Full wwPDB EM Validation Report ⓘ

May 4, 2024 – 12:31 PM EDT

PDB ID	:	8U2Z
EMDB ID	:	EMD-41847
Title	:	TRPV1 in nanodisc bound with diC8-PIP2 in the dilated state
Authors	:	Arnold, W.R.; Julius, D.; Cheng, Y.
Deposited on	:	2023-09-06
Resolution	:	3.60 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:

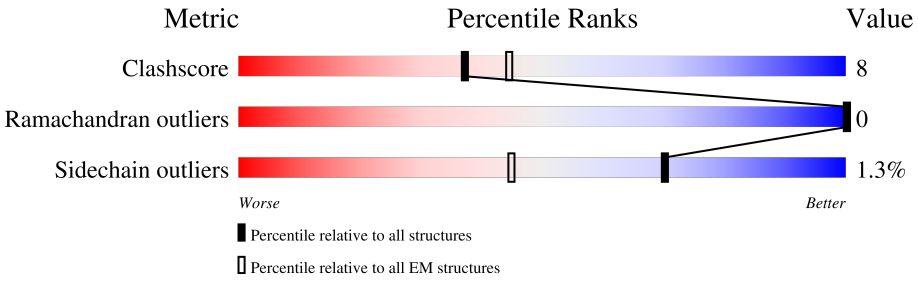
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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 <=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	635	64% 16% • 20%
1	B	635	65% 14% • 20%
1	C	635	65% 15% • 20%
1	D	635	64% 15% • 20%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 34361 atoms, of which 17316 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	510	Total	C	H	N	O	S	0	0
			8269	2704	4143	662	737	23		
1	D	510	Total	C	H	N	O	S	0	0
			8269	2704	4143	662	737	23		
1	B	510	Total	C	H	N	O	S	0	0
			8269	2704	4143	662	737	23		
1	C	510	Total	C	H	N	O	S	0	0
			8269	2704	4143	662	737	23		

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MET	-	initiating methionine	UNP O35433
A	108	GLY	-	expression tag	UNP O35433
A	109	SER	-	expression tag	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	LEU	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	MET	deletion	UNP O35433
A	?	-	GLU	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	THR	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	HIS	deletion	UNP O35433
A	?	-	LYS	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433
A	?	-	ARG	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	ALA	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
D	107	MET	-	initiating methionine	UNP O35433
D	108	GLY	-	expression tag	UNP O35433
D	109	SER	-	expression tag	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	LEU	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	MET	deletion	UNP O35433
D	?	-	GLU	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	THR	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	HIS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	ARG	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	ALA	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
B	107	MET	-	initiating methionine	UNP O35433
B	108	GLY	-	expression tag	UNP O35433
B	109	SER	-	expression tag	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	LEU	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	MET	deletion	UNP O35433
B	?	-	GLU	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433

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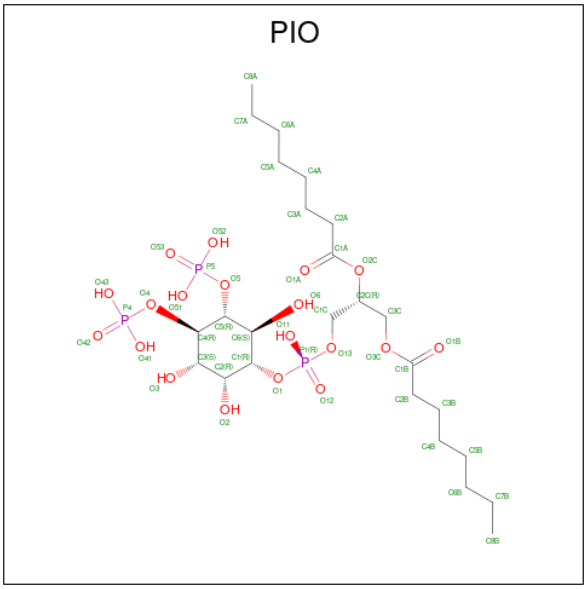
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	HIS	deletion	UNP O35433
B	?	-	LYS	deletion	UNP O35433
B	?	-	CYS	deletion	UNP O35433
B	?	-	ARG	deletion	UNP O35433
B	?	-	GLY	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	ALA	deletion	UNP O35433
B	?	-	CYS	deletion	UNP O35433
B	?	-	LYS	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	GLY	deletion	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
C	107	MET	-	initiating methionine	UNP O35433
C	108	GLY	-	expression tag	UNP O35433
C	109	SER	-	expression tag	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	LEU	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	MET	deletion	UNP O35433
C	?	-	GLU	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	THR	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	HIS	deletion	UNP O35433
C	?	-	LYS	deletion	UNP O35433
C	?	-	CYS	deletion	UNP O35433
C	?	-	ARG	deletion	UNP O35433
C	?	-	GLY	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	ALA	deletion	UNP O35433
C	?	-	CYS	deletion	UNP O35433
C	?	-	LYS	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	GLY	deletion	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433

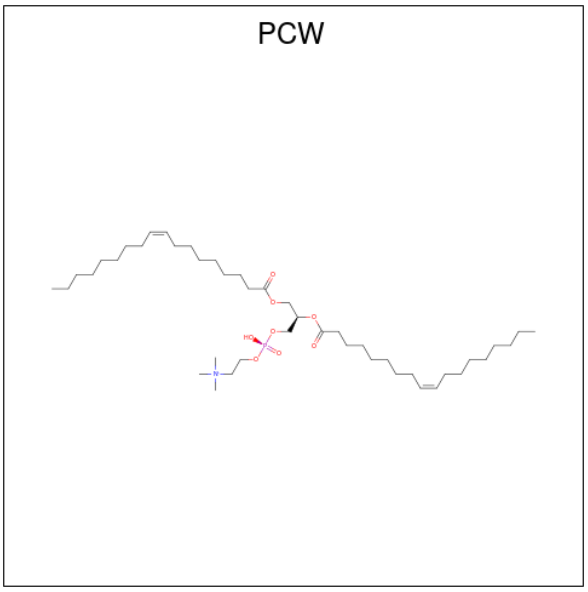
- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5

-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: $C_{25}H_{49}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



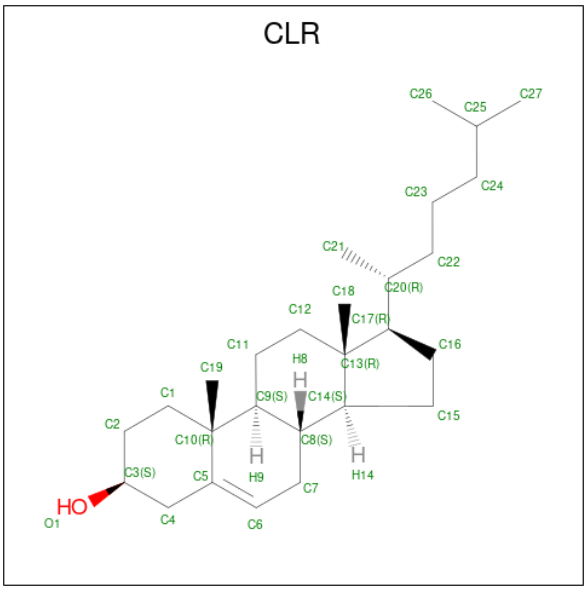
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	O	P	0
			91	25	44	19	3	
2	D	1	Total	C	H	O	P	0
			91	25	44	19	3	
2	B	1	Total	C	H	O	P	0
			91	25	44	19	3	
2	C	1	Total	C	H	O	P	0
			91	25	44	19	3	

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			74	27	46	1	
4	D	1	Total	C	H	O	0
			74	27	46	1	
4	B	1	Total	C	H	O	0
			74	27	46	1	
4	C	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

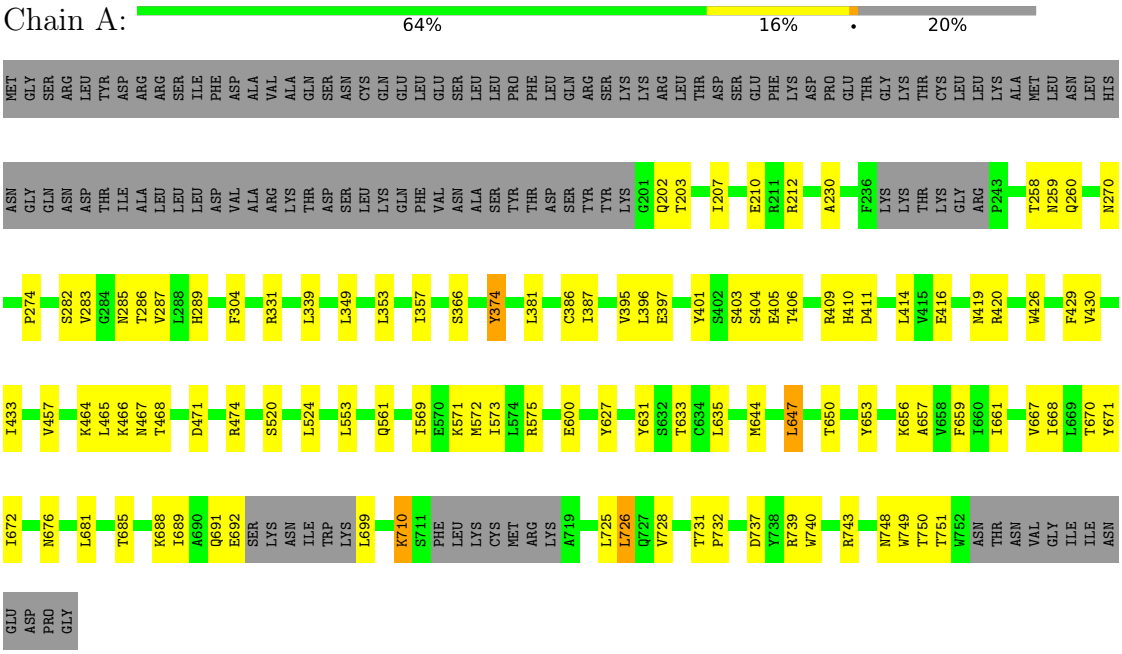
Mol	Chain	Residues	Atoms			AltConf
6	A	6	Total	H	O	0
			18	12	6	
6	D	6	Total	H	O	0
			18	12	6	
6	B	7	Total	H	O	0
			21	14	7	
6	C	5	Total	H	O	0
			15	10	5	

3 Residue-property plots (i)

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

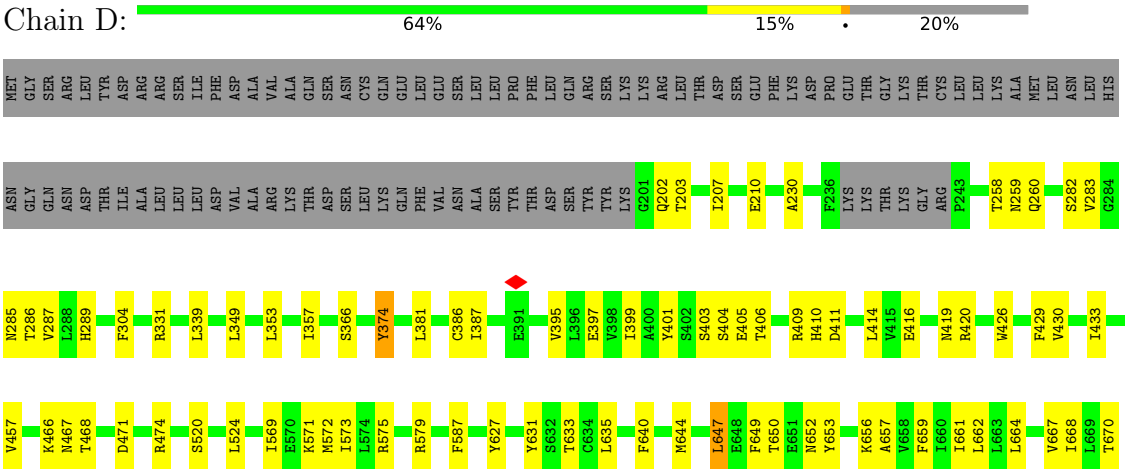
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

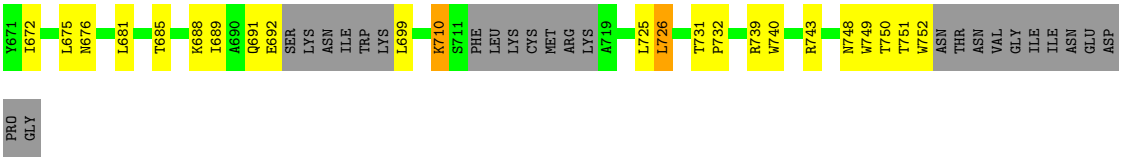
Chain A:



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

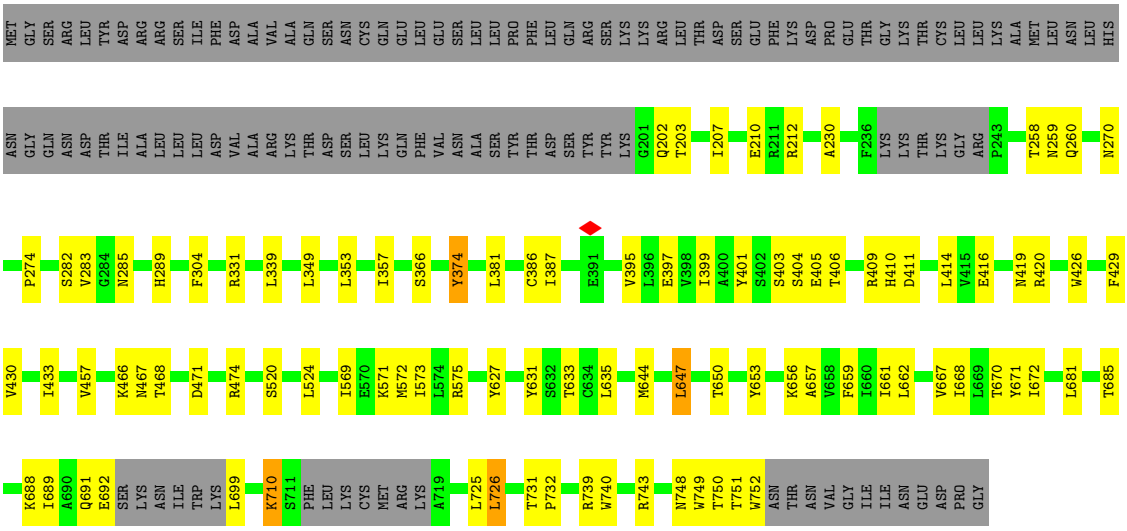
Chain D:





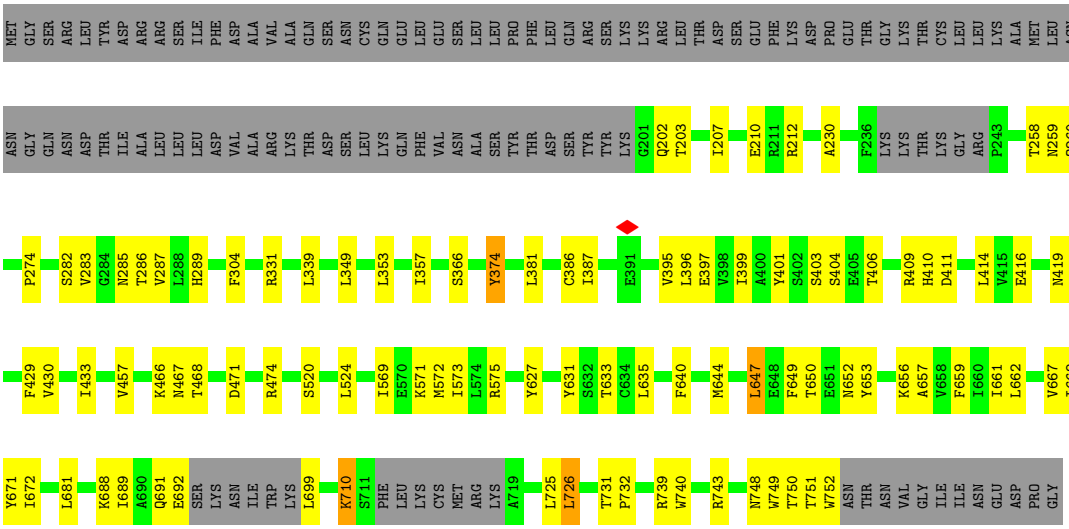
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain B:



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

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	26265	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 ($e^-/Å^2$)	45.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	320.63998, 320.63998, 320.63998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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: PCW, CLR, NA, PIO

