



## Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 05:44 PM EDT

PDB ID : 9CUP / pdb\_00009cup  
EMDB ID : EMD-45938  
Title : BmrCD in inward-facing conformation bound to Hoechst  
Authors : Qingyu, T.; Hassane, S.M.  
Deposited on : 2024-07-26  
Resolution : 3.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

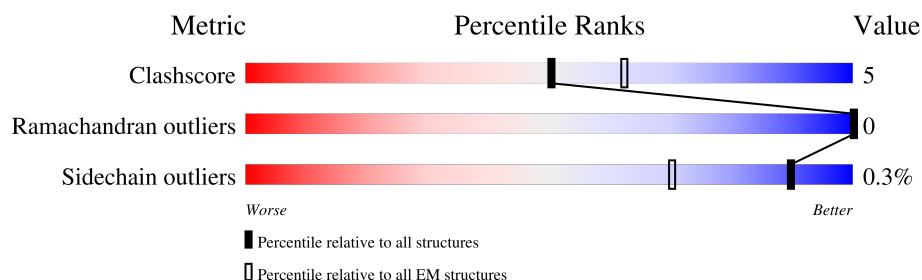
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	D	681	
2	C	607	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22287 atoms, of which 11339 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 YheH.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	D	668	10750	3434	5407	910	979	20	0	0

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 2 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		
2	C	577	9146	2932	4610	756	825	23	0	0

There are 23 discrepancies between the modelled and reference sequences:

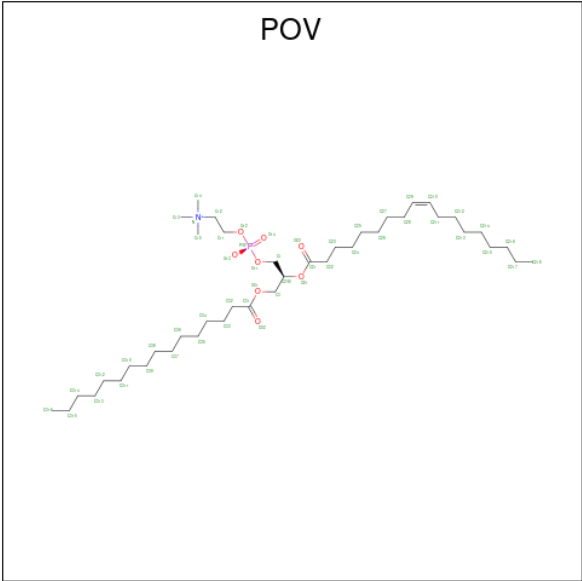
Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	expression tag	UNP O07550
C	-20	GLY	-	expression tag	UNP O07550
C	-19	SER	-	expression tag	UNP O07550
C	-18	SER	-	expression tag	UNP O07550
C	-17	HIS	-	expression tag	UNP O07550
C	-16	HIS	-	expression tag	UNP O07550
C	-15	HIS	-	expression tag	UNP O07550

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Chain	Residue	Modelled	Actual	Comment	Reference
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 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	D	1	Total 119	C 39	H 70	N 1	O 8	P 1	0
3	D	1	Total 22	C 7	H 8	O 6	P 1		0

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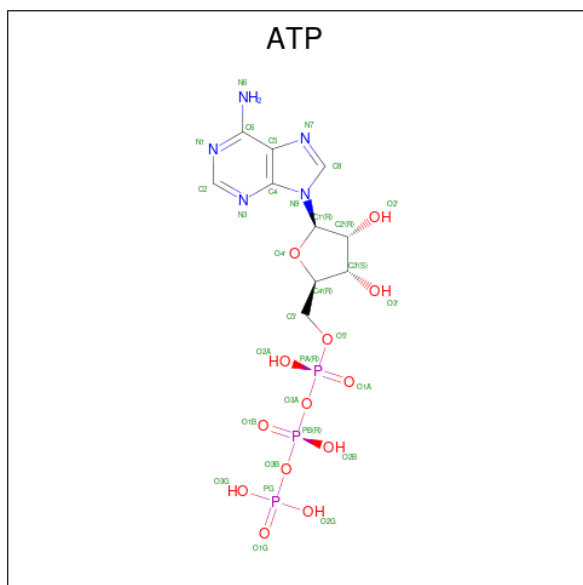
Mol	Chain	Residues	Atoms						AltConf
3	D	1	Total	C	H	N	O	P	0
			107	35	62	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			71	23	38	1	8	1	
3	D	1	Total	C	H	O	P		0
			25	8	10	6	1		
3	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			46	14	22	1	8	1	
3	D	1	Total	C	H	O	P		0
			91	30	52	8	1		
3	D	1	Total	C	H	N	O	P	0
			72	23	40	1	7	1	
3	D	1	Total	C	H	O	P		0
			103	34	60	8	1		
3	D	1	Total	C	H	O	P		0
			25	8	10	6	1		
3	D	1	Total	C	H	O	P		0
			54	18	27	8	1		
3	C	1	Total	C	H	O	P		0
			30	10	11	8	1		
3	C	1	Total	C	H	O	P		0
			48	16	23	8	1		
3	C	1	Total	C	H	O	P		0
			60	20	31	8	1		
3	C	1	Total	C	H	N	O	P	0
			122	39	73	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			110	36	64	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			119	38	71	1	8	1	
3	C	1	Total	C	H	O	P		0
			115	37	69	8	1		
3	C	1	Total	C	H	O	P		0
			97	33	55	8	1		
3	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
3	C	1	Total	C	H	N	O	P	0
			88	28	50	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
3	C	1	Total	C	H	O			0
			41	15	24	2			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

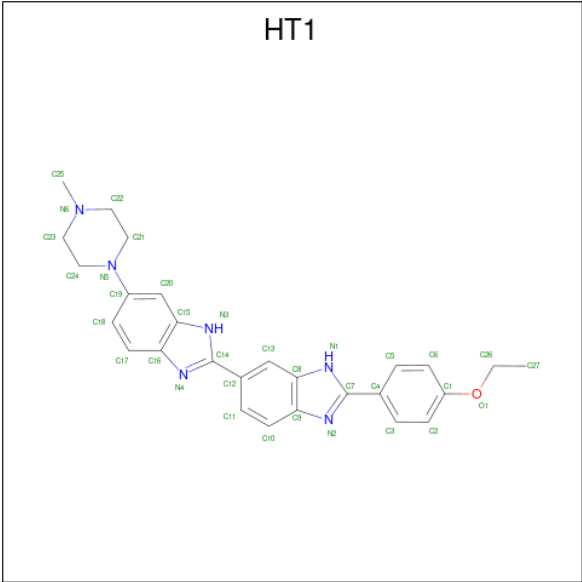


Mol	Chain	Residues	Atoms						AltConf
4	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Mg	0
			1	1	

- Molecule 6 is 2'-(4-ETHOXYPHENYL)-5-(4-METHYL-1-PIPERAZINYL)-2,5'-BI-BENZIMIDAZOLE (CCD ID: HT1) (formula:  $C_{27}H_{28}N_6O$ ) (labeled as "Ligand of Interest" by depositor).

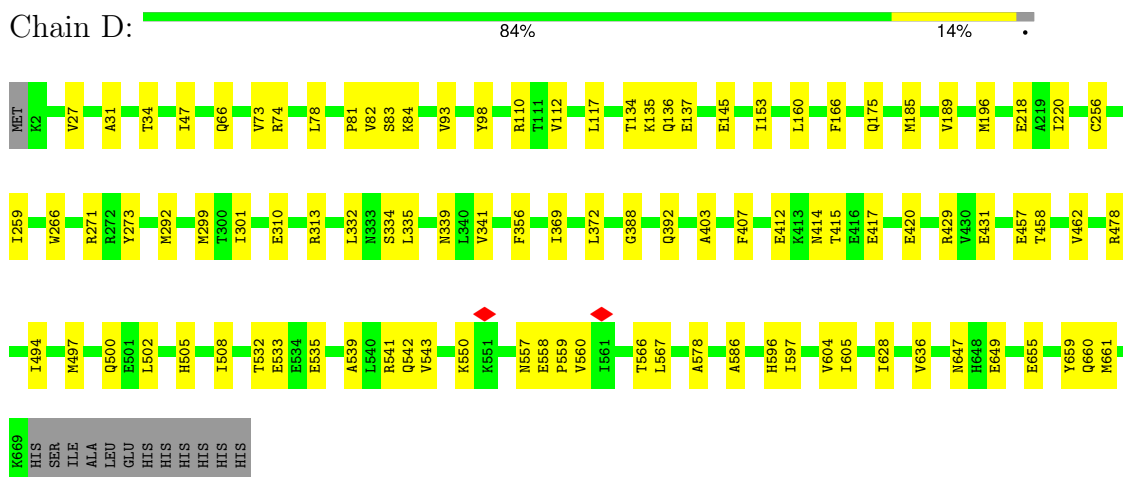


Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	H	N	O	0
			62	27	28	6	1	
6	C	1	Total	C	H	N	O	0
			62	27	28	6	1	

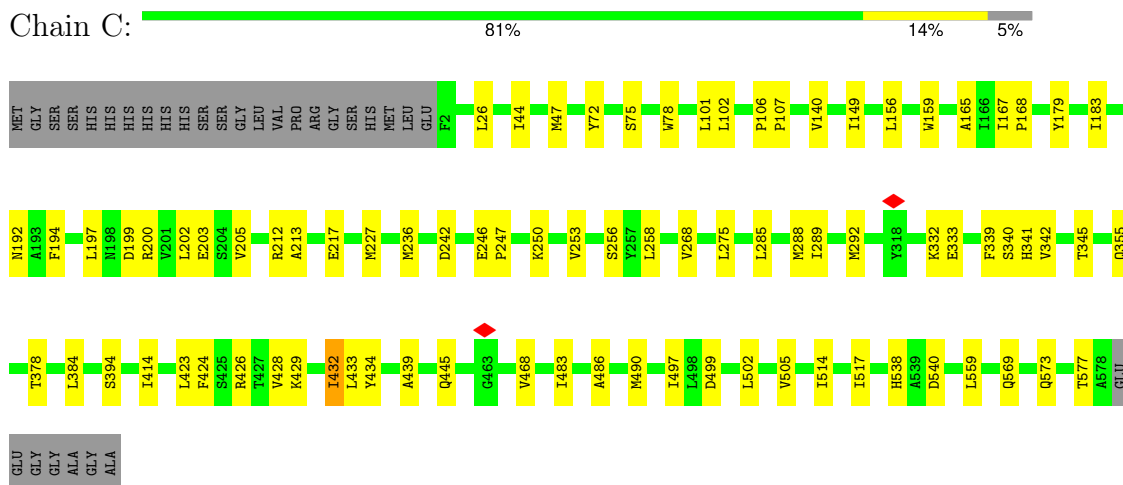
### 3 Residue-property plots

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 YheH



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219934	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	1.053	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.046	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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	D	0.21	0/5444	0.36	0/7347
2	C	0.22	0/4630	0.36	0/6267
All	All	0.22	0/10074	0.36	0/13614

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	D	5343	5407	5406	67	0
2	C	4536	4610	4609	69	0
3	C	498	679	679	5	0
3	D	440	563	563	1	0
4	C	31	12	12	0	0
4	D	31	12	12	0	0
5	D	1	0	0	0	0
6	C	68	56	56	3	0
All	All	10948	11339	11337	120	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 5.

All (120) 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:D:299:MET:HE1	2:C:102:LEU:HD23	1.61	0.83
2:C:246:GLU:N	2:C:246:GLU:OE1	2.19	0.75
2:C:340:SER:O	2:C:341:HIS:ND1	2.24	0.69
1:D:299:MET:HE1	2:C:102:LEU:CD2	2.23	0.69
2:C:333:GLU:N	2:C:333:GLU:OE1	2.25	0.69
1:D:66:GLN:N	1:D:66:GLN:OE1	2.27	0.68
2:C:340:SER:HG	2:C:394:SER:HG	1.44	0.63
2:C:355:GLN:OE1	2:C:355:GLN:N	2.33	0.62
2:C:573:GLN:O	2:C:577:THR:N	2.33	0.61
2:C:426:ARG:NH2	2:C:434:TYR:OH	2.35	0.60
1:D:505:HIS:O	1:D:586:ALA:N	2.38	0.57
2:C:200:ARG:NH1	2:C:203:GLU:OE2	2.38	0.57
1:D:74:ARG:NH2	1:D:145:GLU:OE2	2.38	0.56
1:D:196:MET:HE1	1:D:412:GLU:HB2	1.88	0.56
1:D:566:THR:HG23	1:D:567:LEU:HG	1.85	0.56
2:C:339:PHE:HD2	2:C:342:VAL:HG11	1.70	0.56
1:D:596:HIS:O	1:D:597:ILE:HG23	2.06	0.56
1:D:604:VAL:HG13	1:D:605:ILE:HG23	1.88	0.54
1:D:153:ILE:HG23	2:C:258:LEU:HD21	1.89	0.54
2:C:75:SER:HA	2:C:78:TRP:CD1	2.44	0.53
1:D:266:TRP:HH2	1:D:341:VAL:HG23	1.73	0.53
1:D:541:ARG:NH1	1:D:578:ALA:O	2.41	0.53
1:D:160:LEU:HD13	6:C:616:HT1:H272	1.91	0.53
2:C:159:TRP:N	3:C:612:POV:O13	2.40	0.53
1:D:457:GLU:O	1:D:458:THR:OG1	2.23	0.52
2:C:429:LYS:O	2:C:432:ILE:HG22	2.08	0.52
1:D:462:VAL:CG2	1:D:636:VAL:HG12	2.40	0.52
1:D:535:GLU:O	1:D:539:ALA:N	2.43	0.52
1:D:301:ILE:HD11	2:C:424:PHE:CE2	2.45	0.52
2:C:414:ILE:CG2	2:C:497:ILE:HD12	2.40	0.51
2:C:502:LEU:HB3	2:C:505:VAL:HG22	1.93	0.51
1:D:500:GLN:NE2	2:C:217:GLU:OE1	2.43	0.51
1:D:417:GLU:OE1	1:D:417:GLU:N	2.37	0.50
1:D:81:PRO:O	1:D:82:VAL:HG13	2.12	0.50
2:C:285:LEU:O	2:C:289:ILE:HG23	2.12	0.50
1:D:478:ARG:NH1	1:D:497:MET:O	2.44	0.49
1:D:647:ASN:OD1	1:D:649:GLU:N	2.45	0.49
1:D:175:GLN:NE2	2:C:242:ASP:OD2	2.46	0.49
1:D:310:GLU:OE2	1:D:313:ARG:NH1	2.45	0.49
2:C:423:LEU:HD21	2:C:483:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:MET:O	2:C:212:ARG:NH1	2.39	0.49
1:D:136:GLN:OE1	1:D:137:GLU:N	2.46	0.48
1:D:256:CYS:O	1:D:259:ILE:HG22	2.13	0.48
1:D:494:ILE:HG23	1:D:502:LEU:HD22	1.95	0.48
2:C:569:GLN:OE1	2:C:569:GLN:N	2.43	0.48
1:D:660:GLN:OE1	1:D:661:MET:N	2.47	0.47
2:C:250:LYS:HD3	6:C:616:HT1:H3	1.96	0.47
2:C:192:ASN:OD1	2:C:192:ASN:C	2.57	0.47
2:C:165:ALA:O	2:C:256:SER:OG	2.32	0.47
2:C:345:THR:HG23	2:C:345:THR:O	2.15	0.47
2:C:378:THR:HG23	2:C:499:ASP:OD2	2.15	0.47
1:D:31:ALA:O	1:D:34:THR:HG22	2.15	0.47
2:C:433:LEU:HD22	2:C:439:ALA:HB3	1.97	0.47
1:D:542:GLN:O	1:D:542:GLN:CG	2.63	0.46
1:D:334:SER:OG	1:D:335:LEU:N	2.47	0.46
1:D:628:ILE:O	1:D:628:ILE:CG2	2.63	0.46
1:D:218:GLU:OE2	2:C:194:PHE:CZ	2.69	0.46
1:D:93:VAL:HG12	1:D:110:ARG:HB2	1.98	0.45
1:D:372:LEU:CD2	2:C:44:ILE:HD11	2.45	0.45
1:D:266:TRP:C	1:D:266:TRP:CD1	2.93	0.45
2:C:428:VAL:HG13	2:C:483:ILE:HD11	1.98	0.45
1:D:372:LEU:HD21	2:C:44:ILE:HD11	1.98	0.45
1:D:655:GLU:HA	1:D:659:TYR:HB3	1.99	0.45
1:D:220:ILE:HD11	1:D:403:ALA:HB2	1.99	0.45
1:D:271:ARG:NH2	3:D:702:POV:O13	2.43	0.45
2:C:236:MET:HA	2:C:236:MET:HE2	1.99	0.45
1:D:457:GLU:N	1:D:457:GLU:OE1	2.51	0.44
2:C:149:ILE:HG21	2:C:288:MET:HB2	2.00	0.44
2:C:432:ILE:HD11	2:C:486:ALA:HB1	1.99	0.44
2:C:26:LEU:HD13	2:C:140:VAL:HG11	2.00	0.44
2:C:384:LEU:HD23	2:C:497:ILE:HD11	1.99	0.43
1:D:558:GLU:N	1:D:559:PRO:HD3	2.33	0.43
1:D:27:VAL:HG11	1:D:166:PHE:CE2	2.53	0.43
1:D:47:ILE:HG23	2:C:268:VAL:HG11	1.99	0.43
2:C:197:LEU:HA	2:C:227:MET:HE2	1.99	0.43
2:C:258:LEU:C	2:C:258:LEU:HD23	2.44	0.43
2:C:538:HIS:O	2:C:538:HIS:ND1	2.51	0.43
2:C:428:VAL:HG22	2:C:468:VAL:CG2	2.49	0.43
1:D:273:TYR:HB3	1:D:332:LEU:HD22	2.01	0.42
2:C:540:ASP:OD1	2:C:540:ASP:N	2.41	0.42
1:D:356:PHE:C	2:C:47:MET:HE2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:THR:HG22	1:D:135:LYS:N	2.35	0.42
1:D:550:LYS:O	1:D:557:ASN:ND2	2.52	0.42
1:D:532:THR:OG1	1:D:533:GLU:N	2.52	0.42
2:C:514:ILE:HA	2:C:517:ILE:HG22	2.02	0.42
1:D:98:TYR:CE2	1:D:112:VAL:HG21	2.54	0.42
2:C:236:MET:HE2	2:C:236:MET:N	2.35	0.42
1:D:429:ARG:NH1	1:D:431:GLU:OE2	2.45	0.42
1:D:196:MET:HE1	1:D:412:GLU:CB	2.49	0.42
2:C:332:LYS:N	2:C:332:LYS:HD3	2.35	0.42
1:D:292:MET:HE3	2:C:101:LEU:HD12	2.02	0.41
1:D:369:ILE:HG21	2:C:275:LEU:HD13	2.01	0.41
2:C:167:ILE:N	2:C:168:PRO:HD2	2.35	0.41
2:C:236:MET:HE2	2:C:236:MET:CA	2.51	0.41
1:D:560:VAL:O	1:D:560:VAL:HG12	2.20	0.41
2:C:199:ASP:OD1	2:C:199:ASP:C	2.63	0.41
2:C:253:VAL:HG11	6:C:616:HT1:HN1	1.85	0.41
2:C:292:MET:HE1	3:C:613:POV:H210	2.02	0.41
2:C:414:ILE:HG21	2:C:497:ILE:HD12	2.03	0.41
1:D:508:ILE:HG21	2:C:213:ALA:CB	2.51	0.41
2:C:445:GLN:HA	2:C:445:GLN:OE1	2.20	0.41
1:D:185:MET:O	1:D:189:VAL:HG23	2.21	0.41
2:C:156:LEU:HD22	3:C:608:POV:H1A	2.01	0.41
2:C:179:TYR:O	2:C:183:ILE:HG22	2.21	0.41
1:D:83:SER:O	1:D:84:LYS:HG2	2.20	0.41
1:D:388:GLY:O	1:D:392:GLN:HG2	2.21	0.41
1:D:543:VAL:O	1:D:543:VAL:HG12	2.21	0.41
1:D:136:GLN:CD	1:D:136:GLN:C	2.89	0.41
1:D:339:ASN:HB3	2:C:72:TYR:CD1	2.56	0.41
2:C:246:GLU:HB2	2:C:247:PRO:HD3	2.03	0.41
2:C:258:LEU:HD22	3:C:605:POV:H212	2.02	0.41
2:C:258:LEU:HD22	3:C:605:POV:C212	2.51	0.41
1:D:185:MET:HE3	1:D:407:PHE:HE1	1.85	0.40
2:C:202:LEU:HA	2:C:205:VAL:HG12	2.04	0.40
2:C:439:ALA:CB	2:C:490:MET:HE2	2.51	0.40
1:D:73:VAL:HG13	1:D:78:LEU:HD12	2.03	0.40
1:D:414:ASN:O	1:D:415:THR:HG23	2.22	0.40
1:D:420:GLU:OE1	1:D:420:GLU:N	2.54	0.40
2:C:106:PRO:N	2:C:107:PRO:CD	2.84	0.40
2:C:156:LEU:N	2:C:156:LEU:HD23	2.36	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	D	666/681 (98%)	609 (91%)	57 (9%)	0	100	100
2	C	575/607 (95%)	545 (95%)	30 (5%)	0	100	100
All	All	1241/1288 (96%)	1154 (93%)	87 (7%)	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	D	572/584 (98%)	571 (100%)	1 (0%)	92	96
2	C	486/508 (96%)	484 (100%)	2 (0%)	89	93
All	All	1058/1092 (97%)	1055 (100%)	3 (0%)	90	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	117	LEU
2	C	432	ILE
2	C	559	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	308	GLN
1	D	326	GLN
1	D	355	HIS
1	D	384	GLN
2	C	387	GLN
2	C	481	GLN

