



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 7S88 / pdb_00007s88
EMDB ID : EMD-24890
Title : Open apo-state cryo-EM structure of human TRPV6 in glyco-diosgenin detergent
Authors : Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on : 2021-09-17
Resolution : 2.69 Å(reported)
Based on initial model : 7K4A

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

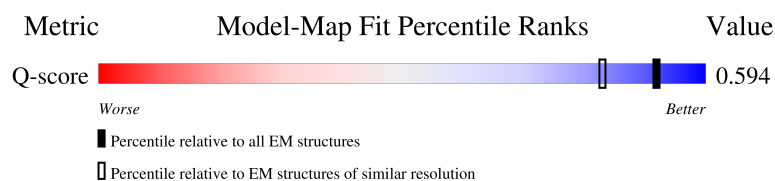
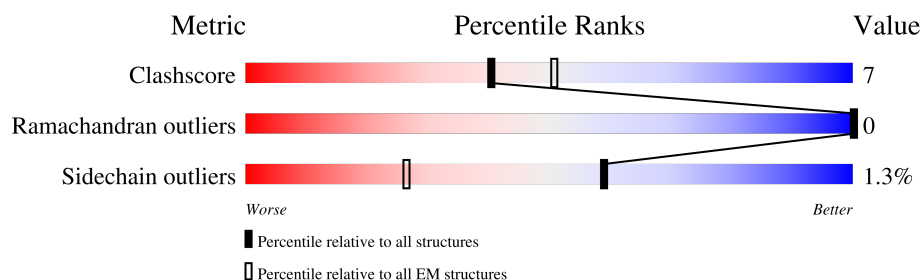
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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	9309 (2.19 - 3.19)

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	683	7% 77% 13% 10%
1	B	683	7% 77% 12% 10%
1	C	683	7% 78% 11% 10%
1	D	683	7% 77% 12% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22201 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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	614	Total	C	N	O	S	0	0
			4935	3186	840	869	40		
1	B	614	Total	C	N	O	S	0	0
			4935	3186	840	869	40		
1	C	614	Total	C	N	O	S	0	0
			4935	3186	840	869	40		
1	D	614	Total	C	N	O	S	0	0
			4935	3186	840	869	40		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	VAL	-	expression tag	UNP Q9H1D0
A	669	PRO	-	expression tag	UNP Q9H1D0
A	670	ARG	-	expression tag	UNP Q9H1D0
A	671	GLY	-	expression tag	UNP Q9H1D0
A	672	SER	-	expression tag	UNP Q9H1D0
A	673	ALA	-	expression tag	UNP Q9H1D0
A	674	ALA	-	expression tag	UNP Q9H1D0
A	675	ALA	-	expression tag	UNP Q9H1D0
A	676	TRP	-	expression tag	UNP Q9H1D0
A	677	SER	-	expression tag	UNP Q9H1D0
A	678	HIS	-	expression tag	UNP Q9H1D0
A	679	PRO	-	expression tag	UNP Q9H1D0
A	680	GLN	-	expression tag	UNP Q9H1D0
A	681	PHE	-	expression tag	UNP Q9H1D0
A	682	GLU	-	expression tag	UNP Q9H1D0
A	683	LYS	-	expression tag	UNP Q9H1D0
B	668	VAL	-	expression tag	UNP Q9H1D0
B	669	PRO	-	expression tag	UNP Q9H1D0
B	670	ARG	-	expression tag	UNP Q9H1D0
B	671	GLY	-	expression tag	UNP Q9H1D0
B	672	SER	-	expression tag	UNP Q9H1D0

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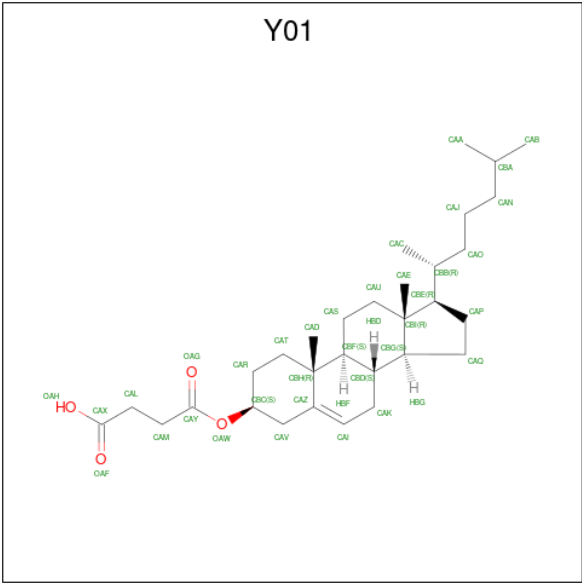
Chain	Residue	Modelled	Actual	Comment	Reference
B	673	ALA	-	expression tag	UNP Q9H1D0
B	674	ALA	-	expression tag	UNP Q9H1D0
B	675	ALA	-	expression tag	UNP Q9H1D0
B	676	TRP	-	expression tag	UNP Q9H1D0
B	677	SER	-	expression tag	UNP Q9H1D0
B	678	HIS	-	expression tag	UNP Q9H1D0
B	679	PRO	-	expression tag	UNP Q9H1D0
B	680	GLN	-	expression tag	UNP Q9H1D0
B	681	PHE	-	expression tag	UNP Q9H1D0
B	682	GLU	-	expression tag	UNP Q9H1D0
B	683	LYS	-	expression tag	UNP Q9H1D0
C	668	VAL	-	expression tag	UNP Q9H1D0
C	669	PRO	-	expression tag	UNP Q9H1D0
C	670	ARG	-	expression tag	UNP Q9H1D0
C	671	GLY	-	expression tag	UNP Q9H1D0
C	672	SER	-	expression tag	UNP Q9H1D0
C	673	ALA	-	expression tag	UNP Q9H1D0
C	674	ALA	-	expression tag	UNP Q9H1D0
C	675	ALA	-	expression tag	UNP Q9H1D0
C	676	TRP	-	expression tag	UNP Q9H1D0
C	677	SER	-	expression tag	UNP Q9H1D0
C	678	HIS	-	expression tag	UNP Q9H1D0
C	679	PRO	-	expression tag	UNP Q9H1D0
C	680	GLN	-	expression tag	UNP Q9H1D0
C	681	PHE	-	expression tag	UNP Q9H1D0
C	682	GLU	-	expression tag	UNP Q9H1D0
C	683	LYS	-	expression tag	UNP Q9H1D0
D	668	VAL	-	expression tag	UNP Q9H1D0
D	669	PRO	-	expression tag	UNP Q9H1D0
D	670	ARG	-	expression tag	UNP Q9H1D0
D	671	GLY	-	expression tag	UNP Q9H1D0
D	672	SER	-	expression tag	UNP Q9H1D0
D	673	ALA	-	expression tag	UNP Q9H1D0
D	674	ALA	-	expression tag	UNP Q9H1D0
D	675	ALA	-	expression tag	UNP Q9H1D0
D	676	TRP	-	expression tag	UNP Q9H1D0
D	677	SER	-	expression tag	UNP Q9H1D0
D	678	HIS	-	expression tag	UNP Q9H1D0
D	679	PRO	-	expression tag	UNP Q9H1D0
D	680	GLN	-	expression tag	UNP Q9H1D0
D	681	PHE	-	expression tag	UNP Q9H1D0
D	682	GLU	-	expression tag	UNP Q9H1D0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	683	LYS	-	expression tag	UNP Q9H1D0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



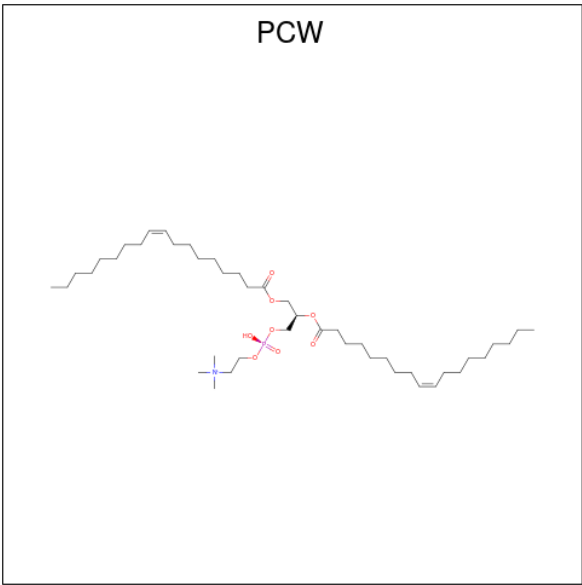
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31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

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

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



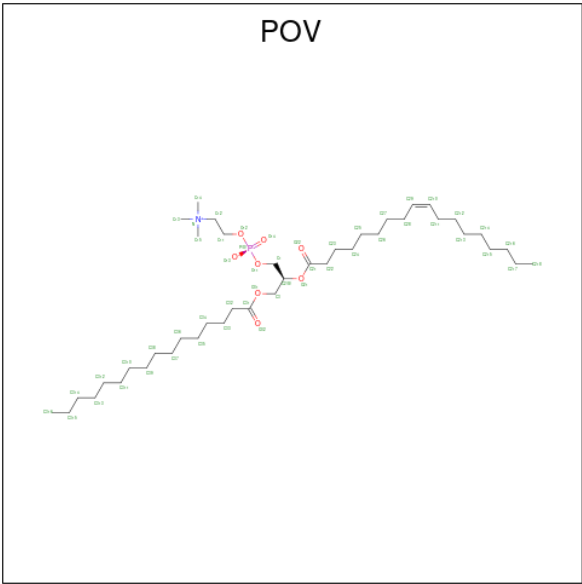
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	C	0
			13	13	
3	A	1	Total	C	0
			14	14	
3	A	1	Total	C	0
			8	8	
3	A	1	Total	C	0
			15	15	
3	A	1	Total	C	0
			8	8	
3	B	1	Total	C	0
			13	13	
3	B	1	Total	C	0
			14	14	
3	B	1	Total	C	0
			8	8	
3	B	1	Total	C	0
			15	15	
3	B	1	Total	C	0
			8	8	

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Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	C	0
			13	13	
3	C	1	Total	C	0
			14	14	
3	C	1	Total	C	0
			8	8	
3	C	1	Total	C	0
			15	15	
3	C	1	Total	C	0
			8	8	
3	D	1	Total	C	0
			15	15	
3	D	1	Total	C	0
			8	8	
3	D	1	Total	C	0
			13	13	
3	D	1	Total	C	0
			14	14	
3	D	1	Total	C	0
			8	8	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	

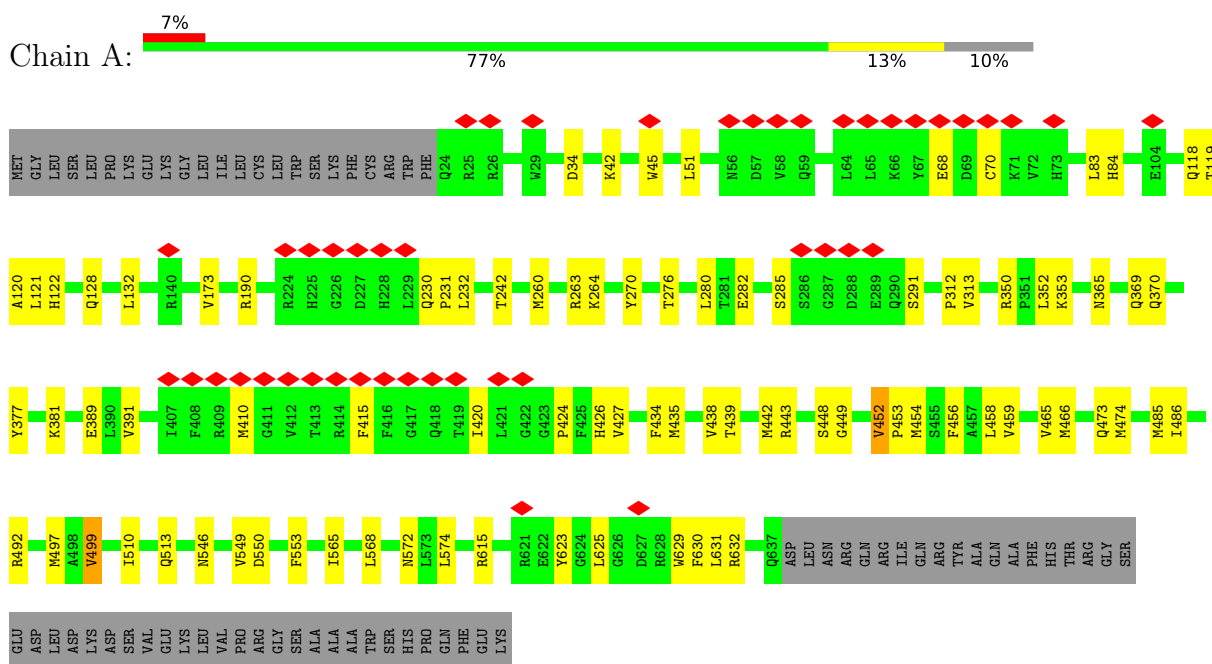
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	36	Total	O	0
			36	36	
6	B	36	Total	O	0
			36	36	
6	C	36	Total	O	0
			36	36	
6	D	36	Total	O	0
			36	36	

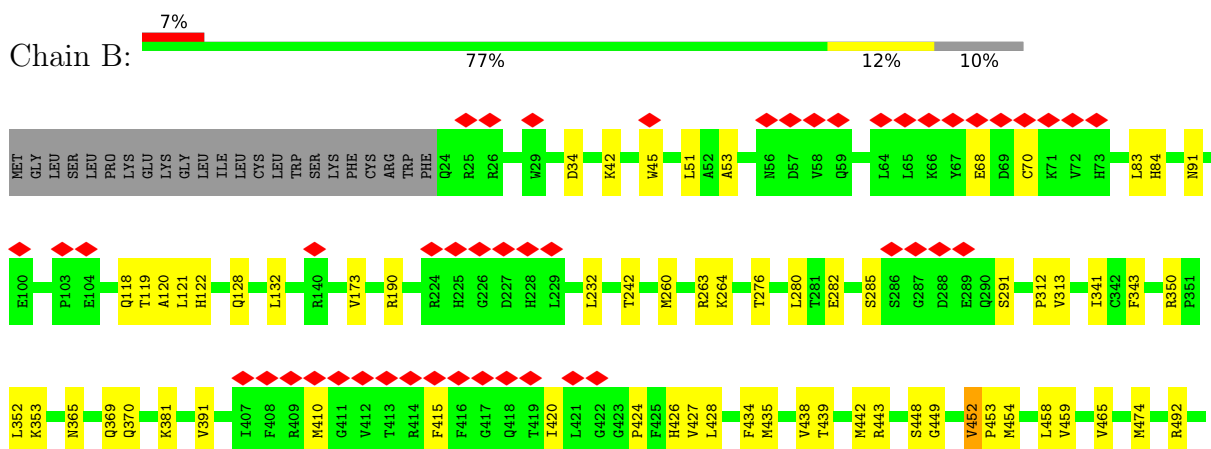
3 Residue-property plots

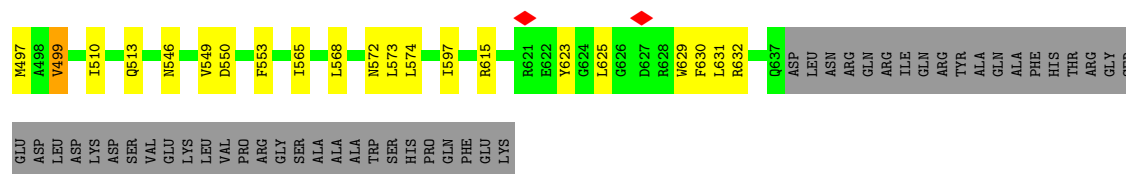
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

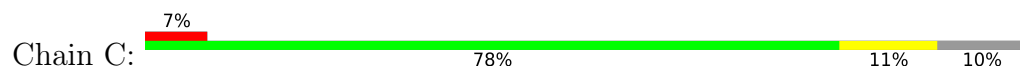


- Molecule 1: Transient receptor potential cation channel subfamily V member 6

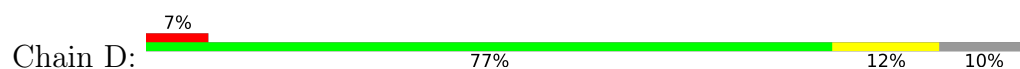




- Molecule 1: Transient receptor potential cation channel subfamily V member 6



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.765	Depositor
Minimum map value	-3.852	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.215	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	211.712, 211.712, 211.712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.827, 0.827, 0.827	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, Y01, PCW, CA

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	0.38	0/5048	0.59	0/6847
1	B	0.38	0/5048	0.59	0/6847
1	C	0.38	0/5048	0.59	0/6847
1	D	0.38	0/5048	0.59	0/6847
All	All	0.38	0/20192	0.59	0/27388

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4935	0	4994	66	0
1	B	4935	0	4994	64	0
1	C	4935	0	4994	61	0
1	D	4935	0	4994	61	0
2	A	105	0	147	9	0
2	B	105	0	147	9	0
2	C	105	0	147	8	0
2	D	105	0	147	7	0
3	A	58	0	90	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	58	0	90	4	0
3	C	58	0	90	2	0
3	D	58	0	90	3	0
4	A	416	0	656	38	0
4	B	416	0	656	38	0
4	C	416	0	656	36	0
4	D	416	0	656	37	0
5	A	1	0	0	0	0
6	A	36	0	0	0	0
6	B	36	0	0	0	0
6	C	36	0	0	0	0
6	D	36	0	0	0	0
All	All	22201	0	23548	320	0

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

All (320) 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:B:424:PRO:HB2	2:B:704:Y01:HAR1	1.73	0.70
1:B:119:THR:H	1:B:122:HIS:HD2	1.45	0.64
1:D:119:THR:H	1:D:122:HIS:HD2	1.45	0.64
1:D:424:PRO:HB2	2:D:708:Y01:HAR1	1.81	0.63
1:C:119:THR:H	1:C:122:HIS:HD2	1.45	0.63
1:B:474:MET:HB3	1:C:492:ARG:HD2	1.81	0.63
1:A:119:THR:H	1:A:122:HIS:HD2	1.45	0.62
1:C:424:PRO:HB2	2:C:704:Y01:HAR1	1.83	0.61
1:A:424:PRO:HB2	2:A:802:Y01:HAR1	1.82	0.61
1:A:492:ARG:HD2	1:D:474:MET:HB3	1.83	0.60
1:B:285:SER:O	1:B:615:ARG:NH1	2.33	0.60
1:A:350:ARG:HH11	4:A:804:POV:H218	1.66	0.60
1:A:459:VAL:HG21	2:A:802:Y01:HAN1	1.82	0.60
1:C:370:GLN:HB2	4:C:706:POV:H217	1.84	0.59
1:C:459:VAL:HG21	2:C:704:Y01:HAN1	1.83	0.59
1:D:350:ARG:HH11	4:D:710:POV:H218	1.67	0.59
1:B:370:GLN:HB2	4:B:706:POV:H217	1.83	0.59
1:C:280:LEU:HD22	1:C:631:LEU:HB2	1.85	0.59
1:C:285:SER:O	1:C:615:ARG:NH1	2.33	0.59
1:D:280:LEU:HD22	1:D:631:LEU:HB2	1.85	0.59
1:D:459:VAL:HG21	2:D:708:Y01:HAN1	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:GLN:HB2	4:D:710:POV:H217	1.84	0.59
1:A:285:SER:O	1:A:615:ARG:NH1	2.33	0.58
1:A:370:GLN:HB2	4:A:804:POV:H217	1.85	0.58
1:B:280:LEU:HD22	1:B:631:LEU:HB2	1.85	0.58
1:A:280:LEU:HD22	1:A:631:LEU:HB2	1.85	0.58
1:C:350:ARG:HH11	4:C:706:POV:H218	1.67	0.58
1:A:623:TYR:HA	1:B:42:LYS:HD2	1.87	0.57
1:B:459:VAL:HG21	2:B:704:Y01:HAN1	1.86	0.57
1:D:448:SER:H	4:D:714:POV:H12	1.70	0.57
1:B:381:LYS:HD2	4:B:714:POV:H1A	1.86	0.57
1:B:448:SER:H	4:B:710:POV:H12	1.69	0.57
1:B:350:ARG:HH11	4:B:706:POV:H218	1.68	0.57
1:A:448:SER:H	4:A:808:POV:H12	1.69	0.57
1:A:474:MET:HB3	1:B:492:ARG:HD2	1.87	0.57
1:C:45:TRP:HA	1:C:51:LEU:HD12	1.87	0.57
1:B:45:TRP:HA	1:B:51:LEU:HD12	1.87	0.57
1:D:285:SER:O	1:D:615:ARG:NH1	2.33	0.57
1:C:448:SER:H	4:C:710:POV:H12	1.69	0.56
1:B:623:TYR:HA	1:C:42:LYS:HD2	1.87	0.56
1:B:420:ILE:HD12	1:B:427:VAL:HG13	1.88	0.56
1:A:420:ILE:HD12	1:A:427:VAL:HG13	1.88	0.56
1:A:190:ARG:HG2	1:A:232:LEU:HD13	1.88	0.56
1:C:474:MET:HB3	1:D:492:ARG:HD2	1.88	0.56
1:B:190:ARG:HG2	1:B:232:LEU:HD13	1.88	0.55
1:D:45:TRP:HA	1:D:51:LEU:HD12	1.87	0.55
1:A:45:TRP:HA	1:A:51:LEU:HD12	1.87	0.55
1:C:420:ILE:HD12	1:C:427:VAL:HG13	1.88	0.55
1:C:190:ARG:HG2	1:C:232:LEU:HD13	1.88	0.55
1:C:623:TYR:HA	1:D:42:LYS:HD2	1.89	0.55
1:A:42:LYS:HD2	1:D:623:TYR:HA	1.89	0.55
1:C:632:ARG:NH1	1:D:34:ASP:OD1	2.37	0.55
1:D:190:ARG:HG2	1:D:232:LEU:HD13	1.88	0.55
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.89	0.54
1:D:420:ILE:HD12	1:D:427:VAL:HG13	1.88	0.54
1:B:449:GLY:H	4:B:706:POV:H22A	1.73	0.54
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.90	0.54
2:C:704:Y01:HAQ1	1:D:565:ILE:HD12	1.89	0.54
1:A:565:ILE:HD12	2:D:708:Y01:HAQ1	1.90	0.53
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.90	0.53
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.90	0.53
1:A:449:GLY:H	4:A:804:POV:H22A	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:GLY:H	4:D:710:POV:H22A	1.74	0.52
1:A:565:ILE:CD1	2:D:708:Y01:HAQ1	2.40	0.52
2:C:704:Y01:HAQ1	1:D:565:ILE:CD1	2.40	0.52
1:A:34:ASP:OD1	1:D:632:ARG:NH1	2.41	0.52
1:C:285:SER:HB3	1:C:291:SER:HB3	1.92	0.52
1:C:449:GLY:H	4:C:706:POV:H22A	1.75	0.52
2:A:802:Y01:HAQ1	1:B:565:ILE:CD1	2.40	0.52
1:B:443:ARG:HG2	4:B:709:POV:H310	1.92	0.51
1:A:285:SER:HB3	1:A:291:SER:HB3	1.92	0.51
1:D:443:ARG:HG2	4:D:713:POV:H310	1.93	0.50
1:A:632:ARG:NH1	1:B:34:ASP:OD1	2.38	0.50
2:B:704:Y01:HAQ1	1:C:565:ILE:HD12	1.93	0.50
1:D:285:SER:HB3	1:D:291:SER:HB3	1.92	0.50
1:B:285:SER:HB3	1:B:291:SER:HB3	1.92	0.50
1:D:381:LYS:HD2	4:D:702:POV:H1A	1.93	0.49
1:B:435:MET:HE1	4:B:706:POV:H31D	1.93	0.49
2:A:802:Y01:HAQ1	1:B:565:ILE:HD12	1.93	0.49
1:C:242:THR:OG1	1:C:282:GLU:OE2	2.23	0.49
1:A:242:THR:OG1	1:A:282:GLU:OE2	2.24	0.49
1:A:497:MET:HE1	1:A:574:LEU:HD22	1.94	0.49
1:A:443:ARG:HG2	4:A:807:POV:H310	1.95	0.49
1:C:443:ARG:HG2	4:C:709:POV:H310	1.94	0.48
2:B:704:Y01:HAQ1	1:C:565:ILE:CD1	2.43	0.48
3:B:715:PCW:H242	3:B:715:PCW:H212	1.60	0.48
1:C:497:MET:HE1	1:C:574:LEU:HD22	1.95	0.48
1:D:497:MET:HE1	1:D:574:LEU:HD22	1.94	0.48
1:D:568:LEU:O	1:D:572:ASN:ND2	2.47	0.48
1:B:497:MET:HE1	1:B:574:LEU:HD22	1.94	0.48
1:C:353:LYS:HE3	1:C:369:GLN:HE21	1.78	0.48
1:B:568:LEU:O	1:B:572:ASN:ND2	2.47	0.48
1:A:353:LYS:HE3	1:A:369:GLN:HE21	1.78	0.48
1:C:263:ARG:NH1	1:C:282:GLU:OE1	2.47	0.48
1:D:353:LYS:HE3	1:D:369:GLN:HE21	1.78	0.48
1:B:625:LEU:HB3	1:B:630:PHE:HE2	1.79	0.48
1:C:568:LEU:O	1:C:572:ASN:ND2	2.46	0.48
1:C:625:LEU:HB3	1:C:630:PHE:HE2	1.79	0.48
1:D:435:MET:HE1	4:D:710:POV:H31D	1.96	0.48
1:A:568:LEU:O	1:A:572:ASN:ND2	2.46	0.48
1:C:270:TYR:OH	1:D:118:GLN:NE2	2.46	0.48
1:A:442:MET:HE1	4:A:804:POV:H38A	1.96	0.47
1:B:353:LYS:HE3	1:B:369:GLN:HE21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:VAL:HG13	2:C:703:Y01:HAA3	1.96	0.47
1:D:442:MET:HE1	4:D:710:POV:H38A	1.96	0.47
1:D:625:LEU:HB3	1:D:630:PHE:HE2	1.79	0.47
1:A:263:ARG:NH1	1:A:282:GLU:OE1	2.47	0.47
1:A:435:MET:HE1	4:A:804:POV:H31D	1.97	0.47
1:A:270:TYR:OH	1:B:118:GLN:NE2	2.47	0.47
1:C:442:MET:HE1	4:C:706:POV:H38A	1.96	0.47
1:B:263:ARG:NH1	1:B:282:GLU:OE1	2.47	0.47
1:A:625:LEU:HB3	1:A:630:PHE:HE2	1.79	0.47
1:D:263:ARG:NH1	1:D:282:GLU:OE1	2.47	0.47
2:C:701:Y01:HAC3	2:C:701:Y01:HAJ2	1.78	0.47
1:A:381:LYS:HD2	4:A:812:POV:H1A	1.97	0.47
1:B:553:PHE:HZ	4:B:702:POV:H35	1.80	0.47
4:B:706:POV:H215	4:B:706:POV:H21B	1.55	0.47
1:C:486:ILE:HD12	2:C:704:Y01:HAD3	1.97	0.47
1:D:242:THR:OG1	1:D:282:GLU:OE2	2.23	0.47
1:A:391:VAL:HG13	2:A:801:Y01:HAA3	1.97	0.46
1:B:438:VAL:HG11	4:B:706:POV:H31A	1.97	0.46
4:A:811:POV:H21B	4:B:707:POV:H316	1.97	0.46
4:A:805:POV:H21E	4:A:805:POV:H212	1.74	0.46
1:C:381:LYS:HD2	4:C:714:POV:H1A	1.97	0.46
1:C:546:ASN:HD22	1:C:549:VAL:HG22	1.81	0.46
1:D:391:VAL:HG13	2:D:707:Y01:HAA3	1.97	0.46
1:B:546:ASN:HD22	1:B:549:VAL:HG22	1.81	0.46
1:B:465:VAL:HB	1:C:499:VAL:HG21	1.97	0.46
1:C:443:ARG:HD3	4:C:706:POV:H21D	1.98	0.46
1:D:264:LYS:HE3	1:D:276:THR:HG21	1.98	0.46
4:C:710:POV:H22A	4:C:710:POV:H25A	1.78	0.46
1:A:377:TYR:OH	1:A:389:GLU:OE1	2.31	0.46
1:A:454:MET:HE2	4:A:807:POV:H316	1.98	0.46
1:C:435:MET:HE1	4:C:706:POV:H31D	1.98	0.45
1:A:264:LYS:HE3	1:A:276:THR:HG21	1.97	0.45
1:B:443:ARG:HD3	4:B:706:POV:H21D	1.99	0.45
1:D:454:MET:HE2	4:D:713:POV:H316	1.98	0.45
1:A:443:ARG:HD3	4:A:804:POV:H21D	1.98	0.45
4:B:706:POV:H22	4:B:706:POV:H2	1.67	0.45
1:C:454:MET:HE2	4:C:709:POV:H316	1.99	0.45
3:B:716:PCW:H182	3:B:716:PCW:H151	1.77	0.45
1:D:546:ASN:HD22	1:D:549:VAL:HG22	1.81	0.45
1:A:486:ILE:HD12	2:A:802:Y01:HAD3	1.99	0.45
1:B:242:THR:OG1	1:B:282:GLU:OE2	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:LYS:HE3	1:C:276:THR:HG21	1.97	0.45
3:C:715:PCW:H212	3:C:715:PCW:H242	1.63	0.45
1:D:486:ILE:HD12	2:D:708:Y01:HAD3	1.99	0.45
1:B:454:MET:HE2	4:B:709:POV:H316	1.99	0.45
1:D:443:ARG:HD3	4:D:710:POV:H21D	1.99	0.45
1:A:546:ASN:HD22	1:A:549:VAL:HG22	1.81	0.45
1:B:264:LYS:HE3	1:B:276:THR:HG21	1.97	0.45
1:B:442:MET:HE1	4:B:706:POV:H38A	1.98	0.45
1:A:550:ASP:HB2	4:D:710:POV:H13	1.99	0.45
2:A:815:Y01:HAC3	2:A:815:Y01:HAJ2	1.78	0.44
4:B:706:POV:H13	1:C:550:ASP:HB2	1.99	0.44
4:B:706:POV:H31E	4:C:702:POV:H27	2.00	0.44
4:C:706:POV:H13	1:D:550:ASP:HB2	1.99	0.44
4:D:710:POV:H29	4:D:714:POV:H13B	1.98	0.44
4:A:804:POV:H21B	4:A:804:POV:H215	1.54	0.44
1:B:465:VAL:HG12	4:B:713:POV:H217	2.00	0.44
4:B:708:POV:H25	4:B:708:POV:H28	1.61	0.44
4:C:710:POV:H36A	4:C:710:POV:H33A	1.72	0.44
4:D:714:POV:H212	4:D:714:POV:H21E	1.65	0.44
4:A:808:POV:H21E	4:A:808:POV:H212	1.65	0.44
4:B:708:POV:H31G	4:B:708:POV:H31D	1.81	0.44
4:B:713:POV:H31C	4:B:713:POV:H39	1.85	0.44
4:C:713:POV:H21B	4:D:711:POV:H316	1.99	0.44
4:A:807:POV:H31F	4:A:807:POV:H31C	1.77	0.44
4:B:706:POV:H22	4:B:706:POV:H25	1.83	0.44
4:A:808:POV:H33A	4:A:808:POV:H36A	1.71	0.44
1:B:428:LEU:HD21	2:B:704:Y01:HBf	2.00	0.44
4:D:710:POV:H25	4:D:710:POV:H22	1.88	0.44
3:A:813:PCW:H212	3:A:813:PCW:H242	1.61	0.44
4:B:713:POV:H25A	4:B:713:POV:H22	1.70	0.44
1:D:84:HIS:HD2	1:D:120:ALA:HB2	1.83	0.44
1:A:449:GLY:N	4:A:804:POV:H22A	2.33	0.44
4:B:710:POV:H33A	4:B:710:POV:H36A	1.70	0.44
1:C:438:VAL:HG11	4:C:706:POV:H31A	2.00	0.44
1:C:439:THR:HB	1:C:453:PRO:HB2	1.99	0.44
1:C:449:GLY:N	4:C:706:POV:H22A	2.33	0.44
4:A:806:POV:H11	4:A:806:POV:H15B	1.83	0.43
4:C:714:POV:H21D	4:C:714:POV:H217	1.74	0.43
1:A:438:VAL:HG11	4:A:804:POV:H31A	1.99	0.43
4:A:804:POV:H13	1:B:550:ASP:HB2	2.00	0.43
4:B:713:POV:H24	4:B:713:POV:H27A	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:615:ARG:HE	1:D:629:TRP:CD1	2.36	0.43
1:B:615:ARG:HE	1:B:629:TRP:CD1	2.36	0.43
4:B:710:POV:H15B	4:B:710:POV:H11A	1.83	0.43
4:C:708:POV:H31D	4:C:708:POV:H31G	1.80	0.43
1:D:438:VAL:HG11	4:D:710:POV:H31A	2.00	0.43
4:D:702:POV:H21D	4:D:702:POV:H217	1.73	0.43
1:C:434:PHE:HD1	4:C:710:POV:H31B	1.84	0.43
1:B:439:THR:HB	1:B:453:PRO:HB2	1.99	0.43
1:A:434:PHE:HD1	4:A:808:POV:H31B	1.84	0.43
1:A:466:MET:HG2	4:A:811:POV:H218	2.00	0.43
1:D:439:THR:HB	1:D:453:PRO:HB2	1.99	0.43
1:B:84:HIS:HD2	1:B:120:ALA:HB2	1.83	0.43
4:B:710:POV:H22A	4:B:710:POV:H25A	1.74	0.43
1:C:84:HIS:HD2	1:C:120:ALA:HB2	1.83	0.43
1:D:449:GLY:N	4:D:710:POV:H22A	2.33	0.43
1:B:449:GLY:N	4:B:706:POV:H22A	2.33	0.43
4:B:710:POV:H212	4:B:710:POV:H21E	1.65	0.43
1:A:260:MET:HE2	1:A:312:PRO:HG3	2.01	0.43
1:A:615:ARG:HE	1:A:629:TRP:CD1	2.36	0.43
4:A:806:POV:H31G	4:A:806:POV:H31D	1.80	0.43
4:B:713:POV:H22A	4:B:713:POV:H2	1.84	0.43
3:C:716:PCW:H182	3:C:716:PCW:H151	1.77	0.43
1:D:260:MET:HE2	1:D:312:PRO:HG3	2.01	0.43
3:D:704:PCW:H182	3:D:704:PCW:H151	1.77	0.43
1:A:84:HIS:HD2	1:A:120:ALA:HB2	1.83	0.42
4:A:804:POV:H29	4:A:808:POV:H13B	2.00	0.42
1:B:350:ARG:NH2	1:C:510:ILE:O	2.52	0.42
1:B:426:HIS:CE1	2:B:703:Y01:HAL1	2.54	0.42
1:C:615:ARG:HE	1:C:629:TRP:CD1	2.36	0.42
4:C:709:POV:H35	4:C:709:POV:H32A	1.86	0.42
4:D:711:POV:H21E	4:D:711:POV:H212	1.75	0.42
4:A:806:POV:H25	4:A:806:POV:H28	1.62	0.42
4:C:706:POV:H29	4:C:710:POV:H13B	2.00	0.42
1:D:434:PHE:HD1	4:D:714:POV:H31B	1.84	0.42
1:A:128:GLN:NE2	1:A:173:VAL:O	2.53	0.42
1:A:439:THR:HB	1:A:453:PRO:HB2	1.99	0.42
1:A:473:GLN:HB3	4:A:811:POV:H15	2.01	0.42
4:A:804:POV:H22	4:A:804:POV:H2	1.65	0.42
4:A:805:POV:H316	4:D:701:POV:H21B	2.00	0.42
4:A:808:POV:H22A	4:A:808:POV:H25A	1.79	0.42
4:B:706:POV:H29	4:B:710:POV:H13B	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:710:POV:H21E	4:C:710:POV:H212	1.65	0.42
3:D:703:PCW:H242	3:D:703:PCW:H212	1.62	0.42
4:D:712:POV:H15B	4:D:712:POV:H11	1.83	0.42
4:A:808:POV:H15B	4:A:808:POV:H11A	1.85	0.42
1:C:410:MET:HB3	1:C:415:PHE:HD2	1.85	0.42
4:C:713:POV:H27A	4:C:713:POV:H24	1.71	0.42
4:D:702:POV:H35A	4:D:702:POV:H32A	1.83	0.42
4:D:713:POV:H31F	4:D:713:POV:H31C	1.76	0.42
1:A:410:MET:HB3	1:A:415:PHE:HD2	1.85	0.42
1:B:128:GLN:NE2	1:B:173:VAL:O	2.53	0.42
4:C:706:POV:H22	4:C:706:POV:H2	1.66	0.42
4:D:714:POV:H25A	4:D:714:POV:H22A	1.77	0.42
1:B:410:MET:HB3	1:B:415:PHE:HD2	1.85	0.42
2:B:701:Y01:HAC3	2:B:701:Y01:HAJ2	1.78	0.42
4:C:710:POV:H15B	4:C:710:POV:H11A	1.84	0.42
1:D:350:ARG:HG3	1:D:352:LEU:HD13	2.02	0.42
1:D:410:MET:HB3	1:D:415:PHE:HD2	1.85	0.42
4:D:710:POV:H215	4:D:710:POV:H21B	1.54	0.42
1:B:260:MET:HE2	1:B:312:PRO:HG3	2.01	0.42
1:C:466:MET:HG2	4:C:713:POV:H218	2.01	0.42
1:C:473:GLN:HB3	4:C:713:POV:H15	2.01	0.42
1:D:510:ILE:HA	1:D:513:GLN:HB2	2.02	0.42
1:A:350:ARG:HG3	1:A:352:LEU:HD13	2.02	0.42
3:A:813:PCW:H231	3:A:813:PCW:H262	1.73	0.42
1:C:128:GLN:NE2	1:C:173:VAL:O	2.53	0.42
1:C:497:MET:SD	2:D:705:Y01:HAB3	2.60	0.42
4:D:710:POV:H22	4:D:710:POV:H2	1.66	0.42
1:A:499:VAL:HG21	1:D:465:VAL:HB	2.02	0.42
3:A:814:PCW:H182	3:A:814:PCW:H151	1.77	0.42
1:C:260:MET:HE2	1:C:312:PRO:HG3	2.01	0.42
1:D:312:PRO:HG2	1:D:313:VAL:HG23	2.02	0.42
1:D:553:PHE:H	4:D:706:POV:H14B	1.85	0.42
1:A:434:PHE:HB3	4:A:808:POV:H313	2.02	0.41
1:D:128:GLN:NE2	1:D:173:VAL:O	2.53	0.41
4:D:713:POV:H15B	4:D:713:POV:H11	1.85	0.41
1:A:230:GLN:HA	1:A:231:PRO:HD3	1.86	0.41
4:A:811:POV:H38	4:A:811:POV:H35A	1.98	0.41
4:B:709:POV:H31F	4:B:709:POV:H31C	1.75	0.41
2:C:703:Y01:HAU2	2:C:703:Y01:HAC1	2.02	0.41
4:C:709:POV:H11	4:C:709:POV:H15B	1.85	0.41
4:D:701:POV:H24	4:D:701:POV:H27A	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:HB3	1:A:70:CYS:H	1.86	0.41
1:A:312:PRO:HG2	1:A:313:VAL:HG23	2.02	0.41
4:A:807:POV:H32A	4:A:807:POV:H35	1.85	0.41
1:B:341:ILE:HG12	4:C:707:POV:H36A	2.01	0.41
1:B:434:PHE:HD1	4:B:710:POV:H31B	1.85	0.41
4:B:713:POV:H21B	4:C:707:POV:H316	2.02	0.41
1:C:434:PHE:HB3	4:C:710:POV:H313	2.02	0.41
1:A:456:PHE:HZ	4:B:702:POV:H21A	1.86	0.41
1:A:510:ILE:HA	1:A:513:GLN:HB2	2.01	0.41
1:A:553:PHE:H	4:A:816:POV:H14B	1.85	0.41
4:C:713:POV:H2	4:C:713:POV:H22A	1.84	0.41
1:B:68:GLU:HB3	1:B:70:CYS:H	1.86	0.41
1:D:68:GLU:HB3	1:D:70:CYS:H	1.86	0.41
1:A:485:MET:HE1	1:B:573:LEU:HG	2.01	0.41
4:A:811:POV:H212	4:A:811:POV:H21E	1.93	0.41
4:A:811:POV:H22A	4:A:811:POV:H2	1.85	0.41
1:B:53:ALA:O	1:B:91:ASN:ND2	2.51	0.41
1:C:553:PHE:H	4:C:702:POV:H14B	1.86	0.41
1:D:53:ALA:O	1:D:91:ASN:ND2	2.51	0.41
1:D:473:GLN:HB3	4:D:701:POV:H15	2.02	0.41
1:A:465:VAL:HB	1:B:499:VAL:HG21	2.03	0.41
1:B:312:PRO:HG2	1:B:313:VAL:HG23	2.02	0.41
1:B:597:ILE:HD13	1:B:597:ILE:HA	1.89	0.41
1:C:68:GLU:HB3	1:C:70:CYS:H	1.85	0.41
1:A:118:GLN:NE2	1:D:270:TYR:OH	2.54	0.41
1:A:426:HIS:CE1	2:A:801:Y01:HAL1	2.56	0.41
4:B:714:POV:H210	4:B:714:POV:H21C	1.94	0.41
3:B:715:PCW:H211	3:B:715:PCW:H182	1.83	0.41
3:B:715:PCW:H231	3:B:715:PCW:H262	1.71	0.41
1:C:510:ILE:HA	1:C:513:GLN:HB2	2.01	0.41
1:D:434:PHE:HB3	4:D:714:POV:H313	2.02	0.41
1:D:516:ASP:HA	1:D:517:PRO:HD3	1.93	0.41
1:D:563:ALA:O	1:D:567:THR:OG1	2.37	0.41
3:D:703:PCW:H262	3:D:703:PCW:H231	1.72	0.41
1:B:350:ARG:HG3	1:B:352:LEU:HD13	2.02	0.41
1:B:632:ARG:NH1	1:C:34:ASP:OD1	2.46	0.41
2:B:703:Y01:HAC1	2:B:703:Y01:HAU2	2.03	0.41
4:B:713:POV:H38	4:B:713:POV:H35A	1.98	0.41
4:D:713:POV:H32A	4:D:713:POV:H35	1.85	0.41
4:C:713:POV:H22	4:C:713:POV:H25A	1.70	0.40
4:D:712:POV:H25	4:D:712:POV:H28	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:VAL:HG13	2:B:703:Y01:HAA3	2.04	0.40
1:C:312:PRO:HG2	1:C:313:VAL:HG23	2.02	0.40
1:B:343:PHE:HE1	4:B:709:POV:H315	1.87	0.40
1:B:510:ILE:HA	1:B:513:GLN:HB2	2.02	0.40
1:C:350:ARG:HG3	1:C:352:LEU:HD13	2.02	0.40
1:C:553:PHE:HZ	4:C:702:POV:H35	1.86	0.40
4:D:701:POV:H2	4:D:701:POV:H22A	1.85	0.40
4:D:711:POV:H211	4:D:711:POV:H28A	1.86	0.40
1:A:553:PHE:HZ	4:A:816:POV:H35	1.86	0.40
4:A:811:POV:H31C	4:A:811:POV:H39	1.85	0.40
4:D:701:POV:H212	4:D:701:POV:H21E	1.94	0.40
2:A:801:Y01:HAC1	2:A:801:Y01:HAU2	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	612/683 (90%)	590 (96%)	22 (4%)	0	100	100
1	B	612/683 (90%)	590 (96%)	22 (4%)	0	100	100
1	C	612/683 (90%)	590 (96%)	22 (4%)	0	100	100
1	D	612/683 (90%)	590 (96%)	22 (4%)	0	100	100
All	All	2448/2732 (90%)	2360 (96%)	88 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/593 (90%)	526 (99%)	7 (1%)	61	83
1	B	533/593 (90%)	526 (99%)	7 (1%)	61	83
1	C	533/593 (90%)	526 (99%)	7 (1%)	61	83
1	D	533/593 (90%)	526 (99%)	7 (1%)	61	83
All	All	2132/2372 (90%)	2104 (99%)	28 (1%)	59	83

