



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 07:34 PM EDT

PDB ID : 9CUS / pdb_00009cus
EMDB ID : EMD-45940
Title : BmrCD in the outward-facing conformation bound to Hoechst
Authors : Tang, Q.; Mchaourab, H.S.
Deposited on : 2024-07-26
Resolution : 3.10 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.dev133
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) : 2.50

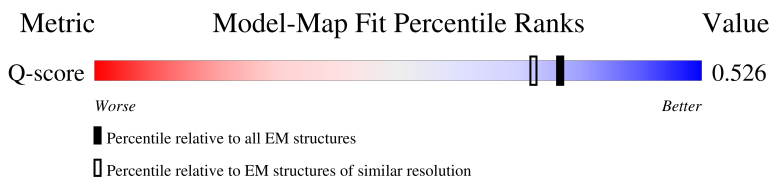
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	C	607	 85% 10% 5%
2	D	681	 88% 10% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21848 atoms, of which 11094 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 Probable multidrug resistance ABC transporter ATP-binding/permease protein YheI.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	C	575	9122	2925	4598	754	822	23	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	expression tag	UNP O07550
C	-20	GLY	-	expression tag	UNP O07550
C	-19	SER	-	expression tag	UNP O07550
C	-18	SER	-	expression tag	UNP O07550
C	-17	HIS	-	expression tag	UNP O07550
C	-16	HIS	-	expression tag	UNP O07550
C	-15	HIS	-	expression tag	UNP O07550
C	-14	HIS	-	expression tag	UNP O07550
C	-13	HIS	-	expression tag	UNP O07550
C	-12	HIS	-	expression tag	UNP O07550
C	-11	SER	-	expression tag	UNP O07550
C	-10	SER	-	expression tag	UNP O07550
C	-9	GLY	-	expression tag	UNP O07550
C	-8	LEU	-	expression tag	UNP O07550
C	-7	VAL	-	expression tag	UNP O07550
C	-6	PRO	-	expression tag	UNP O07550
C	-5	ARG	-	expression tag	UNP O07550
C	-4	GLY	-	expression tag	UNP O07550
C	-3	SER	-	expression tag	UNP O07550
C	-2	HIS	-	expression tag	UNP O07550
C	-1	MET	-	expression tag	UNP O07550
C	0	LEU	-	expression tag	UNP O07550
C	1	GLU	-	expression tag	UNP O07550

- Molecule 2 is a protein called Probable multidrug resistance ABC transporter ATP-binding/permease protein YheH.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	669	Total	C	H	N	O	S	0	0
			10769	3439	5418	911	980	21		

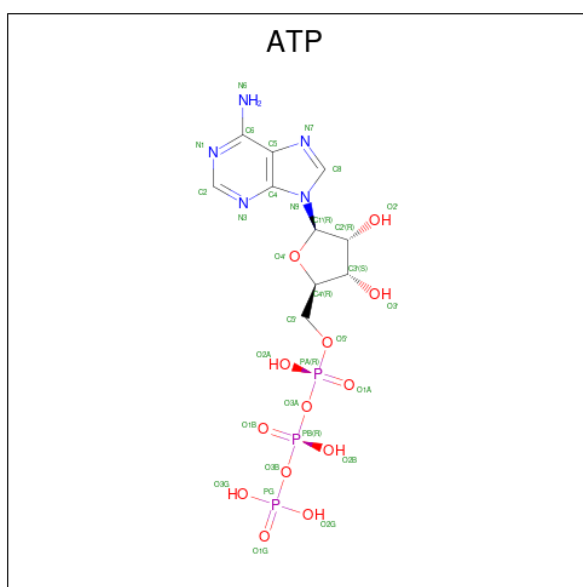
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	674	LEU	-	expression tag	UNP O07549
D	675	GLU	-	expression tag	UNP O07549
D	676	HIS	-	expression tag	UNP O07549
D	677	HIS	-	expression tag	UNP O07549
D	678	HIS	-	expression tag	UNP O07549
D	679	HIS	-	expression tag	UNP O07549
D	680	HIS	-	expression tag	UNP O07549
D	681	HIS	-	expression tag	UNP O07549

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

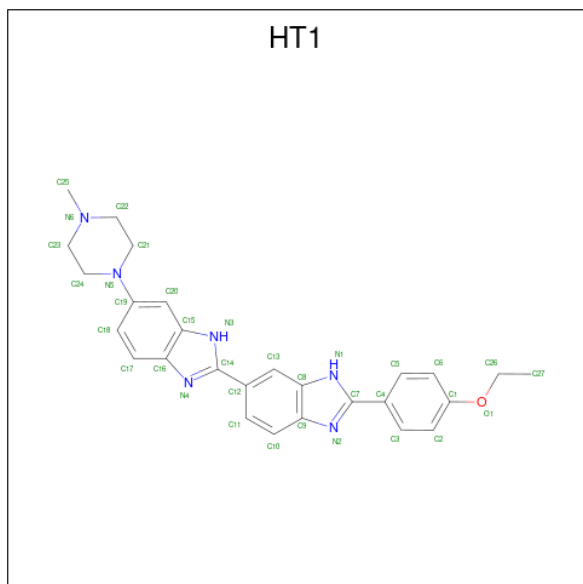
Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



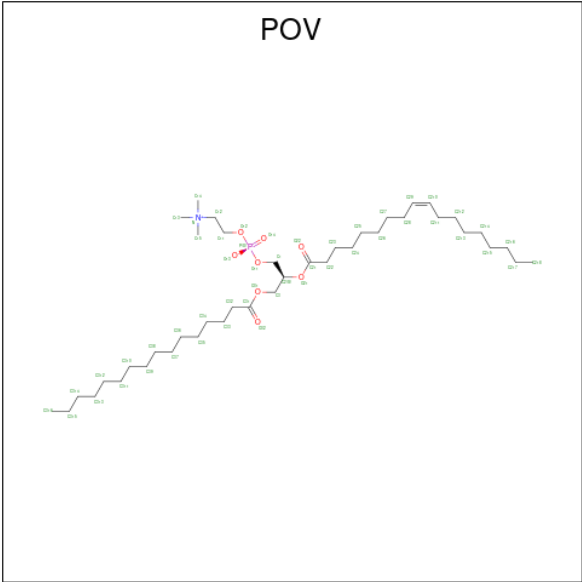
Mol	Chain	Residues	Atoms						AltConf
4	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 5 is 2'-(4-ETHOXYPHENYL)-5-(4-METHYL-1-PIPERAZINYL)-2,5'-BI-BENZIMIDAZOLE (CCD ID: HT1) (formula: C₂₇H₂₈N₆O).



Mol	Chain	Residues	Atoms						AltConf
5	C	1	Total	C	H	N	O		0
			62	27	28	6	1		
5	D	1	Total	C	H	N	O		0
			62	27	28	6	1		

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



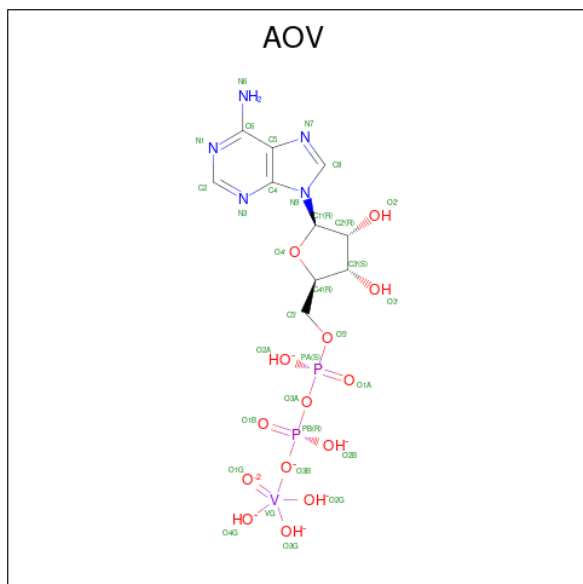
Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	H	O	P	0
			94	31	54	8	1	
6	C	1	Total	C	H	N	O	P
			116	37	69	1	8	1
6	C	1	Total	C	H	N	O	P
			134	42	82	1	8	1
6	C	1	Total	C	H	O	P	0
			44	15	22	6	1	
6	C	1	Total	C	H	O	P	0
			97	32	56	8	1	
6	C	1	Total	C	H	O	P	0
			115	37	69	8	1	
6	C	1	Total	C	H	N	O	P
			69	22	37	1	8	1
6	C	1	Total	C	H			0
			50	19	31			
6	C	1	Total	C	H	O	P	0
			63	21	33	8	1	
6	C	1	Total	C	H	O	P	0
			54	18	27	8	1	
6	D	1	Total	C	H	N	O	P
			98	32	56	1	8	1
6	D	1	Total	C	H	N	O	P
			64	20	34	1	8	1
6	D	1	Total	C	H	N	O	P
			108	34	64	1	8	1
6	D	1	Total	C	H	N	O	P
			134	42	82	1	8	1

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Mol	Chain	Residues	Atoms						AltConf
6	D	1	Total	C	H	O	P	0	
			72	23	40	8	1		
6	D	1	Total	C	H	O	P	0	
			94	31	54	8	1		
6	D	1	Total	C	H	O	P	0	
			84	27	48	8	1		
6	D	1	Total	C	H	O	P	0	
			66	22	35	8	1		
6	D	1	Total	C	H	N	O	P	0
			122	39	73	1	8	1	
6	D	1	Total	C	H	O	P	0	
			78	25	44	8	1		

- Molecule 7 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$).

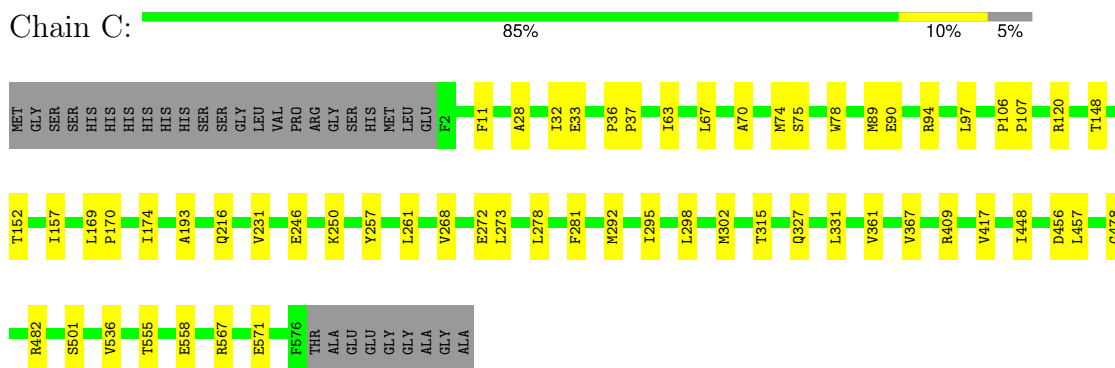


Mol	Chain	Residues	Atoms					AltConf	
7	D	1	Total	C	N	O	P	V	0
			32	10	5	14	2	1	

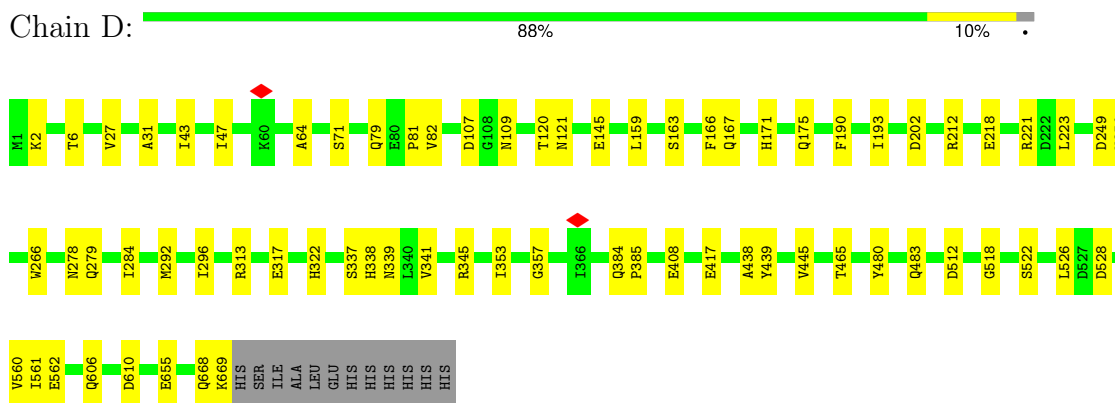
3 Residue-property plots

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: Probable multidrug resistance ABC transporter ATP-binding/permease protein YheI



- Molecule 2: Probable multidrug resistance ABC transporter ATP-binding/permease protein YheH



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27802	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.558	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	310.56, 310.56, 310.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.647, 0.647, 0.647	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HT1, MG, ATP, POV, AOV

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	C	0.13	0/4618	0.26	0/6250
2	D	0.12	0/5452	0.26	0/7357
All	All	0.12	0/10070	0.26	0/13607

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

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	C	4524	4598	4597	39	0
2	D	5351	5418	5418	44	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	31	12	12	0	0
5	C	34	28	28	0	0
5	D	34	28	28	1	0
6	C	356	480	480	0	0
6	D	390	530	530	0	0
7	D	32	0	12	2	0
All	All	10754	11094	11105	80	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 4.

