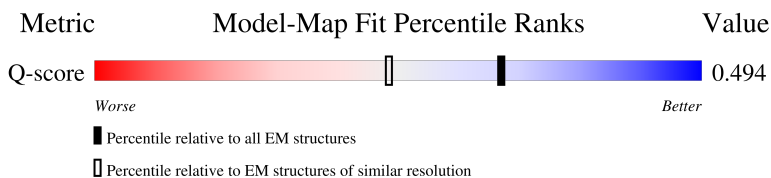
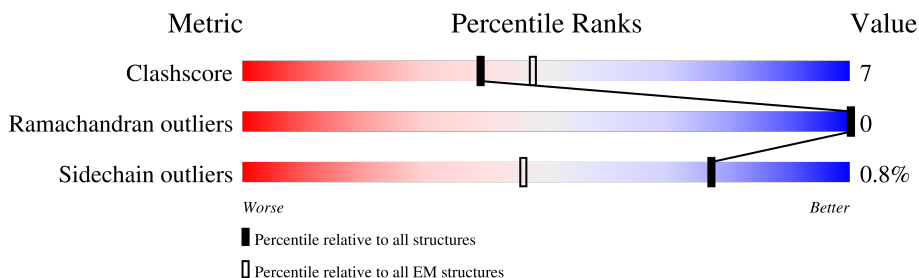
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13205 (2.47 - 3.47)

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	612	<div> <div>11%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
1	B	612	<div> <div>9%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	C	612	<div> <div>12%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
1	D	612	<div> <div>11%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

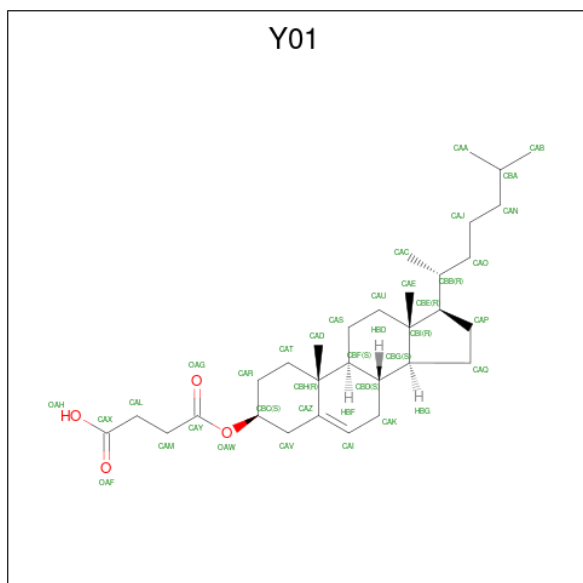
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y01	A	801	X	-	-	-
2	Y01	A	802	X	-	-	-
2	Y01	A	809	X	-	-	-
2	Y01	B	701	X	-	-	-
2	Y01	B	702	X	-	-	-
2	Y01	B	703	X	-	-	-
2	Y01	B	704	X	-	-	-
2	Y01	C	801	X	-	-	-
2	Y01	C	802	X	-	-	-
2	Y01	D	701	X	-	-	-
2	Y01	D	702	X	-	-	-
2	Y01	D	703	X	-	-	-

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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	580	Total 4653	C 3006	N 786	O 823	S 38	0	0
1	B	580	Total 4653	C 3006	N 786	O 823	S 38	0	0
1	C	580	Total 4653	C 3006	N 786	O 823	S 38	0	0
1	D	580	Total 4653	C 3006	N 786	O 823	S 38	0	0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 35	C 31	O 4	0
2	A	1	Total 35	C 31	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	A	1	Total	C				0
			6	6				
3	A	1	Total	C				0
			9	9				
3	A	1	Total	C				0
			6	6				
3	B	1	Total	C				0
			11	11				
3	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	B	1	Total	C				0
			9	9				
3	C	1	Total	C				0
			11	11				
3	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	C	1	Total	C				0
			6	6				
3	C	1	Total	C				0
			9	9				
3	D	1	Total	C				0
			11	11				
3	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	D	1	Total	C				0
			6	6				
3	D	1	Total	C				0
			9	9				

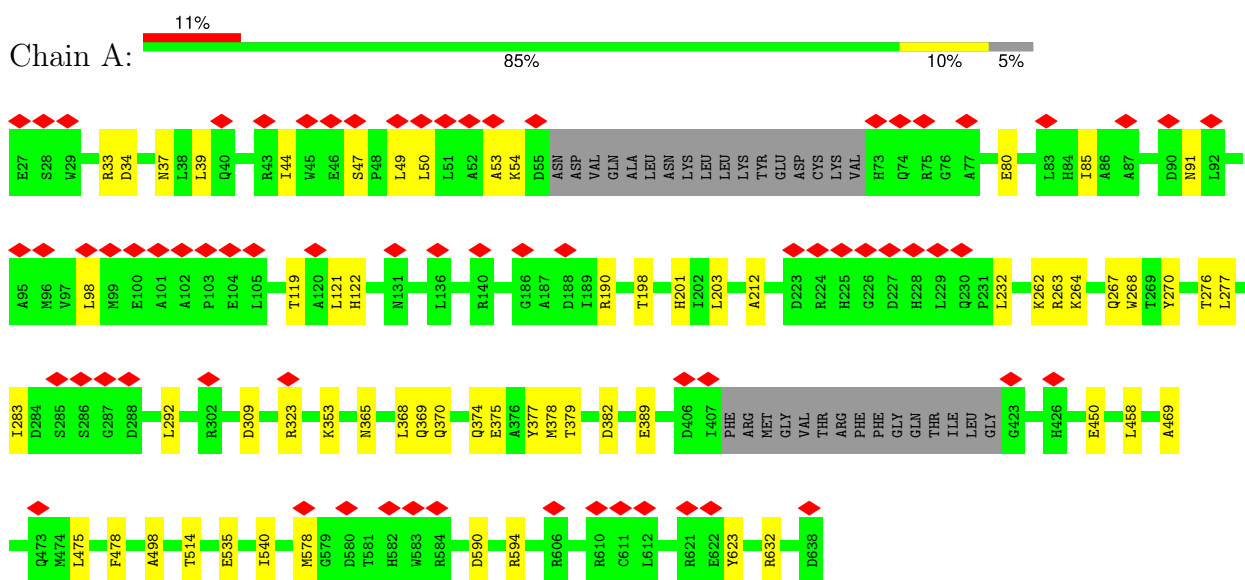
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	

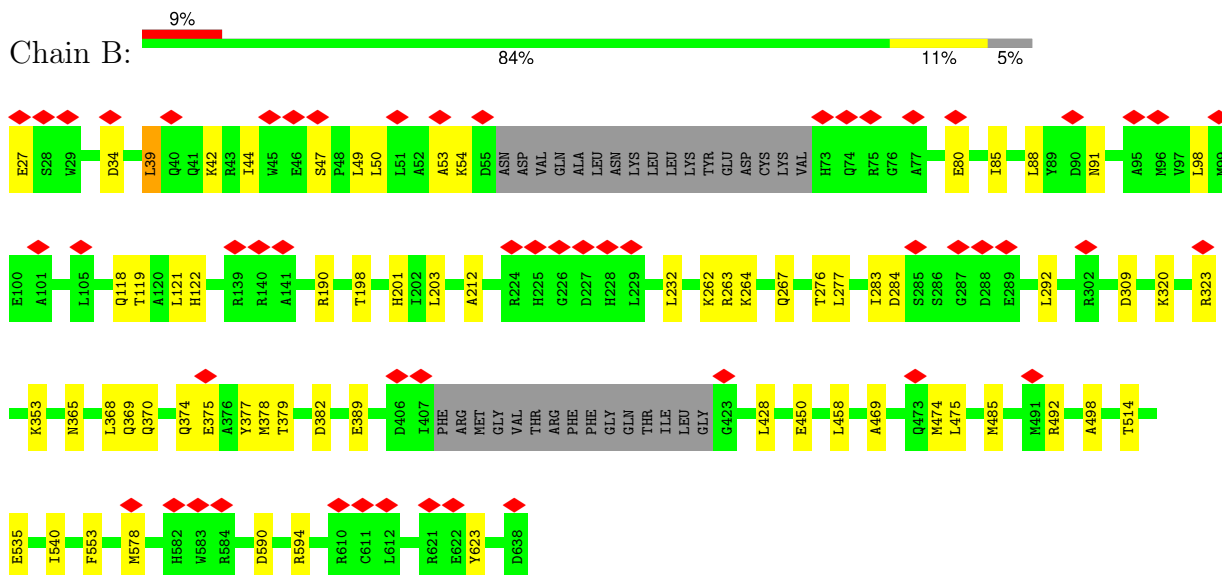
3 Residue-property plots

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

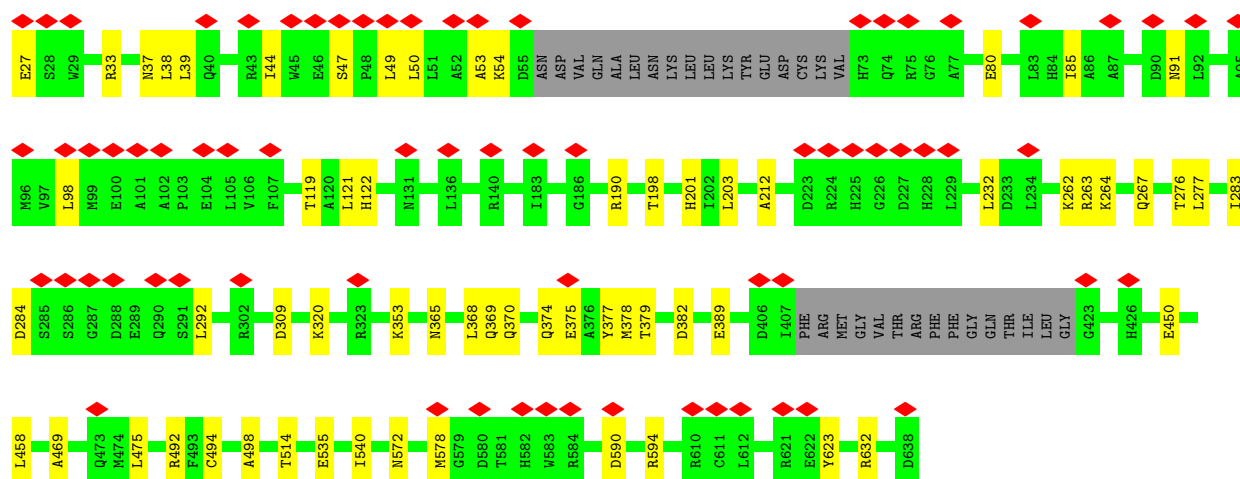
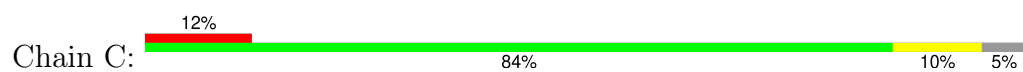
- Molecule 1: Transient receptor potential cation channel subfamily V member 6



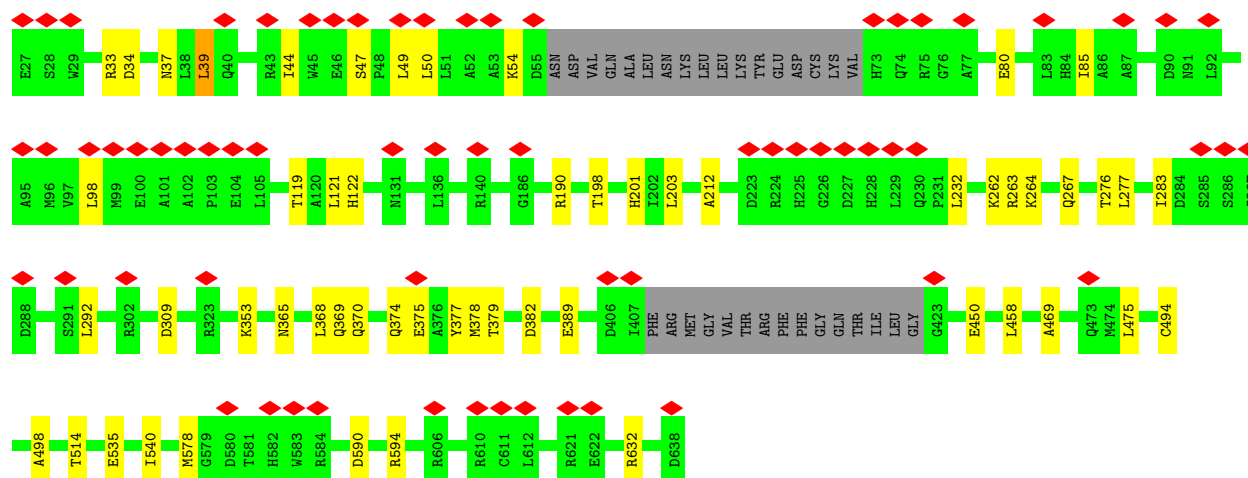
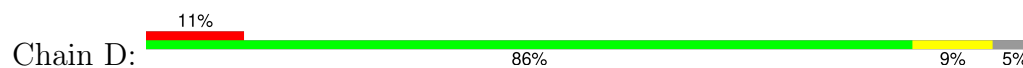
- Molecule 1: Transient receptor potential cation channel subfamily V member 6



- Molecule 1: Transient receptor potential cation channel subfamily V member 6



- Molecule 1: Transient receptor potential cation channel subfamily V member 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0172	Depositor
Map size (\AA)	212.224, 212.224, 212.224	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.829, 0.829, 0.829	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: POV, MG, Y01

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/4760	0.57	0/6460
1	B	0.37	0/4760	0.57	0/6460
1	C	0.37	0/4760	0.57	0/6460
1	D	0.37	0/4760	0.57	0/6460
All	All	0.37	0/19040	0.57	0/25840

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	4653	0	4695	40	0
1	B	4653	0	4695	46	0
1	C	4653	0	4695	41	0
1	D	4653	0	4695	34	0
2	A	105	0	133	32	0
2	B	140	0	177	48	0
2	C	70	0	89	21	0
2	D	105	0	133	33	0
3	A	68	0	103	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	81	1	0
3	C	62	0	92	4	0
3	D	62	0	92	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	19285	0	19680	271	0