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	121	LEU
1	A	132	LEU
1	A	365	ASN
1	A	452	VAL
1	A	458	LEU
1	A	499	VAL
1	B	83	LEU
1	B	121	LEU
1	B	132	LEU
1	B	365	ASN
1	B	452	VAL
1	B	458	LEU
1	B	499	VAL
1	C	83	LEU
1	C	121	LEU
1	C	132	LEU
1	C	365	ASN
1	C	452	VAL
1	C	458	LEU
1	C	499	VAL
1	D	83	LEU
1	D	121	LEU
1	D	132	LEU
1	D	365	ASN
1	D	452	VAL
1	D	458	LEU
1	D	499	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	122	HIS
1	A	174	ASN
1	A	217	ASN
1	A	290	GLN
1	A	365	ASN
1	A	369	GLN
1	B	118	GLN
1	B	122	HIS
1	B	174	ASN
1	B	290	GLN
1	B	369	GLN
1	B	522	HIS
1	C	118	GLN
1	C	122	HIS
1	C	174	ASN
1	C	290	GLN
1	C	365	ASN
1	C	369	GLN
1	D	118	GLN
1	D	122	HIS
1	D	228	HIS
1	D	290	GLN
1	D	365	ASN
1	D	369	GLN
1	D	522	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	A	807	-	51,51,51	1.06	3 (5%)	57,59,59	0.90	3 (5%)
4	POV	A	808	-	51,51,51	1.08	3 (5%)	57,59,59	0.89	3 (5%)
4	POV	B	706	-	51,51,51	1.08	3 (5%)	57,59,59	0.88	3 (5%)
2	Y01	D	707	-	38,38,38	0.58	1 (2%)	57,57,57	0.52	0
4	POV	C	708	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	3 (5%)
4	POV	C	710	-	51,51,51	1.08	3 (5%)	57,59,59	0.89	3 (5%)
3	PCW	D	709	-	12,12,53	0.78	0	11,11,61	0.48	0
4	POV	A	812	-	51,51,51	1.08	3 (5%)	57,59,59	0.88	3 (5%)
4	POV	B	710	-	51,51,51	1.07	3 (5%)	57,59,59	0.88	3 (5%)
2	Y01	C	704	-	38,38,38	0.63	1 (2%)	57,57,57	0.55	0
2	Y01	D	708	-	38,38,38	0.63	1 (2%)	57,57,57	0.55	0
4	POV	A	804	-	51,51,51	1.08	3 (5%)	57,59,59	0.89	3 (5%)
4	POV	D	710	-	51,51,51	1.08	3 (5%)	57,59,59	0.90	3 (5%)
2	Y01	C	701	-	38,38,38	0.52	0	57,57,57	0.90	3 (5%)
4	POV	B	709	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	3 (5%)
4	POV	C	707	-	51,51,51	1.06	3 (5%)	57,59,59	0.96	3 (5%)
4	POV	A	806	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	3 (5%)
4	POV	D	713	-	51,51,51	1.06	3 (5%)	57,59,59	0.90	3 (5%)
4	POV	D	712	-	51,51,51	1.06	3 (5%)	57,59,59	0.91	3 (5%)
3	PCW	C	716	-	7,7,53	0.92	0	6,6,61	0.28	0
2	Y01	C	703	-	38,38,38	0.58	1 (2%)	57,57,57	0.52	0
3	PCW	C	715	-	14,14,53	0.88	0	13,13,61	0.32	0
4	POV	C	709	-	51,51,51	1.06	3 (5%)	57,59,59	0.90	3 (5%)
4	POV	C	713	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	2 (3%)
4	POV	D	702	-	51,51,51	1.08	3 (5%)	57,59,59	0.88	3 (5%)
3	PCW	B	705	-	12,12,53	0.78	0	11,11,61	0.49	0
4	POV	B	713	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	A	811	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	2 (3%)
2	Y01	A	815	-	38,38,38	0.51	0	57,57,57	0.90	3 (5%)
4	POV	B	714	-	51,51,51	1.07	3 (5%)	57,59,59	0.88	3 (5%)
3	PCW	D	715	-	13,13,53	0.87	0	12,12,61	0.33	0
3	PCW	A	814	-	7,7,53	0.92	0	6,6,61	0.28	0
3	PCW	A	803	-	12,12,53	0.78	0	11,11,61	0.50	0
3	PCW	B	711	-	13,13,53	0.87	0	12,12,61	0.33	0
4	POV	D	701	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	2 (3%)
4	POV	D	714	-	51,51,51	1.08	3 (5%)	57,59,59	0.89	3 (5%)
2	Y01	A	801	-	38,38,38	0.58	1 (2%)	57,57,57	0.52	0
2	Y01	B	704	-	38,38,38	0.63	1 (2%)	57,57,57	0.55	0
4	POV	C	714	-	51,51,51	1.07	3 (5%)	57,59,59	0.88	3 (5%)
3	PCW	A	810	-	7,7,53	0.84	0	6,6,61	0.44	0
4	POV	D	711	-	51,51,51	1.06	3 (5%)	57,59,59	0.96	3 (5%)
4	POV	B	702	-	51,51,51	1.08	3 (5%)	57,59,59	0.95	3 (5%)
3	PCW	C	711	-	13,13,53	0.87	0	12,12,61	0.33	0
4	POV	C	706	-	51,51,51	1.08	3 (5%)	57,59,59	0.90	3 (5%)
3	PCW	A	813	-	14,14,53	0.88	0	13,13,61	0.32	0
4	POV	A	805	-	51,51,51	1.06	3 (5%)	57,59,59	0.96	3 (5%)
3	PCW	B	716	-	7,7,53	0.92	0	6,6,61	0.28	0
2	Y01	B	703	-	38,38,38	0.59	1 (2%)	57,57,57	0.53	0
3	PCW	A	809	-	13,13,53	0.87	0	12,12,61	0.33	0
3	PCW	B	715	-	14,14,53	0.88	0	13,13,61	0.32	0
2	Y01	B	701	-	38,38,38	0.51	0	57,57,57	0.90	3 (5%)
3	PCW	C	705	-	12,12,53	0.78	0	11,11,61	0.48	0
3	PCW	D	703	-	14,14,53	0.88	0	13,13,61	0.32	0
2	Y01	A	802	-	38,38,38	0.63	1 (2%)	57,57,57	0.55	0
3	PCW	D	704	-	7,7,53	0.92	0	6,6,61	0.28	0
4	POV	A	816	-	51,51,51	1.08	3 (5%)	57,59,59	0.96	3 (5%)
3	PCW	D	716	-	7,7,53	0.84	0	6,6,61	0.44	0
4	POV	C	702	-	51,51,51	1.08	3 (5%)	57,59,59	0.96	3 (5%)
4	POV	B	707	-	51,51,51	1.06	3 (5%)	57,59,59	0.96	3 (5%)
4	POV	D	706	-	51,51,51	1.09	3 (5%)	57,59,59	0.96	3 (5%)
2	Y01	D	705	-	38,38,38	0.52	0	57,57,57	0.90	3 (5%)
4	POV	B	708	-	51,51,51	1.05	3 (5%)	57,59,59	0.92	3 (5%)
3	PCW	C	712	-	7,7,53	0.84	0	6,6,61	0.44	0
3	PCW	B	712	-	7,7,53	0.84	0	6,6,61	0.44	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	POV	A	807	-	-	33/55/55/55	-
4	POV	A	808	-	-	29/55/55/55	-
4	POV	B	706	-	-	32/55/55/55	-
2	Y01	D	707	-	-	2/19/77/77	0/4/4/4
4	POV	C	708	-	-	29/55/55/55	-
4	POV	C	710	-	-	29/55/55/55	-
3	PCW	D	709	-	-	6/10/10/57	-
4	POV	A	812	-	-	27/55/55/55	-
4	POV	B	710	-	-	29/55/55/55	-
2	Y01	C	704	-	-	6/19/77/77	0/4/4/4
2	Y01	D	708	-	-	6/19/77/77	0/4/4/4
4	POV	A	804	-	-	33/55/55/55	-
4	POV	D	710	-	-	32/55/55/55	-
2	Y01	C	701	-	-	6/19/77/77	0/4/4/4
4	POV	B	709	-	-	30/55/55/55	-
4	POV	C	707	-	-	28/55/55/55	-
4	POV	A	806	-	-	30/55/55/55	-
4	POV	D	713	-	-	33/55/55/55	-
4	POV	D	712	-	-	29/55/55/55	-
3	PCW	C	716	-	-	4/5/5/57	-
2	Y01	C	703	-	-	2/19/77/77	0/4/4/4
3	PCW	C	715	-	-	8/12/12/57	-
4	POV	C	709	-	-	33/55/55/55	-
4	POV	C	713	-	-	29/55/55/55	-
4	POV	D	702	-	-	27/55/55/55	-
3	PCW	B	705	-	-	6/10/10/57	-
4	POV	B	713	-	-	29/55/55/55	-
4	POV	A	811	-	-	28/55/55/55	-
2	Y01	A	815	-	-	6/19/77/77	0/4/4/4
4	POV	B	714	-	-	28/55/55/55	-
3	PCW	D	715	-	-	5/11/11/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	814	-	-	4/5/5/57	-
3	PCW	A	803	-	-	6/10/10/57	-
3	PCW	B	711	-	-	5/11/11/57	-
4	POV	D	701	-	-	29/55/55/55	-
4	POV	D	714	-	-	29/55/55/55	-
2	Y01	A	801	-	-	2/19/77/77	0/4/4/4
2	Y01	B	704	-	-	6/19/77/77	0/4/4/4
4	POV	C	714	-	-	27/55/55/55	-
3	PCW	A	810	-	-	1/5/5/57	-
4	POV	D	711	-	-	28/55/55/55	-
4	POV	B	702	-	-	24/55/55/55	-
3	PCW	C	711	-	-	5/11/11/57	-
4	POV	C	706	-	-	33/55/55/55	-
3	PCW	A	813	-	-	8/12/12/57	-
4	POV	A	805	-	-	27/55/55/55	-
3	PCW	B	716	-	-	4/5/5/57	-
2	Y01	B	703	-	-	2/19/77/77	0/4/4/4
3	PCW	A	809	-	-	5/11/11/57	-
3	PCW	B	715	-	-	8/12/12/57	-
2	Y01	B	701	-	-	6/19/77/77	0/4/4/4
3	PCW	C	705	-	-	6/10/10/57	-
3	PCW	D	703	-	-	8/12/12/57	-
2	Y01	A	802	-	-	6/19/77/77	0/4/4/4
3	PCW	D	704	-	-	4/5/5/57	-
4	POV	A	816	-	-	25/55/55/55	-
3	PCW	D	716	-	-	1/5/5/57	-
4	POV	C	702	-	-	25/55/55/55	-
4	POV	B	707	-	-	28/55/55/55	-
4	POV	D	706	-	-	25/55/55/55	-
2	Y01	D	705	-	-	6/19/77/77	0/4/4/4
4	POV	B	708	-	-	31/55/55/55	-
3	PCW	C	712	-	-	1/5/5/57	-
3	PCW	B	712	-	-	1/5/5/57	-

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	POV	O21-C21	2.92	1.42	1.34
4	A	816	POV	O21-C21	2.90	1.42	1.34
4	B	702	POV	O21-C21	2.90	1.42	1.34
4	D	706	POV	O21-C21	2.90	1.42	1.34
4	A	808	POV	O21-C21	2.86	1.42	1.34
4	B	714	POV	O21-C21	2.85	1.42	1.34
4	D	710	POV	O21-C21	2.85	1.42	1.34
4	D	714	POV	O21-C21	2.85	1.42	1.34
4	C	714	POV	O21-C21	2.85	1.42	1.34
4	C	710	POV	O21-C21	2.84	1.42	1.34
4	B	706	POV	O21-C21	2.84	1.42	1.34
4	B	710	POV	O21-C21	2.84	1.42	1.34
4	D	711	POV	O21-C21	2.84	1.42	1.34
4	A	812	POV	O21-C21	2.83	1.42	1.34
4	C	706	POV	O21-C21	2.83	1.42	1.34
4	D	702	POV	O21-C21	2.83	1.42	1.34
4	B	707	POV	O21-C21	2.83	1.42	1.34
4	A	805	POV	O21-C21	2.83	1.42	1.34
4	A	804	POV	O21-C21	2.82	1.42	1.34
4	A	804	POV	O31-C31	2.82	1.41	1.33
4	C	707	POV	O21-C21	2.81	1.42	1.34
4	C	708	POV	O21-C21	2.80	1.42	1.34
4	D	710	POV	O31-C31	2.79	1.41	1.33
4	B	709	POV	O21-C21	2.79	1.42	1.34
4	B	708	POV	O21-C21	2.78	1.42	1.34
4	C	706	POV	O31-C31	2.78	1.41	1.33
4	D	701	POV	O21-C21	2.77	1.42	1.34
4	A	806	POV	O21-C21	2.77	1.42	1.34
4	D	712	POV	O21-C21	2.77	1.42	1.34
4	A	807	POV	O21-C21	2.77	1.42	1.34
4	A	811	POV	O21-C21	2.77	1.42	1.34
4	C	713	POV	O21-C21	2.76	1.42	1.34
4	B	706	POV	O31-C31	2.76	1.41	1.33
4	D	706	POV	O31-C31	2.76	1.41	1.33
4	C	708	POV	O31-C31	2.76	1.41	1.33
4	D	713	POV	O21-C21	2.75	1.42	1.34
4	B	713	POV	O21-C21	2.75	1.42	1.34
4	C	709	POV	O21-C21	2.75	1.42	1.34
4	D	712	POV	O31-C31	2.74	1.41	1.33
4	A	816	POV	O31-C31	2.74	1.41	1.33
4	B	702	POV	O31-C31	2.72	1.41	1.33
4	B	708	POV	O31-C31	2.72	1.41	1.33
4	A	806	POV	O31-C31	2.71	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	POV	O31-C31	2.71	1.41	1.33
4	A	807	POV	O21-C2	-2.71	1.40	1.46
4	C	713	POV	O31-C31	2.69	1.41	1.33
4	C	709	POV	O21-C2	-2.69	1.40	1.46
4	B	713	POV	O31-C31	2.67	1.41	1.33
4	A	811	POV	O31-C31	2.67	1.41	1.33
4	D	701	POV	O31-C31	2.67	1.41	1.33
4	D	713	POV	O21-C2	-2.66	1.40	1.46
4	B	709	POV	O21-C2	-2.65	1.40	1.46
4	D	714	POV	O21-C2	-2.63	1.40	1.46
4	D	702	POV	O21-C2	-2.61	1.40	1.46
4	C	702	POV	O21-C2	-2.61	1.40	1.46
4	A	808	POV	O21-C2	-2.61	1.40	1.46
4	D	706	POV	O21-C2	-2.61	1.40	1.46
4	C	710	POV	O21-C2	-2.60	1.40	1.46
4	C	714	POV	O21-C2	-2.60	1.40	1.46
4	A	811	POV	O21-C2	-2.60	1.40	1.46
4	A	812	POV	O21-C2	-2.60	1.40	1.46
4	A	816	POV	O21-C2	-2.59	1.40	1.46
4	D	712	POV	O21-C2	-2.59	1.40	1.46
4	C	708	POV	O21-C2	-2.59	1.40	1.46
4	C	713	POV	O21-C2	-2.58	1.40	1.46
4	C	714	POV	O31-C31	2.58	1.40	1.33
4	B	710	POV	O21-C2	-2.57	1.40	1.46
4	B	714	POV	O21-C2	-2.57	1.40	1.46
4	A	806	POV	O21-C2	-2.57	1.40	1.46
4	D	702	POV	O31-C31	2.57	1.40	1.33
4	B	702	POV	O21-C2	-2.57	1.40	1.46
4	B	713	POV	O21-C2	-2.56	1.40	1.46
4	A	812	POV	O31-C31	2.56	1.40	1.33
4	B	708	POV	O21-C2	-2.56	1.40	1.46
4	B	706	POV	O21-C2	-2.55	1.40	1.46
4	D	701	POV	O21-C2	-2.55	1.40	1.46
4	B	714	POV	O31-C31	2.55	1.40	1.33
4	A	807	POV	O31-C31	2.55	1.40	1.33
4	D	713	POV	O31-C31	2.54	1.40	1.33
4	B	709	POV	O31-C31	2.54	1.40	1.33
4	C	706	POV	O21-C2	-2.54	1.40	1.46
4	A	804	POV	O21-C2	-2.53	1.40	1.46
4	C	709	POV	O31-C31	2.52	1.40	1.33
4	D	710	POV	O21-C2	-2.52	1.40	1.46
4	C	707	POV	O31-C31	2.52	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	711	POV	O31-C31	2.52	1.40	1.33
4	A	805	POV	O21-C2	-2.52	1.40	1.46
4	B	707	POV	O31-C31	2.51	1.40	1.33
4	B	707	POV	O21-C2	-2.50	1.40	1.46
4	C	707	POV	O21-C2	-2.50	1.40	1.46
4	A	805	POV	O31-C31	2.48	1.40	1.33
4	D	711	POV	O21-C2	-2.48	1.40	1.46
4	C	710	POV	O31-C31	2.47	1.40	1.33
4	A	808	POV	O31-C31	2.47	1.40	1.33
4	B	710	POV	O31-C31	2.47	1.40	1.33
4	D	714	POV	O31-C31	2.46	1.40	1.33
2	D	707	Y01	OAH-CAX	-2.23	1.23	1.30
2	B	703	Y01	OAH-CAX	-2.22	1.23	1.30
2	A	801	Y01	OAH-CAX	-2.21	1.23	1.30
2	C	703	Y01	OAH-CAX	-2.21	1.23	1.30
2	B	704	Y01	OAH-CAX	-2.09	1.23	1.30
2	D	708	Y01	OAH-CAX	-2.09	1.23	1.30
2	A	802	Y01	OAH-CAX	-2.09	1.23	1.30
2	C	704	Y01	OAH-CAX	-2.08	1.23	1.30

