



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 12:47 AM EST

PDB ID : 7RAU
EMDB ID : EMD-24386
Title : Structure of TRPV3 in complex with osthole
Authors : Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on : 2021-07-02
Resolution : 3.99 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.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) : 2.31.3

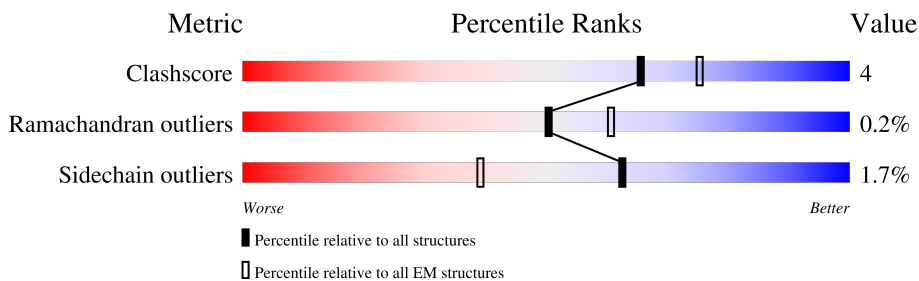
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 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	A	808	
1	B	808	
1	C	808	
1	D	808	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A00	A	901	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A0O	A	902	-	X	-	-
2	A0O	B	901	-	X	-	-
2	A0O	B	902	-	X	-	-
2	A0O	C	901	-	X	-	-
2	A0O	C	902	-	X	-	-
2	A0O	D	901	-	X	-	-
2	A0O	D	902	-	X	-	-

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 20000 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
			Total	C	N	O	S		
1	A	610	4964	3238	818	879	29	0	0
1	B	610	4964	3238	818	879	29	0	0
1	C	610	4964	3238	818	879	29	0	0
1	D	610	4964	3238	818	879	29	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	ASN	conflict	UNP Q8K424
A	564	ALA	TYR	engineered mutation	UNP Q8K424
A	792	LEU	-	expression tag	UNP Q8K424
A	793	VAL	-	expression tag	UNP Q8K424
A	794	PRO	-	expression tag	UNP Q8K424
A	795	ARG	-	expression tag	UNP Q8K424
A	796	GLY	-	expression tag	UNP Q8K424
A	797	SER	-	expression tag	UNP Q8K424
A	798	ALA	-	expression tag	UNP Q8K424
A	799	ALA	-	expression tag	UNP Q8K424
A	800	ALA	-	expression tag	UNP Q8K424
A	801	TRP	-	expression tag	UNP Q8K424
A	802	SER	-	expression tag	UNP Q8K424
A	803	HIS	-	expression tag	UNP Q8K424
A	804	PRO	-	expression tag	UNP Q8K424
A	805	GLN	-	expression tag	UNP Q8K424
A	806	PHE	-	expression tag	UNP Q8K424
A	807	GLU	-	expression tag	UNP Q8K424
A	808	LYS	-	expression tag	UNP Q8K424
B	2	GLY	ASN	conflict	UNP Q8K424
B	564	ALA	TYR	engineered mutation	UNP Q8K424

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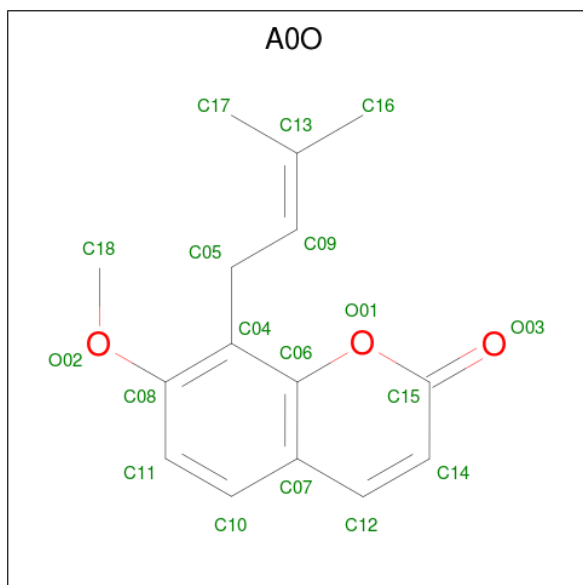
Chain	Residue	Modelled	Actual	Comment	Reference
B	792	LEU	-	expression tag	UNP Q8K424
B	793	VAL	-	expression tag	UNP Q8K424
B	794	PRO	-	expression tag	UNP Q8K424
B	795	ARG	-	expression tag	UNP Q8K424
B	796	GLY	-	expression tag	UNP Q8K424
B	797	SER	-	expression tag	UNP Q8K424
B	798	ALA	-	expression tag	UNP Q8K424
B	799	ALA	-	expression tag	UNP Q8K424
B	800	ALA	-	expression tag	UNP Q8K424
B	801	TRP	-	expression tag	UNP Q8K424
B	802	SER	-	expression tag	UNP Q8K424
B	803	HIS	-	expression tag	UNP Q8K424
B	804	PRO	-	expression tag	UNP Q8K424
B	805	GLN	-	expression tag	UNP Q8K424
B	806	PHE	-	expression tag	UNP Q8K424
B	807	GLU	-	expression tag	UNP Q8K424
B	808	LYS	-	expression tag	UNP Q8K424
C	2	GLY	ASN	conflict	UNP Q8K424
C	564	ALA	TYR	engineered mutation	UNP Q8K424
C	792	LEU	-	expression tag	UNP Q8K424
C	793	VAL	-	expression tag	UNP Q8K424
C	794	PRO	-	expression tag	UNP Q8K424
C	795	ARG	-	expression tag	UNP Q8K424
C	796	GLY	-	expression tag	UNP Q8K424
C	797	SER	-	expression tag	UNP Q8K424
C	798	ALA	-	expression tag	UNP Q8K424
C	799	ALA	-	expression tag	UNP Q8K424
C	800	ALA	-	expression tag	UNP Q8K424
C	801	TRP	-	expression tag	UNP Q8K424
C	802	SER	-	expression tag	UNP Q8K424
C	803	HIS	-	expression tag	UNP Q8K424
C	804	PRO	-	expression tag	UNP Q8K424
C	805	GLN	-	expression tag	UNP Q8K424
C	806	PHE	-	expression tag	UNP Q8K424
C	807	GLU	-	expression tag	UNP Q8K424
C	808	LYS	-	expression tag	UNP Q8K424
D	2	GLY	ASN	conflict	UNP Q8K424
D	564	ALA	TYR	engineered mutation	UNP Q8K424
D	792	LEU	-	expression tag	UNP Q8K424
D	793	VAL	-	expression tag	UNP Q8K424
D	794	PRO	-	expression tag	UNP Q8K424
D	795	ARG	-	expression tag	UNP Q8K424

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Chain	Residue	Modelled	Actual	Comment	Reference
D	796	GLY	-	expression tag	UNP Q8K424
D	797	SER	-	expression tag	UNP Q8K424
D	798	ALA	-	expression tag	UNP Q8K424
D	799	ALA	-	expression tag	UNP Q8K424
D	800	ALA	-	expression tag	UNP Q8K424
D	801	TRP	-	expression tag	UNP Q8K424
D	802	SER	-	expression tag	UNP Q8K424
D	803	HIS	-	expression tag	UNP Q8K424
D	804	PRO	-	expression tag	UNP Q8K424
D	805	GLN	-	expression tag	UNP Q8K424
D	806	PHE	-	expression tag	UNP Q8K424
D	807	GLU	-	expression tag	UNP Q8K424
D	808	LYS	-	expression tag	UNP Q8K424

- Molecule 2 is 7-methoxy-8-(3-methylbut-2-enyl)chromen-2-one (three-letter code: A00) (formula: C₁₅H₁₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			36	30	6	
2	A	1	Total	C	O	0
			36	30	6	
2	B	1	Total	C	O	0
			36	30	6	
2	B	1	Total	C	O	0
			36	30	6	

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Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total	C	O	0
			36	30	6	
2	C	1	Total	C	O	0
			36	30	6	
2	D	1	Total	C	O	0
			36	30	6	
2	D	1	Total	C	O	0
			36	30	6	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63523	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	96.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.451	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.097	Depositor
Map size (\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 (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A00

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	0.34	0/5068	0.55	1/6853 (0.0%)
1	B	0.34	0/5068	0.55	1/6853 (0.0%)
1	C	0.34	0/5068	0.56	1/6853 (0.0%)
1	D	0.34	0/5068	0.55	1/6853 (0.0%)
All	All	0.34	0/20272	0.55	4/27412 (0.0%)