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

All (271) 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)
2:B:701:Y01:CAT	2:B:701:Y01:CBH	1.79	1.61
2:B:702:Y01:CBH	2:B:702:Y01:CAT	1.81	1.58
2:B:704:Y01:CBH	2:B:704:Y01:CAT	1.79	1.58
2:B:703:Y01:CBH	2:B:703:Y01:CAT	1.80	1.58
2:C:801:Y01:CBH	2:C:801:Y01:CAT	1.81	1.57
2:D:701:Y01:CBH	2:D:701:Y01:CAT	1.79	1.55
2:D:703:Y01:CBH	2:D:703:Y01:CAT	1.80	1.55
2:C:802:Y01:CBH	2:C:802:Y01:CAT	1.80	1.54
2:A:802:Y01:CBH	2:A:802:Y01:CAT	1.79	1.54
2:A:809:Y01:CAT	2:A:809:Y01:CBH	1.79	1.53
2:D:702:Y01:CBH	2:D:702:Y01:CAT	1.81	1.52
2:A:801:Y01:CBH	2:A:801:Y01:CAT	1.81	1.52
2:B:701:Y01:CAZ	2:B:701:Y01:CAV	1.90	1.50
2:A:809:Y01:CAZ	2:A:809:Y01:CAV	1.90	1.49
2:B:704:Y01:CAV	2:B:704:Y01:CAZ	1.90	1.49
2:B:703:Y01:CAZ	2:B:703:Y01:CAV	1.91	1.49
2:C:802:Y01:CAZ	2:C:802:Y01:CAV	1.91	1.48
2:A:802:Y01:CAZ	2:A:802:Y01:CAV	1.91	1.47
2:D:701:Y01:CAZ	2:D:701:Y01:CAV	1.90	1.46
2:B:702:Y01:CAV	2:B:702:Y01:CAZ	1.93	1.44
2:D:703:Y01:CAZ	2:D:703:Y01:CAV	1.90	1.44
2:A:801:Y01:CAV	2:A:801:Y01:CAZ	1.93	1.44
2:C:801:Y01:CAZ	2:C:801:Y01:CAV	1.93	1.44
2:D:702:Y01:CAV	2:D:702:Y01:CAZ	1.93	1.42
2:D:701:Y01:CAT	2:D:701:Y01:CAZ	2.46	0.94
2:A:809:Y01:CAT	2:A:809:Y01:CAZ	2.47	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:Y01:CAT	2:B:701:Y01:CAZ	2.47	0.92
2:B:704:Y01:CAT	2:B:704:Y01:CAZ	2.47	0.90
2:A:802:Y01:CAT	2:A:802:Y01:CAZ	2.50	0.89
2:B:703:Y01:CAT	2:B:703:Y01:CAZ	2.51	0.88
2:D:703:Y01:CAT	2:D:703:Y01:CAZ	2.50	0.87
2:C:802:Y01:CAT	2:C:802:Y01:CAZ	2.50	0.87
2:C:801:Y01:CAT	2:C:801:Y01:CBF	2.55	0.84
2:D:702:Y01:CAT	2:D:702:Y01:CAZ	2.56	0.83
2:B:702:Y01:CAT	2:B:702:Y01:CBF	2.56	0.83
2:A:801:Y01:CAT	2:A:801:Y01:CAZ	2.56	0.82
2:B:702:Y01:CAT	2:B:702:Y01:CAZ	2.56	0.82
2:A:801:Y01:CAT	2:A:801:Y01:CBF	2.56	0.82
2:D:702:Y01:CAT	2:D:702:Y01:CBF	2.56	0.82
2:C:801:Y01:CAT	2:C:801:Y01:CAZ	2.57	0.82
2:A:802:Y01:CAT	2:A:802:Y01:CBF	2.62	0.78
2:D:703:Y01:CAT	2:D:703:Y01:CBF	2.62	0.77
2:B:704:Y01:CAT	2:B:704:Y01:CBF	2.63	0.76
2:C:802:Y01:CAT	2:C:802:Y01:CBF	2.63	0.76
2:A:809:Y01:CAT	2:A:809:Y01:CBF	2.64	0.75
2:B:701:Y01:CAT	2:B:701:Y01:CBF	2.64	0.74
2:B:703:Y01:CAT	2:B:703:Y01:CBF	2.65	0.73
2:D:701:Y01:CAT	2:D:701:Y01:CBF	2.65	0.73
1:D:370:GLN:HE22	1:D:450:GLU:H	1.38	0.72
1:C:370:GLN:HE22	1:C:450:GLU:H	1.38	0.71
1:A:370:GLN:HE22	1:A:450:GLU:H	1.38	0.71
1:B:370:GLN:HE22	1:B:450:GLU:H	1.38	0.70
2:A:809:Y01:CBH	2:A:809:Y01:CAV	2.65	0.70
2:B:702:Y01:CBH	2:B:702:Y01:CAV	2.68	0.68
2:D:702:Y01:CBH	2:D:702:Y01:CAV	2.68	0.68
2:B:701:Y01:CBH	2:B:701:Y01:CAV	2.65	0.68
1:B:498:ALA:HB2	2:B:704:Y01:HAJ1	1.76	0.67
1:C:498:ALA:HB2	2:D:701:Y01:HAJ1	1.76	0.67
1:A:270:TYR:OH	1:B:118:GLN:NE2	2.29	0.66
2:A:801:Y01:CBH	2:A:801:Y01:CAV	2.69	0.66
1:A:632:ARG:NH1	1:B:34:ASP:OD1	2.29	0.65
1:A:498:ALA:HB2	2:B:701:Y01:HAJ1	1.81	0.63
2:D:701:Y01:CAV	2:D:701:Y01:CAI	2.74	0.62
1:B:428:LEU:HD11	2:B:703:Y01:HAS1	1.81	0.62
2:B:704:Y01:CBH	2:B:704:Y01:CAV	2.65	0.62
2:A:809:Y01:HAJ1	1:D:498:ALA:HB2	1.82	0.61
2:D:701:Y01:CBH	2:D:701:Y01:CAV	2.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:ARG:NH1	1:D:34:ASP:OD1	2.33	0.60
1:A:578:MET:HE2	1:B:578:MET:HE1	1.83	0.60
2:B:703:Y01:CBH	2:B:703:Y01:CAV	2.68	0.60
1:B:375:GLU:HA	1:B:378:MET:HE3	1.84	0.60
2:B:701:Y01:CAV	2:B:701:Y01:CAI	2.74	0.60
1:A:267:GLN:HE21	1:A:277:LEU:HD22	1.68	0.59
1:B:267:GLN:HE21	1:B:277:LEU:HD22	1.68	0.59
2:B:704:Y01:CAV	2:B:704:Y01:CAI	2.74	0.59
1:A:375:GLU:HA	1:A:378:MET:HE3	1.84	0.59
2:A:809:Y01:CAV	2:A:809:Y01:CAI	2.75	0.59
2:A:801:Y01:CAT	2:A:801:Y01:HAS1	2.33	0.59
1:D:375:GLU:HA	1:D:378:MET:HE3	1.84	0.59
1:C:375:GLU:HA	1:C:378:MET:HE3	1.84	0.58
1:A:623:TYR:HE1	1:B:39:LEU:HD22	1.68	0.58
1:C:309:ASP:OD1	1:C:594:ARG:NH2	2.37	0.58
2:C:801:Y01:CAT	2:C:801:Y01:CAS	2.81	0.58
2:C:801:Y01:CAT	2:C:801:Y01:HAS1	2.34	0.58
1:D:267:GLN:HE21	1:D:277:LEU:HD22	1.68	0.58
1:B:309:ASP:OD1	1:B:594:ARG:NH2	2.37	0.58
1:D:119:THR:H	1:D:122:HIS:HD2	1.51	0.58
1:C:267:GLN:HE21	1:C:277:LEU:HD22	1.67	0.58
1:D:309:ASP:OD1	1:D:594:ARG:NH2	2.37	0.58
1:A:309:ASP:OD1	1:A:594:ARG:NH2	2.37	0.57
2:D:702:Y01:CAT	2:D:702:Y01:HAS1	2.34	0.57
2:C:802:Y01:CBH	2:C:802:Y01:CAV	2.67	0.57
2:D:702:Y01:CAT	2:D:702:Y01:CAS	2.82	0.57
2:A:802:Y01:CBH	2:A:802:Y01:CAV	2.67	0.57
1:B:119:THR:H	1:B:122:HIS:HD2	1.51	0.57
2:A:801:Y01:CAT	2:A:801:Y01:CAS	2.82	0.57
1:A:268:TRP:HB2	1:B:88:LEU:HD21	1.87	0.57
2:C:801:Y01:CBH	2:C:801:Y01:CAV	2.68	0.57
2:D:701:Y01:CAT	2:D:701:Y01:CAD	2.79	0.57
1:D:203:LEU:HD12	1:D:212:ALA:HA	1.87	0.56
1:A:119:THR:H	1:A:122:HIS:HD2	1.51	0.56
2:B:702:Y01:CAT	2:B:702:Y01:CAS	2.84	0.56
1:C:119:THR:H	1:C:122:HIS:HD2	1.51	0.56
2:B:704:Y01:HAC3	2:B:704:Y01:HAA1	1.87	0.56
1:C:203:LEU:HD12	1:C:212:ALA:HA	1.87	0.56
2:A:802:Y01:CAT	2:A:802:Y01:CAD	2.78	0.56
2:A:809:Y01:CAT	2:A:809:Y01:CAD	2.79	0.56
2:D:703:Y01:CAT	2:D:703:Y01:CAD	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:Y01:CAT	2:B:703:Y01:CAD	2.77	0.56
2:C:802:Y01:CAT	2:C:802:Y01:CAD	2.78	0.56
1:A:283:ILE:HG22	1:A:292:LEU:HD22	1.88	0.56
2:A:809:Y01:HAA1	2:A:809:Y01:HAC3	1.88	0.56
2:D:701:Y01:HAC3	2:D:701:Y01:HAA1	1.88	0.56
1:D:283:ILE:HG22	1:D:292:LEU:HD22	1.88	0.56
2:A:802:Y01:CAT	2:A:802:Y01:CAS	2.84	0.55
1:B:203:LEU:HD12	1:B:212:ALA:HA	1.87	0.55
1:C:283:ILE:HG22	1:C:292:LEU:HD22	1.88	0.55
1:B:283:ILE:HG22	1:B:292:LEU:HD22	1.88	0.55
1:B:474:MET:HE2	1:C:492:ARG:HH11	1.71	0.55
2:C:802:Y01:CAT	2:C:802:Y01:CAS	2.85	0.55
1:A:203:LEU:HD12	1:A:212:ALA:HA	1.87	0.55
1:A:368:LEU:HB2	1:B:514:THR:HA	1.88	0.55
2:D:703:Y01:CAT	2:D:703:Y01:CAS	2.85	0.55
2:B:701:Y01:CAT	2:B:701:Y01:CAD	2.79	0.55
2:B:701:Y01:HAA1	2:B:701:Y01:HAC3	1.87	0.54
2:B:702:Y01:HAT1	2:B:702:Y01:HAS1	1.89	0.54
2:B:704:Y01:CAT	2:B:704:Y01:CAD	2.79	0.54
2:D:703:Y01:CBH	2:D:703:Y01:CAV	2.67	0.53
2:D:702:Y01:CAT	2:D:702:Y01:CAD	2.82	0.52
2:B:702:Y01:CAT	2:B:702:Y01:CAD	2.80	0.52
2:D:703:Y01:CAV	2:D:703:Y01:CAI	2.81	0.52
2:B:702:Y01:CAT	2:B:702:Y01:HAS1	2.40	0.52
1:B:578:MET:HE2	1:C:578:MET:HE1	1.93	0.51
1:C:283:ILE:HA	1:C:292:LEU:HB3	1.92	0.51
2:C:801:Y01:CAT	2:C:801:Y01:CAD	2.82	0.51
1:A:623:TYR:CE1	1:B:39:LEU:HD22	2.45	0.51
1:B:283:ILE:HA	1:B:292:LEU:HB3	1.92	0.50
1:B:377:TYR:OH	1:B:389:GLU:OE1	2.28	0.50
1:D:283:ILE:HA	1:D:292:LEU:HB3	1.92	0.50
1:A:283:ILE:HA	1:A:292:LEU:HB3	1.92	0.50
2:C:801:Y01:HAS1	2:C:801:Y01:HAT1	1.93	0.49
1:D:47:SER:HB3	1:D:50:LEU:HB2	1.93	0.49
1:B:47:SER:HB3	1:B:50:LEU:HB2	1.94	0.49
1:A:49:LEU:HD21	1:A:98:LEU:HD11	1.94	0.49
2:D:702:Y01:HAS1	2:D:702:Y01:HAT1	1.94	0.49
2:B:703:Y01:CAT	2:B:703:Y01:CAS	2.91	0.49
1:B:49:LEU:HD21	1:B:98:LEU:HD11	1.94	0.48
1:C:578:MET:HE2	1:D:578:MET:HE1	1.95	0.48
1:D:44:ILE:HG21	1:D:54:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ALA:HB1	1:A:475:LEU:HB3	1.94	0.48
1:C:44:ILE:HG21	1:C:54:LYS:HD2	1.95	0.48
2:A:801:Y01:HAS1	2:A:801:Y01:HAT1	1.95	0.48
1:C:47:SER:HB3	1:C:50:LEU:HB2	1.94	0.48
1:D:49:LEU:HD21	1:D:98:LEU:HD11	1.94	0.48
1:A:47:SER:HB3	1:A:50:LEU:HB2	1.94	0.48
1:C:469:ALA:HB1	1:C:475:LEU:HB3	1.94	0.48
1:C:49:LEU:HD21	1:C:98:LEU:HD11	1.94	0.48
1:D:377:TYR:OH	1:D:389:GLU:OE1	2.28	0.48
1:B:469:ALA:HB1	1:B:475:LEU:HB3	1.94	0.48
2:B:702:Y01:CAZ	2:B:702:Y01:CBC	2.84	0.48
1:C:119:THR:HG23	1:C:121:LEU:H	1.79	0.48
1:D:469:ALA:HB1	1:D:475:LEU:HB3	1.94	0.48
2:A:802:Y01:CAV	2:A:802:Y01:CAI	2.82	0.47
2:C:802:Y01:CAV	2:C:802:Y01:CAI	2.81	0.47
1:A:514:THR:HA	1:D:368:LEU:HB2	1.96	0.47
1:B:44:ILE:HG21	1:B:54:LYS:HD2	1.95	0.47
1:B:590:ASP:OD2	1:B:594:ARG:NH1	2.47	0.47
1:B:284:ASP:OD1	1:B:320:LYS:NZ	2.36	0.47
1:B:485:MET:HE1	1:C:572:ASN:HB2	1.97	0.47
1:A:590:ASP:OD2	1:A:594:ARG:NH1	2.47	0.47
2:B:703:Y01:HAP1	2:B:703:Y01:HAO2	1.46	0.47
1:A:623:TYR:HA	1:B:42:LYS:HE2	1.97	0.47
1:B:623:TYR:CD1	1:C:38:LEU:HB3	2.49	0.47
1:A:44:ILE:HG21	1:A:54:LYS:HD2	1.95	0.47
1:A:119:THR:HG23	1:A:121:LEU:H	1.80	0.47
1:B:119:THR:HG23	1:B:121:LEU:H	1.79	0.47
1:B:535:GLU:HG2	1:B:540:ILE:HD11	1.97	0.47
1:C:590:ASP:OD2	1:C:594:ARG:NH1	2.47	0.47
1:D:119:THR:HG23	1:D:121:LEU:H	1.80	0.47
1:D:190:ARG:HG2	1:D:232:LEU:HD21	1.97	0.47
1:D:590:ASP:OD2	1:D:594:ARG:NH1	2.47	0.46
1:C:190:ARG:HG2	1:C:232:LEU:HD21	1.97	0.46
1:A:535:GLU:HG2	1:A:540:ILE:HD11	1.97	0.46
2:B:703:Y01:CAV	2:B:703:Y01:CAI	2.81	0.46
1:A:190:ARG:HG2	1:A:232:LEU:HD21	1.97	0.46
1:C:377:TYR:OH	1:C:389:GLU:OE1	2.28	0.46
1:C:535:GLU:HG2	1:C:540:ILE:HD11	1.97	0.46
1:B:190:ARG:HG2	1:B:232:LEU:HD21	1.97	0.46
1:D:535:GLU:HG2	1:D:540:ILE:HD11	1.97	0.46
1:C:374:GLN:NE2	1:C:375:GLU:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:705:POV:H33A	3:D:705:POV:H36A	1.67	0.46
2:A:801:Y01:HAE2	2:A:801:Y01:HBB	1.67	0.46
1:A:377:TYR:OH	1:A:389:GLU:OE1	2.28	0.45
1:D:374:GLN:NE2	1:D:375:GLU:HG3	2.31	0.45
1:A:374:GLN:NE2	1:A:375:GLU:HG3	2.31	0.45
2:C:802:Y01:HAP1	2:C:802:Y01:HAO2	1.45	0.45
1:D:377:TYR:HA	1:D:382:ASP:HB3	1.99	0.45
1:B:374:GLN:NE2	1:B:375:GLU:HG3	2.31	0.45
1:C:377:TYR:HA	1:C:382:ASP:HB3	1.98	0.45
1:C:494:CYS:HB2	2:D:701:Y01:HAA2	1.98	0.45
2:A:802:Y01:HAO2	2:A:802:Y01:HAP1	1.53	0.45
1:C:368:LEU:HB2	1:D:514:THR:HA	1.99	0.45
2:D:703:Y01:HAP1	2:D:703:Y01:HAO2	1.48	0.45
3:A:804:POV:H36A	3:A:804:POV:H33A	1.68	0.45
1:A:353:LYS:HE3	1:A:369:GLN:HE21	1.82	0.44
1:D:353:LYS:HE3	1:D:369:GLN:HE21	1.82	0.44
1:B:353:LYS:HE3	1:B:369:GLN:HE21	1.82	0.44
1:B:553:PHE:HA	2:B:701:Y01:HAM1	1.99	0.44
1:B:377:TYR:HA	1:B:382:ASP:HB3	1.98	0.44
2:B:703:Y01:HAB1	2:B:703:Y01:HAJ2	1.84	0.44
1:C:353:LYS:HE3	1:C:369:GLN:HE21	1.82	0.44
1:A:377:TYR:HA	1:A:382:ASP:HB3	1.99	0.44
1:B:323:ARG:NE	1:C:27:GLU:OE1	2.41	0.44
1:A:80:GLU:HG3	1:A:85:ILE:HD11	2.00	0.44
2:A:801:Y01:CAT	2:A:801:Y01:CAD	2.81	0.44
2:B:701:Y01:HAE2	2:B:701:Y01:HBB	1.73	0.44
2:B:702:Y01:CAV	2:B:702:Y01:CAI	2.86	0.44
2:C:801:Y01:CAZ	2:C:801:Y01:CBC	2.86	0.44
2:D:701:Y01:HAA1	2:D:701:Y01:HAJ2	1.79	0.44
1:B:80:GLU:HG3	1:B:85:ILE:HD11	2.00	0.43
3:C:803:POV:H35	3:C:803:POV:H38A	1.79	0.43
2:D:702:Y01:CAZ	2:D:702:Y01:CBC	2.87	0.43
1:B:262:LYS:NZ	1:B:263:ARG:HE	2.17	0.43
1:C:262:LYS:NZ	1:C:263:ARG:HE	2.17	0.43
1:D:262:LYS:NZ	1:D:263:ARG:HE	2.17	0.43
1:D:80:GLU:HG3	1:D:85:ILE:HD11	2.00	0.43
1:A:262:LYS:NZ	1:A:263:ARG:HE	2.17	0.43
2:B:701:Y01:CAT	2:B:701:Y01:CAS	2.97	0.43
1:A:478:PHE:HE2	1:B:492:ARG:HB3	1.84	0.43
1:C:284:ASP:OD1	1:C:320:LYS:NZ	2.36	0.43
1:B:198:THR:H	1:B:201:HIS:CD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:702:Y01:HAE2	2:D:702:Y01:HBB	1.67	0.42
1:A:198:THR:H	1:A:201:HIS:CD2	2.37	0.42
2:A:809:Y01:CAT	2:A:809:Y01:CAS	2.97	0.42
1:C:80:GLU:HG3	1:C:85:ILE:HD11	2.00	0.42
2:A:809:Y01:HAA2	1:D:494:CYS:HB2	2.01	0.42
2:B:704:Y01:HAA1	2:B:704:Y01:HAJ2	1.71	0.42
1:C:264:LYS:HE3	1:C:276:THR:HG21	2.01	0.42
1:C:623:TYR:HE1	1:D:39:LEU:HD22	1.85	0.42
3:D:704:POV:H38A	3:D:704:POV:H35	1.80	0.42
2:A:801:Y01:CAZ	2:A:801:Y01:CBC	2.87	0.42
2:B:701:Y01:HAA1	2:B:701:Y01:HAJ2	1.78	0.42
1:C:198:THR:H	1:C:201:HIS:CD2	2.38	0.42
1:D:198:THR:H	1:D:201:HIS:CD2	2.37	0.42
2:A:809:Y01:HAC3	2:A:809:Y01:HAJ2	1.86	0.41
3:C:804:POV:H36A	3:C:804:POV:H33A	1.66	0.41
2:B:704:Y01:HAC3	2:B:704:Y01:HAJ2	1.84	0.41
1:B:264:LYS:HE3	1:B:276:THR:HG21	2.02	0.41
3:B:705:POV:H35	3:B:705:POV:H38A	1.79	0.41
1:D:264:LYS:HE3	1:D:276:THR:HG21	2.02	0.41
1:A:264:LYS:HE3	1:A:276:THR:HG21	2.02	0.41
1:A:389:GLU:HB3	3:A:806:POV:H312	2.03	0.41
2:B:704:Y01:CAT	2:B:704:Y01:CAS	2.98	0.41
2:D:701:Y01:HAE2	2:D:701:Y01:HBB	1.73	0.41
1:A:34:ASP:OD1	1:D:632:ARG:NH1	2.54	0.41
1:B:368:LEU:HB2	1:C:514:THR:HA	2.03	0.41
1:C:53:ALA:O	1:C:91:ASN:ND2	2.54	0.41
2:C:801:Y01:HAE2	2:C:801:Y01:HBB	1.66	0.41
1:D:389:GLU:HB3	3:D:707:POV:H312	2.02	0.41
2:D:701:Y01:CAT	2:D:701:Y01:CAS	2.98	0.41
1:A:53:ALA:O	1:A:91:ASN:ND2	2.54	0.41
1:B:474:MET:HG2	1:C:492:ARG:NH1	2.36	0.41
1:B:53:ALA:O	1:B:91:ASN:ND2	2.54	0.40
2:B:702:Y01:HAE2	2:B:702:Y01:HBB	1.69	0.40
3:C:803:POV:H37A	3:C:803:POV:H310	1.99	0.40
1:D:33:ARG:O	1:D:37:ASN:ND2	2.54	0.40
1:C:33:ARG:O	1:C:37:ASN:ND2	2.55	0.40
2:C:802:Y01:HAE2	2:C:802:Y01:HBB	1.87	0.40
1:A:33:ARG:O	1:A:37:ASN:ND2	2.55	0.40
1:A:323:ARG:HE	1:B:27:GLU:HB3	1.86	0.40
1:C:389:GLU:HB3	3:C:806:POV:H312	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	574/612 (94%)	562 (98%)	12 (2%)	0	100	100
1	B	574/612 (94%)	562 (98%)	12 (2%)	0	100	100
1	C	574/612 (94%)	562 (98%)	12 (2%)	0	100	100
1	D	574/612 (94%)	562 (98%)	12 (2%)	0	100	100
All	All	2296/2448 (94%)	2248 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	503/531 (95%)	499 (99%)	4 (1%)	79	90
1	B	503/531 (95%)	499 (99%)	4 (1%)	79	90
1	C	503/531 (95%)	499 (99%)	4 (1%)	79	90
1	D	503/531 (95%)	499 (99%)	4 (1%)	79	90
All	All	2012/2124 (95%)	1996 (99%)	16 (1%)	77	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	365	ASN

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Mol	Chain	Res	Type
1	A	379	THR
1	A	458	LEU
1	B	39	LEU
1	B	365	ASN
1	B	379	THR
1	B	458	LEU
1	C	39	LEU
1	C	365	ASN
1	C	379	THR
1	C	458	LEU
1	D	39	LEU
1	D	365	ASN
1	D	379	THR
1	D	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	122	HIS
1	A	165	HIS
1	A	201	HIS
1	A	261	GLN
1	A	267	GLN
1	A	306	GLN
1	A	365	ASN
1	A	369	GLN
1	A	370	GLN
1	A	546	ASN
1	A	587	HIS
1	B	37	ASN
1	B	118	GLN
1	B	122	HIS
1	B	165	HIS
1	B	201	HIS
1	B	261	GLN
1	B	267	GLN
1	B	306	GLN
1	B	365	ASN
1	B	369	GLN
1	B	370	GLN
1	B	546	ASN

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Mol	Chain	Res	Type
1	B	587	HIS
1	C	122	HIS
1	C	165	HIS
1	C	201	HIS
1	C	261	GLN
1	C	267	GLN
1	C	306	GLN
1	C	365	ASN
1	C	369	GLN
1	C	370	GLN
1	C	546	ASN
1	C	587	HIS
1	D	31	GLN
1	D	37	ASN
1	D	122	HIS
1	D	165	HIS
1	D	201	HIS
1	D	261	GLN
1	D	267	GLN
1	D	306	GLN
1	D	365	ASN
1	D	369	GLN
1	D	370	GLN
1	D	546	ASN
1	D	587	HIS

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

Of 33 ligands modelled in this entry, 5 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	A	806	-	8,8,51	0.56	0	7,7,59	0.44	0
3	POV	A	803	-	10,10,51	0.66	0	9,9,59	0.29	0
3	POV	D	705	-	35,35,51	1.16	3 (8%)	41,43,59	1.16	4 (9%)
3	POV	D	707	-	8,8,51	0.57	0	7,7,59	0.43	0
2	Y01	B	702	-	38,38,38	7.83	20 (52%)	57,57,57	3.49	30 (52%)
2	Y01	A	801	-	38,38,38	7.82	20 (52%)	57,57,57	3.50	29 (50%)
3	POV	C	804	-	35,35,51	1.16	3 (8%)	41,43,59	1.17	4 (9%)
3	POV	B	705	-	10,10,51	0.65	0	9,9,59	0.29	0
2	Y01	A	802	-	38,38,38	7.78	21 (55%)	57,57,57	3.65	30 (52%)
3	POV	D	704	-	10,10,51	0.66	0	9,9,59	0.29	0
3	POV	C	805	-	5,5,51	0.55	0	4,4,59	0.24	0
2	Y01	C	802	-	38,38,38	7.77	22 (57%)	57,57,57	3.73	27 (47%)
3	POV	B	707	-	8,8,51	0.57	0	7,7,59	0.45	0
3	POV	D	706	-	5,5,51	0.55	0	4,4,59	0.23	0
3	POV	A	808	-	5,5,51	0.57	0	4,4,59	0.22	0
2	Y01	D	702	-	38,38,38	7.83	20 (52%)	57,57,57	3.52	29 (50%)
3	POV	A	804	-	35,35,51	1.16	3 (8%)	41,43,59	1.15	3 (7%)
3	POV	C	806	-	8,8,51	0.56	0	7,7,59	0.44	0
2	Y01	D	703	-	38,38,38	7.77	22 (57%)	57,57,57	3.71	28 (49%)
2	Y01	D	701	-	38,38,38	7.74	21 (55%)	57,57,57	3.60	30 (52%)
2	Y01	B	704	-	38,38,38	7.74	21 (55%)	57,57,57	3.67	29 (50%)
3	POV	A	805	-	5,5,51	0.56	0	4,4,59	0.22	0
3	POV	C	803	-	10,10,51	0.65	0	9,9,59	0.29	0
2	Y01	B	701	-	38,38,38	7.74	21 (55%)	57,57,57	3.63	27 (47%)
2	Y01	C	801	-	38,38,38	7.81	20 (52%)	57,57,57	3.54	29 (50%)
2	Y01	A	809	-	38,38,38	7.75	21 (55%)	57,57,57	3.62	28 (49%)
3	POV	B	706	-	35,35,51	1.16	3 (8%)	41,43,59	1.12	3 (7%)
2	Y01	B	703	-	38,38,38	7.79	22 (57%)	57,57,57	3.80	24 (42%)

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
3	POV	A	806	-	-	2/6/6/55	-
3	POV	A	803	-	-	6/8/8/55	-
3	POV	D	705	-	-	26/39/39/55	-
3	POV	D	707	-	-	2/6/6/55	-
2	Y01	B	702	-	4/4/12/13	12/19/77/77	0/4/4/4
2	Y01	A	801	-	4/4/12/13	12/19/77/77	0/4/4/4
3	POV	C	804	-	-	26/39/39/55	-
3	POV	B	705	-	-	6/8/8/55	-
2	Y01	A	802	-	4/4/12/13	14/19/77/77	0/4/4/4
3	POV	D	704	-	-	6/8/8/55	-
3	POV	C	805	-	-	2/3/3/55	-
2	Y01	C	802	-	4/4/12/13	14/19/77/77	0/4/4/4
3	POV	B	707	-	-	2/6/6/55	-
3	POV	D	706	-	-	2/3/3/55	-
3	POV	A	808	-	-	2/3/3/55	-
2	Y01	D	702	-	4/4/12/13	12/19/77/77	0/4/4/4
3	POV	A	804	-	-	28/39/39/55	-
3	POV	C	806	-	-	2/6/6/55	-
2	Y01	D	703	-	4/4/12/13	14/19/77/77	0/4/4/4
2	Y01	D	701	-	4/4/12/13	12/19/77/77	0/4/4/4
2	Y01	B	704	-	4/4/12/13	12/19/77/77	0/4/4/4
3	POV	A	805	-	-	2/3/3/55	-
3	POV	C	803	-	-	6/8/8/55	-
2	Y01	B	701	-	4/4/12/13	13/19/77/77	0/4/4/4
2	Y01	C	801	-	4/4/12/13	12/19/77/77	0/4/4/4
2	Y01	A	809	-	4/4/12/13	13/19/77/77	0/4/4/4
3	POV	B	706	-	-	28/39/39/55	-
2	Y01	B	703	-	4/4/12/13	12/19/77/77	0/4/4/4

