



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:14 AM UTC

PDB ID : 6WEK / pdb_00006wek
EMDB ID : EMD-21650
Title : Structure of cGMP-bound WT TAX-4 reconstituted in lipid nanodiscs
Authors : Zheng, X.; Fu, Z.; Su, D.; Zhang, Y.; Li, M.; Pan, Y.; Li, H.; Li, S.; Grassucci, R.A.; Ren, Z.; Hu, Z.; Li, X.; Zhou, M.; Li, G.; Frank, J.; Yang, J.
Deposited on : 2020-04-02
Resolution : 2.70 Å(reported)
Based on initial model : 5H3O

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

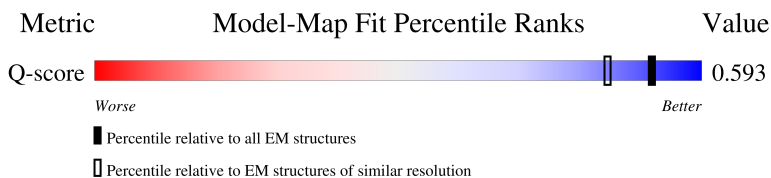
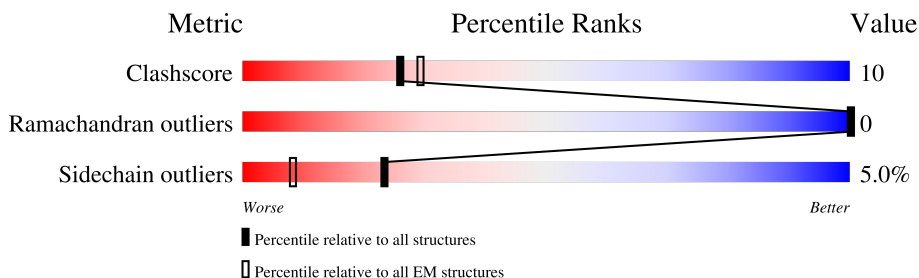
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	733	
1	B	733	
1	C	733	
1	D	733	

2 Entry composition [i](#)

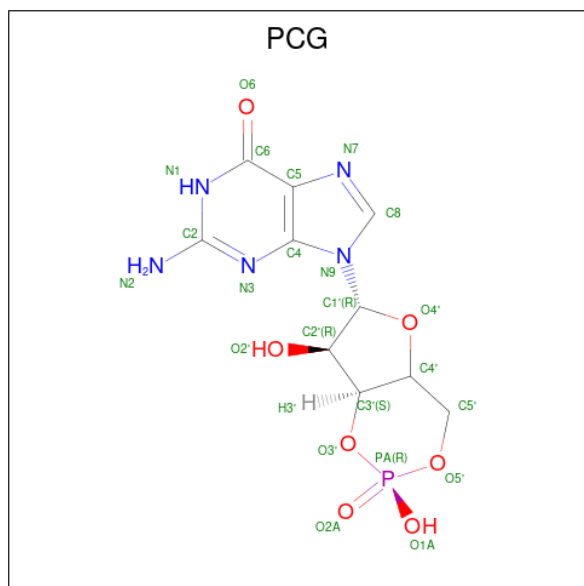
There are 4 unique types of molecules in this entry. The entry contains 17616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	512	Total	C	N	O	S	1	0
			4243	2760	714	745	24		
1	B	512	Total	C	N	O	S	1	0
			4243	2760	714	745	24		
1	C	512	Total	C	N	O	S	1	0
			4243	2760	714	745	24		
1	D	512	Total	C	N	O	S	1	0
			4243	2760	714	745	24		

- Molecule 2 is CYCLIC GUANOSINE MONOPHOSPHATE (CCD ID: PCG) (formula: $C_{10}H_{12}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



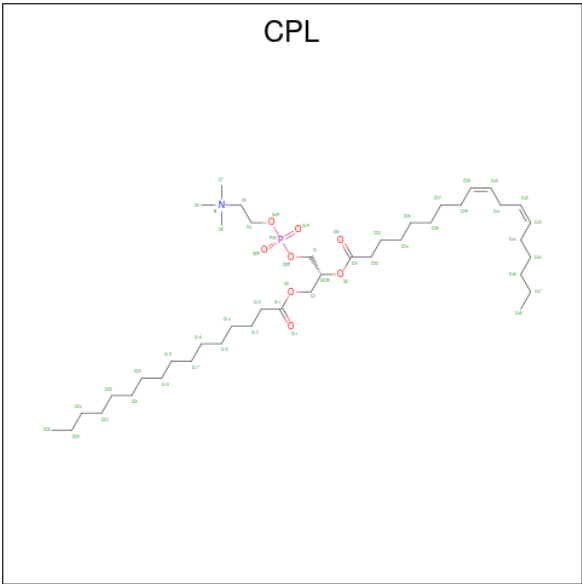
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	B	1	Total	C	N	O	P	0
			23	10	5	7	1	

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Mol	Chain	Residues	Atoms					AltConf
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 (CCD ID: CPL) (formula: C₄₂H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).



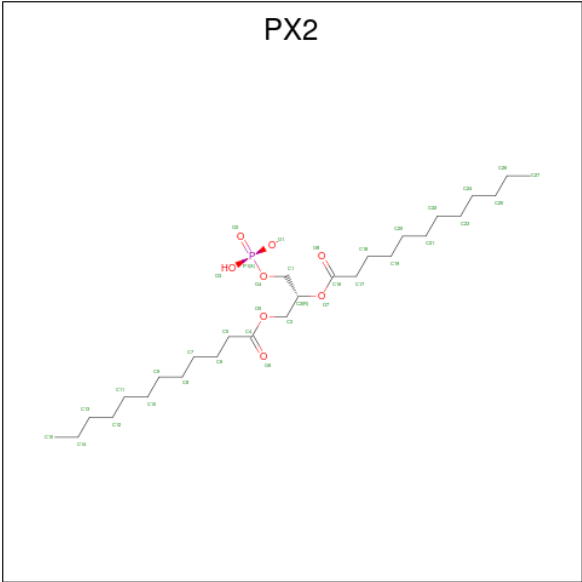
Mol	Chain	Residues	Atoms					AltConf	
3	A	1	Total 38	C 28	N 1	O 8	P 1	0	
3	A	1	Total 8		C 8				0
3	A	1	Total 6		C 6				0
3	A	1	Total 13		C 13				0
3	A	1	Total 12		C 12				0
3	A	1	Total 38	C 29	O 8	P 1			0
3	B	1	Total 38	C 28	N 1	O 8	P 1		0
3	B	1	Total 8		C 8				0
3	B	1	Total 6		C 6				0

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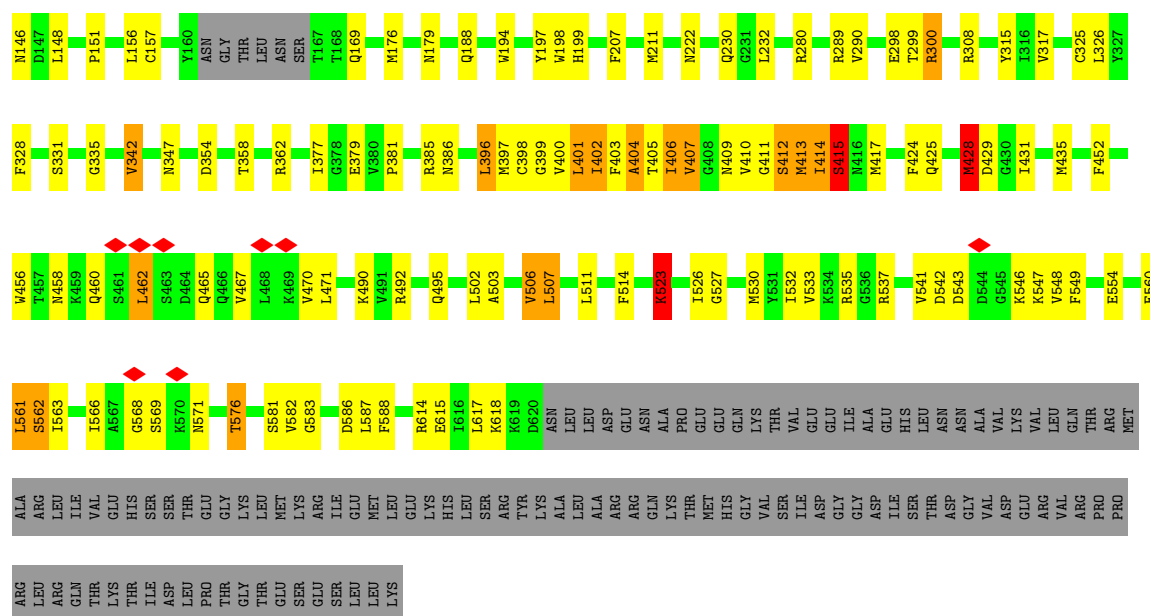
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C			0
			13	13			
3	B	1	Total	C			0
			12	12			
3	B	1	Total	C	O	P	0
			38	29	8	1	
3	C	1	Total	C	N	O	P
			38	28	1	8	1
3	C	1	Total	C			0
			8	8			
3	C	1	Total	C			0
			6	6			
3	C	1	Total	C			0
			13	13			
3	C	1	Total	C			0
			12	12			
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
			6	6			
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	

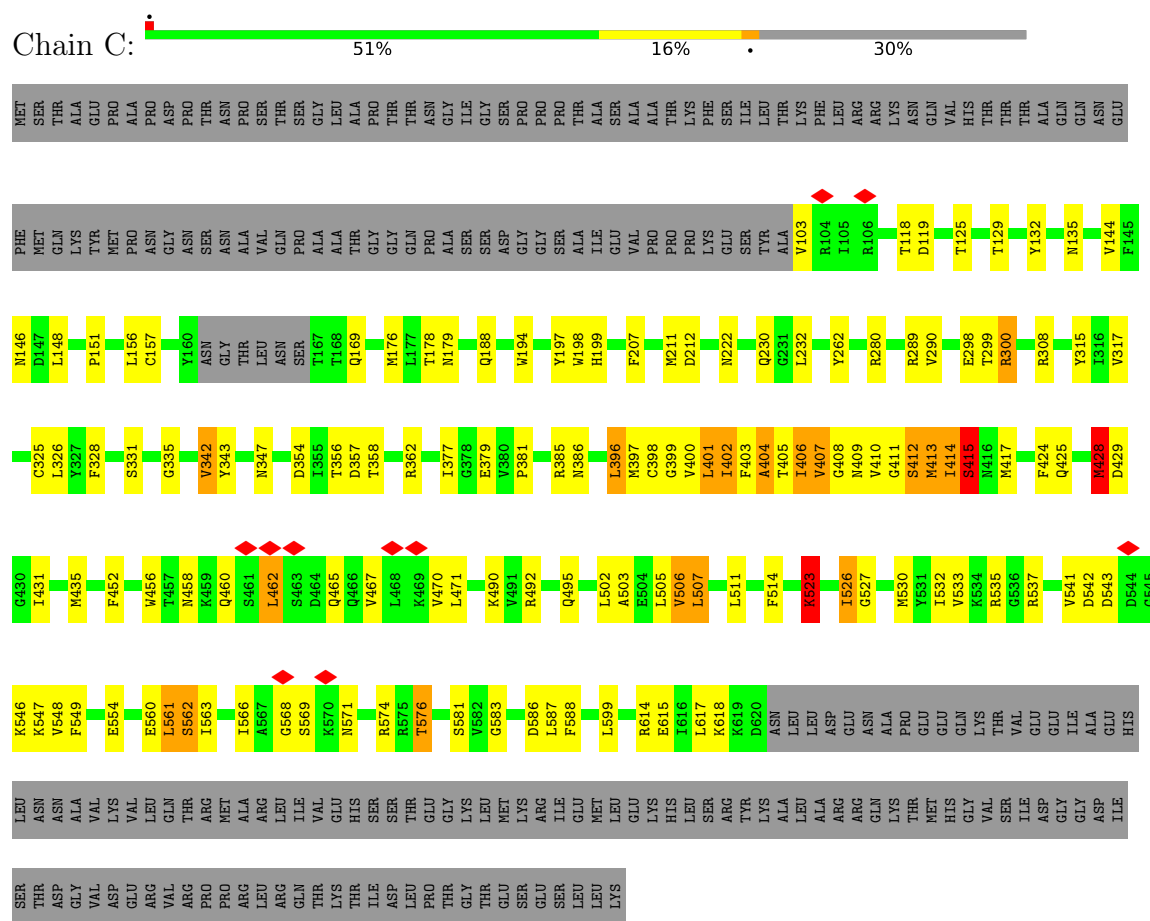
- Molecule 4 is 1,2-DILAULOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$) (labeled as "Ligand of Interest" by depositor).



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	



• Molecule 1: Cyclic nucleotide-gated cation channel



• Molecule 1: Cyclic nucleotide-gated cation channel



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	128685	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 ($e^-/\text{\AA}^2$)	66.03	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.567	Depositor
Minimum map value	-4.132	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.641	Depositor
Map size ($\text{\AA}$)	316.72, 316.72, 316.72	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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, CPL, PX2

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	0.96	40/4345 (0.9%)	0.66	16/5892 (0.3%)
1	B	0.96	40/4345 (0.9%)	0.66	16/5892 (0.3%)
1	C	0.96	41/4345 (0.9%)	0.66	16/5892 (0.3%)
1	D	0.96	40/4345 (0.9%)	0.66	16/5892 (0.3%)
All	All	0.96	161/17380 (0.9%)	0.66	64/23568 (0.3%)

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	CYS	C-O	-13.89	1.07	1.24
1	D	398	CYS	C-O	-13.86	1.07	1.24
1	B	398	CYS	C-O	-13.85	1.07	1.24
1	C	398	CYS	C-O	-13.83	1.07	1.24
1	A	428	MET	C-O	-12.95	1.08	1.24
1	B	428	MET	C-O	-12.93	1.08	1.24
1	D	428	MET	C-O	-12.91	1.09	1.24
1	C	428	MET	C-O	-12.89	1.09	1.24
1	C	399	GLY	C-O	-11.98	1.09	1.23
1	A	399	GLY	C-O	-11.95	1.09	1.23
1	B	399	GLY	C-O	-11.94	1.09	1.23
1	D	399	GLY	C-O	-11.94	1.09	1.23
1	D	409	ASN	C-O	-11.47	1.10	1.24
1	B	409	ASN	C-O	-11.43	1.10	1.24
1	A	409	ASN	C-O	-11.43	1.10	1.24
1	C	409	ASN	C-O	-11.43	1.10	1.24
1	C	404	ALA	C-O	-10.54	1.11	1.24
1	A	404	ALA	C-O	-10.51	1.11	1.24
1	B	404	ALA	C-O	-10.51	1.11	1.24
1	D	404	ALA	C-O	-10.51	1.11	1.24
1	D	406	ILE	CA-C	-10.20	1.40	1.52
1	A	406	ILE	CA-C	-10.19	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	406	ILE	CA-C	-10.19	1.40	1.52
1	B	396	LEU	C-O	-10.18	1.12	1.24
1	C	396	LEU	C-O	-10.18	1.12	1.24
1	A	396	LEU	C-O	-10.17	1.12	1.24
1	D	396	LEU	C-O	-10.15	1.12	1.24
1	C	406	ILE	CA-C	-10.12	1.40	1.52
1	C	409	ASN	CA-C	-9.72	1.40	1.52
1	D	409	ASN	CA-C	-9.70	1.40	1.52
1	B	409	ASN	CA-C	-9.65	1.40	1.52
1	D	415	SER	C-O	-9.64	1.14	1.23
1	C	415	SER	C-O	-9.63	1.14	1.23
1	A	409	ASN	CA-C	-9.63	1.40	1.52
1	A	415	SER	C-O	-9.61	1.14	1.23
1	C	403	PHE	C-O	-9.61	1.11	1.24
1	B	415	SER	C-O	-9.59	1.14	1.23
1	A	403	PHE	C-O	-9.59	1.11	1.24
1	D	403	PHE	C-O	-9.57	1.11	1.24
1	B	403	PHE	C-O	-9.57	1.11	1.24
1	A	404	ALA	CA-C	-8.60	1.42	1.52
1	C	404	ALA	CA-C	-8.56	1.42	1.52
1	B	404	ALA	CA-C	-8.55	1.42	1.52
1	D	404	ALA	CA-C	-8.54	1.42	1.52
1	C	397	MET	C-O	-8.52	1.14	1.24
1	B	397	MET	C-O	-8.47	1.14	1.24
1	A	397	MET	C-O	-8.44	1.14	1.24
1	D	397	MET	C-O	-8.44	1.14	1.24
1	C	413	MET	C-O	-8.31	1.14	1.24
1	B	413	MET	C-O	-8.30	1.14	1.24
1	D	413	MET	C-O	-8.30	1.14	1.24
1	A	413	MET	C-O	-8.29	1.14	1.24
1	C	425	GLN	CA-C	8.15	1.63	1.52
1	B	425	GLN	CA-C	8.14	1.63	1.52
1	D	425	GLN	CA-C	8.11	1.63	1.52
1	A	425	GLN	CA-C	8.09	1.63	1.52
1	A	406	ILE	CA-CB	-8.08	1.44	1.54
1	C	406	ILE	CA-CB	-8.05	1.44	1.54
1	B	406	ILE	CA-CB	-8.02	1.44	1.54
1	D	406	ILE	CA-CB	-7.98	1.44	1.54
1	A	405	THR	C-O	-7.88	1.15	1.24
1	D	405	THR	C-O	-7.86	1.15	1.24
1	B	405	THR	C-O	-7.85	1.15	1.24
1	C	405	THR	C-O	-7.84	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	406	ILE	C-O	-7.82	1.15	1.24
1	C	406	ILE	C-O	-7.78	1.15	1.24
1	B	406	ILE	C-O	-7.77	1.15	1.24
1	A	406	ILE	C-O	-7.72	1.15	1.24
1	D	402	ILE	C-O	-7.67	1.15	1.24
1	B	523	LYS	CA-C	-7.66	1.41	1.52
1	C	523	LYS	CA-C	-7.66	1.41	1.52
1	D	523	LYS	CA-C	-7.65	1.41	1.52
1	A	523	LYS	CA-C	-7.65	1.41	1.52
1	C	402	ILE	C-O	-7.63	1.15	1.24
1	B	402	ILE	C-O	-7.62	1.15	1.24
1	A	402	ILE	C-O	-7.56	1.15	1.24
1	A	410	VAL	C-O	-7.45	1.15	1.24
1	C	410	VAL	C-O	-7.41	1.15	1.24
1	B	410	VAL	C-O	-7.39	1.15	1.24
1	D	410	VAL	C-O	-7.39	1.15	1.24
1	B	399	GLY	CA-C	-7.30	1.44	1.52
1	D	399	GLY	CA-C	-7.30	1.44	1.52
1	C	399	GLY	CA-C	-7.29	1.44	1.52
1	B	410	VAL	CA-CB	-7.25	1.45	1.54
1	A	399	GLY	CA-C	-7.24	1.44	1.52
1	D	410	VAL	CA-CB	-7.23	1.45	1.54
1	A	410	VAL	CA-CB	-7.18	1.45	1.54
1	C	410	VAL	CA-CB	-7.18	1.45	1.54
1	A	413	MET	CA-C	-7.14	1.43	1.52
1	C	413	MET	CA-C	-7.14	1.43	1.52
1	C	414	ILE	C-O	-7.14	1.15	1.24
1	D	414	ILE	C-O	-7.13	1.15	1.24
1	B	413	MET	CA-C	-7.13	1.43	1.52
1	A	414	ILE	C-O	-7.12	1.15	1.24
1	B	414	ILE	C-O	-7.12	1.15	1.24
1	D	413	MET	CA-C	-7.11	1.43	1.52
1	D	398	CYS	CA-C	-6.90	1.43	1.52
1	C	398	CYS	CA-C	-6.88	1.43	1.52
1	B	398	CYS	CA-C	-6.88	1.43	1.52
1	A	398	CYS	CA-C	-6.87	1.43	1.52
1	B	412	SER	CA-C	6.29	1.61	1.52
1	C	412	SER	CA-C	6.28	1.61	1.52
1	D	412	SER	CA-C	6.27	1.61	1.52
1	B	411	GLY	C-O	-6.24	1.16	1.23
1	A	412	SER	CA-C	6.24	1.61	1.52
1	A	411	GLY	C-O	-6.24	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	411	GLY	C-O	-6.20	1.16	1.23
1	A	406	ILE	N-CA	-6.20	1.39	1.46
1	C	411	GLY	C-O	-6.20	1.16	1.23
1	D	406	ILE	N-CA	-6.20	1.39	1.46
1	B	406	ILE	N-CA	-6.19	1.39	1.46
1	D	428	MET	N-CA	-6.19	1.38	1.46
1	C	406	ILE	N-CA	-6.17	1.39	1.46
1	B	428	MET	N-CA	-6.16	1.39	1.46
1	A	428	MET	N-CA	-6.16	1.39	1.46
1	C	428	MET	N-CA	-6.11	1.39	1.46
1	C	415	SER	CA-C	-5.90	1.46	1.53
1	C	398	CYS	CA-CB	-5.90	1.44	1.53
1	B	415	SER	CA-C	-5.88	1.46	1.53
1	D	396	LEU	CA-C	-5.85	1.45	1.52
1	B	398	CYS	CA-CB	-5.85	1.44	1.53
1	A	396	LEU	CA-C	-5.84	1.45	1.52
1	D	415	SER	CA-C	-5.84	1.46	1.53
1	A	415	SER	CA-C	-5.83	1.46	1.53
1	D	398	CYS	CA-CB	-5.80	1.44	1.53
1	A	398	CYS	CA-CB	-5.80	1.44	1.53
1	B	396	LEU	CA-C	-5.80	1.45	1.52
1	C	396	LEU	CA-C	-5.79	1.45	1.52
1	D	401	LEU	CA-C	-5.71	1.45	1.52
1	D	400	VAL	C-O	-5.67	1.17	1.24
1	B	401	LEU	CA-C	-5.66	1.45	1.52
1	C	401	LEU	CA-C	-5.65	1.45	1.52
1	C	400	VAL	C-O	-5.65	1.17	1.24
1	A	401	LEU	CA-C	-5.64	1.45	1.52
1	D	412	SER	C-O	-5.62	1.17	1.24
1	A	400	VAL	C-O	-5.62	1.17	1.24
1	B	400	VAL	C-O	-5.61	1.17	1.24
1	B	412	SER	C-O	-5.61	1.17	1.24
1	C	412	SER	C-O	-5.61	1.17	1.24
1	A	412	SER	C-O	-5.56	1.17	1.24
1	C	523	LYS	C-O	-5.54	1.17	1.24
1	B	523	LYS	C-O	-5.54	1.17	1.24
1	A	523	LYS	C-O	-5.51	1.17	1.24
1	D	523	LYS	C-O	-5.49	1.17	1.24
1	B	410	VAL	CA-C	-5.22	1.46	1.52
1	A	410	VAL	CA-C	-5.21	1.46	1.52
1	C	410	VAL	CA-C	-5.21	1.46	1.52
1	D	410	VAL	CA-C	-5.19	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	ILE	CA-C	-5.18	1.46	1.52
1	A	402	ILE	CA-C	-5.18	1.46	1.52
1	D	402	ILE	CA-C	-5.14	1.46	1.52
1	A	397	MET	CA-C	-5.14	1.46	1.52
1	B	397	MET	CA-C	-5.14	1.46	1.52
1	C	402	ILE	CA-C	-5.13	1.46	1.52
1	C	397	MET	CA-C	-5.10	1.46	1.52
1	D	397	MET	CA-C	-5.08	1.46	1.52
1	A	415	SER	N-CA	-5.07	1.41	1.46
1	C	415	SER	N-CA	-5.05	1.41	1.46
1	C	408	GLY	C-O	-5.05	1.17	1.23
1	B	415	SER	N-CA	-5.05	1.41	1.46
1	D	415	SER	N-CA	-5.03	1.41	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	425	GLN	CA-C-O	10.66	132.15	120.10
1	A	425	GLN	CA-C-O	10.65	132.13	120.10
1	B	425	GLN	CA-C-O	10.64	132.12	120.10
1	C	425	GLN	CA-C-O	10.63	132.11	120.10
1	A	409	ASN	CB-CA-C	-9.42	95.16	110.79
1	B	409	ASN	CB-CA-C	-9.41	95.17	110.79
1	D	409	ASN	CB-CA-C	-9.40	95.18	110.79
1	C	409	ASN	CB-CA-C	-9.38	95.21	110.79
1	A	425	GLN	O-C-N	-8.06	112.79	122.22
1	D	425	GLN	O-C-N	-8.05	112.80	122.22
1	B	425	GLN	O-C-N	-8.04	112.81	122.22
1	C	425	GLN	O-C-N	-8.04	112.81	122.22
1	A	400	VAL	CB-CA-C	-7.38	102.53	111.97
1	B	400	VAL	CB-CA-C	-7.37	102.53	111.97
1	D	400	VAL	CB-CA-C	-7.36	102.55	111.97
1	C	400	VAL	CB-CA-C	-7.35	102.56	111.97
1	C	405	THR	CB-CA-C	-7.03	99.84	110.88
1	A	405	THR	CB-CA-C	-7.02	99.86	110.88
1	B	405	THR	CB-CA-C	-7.02	99.86	110.88
1	D	405	THR	CB-CA-C	-7.01	99.87	110.88
1	D	398	CYS	CB-CA-C	-6.57	99.88	110.79
1	C	398	CYS	CB-CA-C	-6.57	99.89	110.79
1	A	398	CYS	CB-CA-C	-6.57	99.89	110.79
1	B	398	CYS	CB-CA-C	-6.55	99.92	110.79
1	B	523	LYS	N-CA-C	6.21	119.96	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	523	LYS	N-CA-C	6.21	119.96	112.38
1	A	523	LYS	N-CA-C	6.21	119.95	112.38
1	D	523	LYS	N-CA-C	6.19	119.93	112.38
1	B	406	ILE	CB-CA-C	-5.59	104.70	112.02
1	A	406	ILE	CB-CA-C	-5.58	104.72	112.02
1	C	406	ILE	CB-CA-C	-5.57	104.72	112.02
1	D	406	ILE	CB-CA-C	-5.57	104.72	112.02
1	D	406	ILE	N-CA-C	5.55	115.74	110.53
1	B	406	ILE	N-CA-C	5.53	115.73	110.53
1	C	406	ILE	N-CA-C	5.53	115.73	110.53
1	A	406	ILE	N-CA-C	5.53	115.73	110.53
1	D	425	GLN	N-CA-C	5.49	118.03	111.71
1	A	425	GLN	N-CA-C	5.49	118.02	111.71
1	C	425	GLN	N-CA-C	5.47	118.00	111.71
1	B	425	GLN	N-CA-C	5.46	117.99	111.71
1	D	402	ILE	N-CA-C	5.44	116.22	110.72
1	C	402	ILE	N-CA-C	5.43	116.21	110.72
1	A	402	ILE	N-CA-C	5.43	116.20	110.72
1	B	402	ILE	N-CA-C	5.43	116.20	110.72
1	B	399	GLY	CA-C-O	-5.40	115.16	121.00
1	A	399	GLY	CA-C-O	-5.39	115.18	121.00
1	C	410	VAL	CB-CA-C	-5.38	104.88	112.14
1	D	399	GLY	CA-C-O	-5.37	115.20	121.00
1	C	399	GLY	CA-C-O	-5.37	115.20	121.00
1	D	410	VAL	CB-CA-C	-5.34	104.93	112.14
1	B	410	VAL	CB-CA-C	-5.34	104.94	112.14
1	A	410	VAL	CB-CA-C	-5.33	104.94	112.14
1	A	412	SER	O-C-N	-5.33	115.98	122.22
1	B	412	SER	O-C-N	-5.31	116.01	122.22
1	C	412	SER	O-C-N	-5.29	116.03	122.22
1	D	412	SER	O-C-N	-5.29	116.03	122.22
1	A	407	VAL	CB-CA-C	5.15	120.61	112.26
1	C	407	VAL	CB-CA-C	5.14	120.59	112.26
1	B	407	VAL	CB-CA-C	5.14	120.58	112.26
1	D	407	VAL	CB-CA-C	5.13	120.58	112.26
1	D	404	ALA	CB-CA-C	-5.06	102.91	110.90
1	C	404	ALA	CB-CA-C	-5.05	102.92	110.90
1	B	404	ALA	CB-CA-C	-5.05	102.93	110.90
1	A	404	ALA	CB-CA-C	-5.04	102.94	110.90

