



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:04 AM UTC

PDB ID : 6UW6 / pdb_00006uw6
EMDB ID : EMD-20918
Title : Cryo-EM structure of the human TRPV3 K169A mutant determined in lipid nanodisc
Authors : Deng, Z.; Yuan, P.
Deposited on : 2019-11-04
Resolution : 3.66 Å(reported)

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

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

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

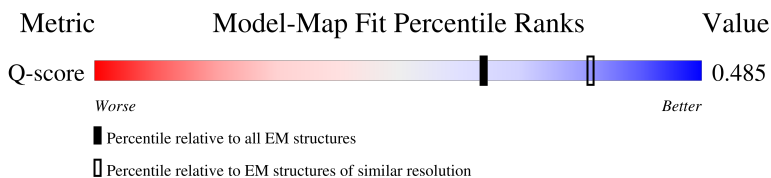
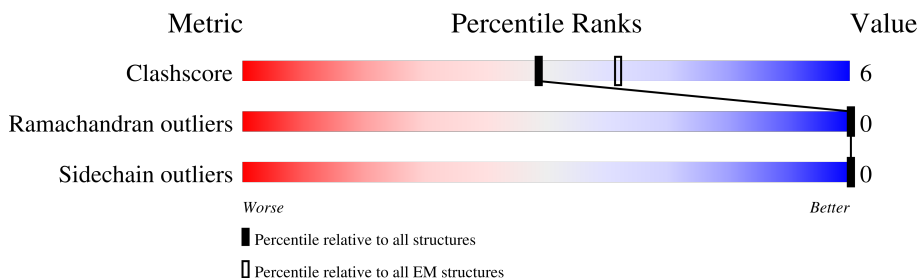
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.66 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	11491 (3.16 - 4.16)

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	790	 66% 10% 24%
1	B	790	 65% 12% 24%
1	C	790	 65% 11% 24%
1	D	790	 66% 10% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20072 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.

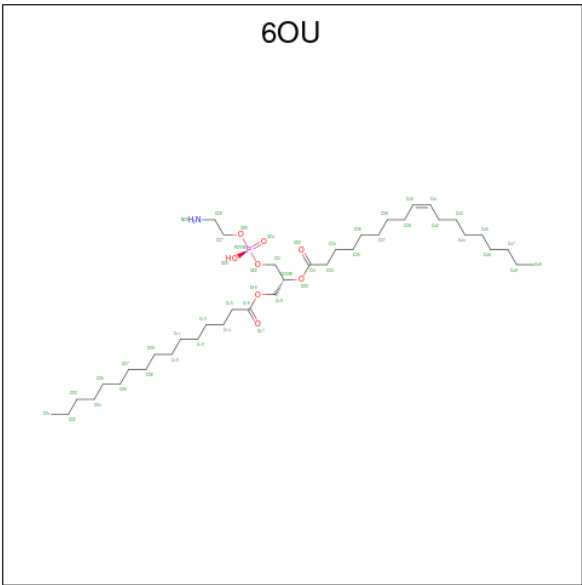
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4910	3200	815	866	29		
1	B	602	Total	C	N	O	S	0	0
			4910	3200	815	866	29		
1	C	602	Total	C	N	O	S	0	0
			4910	3200	815	866	29		
1	D	602	Total	C	N	O	S	0	0
			4910	3200	815	866	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	ILE	variant	UNP Q8NET8
A	169	ALA	LYS	engineered mutation	UNP Q8NET8
B	25	VAL	ILE	variant	UNP Q8NET8
B	169	ALA	LYS	engineered mutation	UNP Q8NET8
C	25	VAL	ILE	variant	UNP Q8NET8
C	169	ALA	LYS	engineered mutation	UNP Q8NET8
D	25	VAL	ILE	variant	UNP Q8NET8
D	169	ALA	LYS	engineered mutation	UNP Q8NET8

- Molecule 2 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-p ropan-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			15	7	1	6	1	
2	A	1	Total	C	O			0
			22	17	5			
2	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	A	1	Total	C	N	O	P	0
			28	18	1	8	1	
2	A	1	Total	C				0
			11	11				
2	B	1	Total	C	N	O	P	0
			15	7	1	6	1	
2	B	1	Total	C	O			0
			22	17	5			
2	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	B	1	Total	C	N	O	P	0
			28	18	1	8	1	
2	B	1	Total	C				0
			11	11				
2	C	1	Total	C	N	O	P	0
			15	7	1	6	1	
2	C	1	Total	C	O			0
			22	17	5			
2	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
2	C	1	Total	C	N	O	P	0
			28	18	1	8	1	

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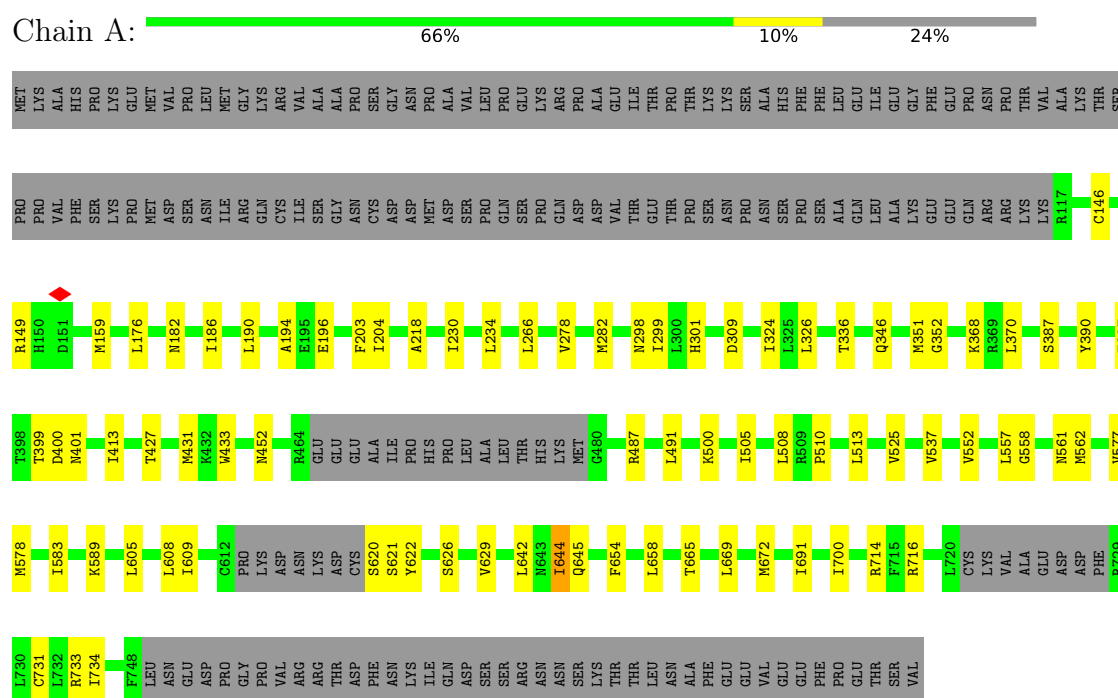
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Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total C 11 11	0
2	D	1	Total C N O P 15 7 1 6 1	0
2	D	1	Total C O 22 17 5	0
2	D	1	Total C N O P 32 22 1 8 1	0
2	D	1	Total C N O P 28 18 1 8 1	0
2	D	1	Total C 11 11	0

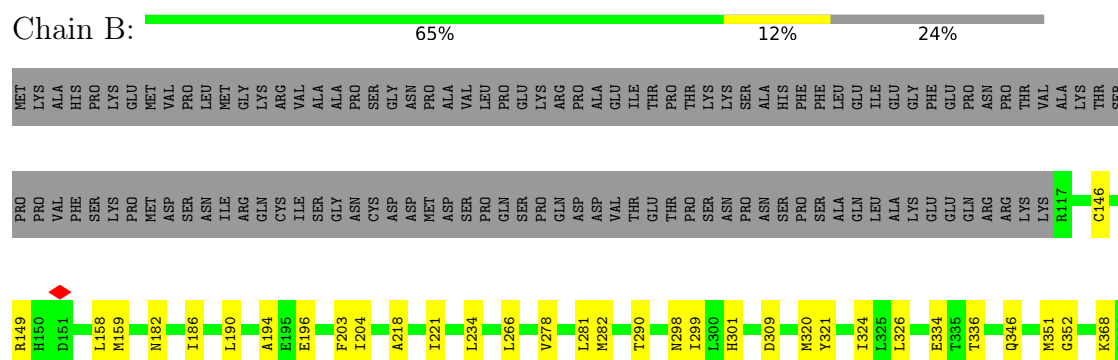
3 Residue-property plots

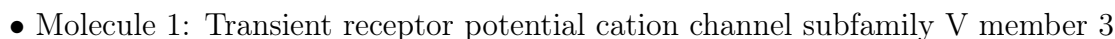
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 3



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D400	D151	PRO	LYS	MET
N401	M159	PRO	VAL	LYS
I413	L176	SER	PHE	HIS
T427	M182	PRO	LYS	LYS
M431	I186	MET	ASP	VAL
W433	L190	SER	SER	PRO
N452	A194	ASN	ILE	LEU
R464	E195	ARG	ARG	GLY
GLU	E196	GLN	LYS	ARG
GLU	F203	ILE	VAL	LYS
ALA	T204	SER	ALA	ALA
ILE	A218	ASN	GLY	PRO
PRO	I230	CYS	SER	SER
PRO	L234	ASP	GLY	GLY
LEU	L266	ASP	ASN	ASN
THR	V278	MET	PRO	PRO
HIS	M282	ASP	ALA	ALA
LYS	T290	PRO	VAL	VAL
MET	N298	GLN	THR	ILE
G480	I299	THR	GLU	THR
R487	H301	PRO	THR	PRO
L491	D309	SER	LYS	LYS
I505	I324	ASN	ASN	SER
L508	L325	SER	SER	HIS
R509	L326	PRO	PHE	PHE
P510	T336	ALA	LEU	LEU
L513	Q346	LEU	ILE	ILE
V537	M351	ALA	GLY	GLU
L541	G352	LYS	GLU	PHE
L548	L370	GLN	GLU	GLU
G558	S387	ARG	ARG	PRO
M562	Y390	LYS	THR	THR
V577	T397	LYS	VAL	ALA
M578	T398	LYS	LYS	LYS
K589		R117	LYS	THR
L605		I123	LYS	SER

L608	C731	R733	I734	F748	LEU	ASN	GLU	ASP	PRO	GLY	PRO	VAL	ARG	THR	ASP	PHE	ASN	LYS	ILE	GLN	ASP	SER	SER	ARG	ASN	ASN	SER	LYS	THR	THR	LEU	ASN	ALA	PHE	GLU	GLU	VAL	GLU	PHE	PRO	GLU	THR	SER	VAL			
I609	L730	L732	L734	L748	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62, 62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6OU