### 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 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	C	606	-	47,47,51	0.52	0	53,55,59	0.50	0
3	POV	D	708	-	23,23,51	0.71	0	29,31,59	0.65	0
3	POV	C	604	-	48,48,51	0.51	0	54,56,59	0.47	0
3	POV	D	707	-	51,51,51	0.50	0	57,59,59	0.46	0
4	ATP	C	614	-	28,33,33	0.73	0	34,52,52	0.91	1 (2%)
3	POV	C	609	-	51,51,51	0.49	0	57,59,59	0.47	0
3	POV	D	706	-	14,14,51	1.01	1 (7%)	17,17,59	1.22	2 (11%)
3	POV	D	705	-	32,32,51	0.62	0	38,40,59	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	POV	D	712	-	14,14,51	1.00	1 (7%)	17,17,59	1.23	2 (11%)
3	POV	D	710	-	31,31,51	0.65	0	36,38,59	0.70	1 (2%)
3	POV	C	612	-	34,34,51	0.60	0	40,42,59	0.57	0
4	ATP	D	714	5	28,33,33	0.77	0	34,52,52	0.79	1 (2%)
3	POV	D	713	-	26,26,51	0.82	1 (3%)	29,31,59	0.95	2 (6%)
3	POV	C	608	-	41,41,51	0.66	1 (2%)	44,46,59	0.83	3 (6%)
3	POV	D	704	-	51,51,51	0.50	0	57,59,59	0.46	0
3	POV	D	709	-	38,38,51	0.69	1 (2%)	41,43,59	0.80	2 (4%)
3	POV	D	702	-	13,13,51	1.04	1 (7%)	16,16,59	1.22	2 (12%)
6	HT1	C	616	-	37,39,39	0.71	0	34,56,56	0.94	2 (5%)
3	POV	C	607	-	45,45,51	0.63	1 (2%)	48,50,59	0.76	2 (4%)
3	POV	D	701	-	48,48,51	0.52	0	54,56,59	0.49	0
3	POV	D	711	-	42,42,51	0.65	1 (2%)	45,47,59	0.78	2 (4%)
3	POV	C	602	-	24,24,51	0.52	0	27,29,59	0.77	1 (3%)
3	POV	C	610	-	51,51,51	0.50	0	57,59,59	0.47	0
3	POV	D	703	-	44,44,51	0.54	0	50,52,59	0.54	0
3	POV	C	601	-	18,18,51	0.55	0	21,23,59	0.74	1 (4%)
3	POV	C	605	-	45,45,51	0.52	0	51,53,59	0.50	0
3	POV	C	611	-	37,37,51	0.57	0	43,45,59	0.53	0
3	POV	C	613	-	16,16,51	0.29	0	16,16,59	0.41	0
3	POV	C	603	-	28,28,51	0.80	1 (3%)	31,33,59	0.94	2 (6%)
6	HT1	C	615	-	37,39,39	0.72	0	34,56,56	0.88	1 (2%)

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	C	606	-	-	16/51/51/55	-
3	POV	D	708	-	-	14/26/26/55	-
3	POV	C	604	-	-	15/52/52/55	-
3	POV	D	707	-	-	21/55/55/55	-
4	ATP	C	614	-	-	9/18/38/38	0/3/3/3
3	POV	C	609	-	-	23/55/55/55	-
3	POV	D	706	-	-	6/13/13/55	-
3	POV	D	705	-	-	16/36/36/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	D	712	-	-	5/13/13/55	-
3	POV	D	710	-	-	16/34/34/55	-
3	POV	C	612	-	-	14/38/38/55	-
4	ATP	D	714	5	-	6/18/38/38	0/3/3/3
3	POV	D	713	-	-	4/28/28/55	-
3	POV	C	608	-	-	8/43/43/55	-
3	POV	D	704	-	-	22/55/55/55	-
3	POV	D	709	-	-	12/40/40/55	-
3	POV	D	702	-	-	1/12/12/55	-
6	HT1	C	616	-	-	7/7/25/25	0/6/6/6
3	POV	C	607	-	-	17/47/47/55	-
3	POV	D	701	-	-	10/52/52/55	-
3	POV	D	711	-	-	12/44/44/55	-
3	POV	C	602	-	-	8/26/26/55	-
3	POV	C	610	-	-	21/55/55/55	-
3	POV	D	703	-	-	16/48/48/55	-
3	POV	C	601	-	-	5/19/19/55	-
3	POV	C	605	-	-	24/49/49/55	-
3	POV	C	611	-	-	13/41/41/55	-
3	POV	C	613	-	-	4/14/14/55	-
3	POV	C	603	-	-	11/30/30/55	-
6	HT1	C	615	-	-	3/7/25/25	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	712	POV	P-O12	3.05	1.66	1.54
3	D	706	POV	P-O12	3.05	1.66	1.54
3	D	709	POV	P-O12	3.05	1.66	1.54
3	D	702	POV	P-O12	3.05	1.66	1.54
3	D	711	POV	P-O12	3.04	1.66	1.54
3	C	603	POV	P-O12	3.04	1.66	1.54
3	D	713	POV	P-O12	3.03	1.66	1.54
3	C	607	POV	P-O12	3.02	1.66	1.54
3	C	608	POV	P-O12	3.02	1.66	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	608	POV	O12-P-O11	-3.57	97.37	106.67
3	D	713	POV	O12-P-O11	-3.52	97.50	106.67
3	C	603	POV	O12-P-O11	-3.51	97.52	106.67
3	D	711	POV	O12-P-O11	-3.45	97.67	106.67
3	D	712	POV	O12-P-O11	-3.43	97.73	106.67
3	C	607	POV	O12-P-O11	-3.43	97.74	106.67
3	D	702	POV	O12-P-O11	-3.40	97.80	106.67
3	D	709	POV	O12-P-O11	-3.39	97.84	106.67
3	D	706	POV	O12-P-O11	-3.39	97.84	106.67
3	D	709	POV	O13-P-O14	2.70	121.35	110.83
3	C	607	POV	O13-P-O14	2.68	121.29	110.83
3	D	706	POV	O13-P-O14	2.67	121.25	110.83
3	D	702	POV	O13-P-O14	2.63	121.10	110.83
3	C	603	POV	O13-P-O14	2.63	121.08	110.83
3	D	713	POV	O13-P-O14	2.62	121.03	110.83
3	C	608	POV	O13-P-O14	2.61	120.98	110.83
3	D	712	POV	O13-P-O14	2.59	120.93	110.83
3	D	711	POV	O13-P-O14	2.58	120.87	110.83
3	C	602	POV	O13-P-O14	2.42	120.28	110.83
3	C	601	POV	O13-P-O14	2.30	119.79	110.83
4	C	614	ATP	C5-C6-N6	2.30	123.81	120.31
6	C	616	HT1	C24-N5-C19	2.28	124.33	118.11
4	D	714	ATP	C5-C6-N6	2.28	123.78	120.31
6	C	615	HT1	C24-N5-C19	2.07	123.77	118.11
6	C	616	HT1	C20-C19-N5	-2.07	119.77	122.11
3	C	608	POV	O11-P-O14	2.03	111.93	106.44
3	D	710	POV	C2-O21-C21	2.01	122.61	117.80

There are no chirality outliers.

All (359) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	703	POV	C1-O11-P-O13
3	D	703	POV	C11-O12-P-O11
3	D	703	POV	C11-O12-P-O14
3	D	704	POV	C11-O12-P-O11
3	D	704	POV	O12-C11-C12-N
3	D	705	POV	C11-O12-P-O14
3	D	705	POV	O12-C11-C12-N
3	D	706	POV	C1-O11-P-O12
3	D	706	POV	C1-O11-P-O13
3	D	706	POV	O11-C1-C2-O21
3	D	707	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	D	707	POV	C1-O11-P-O14
3	D	707	POV	C12-C11-O12-P
3	D	708	POV	C1-O11-P-O12
3	D	708	POV	C1-O11-P-O13
3	D	708	POV	C1-O11-P-O14
3	D	708	POV	C11-O12-P-O14
3	D	708	POV	O12-C11-C12-N
3	D	709	POV	C1-O11-P-O12
3	D	709	POV	C1-O11-P-O13
3	D	709	POV	C1-O11-P-O14
3	D	710	POV	C1-O11-P-O14
3	D	710	POV	C11-O12-P-O11
3	D	710	POV	C11-O12-P-O13
3	D	710	POV	C12-C11-O12-P
3	D	710	POV	C22-C21-O21-C2
3	D	711	POV	C1-O11-P-O12
3	D	711	POV	C1-O11-P-O13
3	D	711	POV	C1-O11-P-O14
3	D	711	POV	C2-C1-O11-P
3	C	604	POV	C1-O11-P-O12
3	C	604	POV	C1-O11-P-O14
3	C	604	POV	O22-C21-O21-C2
3	C	605	POV	C1-O11-P-O13
3	C	605	POV	O12-C11-C12-N
3	C	606	POV	C1-O11-P-O12
3	C	606	POV	C1-O11-P-O13
3	C	606	POV	C11-O12-P-O11
3	C	606	POV	O12-C11-C12-N
3	C	606	POV	C22-C21-O21-C2
3	C	607	POV	C1-O11-P-O12
3	C	607	POV	C1-O11-P-O13
3	C	607	POV	C1-O11-P-O14
3	C	609	POV	C1-O11-P-O12
3	C	609	POV	C1-O11-P-O14
3	C	609	POV	O12-C11-C12-N
3	C	609	POV	C22-C21-O21-C2
3	C	609	POV	O32-C31-O31-C3
3	C	610	POV	C11-O12-P-O11
3	C	610	POV	C2-C1-O11-P
3	C	610	POV	C22-C21-O21-C2
3	C	611	POV	C1-O11-P-O14
3	C	611	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
3	C	611	POV	C11-O12-P-O14
3	C	612	POV	C11-O12-P-O14
3	C	612	POV	O12-C11-C12-N
4	D	714	ATP	C4'-C5'-O5'-PA
4	C	614	ATP	C5'-O5'-PA-O2A
4	C	614	ATP	O4'-C4'-C5'-O5'
3	C	602	POV	O32-C31-O31-C3
3	D	710	POV	O22-C21-O21-C2
3	C	606	POV	O22-C21-O21-C2
3	C	602	POV	C32-C31-O31-C3
3	C	605	POV	C32-C31-O31-C3
3	C	609	POV	C32-C31-O31-C3
3	C	604	POV	C22-C21-O21-C2
3	C	609	POV	O22-C21-O21-C2
3	C	610	POV	O22-C21-O21-C2
3	C	601	POV	O32-C31-O31-C3
3	C	605	POV	O32-C31-O31-C3
3	D	705	POV	C22-C21-O21-C2
3	C	601	POV	C32-C31-O31-C3
4	C	614	ATP	C3'-C4'-C5'-O5'
3	D	703	POV	C2-C1-O11-P
3	D	705	POV	O22-C21-O21-C2
3	C	607	POV	C32-C31-O31-C3
3	C	607	POV	O32-C31-O31-C3
3	D	701	POV	C32-C31-O31-C3
6	C	616	HT1	C2-C1-O1-C26
3	D	704	POV	C311-C310-C39-C38
6	C	616	HT1	C6-C1-O1-C26
3	D	707	POV	C21-C22-C23-C24
3	C	605	POV	C21-C22-C23-C24
3	D	704	POV	C21-C22-C23-C24
3	D	705	POV	C21-C22-C23-C24
3	C	609	POV	C31-C32-C33-C34
6	C	616	HT1	C27-C26-O1-C1
3	D	708	POV	C22-C21-O21-C2
3	C	601	POV	C22-C21-O21-C2
3	D	708	POV	O22-C21-O21-C2
6	C	615	HT1	C2-C1-O1-C26
3	D	709	POV	C32-C31-O31-C3
3	D	709	POV	C22-C21-O21-C2
3	D	709	POV	O22-C21-O21-C2
3	C	601	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	D	702	POV	C1-C2-C3-O31
3	C	612	POV	C32-C31-O31-C3
6	C	615	HT1	C6-C1-O1-C26
3	D	710	POV	C2-C1-O11-P
3	D	701	POV	O32-C31-O31-C3
3	D	701	POV	C33-C34-C35-C36
3	C	606	POV	C21-C22-C23-C24
3	C	607	POV	C37-C38-C39-C310
3	C	609	POV	C311-C312-C313-C314
3	C	610	POV	C39-C310-C311-C312
3	C	607	POV	C35-C36-C37-C38
3	C	609	POV	C33-C34-C35-C36
3	C	609	POV	C2-C3-O31-C31
3	D	711	POV	C36-C37-C38-C39
3	C	612	POV	C32-C33-C34-C35
3	C	603	POV	C22-C21-O21-C2
3	C	605	POV	C33-C34-C35-C36
4	D	714	ATP	C3'-C4'-C5'-O5'
3	D	707	POV	C32-C33-C34-C35
3	D	705	POV	C32-C31-O31-C3
3	D	706	POV	C22-C21-O21-C2
3	C	608	POV	C24-C25-C26-C27
3	C	609	POV	C25-C26-C27-C28
3	D	707	POV	C23-C24-C25-C26
3	D	711	POV	C212-C213-C214-C215
3	C	606	POV	C24-C25-C26-C27
3	C	608	POV	C35-C36-C37-C38
3	C	610	POV	C36-C37-C38-C39
3	D	709	POV	O32-C31-O31-C3
3	C	612	POV	O32-C31-O31-C3
3	C	611	POV	C31-C32-C33-C34
3	C	612	POV	C33-C34-C35-C36
3	D	712	POV	C1-C2-O21-C21
3	D	701	POV	C26-C27-C28-C29
3	C	611	POV	C21-C22-C23-C24
3	D	711	POV	C31-C32-C33-C34
3	C	603	POV	C34-C35-C36-C37
3	C	607	POV	C25-C26-C27-C28
3	C	610	POV	C212-C213-C214-C215
3	D	703	POV	C310-C311-C312-C313
3	C	608	POV	C212-C213-C214-C215
3	D	707	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
3	C	605	POV	C22-C21-O21-C2
3	C	611	POV	C22-C21-O21-C2
3	C	603	POV	O22-C21-O21-C2
3	D	705	POV	O32-C31-O31-C3
3	D	706	POV	O22-C21-O21-C2
3	C	602	POV	C32-C33-C34-C35
3	C	611	POV	C34-C35-C36-C37
3	D	704	POV	C22-C21-O21-C2
3	C	606	POV	C37-C38-C39-C310
3	C	605	POV	C26-C27-C28-C29
3	C	608	POV	O21-C2-C3-O31
3	C	612	POV	O21-C2-C3-O31
3	D	704	POV	C25-C26-C27-C28
3	D	704	POV	C33-C34-C35-C36
3	C	605	POV	C2-C3-O31-C31
3	C	607	POV	C2-C1-O11-P
3	D	704	POV	C23-C24-C25-C26
3	D	703	POV	C34-C35-C36-C37
3	D	704	POV	C211-C212-C213-C214
3	C	609	POV	C37-C38-C39-C310
3	D	711	POV	C210-C211-C212-C213
3	D	708	POV	O11-C1-C2-C3
3	C	610	POV	O11-C1-C2-C3
3	C	605	POV	O22-C21-O21-C2
3	D	711	POV	C33-C34-C35-C36
3	C	613	POV	C211-C212-C213-C214
3	D	705	POV	C31-C32-C33-C34
3	C	610	POV	C32-C31-O31-C3
3	C	603	POV	C1-C2-C3-O31
3	C	608	POV	C32-C31-O31-C3
3	D	701	POV	C22-C21-O21-C2
3	D	707	POV	C311-C312-C313-C314
3	D	705	POV	C24-C25-C26-C27
3	C	604	POV	C25-C26-C27-C28
3	D	710	POV	O11-C1-C2-O21
3	C	603	POV	C32-C31-O31-C3
3	D	701	POV	O21-C2-C3-O31
3	C	601	POV	C22-C23-C24-C25
3	C	611	POV	C311-C310-C39-C38
3	C	607	POV	C34-C35-C36-C37
6	C	616	HT1	C20-C19-N5-C21
3	C	611	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	D	703	POV	C37-C38-C39-C310
3	C	606	POV	C32-C31-O31-C3
3	D	709	POV	O11-C1-C2-C3
3	C	603	POV	O11-C1-C2-C3
3	C	605	POV	O11-C1-C2-C3
3	D	701	POV	C35-C36-C37-C38
3	C	610	POV	C32-C33-C34-C35
3	C	610	POV	O32-C31-O31-C3
3	D	709	POV	C215-C216-C217-C218
3	D	701	POV	C214-C215-C216-C217
3	C	608	POV	O32-C31-O31-C3
3	C	604	POV	C1-C2-C3-O31
3	C	606	POV	C1-C2-C3-O31
3	C	608	POV	C1-C2-C3-O31
3	C	612	POV	C1-C2-C3-O31
3	D	707	POV	C24-C25-C26-C27
3	C	605	POV	C212-C213-C214-C215
3	C	612	POV	C31-C32-C33-C34
3	D	710	POV	C25-C26-C27-C28
3	D	704	POV	O22-C21-O21-C2
3	D	704	POV	C31-C32-C33-C34
3	C	603	POV	O11-C1-C2-O21
3	D	707	POV	C35-C36-C37-C38
3	D	707	POV	C22-C21-O21-C2
3	D	705	POV	C2-C1-O11-P
6	C	615	HT1	C27-C26-O1-C1
3	C	606	POV	O21-C2-C3-O31
3	D	711	POV	C25-C26-C27-C28
4	D	714	ATP	O4'-C4'-C5'-O5'
3	D	704	POV	C213-C214-C215-C216
3	C	605	POV	C31-C32-C33-C34
4	D	714	ATP	PB-O3A-PA-O5'
3	D	707	POV	C213-C214-C215-C216
3	C	609	POV	C212-C213-C214-C215
3	D	711	POV	O31-C31-C32-C33
3	C	610	POV	C33-C34-C35-C36
3	C	609	POV	C35-C36-C37-C38
3	C	609	POV	C211-C212-C213-C214
3	C	603	POV	O32-C31-O31-C3
3	C	603	POV	C32-C33-C34-C35
3	D	701	POV	O22-C21-O21-C2
3	C	603	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	D	708	POV	C3-C2-O21-C21
3	D	710	POV	C1-C2-O21-C21
3	C	606	POV	C1-C2-O21-C21
3	D	710	POV	C210-C211-C212-C213
3	C	604	POV	C22-C23-C24-C25
3	C	606	POV	O32-C31-O31-C3
3	D	701	POV	C1-C2-C3-O31
3	C	612	POV	C12-C11-O12-P
3	C	603	POV	O21-C2-C3-O31
3	C	604	POV	O21-C2-C3-O31
3	D	707	POV	C211-C212-C213-C214
3	C	607	POV	C22-C23-C24-C25
3	D	703	POV	O12-C11-C12-N
3	D	710	POV	O12-C11-C12-N
3	C	611	POV	O12-C11-C12-N
3	D	707	POV	O22-C21-O21-C2
3	D	704	POV	C311-C312-C313-C314
3	D	709	POV	C33-C34-C35-C36
3	D	708	POV	O11-C1-C2-O21
3	D	709	POV	O11-C1-C2-O21
3	C	605	POV	O11-C1-C2-O21
3	C	607	POV	O21-C21-C22-C23
3	C	605	POV	C29-C210-C211-C212
3	C	610	POV	C310-C311-C312-C313
3	D	703	POV	C11-O12-P-O13
3	D	704	POV	C11-O12-P-O14
3	D	708	POV	C11-O12-P-O11
3	D	710	POV	C1-O11-P-O12
3	C	604	POV	C1-O11-P-O13
3	C	604	POV	C11-O12-P-O14
3	C	605	POV	C11-O12-P-O11
3	C	605	POV	C11-O12-P-O13
3	C	605	POV	C11-O12-P-O14
3	C	606	POV	C11-O12-P-O14
3	C	609	POV	C1-O11-P-O13
3	C	609	POV	C11-O12-P-O14
3	C	610	POV	C11-O12-P-O14
3	C	611	POV	C1-O11-P-O12
3	C	612	POV	C11-O12-P-O11
3	C	612	POV	C11-O12-P-O13
4	C	614	ATP	C5'-O5'-PA-O1A
4	C	614	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	C	610	POV	C37-C38-C39-C310
3	D	706	POV	C1-O11-P-O14
3	C	602	POV	C22-C23-C24-C25
3	C	602	POV	C3-C2-O21-C21
6	C	616	HT1	C18-C19-N5-C21
3	D	710	POV	O11-C1-C2-C3
3	C	611	POV	C35-C36-C37-C38
3	C	610	POV	O11-C1-C2-O21
3	D	707	POV	C32-C31-O31-C3
3	D	713	POV	C34-C35-C36-C37
3	D	707	POV	O32-C31-O31-C3
3	D	704	POV	C26-C27-C28-C29
3	D	707	POV	C212-C213-C214-C215
3	D	703	POV	C32-C31-O31-C3
3	C	609	POV	C39-C310-C311-C312
6	C	616	HT1	C18-C19-N5-C24
3	D	704	POV	C32-C31-O31-C3
3	D	705	POV	C26-C27-C28-C29
3	C	612	POV	O11-C1-C2-O21
3	C	608	POV	C32-C33-C34-C35
3	D	703	POV	O32-C31-O31-C3
3	D	704	POV	O32-C31-O31-C3
4	C	614	ATP	PA-O3A-PB-O3B
3	C	613	POV	C212-C213-C214-C215
3	C	607	POV	O31-C31-C32-C33
3	D	704	POV	O21-C2-C3-O31
3	D	708	POV	C21-C22-C23-C24
3	C	604	POV	C21-C22-C23-C24
3	C	609	POV	C2-C1-O11-P
6	C	616	HT1	C20-C19-N5-C24
3	C	607	POV	C310-C311-C312-C313
3	C	609	POV	C213-C214-C215-C216
3	D	704	POV	C310-C311-C312-C313
3	D	703	POV	C24-C25-C26-C27
3	C	613	POV	O22-C21-C22-C23
3	C	613	POV	O21-C21-C22-C23
4	C	614	ATP	PG-O3B-PB-O2B
3	C	602	POV	C23-C24-C25-C26
3	C	604	POV	C35-C36-C37-C38
3	D	704	POV	O11-C1-C2-O21
3	C	602	POV	O11-C1-C2-C3
3	D	709	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
3	C	605	POV	C211-C212-C213-C214
3	C	610	POV	C210-C211-C212-C213
3	D	703	POV	C27-C28-C29-C210
3	D	710	POV	C27-C28-C29-C210
3	D	703	POV	C11-C12-N-C13
3	D	703	POV	C3-C2-O21-C21
3	D	705	POV	C1-C2-O21-C21
3	C	605	POV	C1-C2-O21-C21
4	D	714	ATP	PB-O3B-PG-O2G
3	C	610	POV	C29-C210-C211-C212
3	C	609	POV	C22-C23-C24-C25
3	D	707	POV	C25-C26-C27-C28
3	C	604	POV	O11-C1-C2-O21
3	D	704	POV	C27-C28-C29-C210
3	C	605	POV	C22-C23-C24-C25
3	C	604	POV	C29-C210-C211-C212
3	D	705	POV	O31-C31-C32-C33
3	C	612	POV	O11-C1-C2-C3
3	D	711	POV	O32-C31-C32-C33
3	C	602	POV	O22-C21-O21-C2
3	C	606	POV	C23-C24-C25-C26
3	D	707	POV	C312-C313-C314-C315
4	C	614	ATP	PG-O3B-PB-O1B
4	C	614	ATP	PA-O3A-PB-O1B
3	D	708	POV	O21-C21-C22-C23
3	D	710	POV	C29-C210-C211-C212
3	C	605	POV	C32-C33-C34-C35
3	C	607	POV	C32-C33-C34-C35
3	D	704	POV	C1-C2-C3-O31
3	D	707	POV	O31-C31-C32-C33
3	D	713	POV	O31-C31-C32-C33
3	C	610	POV	O21-C21-C22-C23
3	D	705	POV	C3-C2-O21-C21
3	C	605	POV	C3-C2-O21-C21
3	C	611	POV	C25-C26-C27-C28
3	D	712	POV	O22-C21-O21-C2
3	D	712	POV	O21-C21-C22-C23
3	D	703	POV	C311-C310-C39-C38
3	C	609	POV	C312-C313-C314-C315
3	C	607	POV	C33-C34-C35-C36
3	C	607	POV	C312-C313-C314-C315
3	D	712	POV	C22-C21-O21-C2