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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ASP	CB-CG-OD1	7.47	125.03	118.30
1	C	315	ASP	CB-CG-OD1	7.45	125.01	118.30
1	A	315	ASP	CB-CG-OD1	7.43	124.98	118.30
1	D	315	ASP	CB-CG-OD1	7.37	124.93	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	ASP	Peptide
1	A	436	PHE	Peptide
1	B	414	ASP	Peptide
1	B	436	PHE	Peptide
1	C	414	ASP	Peptide
1	C	436	PHE	Peptide
1	D	414	ASP	Peptide
1	D	436	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4964	0	5053	46	0
1	B	4964	0	5053	44	0
1	C	4964	0	5053	44	0
1	D	4964	0	5053	47	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
All	All	20000	0	20212	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (164) 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:226:ARG:HH12	1:B:742:TRP:HB3	1.57	0.70
1:D:692:TRP:HE1	1:D:696:ARG:HH21	1.42	0.68
1:C:692:TRP:HE1	1:C:696:ARG:HH21	1.42	0.68
1:B:692:TRP:HE1	1:B:696:ARG:HH21	1.42	0.67
1:A:692:TRP:HE1	1:A:696:ARG:HH21	1.42	0.66
1:C:226:ARG:HH12	1:D:742:TRP:HB3	1.63	0.64
1:D:251:ASN:OD1	1:D:295:ARG:NH2	2.33	0.62
1:D:184:LYS:HG2	1:D:230:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ASN:OD1	1:C:295:ARG:NH2	2.33	0.61
1:B:184:LYS:HG2	1:B:230:ILE:HD11	1.82	0.61
1:B:167:THR:HG23	1:B:169:LYS:H	1.65	0.61
1:A:167:THR:HG23	1:A:169:LYS:H	1.65	0.61
1:C:184:LYS:HG2	1:C:230:ILE:HD11	1.82	0.61
1:D:207:GLU:HB2	1:D:215:GLY:HA2	1.83	0.61
1:A:224:GLU:OE2	1:B:383:GLY:N	2.33	0.61
1:A:251:ASN:OD1	1:A:295:ARG:NH2	2.33	0.61
1:A:184:LYS:HG2	1:A:230:ILE:HD11	1.82	0.61
1:D:167:THR:HG23	1:D:169:LYS:H	1.65	0.61
1:B:251:ASN:OD1	1:B:295:ARG:NH2	2.33	0.61
1:C:207:GLU:HB2	1:C:215:GLY:HA2	1.83	0.60
1:A:207:GLU:HB2	1:A:215:GLY:HA2	1.83	0.60
1:C:167:THR:HG23	1:C:169:LYS:H	1.65	0.60
1:B:207:GLU:HB2	1:B:215:GLY:HA2	1.83	0.59
1:B:226:ARG:HH12	1:C:742:TRP:HB3	1.69	0.58
1:C:337:ARG:NH2	1:C:341:GLY:O	2.37	0.57
1:D:337:ARG:NH2	1:D:341:GLY:O	2.37	0.57
1:A:337:ARG:NH2	1:A:341:GLY:O	2.37	0.56
1:B:337:ARG:NH2	1:B:341:GLY:O	2.37	0.56
1:B:193:PHE:O	1:B:197:ASN:ND2	2.39	0.56
1:A:193:PHE:O	1:A:197:ASN:ND2	2.39	0.55
1:D:704:GLU:O	1:D:712:ARG:NH2	2.37	0.55
1:C:224:GLU:OE2	1:D:383:GLY:N	2.38	0.55
1:C:193:PHE:O	1:C:197:ASN:ND2	2.39	0.55
1:A:736:GLU:OE2	1:A:738:LYS:NZ	2.40	0.55
1:B:704:GLU:O	1:B:712:ARG:NH2	2.37	0.55
1:B:736:GLU:OE2	1:B:738:LYS:NZ	2.40	0.55
1:D:736:GLU:OE2	1:D:738:LYS:NZ	2.40	0.55
1:D:193:PHE:O	1:D:197:ASN:ND2	2.39	0.54
1:C:736:GLU:OE2	1:C:738:LYS:NZ	2.40	0.54
1:A:742:TRP:HB3	1:D:226:ARG:HH12	1.71	0.54
1:D:345:LEU:HD13	1:D:360:ILE:HG21	1.90	0.54
1:C:704:GLU:O	1:C:712:ARG:NH2	2.37	0.54
1:A:345:LEU:HD13	1:A:360:ILE:HG21	1.90	0.53
1:B:345:LEU:HD13	1:B:360:ILE:HG21	1.90	0.53
1:A:704:GLU:O	1:A:712:ARG:NH2	2.37	0.52
1:C:345:LEU:HD13	1:C:360:ILE:HG21	1.90	0.52
1:B:224:GLU:OE2	1:C:383:GLY:N	2.44	0.50
1:D:385:VAL:HG22	1:D:737:VAL:HG22	1.94	0.50
1:A:480:SER:HG	1:A:483:GLN:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASN:OD1	1:B:341:GLY:N	2.45	0.50
1:A:338:ASN:OD1	1:A:341:GLY:N	2.45	0.49
1:C:338:ASN:OD1	1:C:341:GLY:N	2.45	0.49
1:D:338:ASN:OD1	1:D:341:GLY:N	2.45	0.49
1:D:148:ARG:O	1:D:150:ARG:NH1	2.46	0.49
1:B:148:ARG:O	1:B:150:ARG:NH1	2.46	0.49
1:C:148:ARG:O	1:C:150:ARG:NH1	2.46	0.49
1:A:148:ARG:O	1:A:150:ARG:NH1	2.46	0.48
1:B:385:VAL:HG22	1:B:737:VAL:HG22	1.94	0.48
1:C:385:VAL:HG22	1:C:737:VAL:HG22	1.94	0.48
1:C:459:SER:OG	1:C:555:MET:SD	2.70	0.48
1:A:459:SER:OG	1:A:555:MET:SD	2.70	0.48
1:A:634:LYS:O	1:A:638:GLY:N	2.46	0.48
1:D:459:SER:OG	1:D:555:MET:SD	2.70	0.48
1:A:385:VAL:HG22	1:A:737:VAL:HG22	1.94	0.48
1:D:634:LYS:O	1:D:638:GLY:N	2.46	0.48
1:A:579:ILE:HG21	1:D:671:ASN:HD21	1.78	0.48
1:D:437:ALA:HA	1:D:440:MET:HB2	1.96	0.47
1:C:642:LEU:HD11	1:D:630:LEU:HD22	1.96	0.47
1:D:574:MET:HG3	1:D:692:TRP:CD1	2.49	0.47
1:A:567:ARG:HB3	1:A:577:VAL:HG21	1.96	0.47
1:B:567:ARG:HB3	1:B:577:VAL:HG21	1.96	0.47
1:A:437:ALA:HA	1:A:440:MET:HB2	1.96	0.47
1:A:383:GLY:N	1:D:224:GLU:OE2	2.47	0.47
1:B:574:MET:HG3	1:B:692:TRP:CD1	2.50	0.47
1:C:567:ARG:HB3	1:C:577:VAL:HG21	1.96	0.47
1:B:642:LEU:HD11	1:C:630:LEU:HD22	1.97	0.47
1:A:574:MET:HG3	1:A:692:TRP:CD1	2.50	0.47
1:B:634:LYS:O	1:B:638:GLY:N	2.46	0.47
1:D:717:MET:SD	1:D:717:MET:N	2.88	0.47
1:B:717:MET:SD	1:B:717:MET:N	2.89	0.46
1:C:574:MET:HG3	1:C:692:TRP:CD1	2.50	0.46
1:D:123:ILE:O	1:D:127:VAL:N	2.43	0.46
1:D:567:ARG:HB3	1:D:577:VAL:HG21	1.96	0.46
1:D:634:LYS:HB3	1:D:639:LEU:HB2	1.97	0.46
1:A:634:LYS:HB3	1:A:639:LEU:HB2	1.98	0.46
1:C:634:LYS:HB3	1:C:639:LEU:HB2	1.97	0.46
1:B:437:ALA:HA	1:B:440:MET:HB2	1.96	0.46
1:C:437:ALA:HA	1:C:440:MET:HB2	1.96	0.46
1:C:717:MET:SD	1:C:717:MET:N	2.88	0.46
1:B:330:ASN:HD22	1:B:331:TRP:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ASN:HD21	1:C:579:ILE:HG21	1.80	0.46
1:C:330:ASN:HD22	1:C:331:TRP:H	1.64	0.46
1:A:717:MET:SD	1:A:717:MET:N	2.88	0.46
1:B:338:ASN:OD1	1:B:342:LEU:N	2.36	0.46
1:C:580:GLN:HA	1:C:583:ILE:HG22	1.99	0.45
1:D:330:ASN:HD22	1:D:331:TRP:H	1.64	0.45
1:A:123:ILE:O	1:A:127:VAL:N	2.43	0.45
1:A:180:ASN:O	1:A:183:THR:OG1	2.35	0.45
1:B:634:LYS:HB3	1:B:639:LEU:HB2	1.98	0.45
1:D:580:GLN:HA	1:D:583:ILE:HG22	1.99	0.45
1:A:330:ASN:HD22	1:A:331:TRP:H	1.64	0.45
1:B:580:GLN:HA	1:B:583:ILE:HG22	1.99	0.45
1:D:156:ASP:O	1:D:160:HIS:N	2.45	0.45
1:D:180:ASN:O	1:D:183:THR:OG1	2.35	0.45
1:D:308:GLU:N	1:D:313:GLN:OE1	2.50	0.45
1:A:604:ALA:O	1:A:607:SER:OG	2.31	0.44
1:B:459:SER:OG	1:B:555:MET:SD	2.70	0.44
1:D:604:ALA:O	1:D:607:SER:OG	2.31	0.44
1:A:642:LEU:HD11	1:B:630:LEU:HD22	1.98	0.44
1:B:180:ASN:O	1:B:183:THR:OG1	2.35	0.44
1:B:308:GLU:N	1:B:313:GLN:OE1	2.50	0.44
1:C:180:ASN:O	1:C:183:THR:OG1	2.35	0.44
1:A:580:GLN:HA	1:A:583:ILE:HG22	1.99	0.44
1:C:260:TYR:OH	1:C:297:ASN:OD1	2.34	0.44
1:D:260:TYR:OH	1:D:297:ASN:OD1	2.34	0.44
1:A:308:GLU:N	1:A:313:GLN:OE1	2.51	0.44
1:A:338:ASN:OD1	1:A:342:LEU:N	2.36	0.44
1:B:233:VAL:O	1:B:237:ALA:N	2.48	0.44
1:C:308:GLU:N	1:C:313:GLN:OE1	2.50	0.44
1:A:650:TYR:HB3	1:A:653:LEU:HB2	2.00	0.43
1:A:260:TYR:OH	1:A:297:ASN:OD1	2.34	0.43
1:B:650:TYR:HB3	1:B:653:LEU:HB2	2.00	0.43
1:B:652:ILE:HG13	1:B:653:LEU:HD12	2.01	0.43
1:C:652:ILE:HG13	1:C:653:LEU:HD12	2.01	0.43
1:A:630:LEU:HD22	1:D:642:LEU:HD11	2.01	0.43
1:C:536:SER:OG	1:C:547:TYR:O	2.37	0.43
1:C:634:LYS:O	1:C:638:GLY:N	2.46	0.43
1:D:650:TYR:HB3	1:D:653:LEU:HB2	2.00	0.43
1:C:233:VAL:O	1:C:237:ALA:N	2.48	0.42
1:D:233:VAL:O	1:D:237:ALA:N	2.48	0.42
1:C:650:TYR:HB3	1:C:653:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ASN:OD1	1:D:342:LEU:N	2.36	0.42
1:D:536:SER:OG	1:D:547:TYR:O	2.37	0.42
1:D:480:SER:HG	1:D:483:GLN:HB2	1.83	0.42
1:A:213:TYR:OH	1:B:754:GLY:N	2.47	0.42
1:B:536:SER:OG	1:B:547:TYR:O	2.37	0.42
1:C:226:ARG:HE	1:C:274:GLN:NE2	2.18	0.42
1:C:123:ILE:O	1:C:127:VAL:N	2.43	0.42
1:A:177:LEU:HD13	1:A:225:ARG:HH11	1.85	0.41
1:B:177:LEU:HD13	1:B:225:ARG:HH11	1.85	0.41
1:A:536:SER:OG	1:A:547:TYR:O	2.37	0.41
1:A:652:ILE:HG13	1:A:653:LEU:HD12	2.01	0.41
1:B:226:ARG:HE	1:B:274:GLN:NE2	2.18	0.41
1:D:652:ILE:HG13	1:D:653:LEU:HD12	2.01	0.41
1:A:233:VAL:O	1:A:237:ALA:N	2.48	0.41
1:D:177:LEU:HD13	1:D:225:ARG:HH11	1.85	0.41
1:C:671:ASN:HD21	1:D:579:ILE:HG21	1.85	0.41
1:A:322:ASP:OD1	1:A:359:TYR:OH	2.38	0.41
1:A:691:ILE:HA	1:A:694:LEU:HB2	2.03	0.41
1:B:691:ILE:HA	1:B:694:LEU:HB2	2.03	0.41
1:C:177:LEU:HD13	1:C:225:ARG:HH11	1.85	0.41
1:D:691:ILE:HA	1:D:694:LEU:HB2	2.03	0.41
1:A:156:ASP:O	1:A:160:HIS:N	2.45	0.41
1:D:322:ASP:OD1	1:D:359:TYR:OH	2.38	0.41
1:B:123:ILE:O	1:B:127:VAL:N	2.43	0.40
1:C:322:ASP:OD1	1:C:359:TYR:OH	2.38	0.40
1:D:226:ARG:HE	1:D:274:GLN:NE2	2.18	0.40
1:C:691:ILE:HA	1:C:694:LEU:HB2	2.03	0.40
1:A:671:ASN:HD21	1:B:579:ILE:HG21	1.86	0.40
1:C:338:ASN:OD1	1:C:342:LEU:N	2.36	0.40
1:C:416:ARG:HE	1:C:694:LEU:HD11	1.87	0.40
1:B:260:TYR:OH	1:B:297:ASN:OD1	2.34	0.40
1:B:322:ASP:OD1	1:B:359:TYR:OH	2.38	0.40
1:D:450:PHE:O	1:D:454:THR:OG1	2.31	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	602/808 (74%)	563 (94%)	38 (6%)	1 (0%)	47	79
1	B	602/808 (74%)	563 (94%)	38 (6%)	1 (0%)	47	79
1	C	602/808 (74%)	563 (94%)	38 (6%)	1 (0%)	47	79
1	D	602/808 (74%)	563 (94%)	38 (6%)	1 (0%)	47	79
All	All	2408/3232 (74%)	2252 (94%)	152 (6%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	413	ILE
1	C	413	ILE
1	D	413	ILE
1	A	413	ILE

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	540/719 (75%)	531 (98%)	9 (2%)	60	78
1	B	540/719 (75%)	531 (98%)	9 (2%)	60	78
1	C	540/719 (75%)	531 (98%)	9 (2%)	60	78
1	D	540/719 (75%)	531 (98%)	9 (2%)	60	78
All	All	2160/2876 (75%)	2124 (98%)	36 (2%)	62	78

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	117	LYS
1	A	330	ASN
1	A	370	LEU
1	A	415	ASN
1	A	647	ASN
1	A	671	ASN
1	A	714	ARG
1	A	717	MET
1	B	116	LYS
1	B	117	LYS
1	B	330	ASN
1	B	370	LEU
1	B	415	ASN
1	B	647	ASN
1	B	671	ASN
1	B	714	ARG
1	B	717	MET
1	C	116	LYS
1	C	117	LYS
1	C	330	ASN
1	C	370	LEU
1	C	415	ASN
1	C	647	ASN
1	C	671	ASN
1	C	714	ARG
1	C	717	MET
1	D	116	LYS
1	D	117	LYS
1	D	330	ASN
1	D	370	LEU
1	D	415	ASN
1	D	647	ASN
1	D	671	ASN
1	D	714	ARG
1	D	717	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS

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Mol	Chain	Res	Type
1	A	197	ASN
1	A	244	HIS
1	A	274	GLN
1	A	330	ASN
1	A	410	ASN
1	A	415	ASN
1	A	483	GLN
1	A	671	ASN
1	A	735	ASN
1	B	160	HIS
1	B	197	ASN
1	B	244	HIS
1	B	274	GLN
1	B	330	ASN
1	B	410	ASN
1	B	415	ASN
1	B	671	ASN
1	B	735	ASN
1	C	160	HIS
1	C	197	ASN
1	C	244	HIS
1	C	274	GLN
1	C	330	ASN
1	C	410	ASN
1	C	415	ASN
1	C	671	ASN
1	C	735	ASN
1	D	160	HIS
1	D	197	ASN
1	D	244	HIS
1	D	274	GLN
1	D	330	ASN
1	D	410	ASN
1	D	415	ASN
1	D	483	GLN
1	D	671	ASN
1	D	735	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	A0O	D	901	-	19,19,19	4.89	12 (63%)	26,26,26	6.94	19 (73%)
2	A0O	B	901	-	19,19,19	4.88	12 (63%)	26,26,26	6.95	19 (73%)
2	A0O	D	902	-	19,19,19	4.79	12 (63%)	26,26,26	7.16	18 (69%)
2	A0O	C	902	-	19,19,19	4.81	12 (63%)	26,26,26	7.19	17 (65%)
2	A0O	C	901	-	19,19,19	4.89	12 (63%)	26,26,26	6.89	19 (73%)
2	A0O	A	901	-	19,19,19	4.90	12 (63%)	26,26,26	6.96	19 (73%)
2	A0O	B	902	-	19,19,19	4.78	11 (57%)	26,26,26	7.14	18 (69%)
2	A0O	A	902	-	19,19,19	4.74	12 (63%)	26,26,26	7.12	17 (65%)

