



Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 05:02 PM EDT

PDB ID : 5IRZ
EMDB ID : EMD-8118
Title : Structure of TRPV1 determined in lipid nanodisc
Authors : Gao, Y.; Cao, E.; Julius, D.; Cheng, Y.
Deposited on : 2016-03-15
Resolution : 3.28 Å(reported)
Based on initial model : 3J5P

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

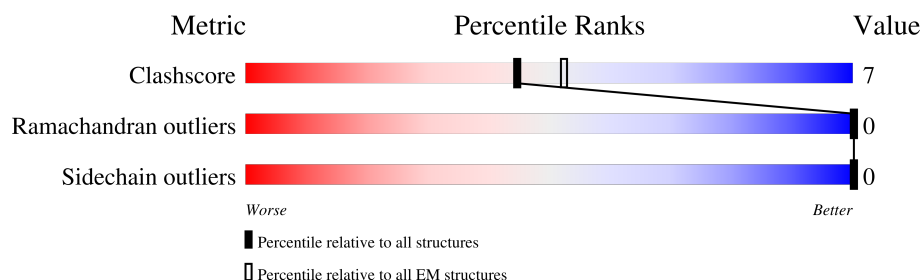
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	636	
1	C	636	
1	D	636	
1	E	636	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13312 atoms, of which 808 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.

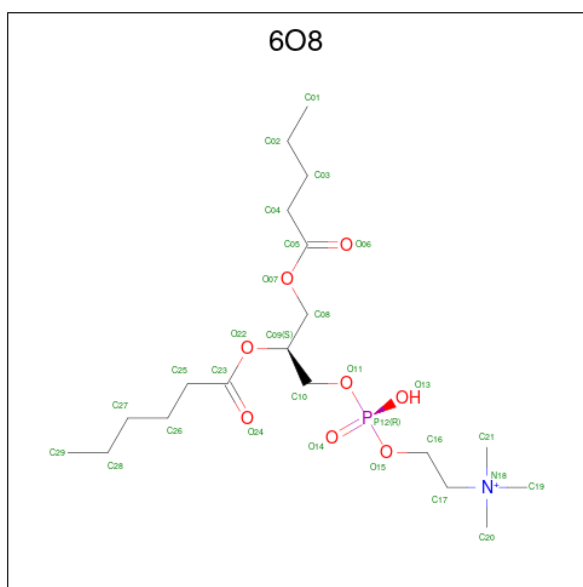
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	394	Total	C	N	O	S	0	0
			2951	1954	483	496	18		
1	E	394	Total	C	N	O	S	0	0
			2951	1954	483	496	18		
1	B	394	Total	C	N	O	S	0	0
			2951	1954	483	496	18		
1	C	394	Total	C	N	O	S	0	0
			2951	1954	483	496	18		

There are 16 discrepancies between the modelled and reference sequences:

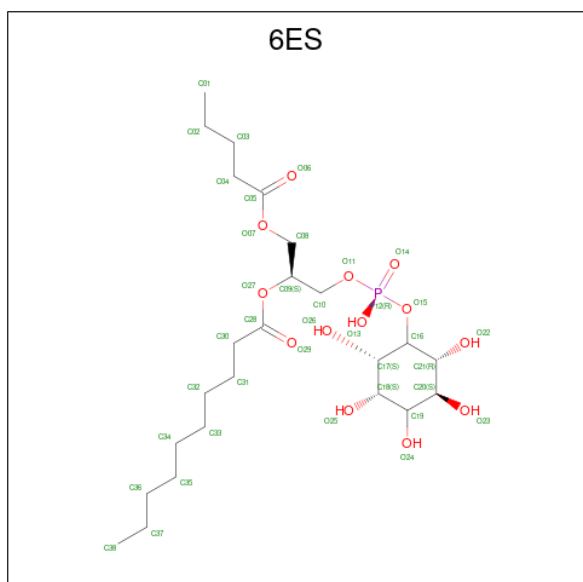
Chain	Residue	Modelled	Actual	Comment	Reference
D	106	ALA	-	expression tag	UNP O35433
D	107	MET	-	expression tag	UNP O35433
D	108	GLY	-	expression tag	UNP O35433
D	109	SER	-	expression tag	UNP O35433
E	106	ALA	-	expression tag	UNP O35433
E	107	MET	-	expression tag	UNP O35433
E	108	GLY	-	expression tag	UNP O35433
E	109	SER	-	expression tag	UNP O35433
B	106	ALA	-	expression tag	UNP O35433
B	107	MET	-	expression tag	UNP O35433
B	108	GLY	-	expression tag	UNP O35433
B	109	SER	-	expression tag	UNP O35433
C	106	ALA	-	expression tag	UNP O35433
C	107	MET	-	expression tag	UNP O35433
C	108	GLY	-	expression tag	UNP O35433
C	109	SER	-	expression tag	UNP O35433

- Molecule 2 is (4R,7S)-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-7-[(pentanoyloxy)methyl]-3,5,8-trioxa-4lambda 5 -phosphatetradecan-1-aminium (three-letter code: 6O8) (formula: C₁₉H₃₉NO₈P).



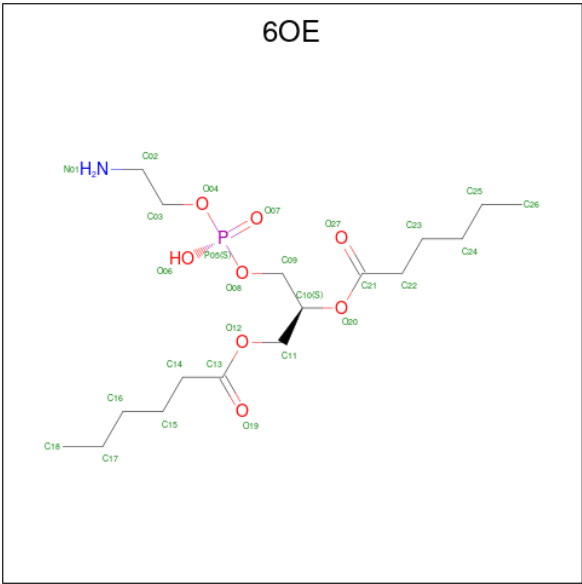
Mol	Chain	Residues	Atoms					AltConf	
2	D	1	Total 65	C 19	H 36	N 1	O 8	P 1	0
2	E	1	Total 65	C 19	H 36	N 1	O 8	P 1	0
2	B	1	Total 65	C 19	H 36	N 1	O 8	P 1	0
2	C	1	Total 65	C 19	H 36	N 1	O 8	P 1	0

- Molecule 3 is (2S)-1-{[(R)-hydroxy{[(1R,2R,3S,4S,5S,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}-3-(pentanoyloxy)propan-2-yl decanoate (three-letter code: 6ES) (formula: C₂₄H₄₅O₁₃P).



Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	H	O	P	0
			80	24	42	13	1	
3	E	1	Total	C	H	O	P	0
			80	24	42	13	1	
3	B	1	Total	C	H	O	P	0
			80	24	42	13	1	
3	C	1	Total	C	H	O	P	0
			80	24	42	13	1	

- Molecule 4 is (2S)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(hexanoyloxy)propyl hexanoate (three-letter code: 6OE) (formula: C₁₇H₃₄NO₈P).



Mol	Chain	Residues	Atoms						AltConf
4	D	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	D	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	D	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	D	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	E	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	E	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	E	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	

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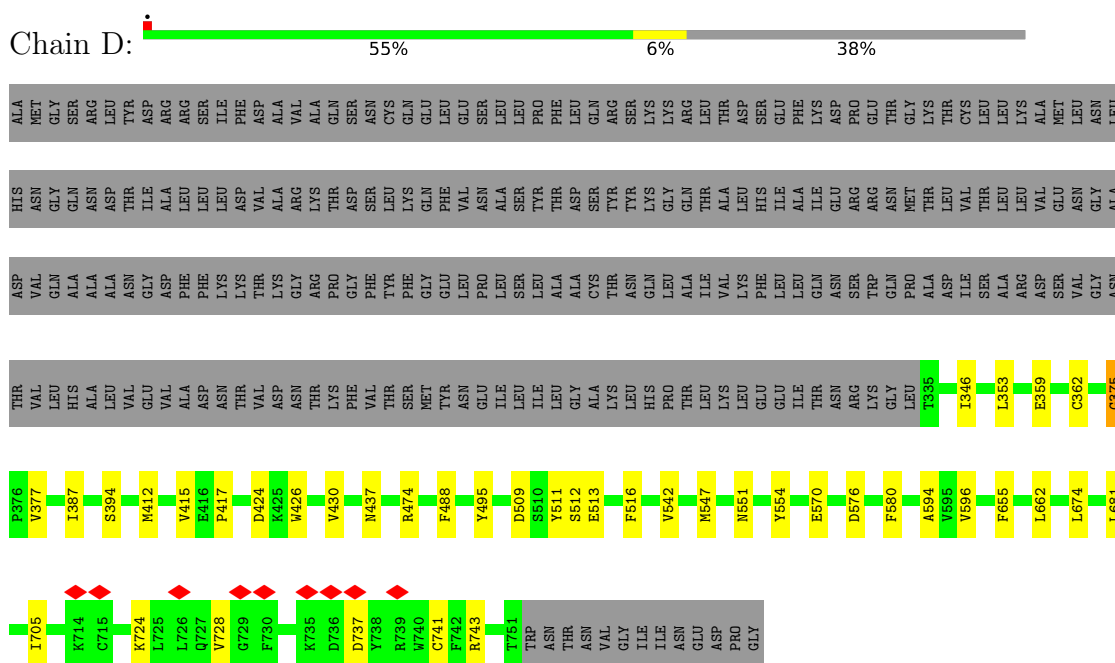
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Mol	Chain	Residues	Atoms						AltConf
4	E	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	B	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	B	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	B	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	B	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	C	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	C	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	C	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	
4	C	1	Total	C	H	N	O	P	0
			232	68	124	4	32	4	

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.

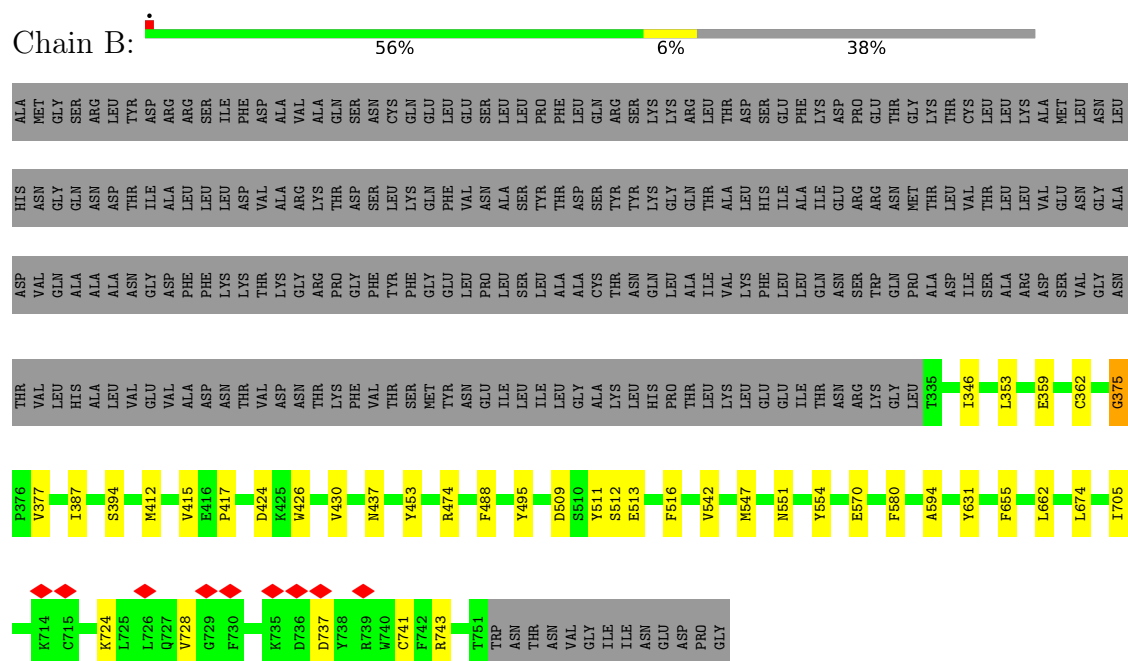
- Molecule 1: Transient receptor potential cation channel subfamily V member 1



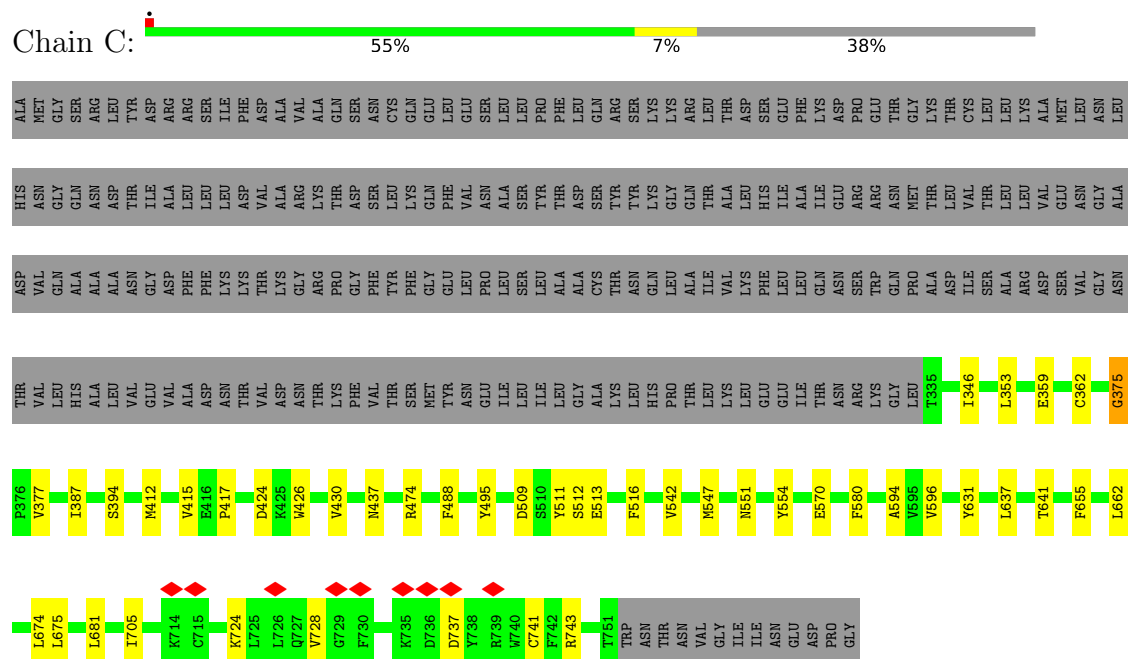
- Molecule 1: Transient receptor potential cation channel subfamily V member 1



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	30689	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed before classification and refinement.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	41132	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.052	Depositor
Minimum map value	-12.106	Depositor
Average map value	-0.308	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (\AA)	233.3952, 233.3952, 233.3952	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6O8, 6ES, 6OE

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	B	0.42	0/3019	0.56	0/4100
1	C	0.42	0/3019	0.56	0/4100
1	D	0.42	0/3019	0.56	0/4100
1	E	0.42	0/3019	0.56	0/4100
All	All	0.42	0/12076	0.56	0/16400