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	0.30	0/4223	0.55	5/5722 (0.1%)
1	B	0.30	0/4223	0.55	5/5722 (0.1%)
1	C	0.30	0/4223	0.55	5/5722 (0.1%)
1	D	0.30	0/4223	0.55	5/5722 (0.1%)
All	All	0.30	0/16892	0.55	20/22888 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	647	LEU	CB-CG-CD2	6.93	122.78	111.00
1	C	647	LEU	CB-CG-CD2	6.92	122.77	111.00
1	A	647	LEU	CB-CG-CD2	6.91	122.75	111.00
1	B	647	LEU	CB-CG-CD2	6.91	122.75	111.00
1	C	644	MET	CB-CG-SD	6.26	131.19	112.40
1	A	644	MET	CB-CG-SD	6.26	131.18	112.40
1	D	644	MET	CB-CG-SD	6.26	131.17	112.40
1	B	644	MET	CB-CG-SD	6.25	131.16	112.40
1	A	726	LEU	CB-CG-CD1	5.67	120.63	111.00
1	C	726	LEU	CB-CG-CD1	5.66	120.62	111.00
1	B	726	LEU	CB-CG-CD1	5.66	120.62	111.00
1	D	726	LEU	CB-CG-CD1	5.64	120.60	111.00
1	B	726	LEU	CB-CG-CD2	5.52	120.38	111.00
1	D	726	LEU	CB-CG-CD2	5.52	120.38	111.00
1	A	726	LEU	CB-CG-CD2	5.49	120.33	111.00
1	C	726	LEU	CB-CG-CD2	5.47	120.31	111.00
1	A	230	ALA	CB-CA-C	5.04	117.67	110.10
1	C	230	ALA	CB-CA-C	5.04	117.66	110.10
1	B	230	ALA	CB-CA-C	5.04	117.65	110.10
1	D	230	ALA	CB-CA-C	5.02	117.63	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4126	4143	4139	77	0
1	B	4126	4143	4139	74	0
1	C	4126	4143	4139	70	0
1	D	4126	4143	4139	70	0
2	A	47	44	44	1	0
2	B	47	44	44	1	0
2	C	47	44	44	1	0
2	D	47	44	44	1	0
3	A	54	84	84	3	0
3	B	108	168	168	4	0
3	C	54	84	84	2	0
4	A	28	46	46	6	0
4	B	28	46	46	9	0
4	C	28	46	46	7	0
4	D	28	46	46	3	0
5	A	1	0	0	0	0
6	A	6	12	0	0	0
6	B	7	14	0	0	0
6	C	5	10	0	0	0
6	D	6	12	0	0	0
All	All	17045	17316	17252	280	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 8.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ILE:HD11	4:B:804:CLR:H211	1.62	0.80
1:C:672:ILE:HD11	4:C:802:CLR:H211	1.64	0.78
1:A:650:THR:O	1:A:656:LYS:NZ	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:THR:O	1:B:656:LYS:NZ	2.18	0.76
1:A:676:ASN:ND2	1:B:569:ILE:HD13	2.00	0.76
1:B:282:SER:O	1:B:331:ARG:NH1	2.18	0.76
1:A:282:SER:O	1:A:331:ARG:NH1	2.18	0.76
1:D:650:THR:O	1:D:656:LYS:NZ	2.18	0.76
1:C:282:SER:O	1:C:331:ARG:NH1	2.18	0.76
1:D:282:SER:O	1:D:331:ARG:NH1	2.18	0.76
1:C:650:THR:O	1:C:656:LYS:NZ	2.18	0.76
1:B:258:THR:OG1	1:B:260:GLN:NE2	2.20	0.74
1:A:258:THR:OG1	1:A:260:GLN:NE2	2.20	0.74
1:A:671:TYR:CE2	4:A:803:CLR:H11	2.22	0.74
1:C:258:THR:OG1	1:C:260:GLN:NE2	2.20	0.74
1:D:258:THR:OG1	1:D:260:GLN:NE2	2.20	0.74
1:A:672:ILE:HD11	4:A:803:CLR:H211	1.69	0.73
1:B:671:TYR:CE2	4:B:804:CLR:H11	2.25	0.71
1:C:671:TYR:CE2	4:C:802:CLR:H11	2.27	0.69
1:A:403:SER:O	1:A:409:ARG:NH2	2.28	0.67
1:C:403:SER:O	1:C:409:ARG:NH2	2.28	0.67
1:B:403:SER:O	1:B:409:ARG:NH2	2.28	0.67
1:D:403:SER:O	1:D:409:ARG:NH2	2.28	0.67
1:C:457:VAL:HG12	1:C:457:VAL:O	1.97	0.65
1:D:457:VAL:HG12	1:D:457:VAL:O	1.97	0.65
1:A:457:VAL:HG12	1:A:457:VAL:O	1.97	0.65
1:B:457:VAL:HG12	1:B:457:VAL:O	1.97	0.64
1:A:668:ILE:HD12	2:B:801:PIO:H5AA	1.81	0.62
1:A:676:ASN:HD21	1:B:569:ILE:HD13	1.66	0.61
1:B:671:TYR:CG	4:B:804:CLR:H111	2.37	0.60
1:C:466:LYS:N	1:C:471:ASP:OD2	2.35	0.59
1:C:671:TYR:CG	4:C:802:CLR:H111	2.38	0.59
1:A:671:TYR:CE1	4:A:803:CLR:H193	2.38	0.59
1:A:671:TYR:CG	4:A:803:CLR:H111	2.38	0.58
1:B:466:LYS:N	1:B:471:ASP:OD2	2.35	0.58
1:D:357:ILE:N	1:D:366:SER:OG	2.36	0.58
1:A:212:ARG:HH22	1:B:752:TRP:HB3	1.67	0.58
1:B:419:ASN:OD1	1:B:420:ARG:N	2.37	0.58
1:C:357:ILE:N	1:C:366:SER:OG	2.36	0.58
1:A:289:HIS:NE2	1:A:339:LEU:HD13	2.19	0.57
1:D:419:ASN:OD1	1:D:420:ARG:N	2.37	0.57
1:C:419:ASN:OD1	1:C:420:ARG:N	2.37	0.57
1:A:466:LYS:N	1:A:471:ASP:OD2	2.35	0.57
1:A:357:ILE:N	1:A:366:SER:OG	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:OD1	1:A:420:ARG:N	2.37	0.57
1:D:466:LYS:N	1:D:471:ASP:OD2	2.35	0.57
1:B:289:HIS:NE2	1:B:339:LEU:HD13	2.19	0.57
1:C:289:HIS:NE2	1:C:339:LEU:HD13	2.19	0.57
1:D:289:HIS:NE2	1:D:339:LEU:HD13	2.19	0.57
1:B:357:ILE:N	1:B:366:SER:OG	2.36	0.56
1:D:647:LEU:HD23	1:D:647:LEU:O	2.07	0.55
1:A:647:LEU:HD23	1:A:647:LEU:O	2.07	0.55
1:B:647:LEU:HD23	1:B:647:LEU:O	2.06	0.55
1:C:647:LEU:HD23	1:C:647:LEU:O	2.07	0.55
1:A:212:ARG:NH2	1:B:752:TRP:CE3	2.75	0.55
1:C:285:ASN:HA	1:C:289:HIS:HD1	1.72	0.55
1:B:285:ASN:HA	1:B:289:HIS:HD1	1.72	0.55
1:B:725:LEU:HD11	1:B:740:TRP:CZ2	2.42	0.55
1:D:725:LEU:HD11	1:D:740:TRP:CZ2	2.42	0.54
1:B:366:SER:O	1:B:739:ARG:NH1	2.40	0.54
1:A:366:SER:O	1:A:739:ARG:NH1	2.40	0.54
1:C:366:SER:O	1:C:739:ARG:NH1	2.40	0.54
1:C:725:LEU:HD11	1:C:740:TRP:CZ2	2.42	0.54
1:A:285:ASN:HA	1:A:289:HIS:HD1	1.72	0.54
1:D:285:ASN:HA	1:D:289:HIS:HD1	1.72	0.54
1:D:366:SER:O	1:D:739:ARG:NH1	2.40	0.54
1:B:671:TYR:CZ	4:B:804:CLR:H193	2.43	0.54
1:A:467:ASN:O	1:A:468:THR:OG1	2.25	0.54
1:A:725:LEU:HD11	1:A:740:TRP:CZ2	2.43	0.53
1:D:381:LEU:HD11	1:D:743:ARG:HD3	1.91	0.53
1:A:381:LEU:HD11	1:A:743:ARG:HD3	1.91	0.53
4:C:802:CLR:H121	4:C:802:CLR:H212	1.91	0.53
4:A:803:CLR:H121	4:A:803:CLR:H212	1.91	0.52
1:A:553:LEU:HD11	1:D:587:PHE:HZ	1.74	0.52
4:D:801:CLR:H121	4:D:801:CLR:H212	1.91	0.52
1:C:381:LEU:HD11	1:C:743:ARG:HD3	1.91	0.52
4:B:804:CLR:H121	4:B:804:CLR:H212	1.91	0.51
2:A:801:PIO:H3B	1:D:662:LEU:HD23	1.92	0.51
1:B:381:LEU:HD11	1:B:743:ARG:HD3	1.91	0.51
1:B:668:ILE:HG23	4:B:804:CLR:C21	2.40	0.51
1:A:349:LEU:O	1:A:353:LEU:HD23	2.11	0.51
1:C:349:LEU:O	1:C:353:LEU:HD23	2.11	0.50
1:D:672:ILE:HD11	4:D:801:CLR:H211	1.91	0.50
1:B:467:ASN:O	1:B:468:THR:OG1	2.25	0.50
1:D:349:LEU:O	1:D:353:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:VAL:O	1:B:457:VAL:CG1	2.60	0.50
1:C:671:TYR:CZ	4:C:802:CLR:H193	2.45	0.50
1:D:467:ASN:O	1:D:468:THR:OG1	2.25	0.50
1:D:429:PHE:O	1:D:433:ILE:HG12	2.12	0.50
1:B:401:TYR:OH	1:B:710:LYS:NZ	2.39	0.50
1:B:429:PHE:O	1:B:433:ILE:HG12	2.12	0.50
1:C:429:PHE:O	1:C:433:ILE:HG12	2.12	0.50
1:B:349:LEU:O	1:B:353:LEU:HD23	2.11	0.49
1:B:671:TYR:CE1	4:B:804:CLR:H193	2.47	0.49
1:C:671:TYR:CE1	4:C:802:CLR:H193	2.47	0.49
1:D:401:TYR:OH	1:D:710:LYS:NZ	2.39	0.49
1:C:457:VAL:O	1:C:457:VAL:CG1	2.60	0.49
1:D:401:TYR:CE1	1:D:710:LYS:NZ	2.81	0.49
1:A:387:ILE:HA	1:A:395:VAL:HG12	1.94	0.49
1:B:387:ILE:HA	1:B:395:VAL:HG12	1.94	0.49
1:C:401:TYR:CE1	1:C:710:LYS:NZ	2.81	0.49
1:D:387:ILE:HA	1:D:395:VAL:HG12	1.94	0.49
1:D:457:VAL:O	1:D:457:VAL:CG1	2.59	0.49
1:C:387:ILE:HA	1:C:395:VAL:HG12	1.94	0.49
1:A:429:PHE:O	1:A:433:ILE:HG12	2.12	0.48
1:A:457:VAL:O	1:A:457:VAL:CG1	2.60	0.48
1:D:653:TYR:OH	1:D:659:PHE:CD2	2.66	0.48
2:D:802:PIO:H3B	1:C:662:LEU:HD23	1.96	0.48
1:A:731:THR:HB	1:A:732:PRO:HD2	1.95	0.48
1:B:662:LEU:HD23	2:C:803:PIO:H3B	1.94	0.48
1:D:283:VAL:HG12	1:D:283:VAL:O	2.13	0.48
1:A:401:TYR:CE1	1:A:710:LYS:NZ	2.81	0.48
1:A:653:TYR:OH	1:A:659:PHE:CD2	2.66	0.48
1:B:212:ARG:NH2	1:C:752:TRP:CE3	2.81	0.48
1:B:401:TYR:CE1	1:B:710:LYS:NZ	2.81	0.48
1:B:731:THR:HB	1:B:732:PRO:HD2	1.96	0.48
1:C:283:VAL:O	1:C:283:VAL:HG12	2.13	0.48
1:A:283:VAL:HG12	1:A:283:VAL:O	2.13	0.48
1:B:569:ILE:O	1:B:573:ILE:HG22	2.14	0.48
3:A:802:PCW:H182	1:D:664:LEU:HD23	1.95	0.47
1:B:283:VAL:HG12	1:B:283:VAL:O	2.13	0.47
1:B:667:VAL:CG1	4:B:804:CLR:H12	2.44	0.47
1:D:731:THR:HB	1:D:732:PRO:HD2	1.95	0.47
1:C:569:ILE:O	1:C:573:ILE:HG22	2.14	0.47
1:D:752:TRP:CE3	1:C:212:ARG:NH2	2.83	0.47
1:A:569:ILE:O	1:A:573:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:THR:O	1:A:751:THR:OG1	2.32	0.47
1:B:653:TYR:OH	1:B:659:PHE:CD2	2.66	0.47
1:C:731:THR:HB	1:C:732:PRO:HD2	1.95	0.47
1:A:471:ASP:OD1	1:A:474:ARG:NH2	2.48	0.47
1:D:569:ILE:O	1:D:573:ILE:HG22	2.14	0.47
1:C:471:ASP:OD1	1:C:474:ARG:NH2	2.48	0.47
1:B:409:ARG:HB2	1:B:409:ARG:CZ	2.46	0.46
1:A:401:TYR:OH	1:A:710:LYS:NZ	2.39	0.46
1:D:409:ARG:CZ	1:D:409:ARG:HB2	2.46	0.46
1:B:471:ASP:OD1	1:B:474:ARG:NH2	2.48	0.46
1:A:572:MET:CE	1:D:675:LEU:HD23	2.46	0.46
1:D:471:ASP:OD1	1:D:474:ARG:NH2	2.48	0.46
1:B:203:THR:O	1:B:207:ILE:HD12	2.16	0.45
1:A:635:LEU:HD12	3:A:802:PCW:H342	1.99	0.45
1:C:409:ARG:HB2	1:C:409:ARG:CZ	2.45	0.45
1:A:409:ARG:HB2	1:A:409:ARG:CZ	2.46	0.45
1:C:203:THR:O	1:C:207:ILE:HD12	2.16	0.45
1:D:203:THR:O	1:D:207:ILE:HD12	2.17	0.45
1:D:635:LEU:HD12	3:C:801:PCW:H342	1.98	0.45
1:B:212:ARG:HH22	1:C:752:TRP:HB3	1.81	0.45
1:C:572:MET:HG3	1:C:681:LEU:HD11	1.98	0.45
1:C:650:THR:O	1:C:650:THR:OG1	2.31	0.45
1:D:406:THR:OG1	1:D:409:ARG:NH2	2.50	0.45
1:C:571:LYS:O	1:C:575:ARG:HB3	2.17	0.45
1:C:653:TYR:OH	1:C:659:PHE:CD2	2.66	0.45
1:D:403:SER:HG	1:D:405:GLU:CD	2.20	0.45
1:A:571:LYS:O	1:A:575:ARG:HB3	2.17	0.45
1:A:689:ILE:HG22	1:A:689:ILE:O	2.17	0.45
1:D:750:THR:O	1:D:751:THR:OG1	2.32	0.45
1:B:571:LYS:O	1:B:575:ARG:HB3	2.17	0.45
3:B:803:PCW:H342	1:C:635:LEU:HD12	1.99	0.45
1:C:689:ILE:O	1:C:689:ILE:HG22	2.17	0.45
1:A:572:MET:HG3	1:A:681:LEU:HD11	1.98	0.45
1:B:397:GLU:HG3	1:B:401:TYR:CE2	2.52	0.44
1:C:397:GLU:HG3	1:C:401:TYR:CE2	2.53	0.44
1:A:203:THR:O	1:A:207:ILE:HD12	2.16	0.44
1:A:406:THR:OG1	1:A:409:ARG:NH2	2.50	0.44
1:B:572:MET:HG3	1:B:681:LEU:HD11	1.98	0.44
1:B:635:LEU:HD12	3:B:802:PCW:H342	1.99	0.44
1:B:689:ILE:HG22	1:B:689:ILE:O	2.17	0.44
1:C:406:THR:OG1	1:C:409:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:GLU:HG3	1:D:401:TYR:CE2	2.53	0.44
1:C:401:TYR:OH	1:C:710:LYS:NZ	2.39	0.44
1:C:467:ASN:O	1:C:468:THR:OG1	2.25	0.44
1:D:572:MET:HG3	1:D:681:LEU:HD11	1.99	0.44
1:D:689:ILE:HG22	1:D:689:ILE:O	2.17	0.44
1:B:571:LYS:HD2	1:B:688:LYS:HD3	1.99	0.44
1:C:571:LYS:HD2	1:C:688:LYS:HD3	1.99	0.44
1:B:657:ALA:O	1:B:661:ILE:HD12	2.18	0.44
1:B:671:TYR:CE2	4:B:804:CLR:H193	2.53	0.44
1:A:561:GLN:O	1:D:579:ARG:NE	2.51	0.44
1:D:571:LYS:O	1:D:575:ARG:HB3	2.17	0.44
1:D:752:TRP:HB3	1:C:212:ARG:HH22	1.81	0.44
1:D:426:TRP:HA	1:D:430:VAL:HB	2.00	0.44
1:C:668:ILE:HG23	4:C:802:CLR:C21	2.47	0.44
1:B:406:THR:OG1	1:B:409:ARG:NH2	2.50	0.43
1:C:426:TRP:HA	1:C:430:VAL:HB	2.00	0.43
1:A:600:GLU:OE2	1:B:457:VAL:HG11	2.18	0.43
1:D:404:SER:HA	1:D:409:ARG:NH2	2.33	0.43
1:D:650:THR:O	1:D:650:THR:OG1	2.31	0.43
1:A:397:GLU:HG3	1:A:401:TYR:CE2	2.52	0.43
1:A:571:LYS:HD2	1:A:688:LYS:HD3	1.99	0.43
1:A:404:SER:HA	1:A:409:ARG:NH2	2.33	0.43
1:D:571:LYS:HD2	1:D:688:LYS:HD3	1.99	0.43
1:C:657:ALA:O	1:C:661:ILE:HD12	2.18	0.43
1:A:426:TRP:HA	1:A:430:VAL:HB	2.00	0.43
1:A:569:ILE:HD13	1:D:676:ASN:ND2	2.34	0.43
1:A:657:ALA:O	1:A:661:ILE:HD12	2.18	0.43
1:A:676:ASN:ND2	1:B:569:ILE:CD1	2.79	0.43
1:D:657:ALA:O	1:D:661:ILE:HD12	2.18	0.43
1:B:426:TRP:HA	1:B:430:VAL:HB	2.00	0.43
1:B:635:LEU:HD12	3:B:802:PCW:C34	2.49	0.43
1:A:635:LEU:HD12	3:A:802:PCW:C34	2.49	0.43
1:A:650:THR:O	1:A:650:THR:OG1	2.31	0.42
1:B:411:ASP:HA	1:B:414:LEU:CD1	2.49	0.42
1:B:404:SER:HA	1:B:409:ARG:NH2	2.33	0.42
1:C:750:THR:O	1:C:751:THR:OG1	2.32	0.42
1:B:416:GLU:OE2	1:B:416:GLU:HA	2.20	0.42
1:C:404:SER:HA	1:C:409:ARG:NH2	2.33	0.42
1:C:416:GLU:OE2	1:C:416:GLU:HA	2.20	0.42
1:A:627:TYR:HB3	1:A:633:THR:HG22	2.02	0.42
1:D:411:ASP:HA	1:D:414:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:SER:O	1:D:524:LEU:HD23	2.20	0.42
1:D:635:LEU:HD12	3:C:801:PCW:C34	2.49	0.42
3:B:803:PCW:C34	1:C:635:LEU:HD12	2.49	0.42
1:C:411:ASP:HA	1:C:414:LEU:CD1	2.49	0.42
1:A:411:ASP:HA	1:A:414:LEU:CD1	2.49	0.42
1:D:202:GLN:NE2	1:D:210:GLU:OE2	2.53	0.42
1:D:416:GLU:OE2	1:D:416:GLU:HA	2.20	0.42
1:B:374:TYR:C	1:B:374:TYR:CD1	2.93	0.42
1:A:553:LEU:HD11	1:D:587:PHE:CZ	2.53	0.42
1:D:374:TYR:CD1	1:D:374:TYR:C	2.94	0.42
1:D:410:HIS:O	1:D:414:LEU:HD12	2.20	0.42
1:C:410:HIS:O	1:C:414:LEU:HD12	2.20	0.42
1:D:748:ASN:OD1	1:D:749:TRP:N	2.53	0.41
1:B:259:ASN:HA	1:B:304:PHE:CZ	2.55	0.41
1:A:374:TYR:CD1	1:A:374:TYR:C	2.93	0.41
1:B:202:GLN:NE2	1:B:210:GLU:OE2	2.53	0.41
1:B:410:HIS:O	1:B:414:LEU:HD12	2.20	0.41
1:B:650:THR:O	1:B:650:THR:OG1	2.31	0.41
1:A:381:LEU:HD21	1:A:726:LEU:HD22	2.03	0.41
1:A:416:GLU:HA	1:A:416:GLU:OE2	2.20	0.41
1:A:520:SER:O	1:A:524:LEU:HD23	2.20	0.41
1:B:627:TYR:HB3	1:B:633:THR:HG22	2.02	0.41
1:C:520:SER:O	1:C:524:LEU:HD23	2.20	0.41
1:A:202:GLN:NE2	1:A:210:GLU:OE2	2.53	0.41
1:D:627:TYR:HB3	1:D:633:THR:HG22	2.02	0.41
1:B:381:LEU:HD21	1:B:726:LEU:HD22	2.03	0.41
1:B:520:SER:O	1:B:524:LEU:HD23	2.20	0.41
1:C:374:TYR:CD1	1:C:374:TYR:C	2.93	0.41
1:C:667:VAL:O	1:C:670:THR:HG22	2.21	0.41
1:A:410:HIS:O	1:A:414:LEU:HD12	2.20	0.41
1:A:748:ASN:OD1	1:A:749:TRP:N	2.53	0.41
1:B:667:VAL:O	1:B:670:THR:HG22	2.21	0.41
1:C:386:CYS:O	1:C:386:CYS:SG	2.79	0.41
1:D:259:ASN:HA	1:D:304:PHE:CZ	2.55	0.41
1:D:667:VAL:O	1:D:670:THR:HG22	2.21	0.41
1:A:259:ASN:HA	1:A:304:PHE:CZ	2.55	0.41
1:C:259:ASN:HA	1:C:304:PHE:CZ	2.55	0.41
1:A:270:ASN:OD1	1:A:274:PRO:HA	2.21	0.41
1:A:386:CYS:SG	1:A:386:CYS:O	2.79	0.41
1:C:202:GLN:NE2	1:C:210:GLU:OE2	2.53	0.41
1:C:286:THR:HG22	1:C:287:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ILE:O	1:C:409:ARG:HD3	2.21	0.41
1:A:464:LYS:HD3	1:A:465:LEU:O	2.21	0.41
1:A:671:TYR:CD1	4:A:803:CLR:H193	2.56	0.41
1:A:685:THR:O	1:A:689:ILE:HG13	2.21	0.41
1:D:381:LEU:HD21	1:D:726:LEU:HD22	2.03	0.41
1:D:386:CYS:SG	1:D:386:CYS:O	2.79	0.41
1:D:668:ILE:HG23	4:D:801:CLR:C21	2.51	0.41
1:B:386:CYS:O	1:B:386:CYS:SG	2.79	0.41
1:C:748:ASN:OD1	1:C:749:TRP:N	2.53	0.41
1:D:286:THR:HG22	1:D:287:VAL:N	2.36	0.41
1:D:652:ASN:OD1	1:D:652:ASN:O	2.40	0.41
1:B:270:ASN:OD1	1:B:274:PRO:HA	2.21	0.41
1:A:395:VAL:HG13	1:A:396:LEU:N	2.36	0.40
1:D:685:THR:O	1:D:689:ILE:HG13	2.21	0.40
1:C:627:TYR:HB3	1:C:633:THR:HG22	2.02	0.40
1:A:286:THR:HG22	1:A:287:VAL:N	2.36	0.40
1:B:685:THR:O	1:B:689:ILE:HG13	2.21	0.40
1:C:640:PHE:HE1	1:C:649:PHE:CE1	2.40	0.40
1:D:399:ILE:O	1:D:409:ARG:HD3	2.21	0.40
1:B:399:ILE:O	1:B:409:ARG:HD3	2.21	0.40
1:B:748:ASN:OD1	1:B:749:TRP:N	2.53	0.40
1:B:750:THR:O	1:B:751:THR:OG1	2.32	0.40
1:C:270:ASN:OD1	1:C:274:PRO:HA	2.21	0.40
1:C:381:LEU:HD21	1:C:726:LEU:HD22	2.03	0.40
1:C:395:VAL:HG13	1:C:396:LEU:N	2.36	0.40
1:A:667:VAL:O	1:A:670:THR:HG22	2.21	0.40
1:A:728:VAL:HG23	1:A:737:ASP:OD2	2.21	0.40
1:D:640:PHE:HE1	1:D:649:PHE:CE1	2.39	0.40
1:B:403:SER:HG	1:B:405:GLU:CD	2.24	0.40
1:A:403:SER:HG	1:A:405:GLU:CD	2.25	0.40
1:C:652:ASN:OD1	1:C:652:ASN:O	2.40	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	502/635 (79%)	461 (92%)	41 (8%)	0	100	100
1	B	502/635 (79%)	461 (92%)	41 (8%)	0	100	100
1	C	502/635 (79%)	461 (92%)	41 (8%)	0	100	100
1	D	502/635 (79%)	461 (92%)	41 (8%)	0	100	100
All	All	2008/2540 (79%)	1844 (92%)	164 (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	449/562 (80%)	443 (99%)	6 (1%)	69	86
1	B	449/562 (80%)	443 (99%)	6 (1%)	69	86
1	C	449/562 (80%)	443 (99%)	6 (1%)	69	86
1	D	449/562 (80%)	443 (99%)	6 (1%)	69	86
All	All	1796/2248 (80%)	1772 (99%)	24 (1%)	70	86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	TYR
1	A	631	TYR
1	A	691	GLN
1	A	692	GLU
1	A	699	LEU
1	A	710	LYS
1	D	374	TYR
1	D	631	TYR
1	D	691	GLN
1	D	692	GLU