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	4243	0	4285	103	0
1	B	4243	0	4285	98	0
1	C	4243	0	4285	105	0
1	D	4243	0	4285	102	0
2	A	23	0	10	1	0
2	B	23	0	10	1	0
2	C	23	0	10	1	0
2	D	23	0	10	1	0
3	A	115	0	162	9	0
3	B	115	0	162	7	0
3	C	115	0	162	6	0
3	D	115	0	162	7	0
4	A	23	0	20	1	0
4	B	23	0	20	2	0
4	C	23	0	20	3	0
4	D	23	0	20	1	0
All	All	17616	0	17908	364	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 10.

All (364) 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:299:THR:HG23	1:D:428:MET:CE	1.35	1.53
1:B:428:MET:CE	1:C:299:THR:HG23	1.40	1.51
1:A:428:MET:CE	1:B:299:THR:HG23	1.41	1.46
1:C:428:MET:CE	1:D:299:THR:HG23	1.57	1.31
1:A:428:MET:HE3	1:B:299:THR:HG23	1.23	1.19
1:B:428:MET:HE3	1:C:299:THR:HG23	1.18	1.14
1:A:299:THR:CG2	1:D:428:MET:CE	2.26	1.13
1:B:428:MET:CE	1:C:299:THR:CG2	2.29	1.10
1:A:428:MET:CE	1:B:299:THR:CG2	2.30	1.09
1:A:299:THR:HG23	1:D:428:MET:HE3	1.08	1.06
1:C:428:MET:HE3	1:D:299:THR:HG23	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ARG:NH2	4:B:807:PX2:O3	1.97	0.97
1:A:299:THR:CG2	1:D:428:MET:HE3	1.93	0.97
1:C:385:ARG:NH2	4:C:807:PX2:O3	1.97	0.96
1:C:537:ARG:NH1	1:D:230[A]:GLN:OE1	1.99	0.96
1:D:385:ARG:NH2	4:D:807:PX2:O3	1.97	0.95
1:A:299:THR:HG23	1:D:428:MET:HE1	1.46	0.94
1:A:428:MET:HE1	1:B:299:THR:HG23	1.50	0.93
1:A:385:ARG:NH2	4:A:807:PX2:O3	2.02	0.92
1:B:428:MET:HE1	1:C:299:THR:HG23	1.52	0.90
1:A:428:MET:HE2	1:B:299:THR:HG23	1.53	0.89
1:B:428:MET:HE3	1:C:299:THR:CG2	1.99	0.87
1:C:428:MET:CE	1:D:299:THR:CG2	2.49	0.87
1:C:428:MET:HE1	1:D:299:THR:HG23	1.53	0.86
1:B:428:MET:HE2	1:C:299:THR:HG23	1.55	0.83
1:D:179:ASN:HD21	1:D:354:ASP:H	1.27	0.83
1:C:179:ASN:HD21	1:C:354:ASP:H	1.27	0.83
1:A:428:MET:HE3	1:B:299:THR:CG2	2.03	0.83
1:A:299:THR:HG23	1:D:428:MET:HE2	1.60	0.82
1:A:179:ASN:HD21	1:A:354:ASP:H	1.27	0.81
1:B:179:ASN:HD21	1:B:354:ASP:H	1.27	0.81
1:B:428:MET:HE1	1:C:299:THR:CG2	2.08	0.81
1:A:537:ARG:NH1	1:B:230[A]:GLN:OE1	2.13	0.81
1:A:299:THR:CG2	1:D:428:MET:HE1	2.03	0.80
1:A:230[A]:GLN:OE1	1:D:537:ARG:NH1	2.14	0.80
1:A:428:MET:HE1	1:B:299:THR:CG2	2.07	0.80
1:B:537:ARG:NH1	1:C:230[A]:GLN:OE1	2.15	0.79
1:A:547:LYS:HE2	1:A:549:PHE:HE1	1.47	0.78
1:B:547:LYS:HE2	1:B:549:PHE:HE1	1.47	0.78
1:D:547:LYS:HE2	1:D:549:PHE:HE1	1.47	0.78
1:C:547:LYS:HE2	1:C:549:PHE:HE1	1.47	0.77
1:A:308:ARG:NH2	1:D:429:ASP:OD2	2.18	0.76
1:B:135:ASN:OD1	1:B:280:ARG:NH1	2.23	0.72
1:C:135:ASN:OD1	1:C:280:ARG:NH1	2.23	0.72
1:D:135:ASN:OD1	1:D:280:ARG:NH1	2.23	0.71
1:A:135:ASN:OD1	1:A:280:ARG:NH1	2.23	0.71
1:A:429:ASP:OD2	1:B:308:ARG:NH2	2.25	0.70
3:A:802:CPL:O31	3:A:802:CPL:HC12	1.93	0.69
3:D:802:CPL:O31	3:D:802:CPL:HC12	1.93	0.69
3:B:802:CPL:O31	3:B:802:CPL:HC12	1.93	0.68
1:C:428:MET:HE1	1:D:299:THR:CG2	2.20	0.68
1:B:429:ASP:OD2	1:C:308:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:802:CPL:HC12	3:C:802:CPL:O31	1.93	0.67
1:C:429:ASP:OD2	1:D:308:ARG:NH2	2.28	0.66
1:B:414:ILE:HG22	1:B:414:ILE:O	1.96	0.65
1:A:414:ILE:O	1:A:414:ILE:HG22	1.96	0.65
1:C:414:ILE:HG22	1:C:414:ILE:O	1.96	0.64
1:B:222:ASN:OD1	1:B:289:ARG:NH2	2.32	0.63
1:D:414:ILE:HG22	1:D:414:ILE:O	1.96	0.63
1:D:458:ASN:HD22	1:D:535:ARG:HH22	1.47	0.63
1:D:222:ASN:OD1	1:D:289:ARG:NH2	2.32	0.63
1:A:222:ASN:OD1	1:A:289:ARG:NH2	2.32	0.62
1:B:562:SER:OG	2:B:801:PCG:O1A	2.17	0.62
1:C:458:ASN:HD22	1:C:535:ARG:HH22	1.47	0.62
1:C:428:MET:HE2	1:D:299:THR:HG23	1.72	0.62
1:C:222:ASN:OD1	1:C:289:ARG:NH2	2.32	0.62
1:B:490:LYS:NZ	1:B:554:GLU:OE1	2.30	0.62
1:A:148:LEU:O	3:A:802:CPL:H122	2.00	0.62
1:A:401:LEU:CD2	1:D:407:VAL:HG22	2.30	0.61
1:C:547:LYS:HG2	1:C:547:LYS:O	2.00	0.61
1:C:562:SER:OG	2:C:801:PCG:O1A	2.17	0.61
1:A:458:ASN:HD22	1:A:535:ARG:HH22	1.47	0.61
1:D:547:LYS:O	1:D:547:LYS:HG2	2.00	0.61
1:B:547:LYS:O	1:B:547:LYS:HG2	2.00	0.61
1:C:157:CYS:HB2	1:C:176:MET:HE2	1.82	0.61
1:A:547:LYS:O	1:A:547:LYS:HG2	2.00	0.61
1:B:458:ASN:HD22	1:B:535:ARG:HH22	1.47	0.60
1:D:157:CYS:HB2	1:D:176:MET:HE2	1.83	0.60
1:D:562:SER:OG	2:D:801:PCG:O1A	2.17	0.60
1:A:562:SER:OG	2:A:801:PCG:O1A	2.17	0.60
1:C:467:VAL:HG13	1:C:471:LEU:HD12	1.84	0.60
1:B:467:VAL:HG13	1:B:471:LEU:HD12	1.84	0.60
1:B:523:LYS:O	1:B:523:LYS:HG2	2.02	0.60
1:D:467:VAL:HG13	1:D:471:LEU:HD12	1.84	0.60
1:A:467:VAL:HG13	1:A:471:LEU:HD12	1.84	0.59
1:A:157:CYS:HB2	1:A:176:MET:HE2	1.82	0.59
1:A:523:LYS:O	1:A:523:LYS:HG2	2.02	0.59
1:B:157:CYS:HB2	1:B:176:MET:HE2	1.82	0.59
1:C:547:LYS:HE2	1:C:549:PHE:CE1	2.34	0.58
1:D:547:LYS:HE2	1:D:549:PHE:CE1	2.34	0.58
1:A:547:LYS:HE2	1:A:549:PHE:CE1	2.34	0.58
1:C:523:LYS:O	1:C:523:LYS:HG2	2.02	0.58
1:B:547:LYS:HE2	1:B:549:PHE:CE1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:O	3:D:802:CPL:H122	2.04	0.58
1:B:462:LEU:HD22	1:B:465:GLN:HG2	1.86	0.57
1:D:462:LEU:HD22	1:D:465:GLN:HG2	1.86	0.57
1:A:407:VAL:HG22	1:B:401:LEU:HD23	1.86	0.57
1:A:490:LYS:NZ	1:A:554:GLU:OE1	2.30	0.57
1:C:148:LEU:O	3:C:802:CPL:H122	2.04	0.57
1:D:523:LYS:HG2	1:D:523:LYS:O	2.02	0.57
1:C:462:LEU:HD22	1:C:465:GLN:HG2	1.86	0.57
1:B:148:LEU:O	3:B:802:CPL:H122	2.04	0.57
1:C:490:LYS:NZ	1:C:554:GLU:OE1	2.30	0.57
1:A:462:LEU:HD22	1:A:465:GLN:HG2	1.86	0.57
1:C:212:ASP:OD2	1:C:262:TYR:OH	2.19	0.56
1:C:542:ASP:OD1	1:C:543:ASP:N	2.39	0.56
1:A:401:LEU:HD23	1:D:407:VAL:HG22	1.87	0.56
1:B:179:ASN:ND2	1:B:354:ASP:H	2.01	0.56
1:C:331:SER:HA	1:C:342:VAL:HG22	1.88	0.55
1:A:407:VAL:HG22	1:B:401:LEU:CD2	2.36	0.55
1:B:542:ASP:OD1	1:B:543:ASP:N	2.39	0.55
1:A:542:ASP:OD1	1:A:543:ASP:N	2.39	0.55
1:D:490:LYS:NZ	1:D:554:GLU:OE1	2.30	0.55
1:D:542:ASP:OD1	1:D:543:ASP:N	2.39	0.55
1:A:199:HIS:CD2	1:A:199:HIS:H	2.25	0.54
1:B:331:SER:HA	1:B:342:VAL:HG22	1.88	0.54
1:C:199:HIS:CD2	1:C:199:HIS:H	2.25	0.54
1:A:331:SER:HA	1:A:342:VAL:HG22	1.88	0.54
1:C:144:VAL:HG21	1:C:325:CYS:HB3	1.90	0.54
1:B:144:VAL:HG21	1:B:325:CYS:HB3	1.90	0.54
1:C:428:MET:HE3	1:D:299:THR:CG2	2.24	0.54
1:D:119:ASP:OD1	1:D:300:ARG:NH2	2.42	0.53
1:D:144:VAL:HG21	1:D:325:CYS:HB3	1.90	0.53
1:D:331:SER:HA	1:D:342:VAL:HG22	1.88	0.53
1:A:527:GLY:HA3	1:A:562:SER:HB2	1.90	0.53
1:B:199:HIS:H	1:B:199:HIS:CD2	2.25	0.53
1:A:144:VAL:HG21	1:A:325:CYS:HB3	1.90	0.53
1:A:179:ASN:ND2	1:A:354:ASP:H	2.01	0.53
1:D:527:GLY:HA3	1:D:562:SER:HB2	1.90	0.53
1:A:561:LEU:HD23	1:A:576:THR:HG21	1.91	0.53
1:D:129:THR:HG23	1:D:290:VAL:HG13	1.91	0.53
1:D:561:LEU:HD23	1:D:576:THR:HG21	1.91	0.53
1:B:119:ASP:OD1	1:B:300:ARG:NH2	2.42	0.53
1:B:561:LEU:HD23	1:B:576:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASP:OD1	1:C:300:ARG:NH2	2.42	0.53
1:C:129:THR:HG23	1:C:290:VAL:HG13	1.91	0.53
1:C:561:LEU:HD23	1:C:576:THR:HG21	1.91	0.53
1:C:156:LEU:HD12	1:C:169:GLN:HB3	1.91	0.53
1:C:527:GLY:HA3	1:C:562:SER:HB2	1.90	0.53
1:D:156:LEU:HD12	1:D:169:GLN:HB3	1.91	0.53
1:A:156:LEU:HD12	1:A:169:GLN:HB3	1.91	0.52
1:B:527:GLY:HA3	1:B:562:SER:HB2	1.90	0.52
1:B:151:PRO:HD2	1:B:197:TYR:CZ	2.45	0.52
1:B:156:LEU:HD12	1:B:169:GLN:HB3	1.91	0.52
1:D:199:HIS:H	1:D:199:HIS:CD2	2.25	0.52
1:A:119:ASP:OD1	1:A:300:ARG:NH2	2.42	0.52
1:D:179:ASN:ND2	1:D:354:ASP:H	2.01	0.52
1:A:151:PRO:HD2	1:A:197:TYR:CZ	2.45	0.52
1:C:151:PRO:HD2	1:C:197:TYR:CZ	2.45	0.52
1:C:179:ASN:ND2	1:C:354:ASP:H	2.01	0.52
1:A:129:THR:HG23	1:A:290:VAL:HG13	1.91	0.51
1:B:129:THR:HG23	1:B:290:VAL:HG13	1.91	0.51
1:B:407:VAL:HG22	1:C:401:LEU:HD23	1.93	0.51
1:D:151:PRO:HD2	1:D:197:TYR:CZ	2.45	0.51
1:B:407:VAL:HG22	1:C:401:LEU:CD2	2.41	0.50
1:A:212:ASP:OD2	1:A:262:TYR:OH	2.19	0.50
1:A:232:LEU:HD21	1:D:582:VAL:HG12	1.95	0.49
1:C:526:ILE:HD11	1:D:601:GLU:HG3	1.94	0.49
1:A:125:THR:HG22	1:A:289:ARG:HD2	1.96	0.48
1:D:503:ALA:O	1:D:506:VAL:HG12	2.14	0.48
1:B:125:THR:HG22	1:B:289:ARG:HD2	1.96	0.48
1:C:125:THR:HG22	1:C:289:ARG:HD2	1.96	0.48
1:C:530:MET:HB3	1:C:563:ILE:HD11	1.96	0.48
1:D:530:MET:HB3	1:D:563:ILE:HD11	1.96	0.48
1:A:329:TRP:CE2	3:A:804:CPL:H132	2.48	0.47
1:C:503:ALA:O	1:C:506:VAL:HG12	2.14	0.47
1:A:396:LEU:HD22	1:D:377:ILE:HD13	1.96	0.47
1:D:125:THR:HG22	1:D:289:ARG:HD2	1.96	0.47
1:B:503:ALA:O	1:B:506:VAL:HG12	2.14	0.47
1:A:503:ALA:O	1:A:506:VAL:HG12	2.14	0.47
1:A:581:SER:OG	1:A:583:GLY:O	2.33	0.47
1:C:514:PHE:CE1	1:C:587:LEU:HD12	2.50	0.47
1:D:533:VAL:HA	1:D:587:LEU:HD23	1.97	0.47
1:C:574:ARG:NH2	1:D:601:GLU:O	2.47	0.47
1:D:179:ASN:HD21	1:D:354:ASP:N	2.05	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:GLN:NE2	1:D:586:ASP:OD2	2.48	0.47
1:B:514:PHE:CE1	1:B:587:LEU:HD12	2.50	0.47
1:B:581:SER:OG	1:B:583:GLY:O	2.33	0.47
1:C:460:GLN:NE2	1:C:586:ASP:OD2	2.48	0.47
1:A:530:MET:HB3	1:A:563:ILE:HD11	1.96	0.46
1:A:533:VAL:HA	1:A:587:LEU:HD23	1.97	0.46
1:C:537:ARG:NH1	1:D:230[A]:GLN:CD	2.70	0.46
1:D:507:LEU:HA	1:D:507:LEU:HD23	1.64	0.46
1:A:514:PHE:CE1	1:A:587:LEU:HD12	2.50	0.46
1:B:530:MET:HB3	1:B:563:ILE:HD11	1.96	0.46
1:D:514:PHE:CE1	1:D:587:LEU:HD12	2.50	0.46
1:A:460:GLN:NE2	1:A:586:ASP:OD2	2.48	0.46
1:C:546:LYS:HG2	1:C:547:LYS:H	1.81	0.46
1:C:492:ARG:HA	1:C:495:GLN:HG2	1.98	0.46
1:A:377:ILE:HD13	1:B:396:LEU:HD22	1.98	0.46
1:C:317:VAL:HG12	3:C:808:CPL:H261	1.98	0.46
1:C:533:VAL:HA	1:C:587:LEU:HD23	1.97	0.46
1:B:460:GLN:NE2	1:B:586:ASP:OD2	2.48	0.46
1:C:179:ASN:HD21	1:C:354:ASP:N	2.05	0.46
1:B:317:VAL:HG12	3:B:808:CPL:H261	1.98	0.46
1:B:385:ARG:NH2	4:B:807:PX2:H1	2.10	0.46
1:B:492:ARG:HA	1:B:495:GLN:HG2	1.98	0.46
1:A:492:ARG:HA	1:A:495:GLN:HG2	1.98	0.46
1:C:581:SER:OG	1:C:583:GLY:O	2.33	0.46
1:D:546:LYS:HG2	1:D:547:LYS:H	1.81	0.46
1:D:581:SER:OG	1:D:583:GLY:O	2.33	0.46
1:B:533:VAL:HA	1:B:587:LEU:HD23	1.97	0.46
1:B:566:ILE:HG22	1:B:568:GLY:H	1.81	0.46
1:C:566:ILE:HG22	1:C:568:GLY:H	1.81	0.46
1:D:317:VAL:HG12	3:D:808:CPL:H261	1.98	0.46
1:D:492:ARG:HA	1:D:495:GLN:HG2	1.98	0.46
1:B:328:PHE:CZ	1:B:362:ARG:HD3	2.51	0.45
1:C:328:PHE:CZ	1:C:362:ARG:HD3	2.51	0.45
1:A:530:MET:HE3	1:A:560:GLU:HB3	1.98	0.45
1:A:566:ILE:HG22	1:A:568:GLY:H	1.81	0.45
1:C:530:MET:HE3	1:C:560:GLU:HB3	1.98	0.45
1:A:328:PHE:CZ	1:A:362:ARG:HD3	2.51	0.45
1:D:328:PHE:CZ	1:D:362:ARG:HD3	2.51	0.45
1:A:317:VAL:HG12	3:A:808:CPL:H261	1.98	0.45
1:B:546:LYS:HG2	1:B:547:LYS:H	1.81	0.45
1:C:452:PHE:HZ	1:D:470:VAL:HG21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:VAL:CG2	1:D:431:ILE:HD11	2.47	0.45
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.64	0.45
3:B:808:CPL:H352	3:B:808:CPL:H322	1.74	0.45
1:D:569:SER:HB2	1:D:617:LEU:HD13	1.99	0.45
1:A:546:LYS:HG2	1:A:547:LYS:H	1.81	0.45
1:C:614:ARG:HG2	1:C:618:LYS:HE3	1.99	0.45
1:B:530:MET:HE3	1:B:560:GLU:HB3	1.98	0.45
1:B:569:SER:HB2	1:B:617:LEU:HD13	1.99	0.45
1:D:132:TYR:CG	1:D:290:VAL:HG21	2.52	0.45
1:D:377:ILE:HG22	1:D:379:GLU:HG2	1.98	0.45
1:A:335:GLY:O	1:A:342:VAL:HG11	2.17	0.44
1:A:377:ILE:HG22	1:A:379:GLU:HG2	1.98	0.44
1:B:377:ILE:HG22	1:B:379:GLU:HG2	1.98	0.44
1:A:132:TYR:CG	1:A:290:VAL:HG21	2.52	0.44
1:B:335:GLY:O	1:B:342:VAL:HG11	2.17	0.44
1:C:527:GLY:HA3	1:C:562:SER:CB	2.47	0.44
1:D:527:GLY:HA3	1:D:562:SER:CB	2.48	0.44
1:D:530:MET:HE3	1:D:560:GLU:HB3	1.98	0.44
1:A:527:GLY:HA3	1:A:562:SER:CB	2.47	0.44
1:D:315:TYR:HE1	3:D:805:CPL:H182	1.82	0.44
1:B:194:TRP:O	1:B:198:TRP:HB3	2.18	0.44
1:D:335:GLY:O	1:D:342:VAL:HG11	2.17	0.44
1:D:566:ILE:HG22	1:D:568:GLY:H	1.82	0.44
1:A:614:ARG:HG2	1:A:618:LYS:HE3	1.98	0.44
1:B:315:TYR:HE1	3:B:805:CPL:H182	1.82	0.44
1:C:315:TYR:HE1	3:C:805:CPL:H182	1.82	0.44
1:B:614:ARG:HG2	1:B:618:LYS:HE3	1.99	0.44
1:C:132:TYR:CG	1:C:290:VAL:HG21	2.53	0.44
1:C:178:THR:OG1	1:C:356:THR:OG1	2.30	0.44
1:A:569:SER:HB2	1:A:617:LEU:HD13	1.99	0.44
1:B:132:TYR:CG	1:B:290:VAL:HG21	2.53	0.44
1:B:315:TYR:CE1	3:B:805:CPL:H182	2.53	0.44
1:C:492:ARG:HA	1:C:495:GLN:HE21	1.82	0.44
1:D:230[A]:GLN:C	1:D:232:LEU:H	2.26	0.44
1:D:415:SER:O	1:D:417:MET:N	2.51	0.44
3:D:802:CPL:HC62	3:D:802:CPL:HC41	1.64	0.44
1:A:470:VAL:HG22	1:D:431:ILE:HD11	1.99	0.44
1:A:492:ARG:HA	1:A:495:GLN:HE21	1.82	0.44
1:B:492:ARG:HA	1:B:495:GLN:HE21	1.82	0.44
1:C:230[A]:GLN:C	1:C:232:LEU:H	2.26	0.44
1:C:315:TYR:CE1	3:C:805:CPL:H182	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:HD13	1:A:406:ILE:HG21	1.64	0.44
1:A:415:SER:O	1:A:417:MET:N	2.51	0.44
3:A:802:CPL:HC62	3:A:802:CPL:HC41	1.64	0.44
1:C:569:SER:HB2	1:C:617:LEU:HD13	1.99	0.44
1:C:599:LEU:HD23	1:C:599:LEU:HA	1.83	0.44
1:D:614:ARG:HG2	1:D:618:LYS:HE3	1.99	0.44
1:B:179:ASN:HD21	1:B:354:ASP:N	2.05	0.43
1:C:407:VAL:HG22	1:D:401:LEU:HD23	2.00	0.43
1:D:152:SER:O	1:D:152:SER:OG	2.36	0.43
1:B:386:ASN:N	1:B:386:ASN:HD22	2.16	0.43
3:D:802:CPL:H321	3:D:802:CPL:H351	1.73	0.43
1:A:505:LEU:HD23	1:A:505:LEU:HA	1.83	0.43
1:B:406:ILE:HG21	1:B:406:ILE:HD13	1.64	0.43
1:C:335:GLY:O	1:C:342:VAL:HG11	2.17	0.43
1:C:415:SER:O	1:C:417:MET:N	2.51	0.43
1:C:507:LEU:HD23	1:C:507:LEU:HA	1.64	0.43
1:A:194:TRP:O	1:A:198:TRP:HB3	2.18	0.43
1:B:386:ASN:HD22	1:B:386:ASN:H	1.67	0.43
3:B:802:CPL:H321	3:B:802:CPL:H351	1.73	0.43
1:C:377:ILE:HG22	1:C:379:GLU:HG2	1.98	0.43
1:A:230[A]:GLN:C	1:A:232:LEU:H	2.26	0.43
3:A:802:CPL:H351	3:A:802:CPL:H321	1.73	0.43
3:C:802:CPL:H351	3:C:802:CPL:H321	1.73	0.43
1:D:492:ARG:HA	1:D:495:GLN:HE21	1.82	0.43
1:C:194:TRP:O	1:C:198:TRP:HB3	2.18	0.43
1:C:386:ASN:HD22	1:C:386:ASN:N	2.16	0.43
1:D:194:TRP:O	1:D:198:TRP:HB3	2.18	0.43
1:C:298:GLU:OE1	1:C:308:ARG:NH1	2.50	0.43
1:A:386:ASN:HD22	1:A:386:ASN:H	1.67	0.43
1:A:502:LEU:O	1:A:506:VAL:HB	2.19	0.43
1:B:230[A]:GLN:C	1:B:232:LEU:H	2.26	0.43
1:B:415:SER:O	1:B:417:MET:N	2.51	0.43
1:C:385:ARG:NH2	4:C:807:PX2:H1	2.13	0.43
1:D:401:LEU:O	1:D:404:ALA:HB3	2.19	0.43
1:A:401:LEU:O	1:A:404:ALA:HB3	2.19	0.43
1:C:386:ASN:HD22	1:C:386:ASN:H	1.67	0.43
1:D:315:TYR:CE1	3:D:805:CPL:H182	2.53	0.43
1:A:298:GLU:OE1	1:A:308:ARG:NH1	2.50	0.42
1:B:298:GLU:OE1	1:B:308:ARG:NH1	2.50	0.42
1:D:148:LEU:HD23	1:D:148:LEU:HA	1.87	0.42
3:A:808:CPL:H352	3:A:808:CPL:H322	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:O	1:B:211:MET:HG2	2.19	0.42
1:B:527:GLY:HA3	1:B:562:SER:CB	2.47	0.42
1:C:541:VAL:HG12	1:C:548:VAL:HG22	2.02	0.42
1:D:541:VAL:HG12	1:D:548:VAL:HG22	2.02	0.42
1:D:502:LEU:O	1:D:506:VAL:HB	2.19	0.42
1:A:386:ASN:HD22	1:A:386:ASN:N	2.16	0.42
1:A:541:VAL:HG12	1:A:548:VAL:HG22	2.01	0.42
1:B:502:LEU:O	1:B:506:VAL:HB	2.19	0.42
1:D:458:ASN:ND2	1:D:535:ARG:HH22	2.16	0.42
1:A:347:ASN:OD1	1:A:381:PRO:HG2	2.20	0.42
1:C:502:LEU:O	1:C:506:VAL:HB	2.19	0.42
1:D:386:ASN:N	1:D:386:ASN:HD22	2.16	0.42
1:D:424:PHE:CZ	1:D:456:TRP:HB2	2.55	0.42
1:B:347:ASN:OD1	1:B:381:PRO:HG2	2.20	0.42
1:B:541:VAL:HG12	1:B:548:VAL:HG22	2.02	0.42
1:D:207:PHE:O	1:D:211:MET:HG2	2.19	0.42
1:A:152:SER:O	1:A:152:SER:OG	2.36	0.42
1:C:401:LEU:O	1:C:404:ALA:HB3	2.19	0.42
1:C:431:ILE:HD12	1:C:452:PHE:CE2	2.55	0.42
1:A:458:ASN:ND2	1:A:535:ARG:HH22	2.16	0.42
1:B:377:ILE:HD13	1:C:396:LEU:HD22	2.02	0.42
1:B:431:ILE:HD12	1:B:452:PHE:CE2	2.55	0.42
1:A:207:PHE:O	1:A:211:MET:HG2	2.19	0.42
1:C:347:ASN:OD1	1:C:381:PRO:HG2	2.20	0.42
1:A:179:ASN:HD21	1:A:354:ASP:N	2.05	0.41
1:C:424:PHE:CZ	1:C:456:TRP:HB2	2.55	0.41
1:D:386:ASN:HD22	1:D:386:ASN:H	1.67	0.41
1:D:431:ILE:HD12	1:D:452:PHE:CE2	2.55	0.41
1:D:298:GLU:OE1	1:D:308:ARG:NH1	2.50	0.41
1:D:358:THR:O	1:D:362:ARG:HG3	2.20	0.41
1:B:358:THR:O	1:B:362:ARG:HG3	2.20	0.41
3:A:802:CPL:HC42	3:A:802:CPL:HC73	1.85	0.41
1:B:401:LEU:O	1:B:404:ALA:HB3	2.19	0.41
1:C:207:PHE:O	1:C:211:MET:HG2	2.19	0.41
1:B:431:ILE:O	1:B:435:MET:HG3	2.21	0.41
1:C:407:VAL:HG22	1:D:401:LEU:CD2	2.50	0.41
1:C:505:LEU:HD23	1:C:505:LEU:HA	1.82	0.41
1:A:431:ILE:HD12	1:A:452:PHE:CE2	2.55	0.41
1:A:582:VAL:HG12	1:B:232:LEU:HD21	2.02	0.41
1:B:507:LEU:HD23	1:B:507:LEU:HA	1.64	0.41
1:D:532:ILE:HB	1:D:588:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:O	1:A:362:ARG:HG3	2.20	0.41
1:A:387:ILE:HD11	3:A:803:CPL:H171	2.02	0.41
1:A:431:ILE:O	1:A:435:MET:HG3	2.21	0.41
1:B:424:PHE:CZ	1:B:456:TRP:HB2	2.55	0.41
1:A:424:PHE:CZ	1:A:456:TRP:HB2	2.55	0.41
1:C:343:TYR:OH	1:C:357:ASP:OD1	2.33	0.41
1:C:358:THR:O	1:C:362:ARG:HG3	2.20	0.41
1:C:406:ILE:HD13	1:C:406:ILE:HG21	1.64	0.41
1:C:532:ILE:HB	1:C:588:PHE:HB2	2.02	0.41
1:D:178:THR:OG1	1:D:356:THR:OG1	2.30	0.41
1:D:431:ILE:O	1:D:435:MET:HG3	2.21	0.41
1:B:146:ASN:HD22	1:B:146:ASN:H	1.69	0.41
1:B:532:ILE:HB	1:B:588:PHE:HB2	2.02	0.41
1:C:386:ASN:HB3	4:C:807:PX2:H10	2.03	0.40
1:A:146:ASN:H	1:A:146:ASN:HD22	1.69	0.40
1:A:377:ILE:CD1	1:B:396:LEU:HD22	2.51	0.40
1:A:532:ILE:HB	1:A:588:PHE:HB2	2.02	0.40
1:D:146:ASN:H	1:D:146:ASN:HD22	1.69	0.40
1:B:582:VAL:HG12	1:C:232:LEU:HD21	2.02	0.40
1:C:146:ASN:HD22	1:C:146:ASN:H	1.69	0.40
1:C:458:ASN:ND2	1:C:535:ARG:HH22	2.16	0.40
1:D:347:ASN:OD1	1:D:381:PRO:HG2	2.20	0.40
1:B:617:LEU:HD23	1:B:617:LEU:HA	1.87	0.40
1:A:475:LEU:HD23	1:A:475:LEU:HA	1.93	0.40
1:C:431:ILE:O	1:C:435:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/733 (69%)	484 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	509/733 (69%)	484 (95%)	25 (5%)	0	100	100
1	C	509/733 (69%)	485 (95%)	24 (5%)	0	100	100
1	D	509/733 (69%)	486 (96%)	23 (4%)	0	100	100
All	All	2036/2932 (69%)	1939 (95%)	97 (5%)	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	465/651 (71%)	442 (95%)	23 (5%)	22	49
1	B	465/651 (71%)	442 (95%)	23 (5%)	22	49
1	C	465/651 (71%)	442 (95%)	23 (5%)	22	49
1	D	465/651 (71%)	442 (95%)	23 (5%)	22	49
All	All	1860/2604 (71%)	1768 (95%)	92 (5%)	23	49