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	375	GLY	Peptide
1	C	375	GLY	Peptide
1	D	375	GLY	Peptide
1	E	375	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2951	0	2788	41	0
1	C	2951	0	2788	46	0
1	D	2951	0	2788	43	0
1	E	2951	0	2788	41	0
2	B	29	36	0	9	0
2	C	29	36	0	9	0
2	D	29	36	0	9	0
2	E	29	36	0	9	0
3	B	38	42	0	10	0
3	C	38	42	0	10	0
3	D	38	42	0	10	0
3	E	38	42	0	10	0
4	B	108	124	0	3	0
4	C	108	124	0	4	0
4	D	108	124	0	3	0
4	E	108	124	0	3	0
All	All	12504	808	11152	161	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 (161) 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:512:SER:N	3:B:802:6ES:O14	1.74	1.21
1:C:512:SER:N	3:C:802:6ES:O14	1.74	1.20
1:D:512:SER:N	3:D:802:6ES:O14	1.73	1.18
1:E:512:SER:N	3:E:802:6ES:O14	1.73	1.17
1:B:516:PHE:HE2	2:B:801:6O8:C20	1.80	0.94
1:C:516:PHE:HE2	2:C:801:6O8:C20	1.80	0.93
1:E:516:PHE:HE2	2:E:801:6O8:C20	1.82	0.92
1:D:516:PHE:HE2	2:D:801:6O8:C20	1.81	0.91
1:C:488:PHE:CZ	2:C:801:6O8:O24	2.26	0.89
1:B:512:SER:CB	3:B:802:6ES:O14	2.23	0.86
1:D:488:PHE:CZ	2:D:801:6O8:O24	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:PHE:CZ	2:E:801:6O8:O24	2.29	0.85
1:D:512:SER:CB	3:D:802:6ES:O14	2.24	0.84
1:B:488:PHE:CZ	2:B:801:6O8:O24	2.29	0.84
1:E:512:SER:CB	3:E:802:6ES:O14	2.26	0.84
1:C:512:SER:CB	3:C:802:6ES:O14	2.27	0.82
1:E:509:ASP:O	3:E:802:6ES:O22	2.01	0.78
1:D:509:ASP:O	3:D:802:6ES:O22	2.01	0.77
1:C:554:TYR:CE2	2:C:801:6O8:C20	2.68	0.77
1:B:509:ASP:O	3:B:802:6ES:O22	2.02	0.75
1:B:554:TYR:CE2	2:B:801:6O8:C20	2.70	0.75
1:C:509:ASP:O	3:C:802:6ES:O22	2.04	0.75
1:D:554:TYR:CE2	2:D:801:6O8:C20	2.71	0.74
1:E:554:TYR:CE2	2:E:801:6O8:C20	2.71	0.73
1:B:511:TYR:HB3	3:B:802:6ES:O06	1.89	0.73
1:E:511:TYR:HB3	3:E:802:6ES:O06	1.88	0.73
1:D:511:TYR:HB3	3:D:802:6ES:O06	1.88	0.72
1:C:516:PHE:CE2	2:C:801:6O8:C20	2.67	0.71
1:C:511:TYR:HB3	3:C:802:6ES:O06	1.92	0.69
1:B:512:SER:CA	3:B:802:6ES:O14	2.41	0.69
1:D:512:SER:CA	3:D:802:6ES:O14	2.41	0.68
1:E:512:SER:CA	3:E:802:6ES:O14	2.42	0.68
1:D:516:PHE:CE2	2:D:801:6O8:C20	2.68	0.67
1:D:426:TRP:HA	1:D:430:VAL:HG12	1.76	0.67
1:E:426:TRP:HA	1:E:430:VAL:HG12	1.76	0.67
1:C:426:TRP:HA	1:C:430:VAL:HG12	1.76	0.66
1:B:426:TRP:HA	1:B:430:VAL:HG12	1.76	0.66
1:C:512:SER:CA	3:C:802:6ES:O14	2.43	0.66
1:C:570:GLU:OE2	3:C:802:6ES:O25	2.17	0.62
1:E:516:PHE:CE2	2:E:801:6O8:C20	2.69	0.61
1:B:516:PHE:CE2	2:B:801:6O8:C20	2.68	0.61
1:B:570:GLU:OE2	3:B:802:6ES:O25	2.18	0.61
1:E:570:GLU:OE2	3:E:802:6ES:O25	2.19	0.60
1:D:570:GLU:OE2	3:D:802:6ES:O25	2.19	0.60
1:C:724:LYS:HG2	1:C:741:CYS:HB3	1.83	0.60
1:D:724:LYS:HG2	1:D:741:CYS:HB3	1.83	0.59
1:C:554:TYR:CZ	2:C:801:6O8:C20	2.85	0.59
1:B:724:LYS:HG2	1:B:741:CYS:HB3	1.83	0.59
1:E:724:LYS:HG2	1:E:741:CYS:HB3	1.83	0.59
1:C:488:PHE:CE1	2:C:801:6O8:O24	2.55	0.58
1:B:488:PHE:CE1	2:B:801:6O8:O24	2.57	0.58
1:D:488:PHE:CE1	2:D:801:6O8:O24	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:PHE:CE1	2:E:801:6O8:O24	2.56	0.58
1:C:437:ASN:OD1	2:C:801:6O8:O06	2.22	0.58
1:E:554:TYR:CZ	2:E:801:6O8:C20	2.88	0.57
1:D:554:TYR:CZ	2:D:801:6O8:C20	2.88	0.56
1:B:554:TYR:CZ	2:B:801:6O8:C20	2.88	0.56
1:B:512:SER:HB2	3:B:802:6ES:O14	2.04	0.56
1:C:516:PHE:CE2	2:C:801:6O8:C16	2.89	0.56
1:E:655:PHE:HD1	4:E:803:6OE:C09	2.19	0.55
1:E:437:ASN:OD1	2:E:801:6O8:O06	2.25	0.55
1:C:512:SER:HB2	3:C:802:6ES:O14	2.06	0.54
1:B:437:ASN:OD1	2:B:801:6O8:O06	2.26	0.54
1:D:512:SER:HB2	3:D:802:6ES:O14	2.05	0.54
1:B:512:SER:HB3	3:B:802:6ES:O14	2.06	0.53
1:B:512:SER:HB2	3:B:802:6ES:P12	2.49	0.53
1:D:655:PHE:HD1	4:D:804:6OE:C09	2.21	0.53
1:D:437:ASN:OD1	2:D:801:6O8:O06	2.26	0.52
1:C:655:PHE:HD1	4:C:806:6OE:C09	2.22	0.52
1:D:512:SER:HB2	3:D:802:6ES:P12	2.49	0.52
1:D:516:PHE:CE2	2:D:801:6O8:C16	2.93	0.52
1:E:516:PHE:CE2	2:E:801:6O8:C16	2.93	0.51
1:B:516:PHE:CE2	2:B:801:6O8:C16	2.93	0.51
1:B:655:PHE:HD1	4:B:806:6OE:C09	2.23	0.51
1:E:512:SER:HB2	3:E:802:6ES:P12	2.50	0.51
1:E:512:SER:HB3	3:E:802:6ES:O14	2.09	0.50
1:C:424:ASP:HB2	1:C:743:ARG:HH21	1.76	0.50
1:B:511:TYR:CB	3:B:802:6ES:O06	2.60	0.50
1:B:424:ASP:HB2	1:B:743:ARG:HH21	1.76	0.49
1:E:512:SER:HB2	3:E:802:6ES:O14	2.07	0.49
1:C:512:SER:HB2	3:C:802:6ES:P12	2.52	0.49
1:C:512:SER:HB3	3:C:802:6ES:O14	2.10	0.49
1:E:511:TYR:CB	3:E:802:6ES:O06	2.59	0.49
1:E:424:ASP:HB2	1:E:743:ARG:HH21	1.77	0.48
1:D:424:ASP:HB2	1:D:743:ARG:HH21	1.76	0.48
1:E:513:GLU:OE1	2:E:801:6O8:C21	2.61	0.48
1:D:512:SER:HB3	3:D:802:6ES:O14	2.07	0.48
1:D:511:TYR:CB	3:D:802:6ES:O06	2.59	0.48
1:D:513:GLU:OE1	2:D:801:6O8:C21	2.62	0.48
1:C:513:GLU:OE1	2:C:801:6O8:C21	2.62	0.48
1:E:375:GLY:O	1:E:377:VAL:N	2.48	0.47
1:C:375:GLY:O	1:C:377:VAL:N	2.48	0.47
1:D:375:GLY:O	1:D:377:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:728:VAL:H	1:E:737:ASP:HA	1.80	0.47
1:C:511:TYR:CB	3:C:802:6ES:O06	2.63	0.47
1:D:728:VAL:H	1:D:737:ASP:HA	1.80	0.47
1:E:655:PHE:CD1	4:E:803:6OE:C09	2.98	0.47
1:B:513:GLU:OE1	2:B:801:6O8:C21	2.63	0.47
1:B:375:GLY:O	1:B:377:VAL:N	2.48	0.46
1:B:728:VAL:H	1:B:737:ASP:HA	1.80	0.46
1:D:430:VAL:HG11	1:D:705:ILE:HG12	1.98	0.45
1:D:594:ALA:HB1	1:B:542:VAL:HG13	1.99	0.45
1:D:415:VAL:HG12	1:D:417:PRO:HD2	1.99	0.45
1:C:728:VAL:H	1:C:737:ASP:HA	1.80	0.45
1:B:594:ALA:HB1	1:C:542:VAL:HG13	1.99	0.45
1:C:415:VAL:HG12	1:C:417:PRO:HD2	1.99	0.45
1:B:415:VAL:HG12	1:B:417:PRO:HD2	1.99	0.45
1:E:415:VAL:HG12	1:E:417:PRO:HD2	1.99	0.45
1:B:495:TYR:CG	1:B:513:GLU:HG2	2.52	0.45
1:E:474:ARG:HB3	4:E:805:6OE:C15	2.47	0.45
1:D:359:GLU:HB3	1:D:362:CYS:HB2	1.99	0.45
1:E:359:GLU:HB3	1:E:362:CYS:HB2	1.99	0.45
1:E:542:VAL:HG11	1:C:662:LEU:HD11	1.98	0.45
1:B:359:GLU:HB3	1:B:362:CYS:HB2	1.99	0.45
1:C:495:TYR:CG	1:C:513:GLU:HG2	2.52	0.45
1:E:353:LEU:HB3	1:E:417:PRO:HG2	1.99	0.44
1:B:430:VAL:HG11	1:B:705:ILE:HG12	1.98	0.44
1:E:430:VAL:HG11	1:E:705:ILE:HG12	1.98	0.44
1:C:430:VAL:HG11	1:C:705:ILE:HG12	1.98	0.44
1:D:495:TYR:CG	1:D:513:GLU:HG2	2.52	0.44
1:E:495:TYR:CG	1:E:513:GLU:HG2	2.52	0.44
1:C:353:LEU:HB3	1:C:417:PRO:HG2	1.99	0.44
1:D:353:LEU:HB3	1:D:417:PRO:HG2	1.99	0.44
1:C:359:GLU:HB3	1:C:362:CYS:HB2	1.99	0.44
1:D:576:ASP:O	1:D:580:PHE:N	2.46	0.44
1:E:453:TYR:CE1	1:C:596:VAL:HG11	2.53	0.44
1:D:542:VAL:HG13	1:E:594:ALA:HB1	1.99	0.43
1:D:580:PHE:HE1	1:D:674:LEU:HB3	1.84	0.43
1:E:542:VAL:HG13	1:C:594:ALA:HB1	2.00	0.43
1:B:353:LEU:HB3	1:B:417:PRO:HG2	1.99	0.43
1:D:474:ARG:HB3	4:D:806:6OE:C15	2.49	0.43
1:D:542:VAL:HG11	1:E:662:LEU:HD11	2.01	0.43
1:D:662:LEU:HD11	1:B:542:VAL:HG11	1.99	0.43
1:C:637:LEU:HD23	1:C:637:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:LEU:HD11	1:C:542:VAL:HG11	2.00	0.43
1:E:580:PHE:HE1	1:E:674:LEU:HB3	1.83	0.43
1:C:631:TYR:CE1	4:C:805:6OE:C22	3.02	0.43
1:D:655:PHE:CD1	4:D:804:6OE:C09	3.02	0.42
1:B:580:PHE:HE1	1:B:674:LEU:HB3	1.84	0.42
1:D:547:MET:HG3	1:D:551:ASN:HD21	1.85	0.42
1:B:474:ARG:HB3	4:B:804:6OE:C15	2.49	0.42
1:B:547:MET:HG3	1:B:551:ASN:HD21	1.85	0.42
1:C:547:MET:HG3	1:C:551:ASN:HD21	1.85	0.42
1:C:387:ILE:O	1:C:394:SER:OG	2.38	0.41
1:C:580:PHE:HE1	1:C:674:LEU:HB3	1.83	0.41
1:E:387:ILE:O	1:E:394:SER:OG	2.38	0.41
1:B:631:TYR:CE1	4:B:805:6OE:C22	3.04	0.41
1:D:346:ILE:HG22	1:D:412:MET:HG2	2.03	0.41
1:B:387:ILE:O	1:B:394:SER:OG	2.38	0.41
1:C:474:ARG:HB3	4:C:804:6OE:C15	2.50	0.41
1:D:387:ILE:O	1:D:394:SER:OG	2.38	0.41
1:D:596:VAL:HG11	1:B:453:TYR:CE1	2.55	0.41
1:D:681:LEU:HD23	1:D:681:LEU:HA	1.93	0.41
1:E:547:MET:HG3	1:E:551:ASN:HD21	1.85	0.41
1:C:681:LEU:HD23	1:C:681:LEU:HA	1.93	0.41
1:B:346:ILE:HG22	1:B:412:MET:HG2	2.03	0.41
1:C:655:PHE:CD1	4:C:806:6OE:C09	3.02	0.40
1:C:346:ILE:HG22	1:C:412:MET:HG2	2.03	0.40
1:C:516:PHE:HE1	1:C:551:ASN:HB3	1.86	0.40
1:E:641:THR:HG23	1:E:675:LEU:HD11	2.04	0.40
1:C:641:THR:HG23	1:C:675:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	392/636 (62%)	362 (92%)	30 (8%)	0	100	100
1	C	392/636 (62%)	363 (93%)	29 (7%)	0	100	100
1	D	392/636 (62%)	363 (93%)	29 (7%)	0	100	100
1	E	392/636 (62%)	363 (93%)	29 (7%)	0	100	100
All	All	1568/2544 (62%)	1451 (92%)	117 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	272/562 (48%)	272 (100%)	0	100	100
1	C	272/562 (48%)	272 (100%)	0	100	100
1	D	272/562 (48%)	272 (100%)	0	100	100
1	E	272/562 (48%)	272 (100%)	0	100	100
All	All	1088/2248 (48%)	1088 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	6OE	C	803	-	26,26,26	1.18	4 (15%)	29,31,31	0.97	2 (6%)
4	6OE	B	803	-	26,26,26	1.18	4 (15%)	29,31,31	0.97	2 (6%)
4	6OE	D	805	-	26,26,26	1.18	4 (15%)	29,31,31	0.98	2 (6%)
4	6OE	D	803	-	26,26,26	1.17	3 (11%)	29,31,31	0.93	2 (6%)
4	6OE	C	806	-	26,26,26	1.16	4 (15%)	29,31,31	0.96	2 (6%)
3	6ES	B	802	-	38,38,38	1.20	3 (7%)	48,50,50	1.31	5 (10%)
3	6ES	E	802	-	38,38,38	1.20	3 (7%)	48,50,50	1.31	5 (10%)
4	6OE	D	804	-	26,26,26	1.16	4 (15%)	29,31,31	0.96	2 (6%)
2	6O8	C	801	-	28,28,28	1.55	7 (25%)	34,36,36	1.28	4 (11%)
4	6OE	B	806	-	26,26,26	1.15	4 (15%)	29,31,31	0.96	2 (6%)
3	6ES	C	802	-	38,38,38	1.20	3 (7%)	48,50,50	1.32	5 (10%)
4	6OE	E	804	-	26,26,26	1.18	4 (15%)	29,31,31	0.98	2 (6%)
4	6OE	B	804	-	26,26,26	1.16	4 (15%)	29,31,31	1.13	2 (6%)
4	6OE	C	805	-	26,26,26	1.17	3 (11%)	29,31,31	0.93	2 (6%)
3	6ES	D	802	-	38,38,38	1.20	3 (7%)	48,50,50	1.31	5 (10%)
2	6O8	E	801	-	28,28,28	1.54	7 (25%)	34,36,36	1.27	4 (11%)
4	6OE	E	806	-	26,26,26	1.17	3 (11%)	29,31,31	0.93	2 (6%)
4	6OE	D	806	-	26,26,26	1.16	4 (15%)	29,31,31	1.13	2 (6%)
4	6OE	C	804	-	26,26,26	1.16	4 (15%)	29,31,31	1.13	2 (6%)
2	6O8	B	801	-	28,28,28	1.55	7 (25%)	34,36,36	1.27	4 (11%)
4	6OE	E	803	-	26,26,26	1.16	4 (15%)	29,31,31	0.96	2 (6%)
4	6OE	B	805	-	26,26,26	1.17	3 (11%)	29,31,31	0.92	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6O8	D	801	-	28,28,28	1.55	7 (25%)	34,36,36	1.27	4 (11%)
4	6OE	E	805	-	26,26,26	1.15	4 (15%)	29,31,31	1.13	2 (6%)

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	6OE	C	803	-	-	13/30/30/30	-
4	6OE	B	803	-	-	13/30/30/30	-
4	6OE	D	805	-	-	13/30/30/30	-
4	6OE	D	803	-	-	9/30/30/30	-
4	6OE	C	806	-	-	15/30/30/30	-
3	6ES	B	802	-	-	13/33/57/57	0/1/1/1
3	6ES	E	802	-	-	13/33/57/57	0/1/1/1
4	6OE	D	804	-	-	15/30/30/30	-
2	6O8	C	801	-	-	13/32/32/32	-
4	6OE	B	806	-	-	15/30/30/30	-
3	6ES	C	802	-	-	13/33/57/57	0/1/1/1
4	6OE	E	804	-	-	13/30/30/30	-
4	6OE	B	804	-	-	10/30/30/30	-
4	6OE	C	805	-	-	9/30/30/30	-
3	6ES	D	802	-	-	13/33/57/57	0/1/1/1
2	6O8	E	801	-	-	13/32/32/32	-
4	6OE	E	806	-	-	9/30/30/30	-
4	6OE	D	806	-	-	10/30/30/30	-
4	6OE	C	804	-	-	10/30/30/30	-
2	6O8	B	801	-	-	13/32/32/32	-
4	6OE	E	803	-	-	15/30/30/30	-
4	6OE	B	805	-	-	9/30/30/30	-
2	6O8	D	801	-	-	14/32/32/32	-
4	6OE	E	805	-	-	10/30/30/30	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	6ES	O27-C09	-2.96	1.39	1.46
3	E	802	6ES	O27-C09	-2.96	1.39	1.46
2	D	801	6O8	O22-C09	-2.94	1.39	1.46
2	E	801	6O8	O22-C09	-2.94	1.39	1.46
2	B	801	6O8	O22-C09	-2.94	1.39	1.46
3	B	802	6ES	O27-C09	-2.94	1.39	1.46
3	C	802	6ES	O27-C09	-2.92	1.39	1.46
2	C	801	6O8	O22-C09	-2.91	1.39	1.46
2	C	801	6O8	C19-N18	-2.90	1.41	1.50
2	D	801	6O8	C19-N18	-2.88	1.41	1.50
2	E	801	6O8	C19-N18	-2.87	1.41	1.50
2	B	801	6O8	C19-N18	-2.86	1.41	1.50
4	D	804	6OE	O20-C10	-2.69	1.39	1.46
2	B	801	6O8	C20-N18	-2.69	1.42	1.50
4	E	806	6OE	O20-C10	-2.68	1.39	1.46
4	C	806	6OE	O20-C10	-2.68	1.39	1.46
2	D	801	6O8	C20-N18	-2.67	1.42	1.50
2	E	801	6O8	C20-N18	-2.67	1.42	1.50
4	E	803	6OE	O20-C10	-2.66	1.39	1.46
2	C	801	6O8	C20-N18	-2.66	1.42	1.50
2	B	801	6O8	C21-N18	-2.66	1.42	1.50
4	B	806	6OE	O20-C10	-2.66	1.39	1.46
2	D	801	6O8	C17-N18	-2.65	1.42	1.51
2	E	801	6O8	C21-N18	-2.65	1.42	1.50
2	B	801	6O8	C17-N18	-2.65	1.42	1.51
2	C	801	6O8	C21-N18	-2.65	1.42	1.50
4	C	805	6OE	O20-C10	-2.65	1.40	1.46
2	C	801	6O8	C17-N18	-2.65	1.42	1.51
2	E	801	6O8	C17-N18	-2.64	1.42	1.51
4	D	803	6OE	O20-C10	-2.64	1.40	1.46
4	E	804	6OE	O20-C10	-2.64	1.40	1.46
4	B	805	6OE	O20-C10	-2.64	1.40	1.46
4	D	805	6OE	O20-C10	-2.64	1.40	1.46
4	B	803	6OE	O20-C10	-2.64	1.40	1.46
2	D	801	6O8	C21-N18	-2.64	1.42	1.50
4	C	803	6OE	O20-C10	-2.61	1.40	1.46
2	D	801	6O8	O07-C08	-2.59	1.39	1.45
2	C	801	6O8	O07-C08	-2.58	1.39	1.45
2	E	801	6O8	O07-C08	-2.56	1.39	1.45
2	B	801	6O8	O07-C08	-2.55	1.39	1.45
3	C	802	6ES	O07-C08	-2.52	1.39	1.45
3	B	802	6ES	O07-C08	-2.52	1.39	1.45
3	D	802	6ES	O07-C08	-2.51	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	802	6ES	O07-C08	-2.46	1.39	1.45
4	C	805	6OE	O12-C13	2.45	1.40	1.33
4	C	803	6OE	O12-C13	2.44	1.40	1.33
4	D	806	6OE	O20-C10	-2.44	1.40	1.46
4	C	804	6OE	O20-C10	-2.44	1.40	1.46
4	D	805	6OE	O12-C13	2.43	1.40	1.33
4	E	805	6OE	O20-C10	-2.43	1.40	1.46
4	D	803	6OE	O12-C13	2.43	1.40	1.33
4	E	806	6OE	O12-C13	2.42	1.40	1.33
4	B	803	6OE	O12-C13	2.42	1.40	1.33
4	E	804	6OE	O12-C13	2.42	1.40	1.33
4	B	805	6OE	O12-C13	2.42	1.40	1.33
4	B	804	6OE	O20-C10	-2.42	1.40	1.46
4	E	805	6OE	O12-C11	-2.38	1.39	1.45
4	C	804	6OE	O12-C11	-2.37	1.39	1.45
4	B	804	6OE	O12-C11	-2.37	1.39	1.45
4	D	806	6OE	O12-C11	-2.36	1.39	1.45
4	C	806	6OE	O12-C13	2.35	1.40	1.33
4	D	804	6OE	O12-C13	2.35	1.40	1.33
4	E	804	6OE	O12-C11	-2.32	1.39	1.45
4	D	805	6OE	O12-C11	-2.32	1.39	1.45
4	B	806	6OE	O12-C13	2.31	1.40	1.33
4	E	803	6OE	O12-C13	2.31	1.40	1.33
4	C	803	6OE	O12-C11	-2.30	1.39	1.45
4	B	803	6OE	O12-C11	-2.29	1.39	1.45
4	D	806	6OE	O12-C13	2.23	1.39	1.33
3	B	802	6ES	O07-C05	2.23	1.39	1.33
4	B	804	6OE	O12-C13	2.22	1.39	1.33
3	D	802	6ES	O07-C05	2.22	1.39	1.33
3	C	802	6ES	O07-C05	2.22	1.39	1.33
4	C	804	6OE	O12-C13	2.21	1.39	1.33
4	E	805	6OE	O12-C13	2.21	1.39	1.33
3	E	802	6ES	O07-C05	2.21	1.39	1.33
4	E	803	6OE	O12-C11	-2.17	1.40	1.45
4	D	804	6OE	O12-C11	-2.17	1.40	1.45
4	B	806	6OE	O12-C11	-2.17	1.40	1.45
4	C	806	6OE	O12-C11	-2.16	1.40	1.45
4	B	804	6OE	O20-C21	2.16	1.40	1.34
4	D	806	6OE	O20-C21	2.15	1.40	1.34
4	E	805	6OE	O20-C21	2.15	1.40	1.34
4	C	804	6OE	O20-C21	2.15	1.40	1.34
4	B	805	6OE	O12-C11	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	805	6OE	O12-C11	-2.12	1.40	1.45
4	D	803	6OE	O12-C11	-2.09	1.40	1.45
2	D	801	6O8	O07-C05	2.09	1.39	1.33
2	B	801	6O8	O07-C05	2.09	1.39	1.33
4	E	806	6OE	O12-C11	-2.09	1.40	1.45
4	B	803	6OE	O20-C21	2.08	1.40	1.34
2	C	801	6O8	O07-C05	2.08	1.39	1.33
4	D	805	6OE	O20-C21	2.08	1.40	1.34
4	C	803	6OE	O20-C21	2.08	1.40	1.34
2	E	801	6O8	O07-C05	2.07	1.39	1.33
4	E	803	6OE	O20-C21	2.07	1.40	1.34
4	B	806	6OE	O20-C21	2.07	1.40	1.34
4	D	804	6OE	O20-C21	2.06	1.40	1.34
4	E	804	6OE	O20-C21	2.06	1.40	1.34
4	C	806	6OE	O20-C21	2.05	1.40	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	6O8	O22-C23-C25	4.59	121.38	111.50
2	E	801	6O8	O22-C23-C25	4.57	121.35	111.50
2	D	801	6O8	O22-C23-C25	4.53	121.27	111.50
2	B	801	6O8	O22-C23-C25	4.53	121.27	111.50
3	E	802	6ES	O27-C28-C30	4.36	120.90	111.50
3	B	802	6ES	O27-C28-C30	4.36	120.90	111.50
3	D	802	6ES	O27-C28-C30	4.35	120.87	111.50
3	C	802	6ES	O27-C28-C30	4.35	120.87	111.50
4	B	804	6OE	O20-C21-C22	4.31	120.79	111.50
4	C	804	6OE	O20-C21-C22	4.31	120.79	111.50
4	D	806	6OE	O20-C21-C22	4.30	120.77	111.50
4	E	805	6OE	O20-C21-C22	4.29	120.76	111.50
4	E	804	6OE	O20-C21-C22	3.42	118.86	111.50
4	C	803	6OE	O20-C21-C22	3.42	118.86	111.50
4	D	805	6OE	O20-C21-C22	3.41	118.85	111.50
4	B	803	6OE	O20-C21-C22	3.39	118.82	111.50
4	E	803	6OE	O20-C21-C22	3.33	118.69	111.50
4	C	806	6OE	O20-C21-C22	3.33	118.68	111.50
4	B	806	6OE	O20-C21-C22	3.33	118.68	111.50
4	D	804	6OE	O20-C21-C22	3.32	118.66	111.50
4	E	806	6OE	O20-C21-C22	2.99	117.95	111.50
4	C	805	6OE	O20-C21-C22	2.97	117.89	111.50
4	D	803	6OE	O20-C21-C22	2.95	117.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	6OE	O20-C21-C22	2.95	117.86	111.50
3	C	802	6ES	O07-C05-C04	2.80	120.71	111.91
3	D	802	6ES	O07-C05-C04	2.79	120.67	111.91
3	E	802	6ES	O07-C05-C04	2.79	120.66	111.91
3	B	802	6ES	O07-C05-C04	2.79	120.65	111.91
4	E	803	6OE	O12-C13-C14	2.51	119.77	111.91
4	B	806	6OE	O12-C13-C14	2.50	119.77	111.91
4	C	806	6OE	O12-C13-C14	2.49	119.73	111.91
2	E	801	6O8	O07-C05-C04	2.48	119.70	111.91
4	D	804	6OE	O12-C13-C14	2.48	119.70	111.91
2	C	801	6O8	C09-O22-C23	-2.48	111.69	117.79
2	D	801	6O8	O07-C05-C04	2.47	119.66	111.91
2	B	801	6O8	O07-C05-C04	2.47	119.66	111.91
4	B	805	6OE	O12-C13-C14	2.47	119.65	111.91
2	C	801	6O8	O07-C05-C04	2.46	119.62	111.91
2	E	801	6O8	C09-O22-C23	-2.46	111.74	117.79
4	E	806	6OE	O12-C13-C14	2.46	119.62	111.91
2	D	801	6O8	C09-O22-C23	-2.46	111.75	117.79
4	D	803	6OE	O12-C13-C14	2.46	119.61	111.91
4	C	805	6OE	O12-C13-C14	2.45	119.61	111.91
2	B	801	6O8	C09-O22-C23	-2.45	111.76	117.79
4	E	805	6OE	O12-C13-C14	2.38	119.38	111.91
4	D	806	6OE	O12-C13-C14	2.37	119.33	111.91
4	B	804	6OE	O12-C13-C14	2.37	119.33	111.91
3	D	802	6ES	C09-O27-C28	-2.36	111.98	117.79
4	C	804	6OE	O12-C13-C14	2.36	119.31	111.91
3	B	802	6ES	C09-O27-C28	-2.36	111.99	117.79
3	C	802	6ES	C09-O27-C28	-2.35	112.00	117.79
3	E	802	6ES	C09-O27-C28	-2.35	112.00	117.79
3	B	802	6ES	O26-C17-C18	-2.33	104.96	110.35
3	E	802	6ES	O26-C17-C18	-2.32	104.99	110.35
3	C	802	6ES	O26-C17-C18	-2.32	104.99	110.35
3	D	802	6ES	O26-C17-C18	-2.31	105.02	110.35
4	D	805	6OE	O12-C13-C14	2.28	119.06	111.91
4	E	804	6OE	O12-C13-C14	2.27	119.04	111.91
4	B	803	6OE	O12-C13-C14	2.26	119.01	111.91
4	C	803	6OE	O12-C13-C14	2.25	118.98	111.91
2	C	801	6O8	P12-O15-C16	-2.20	110.77	121.59
2	B	801	6O8	P12-O15-C16	-2.19	110.80	121.59
2	E	801	6O8	P12-O15-C16	-2.19	110.82	121.59
2	D	801	6O8	P12-O15-C16	-2.18	110.84	121.59
3	E	802	6ES	C20-C21-C16	2.13	114.53	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	6ES	C20-C21-C16	2.12	114.53	109.68
3	C	802	6ES	C20-C21-C16	2.12	114.51	109.68
3	B	802	6ES	C20-C21-C16	2.11	114.50	109.68

There are no chirality outliers.