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Mol	Chain	Res	Type
1	D	699	LEU
1	D	710	LYS
1	B	374	TYR
1	B	631	TYR
1	B	691	GLN
1	B	692	GLU
1	B	699	LEU
1	B	710	LYS
1	C	374	TYR
1	C	631	TYR
1	C	691	GLN
1	C	692	GLU
1	C	699	LEU
1	C	710	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	HIS
1	A	260	GLN
1	D	206	HIS
1	D	260	GLN
1	B	206	HIS
1	B	260	GLN
1	C	206	HIS
1	C	260	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PCW	A	802	-	53,53,53	1.24	8 (15%)	59,61,61	0.90	3 (5%)
2	PIO	C	803	-	47,47,47	1.37	10 (21%)	61,65,65	1.17	3 (4%)
2	PIO	B	801	-	47,47,47	1.37	10 (21%)	61,65,65	1.18	3 (4%)
3	PCW	B	803	-	53,53,53	1.24	8 (15%)	59,61,61	0.90	3 (5%)
4	CLR	B	804	-	31,31,31	3.92	16 (51%)	48,48,48	2.70	19 (39%)
2	PIO	D	802	-	47,47,47	1.37	10 (21%)	61,65,65	1.18	3 (4%)
4	CLR	C	802	-	31,31,31	3.92	16 (51%)	48,48,48	2.71	19 (39%)
4	CLR	A	803	-	31,31,31	3.91	16 (51%)	48,48,48	2.70	19 (39%)
3	PCW	B	802	-	53,53,53	1.25	8 (15%)	59,61,61	0.90	3 (5%)
2	PIO	A	801	-	47,47,47	1.37	10 (21%)	61,65,65	1.17	3 (4%)
4	CLR	D	801	-	31,31,31	3.92	16 (51%)	48,48,48	2.70	19 (39%)
3	PCW	C	801	-	53,53,53	1.24	8 (15%)	59,61,61	0.90	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	802	-	-	30/57/57/57	-
2	PIO	C	803	-	-	20/44/68/68	0/1/1/1
2	PIO	B	801	-	-	20/44/68/68	0/1/1/1
3	PCW	B	803	-	-	30/57/57/57	-
4	CLR	B	804	-	-	5/10/68/68	0/4/4/4
2	PIO	D	802	-	-	20/44/68/68	0/1/1/1
4	CLR	C	802	-	-	5/10/68/68	0/4/4/4
4	CLR	A	803	-	-	5/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	B	802	-	-	30/57/57/57	-
2	PIO	A	801	-	-	20/44/68/68	0/1/1/1
4	CLR	D	801	-	-	5/10/68/68	0/4/4/4
3	PCW	C	801	-	-	30/57/57/57	-

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	801	CLR	C11-C9	10.62	1.71	1.53
4	A	803	CLR	C11-C9	10.60	1.71	1.53
4	B	804	CLR	C11-C9	10.58	1.71	1.53
4	C	802	CLR	C11-C9	10.58	1.71	1.53
4	A	803	CLR	C12-C13	-9.13	1.37	1.54
4	C	802	CLR	C12-C13	-9.13	1.37	1.54
4	D	801	CLR	C12-C13	-9.13	1.37	1.54
4	B	804	CLR	C12-C13	-9.12	1.37	1.54
4	B	804	CLR	C12-C11	7.70	1.69	1.53
4	C	802	CLR	C12-C11	7.70	1.69	1.53
4	D	801	CLR	C12-C11	7.67	1.69	1.53
4	A	803	CLR	C12-C11	7.67	1.69	1.53
4	C	802	CLR	C8-C14	-5.86	1.42	1.53
4	D	801	CLR	C8-C14	-5.85	1.42	1.53
4	B	804	CLR	C8-C14	-5.83	1.42	1.53
4	A	803	CLR	C8-C14	-5.81	1.42	1.53
4	B	804	CLR	C6-C5	-5.53	1.20	1.33
4	D	801	CLR	C6-C5	-5.51	1.20	1.33
4	A	803	CLR	C6-C5	-5.49	1.20	1.33
4	C	802	CLR	C6-C5	-5.49	1.20	1.33
4	B	804	CLR	C10-C9	-5.21	1.47	1.56
4	C	802	CLR	C10-C9	-5.21	1.47	1.56
4	D	801	CLR	C10-C9	-5.20	1.47	1.56
4	A	803	CLR	C10-C9	-5.19	1.47	1.56
4	C	802	CLR	C16-C15	5.01	1.67	1.54
4	A	803	CLR	C16-C15	4.99	1.67	1.54
4	B	804	CLR	C16-C15	4.99	1.67	1.54
4	D	801	CLR	C16-C15	4.98	1.67	1.54
4	C	802	CLR	C2-C3	4.76	1.63	1.51
4	A	803	CLR	C2-C3	4.74	1.63	1.51
4	D	801	CLR	C2-C3	4.73	1.63	1.51
4	B	804	CLR	C2-C3	4.72	1.62	1.51
4	D	801	CLR	C1-C2	4.57	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	804	CLR	C1-C2	4.54	1.63	1.53
4	C	802	CLR	C1-C2	4.54	1.63	1.53
4	A	803	CLR	C1-C2	4.54	1.63	1.53
3	B	802	PCW	O2-C31	3.92	1.45	1.34
3	B	803	PCW	O2-C31	3.90	1.45	1.34
3	C	801	PCW	O2-C31	3.90	1.45	1.34
3	A	802	PCW	O2-C31	3.89	1.45	1.34
2	B	801	PIO	P5-O5	3.17	1.65	1.59
2	D	802	PIO	P4-O4	3.17	1.65	1.59
2	D	802	PIO	P5-O5	3.16	1.65	1.59
2	C	803	PIO	P5-O5	3.16	1.65	1.59
2	A	801	PIO	P5-O5	3.16	1.65	1.59
2	A	801	PIO	P4-O4	3.15	1.65	1.59
2	C	803	PIO	P4-O4	3.15	1.65	1.59
2	B	801	PIO	P4-O4	3.14	1.65	1.59
3	B	802	PCW	O3-C11	2.97	1.42	1.33
3	B	803	PCW	O3-C11	2.95	1.41	1.33
3	C	801	PCW	O3-C11	2.95	1.41	1.33
3	A	802	PCW	O3-C11	2.94	1.41	1.33
4	C	802	CLR	C7-C8	2.76	1.57	1.53
4	A	803	CLR	C7-C8	2.74	1.57	1.53
4	D	801	CLR	C7-C8	2.72	1.57	1.53
4	B	804	CLR	C7-C8	2.72	1.57	1.53
4	C	802	CLR	C7-C6	-2.66	1.44	1.50
4	B	804	CLR	C7-C6	-2.62	1.44	1.50
4	A	803	CLR	C7-C6	-2.61	1.44	1.50
4	C	802	CLR	C13-C17	2.59	1.59	1.55
4	D	801	CLR	C13-C17	2.58	1.59	1.55
4	D	801	CLR	C7-C6	-2.58	1.44	1.50
4	A	803	CLR	C13-C17	2.57	1.59	1.55
4	B	804	CLR	C13-C17	2.55	1.59	1.55
2	B	801	PIO	O2C-C2C	-2.52	1.40	1.46
2	D	802	PIO	O2C-C2C	-2.51	1.40	1.46
2	A	801	PIO	O2C-C2C	-2.50	1.40	1.46
2	C	803	PIO	O2C-C2C	-2.48	1.40	1.46
2	B	801	PIO	O3C-C1B	2.39	1.40	1.33
4	D	801	CLR	C13-C14	-2.39	1.50	1.55
2	C	803	PIO	O3C-C1B	2.39	1.40	1.33
2	A	801	PIO	O3C-C1B	2.39	1.40	1.33
4	A	803	CLR	C13-C14	-2.37	1.50	1.55
2	D	802	PIO	O3C-C1B	2.37	1.40	1.33
4	B	804	CLR	C13-C14	-2.36	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	802	CLR	C13-C14	-2.35	1.50	1.55
4	C	802	CLR	C8-C9	2.24	1.57	1.53
4	B	804	CLR	C8-C9	2.22	1.57	1.53
4	D	801	CLR	C8-C9	2.21	1.57	1.53
3	A	802	PCW	C32-C31	2.21	1.57	1.50
3	C	801	PCW	C32-C31	2.20	1.57	1.50
3	B	803	PCW	C32-C31	2.20	1.57	1.50
3	B	802	PCW	C32-C31	2.20	1.57	1.50
2	C	803	PIO	P5-O51	-2.19	1.46	1.54
2	B	801	PIO	P5-O51	-2.19	1.46	1.54
2	A	801	PIO	P5-O51	-2.19	1.46	1.54
2	B	801	PIO	P4-O43	-2.18	1.46	1.54
2	D	802	PIO	P5-O51	-2.18	1.46	1.54
2	A	801	PIO	P4-O43	-2.18	1.46	1.54
3	C	801	PCW	P-O3P	2.18	1.68	1.59
2	D	802	PIO	P4-O43	-2.17	1.46	1.54
2	C	803	PIO	P4-O43	-2.17	1.46	1.54
4	A	803	CLR	C8-C9	2.17	1.57	1.53
3	A	802	PCW	P-O3P	2.17	1.68	1.59
2	B	801	PIO	O3C-C3C	-2.17	1.40	1.45
3	B	802	PCW	P-O3P	2.16	1.68	1.59
4	A	803	CLR	C15-C14	2.16	1.58	1.54
2	C	803	PIO	O3C-C3C	-2.15	1.40	1.45
2	D	802	PIO	P5-O52	-2.15	1.46	1.54
2	B	801	PIO	P5-O52	-2.15	1.46	1.54
2	C	803	PIO	P5-O52	-2.15	1.46	1.54
3	B	803	PCW	P-O3P	2.15	1.68	1.59
4	D	801	CLR	C15-C14	2.15	1.58	1.54
2	A	801	PIO	P5-O52	-2.15	1.46	1.54
2	A	801	PIO	P4-O41	-2.15	1.46	1.54
3	B	802	PCW	O3-C3	-2.14	1.40	1.45
2	D	802	PIO	P4-O41	-2.14	1.46	1.54
2	A	801	PIO	O3C-C3C	-2.13	1.40	1.45
2	C	803	PIO	P4-O41	-2.13	1.46	1.54
4	B	804	CLR	C15-C14	2.13	1.58	1.54
4	C	802	CLR	C15-C14	2.13	1.58	1.54
2	B	801	PIO	P4-O41	-2.13	1.46	1.54
2	D	802	PIO	O3C-C3C	-2.12	1.40	1.45
3	B	803	PCW	O3-C3	-2.12	1.40	1.45
3	C	801	PCW	O3-C3	-2.12	1.40	1.45
3	A	802	PCW	O3-C3	-2.11	1.40	1.45
2	D	802	PIO	O2C-C1A	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	803	PIO	O2C-C1A	2.09	1.40	1.34
2	A	801	PIO	O2C-C1A	2.08	1.40	1.34
2	B	801	PIO	O2C-C1A	2.06	1.40	1.34
4	A	803	CLR	C4-C5	-2.05	1.47	1.51
3	B	802	PCW	C8-N	-2.05	1.44	1.50
4	B	804	CLR	C4-C5	-2.04	1.47	1.51
4	C	802	CLR	C4-C5	-2.04	1.47	1.51
3	B	802	PCW	C7-N	-2.04	1.44	1.50
3	C	801	PCW	P-O4P	2.03	1.67	1.59
3	C	801	PCW	C7-N	-2.03	1.44	1.50
3	A	802	PCW	P-O4P	2.03	1.67	1.59
3	C	801	PCW	C8-N	-2.03	1.44	1.50
3	A	802	PCW	C7-N	-2.03	1.44	1.50
3	B	803	PCW	P-O4P	2.03	1.67	1.59
3	A	802	PCW	C8-N	-2.02	1.44	1.50
3	B	803	PCW	C8-N	-2.02	1.44	1.50
3	B	802	PCW	P-O4P	2.02	1.67	1.59
4	D	801	CLR	C4-C5	-2.02	1.47	1.51
3	B	803	PCW	C7-N	-2.00	1.44	1.50