All (80) 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:C:555:THR:HG22	1:C:558:GLU:OE1	1.86	0.75
1:C:331:LEU:O	1:C:409:ARG:NH1	2.21	0.73
1:C:555:THR:N	1:C:558:GLU:OE2	2.21	0.72
2:D:223:LEU:O	2:D:223:LEU:HD23	1.93	0.67
1:C:148:THR:O	1:C:152:THR:HG22	1.94	0.67
1:C:456:ASP:OD2	1:C:482:ARG:NH2	2.27	0.66
1:C:33:GLU:OE2	2:D:345:ARG:NH2	2.30	0.65
2:D:171:HIS:NE2	2:D:175:GLN:OE1	2.31	0.63
7:D:702:AOV:VG	7:D:702:AOV:O1G	1.55	0.63
1:C:216:GLN:NE2	2:D:528:ASP:OD2	2.34	0.61
2:D:313:ARG:NH1	2:D:317:GLU:OE2	2.34	0.59
2:D:212:ARG:NH2	2:D:408:GLU:OE2	2.33	0.58
1:C:536:VAL:HG12	1:C:536:VAL:O	2.04	0.57
2:D:606:GLN:NE2	2:D:610:ASP:OD1	2.38	0.57
1:C:63:ILE:O	1:C:67:LEU:HD23	2.05	0.56
2:D:145:GLU:N	2:D:145:GLU:OE2	2.39	0.56
1:C:70:ALA:O	1:C:74:MET:HG3	2.06	0.55
2:D:202:ASP:OD2	2:D:480:TYR:OH	2.24	0.55
2:D:218:GLU:OE1	2:D:221:ARG:NH1	2.40	0.55
2:D:107:ASP:OD1	2:D:121:ASN:ND2	2.36	0.55
1:C:28:ALA:O	1:C:32:ILE:HG12	2.07	0.54
1:C:170:PRO:O	1:C:174:ILE:HG12	2.07	0.54
2:D:655:GLU:OE1	2:D:655:GLU:N	2.40	0.54
1:C:193:ALA:HB1	1:C:231:VAL:HG22	1.90	0.53
1:C:327:GLN:N	1:C:327:GLN:OE1	2.42	0.52
2:D:518:GLY:O	2:D:560:VAL:N	2.36	0.52
1:C:555:THR:HG22	1:C:558:GLU:CD	2.34	0.52
1:C:448:ILE:HD13	1:C:457:LEU:HD11	1.91	0.52
1:C:272:GLU:N	1:C:272:GLU:OE1	2.43	0.51
2:D:163:SER:O	2:D:167:GLN:NE2	2.40	0.51
2:D:27:VAL:HG11	2:D:166:PHE:CE2	2.46	0.51
2:D:337:SER:OG	2:D:338:HIS:N	2.42	0.51
1:C:11:PHE:CG	1:C:89:MET:HE1	2.46	0.50
2:D:43:ILE:HG12	2:D:47:ILE:HD11	1.92	0.50
2:D:64:ALA:HB1	2:D:71:SER:OG	2.12	0.50
1:C:75:SER:HA	1:C:78:TRP:CD1	2.46	0.50
2:D:353:ILE:O	2:D:357:GLY:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLU:OE2	1:C:250:LYS:NZ	2.45	0.49
2:D:31:ALA:HB1	2:D:159:LEU:HD21	1.94	0.49
7:D:702:AOV:O1G	7:D:702:AOV:O4G	2.31	0.49
2:D:417:GLU:HA	2:D:417:GLU:OE1	2.11	0.49
2:D:522:SER:O	2:D:526:LEU:N	2.43	0.48
2:D:249:ASP:OD1	2:D:250:VAL:N	2.47	0.48
1:C:567:ARG:NH1	1:C:571:GLU:OE2	2.48	0.47
1:C:157:ILE:HG21	1:C:281:PHE:HB2	1.95	0.47
1:C:75:SER:CB	2:D:339:ASN:OD1	2.63	0.47
2:D:561:ILE:HG22	2:D:562:GLU:N	2.31	0.46
1:C:361:VAL:HG22	1:C:367:VAL:HG21	1.98	0.45
2:D:2:LYS:O	2:D:6:THR:OG1	2.32	0.45
1:C:417:VAL:HG11	1:C:501:SER:OG	2.17	0.45
2:D:512:ASP:OD1	2:D:512:ASP:N	2.47	0.45
1:C:89:MET:HA	1:C:89:MET:HE2	1.99	0.44
1:C:257:TYR:CE1	1:C:261:LEU:HD12	2.53	0.44
1:C:292:MET:O	1:C:295:ILE:HG22	2.18	0.44
1:C:298:LEU:HD11	1:C:302:MET:HE3	1.99	0.44
2:D:338:HIS:O	2:D:341:VAL:HG12	2.17	0.44
2:D:79:GLN:HG3	2:D:81:PRO:HD3	1.98	0.44
2:D:284:ILE:HG21	2:D:322:HIS:HB2	1.99	0.44
1:C:169:LEU:HB2	1:C:170:PRO:HD3	2.00	0.44
1:C:90:GLU:OE2	1:C:94:ARG:NH2	2.51	0.43
2:D:82:VAL:O	2:D:82:VAL:HG23	2.18	0.43
2:D:266:TRP:C	2:D:266:TRP:CD1	2.97	0.43
1:C:278:LEU:HD22	2:D:47:ILE:HD12	2.00	0.43
2:D:384:GLN:HB2	5:D:703:HT1:H3	2.00	0.42
1:C:106:PRO:N	1:C:107:PRO:CD	2.83	0.42
1:C:97:LEU:HD11	1:C:315:THR:HG21	2.01	0.42
2:D:31:ALA:HB1	2:D:159:LEU:CD2	2.50	0.41
2:D:438:ALA:N	2:D:483:GLN:OE1	2.53	0.41
2:D:439:TYR:HD1	2:D:445:VAL:HG21	1.86	0.41
2:D:109:ASN:ND2	2:D:120:THR:O	2.54	0.41
1:C:36:PRO:N	1:C:37:PRO:HD2	2.35	0.41
1:C:478:GLY:HA3	2:D:465:THR:HG21	2.02	0.41
1:C:456:ASP:OD1	1:C:482:ARG:NH1	2.54	0.41
2:D:292:MET:O	2:D:296:ILE:HD12	2.20	0.41
2:D:190:PHE:O	2:D:193:ILE:HG22	2.20	0.41
2:D:384:GLN:HB3	2:D:385:PRO:HD3	2.03	0.40
2:D:668:GLN:O	2:D:669:LYS:C	2.64	0.40
1:C:120:ARG:NH1	1:C:315:THR:OG1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:VAL:HG22	1:C:273:LEU:HB2	2.03	0.40
2:D:278:ASN:O	2:D:279:GLN:C	2.64	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	C	573/607 (94%)	551 (96%)	22 (4%)	0	100	100
2	D	667/681 (98%)	637 (96%)	30 (4%)	0	100	100
All	All	1240/1288 (96%)	1188 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	485/508 (96%)	485 (100%)	0	100	100
2	D	573/584 (98%)	573 (100%)	0	100	100
All	All	1058/1092 (97%)	1058 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	HIS
2	D	136	GLN
2	D	140	GLN
2	D	596	HIS
2	D	630	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	$\# Z > 2$
7	AOV	D	702	3	32,34,34	1.26	2 (6%)	42,56,56	1.83	9 (21%)
5	HT1	D	703	-	39,39,39	0.32	0	56,56,56	0.70	2 (3%)
6	POV	D	712	-	48,48,51	0.52	0	54,56,59	0.46	0
5	HT1	C	603	-	39,39,39	0.34	0	56,56,56	0.83	2 (3%)
4	ATP	C	602	3	32,33,33	0.43	0	48,52,52	0.67	0
6	POV	C	608	-	40,40,51	0.67	1 (2%)	43,45,59	0.79	2 (4%)
6	POV	C	612	-	29,29,51	0.78	1 (3%)	32,34,59	0.92	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	POV	D	709	-	39,39,51	0.68	1 (2%)	42,44,59	0.82	2 (4%)
6	POV	C	605	-	46,46,51	0.52	0	52,54,59	0.48	0
6	POV	C	607	-	21,21,51	0.83	1 (4%)	24,24,59	1.05	2 (8%)
6	POV	D	708	-	31,31,51	0.75	1 (3%)	34,36,59	0.91	2 (5%)
6	POV	C	611	-	17,17,51	0.24	0	15,15,59	0.21	0
6	POV	D	711	-	30,30,51	0.76	1 (3%)	33,35,59	0.91	2 (6%)
6	POV	D	706	-	43,43,51	0.55	0	49,51,59	0.50	0
6	POV	C	604	-	39,39,51	0.69	1 (2%)	42,44,59	0.80	2 (4%)
6	POV	D	713	-	33,33,51	0.74	1 (3%)	36,38,59	0.88	2 (5%)
6	POV	D	710	-	35,35,51	0.72	1 (2%)	38,40,59	0.83	2 (5%)
6	POV	C	610	-	31,31,51	0.63	0	37,39,59	0.57	0
6	POV	C	609	-	45,45,51	0.64	1 (2%)	48,50,59	0.76	2 (4%)
6	POV	C	613	-	26,26,51	0.82	1 (3%)	29,31,59	0.95	2 (6%)
6	POV	C	606	-	51,51,51	0.50	0	57,59,59	0.45	0
6	POV	D	704	-	41,41,51	0.56	0	47,49,59	0.49	0
6	POV	D	707	-	51,51,51	0.50	0	57,59,59	0.50	0
6	POV	D	705	-	29,29,51	0.64	0	35,37,59	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AOV	D	702	3	-	1/16/39/39	0/3/3/3
5	HT1	D	703	-	-	6/15/25/25	0/6/6/6
6	POV	D	712	-	-	11/52/52/55	-
5	HT1	C	603	-	-	10/15/25/25	0/6/6/6
4	ATP	C	602	3	-	3/22/38/38	0/3/3/3
6	POV	C	608	-	-	10/42/42/55	-
6	POV	C	612	-	-	7/31/31/55	-
6	POV	D	709	-	-	7/41/41/55	-
6	POV	C	605	-	-	14/50/50/55	-
6	POV	C	607	-	-	9/20/20/55	-
6	POV	D	708	-	-	4/33/33/55	-
6	POV	C	611	-	-	4/13/13/55	-
6	POV	D	711	-	-	10/32/32/55	-
6	POV	D	706	-	-	15/47/47/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POV	C	604	-	-	15/41/41/55	-
6	POV	D	713	-	-	15/35/35/55	-
6	POV	D	710	-	-	7/37/37/55	-
6	POV	C	610	-	-	12/35/35/55	-
6	POV	C	609	-	-	12/47/47/55	-
6	POV	C	613	-	-	12/28/28/55	-
6	POV	C	606	-	-	12/55/55/55	-
6	POV	D	704	-	-	22/45/45/55	-
6	POV	D	707	-	-	14/55/55/55	-
6	POV	D	705	-	-	12/33/33/55	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	702	AOV	O1G-VG	-3.35	1.55	1.61
6	D	713	POV	P-O12	3.06	1.66	1.54
6	C	607	POV	P-O12	3.06	1.66	1.54
6	C	604	POV	P-O12	3.06	1.66	1.54
6	D	711	POV	P-O12	3.05	1.66	1.54
6	C	613	POV	P-O12	3.05	1.66	1.54
6	D	709	POV	P-O12	3.04	1.66	1.54
6	D	708	POV	P-O12	3.04	1.66	1.54
6	C	609	POV	P-O12	3.04	1.66	1.54
6	D	710	POV	P-O12	3.04	1.66	1.54
6	C	608	POV	P-O12	3.03	1.66	1.54
6	C	612	POV	P-O12	3.02	1.66	1.54
7	D	702	AOV	C5-N7	-2.78	1.34	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	702	AOV	C5-C4-N3	-5.35	119.35	126.72
7	D	702	AOV	N3-C4-N9	4.50	134.82	127.17
7	D	702	AOV	N3-C2-N1	-4.21	122.21	128.58
6	C	612	POV	O12-P-O11	-3.55	97.41	106.67
7	D	702	AOV	C2-N3-C4	3.54	120.48	111.83
6	D	708	POV	O12-P-O11	-3.48	97.60	106.67
6	C	613	POV	O12-P-O11	-3.46	97.64	106.67
6	D	709	POV	O12-P-O11	-3.46	97.64	106.67
6	C	607	POV	O12-P-O11	-3.45	97.67	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	609	POV	O12-P-O11	-3.45	97.68	106.67
6	C	604	POV	O12-P-O11	-3.44	97.69	106.67
6	D	711	POV	O12-P-O11	-3.44	97.70	106.67
6	D	713	POV	O12-P-O11	-3.43	97.72	106.67
7	D	702	AOV	C5-N7-C8	3.41	108.81	103.45
6	C	608	POV	O12-P-O11	-3.40	97.80	106.67
6	D	710	POV	O12-P-O11	-3.37	97.89	106.67
7	D	702	AOV	N9-C8-N7	-2.67	110.15	113.94
6	D	708	POV	O13-P-O14	2.67	121.24	110.83
6	D	709	POV	O13-P-O14	2.65	121.18	110.83
6	D	713	POV	O13-P-O14	2.65	121.16	110.83
6	C	607	POV	O13-P-O14	2.65	121.16	110.83
6	C	613	POV	O13-P-O14	2.65	121.14	110.83
6	C	612	POV	O13-P-O14	2.63	121.10	110.83
6	C	604	POV	O13-P-O14	2.62	121.06	110.83
6	C	609	POV	O13-P-O14	2.62	121.03	110.83
6	C	608	POV	O13-P-O14	2.62	121.02	110.83
6	D	711	POV	O13-P-O14	2.61	120.99	110.83
6	D	710	POV	O13-P-O14	2.59	120.94	110.83
7	D	702	AOV	C4-C5-N7	-2.53	107.69	110.58
5	D	703	HT1	C24-N5-C19	2.27	124.29	118.11
7	D	702	AOV	C2'-C1'-N9	-2.24	107.73	113.30
5	C	603	HT1	C24-N5-C19	2.19	124.09	118.11
7	D	702	AOV	O3'-C3'-C4'	-2.14	104.92	111.08
5	C	603	HT1	C21-N5-C19	2.05	123.69	118.11
5	D	703	HT1	C21-N5-C19	2.03	123.66	118.11

There are no chirality outliers.