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	0/5015	0.62	4/6780 (0.1%)
1	B	0.38	0/5015	0.62	4/6780 (0.1%)
1	C	0.38	0/5015	0.63	6/6780 (0.1%)
1	D	0.38	0/5015	0.62	4/6780 (0.1%)
All	All	0.38	0/20060	0.62	18/27120 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	GLU	N-CA-C	9.71	121.86	111.28
1	C	196	GLU	N-CA-C	9.71	121.86	111.28
1	D	196	GLU	N-CA-C	9.70	121.85	111.28
1	B	196	GLU	N-CA-C	9.69	121.84	111.28
1	D	218	ALA	N-CA-C	6.91	120.81	112.38
1	C	644	ILE	N-CA-C	6.89	116.90	110.42
1	C	218	ALA	N-CA-C	6.89	120.78	112.38
1	D	644	ILE	N-CA-C	6.88	116.89	110.42
1	B	644	ILE	N-CA-C	6.88	116.88	110.42
1	A	218	ALA	N-CA-C	6.87	120.77	112.38
1	B	218	ALA	N-CA-C	6.87	120.76	112.38
1	A	644	ILE	N-CA-C	6.85	116.86	110.42
1	C	368	LYS	CA-C-N	5.59	132.22	121.54
1	C	368	LYS	C-N-CA	5.59	132.22	121.54
1	B	194	ALA	N-CA-C	-5.19	105.31	111.69
1	C	194	ALA	N-CA-C	-5.18	105.31	111.69
1	A	194	ALA	N-CA-C	-5.16	105.34	111.69
1	D	194	ALA	N-CA-C	-5.15	105.35	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4910	0	4987	56	0
1	B	4910	0	4987	66	0
1	C	4910	0	4987	60	0
1	D	4910	0	4987	60	0
2	A	108	0	0	0	0
2	B	108	0	0	0	0
2	C	108	0	0	0	0
2	D	108	0	0	0	0
All	All	20072	0	19948	232	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 6.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TYR:O	1:A:731:CYS:HA	1.72	0.90
1:C:390:TYR:O	1:C:731:CYS:HA	1.72	0.90
1:B:390:TYR:O	1:B:731:CYS:HA	1.72	0.89
1:D:390:TYR:O	1:D:731:CYS:HA	1.72	0.88
1:B:397:THR:HG22	1:B:397:THR:O	1.81	0.81
1:D:397:THR:O	1:D:397:THR:HG22	1.81	0.79
1:A:397:THR:O	1:A:397:THR:HG22	1.81	0.78
1:C:397:THR:HG22	1:C:397:THR:O	1.81	0.78
1:D:642:LEU:HD23	1:D:642:LEU:O	1.93	0.69
1:B:642:LEU:HD23	1:B:642:LEU:O	1.93	0.69
1:C:642:LEU:O	1:C:642:LEU:HD23	1.93	0.68
1:A:642:LEU:O	1:A:642:LEU:HD23	1.93	0.67
1:D:644:ILE:HD12	1:D:645:GLN:N	2.11	0.66
1:C:644:ILE:HD12	1:C:645:GLN:N	2.11	0.65
1:A:644:ILE:HD12	1:A:645:GLN:N	2.11	0.65
1:B:644:ILE:HD12	1:B:645:GLN:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:VAL:HG12	1:D:282:MET:HE2	1.82	0.61
1:A:278:VAL:HG12	1:A:282:MET:HE2	1.82	0.60
1:C:278:VAL:HG12	1:C:282:MET:HE2	1.81	0.60
1:B:278:VAL:HG12	1:B:282:MET:HE2	1.82	0.60
1:A:298:ASN:ND2	1:A:336:THR:OG1	2.36	0.59
1:B:298:ASN:ND2	1:B:336:THR:OG1	2.36	0.58
1:D:298:ASN:ND2	1:D:336:THR:OG1	2.36	0.58
1:C:298:ASN:ND2	1:C:336:THR:OG1	2.36	0.58
1:A:644:ILE:HG13	1:A:645:GLN:H	1.70	0.57
1:B:644:ILE:HG13	1:B:645:GLN:H	1.70	0.56
1:D:644:ILE:HG13	1:D:645:GLN:H	1.70	0.56
1:C:644:ILE:HG13	1:C:645:GLN:H	1.70	0.55
1:A:583:ILE:HD11	1:D:668:LEU:HD22	1.91	0.54
1:A:714:ARG:O	1:A:716:ARG:NH2	2.41	0.53
1:B:397:THR:O	1:B:397:THR:CG2	2.54	0.53
1:C:714:ARG:O	1:C:716:ARG:NH2	2.41	0.53
1:D:714:ARG:O	1:D:716:ARG:NH2	2.41	0.53
1:B:714:ARG:O	1:B:716:ARG:NH2	2.41	0.53
1:C:427:THR:HG21	1:C:734:ILE:HG21	1.91	0.52
1:D:427:THR:HG21	1:D:734:ILE:HG21	1.91	0.52
1:A:578:MET:HE1	1:D:676:LEU:HD21	1.91	0.52
1:D:346:GLN:NE2	1:D:401:ASN:O	2.43	0.52
1:C:399:THR:OG1	1:C:400:ASP:N	2.43	0.51
1:B:326:LEU:HD22	1:B:370:LEU:HD13	1.92	0.51
1:C:326:LEU:HD22	1:C:370:LEU:HD13	1.92	0.51
1:A:326:LEU:HD22	1:A:370:LEU:HD13	1.92	0.51
1:C:346:GLN:NE2	1:C:401:ASN:O	2.43	0.51
1:A:399:THR:OG1	1:A:400:ASP:N	2.43	0.51
1:B:427:THR:HG21	1:B:734:ILE:HG21	1.91	0.51
1:D:326:LEU:HD22	1:D:370:LEU:HD13	1.93	0.51
1:A:427:THR:HG21	1:A:734:ILE:HG21	1.91	0.51
1:B:399:THR:OG1	1:B:400:ASP:N	2.43	0.51
1:B:346:GLN:NE2	1:B:401:ASN:O	2.43	0.51
1:D:399:THR:OG1	1:D:400:ASP:N	2.43	0.51
1:A:452:ASN:ND2	1:A:558:GLY:O	2.45	0.50
1:C:452:ASN:ND2	1:C:558:GLY:O	2.45	0.50
1:D:452:ASN:ND2	1:D:558:GLY:O	2.45	0.49
1:A:346:GLN:NE2	1:A:401:ASN:O	2.43	0.49
1:A:397:THR:O	1:A:397:THR:CG2	2.54	0.49
1:A:644:ILE:CG1	1:A:645:GLN:N	2.76	0.49
1:B:452:ASN:ND2	1:B:558:GLY:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ILE:HG23	1:A:508:LEU:HD13	1.95	0.48
1:B:505:ILE:HG23	1:B:508:LEU:HD13	1.96	0.48
1:B:644:ILE:CG1	1:B:645:GLN:N	2.76	0.48
1:C:505:ILE:HG23	1:C:508:LEU:HD13	1.95	0.48
1:A:552:VAL:HG21	1:D:608:LEU:HD23	1.95	0.48
1:C:491:LEU:HD22	1:C:537:VAL:HG11	1.96	0.48
1:C:644:ILE:CG1	1:C:645:GLN:N	2.76	0.48
1:D:505:ILE:HG23	1:D:508:LEU:HD13	1.95	0.48
1:D:644:ILE:CG1	1:D:645:GLN:N	2.76	0.48
1:D:644:ILE:CD1	1:D:645:GLN:N	2.77	0.48
1:B:577:VAL:HG21	1:B:691:ILE:HG21	1.96	0.48
1:C:644:ILE:CD1	1:C:645:GLN:N	2.77	0.48
1:A:491:LEU:HD22	1:A:537:VAL:HG11	1.96	0.47
1:B:668:LEU:HD22	1:C:583:ILE:HD11	1.95	0.47
1:C:577:VAL:HG21	1:C:691:ILE:HG21	1.96	0.47
1:A:500:LYS:HE3	1:A:500:LYS:HB2	1.67	0.47
1:B:644:ILE:CD1	1:B:645:GLN:N	2.77	0.47
1:D:491:LEU:HD22	1:D:537:VAL:HG11	1.96	0.47
1:A:577:VAL:HG21	1:A:691:ILE:HG21	1.96	0.47
1:A:644:ILE:CD1	1:A:645:GLN:N	2.77	0.47
1:D:577:VAL:HG21	1:D:691:ILE:HG21	1.96	0.47
1:C:299:ILE:HD11	1:C:324:ILE:HD13	1.97	0.47
1:D:299:ILE:HD11	1:D:324:ILE:HD13	1.97	0.47
1:D:400:ASP:N	1:D:400:ASP:OD2	2.48	0.47
1:C:626:SER:HA	1:C:629:VAL:HG12	1.98	0.46
1:D:387:SER:OG	1:D:733:ARG:NH1	2.49	0.46
1:B:299:ILE:HD11	1:B:324:ILE:HD13	1.97	0.46
1:B:491:LEU:HD22	1:B:537:VAL:HG11	1.96	0.46
1:C:605:LEU:HD21	1:C:658:LEU:HD13	1.98	0.46
1:C:387:SER:OG	1:C:733:ARG:NH1	2.49	0.46
1:C:397:THR:O	1:C:397:THR:CG2	2.54	0.46
1:C:518:SER:O	1:C:518:SER:OG	2.31	0.46
1:D:309:ASP:N	1:D:309:ASP:OD1	2.49	0.46
1:B:605:LEU:HD21	1:B:658:LEU:HD13	1.98	0.46
1:D:605:LEU:HD21	1:D:658:LEU:HD13	1.98	0.46
1:D:351:MET:HE2	1:D:351:MET:HB3	1.83	0.46
1:D:626:SER:HA	1:D:629:VAL:HG12	1.98	0.46
1:D:397:THR:O	1:D:397:THR:CG2	2.54	0.45
1:A:487:ARG:HD2	1:A:537:VAL:HG22	1.97	0.45
1:C:204:ILE:HD11	1:C:234:LEU:HG	1.99	0.45
1:B:387:SER:OG	1:B:733:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:CYS:O	1:A:149:ARG:NH1	2.42	0.45
1:A:620:SER:OG	1:A:621:SER:N	2.47	0.45
1:B:309:ASP:OD1	1:B:309:ASP:N	2.49	0.45
1:D:487:ARG:HD2	1:D:537:VAL:HG22	1.97	0.45
1:A:204:ILE:HD11	1:A:234:LEU:HG	1.99	0.45
1:A:431:MET:HE3	1:A:431:MET:HB2	1.87	0.45
1:A:299:ILE:HD11	1:A:324:ILE:HD13	1.97	0.45
1:B:146:CYS:O	1:B:149:ARG:NH1	2.42	0.45
1:B:620:SER:OG	1:B:621:SER:N	2.47	0.45
1:D:204:ILE:HD11	1:D:234:LEU:HG	1.99	0.45
1:C:487:ARG:HD2	1:C:537:VAL:HG22	1.97	0.45
1:A:182:ASN:OD1	1:A:182:ASN:N	2.50	0.45
1:A:626:SER:HA	1:A:629:VAL:HG12	1.98	0.45
1:C:290:THR:O	1:C:290:THR:OG1	2.35	0.45
1:A:387:SER:OG	1:A:733:ARG:NH1	2.49	0.45
1:A:605:LEU:HD21	1:A:658:LEU:HD13	1.98	0.45
1:A:309:ASP:OD1	1:A:309:ASP:N	2.49	0.45
1:B:204:ILE:HD11	1:B:234:LEU:HG	1.99	0.45
1:B:298:ASN:OD1	1:B:301:HIS:ND1	2.44	0.45
1:C:620:SER:OG	1:C:621:SER:N	2.47	0.45
1:D:620:SER:OG	1:D:621:SER:N	2.47	0.45
1:A:351:MET:HE2	1:A:351:MET:HB3	1.83	0.44
1:B:182:ASN:OD1	1:B:182:ASN:N	2.50	0.44
1:B:626:SER:HA	1:B:629:VAL:HG12	1.98	0.44
1:B:487:ARG:HD2	1:B:537:VAL:HG22	1.97	0.44
1:C:309:ASP:N	1:C:309:ASP:OD1	2.49	0.44
1:C:500:LYS:HB2	1:C:500:LYS:HE3	1.67	0.44
1:B:400:ASP:N	1:B:400:ASP:OD2	2.48	0.44
1:C:665:THR:HA	1:C:669:LEU:HB2	1.99	0.44
1:C:676:LEU:HD21	1:D:578:MET:HE1	1.99	0.44
1:D:562:MET:HE3	1:D:562:MET:HB3	1.84	0.44
1:C:182:ASN:OD1	1:C:182:ASN:N	2.50	0.44
1:D:644:ILE:CD1	1:D:645:GLN:HB2	2.48	0.44
1:B:500:LYS:HB2	1:B:500:LYS:HE3	1.67	0.43
1:B:644:ILE:CD1	1:B:645:GLN:HB2	2.48	0.43
1:D:665:THR:HA	1:D:669:LEU:HB2	1.99	0.43
1:A:352:GLY:HA3	1:A:413:ILE:HG21	2.01	0.43
1:B:433:TRP:HE3	1:B:700:ILE:HD11	1.83	0.43
1:D:433:TRP:HE3	1:D:700:ILE:HD11	1.83	0.43
1:D:541:LEU:HD23	1:D:541:LEU:HA	1.87	0.43
1:A:433:TRP:HE3	1:A:700:ILE:HD11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ASN:OD1	1:D:182:ASN:N	2.50	0.43
1:D:431:MET:HB2	1:D:431:MET:HE3	1.87	0.43
1:B:662:VAL:HG11	1:C:637:ILE:HD13	2.01	0.43
1:C:431:MET:HE3	1:C:431:MET:HB2	1.87	0.43
1:C:609:ILE:HG13	1:C:622:TYR:HB2	2.01	0.43
1:B:290:THR:O	1:B:290:THR:OG1	2.35	0.43
1:D:608:LEU:HD11	1:D:654:PHE:HD1	1.83	0.43
1:C:433:TRP:HE3	1:C:700:ILE:HD11	1.83	0.43
1:C:608:LEU:HD11	1:C:654:PHE:HD1	1.83	0.43
1:C:644:ILE:CD1	1:C:645:GLN:HB2	2.48	0.43
1:B:352:GLY:HA3	1:B:413:ILE:HG21	2.00	0.43
1:B:609:ILE:HG13	1:B:622:TYR:HB2	2.01	0.43
1:C:641:ASP:OD1	1:C:641:ASP:N	2.43	0.43
1:D:609:ILE:HG13	1:D:622:TYR:HB2	2.01	0.43
1:A:644:ILE:CD1	1:A:645:GLN:HB2	2.48	0.43
1:A:609:ILE:HG13	1:A:622:TYR:HB2	2.01	0.43
1:A:608:LEU:HD11	1:A:654:PHE:HD1	1.83	0.43
1:B:457:LEU:HD23	1:B:457:LEU:HA	1.90	0.43
1:B:665:THR:HA	1:B:669:LEU:HB2	1.99	0.43
1:C:159:MET:HE1	1:C:203:PHE:HD1	1.84	0.43
1:C:567:ARG:HE	1:C:567:ARG:HB3	1.68	0.43
1:D:352:GLY:HA3	1:D:413:ILE:HG21	2.00	0.43
1:B:396:ASP:O	1:B:402:SER:OG	2.32	0.42
1:C:548:LEU:HD12	1:C:548:LEU:HA	1.85	0.42
1:D:159:MET:HE1	1:D:203:PHE:HD1	1.84	0.42
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.89	0.42
1:B:351:MET:HE2	1:B:351:MET:HB3	1.83	0.42
1:C:266:LEU:HG	1:C:299:ILE:HD12	2.01	0.42
1:A:298:ASN:OD1	1:A:301:HIS:ND1	2.44	0.42
1:B:320:MET:HE2	1:B:320:MET:HB2	1.85	0.42
1:C:146:CYS:O	1:C:149:ARG:NH1	2.42	0.42
1:C:589:LYS:HB2	1:C:589:LYS:HE3	1.82	0.42
1:B:159:MET:HE1	1:B:203:PHE:HD1	1.84	0.42
1:B:608:LEU:HD11	1:B:654:PHE:HD1	1.83	0.42
1:A:665:THR:HA	1:A:669:LEU:HB2	1.99	0.42
1:B:221:ILE:H	1:B:221:ILE:HG13	1.73	0.42
1:B:510:PRO:HD2	1:B:513:LEU:HD22	2.02	0.42
1:B:589:LYS:HB2	1:B:589:LYS:HE3	1.82	0.42
1:C:352:GLY:HA3	1:C:413:ILE:HG21	2.00	0.42
1:C:510:PRO:HD2	1:C:513:LEU:HD22	2.02	0.42
1:A:159:MET:HE1	1:A:203:PHE:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:PRO:HD2	1:A:513:LEU:HD22	2.02	0.42
1:D:290:THR:O	1:D:290:THR:OG1	2.35	0.42
1:D:658:LEU:HD12	1:D:658:LEU:HA	1.88	0.42
1:A:557:LEU:HD12	1:A:557:LEU:HA	1.88	0.42
1:B:266:LEU:HG	1:B:299:ILE:HD12	2.01	0.42
1:C:670:LEU:O	1:C:674:ILE:HG12	2.20	0.42
1:D:510:PRO:HD2	1:D:513:LEU:HD22	2.02	0.42
1:B:567:ARG:HE	1:B:567:ARG:HB3	1.68	0.42
1:A:589:LYS:HB2	1:A:589:LYS:HE3	1.82	0.41
1:B:670:LEU:O	1:B:674:ILE:HG12	2.20	0.41
1:A:508:LEU:HG	1:A:513:LEU:HD21	2.03	0.41
1:B:453:ILE:HD13	1:B:453:ILE:HA	1.87	0.41
1:B:368:LYS:HA	1:B:368:LYS:HD2	1.89	0.41
1:C:508:LEU:HG	1:C:513:LEU:HD21	2.03	0.41
1:C:644:ILE:HG13	1:C:645:GLN:N	2.35	0.41
1:B:508:LEU:HG	1:B:513:LEU:HD21	2.03	0.41
1:C:662:VAL:HG11	1:D:637:ILE:HD13	2.02	0.41
1:D:266:LEU:HG	1:D:299:ILE:HD12	2.02	0.41
1:B:321:TYR:OH	1:B:334:GLU:OE1	2.38	0.41
1:B:676:LEU:HD21	1:C:578:MET:HE1	2.01	0.41
1:D:123:ILE:HD12	1:D:123:ILE:HA	1.89	0.41
1:A:176:LEU:HD21	1:A:230:ILE:HG21	2.03	0.41
1:A:608:LEU:HD23	1:B:552:VAL:HG21	2.02	0.41
1:C:298:ASN:OD1	1:C:301:HIS:ND1	2.44	0.41
1:B:541:LEU:HD23	1:B:541:LEU:HA	1.87	0.41
1:B:548:LEU:HD12	1:B:548:LEU:HA	1.85	0.41
1:D:508:LEU:HG	1:D:513:LEU:HD21	2.03	0.41
1:A:562:MET:HE3	1:A:562:MET:HB3	1.84	0.41
1:A:658:LEU:HD12	1:A:658:LEU:HA	1.88	0.41
1:B:431:MET:HE3	1:B:431:MET:HB2	1.87	0.41
1:D:670:LEU:O	1:D:674:ILE:HG12	2.20	0.41
1:C:303:LEU:HD22	1:C:317:VAL:HG23	2.03	0.41
1:C:400:ASP:N	1:C:400:ASP:OD2	2.48	0.41
1:D:298:ASN:OD1	1:D:301:HIS:ND1	2.44	0.41
1:A:266:LEU:HG	1:A:299:ILE:HD12	2.01	0.40
1:D:186:ILE:O	1:D:190:LEU:HB2	2.21	0.40
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.93	0.40
1:C:351:MET:HE2	1:C:351:MET:HB3	1.83	0.40
1:D:176:LEU:HD21	1:D:230:ILE:HG21	2.03	0.40
1:B:508:LEU:HG	1:B:513:LEU:HD11	2.04	0.40
1:C:541:LEU:HD23	1:C:541:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:O	1:A:190:LEU:HB2	2.21	0.40
1:B:186:ILE:O	1:B:190:LEU:HB2	2.22	0.40
1:D:548:LEU:HD12	1:D:548:LEU:HA	1.85	0.40
1:D:672:MET:HE2	1:D:672:MET:HB3	1.80	0.40
1:A:368:LYS:HD2	1:A:368:LYS:HA	1.89	0.40
1:A:525:VAL:HG12	1:A:561:ASN:HD21	1.87	0.40
1:A:672:MET:HG3	1:B:681:VAL:HG21	2.03	0.40
1:C:672:MET:HE2	1:C:672:MET:HB3	1.80	0.40
1:D:508:LEU:HG	1:D:513:LEU:HD11	2.04	0.40
1:D:589:LYS:HB2	1:D:589:LYS:HE3	1.82	0.40
1:D:676:LEU:HD23	1:D:676:LEU:HA	1.91	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	594/790 (75%)	544 (92%)	50 (8%)	0	100	100
1	B	594/790 (75%)	544 (92%)	50 (8%)	0	100	100
1	C	594/790 (75%)	543 (91%)	51 (9%)	0	100	100
1	D	594/790 (75%)	545 (92%)	49 (8%)	0	100	100
All	All	2376/3160 (75%)	2176 (92%)	200 (8%)	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	532/702 (76%)	532 (100%)	0	100	100
1	B	532/702 (76%)	532 (100%)	0	100	100
1	C	532/702 (76%)	532 (100%)	0	100	100
1	D	532/702 (76%)	532 (100%)	0	100	100
All	All	2128/2808 (76%)	2128 (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. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	220	ASN
1	A	255	GLN
1	A	314	ASN
1	A	394	ASN
1	A	412	ASN
1	A	417	HIS
1	A	426	HIS
1	A	430	HIS
1	A	646	GLN
1	B	178	ASN
1	B	220	ASN
1	B	255	GLN
1	B	314	ASN
1	B	394	ASN
1	B	426	HIS
1	B	430	HIS
1	B	646	GLN
1	C	178	ASN
1	C	220	ASN
1	C	255	GLN
1	C	314	ASN
1	C	394	ASN
1	C	412	ASN
1	C	417	HIS
1	C	426	HIS
1	C	430	HIS
1	C	646	GLN