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	118	THR
1	A	188	GLN
1	A	300	ARG
1	A	326	LEU
1	A	342	VAL
1	A	402	ILE
1	A	412	SER
1	A	413	MET
1	A	415	SER
1	A	428	MET
1	A	462	LEU
1	A	470	VAL

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Mol	Chain	Res	Type
1	A	506	VAL
1	A	507	LEU
1	A	511	LEU
1	A	523	LYS
1	A	526	ILE
1	A	561	LEU
1	A	562	SER
1	A	571	ASN
1	A	576	THR
1	A	615	GLU
1	B	103	VAL
1	B	118	THR
1	B	188	GLN
1	B	300	ARG
1	B	326	LEU
1	B	342	VAL
1	B	402	ILE
1	B	412	SER
1	B	413	MET
1	B	415	SER
1	B	428	MET
1	B	462	LEU
1	B	470	VAL
1	B	506	VAL
1	B	507	LEU
1	B	511	LEU
1	B	523	LYS
1	B	526	ILE
1	B	561	LEU
1	B	562	SER
1	B	571	ASN
1	B	576	THR
1	B	615	GLU
1	C	103	VAL
1	C	118	THR
1	C	188	GLN
1	C	300	ARG
1	C	326	LEU
1	C	342	VAL
1	C	402	ILE
1	C	412	SER
1	C	413	MET

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Mol	Chain	Res	Type
1	C	415	SER
1	C	428	MET
1	C	462	LEU
1	C	470	VAL
1	C	506	VAL
1	C	507	LEU
1	C	511	LEU
1	C	523	LYS
1	C	526	ILE
1	C	561	LEU
1	C	562	SER
1	C	571	ASN
1	C	576	THR
1	C	615	GLU
1	D	103	VAL
1	D	118	THR
1	D	188	GLN
1	D	300	ARG
1	D	326	LEU
1	D	342	VAL
1	D	402	ILE
1	D	412	SER
1	D	413	MET
1	D	415	SER
1	D	428	MET
1	D	462	LEU
1	D	470	VAL
1	D	506	VAL
1	D	507	LEU
1	D	511	LEU
1	D	523	LYS
1	D	526	ILE
1	D	561	LEU
1	D	562	SER
1	D	571	ASN
1	D	576	THR
1	D	615	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN

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Mol	Chain	Res	Type
1	A	179	ASN
1	A	199	HIS
1	A	323	ASN
1	A	386	ASN
1	A	425	GLN
1	A	426	ASN
1	A	433	GLN
1	A	443	GLN
1	A	466	GLN
1	A	495	GLN
1	A	597	ASN
1	B	146	ASN
1	B	179	ASN
1	B	199	HIS
1	B	323	ASN
1	B	386	ASN
1	B	425	GLN
1	B	426	ASN
1	B	433	GLN
1	B	443	GLN
1	B	495	GLN
1	B	597	ASN
1	C	146	ASN
1	C	169	GLN
1	C	179	ASN
1	C	199	HIS
1	C	323	ASN
1	C	386	ASN
1	C	425	GLN
1	C	426	ASN
1	C	433	GLN
1	C	443	GLN
1	C	495	GLN
1	C	597	ASN
1	D	146	ASN
1	D	179	ASN
1	D	199	HIS
1	D	323	ASN
1	D	386	ASN
1	D	425	GLN
1	D	426	ASN
1	D	433	GLN

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Mol	Chain	Res	Type
1	D	443	GLN
1	D	495	GLN
1	D	597	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](#)

32 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
3	CPL	C	806	-	11,11,51	0.25	0	10,10,59	0.84	0
4	PX2	A	807	-	22,22,35	1.46	4 (18%)	25,27,40	2.30	10 (40%)
3	CPL	A	804	-	5,5,51	0.69	0	4,4,59	0.83	0
3	CPL	C	808	-	37,37,51	1.64	3 (8%)	40,42,59	2.40	14 (35%)
3	CPL	A	805	-	12,12,51	0.56	0	11,11,59	1.15	1 (9%)
3	CPL	D	808	-	37,37,51	1.64	3 (8%)	40,42,59	2.39	14 (35%)
3	CPL	C	804	-	5,5,51	0.24	0	4,4,59	0.65	0
3	CPL	B	804	-	5,5,51	0.24	0	4,4,59	0.65	0
3	CPL	D	802	-	37,37,51	1.49	6 (16%)	43,45,59	2.16	12 (27%)
3	CPL	D	804	-	5,5,51	0.24	0	4,4,59	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PX2	C	807	-	22,22,35	1.46	5 (22%)	25,27,40	2.30	9 (36%)
3	CPL	B	803	-	7,7,51	0.27	0	6,6,59	0.78	0
3	CPL	A	803	-	7,7,51	0.33	0	6,6,59	0.79	0
4	PX2	D	807	-	22,22,35	1.46	4 (18%)	25,27,40	2.30	9 (36%)
3	CPL	C	803	-	7,7,51	0.27	0	6,6,59	0.78	0
4	PX2	B	807	-	22,22,35	1.46	5 (22%)	25,27,40	2.30	9 (36%)
3	CPL	C	802	-	37,37,51	1.49	6 (16%)	43,45,59	2.16	12 (27%)
3	CPL	D	803	-	7,7,51	0.26	0	6,6,59	0.78	0
3	CPL	B	802	-	37,37,51	1.49	6 (16%)	43,45,59	2.16	12 (27%)
3	CPL	D	805	-	12,12,51	0.23	0	11,11,59	0.89	0
3	CPL	A	802	-	37,37,51	1.49	6 (16%)	43,45,59	2.16	12 (27%)
2	PCG	C	801	-	26,26,26	1.80	6 (23%)	39,41,41	2.17	14 (35%)
3	CPL	A	806	-	11,11,51	0.33	0	10,10,59	0.62	0
3	CPL	B	805	-	12,12,51	0.23	0	11,11,59	0.89	0
3	CPL	C	805	-	12,12,51	0.23	0	11,11,59	0.89	0
3	CPL	D	806	-	11,11,51	0.25	0	10,10,59	0.83	0
2	PCG	B	801	-	26,26,26	1.81	6 (23%)	39,41,41	2.16	14 (35%)
3	CPL	B	808	-	37,37,51	1.64	3 (8%)	40,42,59	2.40	14 (35%)
2	PCG	A	801	-	26,26,26	1.82	6 (23%)	39,41,41	2.17	14 (35%)
3	CPL	A	808	-	37,37,51	1.64	3 (8%)	40,42,59	2.40	14 (35%)
3	CPL	B	806	-	11,11,51	0.25	0	10,10,59	0.83	0
2	PCG	D	801	-	26,26,26	1.81	6 (23%)	39,41,41	2.16	14 (35%)

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	CPL	C	806	-	-	3/9/9/55	-
4	PX2	A	807	-	-	11/24/24/37	-
3	CPL	A	804	-	-	1/3/3/55	-
3	CPL	C	808	-	-	17/41/41/55	-
3	CPL	A	805	-	-	9/10/10/55	-
3	CPL	D	808	-	-	17/41/41/55	-
3	CPL	C	804	-	-	1/3/3/55	-
3	CPL	B	804	-	-	1/3/3/55	-
3	CPL	D	802	-	-	17/41/41/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPL	D	804	-	-	1/3/3/55	-
4	PX2	C	807	-	-	11/24/24/37	-
3	CPL	B	803	-	-	3/5/5/55	-
3	CPL	A	803	-	-	3/5/5/55	-
4	PX2	D	807	-	-	11/24/24/37	-
3	CPL	C	803	-	-	3/5/5/55	-
4	PX2	B	807	-	-	11/24/24/37	-
3	CPL	C	802	-	-	17/41/41/55	-
3	CPL	D	803	-	-	3/5/5/55	-
3	CPL	B	802	-	-	17/41/41/55	-
3	CPL	D	805	-	-	9/10/10/55	-
3	CPL	A	802	-	-	17/41/41/55	-
2	PCG	C	801	-	-	0/4/31/31	0/4/4/4
3	CPL	A	806	-	-	5/9/9/55	-
3	CPL	B	805	-	-	9/10/10/55	-
3	CPL	C	805	-	-	9/10/10/55	-
3	CPL	D	806	-	-	3/9/9/55	-
2	PCG	B	801	-	-	0/4/31/31	0/4/4/4
3	CPL	B	808	-	-	17/41/41/55	-
2	PCG	A	801	-	-	0/4/31/31	0/4/4/4
3	CPL	A	808	-	-	17/41/41/55	-
3	CPL	B	806	-	-	3/9/9/55	-
2	PCG	D	801	-	-	0/4/31/31	0/4/4/4

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	808	CPL	O2-C31	6.61	1.53	1.34
3	D	808	CPL	O2-C31	6.61	1.53	1.34
3	B	808	CPL	O2-C31	6.60	1.52	1.34
3	A	808	CPL	O2-C31	6.60	1.52	1.34
3	B	808	CPL	O3-C11	5.54	1.49	1.33
3	A	808	CPL	O3-C11	5.52	1.49	1.33
3	D	808	CPL	O3-C11	5.51	1.49	1.33
3	C	808	CPL	O3-C11	5.49	1.49	1.33
2	A	801	PCG	PA-O5'	5.30	1.63	1.57
2	D	801	PCG	PA-O5'	5.27	1.63	1.57
2	B	801	PCG	PA-O5'	5.25	1.63	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	PCG	PA-O5'	5.20	1.63	1.57
3	B	802	CPL	O2-C31	4.25	1.46	1.34
3	D	802	CPL	O2-C31	4.25	1.46	1.34
3	A	802	CPL	O2-C31	4.24	1.46	1.34
3	C	802	CPL	O2-C31	4.23	1.46	1.34
3	C	802	CPL	O11-C11	-3.95	1.10	1.22
3	D	802	CPL	O11-C11	-3.95	1.10	1.22
3	A	802	CPL	O11-C11	-3.94	1.10	1.22
3	B	802	CPL	O11-C11	-3.94	1.10	1.22
2	C	801	PCG	C5-N7	-3.58	1.31	1.39
2	D	801	PCG	C5-N7	-3.58	1.31	1.39
2	B	801	PCG	C5-N7	-3.56	1.31	1.39
2	A	801	PCG	C5-N7	-3.56	1.31	1.39
3	B	802	CPL	O3-C11	3.16	1.42	1.33
2	C	801	PCG	PA-O3'	3.16	1.63	1.57
3	A	802	CPL	O3-C11	3.16	1.42	1.33
3	C	802	CPL	O3-C11	3.15	1.42	1.33
3	D	802	CPL	O3-C11	3.15	1.42	1.33
2	A	801	PCG	PA-O3'	3.13	1.63	1.57
2	B	801	PCG	PA-O3'	3.11	1.62	1.57
2	D	801	PCG	PA-O3'	3.08	1.62	1.57
4	D	807	PX2	O6-C4	-2.63	1.14	1.22
4	B	807	PX2	O6-C4	-2.63	1.14	1.22
4	A	807	PX2	O6-C4	-2.63	1.14	1.22
4	C	807	PX2	O6-C4	-2.62	1.14	1.22
3	C	802	CPL	C5-N	-2.57	1.43	1.51
3	B	802	CPL	C5-N	-2.56	1.43	1.51
3	D	802	CPL	C5-N	-2.55	1.43	1.51
3	A	802	CPL	C5-N	-2.54	1.43	1.51
4	D	807	PX2	O7-C16	2.47	1.41	1.34
4	C	807	PX2	O7-C16	2.46	1.41	1.34
4	B	807	PX2	O7-C16	2.44	1.41	1.34
4	A	807	PX2	O7-C16	2.42	1.41	1.34
3	D	802	CPL	C7-N	-2.35	1.43	1.50
3	B	802	CPL	C7-N	-2.34	1.43	1.50
3	C	802	CPL	C7-N	-2.32	1.43	1.50
3	A	802	CPL	C7-N	-2.30	1.43	1.50
2	D	801	PCG	O4'-C1'	2.27	1.47	1.42
2	A	801	PCG	O4'-C1'	2.27	1.47	1.42
2	B	801	PCG	O4'-C1'	2.26	1.47	1.42
2	C	801	PCG	O4'-C1'	2.25	1.47	1.42
4	D	807	PX2	O5-C3	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	807	PX2	O5-C3	-2.14	1.40	1.45
4	A	807	PX2	O5-C3	-2.14	1.40	1.45
4	C	807	PX2	O5-C3	-2.13	1.40	1.45
2	A	801	PCG	O3'-C3'	-2.11	1.41	1.44
4	A	807	PX2	C6-C5	-2.11	1.44	1.52
2	B	801	PCG	O3'-C3'	-2.08	1.41	1.44
3	C	808	CPL	C13-C12	-2.08	1.44	1.52
4	C	807	PX2	C6-C5	-2.07	1.44	1.52
4	D	807	PX2	C6-C5	-2.07	1.44	1.52
4	B	807	PX2	C6-C5	-2.07	1.44	1.52
2	C	801	PCG	O3'-C3'	-2.07	1.41	1.44
3	A	808	CPL	C13-C12	-2.06	1.44	1.52
3	B	808	CPL	C13-C12	-2.06	1.44	1.52
3	D	808	CPL	C13-C12	-2.06	1.44	1.52
2	D	801	PCG	O3'-C3'	-2.04	1.41	1.44
3	D	802	CPL	C6-N	-2.04	1.44	1.50
3	A	802	CPL	C6-N	-2.03	1.44	1.50
3	B	802	CPL	C6-N	-2.03	1.44	1.50
3	C	802	CPL	C6-N	-2.03	1.44	1.50
2	D	801	PCG	C4-N9	-2.02	1.32	1.38
2	C	801	PCG	C4-N9	-2.02	1.32	1.38
2	A	801	PCG	C4-N9	-2.01	1.32	1.38
2	B	801	PCG	C4-N9	-2.01	1.33	1.38
4	B	807	PX2	O7-C2	-2.00	1.41	1.46
4	C	807	PX2	O7-C2	-2.00	1.41	1.46