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	POV	O21-C21-C22	4.05	120.24	111.48
4	C	713	POV	O21-C21-C22	4.05	120.23	111.48
4	A	811	POV	O21-C21-C22	4.03	120.20	111.48
4	B	713	POV	O21-C21-C22	4.03	120.20	111.48
4	C	707	POV	O21-C21-C22	3.86	119.83	111.48
4	A	805	POV	O21-C21-C22	3.85	119.82	111.48
4	D	711	POV	O21-C21-C22	3.85	119.81	111.48
4	B	707	POV	O21-C21-C22	3.82	119.74	111.48
4	C	706	POV	O21-C21-C22	3.70	119.49	111.48
4	A	816	POV	O21-C21-C22	3.70	119.48	111.48
4	C	702	POV	O21-C21-C22	3.70	119.48	111.48
4	A	804	POV	O21-C21-C22	3.70	119.48	111.48
4	D	706	POV	O21-C21-C22	3.69	119.46	111.48
4	D	710	POV	O21-C21-C22	3.68	119.44	111.48
4	A	806	POV	O21-C21-C22	3.67	119.42	111.48
4	B	702	POV	O21-C21-C22	3.67	119.41	111.48
4	A	808	POV	O21-C21-C22	3.67	119.41	111.48
4	B	706	POV	O21-C21-C22	3.66	119.40	111.48
4	B	708	POV	O21-C21-C22	3.66	119.39	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	710	POV	O21-C21-C22	3.66	119.39	111.48
4	C	708	POV	O21-C21-C22	3.64	119.36	111.48
4	D	702	POV	O21-C21-C22	3.64	119.36	111.48
4	B	714	POV	O21-C21-C22	3.64	119.36	111.48
4	D	712	POV	O21-C21-C22	3.64	119.36	111.48
4	C	714	POV	O21-C21-C22	3.64	119.35	111.48
4	D	714	POV	O21-C21-C22	3.64	119.35	111.48
4	B	710	POV	O21-C21-C22	3.64	119.35	111.48
4	A	812	POV	O21-C21-C22	3.62	119.32	111.48
4	B	709	POV	O21-C21-C22	3.47	118.99	111.48
4	D	713	POV	O21-C21-C22	3.33	118.68	111.48
4	A	807	POV	O21-C21-C22	3.33	118.68	111.48
4	C	709	POV	O21-C21-C22	3.29	118.60	111.48
2	D	705	Y01	CAL-CAM-CAY	3.28	123.17	113.44
2	A	815	Y01	CAL-CAM-CAY	3.26	123.12	113.44
2	C	701	Y01	CAL-CAM-CAY	3.25	123.09	113.44
2	B	701	Y01	CAL-CAM-CAY	3.25	123.08	113.44
4	D	706	POV	C14-N-C12	2.93	121.56	109.91
4	C	702	POV	C14-N-C12	2.90	121.43	109.91
4	A	816	POV	C14-N-C12	2.90	121.42	109.91
4	B	702	POV	C14-N-C12	2.83	121.17	109.91
4	A	805	POV	C14-N-C12	2.64	120.42	109.91
4	D	701	POV	O31-C31-C32	2.64	119.88	111.83
4	A	811	POV	O31-C31-C32	2.64	119.88	111.83
4	C	702	POV	O31-C31-C32	2.63	119.86	111.83
4	D	711	POV	C14-N-C12	2.63	120.36	109.91
4	C	713	POV	O31-C31-C32	2.63	119.85	111.83
4	D	710	POV	O31-C31-C32	2.62	119.83	111.83
4	D	711	POV	O31-C31-C32	2.62	119.83	111.83
4	B	713	POV	O31-C31-C32	2.62	119.82	111.83
4	A	805	POV	O31-C31-C32	2.62	119.82	111.83
4	C	706	POV	O31-C31-C32	2.61	119.81	111.83
4	D	706	POV	O31-C31-C32	2.61	119.81	111.83
4	C	707	POV	O31-C31-C32	2.61	119.79	111.83
4	B	702	POV	O31-C31-C32	2.61	119.79	111.83
4	A	816	POV	O31-C31-C32	2.61	119.78	111.83
4	B	706	POV	O31-C31-C32	2.61	119.78	111.83
4	B	707	POV	C14-N-C12	2.60	120.26	109.91
4	A	804	POV	O31-C31-C32	2.60	119.77	111.83
4	D	702	POV	O31-C31-C32	2.58	119.70	111.83
4	A	812	POV	O31-C31-C32	2.57	119.68	111.83
4	B	707	POV	O31-C31-C32	2.57	119.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	714	POV	O31-C31-C32	2.56	119.64	111.83
4	C	707	POV	C14-N-C12	2.53	119.98	109.91
4	A	806	POV	O31-C31-C32	2.53	119.54	111.83
4	B	708	POV	O31-C31-C32	2.52	119.52	111.83
4	B	714	POV	O31-C31-C32	2.52	119.51	111.83
4	B	709	POV	O31-C31-C32	2.51	119.49	111.83
4	C	708	POV	O31-C31-C32	2.51	119.49	111.83
4	D	712	POV	O31-C31-C32	2.50	119.46	111.83
4	C	709	POV	O31-C31-C32	2.50	119.45	111.83
4	A	807	POV	O31-C31-C32	2.49	119.44	111.83
4	A	808	POV	O31-C31-C32	2.47	119.36	111.83
4	D	714	POV	O31-C31-C32	2.46	119.33	111.83
4	C	710	POV	O31-C31-C32	2.45	119.32	111.83
4	B	710	POV	O31-C31-C32	2.45	119.31	111.83
4	D	713	POV	O31-C31-C32	2.45	119.30	111.83
4	D	710	POV	C14-N-C12	2.40	119.46	109.91
4	D	714	POV	C14-N-C12	2.40	119.44	109.91
4	A	808	POV	C14-N-C12	2.39	119.41	109.91
4	B	710	POV	C14-N-C12	2.39	119.39	109.91
4	C	710	POV	C14-N-C12	2.37	119.34	109.91
4	C	706	POV	C14-N-C12	2.37	119.33	109.91
4	A	804	POV	C14-N-C12	2.36	119.28	109.91
4	B	714	POV	C14-N-C12	2.33	119.16	109.91
4	D	702	POV	C14-N-C12	2.33	119.15	109.91
4	A	812	POV	C14-N-C12	2.32	119.14	109.91
4	C	714	POV	C14-N-C12	2.32	119.13	109.91
4	B	706	POV	C14-N-C12	2.31	119.07	109.91
4	A	807	POV	C14-N-C12	2.28	118.97	109.91
4	C	709	POV	C14-N-C12	2.28	118.97	109.91
4	B	709	POV	C14-N-C12	2.27	118.94	109.91
4	D	713	POV	C14-N-C12	2.27	118.94	109.91
4	B	708	POV	C14-N-C12	2.21	118.68	109.91
4	A	806	POV	C14-N-C12	2.20	118.66	109.91
4	C	708	POV	C14-N-C12	2.20	118.65	109.91
4	D	712	POV	C14-N-C12	2.19	118.62	109.91
2	C	701	Y01	CAT-CAR-CBC	2.15	113.84	110.33
2	D	705	Y01	CAT-CAR-CBC	2.14	113.83	110.33
2	B	701	Y01	CAT-CAR-CBC	2.13	113.81	110.33
2	A	815	Y01	CAT-CAR-CBC	2.12	113.79	110.33
2	A	815	Y01	OAW-CBC-CAR	-2.08	103.45	108.37
2	D	705	Y01	OAW-CBC-CAR	-2.06	103.49	108.37
2	B	701	Y01	OAW-CBC-CAR	-2.06	103.50	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	Y01	OAW-CBC-CAR	-2.06	103.50	108.37

There are no chirality outliers.

All (1080) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	Y01	CAX-CAL-CAM-CAY
2	C	703	Y01	CAX-CAL-CAM-CAY
2	D	707	Y01	CAX-CAL-CAM-CAY
4	A	804	POV	C11-O12-P-O11
4	A	804	POV	C11-O12-P-O13
4	A	804	POV	O12-C11-C12-N
4	A	804	POV	C22-C21-O21-C2
4	A	804	POV	O22-C21-O21-C2
4	A	805	POV	O12-C11-C12-N
4	A	805	POV	O22-C21-O21-C2
4	A	806	POV	C1-O11-P-O12
4	A	806	POV	C1-O11-P-O13
4	A	806	POV	C1-O11-P-O14
4	A	806	POV	O22-C21-O21-C2
4	A	807	POV	C1-O11-P-O12
4	A	807	POV	C1-O11-P-O13
4	A	807	POV	C11-O12-P-O11
4	A	807	POV	C11-O12-P-O13
4	A	807	POV	O12-C11-C12-N
4	A	808	POV	C1-O11-P-O12
4	A	808	POV	C1-O11-P-O13
4	A	808	POV	O12-C11-C12-N
4	A	811	POV	C1-O11-P-O12
4	A	811	POV	C1-O11-P-O13
4	A	811	POV	C1-O11-P-O14
4	A	811	POV	C22-C21-O21-C2
4	A	811	POV	O22-C21-O21-C2
4	A	812	POV	C1-O11-P-O12
4	A	812	POV	C1-O11-P-O13
4	A	812	POV	C11-O12-P-O14
4	A	812	POV	O21-C2-C3-O31
4	A	816	POV	C1-O11-P-O12
4	A	816	POV	C1-O11-P-O14
4	B	702	POV	C1-O11-P-O12
4	B	702	POV	C1-O11-P-O14
4	B	706	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
4	B	706	POV	C11-O12-P-O13
4	B	706	POV	O12-C11-C12-N
4	B	706	POV	C22-C21-O21-C2
4	B	706	POV	O22-C21-O21-C2
4	B	707	POV	O12-C11-C12-N
4	B	707	POV	O22-C21-O21-C2
4	B	708	POV	C1-O11-P-O12
4	B	708	POV	C1-O11-P-O13
4	B	708	POV	C1-O11-P-O14
4	B	708	POV	C11-O12-P-O11
4	B	708	POV	O22-C21-O21-C2
4	B	709	POV	C1-O11-P-O12
4	B	709	POV	C1-O11-P-O13
4	B	709	POV	C11-O12-P-O11
4	B	709	POV	C11-O12-P-O13
4	B	709	POV	O12-C11-C12-N
4	B	710	POV	C1-O11-P-O12
4	B	710	POV	C1-O11-P-O13
4	B	710	POV	O12-C11-C12-N
4	B	713	POV	C1-O11-P-O12
4	B	713	POV	C1-O11-P-O13
4	B	713	POV	C1-O11-P-O14
4	B	713	POV	C22-C21-O21-C2
4	B	713	POV	O22-C21-O21-C2
4	B	714	POV	C1-O11-P-O12
4	B	714	POV	C1-O11-P-O13
4	B	714	POV	C1-O11-P-O14
4	B	714	POV	C11-O12-P-O14
4	B	714	POV	O21-C2-C3-O31
4	C	702	POV	C1-O11-P-O12
4	C	702	POV	C1-O11-P-O14
4	C	706	POV	C11-O12-P-O11
4	C	706	POV	C11-O12-P-O13
4	C	706	POV	O12-C11-C12-N
4	C	706	POV	C22-C21-O21-C2
4	C	706	POV	O22-C21-O21-C2
4	C	707	POV	O12-C11-C12-N
4	C	707	POV	O22-C21-O21-C2
4	C	708	POV	C1-O11-P-O12
4	C	708	POV	C1-O11-P-O13
4	C	708	POV	C1-O11-P-O14
4	C	708	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
4	C	709	POV	C1-O11-P-O12
4	C	709	POV	C1-O11-P-O13
4	C	709	POV	C11-O12-P-O11
4	C	709	POV	C11-O12-P-O13
4	C	709	POV	O12-C11-C12-N
4	C	710	POV	C1-O11-P-O12
4	C	710	POV	C1-O11-P-O13
4	C	710	POV	O12-C11-C12-N
4	C	713	POV	C1-O11-P-O12
4	C	713	POV	C1-O11-P-O13
4	C	713	POV	C1-O11-P-O14
4	C	713	POV	C22-C21-O21-C2
4	C	713	POV	O22-C21-O21-C2
4	C	714	POV	C1-O11-P-O12
4	C	714	POV	C1-O11-P-O13
4	C	714	POV	C11-O12-P-O14
4	D	701	POV	C1-O11-P-O12
4	D	701	POV	C1-O11-P-O13
4	D	701	POV	C1-O11-P-O14
4	D	701	POV	C22-C21-O21-C2
4	D	701	POV	O22-C21-O21-C2
4	D	702	POV	C1-O11-P-O12
4	D	702	POV	C1-O11-P-O13
4	D	702	POV	C11-O12-P-O14
4	D	702	POV	O21-C2-C3-O31
4	D	706	POV	C1-O11-P-O12
4	D	706	POV	C1-O11-P-O14
4	D	710	POV	C11-O12-P-O11
4	D	710	POV	C11-O12-P-O13
4	D	710	POV	O12-C11-C12-N
4	D	710	POV	C22-C21-O21-C2
4	D	710	POV	O22-C21-O21-C2
4	D	711	POV	O12-C11-C12-N
4	D	711	POV	O22-C21-O21-C2
4	D	712	POV	C1-O11-P-O12
4	D	712	POV	C1-O11-P-O13
4	D	712	POV	C1-O11-P-O14
4	D	712	POV	O22-C21-O21-C2
4	D	713	POV	C1-O11-P-O12
4	D	713	POV	C1-O11-P-O13
4	D	713	POV	C11-O12-P-O11
4	D	713	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
4	D	713	POV	O12-C11-C12-N
4	D	714	POV	C1-O11-P-O12
4	D	714	POV	C1-O11-P-O13
4	D	714	POV	O12-C11-C12-N
4	A	808	POV	O32-C31-O31-C3
4	B	710	POV	O32-C31-O31-C3
4	C	710	POV	O32-C31-O31-C3
4	D	714	POV	O32-C31-O31-C3
4	A	808	POV	C32-C31-O31-C3
4	B	710	POV	C32-C31-O31-C3
4	C	710	POV	C32-C31-O31-C3
4	D	714	POV	C32-C31-O31-C3
4	A	805	POV	C22-C21-O21-C2
4	A	806	POV	C22-C21-O21-C2
4	B	707	POV	C22-C21-O21-C2
4	B	708	POV	C22-C21-O21-C2
4	C	707	POV	C22-C21-O21-C2
4	C	708	POV	C22-C21-O21-C2
4	D	711	POV	C22-C21-O21-C2
4	D	712	POV	C22-C21-O21-C2
2	B	703	Y01	CAX-CAL-CAM-CAY
4	A	811	POV	C32-C31-O31-C3
4	B	713	POV	C32-C31-O31-C3
4	D	701	POV	C32-C31-O31-C3
4	C	713	POV	C32-C31-O31-C3
4	A	811	POV	O32-C31-O31-C3
4	B	713	POV	O32-C31-O31-C3
4	C	713	POV	O32-C31-O31-C3
4	D	701	POV	O32-C31-O31-C3
4	A	804	POV	C212-C213-C214-C215
4	A	812	POV	C22-C23-C24-C25
4	B	714	POV	C22-C23-C24-C25
4	C	706	POV	C212-C213-C214-C215
4	C	714	POV	C22-C23-C24-C25
4	D	702	POV	C22-C23-C24-C25
4	D	710	POV	C212-C213-C214-C215
4	A	808	POV	C33-C34-C35-C36
4	B	706	POV	C212-C213-C214-C215
4	C	707	POV	C212-C213-C214-C215
4	B	710	POV	C33-C34-C35-C36
4	C	710	POV	C33-C34-C35-C36
4	D	711	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
4	D	714	POV	C33-C34-C35-C36
4	B	709	POV	C32-C31-O31-C3
4	D	713	POV	C32-C31-O31-C3
3	B	715	PCW	C21-C22-C23-C24
4	A	805	POV	C212-C213-C214-C215
2	A	815	Y01	CAX-CAL-CAM-CAY
2	B	701	Y01	CAX-CAL-CAM-CAY
2	C	701	Y01	CAX-CAL-CAM-CAY
2	D	705	Y01	CAX-CAL-CAM-CAY
3	A	813	PCW	C21-C22-C23-C24
3	D	703	PCW	C21-C22-C23-C24
3	C	715	PCW	C21-C22-C23-C24
3	C	715	PCW	C23-C24-C25-C26
4	C	714	POV	O21-C2-C3-O31
4	A	807	POV	C32-C31-O31-C3
4	C	709	POV	C32-C31-O31-C3
3	D	703	PCW	C23-C24-C25-C26
4	A	811	POV	C39-C310-C311-C312
4	B	713	POV	C39-C310-C311-C312
4	C	713	POV	C39-C310-C311-C312
4	D	701	POV	C39-C310-C311-C312
3	A	813	PCW	C23-C24-C25-C26
4	D	710	POV	C22-C23-C24-C25
4	A	804	POV	C21-C22-C23-C24
4	C	706	POV	C22-C23-C24-C25
4	A	804	POV	C22-C23-C24-C25
4	A	811	POV	C22-C23-C24-C25
4	B	706	POV	C22-C23-C24-C25
4	B	713	POV	C22-C23-C24-C25
4	C	713	POV	C22-C23-C24-C25
4	D	701	POV	C22-C23-C24-C25
4	A	812	POV	C31-C32-C33-C34
4	B	709	POV	C21-C22-C23-C24
4	C	706	POV	C21-C22-C23-C24
4	C	709	POV	C21-C22-C23-C24
4	C	714	POV	C31-C32-C33-C34
4	D	702	POV	C31-C32-C33-C34
4	D	710	POV	C21-C22-C23-C24
4	B	709	POV	O32-C31-O31-C3
4	D	713	POV	O32-C31-O31-C3
4	A	807	POV	C21-C22-C23-C24
4	B	706	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	B	707	POV	C21-C22-C23-C24
4	B	714	POV	C31-C32-C33-C34
4	D	713	POV	C21-C22-C23-C24
3	B	715	PCW	C23-C24-C25-C26
4	A	805	POV	C21-C22-C23-C24
4	C	707	POV	C21-C22-C23-C24
4	D	711	POV	C21-C22-C23-C24
4	D	701	POV	C35-C36-C37-C38
4	C	713	POV	C35-C36-C37-C38
4	A	807	POV	O32-C31-O31-C3
2	A	802	Y01	CAX-CAL-CAM-CAY
2	B	704	Y01	CAX-CAL-CAM-CAY
2	C	704	Y01	CAX-CAL-CAM-CAY
2	D	708	Y01	CAX-CAL-CAM-CAY
4	A	811	POV	C35-C36-C37-C38
4	B	708	POV	C25-C26-C27-C28
4	C	709	POV	O32-C31-O31-C3
4	B	713	POV	C35-C36-C37-C38
4	D	712	POV	C25-C26-C27-C28
4	A	806	POV	C25-C26-C27-C28
4	A	816	POV	C310-C311-C312-C313
4	B	702	POV	C310-C311-C312-C313
4	C	702	POV	C310-C311-C312-C313
4	C	708	POV	C25-C26-C27-C28
4	D	706	POV	C310-C311-C312-C313
2	A	815	Y01	CAO-CAJ-CAN-CBA
2	A	815	Y01	CAN-CAJ-CAO-CBB
2	B	701	Y01	CAO-CAJ-CAN-CBA
2	B	701	Y01	CAN-CAJ-CAO-CBB
2	C	701	Y01	CAO-CAJ-CAN-CBA
2	C	701	Y01	CAN-CAJ-CAO-CBB
2	D	705	Y01	CAO-CAJ-CAN-CBA
2	D	705	Y01	CAN-CAJ-CAO-CBB
4	B	702	POV	C21-C22-C23-C24
4	C	702	POV	C21-C22-C23-C24
4	D	706	POV	C21-C22-C23-C24
4	B	707	POV	C212-C213-C214-C215
4	A	816	POV	C21-C22-C23-C24
4	B	713	POV	C212-C213-C214-C215
4	C	713	POV	C212-C213-C214-C215
4	A	808	POV	C212-C213-C214-C215
4	C	710	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
4	A	806	POV	C34-C35-C36-C37
4	B	708	POV	C34-C35-C36-C37
4	C	708	POV	C34-C35-C36-C37
4	D	712	POV	C34-C35-C36-C37
4	D	714	POV	C212-C213-C214-C215
4	B	710	POV	C34-C35-C36-C37
4	A	808	POV	C34-C35-C36-C37
4	B	707	POV	C214-C215-C216-C217
4	B	710	POV	C212-C213-C214-C215
4	C	710	POV	C34-C35-C36-C37
4	D	714	POV	C34-C35-C36-C37
4	A	807	POV	C310-C311-C312-C313
4	B	709	POV	C39-C310-C311-C312
4	A	804	POV	C34-C35-C36-C37
4	A	811	POV	C212-C213-C214-C215
4	B	709	POV	C310-C311-C312-C313
4	C	706	POV	C34-C35-C36-C37
4	D	701	POV	C212-C213-C214-C215
4	D	710	POV	C34-C35-C36-C37
4	D	713	POV	C310-C311-C312-C313
4	B	713	POV	C213-C214-C215-C216
4	C	709	POV	C39-C310-C311-C312
4	C	709	POV	C310-C311-C312-C313
4	D	713	POV	C39-C310-C311-C312
4	A	807	POV	C39-C310-C311-C312
4	B	708	POV	C311-C312-C313-C314
4	C	713	POV	C213-C214-C215-C216
4	A	804	POV	C211-C212-C213-C214
4	A	806	POV	C311-C312-C313-C314
4	A	804	POV	C1-C2-C3-O31
4	B	706	POV	C1-C2-C3-O31
4	C	706	POV	C1-C2-C3-O31
4	D	710	POV	C1-C2-C3-O31
4	A	811	POV	C213-C214-C215-C216
4	C	706	POV	C211-C212-C213-C214
4	A	806	POV	C22-C23-C24-C25
4	B	706	POV	C211-C212-C213-C214
4	B	714	POV	C32-C33-C34-C35
4	C	708	POV	C22-C23-C24-C25
4	D	701	POV	C213-C214-C215-C216
4	D	702	POV	C32-C33-C34-C35
4	D	710	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
4	D	712	POV	C22-C23-C24-C25
4	B	706	POV	C34-C35-C36-C37
4	C	708	POV	C311-C312-C313-C314
4	A	812	POV	C32-C33-C34-C35
4	B	710	POV	C36-C37-C38-C39
4	C	714	POV	C32-C33-C34-C35
4	C	714	POV	C36-C37-C38-C39
4	D	702	POV	C36-C37-C38-C39
4	D	712	POV	C311-C312-C313-C314
4	A	808	POV	C36-C37-C38-C39
4	A	812	POV	C36-C37-C38-C39
4	B	708	POV	C22-C23-C24-C25
4	B	714	POV	C310-C311-C312-C313
4	B	714	POV	C36-C37-C38-C39
4	B	714	POV	C37-C38-C39-C310
4	C	710	POV	C36-C37-C38-C39
4	C	714	POV	C310-C311-C312-C313
4	C	714	POV	C37-C38-C39-C310
4	D	702	POV	C37-C38-C39-C310
3	B	715	PCW	C22-C23-C24-C25
4	A	812	POV	C37-C38-C39-C310
4	B	710	POV	C311-C312-C313-C314
4	D	714	POV	C36-C37-C38-C39
3	A	813	PCW	C20-C21-C22-C23
3	D	703	PCW	C20-C21-C22-C23
4	A	812	POV	C310-C311-C312-C313
4	D	702	POV	C310-C311-C312-C313
4	D	712	POV	C37-C38-C39-C310
4	D	714	POV	C311-C312-C313-C314
4	A	806	POV	C37-C38-C39-C310
4	A	808	POV	C311-C312-C313-C314
4	B	707	POV	C22-C23-C24-C25
4	C	708	POV	C37-C38-C39-C310
3	A	813	PCW	C22-C23-C24-C25
4	A	805	POV	C22-C23-C24-C25
4	A	807	POV	C213-C214-C215-C216
4	A	807	POV	C214-C215-C216-C217
4	A	808	POV	C39-C310-C311-C312
4	B	708	POV	C37-C38-C39-C310
4	B	709	POV	C213-C214-C215-C216
4	B	709	POV	C214-C215-C216-C217
4	B	710	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
4	C	707	POV	C22-C23-C24-C25
4	C	709	POV	C213-C214-C215-C216
4	C	709	POV	C214-C215-C216-C217
4	C	710	POV	C39-C310-C311-C312
4	C	710	POV	C311-C312-C313-C314
4	D	711	POV	C22-C23-C24-C25
4	D	713	POV	C213-C214-C215-C216
4	D	713	POV	C214-C215-C216-C217
4	D	714	POV	C39-C310-C311-C312
3	A	809	PCW	C21-C22-C23-C24
3	B	711	PCW	C21-C22-C23-C24
3	C	711	PCW	C21-C22-C23-C24
3	D	715	PCW	C21-C22-C23-C24
2	B	704	Y01	CAO-CAJ-CAN-CBA
2	C	704	Y01	CAO-CAJ-CAN-CBA
2	D	708	Y01	CAO-CAJ-CAN-CBA
3	D	703	PCW	C22-C23-C24-C25
4	A	805	POV	C34-C35-C36-C37
4	B	706	POV	C312-C313-C314-C315
3	C	715	PCW	C22-C23-C24-C25
4	A	805	POV	C312-C313-C314-C315
4	A	808	POV	C24-C25-C26-C27
4	B	707	POV	C34-C35-C36-C37
4	C	707	POV	C34-C35-C36-C37
4	C	710	POV	C24-C25-C26-C27
4	D	711	POV	C312-C313-C314-C315
4	D	711	POV	C34-C35-C36-C37
4	D	714	POV	C24-C25-C26-C27
4	B	706	POV	C32-C31-O31-C3
4	C	706	POV	C32-C31-O31-C3
4	A	807	POV	C212-C213-C214-C215
4	A	812	POV	C23-C24-C25-C26
4	B	709	POV	C212-C213-C214-C215
4	C	709	POV	C212-C213-C214-C215
4	C	713	POV	C37-C38-C39-C310
4	C	714	POV	C23-C24-C25-C26
4	D	701	POV	C37-C38-C39-C310
4	D	713	POV	C212-C213-C214-C215
4	D	714	POV	C35-C36-C37-C38
3	B	715	PCW	C20-C21-C22-C23
3	C	715	PCW	C20-C21-C22-C23
4	B	706	POV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
4	C	706	POV	C26-C27-C28-C29
4	D	710	POV	C26-C27-C28-C29
4	A	808	POV	C35-C36-C37-C38
4	A	811	POV	C37-C38-C39-C310
4	C	710	POV	C35-C36-C37-C38
4	D	702	POV	C23-C24-C25-C26
2	A	802	Y01	CAO-CAJ-CAN-CBA
4	B	708	POV	C32-C33-C34-C35
4	C	707	POV	C312-C313-C314-C315
4	A	804	POV	C31-C32-C33-C34
4	C	706	POV	C31-C32-C33-C34
4	D	710	POV	C31-C32-C33-C34
3	B	705	PCW	C22-C23-C24-C25
4	B	713	POV	C37-C38-C39-C310
4	B	714	POV	C23-C24-C25-C26
3	C	705	PCW	C22-C23-C24-C25
4	B	710	POV	C24-C25-C26-C27
4	B	710	POV	C35-C36-C37-C38
4	A	806	POV	C312-C313-C314-C315
4	B	707	POV	C312-C313-C314-C315
3	A	803	PCW	C22-C23-C24-C25
3	D	709	PCW	C22-C23-C24-C25
4	B	710	POV	C25-C26-C27-C28
4	A	804	POV	C32-C31-O31-C3
4	D	710	POV	C32-C31-O31-C3
4	A	808	POV	O11-C1-C2-O21
4	A	812	POV	O11-C1-C2-O21
4	B	710	POV	O11-C1-C2-O21
4	C	710	POV	O11-C1-C2-O21
4	C	714	POV	O11-C1-C2-O21
4	D	702	POV	O11-C1-C2-O21
4	D	714	POV	O11-C1-C2-O21
4	A	811	POV	C34-C35-C36-C37
4	B	708	POV	C39-C310-C311-C312
4	B	708	POV	C312-C313-C314-C315
4	C	713	POV	C34-C35-C36-C37
4	D	701	POV	C34-C35-C36-C37
4	B	713	POV	C34-C35-C36-C37
4	D	712	POV	C32-C33-C34-C35
4	A	805	POV	C214-C215-C216-C217
4	C	708	POV	C32-C33-C34-C35
4	D	714	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
4	A	804	POV	C26-C27-C28-C29
4	A	808	POV	C26-C27-C28-C29
4	B	710	POV	C26-C27-C28-C29
4	C	710	POV	C26-C27-C28-C29
4	D	714	POV	C26-C27-C28-C29
3	A	809	PCW	C22-C23-C24-C25
3	B	711	PCW	C22-C23-C24-C25
3	C	711	PCW	C22-C23-C24-C25
3	D	715	PCW	C22-C23-C24-C25
4	A	806	POV	C32-C33-C34-C35
4	C	710	POV	C25-C26-C27-C28
4	A	804	POV	C32-C33-C34-C35
4	A	806	POV	C39-C310-C311-C312
4	A	808	POV	C25-C26-C27-C28
4	C	706	POV	C312-C313-C314-C315
4	D	710	POV	C312-C313-C314-C315
3	B	705	PCW	C23-C24-C25-C26
4	C	702	POV	C211-C212-C213-C214
4	B	702	POV	C211-C212-C213-C214
4	C	708	POV	C312-C313-C314-C315
4	D	712	POV	C312-C313-C314-C315
4	A	804	POV	C312-C313-C314-C315
4	C	706	POV	C32-C33-C34-C35
3	D	709	PCW	C23-C24-C25-C26
3	C	705	PCW	C23-C24-C25-C26
4	B	706	POV	C32-C33-C34-C35
4	D	710	POV	C32-C33-C34-C35
4	A	816	POV	C211-C212-C213-C214
4	C	707	POV	C214-C215-C216-C217
4	D	706	POV	C211-C212-C213-C214
4	B	708	POV	C313-C314-C315-C316
2	A	802	Y01	CAM-CAY-OAW-CBC
2	D	708	Y01	CAM-CAY-OAW-CBC
4	A	806	POV	C313-C314-C315-C316
4	C	708	POV	C313-C314-C315-C316
4	A	811	POV	C311-C310-C39-C38
4	B	713	POV	C311-C312-C313-C314
4	C	713	POV	C311-C310-C39-C38
4	C	713	POV	C311-C312-C313-C314
4	D	701	POV	C311-C312-C313-C314
4	B	713	POV	C311-C310-C39-C38
4	D	701	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
3	A	813	PCW	C15-C16-C17-C18
3	C	715	PCW	C15-C16-C17-C18
4	A	811	POV	C311-C312-C313-C314
4	D	711	POV	C214-C215-C216-C217
3	D	703	PCW	C15-C16-C17-C18
4	B	713	POV	C25-C26-C27-C28
3	B	715	PCW	C15-C16-C17-C18
4	A	805	POV	C210-C211-C212-C213
4	A	806	POV	C26-C27-C28-C29
4	B	707	POV	C26-C27-C28-C29
4	C	707	POV	C210-C211-C212-C213
4	D	711	POV	C210-C211-C212-C213
4	D	712	POV	C26-C27-C28-C29
4	C	708	POV	C39-C310-C311-C312
4	D	701	POV	C25-C26-C27-C28
4	A	806	POV	O11-C1-C2-C3
4	A	808	POV	O11-C1-C2-C3
4	B	708	POV	O11-C1-C2-C3
4	C	708	POV	O11-C1-C2-C3
4	D	702	POV	O11-C1-C2-C3
4	D	712	POV	O11-C1-C2-C3
4	D	713	POV	O11-C1-C2-C3
3	A	803	PCW	C23-C24-C25-C26
4	C	713	POV	C25-C26-C27-C28
4	D	712	POV	C313-C314-C315-C316
4	A	811	POV	C25-C26-C27-C28
4	B	706	POV	O32-C31-O31-C3
4	B	706	POV	C31-C32-C33-C34
4	B	708	POV	C31-C32-C33-C34
3	C	705	PCW	C21-C22-C23-C24
4	C	706	POV	O32-C31-O31-C3
2	C	704	Y01	CAM-CAY-OAW-CBC
4	D	712	POV	C39-C310-C311-C312
4	A	804	POV	O32-C31-O31-C3
4	B	709	POV	C1-C2-C3-O31
4	C	714	POV	C1-C2-C3-O31
3	D	709	PCW	C21-C22-C23-C24
4	D	711	POV	C211-C212-C213-C214
4	D	710	POV	O32-C31-O31-C3
4	B	707	POV	C210-C211-C212-C213
4	B	708	POV	C26-C27-C28-C29
3	A	803	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	A	805	POV	C32-C31-O31-C3
4	B	707	POV	C32-C31-O31-C3
3	B	705	PCW	C21-C22-C23-C24
4	B	709	POV	C311-C310-C39-C38
4	A	806	POV	C31-C32-C33-C34
4	C	708	POV	C31-C32-C33-C34
4	D	712	POV	C31-C32-C33-C34
2	B	704	Y01	CAM-CAY-OAW-CBC
4	D	711	POV	C32-C31-O31-C3
4	B	710	POV	C213-C214-C215-C216
4	C	707	POV	C211-C212-C213-C214
4	D	714	POV	C213-C214-C215-C216
4	C	710	POV	C213-C214-C215-C216
4	A	805	POV	C211-C212-C213-C214
4	A	805	POV	C23-C24-C25-C26
4	A	808	POV	C213-C214-C215-C216
4	D	701	POV	C312-C313-C314-C315
4	C	707	POV	C32-C31-O31-C3
4	C	710	POV	C32-C33-C34-C35
4	C	713	POV	C312-C313-C314-C315
4	A	812	POV	C26-C27-C28-C29
4	B	714	POV	C26-C27-C28-C29
4	C	708	POV	C26-C27-C28-C29
4	C	714	POV	C26-C27-C28-C29
4	D	714	POV	C32-C33-C34-C35
4	A	808	POV	C32-C33-C34-C35
4	A	804	POV	C36-C37-C38-C39
4	D	711	POV	C23-C24-C25-C26
4	A	807	POV	O11-C1-C2-O21
4	B	709	POV	O11-C1-C2-O21
4	B	714	POV	O11-C1-C2-O21
4	C	709	POV	O11-C1-C2-O21
4	D	713	POV	O11-C1-C2-O21
4	B	709	POV	C24-C25-C26-C27
4	C	706	POV	C36-C37-C38-C39
4	C	707	POV	C23-C24-C25-C26
4	A	805	POV	C36-C37-C38-C39
4	D	711	POV	C36-C37-C38-C39
4	D	713	POV	C311-C310-C39-C38
4	A	811	POV	C312-C313-C314-C315
4	D	710	POV	C36-C37-C38-C39
4	B	710	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	C	707	POV	C36-C37-C38-C39
4	C	709	POV	C311-C310-C39-C38
3	A	813	PCW	C24-C25-C26-C27
3	B	715	PCW	C24-C25-C26-C27
3	D	703	PCW	C24-C25-C26-C27
4	B	707	POV	C36-C37-C38-C39
4	A	807	POV	C311-C310-C39-C38
4	D	706	POV	C212-C213-C214-C215
3	A	803	PCW	C15-C16-C17-C18
3	B	705	PCW	C15-C16-C17-C18
4	B	713	POV	C312-C313-C314-C315
4	A	816	POV	C212-C213-C214-C215
4	A	816	POV	C22-C23-C24-C25
4	B	708	POV	C212-C213-C214-C215
4	D	706	POV	C22-C23-C24-C25
4	B	702	POV	C22-C23-C24-C25
3	A	814	PCW	C12-C13-C14-C15
3	B	716	PCW	C12-C13-C14-C15
3	C	716	PCW	C12-C13-C14-C15
3	D	704	PCW	C12-C13-C14-C15
4	A	805	POV	C26-C27-C28-C29
4	C	707	POV	C26-C27-C28-C29
4	D	702	POV	C26-C27-C28-C29
4	D	711	POV	C26-C27-C28-C29
3	C	715	PCW	C24-C25-C26-C27
3	D	709	PCW	C15-C16-C17-C18
3	C	705	PCW	C15-C16-C17-C18
4	C	702	POV	C22-C23-C24-C25
4	D	702	POV	C24-C25-C26-C27
4	A	812	POV	C24-C25-C26-C27
4	C	702	POV	C212-C213-C214-C215
4	C	714	POV	C24-C25-C26-C27
4	D	712	POV	C212-C213-C214-C215
4	B	706	POV	C36-C37-C38-C39
4	B	714	POV	C24-C25-C26-C27
4	B	707	POV	C23-C24-C25-C26
4	A	806	POV	C212-C213-C214-C215
2	A	815	Y01	CAJ-CAO-CBB-CAC
2	B	701	Y01	CAJ-CAO-CBB-CAC
2	D	705	Y01	CAJ-CAO-CBB-CAC
4	B	702	POV	C212-C213-C214-C215
4	C	708	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
3	C	705	PCW	C24-C25-C26-C27
3	D	709	PCW	C24-C25-C26-C27
4	A	807	POV	O11-C1-C2-C3
4	A	812	POV	O11-C1-C2-C3
4	B	710	POV	O11-C1-C2-C3
4	B	714	POV	O11-C1-C2-C3
4	C	709	POV	O11-C1-C2-C3
4	C	710	POV	O11-C1-C2-C3
4	C	714	POV	O11-C1-C2-C3
4	D	714	POV	O11-C1-C2-C3
4	B	702	POV	C25-C26-C27-C28
3	A	803	PCW	C24-C25-C26-C27
3	B	705	PCW	C24-C25-C26-C27
4	A	811	POV	C313-C314-C315-C316
4	B	713	POV	C313-C314-C315-C316
2	C	701	Y01	CAJ-CAO-CBB-CAC
3	A	809	PCW	C14-C15-C16-C17
3	B	711	PCW	C14-C15-C16-C17
3	C	711	PCW	C14-C15-C16-C17
3	D	715	PCW	C14-C15-C16-C17
4	A	807	POV	C313-C314-C315-C316
4	C	709	POV	C313-C314-C315-C316
4	D	713	POV	C313-C314-C315-C316
4	C	713	POV	C313-C314-C315-C316
4	A	816	POV	C25-C26-C27-C28
4	B	707	POV	O32-C31-O31-C3
4	C	707	POV	O32-C31-O31-C3
4	D	706	POV	C25-C26-C27-C28
4	B	709	POV	C313-C314-C315-C316
4	D	701	POV	C313-C314-C315-C316
4	A	804	POV	C25-C26-C27-C28
4	D	710	POV	C25-C26-C27-C28
4	A	805	POV	O32-C31-O31-C3
4	D	711	POV	O32-C31-O31-C3
4	B	710	POV	C311-C310-C39-C38
3	A	814	PCW	C14-C15-C16-C17
3	B	716	PCW	C14-C15-C16-C17
3	C	716	PCW	C14-C15-C16-C17
3	D	704	PCW	C14-C15-C16-C17
4	A	804	POV	C213-C214-C215-C216
4	C	702	POV	C25-C26-C27-C28
4	D	713	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
4	B	714	POV	C311-C312-C313-C314
4	C	706	POV	C213-C214-C215-C216
4	D	702	POV	C311-C312-C313-C314
4	A	812	POV	C1-C2-C3-O31
4	B	714	POV	C1-C2-C3-O31
4	D	702	POV	C1-C2-C3-O31
4	A	812	POV	C311-C312-C313-C314
4	C	714	POV	C311-C312-C313-C314
4	A	808	POV	C215-C216-C217-C218
4	C	710	POV	C215-C216-C217-C218
4	B	710	POV	C215-C216-C217-C218
4	D	714	POV	C215-C216-C217-C218
4	C	714	POV	C214-C215-C216-C217
4	B	710	POV	C21-C22-C23-C24
4	A	812	POV	C312-C313-C314-C315
4	B	714	POV	C312-C313-C314-C315
4	A	808	POV	C311-C310-C39-C38
4	A	812	POV	C214-C215-C216-C217
4	D	702	POV	C312-C313-C314-C315
2	A	802	Y01	OAG-CAY-OAW-CBC
2	C	704	Y01	OAG-CAY-OAW-CBC
2	D	708	Y01	OAG-CAY-OAW-CBC
4	B	710	POV	C31-C32-C33-C34
4	A	806	POV	O11-C1-C2-O21
4	B	708	POV	O11-C1-C2-O21
4	C	708	POV	O11-C1-C2-O21
4	D	712	POV	O11-C1-C2-O21
4	C	710	POV	C311-C310-C39-C38
4	D	710	POV	C213-C214-C215-C216
4	D	714	POV	C311-C310-C39-C38
4	D	702	POV	C214-C215-C216-C217
4	A	811	POV	C2-C1-O11-P
4	B	713	POV	C2-C1-O11-P
4	C	713	POV	C2-C1-O11-P
4	D	701	POV	C2-C1-O11-P
4	C	714	POV	C312-C313-C314-C315
4	C	714	POV	C34-C35-C36-C37
4	D	702	POV	C34-C35-C36-C37
4	A	807	POV	O21-C2-C3-O31
4	B	709	POV	O21-C2-C3-O31
4	C	709	POV	O21-C2-C3-O31
4	D	713	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
4	C	702	POV	C36-C37-C38-C39
4	C	709	POV	C312-C313-C314-C315
2	B	704	Y01	OAG-CAY-OAW-CBC
4	A	808	POV	C31-C32-C33-C34
4	C	710	POV	C31-C32-C33-C34
4	D	713	POV	C31-C32-C33-C34
4	D	714	POV	C31-C32-C33-C34
4	A	816	POV	C36-C37-C38-C39
4	A	812	POV	C34-C35-C36-C37
4	B	702	POV	C36-C37-C38-C39
4	B	714	POV	C214-C215-C216-C217
4	A	807	POV	C312-C313-C314-C315
4	B	714	POV	C34-C35-C36-C37
4	D	706	POV	C36-C37-C38-C39
4	B	706	POV	C213-C214-C215-C216
4	D	713	POV	C37-C38-C39-C310
4	B	706	POV	C215-C216-C217-C218
4	B	710	POV	C22-C23-C24-C25
3	A	813	PCW	C14-C15-C16-C17
3	B	715	PCW	C14-C15-C16-C17
4	C	706	POV	C25-C26-C27-C28
4	A	805	POV	C11-C12-N-C14
4	C	707	POV	C11-C12-N-C14
3	C	715	PCW	C14-C15-C16-C17
3	D	703	PCW	C14-C15-C16-C17
4	C	706	POV	C215-C216-C217-C218
4	A	807	POV	C24-C25-C26-C27
4	D	706	POV	C213-C214-C215-C216
4	A	804	POV	C215-C216-C217-C218
4	D	710	POV	C215-C216-C217-C218
4	A	807	POV	C31-C32-C33-C34
4	A	816	POV	C213-C214-C215-C216
4	C	709	POV	C37-C38-C39-C310
4	A	812	POV	C311-C310-C39-C38
4	C	702	POV	C213-C214-C215-C216
4	C	709	POV	C24-C25-C26-C27
4	C	714	POV	C311-C310-C39-C38
4	B	710	POV	C313-C314-C315-C316
4	C	709	POV	C31-C32-C33-C34
4	B	709	POV	C312-C313-C314-C315
4	D	713	POV	C24-C25-C26-C27
4	B	709	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	814	PCW	C16-C17-C18-C19
3	B	716	PCW	C16-C17-C18-C19
3	C	716	PCW	C16-C17-C18-C19
3	D	704	PCW	C16-C17-C18-C19
4	B	702	POV	C33-C34-C35-C36
4	D	702	POV	C311-C310-C39-C38
4	B	702	POV	C213-C214-C215-C216
4	B	714	POV	C311-C310-C39-C38
4	A	816	POV	C33-C34-C35-C36
4	D	706	POV	C33-C34-C35-C36
4	C	702	POV	C33-C34-C35-C36
4	A	807	POV	C37-C38-C39-C310
4	A	808	POV	C313-C314-C315-C316
4	B	706	POV	C210-C211-C212-C213
4	C	706	POV	C210-C211-C212-C213
4	D	710	POV	C210-C211-C212-C213
4	B	709	POV	C37-C38-C39-C310
4	A	804	POV	O11-C1-C2-O21
4	B	706	POV	O11-C1-C2-O21
4	C	706	POV	O11-C1-C2-O21
4	C	710	POV	C313-C314-C315-C316
4	A	805	POV	C1-C2-C3-O31
4	C	707	POV	C1-C2-C3-O31
4	D	711	POV	C1-C2-C3-O31
4	D	713	POV	C1-C2-C3-O31
4	D	714	POV	C313-C314-C315-C316
4	A	804	POV	C12-C11-O12-P
4	B	706	POV	C12-C11-O12-P
4	C	706	POV	C12-C11-O12-P
4	C	713	POV	C12-C11-O12-P
4	D	710	POV	C12-C11-O12-P
4	A	804	POV	C210-C211-C212-C213
4	D	711	POV	C11-C12-N-C14
4	A	816	POV	C37-C38-C39-C310
4	C	702	POV	C37-C38-C39-C310
4	A	811	POV	O12-C11-C12-N
4	A	812	POV	O12-C11-C12-N
4	A	816	POV	O12-C11-C12-N
4	B	702	POV	O12-C11-C12-N
4	B	713	POV	O12-C11-C12-N
4	B	714	POV	O12-C11-C12-N
4	C	702	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
4	C	713	POV	O12-C11-C12-N
4	C	714	POV	O12-C11-C12-N
4	D	701	POV	O12-C11-C12-N
4	D	702	POV	O12-C11-C12-N
4	D	706	POV	O12-C11-C12-N
4	D	706	POV	C37-C38-C39-C310
4	A	806	POV	C311-C310-C39-C38
4	D	712	POV	C311-C310-C39-C38
4	C	708	POV	C311-C310-C39-C38
4	B	707	POV	C11-C12-N-C14
4	B	702	POV	C37-C38-C39-C310
4	B	708	POV	C311-C310-C39-C38
4	B	713	POV	C24-C25-C26-C27
2	C	703	Y01	CAO-CAJ-CAN-CBA
4	D	714	POV	C21-C22-C23-C24
2	A	815	Y01	OAG-CAY-OAW-CBC
2	D	705	Y01	OAG-CAY-OAW-CBC
4	C	714	POV	C212-C213-C214-C215
2	D	707	Y01	CAO-CAJ-CAN-CBA
4	B	714	POV	C212-C213-C214-C215
4	A	812	POV	C35-C36-C37-C38
4	B	708	POV	C35-C36-C37-C38
2	A	801	Y01	CAO-CAJ-CAN-CBA
4	D	701	POV	C24-C25-C26-C27
4	D	702	POV	C35-C36-C37-C38
4	A	812	POV	C212-C213-C214-C215
4	C	714	POV	C35-C36-C37-C38
2	B	701	Y01	OAG-CAY-OAW-CBC
2	C	701	Y01	OAG-CAY-OAW-CBC
4	D	710	POV	O11-C1-C2-O21
4	C	713	POV	C24-C25-C26-C27
4	B	709	POV	C31-C32-C33-C34
3	A	810	PCW	C12-C13-C14-C15
3	D	716	PCW	C12-C13-C14-C15
2	B	703	Y01	CAO-CAJ-CAN-CBA
4	B	714	POV	C35-C36-C37-C38
4	A	805	POV	C11-C12-N-C13
4	C	707	POV	C11-C12-N-C13
3	A	814	PCW	C15-C16-C17-C18
3	B	716	PCW	C15-C16-C17-C18
3	C	716	PCW	C15-C16-C17-C18
3	D	704	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	D	702	POV	C212-C213-C214-C215
4	A	811	POV	C24-C25-C26-C27
4	C	710	POV	C21-C22-C23-C24
3	B	712	PCW	C12-C13-C14-C15
4	A	804	POV	O21-C2-C3-O31
4	A	805	POV	O21-C2-C3-O31
4	B	706	POV	O21-C2-C3-O31
4	C	706	POV	O21-C2-C3-O31
4	D	710	POV	O21-C2-C3-O31
3	C	712	PCW	C12-C13-C14-C15
4	A	807	POV	C1-C2-C3-O31
4	B	707	POV	C1-C2-C3-O31
4	C	709	POV	C1-C2-C3-O31
4	A	808	POV	C37-C38-C39-C310
4	C	708	POV	C35-C36-C37-C38
4	C	710	POV	C37-C38-C39-C310
4	D	712	POV	C35-C36-C37-C38
4	A	804	POV	C1-O11-P-O12
4	A	804	POV	C1-O11-P-O13
4	A	804	POV	C1-O11-P-O14
4	A	805	POV	C11-C12-N-C15
4	A	805	POV	C1-O11-P-O14
4	A	806	POV	C11-O12-P-O11
4	A	807	POV	C1-O11-P-O14
4	A	808	POV	C1-O11-P-O14
4	A	816	POV	C11-C12-N-C13
4	A	816	POV	C1-O11-P-O13
4	B	702	POV	C11-C12-N-C13
4	B	702	POV	C1-O11-P-O13
4	B	706	POV	C1-O11-P-O12
4	B	706	POV	C1-O11-P-O14
4	B	707	POV	C1-O11-P-O14
4	B	708	POV	C11-O12-P-O13
4	B	709	POV	C1-O11-P-O14
4	C	702	POV	C1-O11-P-O13
4	C	706	POV	C1-O11-P-O12
4	C	706	POV	C1-O11-P-O13
4	C	706	POV	C1-O11-P-O14
4	C	707	POV	C1-O11-P-O14
4	C	708	POV	C11-O12-P-O11
4	C	709	POV	C1-O11-P-O14
4	D	706	POV	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
4	D	706	POV	C1-O11-P-O13
4	D	710	POV	C1-O11-P-O12
4	D	710	POV	C1-O11-P-O14
4	D	711	POV	C1-O11-P-O14
4	D	712	POV	C11-O12-P-O11
4	D	713	POV	C1-O11-P-O14
4	D	714	POV	C37-C38-C39-C310
4	A	806	POV	C35-C36-C37-C38
4	A	806	POV	C2-C1-O11-P
4	B	706	POV	C2-C1-O11-P
4	C	706	POV	C2-C1-O11-P
4	C	708	POV	C2-C1-O11-P
4	D	710	POV	C2-C1-O11-P
4	D	712	POV	C2-C1-O11-P
4	D	714	POV	C22-C23-C24-C25
4	A	808	POV	C21-C22-C23-C24
4	A	811	POV	C21-C22-C23-C24
4	B	710	POV	C37-C38-C39-C310
4	C	713	POV	C21-C22-C23-C24
4	B	713	POV	C21-C22-C23-C24
4	D	701	POV	C21-C22-C23-C24
4	B	707	POV	C11-C12-N-C13
4	C	702	POV	C11-C12-N-C13
4	C	707	POV	C11-C12-N-C15
4	D	711	POV	C11-C12-N-C13
4	C	706	POV	O11-C1-C2-C3
4	D	702	POV	C29-C210-C211-C212
4	B	707	POV	C313-C314-C315-C316
4	C	710	POV	C22-C23-C24-C25
4	A	804	POV	C2-C1-O11-P
4	B	708	POV	C2-C1-O11-P
4	C	707	POV	O21-C2-C3-O31
4	D	711	POV	O21-C2-C3-O31
4	B	708	POV	C21-C22-C23-C24
3	A	809	PCW	C15-C16-C17-C18
3	B	711	PCW	C15-C16-C17-C18
3	C	711	PCW	C15-C16-C17-C18
3	D	715	PCW	C15-C16-C17-C18
4	A	816	POV	C11-C12-N-C15
4	D	706	POV	C11-C12-N-C15
4	B	706	POV	C25-C26-C27-C28
3	C	705	PCW	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
4	A	812	POV	C29-C210-C211-C212
4	B	714	POV	C29-C210-C211-C212
4	C	714	POV	C29-C210-C211-C212
4	B	702	POV	C11-C12-N-C15
4	D	711	POV	C11-C12-N-C15
4	B	702	POV	C215-C216-C217-C218
4	A	811	POV	C23-C24-C25-C26
4	A	807	POV	C2-C1-O11-P
4	C	709	POV	C2-C1-O11-P
4	C	713	POV	C23-C24-C25-C26
4	B	713	POV	C23-C24-C25-C26
4	B	708	POV	C27-C28-C29-C210
4	A	804	POV	O11-C1-C2-C3
4	D	710	POV	O11-C1-C2-C3
4	D	701	POV	C23-C24-C25-C26
4	A	816	POV	C215-C216-C217-C218
4	D	706	POV	C215-C216-C217-C218
4	C	702	POV	C11-C12-N-C15
4	C	702	POV	C215-C216-C217-C218
3	A	803	PCW	C19-C20-C21-C22
3	B	705	PCW	C19-C20-C21-C22
4	A	808	POV	C22-C23-C24-C25
4	D	713	POV	C2-C1-O11-P
4	B	707	POV	C11-C12-N-C15
4	D	706	POV	C11-C12-N-C14
3	D	709	PCW	C19-C20-C21-C22
4	A	816	POV	C32-C33-C34-C35
4	D	706	POV	C32-C33-C34-C35
4	B	707	POV	C211-C212-C213-C214
4	C	707	POV	C313-C314-C315-C316
4	C	702	POV	C32-C33-C34-C35
4	A	816	POV	C11-C12-N-C14
4	B	702	POV	C11-C12-N-C14
4	C	702	POV	C11-C12-N-C14
4	B	702	POV	C32-C33-C34-C35
4	D	711	POV	C31-C32-C33-C34
4	B	710	POV	C23-C24-C25-C26
4	C	709	POV	C35-C36-C37-C38
4	B	708	POV	C33-C34-C35-C36
2	B	701	Y01	CAM-CAY-OAW-CBC
4	C	707	POV	C31-C32-C33-C34
4	A	805	POV	C313-C314-C315-C316