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	CLR	C15-C14-C8	-8.04	105.84	119.08
4	C	802	CLR	C15-C14-C8	-8.04	105.84	119.08
4	D	801	CLR	C15-C14-C8	-8.03	105.85	119.08
4	B	804	CLR	C15-C14-C8	-8.03	105.86	119.08
4	C	802	CLR	C7-C8-C9	-6.95	101.30	109.71
4	D	801	CLR	C7-C8-C9	-6.91	101.34	109.71
4	B	804	CLR	C7-C8-C9	-6.90	101.35	109.71
4	A	803	CLR	C7-C8-C9	-6.86	101.40	109.71
4	B	804	CLR	C13-C14-C8	6.02	123.30	114.38
4	D	801	CLR	C13-C14-C8	6.02	123.29	114.38
4	C	802	CLR	C13-C14-C8	5.99	123.25	114.38
4	A	803	CLR	C13-C14-C8	5.98	123.24	114.38
4	A	803	CLR	C11-C9-C10	5.09	119.79	113.08
4	B	804	CLR	C11-C9-C10	5.08	119.77	113.08
4	C	802	CLR	C11-C9-C10	5.08	119.77	113.08
4	D	801	CLR	C11-C9-C10	5.08	119.76	113.08
4	B	804	CLR	C10-C9-C8	-4.48	106.02	112.73
4	A	803	CLR	C10-C9-C8	-4.47	106.03	112.73
4	C	802	CLR	C10-C9-C8	-4.47	106.03	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	801	CLR	C10-C9-C8	-4.45	106.06	112.73
3	C	801	PCW	O2-C31-C32	4.37	120.92	111.50
3	B	803	PCW	O2-C31-C32	4.36	120.89	111.50
3	B	802	PCW	O2-C31-C32	4.36	120.89	111.50
3	A	802	PCW	O2-C31-C32	4.35	120.89	111.50
4	C	802	CLR	C3-C4-C5	4.35	119.41	112.03
4	B	804	CLR	C3-C4-C5	4.34	119.38	112.03
4	A	803	CLR	C3-C4-C5	4.31	119.34	112.03
4	D	801	CLR	C3-C4-C5	4.31	119.34	112.03
4	C	802	CLR	C17-C13-C14	-4.15	95.16	100.07
4	A	803	CLR	C17-C13-C14	-4.13	95.18	100.07
4	B	804	CLR	C17-C13-C14	-4.11	95.20	100.07
4	D	801	CLR	C17-C13-C14	-4.10	95.22	100.07
4	A	803	CLR	C16-C15-C14	-3.83	97.54	105.13
4	B	804	CLR	C16-C15-C14	-3.82	97.55	105.13
4	D	801	CLR	C16-C15-C14	-3.82	97.56	105.13
4	C	802	CLR	C16-C15-C14	-3.81	97.57	105.13
2	C	803	PIO	O2C-C1A-C2A	3.73	119.53	111.50
2	A	801	PIO	O2C-C1A-C2A	3.73	119.53	111.50
2	D	802	PIO	O2C-C1A-C2A	3.72	119.53	111.50
2	B	801	PIO	O2C-C1A-C2A	3.72	119.51	111.50
4	D	801	CLR	C4-C5-C6	-3.63	115.38	120.61
4	A	803	CLR	C4-C5-C6	-3.61	115.41	120.61
4	B	804	CLR	C4-C5-C6	-3.56	115.47	120.61
4	C	802	CLR	C4-C5-C6	-3.55	115.48	120.61
4	A	803	CLR	C8-C7-C6	-3.40	107.85	112.73
4	B	804	CLR	C8-C7-C6	-3.40	107.85	112.73
4	D	801	CLR	C8-C7-C6	-3.39	107.86	112.73
4	C	802	CLR	C8-C7-C6	-3.36	107.90	112.73
4	A	803	CLR	C4-C5-C10	2.94	120.32	116.42
4	D	801	CLR	C4-C5-C10	2.92	120.31	116.42
4	B	804	CLR	C4-C5-C10	2.91	120.29	116.42
4	C	802	CLR	C4-C5-C10	2.91	120.29	116.42
4	A	803	CLR	C14-C8-C9	2.86	112.92	109.09
4	C	802	CLR	C14-C8-C9	2.86	112.92	109.09
4	D	801	CLR	C14-C8-C9	2.86	112.92	109.09
4	B	804	CLR	C14-C8-C9	2.85	112.91	109.09
4	A	803	CLR	C21-C20-C17	-2.79	108.65	112.92
4	B	804	CLR	C21-C20-C17	-2.78	108.66	112.92
4	D	801	CLR	C21-C20-C17	-2.75	108.71	112.92
4	C	802	CLR	C21-C20-C17	-2.75	108.72	112.92
4	C	802	CLR	C16-C17-C20	-2.62	108.09	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	CLR	C16-C17-C20	-2.62	108.09	112.15
4	B	804	CLR	C16-C17-C20	-2.62	108.09	112.15
4	D	801	CLR	C16-C17-C20	-2.60	108.12	112.15
2	B	801	PIO	O3C-C1B-C2B	2.59	120.05	111.91
2	D	802	PIO	O3C-C1B-C2B	2.59	120.04	111.91
2	A	801	PIO	O3C-C1B-C2B	2.58	120.01	111.91
2	C	803	PIO	O3C-C1B-C2B	2.58	120.00	111.91
4	A	803	CLR	C2-C1-C10	2.33	117.78	112.74
4	D	801	CLR	C2-C1-C10	2.32	117.76	112.74
4	B	804	CLR	C2-C1-C10	2.32	117.76	112.74
4	C	802	CLR	C2-C1-C10	2.32	117.76	112.74
2	B	801	PIO	O11-P1-O12	-2.25	101.14	112.24
2	D	802	PIO	O11-P1-O12	-2.24	101.18	112.24
2	A	801	PIO	O11-P1-O12	-2.23	101.19	112.24
2	C	803	PIO	O11-P1-O12	-2.23	101.21	112.24
4	C	802	CLR	C11-C9-C8	-2.22	108.56	111.75
4	D	801	CLR	C11-C9-C8	-2.22	108.56	111.75
3	B	803	PCW	O3-C11-C12	2.21	118.83	111.91
3	C	801	PCW	O3-C11-C12	2.21	118.83	111.91
3	A	802	PCW	O3-C11-C12	2.20	118.82	111.91
4	B	804	CLR	C11-C9-C8	-2.20	108.59	111.75
3	B	802	PCW	O3-C11-C12	2.20	118.81	111.91
4	A	803	CLR	C11-C9-C8	-2.19	108.60	111.75
4	B	804	CLR	C18-C13-C12	-2.18	107.14	110.59
4	D	801	CLR	C18-C13-C12	-2.16	107.17	110.59
4	A	803	CLR	C18-C13-C12	-2.16	107.18	110.59
4	C	802	CLR	C18-C13-C12	-2.15	107.20	110.59
4	C	802	CLR	C12-C13-C14	2.07	110.48	107.27
4	D	801	CLR	C12-C13-C14	2.07	110.48	107.27
4	B	804	CLR	C12-C13-C14	2.07	110.48	107.27
4	A	803	CLR	C12-C13-C14	2.06	110.47	107.27
3	C	801	PCW	C3-C2-C1	-2.05	106.95	111.79
3	A	802	PCW	C3-C2-C1	-2.05	106.95	111.79
3	B	802	PCW	C3-C2-C1	-2.04	106.96	111.79
3	B	803	PCW	C3-C2-C1	-2.04	106.97	111.79
4	B	804	CLR	C19-C10-C9	2.03	114.10	111.68
4	C	802	CLR	C19-C10-C9	2.03	114.10	111.68
4	D	801	CLR	C19-C10-C9	2.01	114.08	111.68
4	A	803	CLR	C19-C10-C9	2.00	114.07	111.68

There are no chirality outliers.

All (220) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PIO	C1-O1-P1-O11
2	A	801	PIO	O1A-C1A-O2C-C2C
2	D	802	PIO	C1-O1-P1-O11
2	D	802	PIO	O1A-C1A-O2C-C2C
2	B	801	PIO	C1-O1-P1-O11
2	B	801	PIO	O1A-C1A-O2C-C2C
2	C	803	PIO	C1-O1-P1-O11
2	C	803	PIO	O1A-C1A-O2C-C2C
3	A	802	PCW	C2-C1-O3P-P
3	A	802	PCW	O4P-C4-C5-N
3	A	802	PCW	C32-C31-O2-C2
3	A	802	PCW	C1-O3P-P-O2P
3	A	802	PCW	C1-O3P-P-O4P
3	A	802	PCW	C4-O4P-P-O1P
3	B	802	PCW	C2-C1-O3P-P
3	B	802	PCW	O4P-C4-C5-N
3	B	802	PCW	C32-C31-O2-C2
3	B	802	PCW	C1-O3P-P-O2P
3	B	802	PCW	C1-O3P-P-O4P
3	B	802	PCW	C4-O4P-P-O1P
3	B	803	PCW	C2-C1-O3P-P
3	B	803	PCW	O4P-C4-C5-N
3	B	803	PCW	C32-C31-O2-C2
3	B	803	PCW	C1-O3P-P-O2P
3	B	803	PCW	C1-O3P-P-O4P
3	B	803	PCW	C4-O4P-P-O1P
3	C	801	PCW	C2-C1-O3P-P
3	C	801	PCW	O4P-C4-C5-N
3	C	801	PCW	C32-C31-O2-C2
3	C	801	PCW	C1-O3P-P-O2P
3	C	801	PCW	C1-O3P-P-O4P
3	C	801	PCW	C4-O4P-P-O1P
3	A	802	PCW	O31-C31-O2-C2
3	B	802	PCW	O31-C31-O2-C2
3	B	803	PCW	O31-C31-O2-C2
3	C	801	PCW	O31-C31-O2-C2
2	A	801	PIO	C2A-C1A-O2C-C2C
2	D	802	PIO	C2A-C1A-O2C-C2C
2	B	801	PIO	C2A-C1A-O2C-C2C
2	C	803	PIO	C2A-C1A-O2C-C2C
2	A	801	PIO	C2B-C1B-O3C-C3C
2	D	802	PIO	C2B-C1B-O3C-C3C
2	B	801	PIO	C2B-C1B-O3C-C3C

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Mol	Chain	Res	Type	Atoms
2	C	803	PIO	C2B-C1B-O3C-C3C
2	A	801	PIO	O1B-C1B-O3C-C3C
2	D	802	PIO	O1B-C1B-O3C-C3C
2	B	801	PIO	O1B-C1B-O3C-C3C
2	C	803	PIO	O1B-C1B-O3C-C3C
3	A	802	PCW	C12-C11-O3-C3
3	B	802	PCW	C12-C11-O3-C3
3	B	803	PCW	C12-C11-O3-C3
3	C	801	PCW	C12-C11-O3-C3
2	A	801	PIO	C1-O1-P1-O13
2	D	802	PIO	C1-O1-P1-O13
2	B	801	PIO	C1-O1-P1-O13
2	C	803	PIO	C1-O1-P1-O13
4	A	803	CLR	C17-C20-C22-C23
4	D	801	CLR	C17-C20-C22-C23
4	B	804	CLR	C17-C20-C22-C23
4	C	802	CLR	C17-C20-C22-C23
4	A	803	CLR	C21-C20-C22-C23
4	D	801	CLR	C21-C20-C22-C23
4	B	804	CLR	C21-C20-C22-C23
4	C	802	CLR	C21-C20-C22-C23
3	A	802	PCW	O11-C11-O3-C3
3	B	802	PCW	O11-C11-O3-C3
3	B	803	PCW	O11-C11-O3-C3
3	C	801	PCW	O11-C11-O3-C3
3	A	802	PCW	C11-C12-C13-C14
3	B	802	PCW	C11-C12-C13-C14
3	B	803	PCW	C11-C12-C13-C14
3	C	801	PCW	C11-C12-C13-C14
3	A	802	PCW	C4-O4P-P-O3P
3	B	802	PCW	C4-O4P-P-O3P
3	B	803	PCW	C4-O4P-P-O3P
3	C	801	PCW	C4-O4P-P-O3P
3	A	802	PCW	C43-C44-C45-C46
3	B	802	PCW	C43-C44-C45-C46
3	B	803	PCW	C43-C44-C45-C46
3	C	801	PCW	C43-C44-C45-C46
2	A	801	PIO	C2B-C3B-C4B-C5B
2	A	801	PIO	C4A-C5A-C6A-C7A
2	D	802	PIO	C2B-C3B-C4B-C5B
2	D	802	PIO	C4A-C5A-C6A-C7A
2	B	801	PIO	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
2	B	801	PIO	C4A-C5A-C6A-C7A
2	C	803	PIO	C4A-C5A-C6A-C7A
2	C	803	PIO	C2B-C3B-C4B-C5B
3	B	803	PCW	C35-C36-C37-C38
3	A	802	PCW	C35-C36-C37-C38
3	B	802	PCW	C35-C36-C37-C38
3	C	801	PCW	C35-C36-C37-C38
4	A	803	CLR	C20-C22-C23-C24
4	D	801	CLR	C20-C22-C23-C24
4	B	804	CLR	C20-C22-C23-C24
4	C	802	CLR	C20-C22-C23-C24
3	B	803	PCW	C21-C22-C23-C24
3	C	801	PCW	C21-C22-C23-C24
3	A	802	PCW	C21-C22-C23-C24
3	B	802	PCW	C21-C22-C23-C24
2	A	801	PIO	C4B-C5B-C6B-C7B
2	D	802	PIO	C4B-C5B-C6B-C7B
2	B	801	PIO	C4B-C5B-C6B-C7B
2	C	803	PIO	C4B-C5B-C6B-C7B
4	A	803	CLR	C23-C24-C25-C26
4	D	801	CLR	C23-C24-C25-C26
4	B	804	CLR	C23-C24-C25-C26
4	C	802	CLR	C23-C24-C25-C26
4	A	803	CLR	C23-C24-C25-C27
4	D	801	CLR	C23-C24-C25-C27
4	B	804	CLR	C23-C24-C25-C27
4	C	802	CLR	C23-C24-C25-C27
3	A	802	PCW	C14-C15-C16-C17
3	B	802	PCW	C14-C15-C16-C17
3	B	803	PCW	C14-C15-C16-C17
3	C	801	PCW	C14-C15-C16-C17
3	B	803	PCW	C24-C25-C26-C27
3	A	802	PCW	C24-C25-C26-C27
3	C	801	PCW	C24-C25-C26-C27
3	B	802	PCW	C24-C25-C26-C27
3	B	802	PCW	C31-C32-C33-C34
3	A	802	PCW	C31-C32-C33-C34
3	B	803	PCW	C31-C32-C33-C34
3	C	801	PCW	C31-C32-C33-C34
2	A	801	PIO	O13-C1C-C2C-C3C
2	D	802	PIO	O13-C1C-C2C-C3C
2	B	801	PIO	O13-C1C-C2C-C3C

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Mol	Chain	Res	Type	Atoms
2	C	803	PIO	O13-C1C-C2C-C3C
3	A	802	PCW	O3P-C1-C2-C3
3	B	802	PCW	O3P-C1-C2-C3
3	B	803	PCW	O3P-C1-C2-C3
3	C	801	PCW	O3P-C1-C2-C3
3	A	802	PCW	C3-C2-O2-C31
3	B	802	PCW	C3-C2-O2-C31
3	B	803	PCW	C3-C2-O2-C31
3	C	801	PCW	C3-C2-O2-C31
2	A	801	PIO	C2C-C1C-O13-P1
2	D	802	PIO	C2C-C1C-O13-P1
2	B	801	PIO	C2C-C1C-O13-P1
2	C	803	PIO	C2C-C1C-O13-P1
2	D	802	PIO	O13-C1C-C2C-O2C
2	C	803	PIO	O13-C1C-C2C-O2C
2	A	801	PIO	C1A-C2A-C3A-C4A
2	D	802	PIO	C1A-C2A-C3A-C4A
2	C	803	PIO	C1A-C2A-C3A-C4A
2	B	801	PIO	C1A-C2A-C3A-C4A
3	A	802	PCW	C4-O4P-P-O2P
3	B	802	PCW	C4-O4P-P-O2P
3	B	803	PCW	C4-O4P-P-O2P
3	C	801	PCW	C4-O4P-P-O2P
2	A	801	PIO	O13-C1C-C2C-O2C
2	B	801	PIO	O13-C1C-C2C-O2C
3	A	802	PCW	O3P-C1-C2-O2
3	B	802	PCW	O3P-C1-C2-O2
3	B	803	PCW	O3P-C1-C2-O2
3	C	801	PCW	O3P-C1-C2-O2
3	A	802	PCW	C44-C45-C46-C47
3	B	802	PCW	C44-C45-C46-C47
3	B	803	PCW	C44-C45-C46-C47
3	C	801	PCW	C44-C45-C46-C47
2	A	801	PIO	C3B-C4B-C5B-C6B
2	C	803	PIO	C3B-C4B-C5B-C6B
2	B	801	PIO	C3B-C4B-C5B-C6B
2	D	802	PIO	C3B-C4B-C5B-C6B
3	C	801	PCW	C22-C23-C24-C25
3	A	802	PCW	C22-C23-C24-C25
3	B	802	PCW	C22-C23-C24-C25
3	B	803	PCW	C22-C23-C24-C25
2	A	801	PIO	C1C-O13-P1-O1