All (244) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	604	POV	C1-O11-P-O12
6	C	604	POV	C1-O11-P-O13
6	C	604	POV	C1-O11-P-O14
6	C	605	POV	C1-O11-P-O12
6	C	605	POV	C1-O11-P-O13
6	C	605	POV	C1-O11-P-O14
6	C	605	POV	C11-O12-P-O11
6	C	605	POV	C11-O12-P-O14
6	C	606	POV	C1-O11-P-O12
6	C	606	POV	C1-O11-P-O13
6	C	606	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
6	C	606	POV	C11-O12-P-O13
6	C	606	POV	C11-O12-P-O14
6	C	606	POV	C12-C11-O12-P
6	C	607	POV	C1-O11-P-O12
6	C	607	POV	C1-O11-P-O13
6	C	610	POV	C11-O12-P-O11
6	C	610	POV	C11-O12-P-O13
6	C	610	POV	C11-O12-P-O14
6	C	613	POV	C1-O11-P-O12
6	C	613	POV	O21-C2-C3-O31
6	D	704	POV	C1-O11-P-O12
6	D	704	POV	C1-O11-P-O13
6	D	704	POV	C2-C1-O11-P
6	D	704	POV	C22-C21-O21-C2
6	D	705	POV	C1-O11-P-O12
6	D	705	POV	C1-O11-P-O14
6	D	705	POV	C11-O12-P-O11
6	D	705	POV	C11-O12-P-O13
6	D	705	POV	C11-O12-P-O14
6	D	705	POV	O12-C11-C12-N
6	D	705	POV	C22-C21-O21-C2
6	D	706	POV	C1-O11-P-O12
6	D	706	POV	C1-O11-P-O13
6	D	706	POV	C1-O11-P-O14
6	D	707	POV	C11-O12-P-O11
6	D	707	POV	C11-O12-P-O13
6	D	707	POV	O12-C11-C12-N
6	D	707	POV	C22-C21-O21-C2
6	D	709	POV	O22-C21-O21-C2
6	D	711	POV	O22-C21-O21-C2
6	D	712	POV	C11-O12-P-O11
6	D	712	POV	C11-O12-P-O13
6	D	713	POV	C1-O11-P-O12
6	D	713	POV	C1-O11-P-O13
6	D	713	POV	C1-O11-P-O14
6	C	613	POV	O22-C21-O21-C2
6	D	704	POV	O22-C21-O21-C2
6	D	705	POV	O22-C21-O21-C2
6	D	707	POV	O22-C21-O21-C2
5	D	703	HT1	C18-C19-N5-C21
6	C	613	POV	C22-C21-O21-C2
6	D	709	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
6	D	711	POV	C22-C21-O21-C2
5	D	703	HT1	C18-C19-N5-C24
6	C	607	POV	C22-C21-O21-C2
6	C	607	POV	O22-C21-O21-C2
5	D	703	HT1	C20-C19-N5-C24
5	D	703	HT1	C20-C19-N5-C21
5	C	603	HT1	C18-C19-N5-C21
6	C	610	POV	C32-C31-O31-C3
5	C	603	HT1	C18-C19-N5-C24
6	C	605	POV	C36-C37-C38-C39
6	C	610	POV	O32-C31-O31-C3
6	D	713	POV	C32-C31-O31-C3
6	C	610	POV	C11-C12-N-C13
6	C	610	POV	C11-C12-N-C15
5	C	603	HT1	C3-C4-C7-N2
5	C	603	HT1	C5-C4-C7-N1
6	C	608	POV	C39-C310-C311-C312
6	D	706	POV	C33-C34-C35-C36
5	C	603	HT1	C3-C4-C7-N1
6	C	609	POV	C311-C312-C313-C314
6	D	710	POV	C311-C310-C39-C38
5	C	603	HT1	C5-C4-C7-N2
6	C	609	POV	C37-C38-C39-C310
6	C	608	POV	C25-C26-C27-C28
6	C	613	POV	C32-C33-C34-C35
6	D	713	POV	C39-C310-C311-C312
6	C	613	POV	C31-C32-C33-C34
6	D	713	POV	O32-C31-O31-C3
6	D	704	POV	C24-C25-C26-C27
6	C	607	POV	C22-C23-C24-C25
6	C	610	POV	C11-C12-N-C14
6	D	709	POV	C311-C312-C313-C314
6	C	612	POV	C32-C33-C34-C35
6	D	707	POV	C23-C24-C25-C26
6	C	605	POV	C24-C25-C26-C27
6	C	608	POV	C33-C34-C35-C36
6	C	604	POV	C25-C26-C27-C28
6	C	609	POV	C36-C37-C38-C39
6	D	712	POV	C22-C21-O21-C2
6	D	704	POV	C31-C32-C33-C34
6	D	706	POV	C35-C36-C37-C38
6	C	609	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	C	611	POV	C24-C25-C26-C27
6	C	607	POV	C1-C2-O21-C21
6	C	607	POV	C21-C22-C23-C24
6	D	704	POV	C22-C23-C24-C25
6	C	611	POV	C310-C311-C312-C313
6	C	612	POV	C37-C38-C39-C310
6	D	712	POV	O21-C2-C3-O31
6	D	707	POV	C2-C1-O11-P
6	D	711	POV	C2-C1-O11-P
6	D	713	POV	C37-C38-C39-C310
6	D	712	POV	O22-C21-O21-C2
6	C	608	POV	C37-C38-C39-C310
6	D	704	POV	C34-C35-C36-C37
6	C	609	POV	C22-C23-C24-C25
6	C	611	POV	C312-C313-C314-C315
6	D	707	POV	C32-C33-C34-C35
6	D	710	POV	C35-C36-C37-C38
6	C	605	POV	C26-C27-C28-C29
6	D	704	POV	C26-C27-C28-C29
5	D	703	HT1	C6-C1-O1-C26
6	C	608	POV	C31-C32-C33-C34
6	C	613	POV	C1-C2-C3-O31
6	D	704	POV	C1-C2-C3-O31
6	D	712	POV	C1-C2-C3-O31
6	D	713	POV	C1-C2-C3-O31
6	C	609	POV	C32-C31-O31-C3
6	D	712	POV	C36-C37-C38-C39
6	C	604	POV	C21-C22-C23-C24
6	C	607	POV	C1-O11-P-O14
6	C	610	POV	C25-C26-C27-C28
6	D	713	POV	C35-C36-C37-C38
6	C	609	POV	C39-C310-C311-C312
6	D	707	POV	C1-C2-O21-C21
5	D	703	HT1	C2-C1-O1-C26
6	C	612	POV	C32-C31-O31-C3
6	D	707	POV	C24-C25-C26-C27
6	C	605	POV	O21-C2-C3-O31
6	C	610	POV	O21-C2-C3-O31
6	D	709	POV	C24-C25-C26-C27
6	C	604	POV	C311-C312-C313-C314
6	D	704	POV	O11-C1-C2-C3
6	D	713	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	C	609	POV	O32-C31-O31-C3
6	D	706	POV	C39-C310-C311-C312
6	D	706	POV	C37-C38-C39-C310
6	C	612	POV	O32-C31-O31-C3
6	D	706	POV	O11-C1-C2-O21
6	C	611	POV	C26-C27-C28-C29
6	D	713	POV	C312-C313-C314-C315
6	D	712	POV	C32-C31-O31-C3
6	C	607	POV	C23-C24-C25-C26
6	D	710	POV	C37-C38-C39-C310
6	D	706	POV	C32-C31-O31-C3
6	C	612	POV	O11-C1-C2-C3
6	D	711	POV	O11-C1-C2-C3
6	D	712	POV	O32-C31-O31-C3
6	D	710	POV	C1-O11-P-O12
6	D	705	POV	C1-C2-O21-C21
6	C	604	POV	O11-C1-C2-O21
6	D	713	POV	O11-C1-C2-O21
6	D	708	POV	C1-C2-C3-O31
6	D	706	POV	C311-C310-C39-C38
6	C	605	POV	C12-C11-O12-P
6	D	704	POV	O21-C2-C3-O31
6	D	706	POV	O32-C31-O31-C3
6	C	608	POV	C21-C22-C23-C24
4	C	602	ATP	PA-O3A-PB-O2B
6	C	605	POV	O12-C11-C12-N
6	C	606	POV	O12-C11-C12-N
6	D	706	POV	O12-C11-C12-N
6	D	707	POV	C22-C23-C24-C25
6	D	708	POV	C37-C38-C39-C310
6	C	606	POV	C24-C25-C26-C27
6	D	709	POV	C23-C24-C25-C26
6	C	608	POV	C35-C36-C37-C38
6	C	609	POV	C313-C314-C315-C316
6	C	612	POV	O11-C1-C2-O21
6	D	704	POV	O11-C1-C2-O21
6	C	608	POV	C311-C312-C313-C314
6	C	608	POV	O21-C2-C3-O31
6	D	708	POV	O21-C2-C3-O31
6	D	713	POV	O21-C2-C3-O31
6	C	610	POV	C1-C2-C3-O31
6	D	704	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
6	C	605	POV	C11-O12-P-O13
6	C	606	POV	C1-O11-P-O14
6	D	704	POV	C11-O12-P-O11
6	D	704	POV	C11-O12-P-O13
6	D	704	POV	C11-O12-P-O14
6	D	705	POV	C1-O11-P-O13
6	D	713	POV	C2-C1-O11-P
6	D	705	POV	C25-C26-C27-C28
6	C	604	POV	C313-C314-C315-C316
6	D	704	POV	C23-C24-C25-C26
6	D	706	POV	O11-C1-C2-C3
6	D	711	POV	O11-C1-C2-O21
5	C	603	HT1	C20-C19-N5-C21
6	C	605	POV	C1-C2-C3-O31
6	D	710	POV	C1-C2-C3-O31
6	D	707	POV	C311-C310-C39-C38
6	C	606	POV	C32-C31-O31-C3
6	C	606	POV	C2-C1-O11-P
6	C	606	POV	O32-C31-O31-C3
6	C	604	POV	C32-C31-O31-C3
6	C	604	POV	O22-C21-O21-C2
6	D	712	POV	C213-C214-C215-C216
4	C	602	ATP	C2'-C1'-N9-C8
6	C	604	POV	O32-C31-O31-C3
6	C	604	POV	C22-C21-O21-C2
6	D	707	POV	O21-C21-C22-C23
6	D	709	POV	C35-C36-C37-C38
6	D	708	POV	C311-C310-C39-C38
6	C	604	POV	C35-C36-C37-C38
6	C	613	POV	O11-C1-C2-C3
5	C	603	HT1	C11-C12-C14-N4
6	C	613	POV	C1-O11-P-O13
6	C	613	POV	C1-O11-P-O14
6	D	710	POV	C1-O11-P-O13
6	D	710	POV	C1-O11-P-O14
6	C	609	POV	C21-C22-C23-C24
6	D	704	POV	C27-C28-C29-C210
6	C	610	POV	C22-C23-C24-C25
6	C	612	POV	O21-C2-C3-O31
6	C	613	POV	O21-C21-C22-C23
6	C	604	POV	O11-C1-C2-C3
6	D	707	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
6	D	704	POV	O21-C21-C22-C23
4	C	602	ATP	PA-O3A-PB-O1B
6	D	712	POV	C214-C215-C216-C217
6	D	706	POV	C36-C37-C38-C39
5	C	603	HT1	C20-C19-N5-C24
6	C	605	POV	C29-C210-C211-C212
6	C	604	POV	C34-C35-C36-C37
6	D	711	POV	O32-C31-O31-C3
6	C	609	POV	O31-C31-C32-C33
6	D	711	POV	O21-C21-C22-C23
6	C	608	POV	C26-C27-C28-C29
6	D	711	POV	C32-C31-O31-C3
6	D	711	POV	C32-C33-C34-C35
6	D	704	POV	O22-C21-C22-C23
6	D	705	POV	O31-C31-C32-C33
6	C	613	POV	O22-C21-C22-C23
6	D	713	POV	C310-C311-C312-C313
5	C	603	HT1	C27-C26-O1-C1
6	D	711	POV	O22-C21-C22-C23
6	C	609	POV	O32-C31-C32-C33
6	D	706	POV	O21-C21-C22-C23
6	D	709	POV	O31-C31-C32-C33
7	D	702	AOV	PA-O3A-PB-O2B

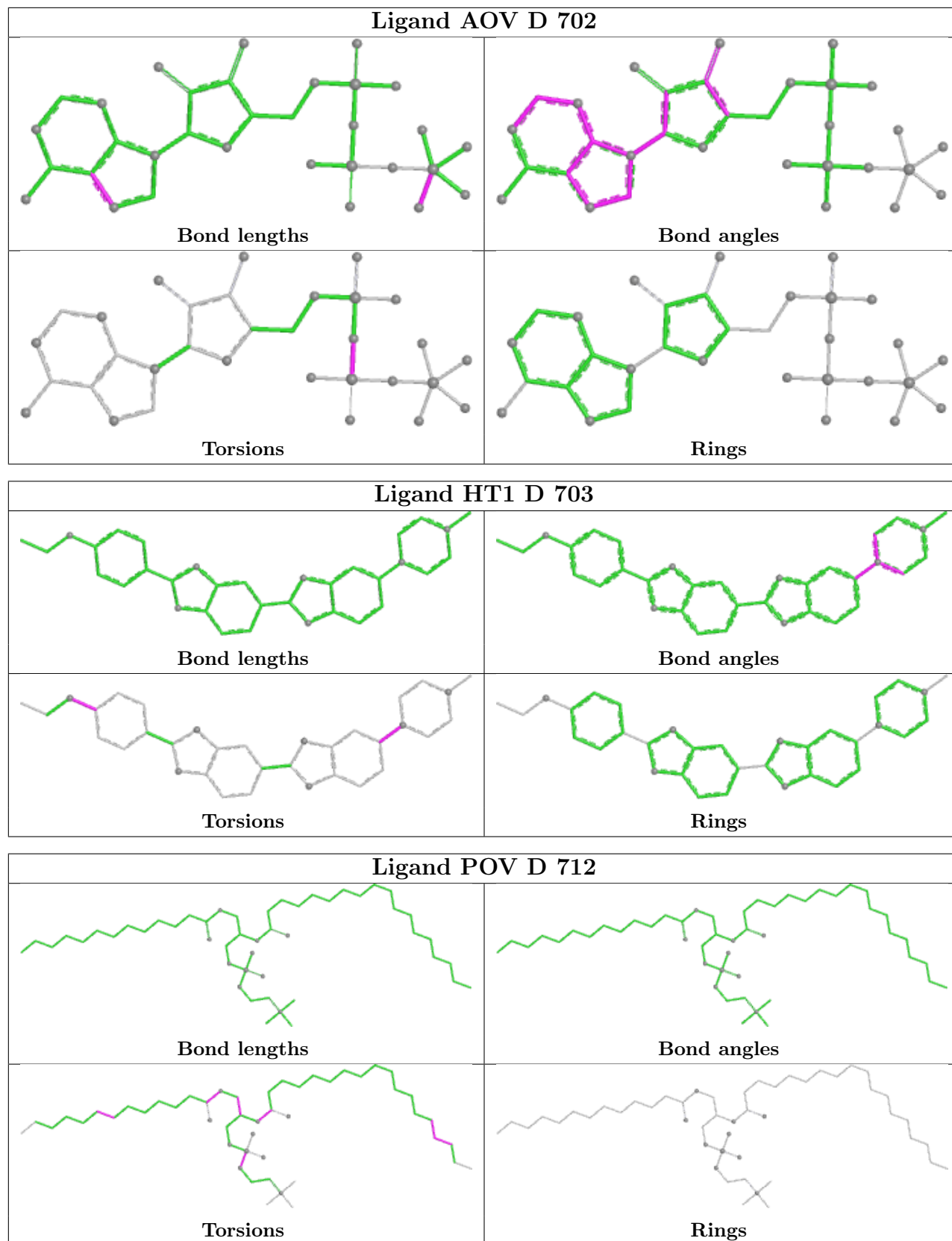
There are no ring outliers.