All (293) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	6O8	C10-O11-P12-O13
2	D	801	6O8	C10-O11-P12-O14
2	D	801	6O8	C16-O15-P12-O14
2	D	801	6O8	C25-C23-O22-C09
2	E	801	6O8	C10-O11-P12-O13
2	E	801	6O8	C10-O11-P12-O14
2	E	801	6O8	C16-O15-P12-O14
2	E	801	6O8	C25-C23-O22-C09
2	B	801	6O8	C10-O11-P12-O13
2	B	801	6O8	C10-O11-P12-O14
2	B	801	6O8	C16-O15-P12-O14
2	B	801	6O8	C25-C23-O22-C09
2	C	801	6O8	C10-O11-P12-O13
2	C	801	6O8	C10-O11-P12-O14
2	C	801	6O8	C16-O15-P12-O14
2	C	801	6O8	C25-C23-O22-C09
3	D	802	6ES	C10-O11-P12-O13
3	D	802	6ES	C10-O11-P12-O15
3	E	802	6ES	C10-O11-P12-O13
3	E	802	6ES	C10-O11-P12-O15
3	B	802	6ES	C10-O11-P12-O13
3	B	802	6ES	C10-O11-P12-O15
3	C	802	6ES	C10-O11-P12-O13
3	C	802	6ES	C10-O11-P12-O15
4	D	803	6OE	N01-C02-C03-O04
4	D	803	6OE	C03-O04-P05-O06
4	D	803	6OE	C03-O04-P05-O07
4	D	804	6OE	C03-O04-P05-O06
4	D	805	6OE	C03-O04-P05-O08
4	D	805	6OE	C09-O08-P05-O07
4	D	806	6OE	N01-C02-C03-O04
4	D	806	6OE	C03-O04-P05-O08
4	D	806	6OE	C09-O08-P05-O07
4	E	803	6OE	C03-O04-P05-O06

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Mol	Chain	Res	Type	Atoms
4	E	804	6OE	C03-O04-P05-O08
4	E	804	6OE	C09-O08-P05-O07
4	E	805	6OE	N01-C02-C03-O04
4	E	805	6OE	C03-O04-P05-O08
4	E	805	6OE	C09-O08-P05-O07
4	E	806	6OE	N01-C02-C03-O04
4	E	806	6OE	C03-O04-P05-O06
4	E	806	6OE	C03-O04-P05-O07
4	B	803	6OE	C03-O04-P05-O08
4	B	803	6OE	C09-O08-P05-O07
4	B	804	6OE	N01-C02-C03-O04
4	B	804	6OE	C03-O04-P05-O08
4	B	804	6OE	C09-O08-P05-O07
4	B	805	6OE	N01-C02-C03-O04
4	B	805	6OE	C03-O04-P05-O06
4	B	805	6OE	C03-O04-P05-O07
4	B	806	6OE	C03-O04-P05-O06
4	C	803	6OE	C03-O04-P05-O08
4	C	803	6OE	C09-O08-P05-O07
4	C	804	6OE	N01-C02-C03-O04
4	C	804	6OE	C03-O04-P05-O08
4	C	804	6OE	C09-O08-P05-O07
4	C	805	6OE	N01-C02-C03-O04
4	C	805	6OE	C03-O04-P05-O06
4	C	805	6OE	C03-O04-P05-O07
4	C	806	6OE	C03-O04-P05-O06
2	D	801	6O8	O06-C05-O07-C08
2	E	801	6O8	O06-C05-O07-C08
2	B	801	6O8	O06-C05-O07-C08
2	C	801	6O8	O06-C05-O07-C08
2	D	801	6O8	O24-C23-O22-C09
2	E	801	6O8	O24-C23-O22-C09
2	B	801	6O8	O24-C23-O22-C09
2	C	801	6O8	O24-C23-O22-C09
2	D	801	6O8	C04-C05-O07-C08
2	E	801	6O8	C04-C05-O07-C08
2	B	801	6O8	C04-C05-O07-C08
2	C	801	6O8	C04-C05-O07-C08
4	D	806	6OE	C14-C13-O12-C11
4	E	805	6OE	C14-C13-O12-C11
4	B	804	6OE	C14-C13-O12-C11
4	C	804	6OE	C14-C13-O12-C11

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Mol	Chain	Res	Type	Atoms
4	D	803	6OE	C14-C13-O12-C11
4	E	806	6OE	C14-C13-O12-C11
4	B	805	6OE	C14-C13-O12-C11
4	C	805	6OE	C14-C13-O12-C11
4	D	806	6OE	O19-C13-O12-C11
4	E	805	6OE	O19-C13-O12-C11
4	B	804	6OE	O19-C13-O12-C11
4	C	804	6OE	O19-C13-O12-C11
4	D	803	6OE	O19-C13-O12-C11
4	E	806	6OE	O19-C13-O12-C11
4	C	805	6OE	O19-C13-O12-C11
4	B	805	6OE	O19-C13-O12-C11
4	D	804	6OE	C22-C21-O20-C10
4	B	806	6OE	C22-C21-O20-C10
4	C	806	6OE	C22-C21-O20-C10
4	D	805	6OE	C14-C13-O12-C11
4	E	804	6OE	C14-C13-O12-C11
4	B	803	6OE	C14-C13-O12-C11
4	C	803	6OE	C14-C13-O12-C11
4	E	803	6OE	C22-C21-O20-C10
4	D	804	6OE	C13-C14-C15-C16
4	E	803	6OE	C13-C14-C15-C16
4	B	806	6OE	C13-C14-C15-C16
4	C	806	6OE	C13-C14-C15-C16
4	D	805	6OE	O19-C13-O12-C11
4	E	804	6OE	O19-C13-O12-C11
4	B	803	6OE	O19-C13-O12-C11
4	C	803	6OE	O19-C13-O12-C11
3	D	802	6ES	C02-C03-C04-C05
3	E	802	6ES	C02-C03-C04-C05
3	B	802	6ES	C02-C03-C04-C05
3	C	802	6ES	C02-C03-C04-C05
4	D	804	6OE	O27-C21-O20-C10
4	E	803	6OE	O27-C21-O20-C10
4	B	806	6OE	O27-C21-O20-C10
4	C	806	6OE	O27-C21-O20-C10
2	D	801	6O8	C10-O11-P12-O15
2	E	801	6O8	C10-O11-P12-O15
2	B	801	6O8	C10-O11-P12-O15
2	C	801	6O8	C10-O11-P12-O15
4	D	803	6OE	C03-O04-P05-O08
4	D	805	6OE	C09-O08-P05-O04

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Mol	Chain	Res	Type	Atoms
4	D	806	6OE	C09-O08-P05-O04
4	E	804	6OE	C09-O08-P05-O04
4	E	805	6OE	C09-O08-P05-O04
4	E	806	6OE	C03-O04-P05-O08
4	B	803	6OE	C09-O08-P05-O04
4	B	804	6OE	C09-O08-P05-O04
4	B	805	6OE	C03-O04-P05-O08
4	C	803	6OE	C09-O08-P05-O04
4	C	804	6OE	C09-O08-P05-O04
4	C	805	6OE	C03-O04-P05-O08
3	D	802	6ES	C30-C28-O27-C09
3	E	802	6ES	C30-C28-O27-C09
3	B	802	6ES	C30-C28-O27-C09
3	C	802	6ES	C30-C28-O27-C09
3	D	802	6ES	C32-C33-C34-C35
3	E	802	6ES	C32-C33-C34-C35
3	C	802	6ES	C32-C33-C34-C35
4	D	804	6OE	C14-C13-O12-C11
4	E	803	6OE	C14-C13-O12-C11
4	B	806	6OE	C14-C13-O12-C11
4	C	806	6OE	C14-C13-O12-C11
3	B	802	6ES	C32-C33-C34-C35
3	D	802	6ES	O29-C28-O27-C09
3	E	802	6ES	O29-C28-O27-C09
3	B	802	6ES	O29-C28-O27-C09
3	C	802	6ES	O29-C28-O27-C09
3	D	802	6ES	C30-C31-C32-C33
3	E	802	6ES	C30-C31-C32-C33
3	B	802	6ES	C30-C31-C32-C33
3	C	802	6ES	C30-C31-C32-C33
4	D	804	6OE	O19-C13-O12-C11
4	E	803	6OE	O19-C13-O12-C11
4	B	806	6OE	O19-C13-O12-C11
4	C	806	6OE	O19-C13-O12-C11
3	D	802	6ES	C04-C05-O07-C08
3	E	802	6ES	C04-C05-O07-C08
3	B	802	6ES	C04-C05-O07-C08
3	C	802	6ES	C04-C05-O07-C08
4	D	803	6OE	C13-C14-C15-C16
4	E	806	6OE	C13-C14-C15-C16
4	B	805	6OE	C13-C14-C15-C16
4	C	805	6OE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	D	802	6ES	O06-C05-O07-C08
3	E	802	6ES	O06-C05-O07-C08
3	B	802	6ES	O06-C05-O07-C08
3	C	802	6ES	O06-C05-O07-C08
4	D	804	6OE	C03-O04-P05-O08
4	E	803	6OE	C03-O04-P05-O08
4	B	806	6OE	C03-O04-P05-O08
4	C	806	6OE	C03-O04-P05-O08
2	D	801	6O8	C09-C10-O11-P12
2	E	801	6O8	C09-C10-O11-P12
2	B	801	6O8	C09-C10-O11-P12
2	C	801	6O8	C09-C10-O11-P12
4	D	806	6OE	O08-C09-C10-C11
4	E	805	6OE	O08-C09-C10-C11
4	B	804	6OE	O08-C09-C10-C11
4	C	804	6OE	O08-C09-C10-C11
3	D	802	6ES	C33-C34-C35-C36
3	E	802	6ES	C33-C34-C35-C36
3	C	802	6ES	C33-C34-C35-C36
3	B	802	6ES	C33-C34-C35-C36
4	D	804	6OE	O08-C09-C10-O20
4	E	803	6OE	O08-C09-C10-O20
4	B	806	6OE	O08-C09-C10-O20
4	C	806	6OE	O08-C09-C10-O20
2	D	801	6O8	C16-O15-P12-O11
2	E	801	6O8	C16-O15-P12-O11
2	B	801	6O8	C16-O15-P12-O11
2	C	801	6O8	C16-O15-P12-O11
2	D	801	6O8	C16-O15-P12-O13
2	E	801	6O8	C16-O15-P12-O13
2	B	801	6O8	C16-O15-P12-O13
2	C	801	6O8	C16-O15-P12-O13
3	D	802	6ES	C10-O11-P12-O14
3	E	802	6ES	C10-O11-P12-O14
3	B	802	6ES	C10-O11-P12-O14
3	C	802	6ES	C10-O11-P12-O14
4	D	804	6OE	C03-O04-P05-O07
4	D	805	6OE	C09-O08-P05-O06
4	D	806	6OE	C03-O04-P05-O06
4	E	803	6OE	C03-O04-P05-O07
4	E	804	6OE	C09-O08-P05-O06
4	E	805	6OE	C03-O04-P05-O06

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Mol	Chain	Res	Type	Atoms
4	B	803	6OE	C09-O08-P05-O06
4	B	804	6OE	C03-O04-P05-O06
4	B	806	6OE	C03-O04-P05-O07
4	C	803	6OE	C09-O08-P05-O06
4	C	804	6OE	C03-O04-P05-O06
4	C	806	6OE	C03-O04-P05-O07
4	D	804	6OE	O08-C09-C10-C11
4	E	803	6OE	O08-C09-C10-C11
4	B	806	6OE	O08-C09-C10-C11
4	C	806	6OE	O08-C09-C10-C11
4	D	806	6OE	O08-C09-C10-O20
4	E	805	6OE	O08-C09-C10-O20
4	B	804	6OE	O08-C09-C10-O20
4	C	804	6OE	O08-C09-C10-O20
2	D	801	6O8	O15-C16-C17-N18
2	E	801	6O8	O15-C16-C17-N18
2	B	801	6O8	O15-C16-C17-N18
2	C	801	6O8	O15-C16-C17-N18
4	D	805	6OE	C09-C10-O20-C21
4	D	805	6OE	C11-C10-O20-C21
4	E	804	6OE	C11-C10-O20-C21
4	B	803	6OE	C09-C10-O20-C21
4	B	803	6OE	C11-C10-O20-C21
4	C	803	6OE	C11-C10-O20-C21
4	D	805	6OE	O27-C21-O20-C10
4	E	804	6OE	O27-C21-O20-C10
4	B	803	6OE	O27-C21-O20-C10
4	C	803	6OE	O27-C21-O20-C10
4	D	805	6OE	C22-C21-O20-C10
4	D	804	6OE	C09-O08-P05-O04
4	E	803	6OE	C09-O08-P05-O04
4	B	806	6OE	C09-O08-P05-O04
4	C	806	6OE	C09-O08-P05-O04
4	E	804	6OE	C22-C21-O20-C10
4	B	803	6OE	C22-C21-O20-C10
4	D	804	6OE	N01-C02-C03-O04
4	E	803	6OE	N01-C02-C03-O04
4	B	806	6OE	N01-C02-C03-O04
4	C	806	6OE	N01-C02-C03-O04
4	D	805	6OE	C22-C23-C24-C25
4	E	804	6OE	C22-C23-C24-C25
4	B	803	6OE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	C	803	6OE	C22-C23-C24-C25
4	D	804	6OE	C14-C15-C16-C17
4	C	803	6OE	C22-C21-O20-C10
4	B	806	6OE	C14-C15-C16-C17
4	C	806	6OE	C14-C15-C16-C17
4	E	803	6OE	C14-C15-C16-C17
4	E	804	6OE	C09-C10-O20-C21
4	C	803	6OE	C09-C10-O20-C21
4	D	803	6OE	O20-C10-C11-O12
4	E	806	6OE	O20-C10-C11-O12
4	B	805	6OE	O20-C10-C11-O12
4	C	805	6OE	O20-C10-C11-O12
4	D	803	6OE	C09-C10-C11-O12
4	E	806	6OE	C09-C10-C11-O12
4	B	805	6OE	C09-C10-C11-O12
4	C	805	6OE	C09-C10-C11-O12
4	D	805	6OE	O08-C09-C10-C11
4	E	804	6OE	O08-C09-C10-C11
4	B	803	6OE	O08-C09-C10-C11
4	C	803	6OE	O08-C09-C10-C11
3	D	802	6ES	O27-C28-C30-C31
3	B	802	6ES	O27-C28-C30-C31
4	B	806	6OE	C23-C24-C25-C26
4	E	803	6OE	C23-C24-C25-C26
4	C	806	6OE	C23-C24-C25-C26
3	E	802	6ES	O27-C28-C30-C31
3	C	802	6ES	O27-C28-C30-C31
4	D	804	6OE	C23-C24-C25-C26
4	D	805	6OE	O08-C09-C10-O20
4	E	804	6OE	O08-C09-C10-O20
4	B	803	6OE	O08-C09-C10-O20
4	C	803	6OE	O08-C09-C10-O20
2	C	801	6O8	C25-C26-C27-C28
2	E	801	6O8	C25-C26-C27-C28
2	B	801	6O8	C25-C26-C27-C28
2	D	801	6O8	C25-C26-C27-C28
3	B	802	6ES	O29-C28-C30-C31
3	D	802	6ES	O29-C28-C30-C31
4	D	806	6OE	C09-O08-P05-O06
4	E	805	6OE	C09-O08-P05-O06
4	B	804	6OE	C09-O08-P05-O06
4	C	804	6OE	C09-O08-P05-O06

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	E	802	6ES	O29-C28-C30-C31
3	C	802	6ES	O29-C28-C30-C31
4	D	804	6OE	C02-C03-O04-P05
4	E	803	6OE	C02-C03-O04-P05
4	B	806	6OE	C02-C03-O04-P05
4	C	806	6OE	C02-C03-O04-P05
2	D	801	6O8	C03-C04-C05-O07

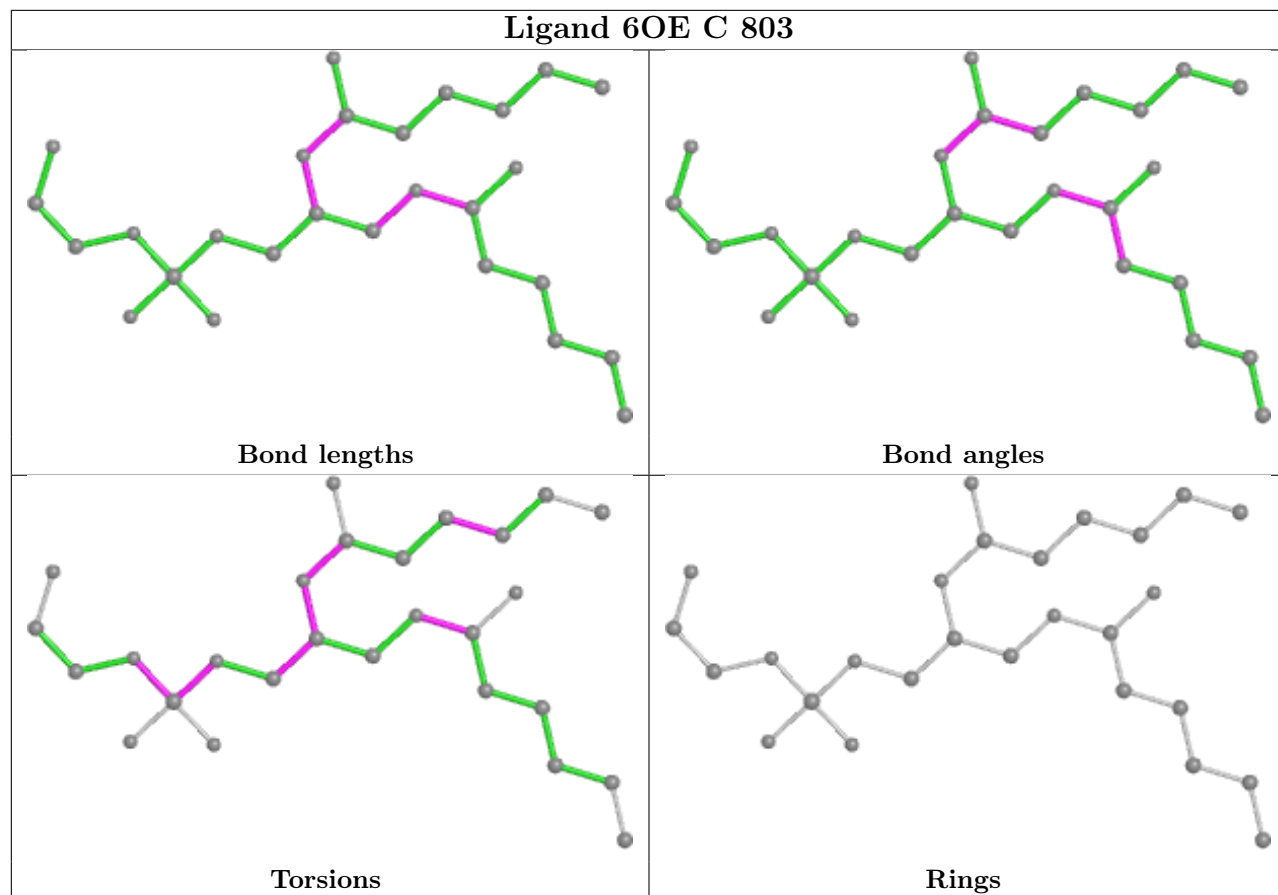
There are no ring outliers.

