



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 06:03 PM EDT

PDB ID : 7N15
EMDB ID : EMD-24113
Title : Structure of TAX-4_R421W w/cGMP open state
Authors : Zheng, X.; Li, H.; Hu, Z.; Su, D.; Yang, J.
Deposited on : 2021-05-27
Resolution : 2.90 Å(reported)
Based on initial model : 6WEK

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.39

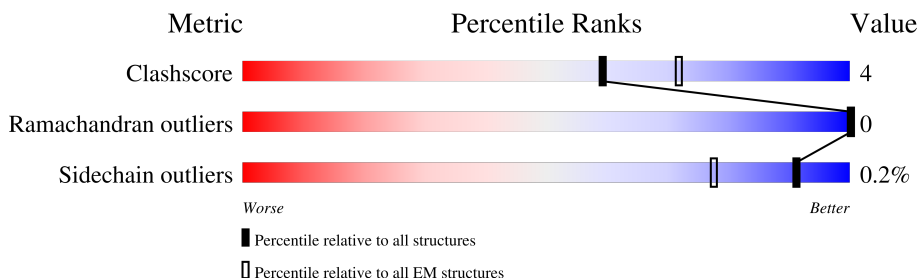
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	
1	B	738	
1	C	738	
1	D	738	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclic nucleotide-gated cation channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	520	Total	C	N	O	S	0	0
			4295	2795	720	756	24		
1	B	520	Total	C	N	O	S	0	0
			4295	2795	720	756	24		
1	C	520	Total	C	N	O	S	0	0
			4295	2795	720	756	24		
1	D	520	Total	C	N	O	S	0	0
			4295	2795	720	756	24		

There are 24 discrepancies between the modelled and reference sequences:

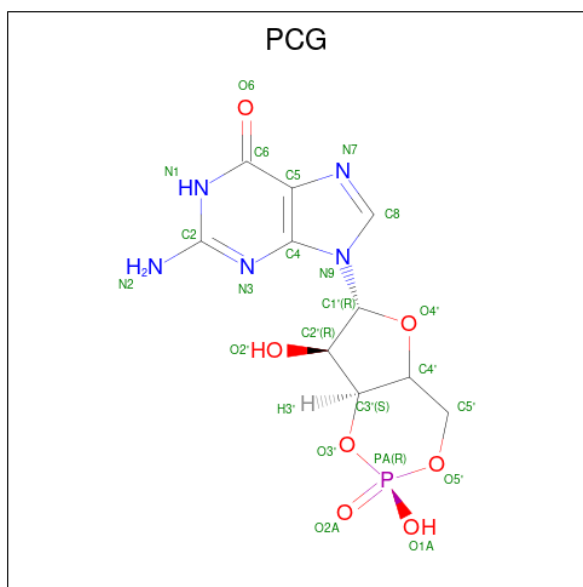
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q03611
A	-3	GLY	-	expression tag	UNP Q03611
A	-2	GLY	-	expression tag	UNP Q03611
A	-1	GLY	-	expression tag	UNP Q03611
A	0	SER	-	expression tag	UNP Q03611
A	421	TRP	ARG	engineered mutation	UNP Q03611
B	-4	GLY	-	expression tag	UNP Q03611
B	-3	GLY	-	expression tag	UNP Q03611
B	-2	GLY	-	expression tag	UNP Q03611
B	-1	GLY	-	expression tag	UNP Q03611
B	0	SER	-	expression tag	UNP Q03611
B	421	TRP	ARG	engineered mutation	UNP Q03611
C	-4	GLY	-	expression tag	UNP Q03611
C	-3	GLY	-	expression tag	UNP Q03611
C	-2	GLY	-	expression tag	UNP Q03611
C	-1	GLY	-	expression tag	UNP Q03611
C	0	SER	-	expression tag	UNP Q03611
C	421	TRP	ARG	engineered mutation	UNP Q03611
D	-4	GLY	-	expression tag	UNP Q03611
D	-3	GLY	-	expression tag	UNP Q03611
D	-2	GLY	-	expression tag	UNP Q03611
D	-1	GLY	-	expression tag	UNP Q03611

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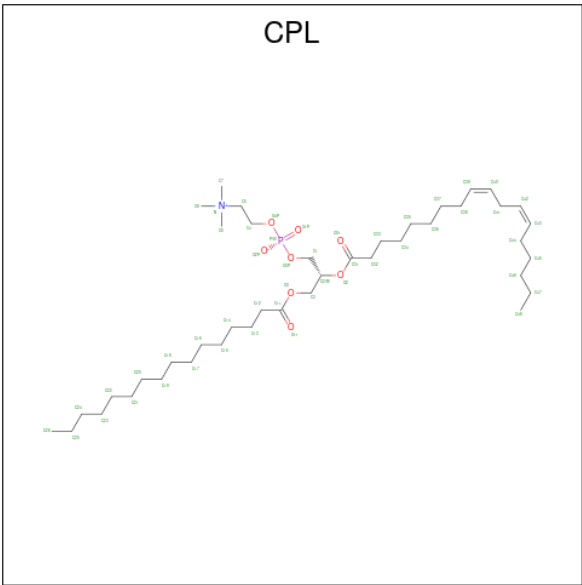
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q03611
D	421	TRP	ARG	engineered mutation	UNP Q03611

- Molecule 2 is CYCLIC GUANOSINE MONOPHOSPHATE (three-letter code: PCG) (formula: $C_{10}H_{12}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 3 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



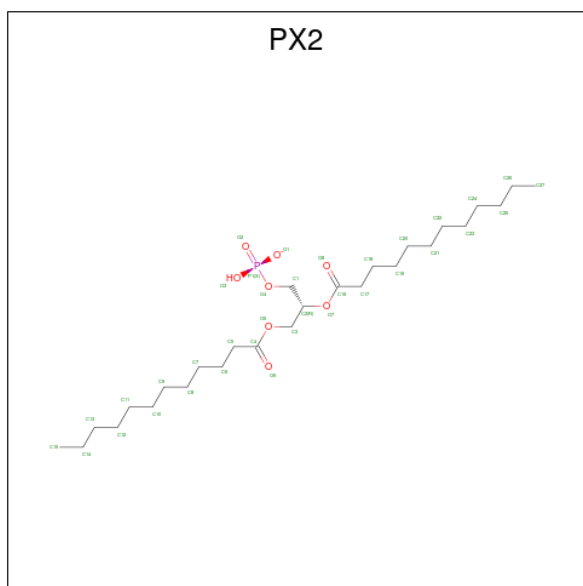
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	A	1	Total	C				0
			8	8				
3	A	1	Total	C				0
			13	13				
3	A	1	Total	C				0
			12	12				
3	A	1	Total	C	O	P		0
			38	29	8	1		
3	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	B	1	Total	C				0
			8	8				
3	B	1	Total	C				0
			13	13				
3	B	1	Total	C				0
			12	12				
3	B	1	Total	C	O	P		0
			38	29	8	1		
3	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	C	1	Total	C				0
			8	8				
3	C	1	Total	C				0
			13	13				
3	C	1	Total	C				0
			12	12				

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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	O	P	0
			38	29	8	1	
3	D	1	Total	C	N	O	P
			38	28	1	8	1
3	D	1	Total	C			0
			8	8			
3	D	1	Total	C			0
			13	13			
3	D	1	Total	C			0
			12	12			
3	D	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 4 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: C₂₇H₅₂O₈P) (labeled as "Ligand of Interest" by depositor).

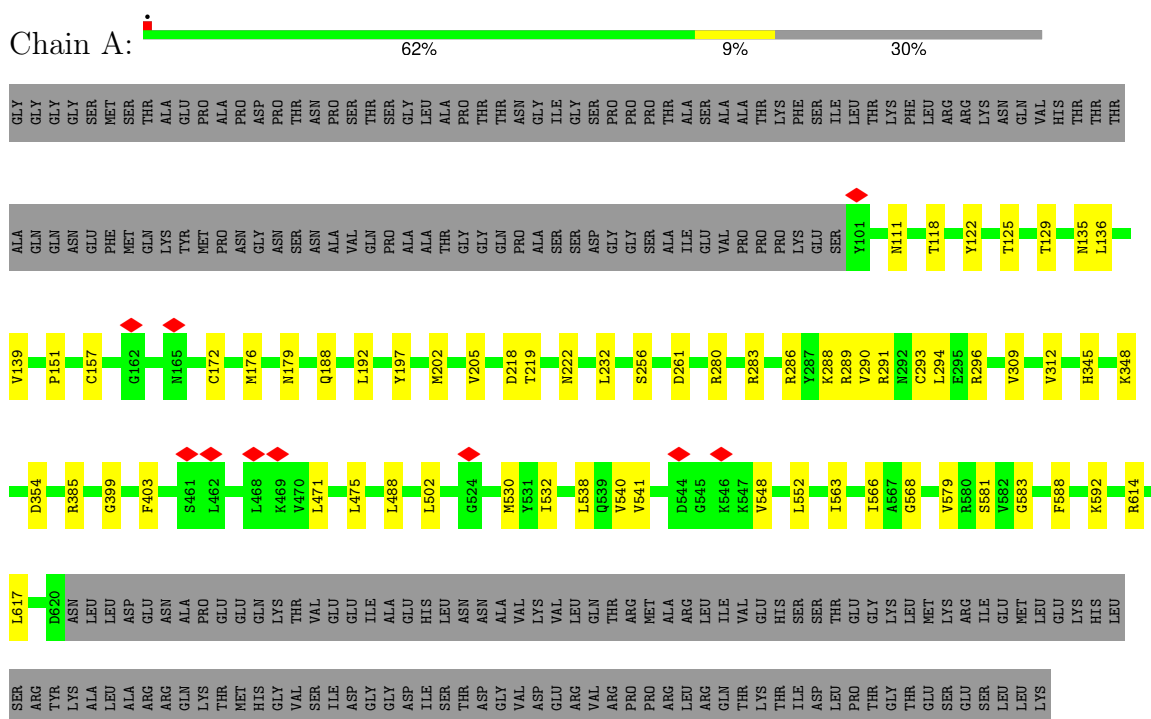


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			23	14	8	1	
4	B	1	Total	C	O	P	0
			23	14	8	1	
4	C	1	Total	C	O	P	0
			23	14	8	1	
4	D	1	Total	C	O	P	0
			23	14	8	1	

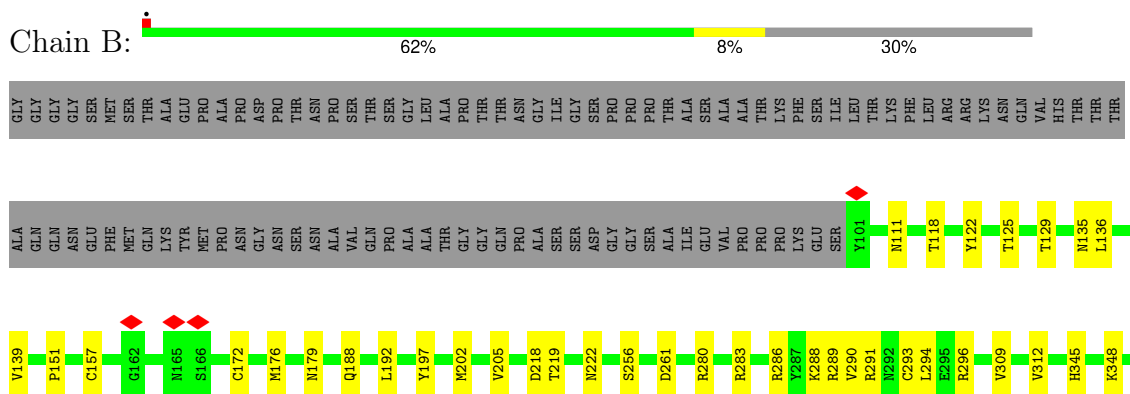
3 Residue-property plots

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.

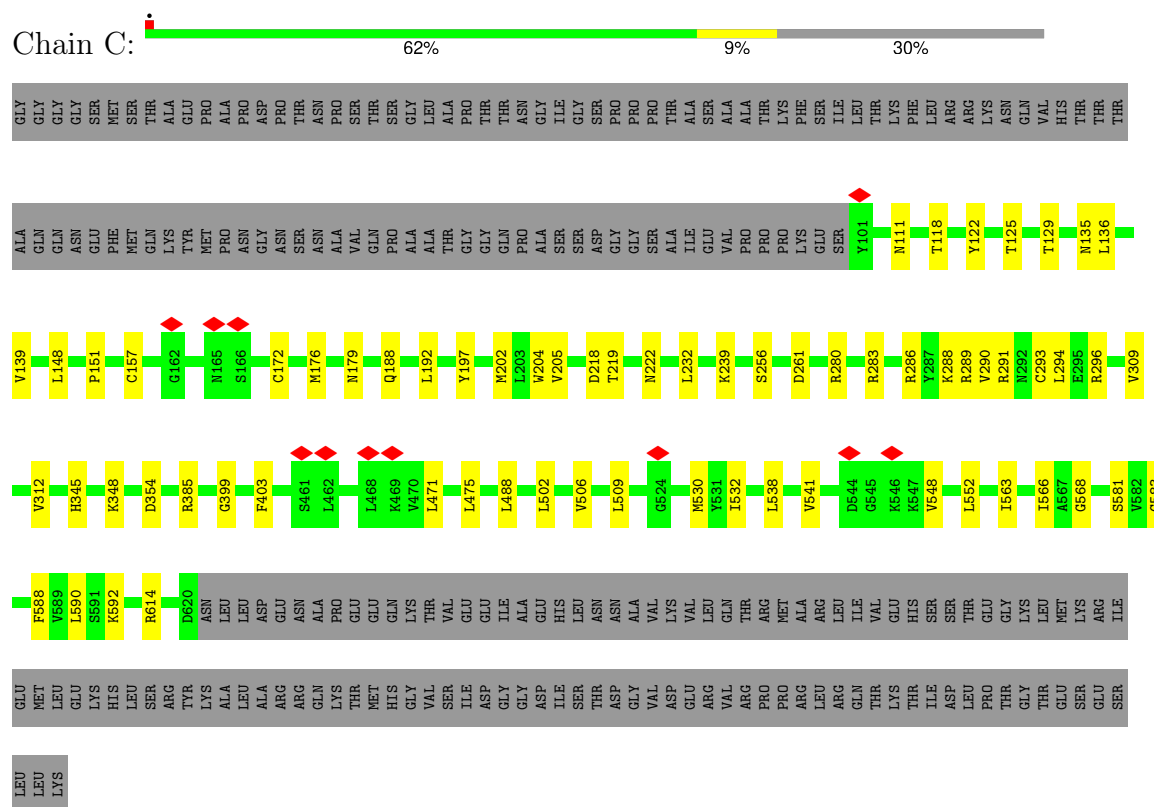
• Molecule 1: Cyclic nucleotide-gated cation channel



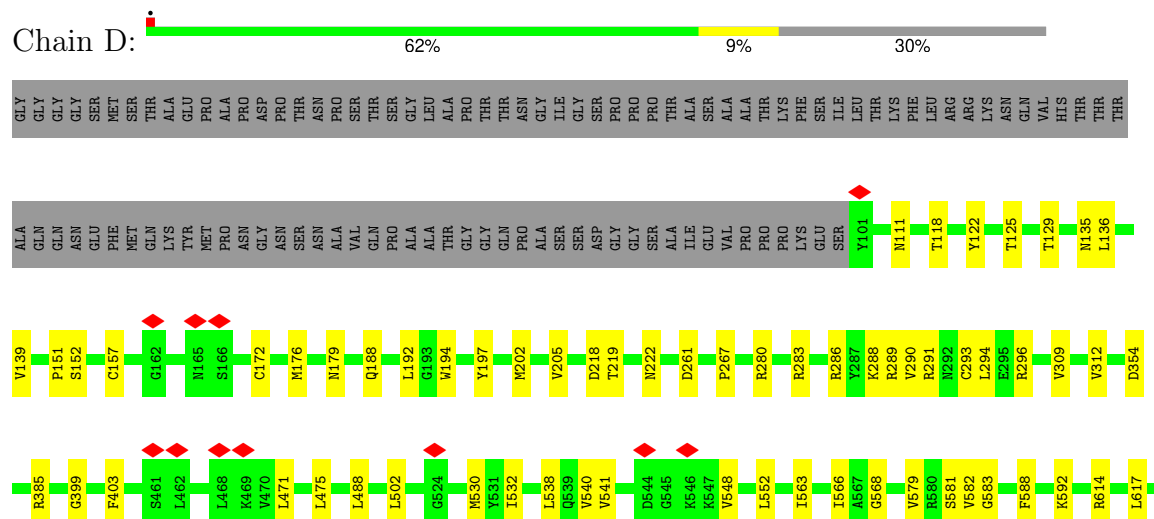
• Molecule 1: Cyclic nucleotide-gated cation channel



- Molecule 1: Cyclic nucleotide-gated cation channel



- Molecule 1: Cyclic nucleotide-gated cation channel



De200	ASN	LEU	LEU	ASP	GLU	ASN	ALA	PRO	GLU	GLU	GLN	LYS	THR	VAL	GLU	ILE	ALA	GLU	HIS	LEU	ASN	ASN	ALA	VAL	LYS	VAL	LEU	GLN	THR	ARG	ARG	MET	ALA	ARG	LEU	ILE	VAL	GLU	HIS	SER	SER	THR	GLU	GLY	LYS	LEU	MET	LYS	ARG	ILE	GLU	MET	LEU	GLU	LYS	HIS	LEU	SER	ARG
	TYR	LYS	ALA	LEU	ALA	ARG	ARG	GLN	LYS	THR	MET	HIS	GLY	VAL	SER	ILE	ASP	GLY	ASP	ILE	SER	THR	ASP	GLY	VAL	VAL	ASP	GLU	ARG	VAL	ARG	PRO	PRO	ARG	LEU	ARG	GLN	THR	THR	LYS	THR	ILE	ASP	LEU	PHO	THR	GLY	THR	GLU	SER	GLU	SER	LEU	LEU	LYS				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	284615	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 ($e^-/\text{\AA}^2$)	69.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.882	Depositor
Minimum map value	-4.576	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.180	Depositor
Recommended contour level	0.45	Depositor
Map size (\AA)	245.68, 245.68, 245.68	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCG, PX2, CPL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/4401	0.55	1/5973 (0.0%)
1	B	0.37	0/4401	0.55	1/5973 (0.0%)
1	C	0.37	0/4401	0.55	1/5973 (0.0%)
1	D	0.37	0/4401	0.55	1/5973 (0.0%)
All	All	0.37	0/17604	0.55	4/23892 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	LEU	CA-CB-CG	5.57	128.10	115.30
1	D	136	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	136	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	136	LEU	CA-CB-CG	5.54	128.05	115.30