2 monomers are involved in 3 short contacts:

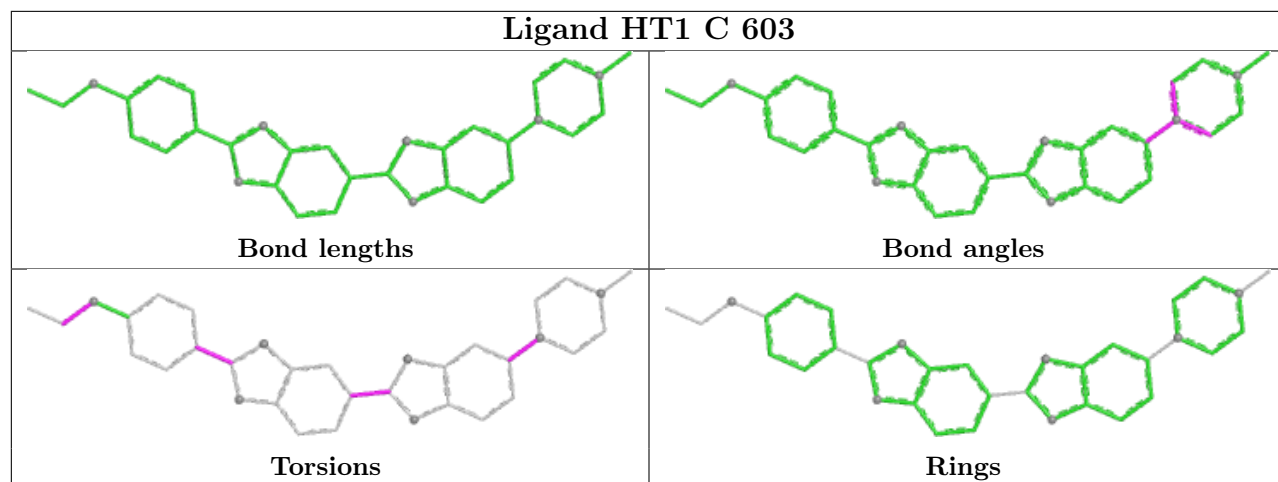
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	702	AOV	2	0
5	D	703	HT1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

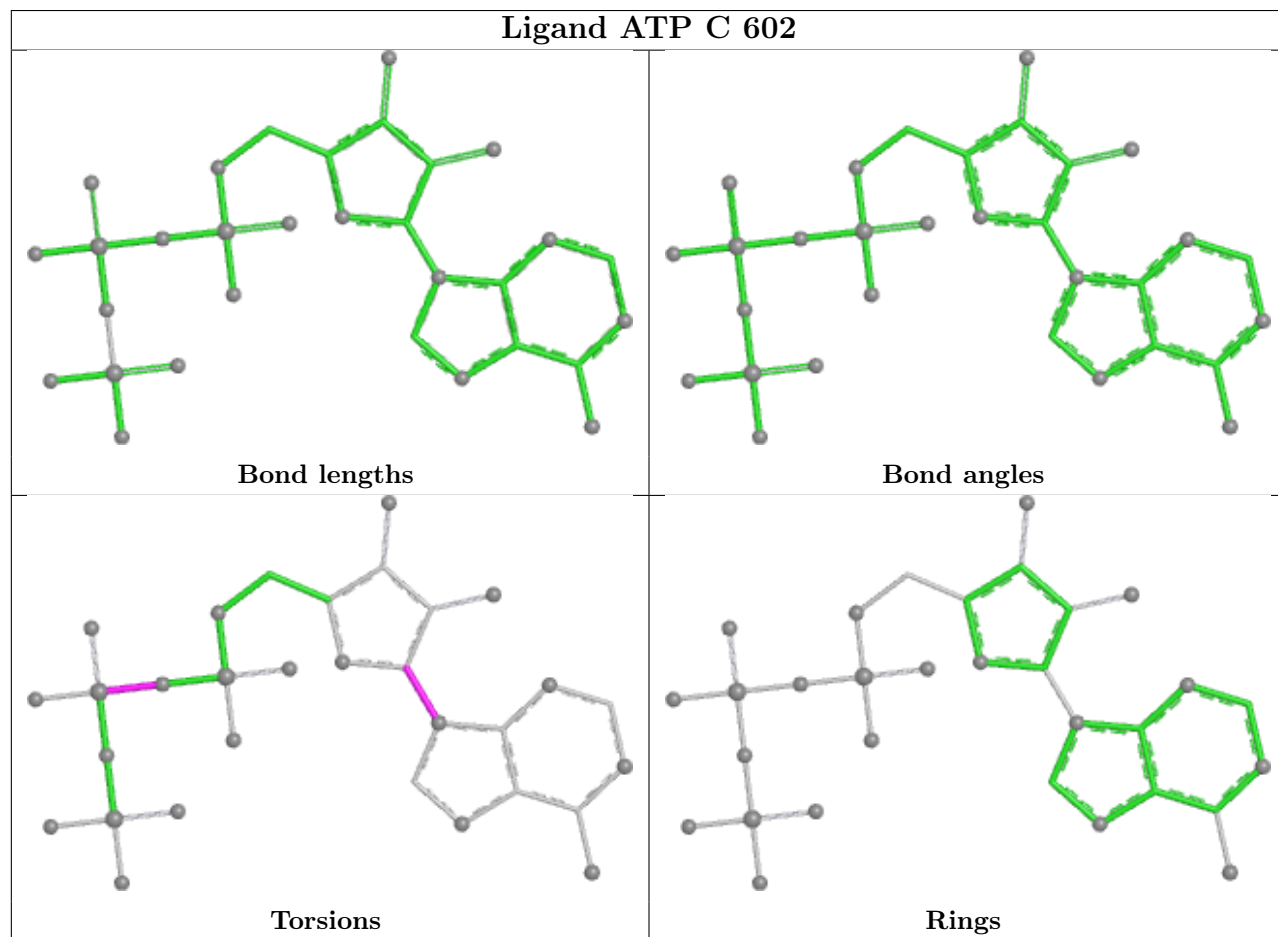
equivalents in the CSD to analyse the geometry.

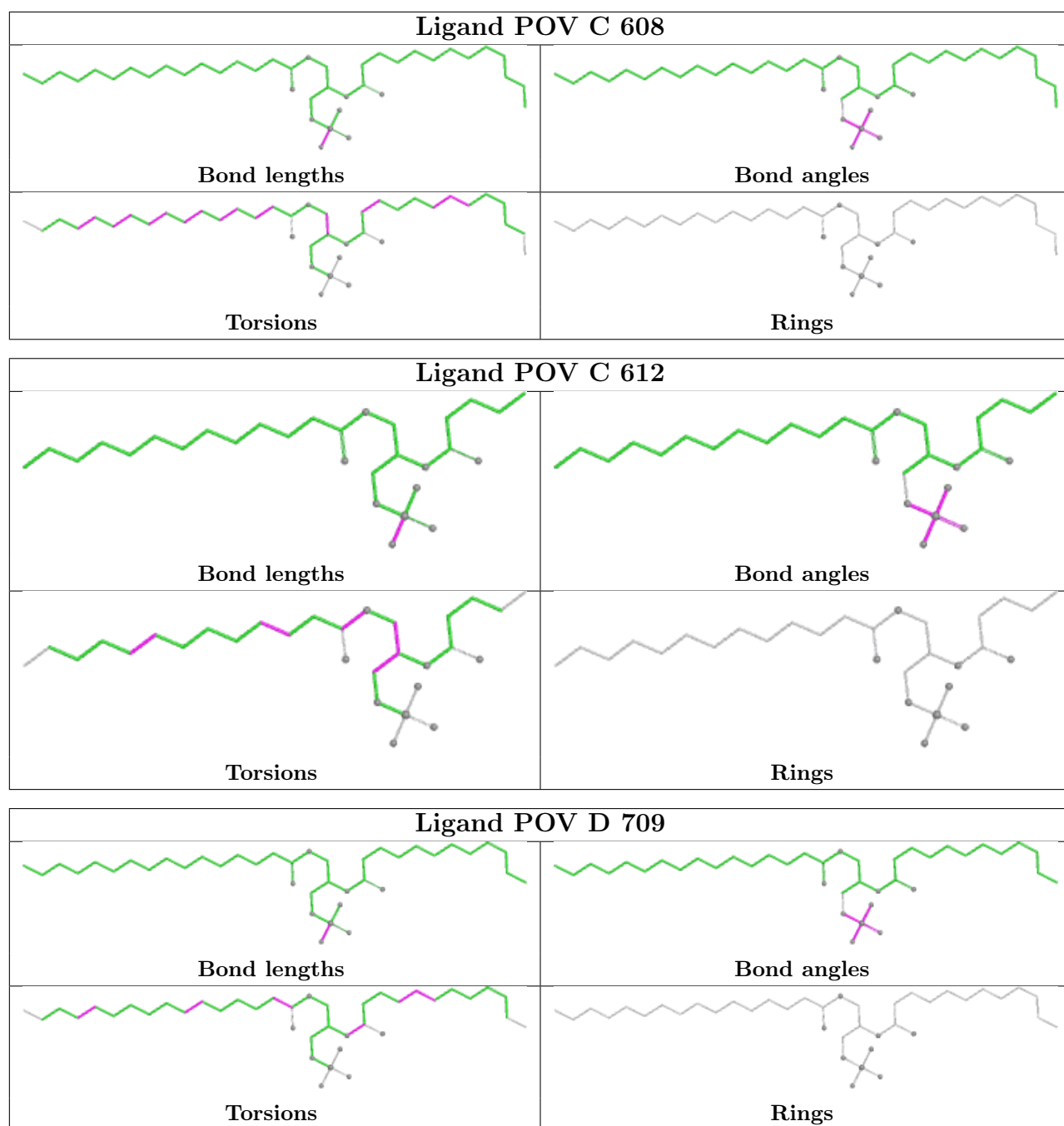


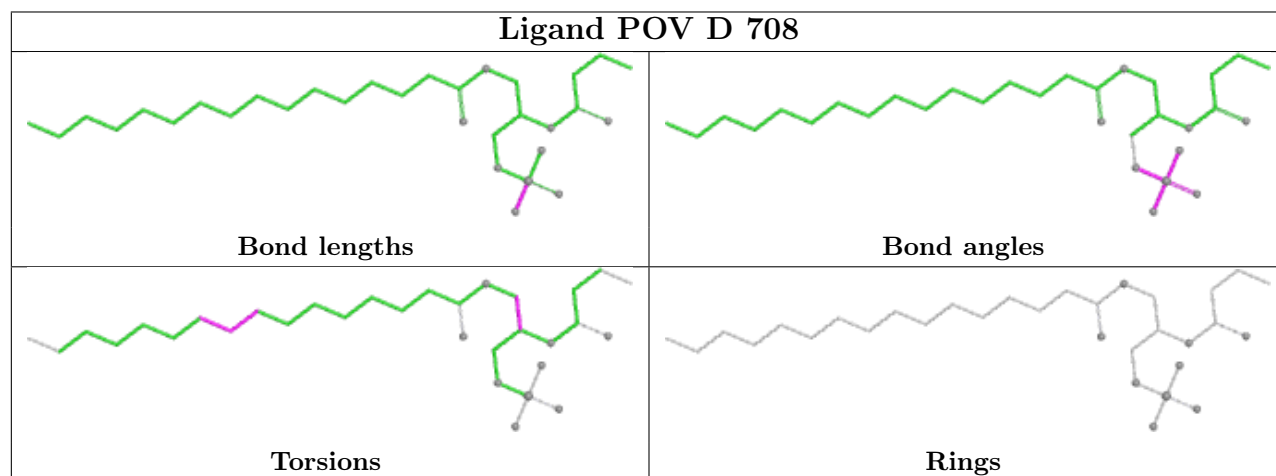
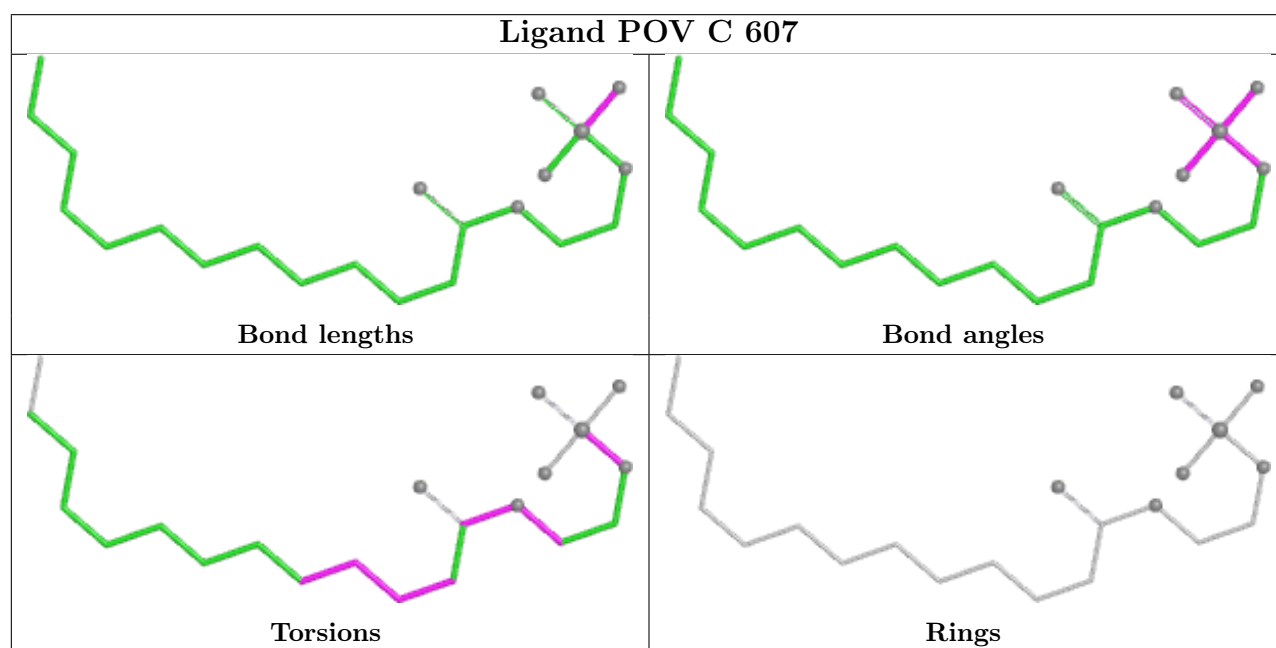
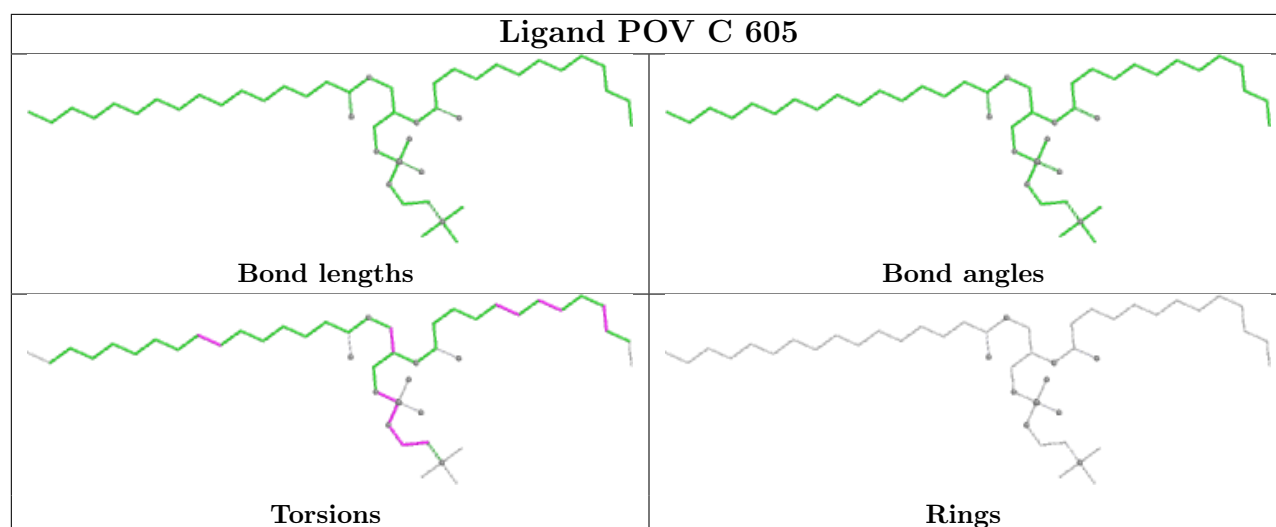
Ligand HT1 C 603