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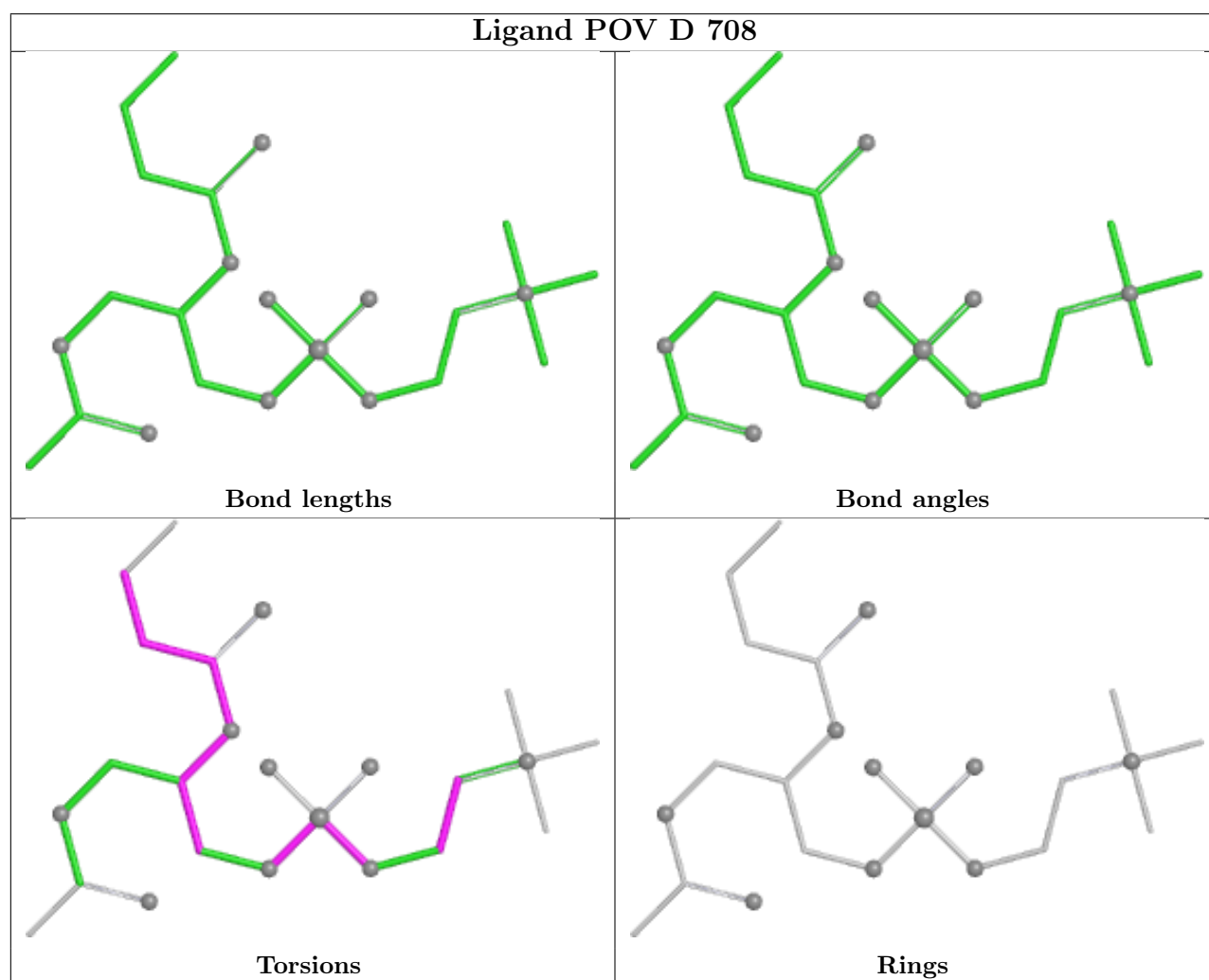
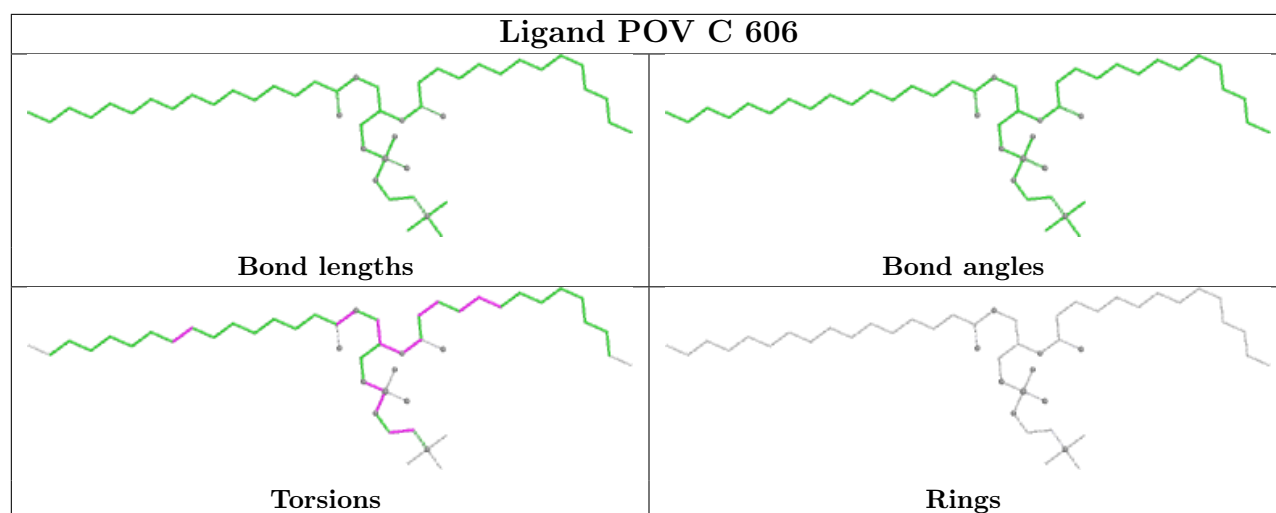
Mol	Chain	Res	Type	Atoms
3	D	707	POV	O32-C31-C32-C33
3	D	713	POV	O32-C31-C32-C33
3	C	610	POV	C22-C23-C24-C25
3	D	705	POV	O32-C31-C32-C33
3	C	610	POV	O22-C21-C22-C23
3	D	713	POV	O21-C21-C22-C23
3	C	605	POV	O21-C21-C22-C23
3	C	604	POV	O11-C1-C2-C3
3	D	708	POV	O22-C21-C22-C23
3	D	712	POV	O22-C21-C22-C23
4	D	714	ATP	PB-O3A-PA-O1A
3	D	705	POV	C25-C26-C27-C28

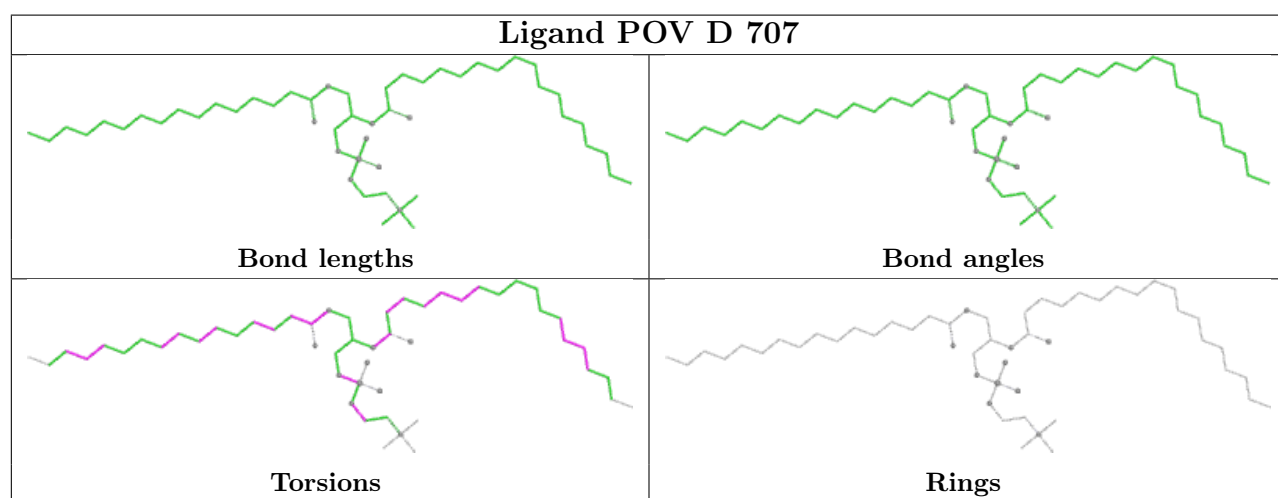
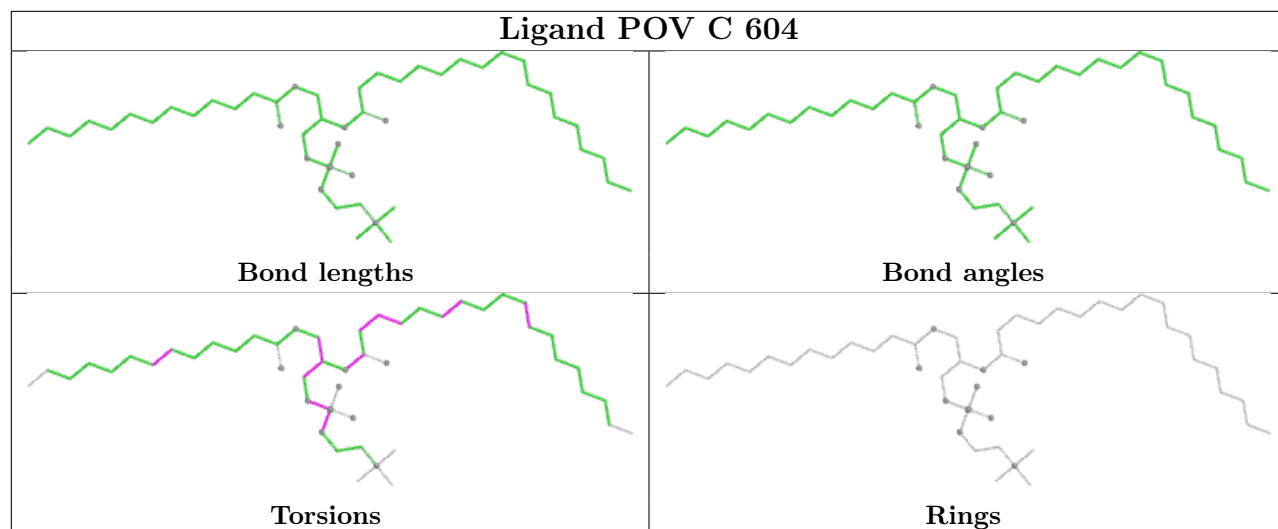
There are no ring outliers.