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	CPL	O3-C11-C12	6.53	131.73	111.83
3	B	802	CPL	O3-C11-C12	6.51	131.69	111.83
3	C	802	CPL	O3-C11-C12	6.51	131.68	111.83
3	D	802	CPL	O3-C11-C12	6.51	131.68	111.83
3	A	802	CPL	O2-C31-C32	6.03	124.53	111.48
3	D	802	CPL	O2-C31-C32	6.03	124.52	111.48
3	B	802	CPL	O2-C31-C32	6.02	124.50	111.48
3	C	802	CPL	O2-C31-C32	6.01	124.49	111.48
2	A	801	PCG	C2-N3-C4	5.83	122.35	112.30
2	B	801	PCG	C2-N3-C4	5.81	122.30	112.30
2	D	801	PCG	C2-N3-C4	5.81	122.30	112.30
2	C	801	PCG	C2-N3-C4	5.80	122.29	112.30
3	B	808	CPL	C20-C19-C18	-5.52	86.49	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	808	CPL	C20-C19-C18	-5.51	86.50	114.37
3	C	808	CPL	C20-C19-C18	-5.51	86.53	114.37
3	D	808	CPL	C20-C19-C18	-5.51	86.53	114.37
3	A	808	CPL	C2-O2-C31	5.46	130.86	117.80
3	B	808	CPL	C2-O2-C31	5.45	130.84	117.80
3	C	808	CPL	C2-O2-C31	5.42	130.78	117.80
3	D	808	CPL	C2-O2-C31	5.42	130.76	117.80
2	D	801	PCG	C5-C4-N3	-5.40	119.80	128.39
2	A	801	PCG	C5-C4-N3	-5.39	119.81	128.39
2	B	801	PCG	C5-C4-N3	-5.39	119.81	128.39
2	C	801	PCG	C5-C4-N3	-5.37	119.84	128.39
4	D	807	PX2	O5-C4-O6	-5.09	110.89	123.63
4	B	807	PX2	O5-C4-O6	-5.09	110.89	123.63
4	A	807	PX2	O5-C4-O6	-5.08	110.93	123.63
4	C	807	PX2	O5-C4-O6	-5.07	110.93	123.63
3	A	802	CPL	O3-C3-C2	5.00	122.82	108.40
3	C	802	CPL	O3-C3-C2	5.00	122.81	108.40
3	B	802	CPL	O3-C3-C2	5.00	122.81	108.40
3	D	802	CPL	O3-C3-C2	4.99	122.79	108.40
3	D	808	CPL	O3-C11-C12	4.89	126.75	111.83
3	B	808	CPL	O3-C11-C12	4.89	126.73	111.83
3	A	808	CPL	O3-C11-C12	4.88	126.72	111.83
3	C	808	CPL	O3-C11-C12	4.88	126.71	111.83
4	A	807	PX2	O7-C16-C17	4.45	121.10	111.48
4	B	807	PX2	O7-C16-C17	4.45	121.10	111.48
4	C	807	PX2	O7-C16-C17	4.44	121.09	111.48
4	D	807	PX2	O7-C16-C17	4.44	121.08	111.48
3	C	808	CPL	O2-C31-C32	4.18	120.52	111.48
3	B	808	CPL	O2-C31-C32	4.17	120.50	111.48
3	A	808	CPL	O2-C31-C32	4.16	120.48	111.48
3	D	808	CPL	O2-C31-C32	4.16	120.47	111.48
3	A	808	CPL	O3-C3-C2	3.97	119.85	108.40
3	B	808	CPL	O3-C3-C2	3.97	119.84	108.40
3	C	808	CPL	O3-C3-C2	3.97	119.84	108.40
3	D	808	CPL	O3-C3-C2	3.97	119.83	108.40
4	A	807	PX2	O1-P1-O4	-3.93	96.41	106.67
4	D	807	PX2	O1-P1-O4	-3.92	96.44	106.67
4	B	807	PX2	O1-P1-O4	-3.91	96.47	106.67
4	C	807	PX2	O1-P1-O4	-3.90	96.50	106.67
4	C	807	PX2	O7-C16-O8	-3.88	114.63	123.70
4	D	807	PX2	O7-C16-O8	-3.88	114.64	123.70
4	B	807	PX2	O7-C16-O8	-3.87	114.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	807	PX2	O7-C16-O8	-3.86	114.68	123.70
2	C	801	PCG	O3'-C3'-C4'	-3.79	107.85	110.71
2	B	801	PCG	O3'-C3'-C4'	-3.75	107.88	110.71
2	D	801	PCG	O3'-C3'-C4'	-3.74	107.89	110.71
2	A	801	PCG	O3'-C3'-C4'	-3.74	107.89	110.71
3	C	808	CPL	C22-C21-C20	-3.72	95.56	114.37
3	A	808	CPL	C22-C21-C20	-3.71	95.61	114.37
3	A	802	CPL	O3-C11-O11	-3.71	114.34	123.63
3	B	808	CPL	C22-C21-C20	-3.71	95.62	114.37
3	D	808	CPL	C22-C21-C20	-3.71	95.63	114.37
3	B	802	CPL	O3-C11-O11	-3.70	114.37	123.63
3	C	802	CPL	O3-C11-O11	-3.70	114.37	123.63
3	D	802	CPL	O3-C11-O11	-3.69	114.39	123.63
2	C	801	PCG	C2-N1-C6	-3.69	118.42	125.11
2	B	801	PCG	C2-N1-C6	-3.67	118.45	125.11
2	A	801	PCG	C2-N1-C6	-3.66	118.47	125.11
2	D	801	PCG	C2-N1-C6	-3.66	118.47	125.11
3	C	808	CPL	C3-C2-C1	-3.66	103.26	111.78
3	D	808	CPL	C3-C2-C1	-3.64	103.29	111.78
3	B	808	CPL	C3-C2-C1	-3.64	103.30	111.78
3	A	808	CPL	C3-C2-C1	-3.64	103.30	111.78
3	B	808	CPL	C14-C13-C12	-3.63	99.80	113.13
3	A	808	CPL	C14-C13-C12	-3.62	99.82	113.13
3	C	808	CPL	C14-C13-C12	-3.62	99.84	113.13
3	D	808	CPL	C14-C13-C12	-3.61	99.86	113.13
2	D	801	PCG	N9-C4-N3	3.37	132.70	125.95
2	A	801	PCG	N9-C4-N3	3.36	132.67	125.95
2	B	801	PCG	N9-C4-N3	3.35	132.66	125.95
2	C	801	PCG	N9-C4-N3	3.33	132.62	125.95
2	C	801	PCG	O1A-PA-O2A	3.24	118.52	108.56
2	A	801	PCG	O1A-PA-O2A	3.24	118.51	108.56
2	B	801	PCG	O1A-PA-O2A	3.23	118.50	108.56
2	D	801	PCG	O1A-PA-O2A	3.22	118.47	108.56
4	A	807	PX2	C3-O5-C4	3.20	128.82	117.12
4	D	807	PX2	C3-O5-C4	3.19	128.79	117.12
4	C	807	PX2	C3-O5-C4	3.19	128.77	117.12
4	B	807	PX2	C3-O5-C4	3.18	128.74	117.12
3	A	802	CPL	O2P-P-O3P	3.17	121.93	107.57
3	C	808	CPL	O11-C11-C12	-3.17	111.39	123.78
3	C	802	CPL	O2P-P-O3P	3.17	121.92	107.57
3	A	808	CPL	O11-C11-C12	-3.16	111.41	123.78
3	D	808	CPL	O11-C11-C12	-3.16	111.42	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	CPL	O2P-P-O3P	3.16	121.89	107.57
3	B	808	CPL	O11-C11-C12	-3.16	111.43	123.78
3	D	802	CPL	O2P-P-O3P	3.15	121.86	107.57
3	D	802	CPL	O4P-P-O1P	3.14	121.38	108.94
3	B	802	CPL	O4P-P-O1P	3.14	121.38	108.94
3	A	802	CPL	O4P-P-O1P	3.14	121.37	108.94
3	C	802	CPL	O4P-P-O1P	3.13	121.34	108.94
3	C	808	CPL	C24-C23-C22	-3.09	98.74	114.37
3	A	808	CPL	C24-C23-C22	-3.09	98.76	114.37
3	D	808	CPL	C24-C23-C22	-3.09	98.77	114.37
3	B	808	CPL	C24-C23-C22	-3.09	98.77	114.37
3	C	802	CPL	C4-C5-N	-2.91	106.48	115.82
3	D	802	CPL	C4-C5-N	-2.91	106.48	115.82
3	B	802	CPL	C4-C5-N	-2.90	106.52	115.82
3	A	802	CPL	C4-C5-N	-2.90	106.52	115.82
4	D	807	PX2	O5-C4-C5	2.83	120.47	111.83
4	B	807	PX2	O5-C4-C5	2.82	120.44	111.83
4	C	807	PX2	O5-C4-C5	2.82	120.43	111.83
4	A	807	PX2	O5-C4-C5	2.82	120.43	111.83
3	A	808	CPL	C18-C17-C16	-2.80	100.19	114.37
3	D	808	CPL	C18-C17-C16	-2.80	100.20	114.37
3	C	808	CPL	C18-C17-C16	-2.80	100.21	114.37
3	B	808	CPL	C18-C17-C16	-2.80	100.21	114.37
2	D	801	PCG	O3'-C3'-C2'	-2.75	112.91	115.61
2	C	801	PCG	O3'-C3'-C2'	-2.73	112.92	115.61
2	A	801	PCG	O3'-C3'-C2'	-2.71	112.95	115.61
2	B	801	PCG	O3'-C3'-C2'	-2.69	112.97	115.61
4	D	807	PX2	O3-P1-O4	2.59	113.42	106.67
4	B	807	PX2	O3-P1-O4	2.59	113.42	106.67
2	C	801	PCG	N9-C8-N7	-2.59	108.60	113.40
4	C	807	PX2	O3-P1-O4	2.59	113.42	106.67
2	B	801	PCG	N9-C8-N7	-2.57	108.64	113.40
2	A	801	PCG	N9-C8-N7	-2.57	108.64	113.40
2	D	801	PCG	N9-C8-N7	-2.57	108.64	113.40
4	A	807	PX2	O3-P1-O4	2.56	113.34	106.67
3	B	808	CPL	P-O3P-C1	2.56	136.00	121.35
3	D	808	CPL	P-O3P-C1	2.55	135.99	121.35
3	A	808	CPL	P-O3P-C1	2.55	135.98	121.35
3	C	808	CPL	P-O3P-C1	2.55	135.94	121.35
3	C	808	CPL	O31-C31-C32	-2.55	113.82	123.78
3	D	808	CPL	O31-C31-C32	-2.55	113.83	123.78
3	A	808	CPL	O31-C31-C32	-2.54	113.85	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	808	CPL	O31-C31-C32	-2.54	113.87	123.78
2	A	801	PCG	C5-C6-N1	2.53	119.69	113.25
2	C	801	PCG	C5-C6-N1	2.52	119.68	113.25
3	A	802	CPL	O11-C11-C12	-2.52	113.91	123.78
3	D	802	CPL	O11-C11-C12	-2.52	113.92	123.78
3	B	802	CPL	O11-C11-C12	-2.52	113.93	123.78
3	C	802	CPL	O11-C11-C12	-2.52	113.93	123.78
2	B	801	PCG	C5-C6-N1	2.52	119.66	113.25
2	D	801	PCG	C5-C6-N1	2.51	119.63	113.25
4	B	807	PX2	C6-C5-C4	-2.49	104.57	113.69
2	C	801	PCG	C8-N7-C5	2.49	108.69	104.26
4	D	807	PX2	C6-C5-C4	-2.48	104.59	113.69
4	C	807	PX2	C6-C5-C4	-2.48	104.59	113.69
2	D	801	PCG	C8-N7-C5	2.48	108.68	104.26
2	B	801	PCG	C8-N7-C5	2.48	108.68	104.26
4	A	807	PX2	C6-C5-C4	-2.48	104.61	113.69
2	A	801	PCG	C8-N7-C5	2.47	108.66	104.26
3	A	805	CPL	C22-C21-C20	-2.46	101.93	114.37
3	A	802	CPL	C8-N-C6	2.44	115.38	108.98
3	B	802	CPL	C8-N-C6	2.41	115.30	108.98
3	C	802	CPL	C8-N-C6	2.40	115.29	108.98
3	D	802	CPL	C8-N-C6	2.40	115.28	108.98
4	A	807	PX2	O5-C3-C2	-2.35	101.62	108.40
2	D	801	PCG	O6-C6-C5	-2.34	120.35	126.53
2	A	801	PCG	O6-C6-C5	-2.34	120.35	126.53
2	B	801	PCG	O6-C6-C5	-2.32	120.40	126.53
4	C	807	PX2	O5-C3-C2	-2.32	101.71	108.40
4	B	807	PX2	O5-C3-C2	-2.32	101.72	108.40
2	C	801	PCG	O6-C6-C5	-2.31	120.42	126.53
4	D	807	PX2	O5-C3-C2	-2.31	101.74	108.40
2	B	801	PCG	C4-C5-N7	-2.26	107.09	110.67
2	D	801	PCG	C4-C5-N7	-2.25	107.10	110.67
2	C	801	PCG	C4-C5-N7	-2.25	107.11	110.67
2	A	801	PCG	C4-C5-N7	-2.25	107.11	110.67
2	B	801	PCG	C4'-O4'-C1'	-2.23	104.55	109.47
2	C	801	PCG	C4'-O4'-C1'	-2.22	104.55	109.47
2	D	801	PCG	C4'-O4'-C1'	-2.22	104.56	109.47
2	A	801	PCG	C4'-O4'-C1'	-2.22	104.57	109.47
3	A	802	CPL	C17-C16-C15	-2.20	103.26	114.37
3	D	802	CPL	C17-C16-C15	-2.19	103.28	114.37
3	B	802	CPL	C17-C16-C15	-2.19	103.30	114.37
3	C	802	CPL	C17-C16-C15	-2.19	103.31	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	CPL	O2P-P-O4P	-2.12	97.95	107.57
3	D	802	CPL	C14-C13-C12	-2.12	105.34	113.13
3	C	802	CPL	O2P-P-O4P	-2.11	97.99	107.57
3	B	802	CPL	O2P-P-O4P	-2.11	98.01	107.57
3	A	802	CPL	C14-C13-C12	-2.11	105.38	113.13
3	B	802	CPL	C14-C13-C12	-2.11	105.38	113.13
3	D	802	CPL	O2P-P-O4P	-2.11	98.02	107.57
3	C	802	CPL	C14-C13-C12	-2.10	105.41	113.13
3	D	808	CPL	C15-C14-C13	-2.07	103.89	114.37
3	A	808	CPL	C15-C14-C13	-2.07	103.89	114.37
3	B	808	CPL	C15-C14-C13	-2.07	103.92	114.37
3	C	808	CPL	C15-C14-C13	-2.06	103.96	114.37
2	C	801	PCG	N2-C2-N1	2.04	121.06	116.76
2	A	801	PCG	N2-C2-N1	2.02	121.03	116.76
2	B	801	PCG	N2-C2-N1	2.02	121.03	116.76
2	D	801	PCG	N2-C2-N1	2.01	121.00	116.76
4	A	807	PX2	C18-C17-C16	-2.01	106.34	113.69

There are no chirality outliers.

All (246) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	CPL	C4-O4P-P-O1P
3	A	802	CPL	C4-O4P-P-O3P
3	A	808	CPL	C32-C31-O2-C2
3	A	808	CPL	C4-O4P-P-O1P
3	A	808	CPL	C4-O4P-P-O2P
3	B	802	CPL	C4-O4P-P-O1P
3	B	802	CPL	C4-O4P-P-O3P
3	B	808	CPL	C32-C31-O2-C2
3	B	808	CPL	C4-O4P-P-O1P
3	B	808	CPL	C4-O4P-P-O2P
3	C	802	CPL	C4-O4P-P-O1P
3	C	802	CPL	C4-O4P-P-O3P
3	C	808	CPL	C32-C31-O2-C2
3	C	808	CPL	C4-O4P-P-O1P
3	C	808	CPL	C4-O4P-P-O2P
3	D	802	CPL	C4-O4P-P-O1P
3	D	802	CPL	C4-O4P-P-O3P
3	D	808	CPL	C32-C31-O2-C2
3	D	808	CPL	C4-O4P-P-O1P
3	D	808	CPL	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
4	A	807	PX2	C17-C16-O7-C2
4	B	807	PX2	C17-C16-O7-C2
4	C	807	PX2	C17-C16-O7-C2
4	D	807	PX2	C17-C16-O7-C2
3	A	802	CPL	O31-C31-O2-C2
3	A	808	CPL	O31-C31-O2-C2
3	B	802	CPL	O31-C31-O2-C2
3	B	808	CPL	O31-C31-O2-C2
3	C	802	CPL	O31-C31-O2-C2
3	C	808	CPL	O31-C31-O2-C2
3	D	802	CPL	O31-C31-O2-C2
3	D	808	CPL	O31-C31-O2-C2
4	A	807	PX2	O8-C16-O7-C2
4	B	807	PX2	O8-C16-O7-C2
4	C	807	PX2	O8-C16-O7-C2
4	D	807	PX2	O8-C16-O7-C2
3	A	808	CPL	C12-C11-O3-C3
3	B	808	CPL	C12-C11-O3-C3
3	C	808	CPL	C12-C11-O3-C3
3	D	808	CPL	C12-C11-O3-C3
3	A	802	CPL	C32-C31-O2-C2
3	B	802	CPL	C32-C31-O2-C2
3	C	802	CPL	C32-C31-O2-C2
3	D	802	CPL	C32-C31-O2-C2
3	A	808	CPL	C32-C33-C34-C35
3	B	808	CPL	C32-C33-C34-C35
3	C	808	CPL	C32-C33-C34-C35
3	D	808	CPL	C32-C33-C34-C35
3	A	808	CPL	O11-C11-O3-C3
3	B	808	CPL	O11-C11-O3-C3
3	C	808	CPL	O11-C11-O3-C3
3	D	808	CPL	O11-C11-O3-C3
3	A	806	CPL	C16-C17-C18-C19
3	A	802	CPL	C32-C33-C34-C35
3	B	802	CPL	C32-C33-C34-C35
3	C	802	CPL	C32-C33-C34-C35
3	D	802	CPL	C32-C33-C34-C35
3	A	806	CPL	C18-C19-C20-C21
4	B	807	PX2	C5-C4-O5-C3
4	C	807	PX2	C5-C4-O5-C3
4	D	807	PX2	C5-C4-O5-C3
4	A	807	PX2	C5-C4-O5-C3

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Mol	Chain	Res	Type	Atoms
4	A	807	PX2	O6-C4-O5-C3
4	B	807	PX2	O6-C4-O5-C3
4	C	807	PX2	O6-C4-O5-C3
4	D	807	PX2	O6-C4-O5-C3
3	A	805	CPL	C14-C15-C16-C17
3	B	805	CPL	C14-C15-C16-C17
3	C	805	CPL	C14-C15-C16-C17
3	D	805	CPL	C14-C15-C16-C17
3	B	808	CPL	C11-C12-C13-C14
3	C	808	CPL	C11-C12-C13-C14
3	A	808	CPL	C11-C12-C13-C14
3	D	808	CPL	C11-C12-C13-C14
3	A	808	CPL	C12-C13-C14-C15
3	B	808	CPL	C12-C13-C14-C15
3	C	808	CPL	C12-C13-C14-C15
3	D	808	CPL	C12-C13-C14-C15
3	A	805	CPL	C20-C21-C22-C23
3	A	808	CPL	C15-C16-C17-C18
3	B	808	CPL	C15-C16-C17-C18
3	C	808	CPL	C15-C16-C17-C18
3	D	808	CPL	C15-C16-C17-C18
3	A	805	CPL	C17-C18-C19-C20
3	A	805	CPL	C18-C19-C20-C21
3	B	805	CPL	C18-C19-C20-C21
3	B	805	CPL	C20-C21-C22-C23
3	C	805	CPL	C18-C19-C20-C21
3	C	805	CPL	C20-C21-C22-C23
3	D	805	CPL	C18-C19-C20-C21
3	D	805	CPL	C20-C21-C22-C23
3	B	802	CPL	C31-C32-C33-C34
3	C	802	CPL	C31-C32-C33-C34
3	D	802	CPL	C31-C32-C33-C34
3	A	806	CPL	C20-C21-C22-C23
3	A	802	CPL	C31-C32-C33-C34
3	B	806	CPL	C18-C19-C20-C21
3	C	806	CPL	C18-C19-C20-C21
3	D	806	CPL	C18-C19-C20-C21
3	A	804	CPL	C13-C14-C15-C16
3	A	802	CPL	O3P-C1-C2-C3
3	B	802	CPL	O3P-C1-C2-C3
3	C	802	CPL	O3P-C1-C2-C3
3	D	802	CPL	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
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	807	PX2	C1-C2-C3-O5
4	B	807	PX2	C1-C2-C3-O5
4	C	807	PX2	C1-C2-C3-O5
4	D	807	PX2	C1-C2-C3-O5
3	A	803	CPL	C14-C15-C16-C17
3	A	803	CPL	C16-C17-C18-C19
3	B	803	CPL	C14-C15-C16-C17
3	C	803	CPL	C14-C15-C16-C17
3	D	803	CPL	C14-C15-C16-C17
3	A	802	CPL	C1-C2-O2-C31
3	B	802	CPL	C1-C2-O2-C31
3	C	802	CPL	C1-C2-O2-C31
3	D	802	CPL	C1-C2-O2-C31
3	B	805	CPL	C13-C14-C15-C16
3	D	805	CPL	C13-C14-C15-C16
3	C	805	CPL	C13-C14-C15-C16
3	A	805	CPL	C19-C20-C21-C22
3	B	803	CPL	C15-C16-C17-C18
3	C	803	CPL	C15-C16-C17-C18
3	D	803	CPL	C15-C16-C17-C18
3	A	805	CPL	C12-C13-C14-C15
3	A	806	CPL	C12-C13-C14-C15
3	B	802	CPL	C12-C11-O3-C3
3	A	805	CPL	C13-C14-C15-C16
3	A	802	CPL	C12-C11-O3-C3
3	C	802	CPL	C12-C11-O3-C3
3	D	802	CPL	C12-C11-O3-C3
3	A	808	CPL	O3P-C1-C2-C3
3	B	808	CPL	O3P-C1-C2-C3
3	C	808	CPL	O3P-C1-C2-C3
3	D	808	CPL	O3P-C1-C2-C3
3	B	806	CPL	C12-C13-C14-C15
3	C	806	CPL	C12-C13-C14-C15
3	D	806	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	802	CPL	O11-C11-O3-C3
3	B	802	CPL	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
3	C	802	CPL	O11-C11-O3-C3
3	A	802	CPL	O11-C11-O3-C3
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	A	808	CPL	C19-C20-C21-C22
3	B	808	CPL	C19-C20-C21-C22
3	D	808	CPL	C19-C20-C21-C22
3	C	808	CPL	C19-C20-C21-C22
4	A	807	PX2	O7-C2-C3-O5
4	B	807	PX2	O7-C2-C3-O5
4	C	807	PX2	O7-C2-C3-O5
4	D	807	PX2	O7-C2-C3-O5
3	A	802	CPL	O4P-C4-C5-N
3	B	802	CPL	O4P-C4-C5-N
3	C	802	CPL	O4P-C4-C5-N
3	D	802	CPL	O4P-C4-C5-N
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	805	CPL	C16-C17-C18-C19
3	A	802	CPL	C19-C20-C21-C22
3	A	802	CPL	C4-O4P-P-O2P
3	A	808	CPL	C4-O4P-P-O3P
3	B	802	CPL	C4-O4P-P-O2P
3	B	808	CPL	C4-O4P-P-O3P
3	C	802	CPL	C4-O4P-P-O2P
3	C	808	CPL	C4-O4P-P-O3P
3	D	802	CPL	C4-O4P-P-O2P
3	D	808	CPL	C4-O4P-P-O3P
4	A	807	PX2	C1-C2-O7-C16
4	B	807	PX2	C1-C2-O7-C16
4	C	807	PX2	C1-C2-O7-C16
4	D	807	PX2	C1-C2-O7-C16
3	B	805	CPL	C15-C16-C17-C18
3	C	805	CPL	C15-C16-C17-C18
3	D	805	CPL	C15-C16-C17-C18
3	C	802	CPL	C18-C19-C20-C21
4	A	807	PX2	O7-C16-C17-C18
4	B	807	PX2	O7-C16-C17-C18
4	C	807	PX2	O7-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	D	807	PX2	O7-C16-C17-C18
3	B	802	CPL	C18-C19-C20-C21
3	D	802	CPL	C18-C19-C20-C21
3	B	808	CPL	C23-C24-C25-C26
3	C	808	CPL	C23-C24-C25-C26
3	A	808	CPL	C23-C24-C25-C26
3	A	802	CPL	C18-C19-C20-C21
3	D	808	CPL	C23-C24-C25-C26
3	C	805	CPL	C19-C20-C21-C22
3	B	805	CPL	C19-C20-C21-C22
3	D	805	CPL	C19-C20-C21-C22
3	B	808	CPL	C35-C36-C37-C38
3	C	808	CPL	C35-C36-C37-C38
3	D	808	CPL	C35-C36-C37-C38
3	A	808	CPL	C35-C36-C37-C38
4	A	807	PX2	C3-C2-O7-C16
4	B	807	PX2	C3-C2-O7-C16
4	C	807	PX2	C3-C2-O7-C16
4	D	807	PX2	C3-C2-O7-C16
3	A	803	CPL	C15-C16-C17-C18
3	B	802	CPL	C20-C21-C22-C23
3	C	802	CPL	C20-C21-C22-C23
3	D	802	CPL	C20-C21-C22-C23
4	D	807	PX2	C6-C7-C8-C9
3	A	802	CPL	C20-C21-C22-C23
4	A	807	PX2	C6-C7-C8-C9
4	B	807	PX2	C6-C7-C8-C9
4	C	807	PX2	C6-C7-C8-C9
3	A	808	CPL	C1-C2-C3-O3
3	B	808	CPL	C1-C2-C3-O3
3	C	808	CPL	C1-C2-C3-O3
3	D	808	CPL	C1-C2-C3-O3
4	C	807	PX2	C5-C6-C7-C8
3	D	803	CPL	C16-C17-C18-C19
4	B	807	PX2	C5-C6-C7-C8
4	D	807	PX2	C5-C6-C7-C8
3	B	803	CPL	C16-C17-C18-C19
3	C	803	CPL	C16-C17-C18-C19
4	A	807	PX2	C5-C6-C7-C8
3	A	805	CPL	C21-C22-C23-C24
3	A	806	CPL	C15-C16-C17-C18
3	C	806	CPL	C17-C18-C19-C20