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	A	4295	0	4329	38	0
1	B	4295	0	4329	37	0
1	C	4295	0	4329	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4295	0	4329	39	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
3	A	109	0	154	2	0
3	B	109	0	154	2	0
3	C	109	0	154	2	0
3	D	109	0	154	2	0
4	A	23	0	20	1	0
4	B	23	0	20	1	0
4	C	23	0	20	1	0
4	D	23	0	20	1	0
All	All	17800	0	18056	157	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 (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:O	1:A:139:VAL:HB	1.96	0.66
1:C:135:ASN:O	1:C:139:VAL:HB	1.96	0.66
1:D:135:ASN:O	1:D:139:VAL:HB	1.96	0.66
1:B:135:ASN:O	1:B:139:VAL:HB	1.96	0.64
1:D:179:ASN:HD21	1:D:354:ASP:H	1.47	0.62
1:B:188:GLN:HE21	1:B:192:LEU:HD21	1.65	0.61
1:C:188:GLN:HE21	1:C:192:LEU:HD21	1.65	0.61
1:A:179:ASN:HD21	1:A:354:ASP:H	1.47	0.61
1:C:179:ASN:HD21	1:C:354:ASP:H	1.47	0.61
1:D:188:GLN:HE21	1:D:192:LEU:HD21	1.65	0.60
1:A:188:GLN:HE21	1:A:192:LEU:HD21	1.65	0.60
1:B:179:ASN:HD21	1:B:354:ASP:H	1.47	0.60
1:A:111:ASN:OD1	1:A:111:ASN:O	2.20	0.59
1:D:111:ASN:O	1:D:111:ASN:OD1	2.20	0.59
1:B:111:ASN:O	1:B:111:ASN:OD1	2.20	0.59
1:C:111:ASN:O	1:C:111:ASN:OD1	2.20	0.58
1:B:125:THR:HG22	1:B:289:ARG:HD2	1.86	0.58
1:C:125:THR:HG22	1:C:289:ARG:HD2	1.86	0.58
1:A:125:THR:HG22	1:A:289:ARG:HD2	1.86	0.57
1:D:125:THR:HG22	1:D:289:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ASN:OD1	1:C:289:ARG:NH2	2.40	0.55
1:B:222:ASN:OD1	1:B:289:ARG:NH2	2.40	0.55
1:D:222:ASN:OD1	1:D:289:ARG:NH2	2.40	0.55
1:A:222:ASN:OD1	1:A:289:ARG:NH2	2.40	0.55
1:A:261:ASP:OD1	1:A:283:ARG:NH2	2.40	0.55
1:B:261:ASP:OD1	1:B:283:ARG:NH2	2.40	0.55
1:B:129:THR:HG23	1:B:290:VAL:HG13	1.89	0.55
1:C:122:TYR:HB2	1:C:296:ARG:HH21	1.72	0.54
1:D:122:TYR:HB2	1:D:296:ARG:HH21	1.73	0.54
1:C:129:THR:HG23	1:C:290:VAL:HG13	1.89	0.54
1:A:129:THR:HG23	1:A:290:VAL:HG13	1.89	0.54
1:B:122:TYR:HB2	1:B:296:ARG:HH21	1.72	0.54
1:C:261:ASP:OD1	1:C:283:ARG:NH2	2.40	0.54
1:D:261:ASP:OD1	1:D:283:ARG:NH2	2.40	0.54
1:A:122:TYR:HB2	1:A:296:ARG:HH21	1.72	0.54
1:A:385:ARG:NH2	4:A:806:PX2:O3	2.42	0.53
1:B:385:ARG:NH2	4:B:806:PX2:O3	2.42	0.53
1:D:129:THR:HG23	1:D:290:VAL:HG13	1.89	0.53
1:C:566:ILE:HG22	1:C:568:GLY:H	1.73	0.53
1:A:566:ILE:HG22	1:A:568:GLY:H	1.74	0.52
1:D:385:ARG:NH2	4:D:806:PX2:O3	2.42	0.52
1:C:385:ARG:NH2	4:C:806:PX2:O3	2.42	0.52
1:B:566:ILE:HG22	1:B:568:GLY:H	1.74	0.52
1:D:566:ILE:HG22	1:D:568:GLY:H	1.73	0.52
1:A:532:ILE:HB	1:A:588:PHE:HB2	1.92	0.52
1:D:532:ILE:HB	1:D:588:PHE:HB2	1.92	0.52
1:C:532:ILE:HB	1:C:588:PHE:HB2	1.92	0.51
1:D:202:MET:HA	1:D:205:VAL:HG12	1.93	0.51
1:C:202:MET:HA	1:C:205:VAL:HG12	1.93	0.51
1:D:157:CYS:N	1:D:172:CYS:SG	2.84	0.51
1:A:202:MET:HA	1:A:205:VAL:HG12	1.93	0.50
1:B:471:LEU:HD22	1:B:475:LEU:HD23	1.93	0.50
1:A:157:CYS:N	1:A:172:CYS:SG	2.85	0.50
1:B:532:ILE:HB	1:B:588:PHE:HB2	1.92	0.50
1:C:157:CYS:N	1:C:172:CYS:SG	2.85	0.50
1:C:471:LEU:HD22	1:C:475:LEU:HD23	1.93	0.50
1:B:202:MET:HA	1:B:205:VAL:HG12	1.93	0.50
1:D:471:LEU:HD22	1:D:475:LEU:HD23	1.93	0.50
1:A:399:GLY:O	1:A:403:PHE:HB2	2.11	0.50
1:B:157:CYS:N	1:B:172:CYS:SG	2.84	0.50
1:D:399:GLY:O	1:D:403:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:GLY:O	1:B:403:PHE:HB2	2.11	0.50
1:D:566:ILE:HG23	1:D:614:ARG:HH21	1.77	0.50
1:B:566:ILE:HG23	1:B:614:ARG:HH21	1.76	0.50
1:C:399:GLY:O	1:C:403:PHE:HB2	2.11	0.49
1:A:471:LEU:HD22	1:A:475:LEU:HD23	1.94	0.49
1:B:530:MET:HB3	1:B:563:ILE:HD11	1.95	0.48
1:C:566:ILE:HG23	1:C:614:ARG:HH21	1.77	0.48
1:A:566:ILE:HG23	1:A:614:ARG:HH21	1.77	0.48
1:C:530:MET:HB3	1:C:563:ILE:HD11	1.95	0.48
1:A:563:ILE:O	1:A:592:LYS:NZ	2.47	0.48
1:B:541:VAL:HG12	1:B:548:VAL:HG22	1.96	0.48
1:D:563:ILE:O	1:D:592:LYS:NZ	2.47	0.48
1:C:541:VAL:HG12	1:C:548:VAL:HG22	1.96	0.47
1:A:530:MET:HB3	1:A:563:ILE:HD11	1.95	0.47
1:D:288:LYS:HG3	1:D:291:ARG:HH21	1.80	0.47
1:D:530:MET:HB3	1:D:563:ILE:HD11	1.95	0.47
1:B:563:ILE:O	1:B:592:LYS:NZ	2.47	0.47
1:A:256:SER:O	1:A:256:SER:OG	2.33	0.46
1:A:541:VAL:HG12	1:A:548:VAL:HG22	1.96	0.46
1:D:541:VAL:HG12	1:D:548:VAL:HG22	1.96	0.46
1:C:309:VAL:HA	1:C:312:VAL:HG12	1.98	0.46
1:A:288:LYS:HG3	1:A:291:ARG:HH21	1.80	0.46
1:C:288:LYS:HG3	1:C:291:ARG:HH21	1.80	0.46
1:C:563:ILE:O	1:C:592:LYS:NZ	2.47	0.46
1:B:219:THR:HB	1:B:286:ARG:HH12	1.81	0.46
1:D:309:VAL:HA	1:D:312:VAL:HG12	1.98	0.46
1:B:288:LYS:HG3	1:B:291:ARG:HH21	1.80	0.46
1:C:294:LEU:HD21	3:C:804:CPL:H141	1.98	0.46
1:A:309:VAL:HA	1:A:312:VAL:HG12	1.98	0.46
1:B:309:VAL:HA	1:B:312:VAL:HG12	1.98	0.46
1:C:581:SER:OG	1:C:583:GLY:O	2.32	0.45
1:D:294:LEU:HD21	3:D:804:CPL:H141	1.98	0.45
1:B:256:SER:O	1:B:256:SER:OG	2.33	0.45
1:C:172:CYS:HA	1:C:176:MET:HE2	1.98	0.45
1:C:219:THR:HB	1:C:286:ARG:HH12	1.81	0.45
1:D:219:THR:HB	1:D:286:ARG:HH12	1.81	0.45
1:C:111:ASN:OD1	1:C:111:ASN:C	2.55	0.45
1:A:219:THR:HB	1:A:286:ARG:HH12	1.81	0.45
1:B:294:LEU:HD21	3:B:804:CPL:H141	1.98	0.45
1:C:345:HIS:O	1:C:348:LYS:NZ	2.42	0.45
1:B:111:ASN:OD1	1:B:111:ASN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:OD1	1:A:111:ASN:C	2.55	0.44
1:A:294:LEU:HD21	3:A:804:CPL:H141	1.98	0.44
1:D:581:SER:OG	1:D:583:GLY:O	2.32	0.44
1:D:111:ASN:OD1	1:D:111:ASN:C	2.55	0.44
1:B:172:CYS:HA	1:B:176:MET:HE2	1.99	0.44
1:D:172:CYS:HA	1:D:176:MET:HE2	1.98	0.44
1:D:125:THR:HB	1:D:293:CYS:HB2	2.00	0.43
1:C:256:SER:O	1:C:256:SER:OG	2.33	0.43
1:D:152:SER:O	1:D:152:SER:OG	2.36	0.43
1:C:125:THR:HB	1:C:293:CYS:HB2	2.00	0.43
1:A:172:CYS:HA	1:A:176:MET:HE2	1.99	0.43
3:D:802:CPL:HC62	3:D:802:CPL:HC41	1.87	0.43
1:D:192:LEU:HD23	1:D:192:LEU:HA	1.91	0.43
1:D:151:PRO:HD2	1:D:197:TYR:CZ	2.54	0.42
1:A:151:PRO:HD2	1:A:197:TYR:CZ	2.54	0.42
1:B:581:SER:OG	1:B:583:GLY:O	2.32	0.42
1:C:538:LEU:HB2	1:C:552:LEU:HB2	2.01	0.42
1:B:125:THR:HB	1:B:293:CYS:HB2	2.00	0.42
1:B:151:PRO:HD2	1:B:197:TYR:CZ	2.54	0.42
1:A:125:THR:HB	1:A:293:CYS:HB2	2.00	0.42
1:B:488:LEU:HD13	1:B:502:LEU:HD11	2.01	0.42
1:A:488:LEU:HD13	1:A:502:LEU:HD11	2.01	0.42
1:C:192:LEU:HD23	1:C:192:LEU:HA	1.91	0.42
1:A:232:LEU:HD21	1:D:582:VAL:HG12	2.01	0.42
1:A:345:HIS:O	1:A:348:LYS:NZ	2.42	0.42
1:B:582:VAL:HG12	1:C:232:LEU:HD21	2.02	0.42
1:C:151:PRO:HD2	1:C:197:TYR:CZ	2.54	0.42
1:D:538:LEU:HB2	1:D:552:LEU:HB2	2.01	0.42
1:B:538:LEU:HB2	1:B:552:LEU:HB2	2.01	0.41
3:B:802:CPL:HC62	3:B:802:CPL:HC41	1.87	0.41
1:A:581:SER:OG	1:A:583:GLY:O	2.32	0.41
1:A:617:LEU:HD23	1:A:617:LEU:HA	1.94	0.41
1:C:148:LEU:O	1:C:204:TRP:NE1	2.47	0.41
1:D:139:VAL:HG21	1:D:280:ARG:HB2	2.02	0.41
1:B:345:HIS:O	1:B:348:LYS:NZ	2.42	0.41
1:C:488:LEU:HD13	1:C:502:LEU:HD11	2.01	0.41
1:D:194:TRP:NE1	1:D:267:PRO:O	2.42	0.41
1:D:617:LEU:HD23	1:D:617:LEU:HA	1.94	0.41
1:A:538:LEU:HB2	1:A:552:LEU:HB2	2.01	0.41
3:A:802:CPL:HC62	3:A:802:CPL:HC41	1.87	0.41
1:B:139:VAL:HG21	1:B:280:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:O	1:B:506:VAL:HB	2.21	0.41
3:C:802:CPL:HC41	3:C:802:CPL:HC62	1.87	0.41
1:C:218:ASP:OD1	1:C:289:ARG:NH1	2.54	0.41
1:D:488:LEU:HD13	1:D:502:LEU:HD11	2.01	0.41
1:B:218:ASP:OD1	1:B:289:ARG:NH1	2.54	0.40
1:C:502:LEU:O	1:C:506:VAL:HB	2.21	0.40
1:D:218:ASP:OD1	1:D:289:ARG:NH1	2.54	0.40
1:A:540:VAL:HG22	1:A:579:VAL:HG12	2.03	0.40
1:C:509:LEU:HD23	1:C:590:LEU:HB2	2.03	0.40
1:A:139:VAL:HG21	1:A:280:ARG:HB2	2.02	0.40
1:C:239:LYS:HE2	1:C:239:LYS:HB3	1.95	0.40
1:A:218:ASP:OD1	1:A:289:ARG:NH1	2.54	0.40
1:C:139:VAL:HG21	1:C:280:ARG:HB2	2.02	0.40
1:D:540:VAL:HG22	1:D:579:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/738 (70%)	506 (98%)	12 (2%)	0	100	100
1	B	518/738 (70%)	506 (98%)	12 (2%)	0	100	100
1	C	518/738 (70%)	506 (98%)	12 (2%)	0	100	100
1	D	518/738 (70%)	506 (98%)	12 (2%)	0	100	100
All	All	2072/2952 (70%)	2024 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/652 (72%)	469 (100%)	1 (0%)	92	98
1	B	470/652 (72%)	469 (100%)	1 (0%)	92	98
1	C	470/652 (72%)	469 (100%)	1 (0%)	92	98
1	D	470/652 (72%)	469 (100%)	1 (0%)	92	98
All	All	1880/2608 (72%)	1876 (100%)	4 (0%)	91	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	THR
1	B	118	THR
1	C	118	THR
1	D	118	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	188	GLN
1	A	199	HIS
1	A	426	ASN
1	A	458	ASN
1	A	565	ASN
1	B	179	ASN
1	B	188	GLN
1	B	199	HIS
1	B	426	ASN
1	B	458	ASN
1	B	565	ASN
1	C	179	ASN
1	C	188	GLN
1	C	199	HIS