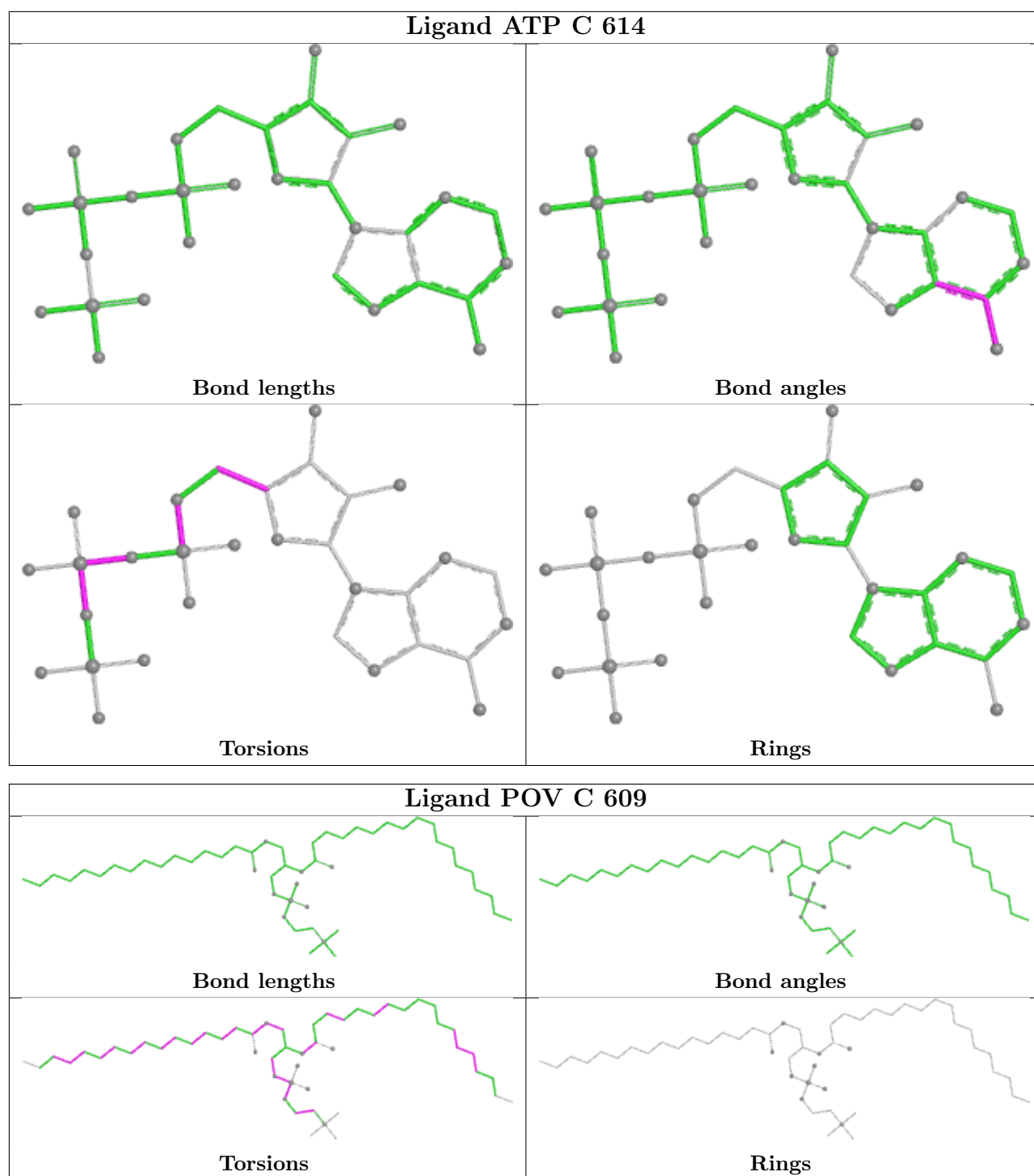
6 monomers are involved in 9 short contacts:

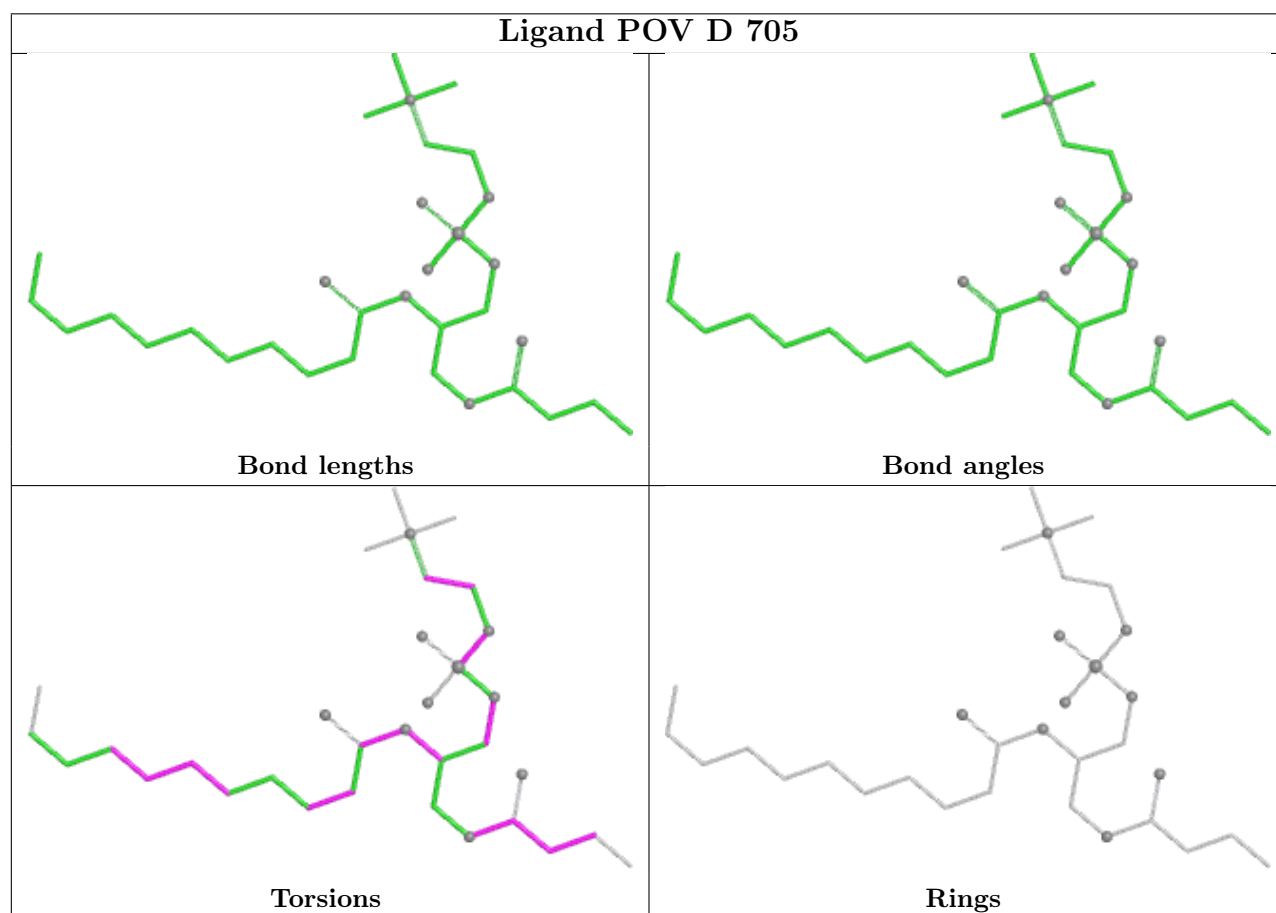
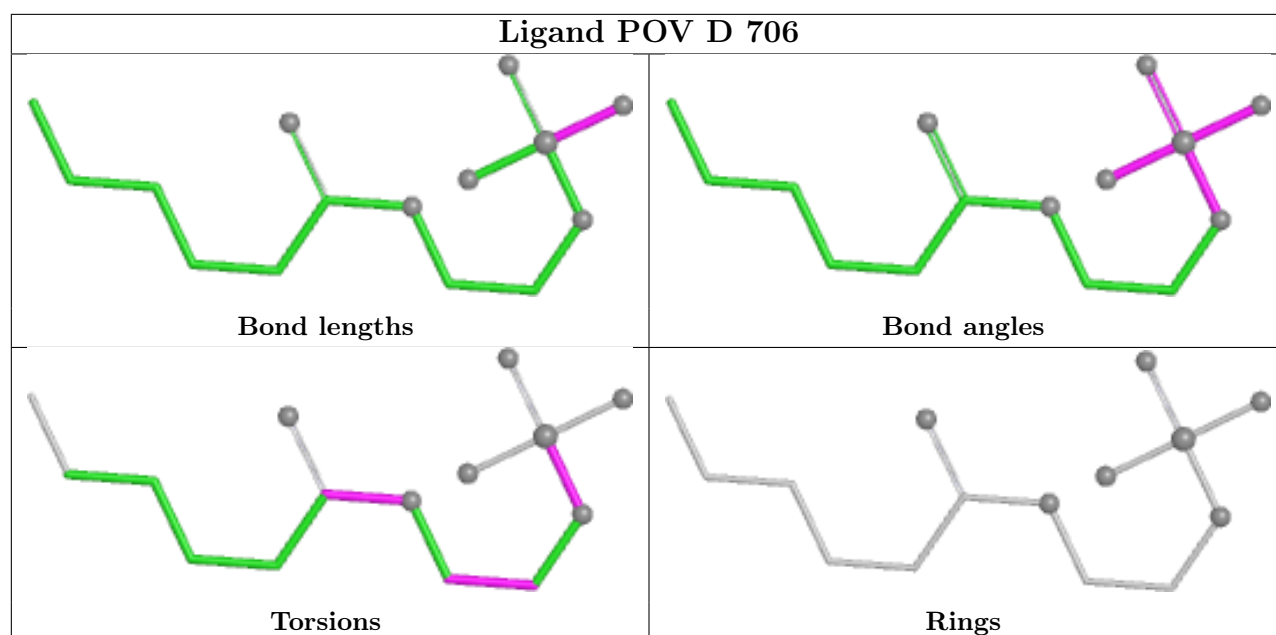
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	612	POV	1	0
3	C	608	POV	1	0
3	D	702	POV	1	0
6	C	616	HT1	3	0
3	C	605	POV	2	0
3	C	613	POV	1	0

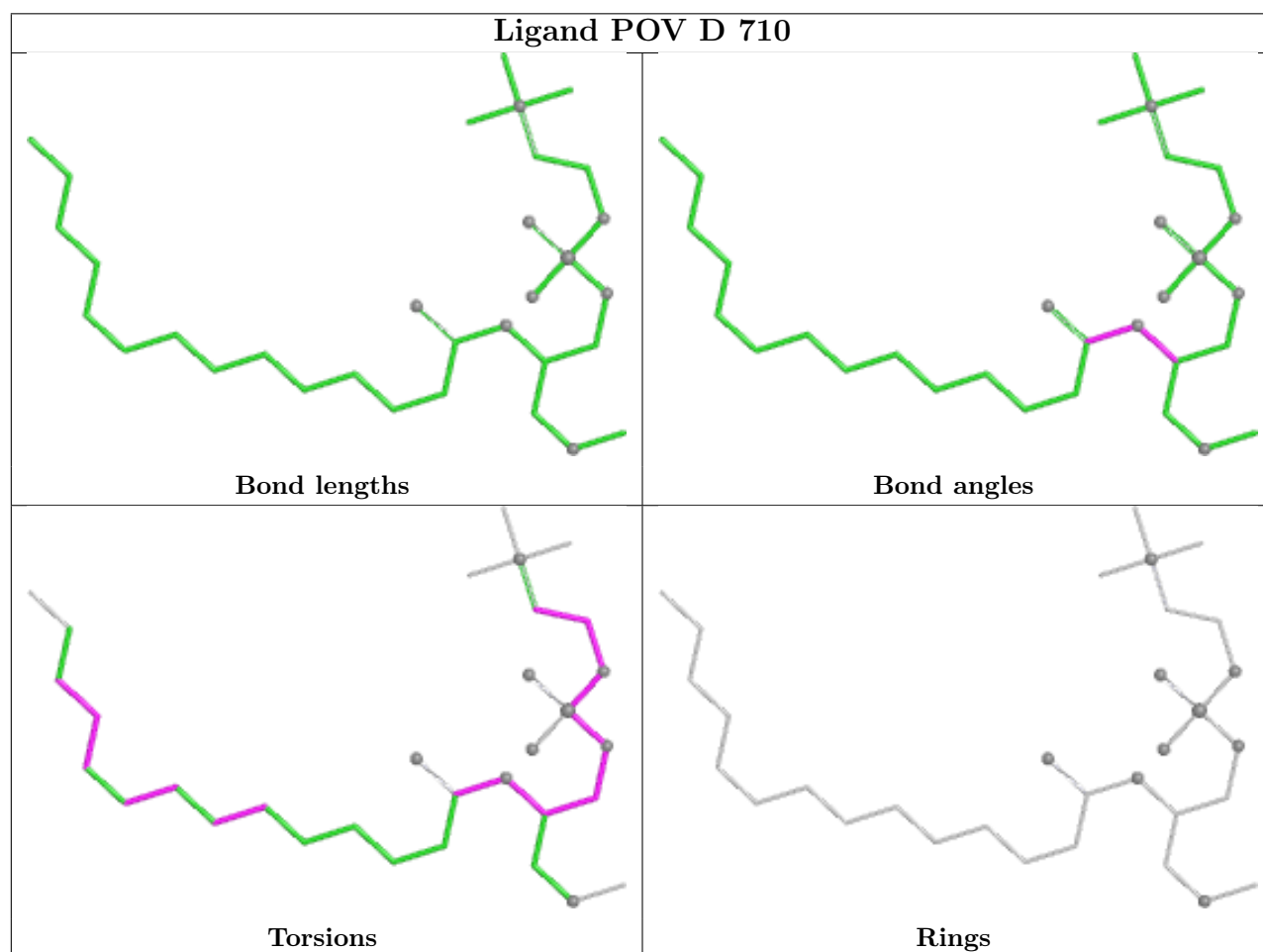
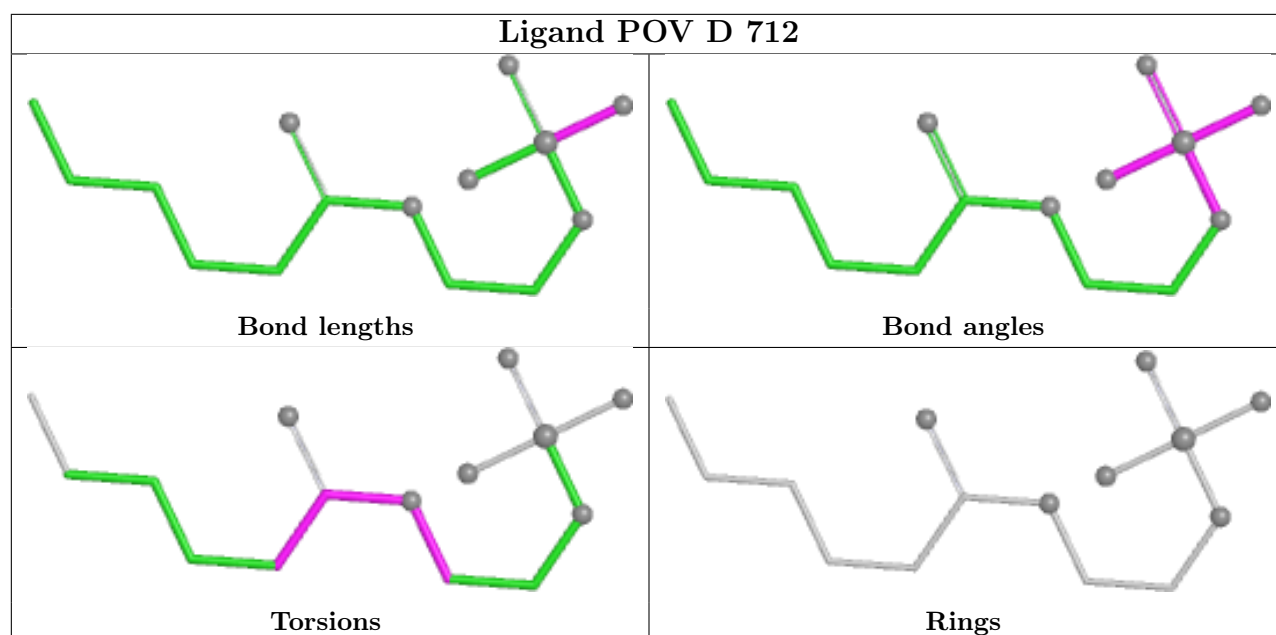
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



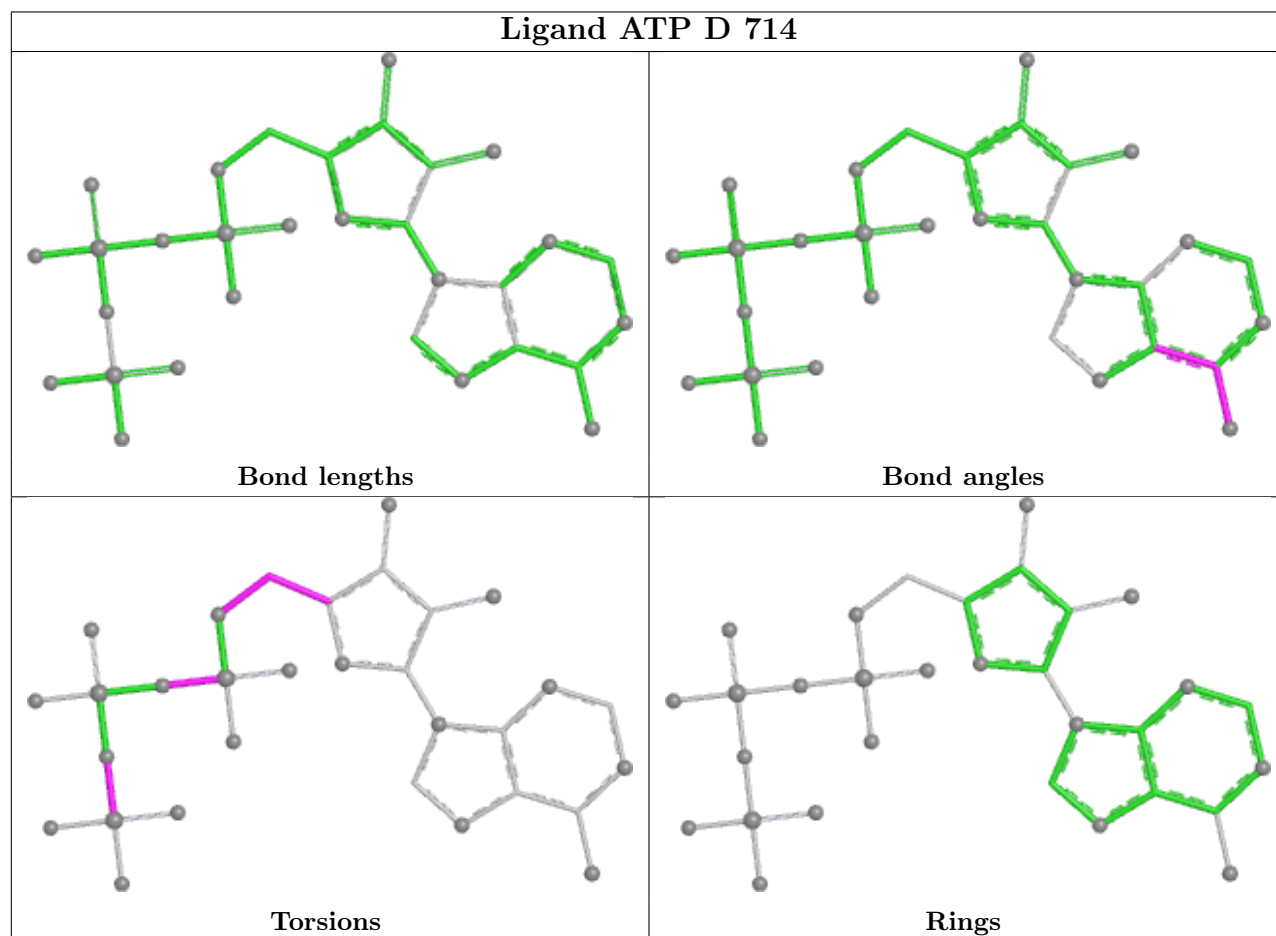
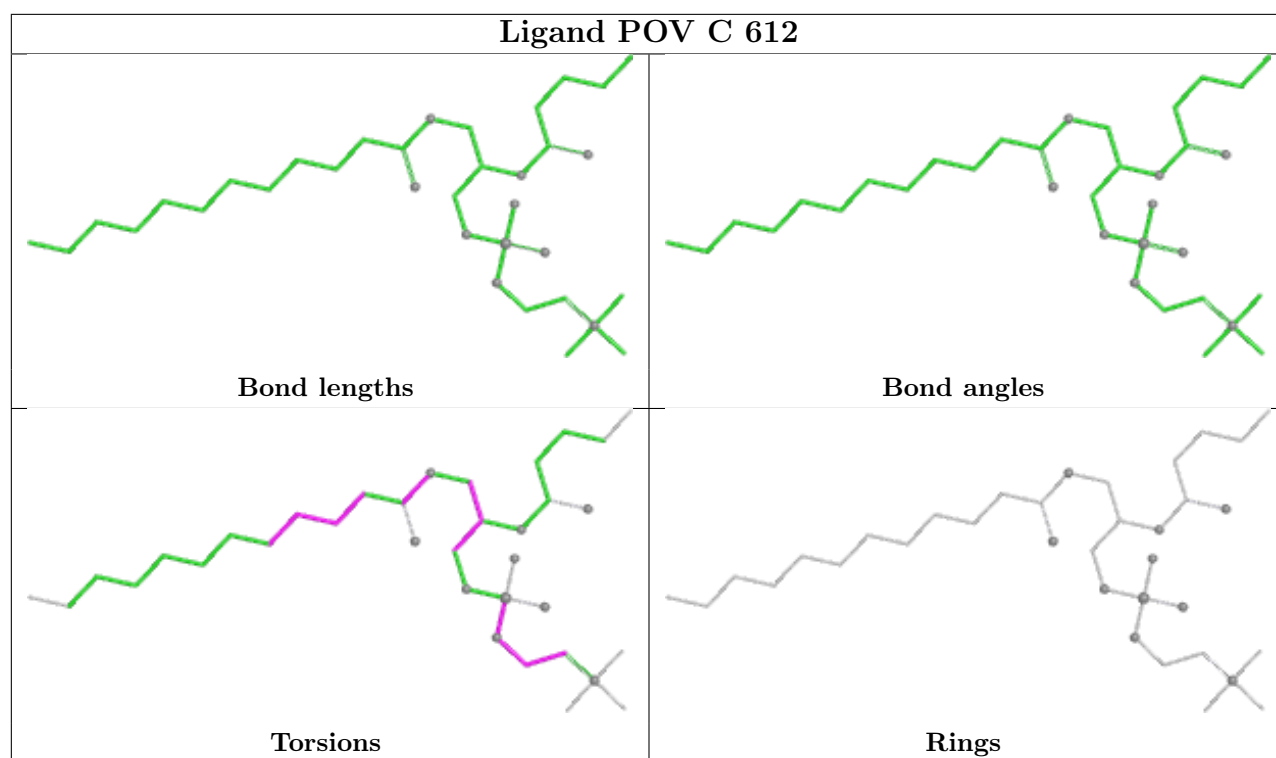