All (263) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	Y01	CAK-CBD	-22.92	1.16	1.53
2	C	802	Y01	CAK-CBD	-22.76	1.16	1.53
2	A	802	Y01	CAK-CBD	-22.76	1.16	1.53
2	D	703	Y01	CAK-CBD	-22.74	1.16	1.53
2	A	809	Y01	CAK-CBD	-22.68	1.16	1.53
2	B	701	Y01	CAK-CBD	-22.62	1.16	1.53
2	D	701	Y01	CAK-CBD	-22.61	1.16	1.53
2	B	702	Y01	CAK-CBD	-22.58	1.16	1.53
2	D	702	Y01	CAK-CBD	-22.58	1.16	1.53
2	B	704	Y01	CAK-CBD	-22.57	1.16	1.53
2	A	801	Y01	CAK-CBD	-22.54	1.16	1.53
2	C	801	Y01	CAK-CBD	-22.48	1.16	1.53
2	D	702	Y01	CAV-CAZ	20.86	1.93	1.51
2	A	801	Y01	CAV-CAZ	20.86	1.93	1.51
2	B	702	Y01	CAV-CAZ	20.75	1.93	1.51
2	C	801	Y01	CAV-CAZ	20.74	1.93	1.51
2	A	802	Y01	CBD-CBG	-20.15	1.15	1.53
2	B	702	Y01	CBD-CBG	-20.10	1.15	1.53
2	D	703	Y01	CBD-CBG	-20.08	1.15	1.53
2	D	701	Y01	CBD-CBG	-20.05	1.15	1.53
2	C	802	Y01	CBD-CBG	-19.98	1.16	1.53
2	C	801	Y01	CBD-CBG	-19.97	1.16	1.53
2	A	809	Y01	CBD-CBG	-19.94	1.16	1.53
2	B	703	Y01	CBD-CBG	-19.92	1.16	1.53
2	B	701	Y01	CBD-CBG	-19.88	1.16	1.53
2	D	702	Y01	CBD-CBG	-19.87	1.16	1.53
2	B	704	Y01	CBD-CBG	-19.83	1.16	1.53
2	A	802	Y01	CAV-CAZ	19.81	1.91	1.51
2	A	801	Y01	CBD-CBG	-19.78	1.16	1.53
2	B	703	Y01	CAV-CAZ	19.71	1.91	1.51
2	C	802	Y01	CAV-CAZ	19.63	1.91	1.51
2	D	703	Y01	CAV-CAZ	19.59	1.90	1.51
2	A	809	Y01	CAV-CAZ	19.19	1.90	1.51
2	B	701	Y01	CAV-CAZ	19.15	1.90	1.51
2	B	704	Y01	CAV-CAZ	19.14	1.90	1.51
2	D	701	Y01	CAV-CAZ	19.13	1.90	1.51
2	B	701	Y01	CBH-CAZ	-16.76	1.20	1.52
2	D	701	Y01	CBH-CAZ	-16.75	1.20	1.52
2	A	809	Y01	CBH-CAZ	-16.72	1.21	1.52
2	B	704	Y01	CBH-CAZ	-16.69	1.21	1.52
2	A	802	Y01	CBH-CAZ	-16.63	1.21	1.52
2	C	802	Y01	CBH-CAZ	-16.57	1.21	1.52
2	D	703	Y01	CBH-CAZ	-16.49	1.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	Y01	CBH-CAZ	-16.19	1.22	1.52
2	A	801	Y01	CBH-CAZ	-15.36	1.23	1.52
2	D	702	Y01	CBH-CAZ	-15.27	1.23	1.52
2	B	702	Y01	CBH-CAZ	-15.25	1.23	1.52
2	C	801	Y01	CBH-CAZ	-15.22	1.23	1.52
2	C	801	Y01	CAT-CBH	15.06	1.81	1.54
2	B	702	Y01	CAT-CBH	15.05	1.81	1.54
2	D	702	Y01	CAT-CBH	15.04	1.81	1.54
2	A	801	Y01	CAT-CBH	14.89	1.81	1.54
2	B	703	Y01	CAT-CBH	14.26	1.80	1.54
2	C	802	Y01	CAT-CBH	14.19	1.80	1.54
2	D	703	Y01	CAT-CBH	14.09	1.80	1.54
2	A	802	Y01	CAT-CBH	14.04	1.79	1.54
2	B	704	Y01	CAT-CBH	13.81	1.79	1.54
2	A	809	Y01	CAT-CBH	13.79	1.79	1.54
2	B	701	Y01	CAT-CBH	13.77	1.79	1.54
2	D	701	Y01	CAT-CBH	13.70	1.79	1.54
2	A	801	Y01	CAU-CBI	-12.69	1.32	1.54
2	C	801	Y01	CAU-CBI	-12.61	1.32	1.54
2	D	702	Y01	CAU-CBI	-12.61	1.32	1.54
2	B	702	Y01	CAU-CBI	-12.48	1.32	1.54
2	B	703	Y01	CAU-CBI	-12.03	1.33	1.54
2	D	703	Y01	CAU-CBI	-11.99	1.33	1.54
2	B	704	Y01	CAU-CBI	-11.98	1.33	1.54
2	C	802	Y01	CAU-CBI	-11.95	1.33	1.54
2	B	701	Y01	CAU-CBI	-11.87	1.33	1.54
2	A	802	Y01	CAU-CBI	-11.85	1.33	1.54
2	D	701	Y01	CAU-CBI	-11.83	1.33	1.54
2	A	809	Y01	CAU-CBI	-11.83	1.33	1.54
2	B	704	Y01	CBI-CBG	8.89	1.71	1.55
2	B	701	Y01	CBI-CBE	8.79	1.71	1.55
2	D	701	Y01	CBI-CBE	8.78	1.71	1.55
2	B	701	Y01	CBI-CBG	8.78	1.71	1.55
2	B	704	Y01	CBI-CBE	8.75	1.71	1.55
2	A	809	Y01	CBI-CBG	8.72	1.71	1.55
2	A	809	Y01	CBI-CBE	8.72	1.71	1.55
2	D	701	Y01	CBI-CBG	8.69	1.71	1.55
2	C	802	Y01	CBI-CBE	8.54	1.70	1.55
2	D	703	Y01	CBI-CBE	8.53	1.70	1.55
2	B	703	Y01	CBI-CBE	8.46	1.70	1.55
2	A	801	Y01	CBI-CBE	8.44	1.70	1.55
2	D	702	Y01	CBI-CBE	8.39	1.70	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	Y01	CBI-CBE	8.37	1.70	1.55
2	C	801	Y01	CBI-CBE	8.26	1.70	1.55
2	C	801	Y01	CBI-CBG	8.26	1.70	1.55
2	A	801	Y01	CBI-CBG	8.25	1.70	1.55
2	D	702	Y01	CBI-CBG	8.25	1.70	1.55
2	B	702	Y01	CBI-CBG	8.24	1.70	1.55
2	A	802	Y01	CBI-CBG	8.11	1.69	1.55
2	B	702	Y01	CBI-CBE	8.09	1.69	1.55
2	D	703	Y01	CBI-CBG	8.09	1.69	1.55
2	C	802	Y01	CBI-CBG	8.07	1.69	1.55
2	B	703	Y01	CBI-CBG	8.07	1.69	1.55
2	D	702	Y01	CAQ-CAP	6.95	1.73	1.54
2	A	801	Y01	CAQ-CAP	6.95	1.73	1.54
2	C	801	Y01	CAQ-CAP	6.87	1.72	1.54
2	B	702	Y01	CAQ-CAP	6.87	1.72	1.54
2	B	703	Y01	CAQ-CAP	6.67	1.72	1.54
2	C	802	Y01	CAQ-CAP	6.65	1.72	1.54
2	A	802	Y01	CAQ-CAP	6.64	1.72	1.54
2	D	703	Y01	CAQ-CAP	6.60	1.72	1.54
2	B	701	Y01	CAQ-CAP	6.56	1.71	1.54
2	A	809	Y01	CAQ-CAP	6.53	1.71	1.54
2	D	701	Y01	CAQ-CAP	6.49	1.71	1.54
2	B	704	Y01	CAQ-CAP	6.49	1.71	1.54
2	D	702	Y01	CAI-CAZ	5.70	1.44	1.33
2	B	702	Y01	CAI-CAZ	5.68	1.44	1.33
2	A	801	Y01	CAI-CAZ	5.67	1.44	1.33
2	C	801	Y01	CAI-CAZ	5.64	1.44	1.33
2	D	701	Y01	CAQ-CBG	5.57	1.65	1.54
2	A	809	Y01	CAQ-CBG	5.53	1.65	1.54
2	B	701	Y01	CAQ-CBG	5.48	1.65	1.54
2	B	704	Y01	CAQ-CBG	5.46	1.65	1.54
2	B	702	Y01	CAQ-CBG	5.40	1.65	1.54
2	B	703	Y01	CAQ-CBG	5.39	1.65	1.54
2	A	801	Y01	CAQ-CBG	5.36	1.65	1.54
2	D	702	Y01	CAQ-CBG	5.36	1.65	1.54
2	C	801	Y01	CAQ-CBG	5.33	1.65	1.54
2	B	702	Y01	CAU-CAS	-5.30	1.42	1.53
2	C	801	Y01	CAU-CAS	-5.18	1.43	1.53
2	C	802	Y01	CAQ-CBG	5.17	1.64	1.54
2	D	703	Y01	CAQ-CBG	5.17	1.64	1.54
2	A	802	Y01	CAQ-CBG	5.14	1.64	1.54
2	B	703	Y01	CAI-CAZ	5.08	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	702	Y01	CAU-CAS	-5.07	1.43	1.53
2	A	801	Y01	CAU-CAS	-4.96	1.43	1.53
2	B	704	Y01	CAI-CAZ	4.82	1.42	1.33
2	A	809	Y01	CAI-CAZ	4.81	1.42	1.33
2	B	701	Y01	CAI-CAZ	4.81	1.42	1.33
2	B	701	Y01	OAW-CAY	4.80	1.47	1.34
2	D	701	Y01	OAW-CAY	4.79	1.47	1.34
2	B	704	Y01	OAW-CAY	4.79	1.47	1.34
2	A	809	Y01	OAW-CAY	4.77	1.47	1.34
2	D	701	Y01	CAI-CAZ	4.72	1.42	1.33
2	A	802	Y01	CAU-CAS	-4.71	1.44	1.53
2	C	802	Y01	CAI-CAZ	4.64	1.42	1.33
2	D	703	Y01	CAU-CAS	-4.61	1.44	1.53
2	A	802	Y01	CAI-CAZ	4.61	1.42	1.33
2	D	703	Y01	CAI-CAZ	4.59	1.42	1.33
2	C	802	Y01	CAU-CAS	-4.55	1.44	1.53
2	B	703	Y01	CAU-CAS	-4.55	1.44	1.53
2	D	701	Y01	CAU-CAS	-4.52	1.44	1.53
2	B	701	Y01	CAU-CAS	-4.48	1.44	1.53
2	A	809	Y01	CAU-CAS	-4.48	1.44	1.53
2	B	704	Y01	CAU-CAS	-4.48	1.44	1.53
2	D	701	Y01	CAT-CAR	4.34	1.62	1.53
2	B	701	Y01	CAT-CAR	4.31	1.62	1.53
2	B	704	Y01	CAT-CAR	4.30	1.62	1.53
2	A	809	Y01	CAT-CAR	4.29	1.62	1.53
2	B	703	Y01	CAT-CAR	4.28	1.61	1.53
2	B	703	Y01	OAW-CAY	4.27	1.46	1.34
2	C	802	Y01	OAW-CAY	4.25	1.46	1.34
2	D	703	Y01	OAW-CAY	4.15	1.46	1.34
2	A	802	Y01	OAW-CAY	4.14	1.46	1.34
2	B	704	Y01	CBH-CBF	-4.00	1.49	1.56
2	A	809	Y01	CBH-CBF	-3.98	1.49	1.56
2	B	701	Y01	CBH-CBF	-3.97	1.49	1.56
2	A	801	Y01	CBB-CBE	-3.92	1.47	1.54
2	D	703	Y01	CAT-CAR	3.91	1.61	1.53
2	B	702	Y01	CBB-CBE	-3.90	1.47	1.54
2	C	801	Y01	CBB-CBE	-3.89	1.47	1.54
2	C	802	Y01	CBD-CBF	-3.88	1.46	1.53
2	A	802	Y01	CAT-CAR	3.86	1.61	1.53
2	D	703	Y01	CBD-CBF	-3.86	1.46	1.53
2	B	702	Y01	OAW-CAY	3.85	1.45	1.34
2	B	703	Y01	CBD-CBF	-3.84	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	Y01	CBH-CBF	-3.83	1.49	1.56
2	D	702	Y01	CBB-CBE	-3.82	1.47	1.54
2	C	802	Y01	CAT-CAR	3.80	1.61	1.53
2	A	802	Y01	CBD-CBF	-3.78	1.46	1.53
2	A	802	Y01	CBB-CBE	-3.76	1.48	1.54
2	D	703	Y01	CBB-CBE	-3.73	1.48	1.54
2	C	802	Y01	CBB-CBE	-3.70	1.48	1.54
2	B	703	Y01	CBB-CBE	-3.70	1.48	1.54
2	B	704	Y01	CBD-CBF	-3.68	1.46	1.53
2	B	702	Y01	CBD-CBF	-3.66	1.46	1.53
2	B	701	Y01	CBD-CBF	-3.62	1.46	1.53
2	A	809	Y01	CBD-CBF	-3.56	1.46	1.53
2	D	703	Y01	CBH-CBF	-3.48	1.50	1.56
2	A	801	Y01	OAW-CAY	3.47	1.44	1.34
2	A	802	Y01	CBH-CBF	-3.47	1.50	1.56
2	A	801	Y01	CBD-CBF	-3.46	1.47	1.53
2	D	701	Y01	CBD-CBF	-3.44	1.47	1.53
2	D	702	Y01	OAW-CAY	3.43	1.44	1.34
2	D	702	Y01	CBD-CBF	-3.42	1.47	1.53
2	C	801	Y01	OAW-CAY	3.35	1.43	1.34
2	C	801	Y01	CBD-CBF	-3.33	1.47	1.53
2	D	701	Y01	CBB-CBE	-3.33	1.48	1.54
2	C	802	Y01	CBH-CBF	-3.32	1.50	1.56
2	B	703	Y01	CBH-CBF	-3.32	1.50	1.56
2	A	801	Y01	CAT-CAR	3.30	1.60	1.53
2	D	702	Y01	CAT-CAR	3.25	1.59	1.53
2	B	702	Y01	CAT-CAR	3.22	1.59	1.53
2	B	704	Y01	CBB-CBE	-3.21	1.48	1.54
2	B	701	Y01	CBB-CBE	-3.18	1.48	1.54
2	C	801	Y01	CAT-CAR	3.18	1.59	1.53
2	A	809	Y01	CBB-CBE	-3.13	1.49	1.54
3	B	706	POV	O21-C2	-2.89	1.39	1.46
3	C	804	POV	O21-C2	-2.88	1.39	1.46
3	D	705	POV	O21-C2	-2.88	1.39	1.46
3	A	804	POV	O21-C2	-2.87	1.39	1.46
2	B	703	Y01	OAW-CBC	2.79	1.53	1.46
2	B	704	Y01	CAO-CBB	2.73	1.61	1.54
2	C	802	Y01	CAO-CBB	2.73	1.61	1.54
2	D	703	Y01	CAO-CBB	2.72	1.61	1.54
2	A	801	Y01	OAW-CBC	2.71	1.53	1.46
2	A	802	Y01	CAS-CBF	-2.69	1.49	1.53
2	B	701	Y01	CAO-CBB	2.68	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	Y01	CAO-CBB	2.67	1.61	1.54
3	B	706	POV	O21-C21	2.67	1.41	1.34
3	A	804	POV	O21-C21	2.66	1.41	1.34
2	D	702	Y01	OAW-CBC	2.66	1.52	1.46
3	C	804	POV	O21-C21	2.65	1.41	1.34
2	A	809	Y01	CAO-CBB	2.64	1.60	1.54
2	A	802	Y01	CAO-CBB	2.64	1.60	1.54
3	D	705	POV	O21-C21	2.64	1.41	1.34
2	D	701	Y01	CAS-CBF	-2.63	1.49	1.53
2	D	703	Y01	CAS-CBF	-2.63	1.49	1.53
2	B	702	Y01	CBH-CBF	-2.62	1.51	1.56
2	C	801	Y01	CAR-CBC	-2.62	1.44	1.51
2	D	701	Y01	CAO-CBB	2.60	1.60	1.54
2	B	703	Y01	CAS-CBF	-2.59	1.49	1.53
2	B	702	Y01	OAW-CBC	2.58	1.52	1.46
2	A	801	Y01	CAR-CBC	-2.57	1.44	1.51
2	D	702	Y01	CAR-CBC	-2.56	1.44	1.51
2	B	701	Y01	CAS-CBF	-2.52	1.49	1.53
2	A	809	Y01	CAS-CBF	-2.51	1.49	1.53
2	B	702	Y01	CAR-CBC	-2.49	1.44	1.51
2	C	801	Y01	OAW-CBC	2.48	1.52	1.46
2	C	802	Y01	OAW-CBC	2.44	1.52	1.46
2	C	801	Y01	CBH-CBF	-2.44	1.52	1.56
2	C	802	Y01	CAS-CBF	-2.44	1.49	1.53
3	D	705	POV	O31-C31	2.43	1.40	1.33
3	B	706	POV	O31-C31	2.43	1.40	1.33
3	C	804	POV	O31-C31	2.42	1.40	1.33
3	A	804	POV	O31-C31	2.41	1.40	1.33
2	D	702	Y01	CBH-CBF	-2.38	1.52	1.56
2	B	704	Y01	CAS-CBF	-2.38	1.49	1.53
2	D	703	Y01	OAW-CBC	2.37	1.52	1.46
2	B	703	Y01	CAV-CBC	-2.34	1.46	1.52
2	A	802	Y01	OAW-CBC	2.31	1.52	1.46
2	A	801	Y01	CAO-CBB	2.31	1.60	1.54
2	C	802	Y01	CAV-CBC	-2.30	1.47	1.52
2	A	801	Y01	CBH-CBF	-2.26	1.52	1.56
2	D	703	Y01	CAV-CBC	-2.23	1.47	1.52
2	B	701	Y01	OAW-CBC	2.21	1.51	1.46
2	D	701	Y01	OAW-CBC	2.20	1.51	1.46
2	C	801	Y01	CAO-CBB	2.19	1.59	1.54
2	A	809	Y01	OAW-CBC	2.19	1.51	1.46
2	D	702	Y01	CAO-CBB	2.18	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	Y01	CAO-CBB	2.18	1.59	1.54
2	D	701	Y01	CAM-CAY	2.18	1.57	1.50
2	B	704	Y01	OAW-CBC	2.16	1.51	1.46
2	A	802	Y01	CAV-CBC	-2.16	1.47	1.52
2	B	704	Y01	CAM-CAY	2.15	1.56	1.50
2	A	809	Y01	CAM-CAY	2.09	1.56	1.50
2	B	703	Y01	CAE-CBI	2.09	1.57	1.54
2	B	701	Y01	CAM-CAY	2.08	1.56	1.50
2	D	703	Y01	CAE-CBI	2.07	1.57	1.54
2	C	802	Y01	CAE-CBI	2.03	1.57	1.54