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Mol	Chain	Res	Type
1	C	426	ASN
1	C	458	ASN
1	C	565	ASN
1	D	179	ASN
1	D	188	GLN
1	D	426	ASN
1	D	458	ASN
1	D	565	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](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PX2	C	806	-	22,22,35	1.27	4 (18%)	25,27,40	1.44	2 (8%)
3	CPL	B	807	-	37,37,51	0.99	4 (10%)	40,42,59	1.18	2 (5%)
2	PCG	D	801	-	22,26,26	2.21	4 (18%)	25,41,41	2.41	8 (32%)
2	PCG	C	801	-	22,26,26	2.21	4 (18%)	25,41,41	2.42	8 (32%)
3	CPL	B	803	-	7,7,51	0.28	0	6,6,59	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CPL	D	807	-	37,37,51	0.99	4 (10%)	40,42,59	1.18	2 (5%)
3	CPL	D	804	-	12,12,51	0.25	0	11,11,59	0.84	0
3	CPL	D	803	-	7,7,51	0.29	0	6,6,59	0.75	0
3	CPL	C	803	-	7,7,51	0.29	0	6,6,59	0.75	0
3	CPL	C	807	-	37,37,51	0.99	4 (10%)	40,42,59	1.18	2 (5%)
3	CPL	D	805	-	11,11,51	0.27	0	10,10,59	0.82	0
2	PCG	A	801	-	22,26,26	2.21	4 (18%)	25,41,41	2.42	8 (32%)
3	CPL	A	807	-	37,37,51	0.99	4 (10%)	40,42,59	1.18	2 (5%)
3	CPL	A	803	-	7,7,51	0.29	0	6,6,59	0.75	0
4	PX2	D	806	-	22,22,35	1.26	4 (18%)	25,27,40	1.44	2 (8%)
3	CPL	B	804	-	12,12,51	0.25	0	11,11,59	0.84	0
3	CPL	A	804	-	12,12,51	0.25	0	11,11,59	0.84	0
3	CPL	A	802	-	37,37,51	1.13	4 (10%)	43,45,59	0.99	2 (4%)
3	CPL	B	802	-	37,37,51	1.13	4 (10%)	43,45,59	0.99	2 (4%)
3	CPL	D	802	-	37,37,51	1.13	4 (10%)	43,45,59	0.99	2 (4%)
3	CPL	A	805	-	11,11,51	0.27	0	10,10,59	0.81	0
4	PX2	A	806	-	22,22,35	1.26	4 (18%)	25,27,40	1.44	2 (8%)
3	CPL	C	804	-	12,12,51	0.25	0	11,11,59	0.84	0
2	PCG	B	801	-	22,26,26	2.21	4 (18%)	25,41,41	2.42	8 (32%)
3	CPL	C	802	-	37,37,51	1.14	4 (10%)	43,45,59	1.00	2 (4%)
3	CPL	B	805	-	11,11,51	0.27	0	10,10,59	0.82	0
4	PX2	B	806	-	22,22,35	1.26	4 (18%)	25,27,40	1.44	2 (8%)
3	CPL	C	805	-	11,11,51	0.27	0	10,10,59	0.81	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
4	PX2	C	806	-	-	11/24/24/37	-
3	CPL	B	807	-	-	19/41/41/55	-
2	PCG	D	801	-	-	0/0/31/31	0/4/4/4
2	PCG	C	801	-	-	0/0/31/31	0/4/4/4
3	CPL	B	803	-	-	4/5/5/55	-
3	CPL	D	807	-	-	19/41/41/55	-
3	CPL	D	804	-	-	7/10/10/55	-
3	CPL	D	803	-	-	4/5/5/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPL	C	803	-	-	4/5/5/55	-
3	CPL	C	807	-	-	19/41/41/55	-
3	CPL	D	805	-	-	5/9/9/55	-
2	PCG	A	801	-	-	0/0/31/31	0/4/4/4
3	CPL	A	807	-	-	19/41/41/55	-
3	CPL	A	803	-	-	4/5/5/55	-
4	PX2	D	806	-	-	11/24/24/37	-
3	CPL	B	804	-	-	7/10/10/55	-
3	CPL	A	804	-	-	7/10/10/55	-
3	CPL	A	802	-	-	13/41/41/55	-
3	CPL	B	802	-	-	13/41/41/55	-
3	CPL	D	802	-	-	13/41/41/55	-
3	CPL	A	805	-	-	5/9/9/55	-
4	PX2	A	806	-	-	11/24/24/37	-
3	CPL	C	804	-	-	7/10/10/55	-
2	PCG	B	801	-	-	0/0/31/31	0/4/4/4
3	CPL	C	802	-	-	13/41/41/55	-
3	CPL	B	805	-	-	5/9/9/55	-
4	PX2	B	806	-	-	11/24/24/37	-
3	CPL	C	805	-	-	5/9/9/55	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	PCG	PA-O5'	5.49	1.63	1.57
2	A	801	PCG	PA-O5'	5.48	1.63	1.57
2	D	801	PCG	PA-O5'	5.48	1.63	1.57
2	C	801	PCG	PA-O5'	5.46	1.63	1.57
2	C	801	PCG	O4'-C1'	5.11	1.47	1.40
2	A	801	PCG	O4'-C1'	5.11	1.47	1.40
2	D	801	PCG	O4'-C1'	5.10	1.47	1.40
2	B	801	PCG	O4'-C1'	5.07	1.47	1.40
2	C	801	PCG	C5-C6	-4.14	1.39	1.47
2	D	801	PCG	C5-C6	-4.14	1.39	1.47
2	A	801	PCG	C5-C6	-4.13	1.39	1.47
2	B	801	PCG	C5-C6	-4.13	1.39	1.47
2	C	801	PCG	PA-O3'	3.33	1.63	1.57
2	B	801	PCG	PA-O3'	3.32	1.63	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	PCG	PA-O3'	3.32	1.63	1.57
2	A	801	PCG	PA-O3'	3.32	1.63	1.57
3	C	802	CPL	O2-C2	-2.74	1.40	1.46
3	A	802	CPL	O2-C2	-2.73	1.40	1.46
3	B	802	CPL	O2-C2	-2.71	1.40	1.46
3	D	802	CPL	O2-C2	-2.71	1.40	1.46
4	C	806	PX2	O7-C2	-2.62	1.40	1.46
4	D	806	PX2	O7-C2	-2.60	1.40	1.46
4	A	806	PX2	O7-C2	-2.60	1.40	1.46
4	B	806	PX2	O7-C2	-2.58	1.40	1.46
3	C	807	CPL	O2-C2	-2.51	1.40	1.46
3	A	807	CPL	O2-C2	-2.50	1.40	1.46
3	B	807	CPL	O2-C2	-2.47	1.40	1.46
3	D	807	CPL	O2-C2	-2.46	1.40	1.46
3	B	802	CPL	O3-C11	2.45	1.40	1.33
3	A	802	CPL	O3-C11	2.44	1.40	1.33
3	C	802	CPL	O3-C11	2.44	1.40	1.33
3	D	802	CPL	O3-C11	2.44	1.40	1.33
4	B	806	PX2	O5-C4	2.42	1.40	1.33
4	C	806	PX2	O5-C4	2.42	1.40	1.33
4	A	806	PX2	O5-C4	2.42	1.40	1.33
4	D	806	PX2	O5-C4	2.42	1.40	1.33
3	C	807	CPL	O2-C31	2.39	1.41	1.34
3	A	807	CPL	O2-C31	2.37	1.41	1.34
3	B	807	CPL	O2-C31	2.37	1.41	1.34
3	D	807	CPL	O2-C31	2.37	1.41	1.34
4	B	806	PX2	O7-C16	2.37	1.41	1.34
4	D	806	PX2	O7-C16	2.36	1.40	1.34
4	C	806	PX2	O7-C16	2.36	1.40	1.34
4	A	806	PX2	O7-C16	2.36	1.40	1.34
3	D	807	CPL	O3-C11	2.33	1.40	1.33
3	A	807	CPL	O3-C11	2.31	1.40	1.33
3	C	807	CPL	O3-C11	2.31	1.40	1.33
3	B	807	CPL	O3-C11	2.31	1.40	1.33
3	A	807	CPL	O3-C3	-2.23	1.40	1.45
3	C	807	CPL	O3-C3	-2.22	1.40	1.45
3	B	807	CPL	O3-C3	-2.21	1.40	1.45
3	A	802	CPL	O2-C31	2.20	1.40	1.34
3	C	802	CPL	O2-C31	2.19	1.40	1.34
3	D	802	CPL	O2-C31	2.19	1.40	1.34
3	D	807	CPL	O3-C3	-2.19	1.40	1.45
4	C	806	PX2	O5-C3	-2.19	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	CPL	O2-C31	2.19	1.40	1.34
4	A	806	PX2	O5-C3	-2.17	1.40	1.45
3	C	802	CPL	O3-C3	-2.16	1.40	1.45
3	D	802	CPL	O3-C3	-2.16	1.40	1.45
4	B	806	PX2	O5-C3	-2.15	1.40	1.45
3	A	802	CPL	O3-C3	-2.15	1.40	1.45
3	B	802	CPL	O3-C3	-2.14	1.40	1.45
4	D	806	PX2	O5-C3	-2.14	1.40	1.45

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	PCG	C4'-O4'-C1'	-7.42	103.13	109.92
2	C	801	PCG	C4'-O4'-C1'	-7.41	103.14	109.92
2	A	801	PCG	C4'-O4'-C1'	-7.39	103.16	109.92
2	D	801	PCG	C4'-O4'-C1'	-7.36	103.19	109.92
4	B	806	PX2	O7-C16-C17	4.77	121.80	111.48
4	D	806	PX2	O7-C16-C17	4.76	121.79	111.48
4	A	806	PX2	O7-C16-C17	4.76	121.78	111.48
4	C	806	PX2	O7-C16-C17	4.75	121.75	111.48
3	B	807	CPL	O2-C31-C32	4.10	120.36	111.48
3	A	807	CPL	O2-C31-C32	4.10	120.36	111.48
3	C	807	CPL	O2-C31-C32	4.10	120.34	111.48
3	D	807	CPL	O2-C31-C32	4.10	120.34	111.48
2	A	801	PCG	O3'-C3'-C4'	-3.70	107.92	110.71
2	B	801	PCG	O3'-C3'-C4'	-3.70	107.92	110.71
2	C	801	PCG	O3'-C3'-C4'	-3.69	107.93	110.71
2	D	801	PCG	O3'-C3'-C4'	-3.67	107.94	110.71
2	D	801	PCG	C2-N1-C6	-3.66	118.42	125.11
2	C	801	PCG	C2-N1-C6	-3.64	118.44	125.11
2	A	801	PCG	C2-N1-C6	-3.64	118.44	125.11
2	B	801	PCG	C2-N1-C6	-3.64	118.44	125.11
2	B	801	PCG	C8-N7-C5	3.53	108.55	102.55
2	C	801	PCG	C8-N7-C5	3.53	108.55	102.55
2	A	801	PCG	C8-N7-C5	3.53	108.55	102.55
2	D	801	PCG	C8-N7-C5	3.51	108.52	102.55
3	A	802	CPL	O2-C31-C32	3.46	118.96	111.48
3	C	802	CPL	O2-C31-C32	3.45	118.94	111.48
3	D	802	CPL	O2-C31-C32	3.45	118.94	111.48
3	B	802	CPL	O2-C31-C32	3.45	118.94	111.48
2	B	801	PCG	O1A-PA-O2A	3.31	118.72	108.56
2	C	801	PCG	O1A-PA-O2A	3.29	118.68	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	PCG	O1A-PA-O2A	3.29	118.68	108.56
2	A	801	PCG	O1A-PA-O2A	3.29	118.67	108.56
2	C	801	PCG	O3'-C3'-C2'	-3.03	112.64	115.61
2	A	801	PCG	O3'-C3'-C2'	-3.00	112.67	115.61
2	B	801	PCG	O3'-C3'-C2'	-2.99	112.68	115.61
2	D	801	PCG	O3'-C3'-C2'	-2.98	112.68	115.61
2	B	801	PCG	C5-C6-N1	2.83	119.47	114.07
2	D	801	PCG	C5-C6-N1	2.82	119.46	114.07
2	A	801	PCG	C5-C6-N1	2.82	119.44	114.07
2	C	801	PCG	C5-C6-N1	2.81	119.44	114.07
3	A	807	CPL	O3-C11-C12	2.75	120.22	111.83
3	C	807	CPL	O3-C11-C12	2.75	120.21	111.83
3	D	807	CPL	O3-C11-C12	2.74	120.18	111.83
3	B	807	CPL	O3-C11-C12	2.74	120.18	111.83
4	C	806	PX2	O5-C4-C5	2.64	119.90	111.83
4	B	806	PX2	O5-C4-C5	2.64	119.88	111.83
4	A	806	PX2	O5-C4-C5	2.64	119.87	111.83
4	D	806	PX2	O5-C4-C5	2.63	119.86	111.83
3	C	802	CPL	O3-C11-C12	2.60	119.76	111.83
3	D	802	CPL	O3-C11-C12	2.59	119.73	111.83
3	A	802	CPL	O3-C11-C12	2.59	119.72	111.83
3	B	802	CPL	O3-C11-C12	2.58	119.70	111.83
2	C	801	PCG	O5'-PA-O3'	-2.12	102.87	105.70
2	B	801	PCG	O5'-PA-O3'	-2.09	102.90	105.70
2	A	801	PCG	O5'-PA-O3'	-2.09	102.90	105.70
2	D	801	PCG	O5'-PA-O3'	-2.08	102.92	105.70

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	CPL	O4P-C4-C5-N
3	A	802	CPL	C4-O4P-P-O1P
3	A	802	CPL	C4-O4P-P-O2P
3	A	802	CPL	C4-O4P-P-O3P
3	A	807	CPL	C32-C31-O2-C2
3	A	807	CPL	C1-O3P-P-O2P
3	A	807	CPL	C4-O4P-P-O2P
3	A	807	CPL	C4-O4P-P-O3P
3	B	802	CPL	O4P-C4-C5-N
3	B	802	CPL	C4-O4P-P-O1P
3	B	802	CPL	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	B	802	CPL	C4-O4P-P-O3P
3	B	807	CPL	C32-C31-O2-C2
3	B	807	CPL	C1-O3P-P-O2P
3	B	807	CPL	C4-O4P-P-O2P
3	B	807	CPL	C4-O4P-P-O3P
3	C	802	CPL	O4P-C4-C5-N
3	C	802	CPL	C4-O4P-P-O1P
3	C	802	CPL	C4-O4P-P-O2P
3	C	802	CPL	C4-O4P-P-O3P
3	C	807	CPL	C32-C31-O2-C2
3	C	807	CPL	C1-O3P-P-O2P
3	C	807	CPL	C4-O4P-P-O2P
3	C	807	CPL	C4-O4P-P-O3P
3	D	802	CPL	O4P-C4-C5-N
3	D	802	CPL	C4-O4P-P-O1P
3	D	802	CPL	C4-O4P-P-O2P
3	D	802	CPL	C4-O4P-P-O3P
3	D	807	CPL	C32-C31-O2-C2
3	D	807	CPL	C1-O3P-P-O2P
3	D	807	CPL	C4-O4P-P-O2P
3	D	807	CPL	C4-O4P-P-O3P
4	A	806	PX2	C1-O4-P1-O1
4	A	806	PX2	C1-O4-P1-O2
4	A	806	PX2	O8-C16-O7-C2
4	A	806	PX2	C17-C16-O7-C2
4	B	806	PX2	C1-O4-P1-O1
4	B	806	PX2	C1-O4-P1-O2
4	B	806	PX2	O8-C16-O7-C2
4	B	806	PX2	C17-C16-O7-C2
4	C	806	PX2	C1-O4-P1-O1
4	C	806	PX2	C1-O4-P1-O2
4	C	806	PX2	O8-C16-O7-C2
4	C	806	PX2	C17-C16-O7-C2
4	D	806	PX2	C1-O4-P1-O1
4	D	806	PX2	C1-O4-P1-O2
4	D	806	PX2	O8-C16-O7-C2
4	D	806	PX2	C17-C16-O7-C2
3	A	807	CPL	O31-C31-O2-C2
3	B	807	CPL	O31-C31-O2-C2
3	C	807	CPL	O31-C31-O2-C2
3	D	807	CPL	O31-C31-O2-C2
3	A	807	CPL	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
3	B	807	CPL	O11-C11-O3-C3
3	C	807	CPL	O11-C11-O3-C3
3	D	807	CPL	O11-C11-O3-C3
3	A	807	CPL	C12-C11-O3-C3
3	B	807	CPL	C12-C11-O3-C3
3	C	807	CPL	C12-C11-O3-C3
3	D	807	CPL	C12-C11-O3-C3
4	A	806	PX2	C5-C4-O5-C3
4	B	806	PX2	C5-C4-O5-C3
4	C	806	PX2	C5-C4-O5-C3
4	D	806	PX2	C5-C4-O5-C3
4	A	806	PX2	O6-C4-O5-C3
4	B	806	PX2	O6-C4-O5-C3
4	C	806	PX2	O6-C4-O5-C3
4	D	806	PX2	O6-C4-O5-C3
3	A	802	CPL	C31-C32-C33-C34
3	A	807	CPL	C31-C32-C33-C34
3	B	802	CPL	C31-C32-C33-C34
3	B	807	CPL	C31-C32-C33-C34
3	C	802	CPL	C31-C32-C33-C34
3	C	807	CPL	C31-C32-C33-C34
3	D	802	CPL	C31-C32-C33-C34
3	D	807	CPL	C31-C32-C33-C34
3	A	804	CPL	C16-C17-C18-C19
3	B	804	CPL	C16-C17-C18-C19
3	C	804	CPL	C16-C17-C18-C19
3	D	804	CPL	C16-C17-C18-C19
3	A	805	CPL	C18-C19-C20-C21
3	B	805	CPL	C18-C19-C20-C21
3	C	805	CPL	C18-C19-C20-C21
3	D	805	CPL	C18-C19-C20-C21
3	A	807	CPL	C19-C20-C21-C22
3	B	807	CPL	C19-C20-C21-C22
3	C	807	CPL	C19-C20-C21-C22
3	D	807	CPL	C19-C20-C21-C22
3	A	804	CPL	C14-C15-C16-C17
3	B	804	CPL	C14-C15-C16-C17
3	C	804	CPL	C14-C15-C16-C17
3	D	804	CPL	C14-C15-C16-C17
3	A	807	CPL	C11-C12-C13-C14
3	B	807	CPL	C11-C12-C13-C14
3	C	807	CPL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	D	807	CPL	C11-C12-C13-C14
4	A	806	PX2	C16-C17-C18-C19
4	B	806	PX2	C16-C17-C18-C19
4	C	806	PX2	C16-C17-C18-C19
4	D	806	PX2	C16-C17-C18-C19
3	A	805	CPL	C13-C14-C15-C16
3	B	805	CPL	C13-C14-C15-C16
3	C	805	CPL	C13-C14-C15-C16
3	D	805	CPL	C13-C14-C15-C16
3	A	802	CPL	C15-C16-C17-C18
3	B	802	CPL	C15-C16-C17-C18
3	C	802	CPL	C15-C16-C17-C18
3	D	802	CPL	C15-C16-C17-C18
3	A	804	CPL	C13-C14-C15-C16
3	B	804	CPL	C13-C14-C15-C16
3	C	804	CPL	C13-C14-C15-C16
3	D	804	CPL	C13-C14-C15-C16
4	A	806	PX2	C4-C5-C6-C7
4	B	806	PX2	C4-C5-C6-C7
4	C	806	PX2	C4-C5-C6-C7
4	D	806	PX2	C4-C5-C6-C7
3	B	807	CPL	C18-C19-C20-C21
3	D	807	CPL	C18-C19-C20-C21
3	A	807	CPL	C18-C19-C20-C21
3	C	807	CPL	C18-C19-C20-C21
3	A	807	CPL	C22-C23-C24-C25
3	B	807	CPL	C22-C23-C24-C25
3	C	807	CPL	C22-C23-C24-C25
3	D	807	CPL	C22-C23-C24-C25
3	A	804	CPL	C12-C13-C14-C15
3	B	804	CPL	C12-C13-C14-C15
3	D	804	CPL	C12-C13-C14-C15
3	C	804	CPL	C12-C13-C14-C15
4	A	806	PX2	C5-C6-C7-C8
4	B	806	PX2	C5-C6-C7-C8
4	C	806	PX2	C5-C6-C7-C8
4	D	806	PX2	C5-C6-C7-C8
3	A	807	CPL	C23-C24-C25-C26
3	B	807	CPL	C23-C24-C25-C26
3	C	807	CPL	C23-C24-C25-C26
3	D	807	CPL	C23-C24-C25-C26
3	A	804	CPL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
3	B	804	CPL	C18-C19-C20-C21
3	C	804	CPL	C18-C19-C20-C21
3	D	804	CPL	C18-C19-C20-C21
3	D	803	CPL	C16-C17-C18-C19
3	A	803	CPL	C16-C17-C18-C19
3	B	803	CPL	C16-C17-C18-C19
3	C	803	CPL	C16-C17-C18-C19
4	B	806	PX2	C17-C18-C19-C20
4	A	806	PX2	C17-C18-C19-C20
4	C	806	PX2	C17-C18-C19-C20
4	D	806	PX2	C17-C18-C19-C20
3	A	805	CPL	C12-C13-C14-C15
3	B	805	CPL	C12-C13-C14-C15
3	C	805	CPL	C12-C13-C14-C15
3	D	805	CPL	C12-C13-C14-C15
3	D	807	CPL	C15-C16-C17-C18
3	A	807	CPL	C15-C16-C17-C18
3	B	803	CPL	C15-C16-C17-C18
3	C	807	CPL	C15-C16-C17-C18
3	A	803	CPL	C15-C16-C17-C18
3	B	807	CPL	C15-C16-C17-C18
3	C	803	CPL	C15-C16-C17-C18
3	D	803	CPL	C15-C16-C17-C18
3	A	802	CPL	O3P-C1-C2-C3
3	A	807	CPL	O3P-C1-C2-C3
3	B	802	CPL	O3P-C1-C2-C3
3	B	807	CPL	O3P-C1-C2-C3
3	C	802	CPL	O3P-C1-C2-C3
3	C	807	CPL	O3P-C1-C2-C3
3	D	802	CPL	O3P-C1-C2-C3
3	D	807	CPL	O3P-C1-C2-C3
3	A	807	CPL	C1-C2-C3-O3
3	B	807	CPL	C1-C2-C3-O3
3	C	807	CPL	C1-C2-C3-O3
3	D	807	CPL	C1-C2-C3-O3
3	A	802	CPL	O3P-C1-C2-O2
3	B	802	CPL	O3P-C1-C2-O2
3	C	802	CPL	O3P-C1-C2-O2
3	D	802	CPL	O3P-C1-C2-O2
3	B	803	CPL	C13-C14-C15-C16
3	D	803	CPL	C13-C14-C15-C16
3	A	803	CPL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	C	803	CPL	C13-C14-C15-C16
3	A	802	CPL	C19-C20-C21-C22
3	B	802	CPL	C19-C20-C21-C22
3	C	802	CPL	C19-C20-C21-C22
3	D	802	CPL	C19-C20-C21-C22
3	A	807	CPL	O3P-C1-C2-O2
3	B	807	CPL	O3P-C1-C2-O2
3	C	807	CPL	O3P-C1-C2-O2
3	D	807	CPL	O3P-C1-C2-O2
3	D	804	CPL	C15-C16-C17-C18
3	A	804	CPL	C15-C16-C17-C18
3	B	804	CPL	C15-C16-C17-C18
3	C	804	CPL	C15-C16-C17-C18
3	A	807	CPL	O2-C2-C3-O3
3	B	807	CPL	O2-C2-C3-O3
3	C	807	CPL	O2-C2-C3-O3
3	D	807	CPL	O2-C2-C3-O3
3	A	807	CPL	C1-O3P-P-O4P
3	B	807	CPL	C1-O3P-P-O4P
3	C	807	CPL	C1-O3P-P-O4P
3	D	807	CPL	C1-O3P-P-O4P
3	B	802	CPL	C18-C19-C20-C21
3	C	802	CPL	C18-C19-C20-C21
3	D	802	CPL	C18-C19-C20-C21
3	A	802	CPL	C18-C19-C20-C21
4	A	806	PX2	C1-O4-P1-O3
4	B	806	PX2	C1-O4-P1-O3
4	C	806	PX2	C1-O4-P1-O3
4	D	806	PX2	C1-O4-P1-O3
3	D	802	CPL	C17-C18-C19-C20
3	A	802	CPL	C17-C18-C19-C20
3	C	802	CPL	C17-C18-C19-C20
3	B	802	CPL	C17-C18-C19-C20
3	B	805	CPL	C17-C18-C19-C20
3	C	805	CPL	C17-C18-C19-C20
3	A	805	CPL	C17-C18-C19-C20
3	D	805	CPL	C17-C18-C19-C20
3	A	802	CPL	O11-C11-O3-C3
3	B	802	CPL	O11-C11-O3-C3
3	C	802	CPL	O11-C11-O3-C3
3	D	802	CPL	O11-C11-O3-C3
3	D	803	CPL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	A	803	CPL	C14-C15-C16-C17
3	B	803	CPL	C14-C15-C16-C17
3	C	803	CPL	C14-C15-C16-C17
3	A	804	CPL	C17-C18-C19-C20
3	B	804	CPL	C17-C18-C19-C20
3	C	804	CPL	C17-C18-C19-C20
3	D	804	CPL	C17-C18-C19-C20
3	A	802	CPL	C12-C11-O3-C3
3	B	802	CPL	C12-C11-O3-C3
3	C	802	CPL	C12-C11-O3-C3
3	D	802	CPL	C12-C11-O3-C3
3	D	805	CPL	C16-C17-C18-C19
3	A	805	CPL	C16-C17-C18-C19
3	B	805	CPL	C16-C17-C18-C19
3	C	805	CPL	C16-C17-C18-C19