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Mol	Chain	Res	Type	Atoms
2	D	802	PIO	C1C-O13-P1-O1
2	B	801	PIO	C1C-O13-P1-O1
2	C	803	PIO	C1C-O13-P1-O1
3	B	803	PCW	C45-C46-C47-C48
3	A	802	PCW	C45-C46-C47-C48
3	B	802	PCW	C45-C46-C47-C48
3	C	801	PCW	C45-C46-C47-C48
2	A	801	PIO	C2A-C3A-C4A-C5A
2	C	803	PIO	C2A-C3A-C4A-C5A
2	D	802	PIO	C2A-C3A-C4A-C5A
2	B	801	PIO	C2A-C3A-C4A-C5A
3	A	802	PCW	C32-C33-C34-C35
3	B	802	PCW	C32-C33-C34-C35
3	B	803	PCW	C32-C33-C34-C35
3	C	801	PCW	C32-C33-C34-C35
3	A	802	PCW	C17-C18-C19-C20
3	B	802	PCW	C17-C18-C19-C20
3	B	803	PCW	C17-C18-C19-C20
3	C	801	PCW	C17-C18-C19-C20
2	A	801	PIO	C1-O1-P1-O12
2	D	802	PIO	C1-O1-P1-O12
2	B	801	PIO	C1-O1-P1-O12
2	C	803	PIO	C1-O1-P1-O12
2	A	801	PIO	C5-O5-P5-O53
2	D	802	PIO	C5-O5-P5-O53
2	B	801	PIO	C5-O5-P5-O53
2	C	803	PIO	C5-O5-P5-O53
2	A	801	PIO	O3C-C1B-C2B-C3B
3	B	803	PCW	C41-C42-C43-C44
2	D	802	PIO	O3C-C1B-C2B-C3B
2	B	801	PIO	O3C-C1B-C2B-C3B
2	C	803	PIO	O3C-C1B-C2B-C3B
3	A	802	PCW	C41-C42-C43-C44
3	C	801	PCW	C41-C42-C43-C44
3	B	802	PCW	C41-C42-C43-C44
3	A	802	PCW	O3-C11-C12-C13
3	B	802	PCW	O3-C11-C12-C13
3	B	803	PCW	O3-C11-C12-C13
3	C	801	PCW	O3-C11-C12-C13
2	D	802	PIO	O1B-C1B-C2B-C3B
2	A	801	PIO	O1B-C1B-C2B-C3B
2	B	801	PIO	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
2	C	803	PIO	O1B-C1B-C2B-C3B
3	A	802	PCW	C5-C4-O4P-P
3	B	802	PCW	C5-C4-O4P-P
3	B	803	PCW	C5-C4-O4P-P
3	C	801	PCW	C5-C4-O4P-P
3	A	802	PCW	O11-C11-C12-C13
3	B	802	PCW	O11-C11-C12-C13
3	B	803	PCW	O11-C11-C12-C13
3	C	801	PCW	O11-C11-C12-C13

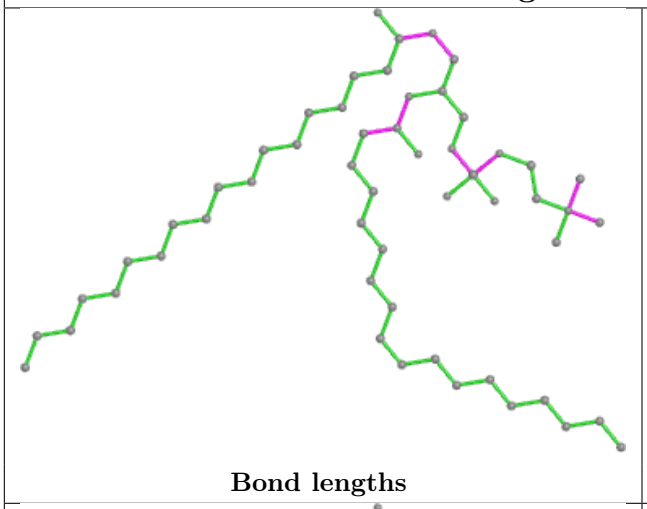
There are no ring outliers.

12 monomers are involved in 38 short contacts:

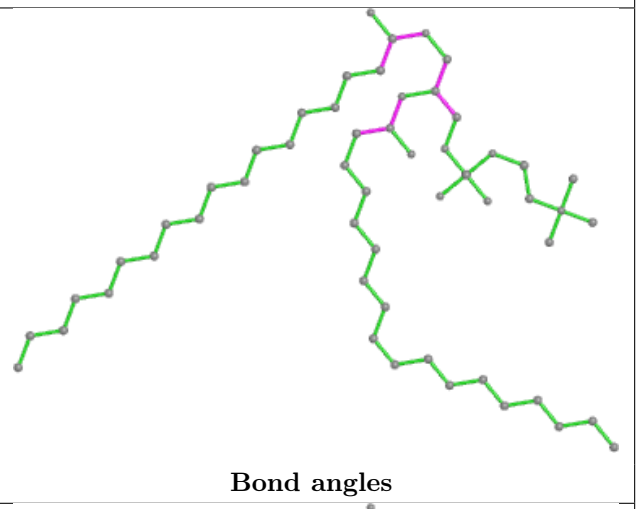
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PCW	3	0
2	C	803	PIO	1	0
2	B	801	PIO	1	0
3	B	803	PCW	2	0
4	B	804	CLR	9	0
2	D	802	PIO	1	0
4	C	802	CLR	7	0
4	A	803	CLR	6	0
3	B	802	PCW	2	0
2	A	801	PIO	1	0
4	D	801	CLR	3	0
3	C	801	PCW	2	0