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Mol	Chain	Res	Type
1	D	178	ASN
1	D	220	ASN
1	D	255	GLN
1	D	314	ASN
1	D	394	ASN
1	D	412	ASN
1	D	426	HIS
1	D	430	HIS
1	D	646	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
2	6OU	A	801	-	14,14,48	2.17	8 (57%)	16,17,53	0.87	0
2	6OU	C	802	-	21,21,48	2.45	8 (38%)	23,23,53	1.39	2 (8%)
2	6OU	D	805	-	10,10,48	1.74	2 (20%)	9,9,53	0.78	0
2	6OU	A	802	-	21,21,48	2.45	8 (38%)	23,23,53	1.39	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6OU	B	803	-	31,31,48	2.33	12 (38%)	34,36,53	1.22	2 (5%)
2	6OU	C	805	-	10,10,48	1.74	2 (20%)	9,9,53	0.79	0
2	6OU	A	803	-	31,31,48	2.33	12 (38%)	34,36,53	1.23	2 (5%)
2	6OU	D	803	-	31,31,48	2.33	12 (38%)	34,36,53	1.22	2 (5%)
2	6OU	B	801	-	14,14,48	2.17	8 (57%)	16,17,53	0.87	0
2	6OU	B	805	-	10,10,48	1.74	2 (20%)	9,9,53	0.78	0
2	6OU	B	804	-	27,27,48	2.39	12 (44%)	30,32,53	1.34	2 (6%)
2	6OU	B	802	-	21,21,48	2.45	8 (38%)	23,23,53	1.39	2 (8%)
2	6OU	C	804	-	27,27,48	2.39	12 (44%)	30,32,53	1.34	2 (6%)
2	6OU	A	805	-	10,10,48	1.74	2 (20%)	9,9,53	0.78	0
2	6OU	D	801	-	14,14,48	2.17	8 (57%)	16,17,53	0.86	0
2	6OU	D	804	-	27,27,48	2.39	12 (44%)	30,32,53	1.34	2 (6%)
2	6OU	D	802	-	21,21,48	2.46	8 (38%)	23,23,53	1.39	2 (8%)
2	6OU	C	803	-	31,31,48	2.33	12 (38%)	34,36,53	1.23	2 (5%)
2	6OU	A	804	-	27,27,48	2.39	12 (44%)	30,32,53	1.34	2 (6%)
2	6OU	C	801	-	14,14,48	2.17	8 (57%)	16,17,53	0.87	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
2	6OU	A	801	-	-	8/14/14/52	-
2	6OU	C	802	-	-	7/23/23/52	-
2	6OU	D	805	-	-	3/8/8/52	-
2	6OU	A	802	-	-	7/23/23/52	-
2	6OU	B	803	-	-	11/35/35/52	-
2	6OU	C	805	-	-	3/8/8/52	-
2	6OU	A	803	-	-	11/35/35/52	-
2	6OU	D	803	-	-	11/35/35/52	-
2	6OU	B	801	-	-	8/14/14/52	-
2	6OU	B	805	-	-	3/8/8/52	-
2	6OU	B	804	-	-	15/31/31/52	-
2	6OU	B	802	-	-	7/23/23/52	-
2	6OU	C	804	-	-	15/31/31/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6OU	A	805	-	-	3/8/8/52	-
2	6OU	D	801	-	-	8/14/14/52	-
2	6OU	D	804	-	-	15/31/31/52	-
2	6OU	D	802	-	-	7/23/23/52	-
2	6OU	C	803	-	-	11/35/35/52	-
2	6OU	A	804	-	-	15/31/31/52	-
2	6OU	C	801	-	-	8/14/14/52	-

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	6OU	O18-C16	4.76	1.47	1.33
2	D	802	6OU	O18-C16	4.75	1.47	1.33
2	B	802	6OU	O18-C16	4.74	1.47	1.33
2	C	802	6OU	O18-C16	4.74	1.47	1.33
2	C	804	6OU	O18-C16	4.71	1.47	1.33
2	B	804	6OU	O18-C16	4.70	1.47	1.33
2	A	804	6OU	O18-C16	4.69	1.47	1.33
2	D	804	6OU	O18-C16	4.69	1.47	1.33
2	B	803	6OU	O30-C31	4.66	1.47	1.34
2	A	803	6OU	O30-C31	4.66	1.47	1.34
2	D	803	6OU	O30-C31	4.66	1.47	1.34
2	C	803	6OU	O30-C31	4.65	1.47	1.34
2	B	803	6OU	O18-C16	4.62	1.46	1.33
2	D	802	6OU	O30-C31	4.62	1.47	1.34
2	C	803	6OU	O18-C16	4.61	1.46	1.33
2	D	804	6OU	O30-C31	4.61	1.47	1.34
2	A	803	6OU	O18-C16	4.61	1.46	1.33
2	D	803	6OU	O18-C16	4.60	1.46	1.33
2	A	802	6OU	O30-C31	4.60	1.47	1.34
2	A	804	6OU	O30-C31	4.59	1.47	1.34
2	C	804	6OU	O30-C31	4.59	1.47	1.34
2	B	804	6OU	O30-C31	4.59	1.47	1.34
2	B	802	6OU	O30-C31	4.59	1.47	1.34
2	C	802	6OU	O30-C31	4.58	1.47	1.34
2	B	802	6OU	C21-C20	3.97	1.60	1.51
2	C	802	6OU	C21-C20	3.97	1.60	1.51
2	D	802	6OU	C21-C20	3.97	1.60	1.51
2	A	802	6OU	C21-C20	3.96	1.60	1.51
2	D	803	6OU	P23-O26	3.62	1.73	1.59
2	A	803	6OU	P23-O26	3.60	1.73	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	803	6OU	P23-O26	3.60	1.73	1.59
2	C	803	6OU	P23-O26	3.60	1.73	1.59
2	C	804	6OU	P23-O22	3.58	1.73	1.59
2	B	803	6OU	P23-O22	3.58	1.73	1.59
2	A	804	6OU	P23-O22	3.58	1.73	1.59
2	B	804	6OU	P23-O22	3.57	1.73	1.59
2	D	804	6OU	P23-O22	3.57	1.73	1.59
2	A	803	6OU	P23-O22	3.57	1.73	1.59
2	C	803	6OU	P23-O22	3.56	1.73	1.59
2	D	803	6OU	P23-O22	3.55	1.73	1.59
2	C	804	6OU	P23-O26	3.50	1.73	1.59
2	A	804	6OU	P23-O26	3.49	1.73	1.59
2	B	804	6OU	P23-O26	3.49	1.73	1.59
2	D	804	6OU	P23-O26	3.49	1.73	1.59
2	D	803	6OU	C15-C16	3.48	1.60	1.50
2	C	803	6OU	C15-C16	3.48	1.60	1.50
2	A	803	6OU	C15-C16	3.46	1.60	1.50
2	D	801	6OU	P23-O22	3.46	1.72	1.59
2	B	803	6OU	C15-C16	3.45	1.60	1.50
2	A	801	6OU	P23-O22	3.45	1.72	1.59
2	C	801	6OU	P23-O22	3.45	1.72	1.59
2	B	801	6OU	P23-O22	3.44	1.72	1.59
2	C	802	6OU	C33-C31	3.43	1.60	1.50
2	B	803	6OU	C33-C31	3.42	1.60	1.50
2	D	802	6OU	C15-C16	3.42	1.60	1.50
2	A	803	6OU	C33-C31	3.41	1.60	1.50
2	B	802	6OU	C15-C16	3.41	1.60	1.50
2	B	802	6OU	C33-C31	3.41	1.60	1.50
2	A	802	6OU	C33-C31	3.41	1.60	1.50
2	A	802	6OU	C15-C16	3.40	1.60	1.50
2	C	802	6OU	C15-C16	3.39	1.60	1.50
2	B	804	6OU	C33-C31	3.39	1.60	1.50
2	C	803	6OU	C33-C31	3.39	1.60	1.50
2	D	803	6OU	C33-C31	3.39	1.60	1.50
2	A	804	6OU	C33-C31	3.39	1.60	1.50
2	D	802	6OU	C33-C31	3.38	1.60	1.50
2	D	804	6OU	C33-C31	3.38	1.60	1.50
2	C	804	6OU	C33-C31	3.37	1.60	1.50
2	C	801	6OU	P23-O26	3.35	1.72	1.59
2	A	801	6OU	P23-O26	3.33	1.72	1.59
2	B	801	6OU	P23-O26	3.33	1.72	1.59
2	D	801	6OU	P23-O26	3.33	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	804	6OU	C15-C16	3.32	1.60	1.50
2	B	804	6OU	C15-C16	3.32	1.60	1.50
2	A	804	6OU	C15-C16	3.31	1.60	1.50
2	C	804	6OU	C15-C16	3.29	1.60	1.50
2	C	801	6OU	C15-C16	3.29	1.60	1.49
2	B	801	6OU	C15-C16	3.28	1.60	1.49
2	A	801	6OU	C15-C16	3.27	1.60	1.49
2	D	801	6OU	C15-C16	3.26	1.60	1.49
2	A	804	6OU	C19-C20	3.22	1.60	1.50
2	C	804	6OU	C19-C20	3.21	1.60	1.50
2	D	804	6OU	C19-C20	3.21	1.60	1.50
2	B	804	6OU	C19-C20	3.19	1.60	1.50
2	A	803	6OU	C21-C20	3.17	1.60	1.50
2	C	803	6OU	C21-C20	3.16	1.60	1.50
2	D	803	6OU	C21-C20	3.16	1.60	1.50
2	D	803	6OU	C19-C20	3.15	1.60	1.50
2	B	803	6OU	C21-C20	3.15	1.60	1.50
2	C	803	6OU	C19-C20	3.14	1.60	1.50
2	A	803	6OU	C19-C20	3.13	1.60	1.50
2	B	803	6OU	C19-C20	3.12	1.60	1.50
2	D	802	6OU	C19-C20	3.10	1.60	1.50
2	A	802	6OU	C19-C20	3.09	1.60	1.50
2	B	802	6OU	C19-C20	3.09	1.60	1.50
2	C	802	6OU	C19-C20	3.08	1.60	1.50
2	A	804	6OU	C21-C20	3.07	1.60	1.50
2	B	804	6OU	C21-C20	3.07	1.60	1.50
2	D	804	6OU	C21-C20	3.07	1.60	1.50
2	C	804	6OU	C21-C20	3.05	1.60	1.50
2	A	801	6OU	O18-C16	2.78	1.46	1.33
2	D	801	6OU	O18-C16	2.78	1.46	1.33
2	C	801	6OU	O18-C16	2.78	1.46	1.33
2	B	801	6OU	O18-C16	2.77	1.46	1.33
2	B	803	6OU	C28-C27	2.69	1.60	1.49
2	A	803	6OU	C28-C27	2.68	1.60	1.49
2	C	803	6OU	C28-C27	2.68	1.60	1.49
2	D	803	6OU	C28-C27	2.68	1.60	1.49
2	A	804	6OU	C28-C27	2.64	1.60	1.49
2	B	804	6OU	C28-C27	2.63	1.60	1.49
2	C	804	6OU	C28-C27	2.63	1.60	1.49
2	D	804	6OU	C28-C27	2.62	1.60	1.49
2	D	801	6OU	C28-C27	2.54	1.60	1.49
2	C	801	6OU	C28-C27	2.54	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	6OU	C28-C27	2.54	1.60	1.49
2	A	801	6OU	C28-C27	2.53	1.60	1.49
2	B	803	6OU	C14-C15	2.34	1.60	1.52
2	C	803	6OU	C14-C15	2.33	1.60	1.52
2	D	801	6OU	C20-C19	2.33	1.60	1.51
2	A	803	6OU	C14-C15	2.32	1.60	1.52
2	A	801	6OU	C20-C19	2.32	1.60	1.51
2	A	804	6OU	C34-C33	2.31	1.60	1.52
2	A	801	6OU	C20-C21	2.31	1.60	1.51
2	B	801	6OU	C20-C21	2.31	1.60	1.51
2	B	801	6OU	C20-C19	2.30	1.60	1.51
2	D	803	6OU	C14-C15	2.30	1.60	1.52
2	C	801	6OU	C20-C19	2.30	1.60	1.51
2	C	804	6OU	C34-C33	2.30	1.60	1.52
2	C	801	6OU	C20-C21	2.30	1.60	1.51
2	D	804	6OU	C34-C33	2.30	1.60	1.52
2	D	804	6OU	P23-O24	2.29	1.58	1.50
2	B	804	6OU	C34-C33	2.29	1.60	1.52
2	B	804	6OU	P23-O24	2.29	1.58	1.50
2	D	803	6OU	C34-C33	2.29	1.60	1.52
2	C	803	6OU	C34-C33	2.29	1.60	1.52
2	C	804	6OU	P23-O24	2.29	1.58	1.50
2	D	801	6OU	C20-C21	2.28	1.60	1.51
2	A	803	6OU	C34-C33	2.28	1.60	1.52
2	C	803	6OU	P23-O24	2.28	1.58	1.50
2	B	803	6OU	C34-C33	2.28	1.60	1.52
2	A	804	6OU	P23-O24	2.28	1.58	1.50
2	B	802	6OU	C14-C15	2.27	1.60	1.52
2	C	802	6OU	C14-C15	2.26	1.60	1.52
2	B	802	6OU	C34-C33	2.26	1.60	1.52
2	D	802	6OU	C34-C33	2.26	1.60	1.52
2	D	803	6OU	P23-O24	2.26	1.58	1.50
2	A	802	6OU	C14-C15	2.26	1.60	1.52
2	D	802	6OU	C14-C15	2.26	1.60	1.52
2	A	803	6OU	P23-O24	2.25	1.58	1.50
2	B	803	6OU	P23-O24	2.24	1.58	1.50
2	A	802	6OU	C34-C33	2.24	1.60	1.52
2	C	802	6OU	C34-C33	2.24	1.60	1.52
2	C	804	6OU	C14-C15	2.23	1.60	1.52
2	D	804	6OU	C14-C15	2.21	1.60	1.52
2	A	804	6OU	C14-C15	2.21	1.60	1.52
2	D	801	6OU	P23-O24	2.20	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	804	6OU	C14-C15	2.20	1.60	1.52
2	A	801	6OU	P23-O24	2.19	1.58	1.50
2	B	801	6OU	P23-O24	2.19	1.58	1.50
2	C	801	6OU	P23-O24	2.18	1.58	1.50
2	D	805	6OU	C42-C41	2.05	1.60	1.50
2	B	805	6OU	C42-C41	2.04	1.60	1.50
2	A	805	6OU	C42-C41	2.04	1.60	1.50
2	C	805	6OU	C42-C41	2.04	1.60	1.50
2	C	805	6OU	C38-C39	2.02	1.60	1.52
2	A	805	6OU	C38-C39	2.01	1.60	1.52
2	B	805	6OU	C38-C39	2.01	1.60	1.52
2	D	805	6OU	C38-C39	2.01	1.60	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	804	6OU	O30-C31-C33	4.51	121.24	111.48
2	C	804	6OU	O30-C31-C33	4.51	121.23	111.48
2	D	804	6OU	O30-C31-C33	4.50	121.21	111.48
2	A	804	6OU	O30-C31-C33	4.50	121.21	111.48
2	C	803	6OU	O30-C31-C33	4.37	120.94	111.48
2	A	803	6OU	O30-C31-C33	4.36	120.91	111.48
2	B	803	6OU	O30-C31-C33	4.36	120.91	111.48
2	D	803	6OU	O30-C31-C33	4.35	120.90	111.48
2	B	802	6OU	O30-C31-C33	3.91	119.95	111.48
2	A	802	6OU	O30-C31-C33	3.91	119.93	111.48
2	C	802	6OU	O30-C31-C33	3.90	119.93	111.48
2	D	802	6OU	O30-C31-C33	3.89	119.90	111.48
2	D	804	6OU	O18-C16-C15	3.16	121.46	111.83
2	B	804	6OU	O18-C16-C15	3.15	121.44	111.83
2	A	804	6OU	O18-C16-C15	3.15	121.43	111.83
2	C	804	6OU	O18-C16-C15	3.15	121.43	111.83
2	C	802	6OU	O18-C16-C15	3.04	121.09	111.83
2	A	802	6OU	O18-C16-C15	3.03	121.07	111.83
2	B	802	6OU	O18-C16-C15	3.03	121.06	111.83
2	D	802	6OU	O18-C16-C15	3.02	121.03	111.83
2	B	803	6OU	O18-C16-C15	2.54	119.57	111.83
2	C	803	6OU	O18-C16-C15	2.53	119.56	111.83
2	A	803	6OU	O18-C16-C15	2.53	119.55	111.83
2	D	803	6OU	O18-C16-C15	2.53	119.54	111.83

There are no chirality outliers.