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	A0O	D	901	-	-	2/7/7/7	0/2/2/2
2	A0O	B	901	-	-	2/7/7/7	0/2/2/2
2	A0O	D	902	-	-	2/7/7/7	0/2/2/2
2	A0O	C	902	-	-	3/7/7/7	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A00	C	901	-	-	2/7/7/7	0/2/2/2
2	A00	A	901	-	-	2/7/7/7	0/2/2/2
2	A00	B	902	-	-	2/7/7/7	0/2/2/2
2	A00	A	902	-	-	2/7/7/7	0/2/2/2

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	A00	C06-C04	10.13	1.56	1.39
2	A	901	A00	C06-C04	10.13	1.56	1.39
2	C	901	A00	C06-C04	10.09	1.56	1.39
2	D	901	A00	C06-C04	10.07	1.56	1.39
2	C	902	A00	C06-C04	9.97	1.55	1.39
2	D	902	A00	C06-C04	9.92	1.55	1.39
2	B	902	A00	C06-C04	9.88	1.55	1.39
2	A	902	A00	C06-C04	9.76	1.55	1.39
2	D	901	A00	C07-C12	9.49	1.64	1.44
2	D	902	A00	C07-C12	9.49	1.64	1.44
2	C	901	A00	C07-C12	9.48	1.64	1.44
2	C	902	A00	C07-C12	9.48	1.64	1.44
2	B	902	A00	C07-C12	9.47	1.64	1.44
2	B	901	A00	C07-C12	9.47	1.64	1.44
2	A	901	A00	C07-C12	9.45	1.64	1.44
2	A	902	A00	C07-C12	9.37	1.64	1.44
2	C	902	A00	C08-C04	7.96	1.51	1.40
2	A	901	A00	C08-C04	7.93	1.51	1.40
2	D	901	A00	C08-C04	7.88	1.51	1.40
2	C	901	A00	C08-C04	7.86	1.51	1.40
2	B	901	A00	C08-C04	7.82	1.51	1.40
2	D	902	A00	C08-C04	7.80	1.51	1.40
2	B	902	A00	C08-C04	7.77	1.51	1.40
2	A	902	A00	C08-C04	7.50	1.50	1.40
2	A	902	A00	O01-C15	-7.16	1.26	1.38
2	B	902	A00	O01-C15	-7.07	1.26	1.38
2	D	902	A00	O01-C15	-7.05	1.26	1.38
2	C	902	A00	O01-C15	-7.00	1.26	1.38
2	A	901	A00	O01-C15	-6.96	1.26	1.38
2	D	901	A00	O01-C15	-6.95	1.26	1.38
2	C	901	A00	O01-C15	-6.91	1.26	1.38
2	B	901	A00	O01-C15	-6.87	1.26	1.38
2	C	901	A00	C11-C10	-6.44	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	A0O	C10-C07	-6.40	1.29	1.41
2	D	901	A0O	C10-C07	-6.38	1.29	1.41
2	D	901	A0O	C11-C10	-6.38	1.27	1.38
2	A	901	A0O	C11-C10	-6.37	1.27	1.38
2	B	901	A0O	C11-C10	-6.37	1.27	1.38
2	B	901	A0O	C10-C07	-6.36	1.29	1.41
2	C	902	A0O	C11-C10	-6.35	1.27	1.38
2	C	901	A0O	C10-C07	-6.34	1.29	1.41
2	A	902	A0O	C11-C10	-6.32	1.27	1.38
2	D	902	A0O	C11-C10	-6.29	1.27	1.38
2	B	902	A0O	C11-C10	-6.23	1.27	1.38
2	B	902	A0O	C10-C07	-5.95	1.30	1.41
2	C	902	A0O	C10-C07	-5.92	1.30	1.41
2	A	902	A0O	C10-C07	-5.89	1.30	1.41
2	D	902	A0O	C10-C07	-5.89	1.30	1.41
2	C	901	A0O	C07-C06	4.75	1.50	1.41
2	A	902	A0O	C07-C06	4.74	1.50	1.41
2	A	901	A0O	C07-C06	4.74	1.50	1.41
2	D	901	A0O	C07-C06	4.72	1.50	1.41
2	B	901	A0O	C07-C06	4.71	1.50	1.41
2	C	902	A0O	C07-C06	4.69	1.50	1.41
2	D	902	A0O	C07-C06	4.67	1.50	1.41
2	B	902	A0O	C07-C06	4.66	1.50	1.41
2	C	901	A0O	C05-C04	4.38	1.56	1.51
2	D	901	A0O	C05-C04	4.36	1.56	1.51
2	A	901	A0O	C05-C04	4.29	1.56	1.51
2	B	901	A0O	C05-C04	4.19	1.56	1.51
2	D	902	A0O	C05-C04	3.31	1.55	1.51
2	C	902	A0O	C05-C04	3.29	1.55	1.51
2	B	902	A0O	C05-C04	3.16	1.55	1.51
2	A	902	A0O	C05-C04	3.12	1.55	1.51
2	B	901	A0O	O02-C08	2.66	1.41	1.37
2	B	901	A0O	O01-C06	-2.65	1.34	1.38
2	A	901	A0O	O02-C08	2.64	1.41	1.37
2	A	902	A0O	O01-C06	-2.64	1.34	1.38
2	B	902	A0O	O01-C06	-2.63	1.34	1.38
2	D	901	A0O	O01-C06	-2.63	1.34	1.38
2	C	901	A0O	O02-C08	2.63	1.41	1.37
2	A	901	A0O	O01-C06	-2.62	1.34	1.38
2	C	901	A0O	O01-C06	-2.60	1.34	1.38
2	B	902	A0O	O02-C08	2.60	1.41	1.37
2	C	902	A0O	O02-C08	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	A00	O02-C08	2.58	1.41	1.37
2	D	902	A00	O01-C06	-2.57	1.34	1.38
2	D	902	A00	O02-C08	2.56	1.41	1.37
2	C	902	A00	O01-C06	-2.48	1.34	1.38
2	A	902	A00	O02-C08	2.39	1.41	1.37
2	D	901	A00	C05-C09	2.29	1.55	1.50
2	C	901	A00	C05-C09	2.28	1.55	1.50
2	A	902	A00	C14-C15	-2.22	1.39	1.44
2	A	901	A00	C05-C09	2.22	1.55	1.50
2	B	901	A00	C05-C09	2.21	1.55	1.50
2	D	902	A00	C14-C15	-2.20	1.39	1.44
2	B	902	A00	C14-C15	-2.19	1.39	1.44
2	C	902	A00	C14-C15	-2.18	1.39	1.44
2	B	901	A00	C14-C15	-2.08	1.39	1.44
2	D	901	A00	C14-C15	-2.06	1.40	1.44
2	A	901	A00	C14-C15	-2.06	1.40	1.44
2	C	901	A00	C14-C15	-2.05	1.40	1.44
2	C	902	A00	C05-C09	2.03	1.55	1.50
2	D	902	A00	C05-C09	2.03	1.55	1.50
2	A	902	A00	C05-C09	2.01	1.55	1.50