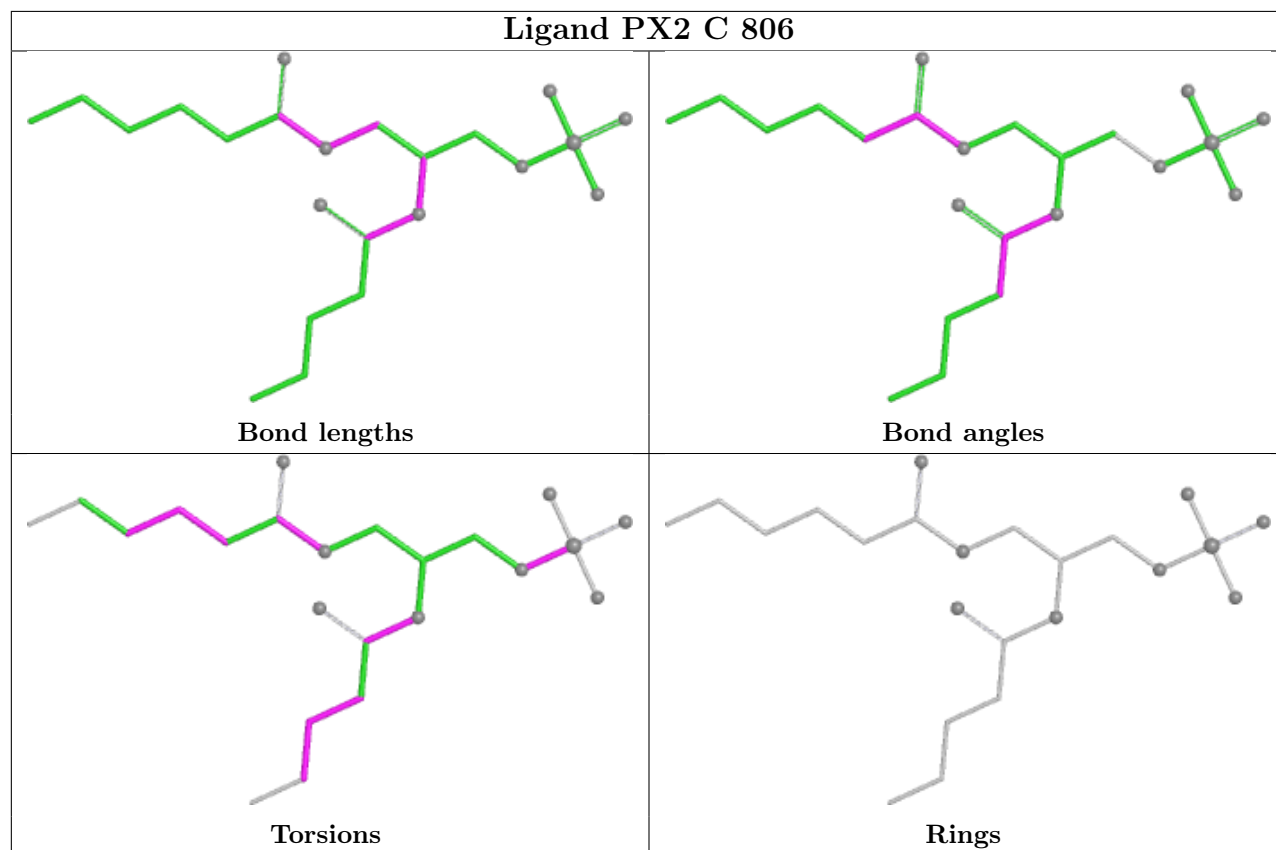
There are no ring outliers.

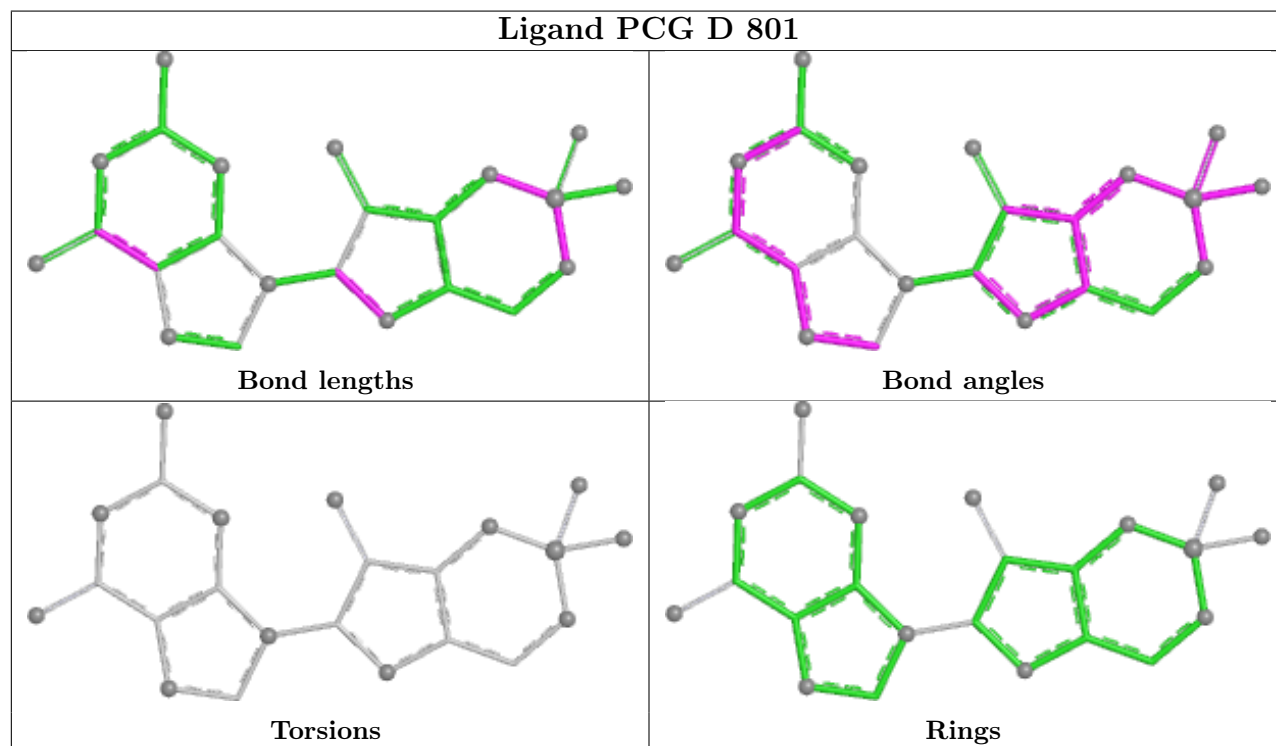
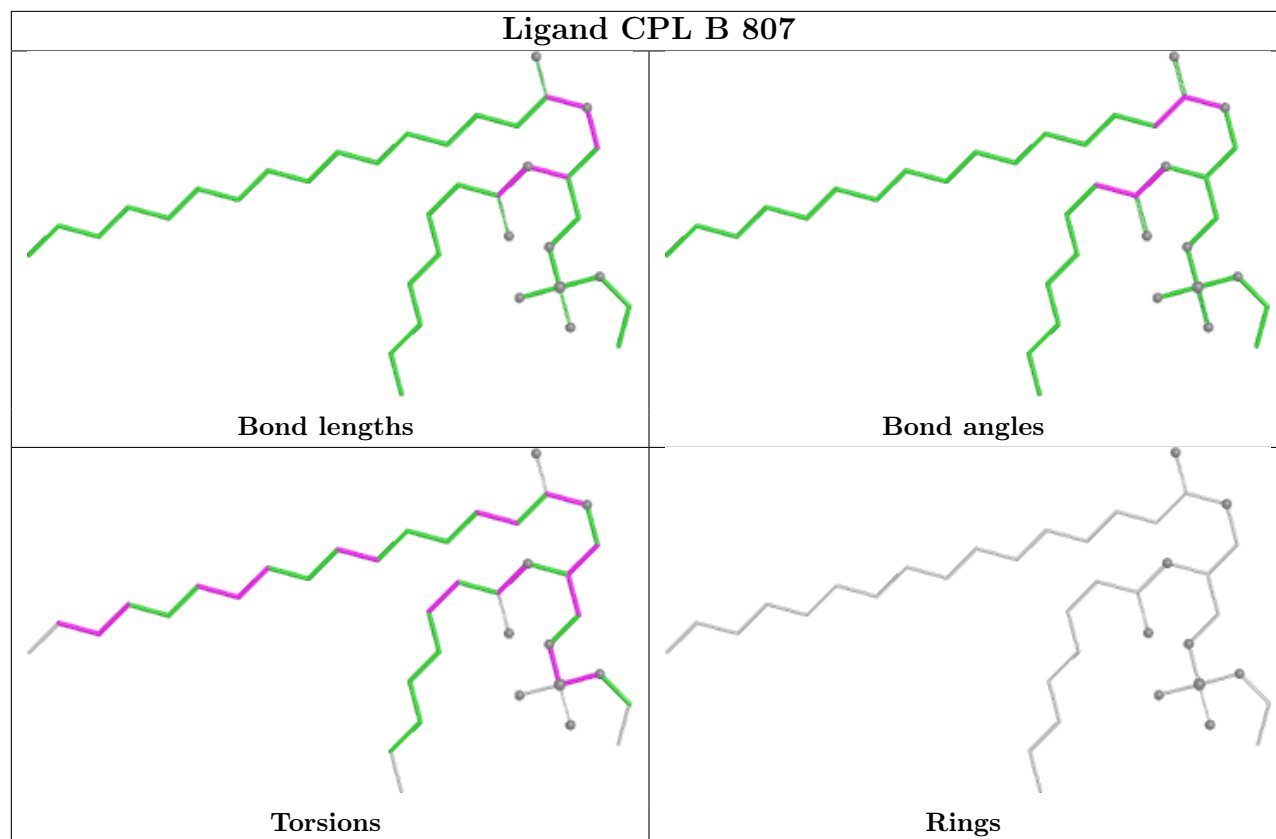
12 monomers are involved in 12 short contacts:

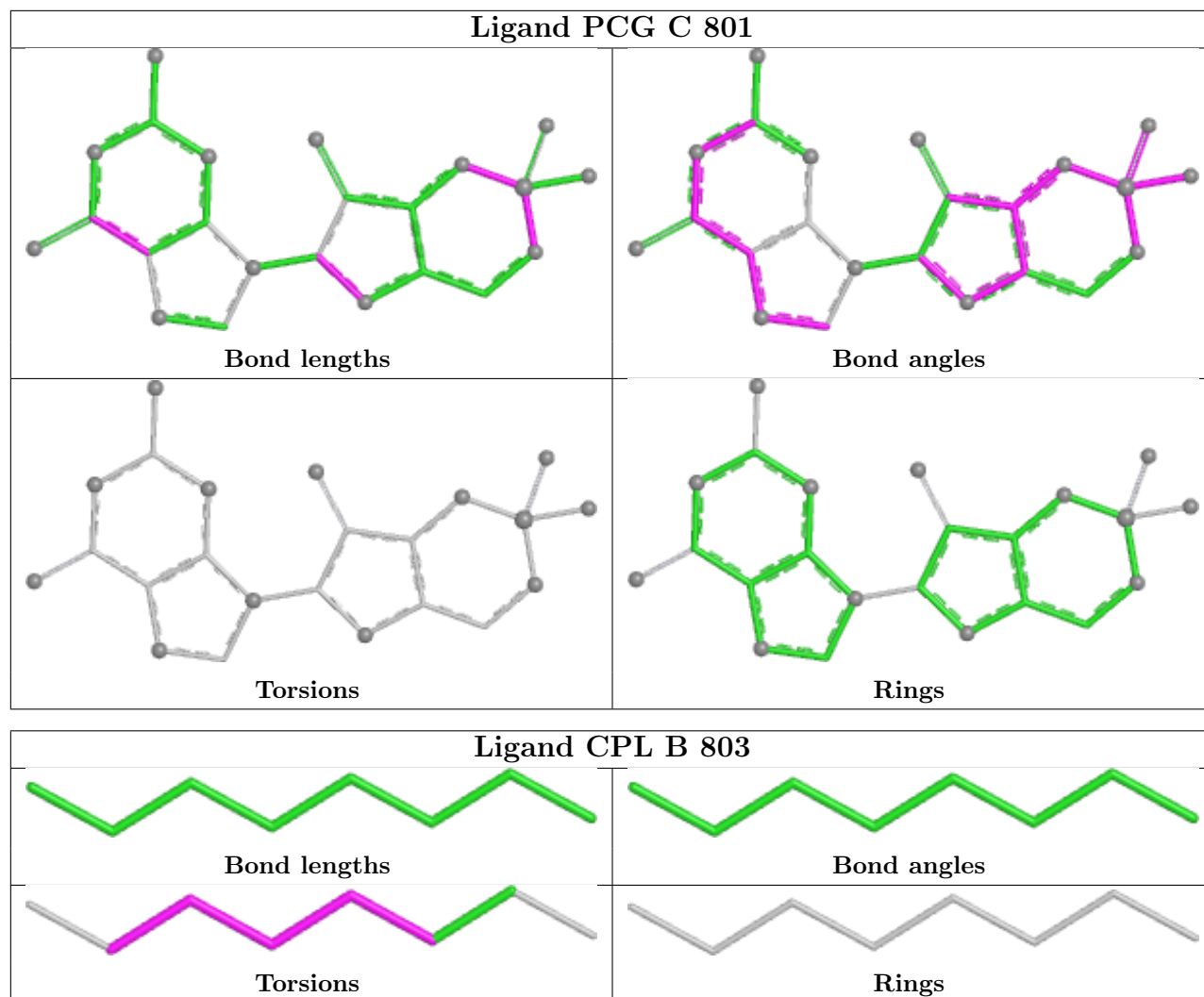
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	806	PX2	1	0
3	D	804	CPL	1	0
4	D	806	PX2	1	0
3	B	804	CPL	1	0
3	A	804	CPL	1	0
3	A	802	CPL	1	0
3	B	802	CPL	1	0
3	D	802	CPL	1	0
4	A	806	PX2	1	0
3	C	804	CPL	1	0
3	C	802	CPL	1	0
4	B	806	PX2	1	0