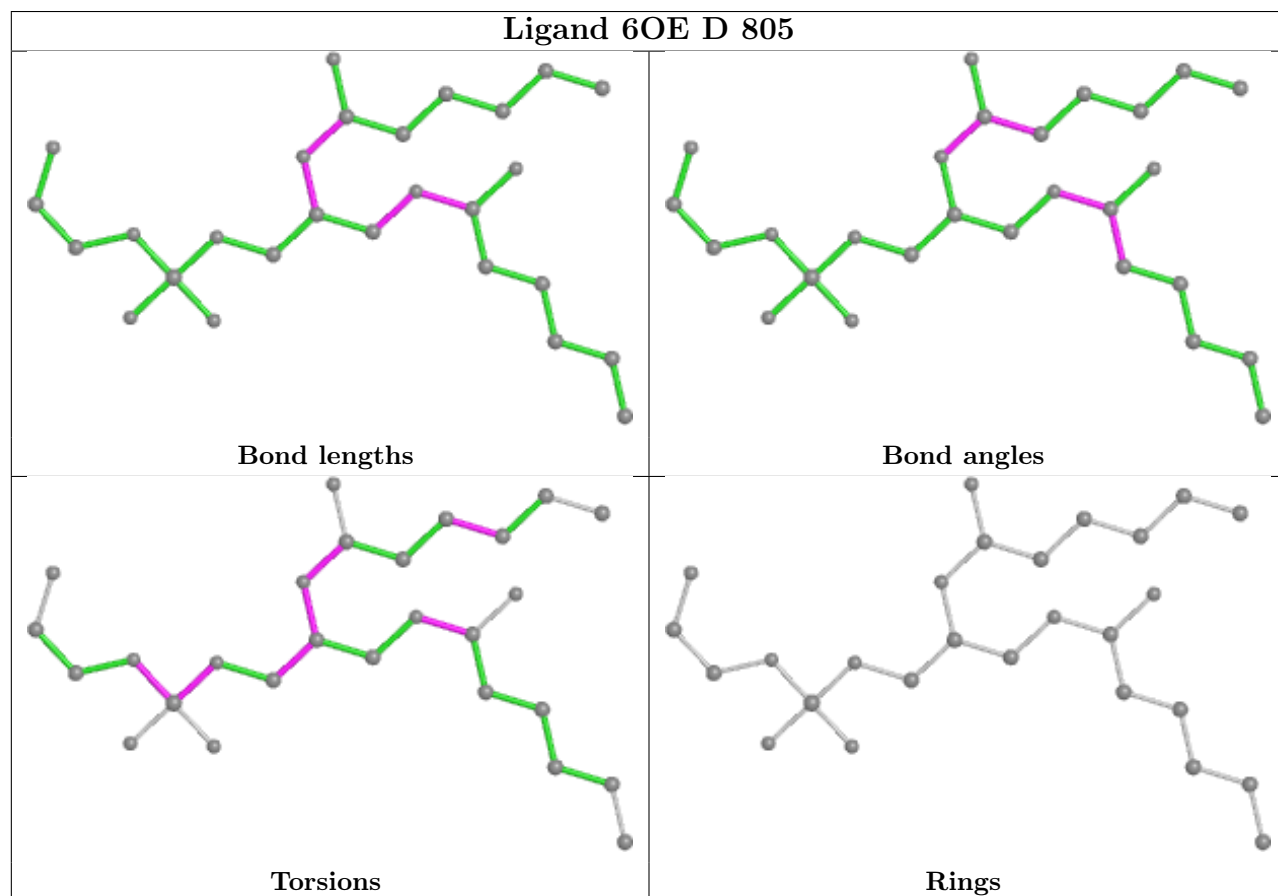
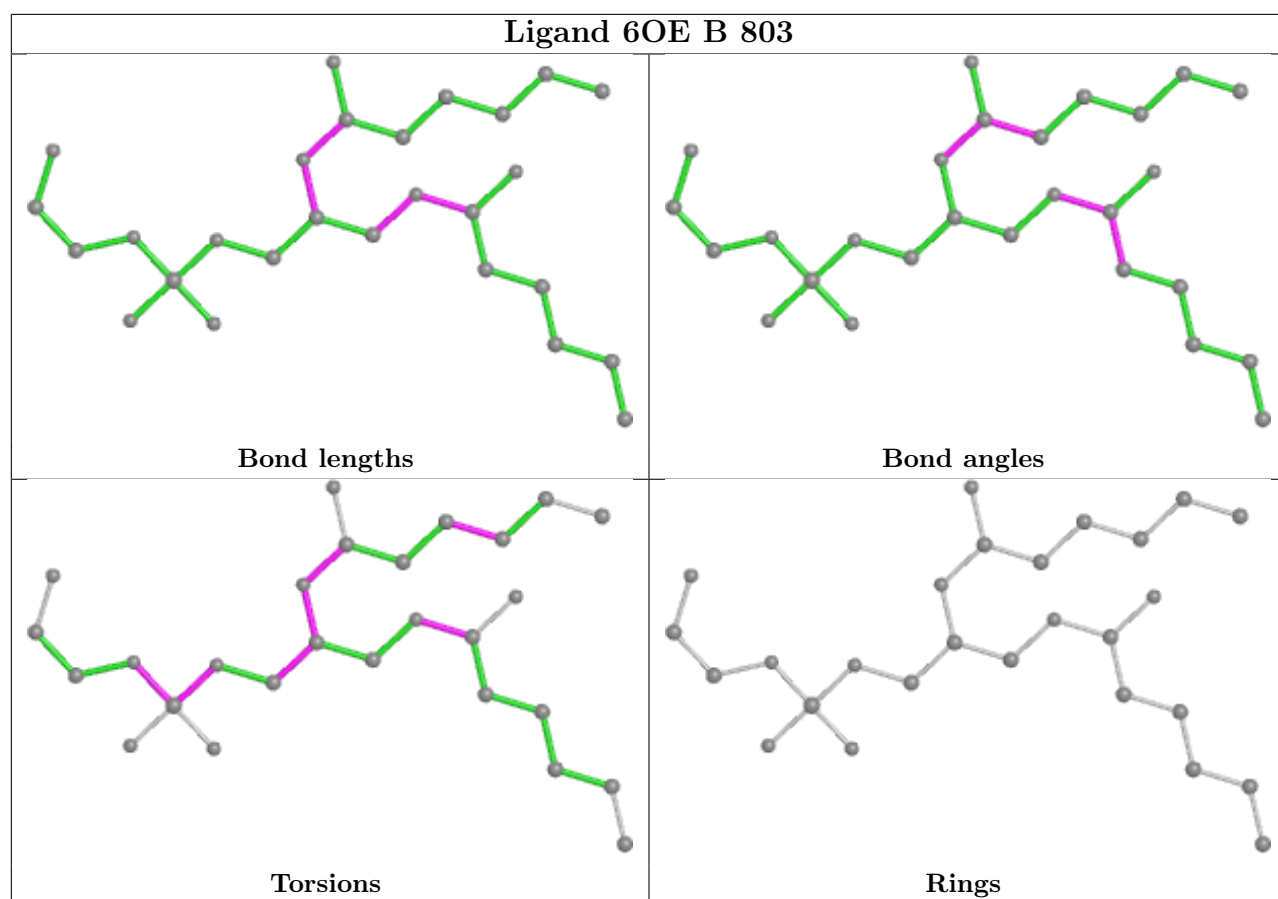
18 monomers are involved in 89 short contacts:

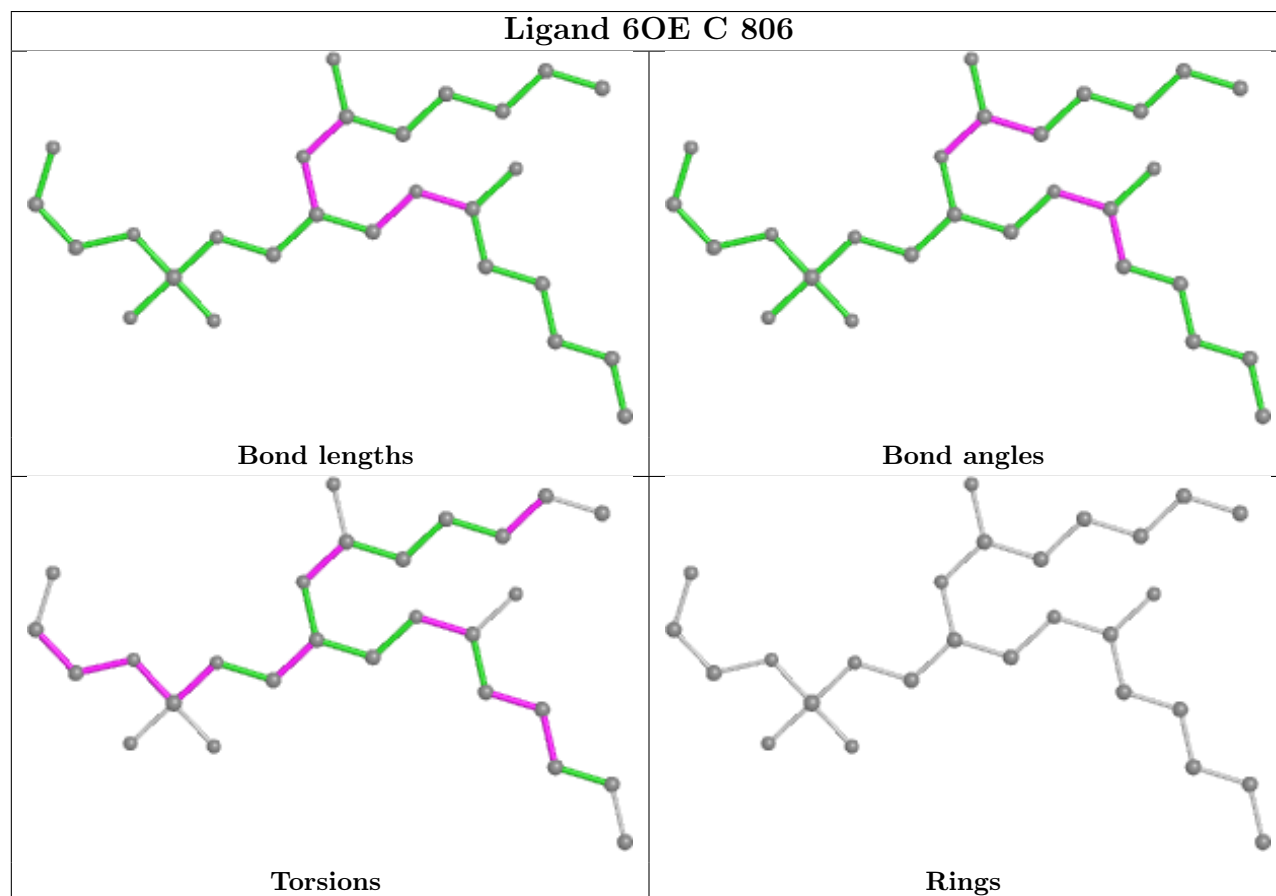
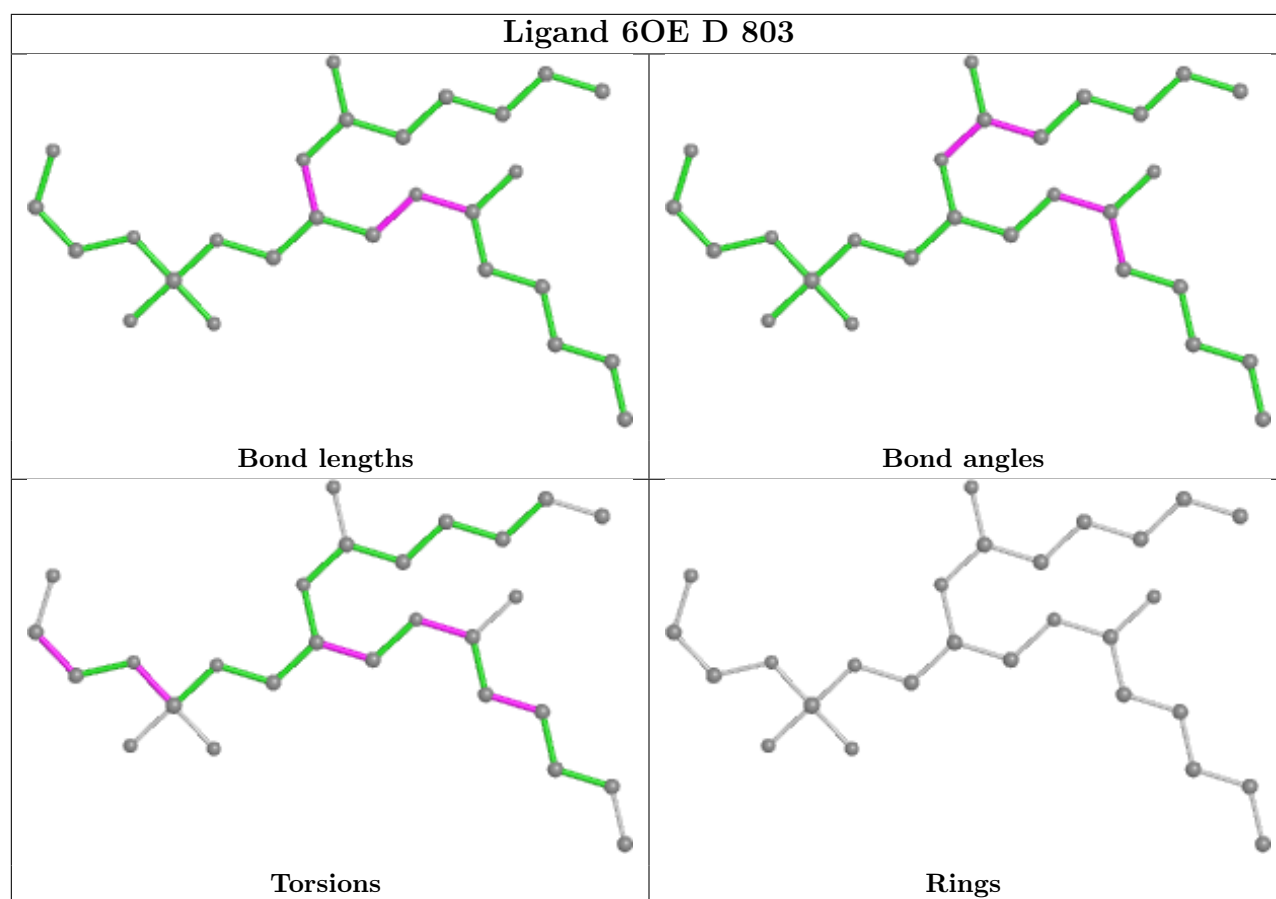
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	806	6OE	2	0
3	B	802	6ES	10	0
3	E	802	6ES	10	0
4	D	804	6OE	2	0
2	C	801	6O8	9	0
4	B	806	6OE	1	0
3	C	802	6ES	10	0
4	B	804	6OE	1	0
4	C	805	6OE	1	0
3	D	802	6ES	10	0
2	E	801	6O8	9	0
4	D	806	6OE	1	0
4	C	804	6OE	1	0
2	B	801	6O8	9	0
4	E	803	6OE	2	0
4	B	805	6OE	1	0
2	D	801	6O8	9	0
4	E	805	6OE	1	0

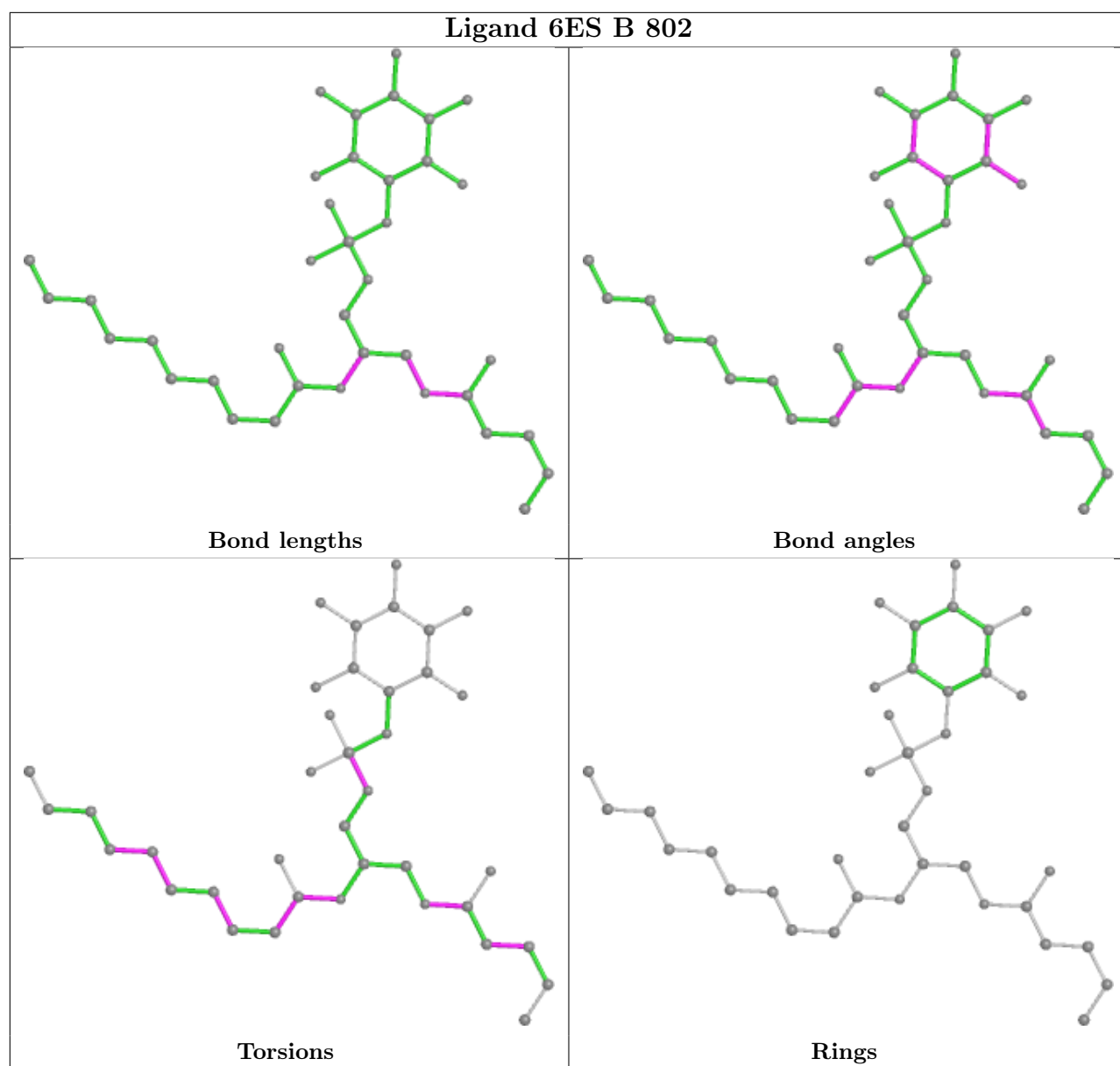
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

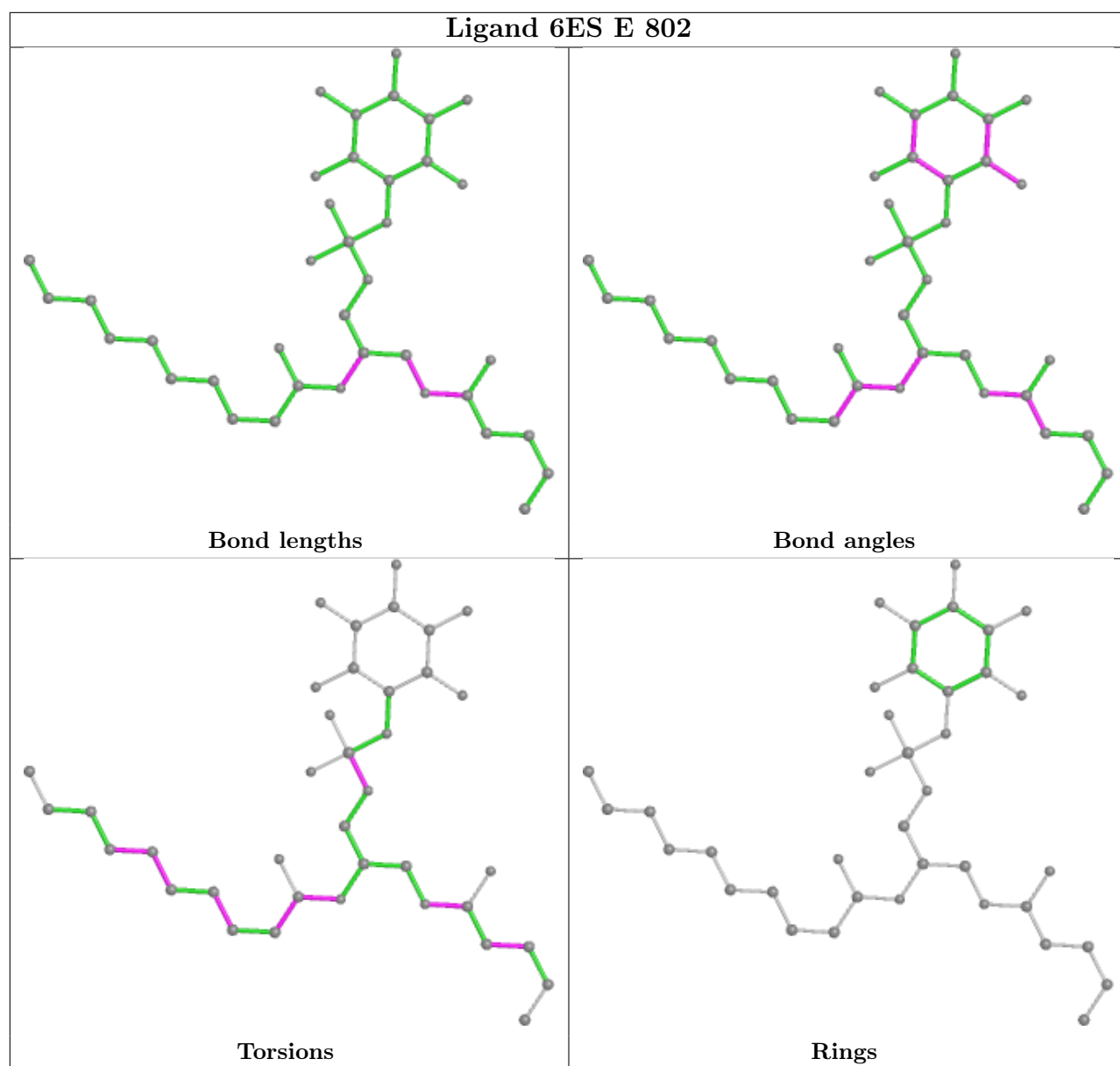
equivalents in the CSD to analyse the geometry.

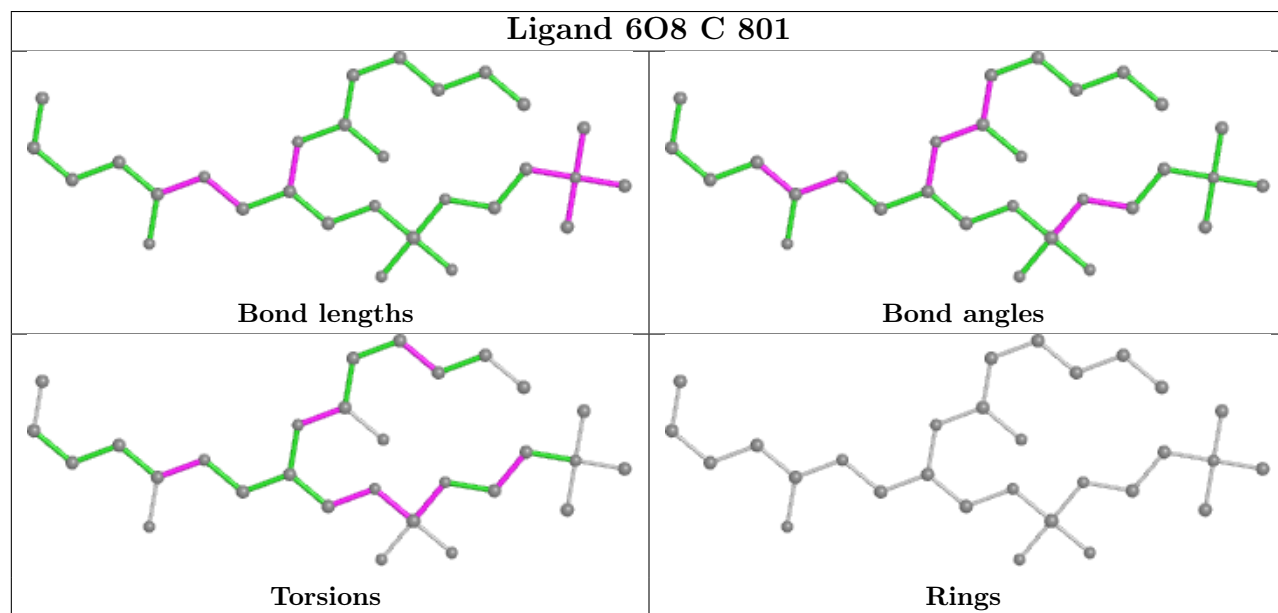
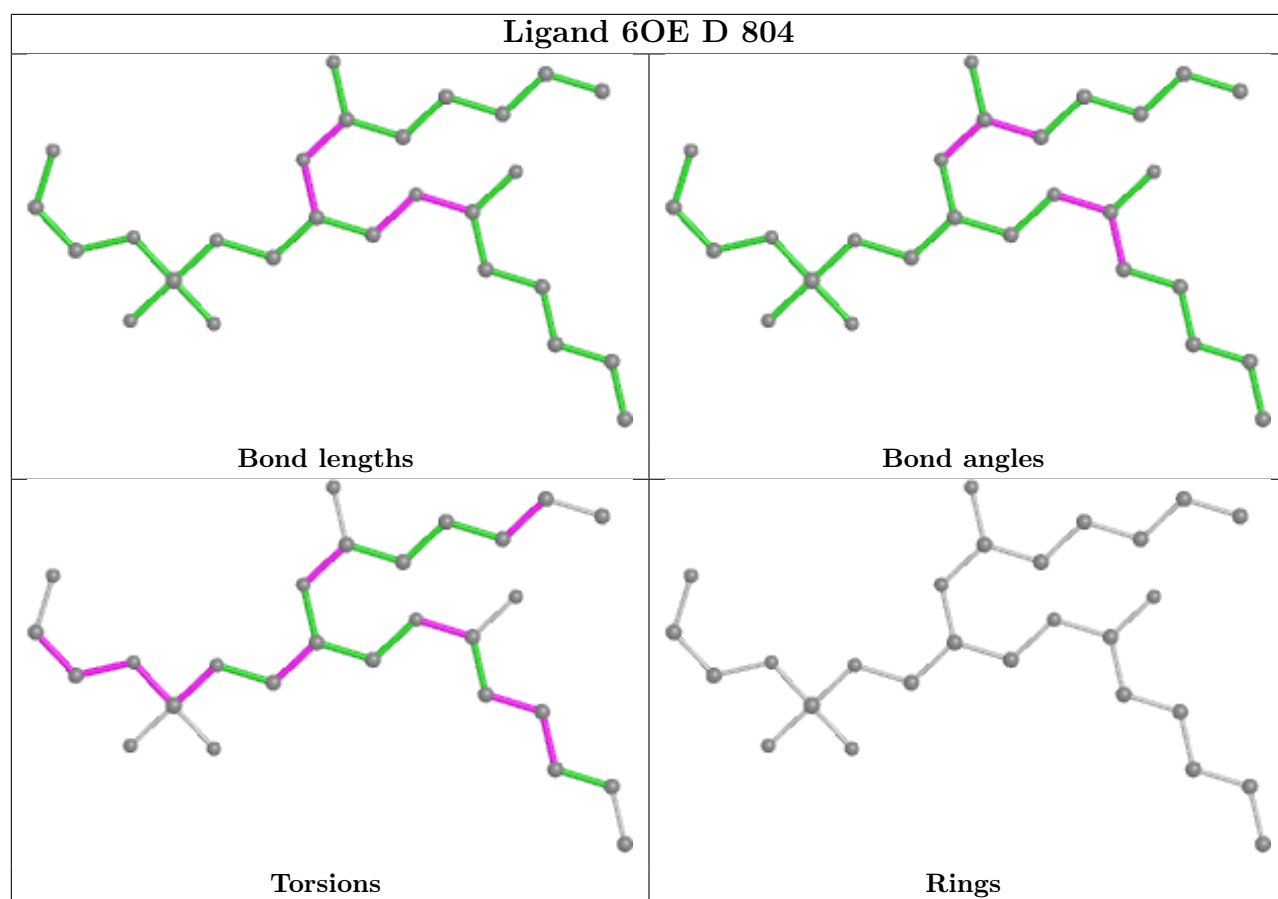