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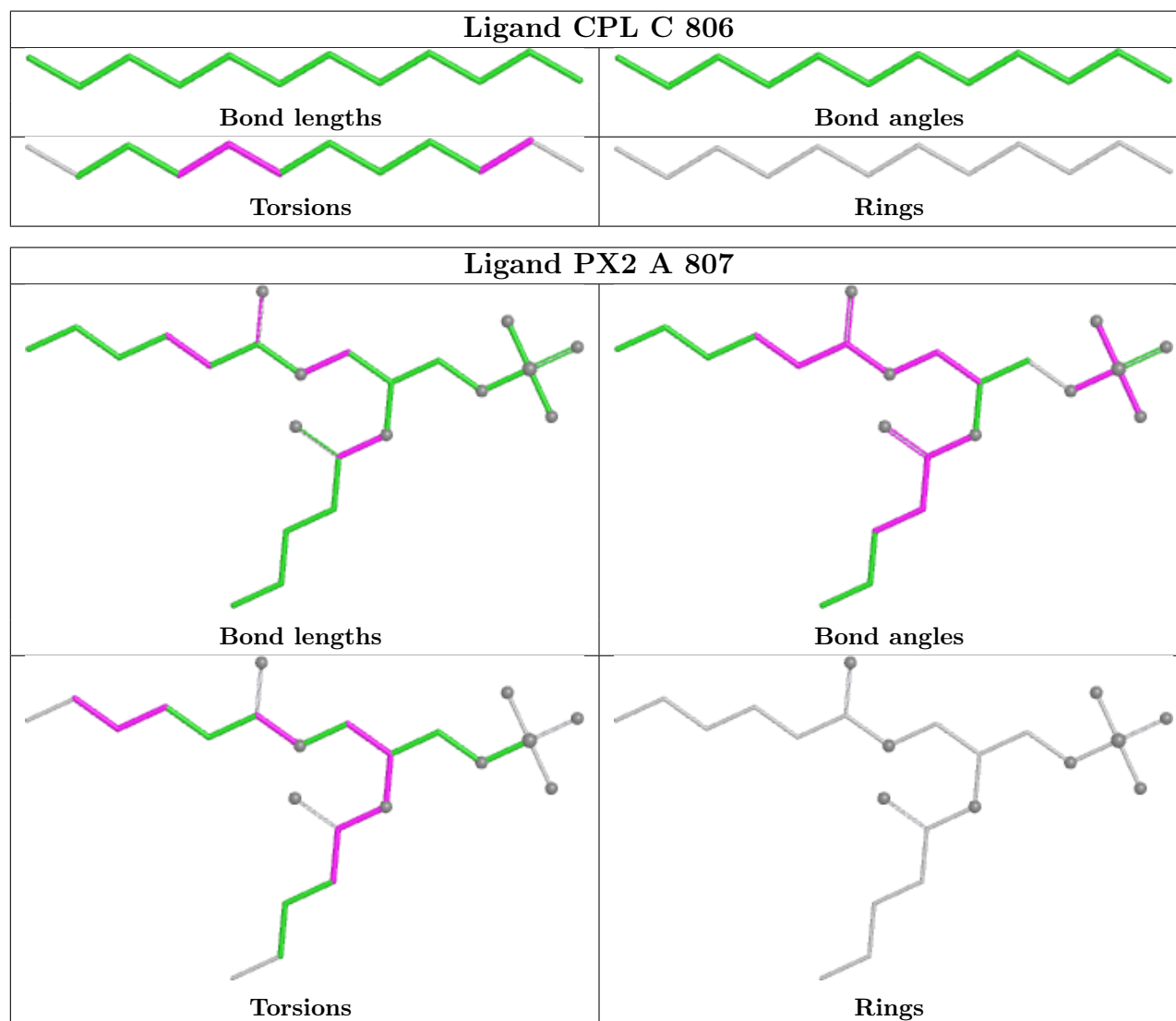
Mol	Chain	Res	Type	Atoms
3	B	806	CPL	C17-C18-C19-C20
3	D	806	CPL	C17-C18-C19-C20
3	C	805	CPL	C17-C18-C19-C20
3	B	805	CPL	C17-C18-C19-C20
3	D	805	CPL	C17-C18-C19-C20
3	A	808	CPL	O3P-C1-C2-O2
3	B	808	CPL	O3P-C1-C2-O2
3	C	808	CPL	O3P-C1-C2-O2
3	D	808	CPL	O3P-C1-C2-O2
3	B	805	CPL	C21-C22-C23-C24
3	C	805	CPL	C21-C22-C23-C24
3	D	805	CPL	C21-C22-C23-C24
3	D	802	CPL	C15-C16-C17-C18
3	A	802	CPL	C15-C16-C17-C18
3	B	802	CPL	C15-C16-C17-C18
3	C	802	CPL	C15-C16-C17-C18

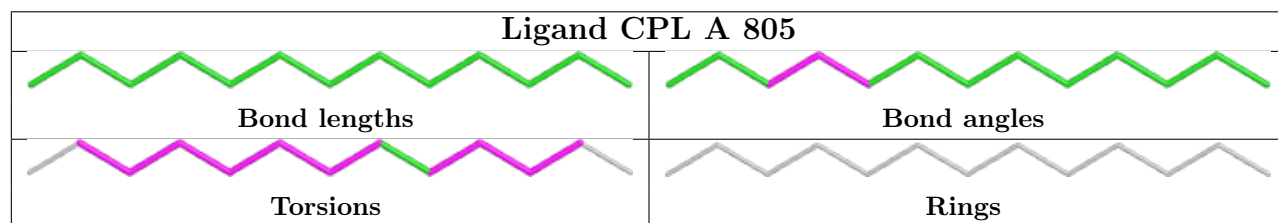
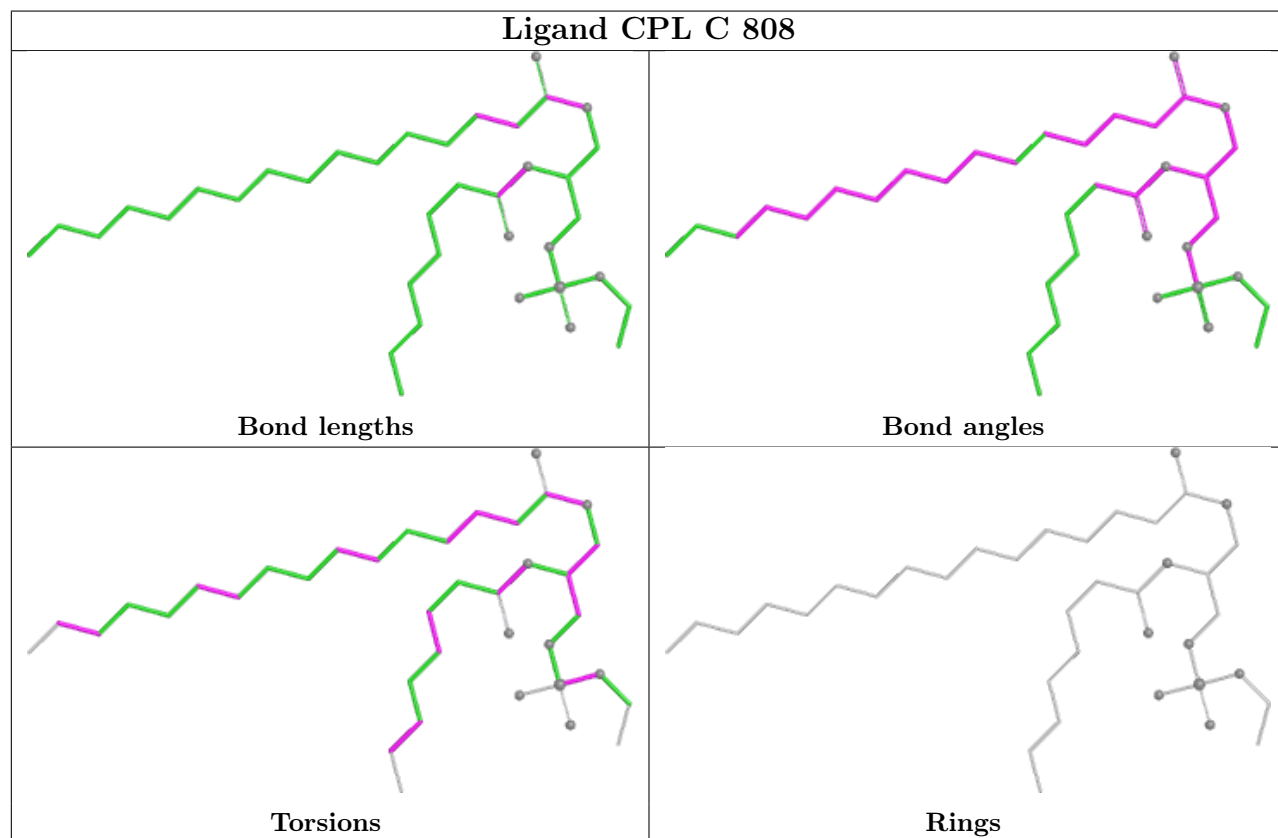
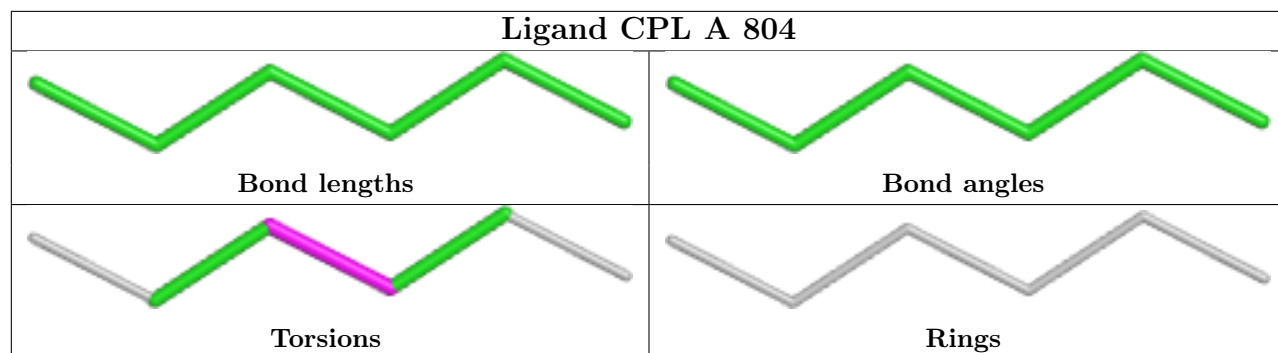
There are no ring outliers.

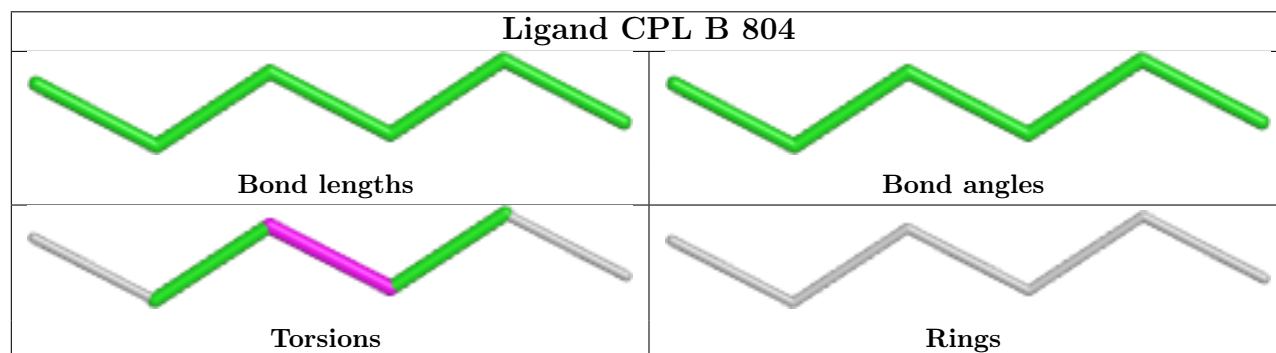
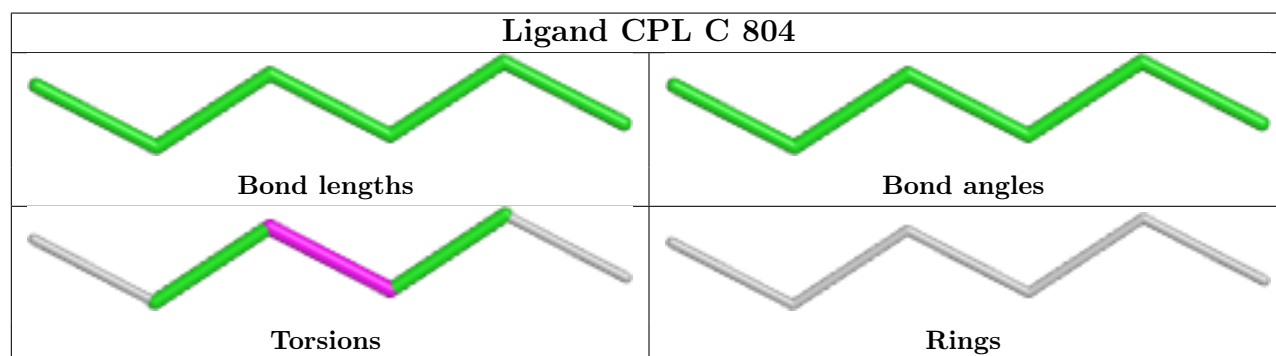
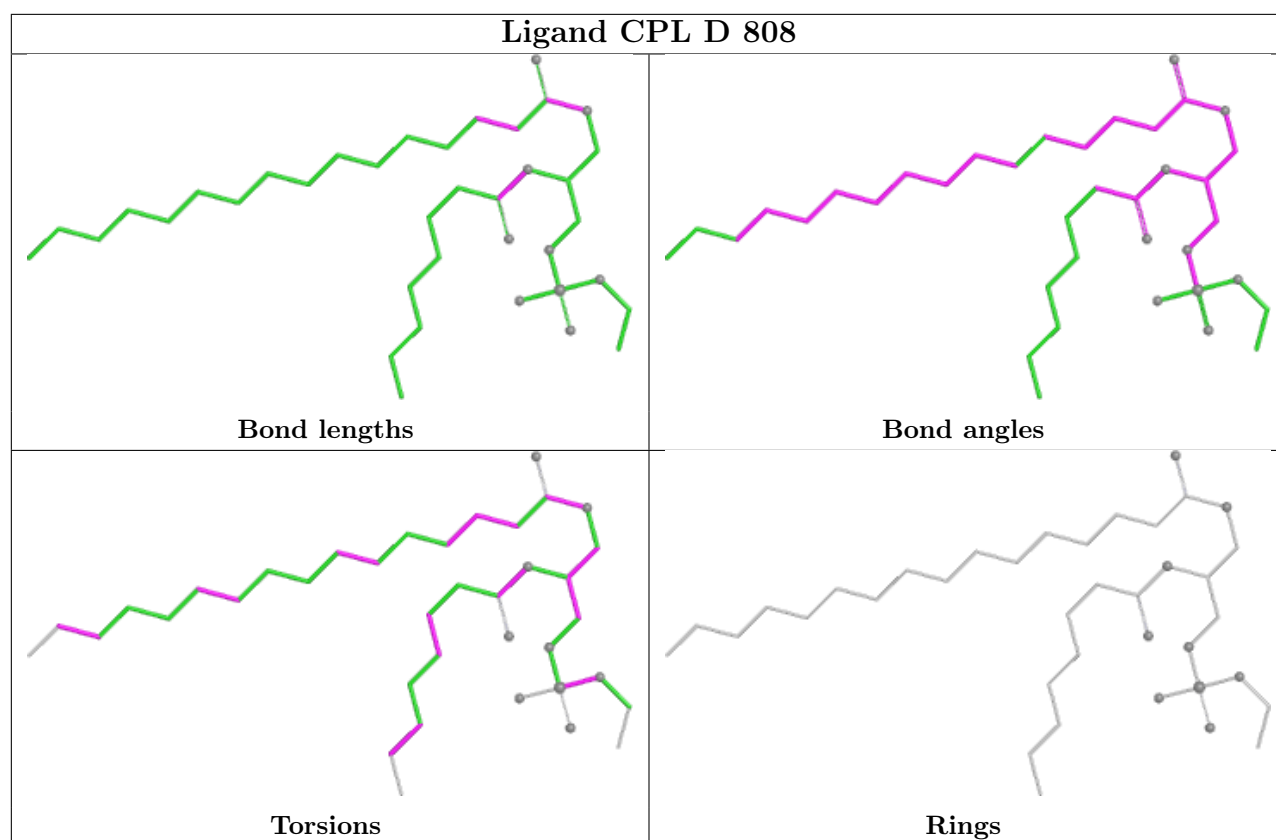
21 monomers are involved in 40 short contacts:

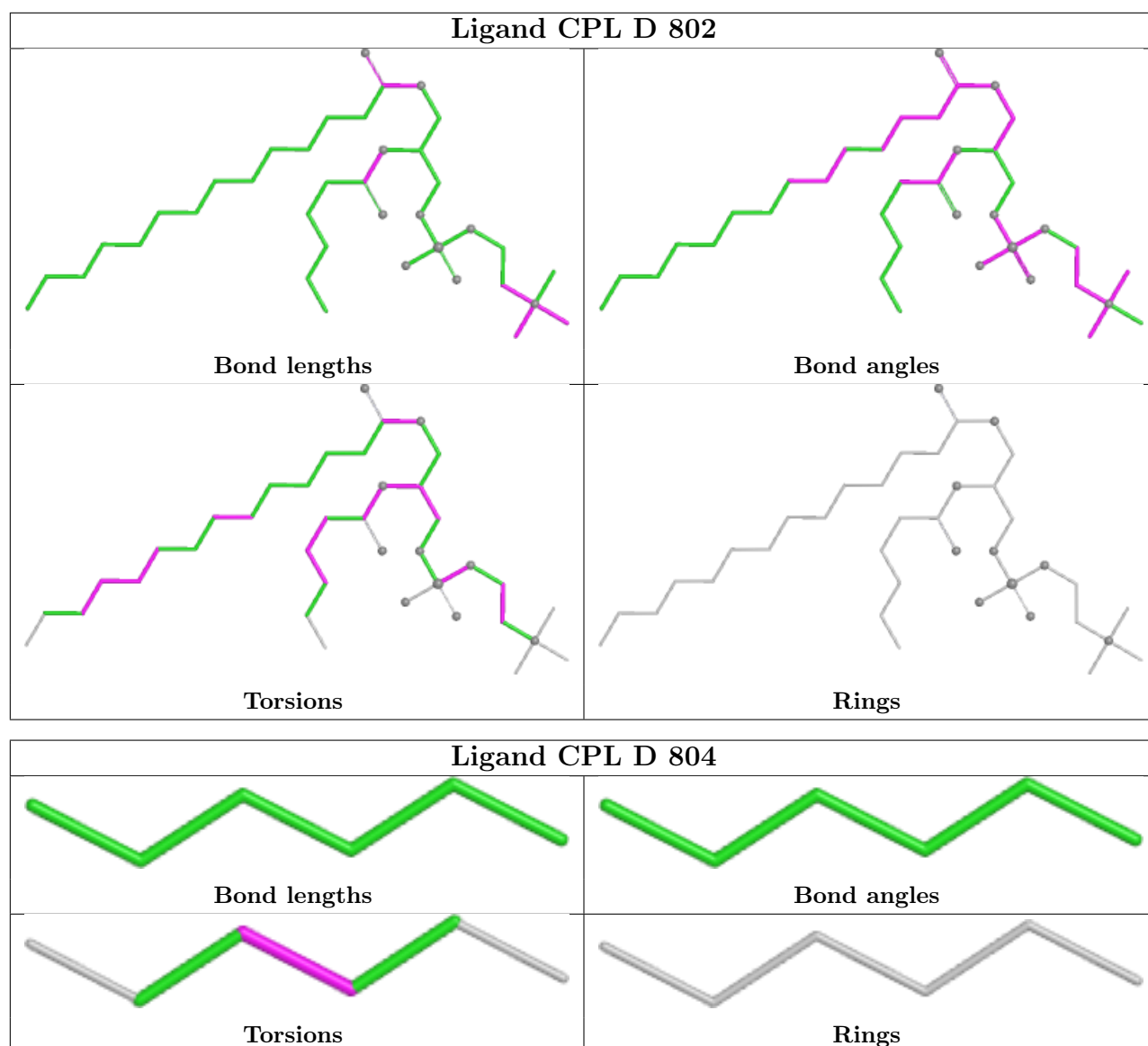
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	PX2	1	0
3	A	804	CPL	1	0
3	C	808	CPL	1	0
3	D	808	CPL	1	0
3	D	802	CPL	4	0
4	C	807	PX2	3	0
3	A	803	CPL	1	0
4	D	807	PX2	1	0
4	B	807	PX2	2	0
3	C	802	CPL	3	0
3	B	802	CPL	3	0
3	D	805	CPL	2	0
3	A	802	CPL	5	0
2	C	801	PCG	1	0
3	B	805	CPL	2	0
3	C	805	CPL	2	0
2	B	801	PCG	1	0
3	B	808	CPL	2	0
2	A	801	PCG	1	0
3	A	808	CPL	2	0
2	D	801	PCG	1	0