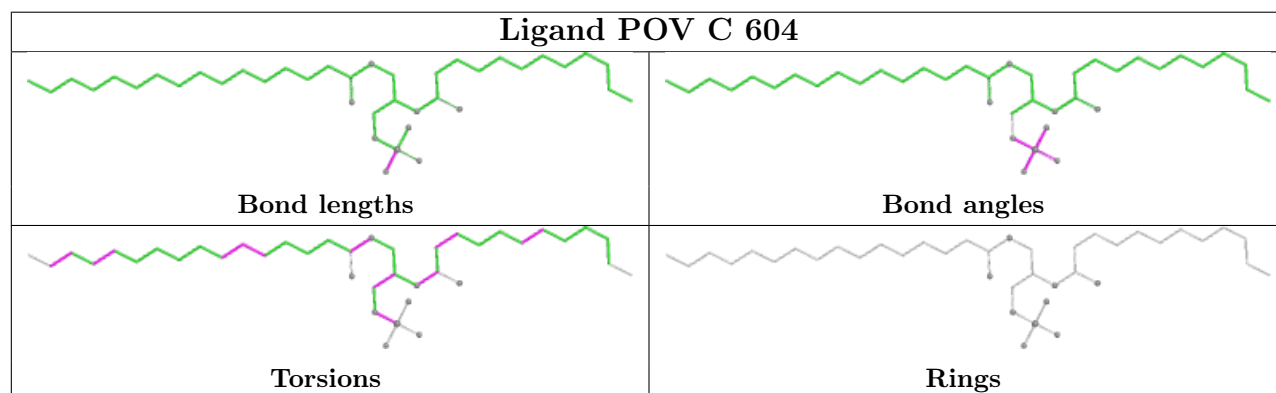
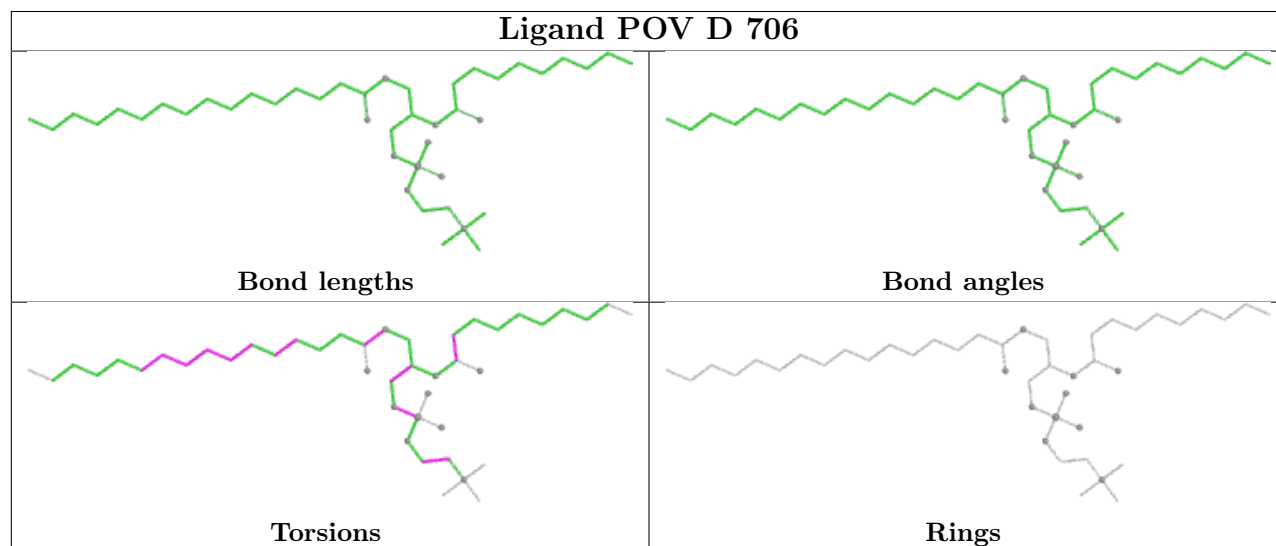
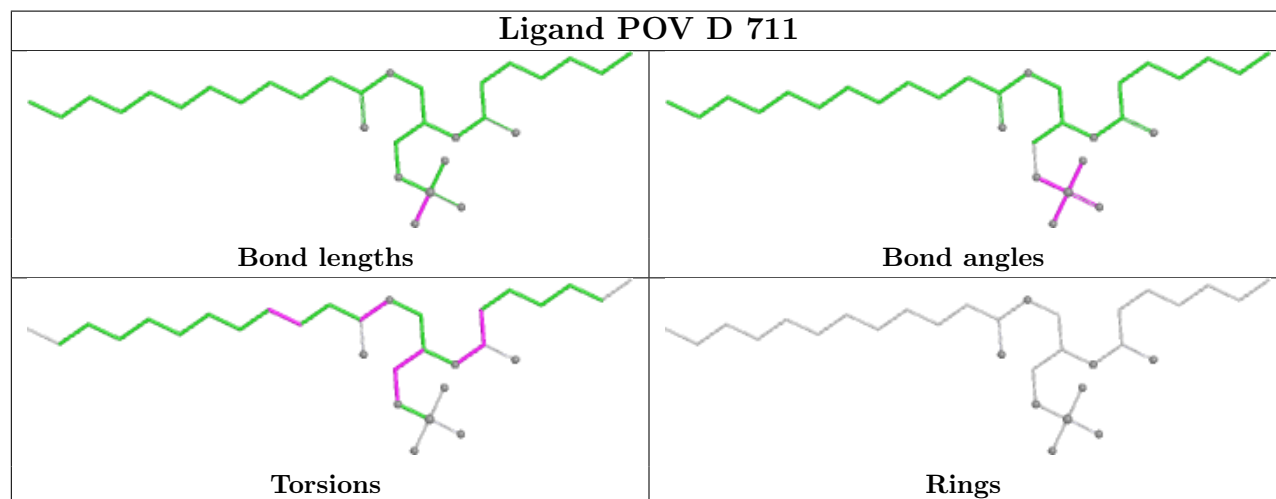
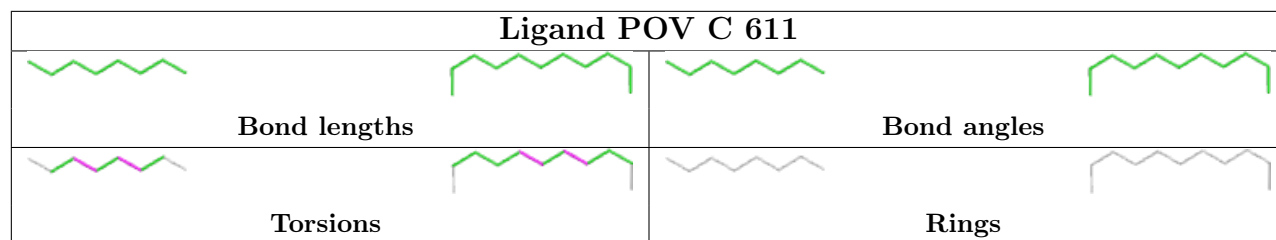


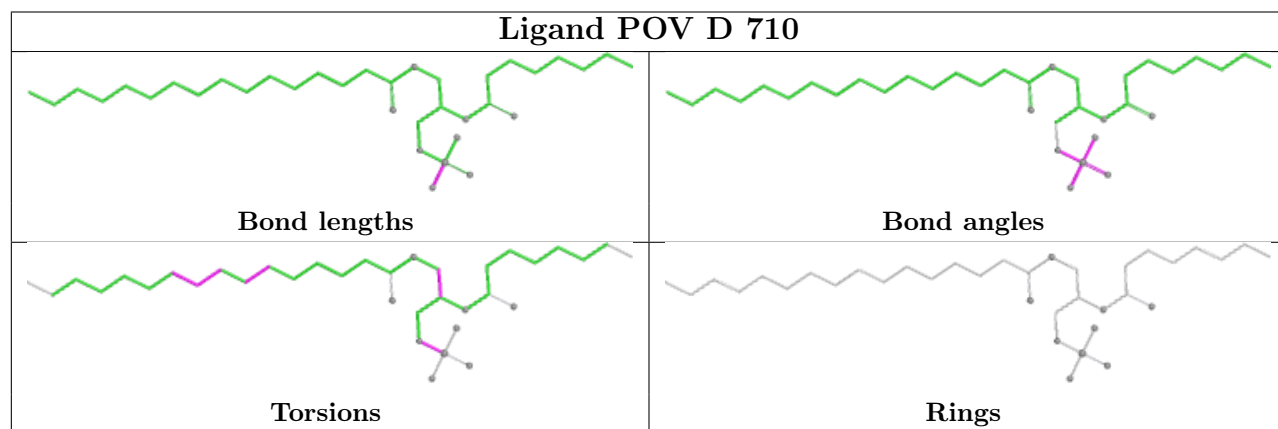
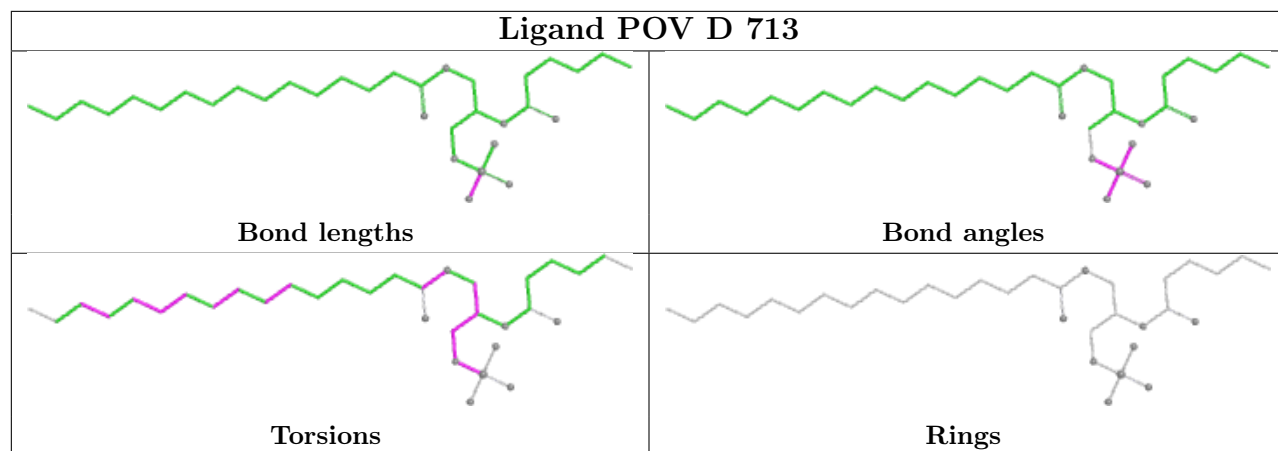
Ligand ATP C 602