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

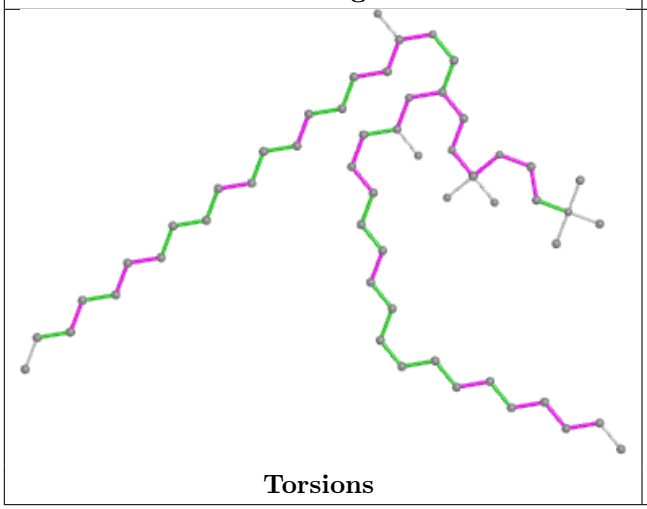
Ligand PCW A 802



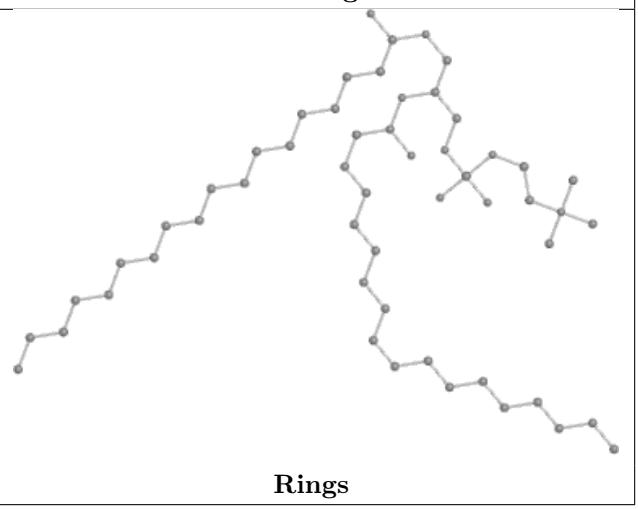
Bond lengths



Bond angles

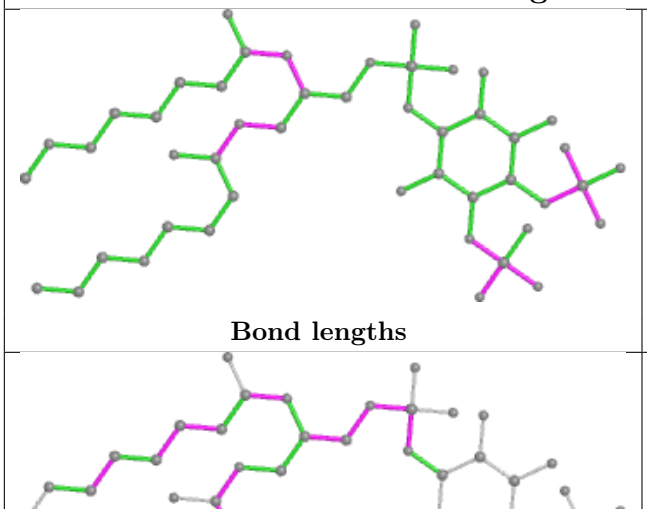


Torsions

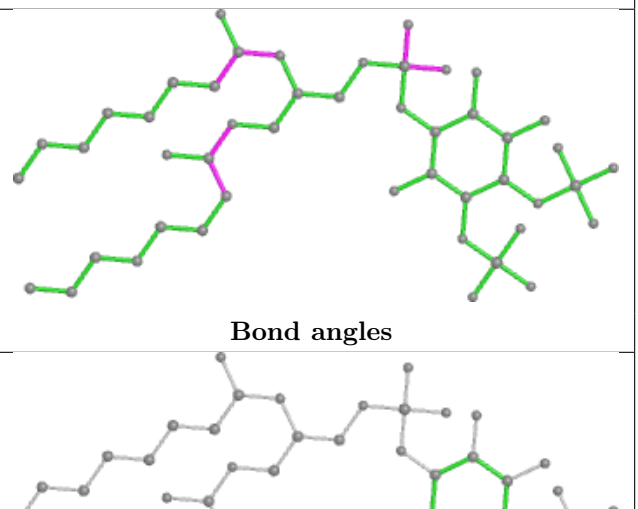


Rings

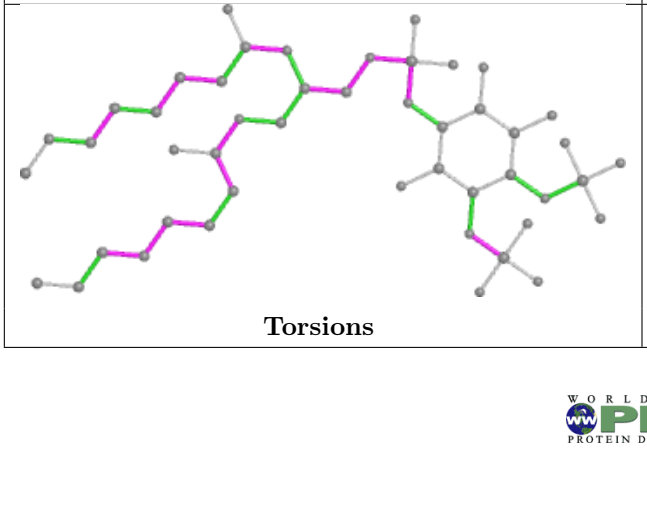
Ligand PIO C 803



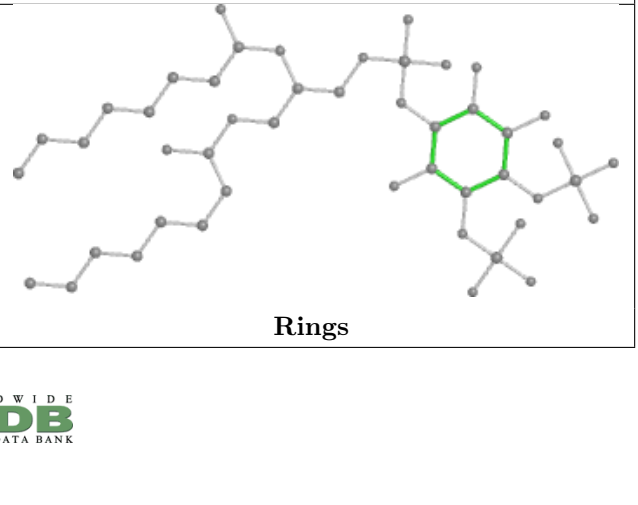
Bond lengths



Bond angles

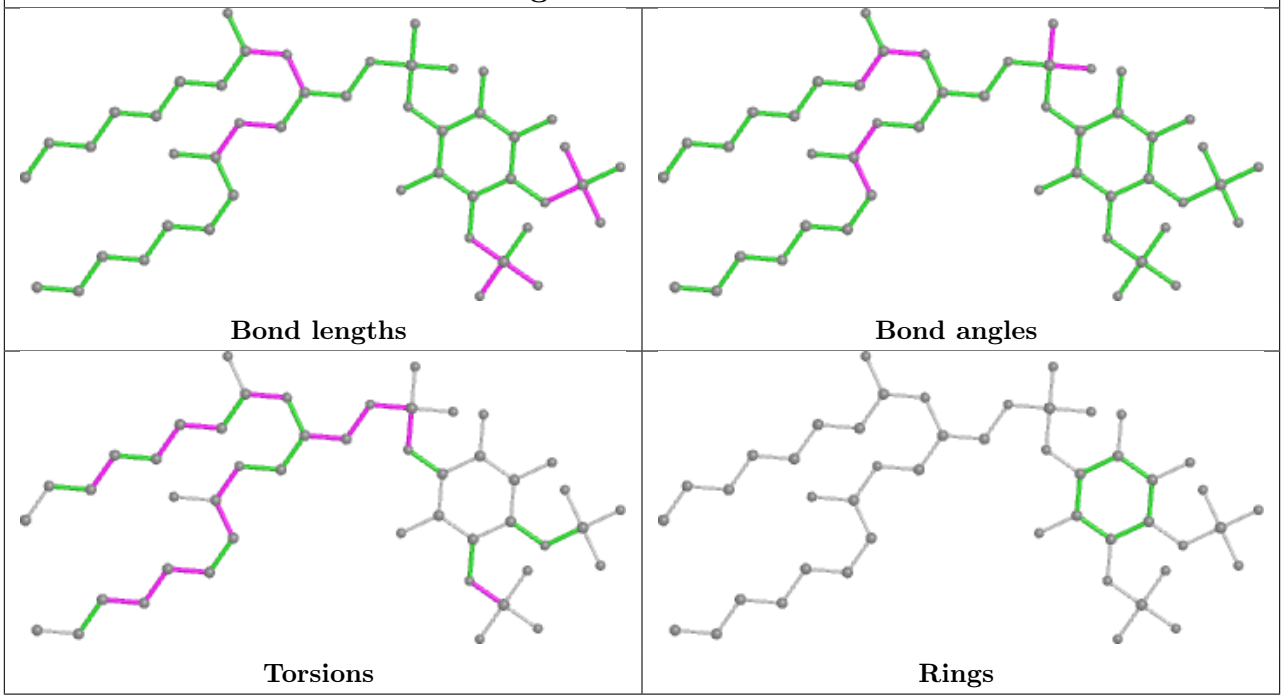


Torsions

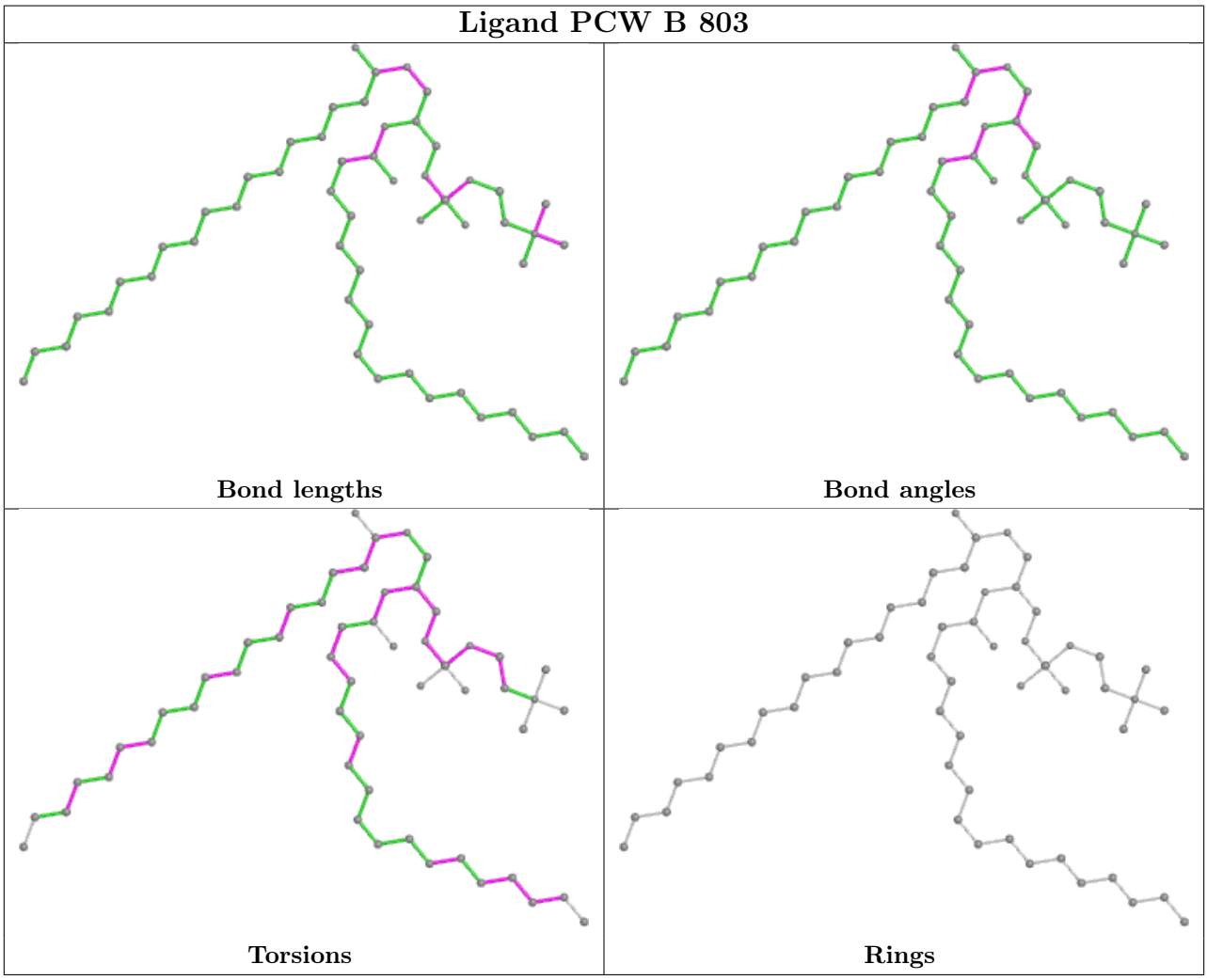


Rings

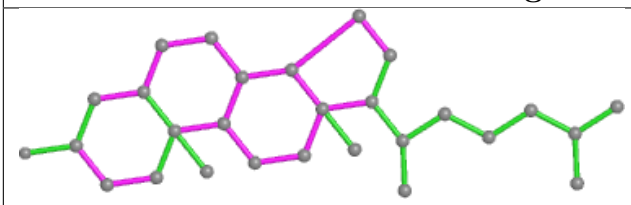
Ligand PIO B 801



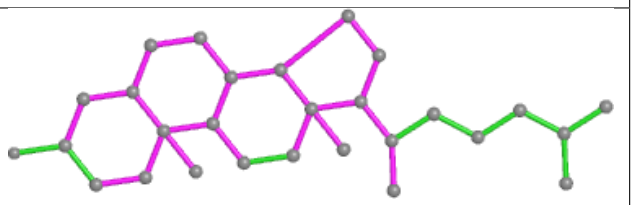
Ligand PCW B 803



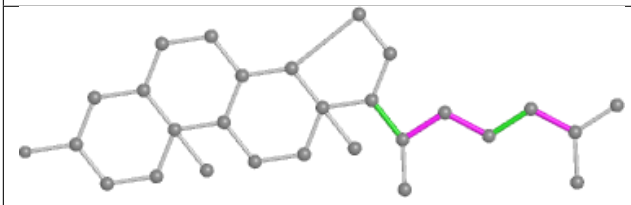
Ligand CLR B 804



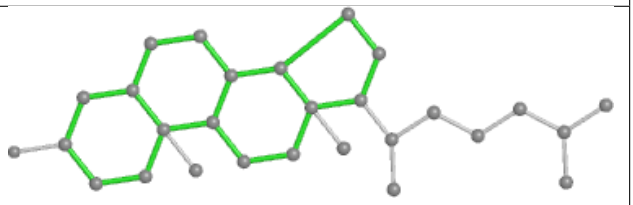
Bond lengths



Bond angles

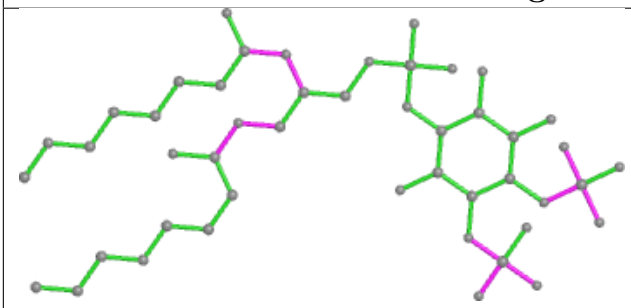


Torsions

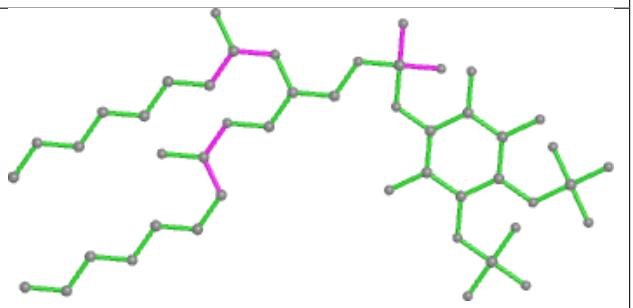


Rings

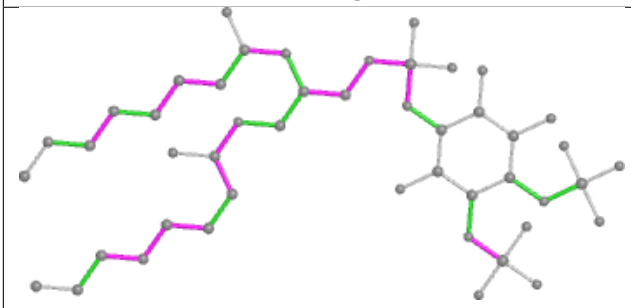
Ligand PIO D 802



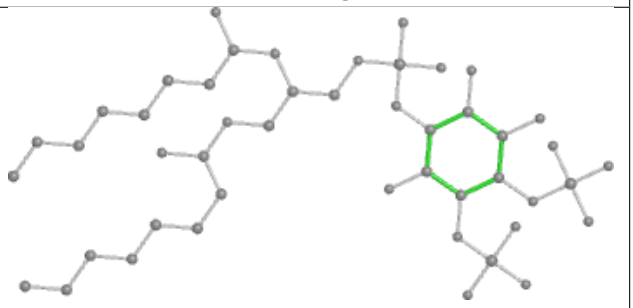
Bond lengths



Bond angles

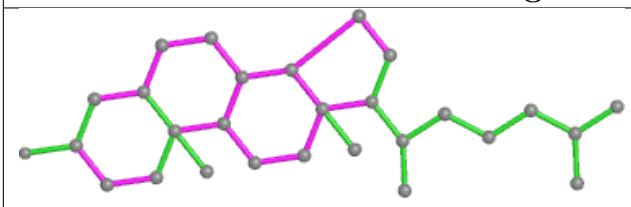


Torsions