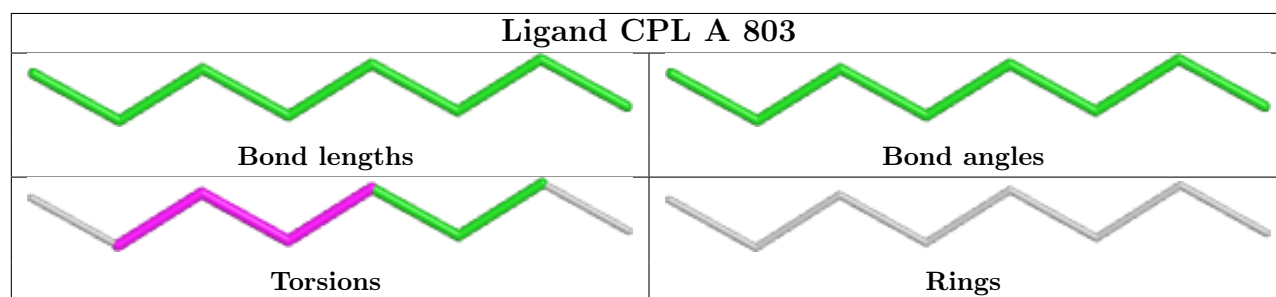
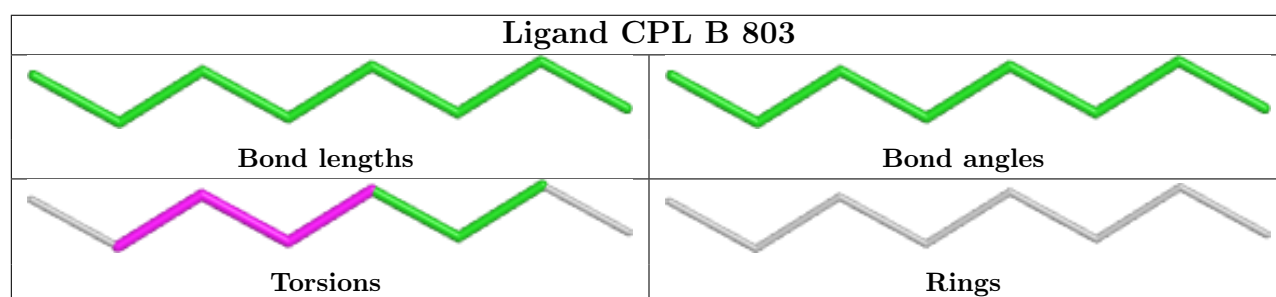
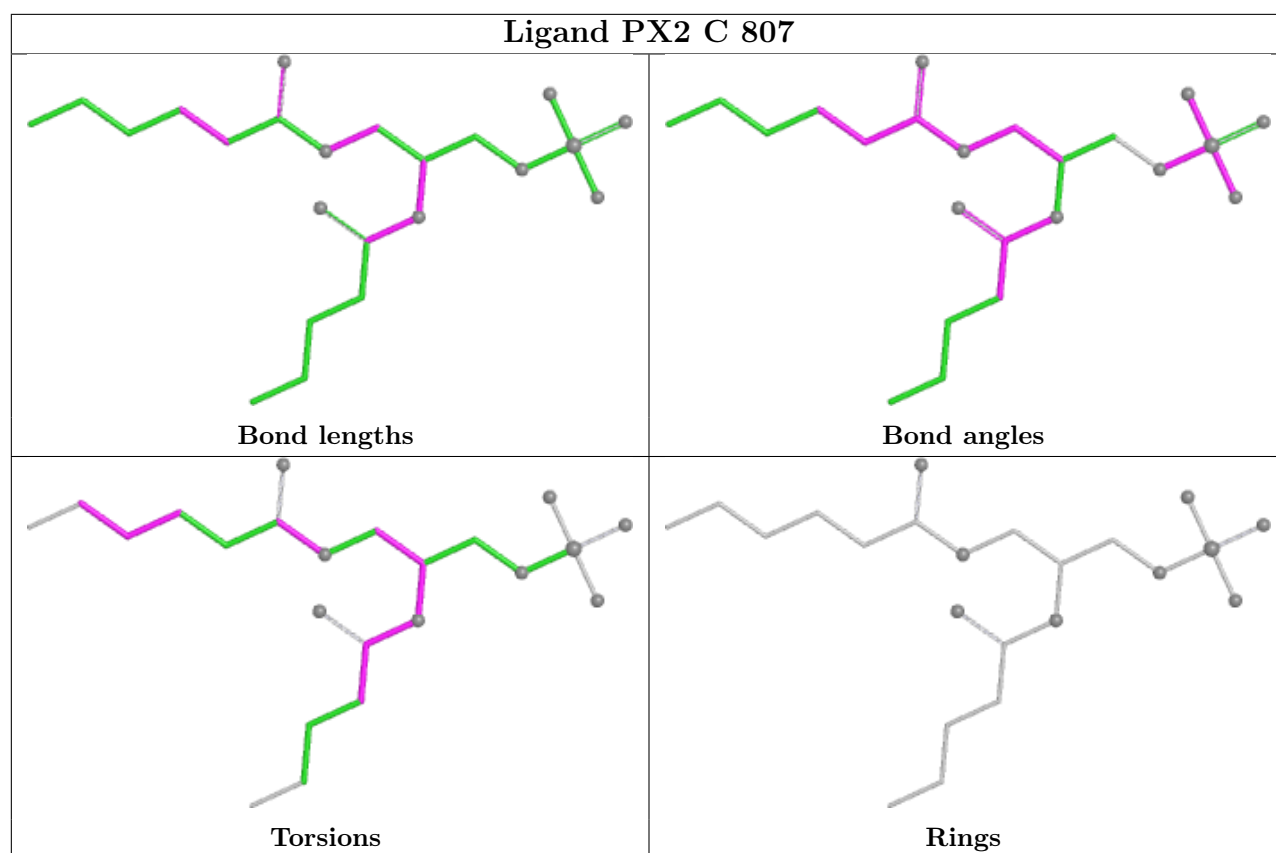
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

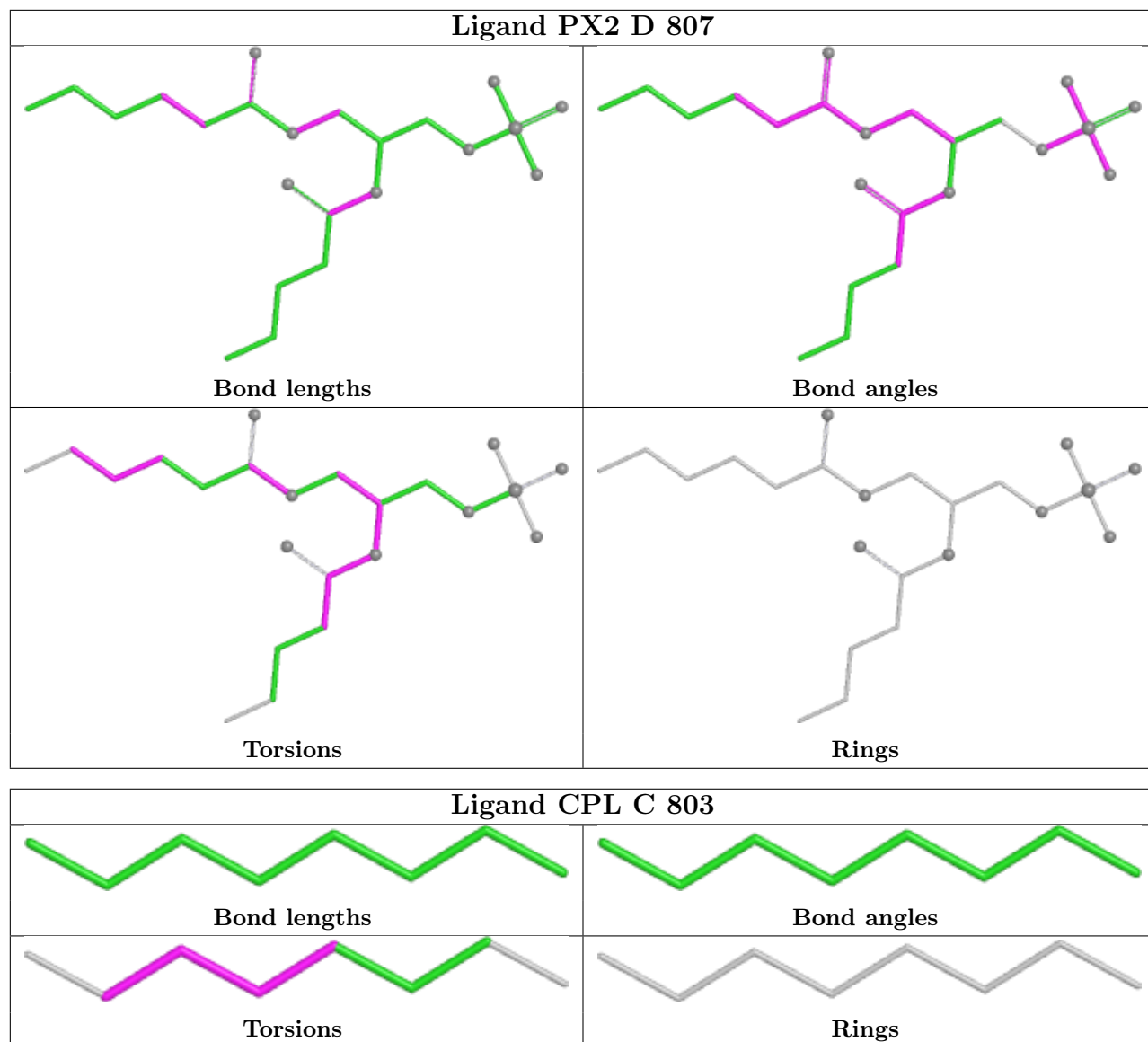


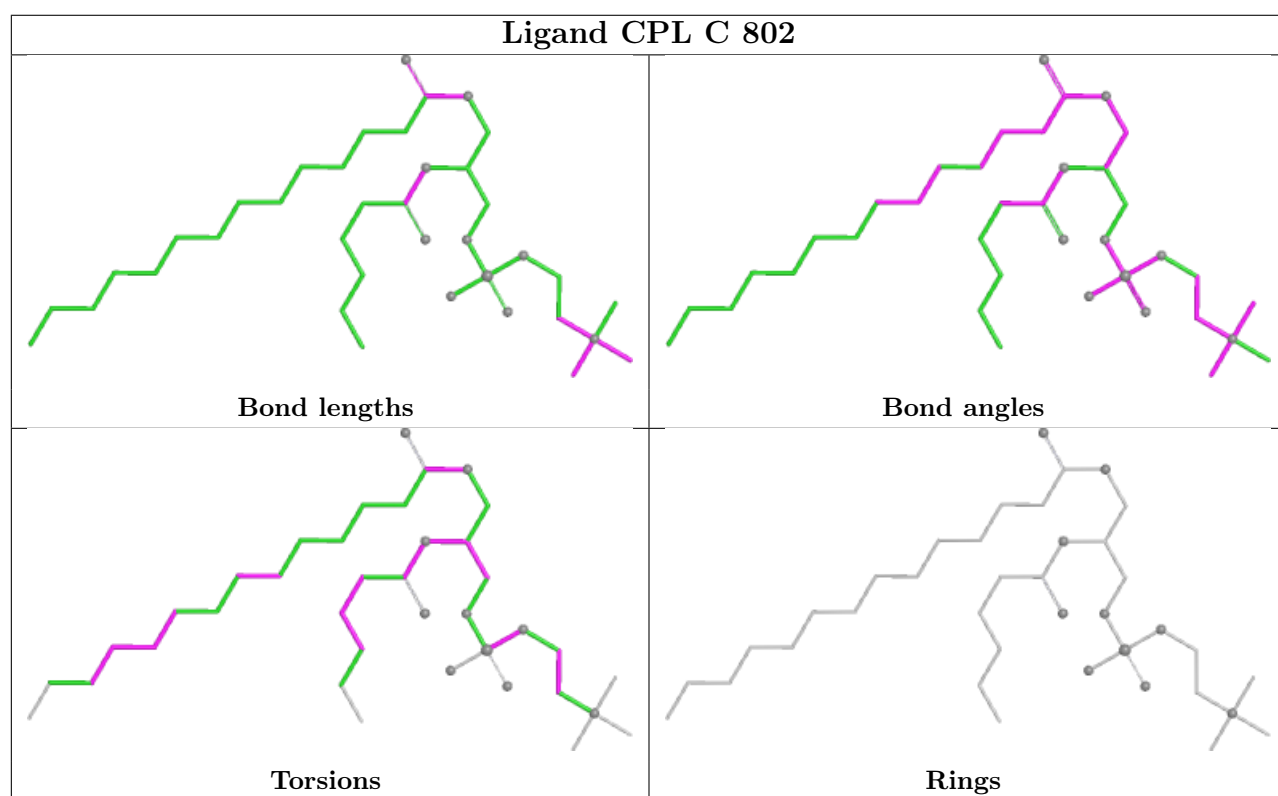
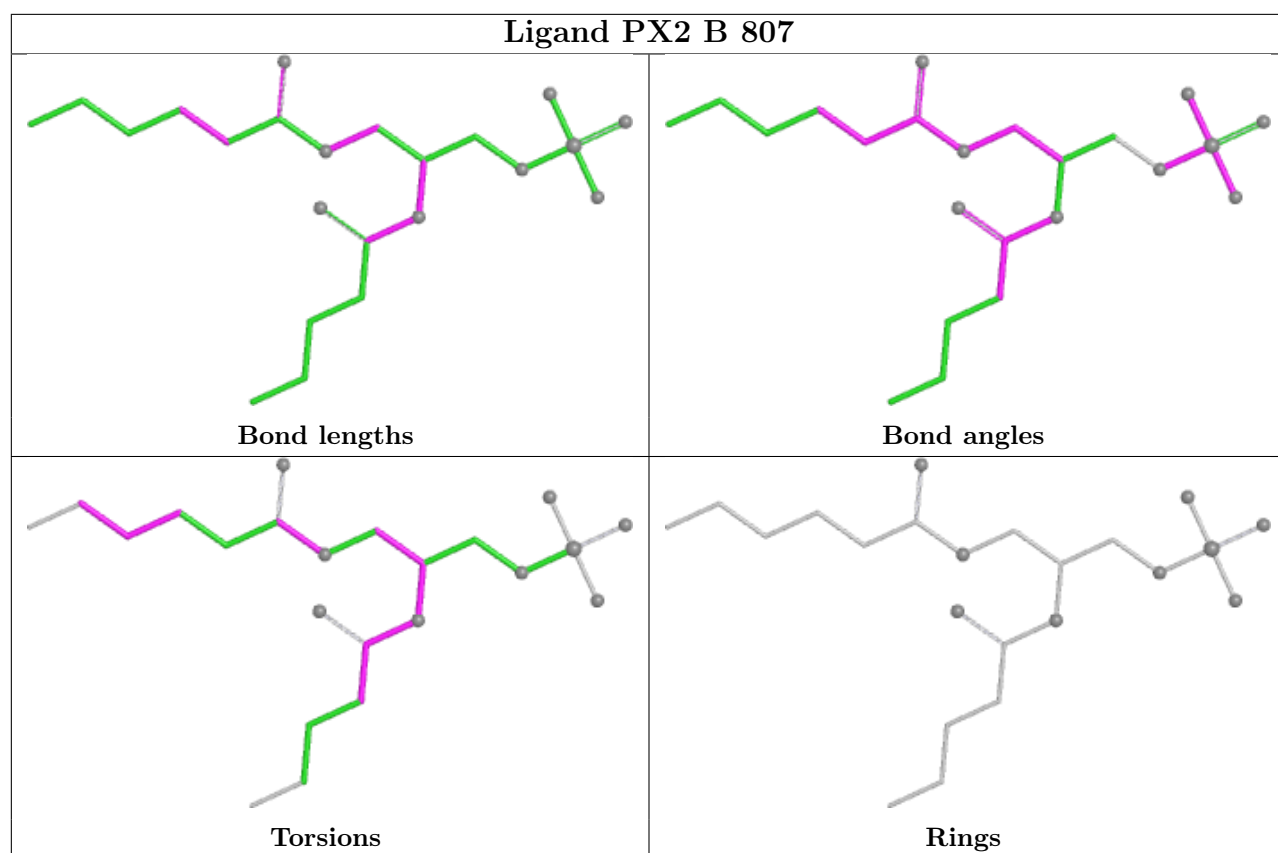


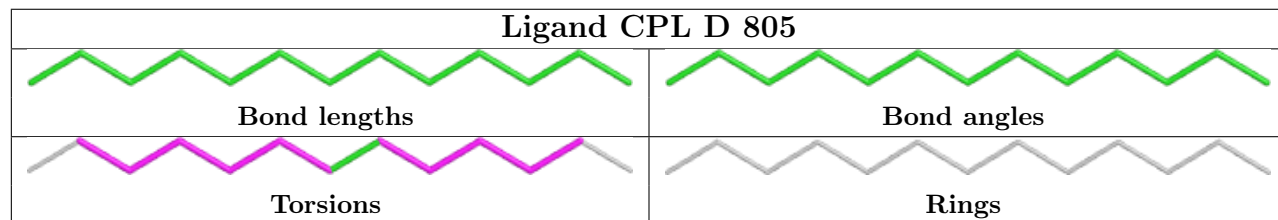
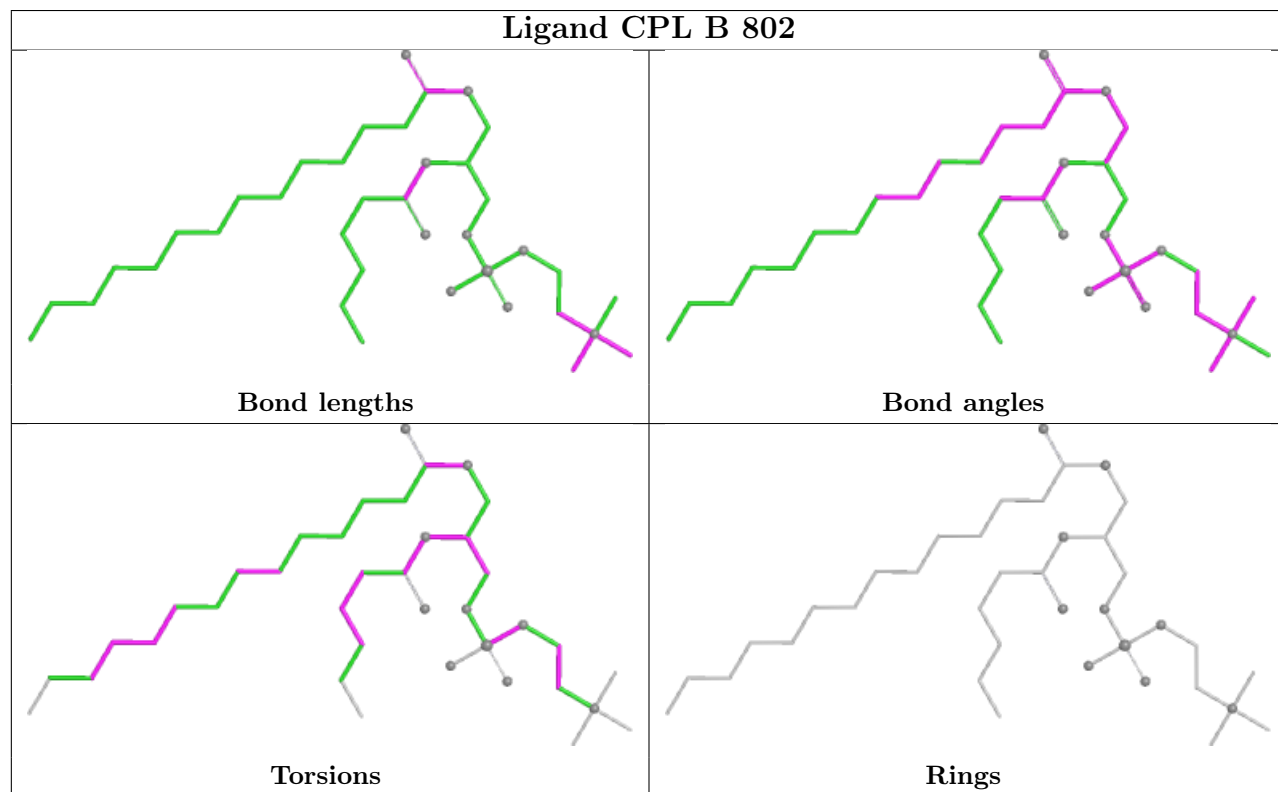
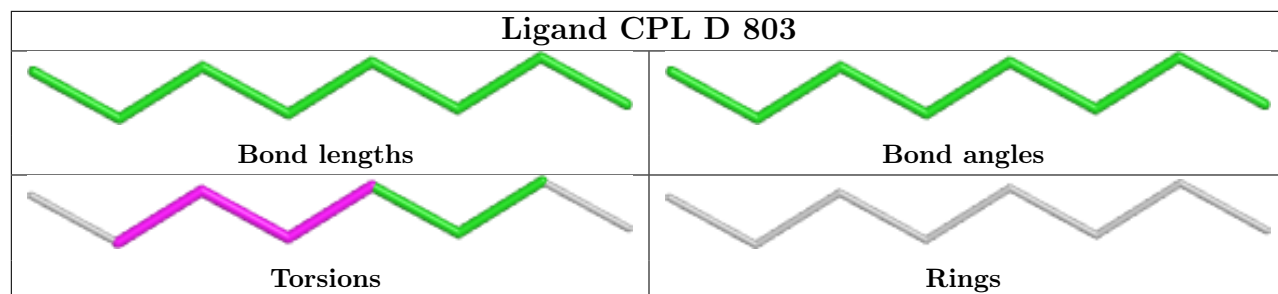


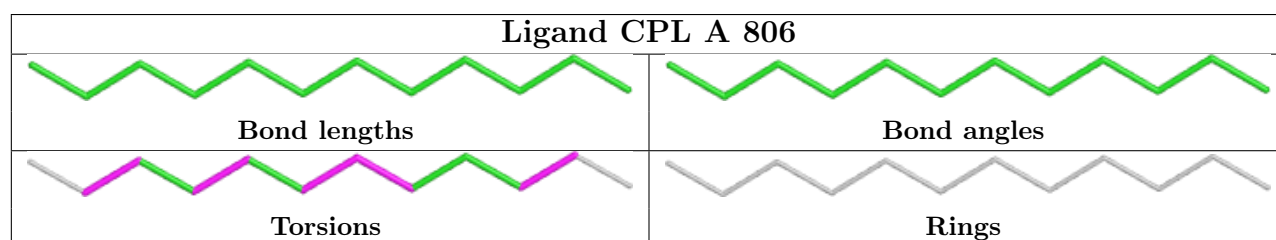
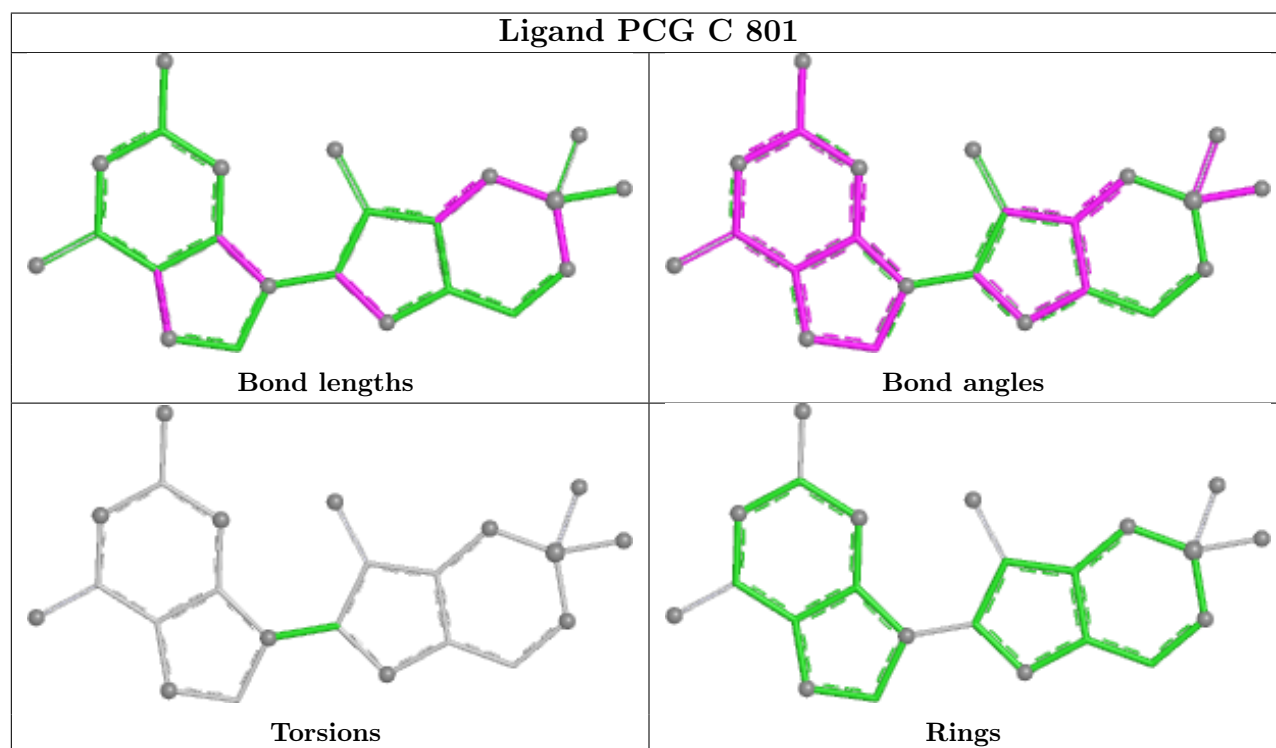
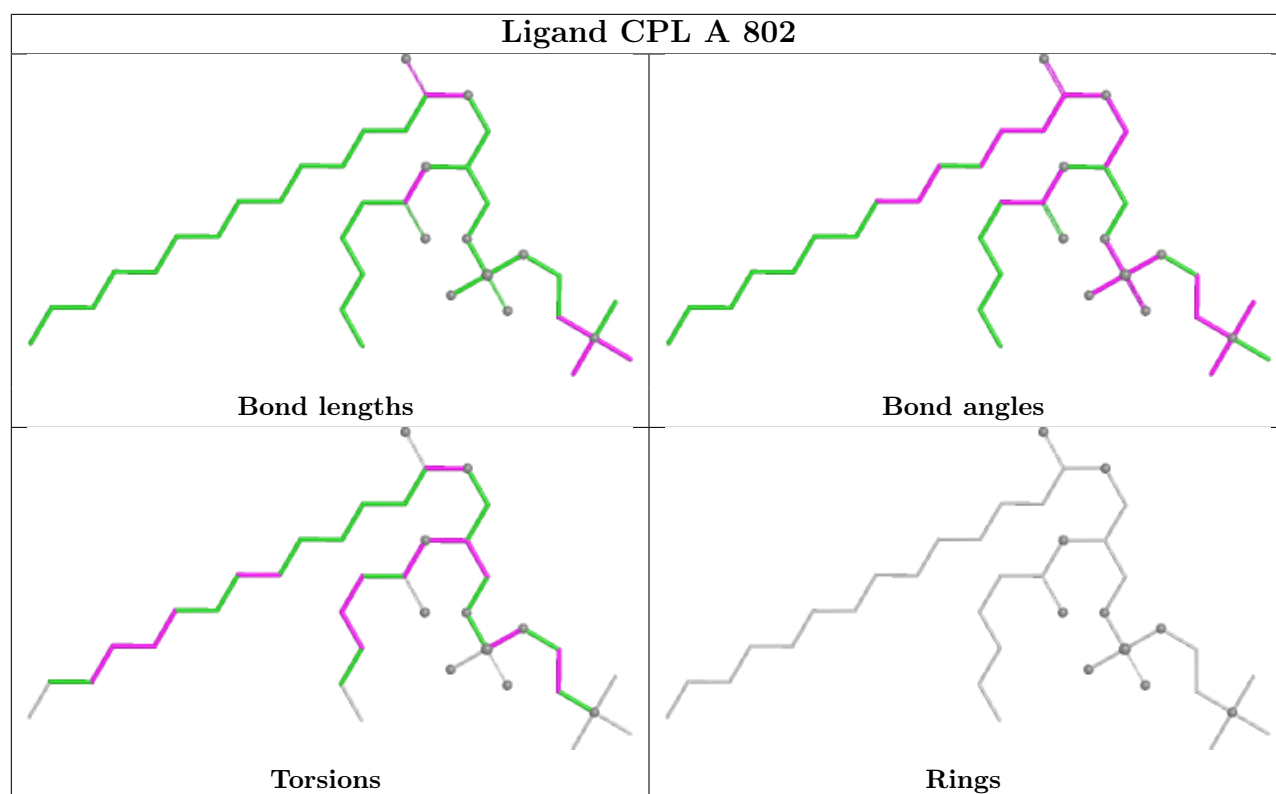