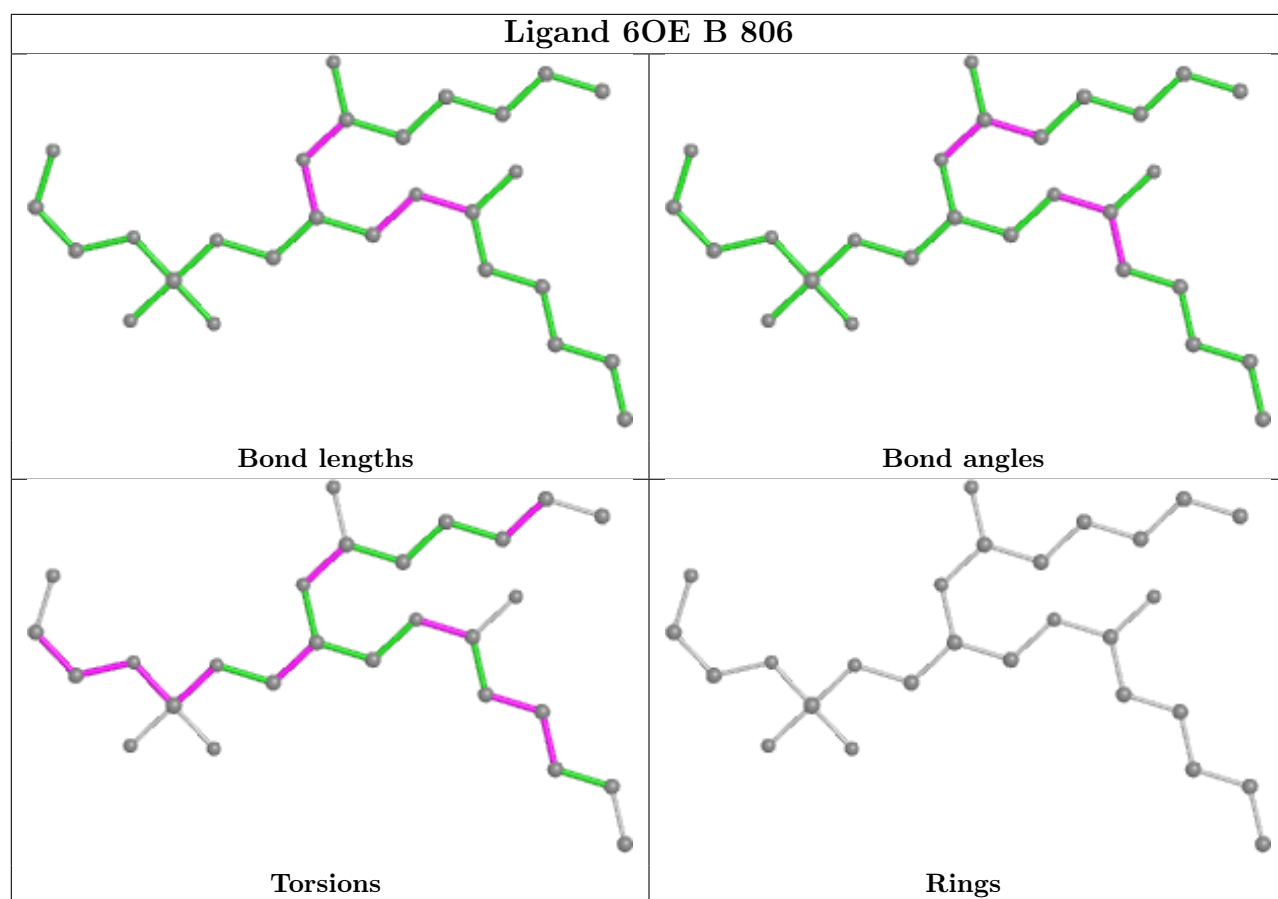


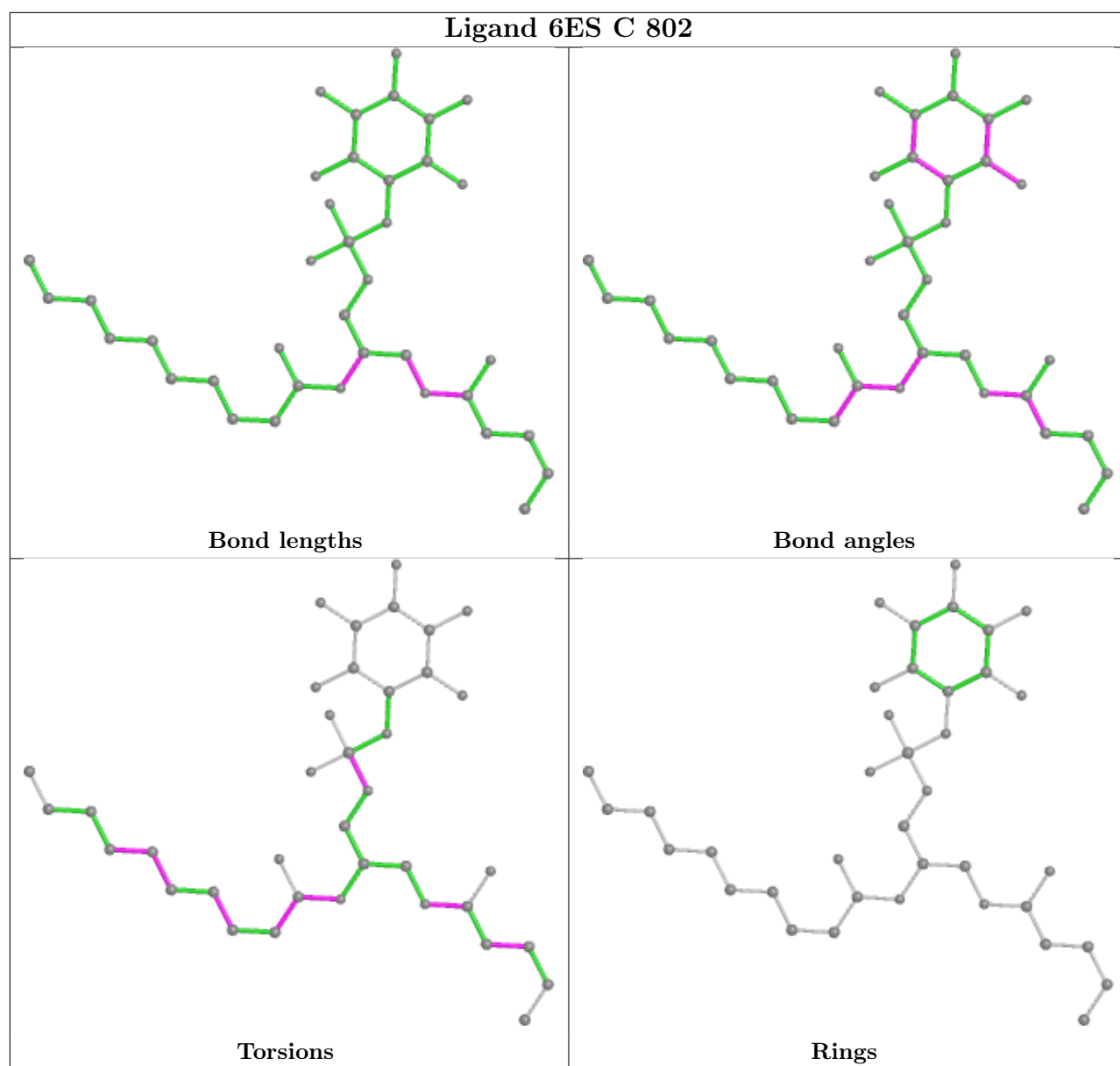


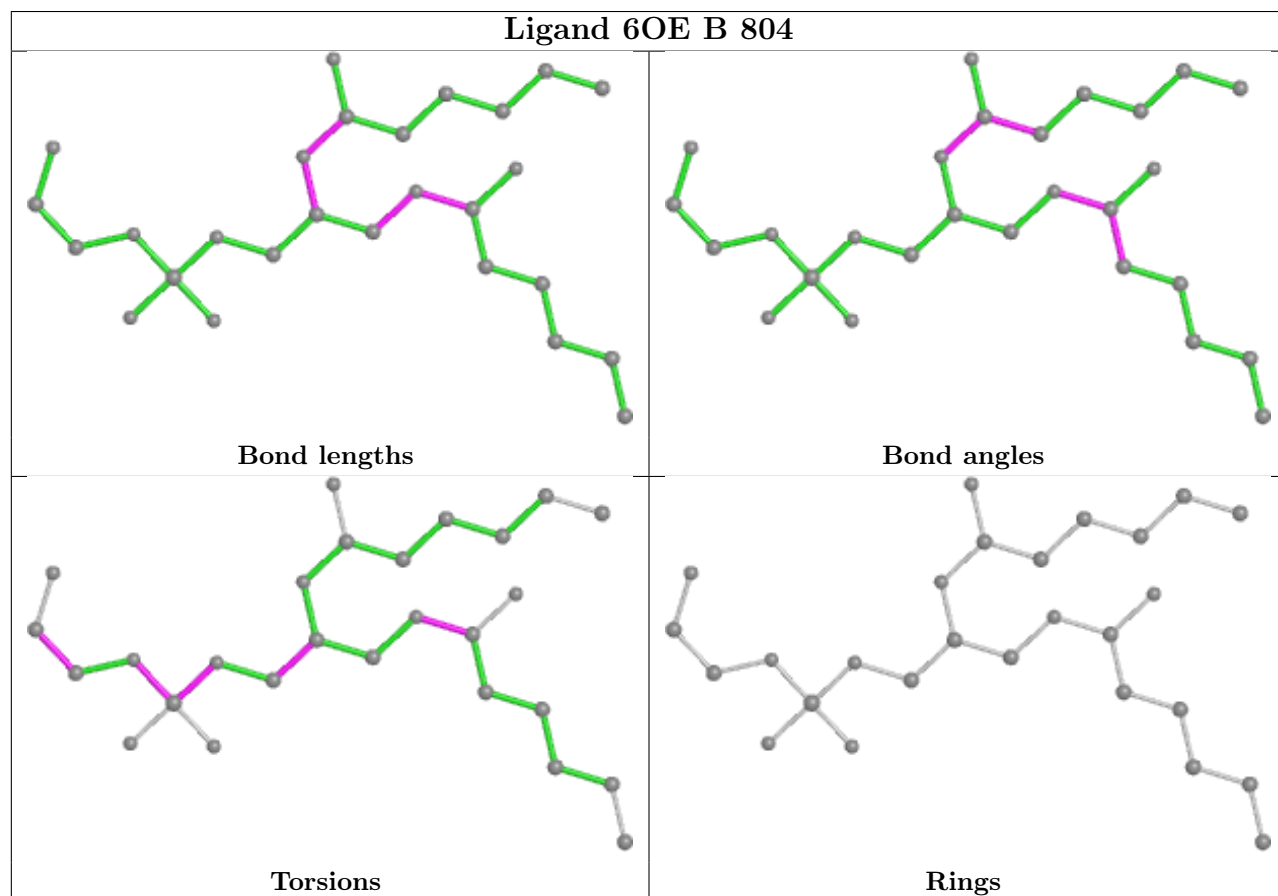
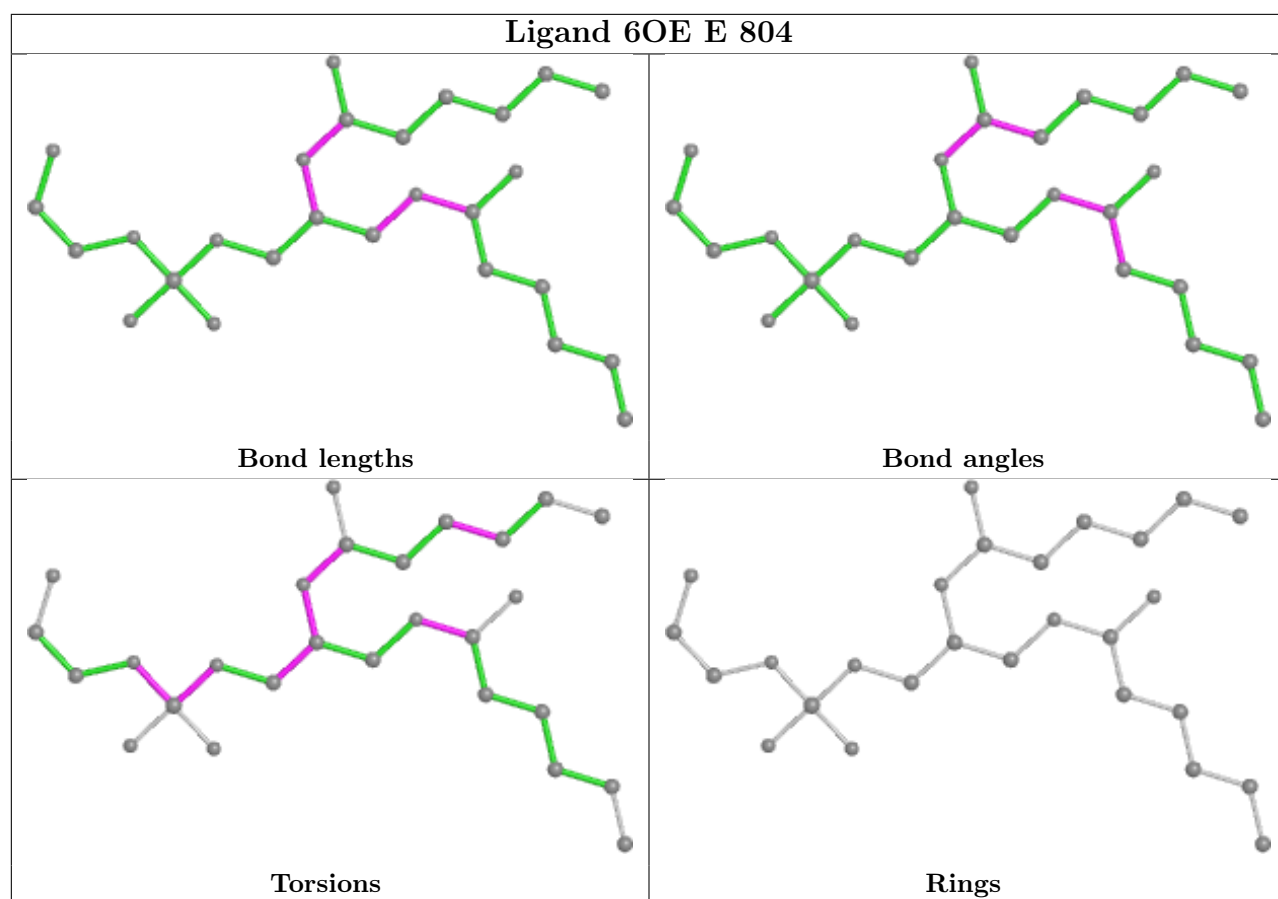