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	A00	O01-C06-C04	25.21	144.57	115.96
2	C	902	A00	O01-C06-C04	25.20	144.56	115.96
2	B	902	A00	O01-C06-C04	25.10	144.44	115.96
2	D	902	A00	O01-C06-C04	25.09	144.43	115.96
2	A	901	A00	O01-C06-C04	24.94	144.26	115.96
2	D	901	A00	O01-C06-C04	24.93	144.25	115.96
2	B	901	A00	O01-C06-C04	24.78	144.07	115.96
2	C	901	A00	O01-C06-C04	24.72	144.01	115.96
2	D	902	A00	C06-O01-C15	13.98	133.93	121.99
2	B	902	A00	C06-O01-C15	13.94	133.90	121.99
2	C	902	A00	C06-O01-C15	13.92	133.88	121.99
2	B	901	A00	C06-O01-C15	13.86	133.83	121.99
2	A	901	A00	C06-O01-C15	13.68	133.68	121.99
2	A	902	A00	C06-O01-C15	13.63	133.63	121.99
2	C	901	A00	C06-O01-C15	13.59	133.60	121.99
2	D	901	A00	C06-O01-C15	13.58	133.59	121.99
2	C	902	A00	O02-C08-C04	9.16	125.05	115.35
2	A	902	A00	C07-C06-C04	-9.12	102.75	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	902	A00	C07-C06-C04	-9.01	102.99	121.91
2	C	902	A00	C07-C06-C04	-9.00	103.00	121.91
2	B	902	A00	C07-C06-C04	-9.00	103.01	121.91
2	A	902	A00	C08-C04-C06	8.78	127.14	116.63
2	D	902	A00	O02-C08-C04	8.72	124.58	115.35
2	B	902	A00	C08-C04-C06	8.72	127.07	116.63
2	D	902	A00	C08-C04-C06	8.69	127.04	116.63
2	C	902	A00	C08-C04-C06	8.69	127.03	116.63
2	B	901	A00	C07-C06-C04	-8.56	103.94	121.91
2	A	901	A00	C07-C06-C04	-8.55	103.95	121.91
2	B	902	A00	O02-C08-C04	8.53	124.38	115.35
2	D	901	A00	C07-C06-C04	-8.51	104.04	121.91
2	C	901	A00	C07-C06-C04	-8.47	104.12	121.91
2	A	901	A00	O02-C08-C04	8.41	124.25	115.35
2	B	901	A00	O02-C08-C04	8.34	124.18	115.35
2	D	901	A00	O02-C08-C04	8.28	124.11	115.35
2	D	901	A00	O01-C06-C07	-8.27	111.72	120.56
2	A	901	A00	O01-C06-C07	-8.21	111.78	120.56
2	C	901	A00	O02-C08-C04	8.17	123.99	115.35
2	C	901	A00	O01-C06-C07	-8.13	111.87	120.56
2	B	901	A00	O01-C06-C07	-8.02	111.99	120.56
2	A	902	A00	O02-C08-C04	7.82	123.63	115.35
2	B	901	A00	C08-C04-C06	7.78	125.95	116.63
2	A	901	A00	C08-C04-C06	7.77	125.94	116.63
2	D	901	A00	C08-C04-C06	7.73	125.89	116.63
2	C	901	A00	C08-C04-C06	7.61	125.75	116.63
2	C	902	A00	O01-C06-C07	-7.60	112.44	120.56
2	B	902	A00	O01-C06-C07	-7.50	112.55	120.56
2	D	902	A00	O01-C06-C07	-7.47	112.58	120.56
2	A	902	A00	O01-C06-C07	-7.38	112.68	120.56
2	A	902	A00	C10-C07-C06	6.54	127.49	119.76
2	C	902	A00	C11-C08-C04	-6.42	111.75	120.54
2	D	902	A00	C10-C07-C06	6.37	127.28	119.76
2	B	902	A00	C11-C08-C04	-6.33	111.86	120.54
2	D	902	A00	C11-C08-C04	-6.33	111.87	120.54
2	B	902	A00	C10-C07-C06	6.31	127.22	119.76
2	A	901	A00	C11-C08-C04	-6.30	111.92	120.54
2	C	902	A00	C10-C07-C06	6.29	127.19	119.76
2	D	902	A00	C05-C09-C13	-6.27	119.97	127.59
2	D	901	A00	C11-C08-C04	-6.25	111.98	120.54
2	B	901	A00	C11-C08-C04	-6.24	111.99	120.54
2	C	902	A00	C05-C09-C13	-6.21	120.03	127.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	A00	C05-C09-C13	-6.20	120.05	127.59
2	B	902	A00	C05-C09-C13	-6.19	120.06	127.59
2	C	901	A00	C11-C08-C04	-6.16	112.11	120.54
2	A	902	A00	C11-C08-C04	-6.08	112.22	120.54
2	B	901	A00	C10-C07-C06	6.02	126.88	119.76
2	A	901	A00	C10-C07-C06	5.98	126.83	119.76
2	D	901	A00	C10-C07-C06	5.96	126.81	119.76
2	C	901	A00	C10-C07-C06	5.93	126.77	119.76
2	A	902	A00	C06-C07-C12	-4.37	113.20	117.52
2	B	902	A00	C06-C07-C12	-4.26	113.31	117.52
2	A	901	A00	C05-C09-C13	-4.26	122.41	127.59
2	D	901	A00	C05-C09-C13	-4.25	122.42	127.59
2	D	902	A00	C06-C07-C12	-4.24	113.33	117.52
2	C	901	A00	C05-C09-C13	-4.11	122.59	127.59
2	B	901	A00	C05-C09-C13	-4.11	122.59	127.59
2	C	902	A00	C06-C07-C12	-4.01	113.56	117.52
2	A	902	A00	C05-C04-C08	-3.93	115.54	121.67
2	A	902	A00	C18-O02-C08	-3.57	112.14	117.53
2	B	902	A00	C05-C04-C08	-3.46	116.27	121.67
2	C	901	A00	O03-C15-C14	-3.40	119.68	126.00
2	D	902	A00	C05-C04-C08	-3.38	116.40	121.67
2	D	901	A00	O03-C15-C14	-3.38	119.72	126.00
2	A	901	A00	O03-C15-C14	-3.37	119.73	126.00
2	B	901	A00	O03-C15-C14	-3.36	119.75	126.00
2	B	902	A00	C18-O02-C08	-3.36	112.45	117.53
2	B	901	A00	C06-C07-C12	-3.30	114.26	117.52
2	C	901	A00	C06-C07-C12	-3.29	114.27	117.52
2	A	902	A00	O01-C15-O03	3.28	120.62	116.44
2	B	901	A00	C05-C04-C08	-3.27	116.58	121.67
2	A	901	A00	C06-C07-C12	-3.27	114.29	117.52
2	D	902	A00	C18-O02-C08	-3.25	112.62	117.53
2	D	901	A00	C05-C04-C08	-3.25	116.61	121.67
2	C	902	A00	C18-O02-C08	-3.24	112.63	117.53
2	C	902	A00	C05-C04-C08	-3.24	116.62	121.67
2	D	901	A00	C06-C07-C12	-3.23	114.33	117.52
2	A	901	A00	C05-C04-C08	-3.20	116.69	121.67
2	B	902	A00	O01-C15-O03	3.14	120.45	116.44
2	C	902	A00	O03-C15-C14	-3.14	120.17	126.00
2	C	901	A00	C05-C04-C08	-3.10	116.84	121.67
2	A	902	A00	O03-C15-C14	-3.07	120.30	126.00
2	A	901	A00	C10-C11-C08	3.05	125.86	120.06
2	D	902	A00	O03-C15-C14	-3.02	120.38	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	A00	O01-C15-O03	3.02	120.29	116.44
2	D	901	A00	C10-C11-C08	3.02	125.80	120.06
2	B	902	A00	O03-C15-C14	-3.02	120.39	126.00
2	B	901	A00	C10-C11-C08	3.01	125.78	120.06
2	D	902	A00	O01-C15-O03	3.00	120.27	116.44
2	C	901	A00	C10-C11-C08	2.99	125.74	120.06
2	C	902	A00	C11-C10-C07	2.92	125.69	121.74
2	B	902	A00	C11-C10-C07	2.87	125.62	121.74
2	C	902	A00	C05-C04-C06	-2.85	116.34	121.37
2	D	902	A00	C11-C10-C07	2.81	125.55	121.74
2	A	902	A00	C11-C10-C07	2.81	125.54	121.74
2	C	901	A00	C11-C10-C07	2.79	125.51	121.74
2	A	901	A00	C11-C10-C07	2.78	125.50	121.74
2	D	901	A00	C11-C10-C07	2.77	125.49	121.74
2	C	902	A00	C10-C11-C08	2.77	125.32	120.06
2	B	901	A00	C11-C10-C07	2.75	125.46	121.74
2	D	902	A00	C10-C11-C08	2.74	125.27	120.06
2	D	902	A00	C05-C04-C06	-2.73	116.55	121.37
2	D	901	A00	O01-C15-O03	2.71	119.90	116.44
2	A	901	A00	O01-C15-O03	2.70	119.89	116.44
2	B	902	A00	C10-C11-C08	2.70	125.21	120.06
2	C	901	A00	O01-C15-O03	2.68	119.86	116.44
2	B	902	A00	C05-C04-C06	-2.68	116.65	121.37
2	B	901	A00	O01-C15-O03	2.64	119.81	116.44
2	A	902	A00	C10-C11-C08	2.52	124.86	120.06
2	A	902	A00	C05-C04-C06	-2.30	117.31	121.37
2	A	901	A00	C05-C04-C06	-2.26	117.38	121.37
2	C	901	A00	C05-C04-C06	-2.24	117.41	121.37
2	D	901	A00	C18-O02-C08	-2.21	114.19	117.53
2	B	901	A00	C05-C04-C06	-2.21	117.48	121.37
2	C	901	A00	O01-C15-C14	2.20	120.47	117.12
2	D	901	A00	C05-C04-C06	-2.19	117.50	121.37
2	B	901	A00	O01-C15-C14	2.19	120.45	117.12
2	B	901	A00	C18-O02-C08	-2.17	114.25	117.53
2	B	901	A00	C16-C13-C17	2.15	119.35	114.60
2	A	901	A00	O01-C15-C14	2.14	120.38	117.12
2	D	901	A00	O01-C15-C14	2.14	120.38	117.12
2	C	901	A00	C16-C13-C17	2.12	119.30	114.60
2	A	901	A00	C18-O02-C08	-2.08	114.38	117.53
2	C	901	A00	C18-O02-C08	-2.08	114.39	117.53
2	A	901	A00	C16-C13-C17	2.06	119.16	114.60
2	D	901	A00	C16-C13-C17	2.05	119.14	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	902	A00	C16-C13-C17	2.02	119.07	114.60
2	B	902	A00	C16-C13-C17	2.01	119.03	114.60

There are no chirality outliers.

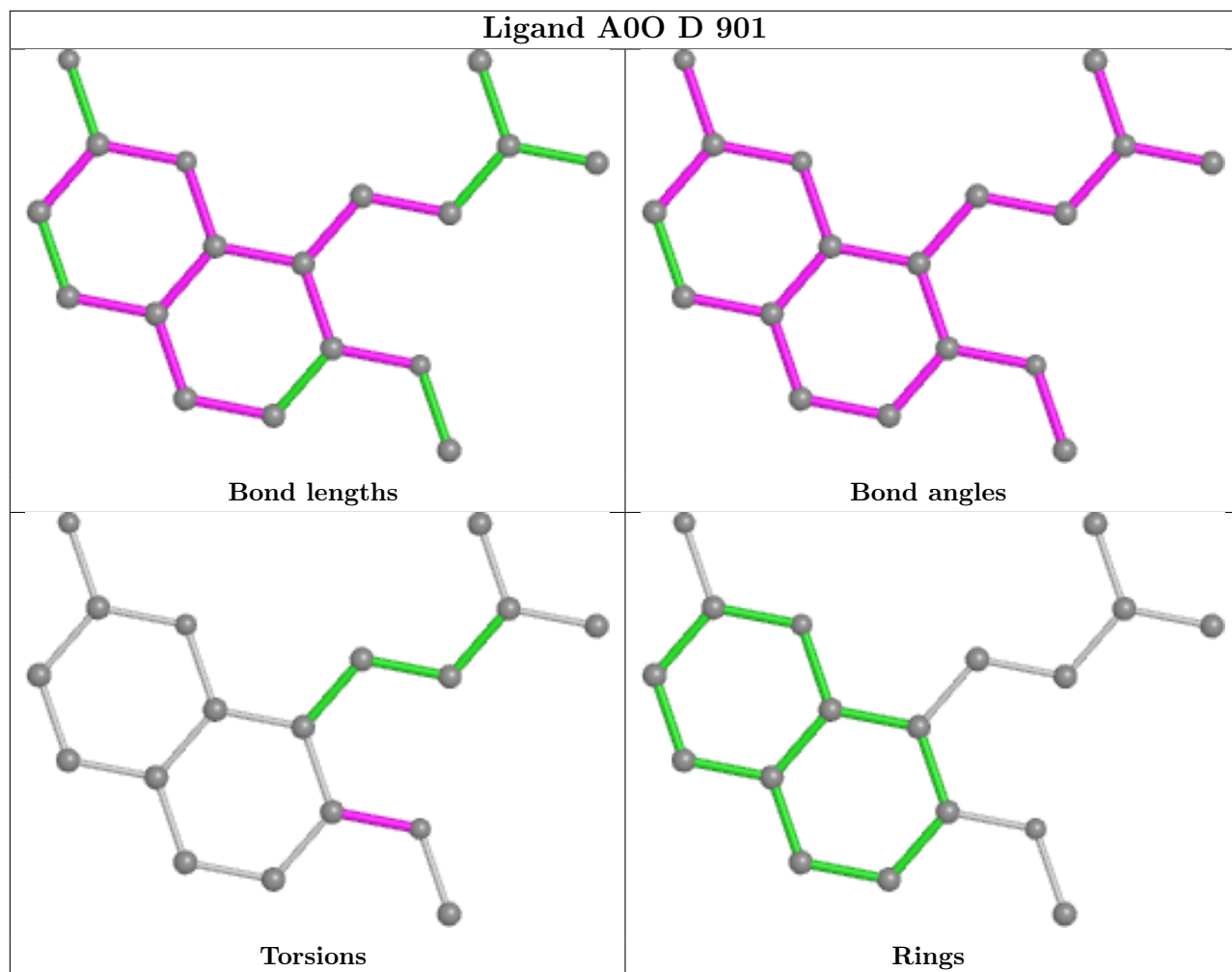
All (17) torsion outliers are listed below:

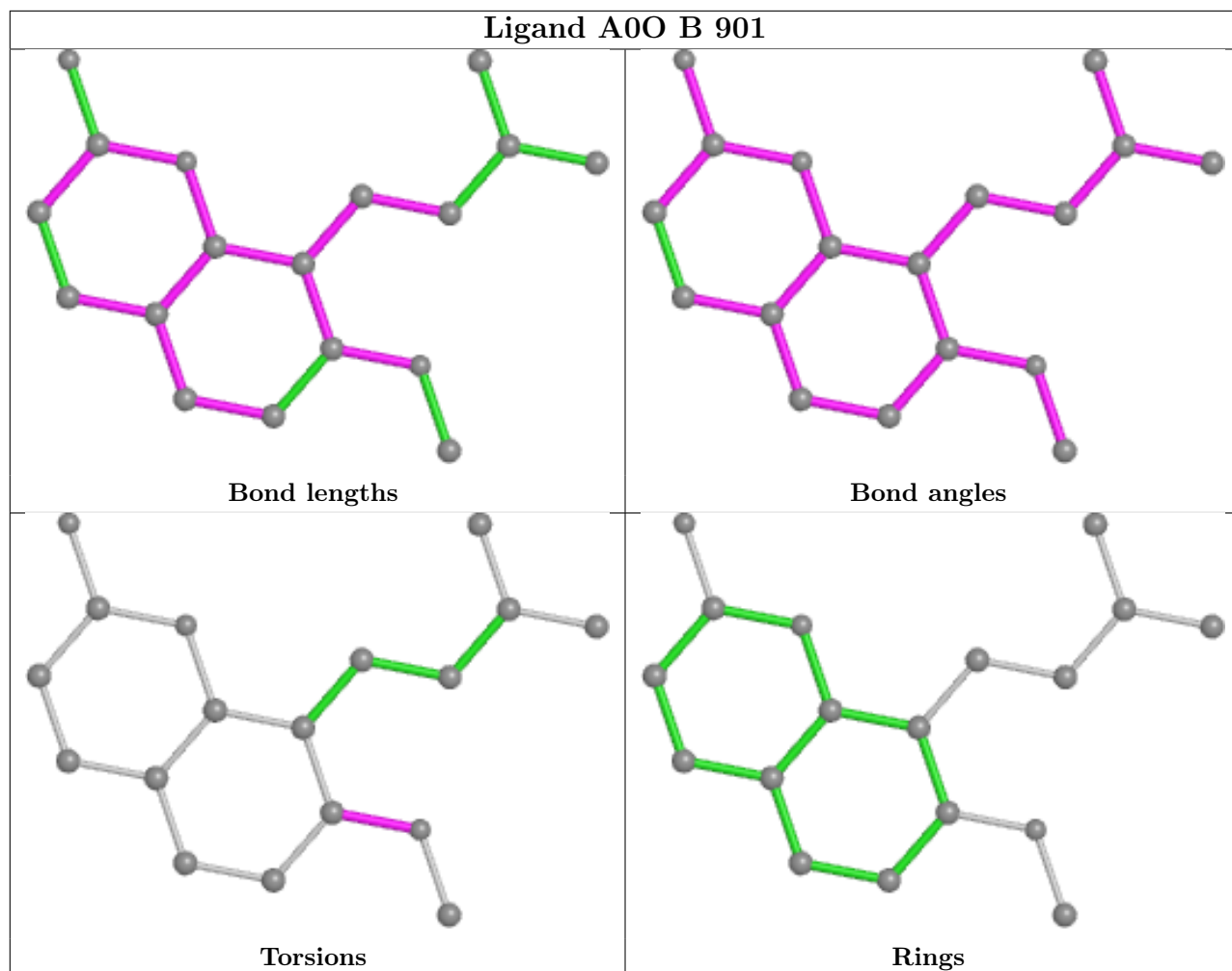
Mol	Chain	Res	Type	Atoms
2	A	902	A00	C11-C08-O02-C18
2	B	902	A00	C11-C08-O02-C18
2	C	902	A00	C11-C08-O02-C18
2	D	902	A00	C11-C08-O02-C18
2	B	902	A00	C04-C08-O02-C18
2	A	902	A00	C04-C08-O02-C18
2	C	902	A00	C04-C08-O02-C18
2	D	902	A00	C04-C08-O02-C18
2	B	901	A00	C11-C08-O02-C18
2	B	901	A00	C04-C08-O02-C18
2	D	901	A00	C11-C08-O02-C18
2	A	901	A00	C11-C08-O02-C18
2	C	901	A00	C11-C08-O02-C18
2	A	901	A00	C04-C08-O02-C18
2	D	901	A00	C04-C08-O02-C18
2	C	901	A00	C04-C08-O02-C18
2	C	902	A00	C08-C04-C05-C09