All (354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	Y01	CAD-CBH-CBF	-13.01	97.06	111.66
2	B	701	Y01	CAD-CBH-CBF	-12.80	97.30	111.66
2	A	809	Y01	CAD-CBH-CBF	-12.72	97.38	111.66
2	D	701	Y01	CAD-CBH-CBF	-12.66	97.46	111.66
2	B	703	Y01	CAD-CBH-CBF	-12.23	97.94	111.66
2	A	802	Y01	CAD-CBH-CBF	-11.61	98.63	111.66
2	C	802	Y01	CAD-CBH-CBF	-11.51	98.74	111.66
2	D	703	Y01	CAD-CBH-CBF	-11.48	98.78	111.66
2	B	702	Y01	CAD-CBH-CBF	-9.33	101.19	111.66
2	C	801	Y01	CAD-CBH-CBF	-9.25	101.28	111.66
2	D	702	Y01	CAD-CBH-CBF	-8.99	101.57	111.66
2	C	801	Y01	CAK-CBD-CBF	8.69	119.76	109.72
2	A	801	Y01	CAD-CBH-CBF	-8.56	102.06	111.66
2	D	702	Y01	CAK-CBD-CBF	8.49	119.53	109.72
2	B	703	Y01	CAU-CBI-CBE	-8.40	104.23	116.60
2	A	801	Y01	CAK-CBD-CBF	8.32	119.34	109.72
2	C	802	Y01	CAU-CBI-CBE	-8.11	104.65	116.60
2	A	802	Y01	CAK-CBD-CBF	8.05	119.02	109.72
2	B	702	Y01	CAK-CBD-CBF	8.00	118.97	109.72
2	D	703	Y01	CAU-CBI-CBE	-8.00	104.82	116.60
2	D	703	Y01	CAK-CBD-CBF	7.85	118.80	109.72
2	A	802	Y01	CAU-CBI-CBE	-7.69	105.27	116.60
2	B	703	Y01	CAK-CBD-CBF	7.67	118.59	109.72
2	B	704	Y01	CAK-CBD-CBF	7.60	118.50	109.72
2	C	802	Y01	CAK-CBD-CBF	7.58	118.48	109.72
2	B	701	Y01	CAK-CBD-CBF	7.48	118.36	109.72
2	A	809	Y01	CAK-CBD-CBF	7.40	118.27	109.72
2	D	701	Y01	CAK-CAI-CAZ	-7.35	112.61	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	Y01	CAV-CAZ-CAI	-7.31	110.66	120.57
2	D	701	Y01	CAV-CAZ-CAI	-7.30	110.67	120.57
2	B	704	Y01	CAV-CAZ-CAI	-7.28	110.71	120.57
2	B	704	Y01	CBD-CAK-CAI	7.26	122.82	112.76
2	D	701	Y01	CAK-CBD-CBF	7.19	118.03	109.72
2	A	809	Y01	CAV-CAZ-CAI	-7.16	110.86	120.57
2	B	701	Y01	CBD-CAK-CAI	7.15	122.67	112.76
2	A	801	Y01	OAW-CBC-CAV	7.12	122.71	108.04
2	C	802	Y01	CBG-CBI-CBE	7.11	108.26	100.10
2	B	702	Y01	CBD-CAK-CAI	7.09	122.59	112.76
2	B	702	Y01	OAW-CBC-CAV	7.08	122.61	108.04
2	A	809	Y01	CBD-CAK-CAI	7.02	122.49	112.76
2	D	702	Y01	OAW-CBC-CAV	6.96	122.37	108.04
2	B	703	Y01	CAS-CBF-CBH	6.95	121.65	113.08
2	C	801	Y01	CAT-CBH-CBF	-6.88	99.64	108.74
2	B	703	Y01	CBG-CBI-CBE	6.86	107.97	100.10
2	A	809	Y01	CAK-CAI-CAZ	-6.86	113.43	125.02
2	C	801	Y01	OAW-CBC-CAV	6.82	122.09	108.04
2	B	703	Y01	CBD-CAK-CAI	6.80	122.19	112.76
2	B	702	Y01	CBF-CBH-CAZ	6.80	119.61	109.65
2	B	704	Y01	CAK-CAI-CAZ	-6.79	113.55	125.02
2	B	701	Y01	CAK-CAI-CAZ	-6.78	113.58	125.02
2	D	703	Y01	CBG-CBI-CBE	6.76	107.86	100.10
2	A	802	Y01	CAS-CBF-CBH	6.75	121.41	113.08
2	C	802	Y01	CBF-CBH-CAZ	6.66	119.41	109.65
2	D	703	Y01	CAS-CBF-CBH	6.66	121.30	113.08
2	A	802	Y01	CBF-CBH-CAZ	6.66	119.40	109.65
2	C	801	Y01	CBF-CBH-CAZ	6.63	119.36	109.65
2	A	801	Y01	CBD-CAK-CAI	6.62	121.93	112.76
2	D	702	Y01	CBF-CBH-CAZ	6.57	119.27	109.65
2	D	703	Y01	CBF-CBH-CAZ	6.56	119.26	109.65
2	D	702	Y01	CBG-CBI-CBE	6.56	107.62	100.10
2	D	702	Y01	CAT-CBH-CBF	-6.56	100.06	108.74
2	A	801	Y01	CBG-CBI-CBE	6.55	107.62	100.10
2	D	701	Y01	CBD-CAK-CAI	6.52	121.80	112.76
2	A	801	Y01	CBF-CBH-CAZ	6.51	119.19	109.65
2	C	802	Y01	CAS-CBF-CBH	6.51	121.11	113.08
2	A	809	Y01	CAE-CBI-CBE	-6.50	99.89	111.68
2	B	702	Y01	CAT-CBH-CBF	-6.45	100.20	108.74
2	D	702	Y01	CBD-CAK-CAI	6.44	121.69	112.76
2	B	701	Y01	CAE-CBI-CBE	-6.44	99.99	111.68
2	D	701	Y01	CAE-CBI-CBE	-6.42	100.04	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	Y01	CAK-CAI-CAZ	-6.36	114.28	125.02
2	C	801	Y01	CBD-CAK-CAI	6.36	121.57	112.76
2	A	801	Y01	CAT-CBH-CBF	-6.36	100.33	108.74
2	B	703	Y01	CBF-CBH-CAZ	6.25	118.80	109.65
2	C	801	Y01	CBG-CBI-CBE	6.21	107.23	100.10
2	D	703	Y01	CBD-CAK-CAI	6.20	121.35	112.76
2	A	802	Y01	CBD-CAK-CAI	6.08	121.19	112.76
2	C	802	Y01	CBD-CAK-CAI	6.07	121.17	112.76
2	B	704	Y01	CAE-CBI-CBE	-6.01	100.77	111.68
2	B	704	Y01	CAS-CBF-CBH	5.99	120.48	113.08
2	B	703	Y01	CAS-CAU-CBI	5.95	122.77	112.74
2	B	703	Y01	OAW-CBC-CAR	5.94	122.41	108.37
2	A	802	Y01	CBG-CBI-CBE	5.94	106.91	100.10
2	C	802	Y01	CAK-CAI-CAZ	-5.90	115.05	125.02
2	A	801	Y01	CAK-CAI-CAZ	-5.87	115.11	125.02
2	D	702	Y01	CAK-CAI-CAZ	-5.78	115.26	125.02
2	C	802	Y01	CAS-CAU-CBI	5.77	122.47	112.74
2	D	703	Y01	CAS-CAU-CBI	5.74	122.42	112.74
2	D	701	Y01	CAS-CBF-CBH	5.73	120.16	113.08
2	B	704	Y01	CAS-CAU-CBI	5.73	122.41	112.74
2	A	801	Y01	CAU-CBI-CBE	-5.71	108.19	116.60
2	D	701	Y01	CAS-CAU-CBI	5.71	122.37	112.74
2	A	809	Y01	CAS-CAU-CBI	5.70	122.35	112.74
2	B	701	Y01	CAS-CAU-CBI	5.66	122.28	112.74
2	D	703	Y01	CAK-CAI-CAZ	-5.65	115.48	125.02
2	B	702	Y01	CAK-CAI-CAZ	-5.63	115.51	125.02
2	C	801	Y01	CAK-CAI-CAZ	-5.61	115.54	125.02
2	B	701	Y01	OAW-CAY-CAM	5.61	123.62	111.48
2	A	809	Y01	CAS-CBF-CBH	5.61	120.00	113.08
2	A	802	Y01	CAS-CAU-CBI	5.61	122.21	112.74
2	D	702	Y01	CAU-CBI-CBE	-5.58	108.38	116.60
2	A	809	Y01	OAW-CAY-CAM	5.57	123.54	111.48
2	B	701	Y01	CAS-CBF-CBH	5.57	119.95	113.08
2	C	802	Y01	CBC-OAW-CAY	5.56	131.11	117.80
2	A	802	Y01	CBC-OAW-CAY	5.51	130.97	117.80
2	D	701	Y01	OAW-CAY-CAM	5.49	123.36	111.48
2	B	703	Y01	CBC-OAW-CAY	5.47	130.89	117.80
2	B	704	Y01	OAW-CAY-CAM	5.47	123.32	111.48
2	B	702	Y01	CAC-CBB-CAO	-5.47	101.88	110.34
2	A	809	Y01	CBG-CBI-CBE	5.46	106.36	100.10
2	B	702	Y01	CBG-CBI-CBE	5.43	106.33	100.10
2	D	703	Y01	CBC-OAW-CAY	5.43	130.79	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	Y01	CBG-CBI-CBE	5.40	106.29	100.10
2	D	702	Y01	CAS-CAU-CBI	5.38	121.82	112.74
2	C	801	Y01	CAC-CBB-CAO	-5.37	102.02	110.34
2	B	704	Y01	CBG-CBI-CBE	5.36	106.25	100.10
2	D	703	Y01	OAW-CBC-CAR	5.32	120.95	108.37
2	B	702	Y01	CAS-CAU-CBI	5.32	121.71	112.74
2	C	801	Y01	CAS-CAU-CBI	5.31	121.70	112.74
2	B	702	Y01	CAK-CBD-CBG	5.30	118.44	110.93
2	A	802	Y01	CAK-CAI-CAZ	-5.30	116.08	125.02
2	D	702	Y01	CAC-CBB-CAO	-5.29	102.15	110.34
2	A	801	Y01	CAS-CAU-CBI	5.28	121.64	112.74
2	B	702	Y01	CAU-CBI-CBE	-5.26	108.85	116.60
2	D	701	Y01	CBG-CBI-CBE	5.25	106.13	100.10
2	C	801	Y01	CAU-CBI-CBE	-5.25	108.87	116.60
2	C	802	Y01	OAW-CBC-CAR	5.24	120.75	108.37
2	A	802	Y01	OAW-CBC-CAR	5.13	120.49	108.37
2	D	702	Y01	CAK-CBD-CBG	5.02	118.04	110.93
2	B	703	Y01	CAV-CAZ-CAI	-4.99	113.81	120.57
2	A	801	Y01	CAC-CBB-CAO	-4.96	102.66	110.34
2	A	801	Y01	CAK-CBD-CBG	4.94	117.92	110.93
2	C	801	Y01	CAK-CBD-CBG	4.82	117.75	110.93
2	B	704	Y01	CBF-CBH-CAZ	4.77	116.64	109.65
2	B	702	Y01	CAS-CBF-CBH	4.73	118.92	113.08
2	A	809	Y01	CBF-CBH-CAZ	4.71	116.54	109.65
2	D	701	Y01	CAT-CAR-CBC	4.70	118.00	110.33
2	B	701	Y01	CBF-CBH-CAZ	4.69	116.51	109.65
2	A	809	Y01	CAT-CAR-CBC	4.64	117.91	110.33
2	D	701	Y01	CBF-CBH-CAZ	4.64	116.45	109.65
2	B	704	Y01	CAT-CAR-CBC	4.64	117.90	110.33
2	B	701	Y01	CAT-CAR-CBC	4.58	117.80	110.33
2	B	704	Y01	CAR-CBC-CAV	4.57	117.33	110.97
2	C	802	Y01	CAT-CAR-CBC	4.56	117.77	110.33
2	C	801	Y01	CAS-CBF-CBH	4.54	118.69	113.08
2	D	701	Y01	CAR-CBC-CAV	4.54	117.29	110.97
2	B	703	Y01	CAT-CAR-CBC	4.54	117.73	110.33
2	D	703	Y01	CAV-CAZ-CAI	-4.52	114.44	120.57
2	A	809	Y01	CAR-CBC-CAV	4.49	117.22	110.97
2	C	801	Y01	CAV-CAZ-CAI	-4.49	114.49	120.57
2	B	701	Y01	CAR-CBC-CAV	4.44	117.14	110.97
2	D	703	Y01	CAC-CBB-CBE	-4.40	106.28	112.88
2	D	702	Y01	CAS-CBF-CBH	4.37	118.48	113.08
2	A	801	Y01	CAS-CBF-CBH	4.29	118.37	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	Y01	CAT-CAR-CBC	4.27	117.29	110.33
2	A	802	Y01	CAT-CAR-CBC	4.26	117.28	110.33
2	A	802	Y01	CBH-CBF-CBD	4.25	118.92	112.71
2	C	802	Y01	CAV-CAZ-CAI	-4.23	114.84	120.57
2	A	802	Y01	CAU-CBI-CBG	4.21	113.55	107.25
2	C	802	Y01	OAW-CAY-CAM	4.20	120.57	111.48
2	D	703	Y01	CBH-CBF-CBD	4.18	118.82	112.71
2	B	703	Y01	CBH-CBF-CBD	4.17	118.81	112.71
2	A	801	Y01	CAV-CAZ-CAI	-4.16	114.93	120.57
2	B	703	Y01	CAC-CBB-CBE	-4.15	106.65	112.88
2	A	809	Y01	CBH-CBF-CBD	4.15	118.78	112.71
2	B	701	Y01	CBH-CBF-CBD	4.14	118.76	112.71
2	B	704	Y01	CBH-CBF-CBD	4.13	118.74	112.71
2	C	802	Y01	CAC-CBB-CBE	-4.11	106.71	112.88
2	C	802	Y01	CBC-CAV-CAZ	4.10	117.51	111.45
2	C	802	Y01	CBH-CBF-CBD	4.10	118.70	112.71
2	B	703	Y01	OAW-CAY-CAM	4.08	120.31	111.48
2	B	702	Y01	CAV-CAZ-CAI	-4.01	115.13	120.57
2	D	701	Y01	CBH-CBF-CBD	3.95	118.49	112.71
2	D	703	Y01	OAW-CAY-CAM	3.95	120.03	111.48
2	D	702	Y01	CAV-CAZ-CAI	-3.95	115.22	120.57
2	D	703	Y01	CAU-CBI-CBG	3.94	113.14	107.25
2	A	802	Y01	CAV-CAZ-CAI	-3.94	115.23	120.57
2	B	703	Y01	CAU-CBI-CBG	3.88	113.05	107.25
2	C	802	Y01	CAU-CBI-CBG	3.87	113.04	107.25
2	A	802	Y01	OAW-CAY-CAM	3.86	119.83	111.48
2	A	802	Y01	CAC-CBB-CBE	-3.85	107.10	112.88
2	A	801	Y01	CAO-CBB-CBE	3.82	118.24	110.33
2	C	801	Y01	CAE-CBI-CBE	-3.81	104.76	111.68
2	B	704	Y01	CAU-CBI-CBE	-3.81	110.99	116.60
2	A	802	Y01	CBC-CAV-CAZ	3.80	117.06	111.45
2	B	702	Y01	CAU-CBI-CBG	3.78	112.90	107.25
2	D	703	Y01	CBC-CAV-CAZ	3.73	116.96	111.45
2	A	801	Y01	OAW-CAY-CAM	3.71	119.52	111.48
3	D	705	POV	O21-C21-C22	3.70	119.48	111.48
3	C	804	POV	O21-C21-C22	3.69	119.47	111.48
3	A	804	POV	O21-C21-C22	3.66	119.39	111.48
2	B	701	Y01	CBC-CAV-CAZ	3.63	116.81	111.45
2	D	703	Y01	CAQ-CBG-CBI	-3.63	99.57	103.84
3	B	706	POV	O21-C21-C22	3.62	119.30	111.48
2	D	702	Y01	CAE-CBI-CBE	-3.61	105.12	111.68
2	C	802	Y01	CAO-CBB-CBE	3.60	117.80	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	Y01	OAW-CAY-CAM	3.59	119.24	111.48
2	D	703	Y01	CAO-CBB-CBE	3.50	117.59	110.33
2	C	801	Y01	CAU-CBI-CBG	3.50	112.48	107.25
2	D	701	Y01	CAU-CBI-CBE	-3.50	111.45	116.60
2	B	703	Y01	CAO-CBB-CBE	3.49	117.57	110.33
2	A	809	Y01	CBC-CAV-CAZ	3.49	116.61	111.45
2	D	702	Y01	CAO-CBB-CBE	3.46	117.50	110.33
2	D	702	Y01	CAU-CBI-CBG	3.44	112.39	107.25
2	A	809	Y01	CAU-CBI-CBE	-3.41	111.58	116.60
2	C	801	Y01	CAO-CBB-CBE	3.41	117.39	110.33
2	B	704	Y01	CBC-CAV-CAZ	3.41	116.48	111.45
2	C	802	Y01	CAQ-CBG-CBI	-3.40	99.85	103.84
2	C	801	Y01	OAW-CAY-OAG	-3.39	115.79	123.70
2	A	801	Y01	CAU-CBI-CBG	3.38	112.30	107.25
2	D	702	Y01	OAW-CAY-CAM	3.37	118.77	111.48
2	B	701	Y01	CAU-CBI-CBE	-3.37	111.64	116.60
2	A	801	Y01	CAE-CBI-CBE	-3.36	105.58	111.68
2	A	802	Y01	CAQ-CBG-CBI	-3.35	99.89	103.84
2	B	702	Y01	CAE-CBI-CBE	-3.35	105.61	111.68
2	B	703	Y01	CAP-CBE-CBI	3.34	107.77	103.84
2	A	801	Y01	CBC-OAW-CAY	3.34	125.78	117.80
2	D	701	Y01	CBI-CBG-CBD	3.32	119.13	114.41
2	A	801	Y01	OAW-CAY-OAG	-3.29	116.02	123.70
2	D	701	Y01	CBC-CAV-CAZ	3.29	116.31	111.45
2	A	809	Y01	CBI-CBG-CBD	3.26	119.05	114.41
2	B	704	Y01	CBI-CBG-CBD	3.26	119.04	114.41
2	B	703	Y01	CBC-CAV-CAZ	3.25	116.25	111.45
2	B	701	Y01	CBI-CBG-CBD	3.25	119.03	114.41
2	C	802	Y01	CAP-CBE-CBI	3.23	107.64	103.84
2	D	701	Y01	CAU-CBI-CBG	3.23	112.08	107.25
2	A	802	Y01	CAO-CBB-CBE	3.18	116.92	110.33
2	D	703	Y01	CAP-CBE-CBI	3.15	107.54	103.84
2	A	809	Y01	CAU-CBI-CBG	3.15	111.95	107.25
2	B	704	Y01	CAU-CBI-CBG	3.12	111.91	107.25
2	C	802	Y01	CBI-CBG-CBD	3.11	118.83	114.41
2	B	703	Y01	CBI-CBG-CBD	3.11	118.82	114.41
2	B	701	Y01	CAU-CBI-CBG	3.10	111.89	107.25
2	A	801	Y01	CBI-CBE-CBB	-3.10	114.71	119.50
2	B	702	Y01	CBC-OAW-CAY	3.07	125.14	117.80
2	C	801	Y01	CAD-CBH-CAT	3.02	114.03	109.43
2	D	702	Y01	CBC-OAW-CAY	3.01	125.00	117.80
2	D	702	Y01	CAD-CBH-CAT	3.00	114.00	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	Y01	CAQ-CBG-CBI	-3.00	100.31	103.84
2	B	704	Y01	CAD-CBH-CAT	2.99	113.98	109.43
2	D	702	Y01	OAW-CAY-OAG	-2.96	116.78	123.70
2	D	702	Y01	CBI-CBE-CBB	-2.95	114.94	119.50
2	C	801	Y01	CBI-CBE-CBB	-2.95	114.95	119.50
2	A	801	Y01	CAD-CBH-CAT	2.93	113.89	109.43
2	A	809	Y01	CAD-CBH-CAT	2.92	113.88	109.43
2	D	703	Y01	CBI-CBG-CBD	2.92	118.56	114.41
2	C	801	Y01	CAR-CAT-CBH	2.91	118.99	112.78
2	B	702	Y01	CBI-CBE-CBB	-2.91	115.00	119.50
2	B	701	Y01	CAD-CBH-CAT	2.90	113.85	109.43
2	D	701	Y01	CAD-CBH-CAT	2.89	113.83	109.43
2	A	802	Y01	CAT-CBH-CBF	-2.88	104.92	108.74
2	D	702	Y01	CAR-CAT-CBH	2.87	118.90	112.78
2	A	802	Y01	CBI-CBE-CBB	-2.86	115.08	119.50
2	B	703	Y01	CBI-CBE-CBB	-2.85	115.10	119.50
2	A	802	Y01	CAU-CAS-CBF	-2.84	108.31	113.14
2	A	801	Y01	CAR-CAT-CBH	2.83	118.81	112.78
2	B	702	Y01	CAO-CBB-CBE	2.81	116.16	110.33
2	B	703	Y01	CAU-CAS-CBF	-2.81	108.36	113.14
2	D	701	Y01	CAD-CBH-CAZ	2.80	112.66	108.38
2	D	703	Y01	CAT-CBH-CBF	-2.78	105.06	108.74
2	D	703	Y01	CAU-CAS-CBF	-2.78	108.42	113.14
2	C	802	Y01	CAU-CAS-CBF	-2.77	108.43	113.14
2	A	809	Y01	CAD-CBH-CAZ	2.76	112.60	108.38
2	C	802	Y01	CAT-CBH-CBF	-2.74	105.11	108.74
2	B	704	Y01	CAD-CBH-CAZ	2.73	112.56	108.38
2	B	704	Y01	CAK-CBD-CBG	2.71	114.77	110.93
2	B	701	Y01	CAD-CBH-CAZ	2.71	112.52	108.38
2	B	701	Y01	CAO-CBB-CBE	2.71	115.94	110.33
2	C	802	Y01	CBI-CBE-CBB	-2.70	115.33	119.50
2	C	801	Y01	CAT-CBH-CAZ	2.69	113.39	108.74
2	B	702	Y01	CBH-CBF-CBD	2.69	116.65	112.71
2	C	801	Y01	CBC-OAW-CAY	2.68	124.20	117.80
2	B	701	Y01	CAK-CBD-CBG	2.67	114.71	110.93
2	A	802	Y01	CAK-CBD-CBG	2.66	114.70	110.93
2	B	702	Y01	CAP-CBE-CBB	-2.66	108.15	112.18
3	D	705	POV	C14-N-C12	2.65	120.45	109.91
3	A	804	POV	C14-N-C12	2.65	120.43	109.91
3	B	706	POV	O31-C31-C32	2.65	119.90	111.83
3	C	804	POV	C14-N-C12	2.64	120.40	109.91
2	B	704	Y01	CAO-CBB-CBE	2.63	115.78	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	Y01	CBI-CBE-CBB	-2.62	115.45	119.50
2	D	701	Y01	CAO-CBB-CBE	2.62	115.76	110.33
3	B	706	POV	C14-N-C12	2.62	120.33	109.91
3	A	804	POV	O31-C31-C32	2.61	119.81	111.83
3	C	804	POV	O31-C31-C32	2.59	119.73	111.83
2	B	702	Y01	CAQ-CAP-CBE	2.59	110.21	105.14
2	C	801	Y01	CAP-CBE-CBB	-2.57	108.28	112.18
2	B	702	Y01	OAW-CAY-CAM	2.57	117.04	111.48
2	A	809	Y01	CAO-CBB-CBE	2.56	115.64	110.33
3	D	705	POV	O31-C31-C32	2.54	119.59	111.83
2	A	809	Y01	CAP-CBE-CBB	-2.49	108.41	112.18
2	D	702	Y01	CAT-CBH-CAZ	2.47	113.00	108.74
2	A	809	Y01	CAK-CBD-CBG	2.44	114.38	110.93
2	A	802	Y01	CAP-CBE-CBI	2.43	106.70	103.84
2	A	801	Y01	CAT-CBH-CAZ	2.42	112.92	108.74
2	B	702	Y01	CAR-CAT-CBH	2.40	117.90	112.78
2	B	701	Y01	CAP-CBE-CBB	-2.40	108.55	112.18
2	B	704	Y01	CAC-CBB-CAO	-2.39	106.64	110.34
2	D	702	Y01	CAP-CBE-CBB	-2.39	108.56	112.18
2	B	702	Y01	CAD-CBH-CAT	2.39	113.07	109.43
2	B	701	Y01	OAW-CBC-CAR	2.37	113.97	108.37
2	D	701	Y01	OAW-CAY-OAG	-2.36	118.18	123.70
2	B	702	Y01	CAT-CBH-CAZ	2.36	112.81	108.74
2	B	701	Y01	CAP-CBE-CBI	-2.36	101.07	103.84
2	D	701	Y01	CBH-CAZ-CAI	-2.35	119.50	122.93
2	B	704	Y01	OAW-CAY-OAG	-2.34	118.23	123.70
2	B	704	Y01	CAC-CBB-CBE	-2.34	109.37	112.88
2	B	702	Y01	CAT-CAR-CBC	-2.33	106.53	110.33
2	D	701	Y01	OAW-CBC-CAR	2.33	113.88	108.37
2	D	703	Y01	CAD-CBH-CAT	2.32	112.97	109.43
2	B	702	Y01	CBH-CAZ-CAI	-2.32	119.54	122.93
2	A	809	Y01	CAP-CBE-CBI	-2.32	101.11	103.84
2	A	809	Y01	OAW-CBC-CAR	2.32	113.86	108.37
2	A	802	Y01	CAD-CBH-CAT	2.32	112.96	109.43
2	A	801	Y01	CAP-CBE-CBB	-2.31	108.68	112.18
2	D	702	Y01	CAQ-CAP-CBE	2.30	109.65	105.14
2	A	809	Y01	OAW-CAY-OAG	-2.30	118.34	123.70
2	B	704	Y01	OAW-CBC-CAR	2.29	113.78	108.37
2	A	802	Y01	CAR-CBC-CAV	2.28	114.15	110.97
2	B	704	Y01	CAP-CBE-CBB	-2.27	108.74	112.18
2	A	801	Y01	CBI-CBG-CBD	2.27	117.63	114.41
2	B	701	Y01	OAW-CAY-OAG	-2.25	118.44	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	Y01	CBI-CBG-CBD	2.24	117.60	114.41
2	B	704	Y01	CAE-CBI-CBG	2.24	115.73	111.68
2	D	701	Y01	CAC-CBB-CBE	-2.23	109.53	112.88
2	C	802	Y01	CAD-CBH-CAT	2.21	112.80	109.43
2	D	701	Y01	CAP-CBE-CBB	-2.20	108.85	112.18
2	D	703	Y01	CAR-CBC-CAV	2.20	114.03	110.97
2	C	802	Y01	CAR-CBC-CAV	2.20	114.03	110.97
2	C	801	Y01	CBI-CBG-CBD	2.19	117.52	114.41
2	D	702	Y01	CBH-CAZ-CAI	-2.18	119.74	122.93
2	B	702	Y01	CAQ-CBG-CBD	2.18	122.57	119.10
2	D	702	Y01	CBH-CBF-CBD	2.17	115.88	112.71
2	A	802	Y01	CAQ-CBG-CBD	2.16	122.55	119.10
2	C	801	Y01	CAQ-CAP-CBE	2.16	109.37	105.14
2	A	801	Y01	CAQ-CAP-CBE	2.15	109.36	105.14
2	C	801	Y01	CBH-CBF-CBD	2.15	115.86	112.71
2	C	801	Y01	CBH-CAZ-CAI	-2.15	119.79	122.93
2	D	701	Y01	CAC-CBB-CAO	-2.15	107.02	110.34
2	D	702	Y01	CBI-CBG-CBD	2.14	117.45	114.41
2	A	801	Y01	CBH-CAZ-CAI	-2.12	119.83	122.93
2	A	801	Y01	CBH-CBF-CBD	2.12	115.81	112.71
2	B	702	Y01	CAR-CBC-CAV	2.11	113.91	110.97
2	A	809	Y01	CAC-CBB-CAO	-2.10	107.09	110.34
2	D	703	Y01	CAK-CBD-CBG	2.09	113.89	110.93
2	A	809	Y01	CBH-CAZ-CAI	-2.06	119.93	122.93
2	B	701	Y01	CAC-CBB-CAO	-2.04	107.19	110.34
2	D	701	Y01	CAK-CBD-CBG	2.03	113.81	110.93
3	C	804	POV	C3-C2-C1	-2.02	107.07	111.78
2	D	701	Y01	OAH-CAX-CAL	2.02	120.39	114.00
2	B	704	Y01	OAH-CAX-CAL	2.02	120.39	114.00
2	A	802	Y01	OAH-CAX-CAL	2.02	120.38	114.00
3	D	705	POV	C3-C2-C1	-2.01	107.09	111.78
2	D	701	Y01	CAP-CBE-CBI	-2.01	101.47	103.84

All (48) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	Y01	CBF
2	A	801	Y01	CBD
2	A	801	Y01	CBC
2	A	801	Y01	CBG
2	A	802	Y01	CBF
2	A	802	Y01	CBD

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Mol	Chain	Res	Type	Atom
2	A	802	Y01	CBC
2	A	802	Y01	CBG
2	A	809	Y01	CBF
2	A	809	Y01	CBD
2	A	809	Y01	CBC
2	A	809	Y01	CBG
2	B	701	Y01	CBF
2	B	701	Y01	CBD
2	B	701	Y01	CBC
2	B	701	Y01	CBG
2	B	702	Y01	CBF
2	B	702	Y01	CBD
2	B	702	Y01	CBC
2	B	702	Y01	CBG
2	B	703	Y01	CBF
2	B	703	Y01	CBD
2	B	703	Y01	CBC
2	B	703	Y01	CBG
2	B	704	Y01	CBF
2	B	704	Y01	CBD
2	B	704	Y01	CBC
2	B	704	Y01	CBG
2	C	801	Y01	CBF
2	C	801	Y01	CBD
2	C	801	Y01	CBC
2	C	801	Y01	CBG
2	C	802	Y01	CBF
2	C	802	Y01	CBD
2	C	802	Y01	CBC
2	C	802	Y01	CBG
2	D	701	Y01	CBF
2	D	701	Y01	CBD
2	D	701	Y01	CBC
2	D	701	Y01	CBG
2	D	702	Y01	CBF
2	D	702	Y01	CBD
2	D	702	Y01	CBC
2	D	702	Y01	CBG
2	D	703	Y01	CBF
2	D	703	Y01	CBD
2	D	703	Y01	CBC
2	D	703	Y01	CBG