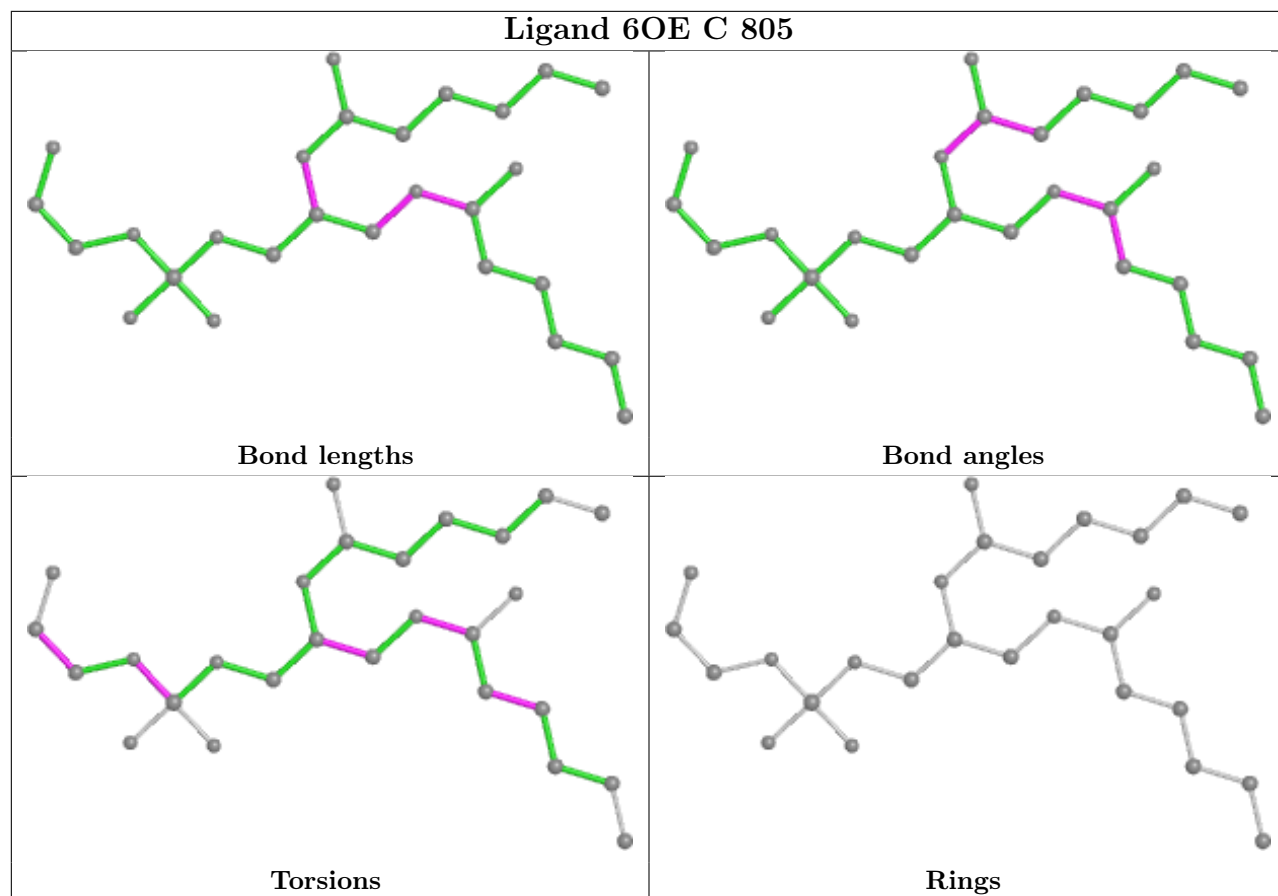


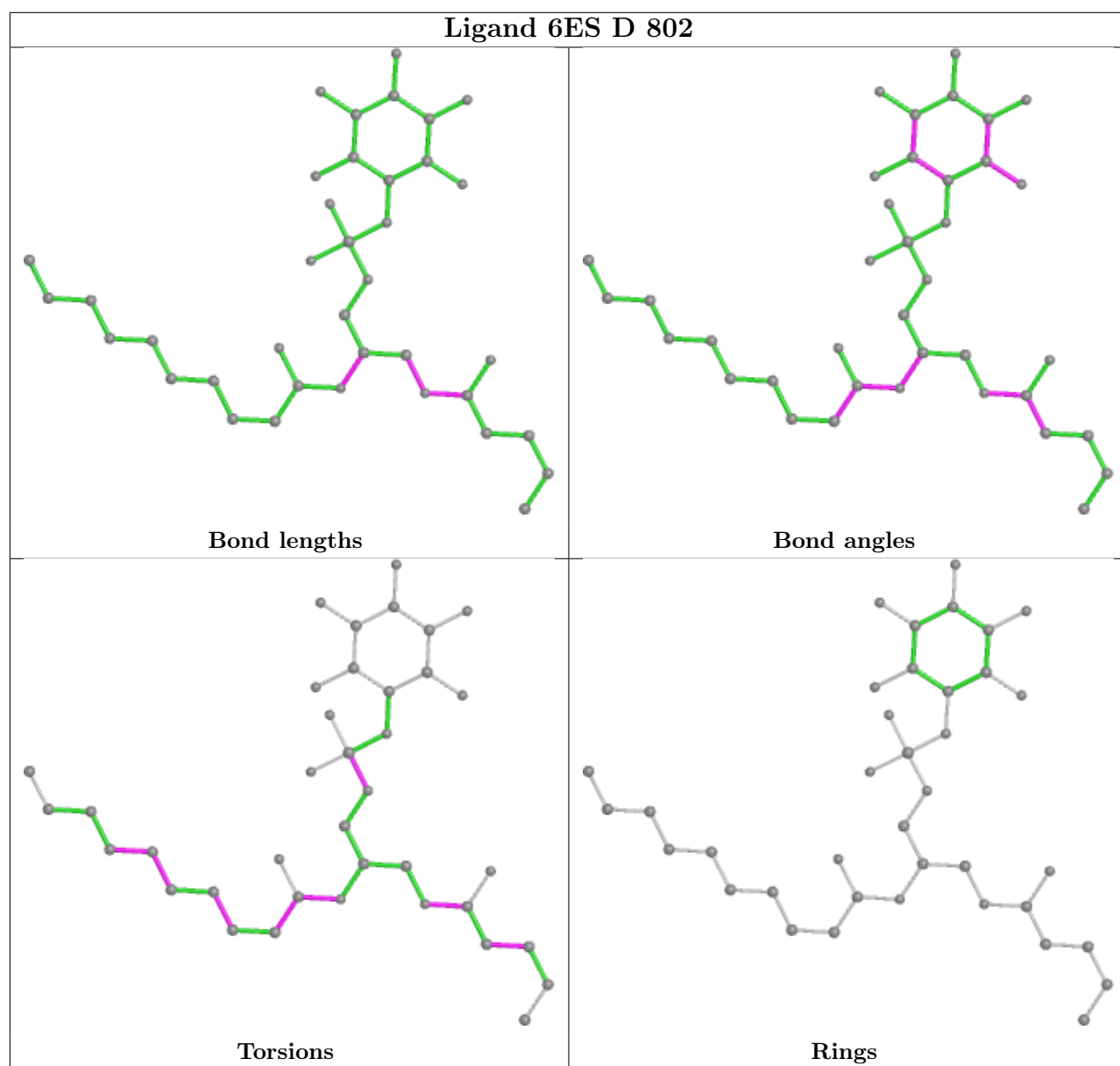




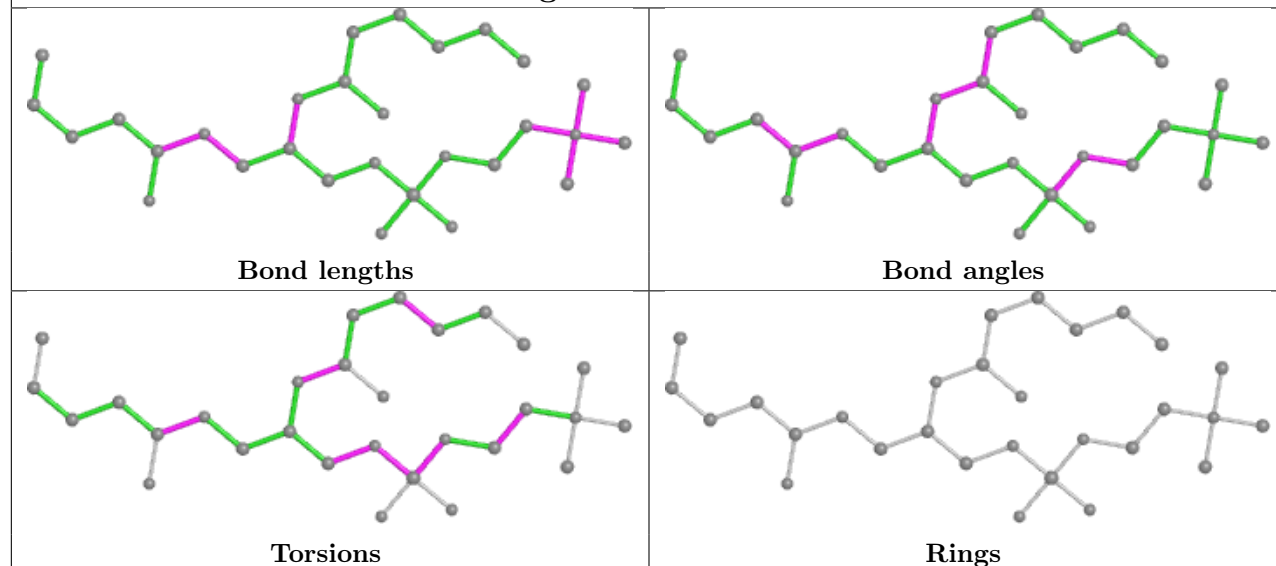




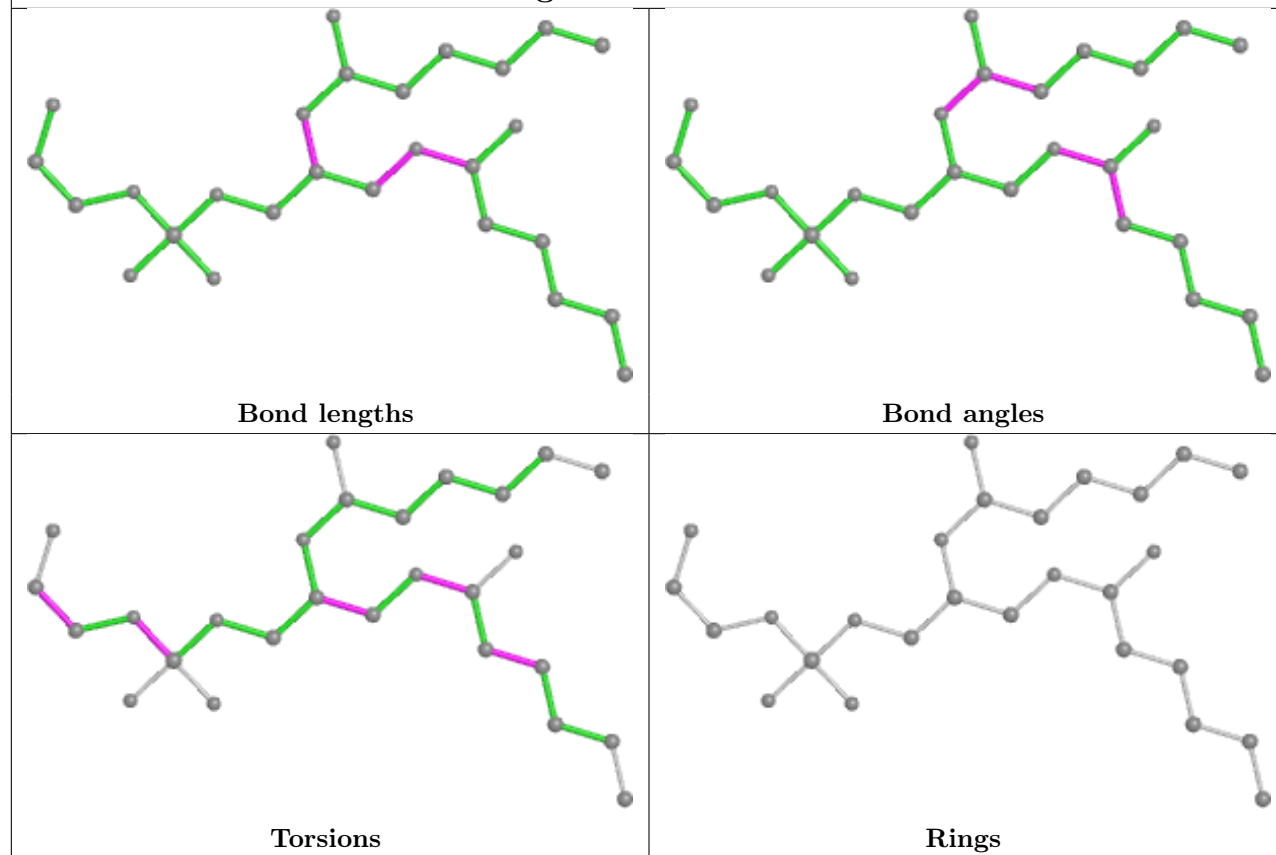


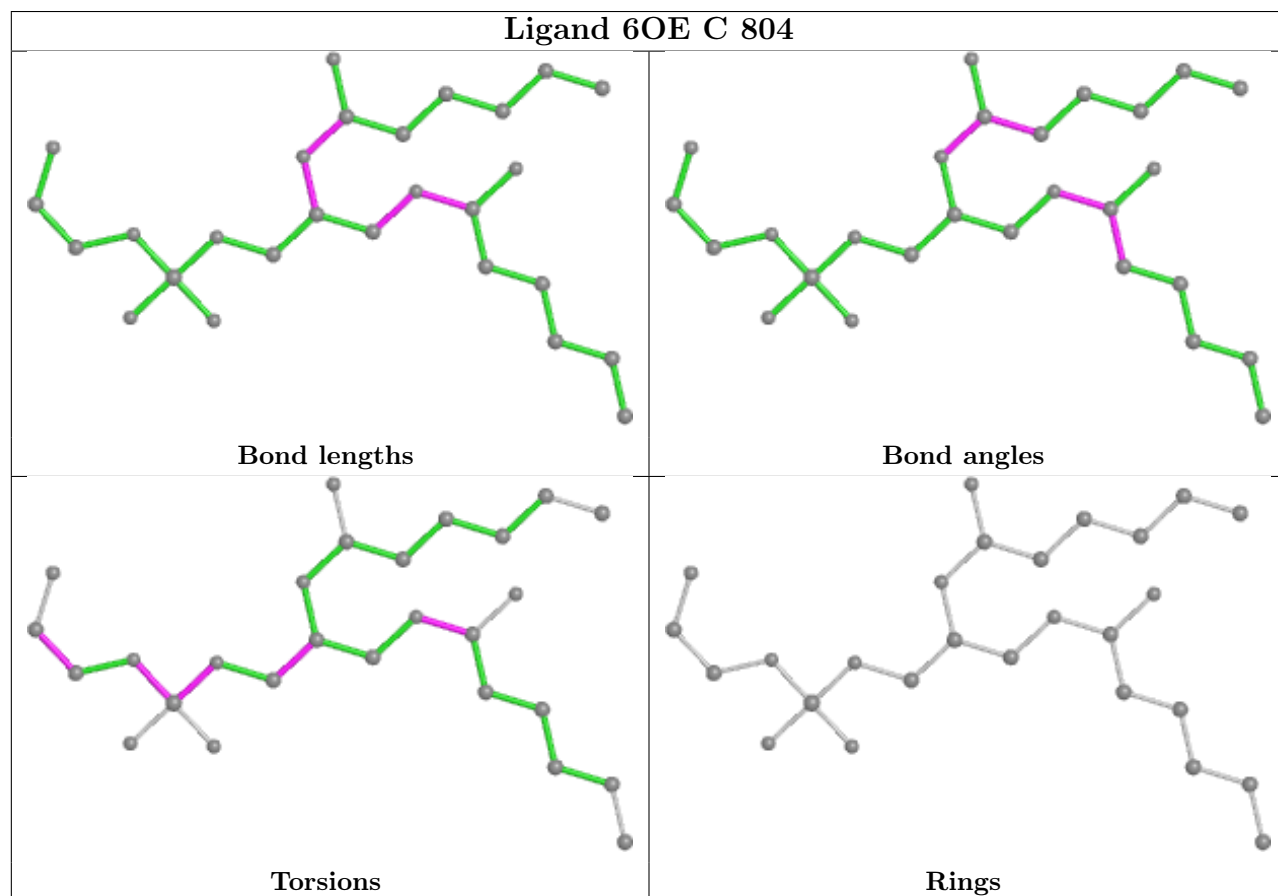
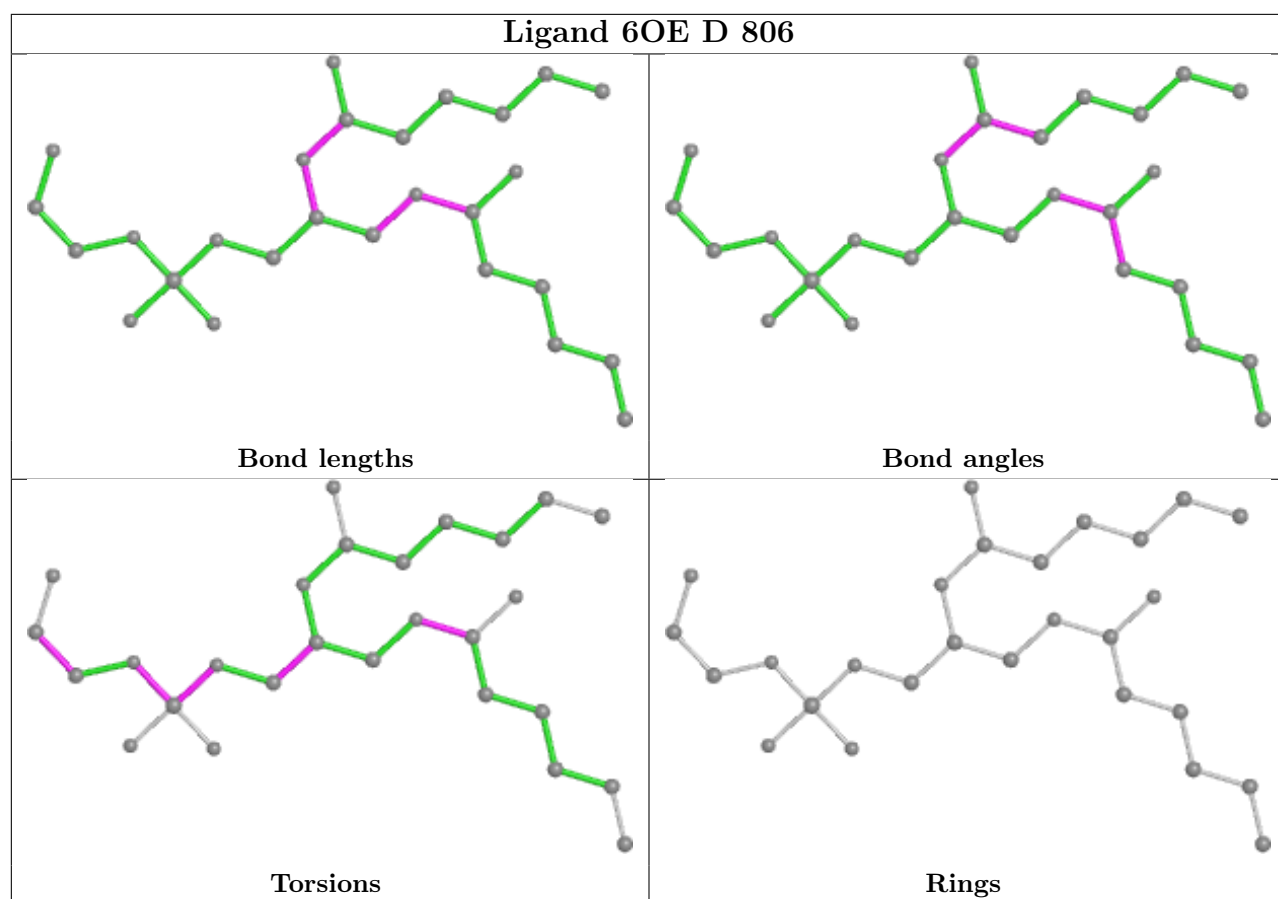


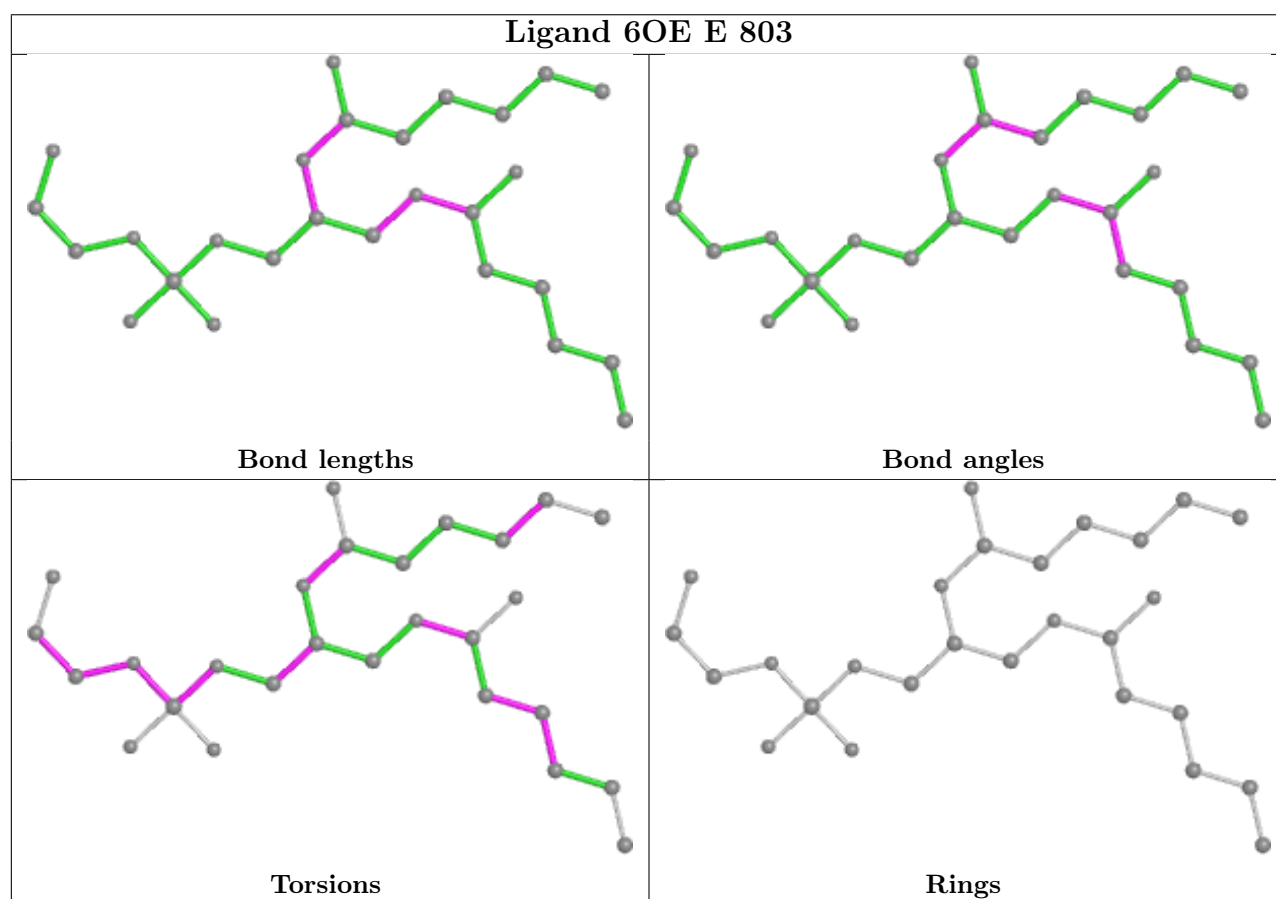
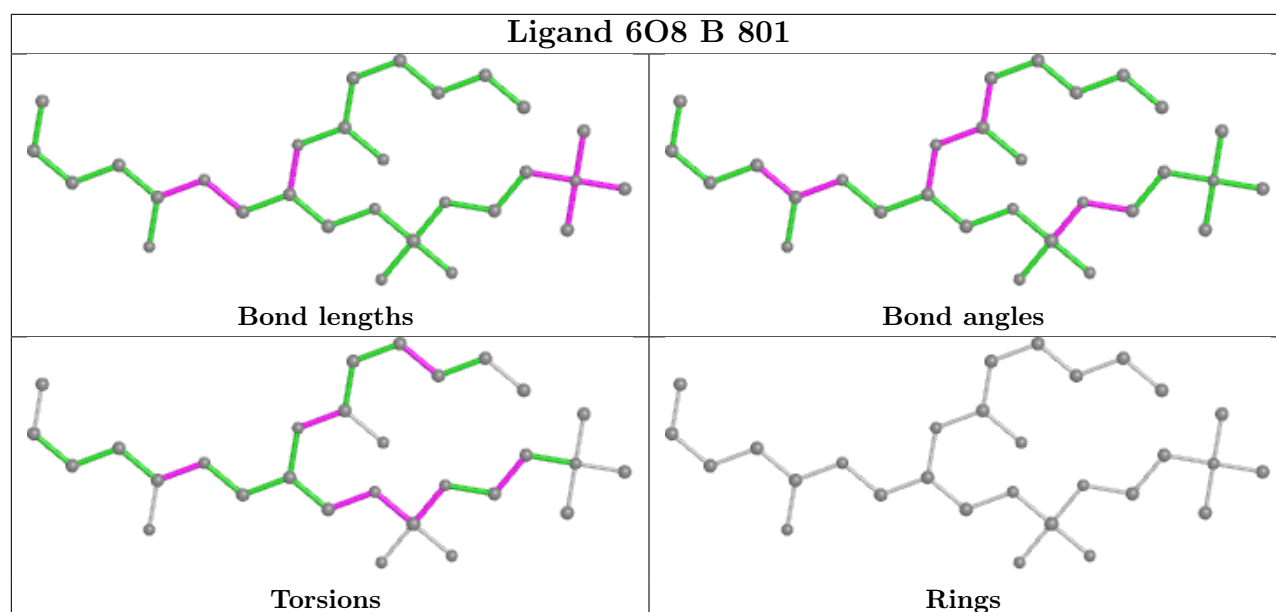
Ligand 6O8 E 801