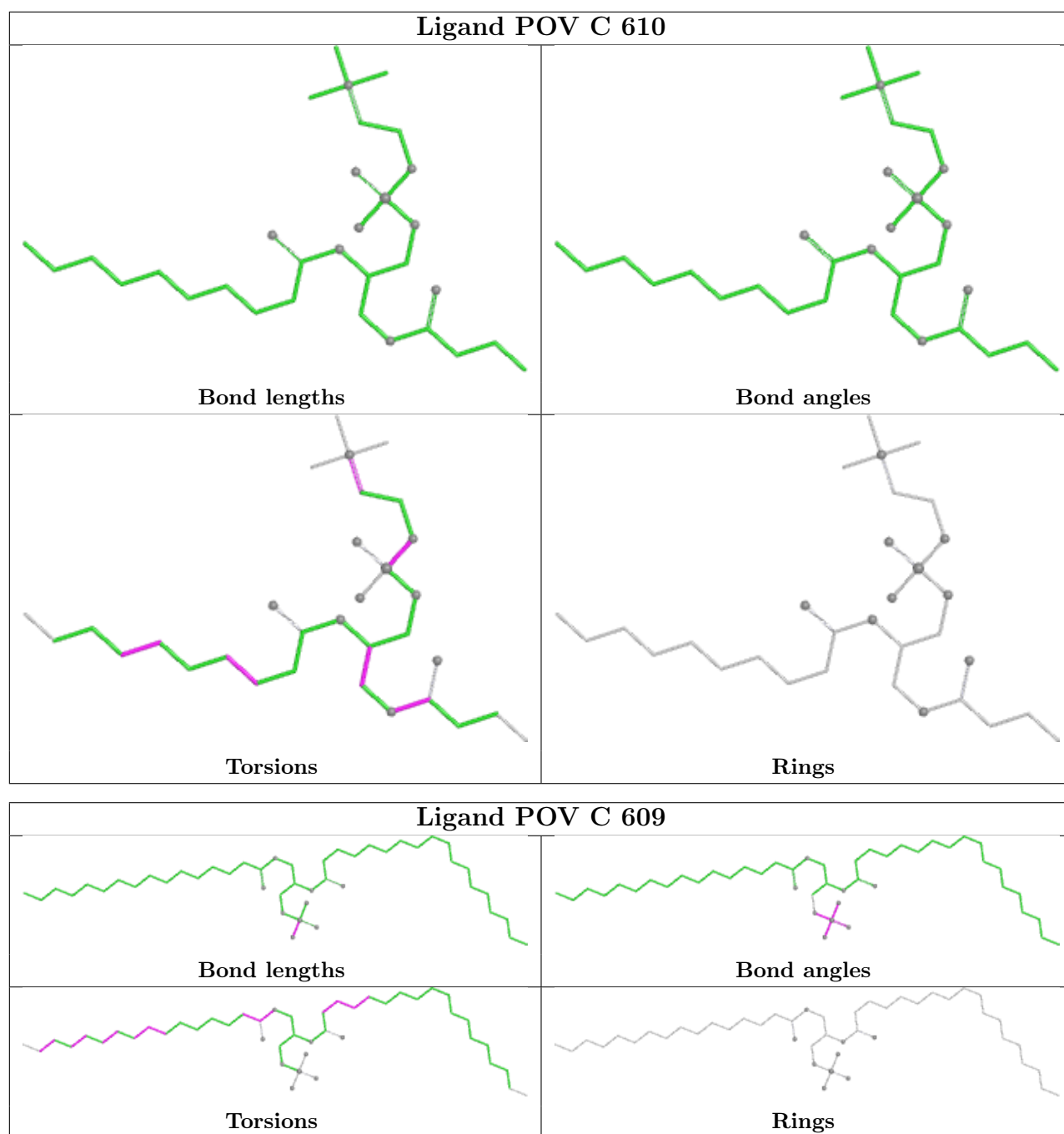


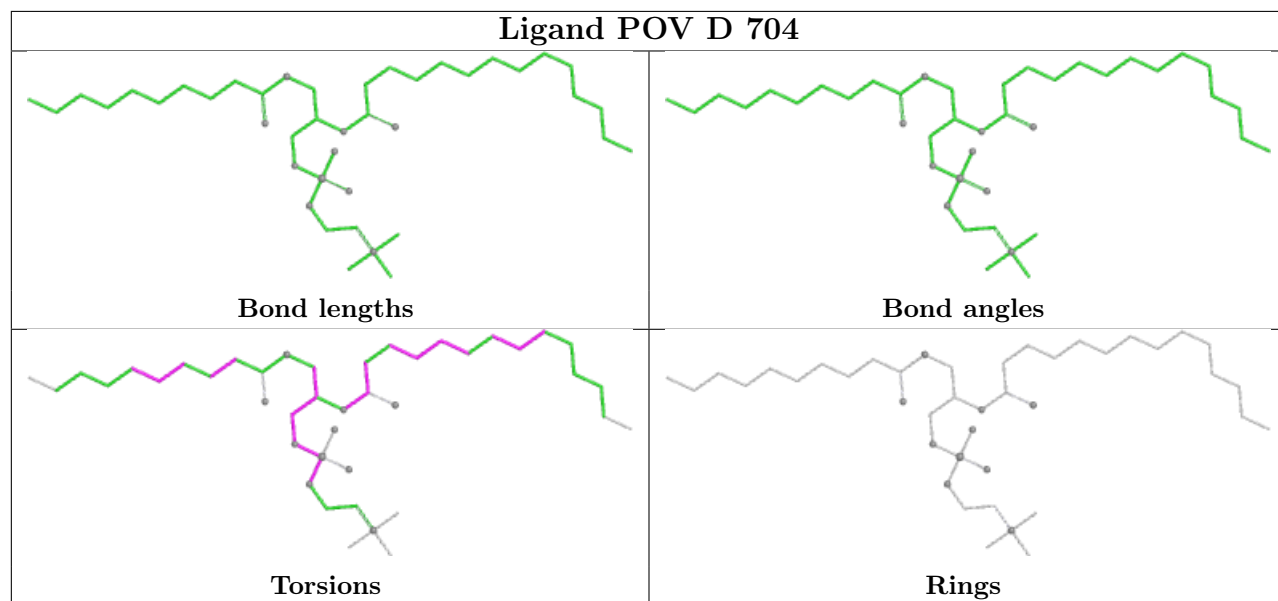
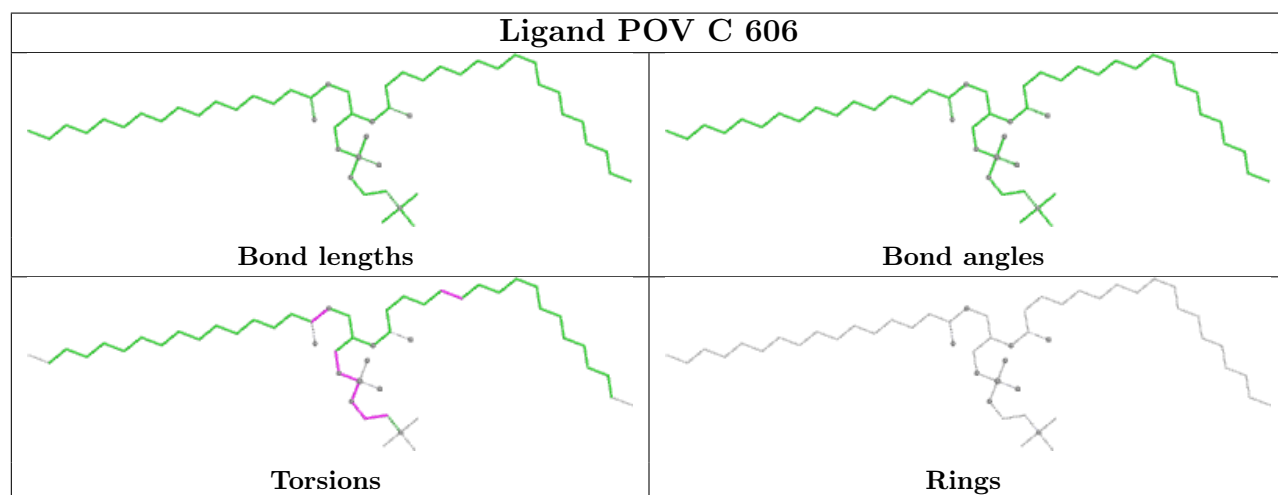
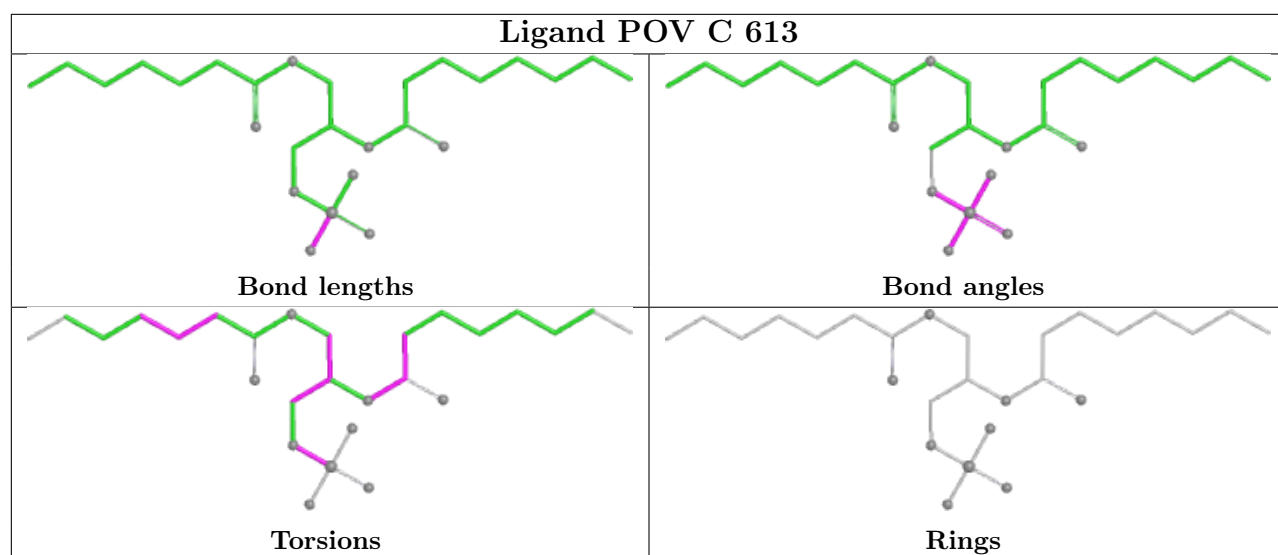


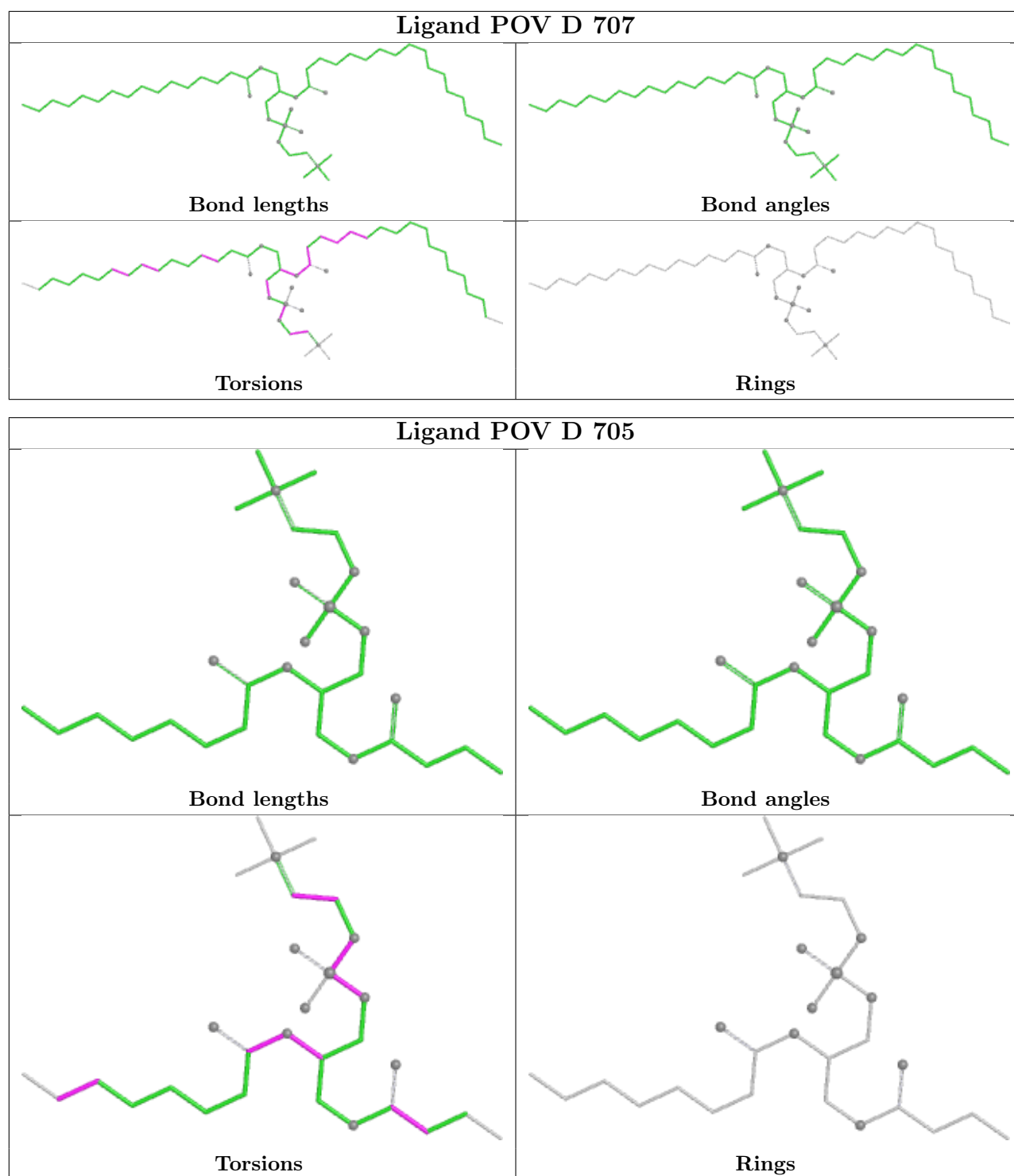












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

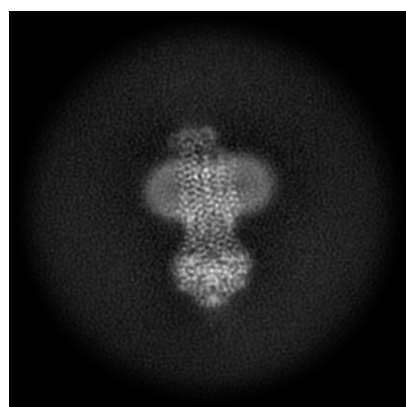
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45940. These allow visual inspection of the internal detail of the map and identification of artifacts.