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	6OU	C21-O22-P23-O24
2	A	801	6OU	C21-O22-P23-O25
2	A	801	6OU	C21-O22-P23-O26
2	A	801	6OU	C27-O26-P23-O22
2	A	801	6OU	C27-O26-P23-O24
2	A	801	6OU	C27-O26-P23-O25
2	A	803	6OU	O18-C19-C20-O30
2	A	803	6OU	C21-O22-P23-O24
2	A	803	6OU	C21-O22-P23-O25
2	A	803	6OU	O26-C27-C28-N29
2	A	804	6OU	C21-O22-P23-O24
2	A	804	6OU	C21-O22-P23-O26
2	A	804	6OU	C27-O26-P23-O22
2	A	804	6OU	C27-O26-P23-O24
2	A	804	6OU	C27-O26-P23-O25
2	A	804	6OU	O26-C27-C28-N29
2	B	801	6OU	C21-O22-P23-O24
2	B	801	6OU	C21-O22-P23-O25
2	B	801	6OU	C21-O22-P23-O26
2	B	801	6OU	C27-O26-P23-O22
2	B	801	6OU	C27-O26-P23-O24
2	B	801	6OU	C27-O26-P23-O25
2	B	803	6OU	O18-C19-C20-O30
2	B	803	6OU	C21-O22-P23-O24
2	B	803	6OU	C21-O22-P23-O25
2	B	803	6OU	O26-C27-C28-N29
2	B	804	6OU	C21-O22-P23-O24
2	B	804	6OU	C21-O22-P23-O26
2	B	804	6OU	C27-O26-P23-O22
2	B	804	6OU	C27-O26-P23-O24
2	B	804	6OU	C27-O26-P23-O25
2	B	804	6OU	O26-C27-C28-N29
2	C	801	6OU	C21-O22-P23-O24
2	C	801	6OU	C21-O22-P23-O25
2	C	801	6OU	C21-O22-P23-O26
2	C	801	6OU	C27-O26-P23-O22
2	C	801	6OU	C27-O26-P23-O24
2	C	801	6OU	C27-O26-P23-O25
2	C	803	6OU	O18-C19-C20-O30
2	C	803	6OU	C21-O22-P23-O24
2	C	803	6OU	C21-O22-P23-O25
2	C	803	6OU	O26-C27-C28-N29

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Mol	Chain	Res	Type	Atoms
2	C	804	6OU	C21-O22-P23-O24
2	C	804	6OU	C21-O22-P23-O26
2	C	804	6OU	C27-O26-P23-O22
2	C	804	6OU	C27-O26-P23-O24
2	C	804	6OU	C27-O26-P23-O25
2	C	804	6OU	O26-C27-C28-N29
2	D	801	6OU	C21-O22-P23-O24
2	D	801	6OU	C21-O22-P23-O25
2	D	801	6OU	C21-O22-P23-O26
2	D	801	6OU	C27-O26-P23-O22
2	D	801	6OU	C27-O26-P23-O24
2	D	801	6OU	C27-O26-P23-O25
2	D	803	6OU	O18-C19-C20-O30
2	D	803	6OU	C21-O22-P23-O24
2	D	803	6OU	C21-O22-P23-O25
2	D	803	6OU	O26-C27-C28-N29
2	D	804	6OU	C21-O22-P23-O24
2	D	804	6OU	C21-O22-P23-O26
2	D	804	6OU	C27-O26-P23-O22
2	D	804	6OU	C27-O26-P23-O24
2	D	804	6OU	C27-O26-P23-O25
2	D	804	6OU	O26-C27-C28-N29
2	A	802	6OU	C15-C16-O18-C19
2	B	802	6OU	C15-C16-O18-C19
2	C	802	6OU	C15-C16-O18-C19
2	D	802	6OU	C15-C16-O18-C19
2	A	802	6OU	O17-C16-O18-C19
2	B	802	6OU	O17-C16-O18-C19
2	C	802	6OU	O17-C16-O18-C19
2	D	802	6OU	O17-C16-O18-C19
2	A	801	6OU	C15-C16-O18-C19
2	B	801	6OU	C15-C16-O18-C19
2	C	801	6OU	C15-C16-O18-C19
2	D	801	6OU	C15-C16-O18-C19
2	A	801	6OU	O17-C16-O18-C19
2	B	801	6OU	O17-C16-O18-C19
2	C	801	6OU	O17-C16-O18-C19
2	D	801	6OU	O17-C16-O18-C19
2	A	805	6OU	C40-C41-C42-C43
2	B	805	6OU	C40-C41-C42-C43
2	C	805	6OU	C40-C41-C42-C43
2	D	805	6OU	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
2	A	804	6OU	O30-C20-C21-O22
2	B	804	6OU	O30-C20-C21-O22
2	C	804	6OU	O30-C20-C21-O22
2	D	804	6OU	O30-C20-C21-O22
2	A	802	6OU	O18-C19-C20-O30
2	B	802	6OU	O18-C19-C20-O30
2	C	802	6OU	O18-C19-C20-O30
2	D	802	6OU	O18-C19-C20-O30
2	A	802	6OU	C10-C11-C12-C13
2	B	802	6OU	C10-C11-C12-C13
2	C	802	6OU	C10-C11-C12-C13
2	D	802	6OU	C10-C11-C12-C13
2	A	802	6OU	C31-C33-C34-C35
2	B	802	6OU	C31-C33-C34-C35
2	C	802	6OU	C31-C33-C34-C35
2	D	802	6OU	C31-C33-C34-C35
2	A	804	6OU	O18-C19-C20-C21
2	B	804	6OU	O18-C19-C20-C21
2	C	804	6OU	O18-C19-C20-C21
2	D	804	6OU	O18-C19-C20-C21
2	D	802	6OU	C13-C14-C15-C16
2	A	802	6OU	C13-C14-C15-C16
2	B	802	6OU	C13-C14-C15-C16
2	C	802	6OU	C13-C14-C15-C16
2	A	803	6OU	O30-C20-C21-O22
2	B	803	6OU	O30-C20-C21-O22
2	C	803	6OU	O30-C20-C21-O22
2	D	803	6OU	O30-C20-C21-O22
2	A	803	6OU	C12-C13-C14-C15
2	C	803	6OU	C12-C13-C14-C15
2	B	803	6OU	C12-C13-C14-C15
2	D	803	6OU	C12-C13-C14-C15
2	A	804	6OU	C31-C33-C34-C35
2	B	804	6OU	C31-C33-C34-C35
2	C	804	6OU	C31-C33-C34-C35
2	D	804	6OU	C31-C33-C34-C35
2	A	804	6OU	C19-C20-C21-O22
2	B	804	6OU	C19-C20-C21-O22
2	C	804	6OU	C19-C20-C21-O22
2	D	804	6OU	C19-C20-C21-O22
2	B	803	6OU	C36-C37-C38-C39
2	C	803	6OU	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
2	D	803	6OU	C36-C37-C38-C39
2	A	803	6OU	C36-C37-C38-C39
2	A	802	6OU	O18-C19-C20-C21
2	B	802	6OU	O18-C19-C20-C21
2	C	802	6OU	O18-C19-C20-C21
2	D	802	6OU	O18-C19-C20-C21
2	A	803	6OU	C19-C20-C21-O22
2	B	803	6OU	C19-C20-C21-O22
2	C	803	6OU	C19-C20-C21-O22
2	D	803	6OU	C19-C20-C21-O22
2	A	803	6OU	O18-C19-C20-C21
2	B	803	6OU	O18-C19-C20-C21
2	C	803	6OU	O18-C19-C20-C21
2	D	803	6OU	O18-C19-C20-C21
2	A	804	6OU	O18-C19-C20-O30
2	B	804	6OU	O18-C19-C20-O30
2	C	804	6OU	O18-C19-C20-O30
2	D	804	6OU	O18-C19-C20-O30
2	A	804	6OU	C15-C16-O18-C19
2	B	804	6OU	C15-C16-O18-C19
2	C	804	6OU	C15-C16-O18-C19
2	D	804	6OU	C15-C16-O18-C19
2	B	804	6OU	O17-C16-O18-C19
2	A	804	6OU	O17-C16-O18-C19
2	A	803	6OU	C21-O22-P23-O26
2	A	804	6OU	C21-O22-P23-O25
2	B	803	6OU	C21-O22-P23-O26
2	B	804	6OU	C21-O22-P23-O25
2	C	803	6OU	C21-O22-P23-O26
2	C	804	6OU	C21-O22-P23-O25
2	D	803	6OU	C21-O22-P23-O26
2	D	804	6OU	C21-O22-P23-O25
2	C	804	6OU	O17-C16-O18-C19
2	D	804	6OU	O17-C16-O18-C19
2	B	804	6OU	C12-C13-C14-C15
2	A	804	6OU	C12-C13-C14-C15
2	C	804	6OU	C12-C13-C14-C15
2	D	804	6OU	C12-C13-C14-C15
2	A	805	6OU	C38-C39-C40-C41
2	B	805	6OU	C38-C39-C40-C41
2	C	805	6OU	C38-C39-C40-C41
2	D	805	6OU	C38-C39-C40-C41

Continued on next page...

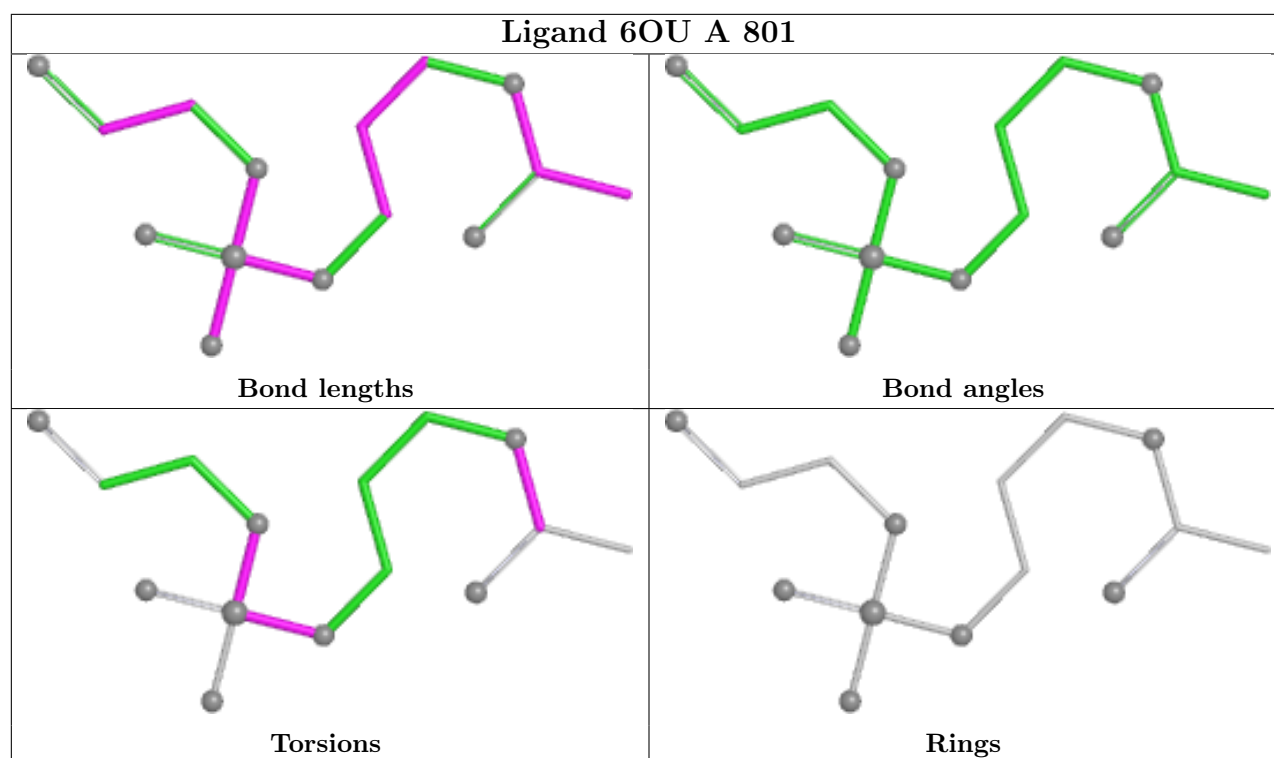
Continued from previous page...

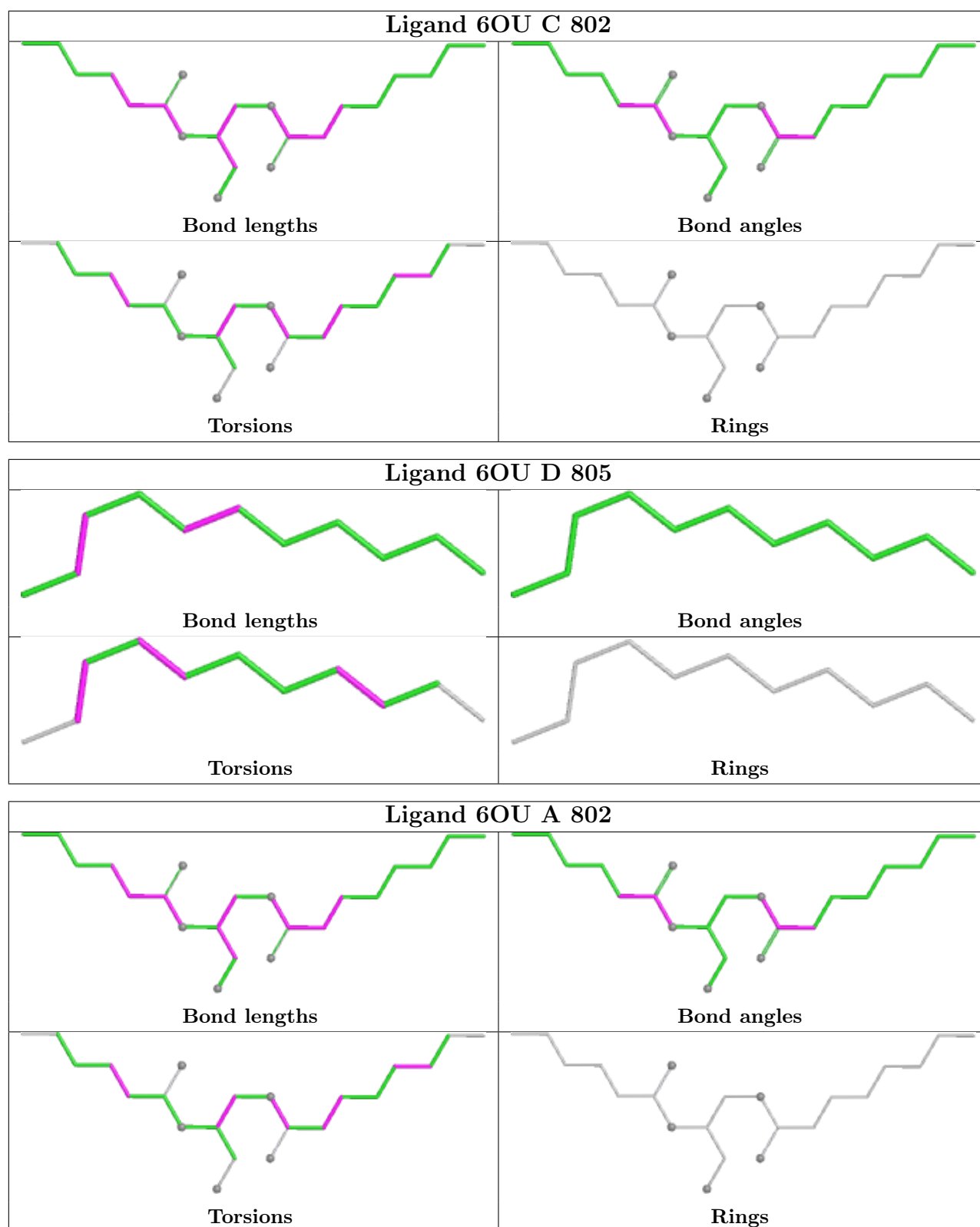
Mol	Chain	Res	Type	Atoms
2	A	805	6OU	C34-C35-C36-C37
2	C	805	6OU	C34-C35-C36-C37
2	D	805	6OU	C34-C35-C36-C37
2	B	805	6OU	C34-C35-C36-C37
2	A	803	6OU	C14-C15-C16-O18
2	B	803	6OU	C14-C15-C16-O18
2	C	803	6OU	C14-C15-C16-O18
2	D	803	6OU	C14-C15-C16-O18