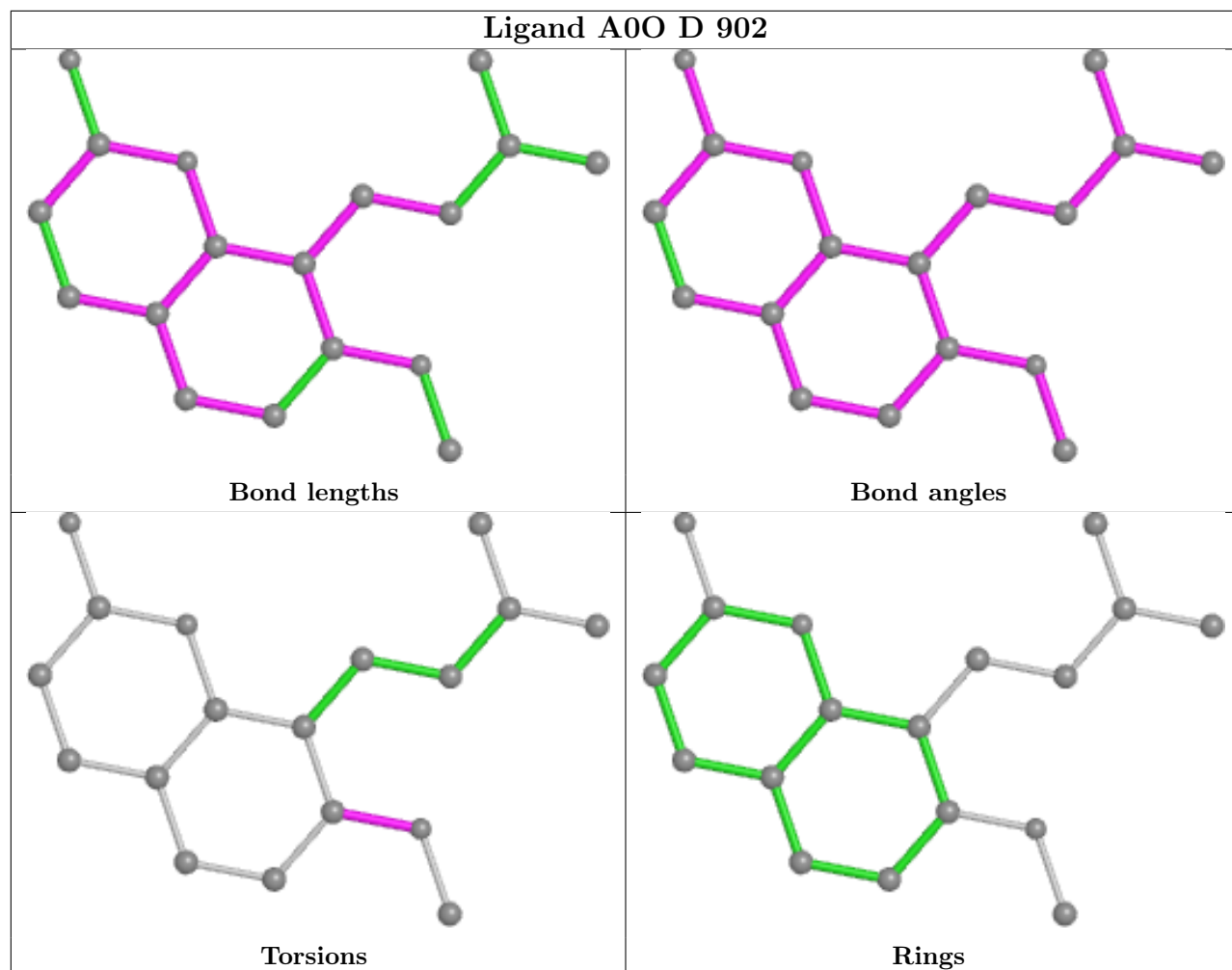
There are no ring outliers.

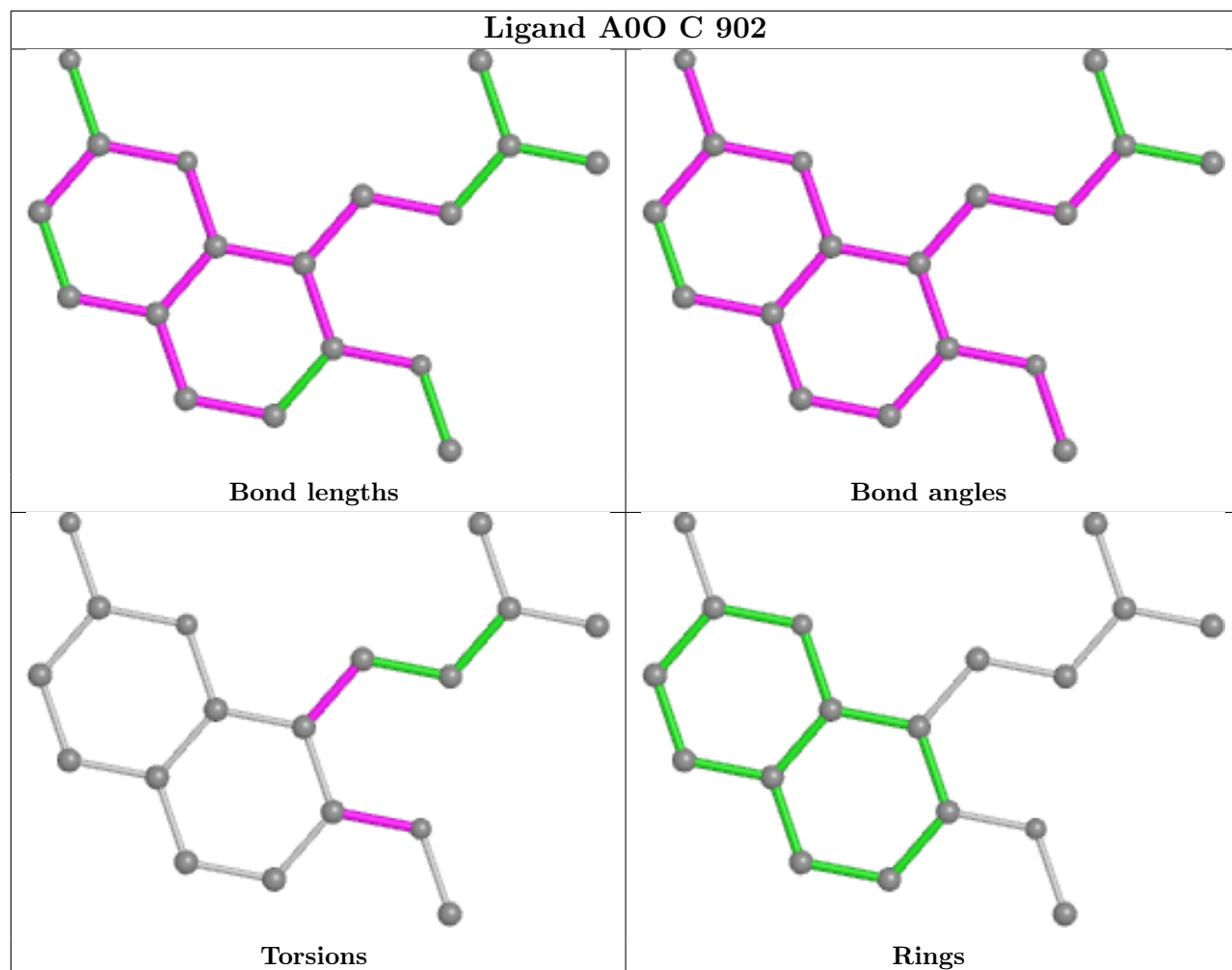
No monomer is involved in short contacts.

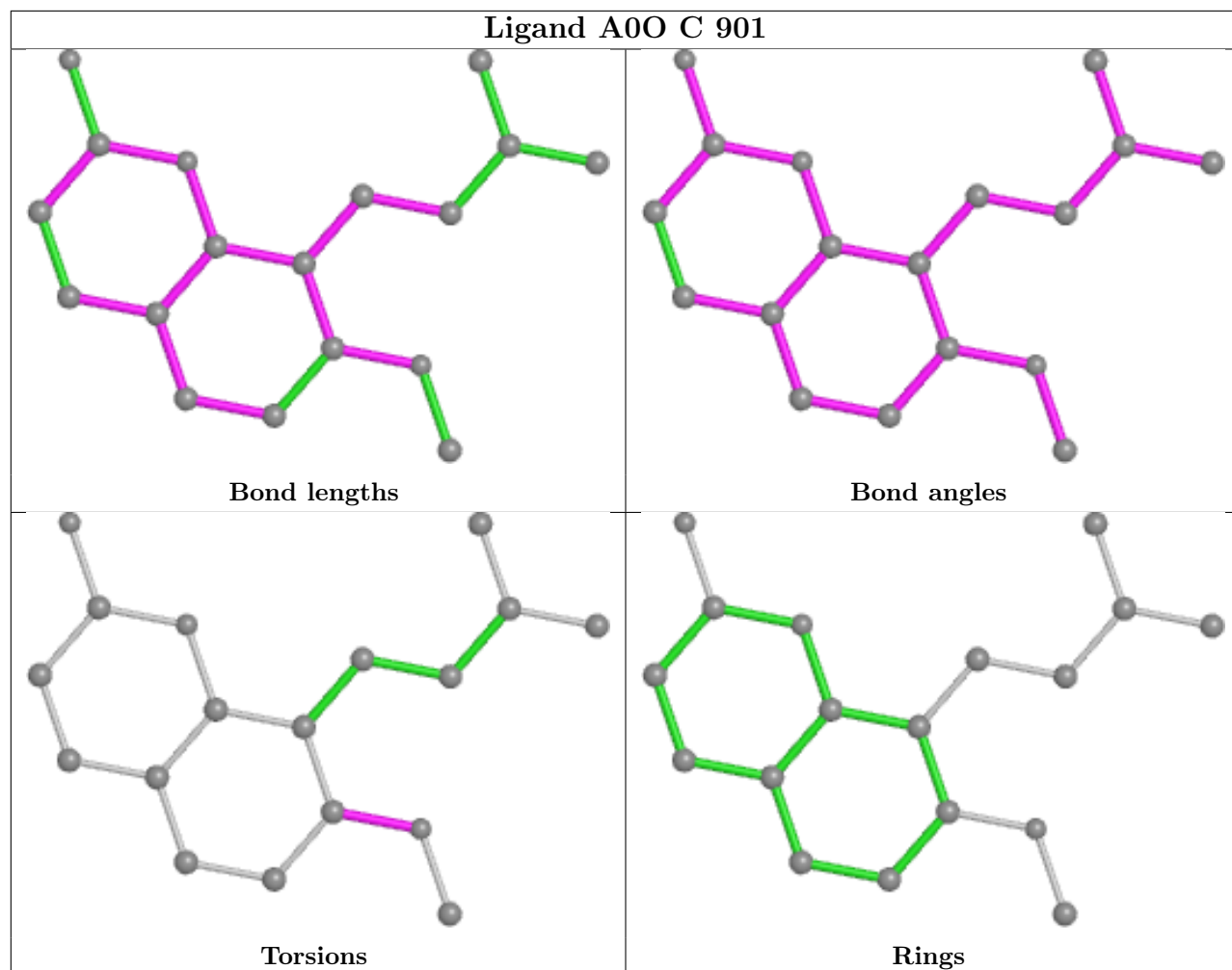
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