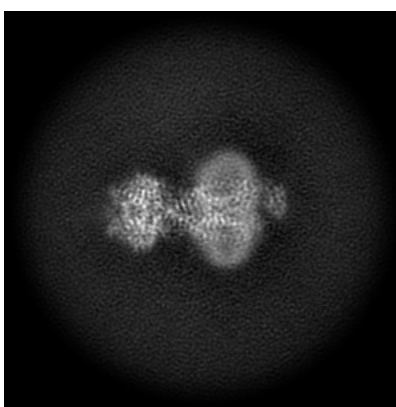
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

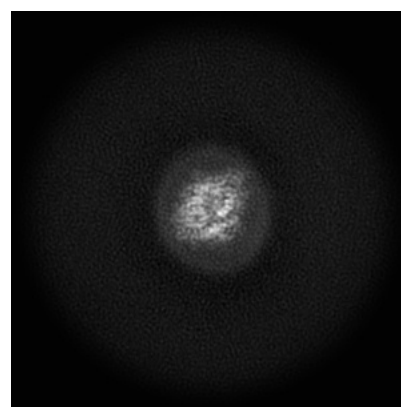
6.1.1 Primary map



X



Y

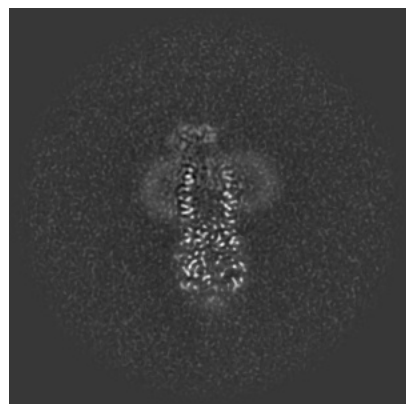


Z

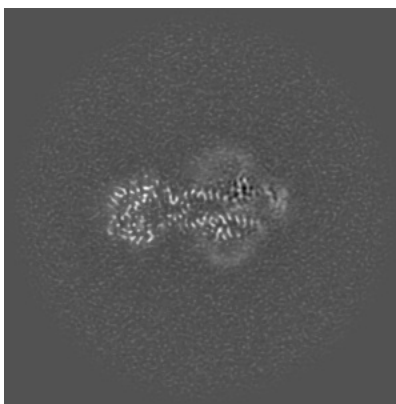
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

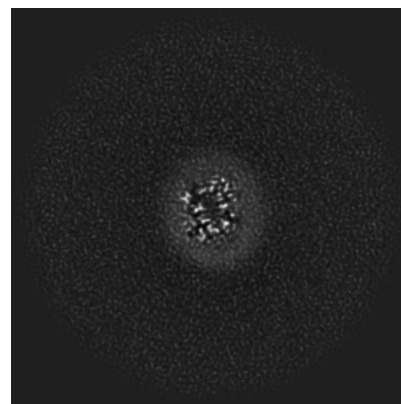
6.2.1 Primary map



X Index: 240



Y Index: 240

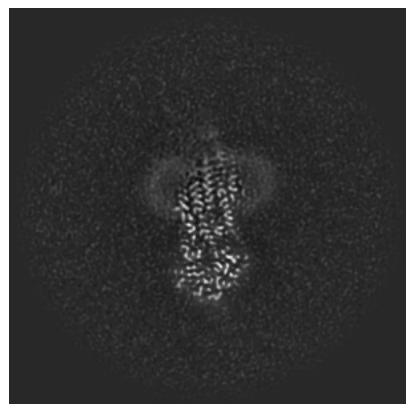


Z Index: 240

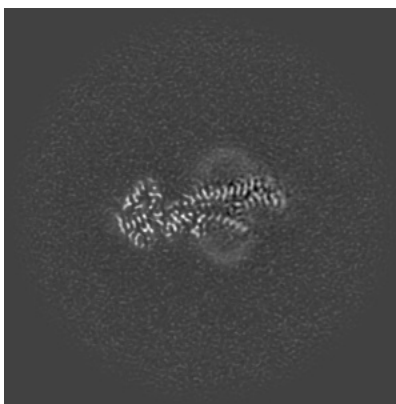
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

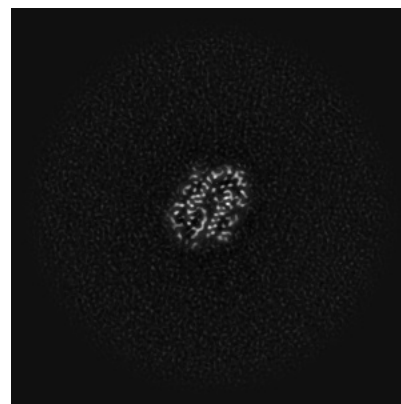
6.3.1 Primary map



X Index: 228



Y Index: 222

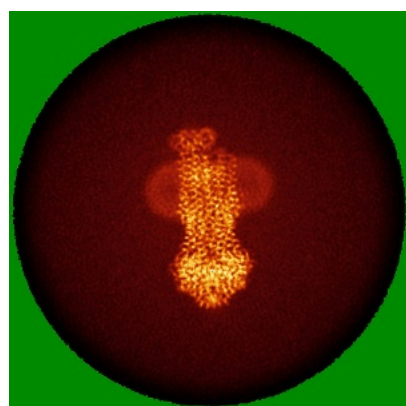


Z Index: 167

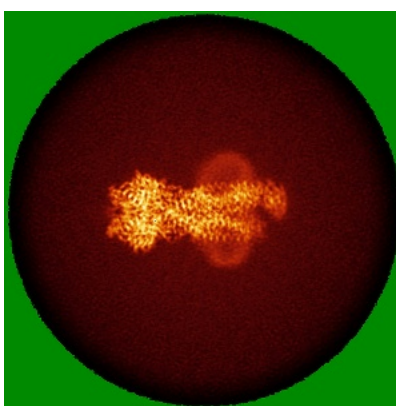
The images above show the largest variance slices of the map in three orthogonal directions.

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

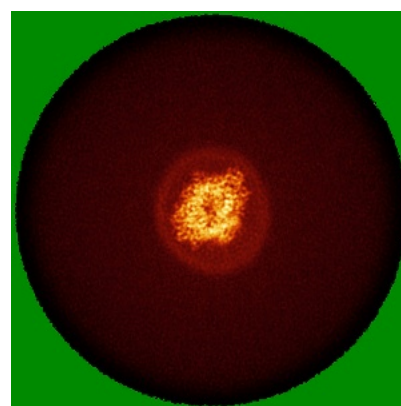
6.4.1 Primary map



X



Y

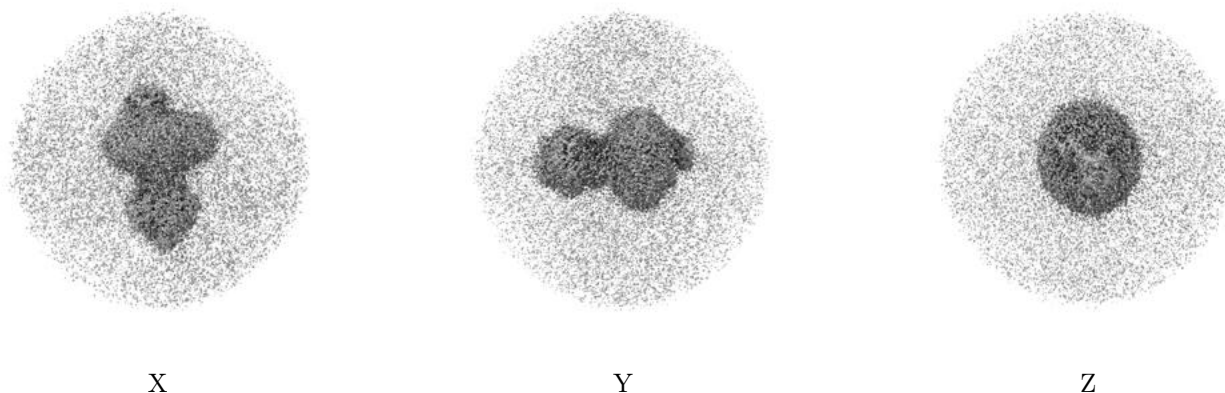


Z

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

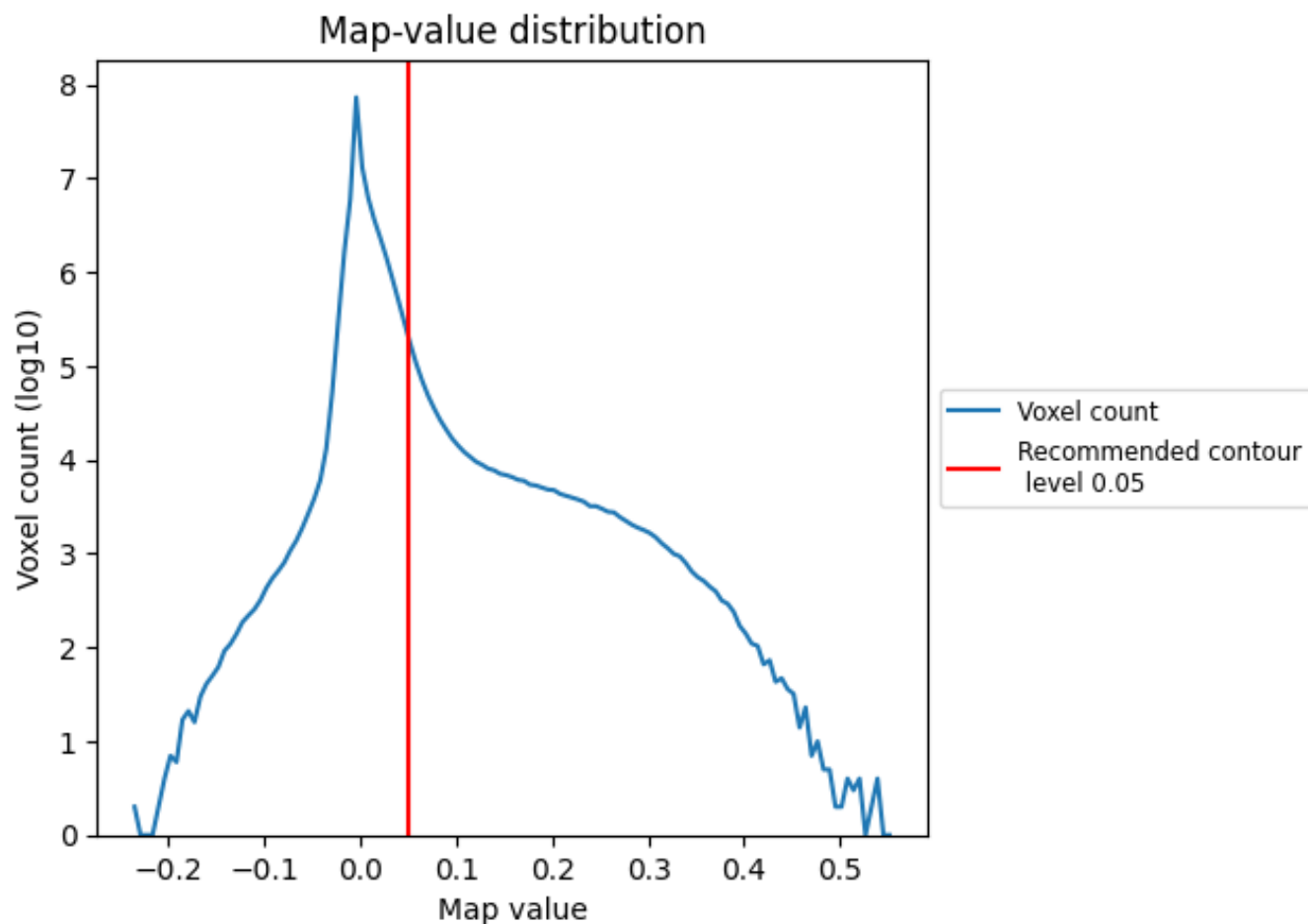
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

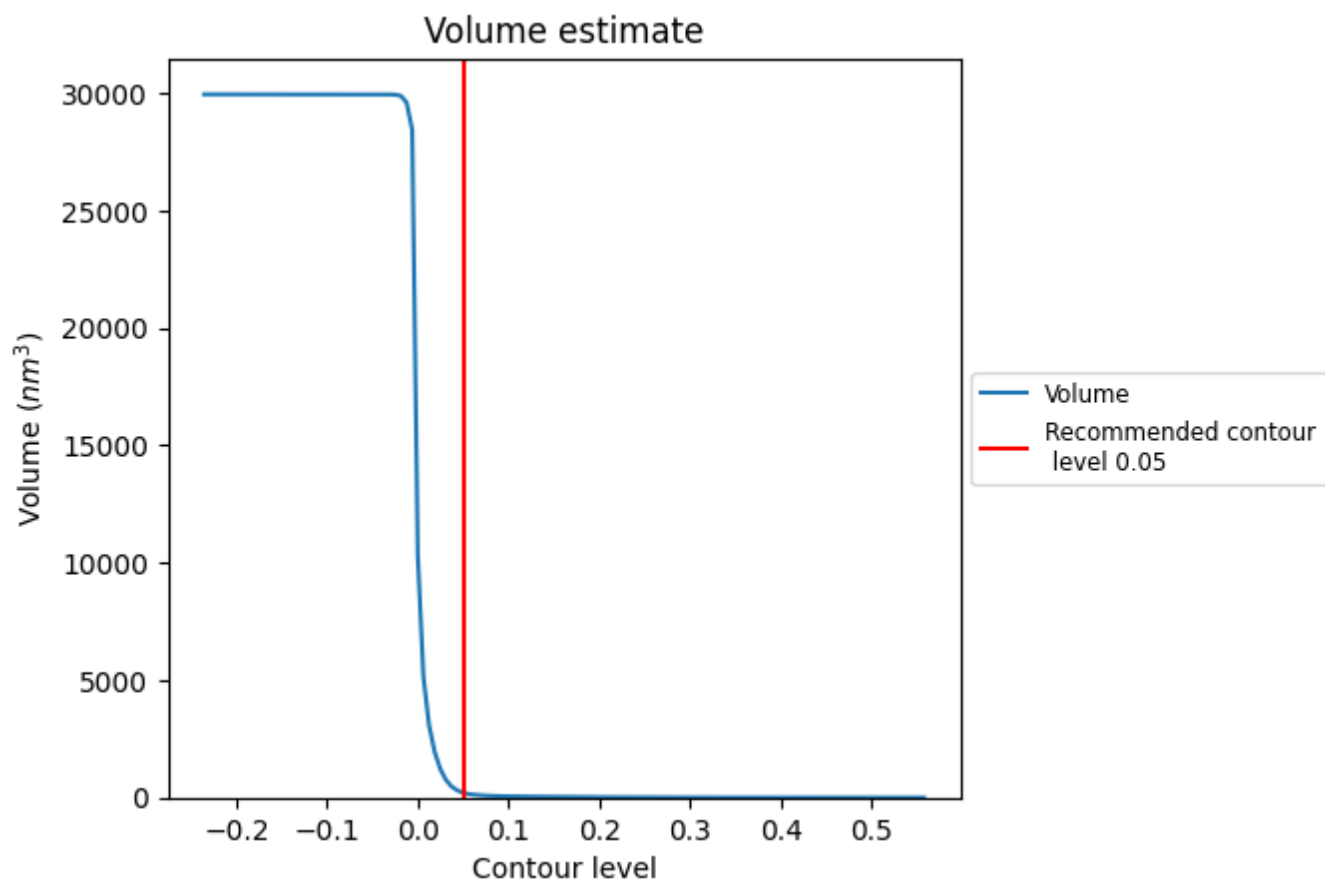
This section contains the results of statistical analysis of the map.