All (300) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	Y01	CAV-CBC-OAW-CAY
2	A	801	Y01	CAM-CAY-OAW-CBC
2	A	802	Y01	CAR-CBC-OAW-CAY
2	A	809	Y01	CAV-CBC-OAW-CAY
2	A	809	Y01	OAG-CAY-OAW-CBC
2	A	809	Y01	CAM-CAY-OAW-CBC
2	B	701	Y01	CAV-CBC-OAW-CAY
2	B	701	Y01	OAG-CAY-OAW-CBC
2	B	701	Y01	CAM-CAY-OAW-CBC
2	B	702	Y01	CAV-CBC-OAW-CAY
2	B	703	Y01	CAO-CBB-CBE-CAP
2	B	703	Y01	CAC-CBB-CBE-CBI
2	B	703	Y01	CAR-CBC-OAW-CAY
2	B	704	Y01	CAV-CBC-OAW-CAY
2	B	704	Y01	OAG-CAY-OAW-CBC
2	B	704	Y01	CAM-CAY-OAW-CBC
2	C	801	Y01	CAV-CBC-OAW-CAY
2	C	801	Y01	CAM-CAY-OAW-CBC
2	C	802	Y01	CAO-CBB-CBE-CAP
2	C	802	Y01	CAC-CBB-CBE-CBI
2	C	802	Y01	CAR-CBC-OAW-CAY
2	D	701	Y01	CAV-CBC-OAW-CAY
2	D	701	Y01	OAG-CAY-OAW-CBC
2	D	701	Y01	CAM-CAY-OAW-CBC
2	D	702	Y01	CAV-CBC-OAW-CAY
2	D	703	Y01	CAO-CBB-CBE-CAP
2	D	703	Y01	CAC-CBB-CBE-CBI
2	D	703	Y01	CAR-CBC-OAW-CAY
3	A	804	POV	C1-O11-P-O13
3	B	706	POV	C1-O11-P-O13
3	B	706	POV	C11-O12-P-O11
3	B	706	POV	C11-O12-P-O14
3	C	804	POV	C1-O11-P-O12
3	C	804	POV	C1-O11-P-O13
3	C	804	POV	C1-O11-P-O14
3	D	705	POV	C1-O11-P-O12
3	D	705	POV	C1-O11-P-O13
3	D	705	POV	C1-O11-P-O14
3	A	804	POV	O32-C31-O31-C3
3	B	706	POV	O32-C31-O31-C3
3	C	804	POV	O32-C31-O31-C3
2	B	703	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
2	C	802	Y01	CAC-CBB-CBE-CAP
2	D	703	Y01	CAC-CBB-CBE-CAP
2	A	801	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	CAC-CBB-CBE-CBI
2	B	702	Y01	CAC-CBB-CBE-CBI
2	C	801	Y01	CAC-CBB-CBE-CBI
2	D	702	Y01	CAC-CBB-CBE-CBI
2	A	801	Y01	CAO-CBB-CBE-CBI
2	C	802	Y01	CAO-CBB-CBE-CBI
3	D	705	POV	O32-C31-O31-C3
2	A	801	Y01	OAG-CAY-OAW-CBC
2	C	801	Y01	OAG-CAY-OAW-CBC
2	D	702	Y01	OAG-CAY-OAW-CBC
2	D	702	Y01	CAM-CAY-OAW-CBC
2	A	802	Y01	CAJ-CAO-CBB-CAC
2	B	703	Y01	CAJ-CAO-CBB-CAC
2	C	802	Y01	CAJ-CAO-CBB-CAC
2	A	802	Y01	CAC-CBB-CBE-CAP
2	A	802	Y01	CAO-CBB-CBE-CAP
2	A	802	Y01	CAO-CBB-CBE-CBI
2	B	703	Y01	CAO-CBB-CBE-CBI
2	C	801	Y01	CAO-CBB-CBE-CBI
2	D	702	Y01	CAO-CBB-CBE-CBI
2	D	703	Y01	CAO-CBB-CBE-CBI
3	A	804	POV	C32-C31-O31-C3
3	B	706	POV	C32-C31-O31-C3
3	C	804	POV	C32-C31-O31-C3
3	D	705	POV	C32-C31-O31-C3
2	D	703	Y01	CAJ-CAO-CBB-CAC
2	B	704	Y01	CAC-CBB-CBE-CBI
2	B	702	Y01	CAM-CAY-OAW-CBC
2	D	701	Y01	CAC-CBB-CBE-CBI
2	C	802	Y01	CAJ-CAO-CBB-CBE
2	B	703	Y01	CAJ-CAO-CBB-CBE
2	B	702	Y01	OAG-CAY-OAW-CBC
2	A	801	Y01	CAC-CBB-CBE-CAP
2	B	702	Y01	CAO-CBB-CBE-CBI
2	B	704	Y01	CAO-CBB-CBE-CBI
2	A	809	Y01	CAJ-CAO-CBB-CAC
2	B	701	Y01	CAJ-CAO-CBB-CAC
2	B	704	Y01	CAJ-CAO-CBB-CAC
2	D	701	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
2	B	701	Y01	CAC-CBB-CBE-CBI
2	D	701	Y01	CAO-CBB-CBE-CBI
2	B	701	Y01	CAO-CBB-CBE-CBI
2	D	703	Y01	CAJ-CAO-CBB-CBE
2	A	809	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	CAO-CAJ-CAN-CBA
2	A	809	Y01	CAO-CAJ-CAN-CBA
2	B	701	Y01	CAO-CAJ-CAN-CBA
2	B	702	Y01	CAO-CAJ-CAN-CBA
2	D	701	Y01	CAO-CAJ-CAN-CBA
3	C	804	POV	C33-C34-C35-C36
2	D	703	Y01	CAO-CAJ-CAN-CBA
2	C	802	Y01	CAO-CAJ-CAN-CBA
2	A	801	Y01	CAX-CAL-CAM-CAY
2	B	702	Y01	CAX-CAL-CAM-CAY
2	B	704	Y01	CAX-CAL-CAM-CAY
2	C	801	Y01	CAX-CAL-CAM-CAY
2	D	701	Y01	CAX-CAL-CAM-CAY
2	D	702	Y01	CAX-CAL-CAM-CAY
3	C	803	POV	C35-C36-C37-C38
3	A	803	POV	C35-C36-C37-C38
3	B	705	POV	C35-C36-C37-C38
3	D	704	POV	C35-C36-C37-C38
2	C	801	Y01	CAO-CAJ-CAN-CBA
3	A	804	POV	C33-C34-C35-C36
2	B	703	Y01	CAO-CAJ-CAN-CBA
2	D	702	Y01	CAO-CAJ-CAN-CBA
2	A	809	Y01	CAO-CBB-CBE-CBI
2	A	809	Y01	CAX-CAL-CAM-CAY
2	B	701	Y01	CAX-CAL-CAM-CAY
2	A	801	Y01	CAO-CAJ-CAN-CBA
2	B	704	Y01	CAO-CAJ-CAN-CBA
3	C	804	POV	C22-C21-O21-C2
3	D	705	POV	C22-C21-O21-C2
3	C	804	POV	O22-C21-O21-C2
3	D	705	POV	O22-C21-O21-C2
3	B	706	POV	C33-C34-C35-C36
3	D	705	POV	C33-C34-C35-C36
2	B	704	Y01	CAN-CAJ-CAO-CBB
3	A	804	POV	O22-C21-O21-C2
3	A	804	POV	C22-C21-O21-C2
3	B	706	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	B	703	Y01	CAN-CAJ-CAO-CBB
2	C	802	Y01	CAN-CAJ-CAO-CBB
3	B	706	POV	O22-C21-O21-C2
2	A	802	Y01	CAJ-CAO-CBB-CBE
2	D	702	Y01	CAC-CBB-CBE-CAP
3	D	705	POV	C31-C32-C33-C34
3	A	804	POV	C31-C32-C33-C34
3	B	706	POV	C31-C32-C33-C34
3	C	804	POV	C31-C32-C33-C34
3	A	803	POV	C311-C310-C39-C38
3	B	705	POV	C311-C310-C39-C38
3	C	803	POV	C311-C310-C39-C38
3	D	704	POV	C311-C310-C39-C38
2	C	802	Y01	CAM-CAY-OAW-CBC
3	D	705	POV	C34-C35-C36-C37
3	A	804	POV	C34-C35-C36-C37
3	C	804	POV	C22-C23-C24-C25
3	B	706	POV	C22-C23-C24-C25
3	D	705	POV	C22-C23-C24-C25
2	D	703	Y01	CAN-CAJ-CAO-CBB
3	A	804	POV	C22-C23-C24-C25
3	B	706	POV	C34-C35-C36-C37
3	C	804	POV	C34-C35-C36-C37
2	B	702	Y01	CAC-CBB-CBE-CAP
2	B	704	Y01	CAC-CBB-CBE-CAP
2	C	801	Y01	CAC-CBB-CBE-CAP
2	A	802	Y01	CAM-CAY-OAW-CBC
2	D	703	Y01	CAM-CAY-OAW-CBC
2	A	802	Y01	OAG-CAY-OAW-CBC
3	C	804	POV	C24-C25-C26-C27
3	D	705	POV	C24-C25-C26-C27
3	A	804	POV	C11-C12-N-C14
3	A	804	POV	C11-C12-N-C15
3	B	706	POV	C11-C12-N-C14
3	C	804	POV	C11-C12-N-C14
3	C	804	POV	C11-C12-N-C15
3	D	705	POV	C11-C12-N-C14
3	D	705	POV	C11-C12-N-C15
3	A	804	POV	C24-C25-C26-C27
3	B	706	POV	C24-C25-C26-C27
2	A	802	Y01	CAN-CAJ-CAO-CBB
2	B	701	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
2	D	701	Y01	CAN-CAJ-CAO-CBB
3	A	804	POV	C23-C24-C25-C26
3	B	706	POV	C23-C24-C25-C26
3	C	804	POV	C23-C24-C25-C26
3	A	804	POV	C21-C22-C23-C24
3	B	706	POV	C21-C22-C23-C24
3	C	804	POV	C21-C22-C23-C24
3	D	705	POV	C21-C22-C23-C24
3	D	705	POV	C23-C24-C25-C26
2	A	801	Y01	CAN-CAJ-CAO-CBB
3	A	803	POV	C37-C38-C39-C310
3	C	803	POV	C37-C38-C39-C310
3	D	704	POV	C37-C38-C39-C310
3	B	705	POV	C37-C38-C39-C310
2	D	703	Y01	OAG-CAY-OAW-CBC
2	C	801	Y01	CAN-CAJ-CAO-CBB
3	B	706	POV	C11-C12-N-C15
2	C	802	Y01	OAG-CAY-OAW-CBC
2	D	702	Y01	CAN-CAJ-CAO-CBB
2	B	702	Y01	CAN-CAJ-CAO-CBB
2	A	809	Y01	CAN-CAJ-CAO-CBB
2	D	701	Y01	CAC-CBB-CBE-CAP
3	A	804	POV	C11-C12-N-C13
3	B	706	POV	C11-C12-N-C13
3	C	804	POV	C11-C12-N-C13
3	D	705	POV	C11-C12-N-C13
2	A	809	Y01	CAC-CBB-CBE-CAP
2	B	701	Y01	CAC-CBB-CBE-CAP
2	A	801	Y01	CAO-CBB-CBE-CAP
3	A	804	POV	C36-C37-C38-C39
3	D	705	POV	C36-C37-C38-C39
3	C	804	POV	C36-C37-C38-C39
3	B	706	POV	C36-C37-C38-C39
3	C	805	POV	C213-C214-C215-C216
3	A	803	POV	C310-C311-C312-C313
3	D	704	POV	C310-C311-C312-C313
3	B	705	POV	C310-C311-C312-C313
3	C	803	POV	C310-C311-C312-C313
3	A	805	POV	C213-C214-C215-C216
3	A	808	POV	C213-C214-C215-C216
3	D	706	POV	C213-C214-C215-C216
3	C	805	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
3	D	706	POV	C214-C215-C216-C217
3	A	805	POV	C214-C215-C216-C217
3	A	808	POV	C214-C215-C216-C217
3	A	803	POV	C39-C310-C311-C312
3	B	705	POV	C39-C310-C311-C312
3	C	803	POV	C39-C310-C311-C312
3	D	704	POV	C39-C310-C311-C312
3	B	706	POV	C37-C38-C39-C310
3	C	804	POV	C37-C38-C39-C310
3	A	804	POV	C37-C38-C39-C310
2	B	704	Y01	CAO-CBB-CBE-CAP
2	D	702	Y01	CAO-CBB-CBE-CAP
3	D	705	POV	C37-C38-C39-C310
2	D	701	Y01	CAO-CBB-CBE-CAP
2	A	809	Y01	CAJ-CAN-CBA-CAA
2	B	701	Y01	CAJ-CAN-CBA-CAA
2	C	801	Y01	CAO-CBB-CBE-CAP
3	B	707	POV	C311-C310-C39-C38
2	B	701	Y01	CAO-CBB-CBE-CAP
2	B	702	Y01	CAO-CBB-CBE-CAP
2	D	701	Y01	CAJ-CAN-CBA-CAA
2	A	809	Y01	CAO-CBB-CBE-CAP
2	B	704	Y01	CAJ-CAN-CBA-CAA
3	A	806	POV	C313-C314-C315-C316
3	B	706	POV	C32-C33-C34-C35
3	C	804	POV	C32-C33-C34-C35
3	D	707	POV	C311-C310-C39-C38
3	C	806	POV	C311-C310-C39-C38
3	A	804	POV	C1-O11-P-O12
3	A	804	POV	C1-O11-P-O14
3	A	804	POV	C11-O12-P-O11
3	A	804	POV	C11-O12-P-O13
3	A	804	POV	C11-O12-P-O14
3	B	706	POV	C1-O11-P-O12
3	B	706	POV	C1-O11-P-O14
3	B	706	POV	C11-O12-P-O13
3	C	804	POV	C11-O12-P-O11
3	C	804	POV	C11-O12-P-O13
3	C	804	POV	C11-O12-P-O14
3	D	705	POV	C11-O12-P-O11
3	D	705	POV	C11-O12-P-O13
3	D	705	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
3	C	804	POV	C35-C36-C37-C38
3	A	804	POV	C32-C33-C34-C35
3	D	707	POV	C313-C314-C315-C316
3	A	806	POV	C311-C310-C39-C38
2	C	802	Y01	CAX-CAL-CAM-CAY
3	B	707	POV	C313-C314-C315-C316
3	B	706	POV	C35-C36-C37-C38
3	A	804	POV	C35-C36-C37-C38
3	D	705	POV	C32-C33-C34-C35
3	D	705	POV	C35-C36-C37-C38
2	B	703	Y01	OAG-CAY-OAW-CBC
2	A	809	Y01	CAJ-CAN-CBA-CAB
3	A	803	POV	C33-C34-C35-C36
2	C	801	Y01	CAM-CAL-CAX-OAH
2	D	702	Y01	CAM-CAL-CAX-OAH
2	A	802	Y01	CAM-CAL-CAX-OAH
2	A	801	Y01	CAM-CAL-CAX-OAH
2	B	702	Y01	CAM-CAL-CAX-OAH
2	B	703	Y01	CAM-CAL-CAX-OAF
3	B	705	POV	C33-C34-C35-C36
3	C	803	POV	C33-C34-C35-C36
3	D	704	POV	C33-C34-C35-C36
2	D	703	Y01	CAM-CAL-CAX-OAH
2	B	702	Y01	CAM-CAL-CAX-OAF
3	C	806	POV	C313-C314-C315-C316
2	A	801	Y01	CAM-CAL-CAX-OAF
2	C	802	Y01	CAM-CAL-CAX-OAH
2	C	802	Y01	CAM-CAL-CAX-OAF
2	D	702	Y01	CAM-CAL-CAX-OAF
2	C	801	Y01	CAM-CAL-CAX-OAF
2	D	703	Y01	CAM-CAL-CAX-OAF
3	B	706	POV	O11-C1-C2-C3
2	B	703	Y01	CAM-CAL-CAX-OAH
3	A	804	POV	O21-C21-C22-C23
3	B	706	POV	O21-C21-C22-C23
3	D	705	POV	O21-C21-C22-C23
2	B	701	Y01	CAJ-CAN-CBA-CAB
2	A	802	Y01	CAM-CAL-CAX-OAF
3	C	804	POV	O21-C21-C22-C23
2	A	802	Y01	CAX-CAL-CAM-CAY
2	D	703	Y01	CAX-CAL-CAM-CAY
3	A	804	POV	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	A	804	POV	O11-C1-C2-C3
3	B	706	POV	O31-C31-C32-C33
3	D	705	POV	O31-C31-C32-C33
3	C	804	POV	O31-C31-C32-C33
3	B	706	POV	O32-C31-C32-C33
3	A	804	POV	O32-C31-C32-C33

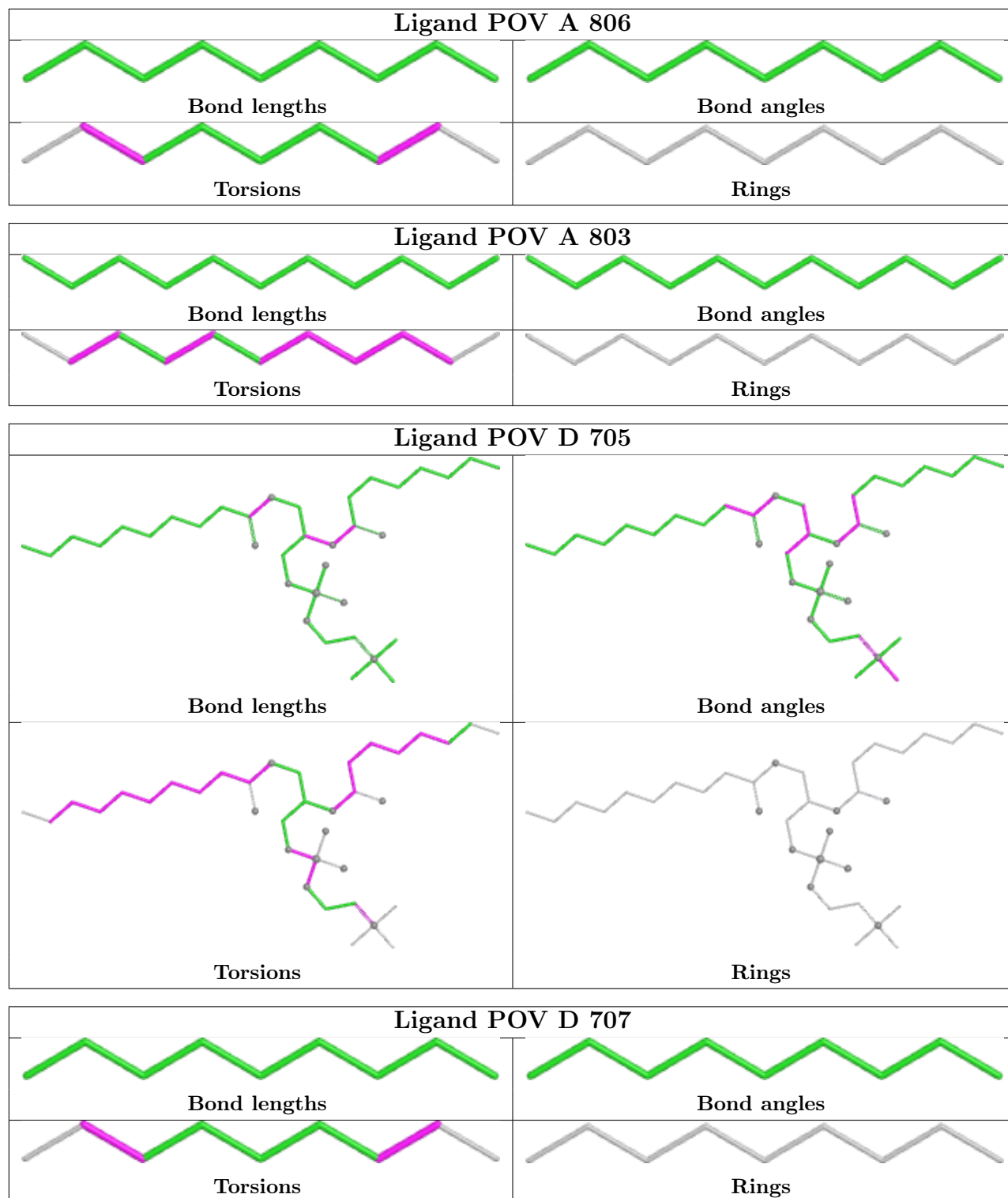
There are no ring outliers.

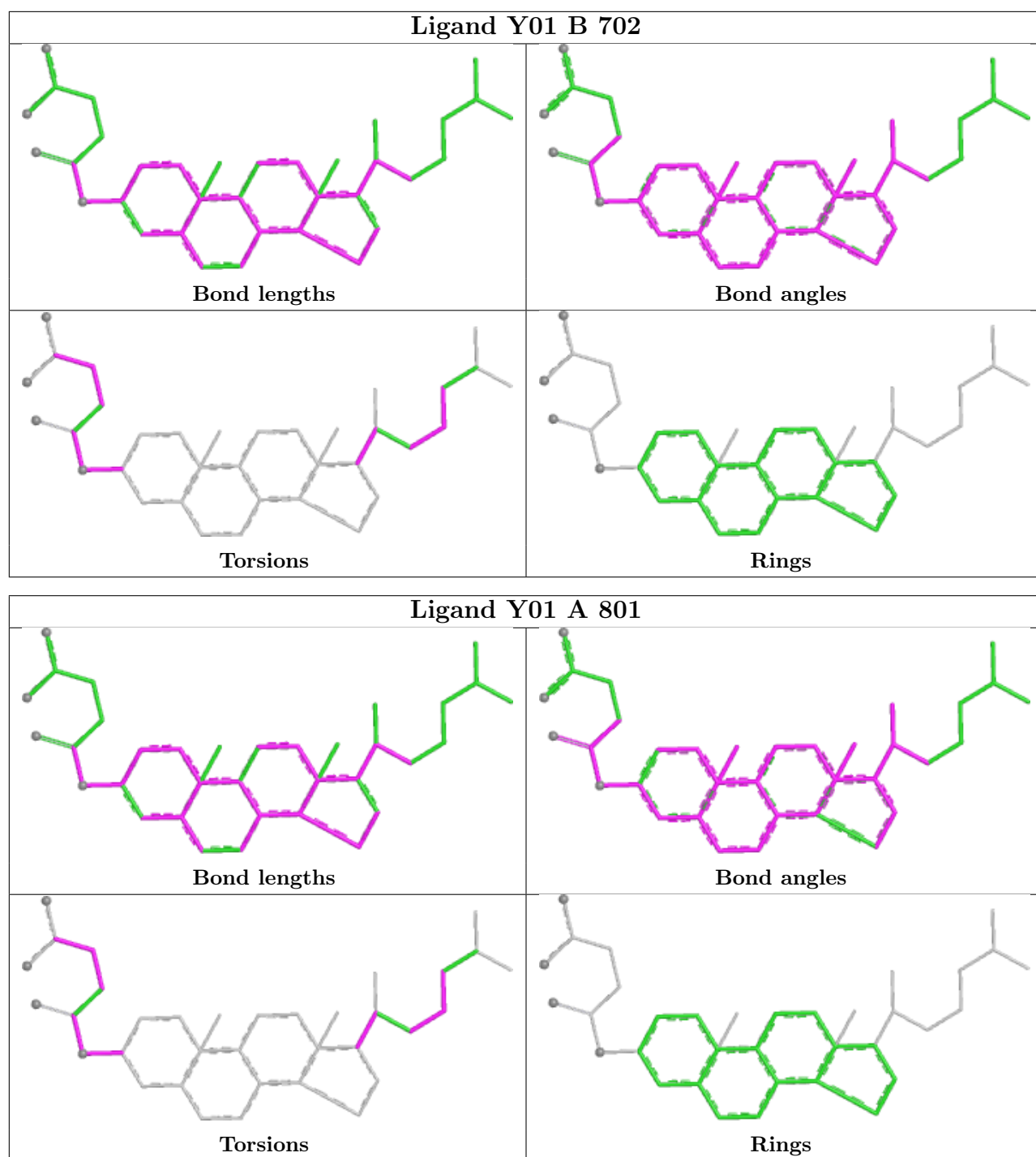
21 monomers are involved in 144 short contacts:

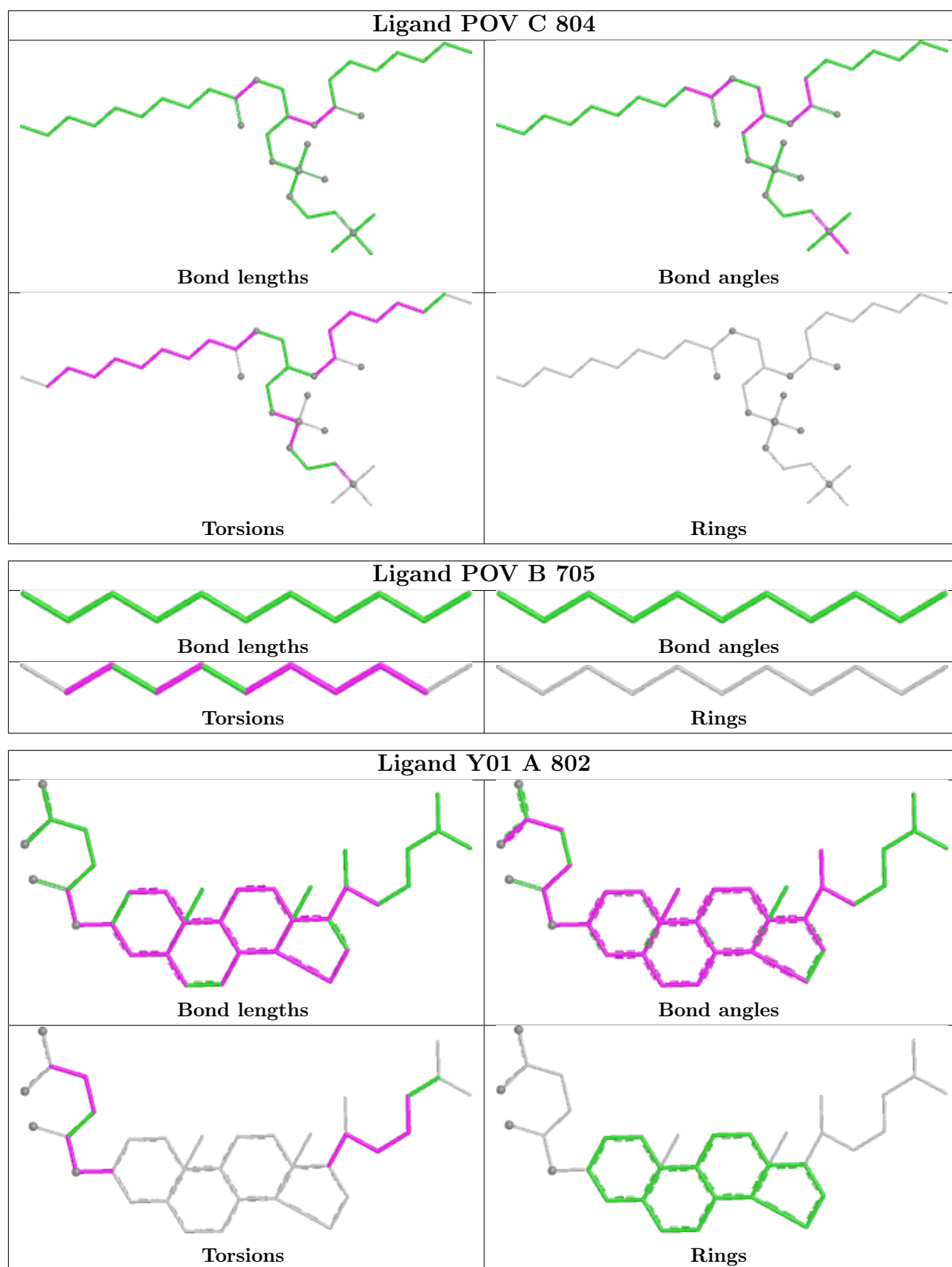
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	806	POV	1	0
3	D	705	POV	1	0
3	D	707	POV	1	0
2	B	702	Y01	12	0
2	A	801	Y01	11	0
3	C	804	POV	1	0
3	B	705	POV	1	0
2	A	802	Y01	9	0
3	D	704	POV	1	0
2	C	802	Y01	10	0
2	D	702	Y01	11	0
3	A	804	POV	1	0
3	C	806	POV	1	0
2	D	703	Y01	9	0
2	D	701	Y01	13	0
2	B	704	Y01	12	0
3	C	803	POV	2	0
2	B	701	Y01	13	0
2	C	801	Y01	11	0
2	A	809	Y01	12	0
2	B	703	Y01	11	0