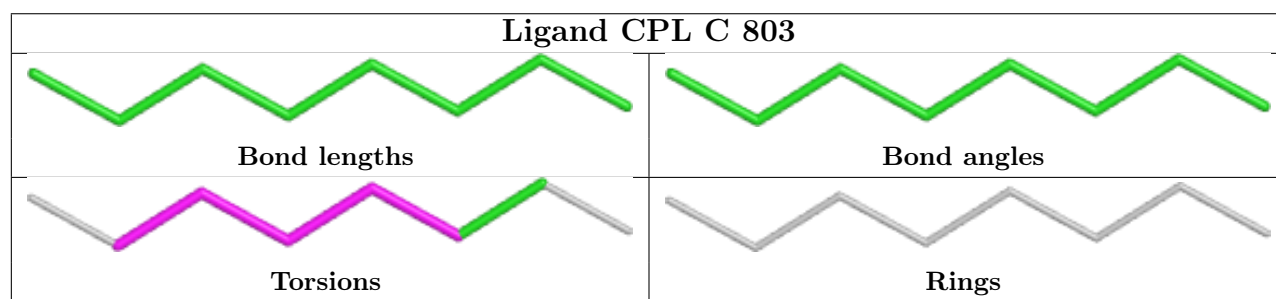
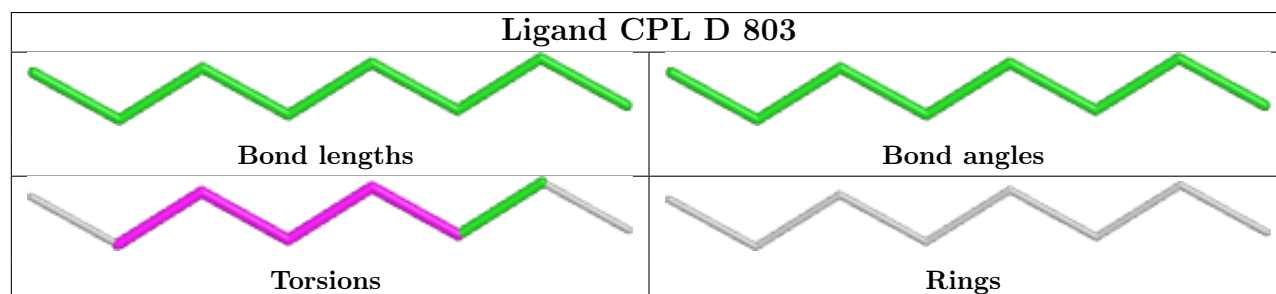
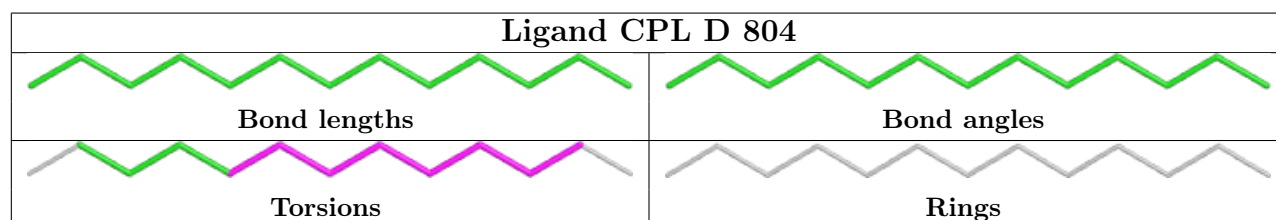
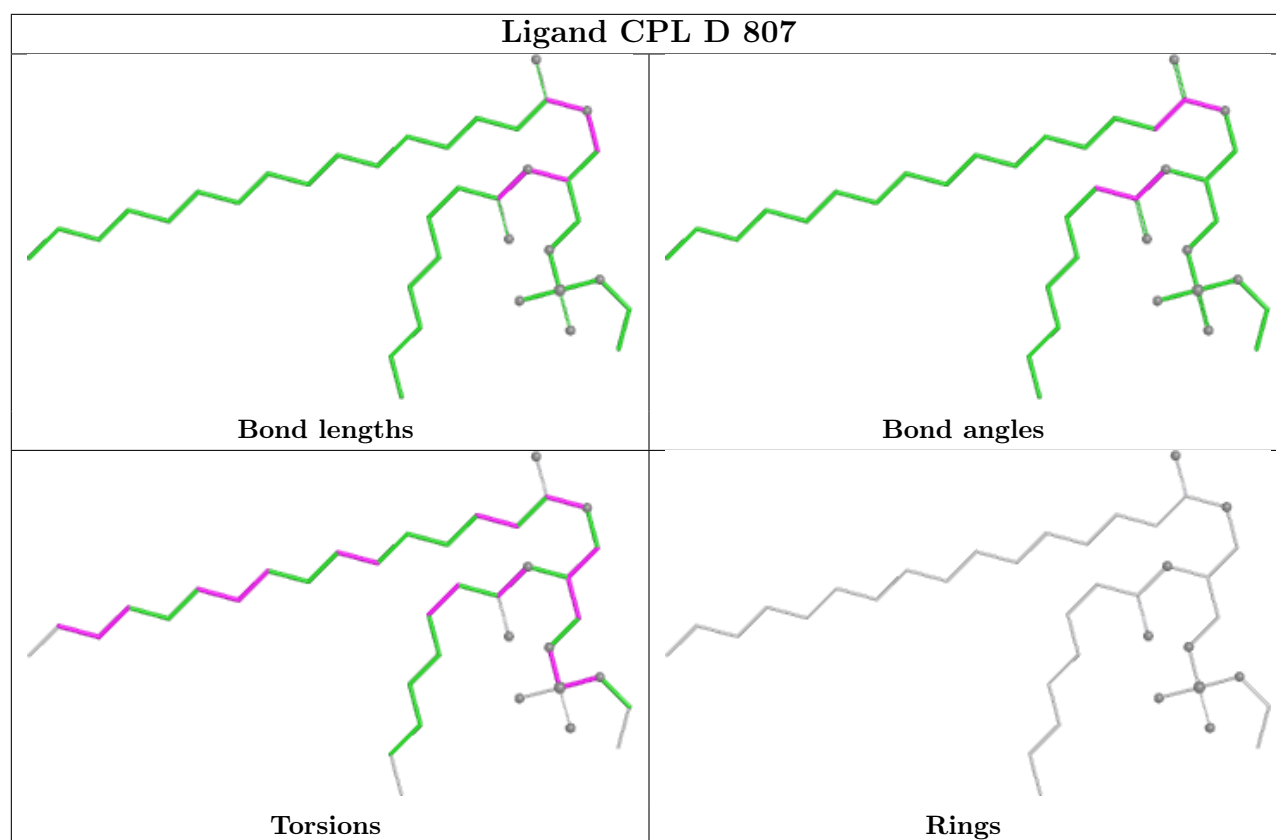
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

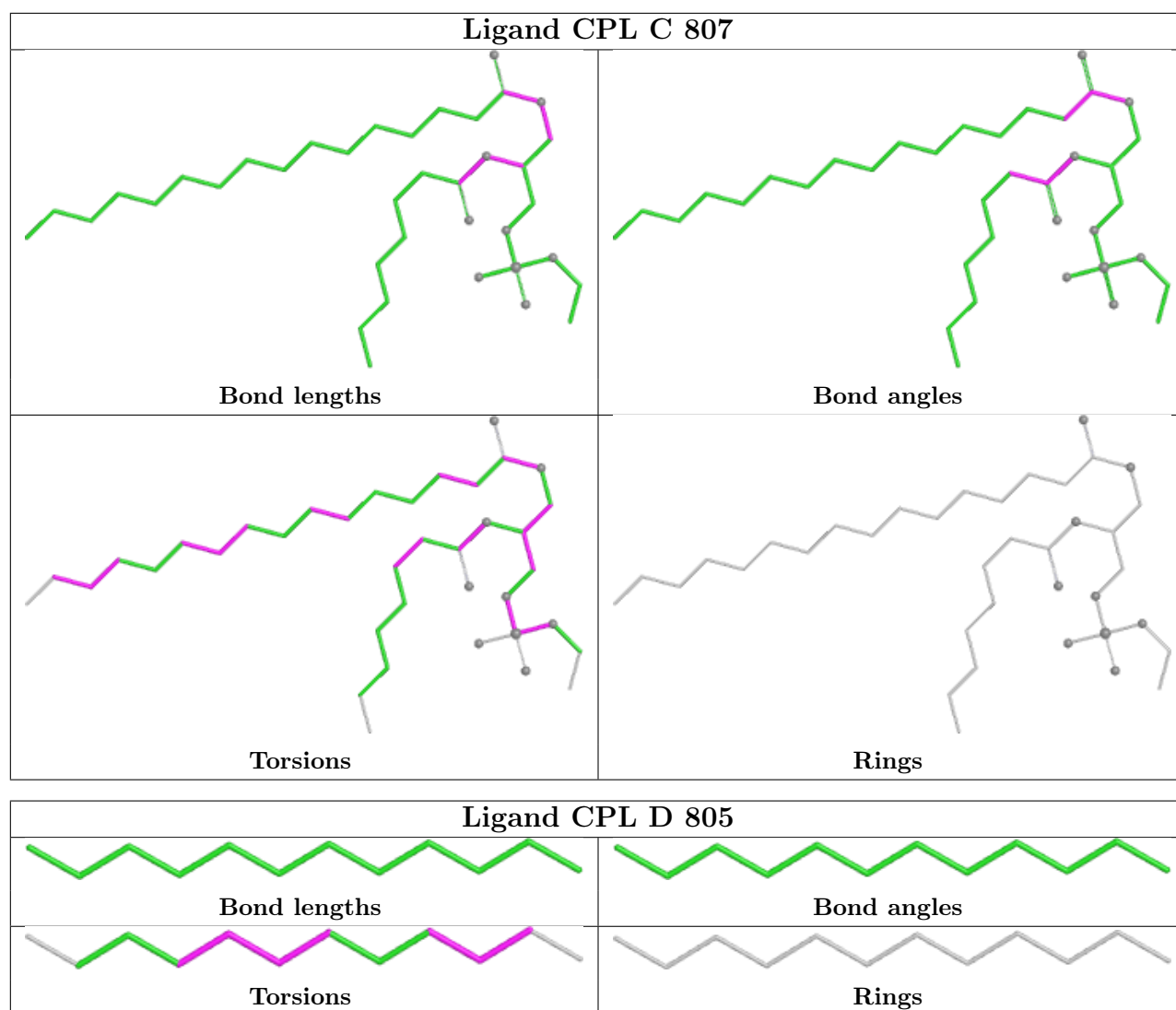
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

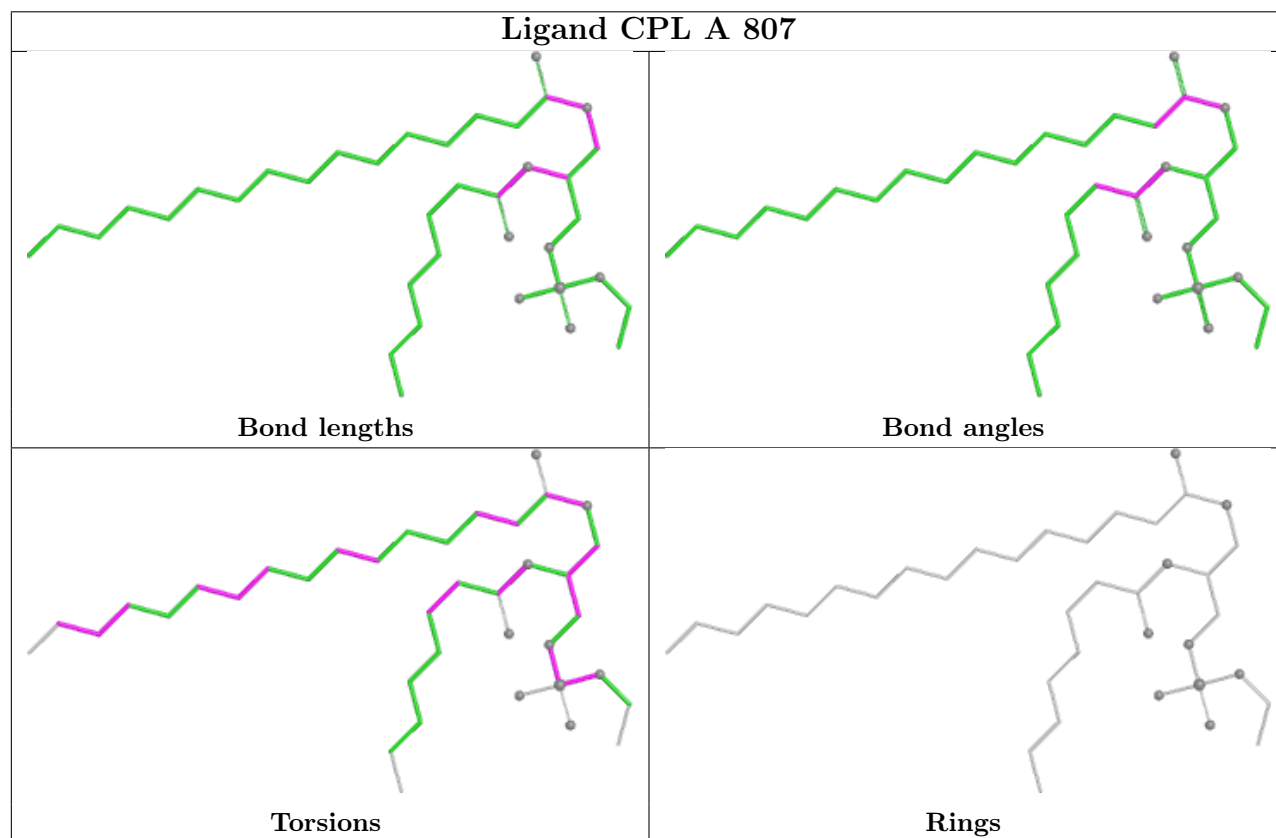
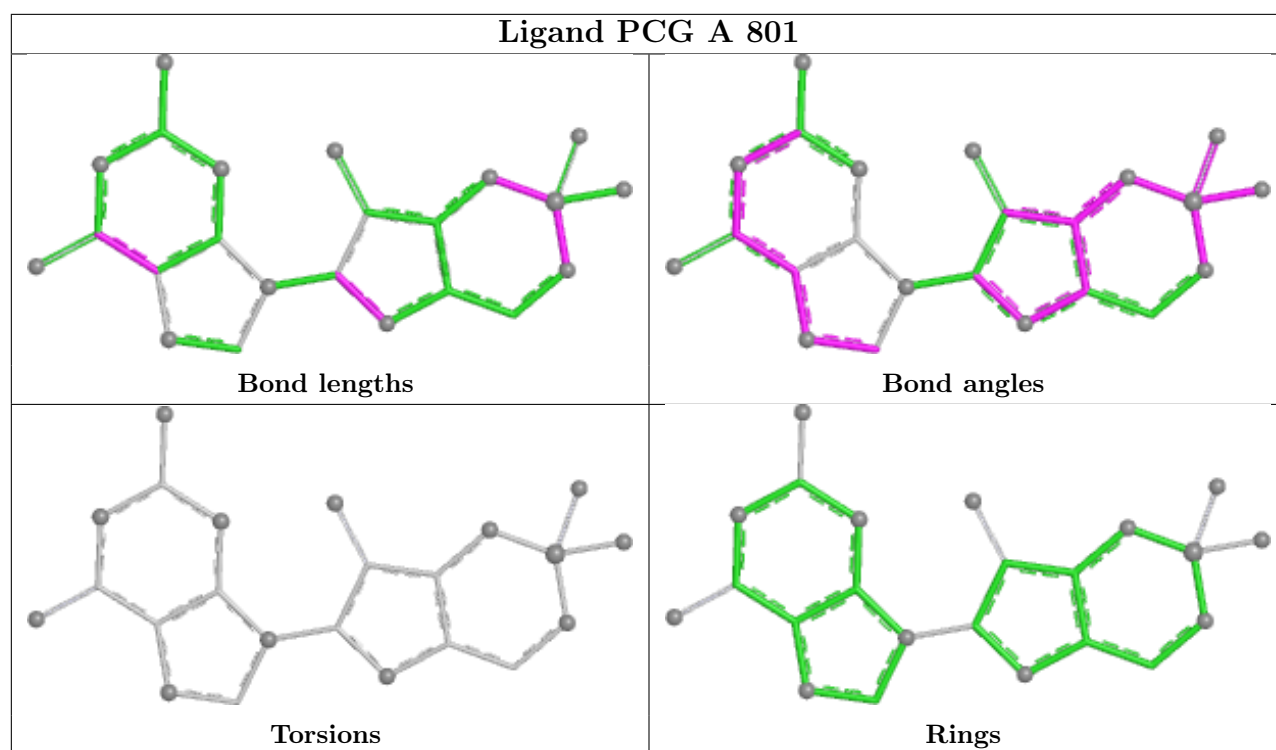


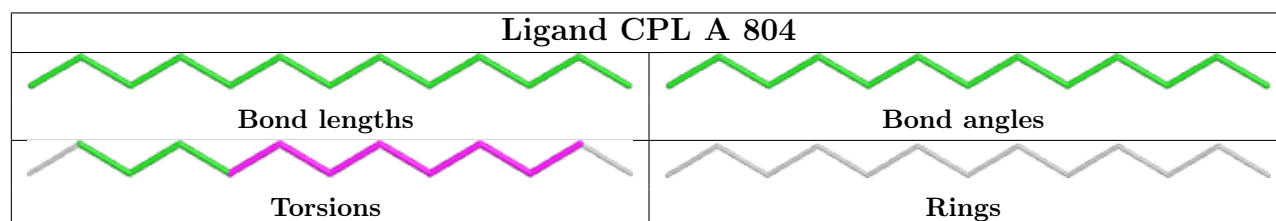
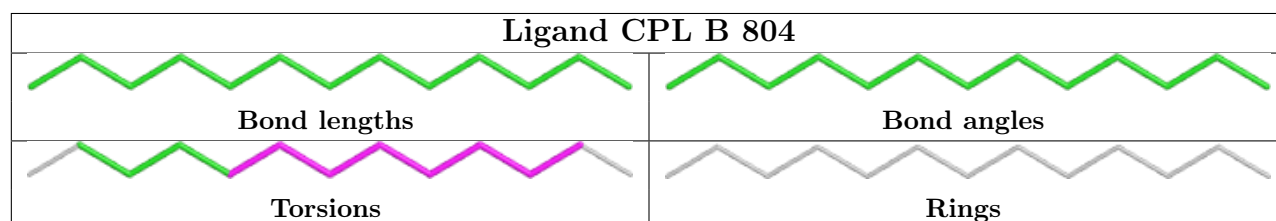
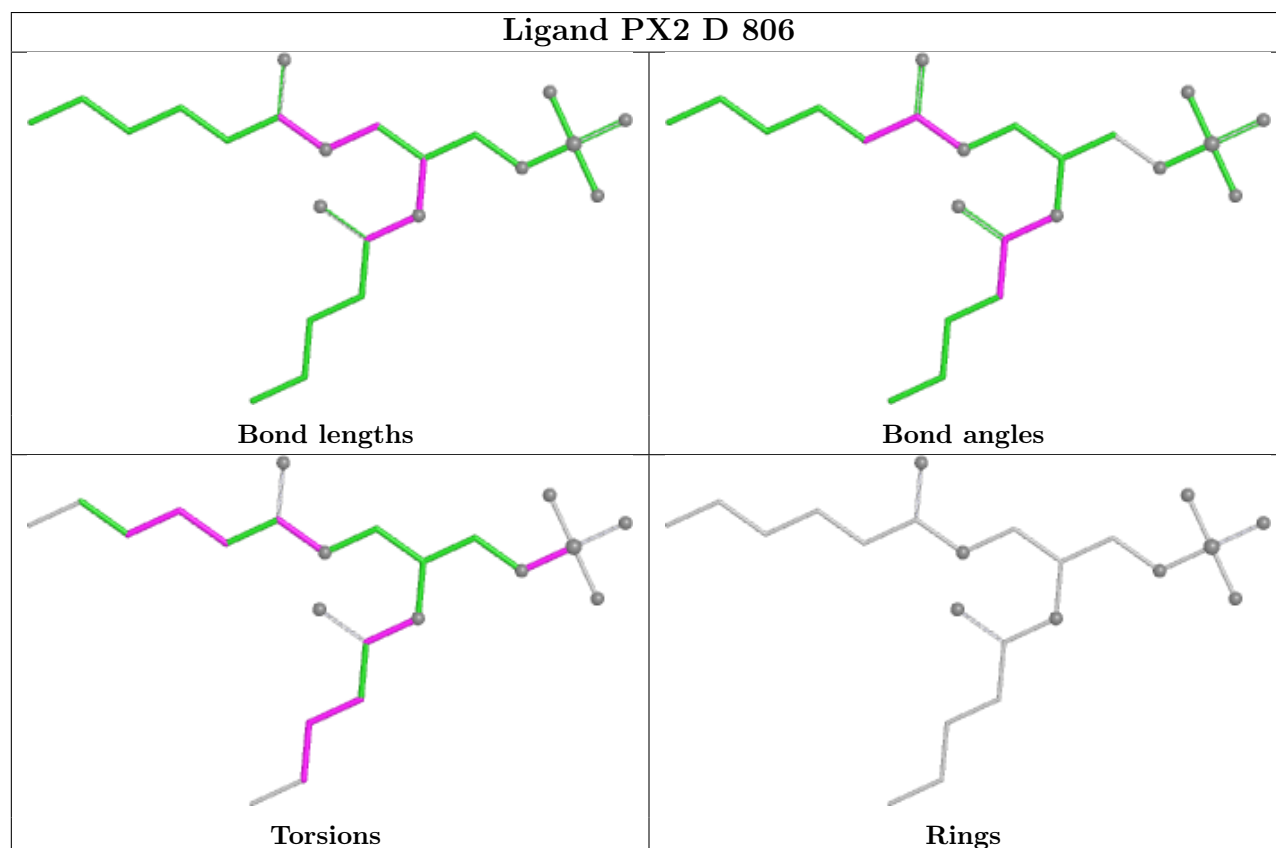
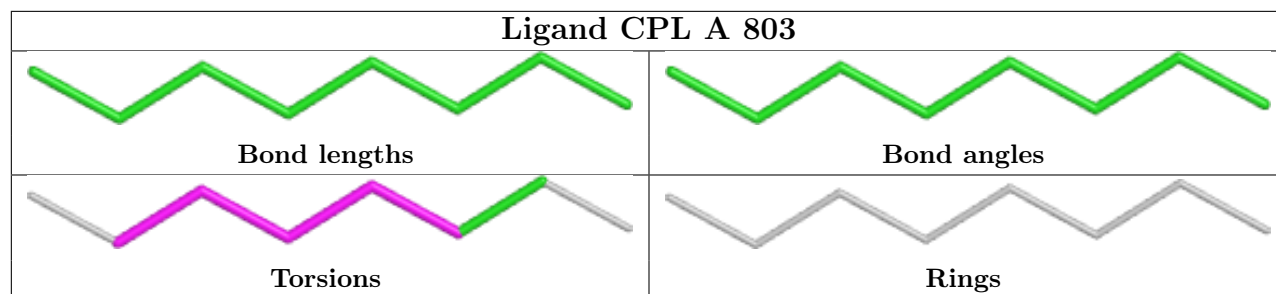