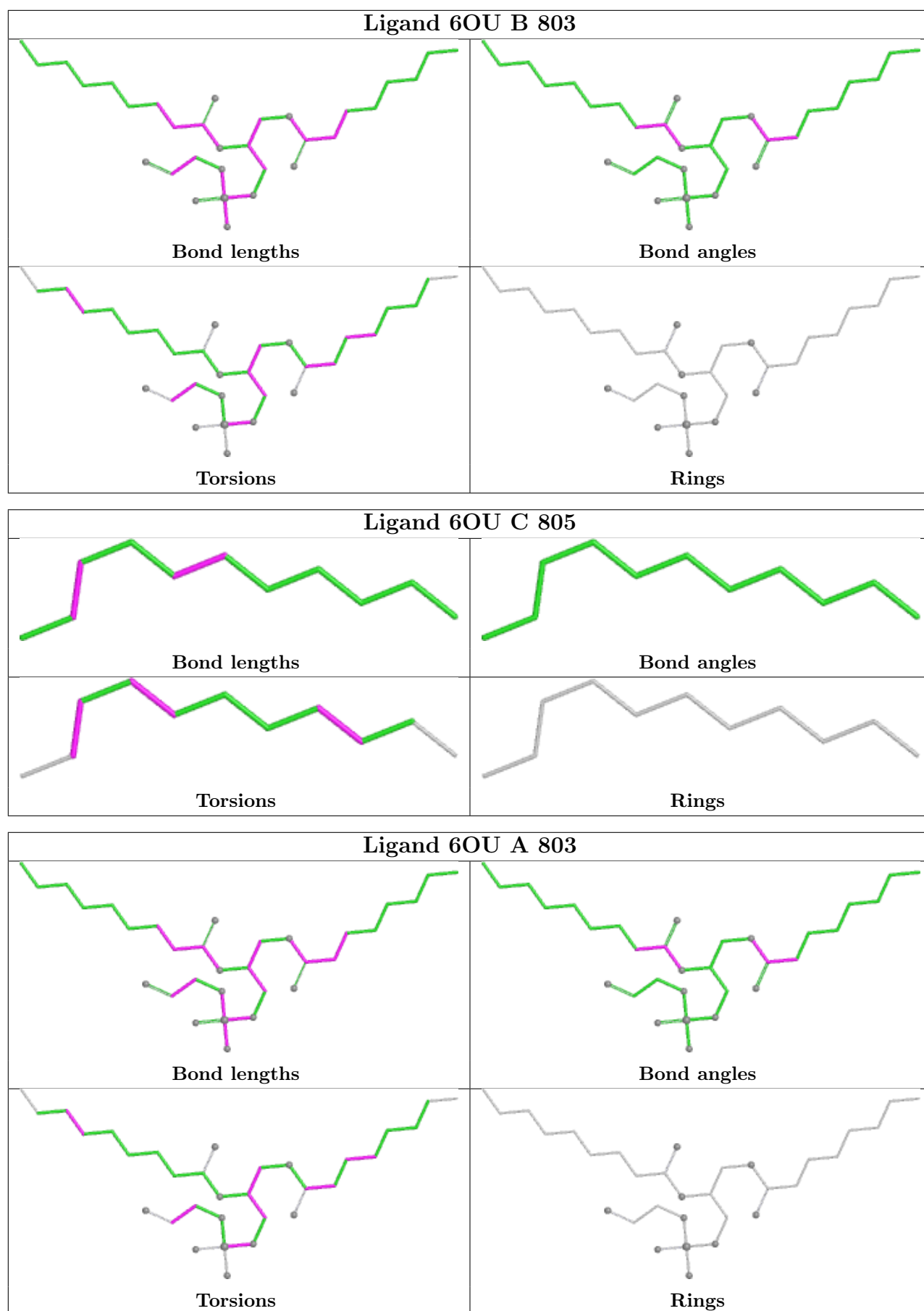
There are no ring outliers.

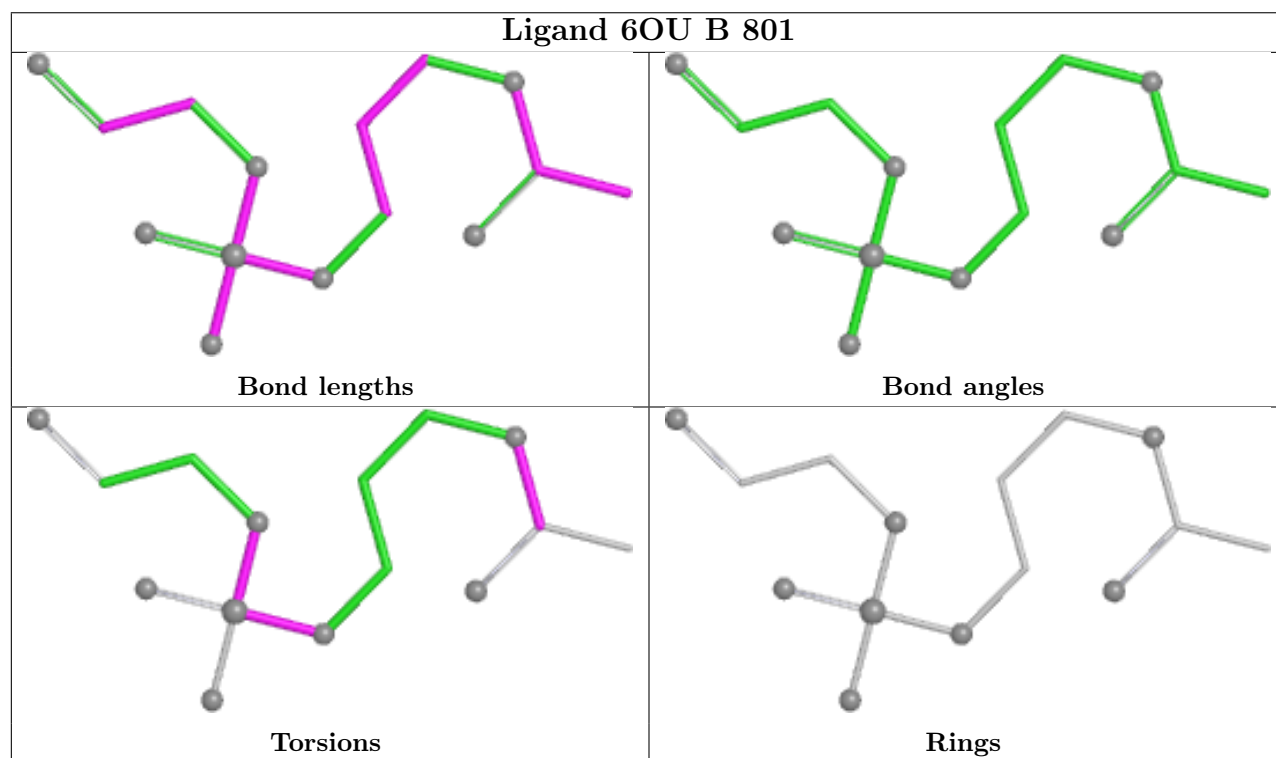
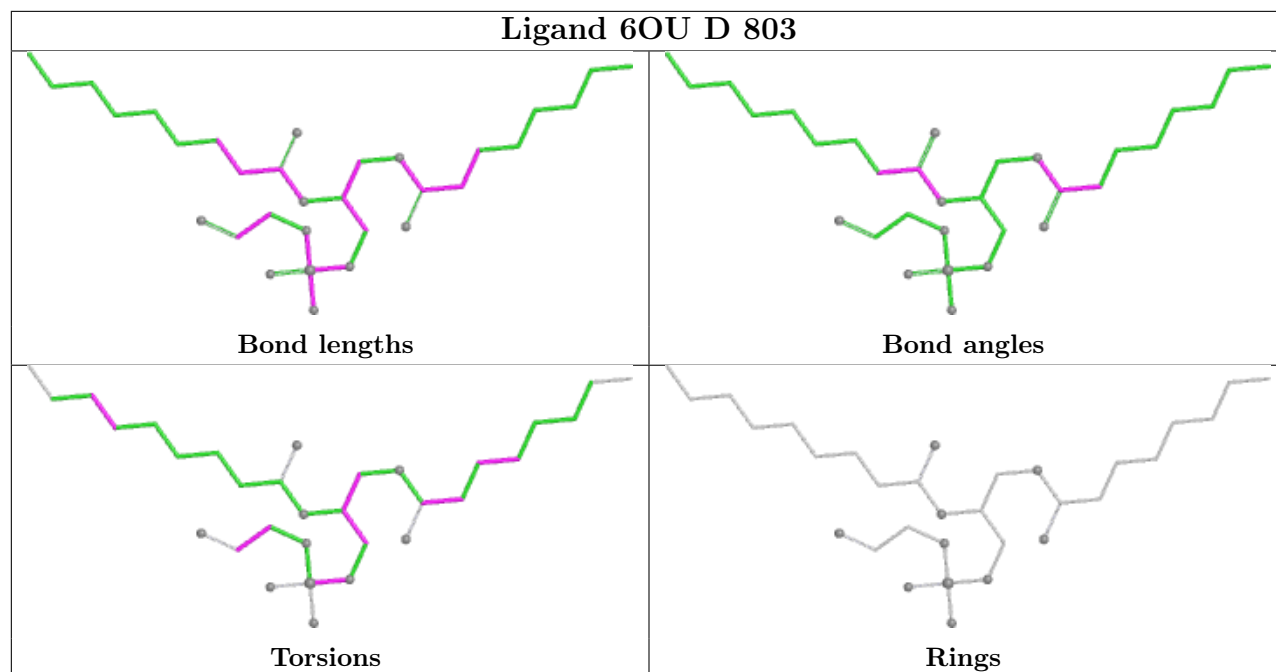
No monomer is involved in short contacts.

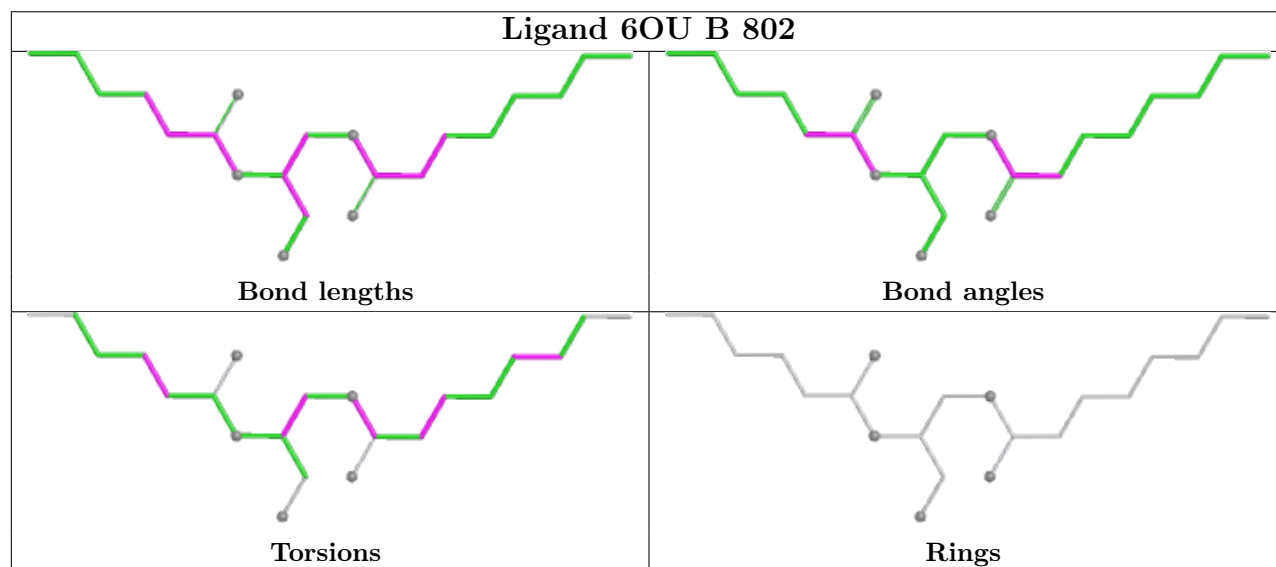
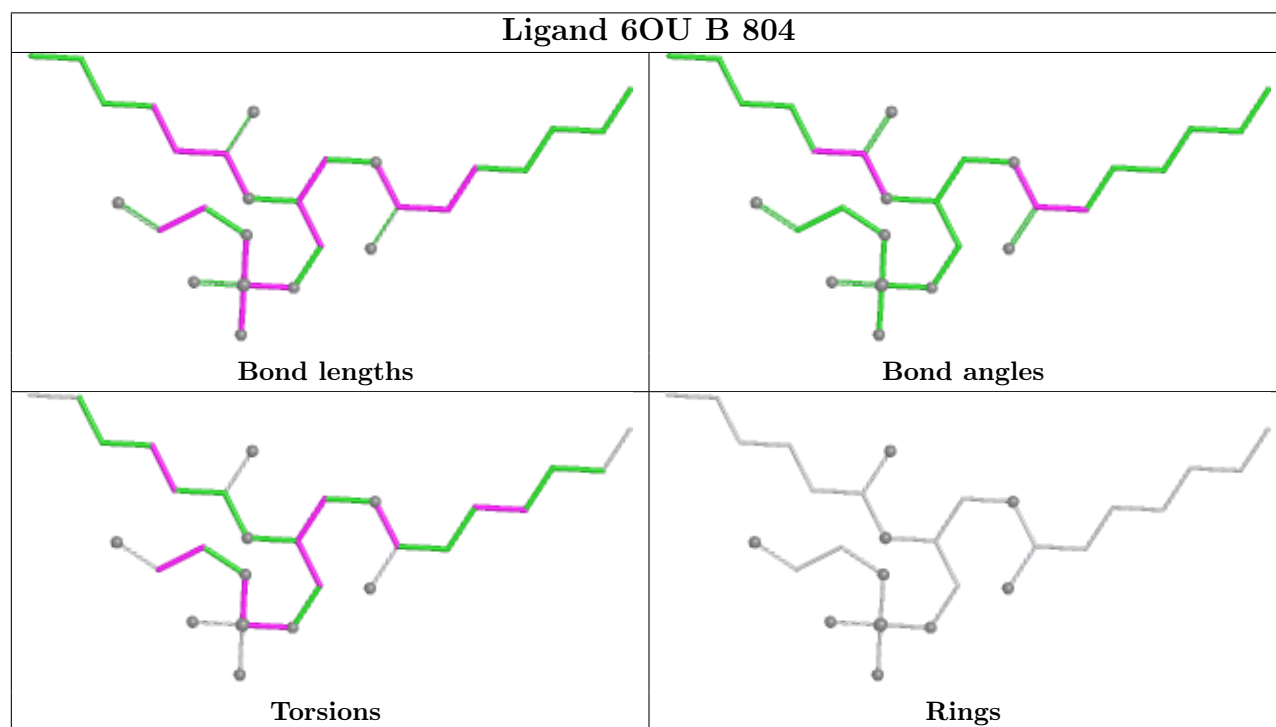
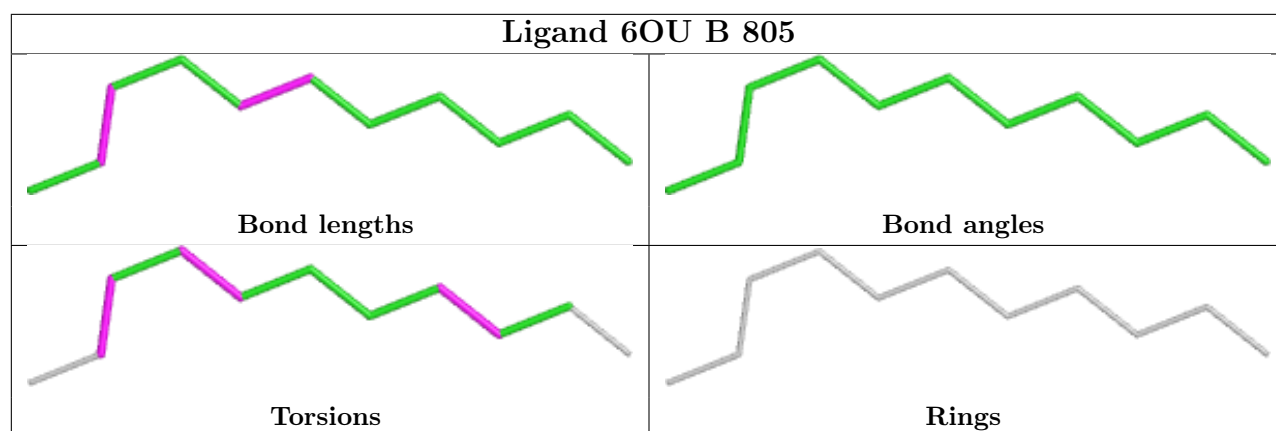
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