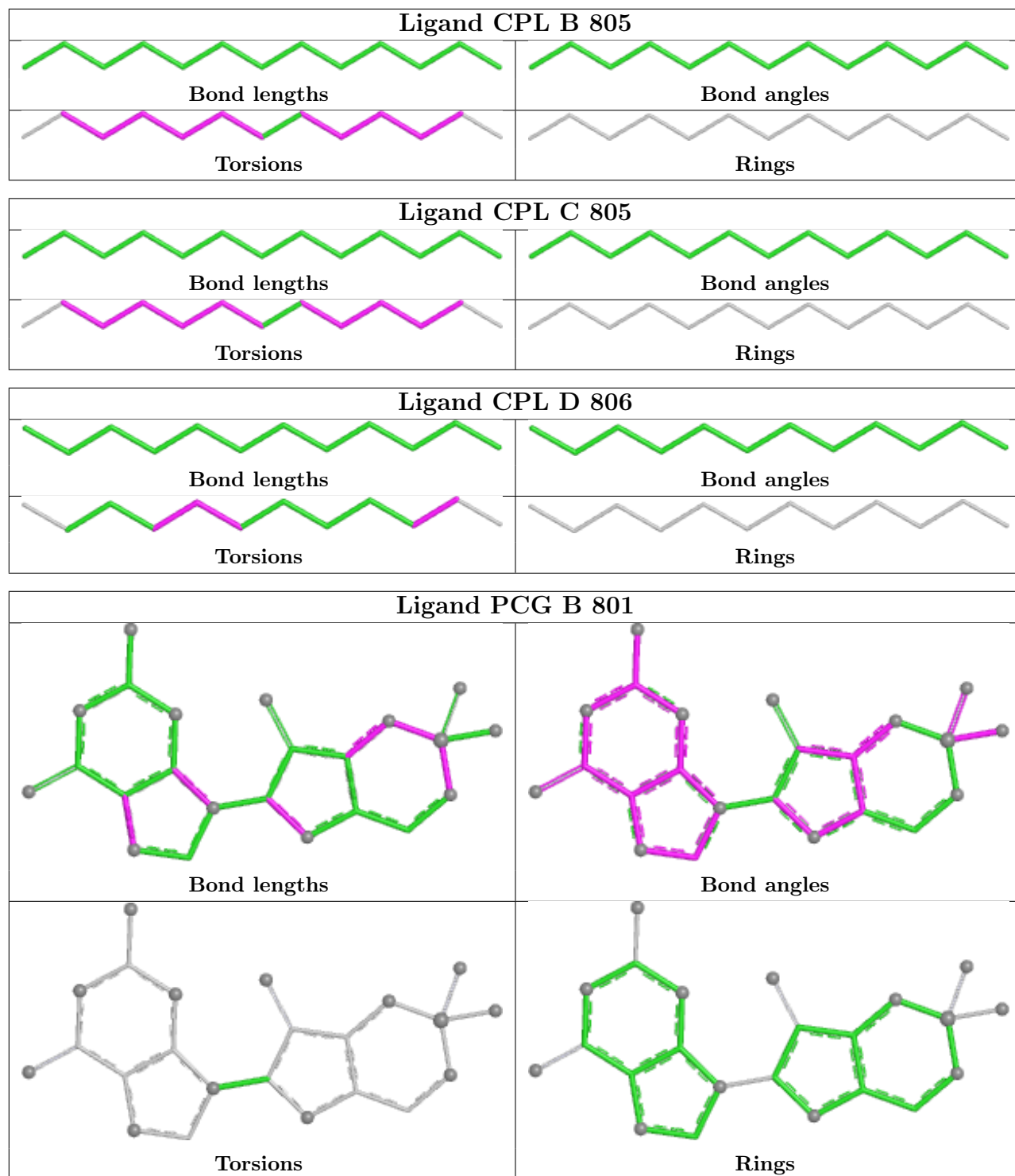


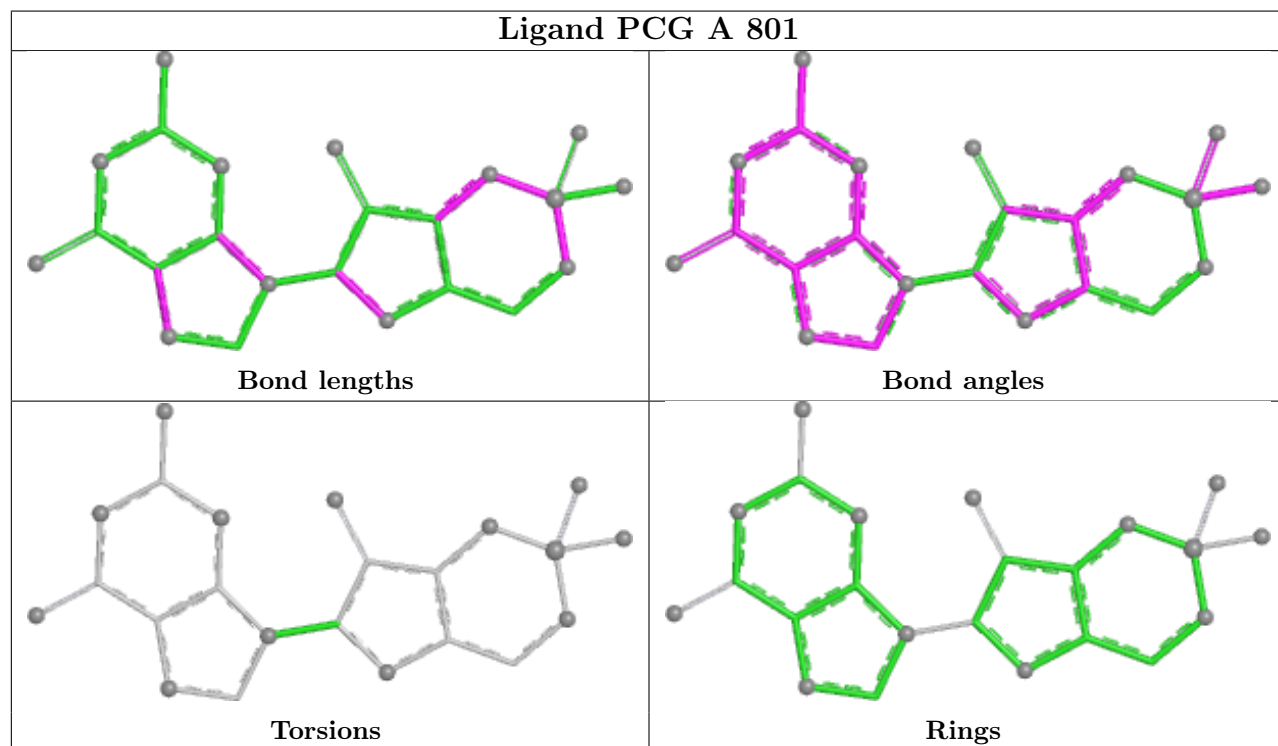
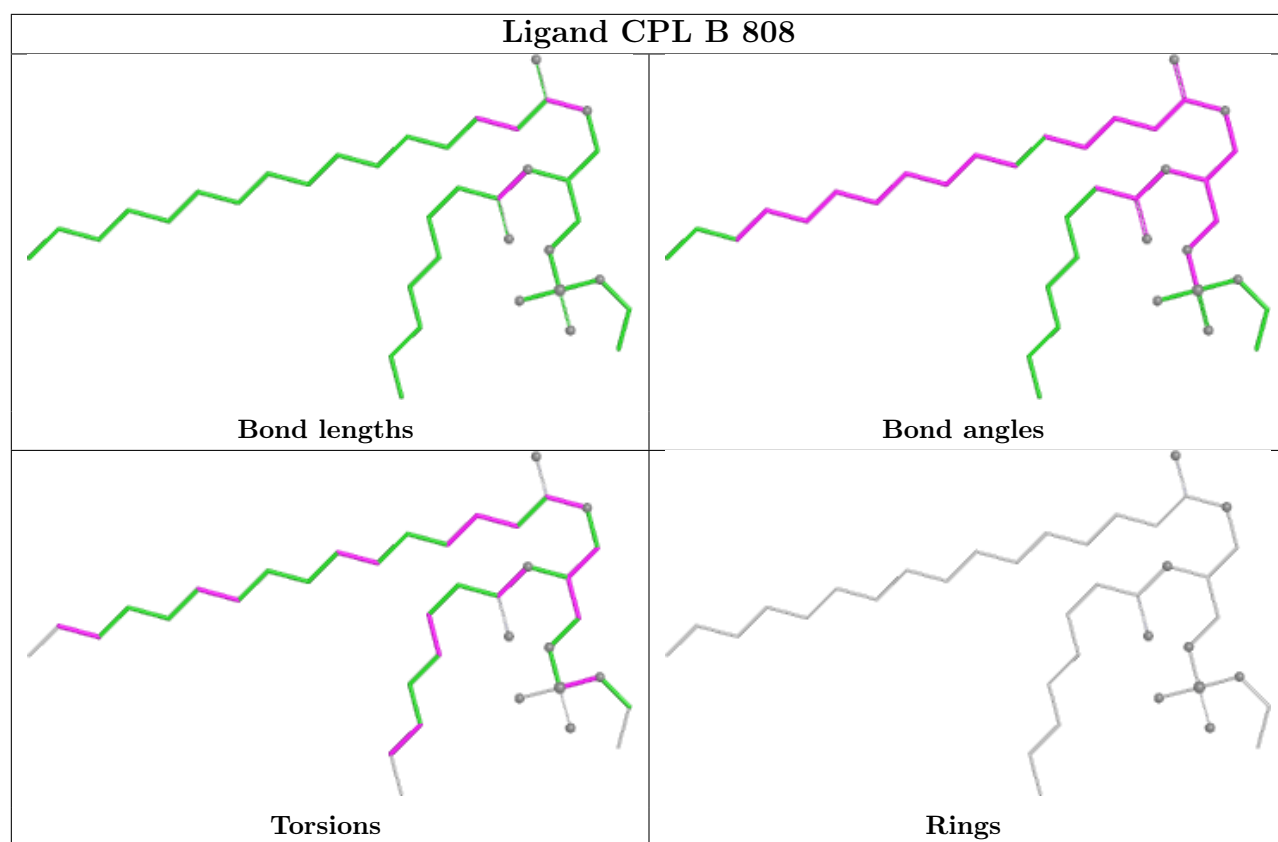


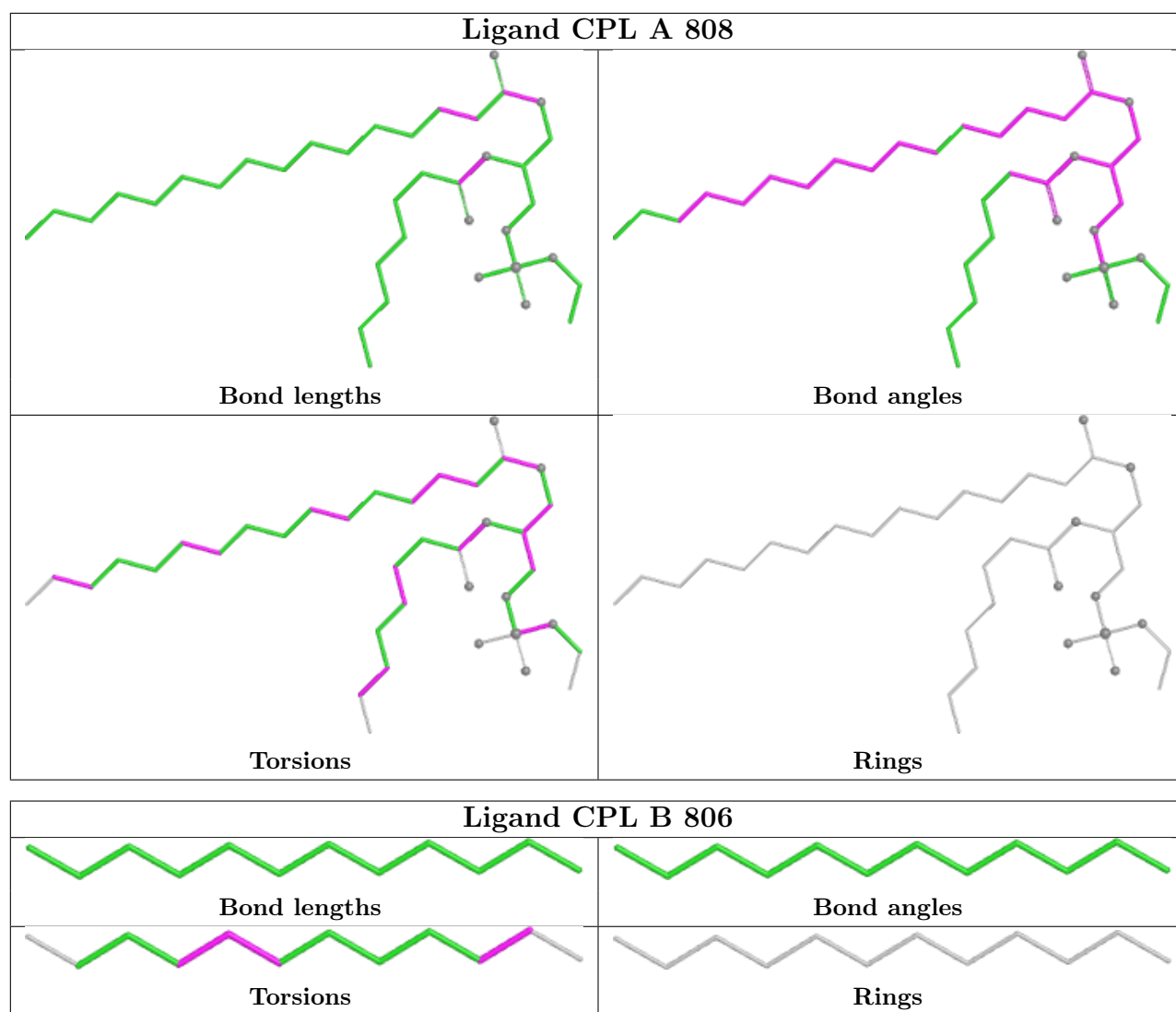


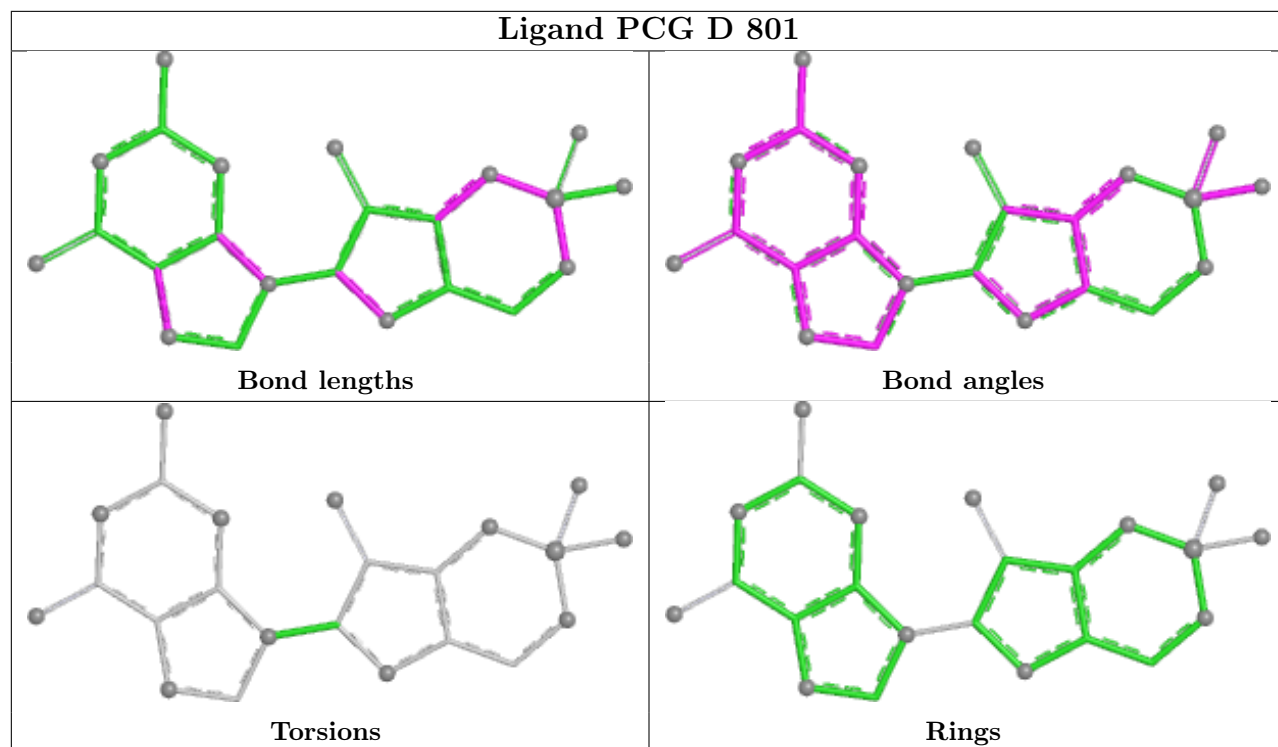












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

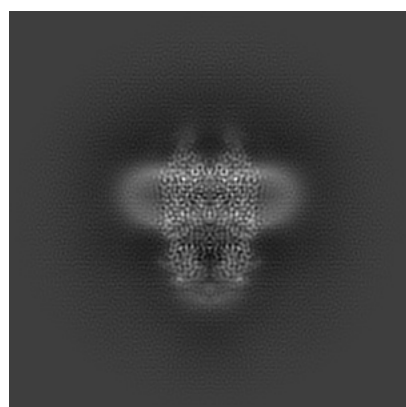
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21650. These allow visual inspection of the internal detail of the map and identification of artifacts.

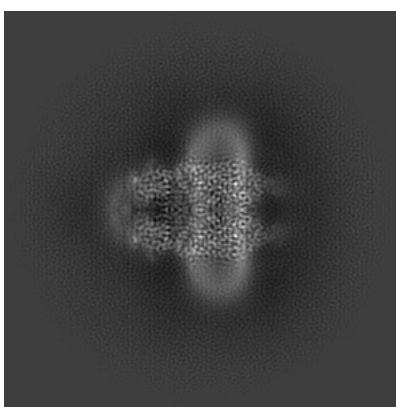
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

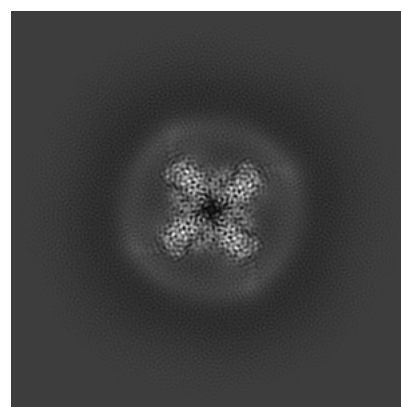
6.1.1 Primary map



X



Y

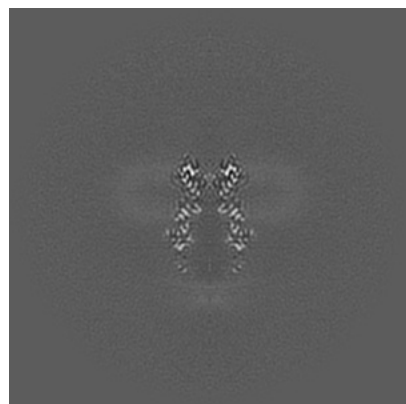


Z

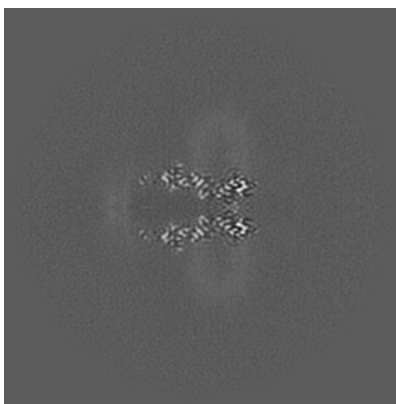
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

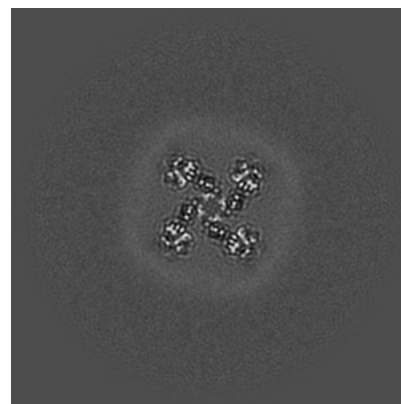
6.2.1 Primary map



X Index: 148



Y Index: 148

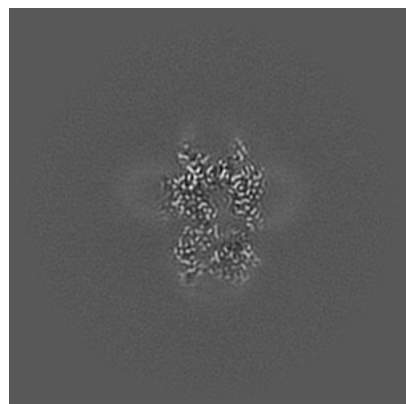


Z Index: 148

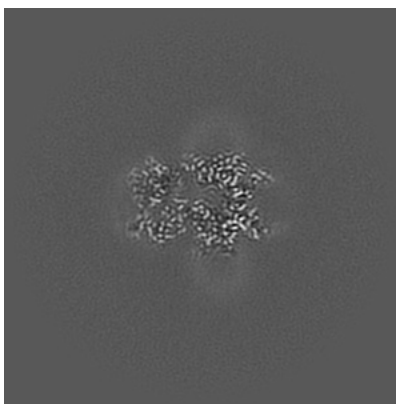
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

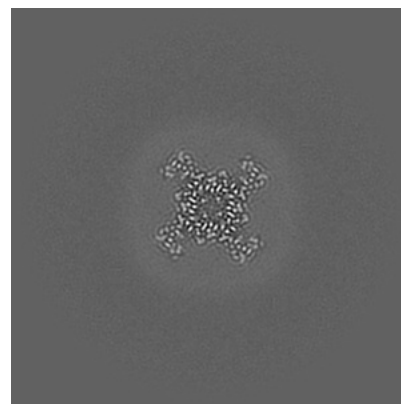
6.3.1 Primary map



X Index: 129



Y Index: 167

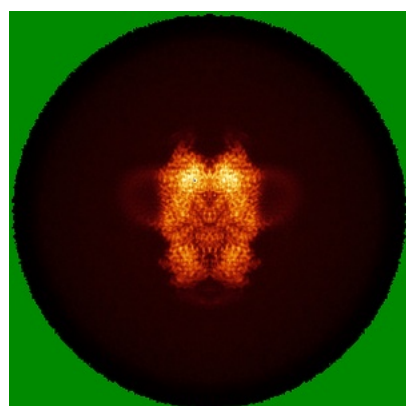


Z Index: 173

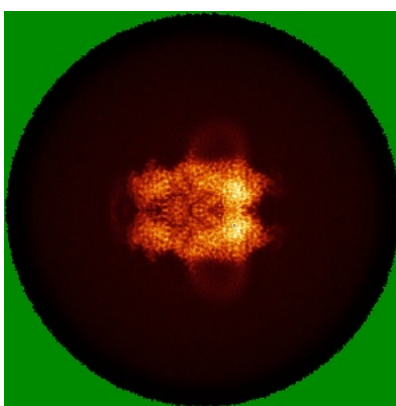
The images above show the largest variance slices of the map in three orthogonal directions.