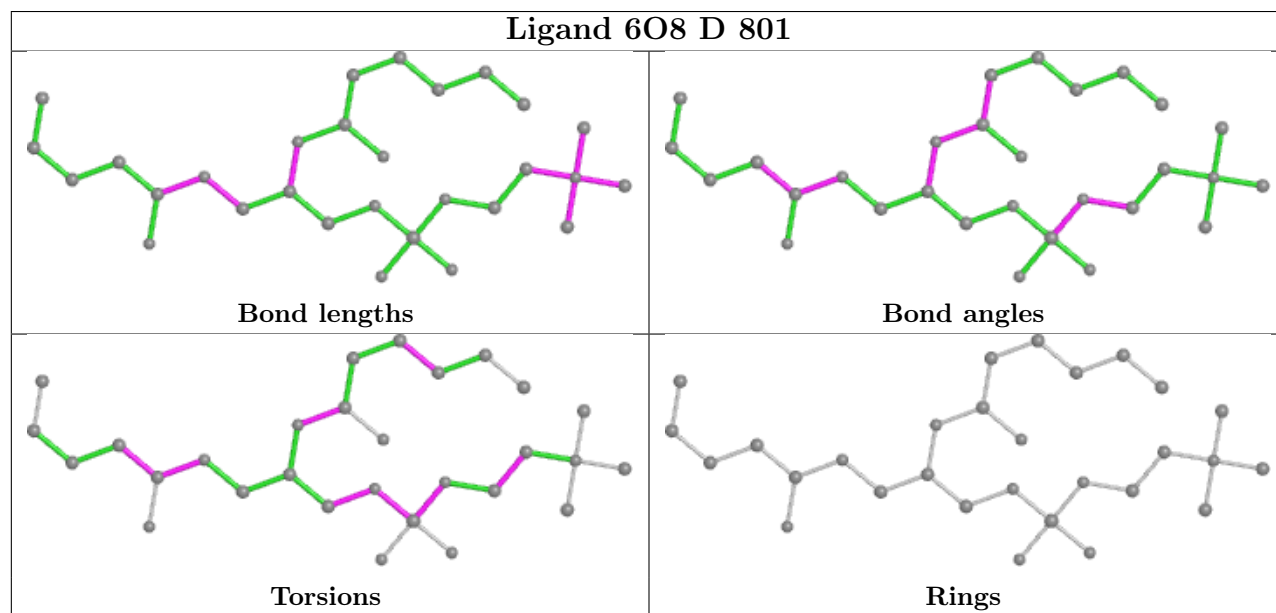
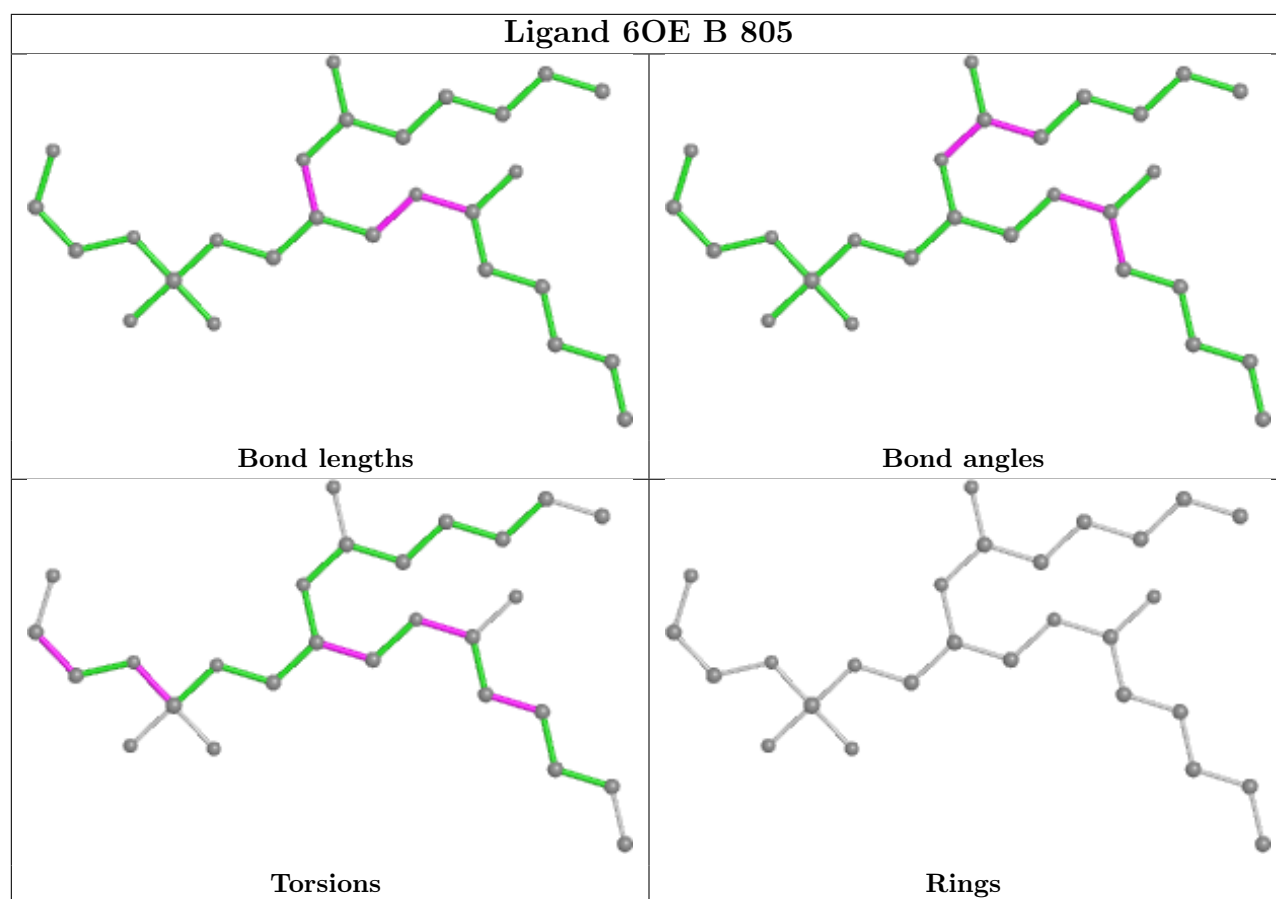


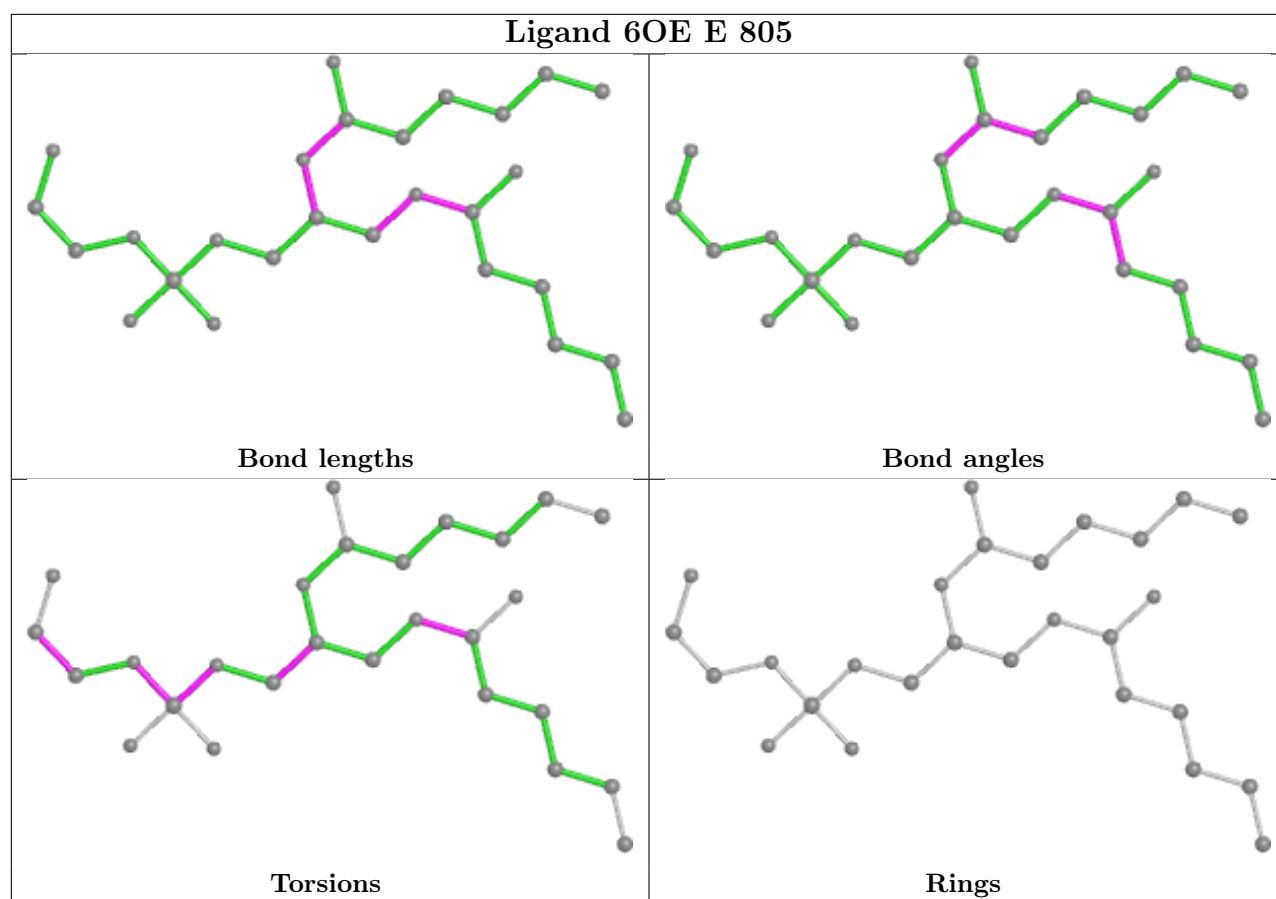
Ligand 6OE E 806











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.

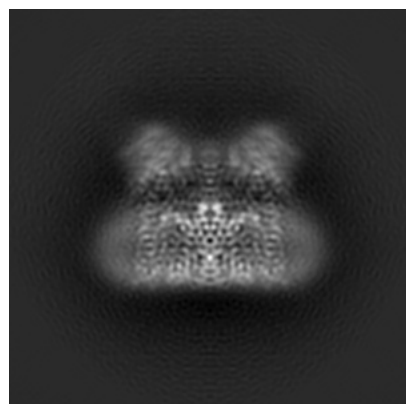
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8118. These allow visual inspection of the internal detail of the map and identification of artifacts.

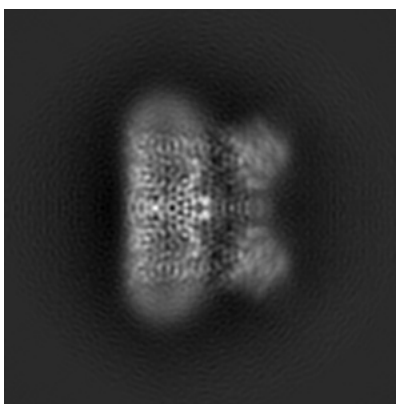
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

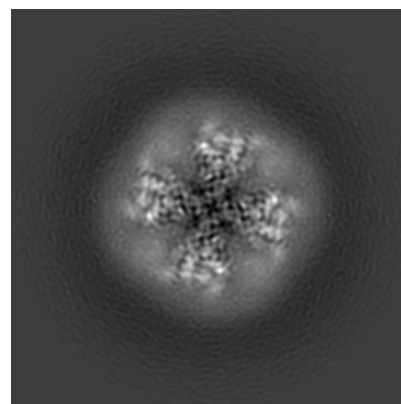
6.1.1 Primary map



X

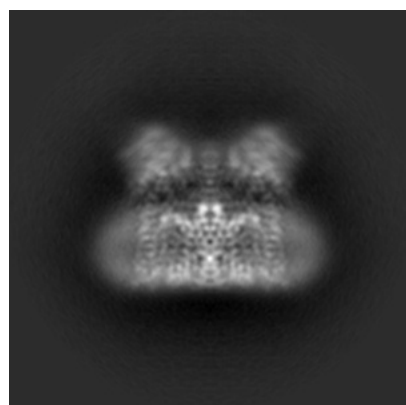


Y

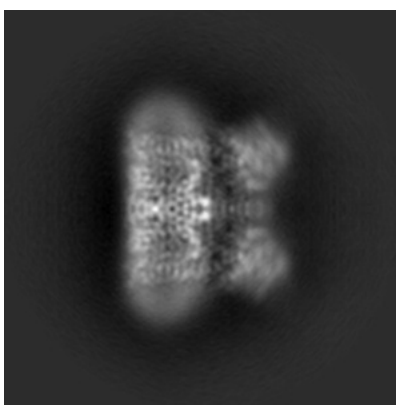


Z

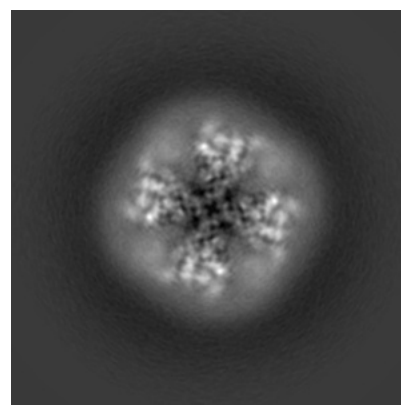
6.1.2 Raw map



X



Y

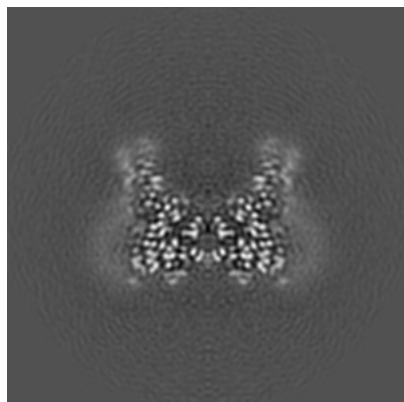


Z

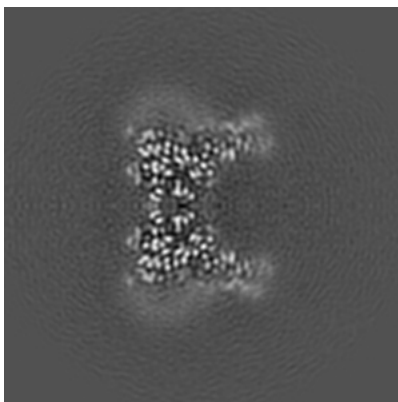
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

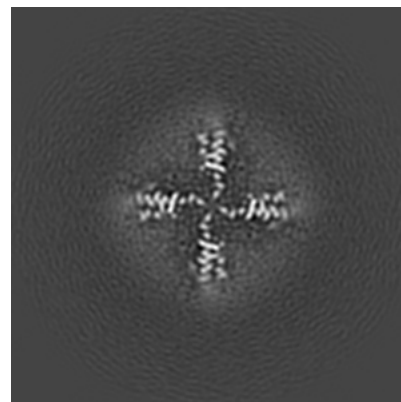
6.2.1 Primary map



X Index: 96

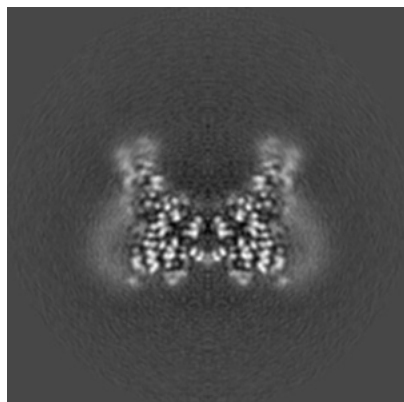


Y Index: 96

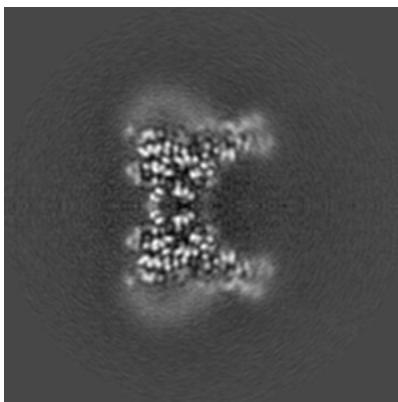


Z Index: 96

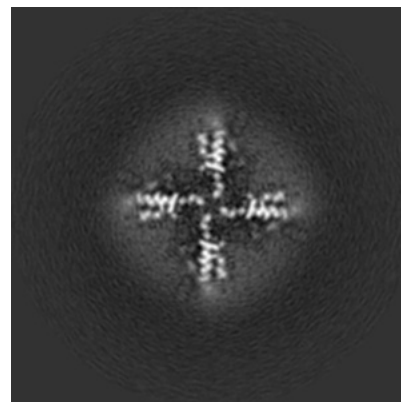
6.2.2 Raw map



X Index: 96



Y Index: 96

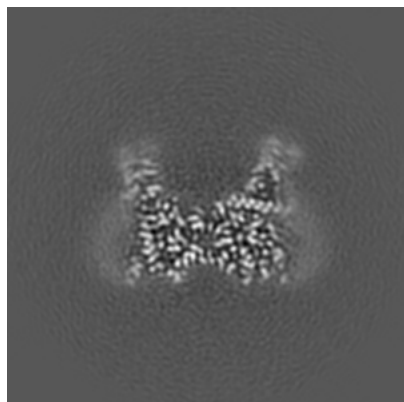


Z Index: 96

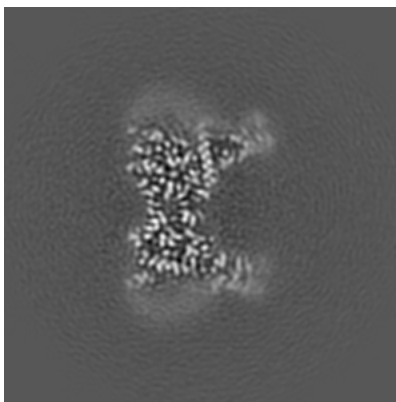
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

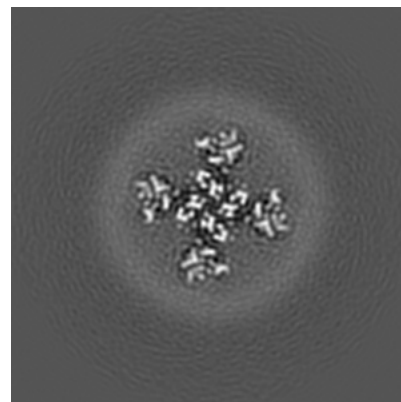
6.3.1 Primary map



X Index: 98

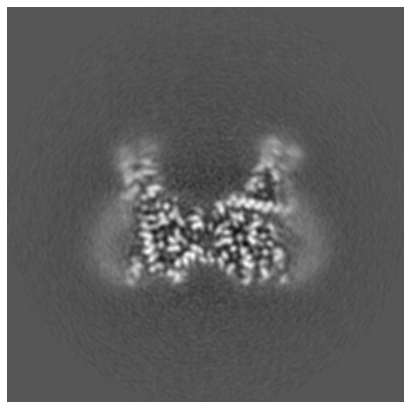


Y Index: 94

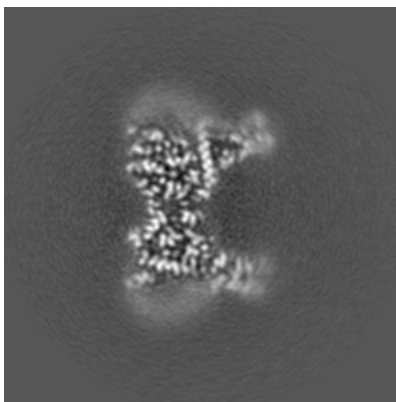


Z Index: 83

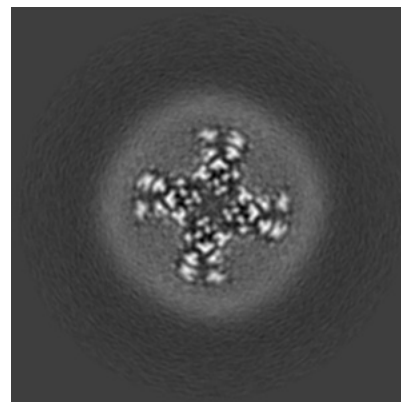
6.3.2 Raw map



X Index: 98



Y Index: 94

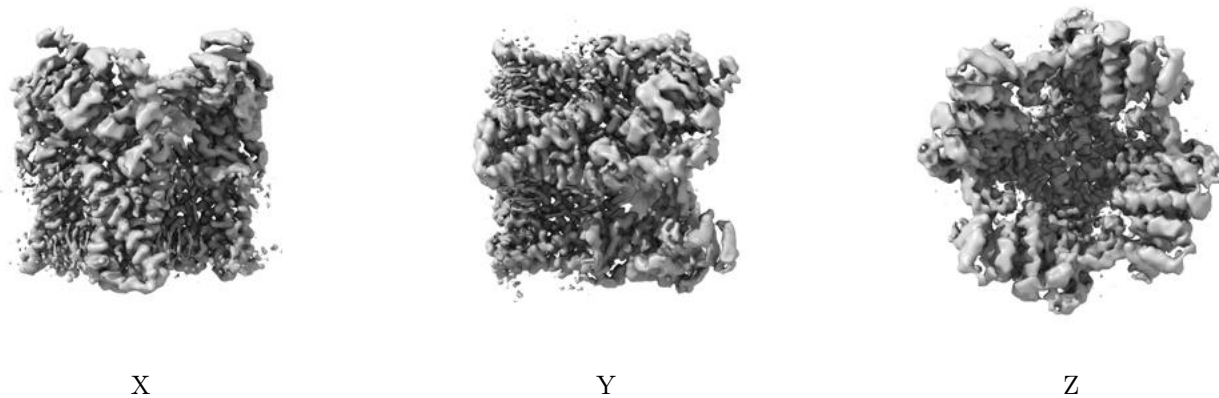


Z Index: 67

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

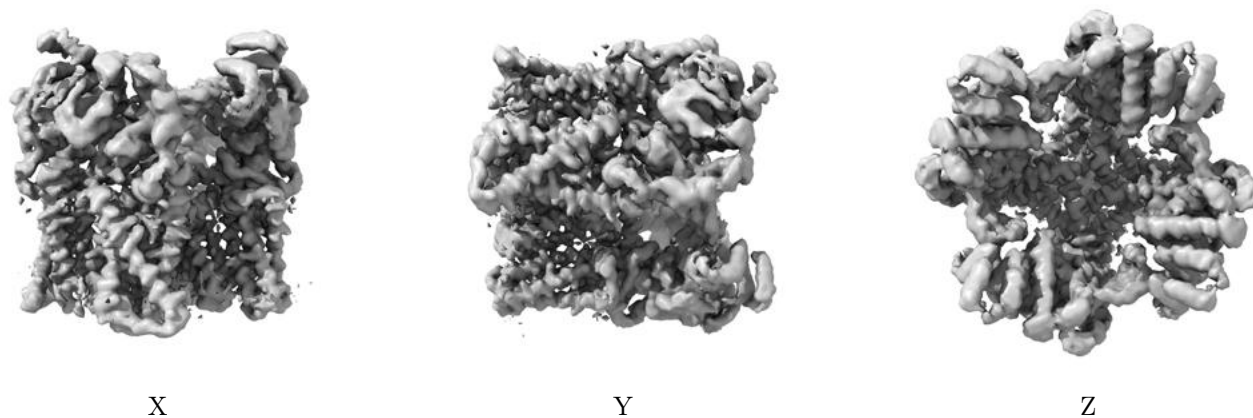
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