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.

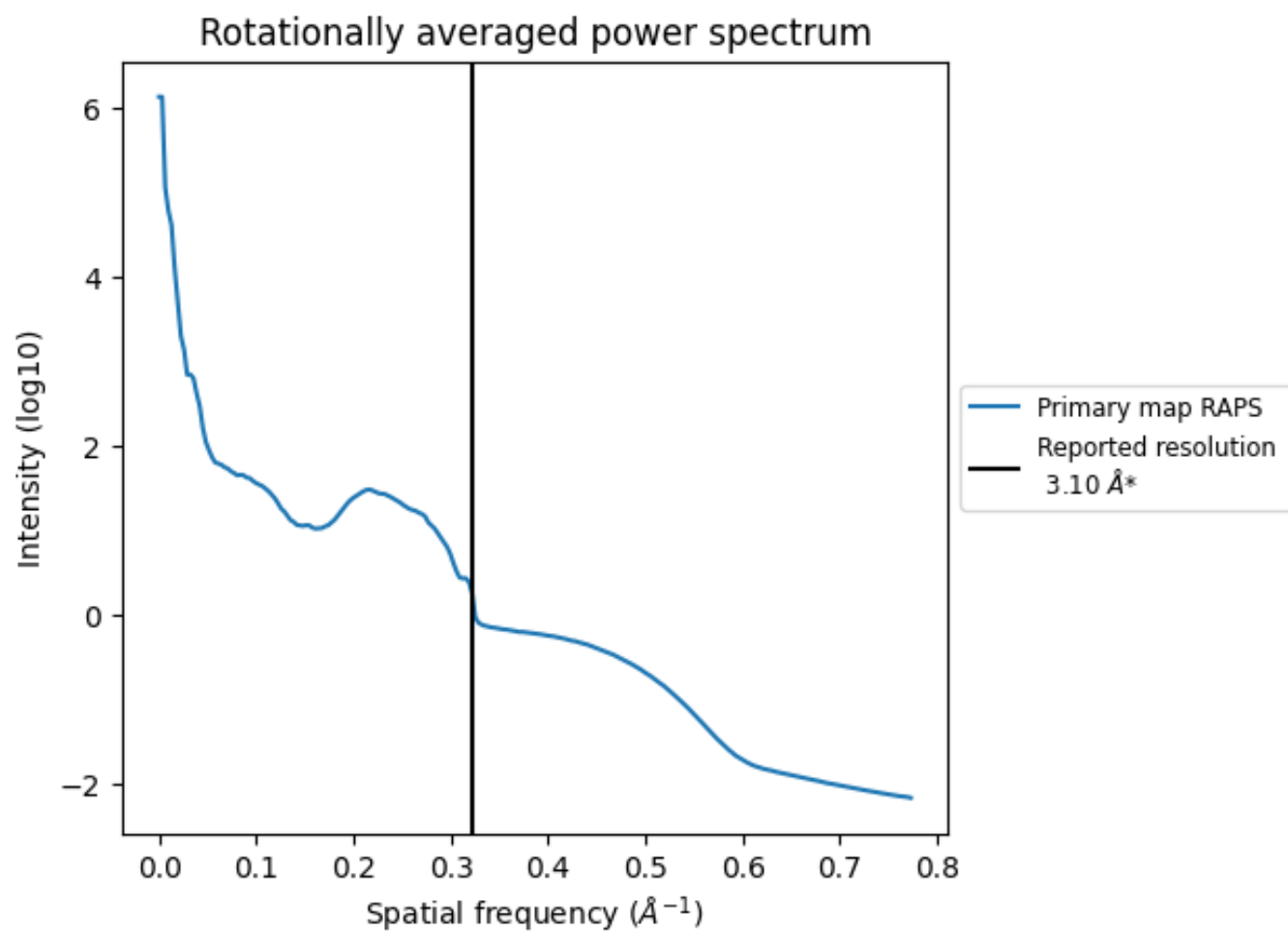
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm³; this corresponds to an approximate mass of 187 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 0.323 Å⁻¹

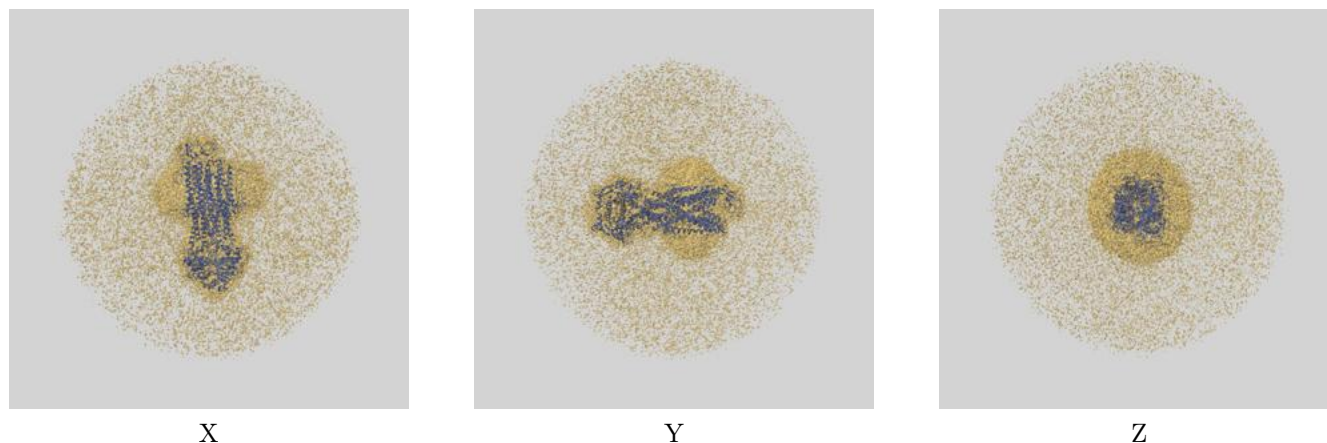
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

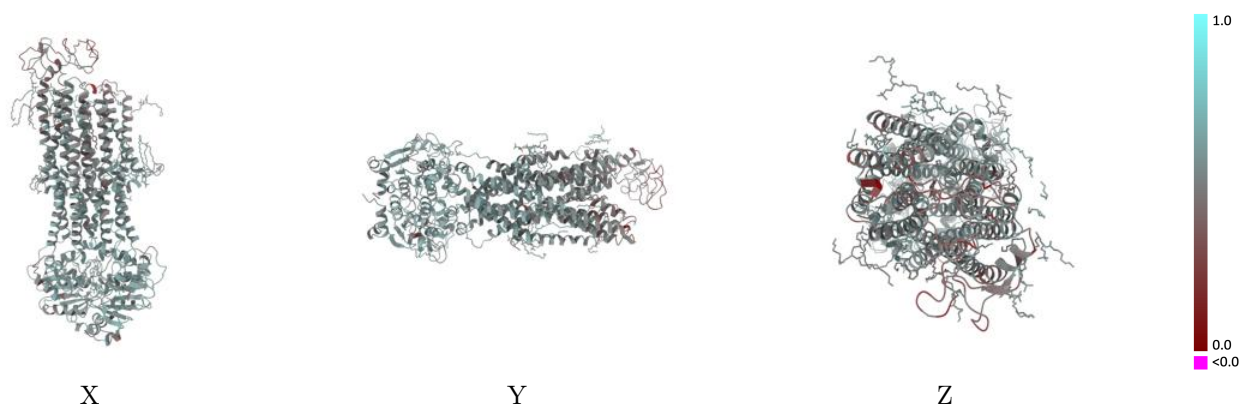
This section contains information regarding the fit between EMDB map EMD-45940 and PDB model 9CUS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



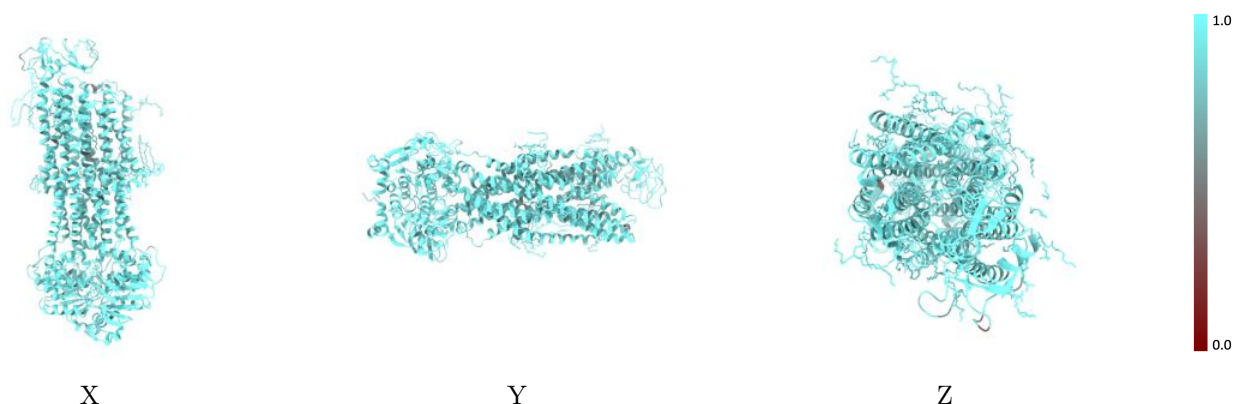
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



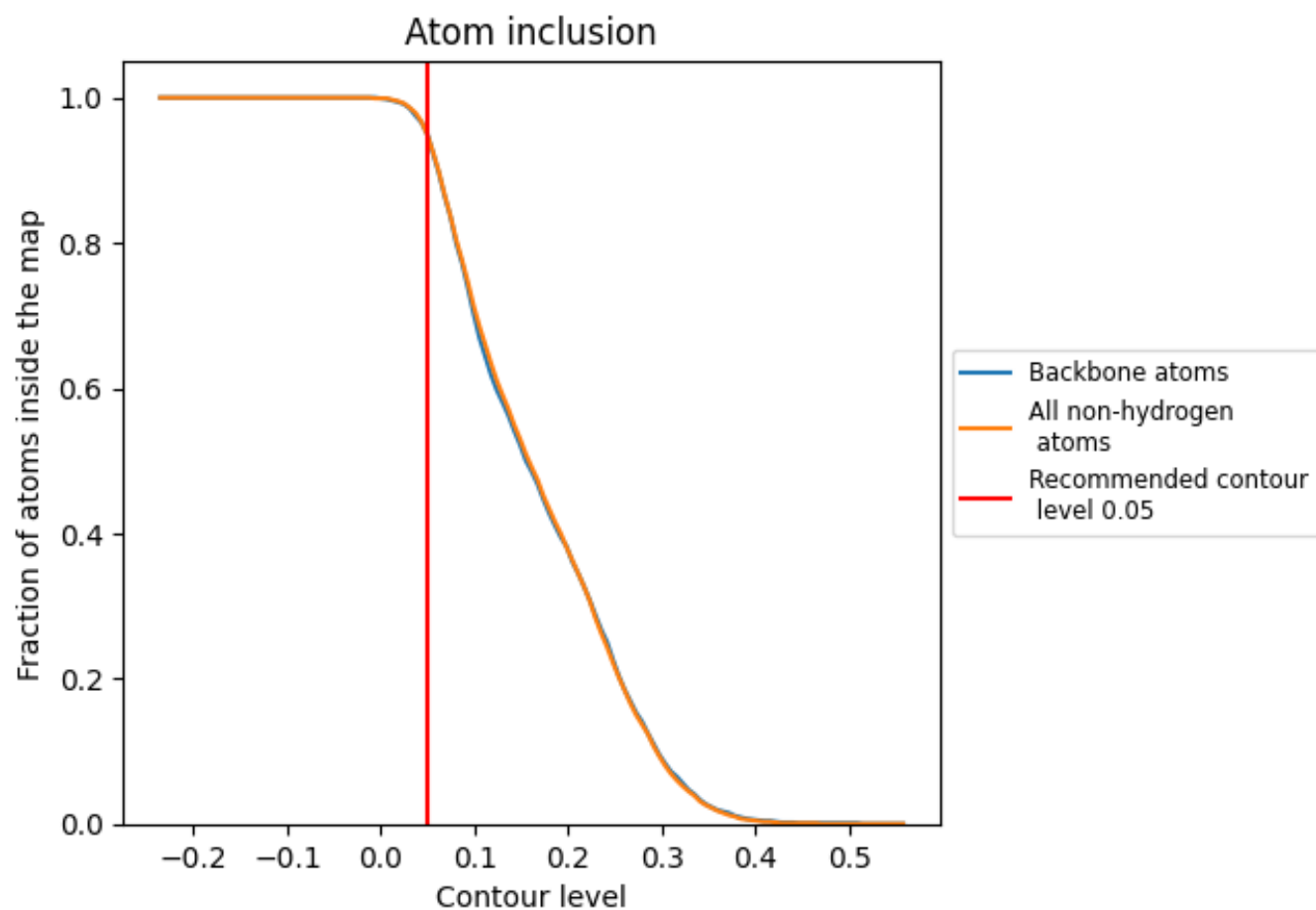
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.5260
C	0.9500	0.5380
D	0.9440	0.5160