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Mol	Chain	Res	Type	Atoms
4	B	706	POV	O11-C1-C2-C3
4	A	805	POV	C31-C32-C33-C34
4	A	806	POV	C27-C28-C29-C210
4	C	708	POV	C27-C28-C29-C210
4	D	712	POV	C27-C28-C29-C210
4	A	807	POV	C35-C36-C37-C38
4	B	707	POV	C32-C33-C34-C35
4	A	807	POV	C11-C12-N-C14
4	B	709	POV	C11-C12-N-C14
4	C	709	POV	C11-C12-N-C14
4	D	713	POV	C11-C12-N-C14
4	D	713	POV	C11-C12-N-C15
4	D	711	POV	C313-C314-C315-C316
4	B	714	POV	C213-C214-C215-C216
4	B	707	POV	C31-C32-C33-C34
4	D	702	POV	C213-C214-C215-C216
4	A	812	POV	C213-C214-C215-C216
4	C	714	POV	C213-C214-C215-C216
4	C	708	POV	C33-C34-C35-C36
4	D	701	POV	C214-C215-C216-C217
4	D	712	POV	C33-C34-C35-C36
4	B	709	POV	C2-C1-O11-P
4	C	708	POV	C211-C212-C213-C214
4	A	806	POV	C33-C34-C35-C36
4	A	807	POV	C11-C12-N-C15
4	B	709	POV	C11-C12-N-C15
4	C	709	POV	C11-C12-N-C15
2	C	701	Y01	CAM-CAY-OAW-CBC
4	C	708	POV	C21-C22-C23-C24
4	B	708	POV	C24-C25-C26-C27
2	A	815	Y01	CAM-CAY-OAW-CBC
4	D	712	POV	C21-C22-C23-C24
4	A	807	POV	C11-C12-N-C13
4	B	709	POV	C11-C12-N-C13
4	C	709	POV	C11-C12-N-C13
4	D	713	POV	C11-C12-N-C13
4	A	805	POV	C39-C310-C311-C312
4	D	712	POV	C24-C25-C26-C27
4	C	708	POV	C24-C25-C26-C27
4	B	707	POV	O21-C2-C3-O31
4	C	706	POV	C27-C28-C29-C210
4	D	714	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
4	A	806	POV	C24-C25-C26-C27
4	D	712	POV	C211-C212-C213-C214
4	B	713	POV	C214-C215-C216-C217
4	A	804	POV	C27-C28-C29-C210
4	A	816	POV	C29-C210-C211-C212
4	B	713	POV	C27-C28-C29-C210
4	D	701	POV	C27-C28-C29-C210
4	D	706	POV	C29-C210-C211-C212
4	A	806	POV	C21-C22-C23-C24
3	A	809	PCW	C19-C20-C21-C22
3	B	711	PCW	C19-C20-C21-C22
3	C	711	PCW	C19-C20-C21-C22
3	D	715	PCW	C19-C20-C21-C22
4	A	808	POV	C27-C28-C29-C210
4	B	702	POV	C29-C210-C211-C212
4	B	706	POV	C27-C28-C29-C210
4	C	710	POV	C27-C28-C29-C210
4	C	713	POV	C27-C28-C29-C210
4	D	710	POV	C27-C28-C29-C210
4	A	806	POV	C211-C212-C213-C214
2	D	705	Y01	CAM-CAY-OAW-CBC
4	A	811	POV	C27-C28-C29-C210
4	B	710	POV	C27-C28-C29-C210
4	C	707	POV	C32-C33-C34-C35
4	C	709	POV	C34-C35-C36-C37
4	D	711	POV	C39-C310-C311-C312
3	C	715	PCW	C16-C17-C18-C19
4	A	807	POV	C34-C35-C36-C37
4	A	807	POV	C29-C210-C211-C212
4	A	807	POV	C27-C28-C29-C210
4	B	709	POV	C29-C210-C211-C212
4	C	702	POV	C29-C210-C211-C212
4	C	709	POV	C29-C210-C211-C212
4	C	709	POV	C27-C28-C29-C210
4	D	713	POV	C29-C210-C211-C212
4	D	713	POV	C27-C28-C29-C210
4	A	811	POV	C12-C11-O12-P
4	B	713	POV	C12-C11-O12-P
4	D	701	POV	C12-C11-O12-P
4	C	713	POV	C214-C215-C216-C217
4	D	711	POV	C32-C33-C34-C35
4	A	816	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
4	B	702	POV	O21-C2-C3-O31
4	B	708	POV	O21-C2-C3-O31
4	C	708	POV	O21-C2-C3-O31
4	D	706	POV	O21-C2-C3-O31
4	D	713	POV	C34-C35-C36-C37
2	C	704	Y01	CAM-CAL-CAX-OAH
4	B	714	POV	C25-C26-C27-C28
4	D	713	POV	C35-C36-C37-C38
4	B	709	POV	C27-C28-C29-C210
3	A	813	PCW	C16-C17-C18-C19
3	B	715	PCW	C16-C17-C18-C19
3	D	703	PCW	C16-C17-C18-C19
4	C	713	POV	C33-C34-C35-C36
4	D	701	POV	C33-C34-C35-C36
4	C	707	POV	C39-C310-C311-C312
2	A	802	Y01	CAM-CAL-CAX-OAH
2	C	704	Y01	CAM-CAL-CAX-OAF
2	D	708	Y01	CAM-CAL-CAX-OAH
4	A	804	POV	O21-C21-C22-C23
4	B	702	POV	O21-C21-C22-C23
4	D	706	POV	O21-C21-C22-C23
4	A	816	POV	O21-C21-C22-C23
4	C	702	POV	O21-C21-C22-C23
4	C	706	POV	O21-C21-C22-C23
4	A	811	POV	C33-C34-C35-C36
4	B	713	POV	C33-C34-C35-C36
2	D	708	Y01	CAM-CAL-CAX-OAF
2	A	802	Y01	CAM-CAL-CAX-OAF
2	B	704	Y01	CAM-CAL-CAX-OAH
4	B	706	POV	O21-C21-C22-C23
4	D	714	POV	C23-C24-C25-C26
4	A	811	POV	C214-C215-C216-C217
4	A	806	POV	O21-C2-C3-O31
4	C	702	POV	O21-C2-C3-O31
4	D	712	POV	O21-C2-C3-O31
4	D	710	POV	O21-C21-C22-C23
4	A	807	POV	C26-C27-C28-C29
4	C	709	POV	C26-C27-C28-C29
4	D	713	POV	C26-C27-C28-C29
4	B	702	POV	C311-C312-C313-C314
4	B	708	POV	C310-C311-C312-C313
4	A	805	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	B	708	POV	C211-C212-C213-C214
4	B	707	POV	O21-C21-C22-C23
2	B	704	Y01	CAM-CAL-CAX-OAF
4	D	714	POV	C214-C215-C216-C217
4	B	710	POV	C214-C215-C216-C217
4	B	707	POV	C24-C25-C26-C27
4	D	711	POV	O21-C21-C22-C23
4	C	707	POV	O21-C21-C22-C23
4	A	806	POV	C310-C311-C312-C313
4	C	710	POV	C23-C24-C25-C26
4	A	808	POV	C214-C215-C216-C217
4	C	710	POV	C214-C215-C216-C217
4	D	702	POV	C25-C26-C27-C28
4	A	805	POV	O21-C21-C22-C23
4	C	702	POV	O22-C21-C22-C23
4	C	714	POV	C25-C26-C27-C28
4	A	804	POV	O22-C21-C22-C23
4	B	702	POV	O22-C21-C22-C23
4	B	706	POV	O22-C21-C22-C23
4	A	816	POV	O22-C21-C22-C23
4	A	816	POV	C311-C312-C313-C314
4	D	706	POV	C311-C312-C313-C314
4	D	706	POV	C24-C25-C26-C27
4	C	706	POV	O22-C21-C22-C23
4	D	706	POV	O22-C21-C22-C23
4	B	707	POV	C37-C38-C39-C310
4	A	812	POV	C25-C26-C27-C28
4	A	816	POV	C24-C25-C26-C27
4	C	702	POV	C24-C25-C26-C27
4	D	710	POV	O22-C21-C22-C23
4	C	702	POV	C311-C312-C313-C314
4	C	707	POV	C37-C38-C39-C310
4	B	713	POV	O21-C21-C22-C23
4	C	713	POV	O21-C21-C22-C23
4	D	701	POV	O21-C21-C22-C23
4	D	711	POV	O22-C21-C22-C23

There are no ring outliers.