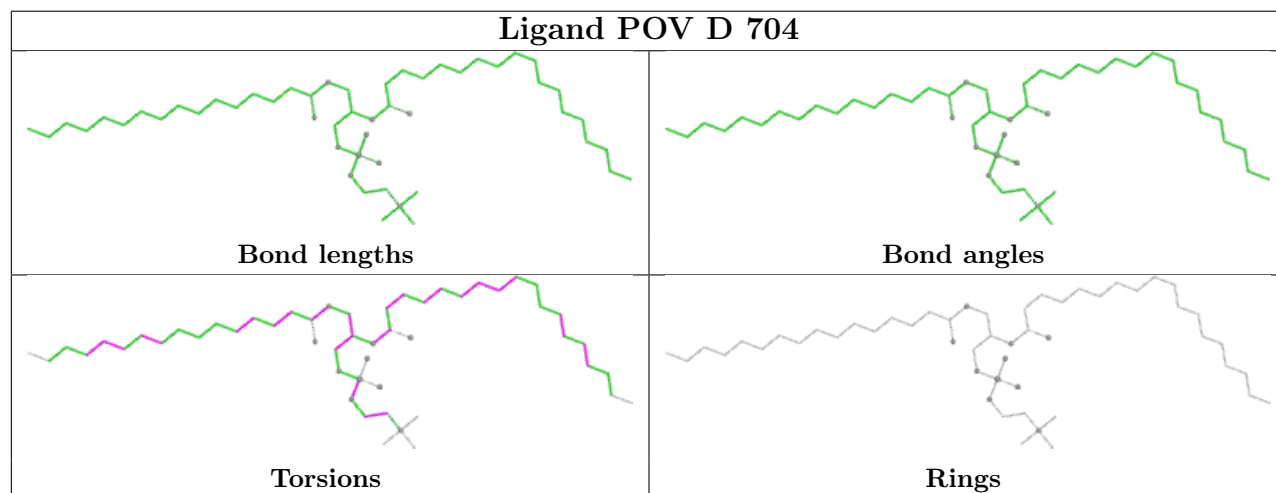
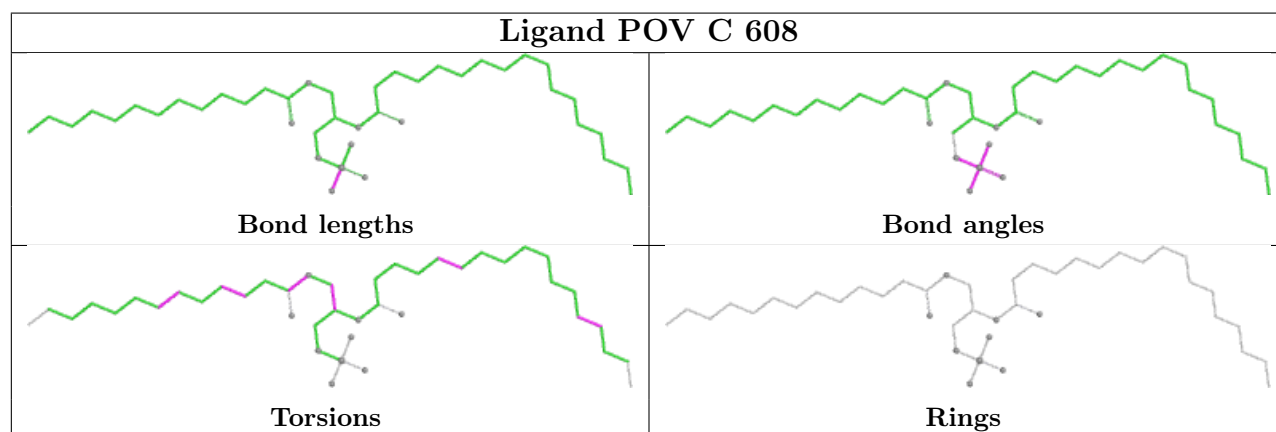
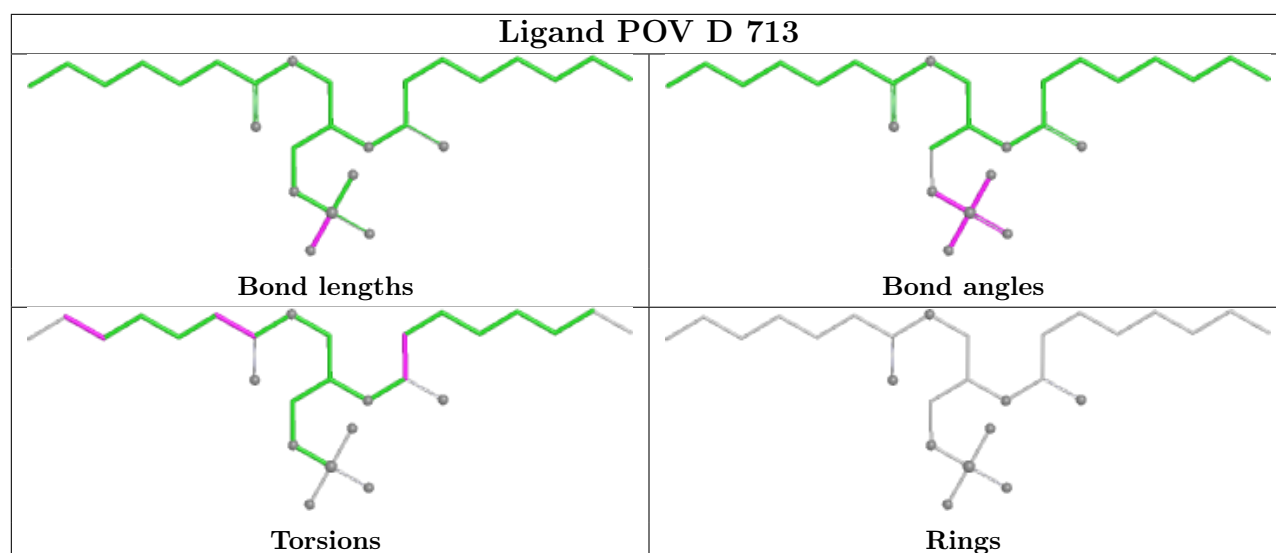


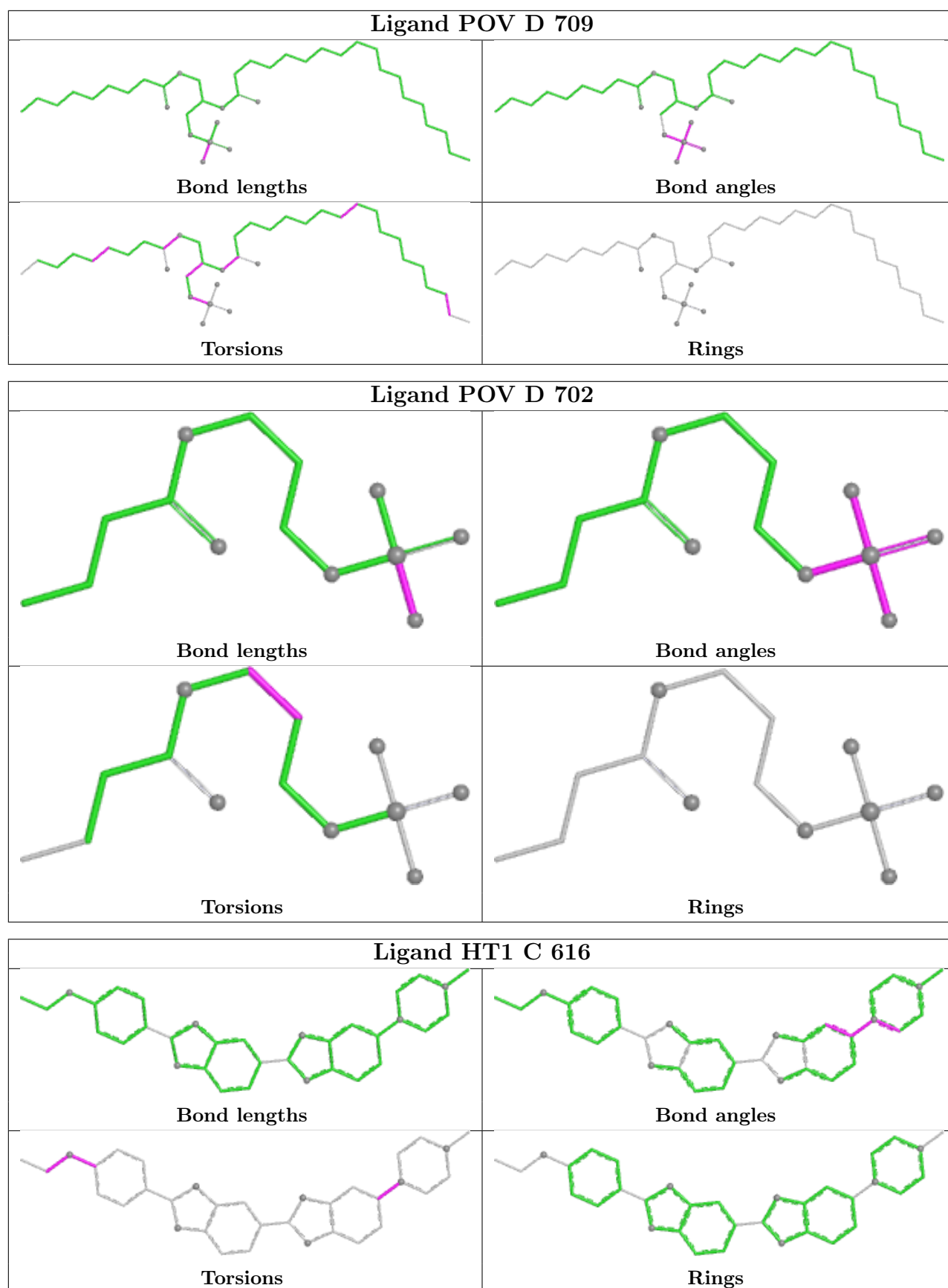


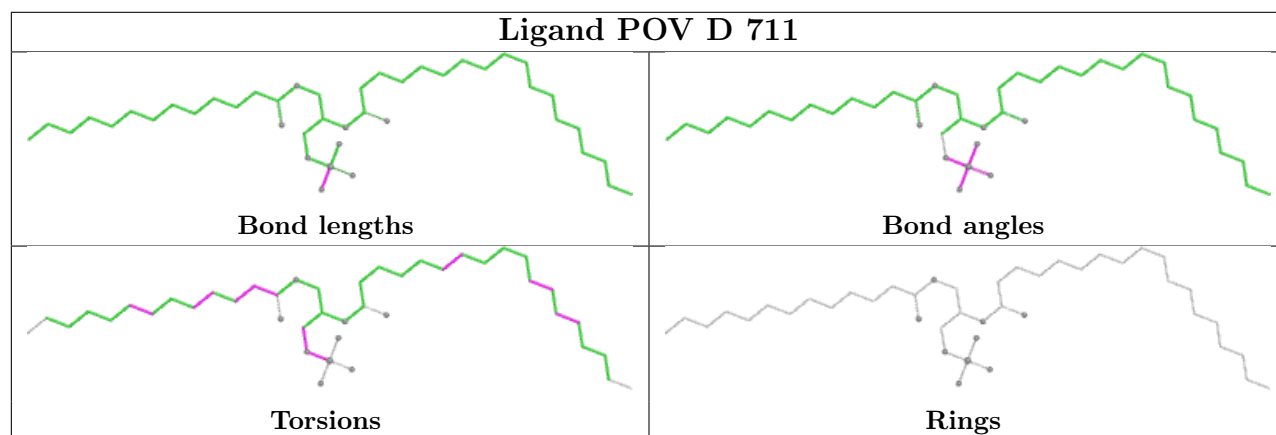
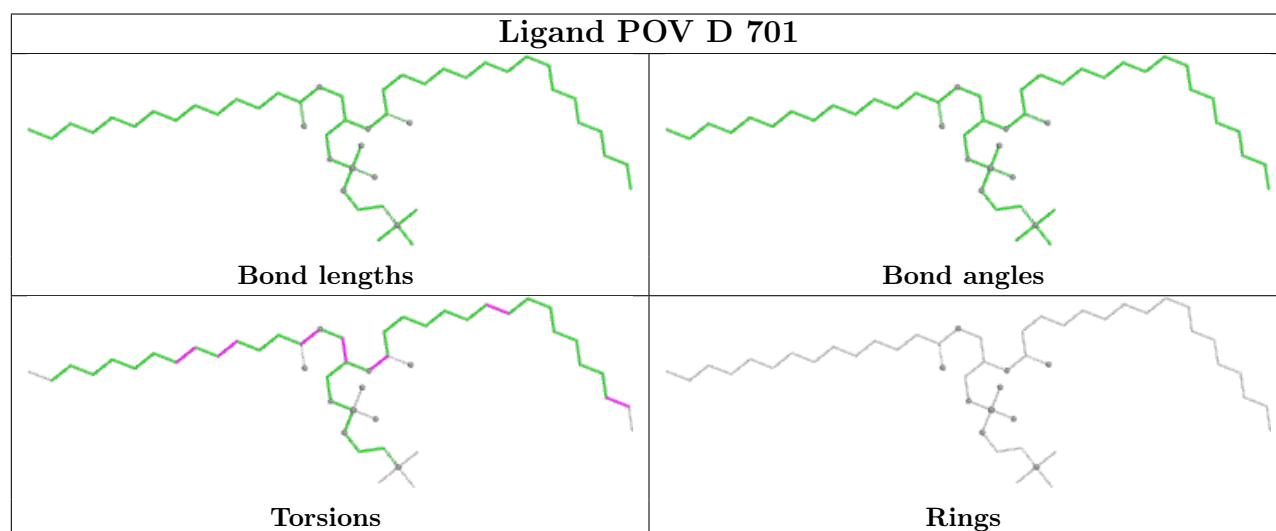
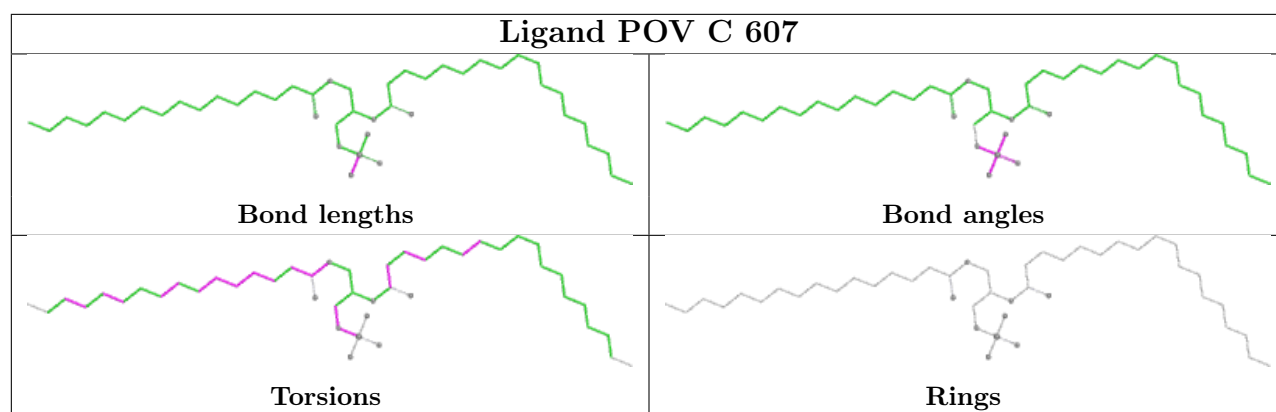