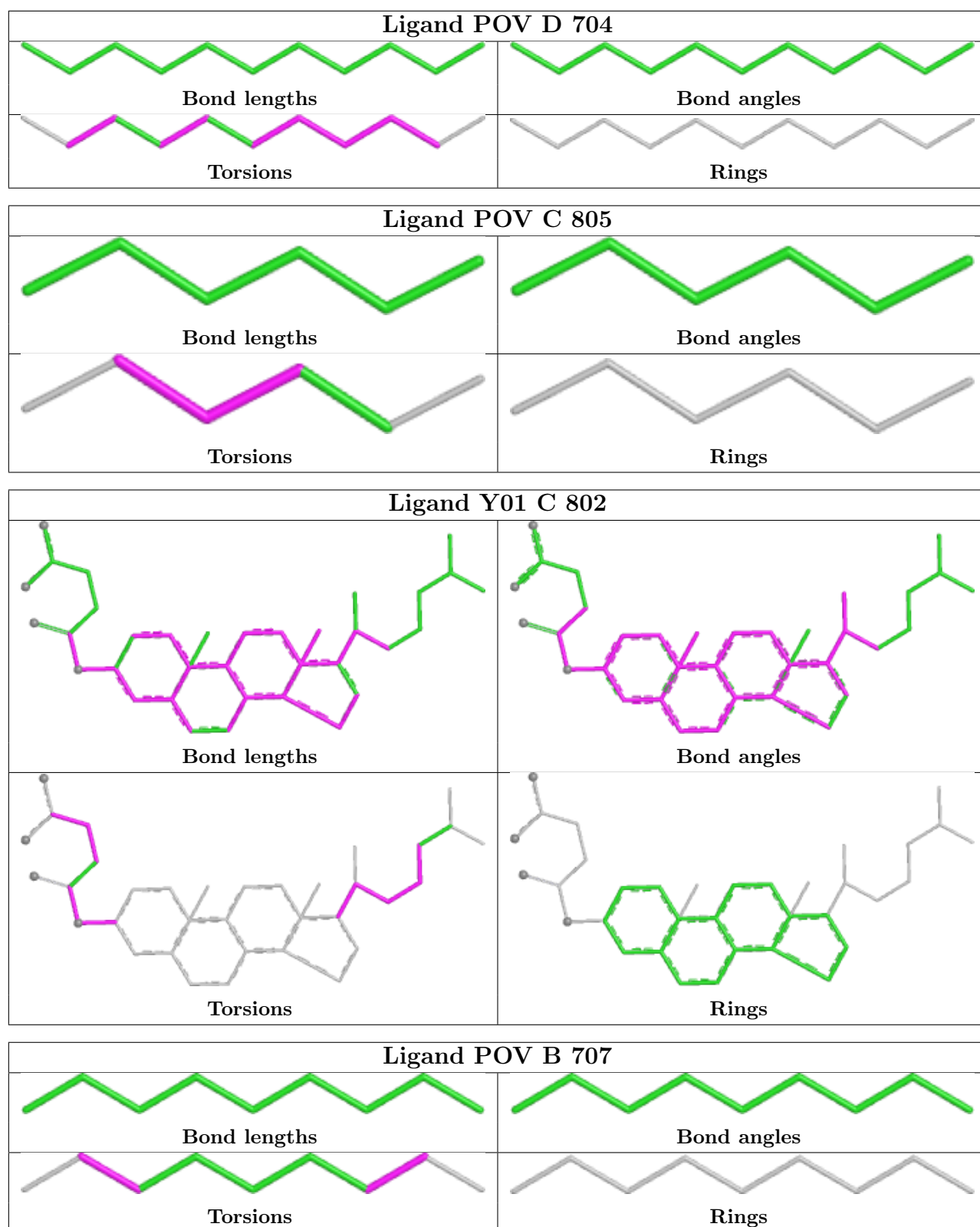
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

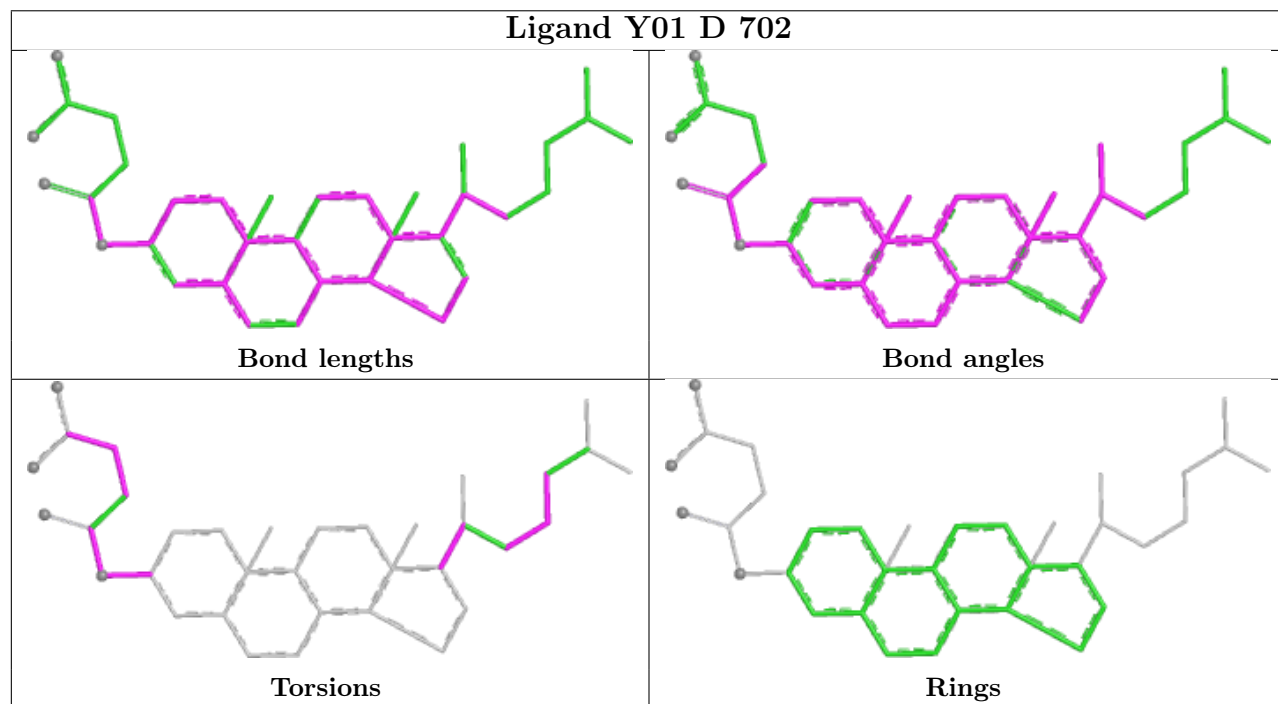
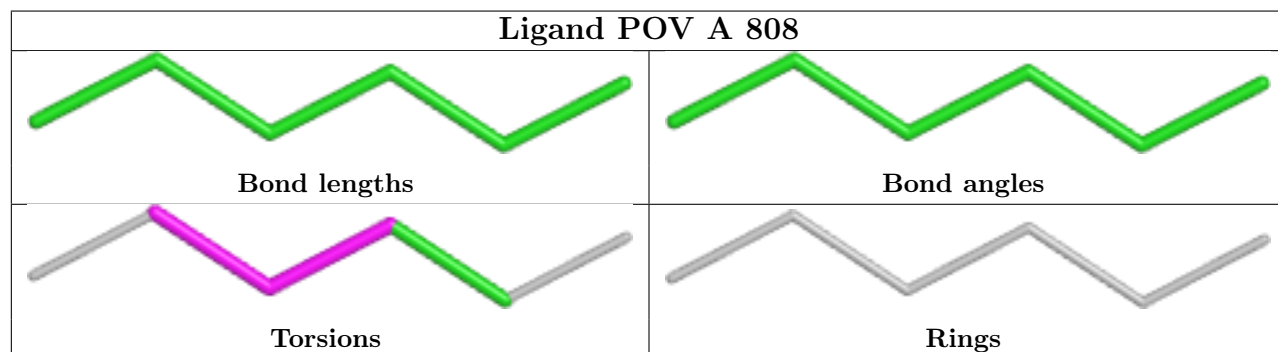
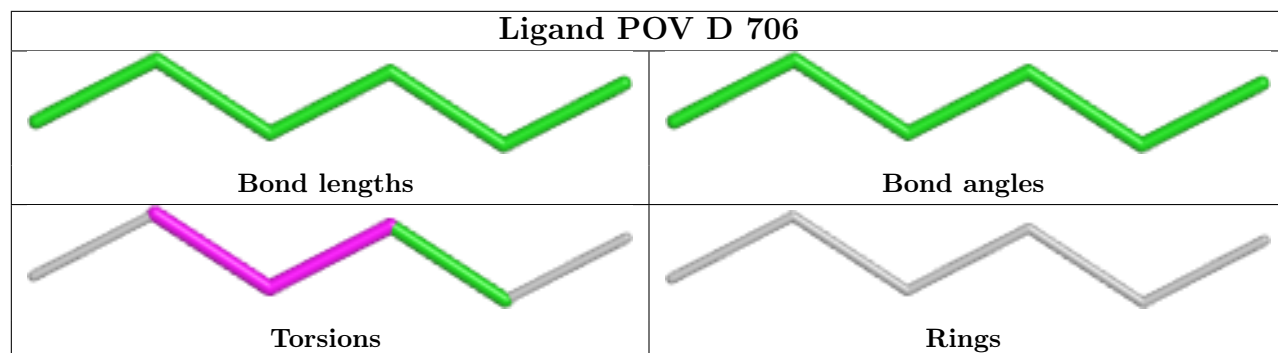
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

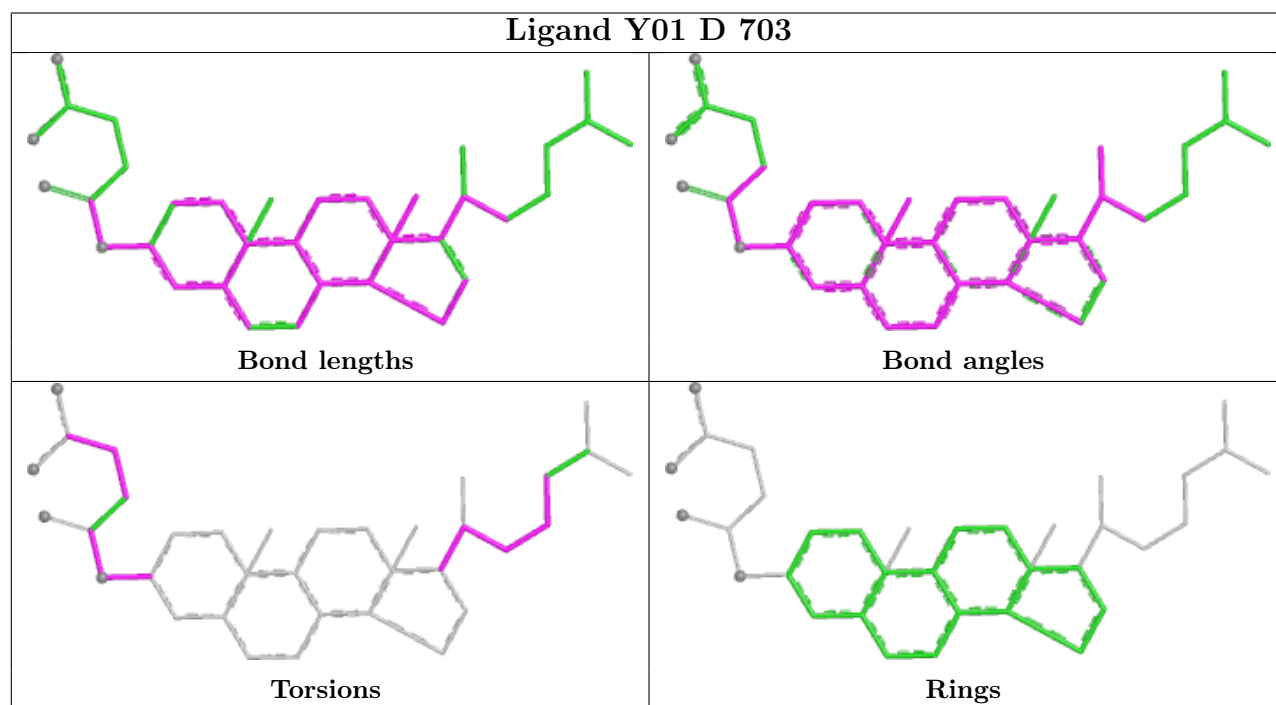
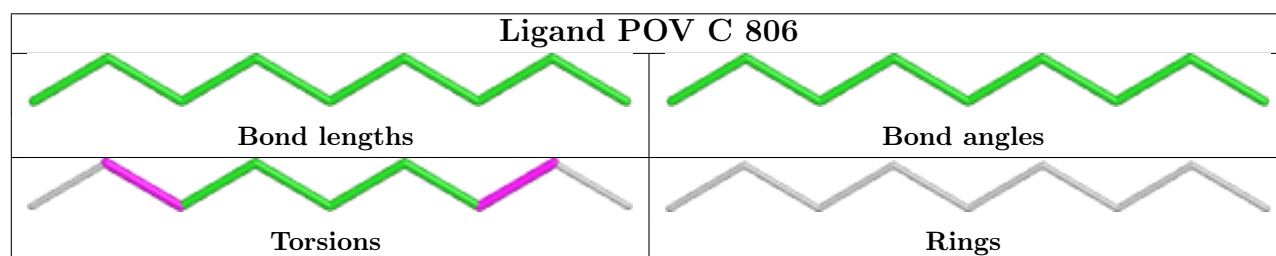
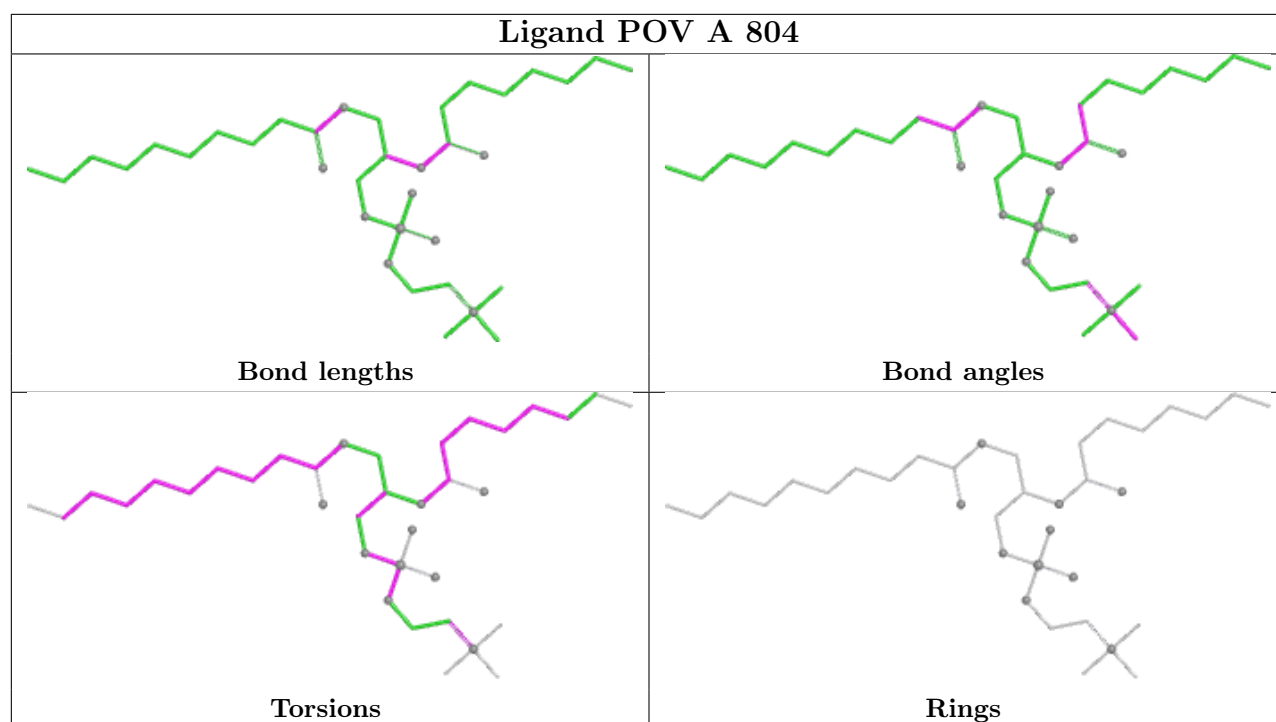


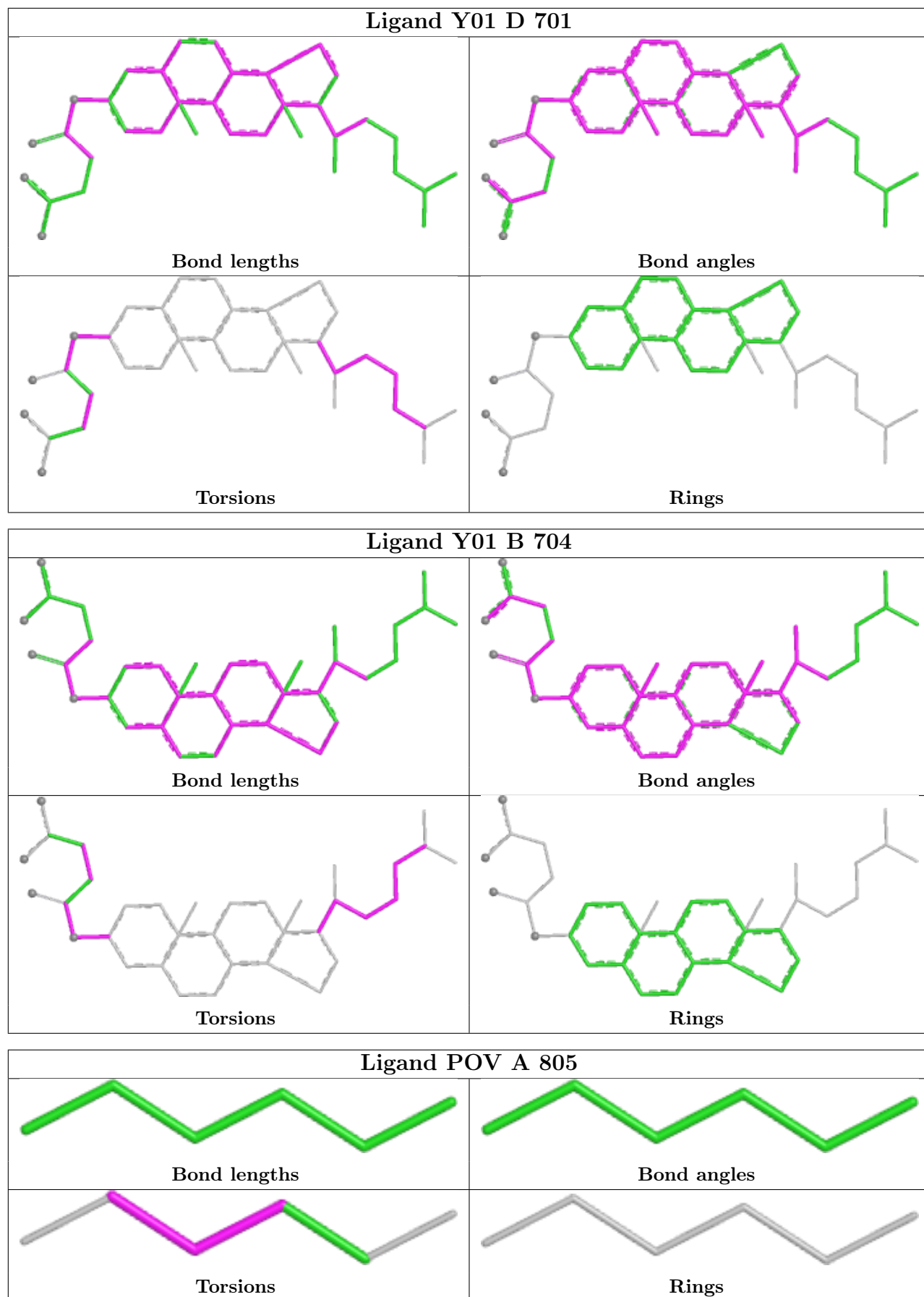


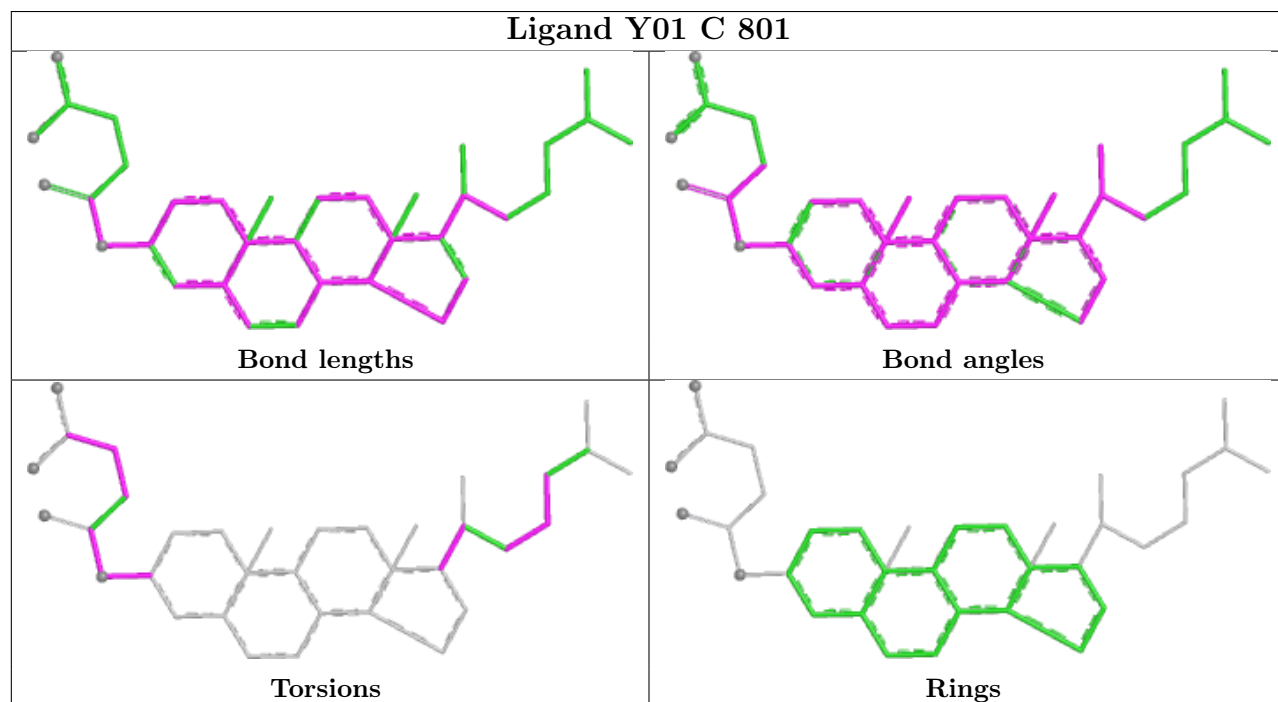
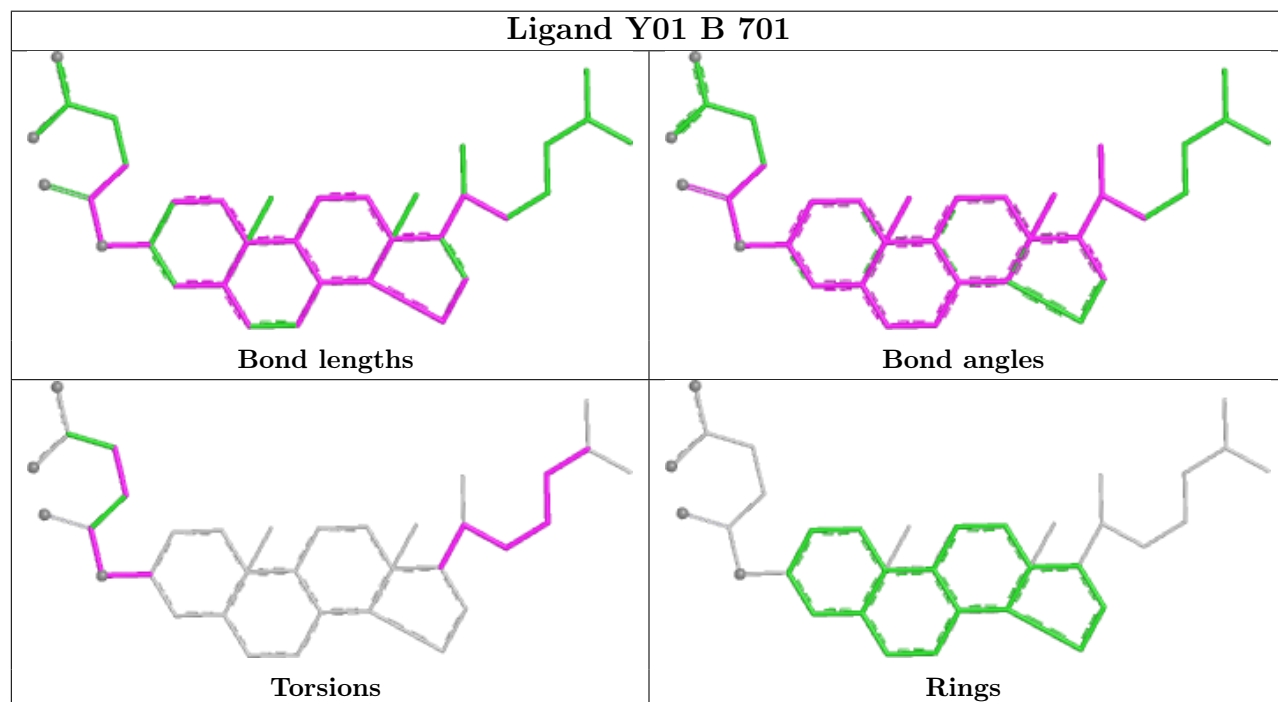
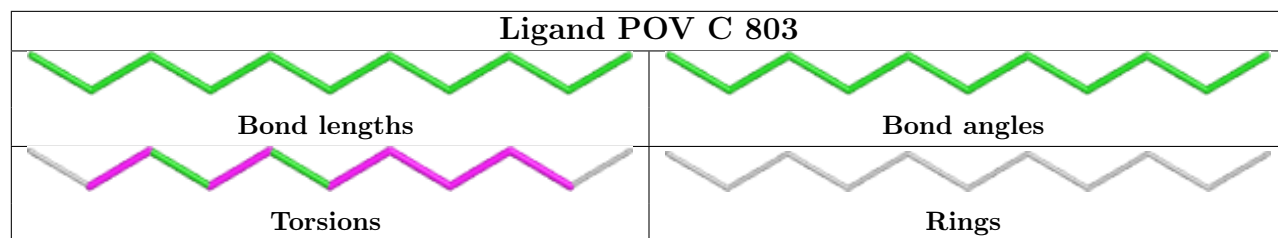