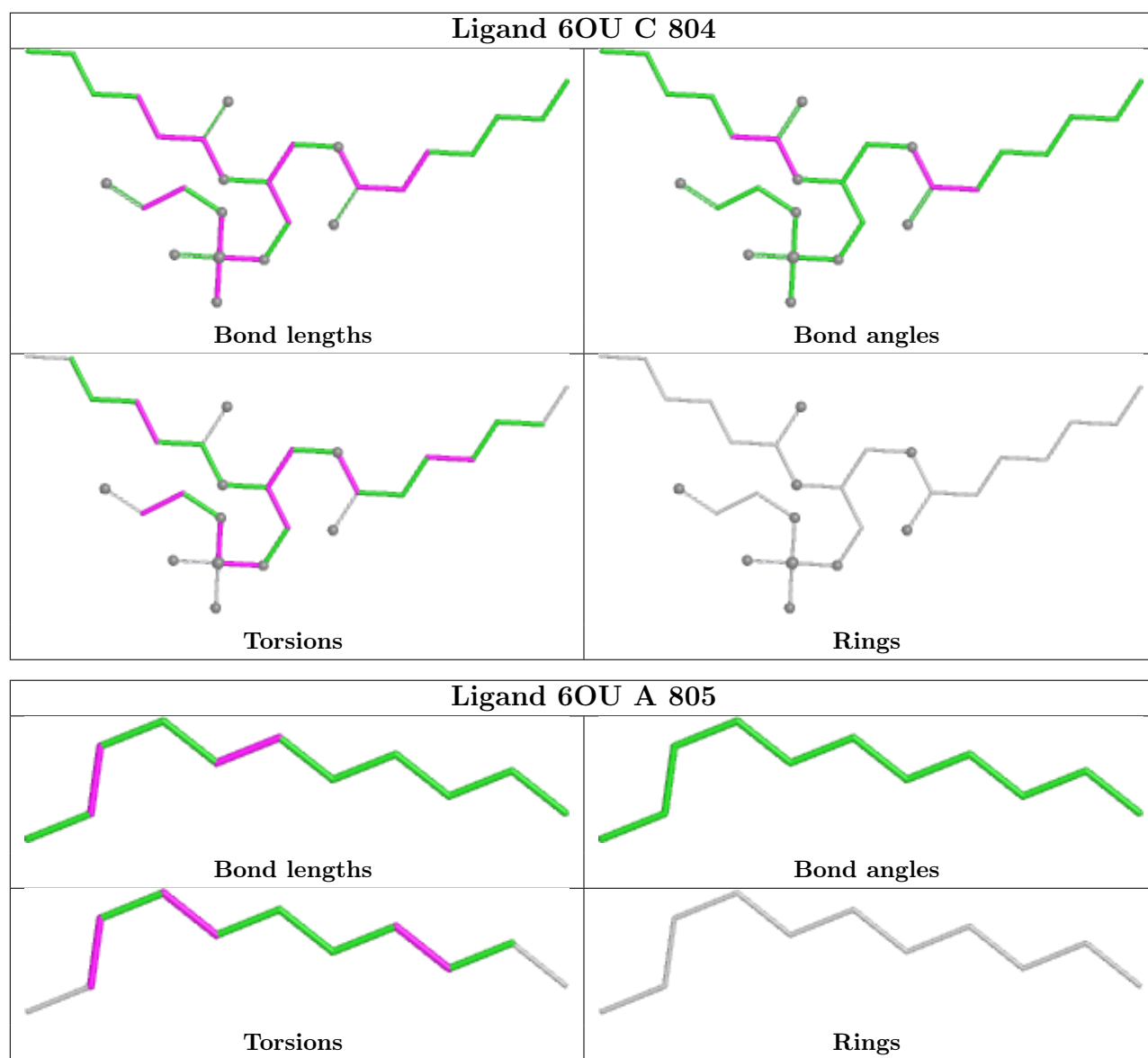


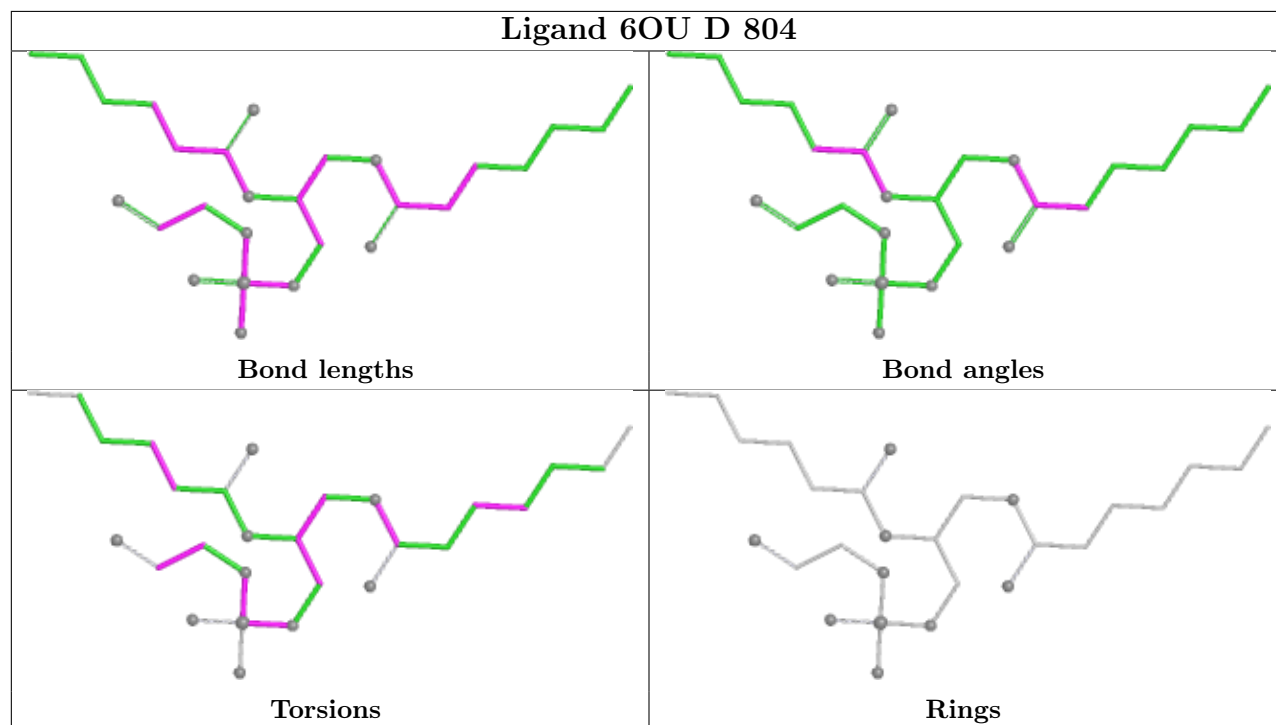
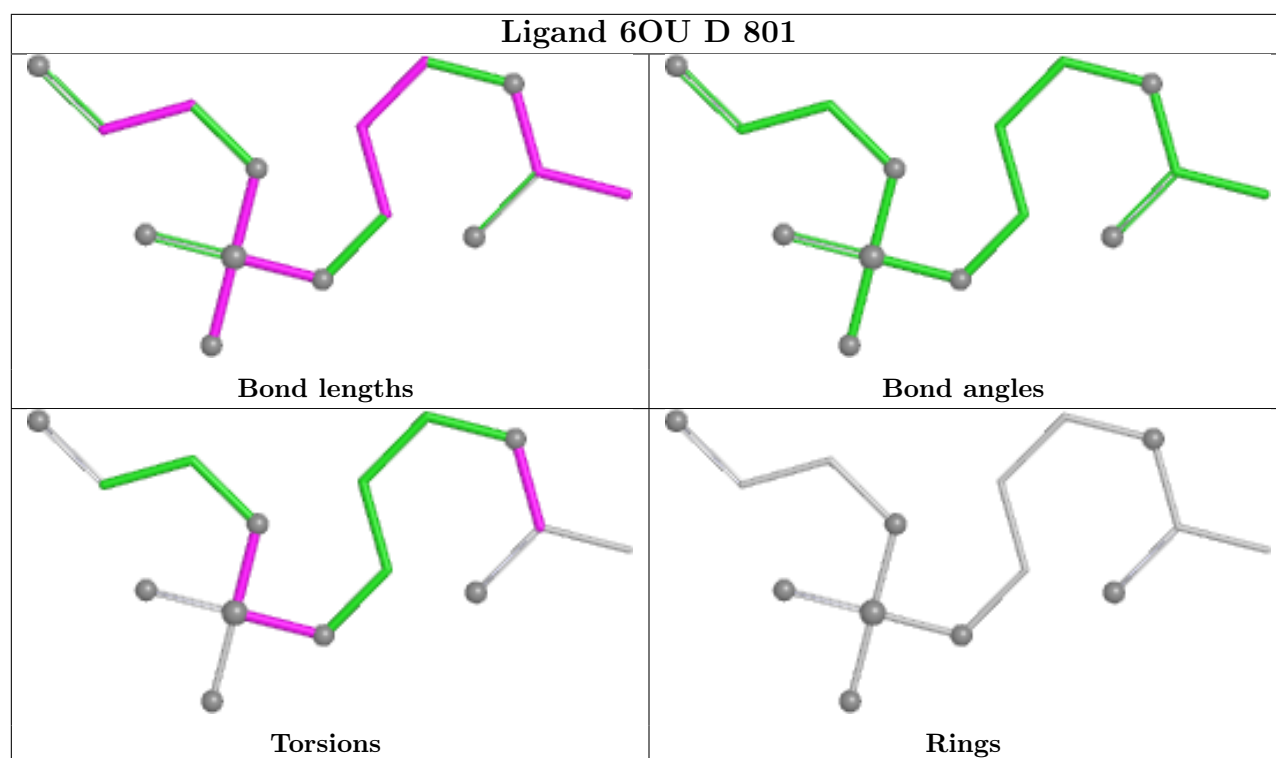


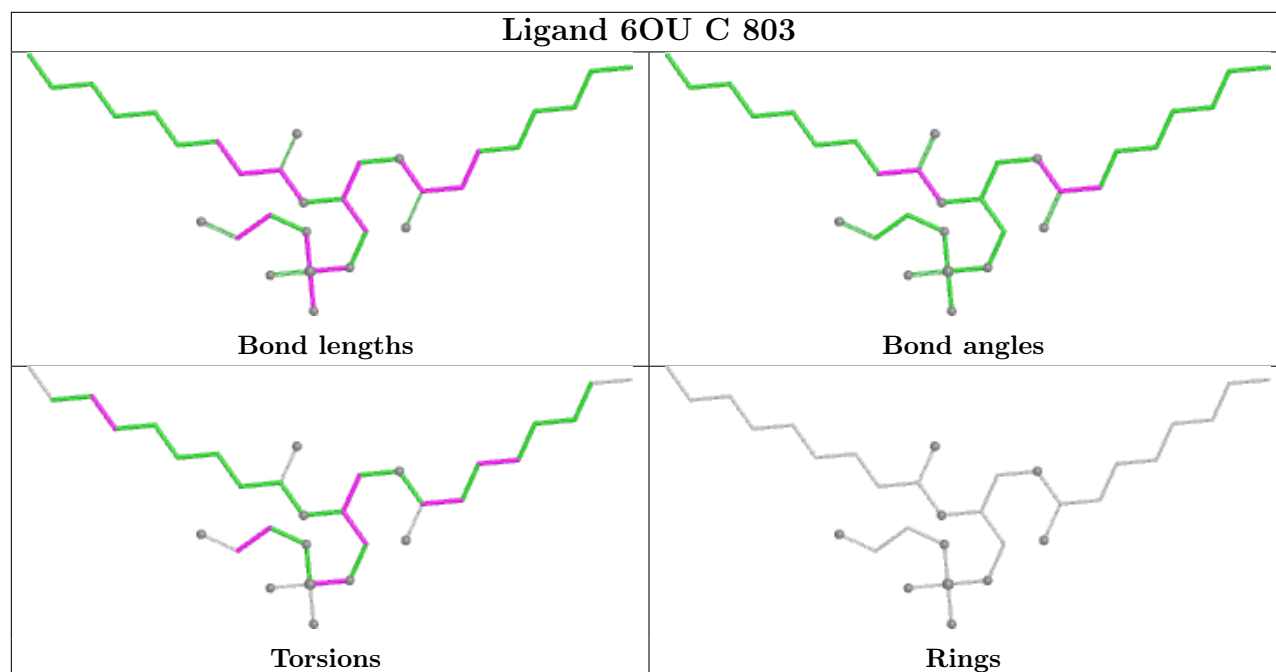
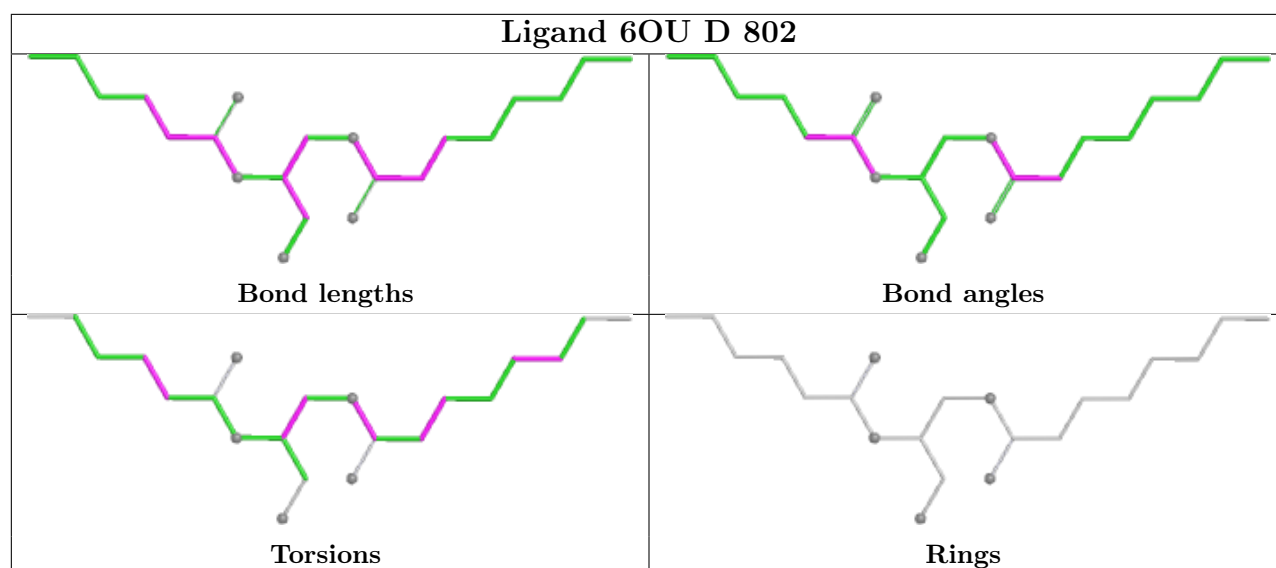