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

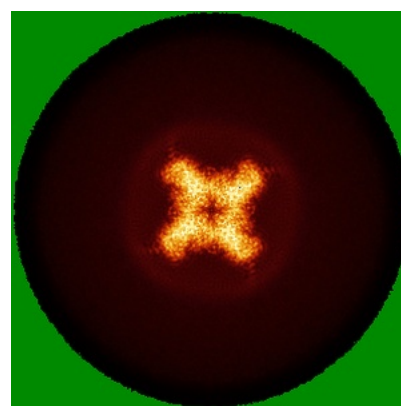
6.4.1 Primary map



X



Y

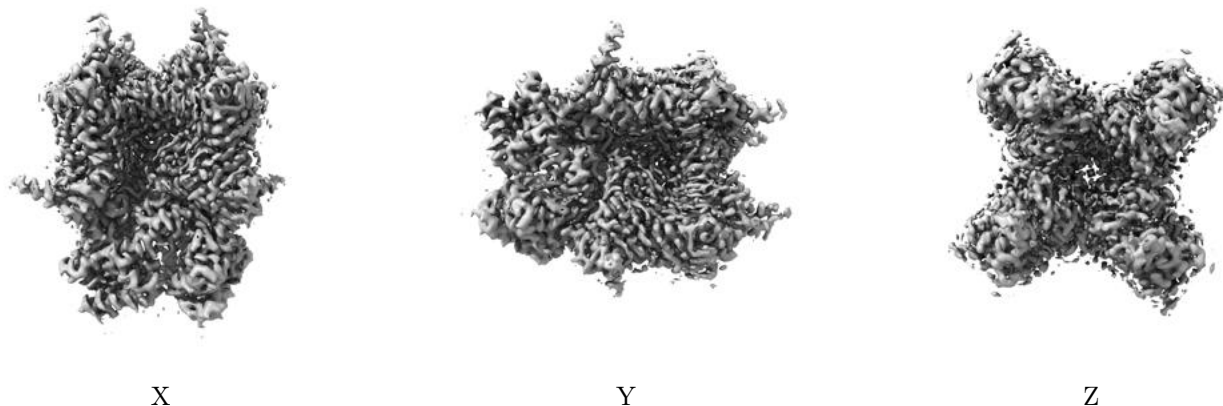


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.641. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

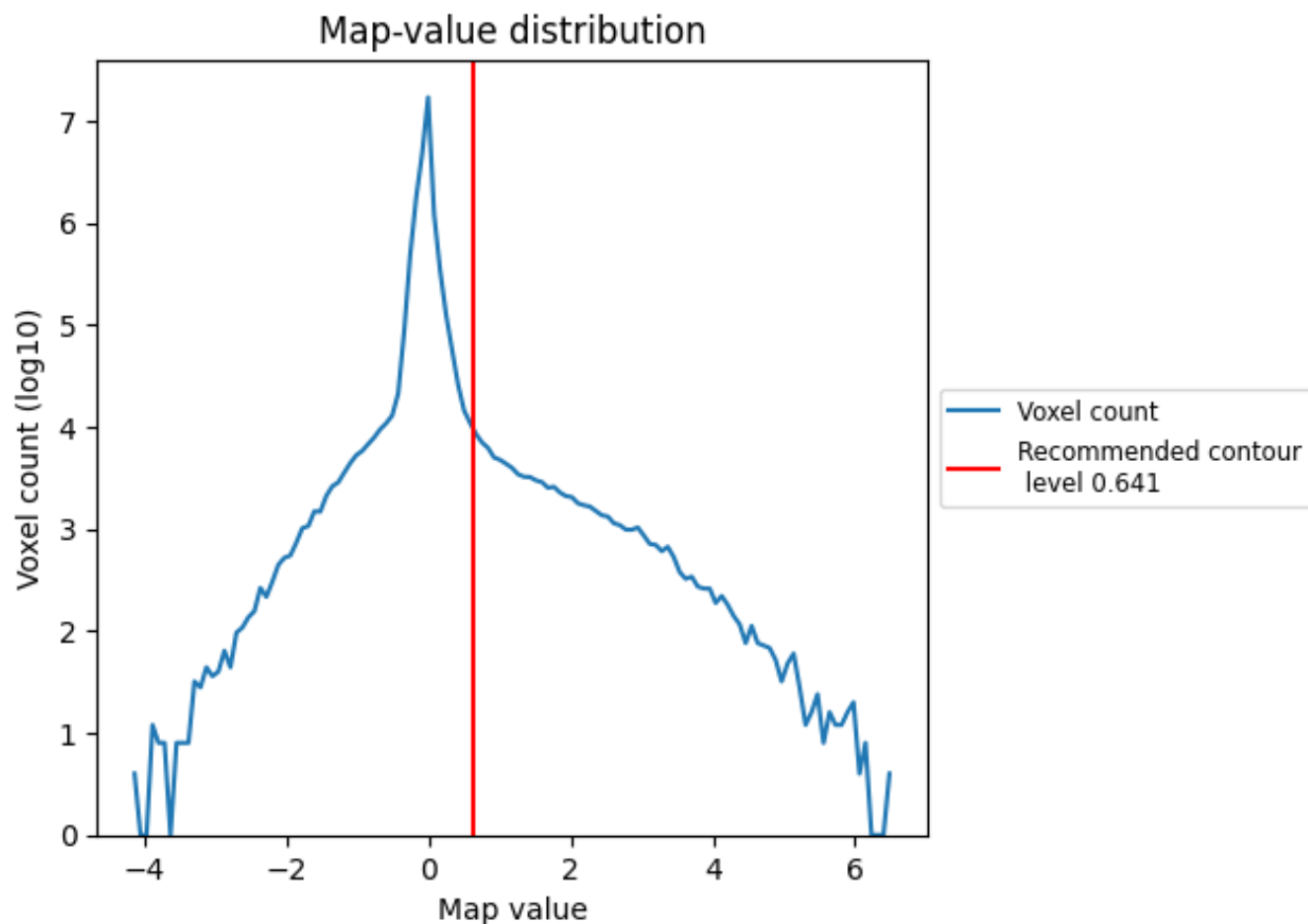
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

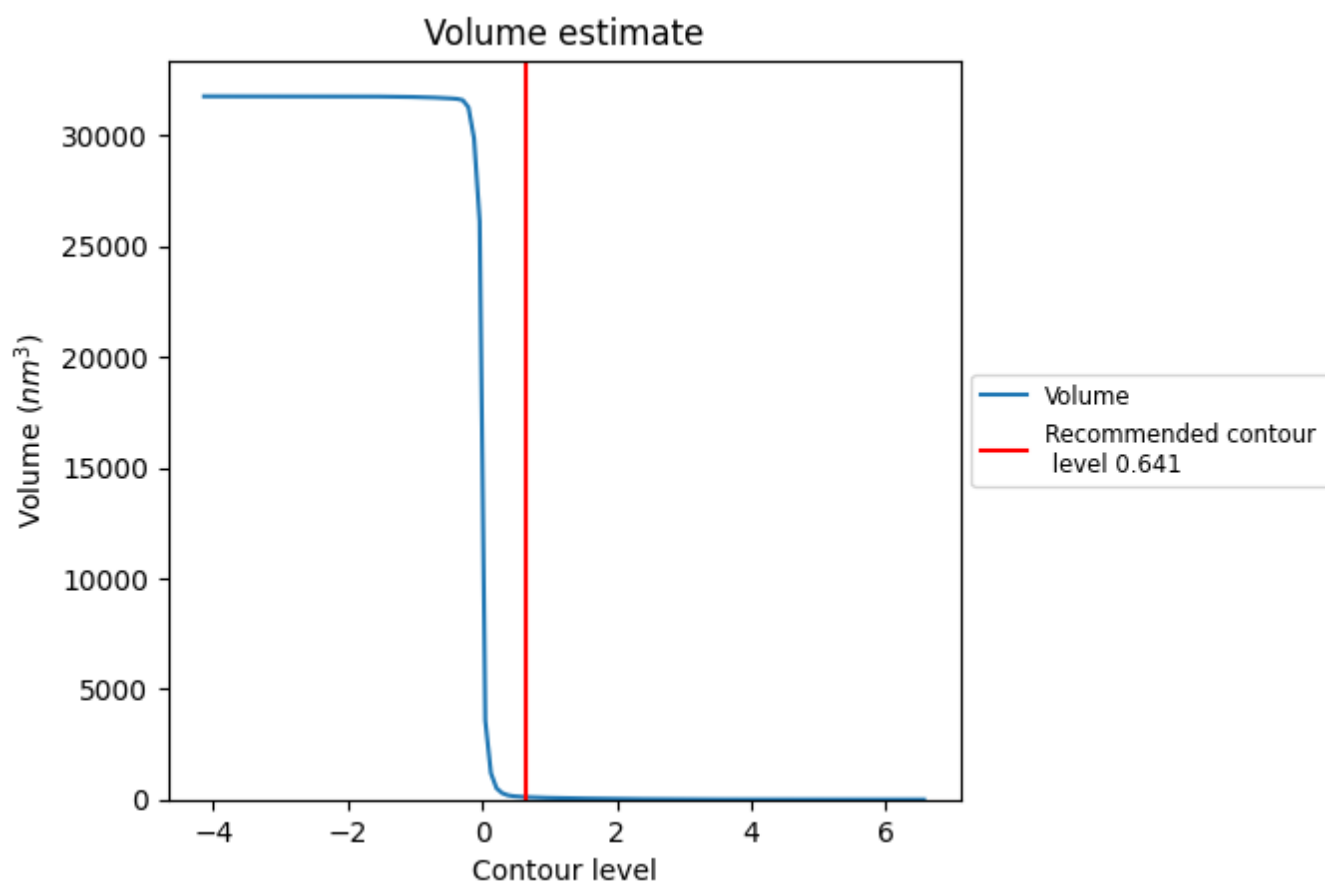
This section contains the results of statistical analysis of the map.

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.

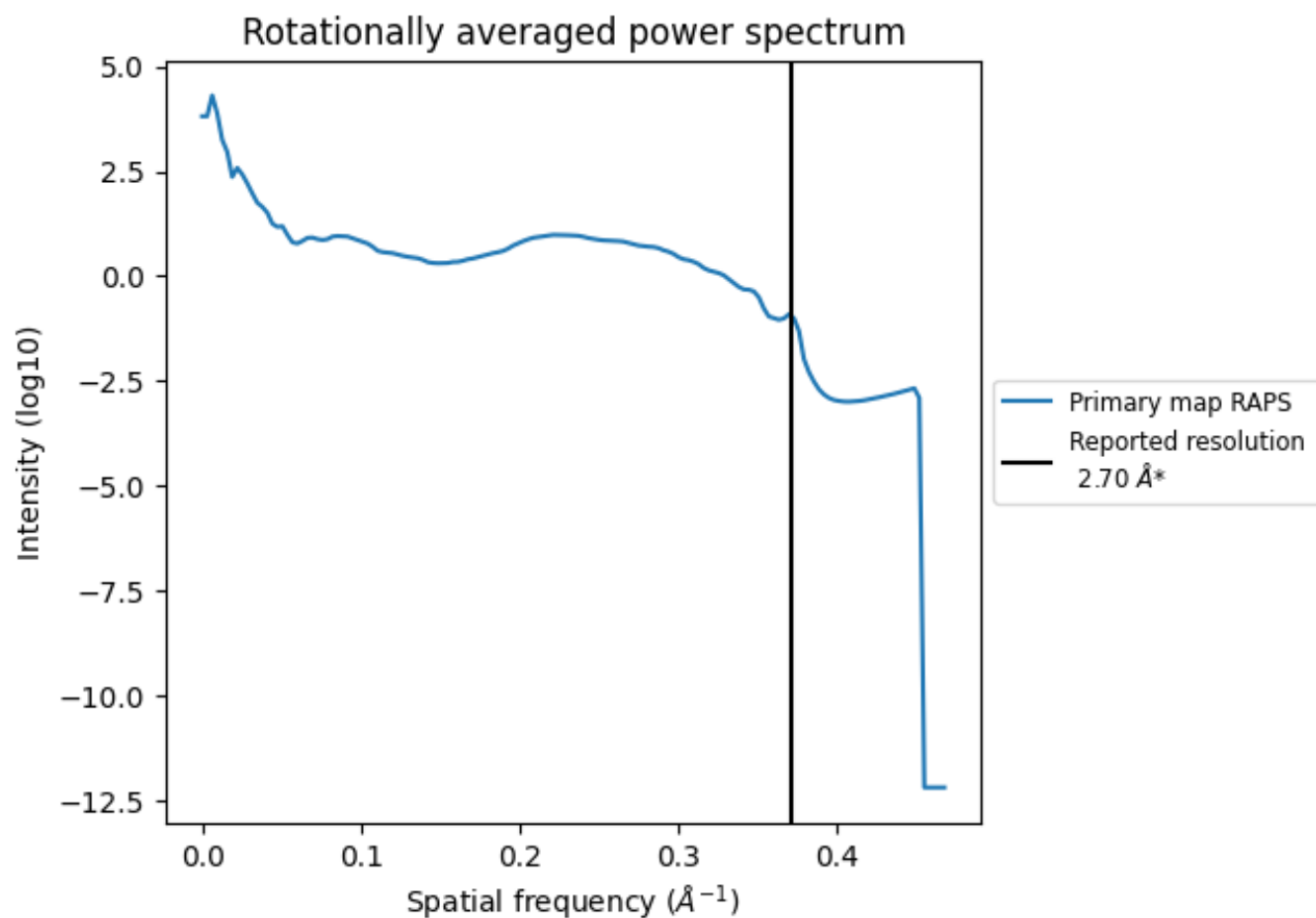
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 0.370 Å⁻¹

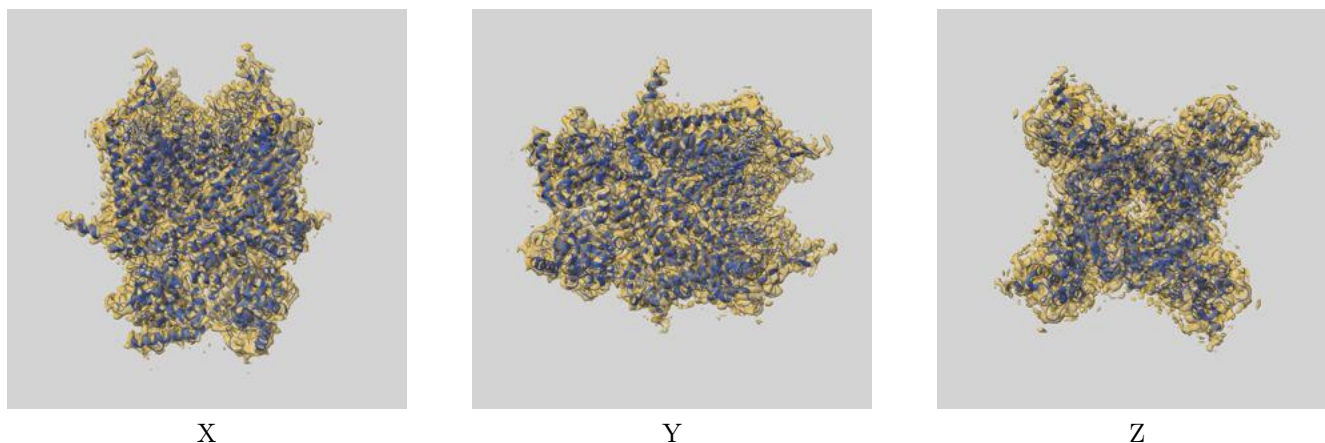
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

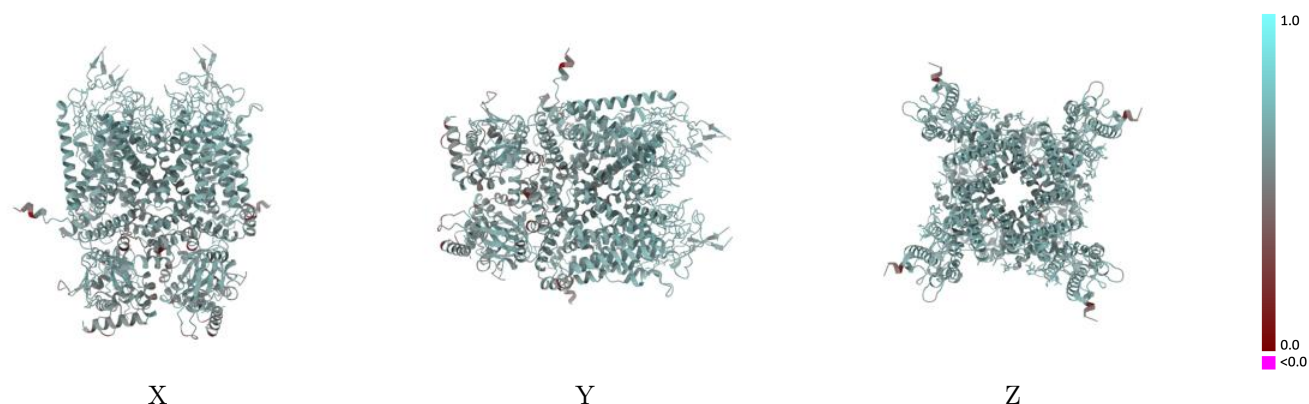
This section contains information regarding the fit between EMDB map EMD-21650 and PDB model 6WEK. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



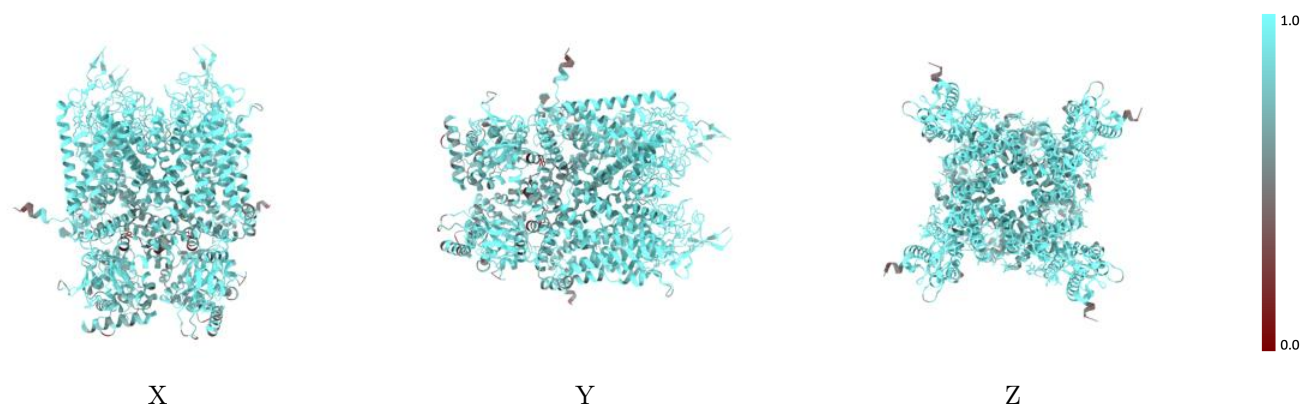
The images above show the 3D surface view of the map at the recommended contour level 0.641 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



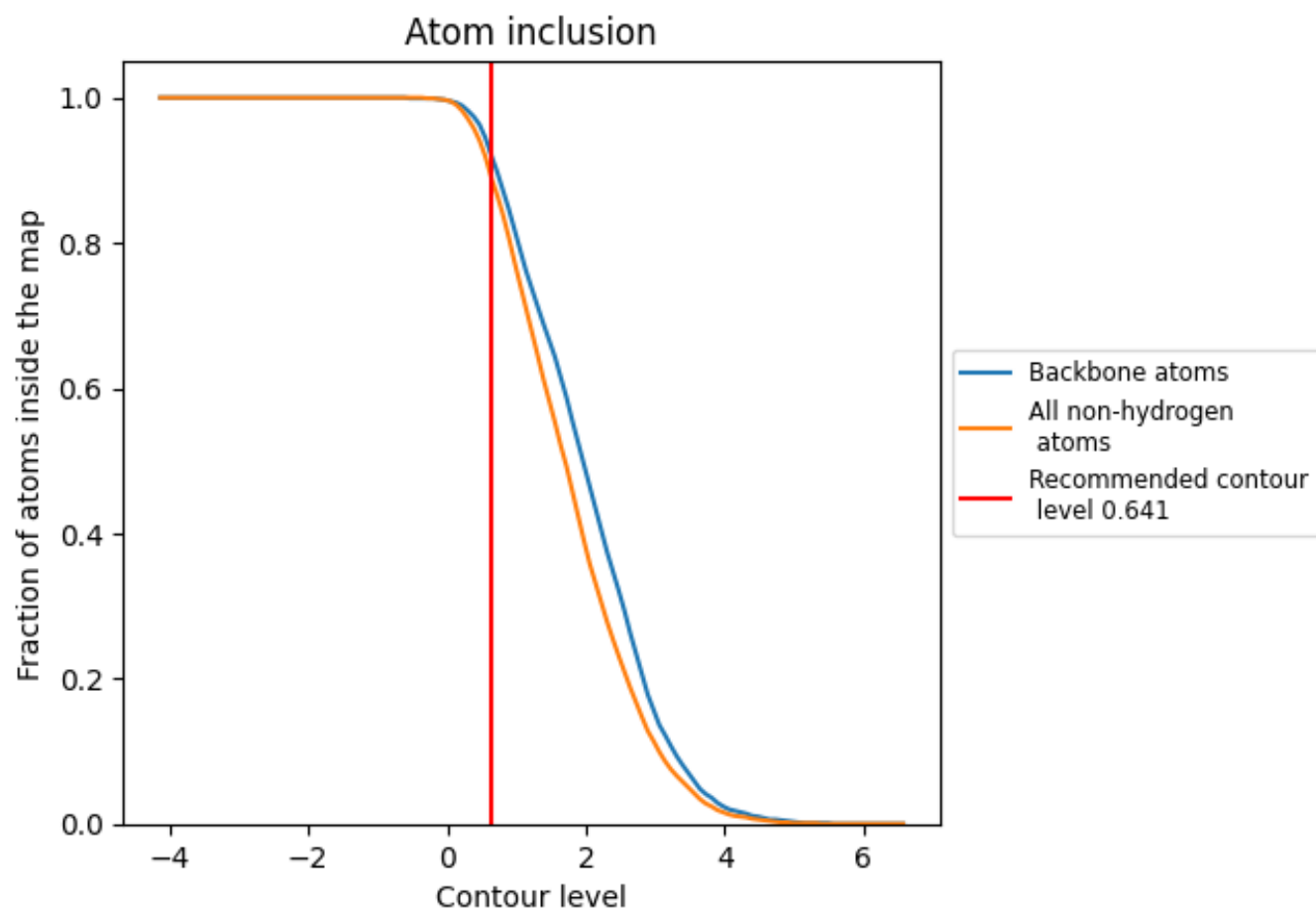
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.641).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.641) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.5930
A	0.8870	0.5920
B	0.8890	0.5940
C	0.8870	0.5940
D	0.8900	0.5910