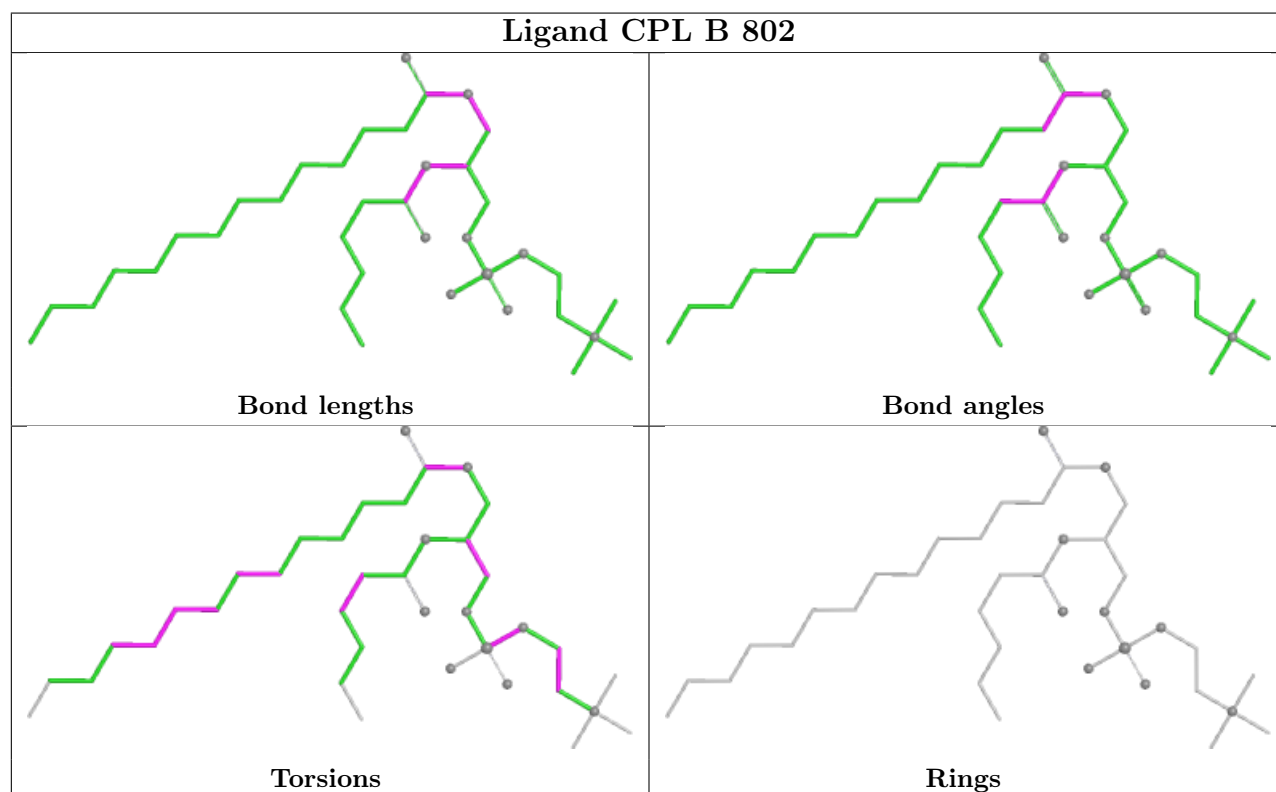
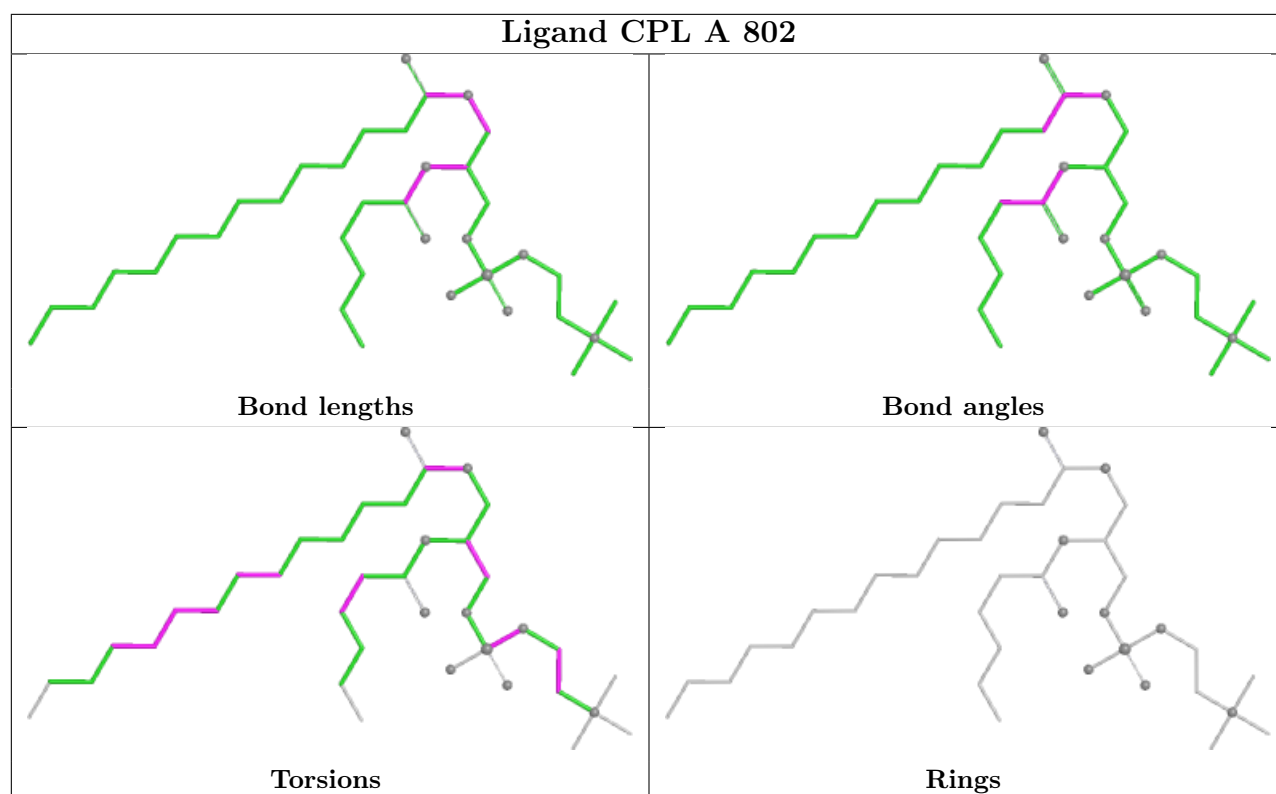