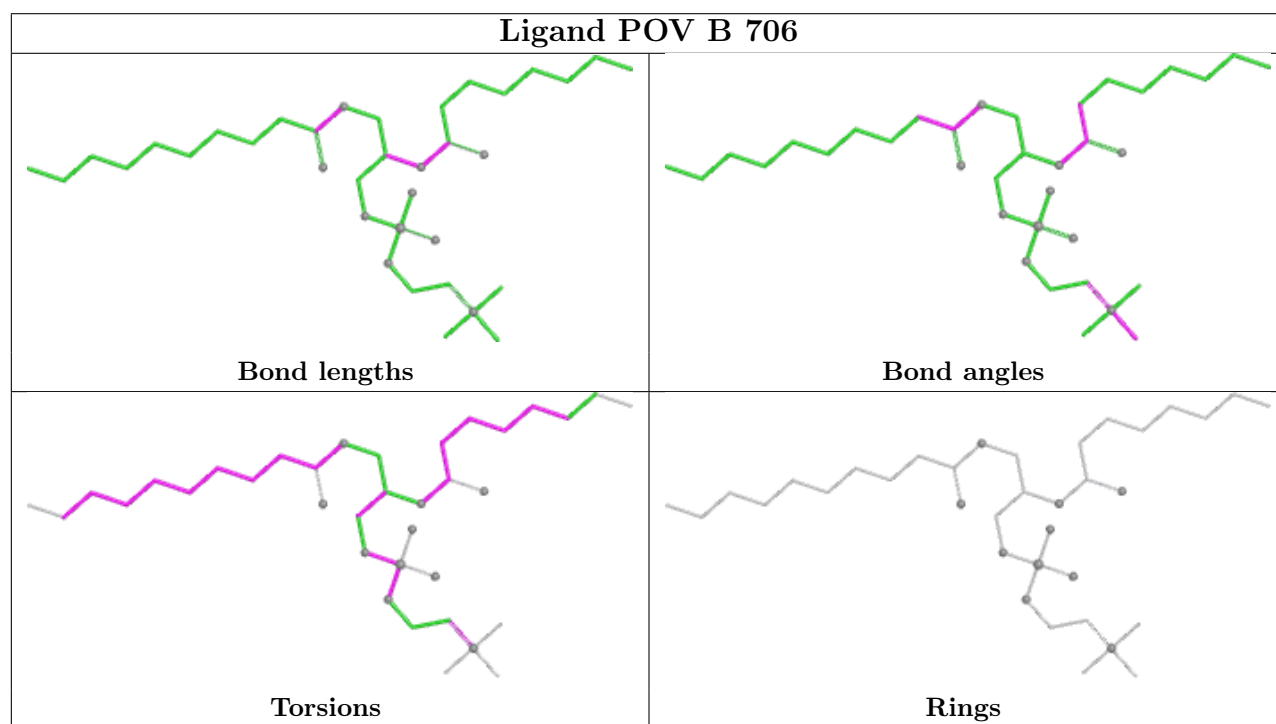
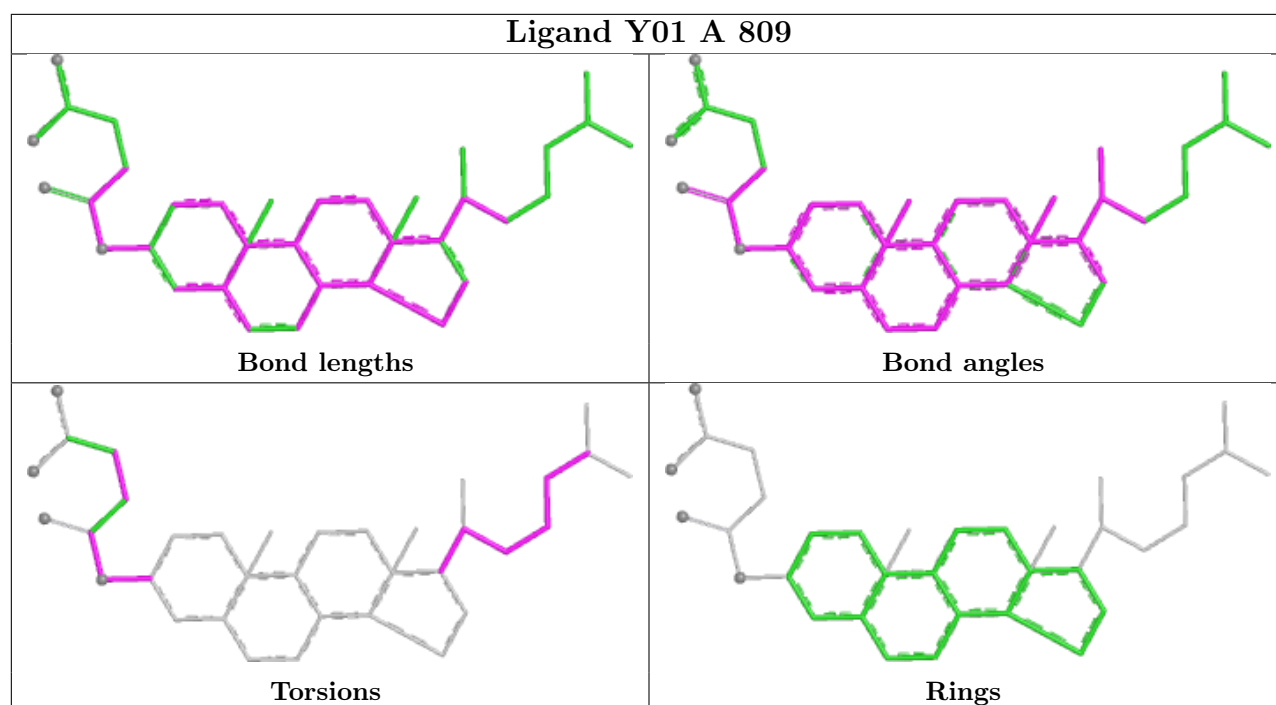


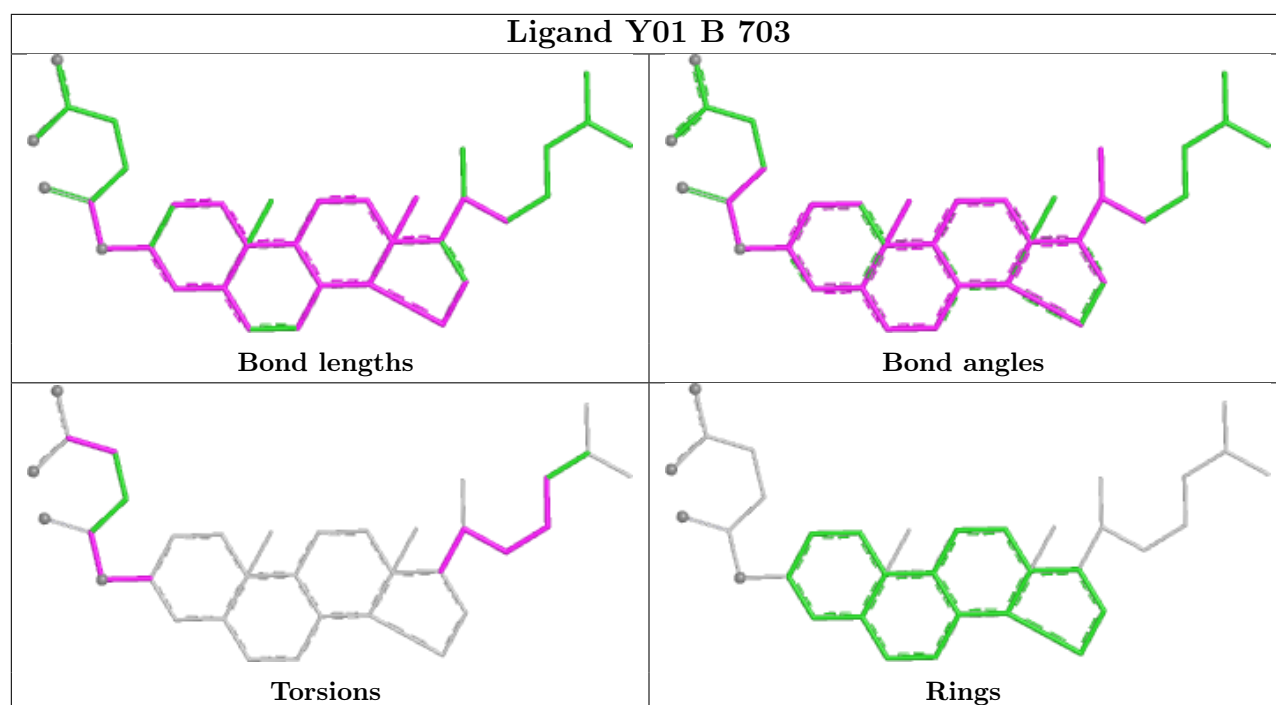












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

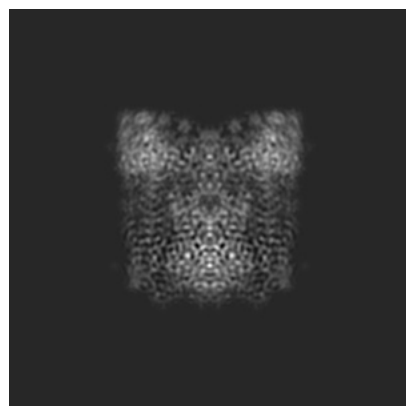
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49646. These allow visual inspection of the internal detail of the map and identification of artifacts.

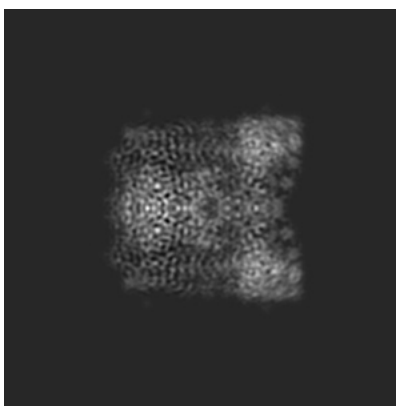
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

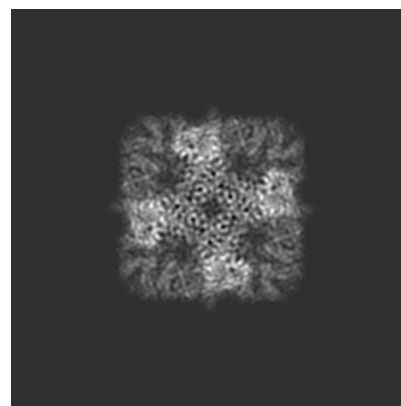
6.1.1 Primary map



X

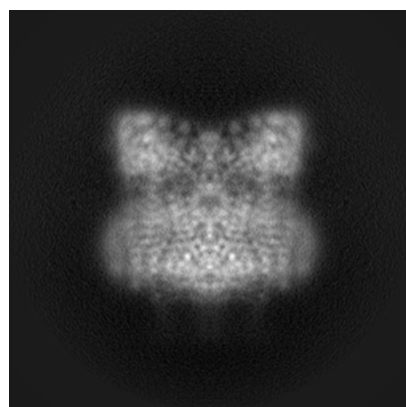


Y

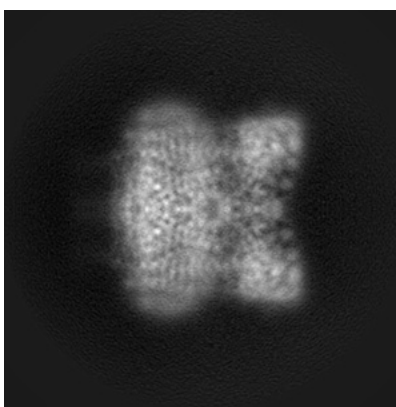


Z

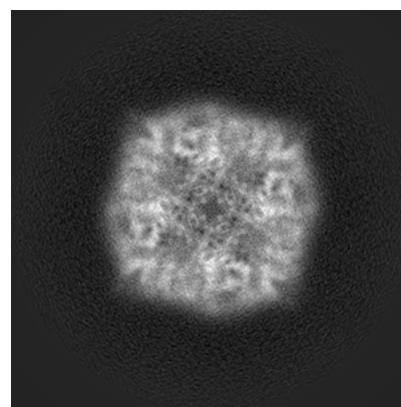
6.1.2 Raw map



X



Y



Z

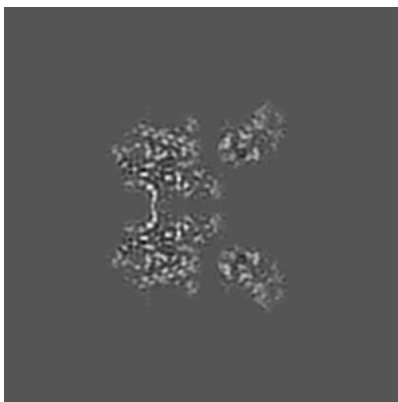
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

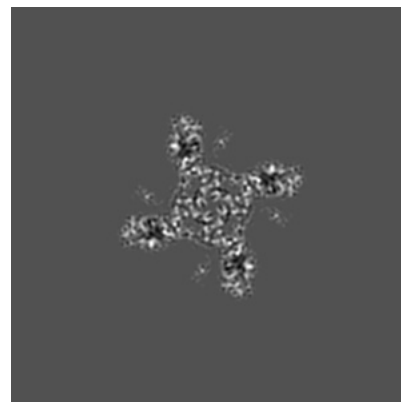
6.2.1 Primary map



X Index: 128



Y Index: 128

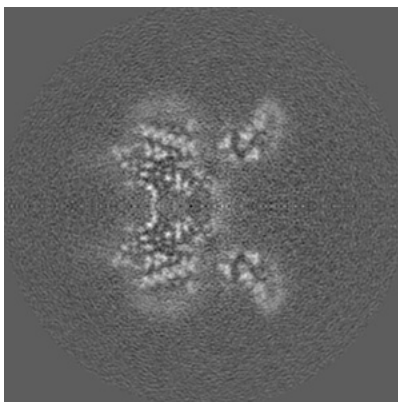


Z Index: 128

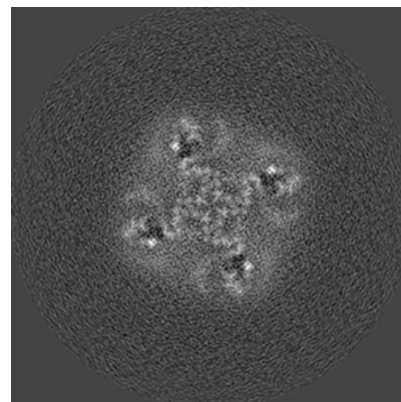
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

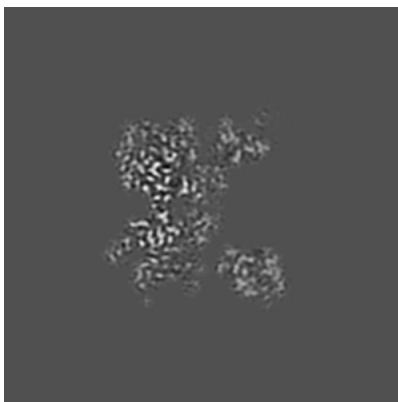
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

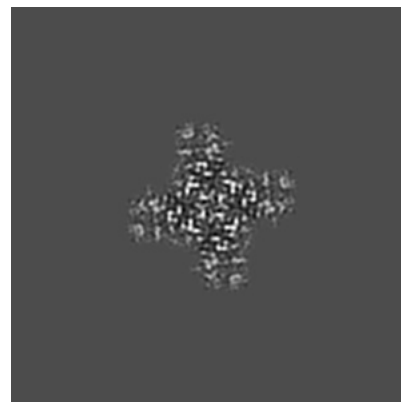
6.3.1 Primary map



X Index: 132



Y Index: 132

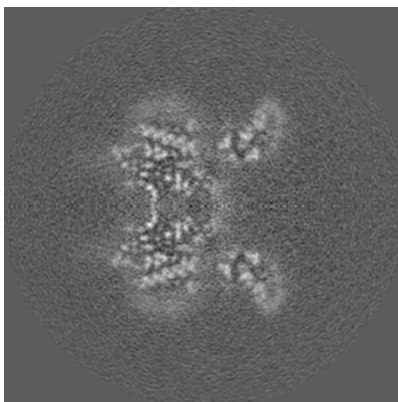


Z Index: 97

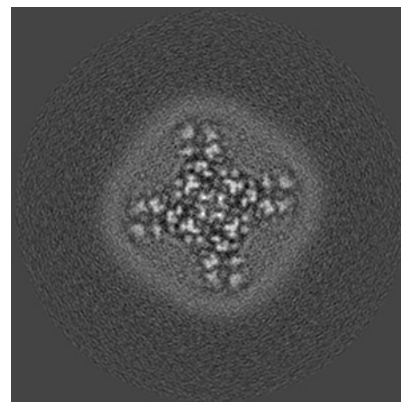
6.3.2 Raw map



X Index: 128



Y Index: 128

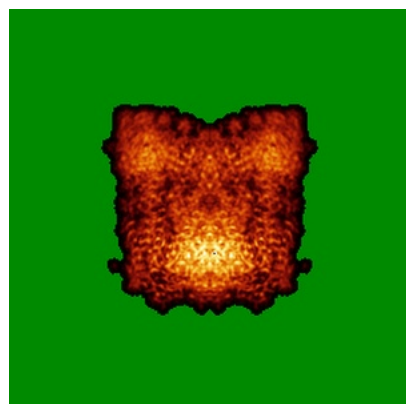


Z Index: 97

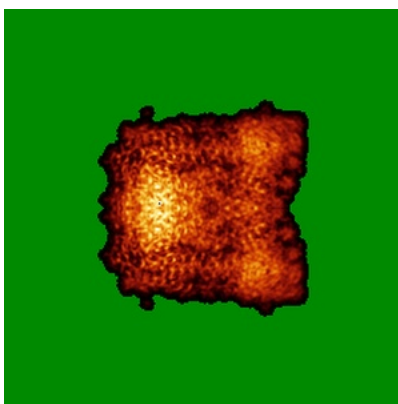
The images above show the largest variance slices of the map in three orthogonal directions.

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

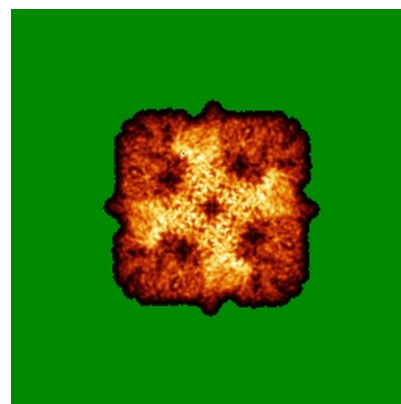
6.4.1 Primary map



X

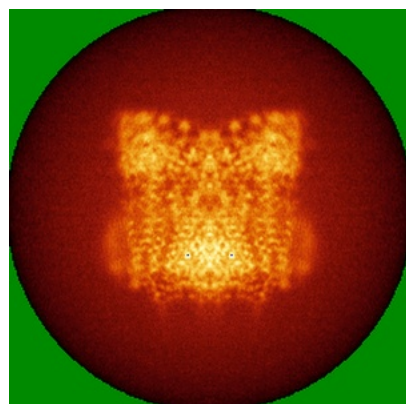


Y

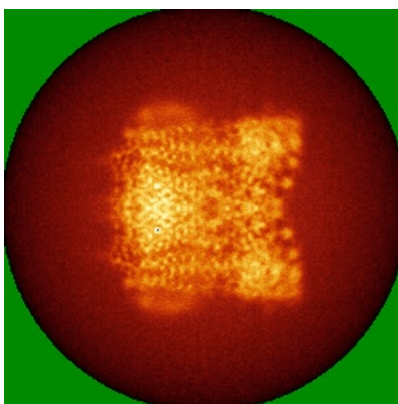


Z

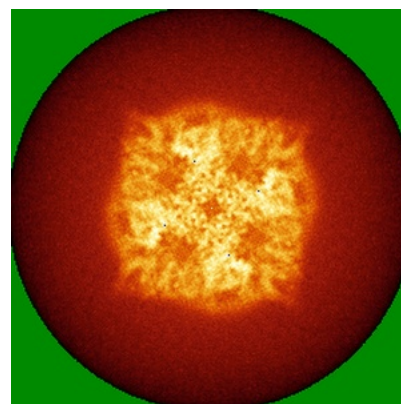
6.4.2 Raw map



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.

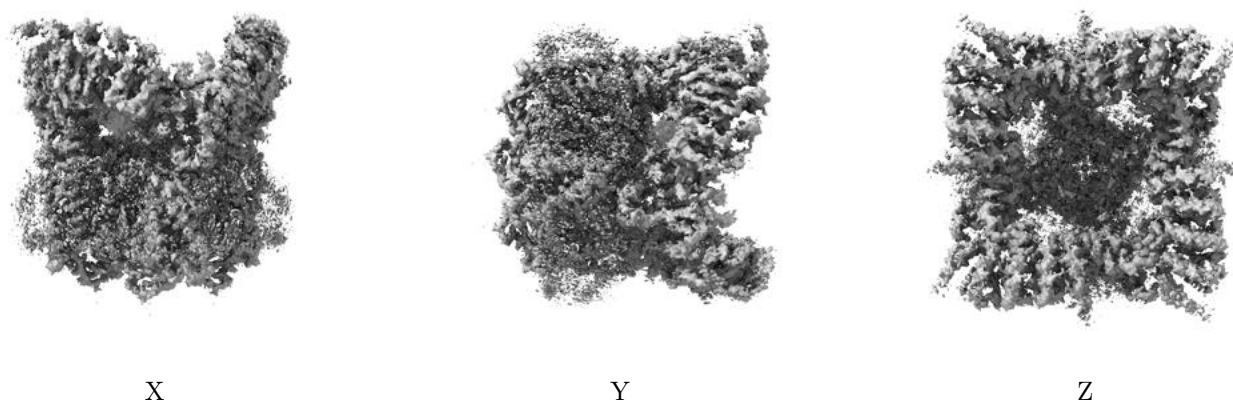
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0172. 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.