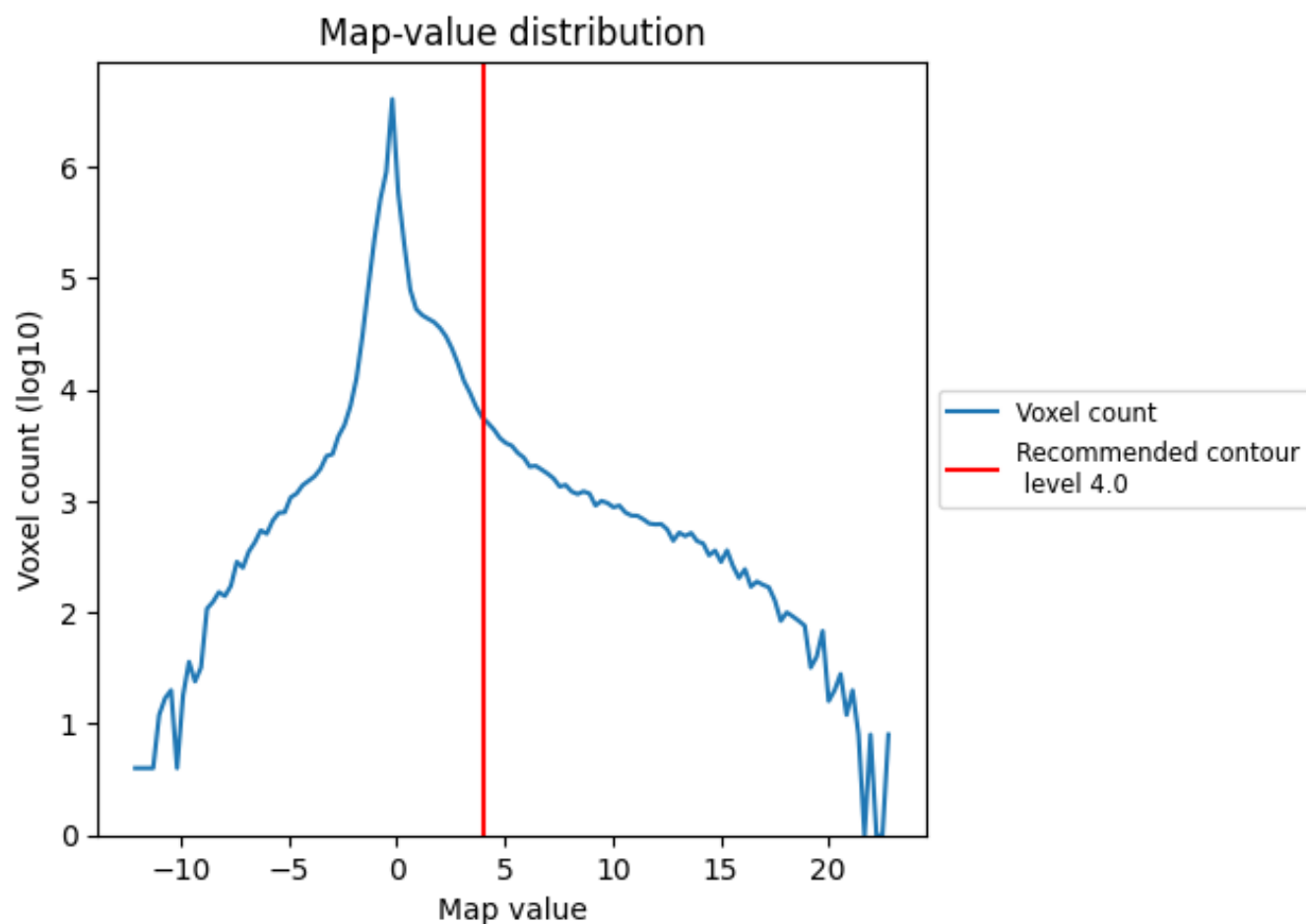
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

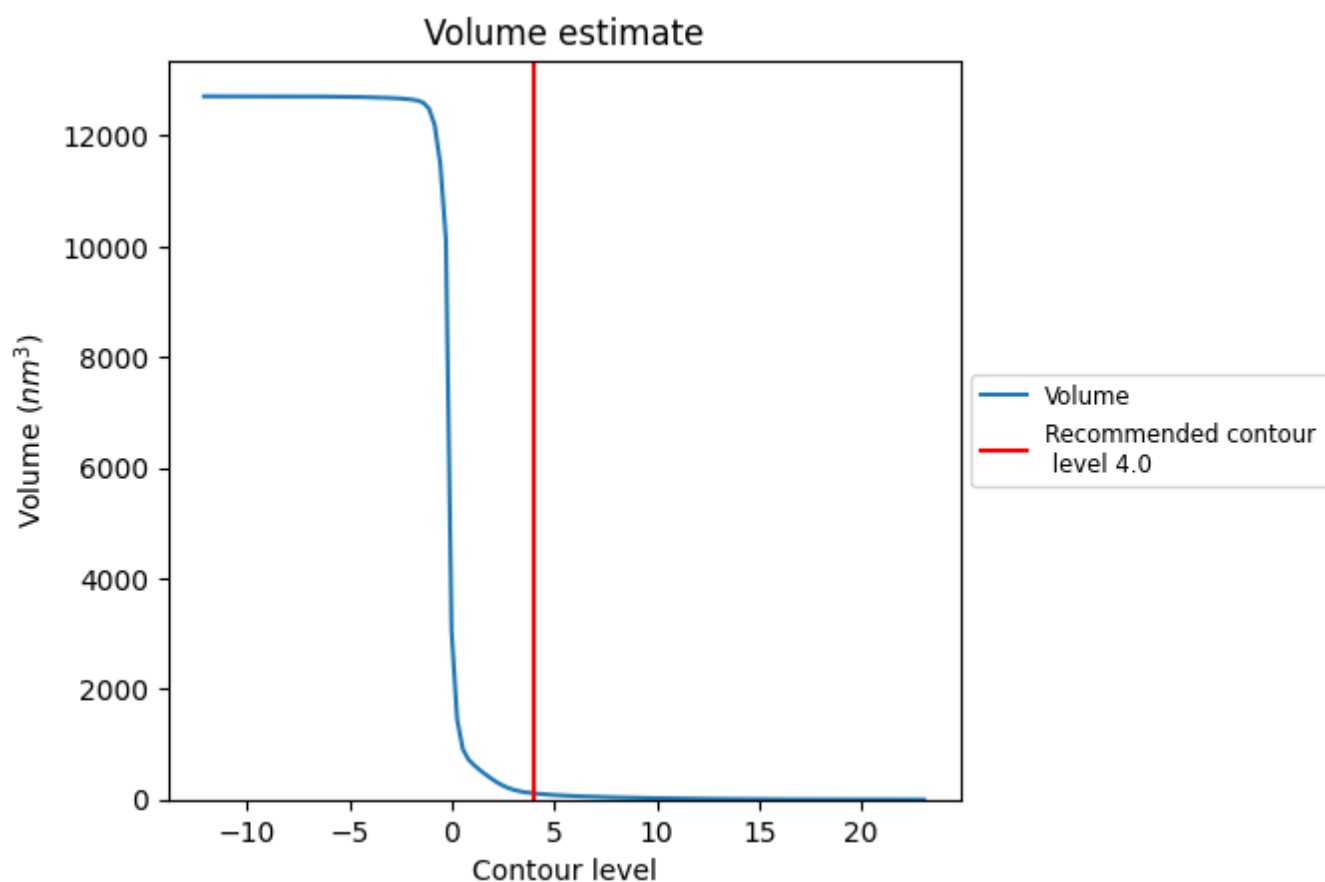
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

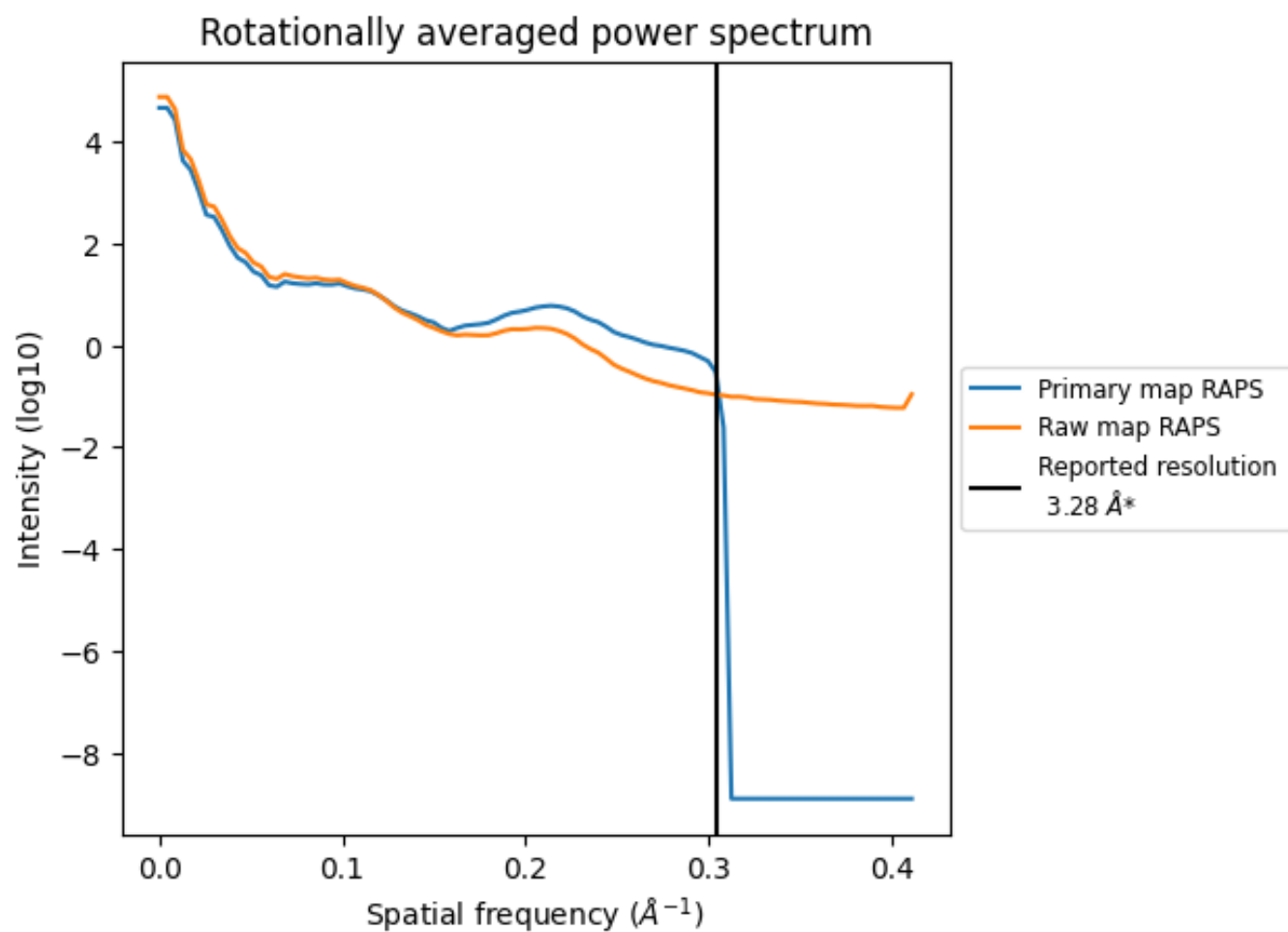
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

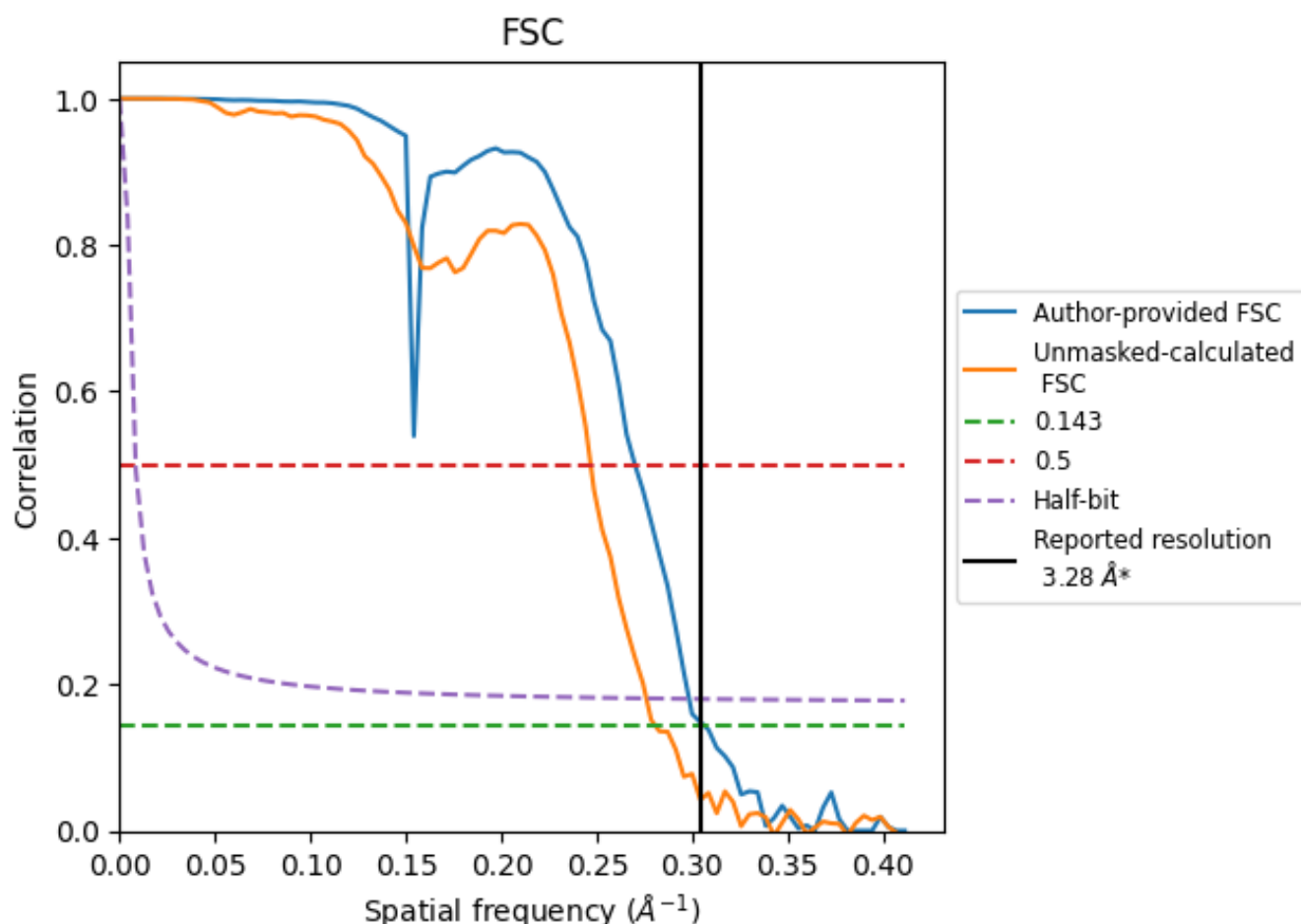


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

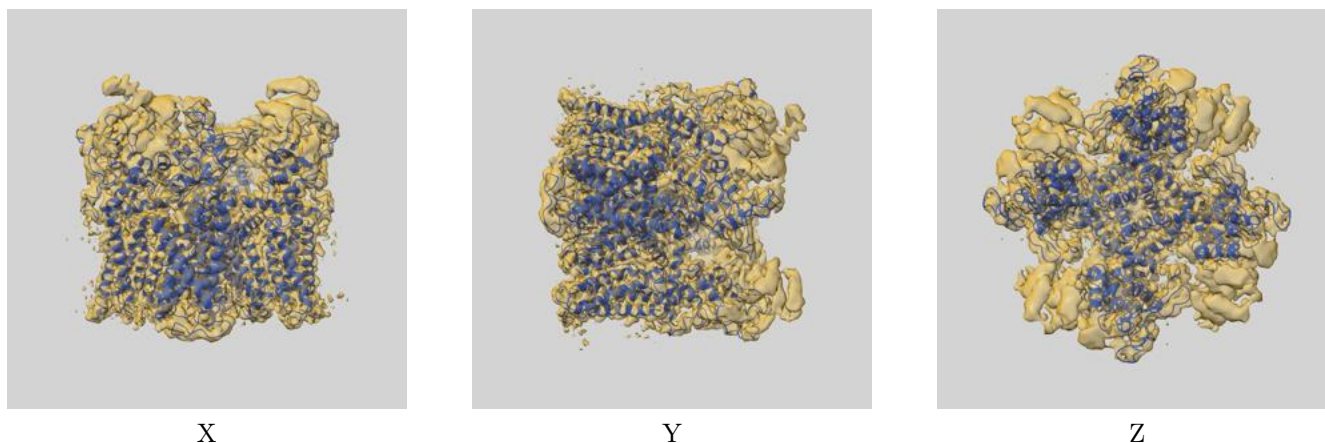
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.26	3.70	3.35
Unmasked-calculated*	3.56	4.05	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

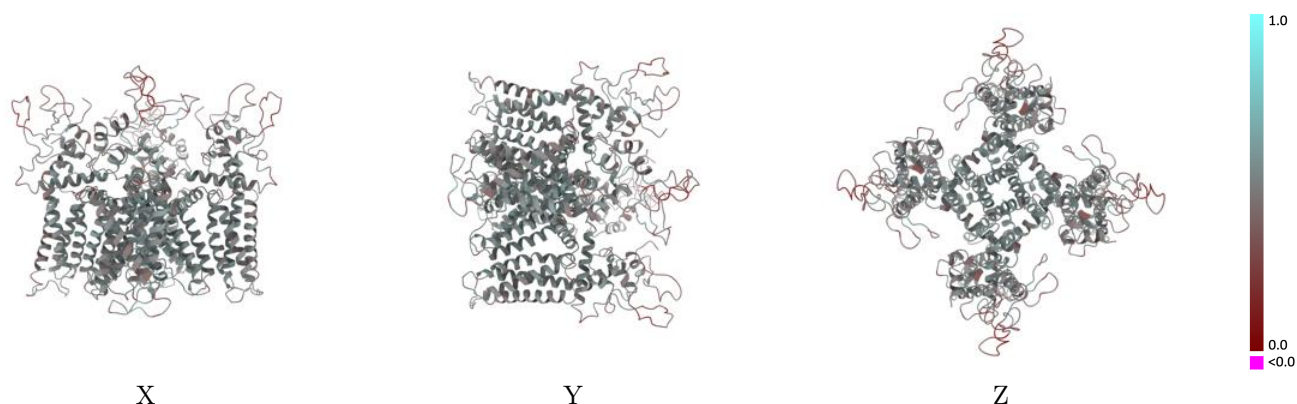
This section contains information regarding the fit between EMDB map EMD-8118 and PDB model 5IRZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



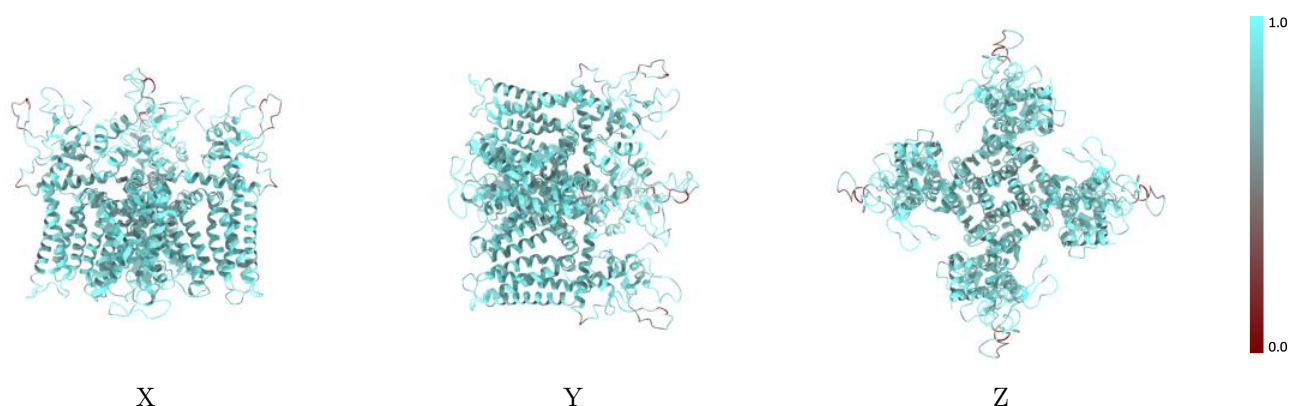
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



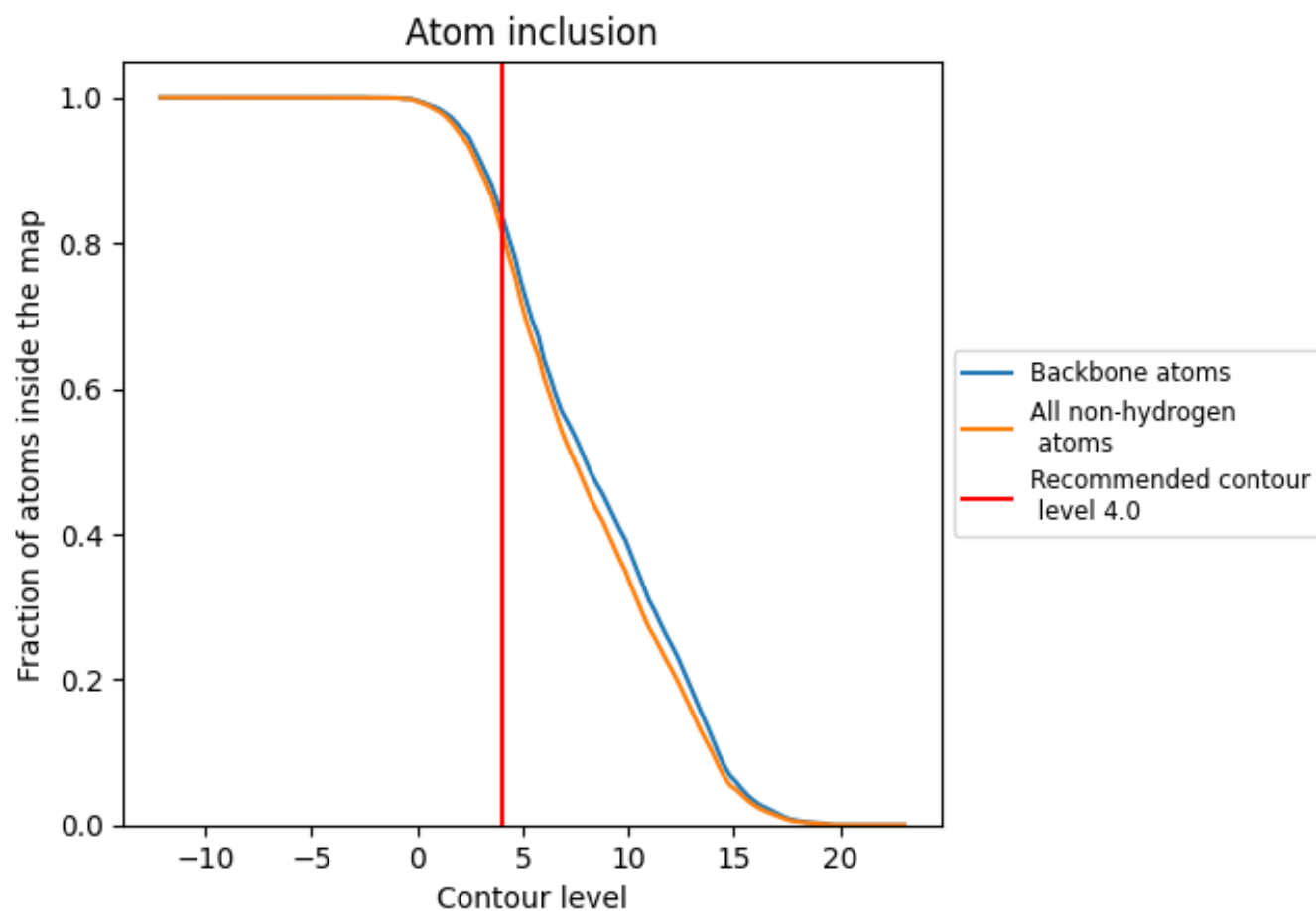
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8195	<div><div></div></div> 0.4870
B	<div><div></div></div> 0.8283	<div><div></div></div> 0.4870
C	<div><div></div></div> 0.8257	<div><div></div></div> 0.4870
D	<div><div></div></div> 0.8270	<div><div></div></div> 0.4870
E	<div><div></div></div> 0.8257	<div><div></div></div> 0.4870