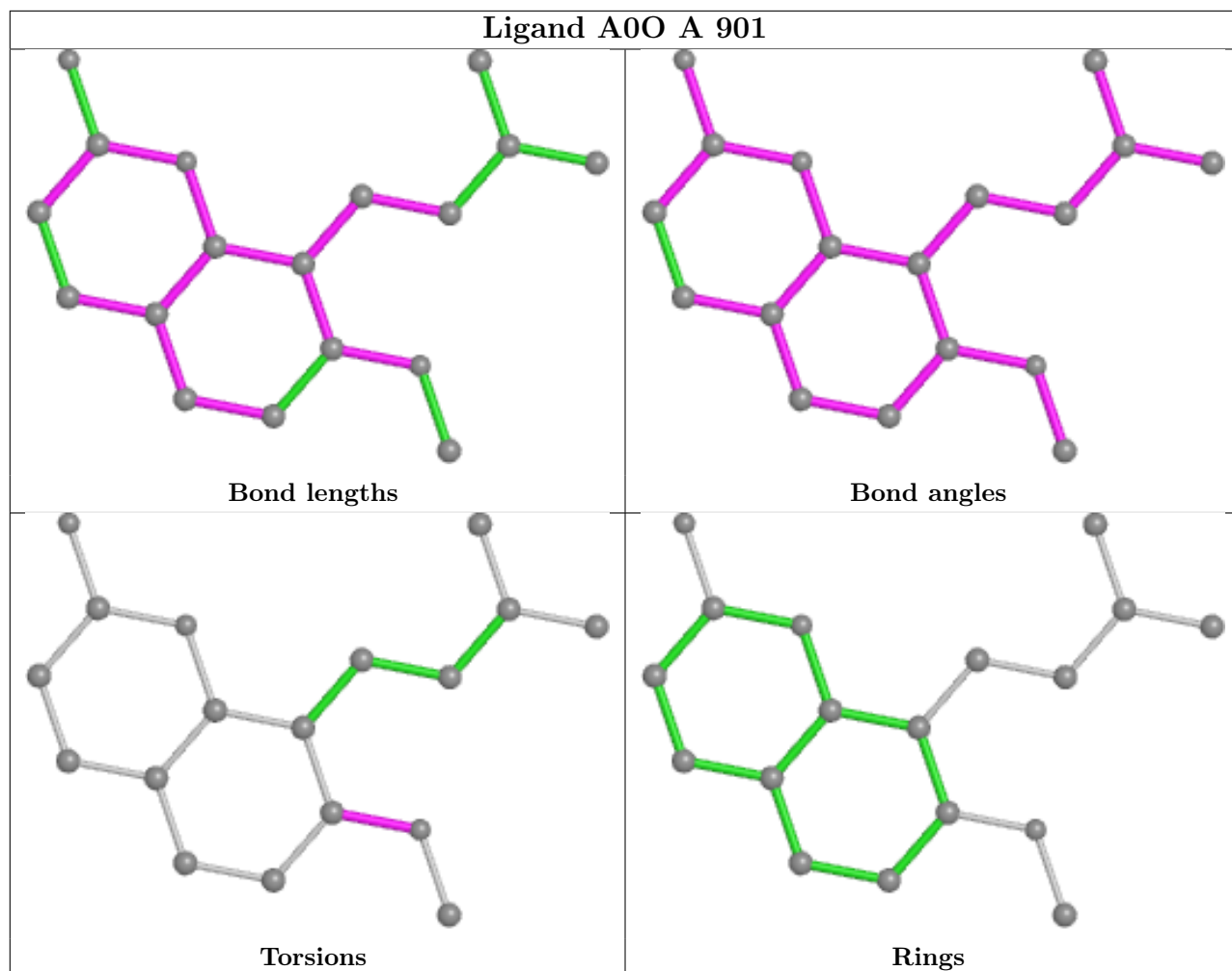


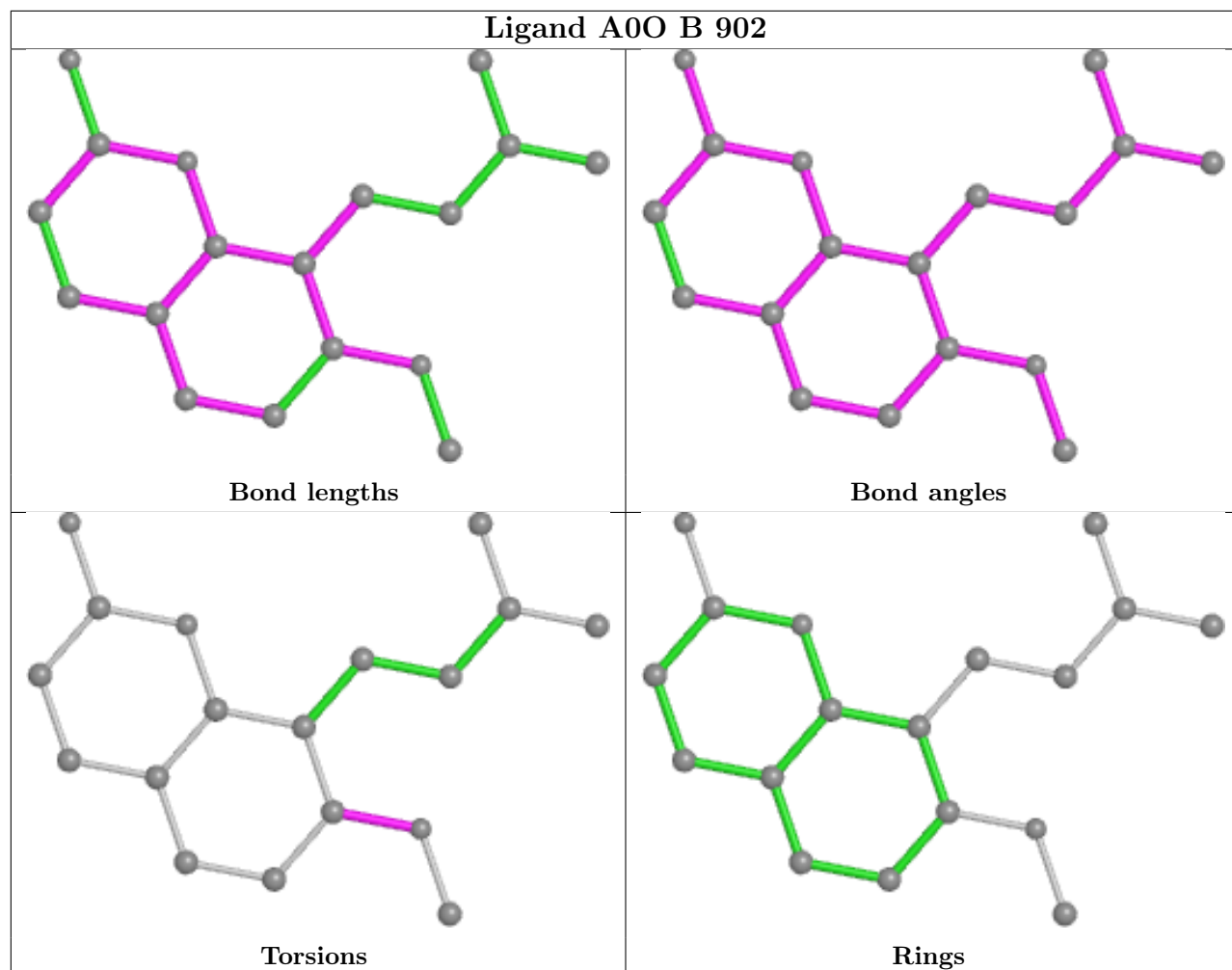


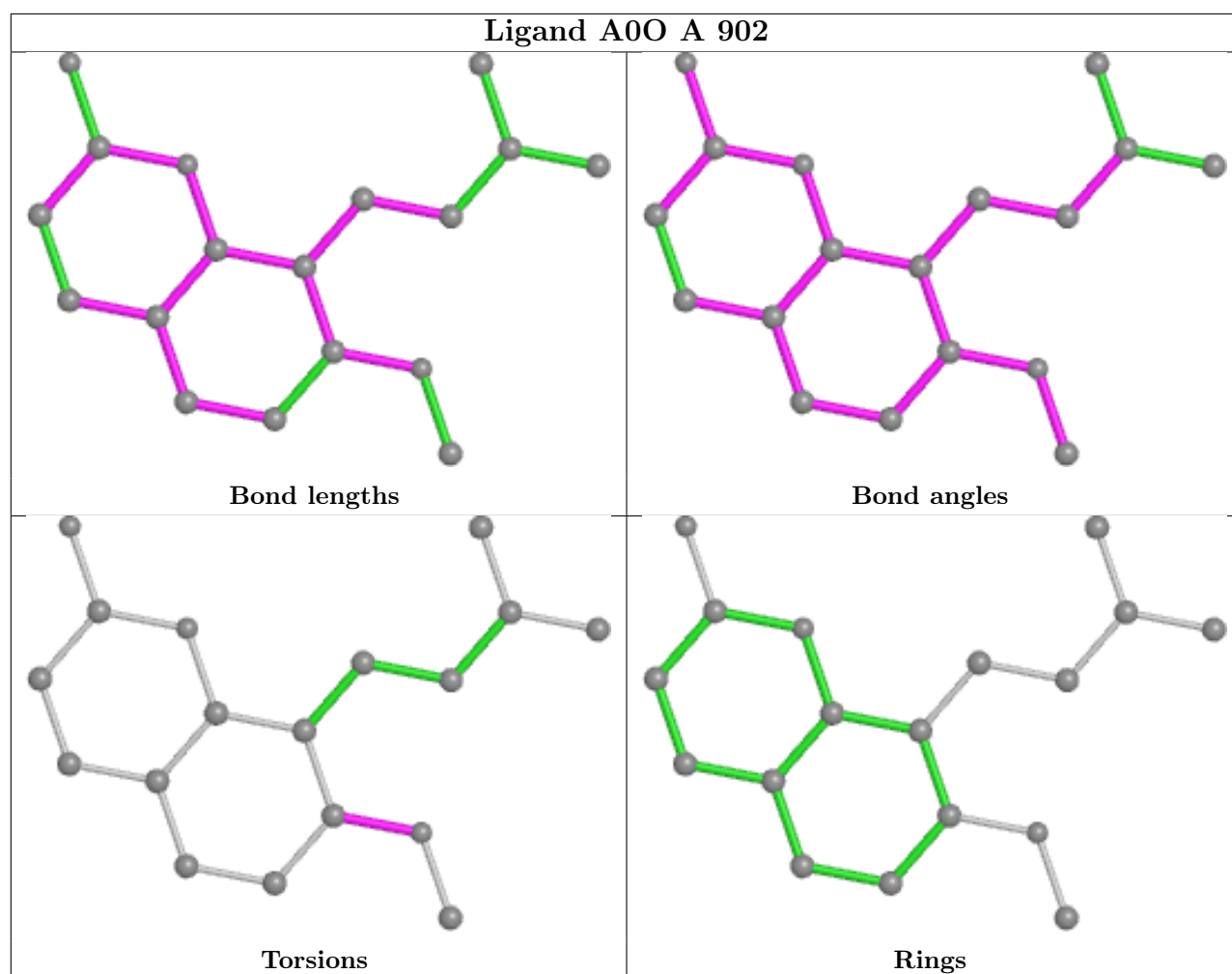












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

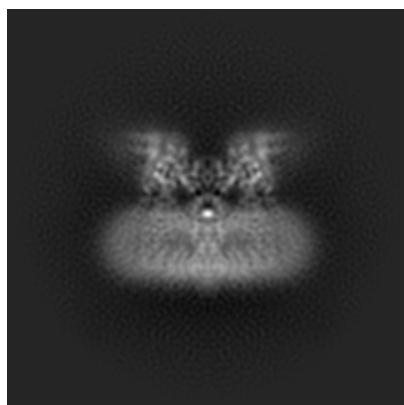
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24386. These allow visual inspection of the internal detail of the map and identification of artifacts.