52 monomers are involved in 189 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	POV	4	0

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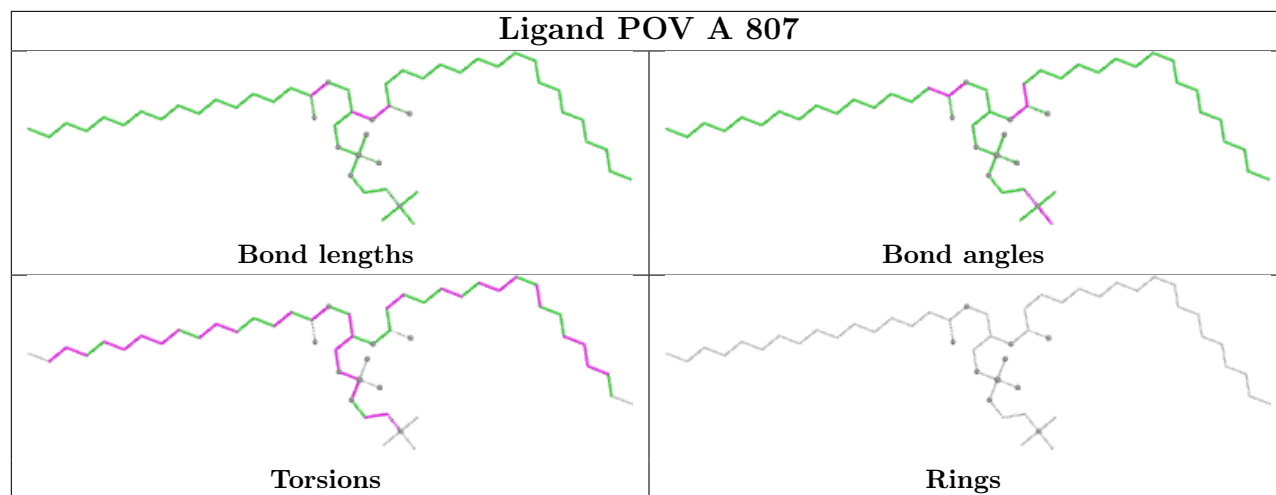
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	808	POV	8	0
4	B	706	POV	14	0
2	D	707	Y01	1	0
4	C	708	POV	1	0
4	C	710	POV	8	0
4	A	812	POV	1	0
4	B	710	POV	7	0
2	C	704	Y01	5	0
2	D	708	Y01	5	0
4	A	804	POV	12	0
4	D	710	POV	13	0
2	C	701	Y01	1	0
4	B	709	POV	4	0
4	C	707	POV	2	0
4	A	806	POV	3	0
4	D	713	POV	5	0
4	D	712	POV	2	0
3	C	716	PCW	1	0
2	C	703	Y01	2	0
3	C	715	PCW	1	0
4	C	709	POV	4	0
4	C	713	POV	6	0
4	D	702	POV	3	0
4	B	713	POV	7	0
4	A	811	POV	7	0
2	A	815	Y01	1	0
4	B	714	POV	2	0
3	A	814	PCW	1	0
4	D	701	POV	5	0
4	D	714	POV	6	0
2	A	801	Y01	3	0
2	B	704	Y01	5	0
4	C	714	POV	2	0
4	D	711	POV	3	0
4	B	702	POV	2	0
4	C	706	POV	11	0
3	A	813	PCW	2	0
4	A	805	POV	2	0
3	B	716	PCW	1	0
2	B	703	Y01	3	0
3	B	715	PCW	3	0
2	B	701	Y01	1	0

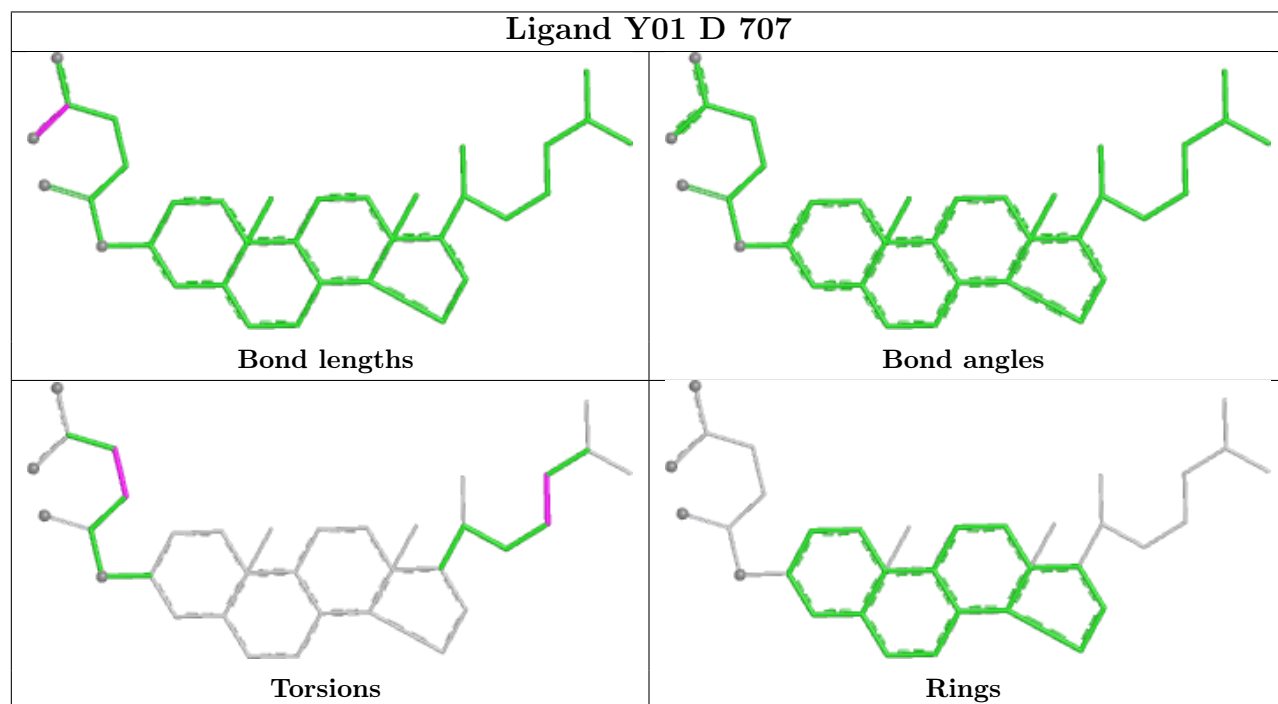
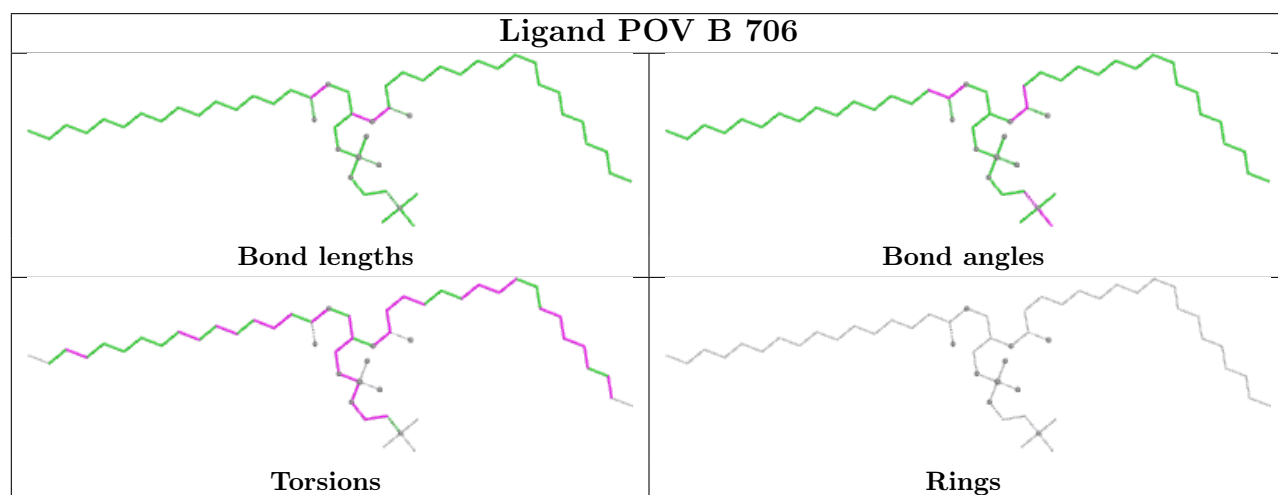
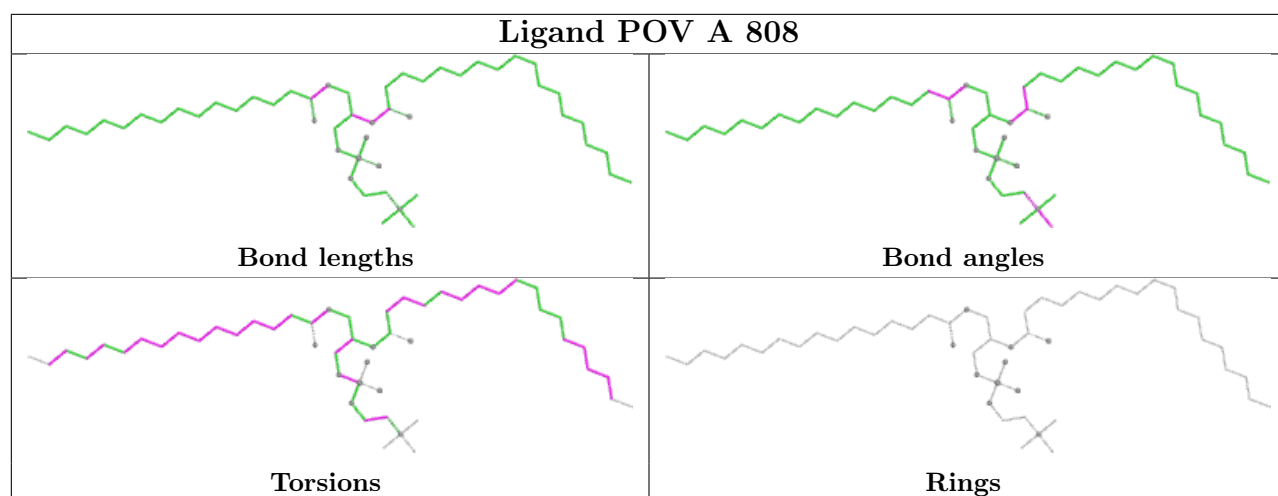
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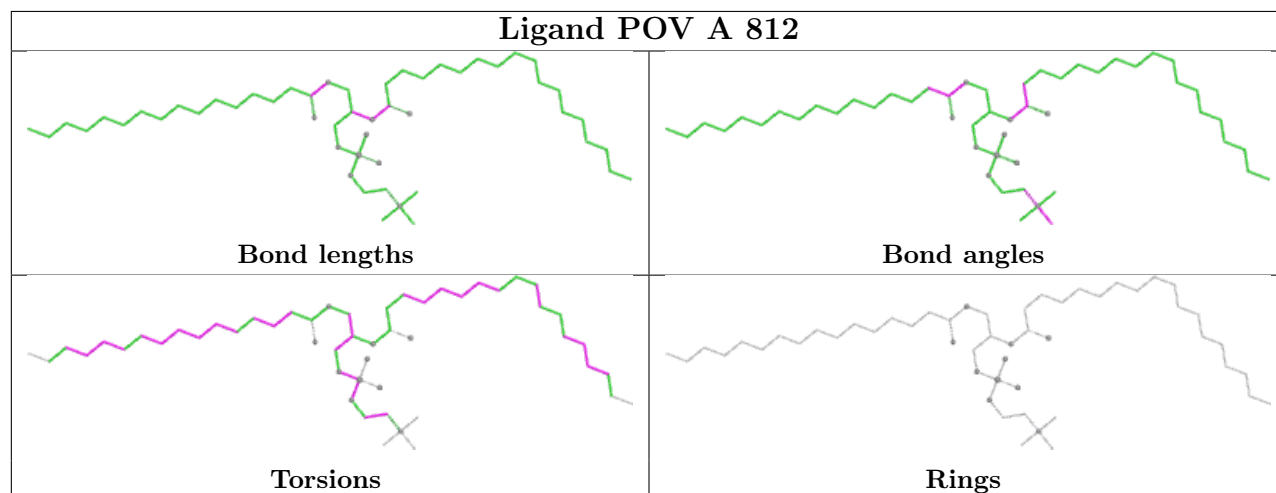
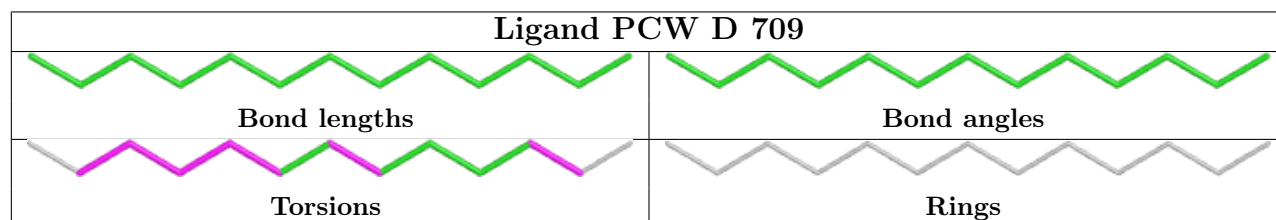
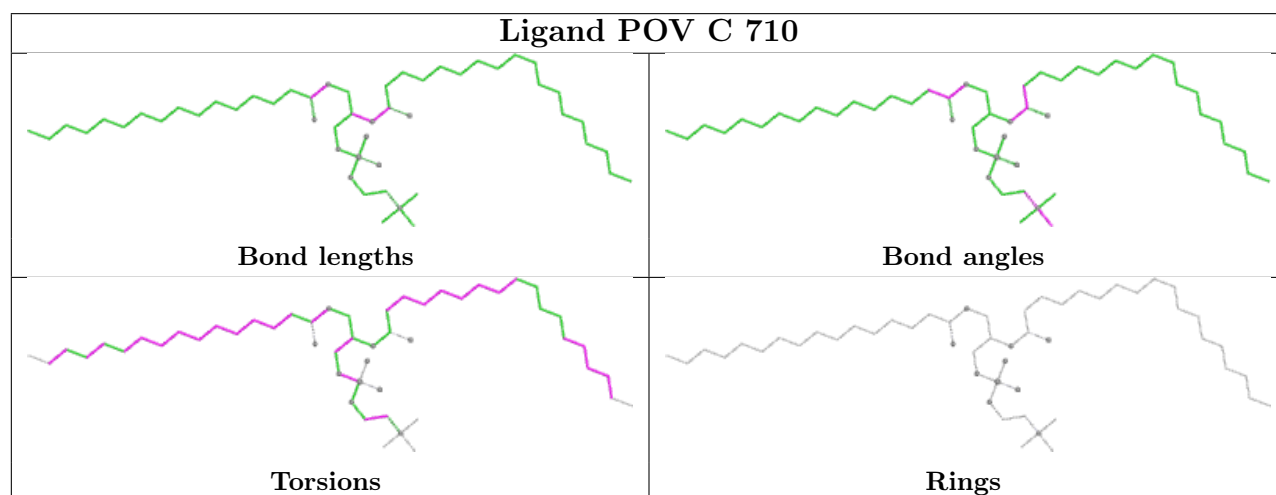
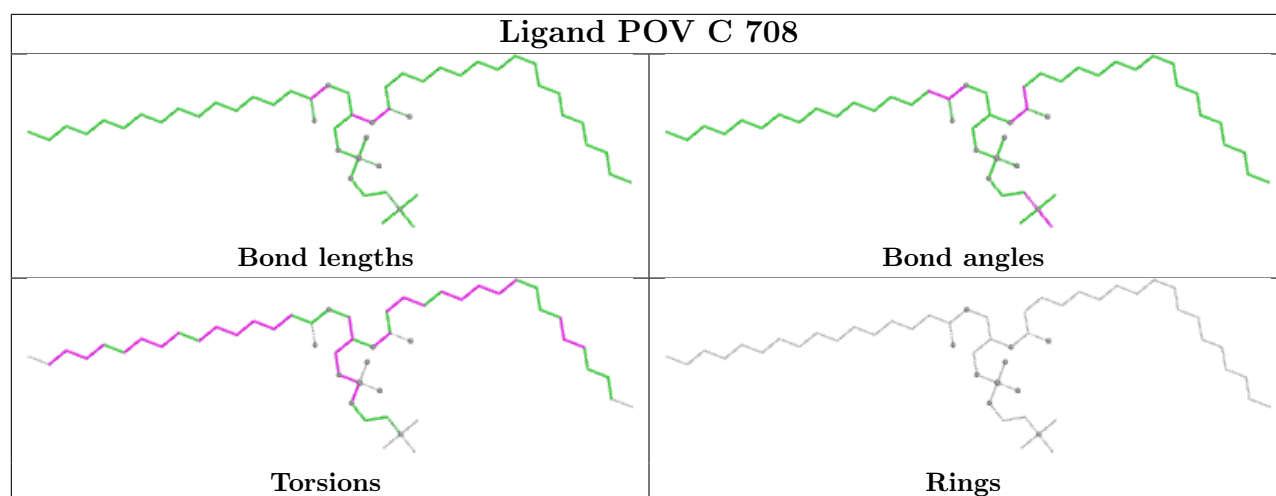
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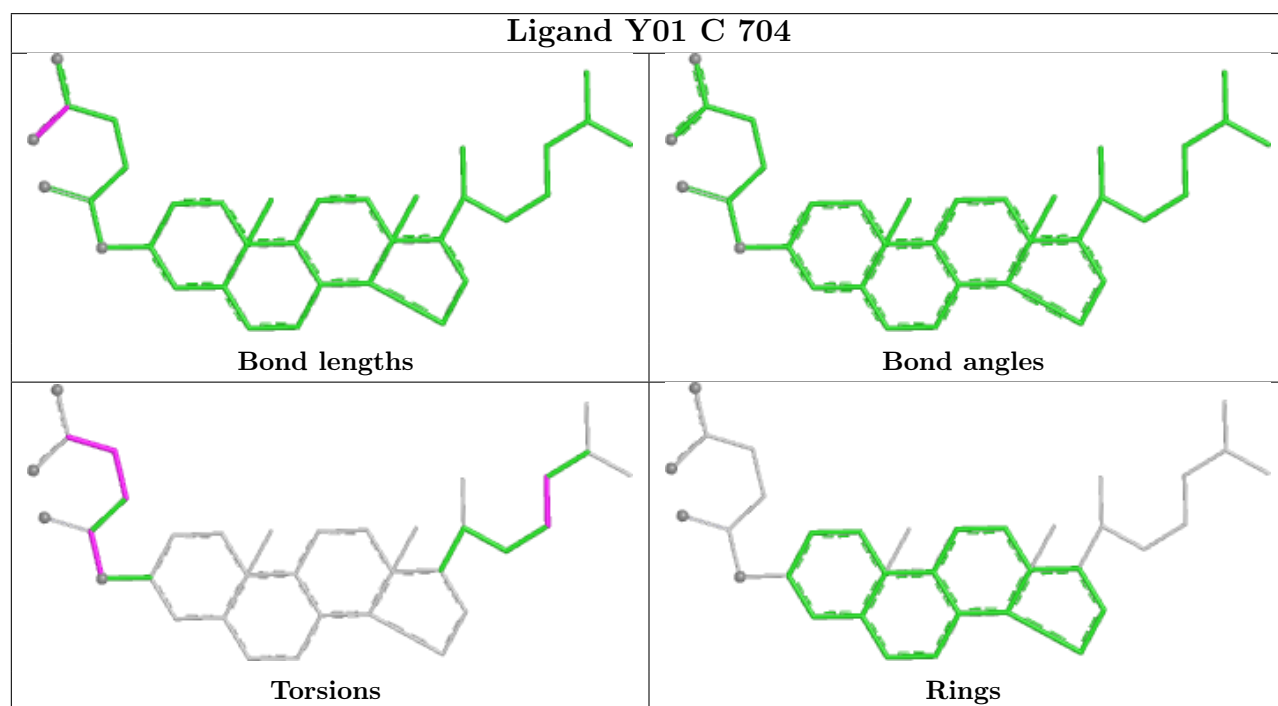
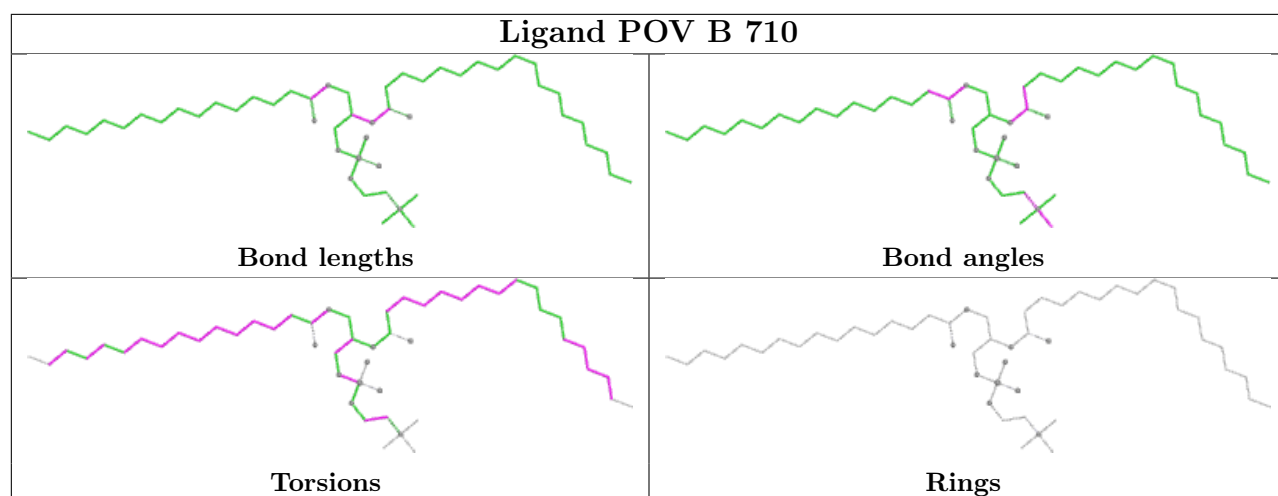
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	703	PCW	2	0
2	A	802	Y01	5	0
3	D	704	PCW	1	0
4	A	816	POV	2	0
4	C	702	POV	3	0
4	B	707	POV	1	0
4	D	706	POV	1	0
2	D	705	Y01	1	0
4	B	708	POV	2	0

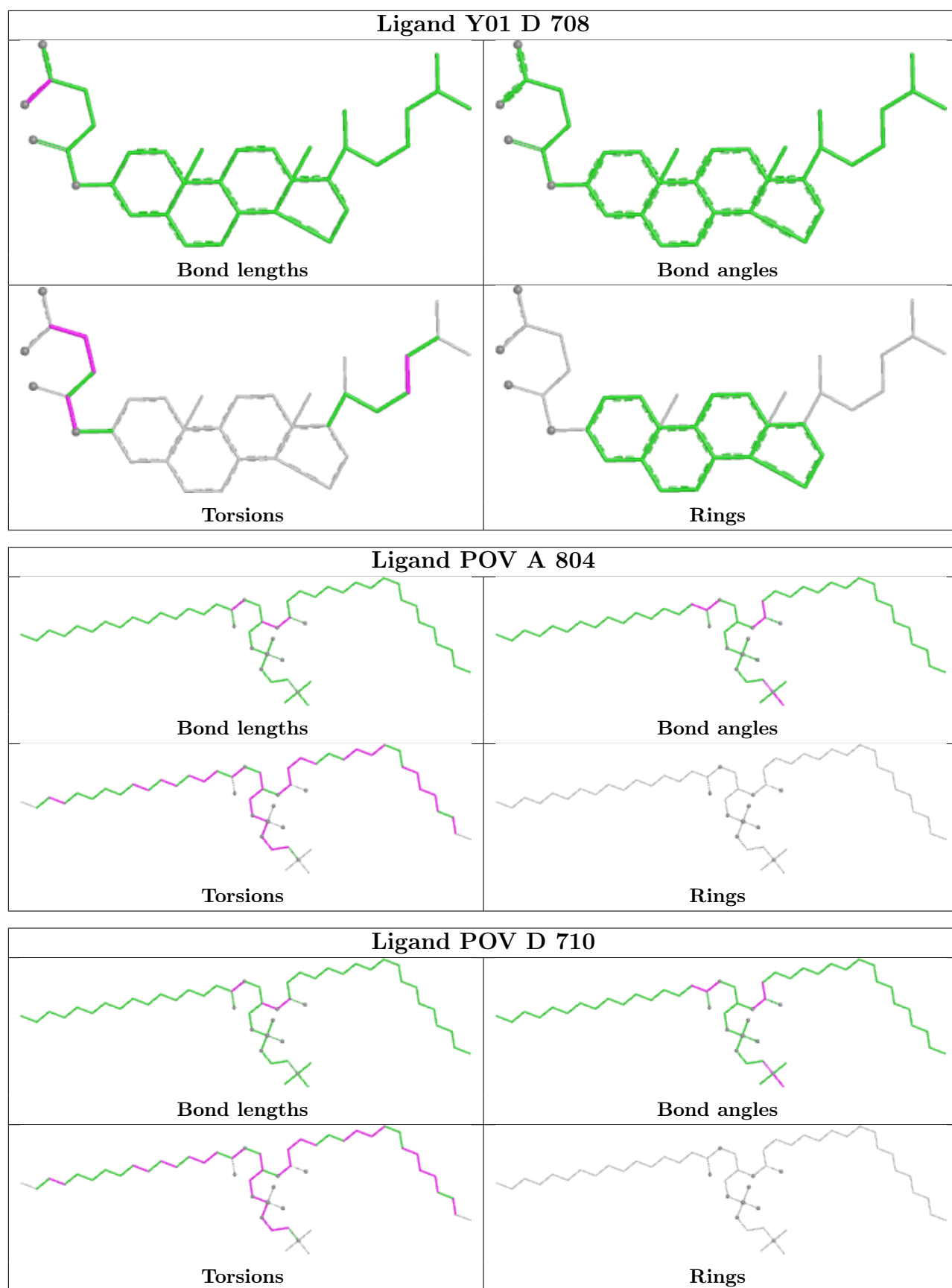
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