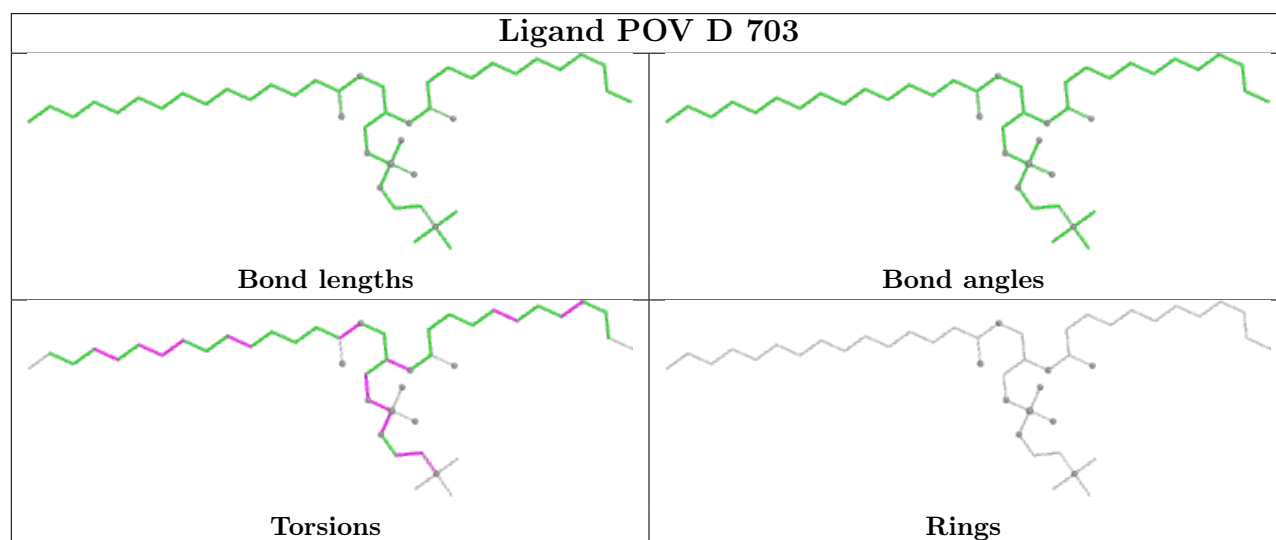
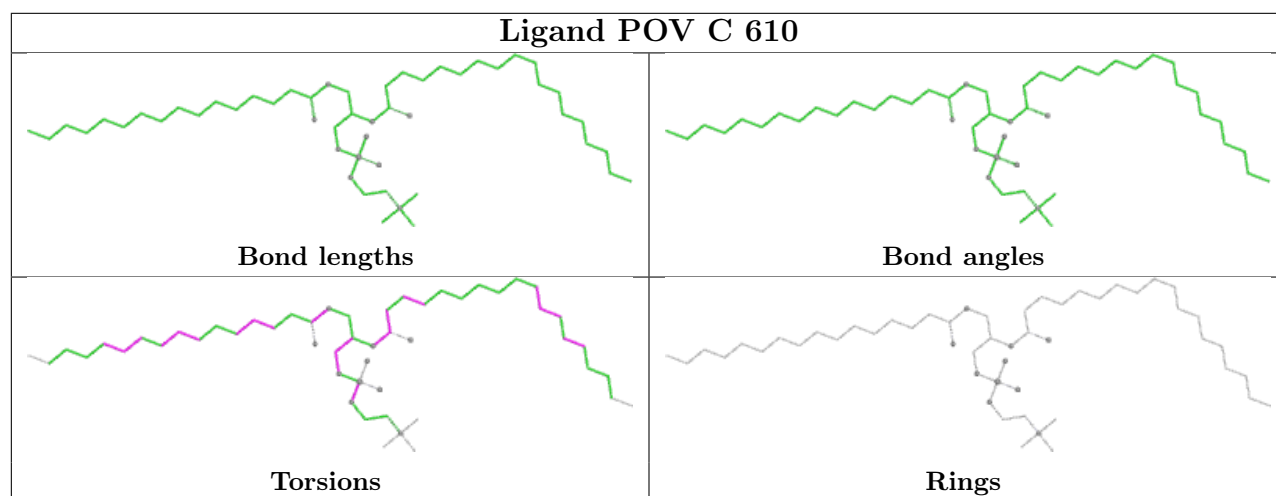
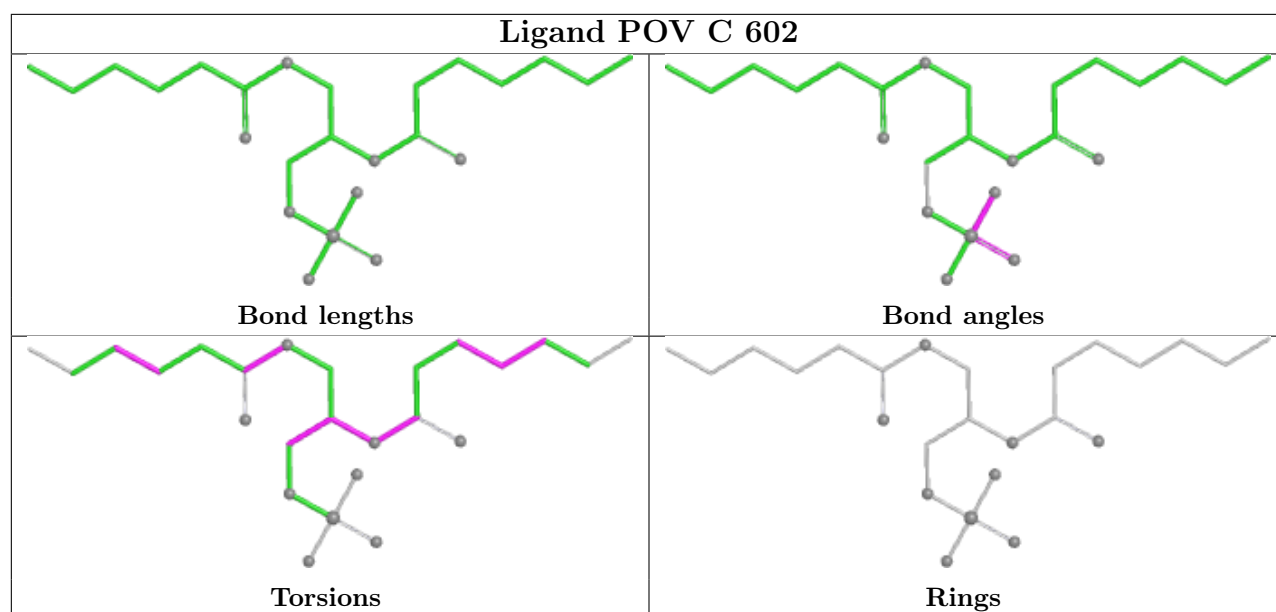


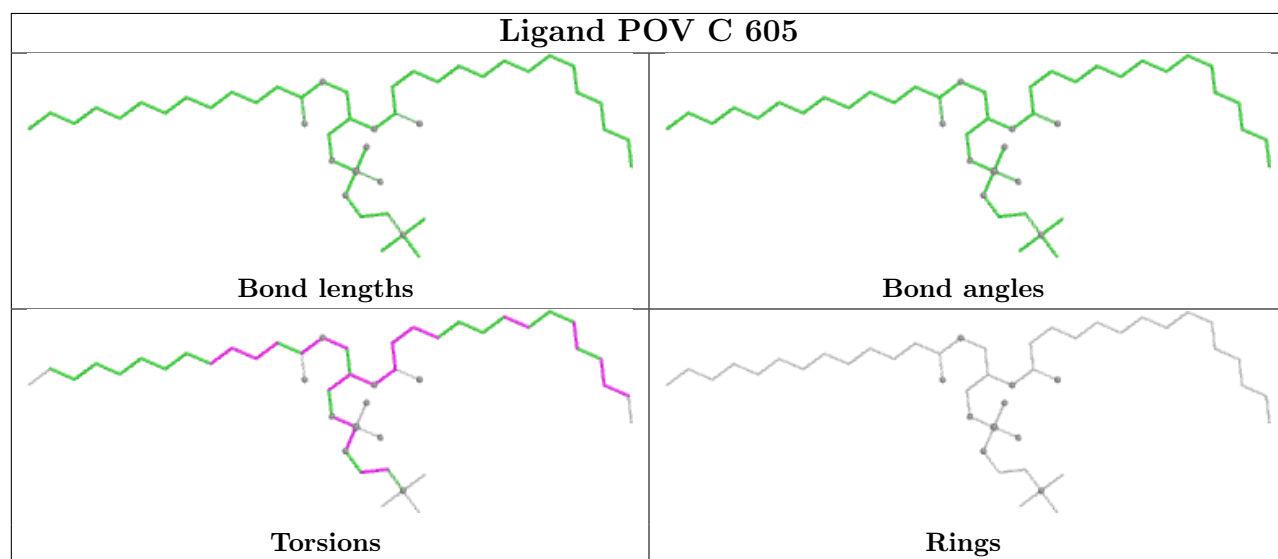
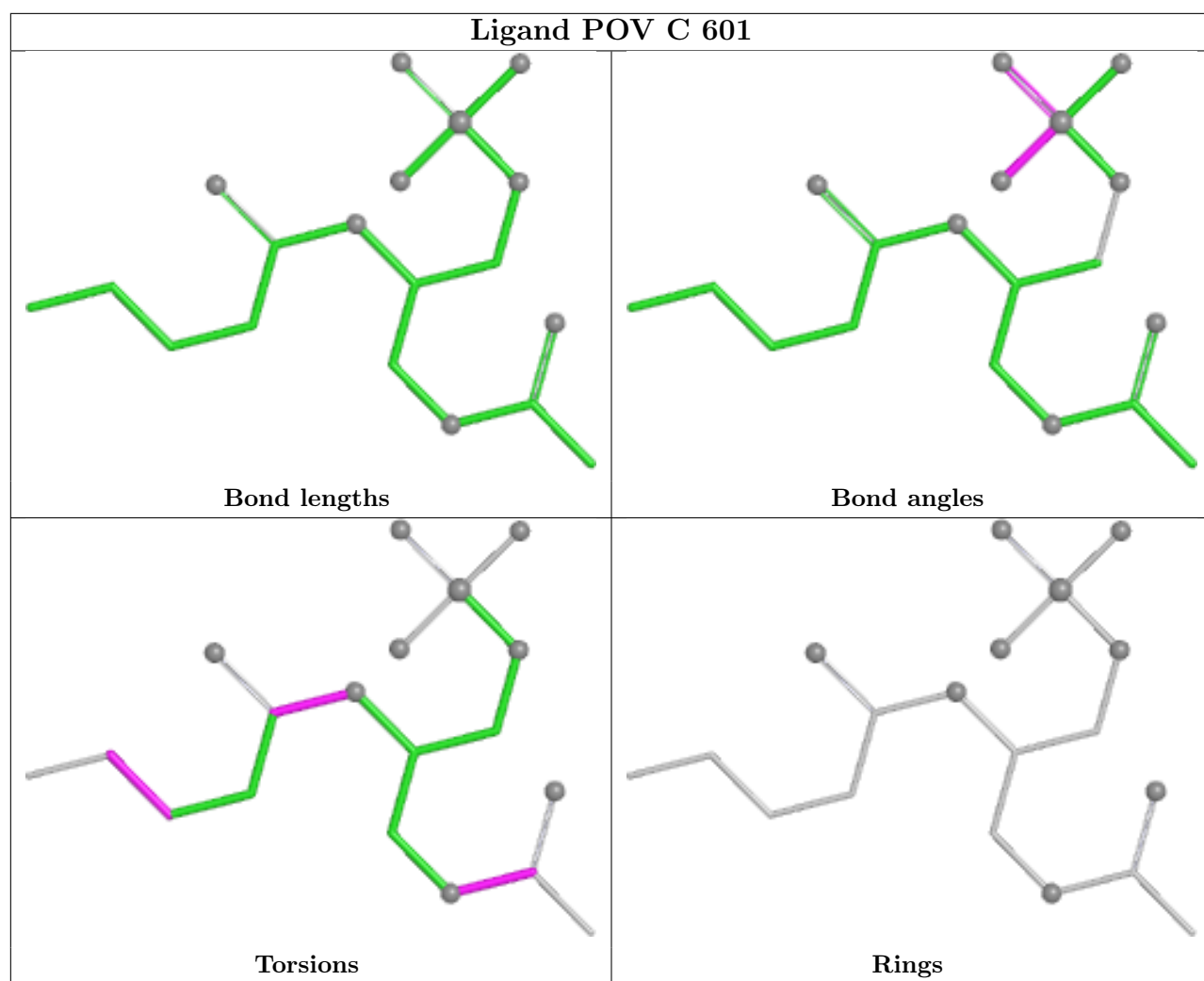


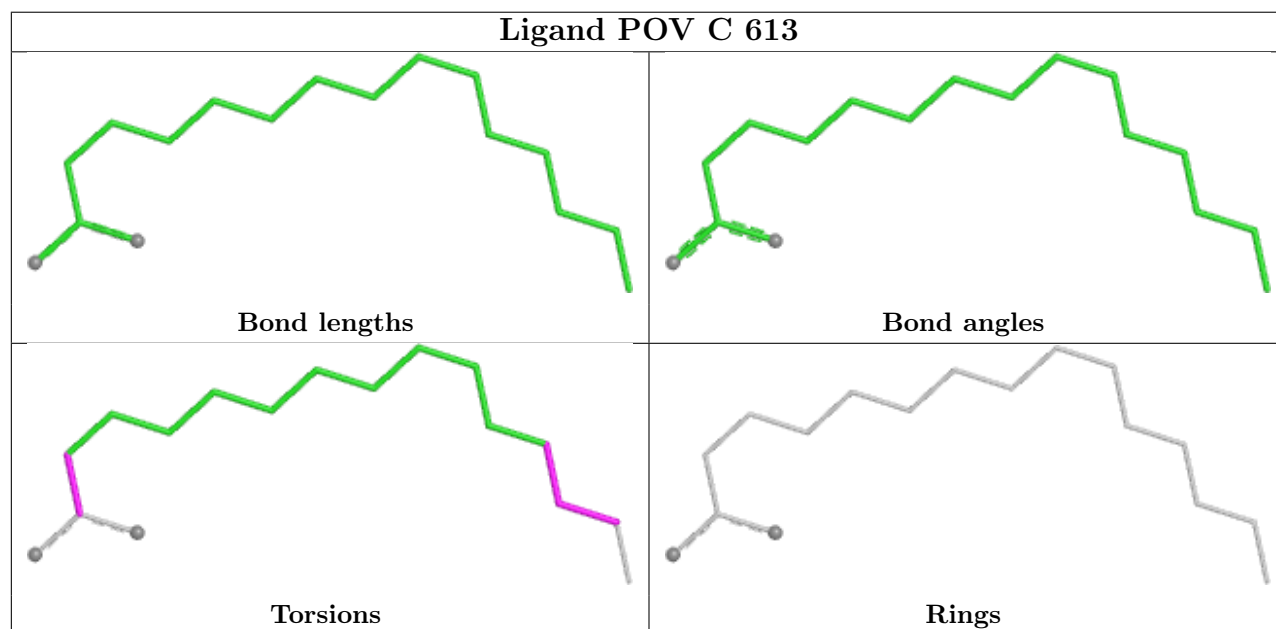
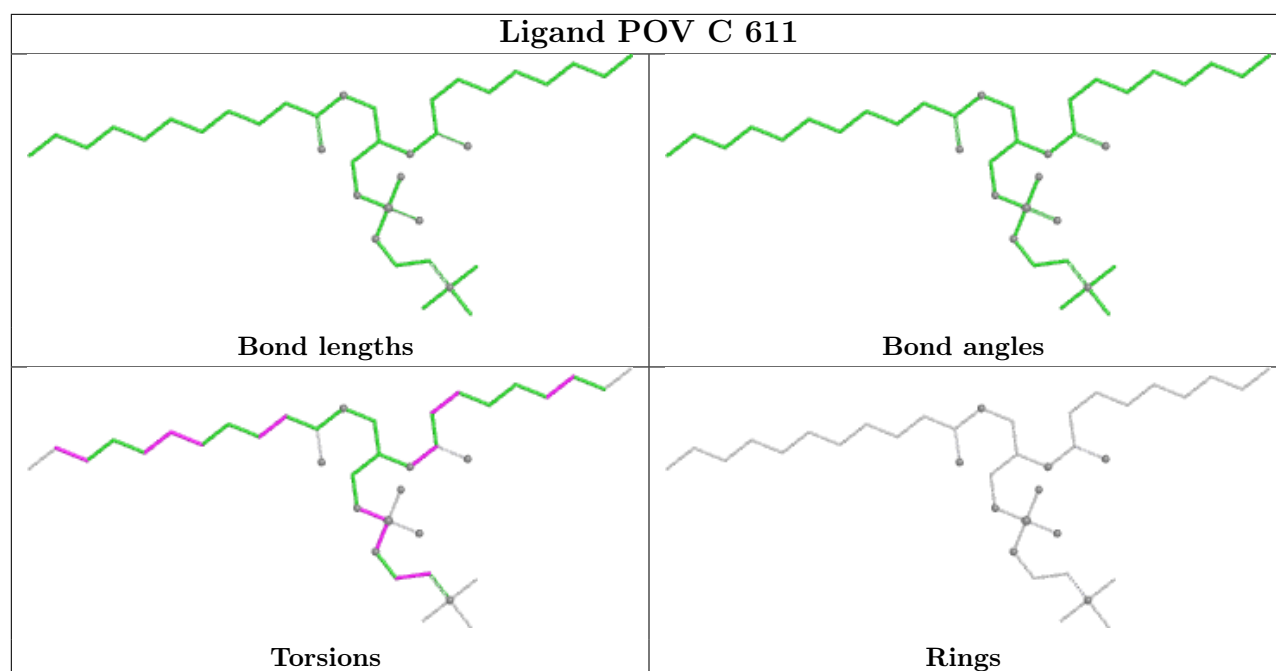


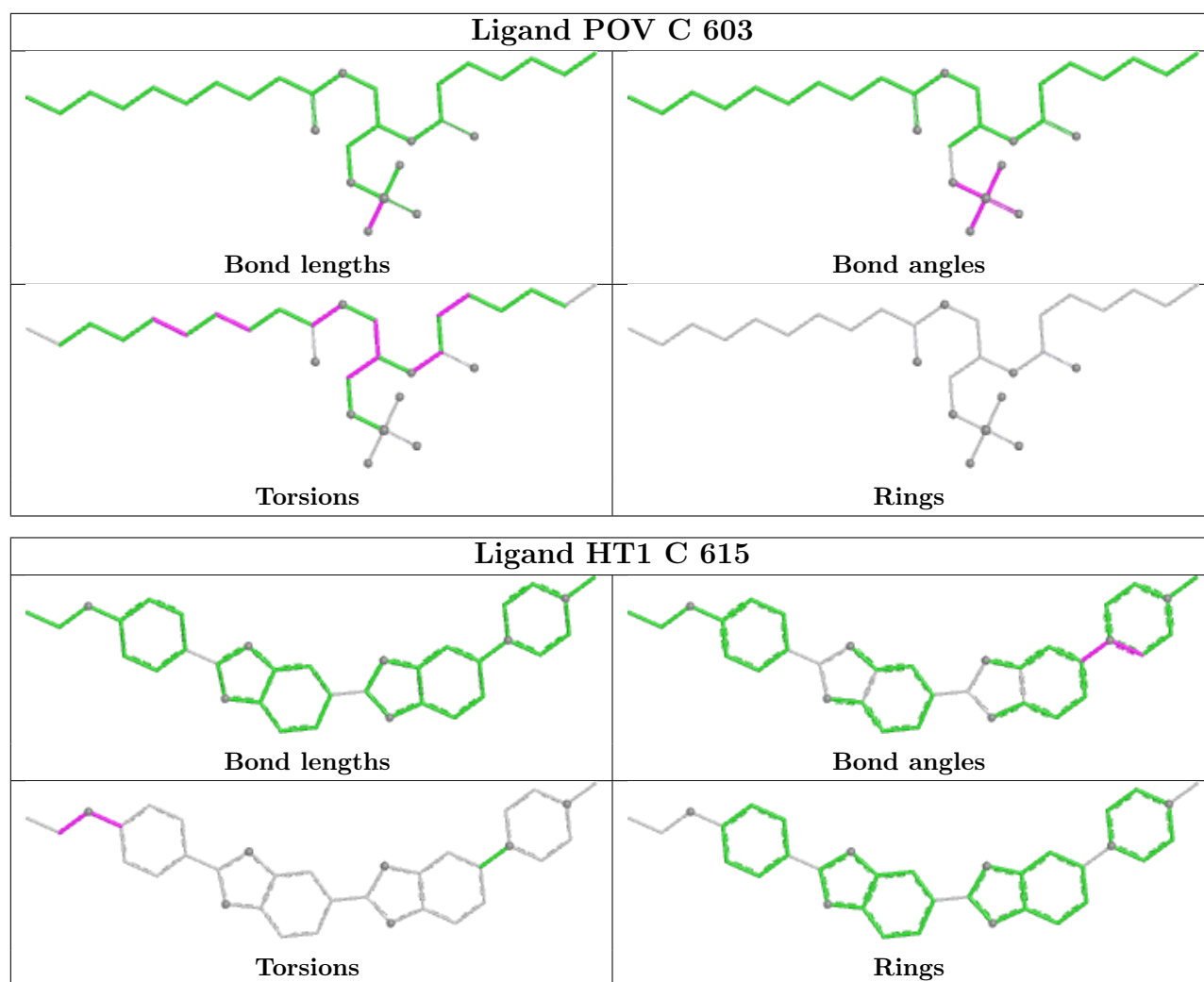












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



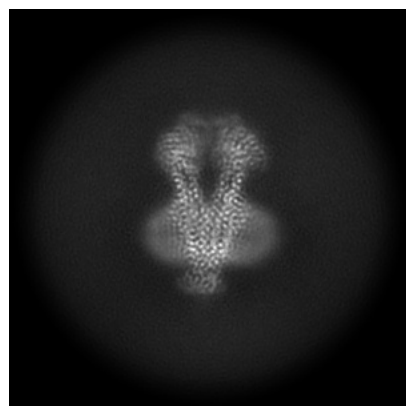
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45938. These allow visual inspection of the internal detail of the map and identification of artifacts.