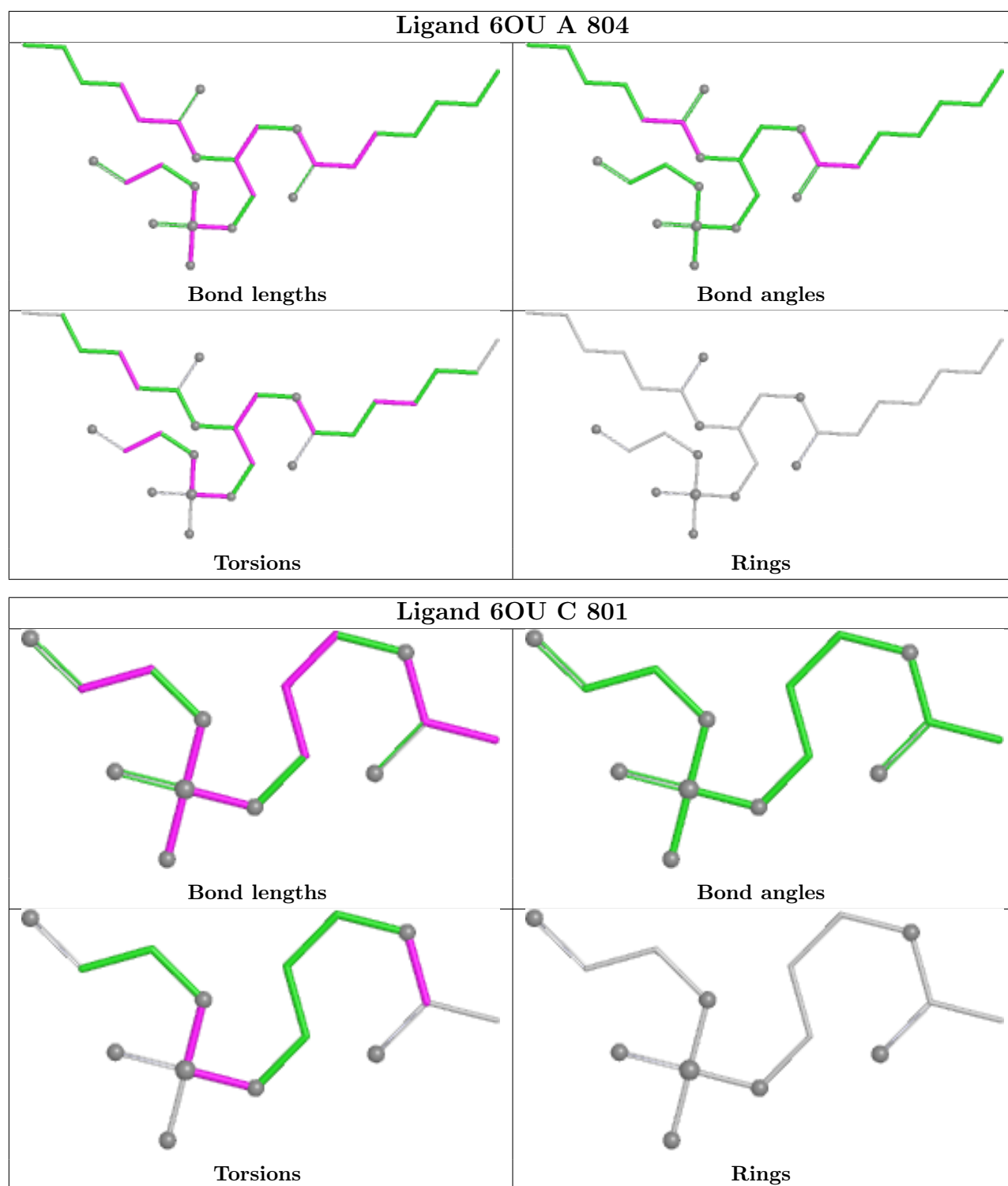












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

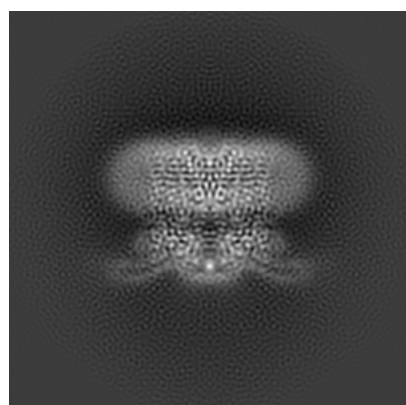
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20918. These allow visual inspection of the internal detail of the map and identification of artifacts.

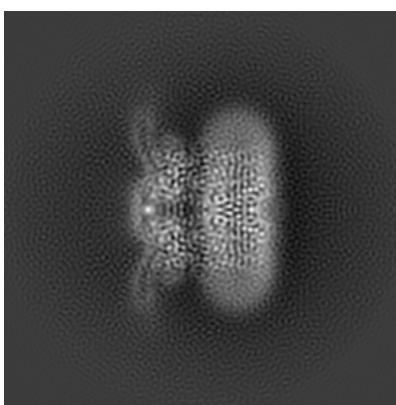
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

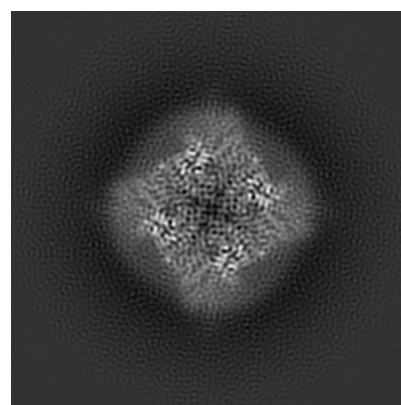
6.1.1 Primary map



X



Y

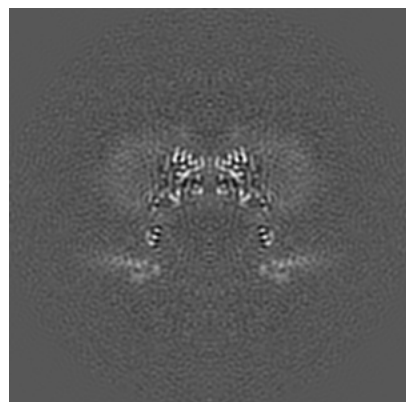


Z

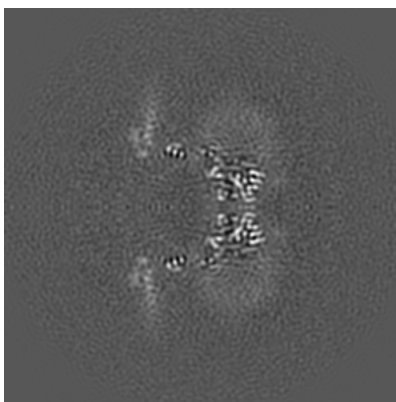
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

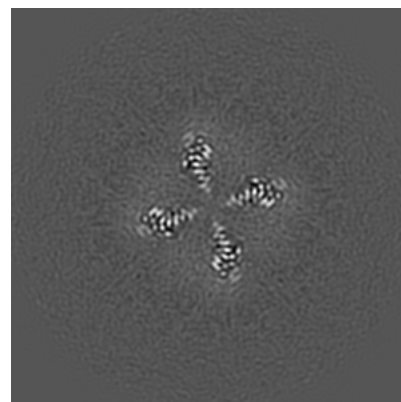
6.2.1 Primary map



X Index: 128



Y Index: 128

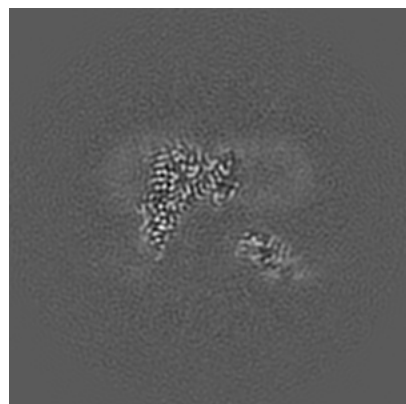


Z Index: 128

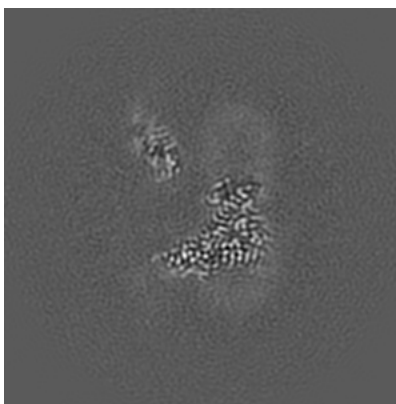
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

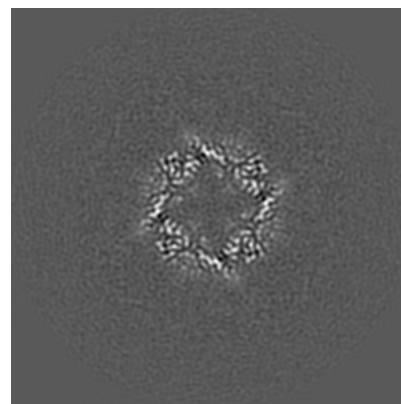
6.3.1 Primary map



X Index: 136



Y Index: 120

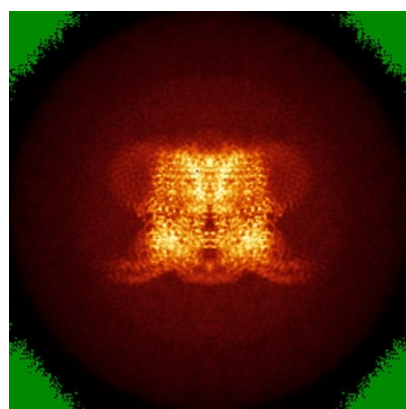


Z Index: 109

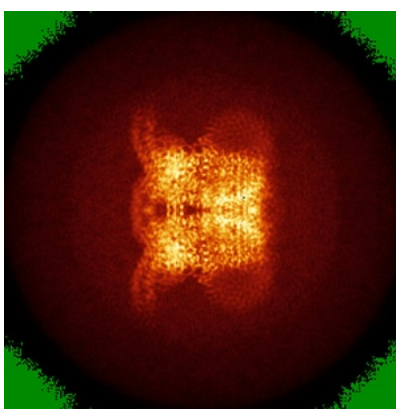
The images above show the largest variance slices of the map in three orthogonal directions.

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

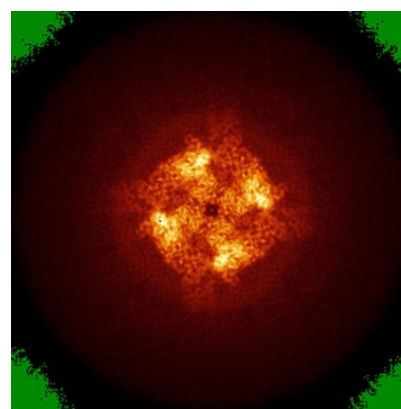
6.4.1 Primary map



X



Y

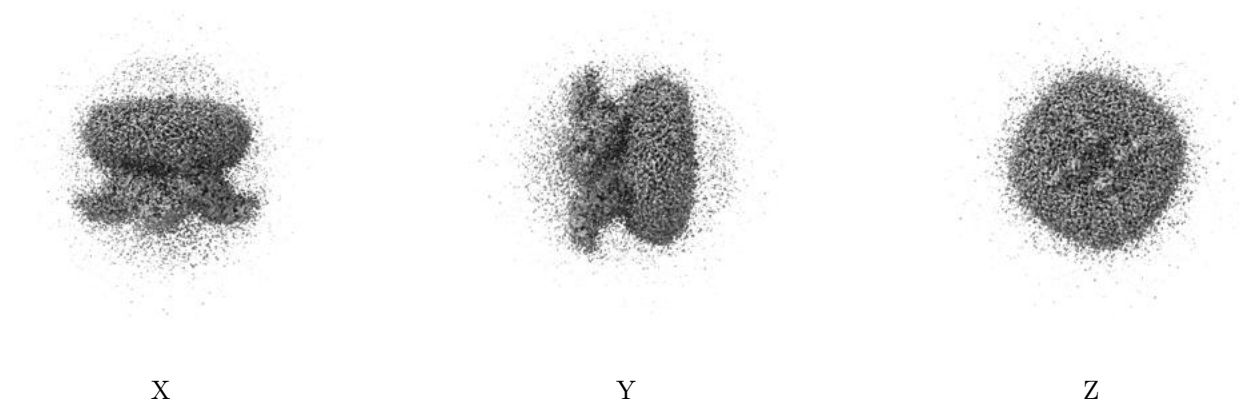


Z

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

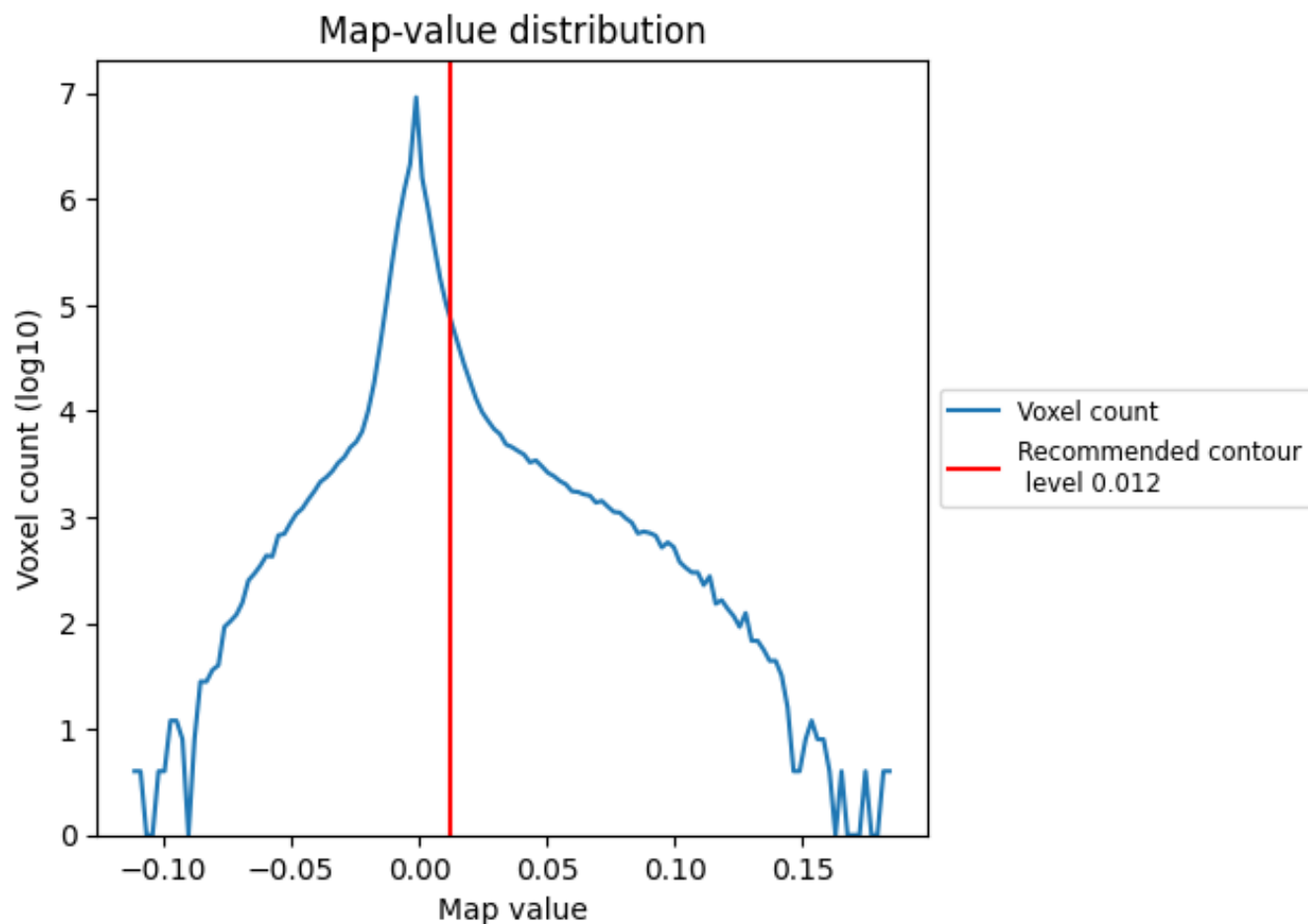
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