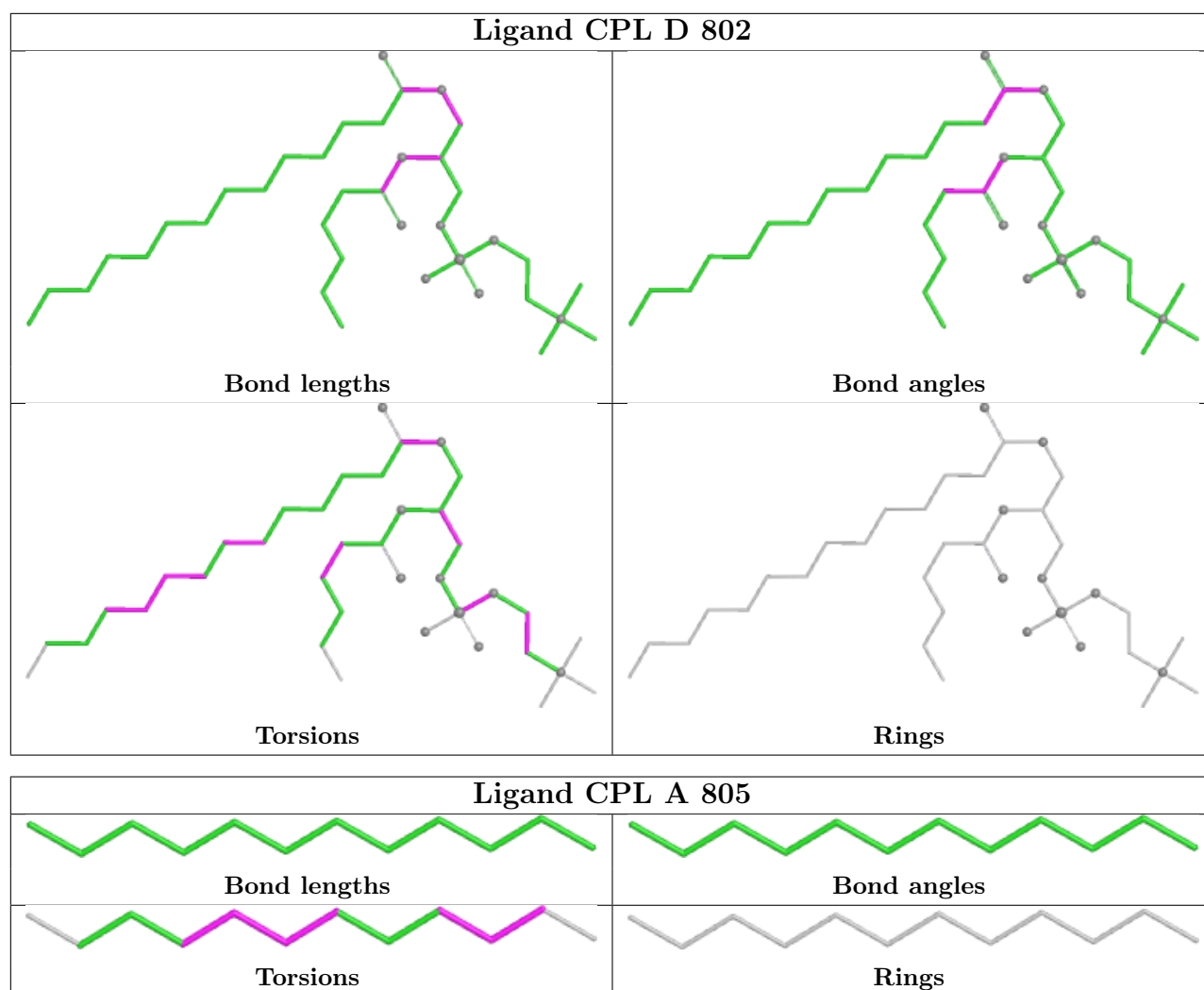


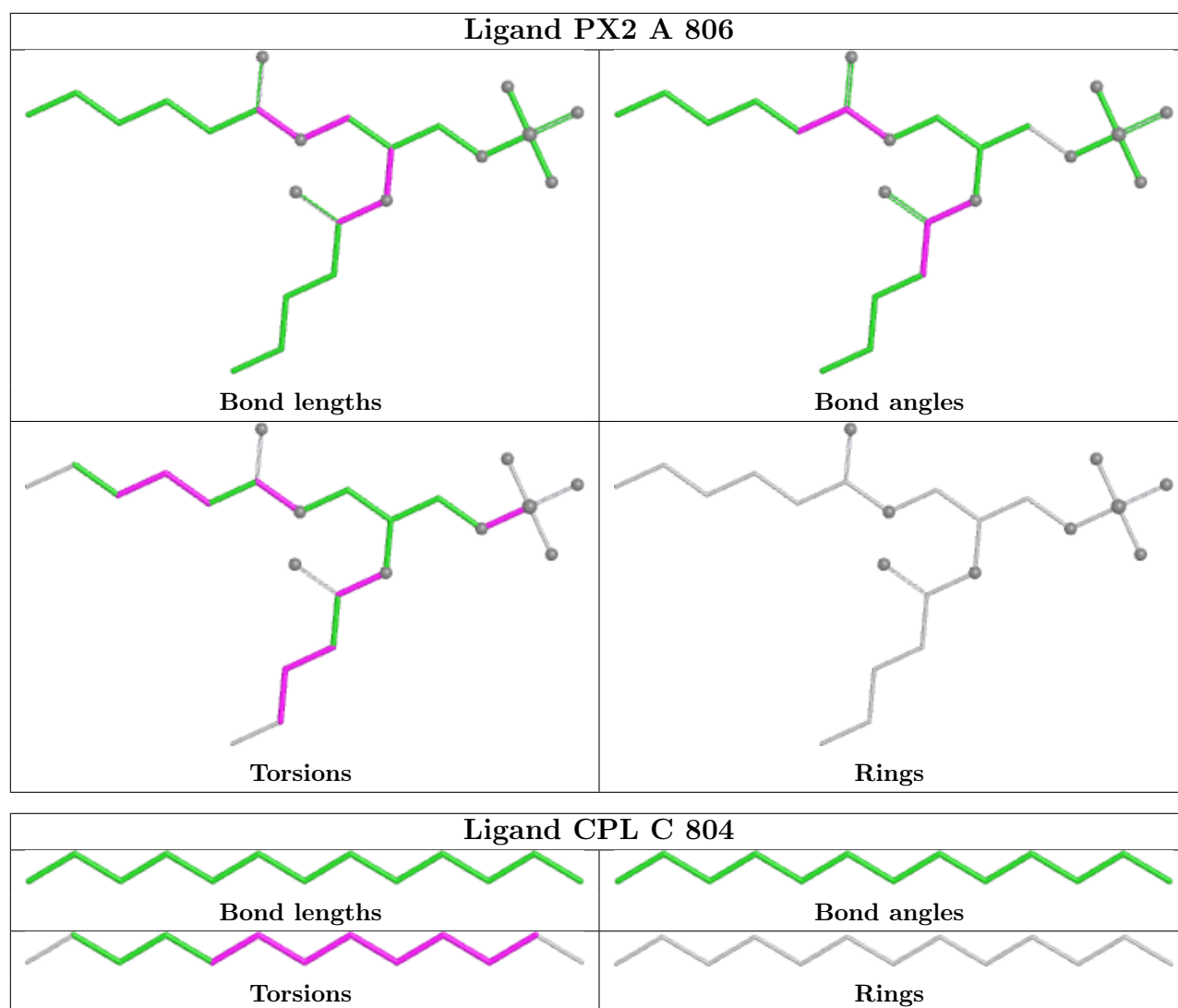


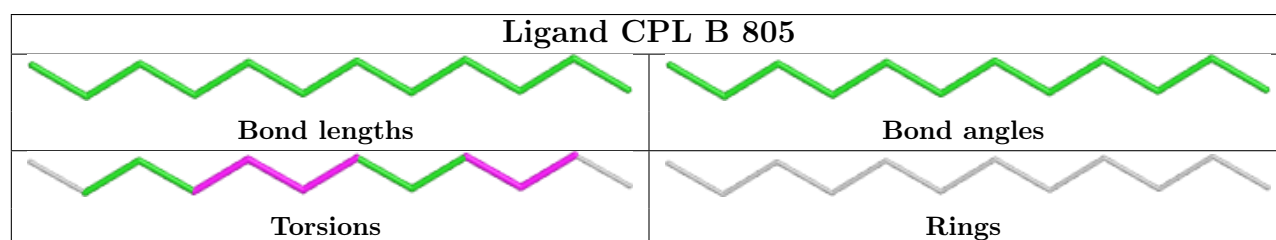
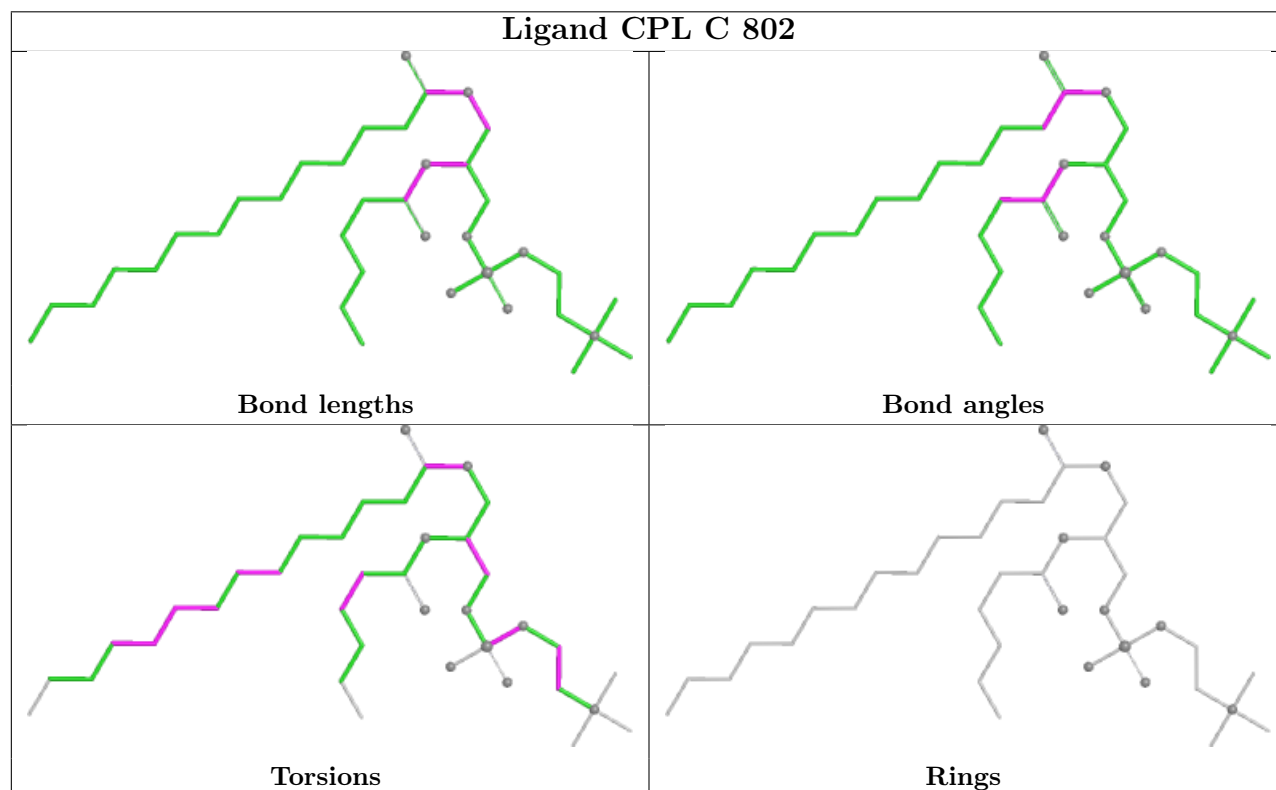
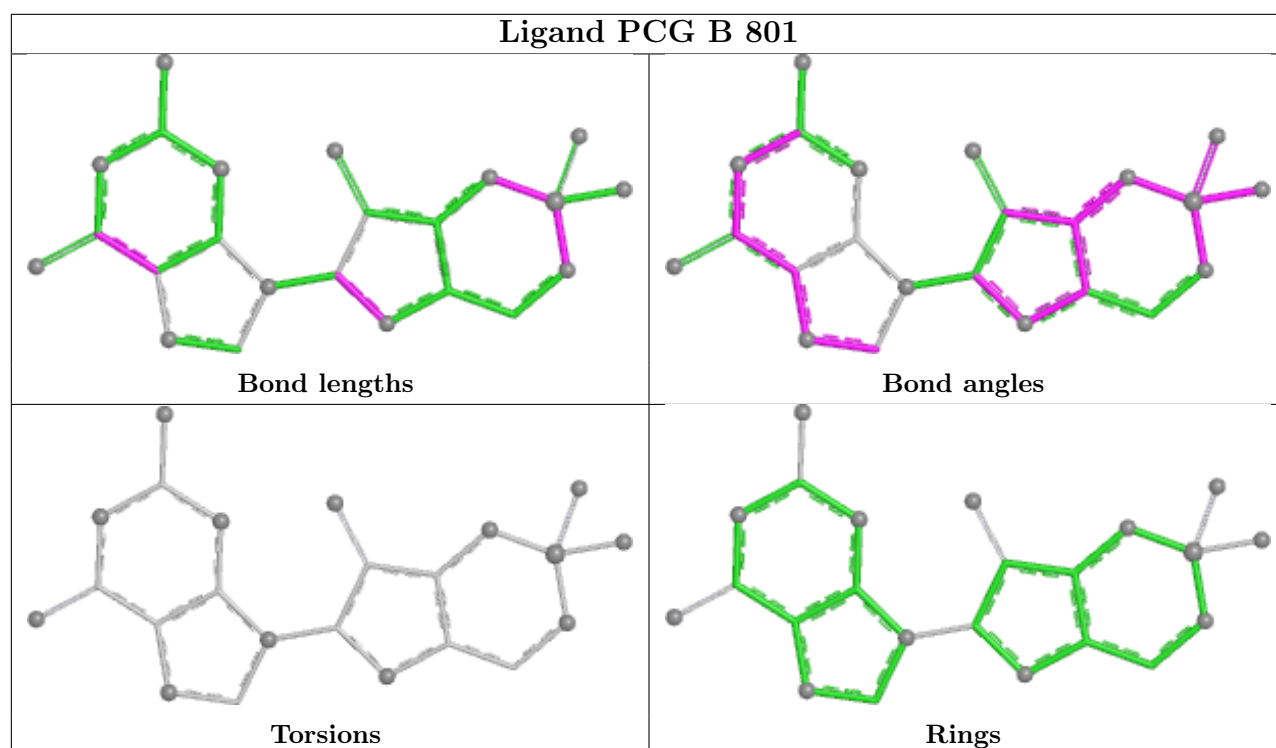


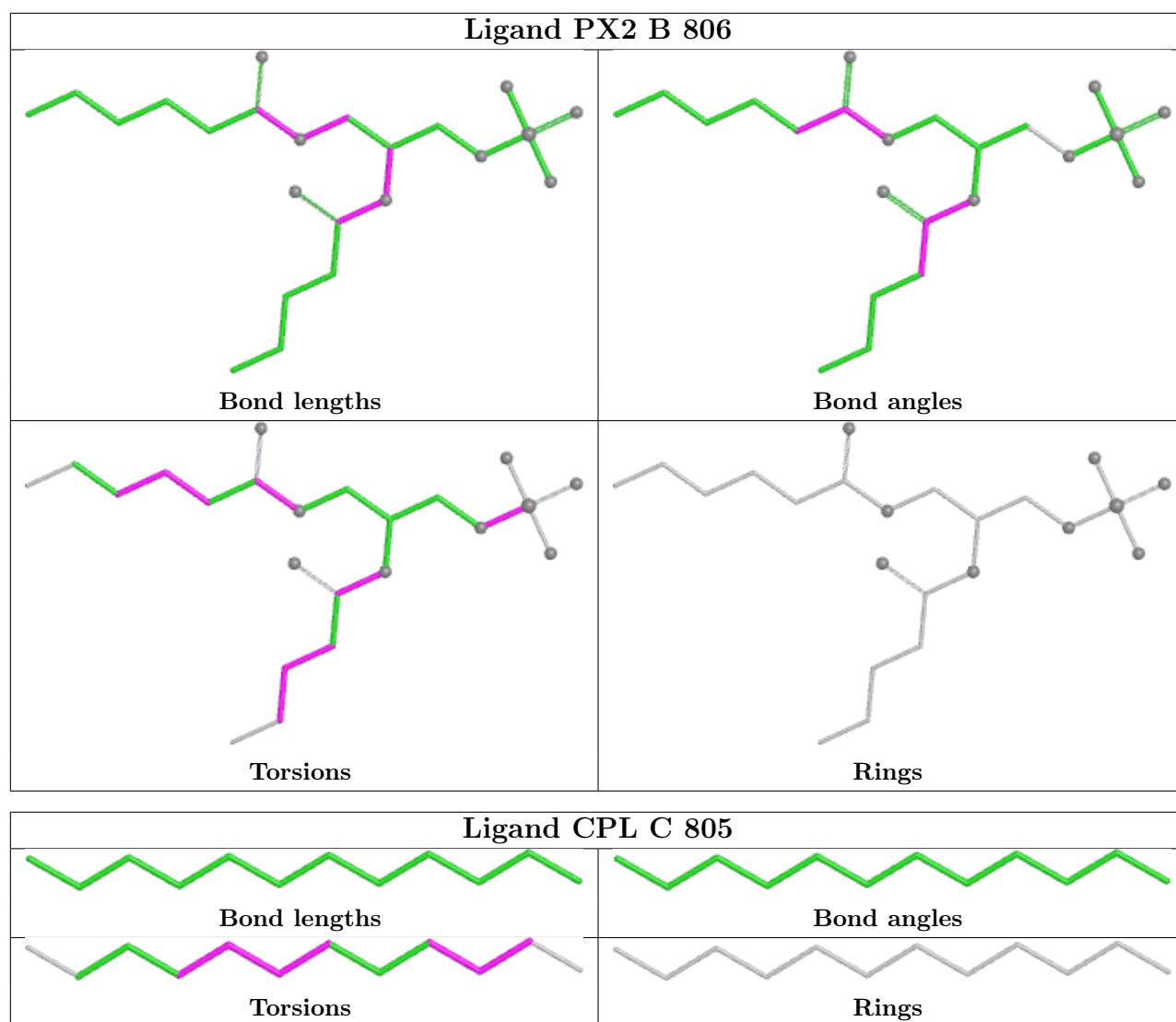












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

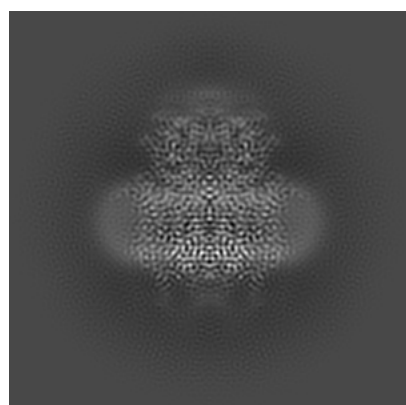
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24113. These allow visual inspection of the internal detail of the map and identification of artifacts.

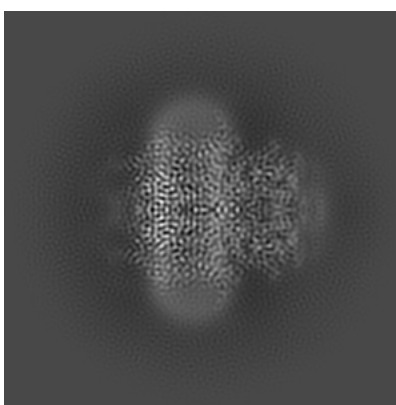
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

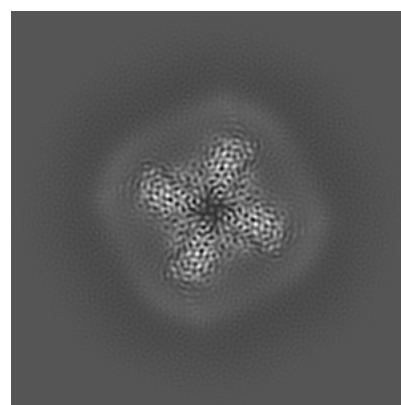
6.1.1 Primary map



X



Y

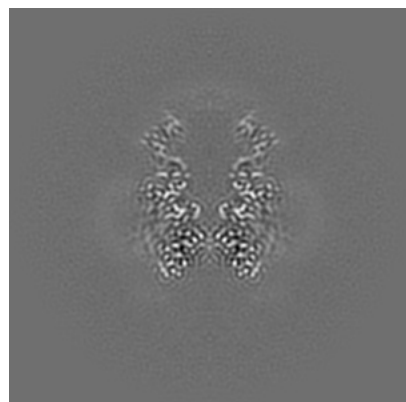


Z

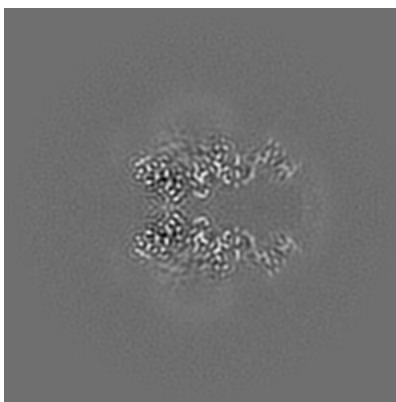
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

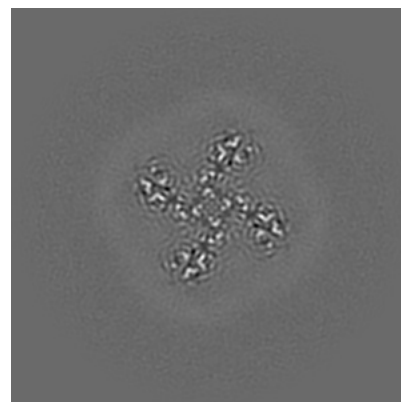
6.2.1 Primary map



X Index: 148



Y Index: 148

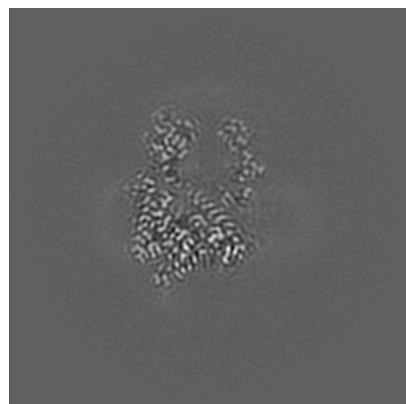


Z Index: 148

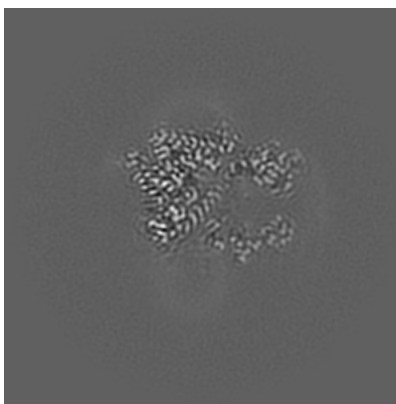
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

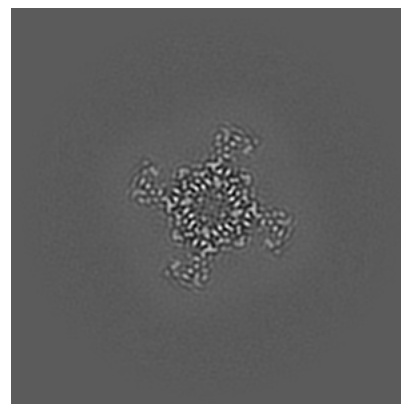
6.3.1 Primary map



X Index: 137



Y Index: 137

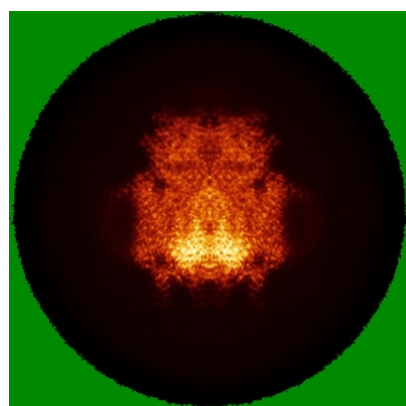


Z Index: 117

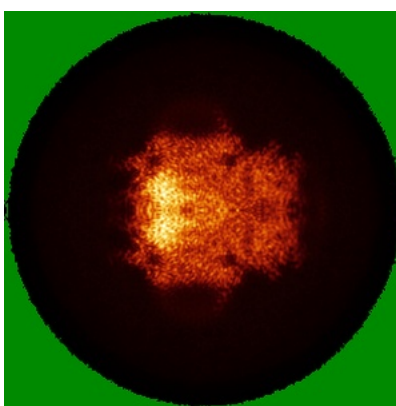
The images above show the largest variance slices of the map in three orthogonal directions.

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

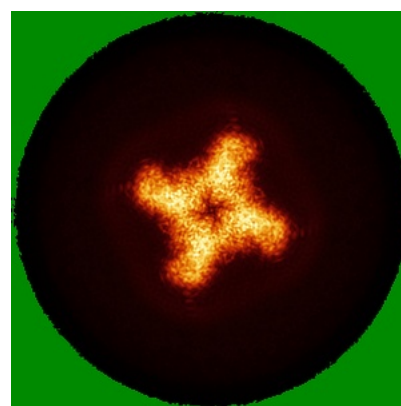
6.4.1 Primary map



X



Y

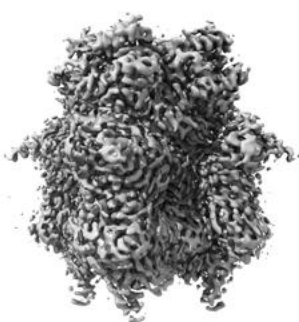


Z

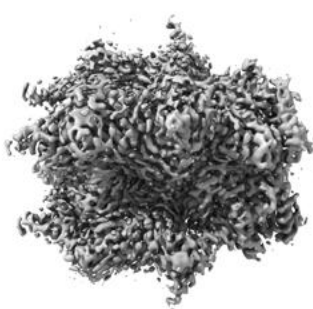
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

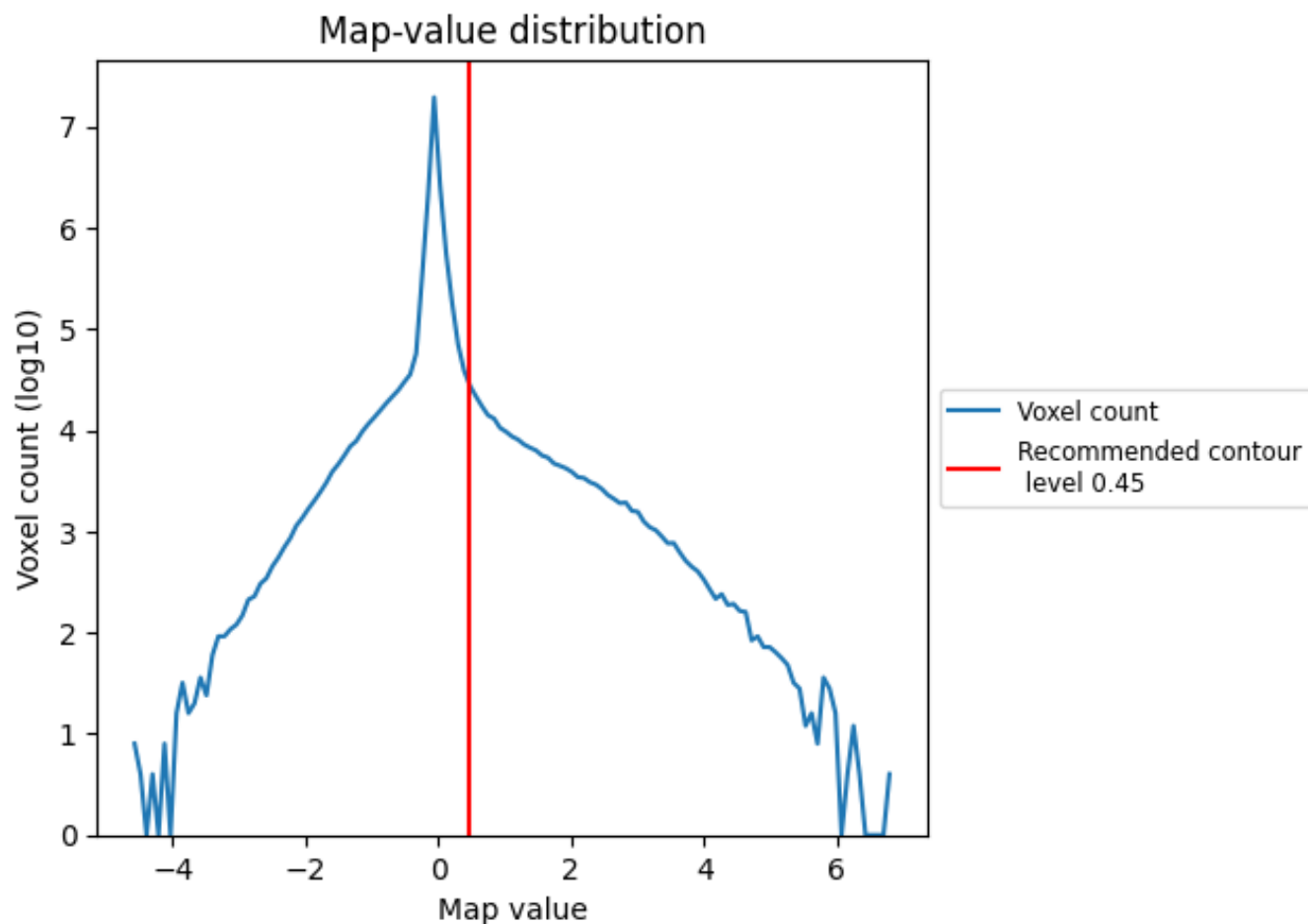
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