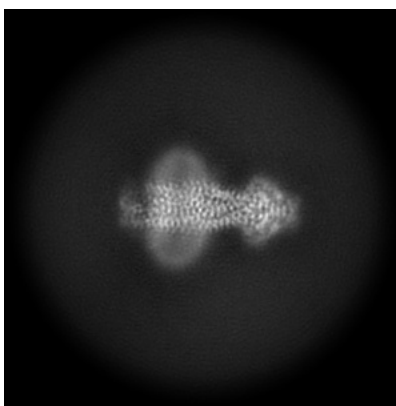
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

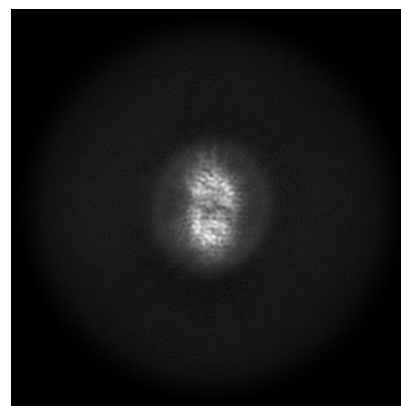
#### 6.1.1 Primary map



X

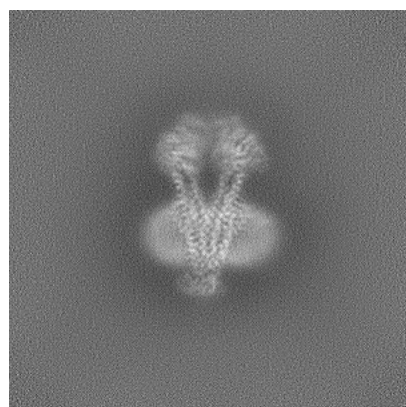


Y

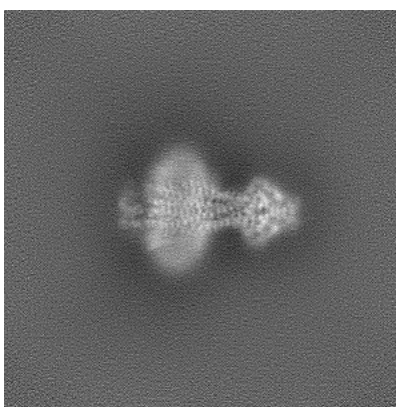


Z

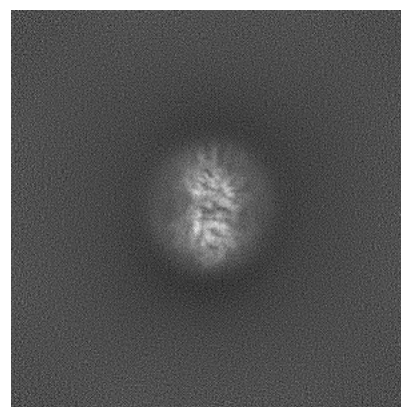
#### 6.1.2 Raw map



X



Y



Z

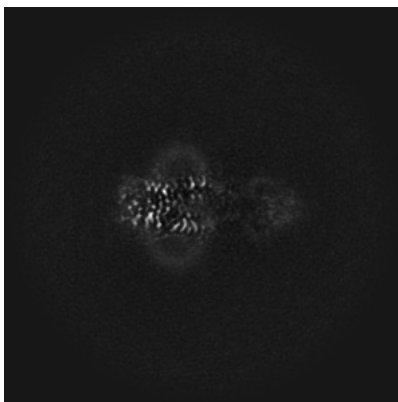
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

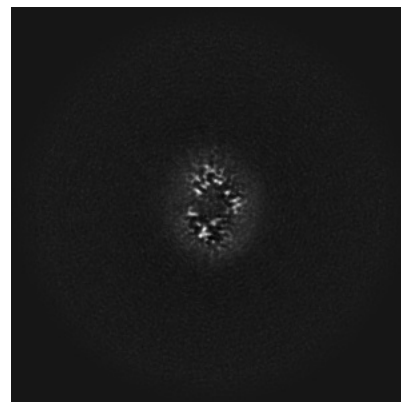
### 6.2.1 Primary map



X Index: 240

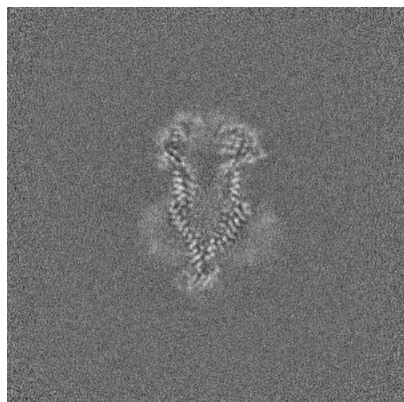


Y Index: 240

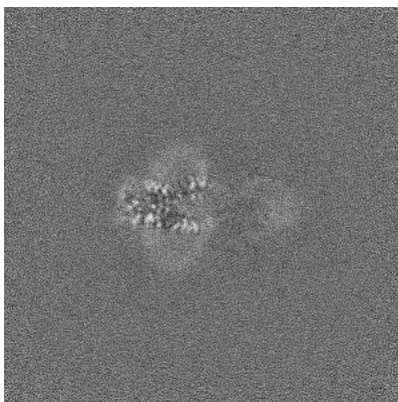


Z Index: 240

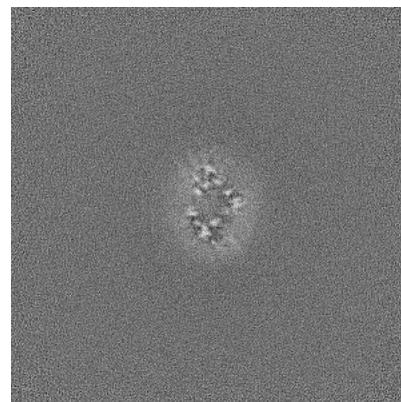
### 6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

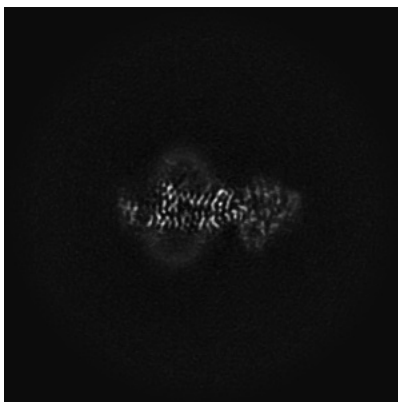
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

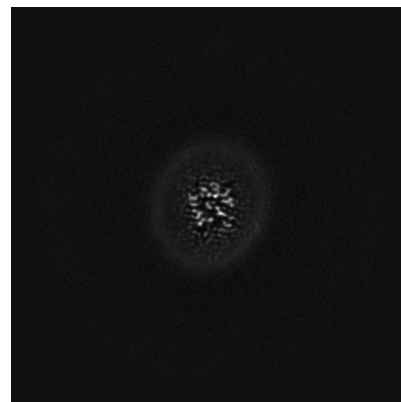
### 6.3.1 Primary map



X Index: 238

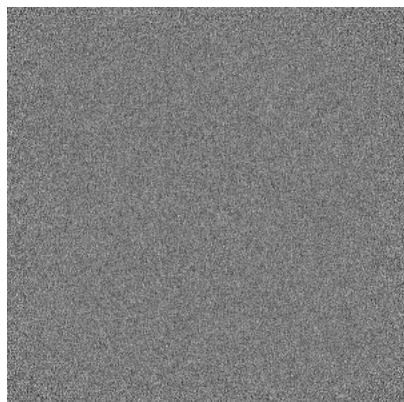


Y Index: 218

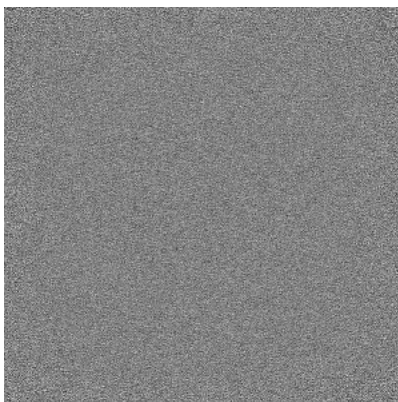


Z Index: 196

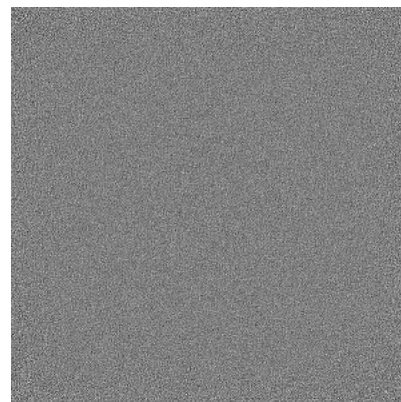
### 6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 479

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

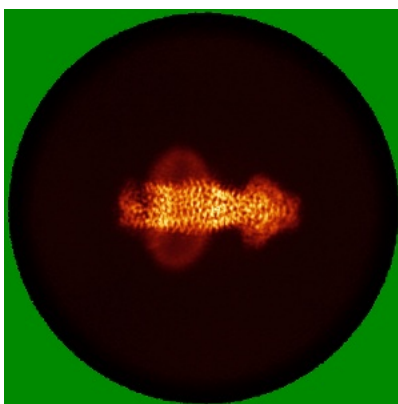


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

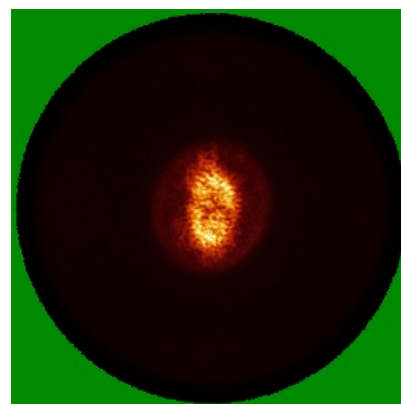
### 6.4.1 Primary map



X

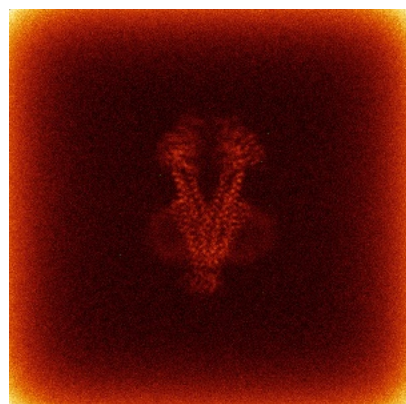


Y

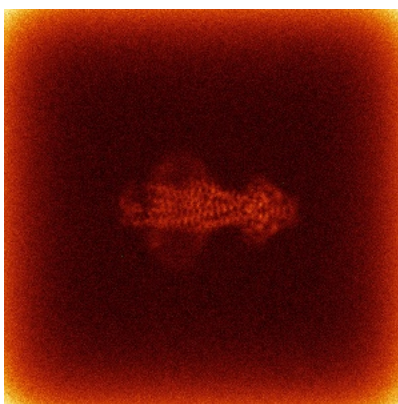


Z

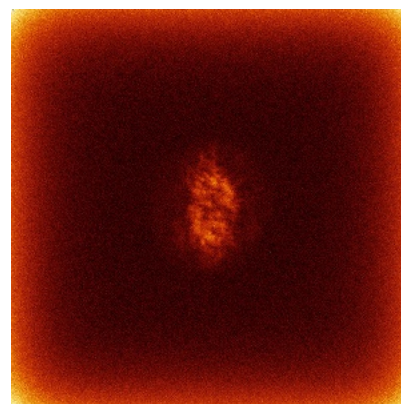
### 6.4.2 Raw map



X



Y

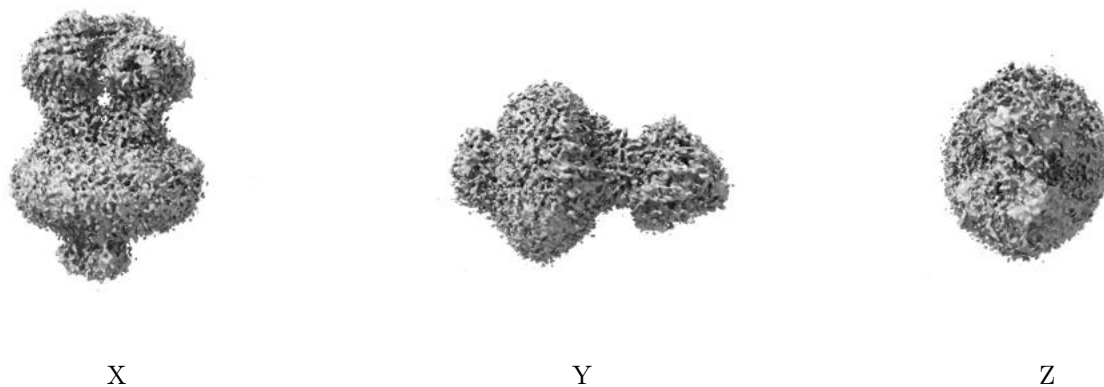


Z

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.

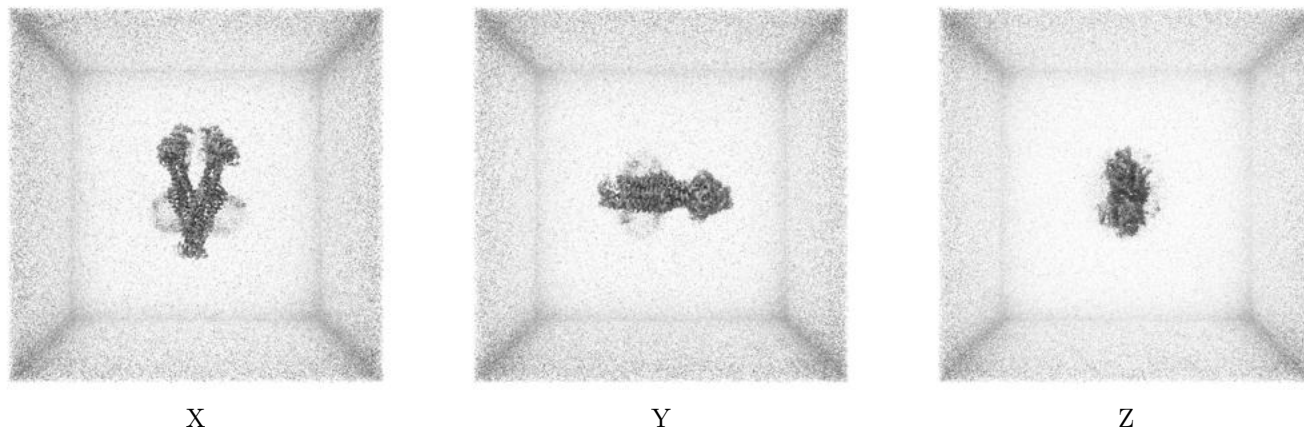
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.046. 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.

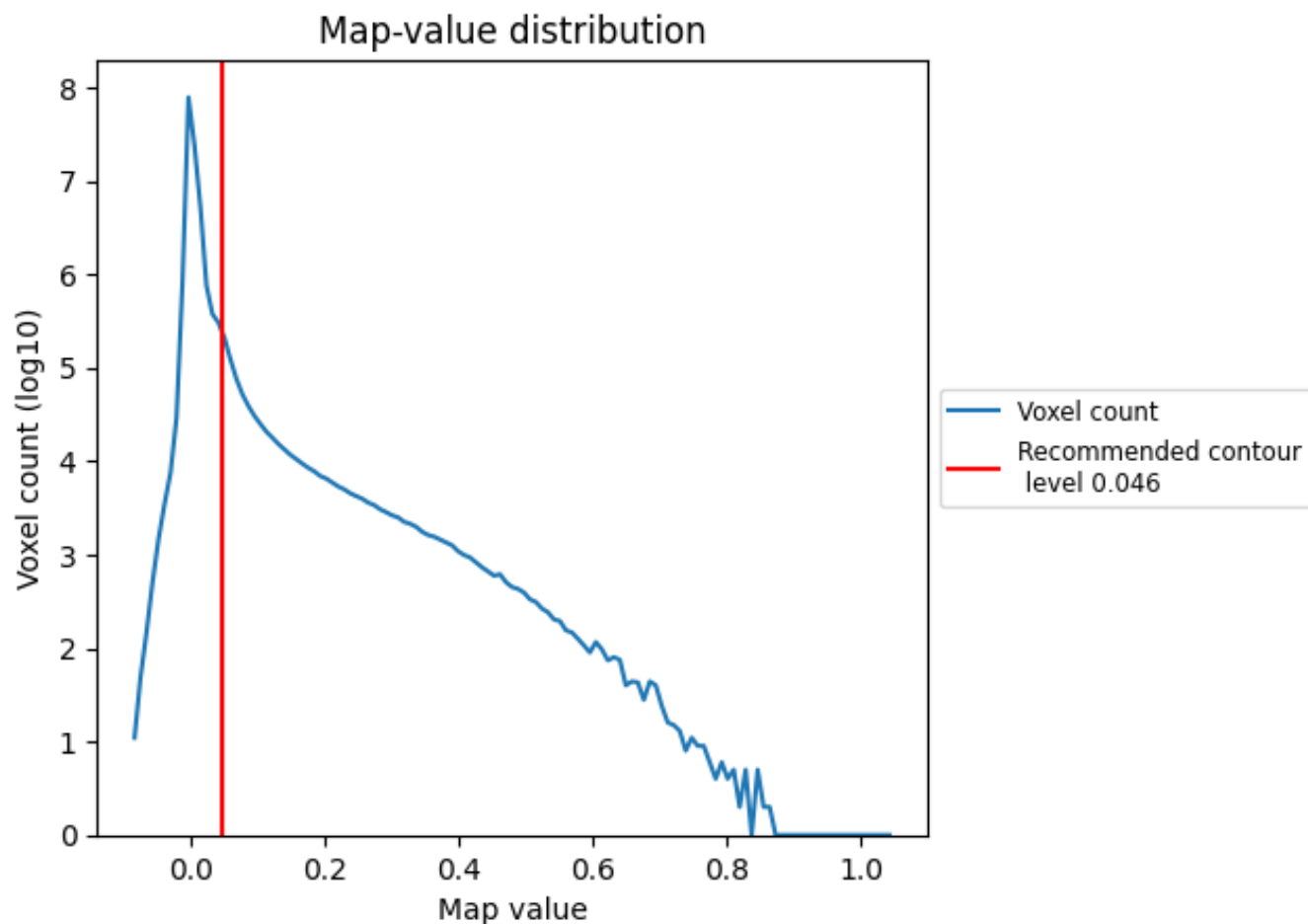
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

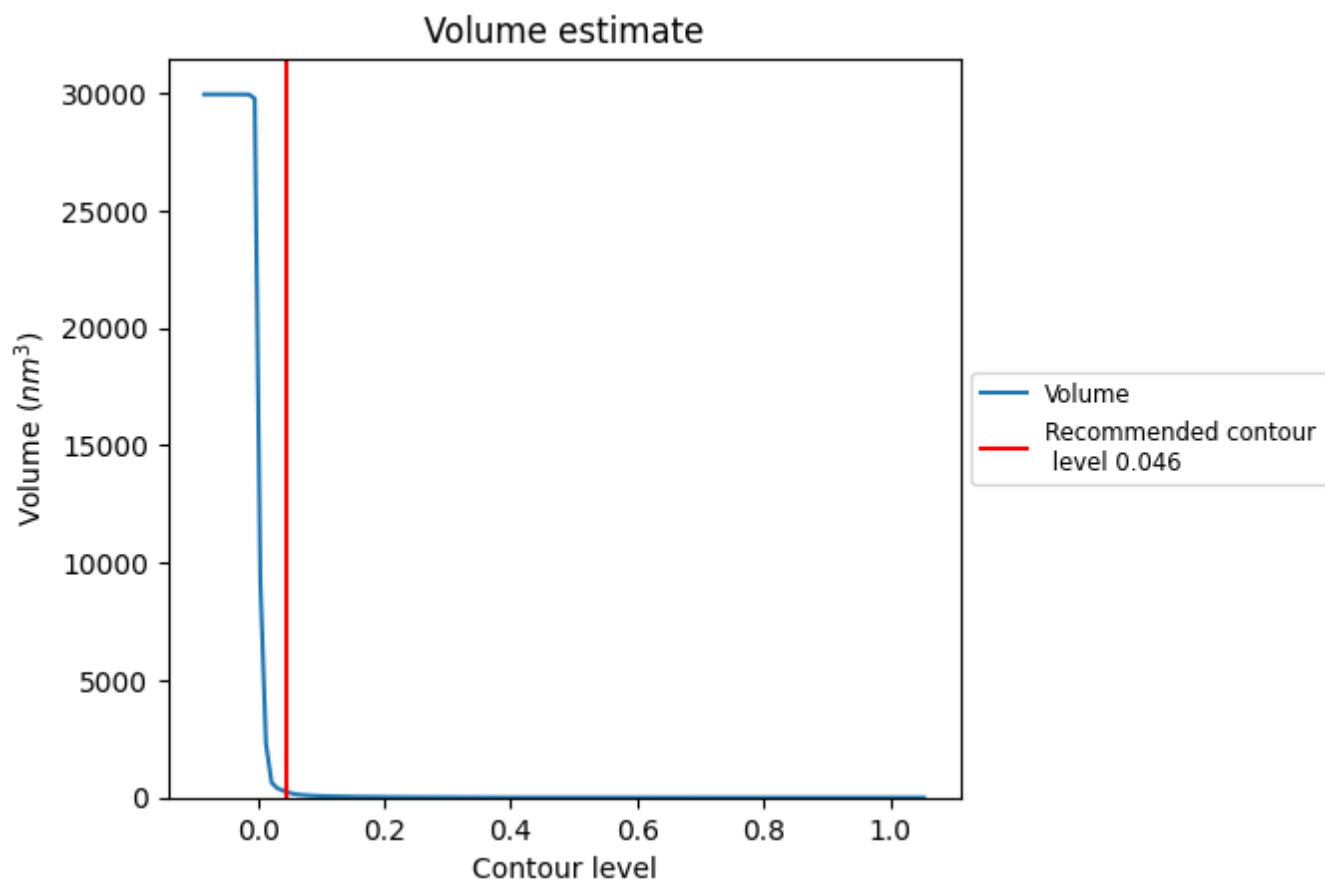
This section contains the results of statistical analysis of the map.