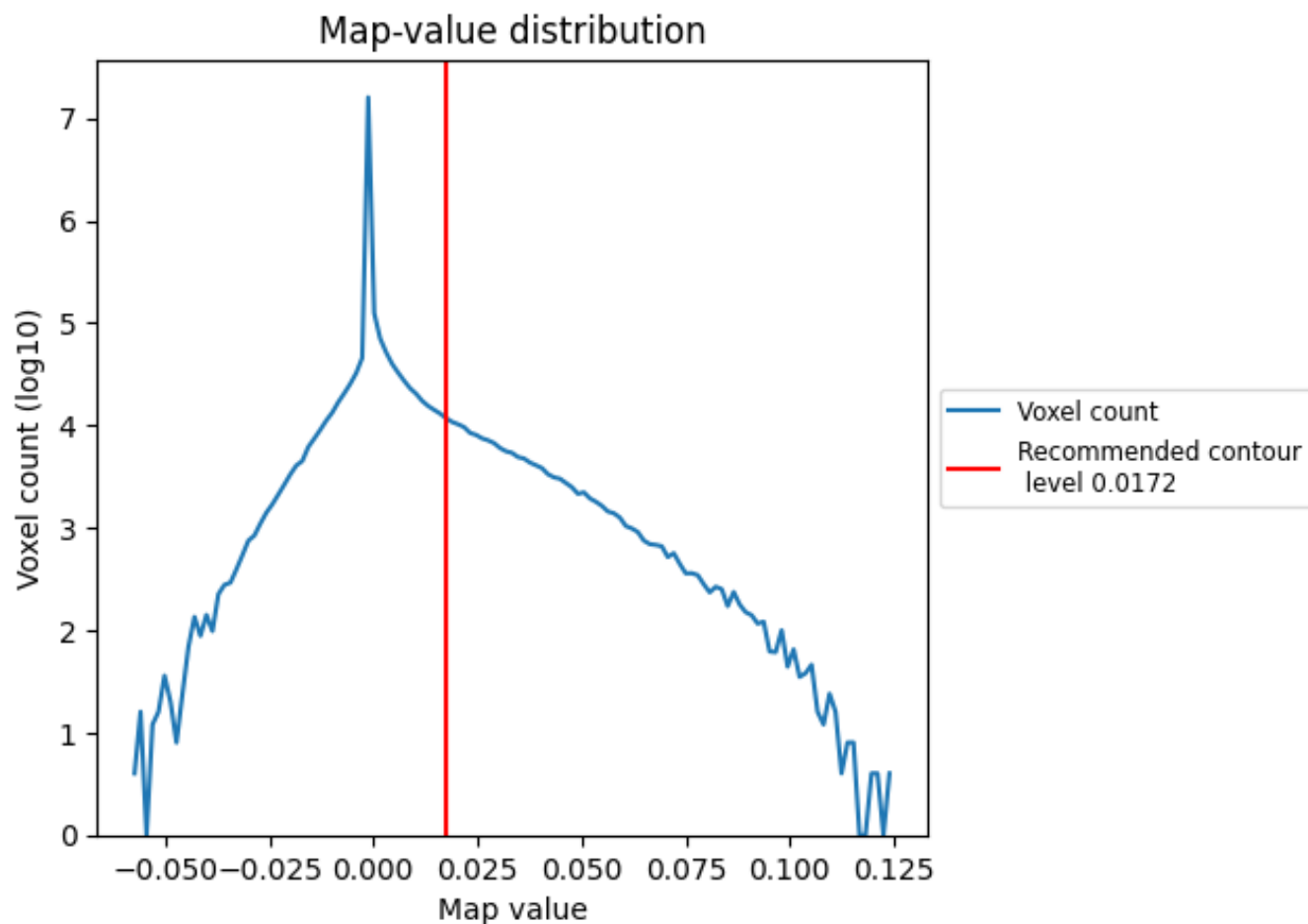
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

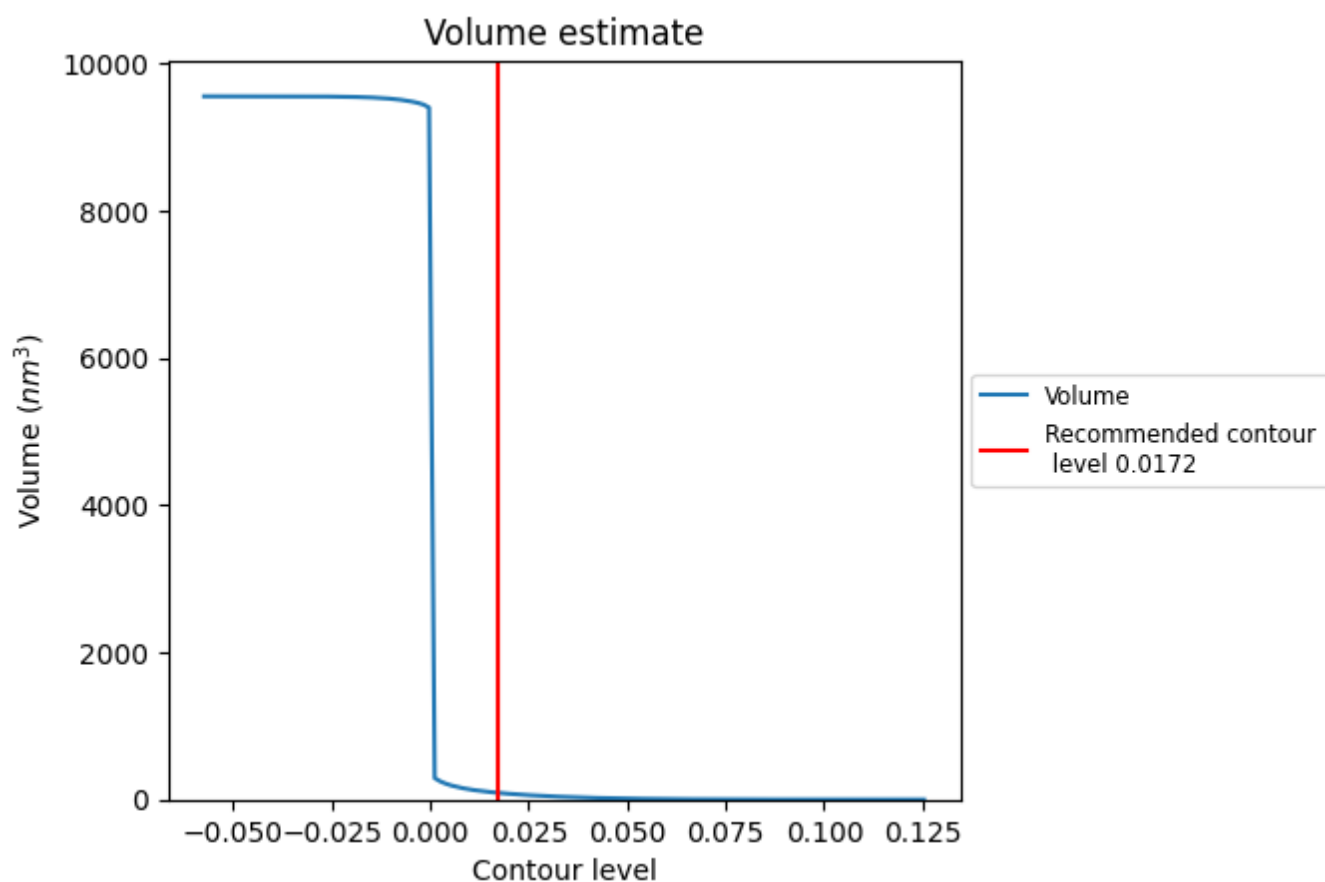
This section contains the results of statistical analysis of the map.

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.

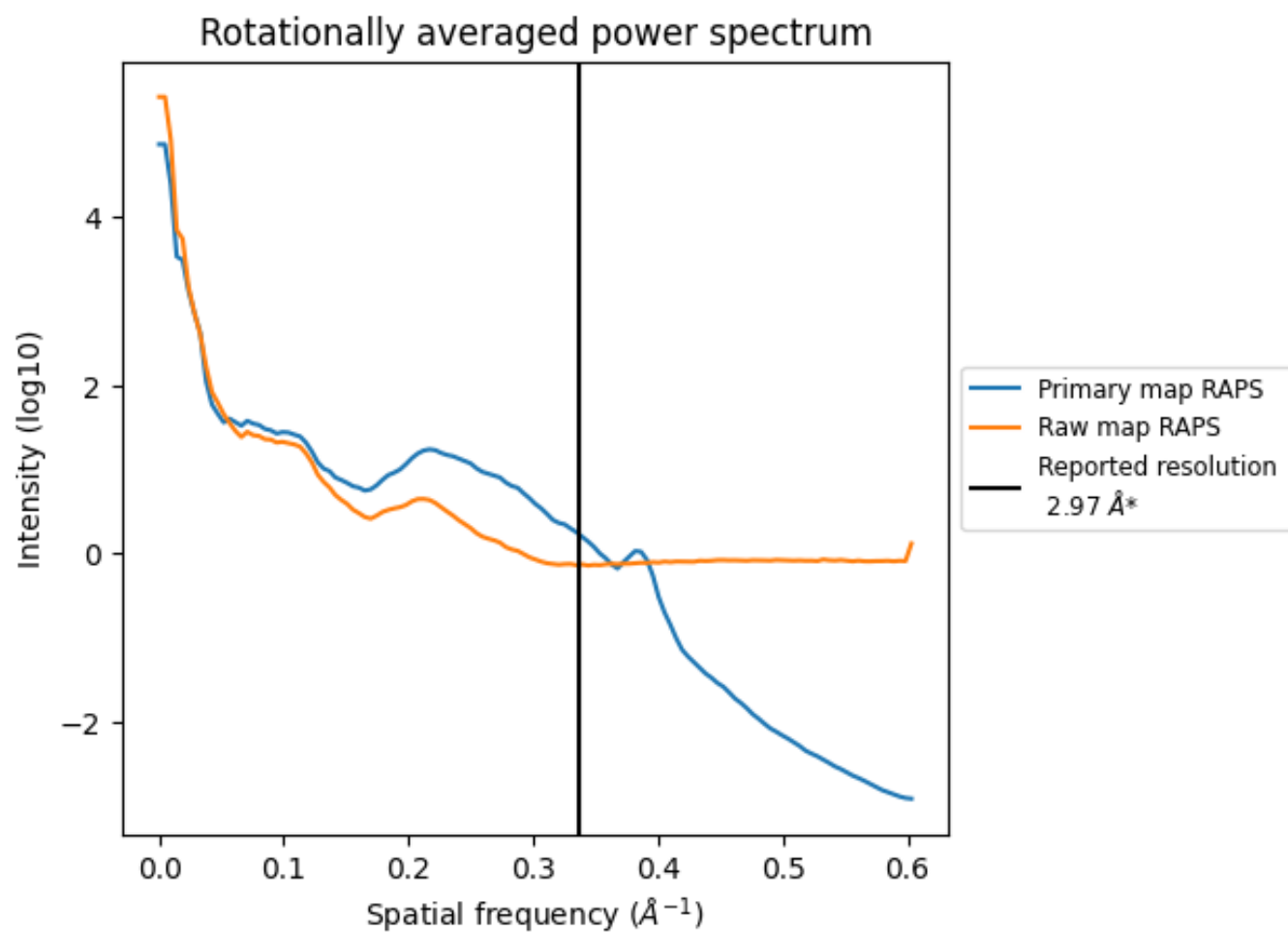
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm³; this corresponds to an approximate mass of 83 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 ⓘ

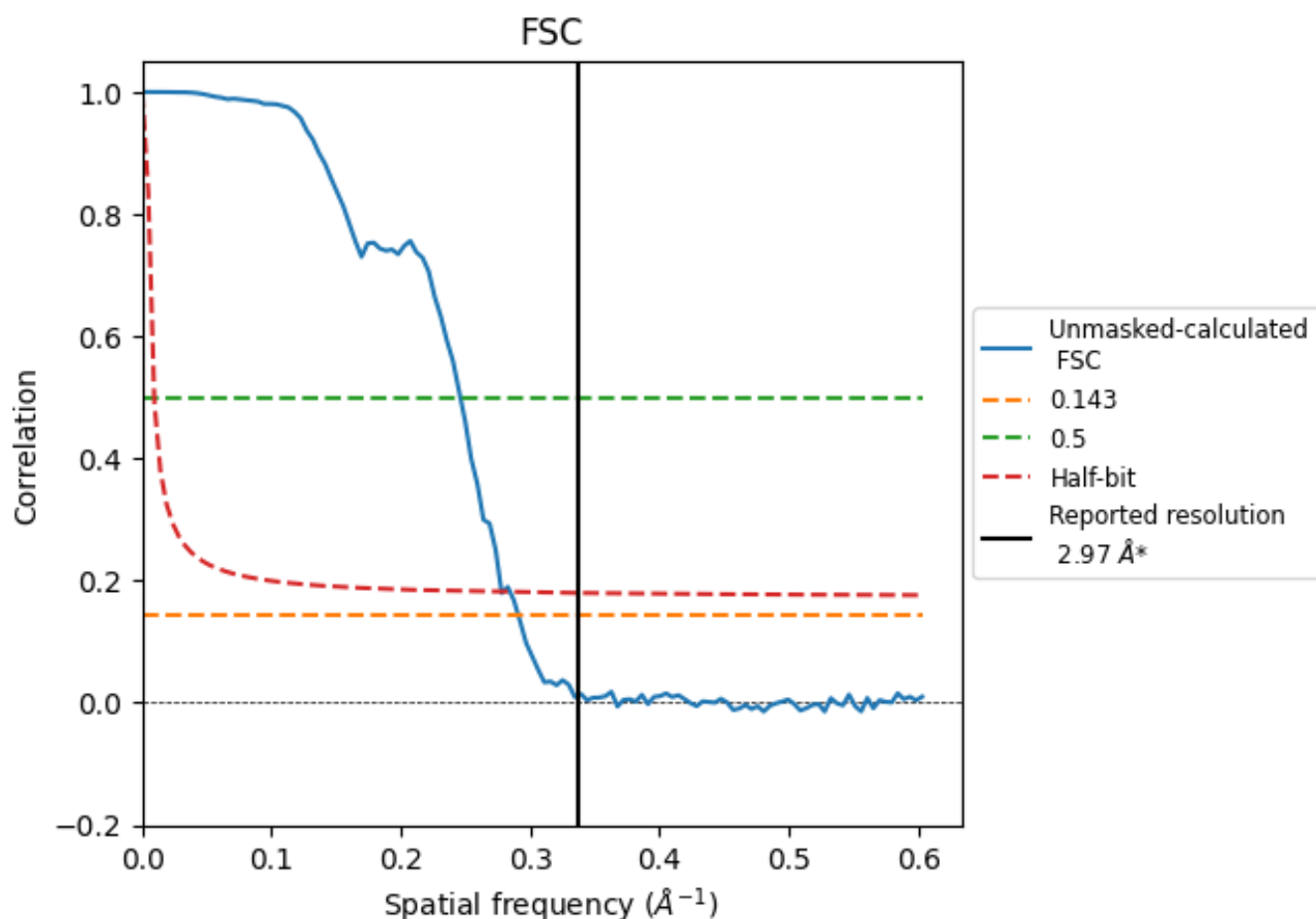


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

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 0.337 \AA^{-1}

8.2 Resolution estimates [i](#)

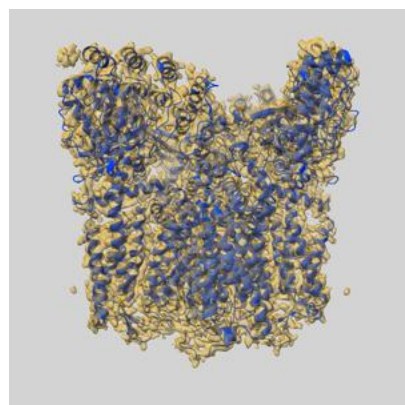
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.07	3.60

*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 3.44 differs from the reported value 2.97 by more than 10 %

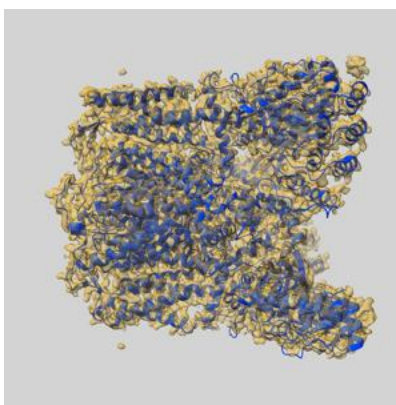
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49646 and PDB model 9NQ9. Per-residue inclusion information can be found in section 3 on page 7.

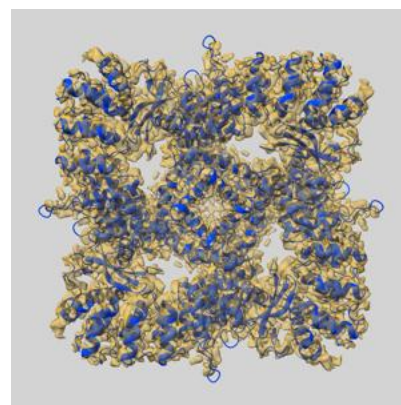
9.1 Map-model overlay [i](#)



X



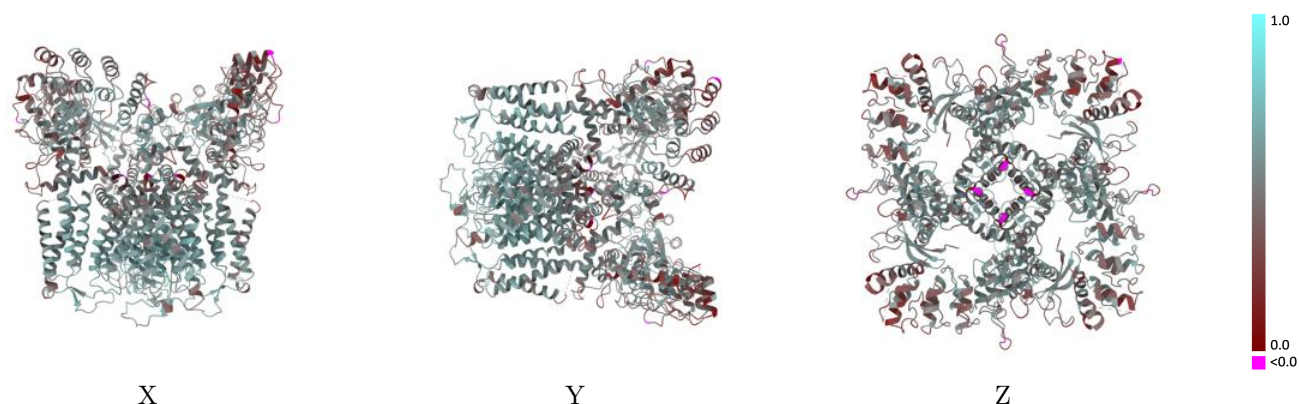
Y



Z

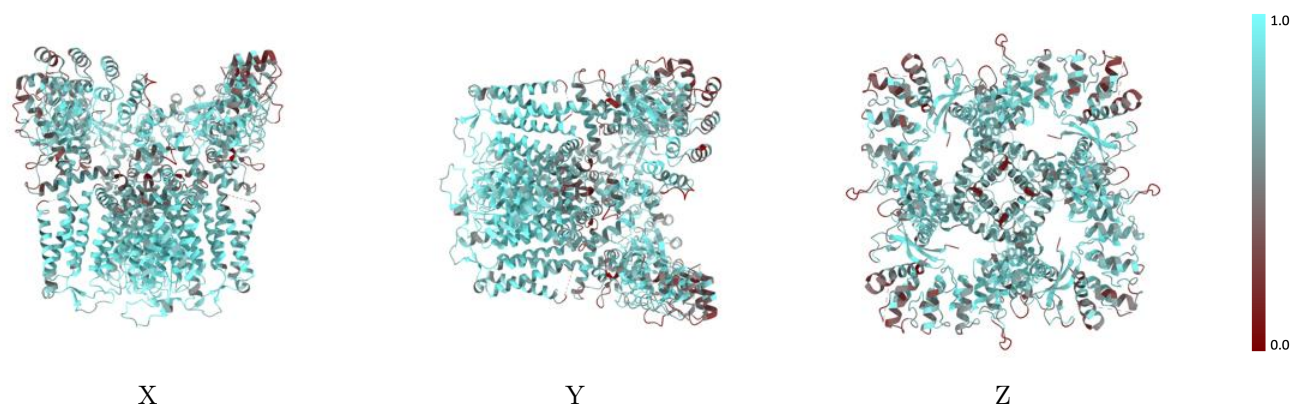
The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



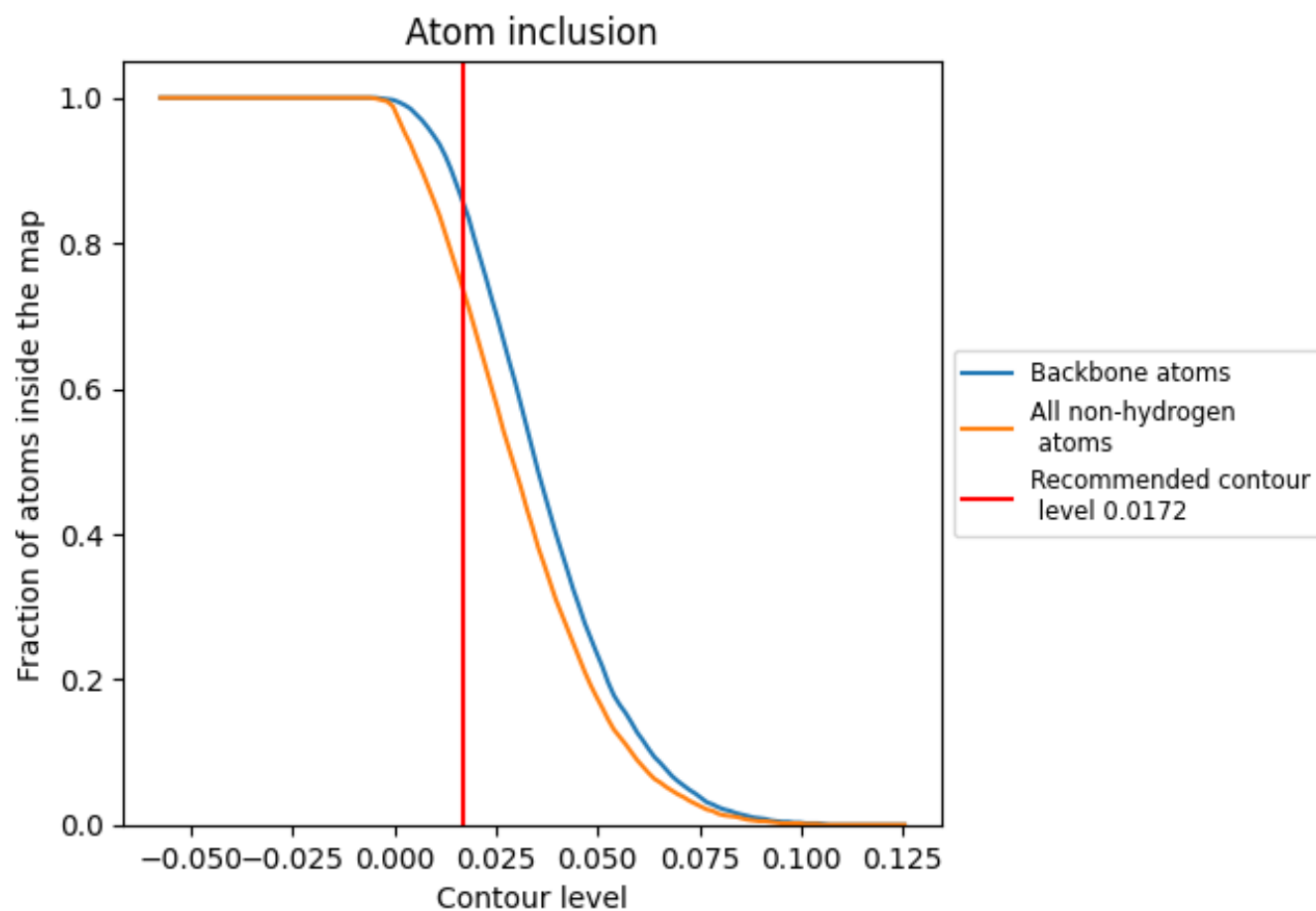
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0172).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 73% 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 (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7320	<div></div> 0.4940
A	<div></div> 0.7250	<div></div> 0.4910
B	<div></div> 0.7410	<div></div> 0.5050
C	<div></div> 0.7270	<div></div> 0.4870
D	<div></div> 0.7340	<div></div> 0.4940