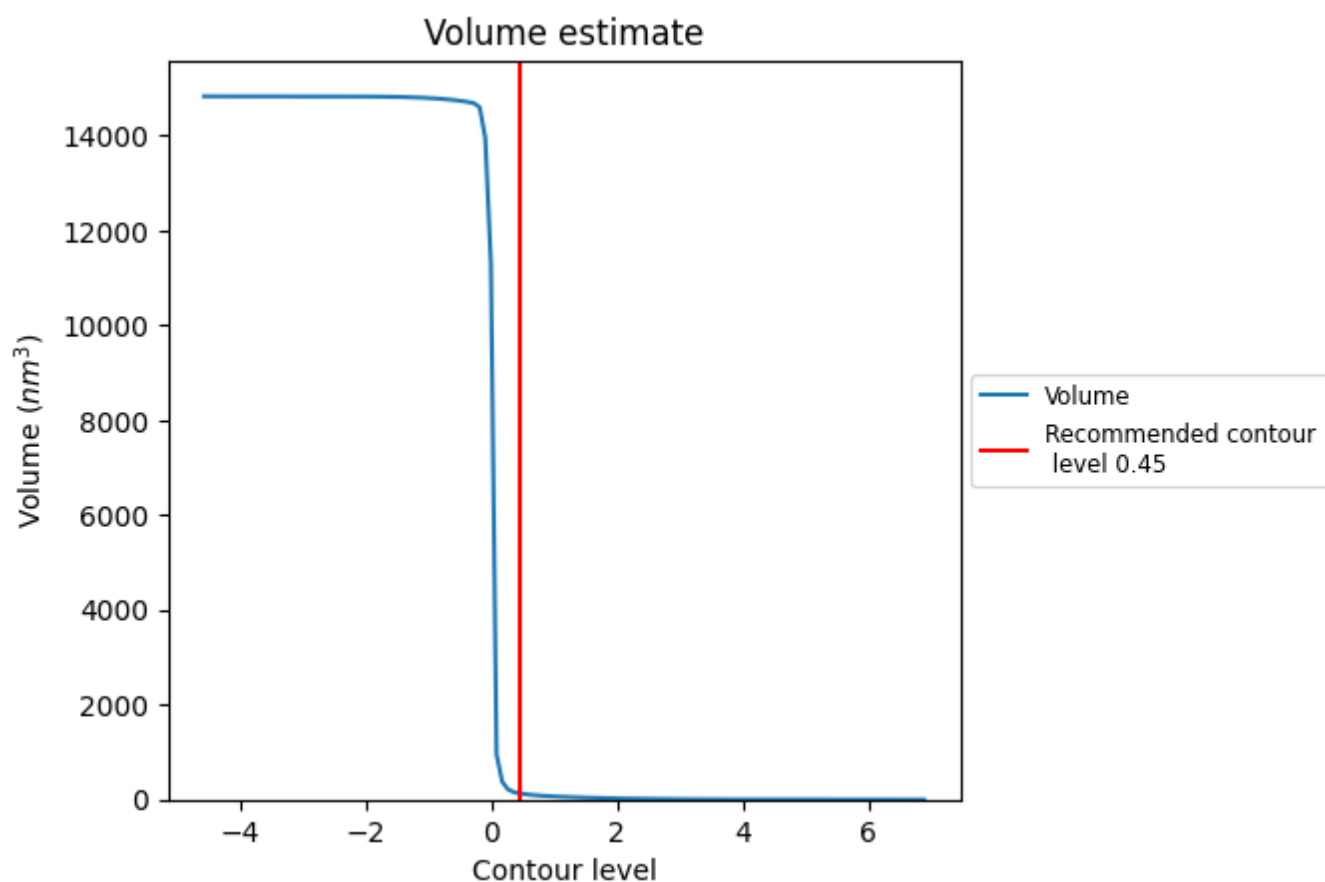
This section contains the results of statistical analysis of the map.

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.

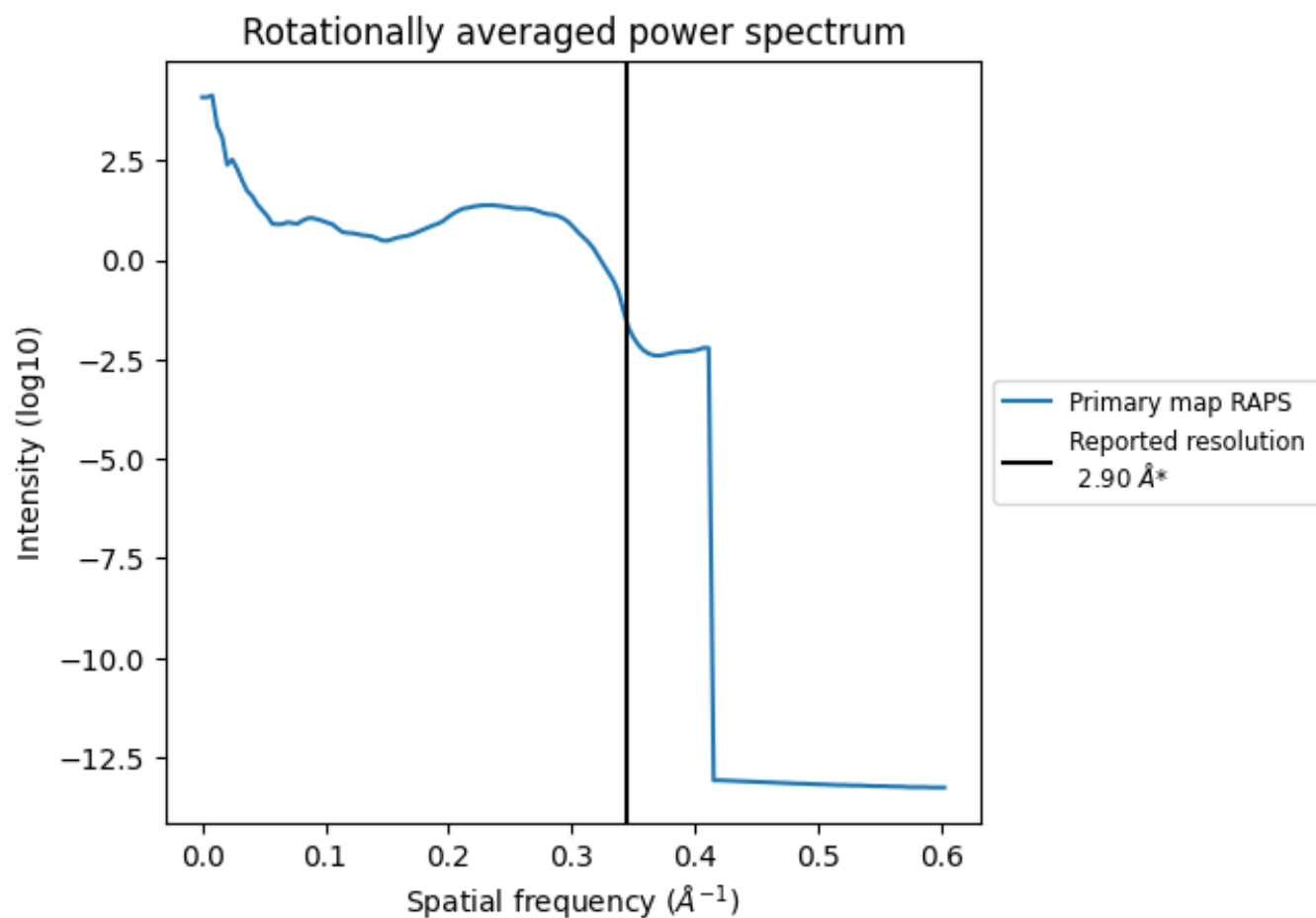
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm^3 ; this corresponds to an approximate mass of 117 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 0.345 Å⁻¹

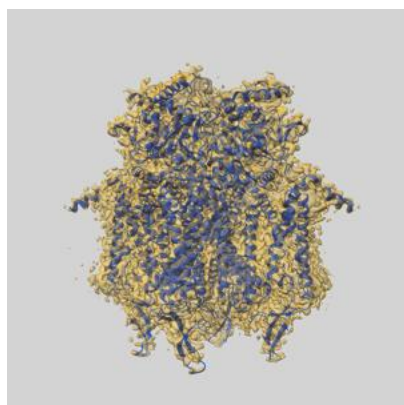
8 Fourier-Shell correlation

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

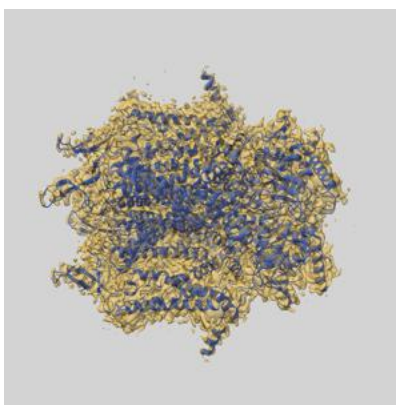
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24113 and PDB model 7N15. Per-residue inclusion information can be found in section [3](#) on page [7](#).

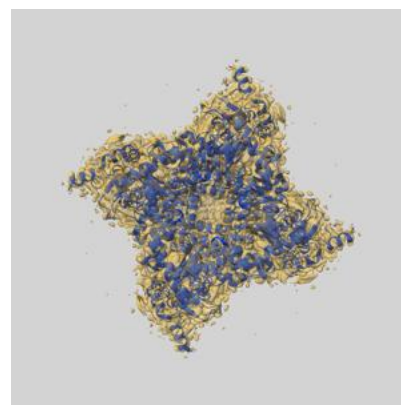
9.1 Map-model overlay [i](#)



X



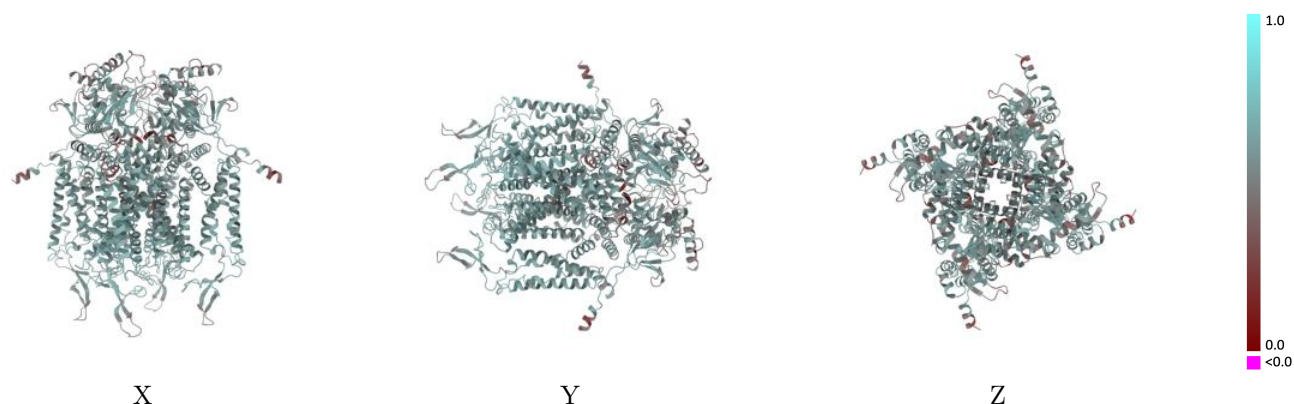
Y



Z

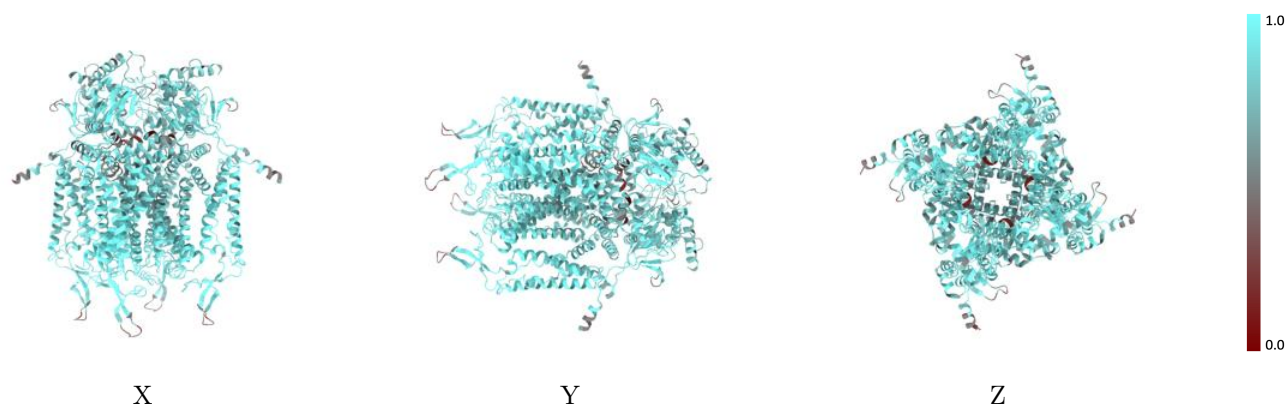
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



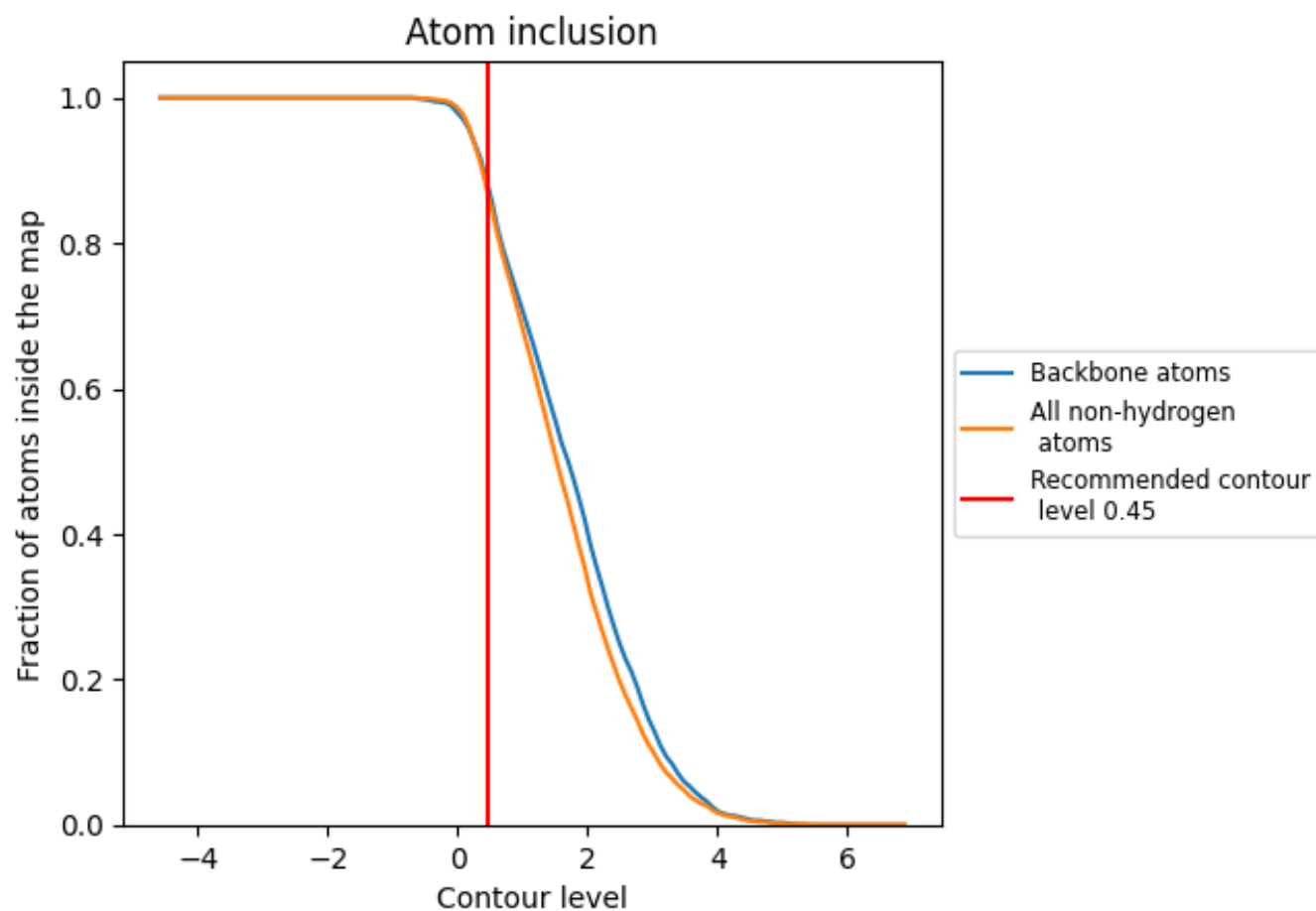
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8740	<div></div> 0.5710
A	<div></div> 0.8740	<div></div> 0.5710
B	<div></div> 0.8740	<div></div> 0.5710
C	<div></div> 0.8740	<div></div> 0.5720
D	<div></div> 0.8750	<div></div> 0.5710