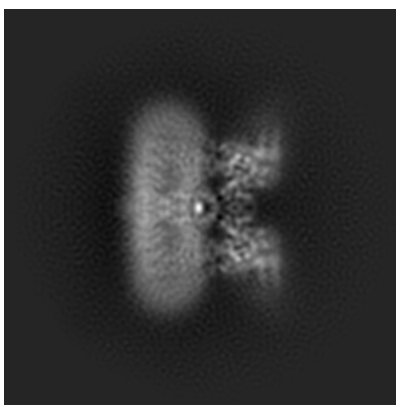
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

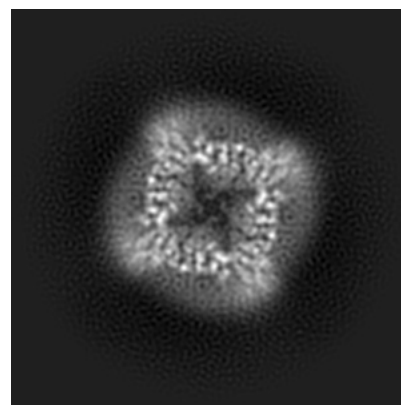
6.1.1 Primary map



X



Y

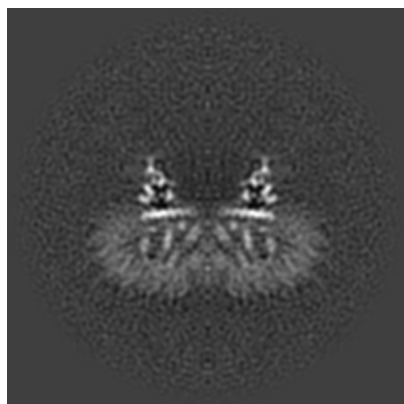


Z

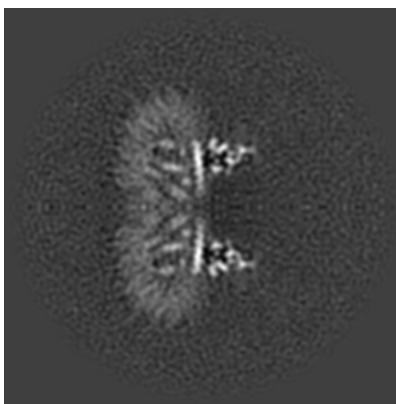
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

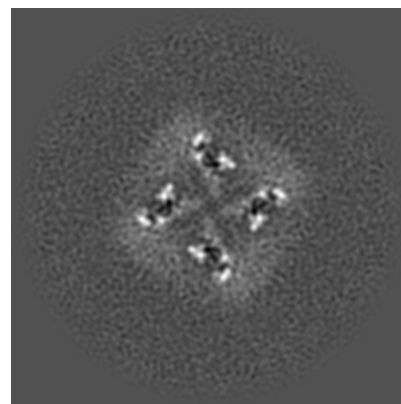
6.2.1 Primary map



X Index: 128



Y Index: 128

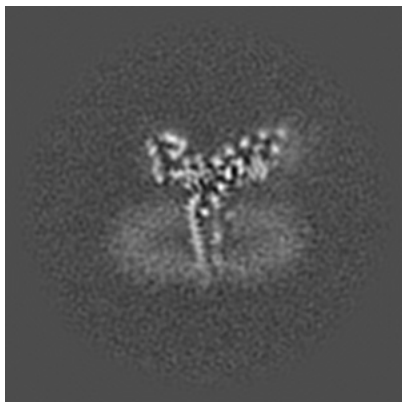


Z Index: 128

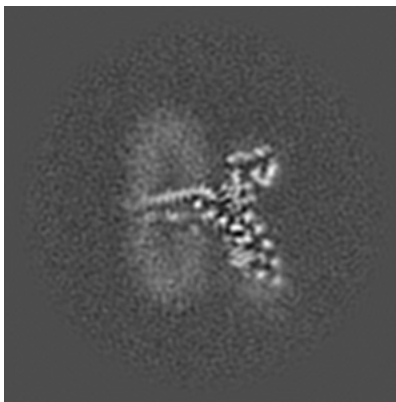
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

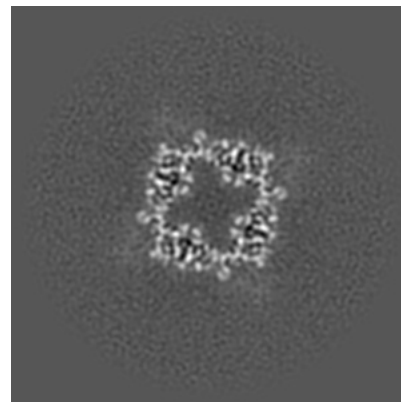
6.3.1 Primary map



X Index: 96



Y Index: 96

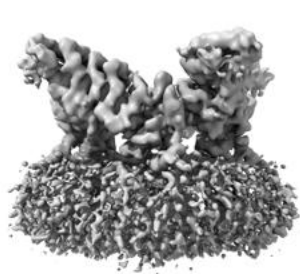


Z Index: 149

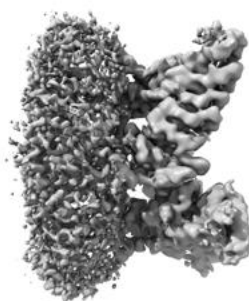
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

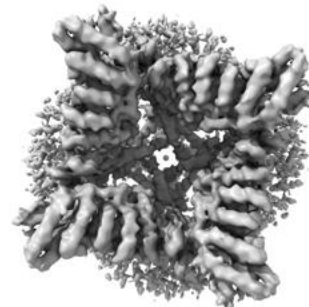
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.097. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

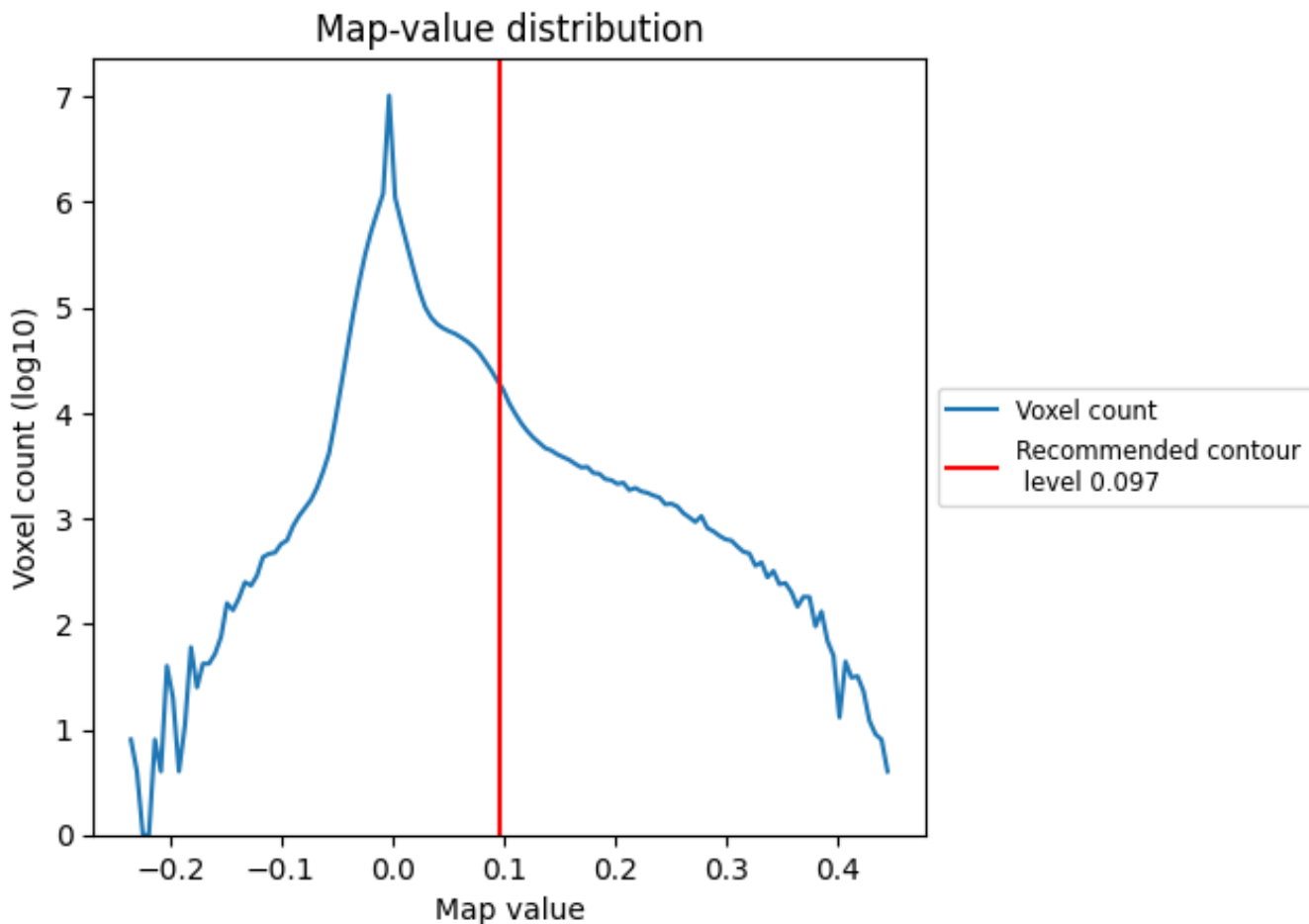
6.5 Mask visualisation

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

7 Map analysis [i](#)

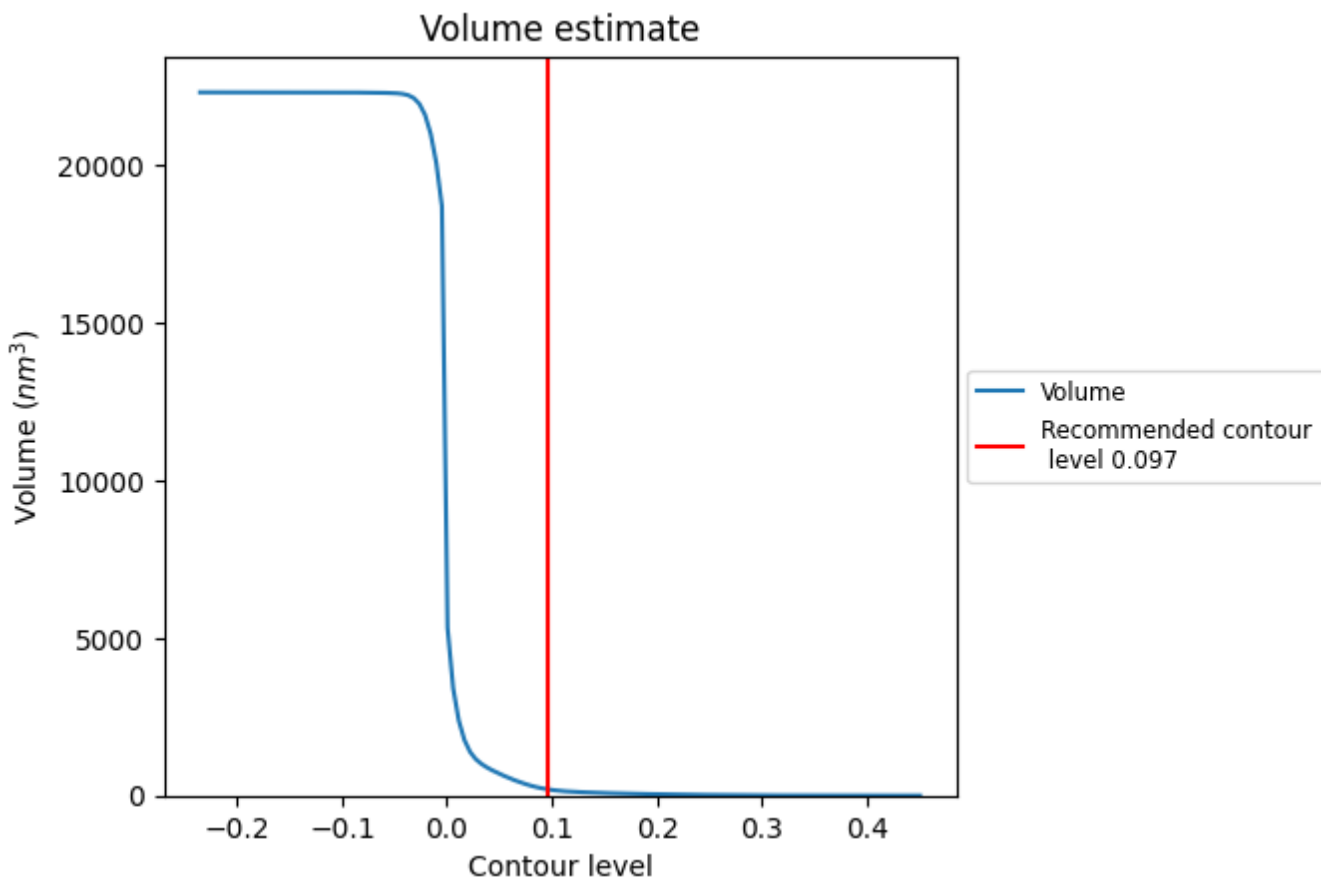
This section contains the results of statistical analysis of the map.

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.