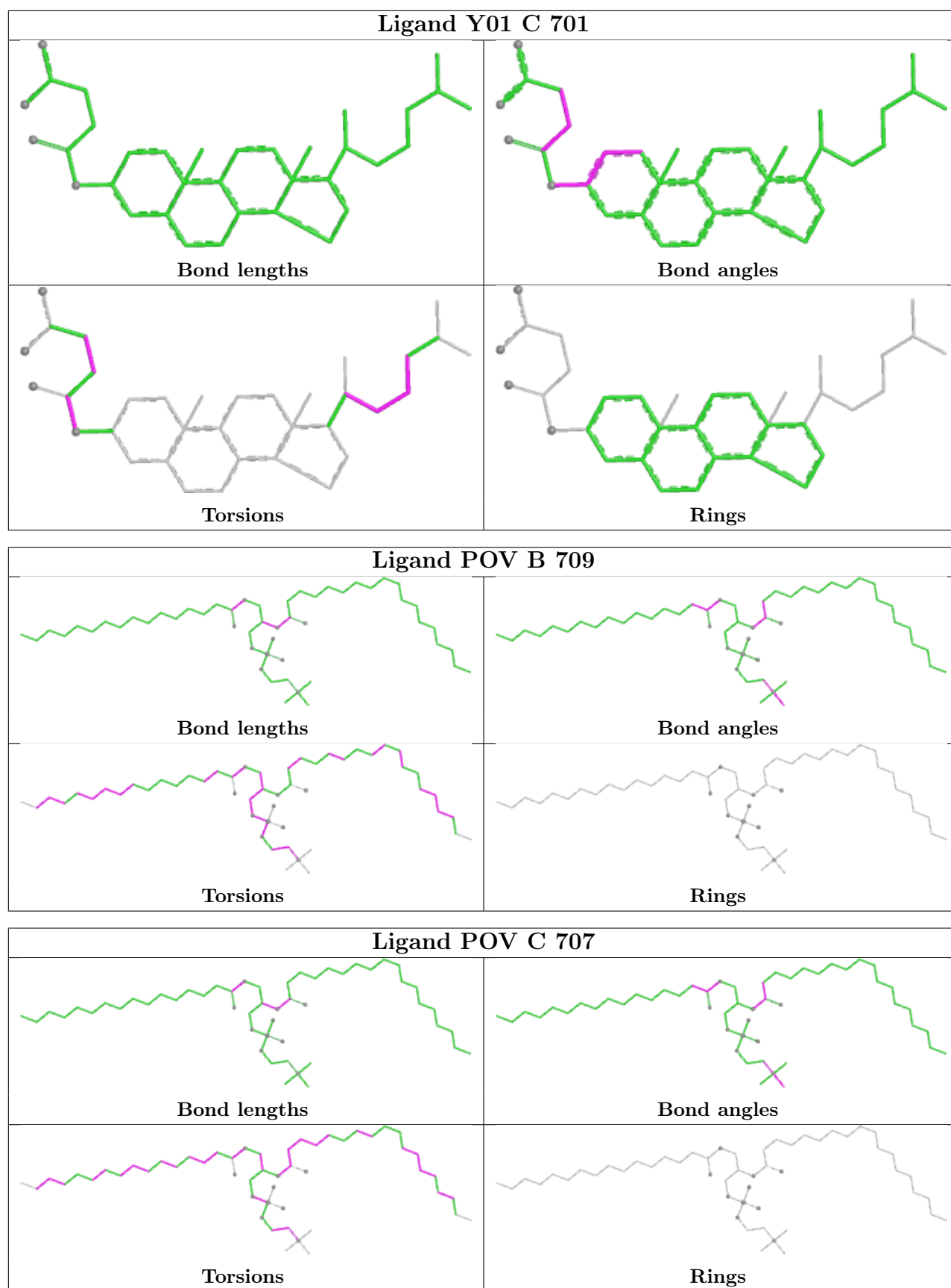


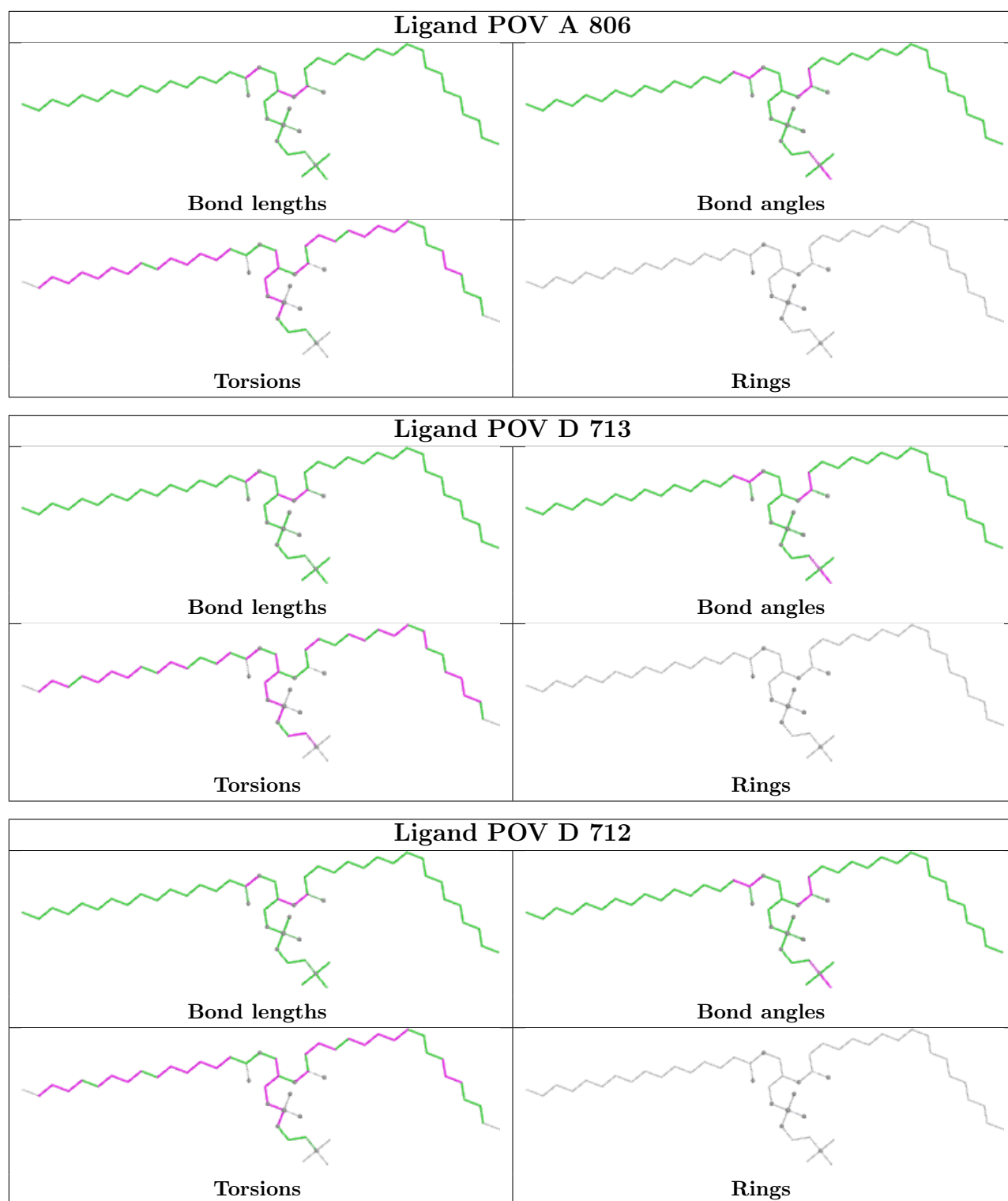


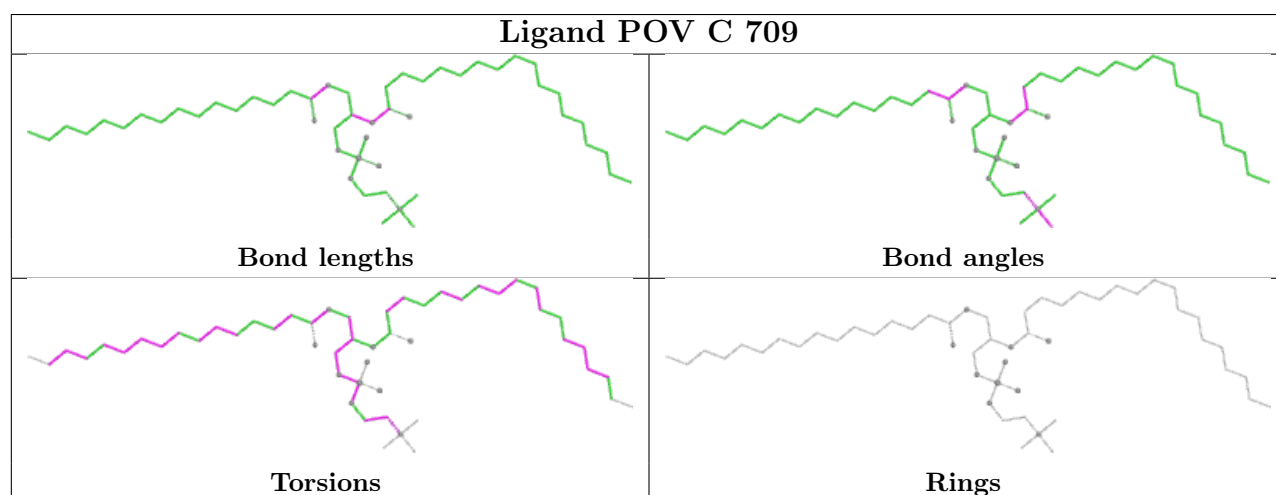
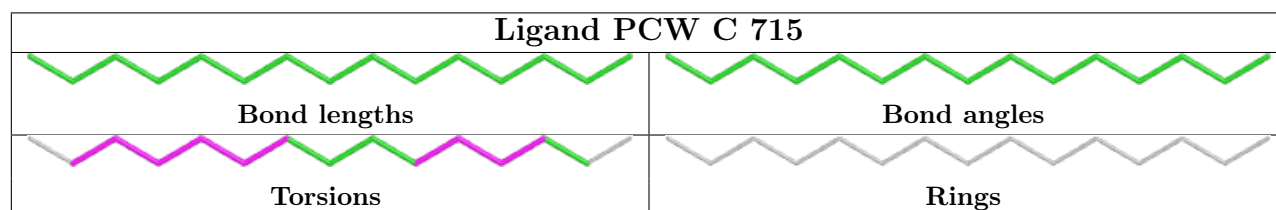
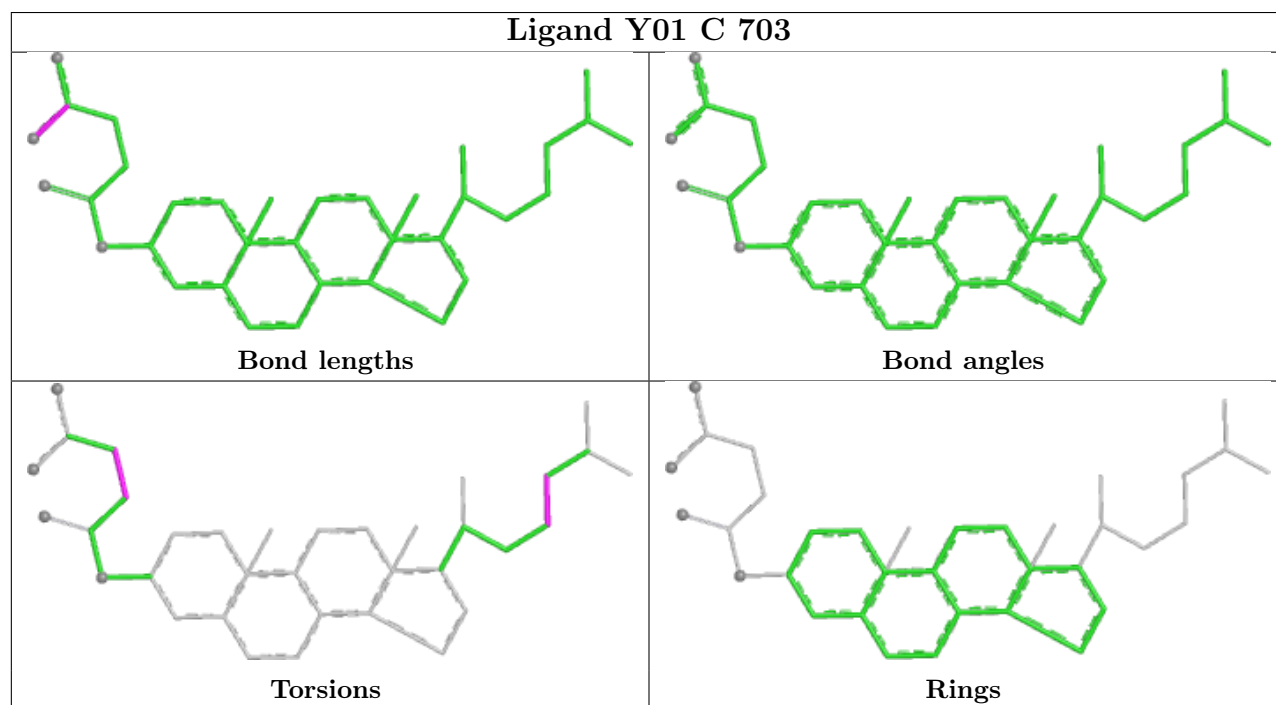
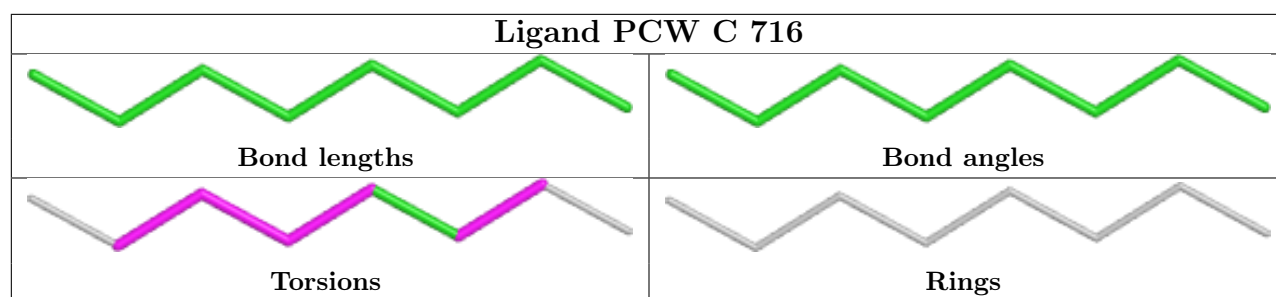


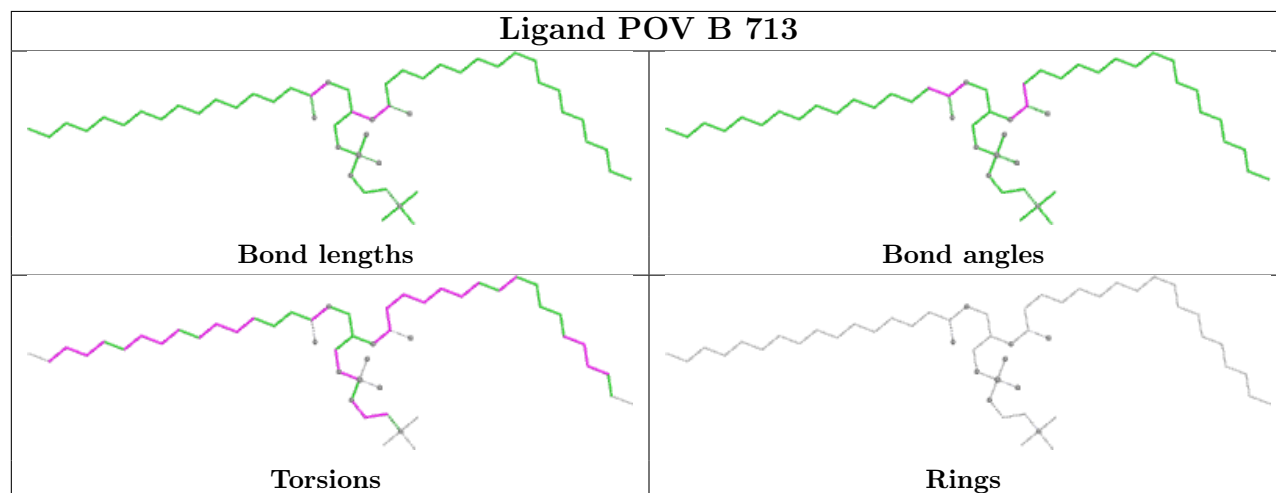
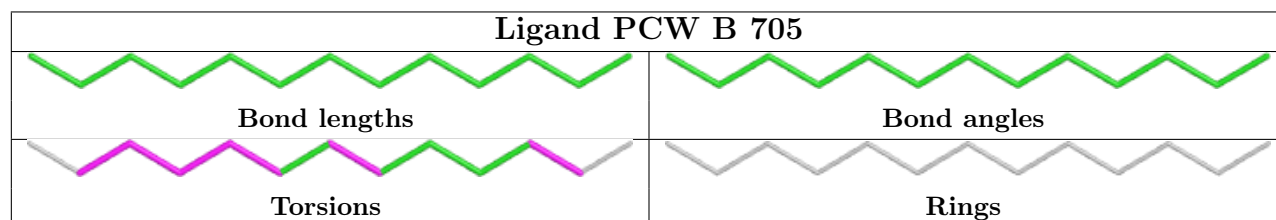
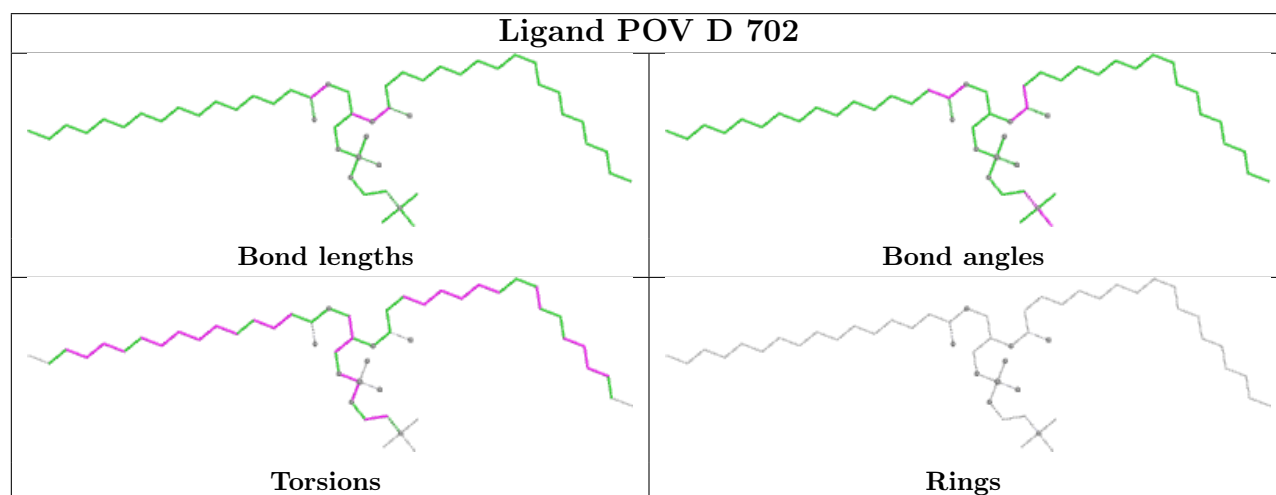
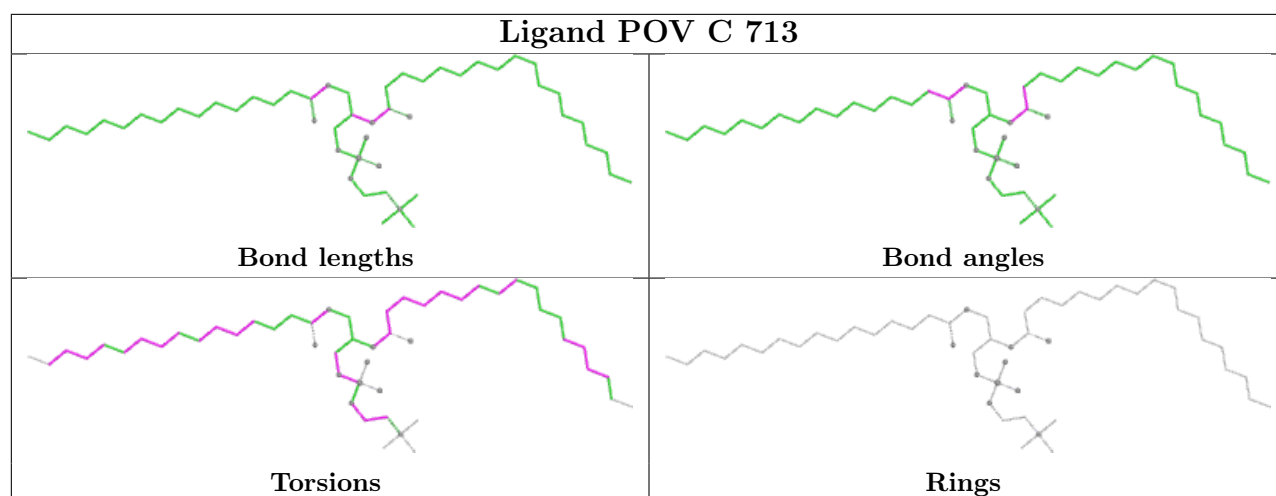


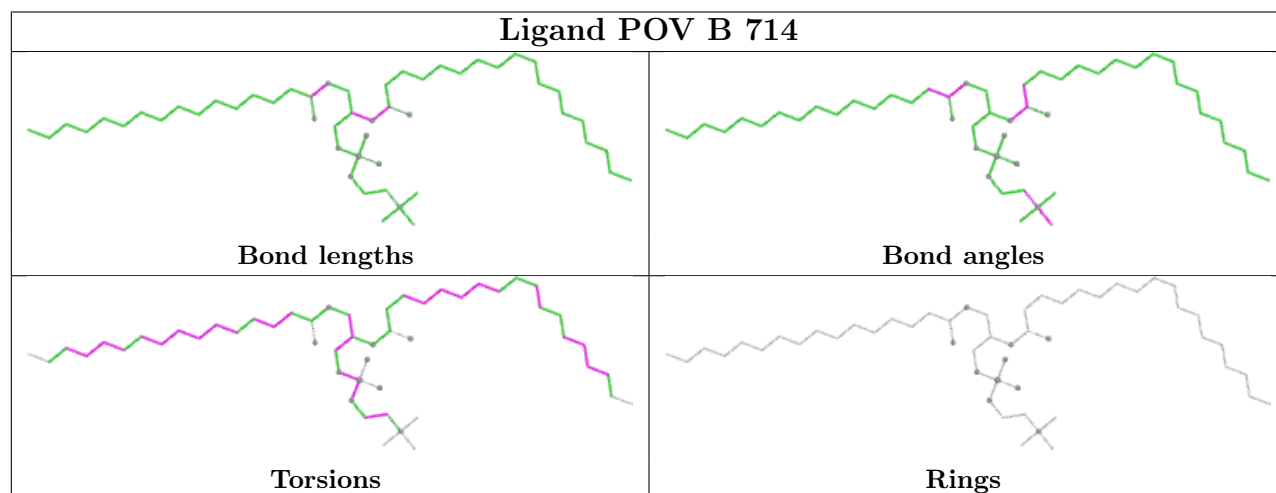
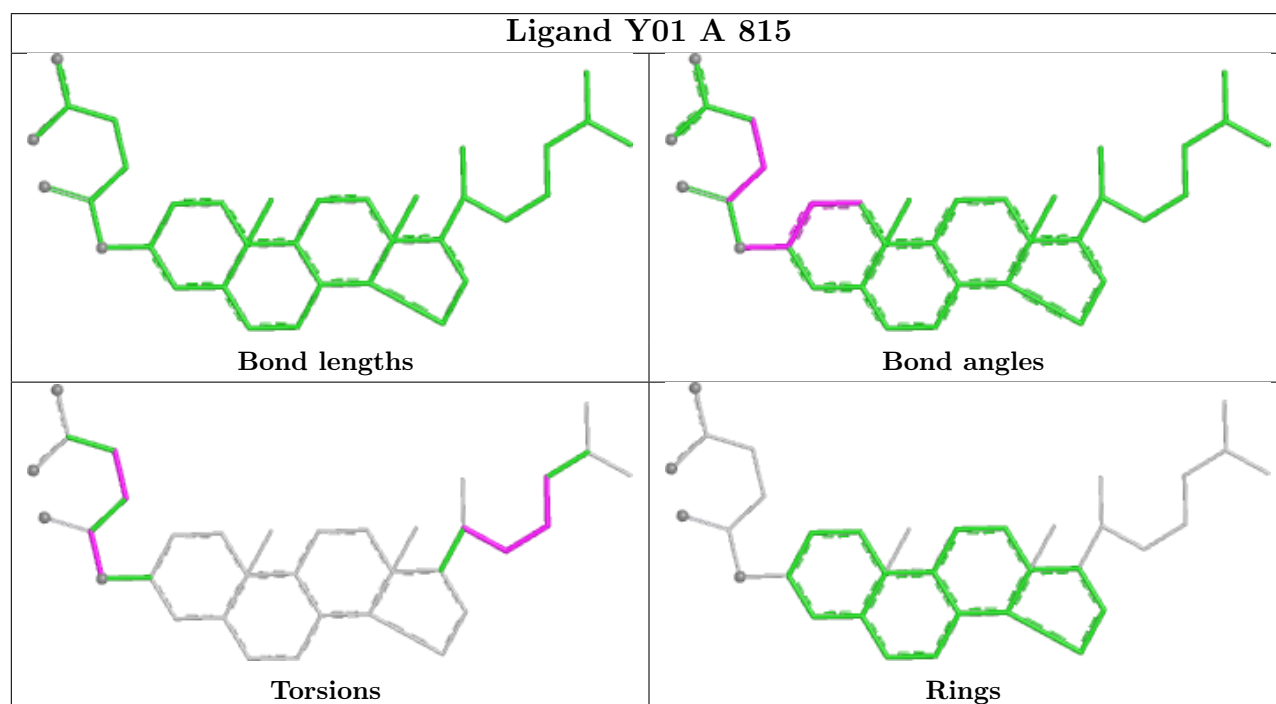
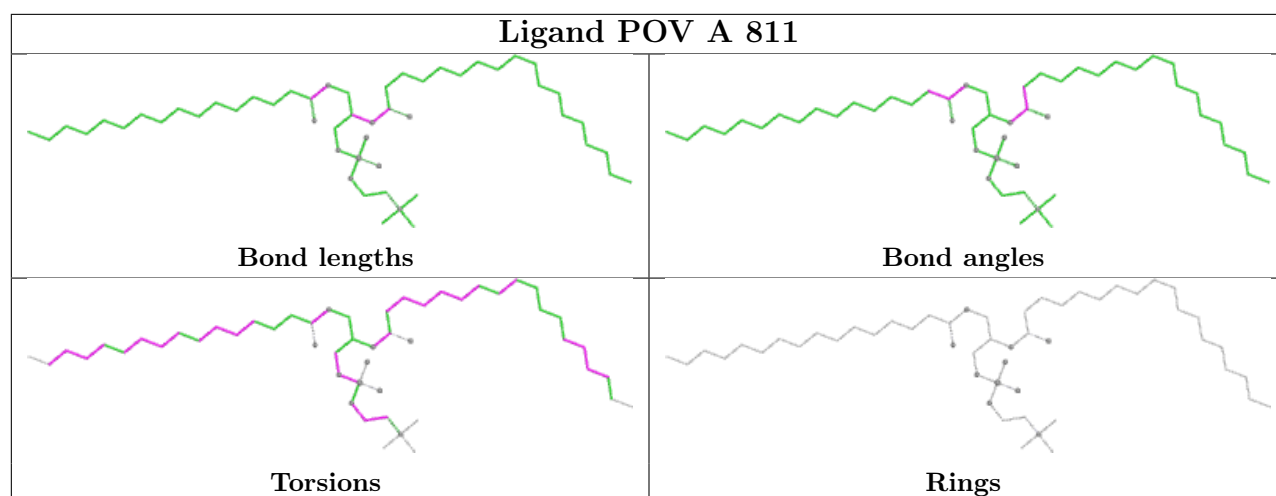






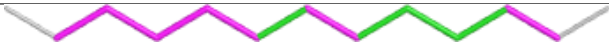




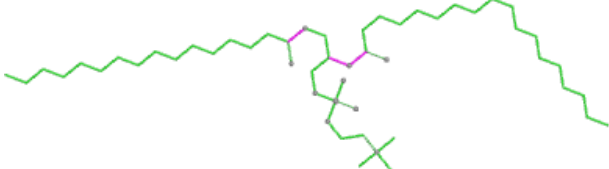
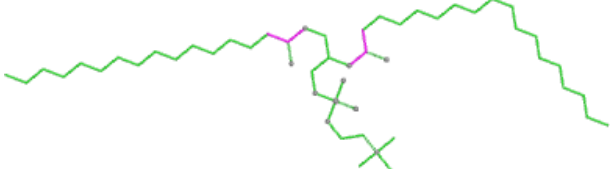
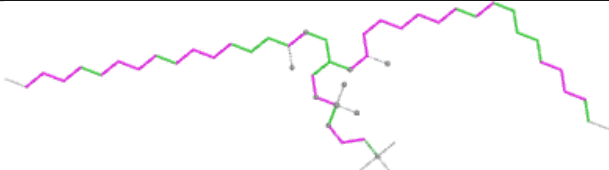
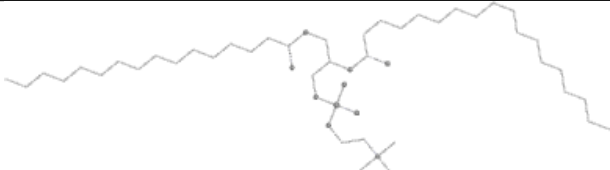


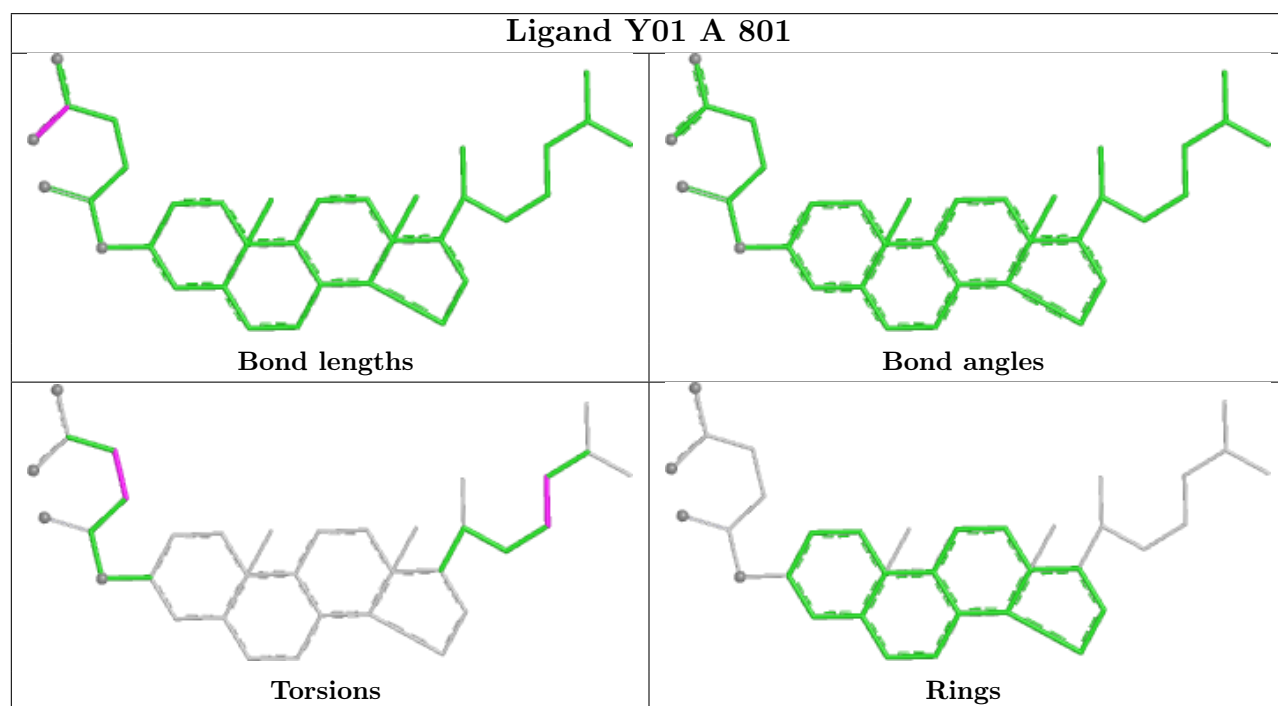
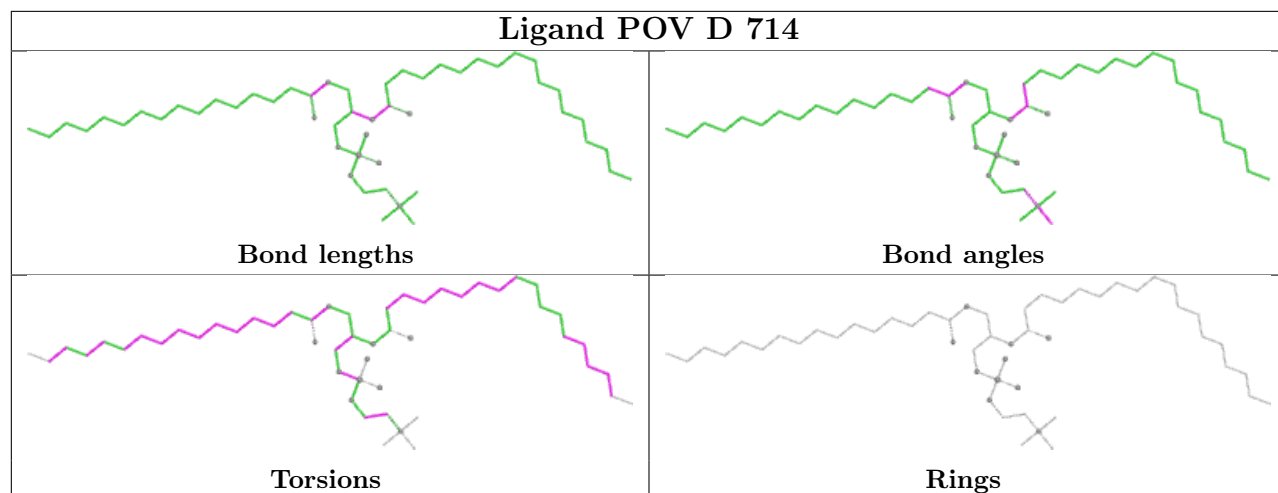
Ligand PCW D 715	
 Bond lengths	 Bond angles
 Torsions	 Rings

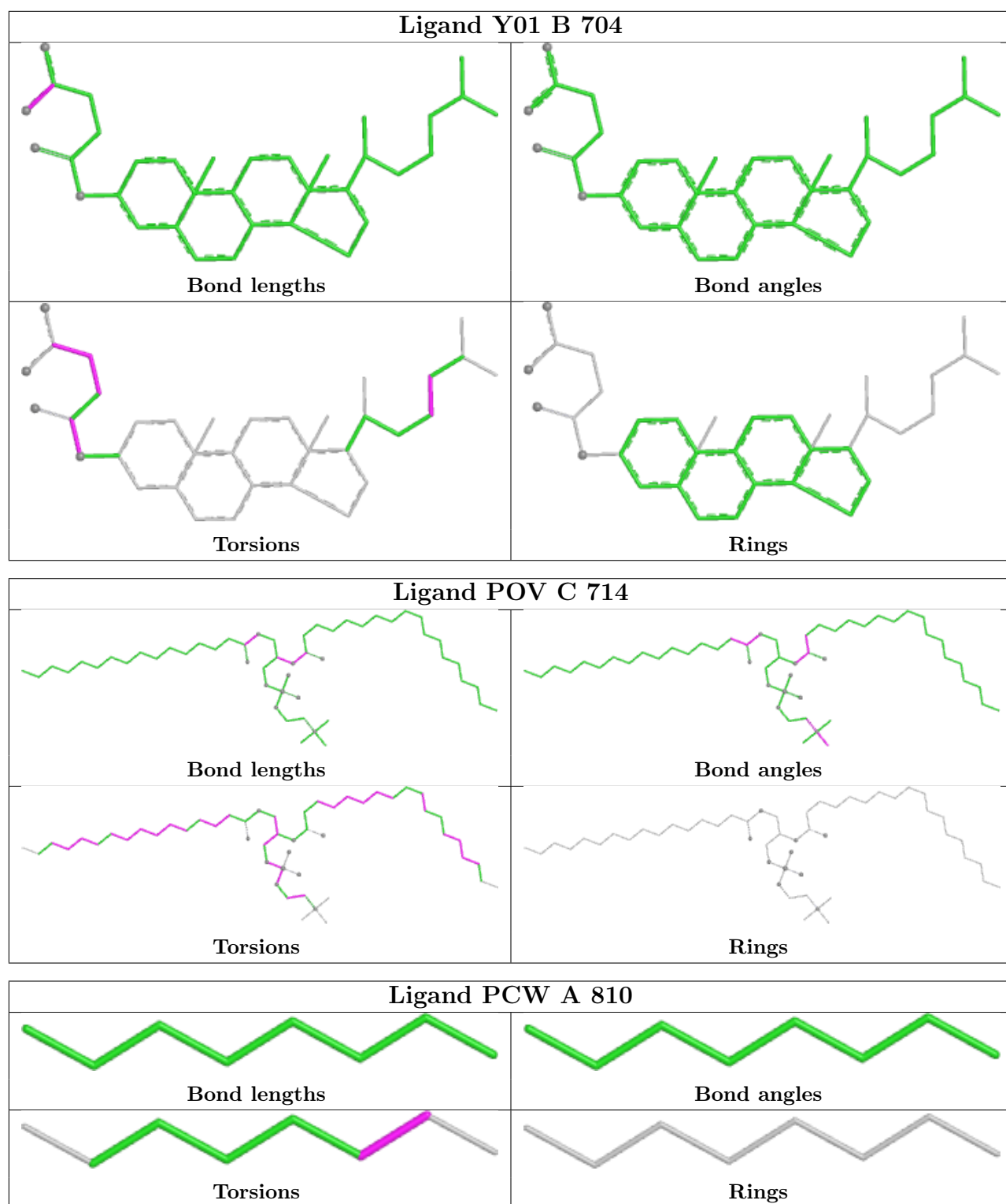
Ligand PCW A 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