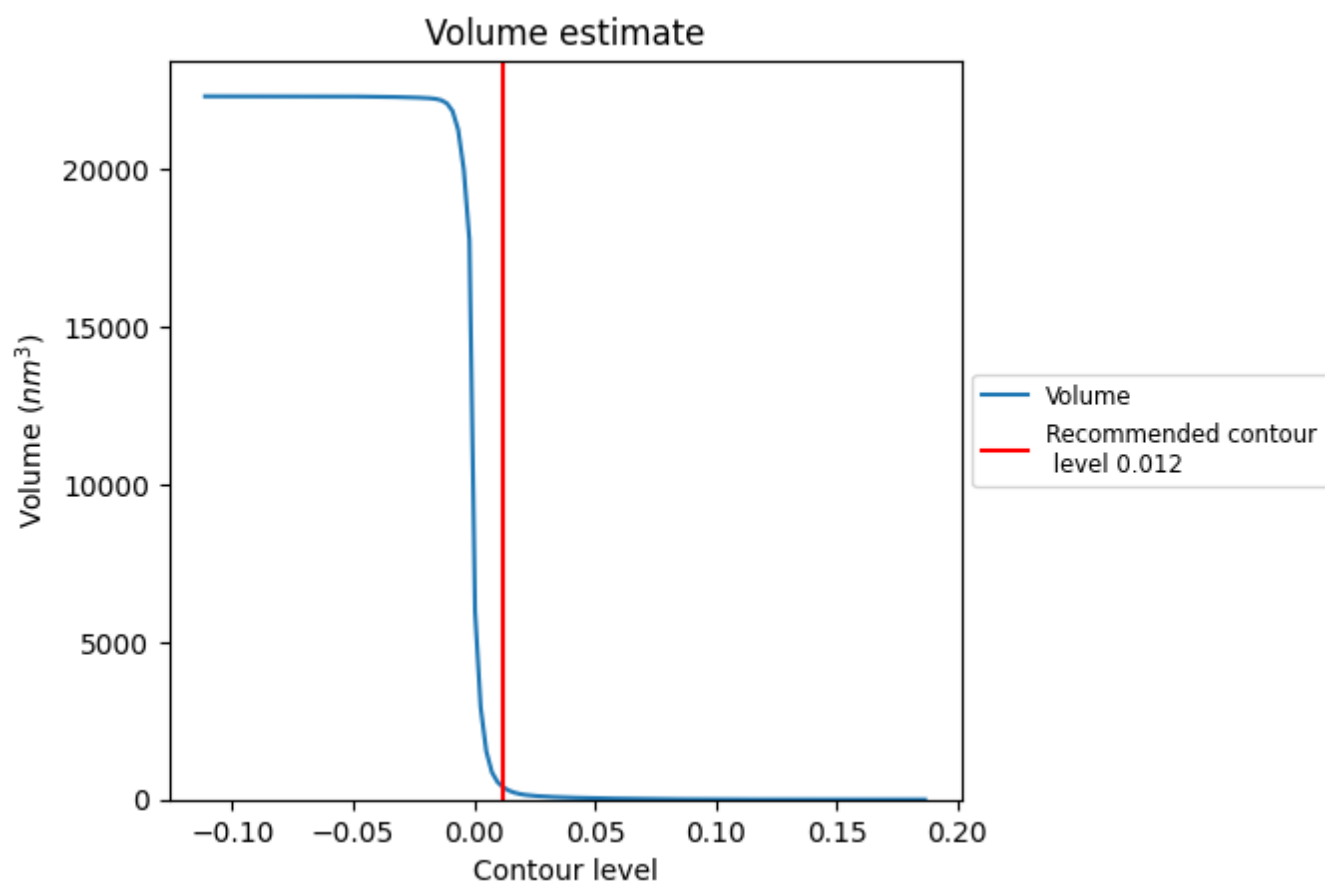
This section contains the results of statistical analysis of the map.

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.

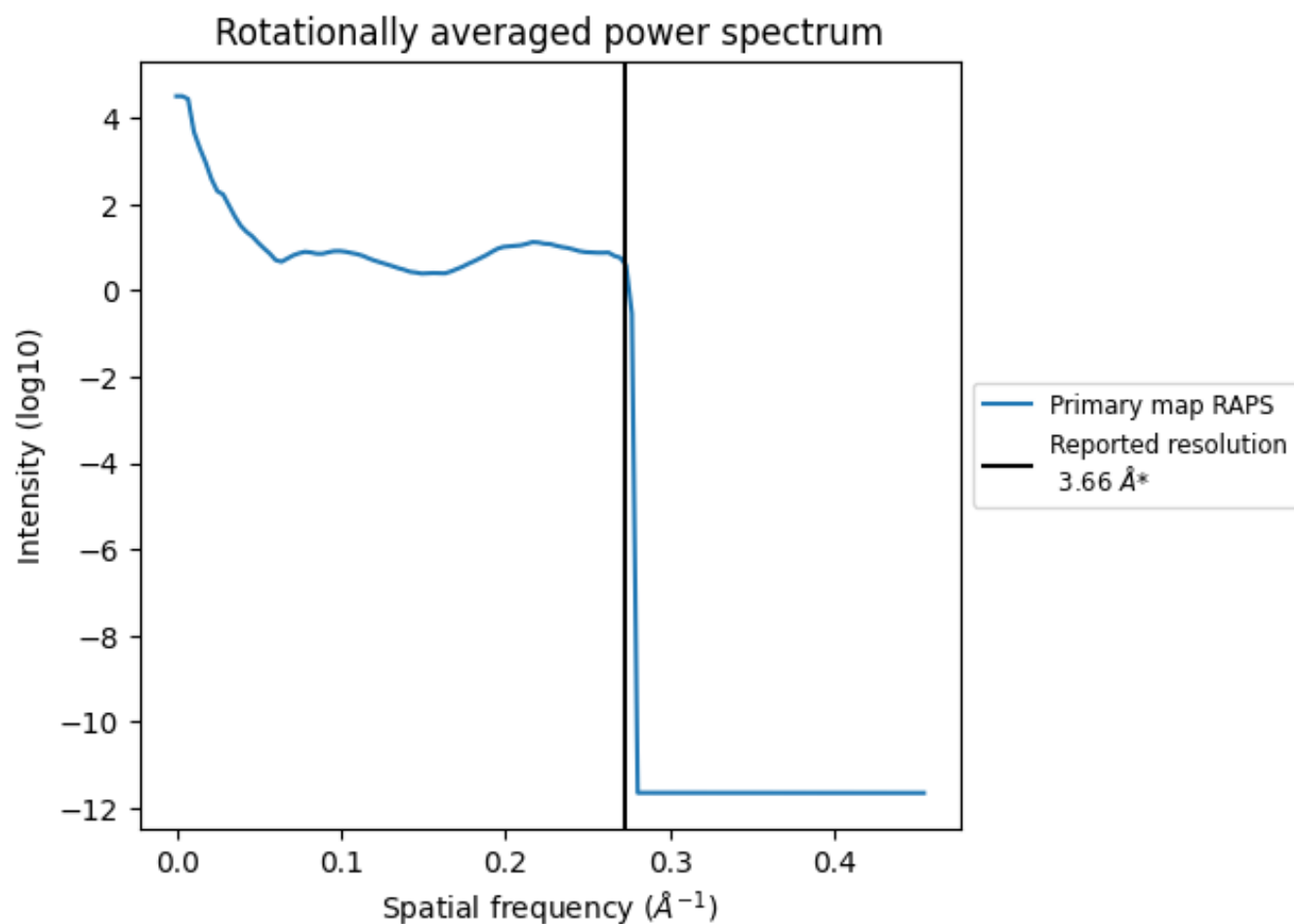
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 396 nm^3 ; this corresponds to an approximate mass of 358 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 0.273 $\text{\AA}^{-1}$

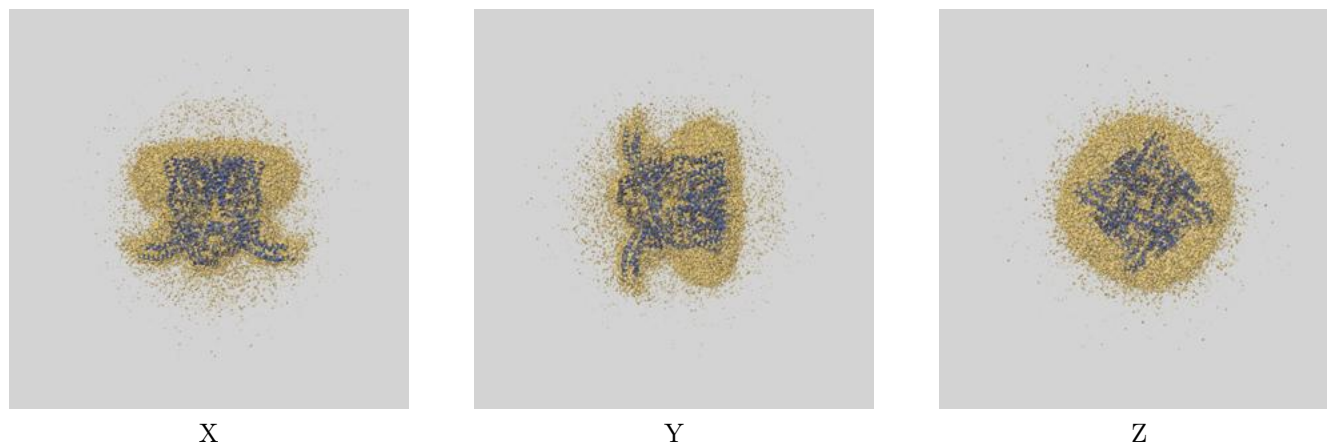
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

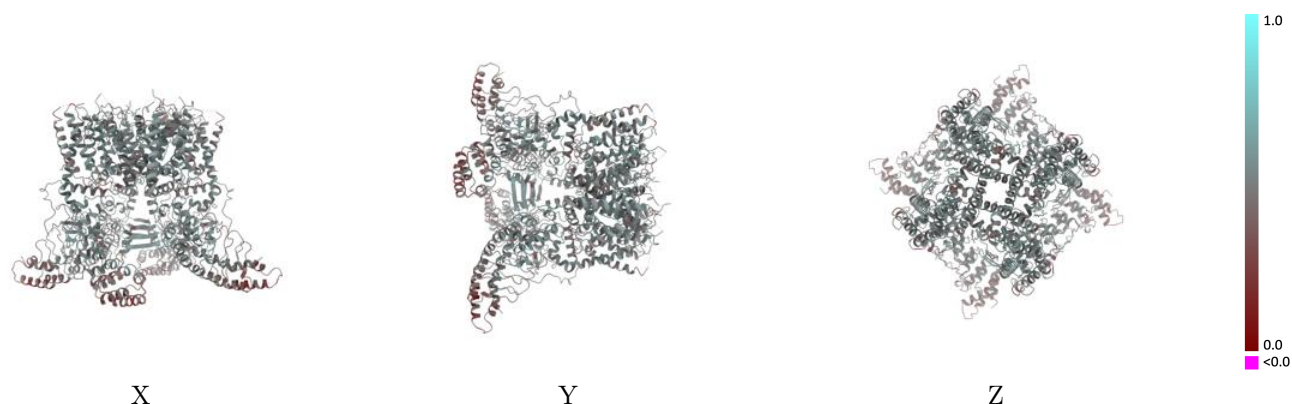
This section contains information regarding the fit between EMDB map EMD-20918 and PDB model 6UW6. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



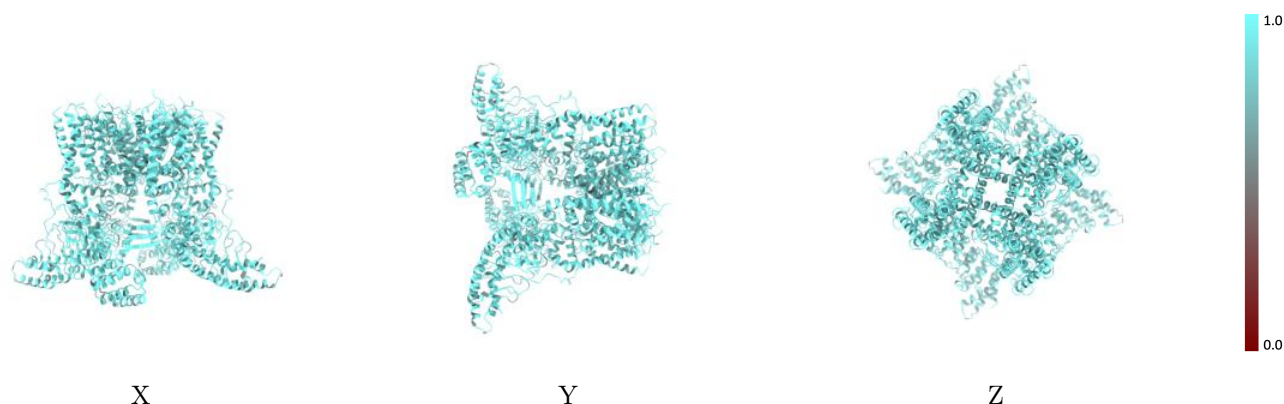
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



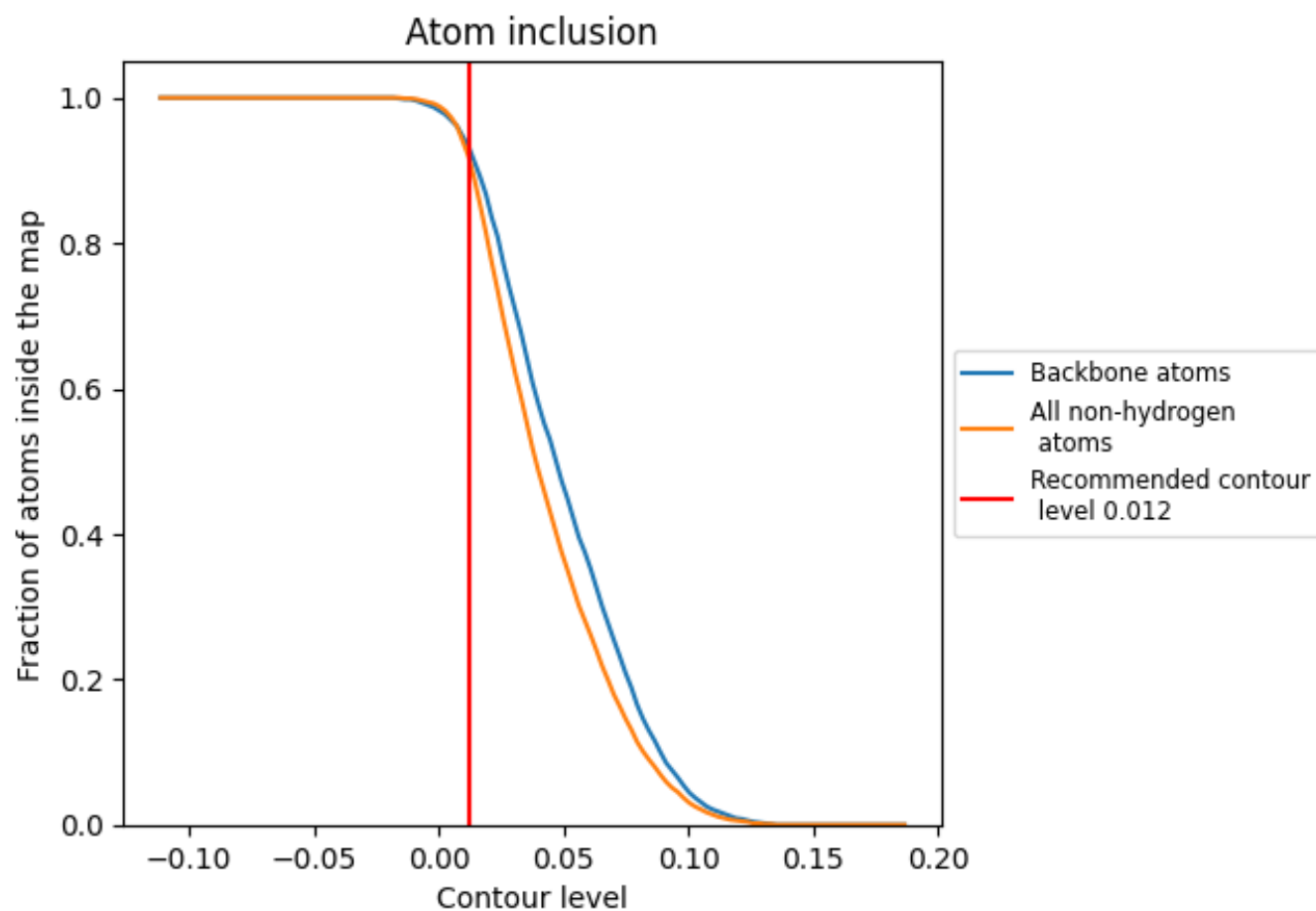
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.4850
A	0.9190	0.4820
B	0.9190	0.4860
C	0.9180	0.4850
D	0.9230	0.4860