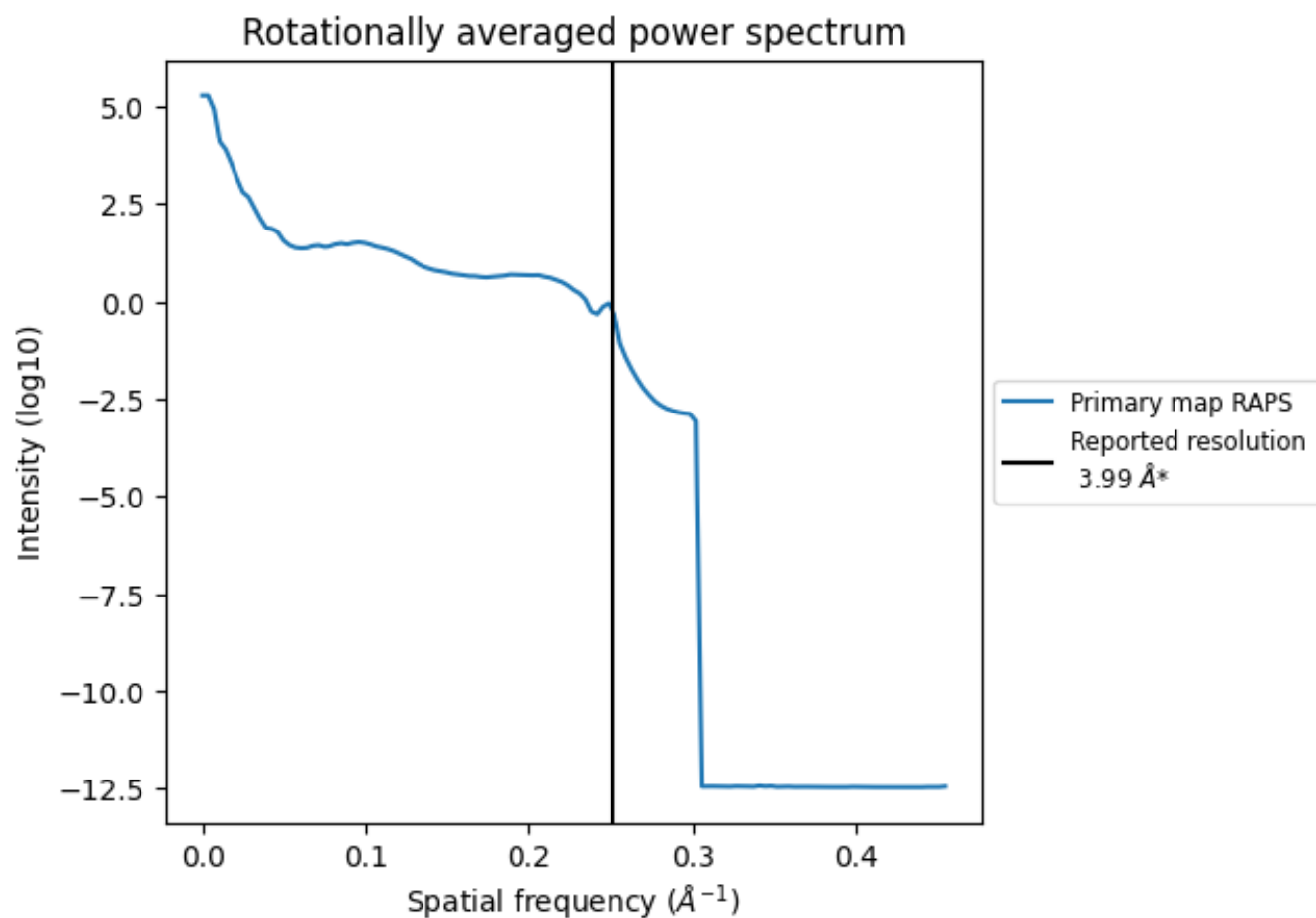
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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 i



*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

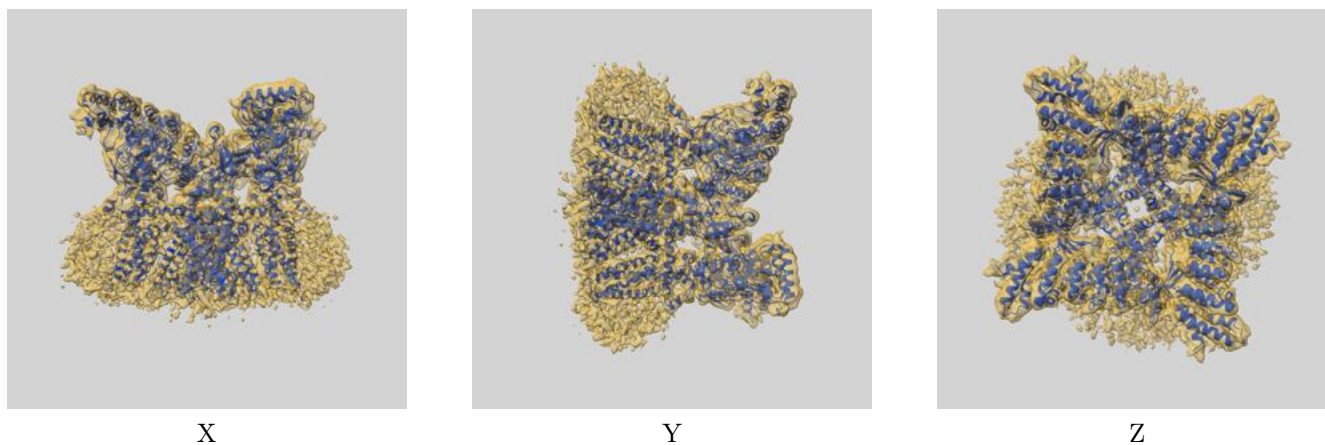
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

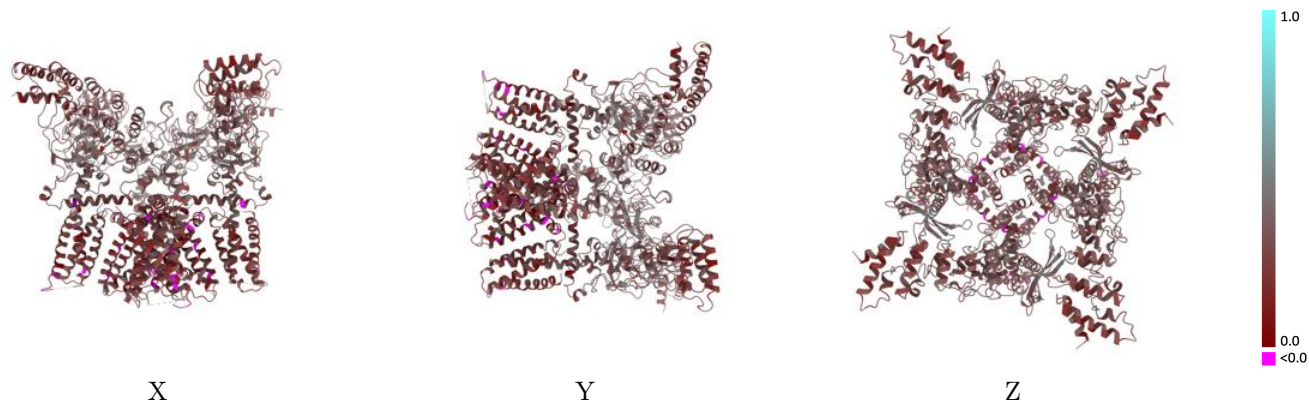
This section contains information regarding the fit between EMDB map EMD-24386 and PDB model 7RAU. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



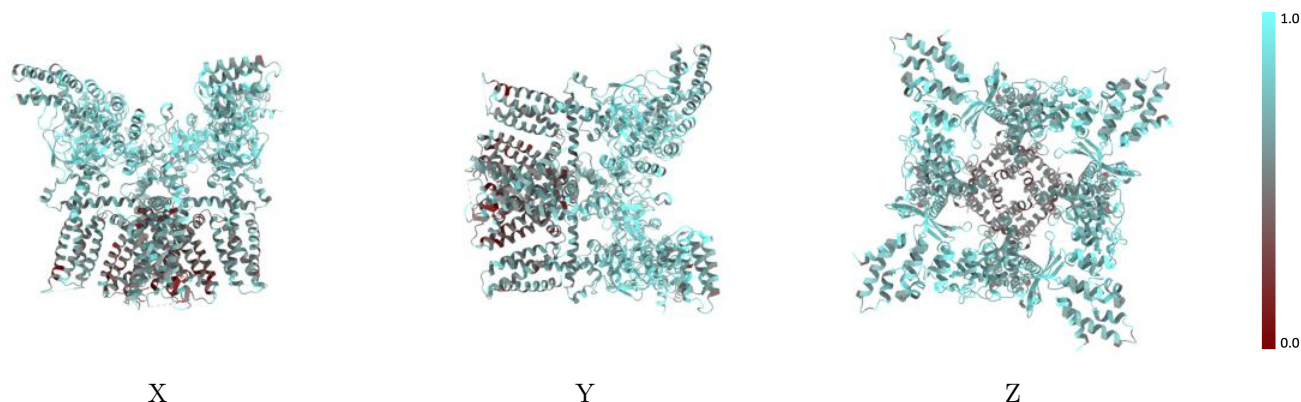
The images above show the 3D surface view of the map at the recommended contour level 0.097 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



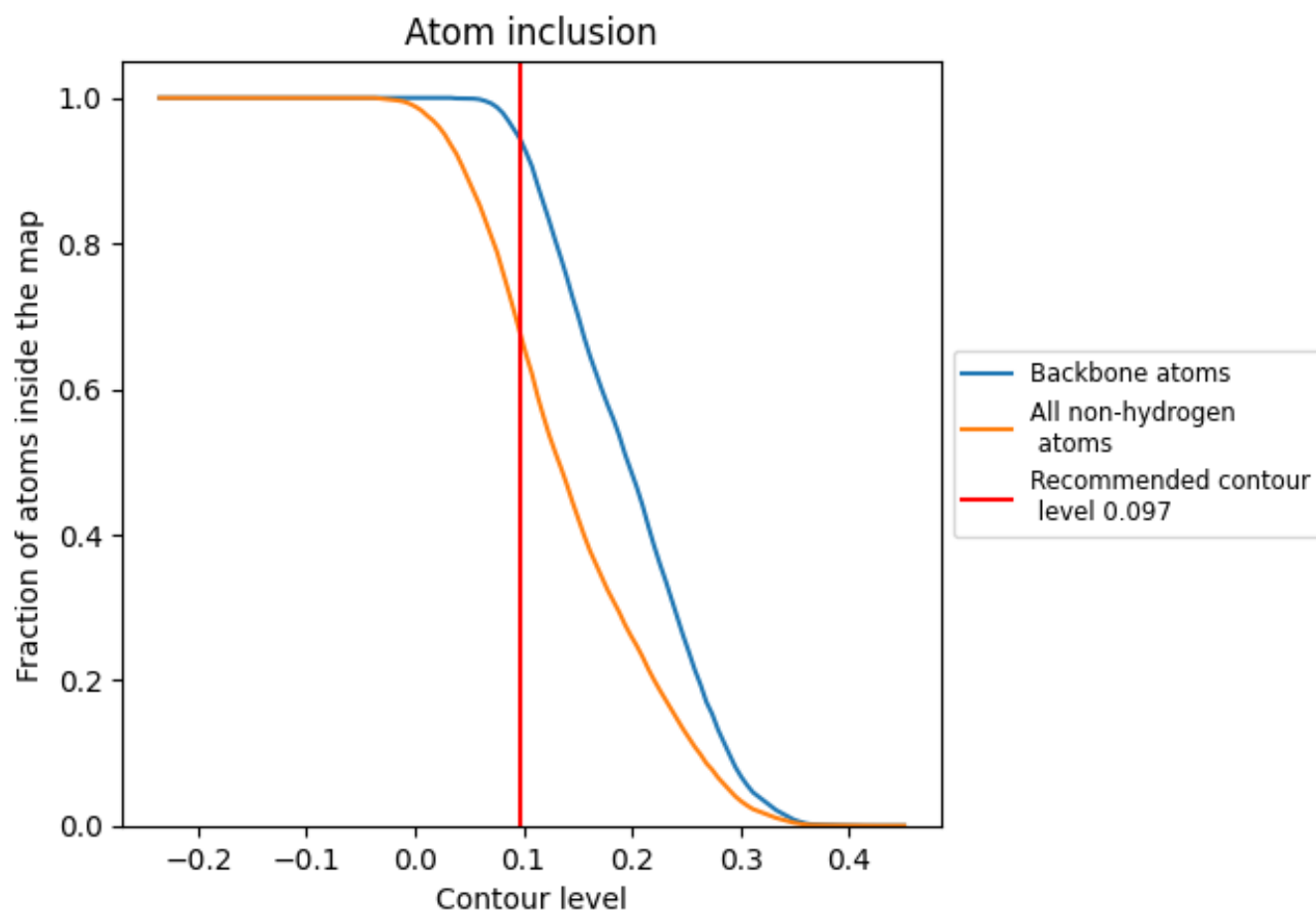
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.097).







9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 68% 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 (0.097) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6757	 0.2980
A	 0.6760	 0.2990
B	 0.6771	 0.2980
C	 0.6740	 0.2990
D	 0.6758	 0.2970