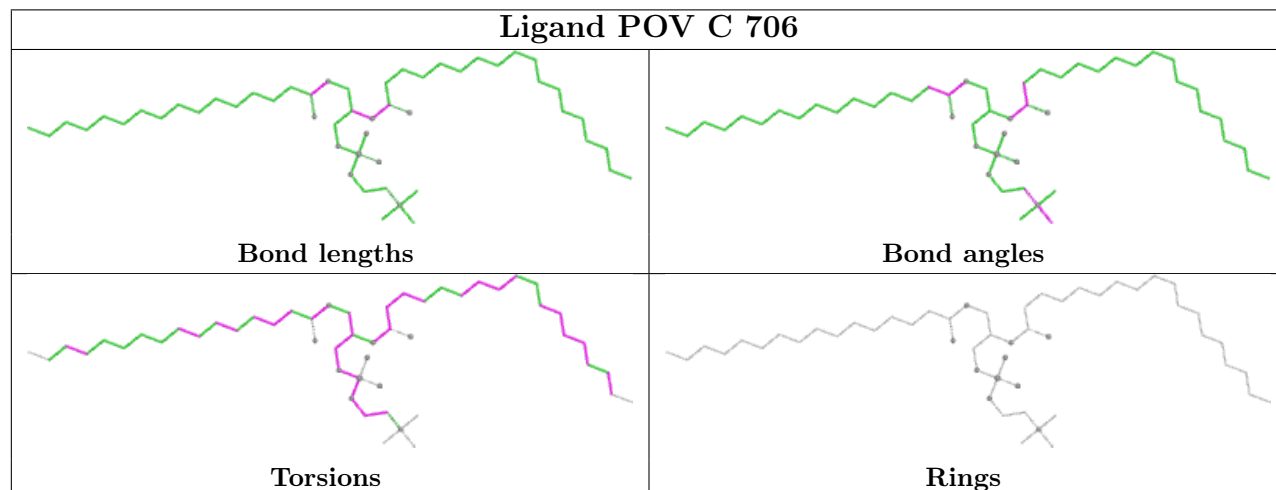
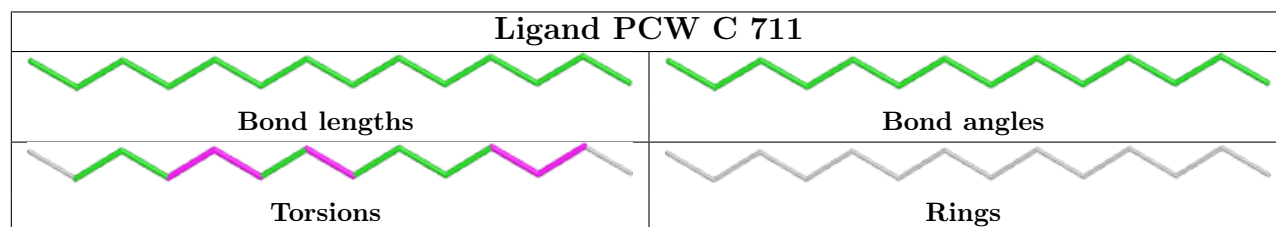
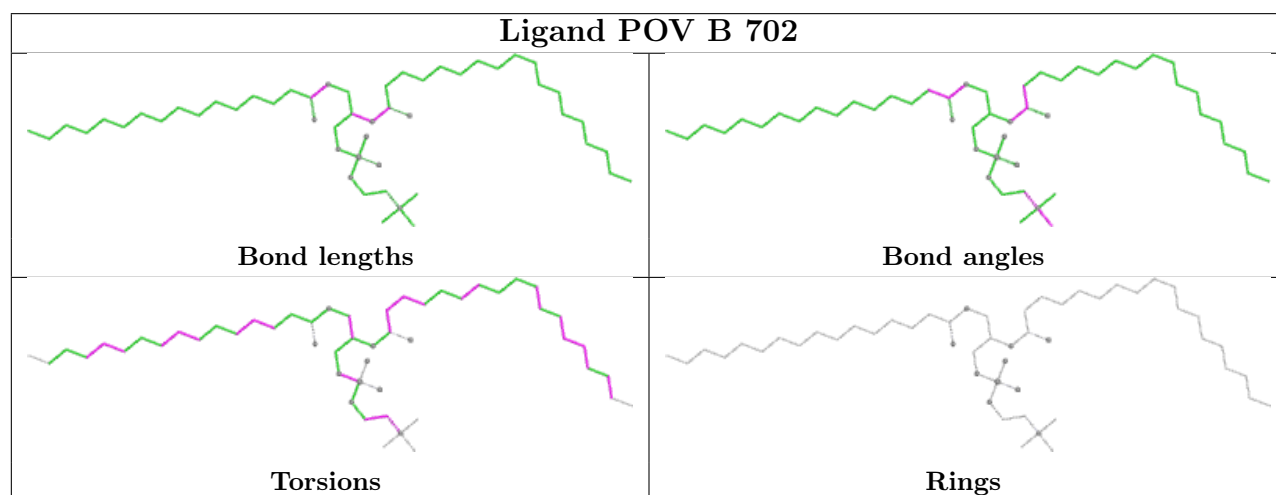
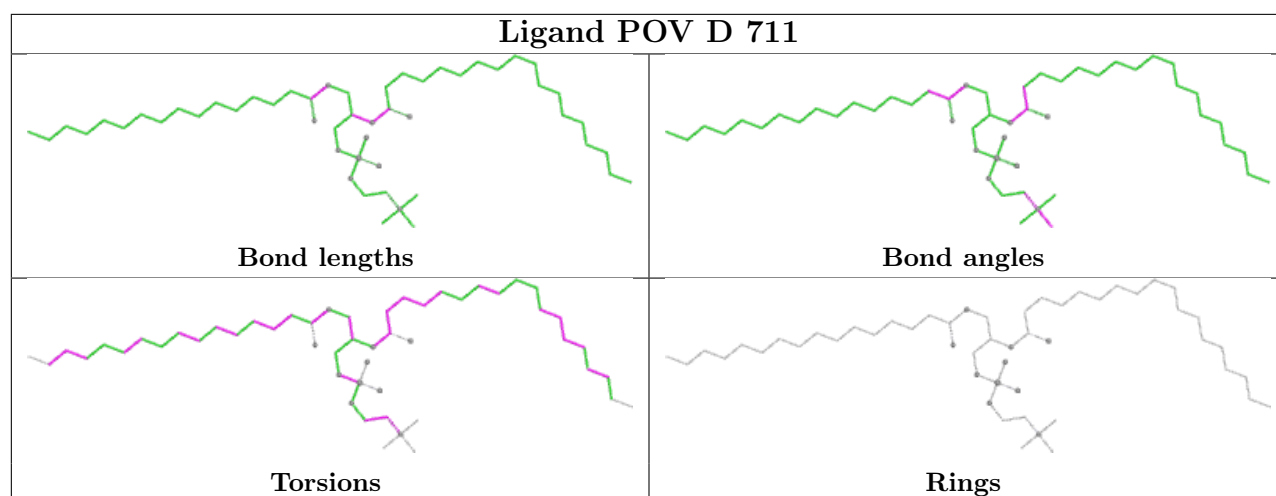
Ligand PCW A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

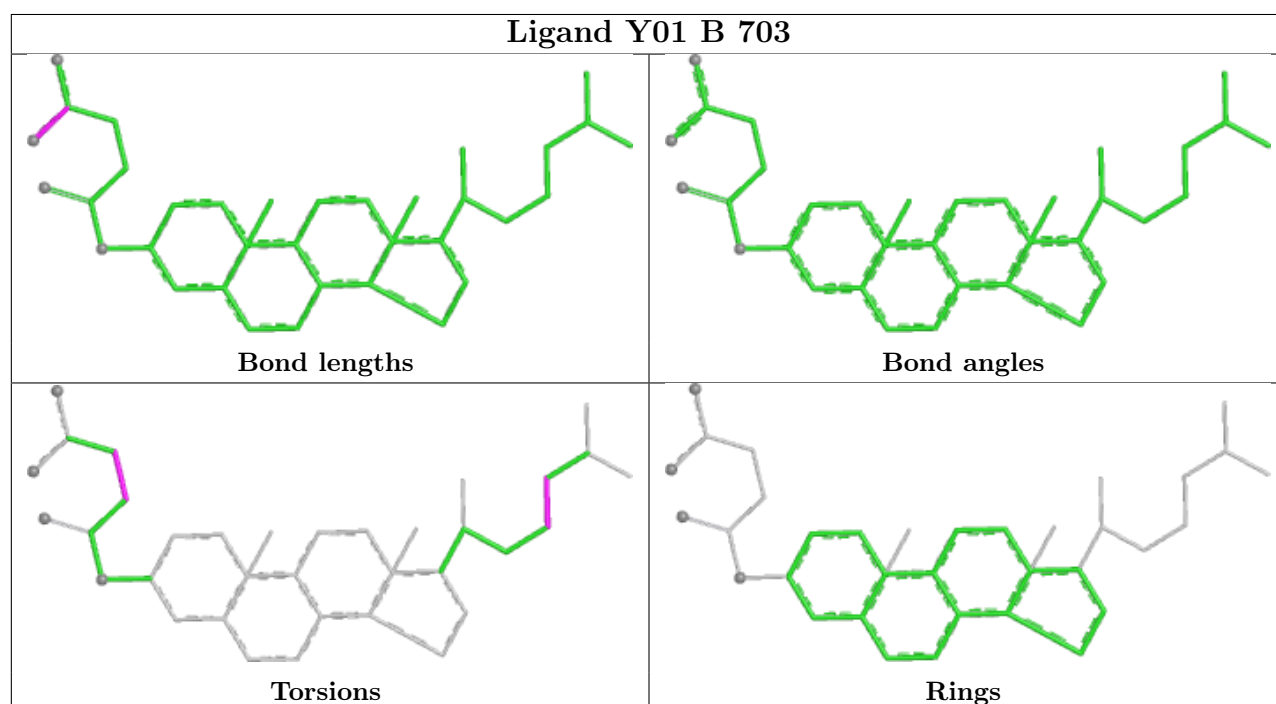
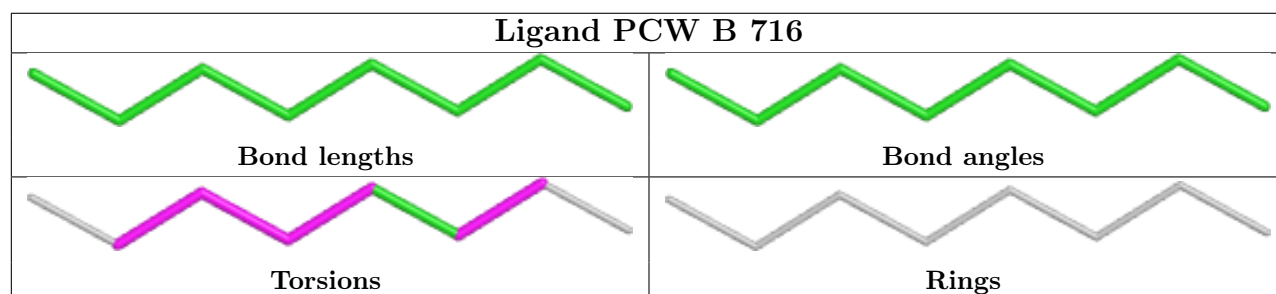
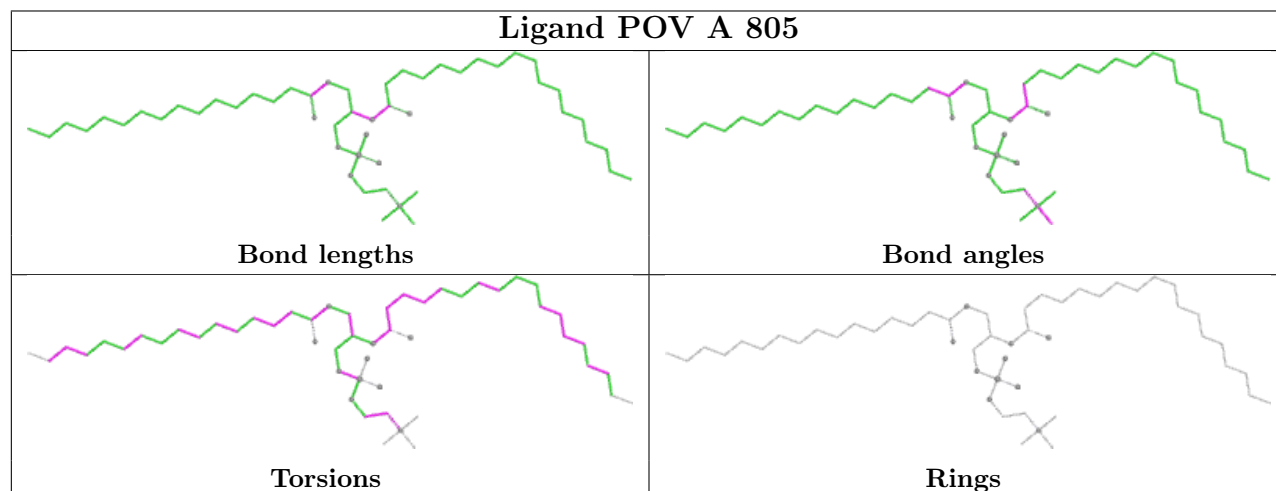
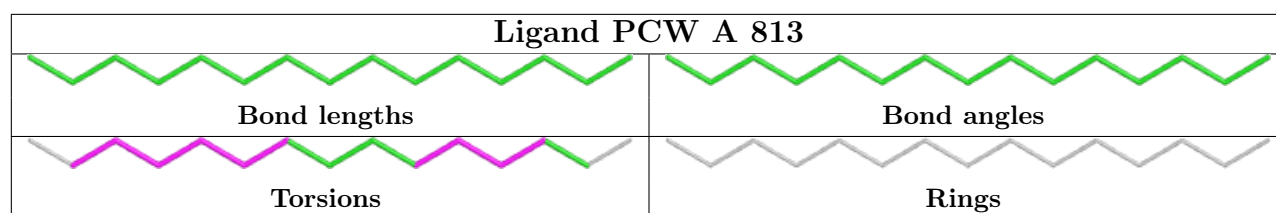
Ligand PCW B 711	
 Bond lengths	 Bond angles
 Torsions	 Rings

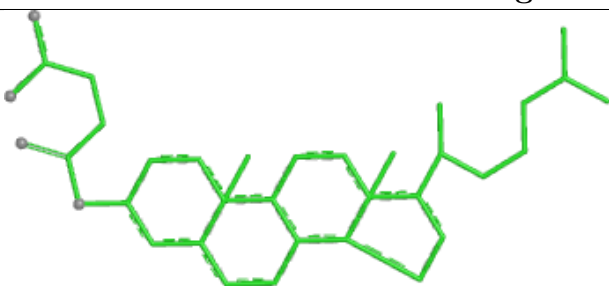
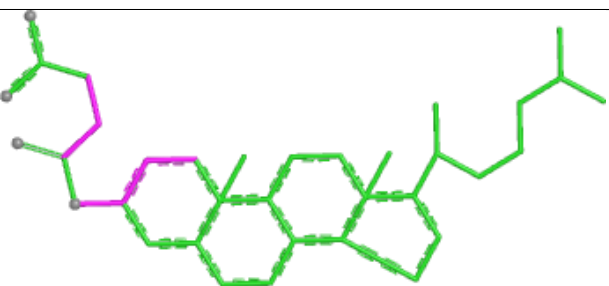
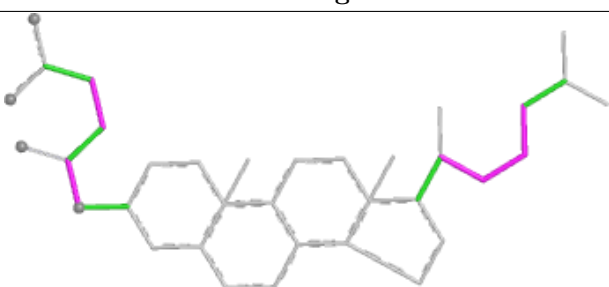
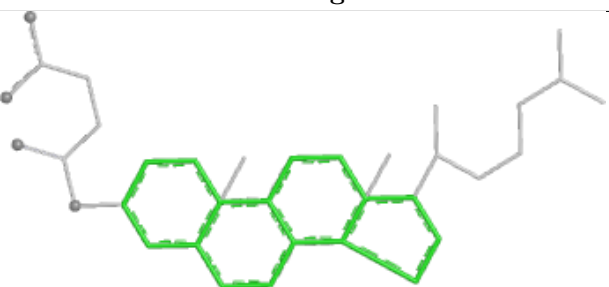
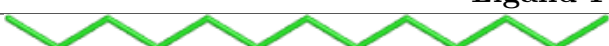
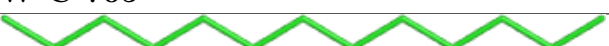
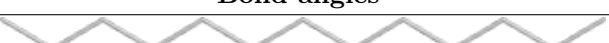
Ligand POV D 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

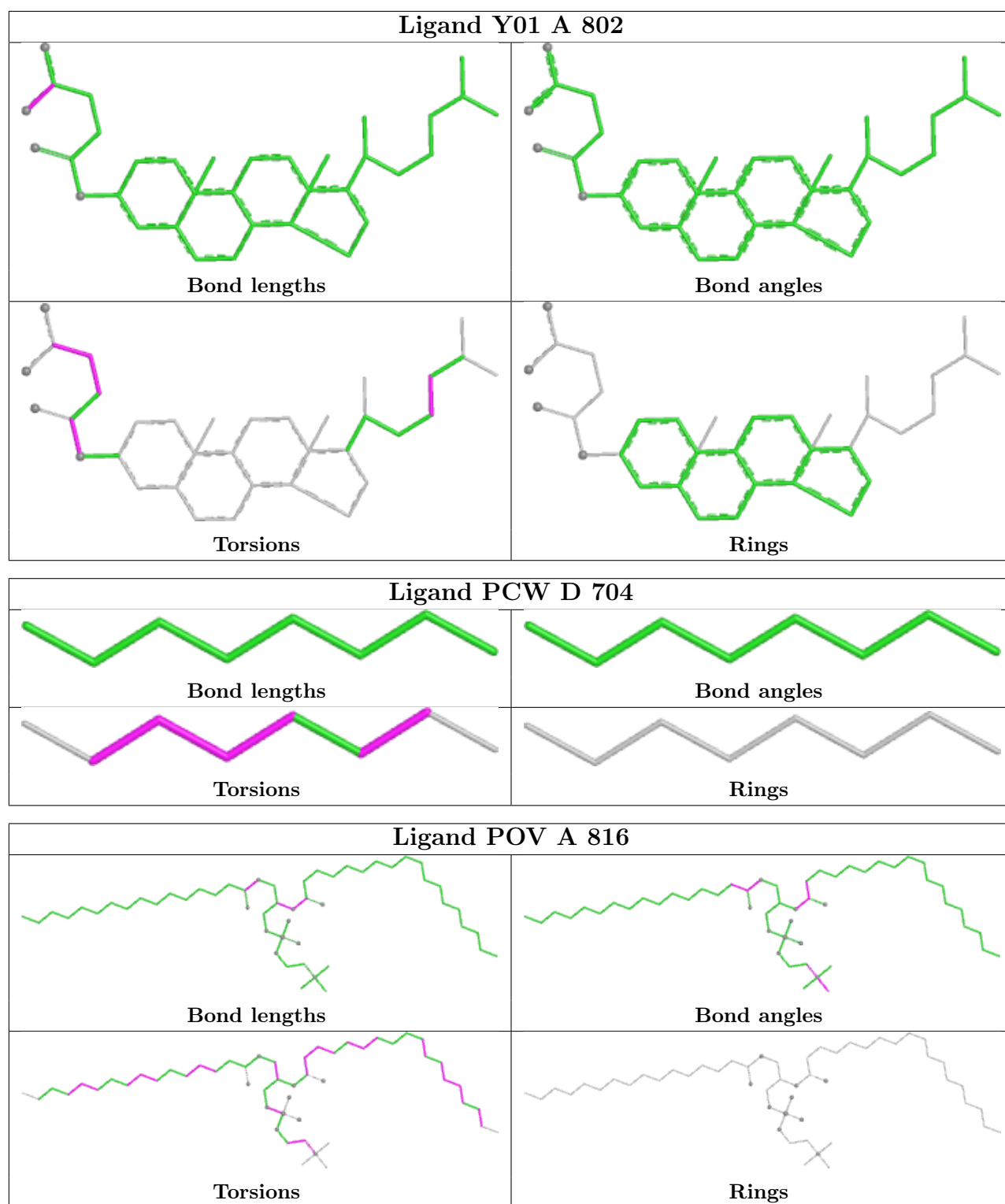


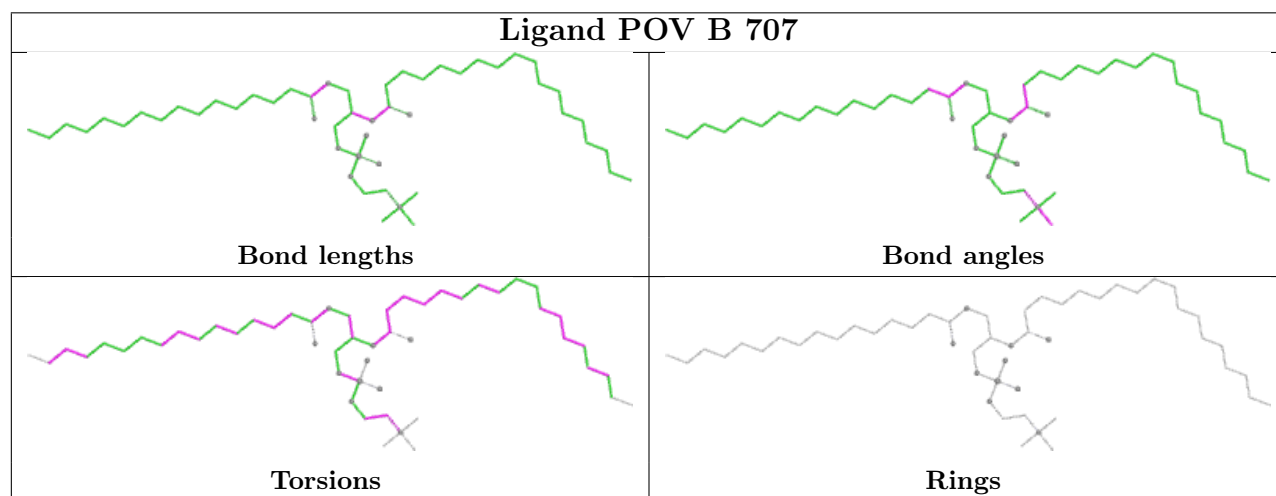
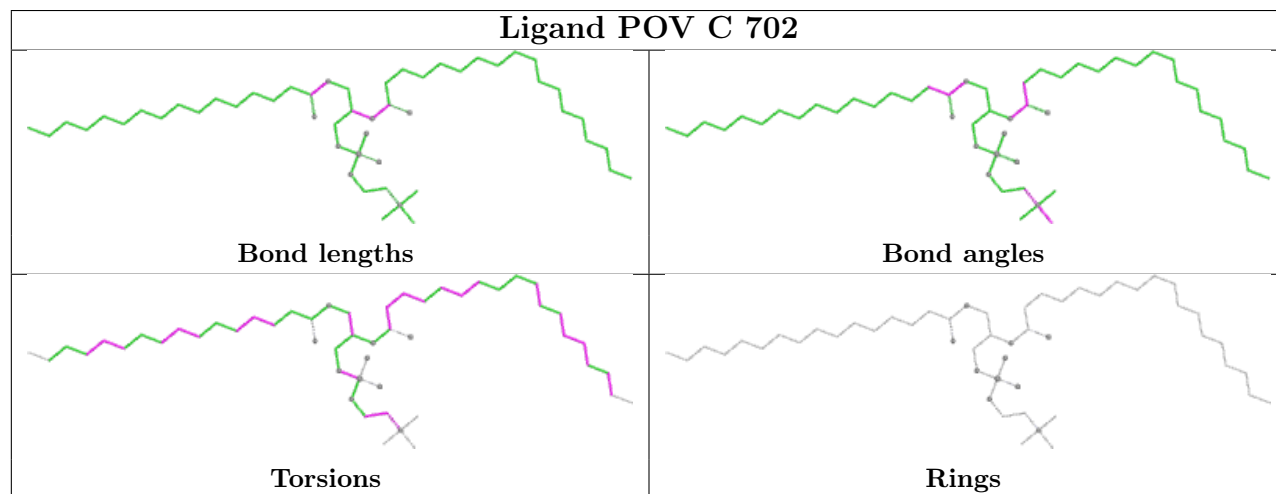
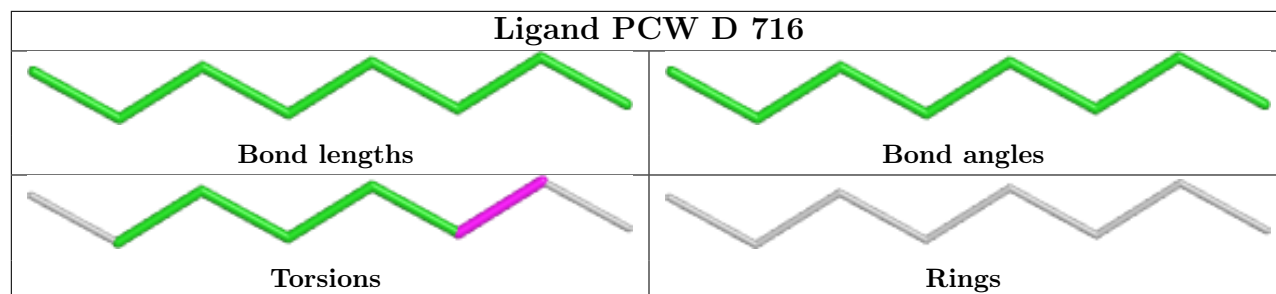


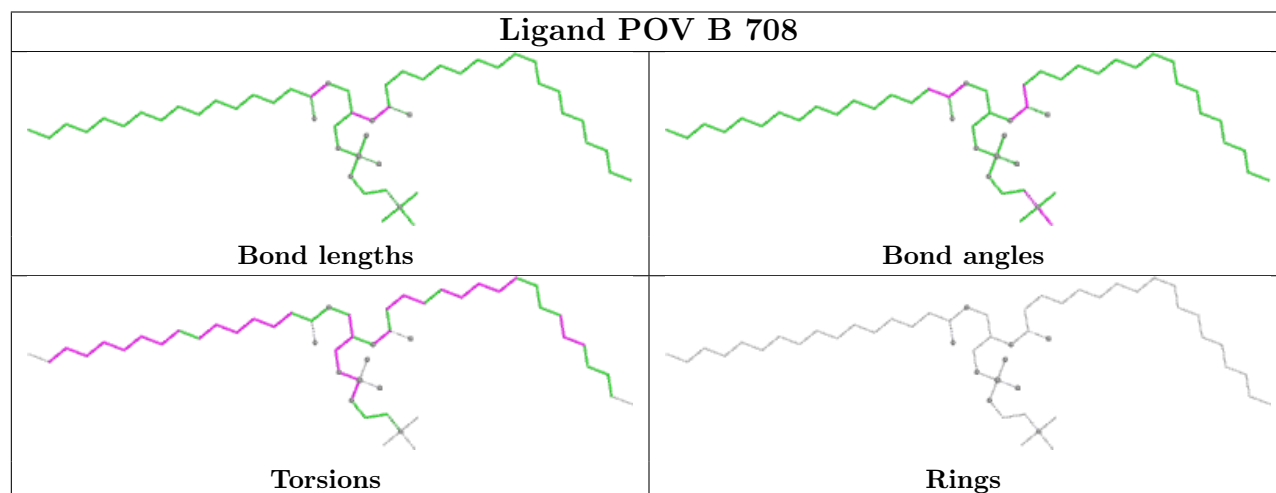
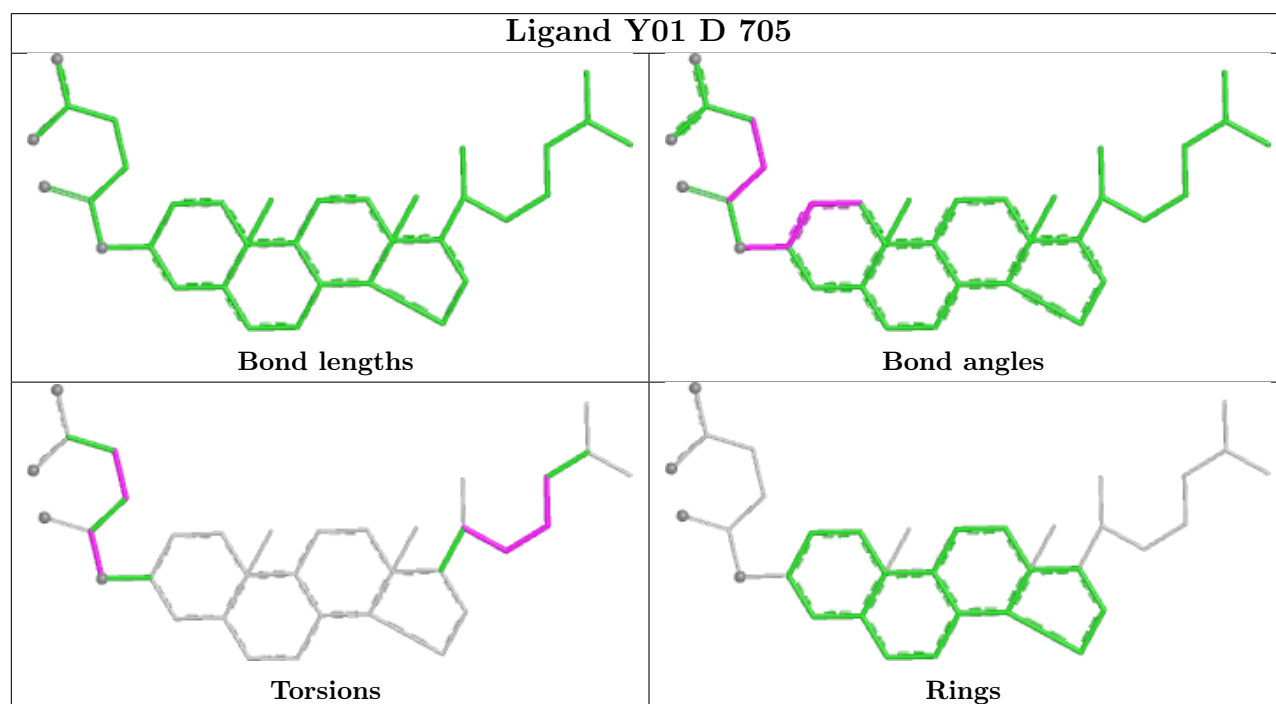
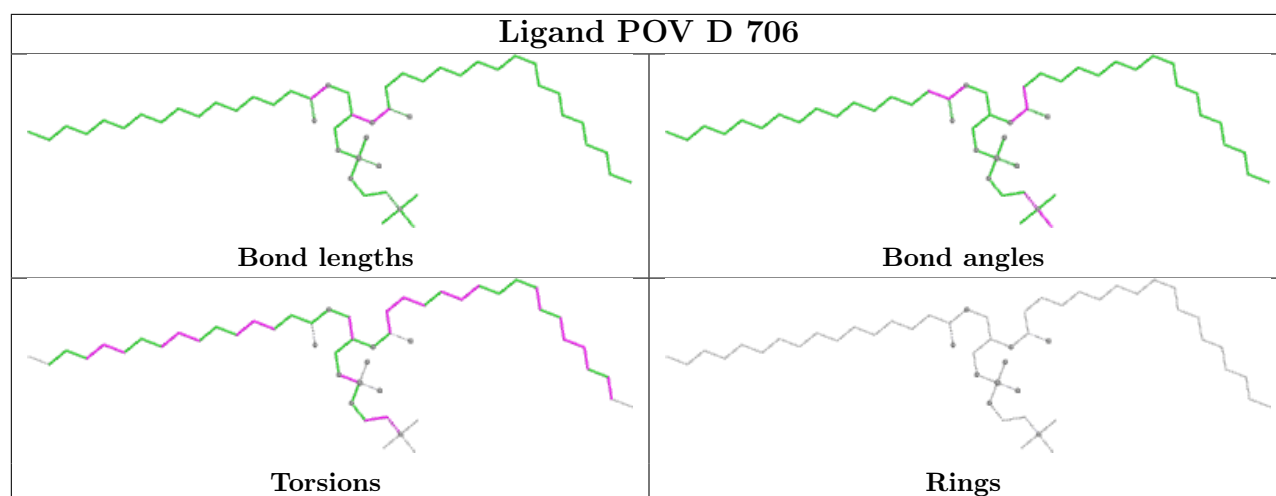


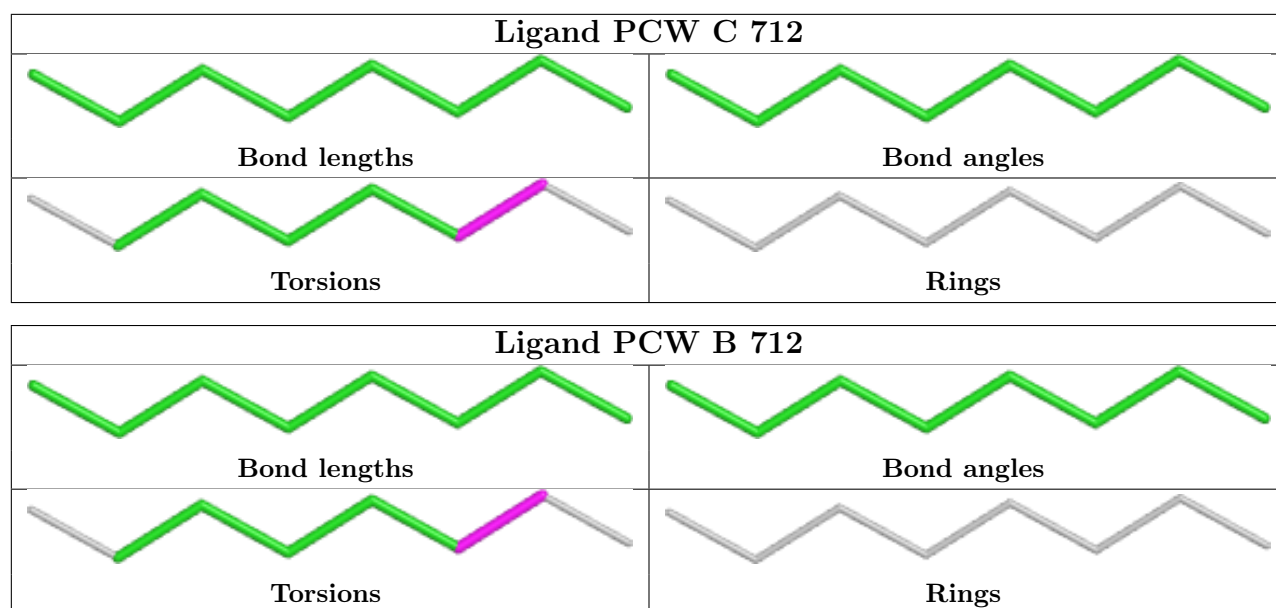


Ligand PCW A 809	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PCW B 715	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand Y01 B 701	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PCW C 705	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PCW D 703	
 Bond lengths	 Bond angles
 Torsions	 Rings









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.