### 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.

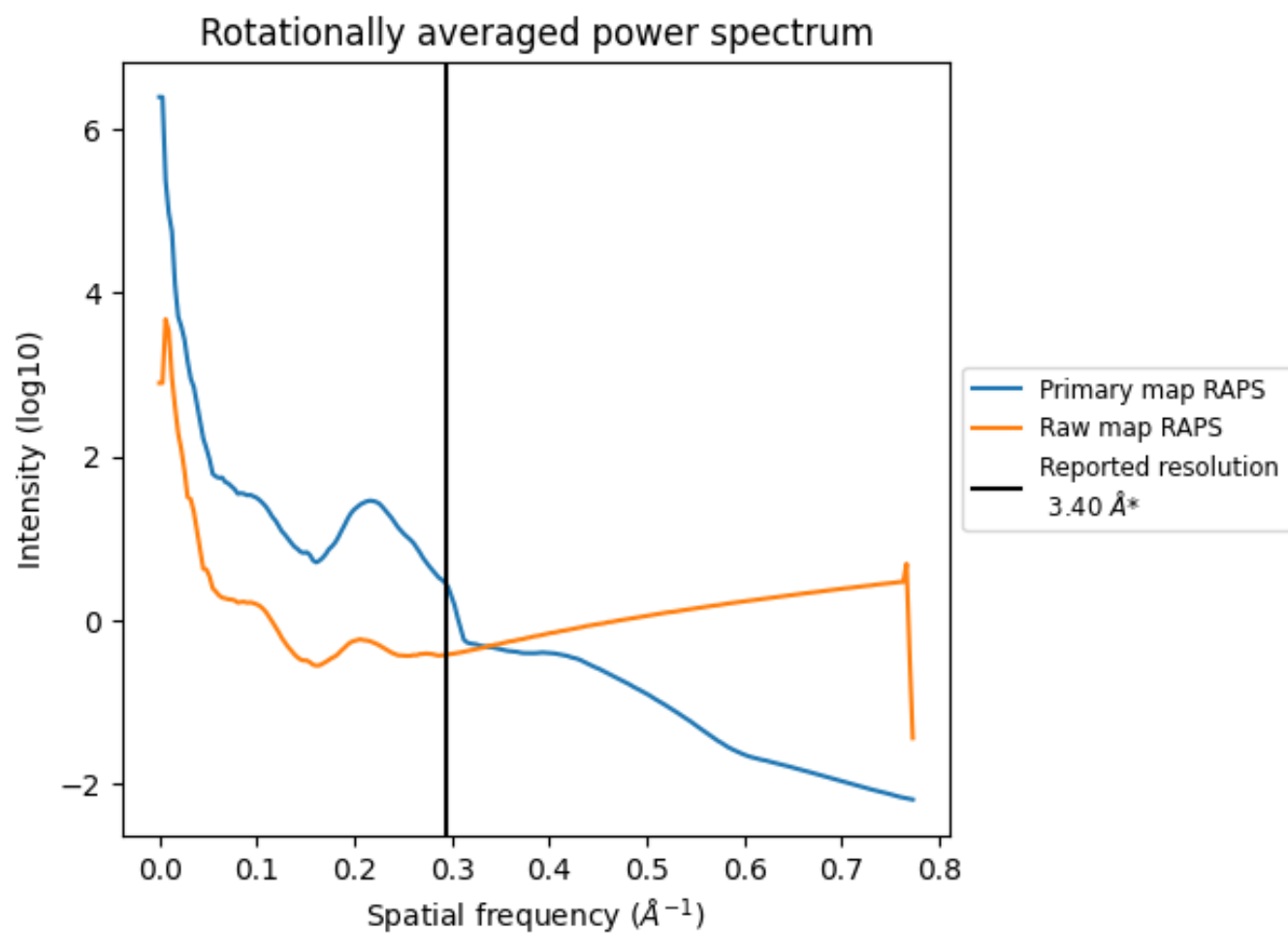
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm<sup>3</sup>; this corresponds to an approximate mass of 217 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



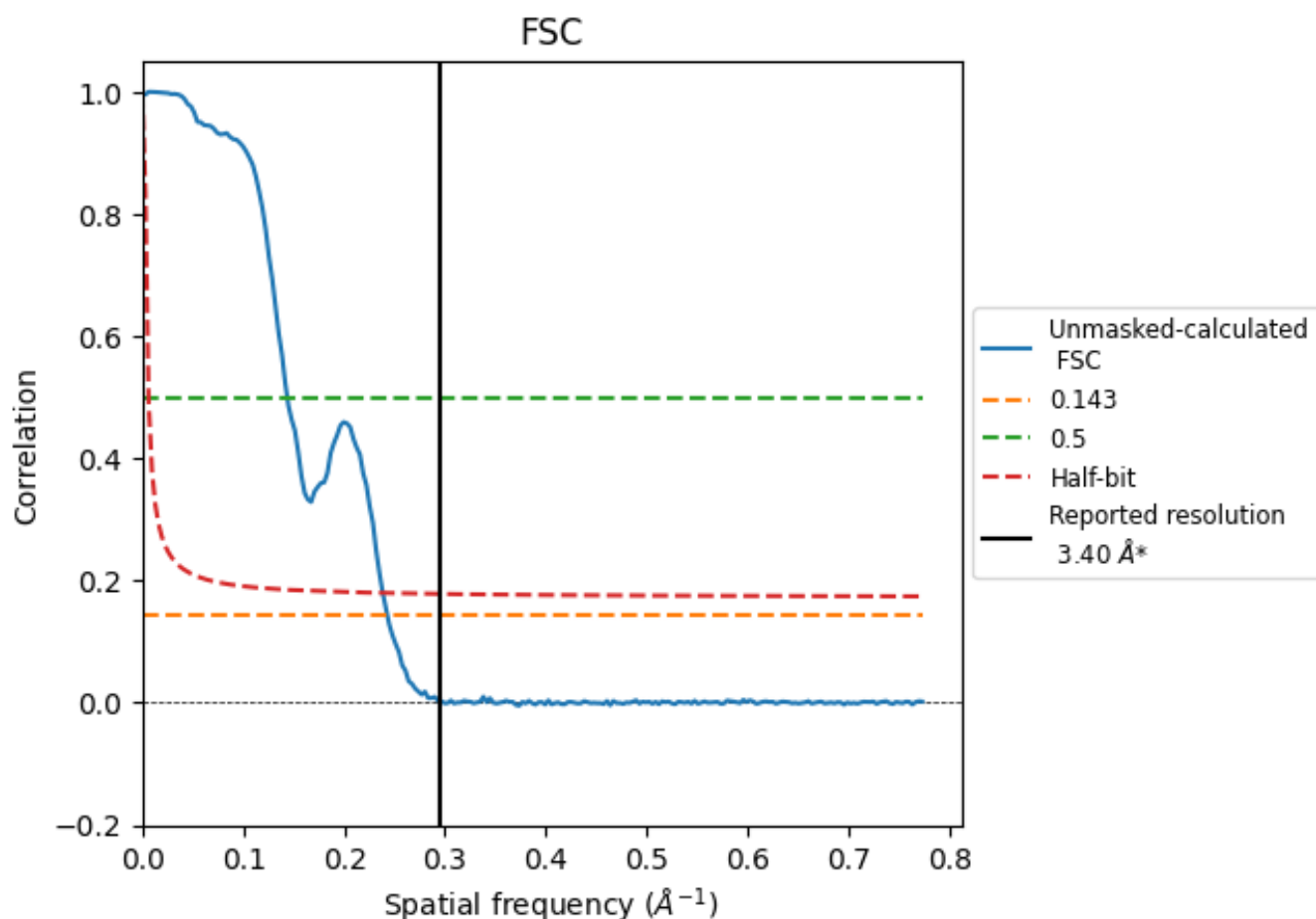
\*Reported resolution corresponds to spatial frequency of  $0.294 \text{ \AA}^{-1}$



## 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 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

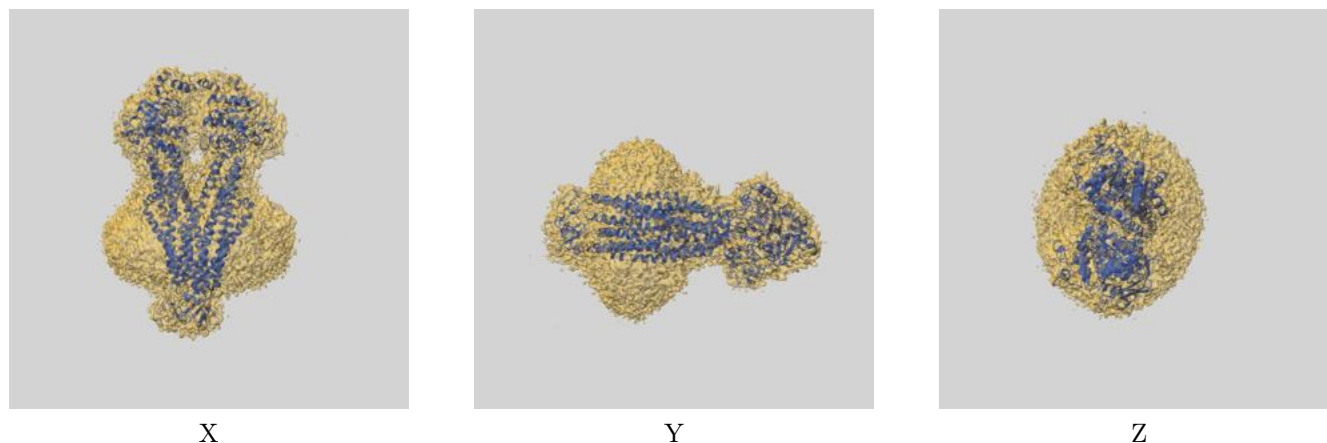
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.12	6.96	4.20

\*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 4.12 differs from the reported value 3.4 by more than 10 %

## 9 Map-model fit [i](#)

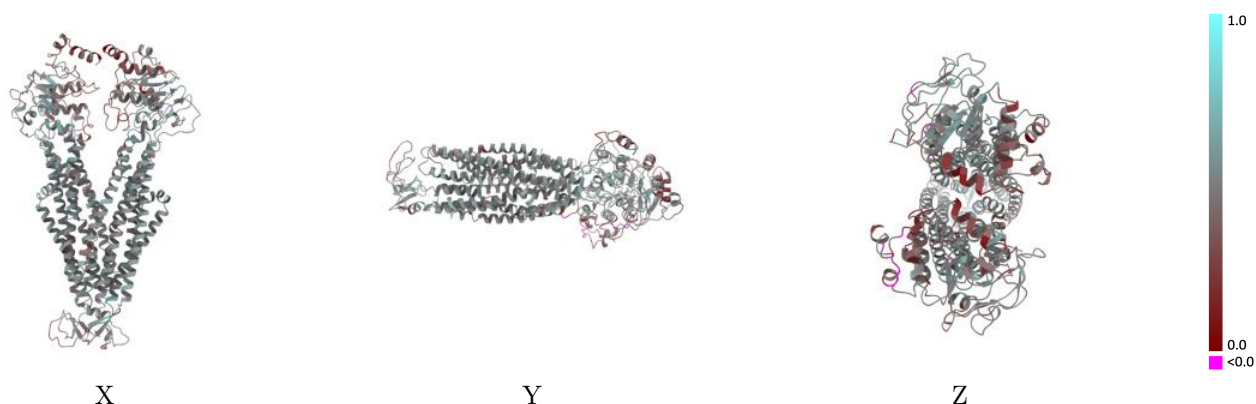
This section contains information regarding the fit between EMDB map EMD-45938 and PDB model 9CUP. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



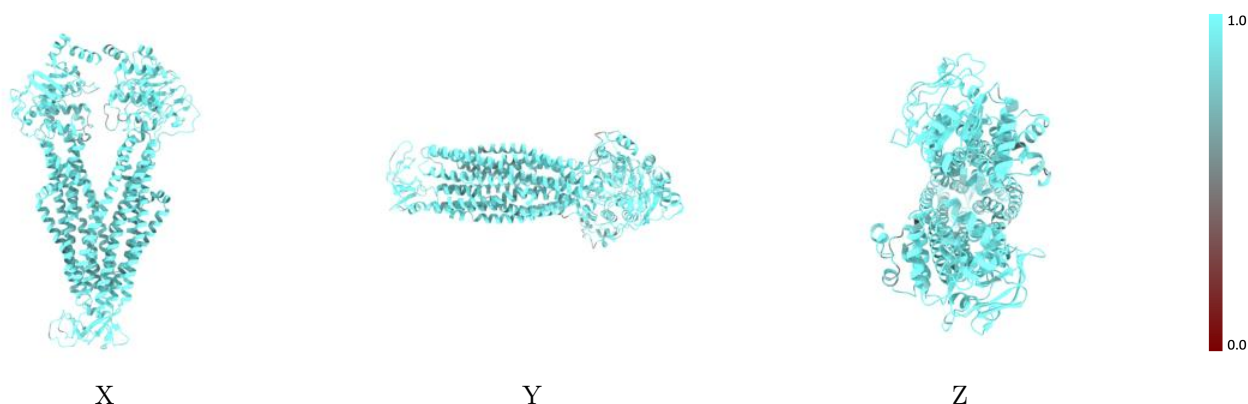
The images above show the 3D surface view of the map at the recommended contour level 0.046 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



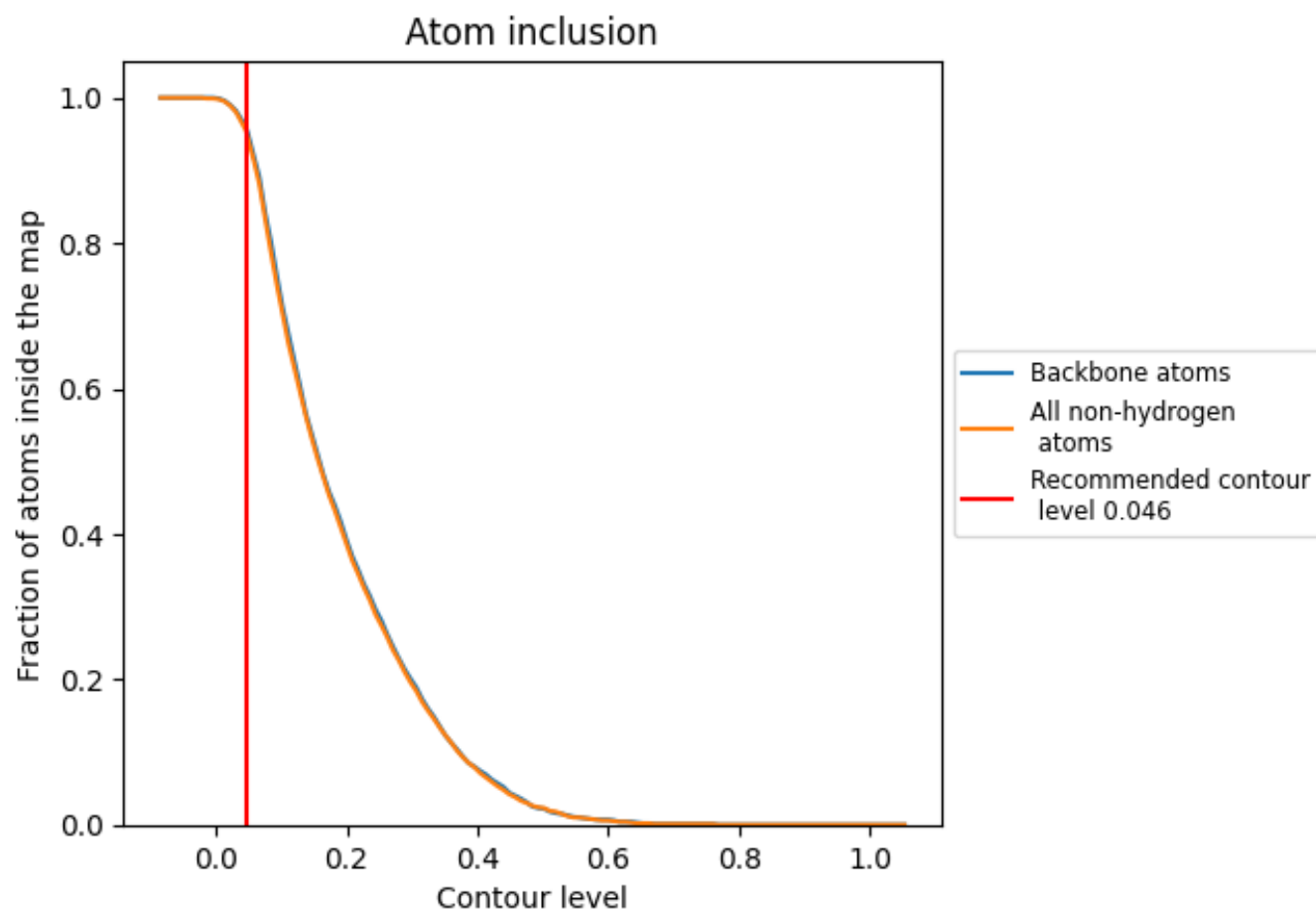
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.046).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.046) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9550	<div></div> 0.4670
C	<div></div> 0.9510	<div></div> 0.4730
D	<div></div> 0.9520	<div></div> 0.4620