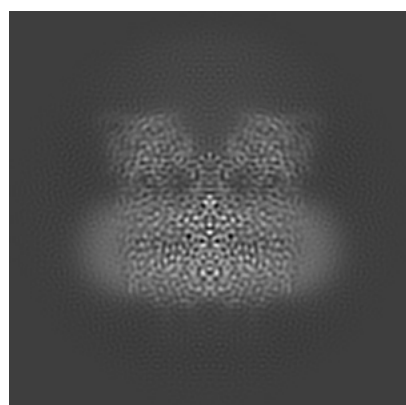
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24890. These allow visual inspection of the internal detail of the map and identification of artifacts.

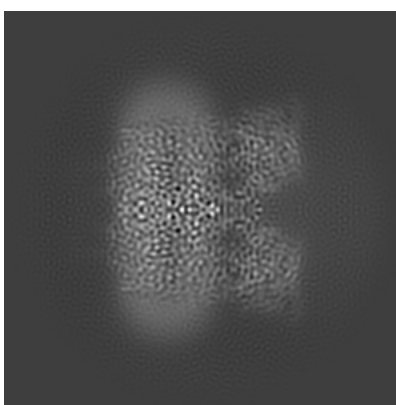
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

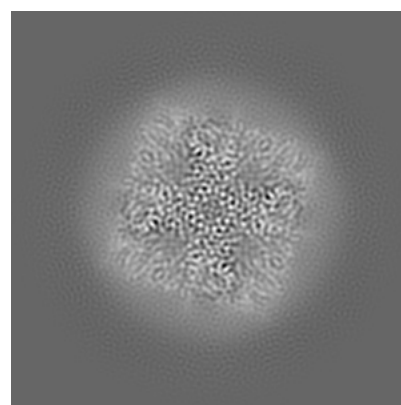
6.1.1 Primary map



X



Y

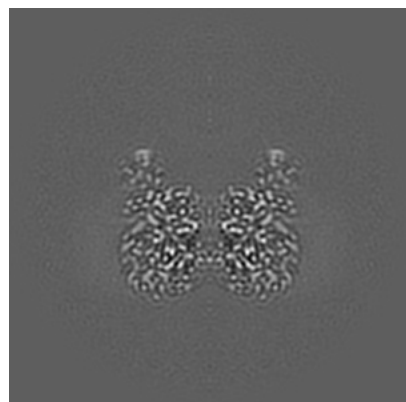


Z

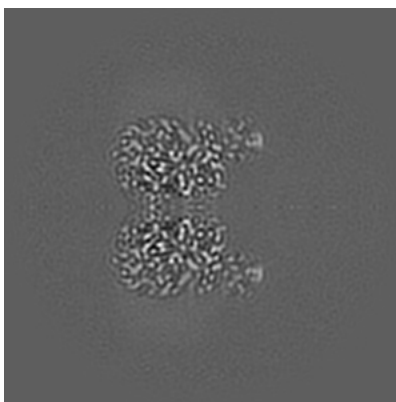
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

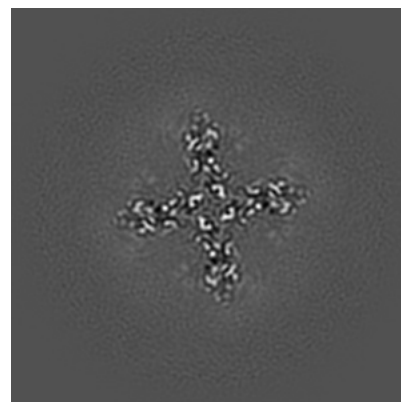
6.2.1 Primary map



X Index: 128



Y Index: 128

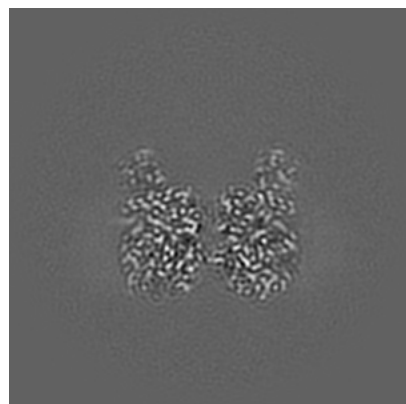


Z Index: 128

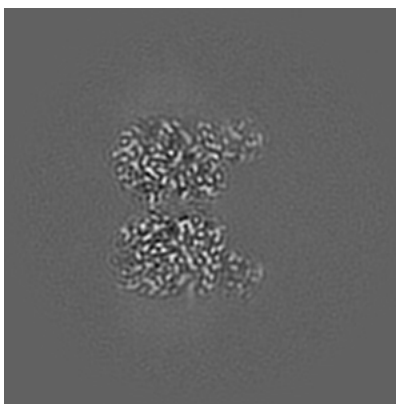
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

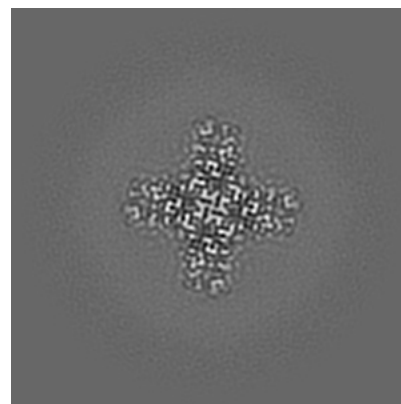
6.3.1 Primary map



X Index: 129



Y Index: 127

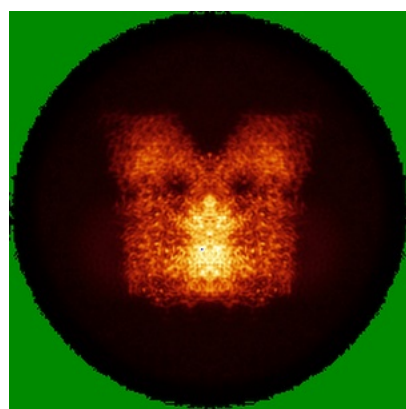


Z Index: 95

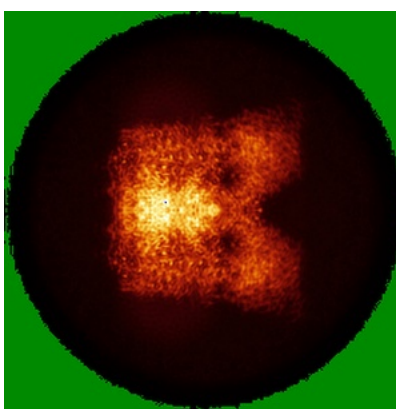
The images above show the largest variance slices of the map in three orthogonal directions.

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

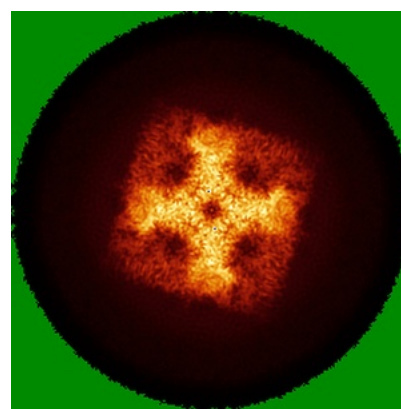
6.4.1 Primary map



X



Y

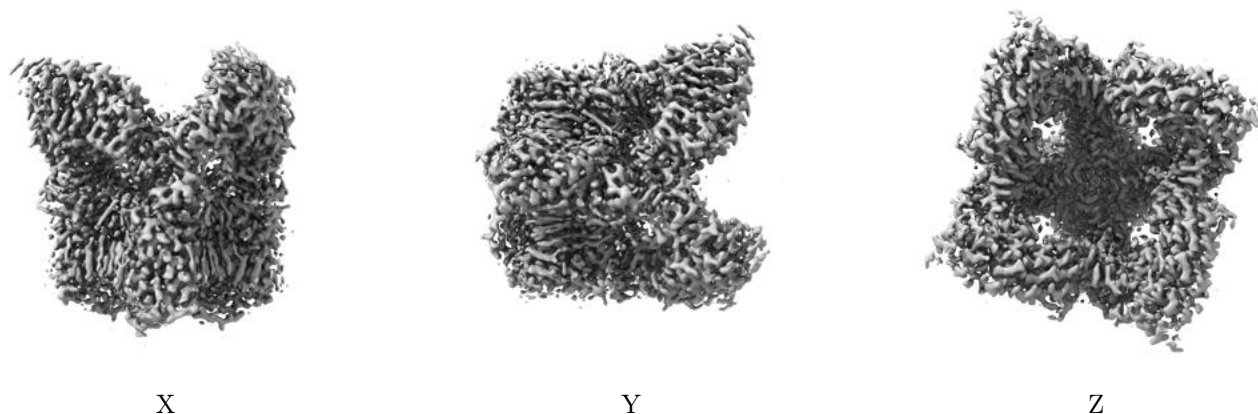


Z

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

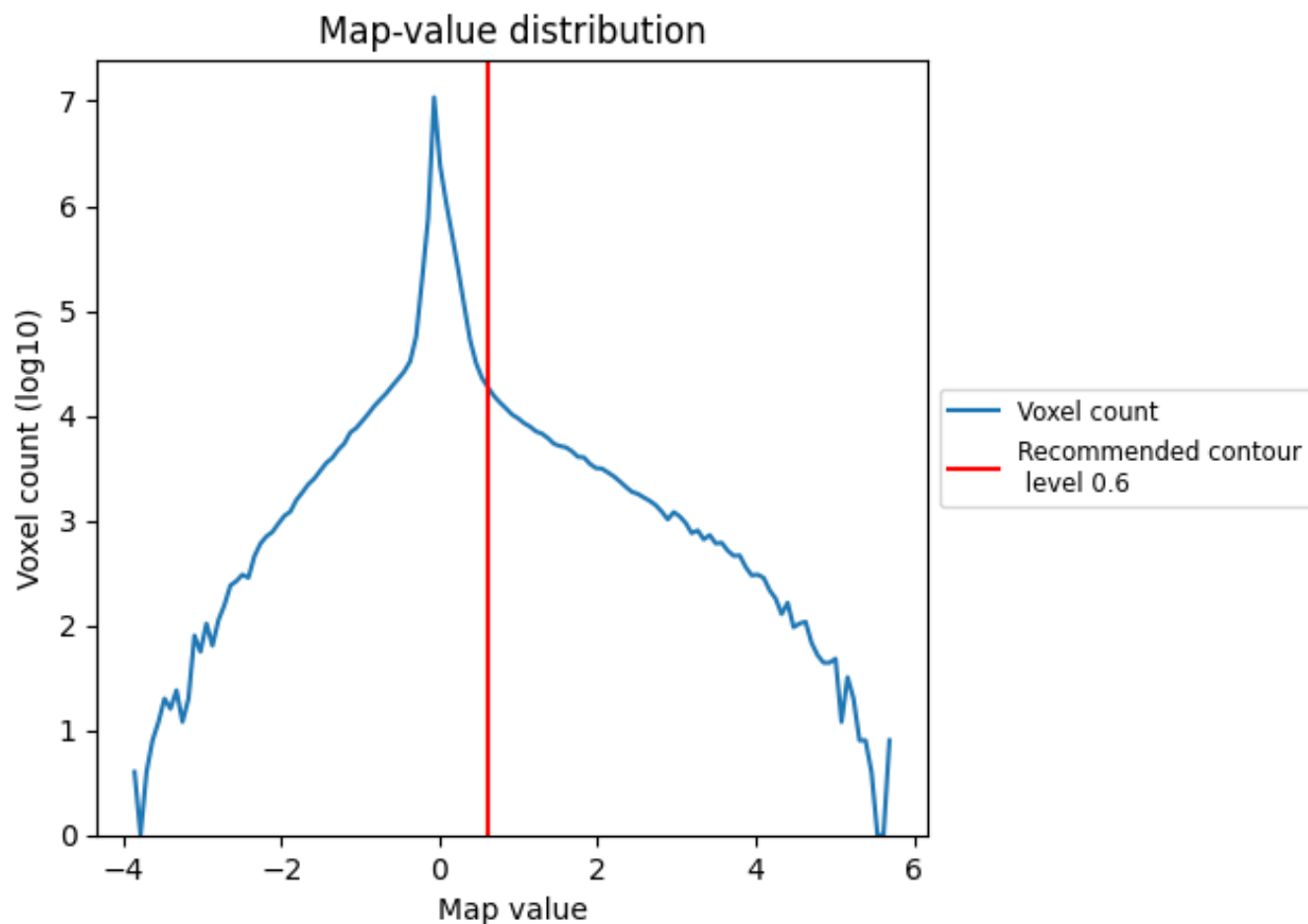
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

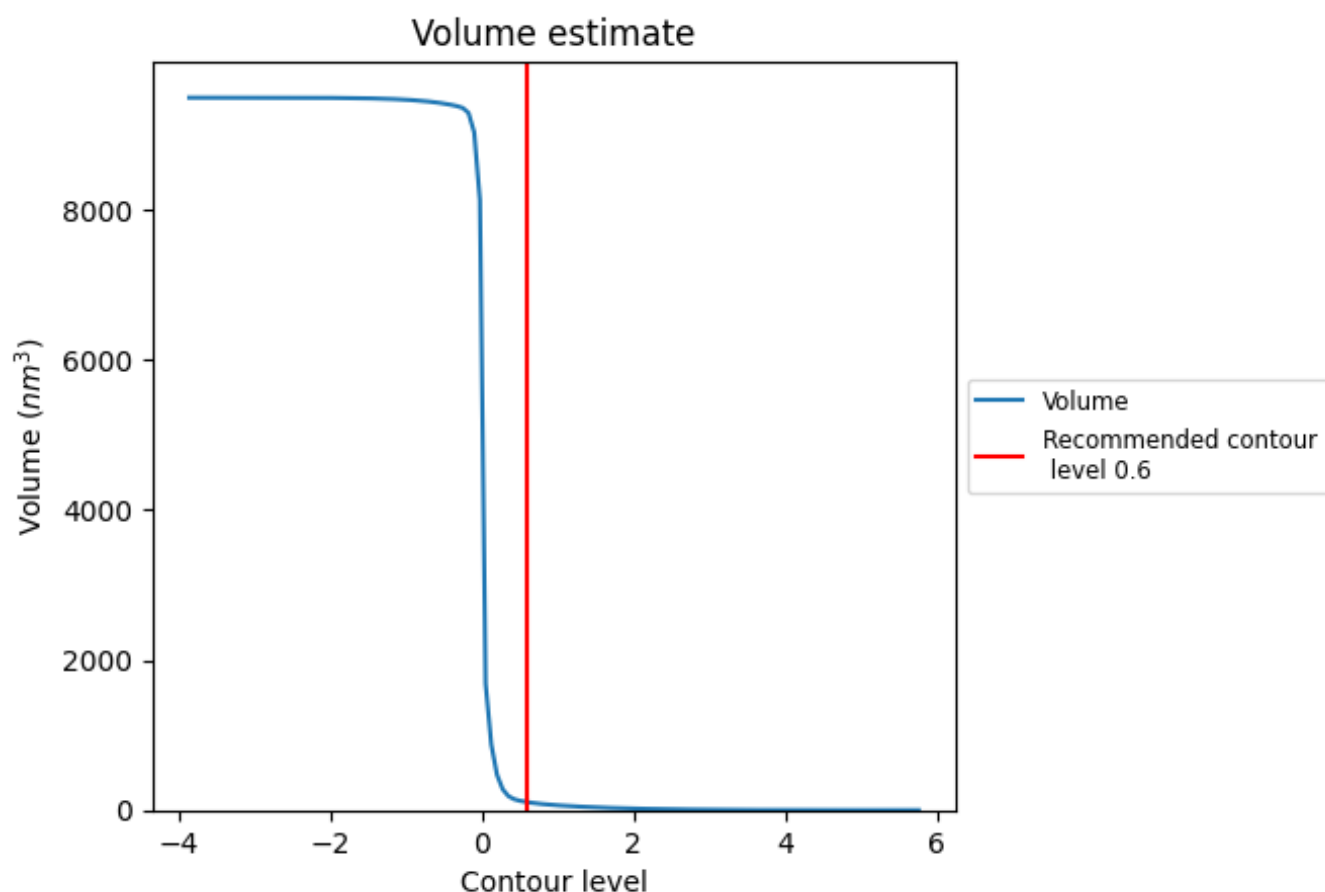
This section contains the results of statistical analysis of the map.

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.

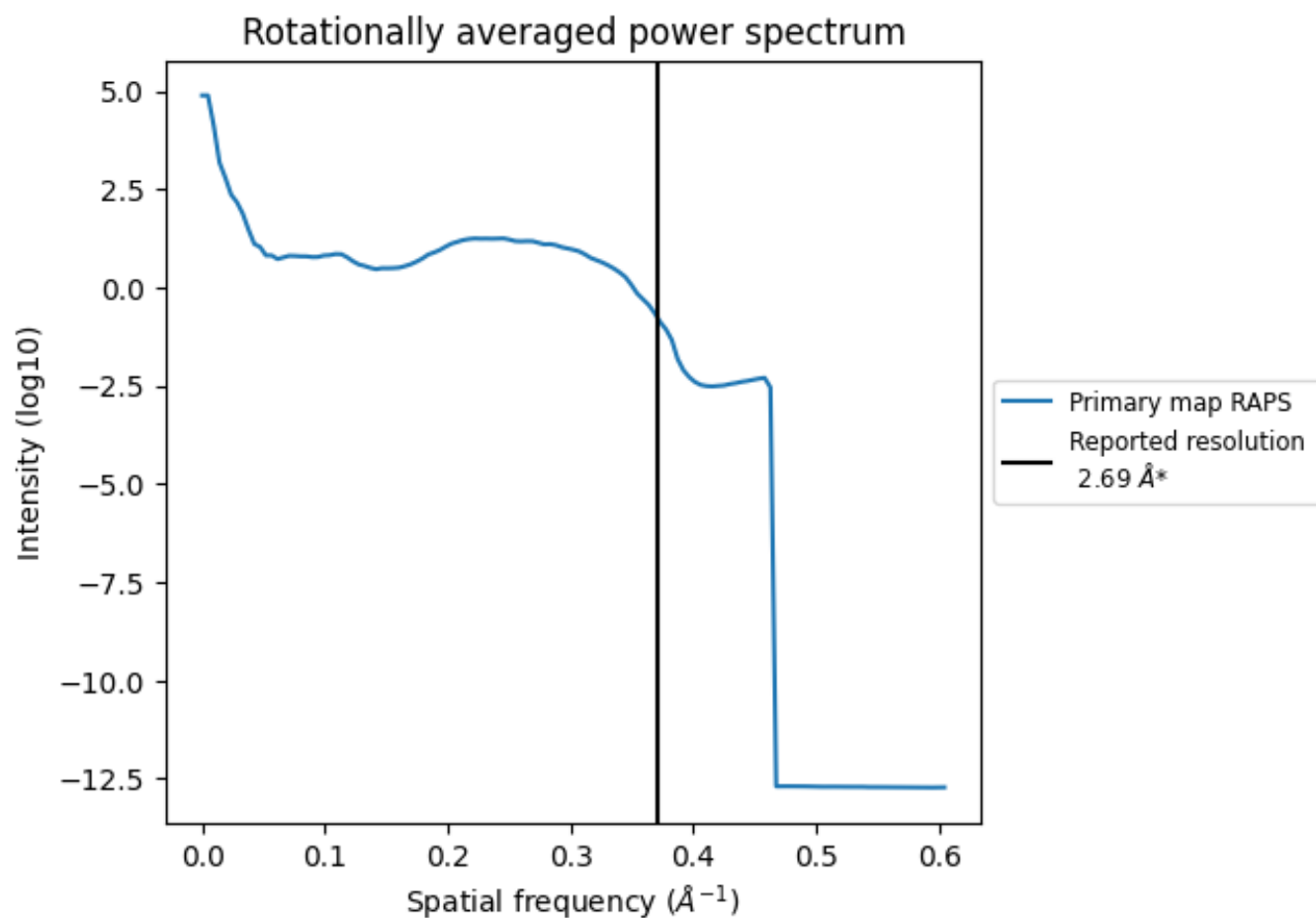
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm^3 ; this corresponds to an approximate mass of 97 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 0.372 Å⁻¹

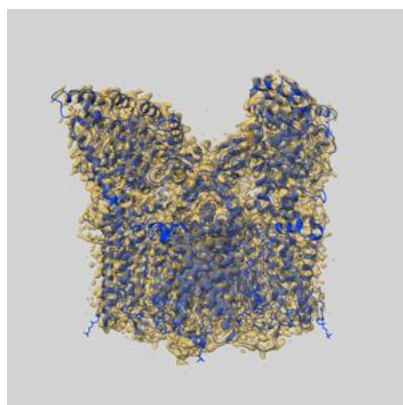
8 Fourier-Shell correlation

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

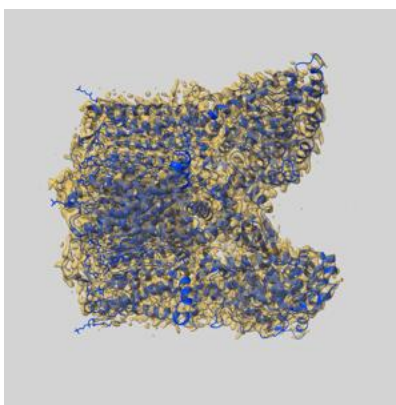
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24890 and PDB model 7S88. Per-residue inclusion information can be found in section 3 on page 10.

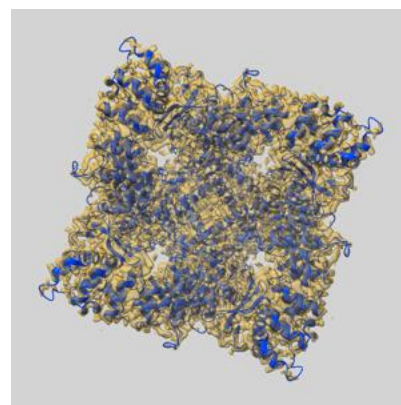
9.1 Map-model overlay [i](#)



X



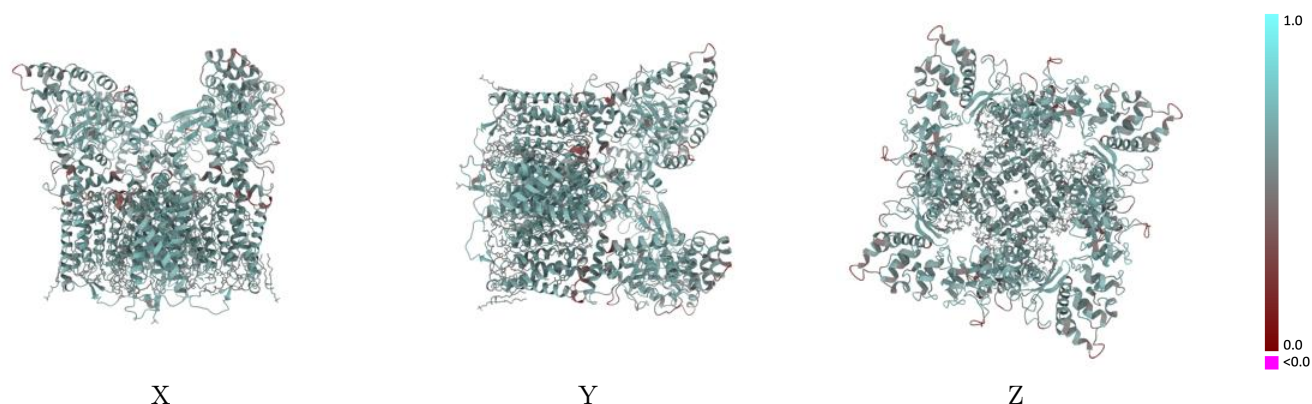
Y



Z

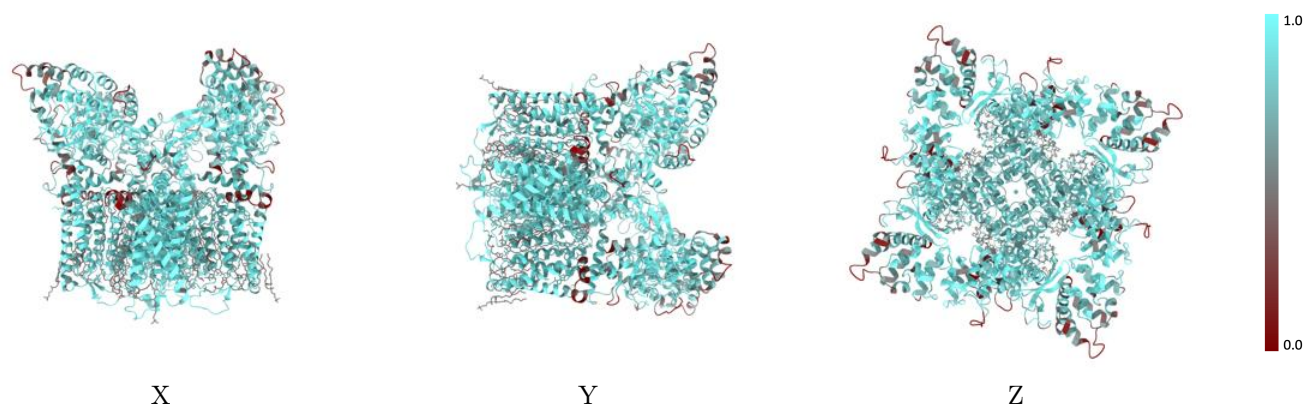
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



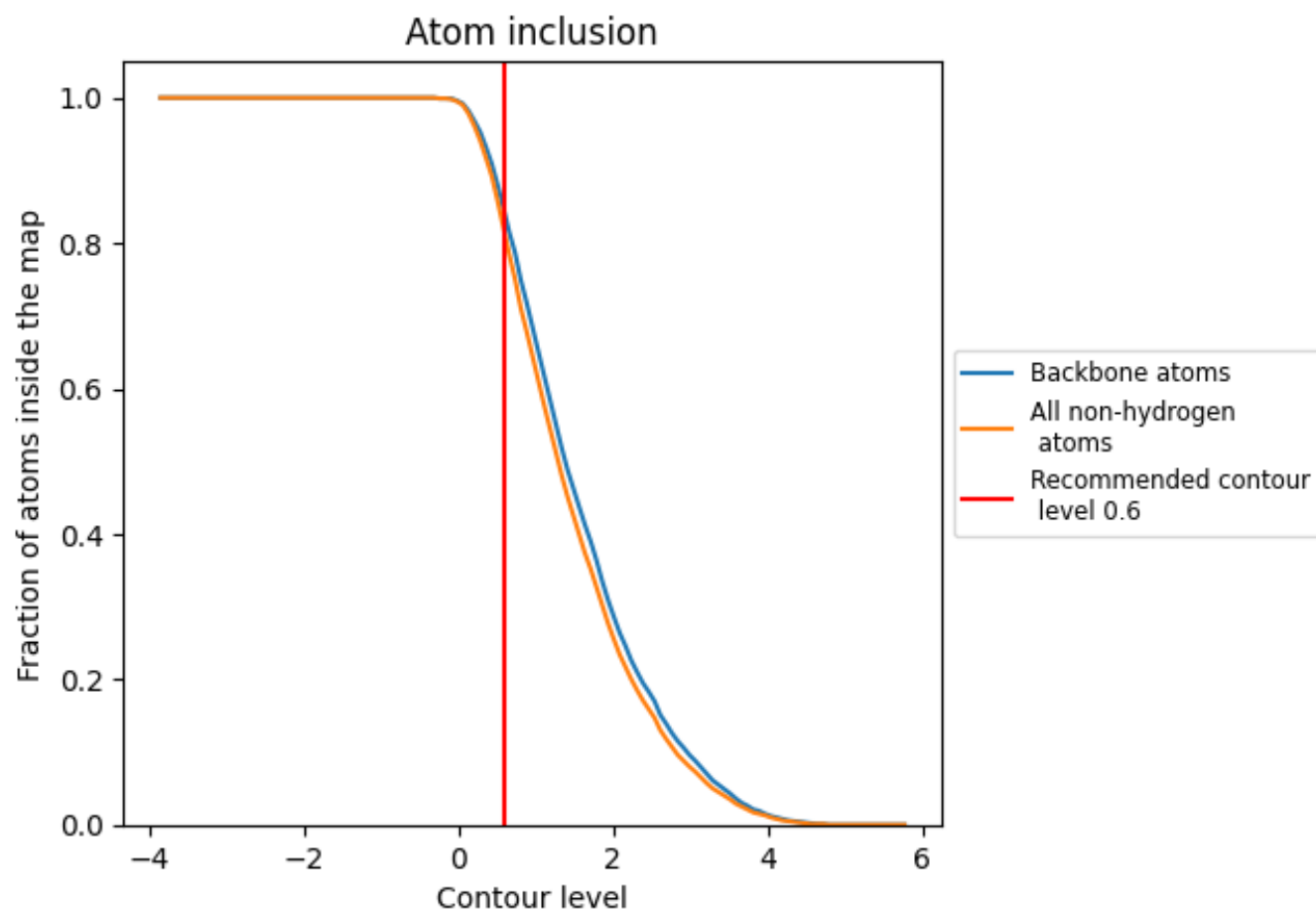
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.5940
A	0.8160	0.5930
B	0.8180	0.5960
C	0.8160	0.5940
D	0.8170	0.5930