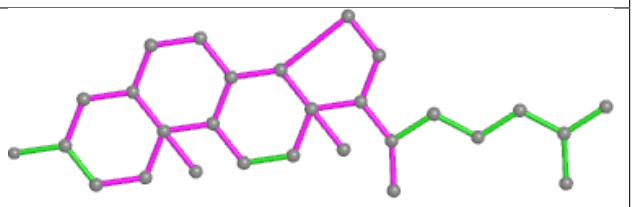


Rings

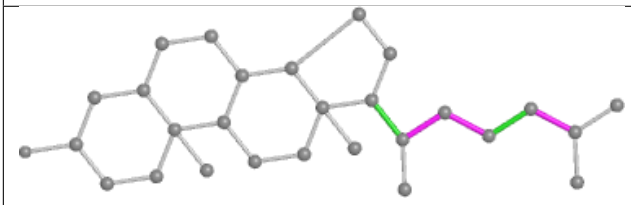
Ligand CLR C 802



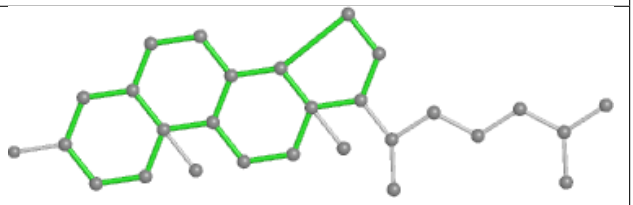
Bond lengths



Bond angles

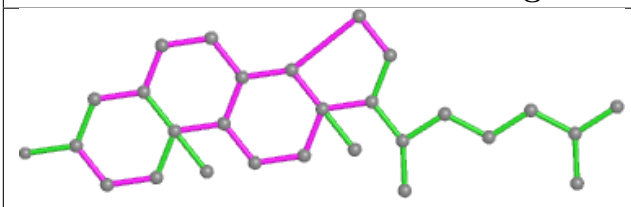


Torsions

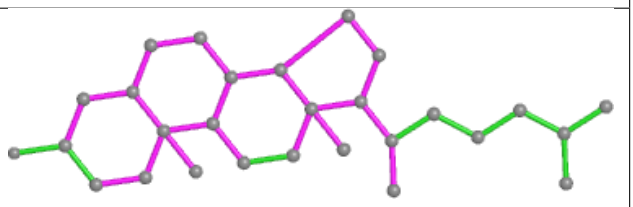


Rings

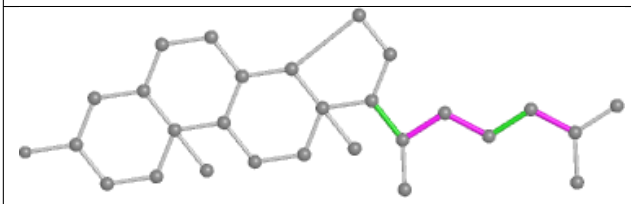
Ligand CLR A 803



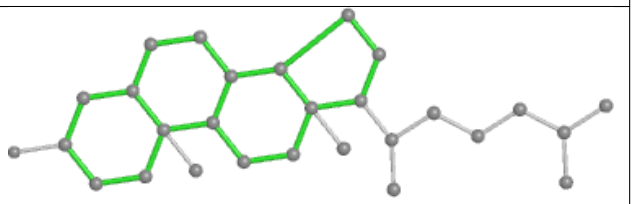
Bond lengths



Bond angles

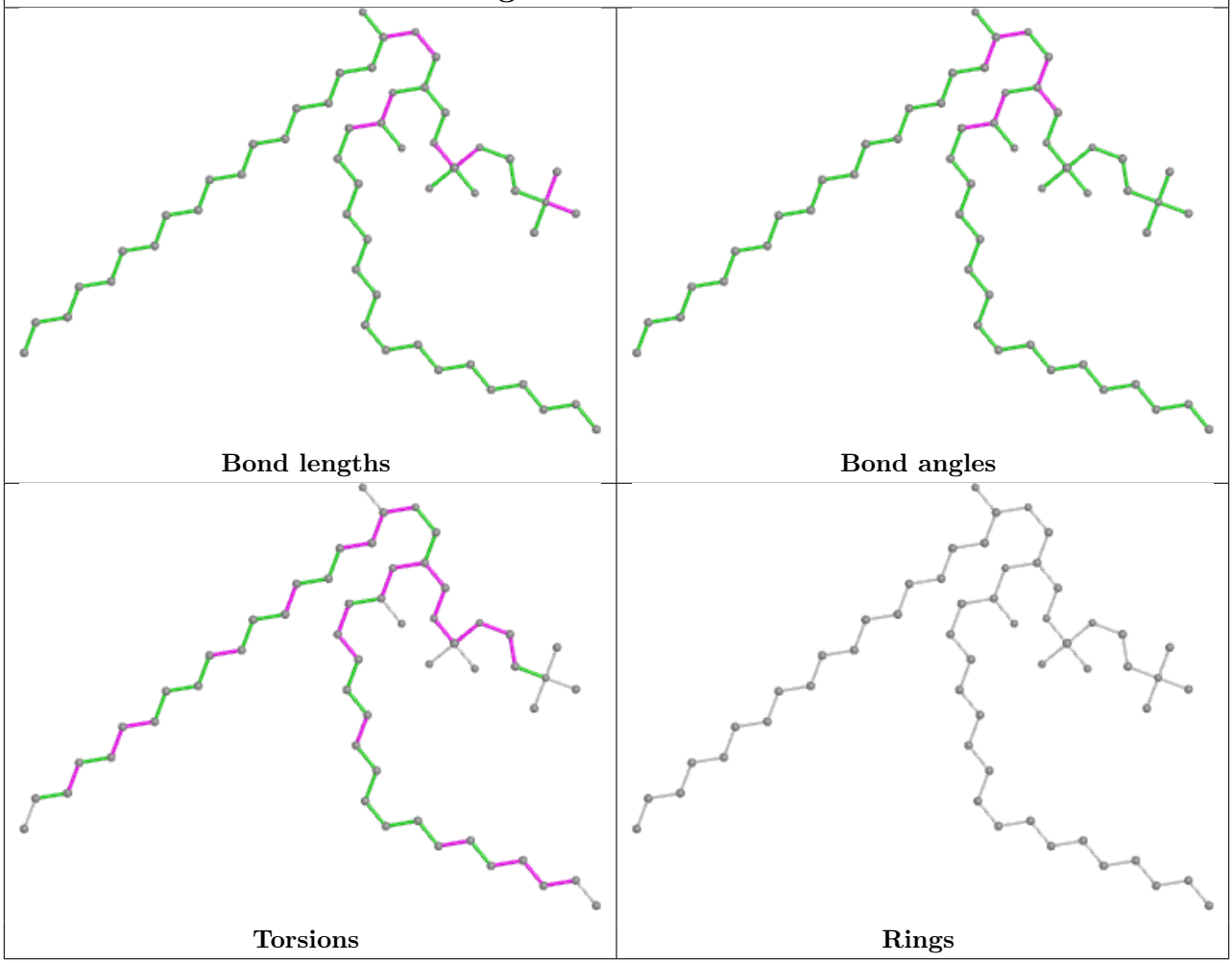


Torsions

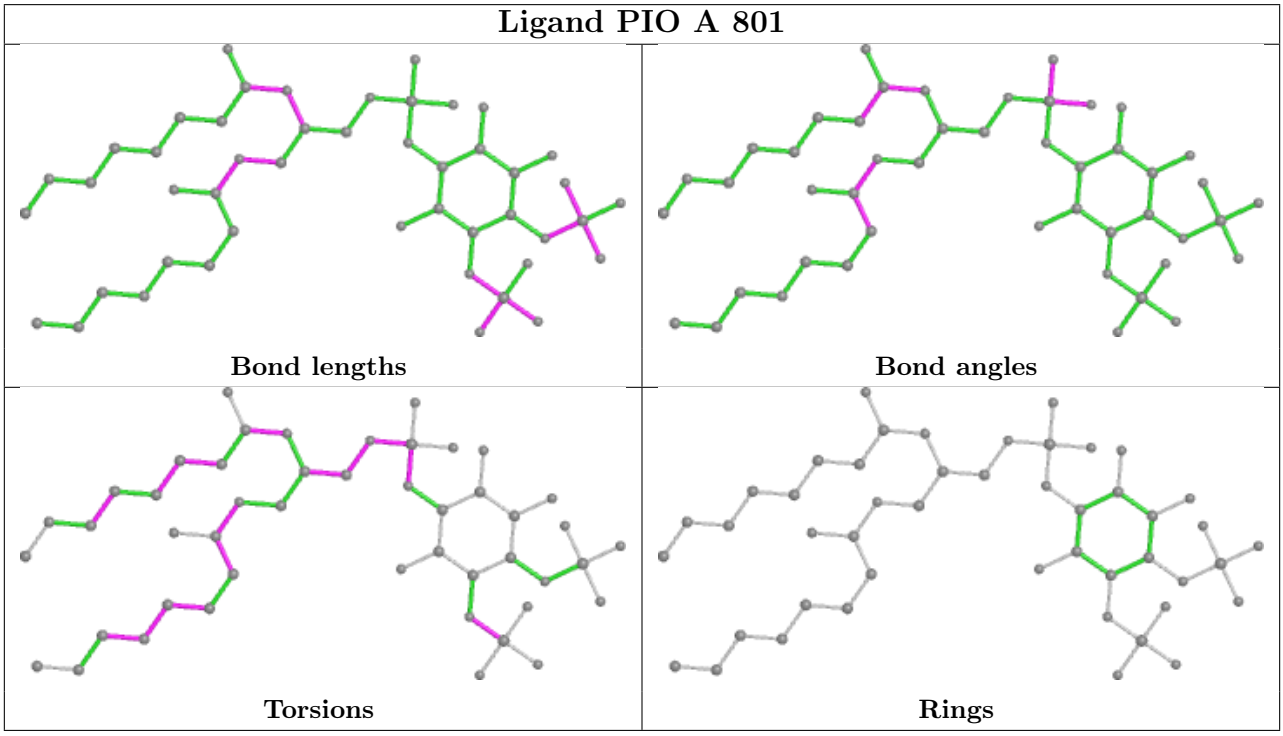


Rings

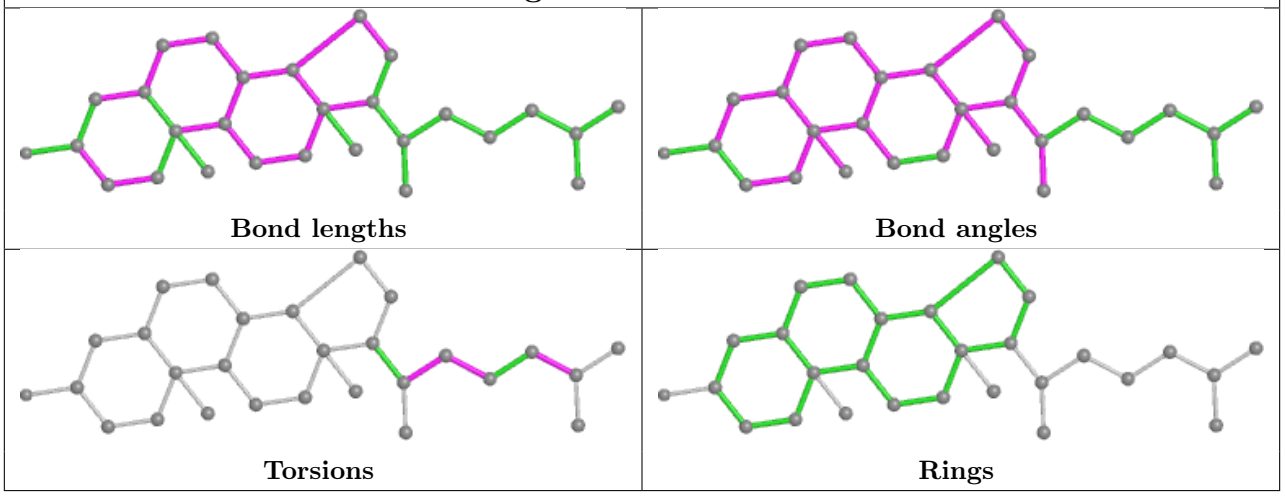
Ligand PCW B 802



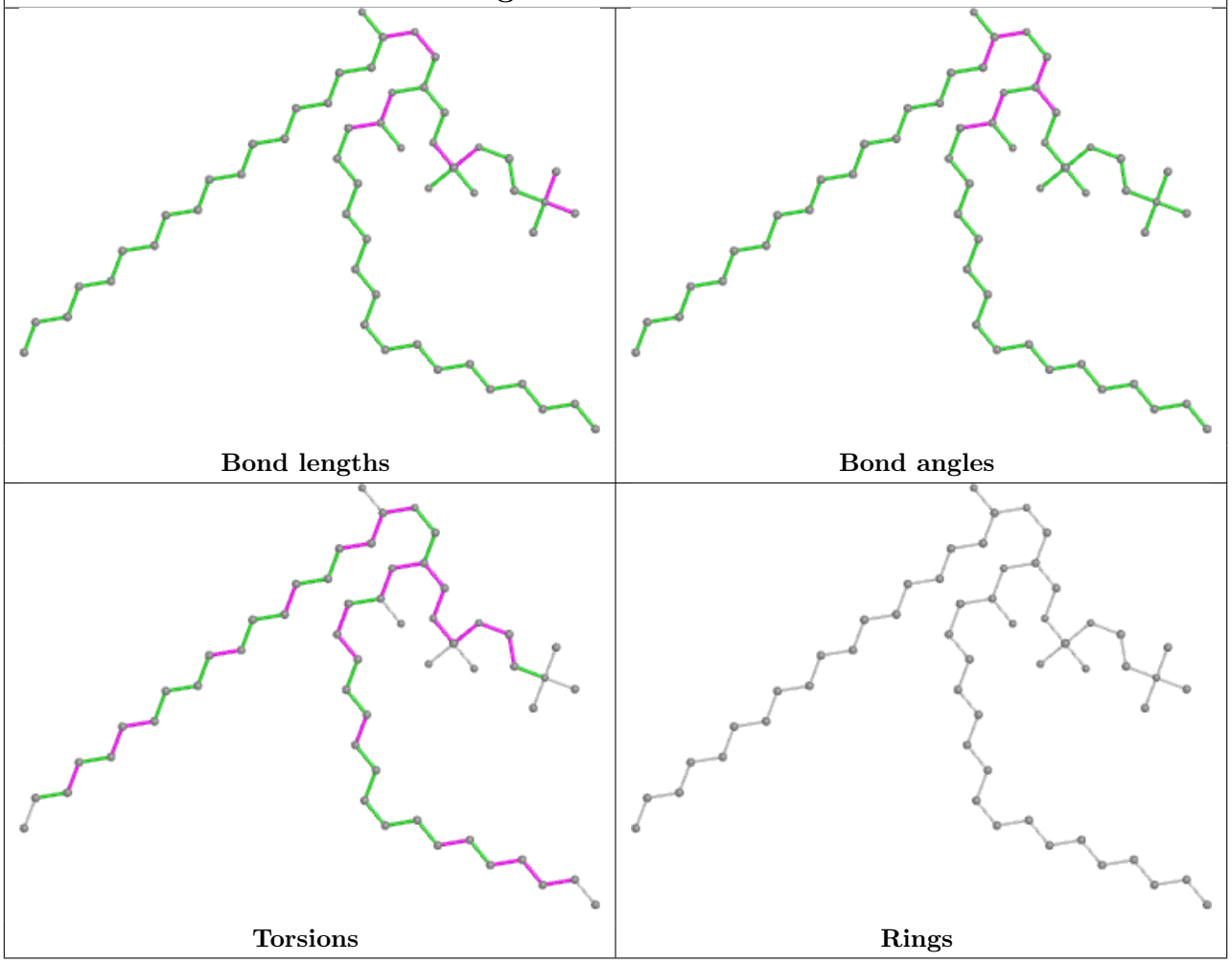
Ligand PIO A 801



Ligand CLR D 801



Ligand PCW C 801



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.

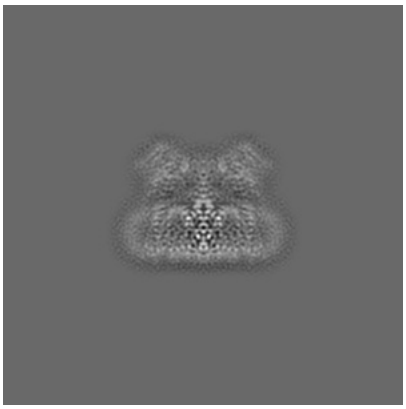
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41847. These allow visual inspection of the internal detail of the map and identification of artifacts.

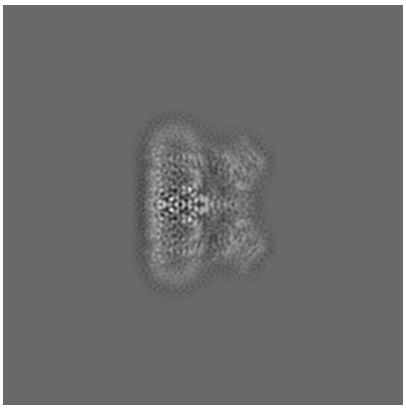
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

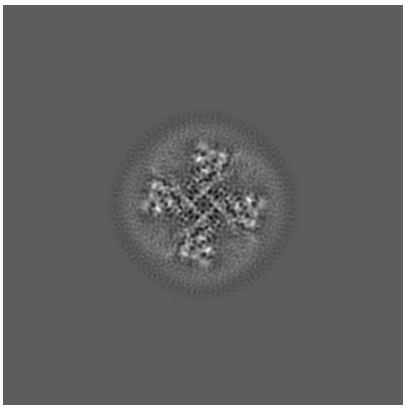
6.1.1 Primary map



X

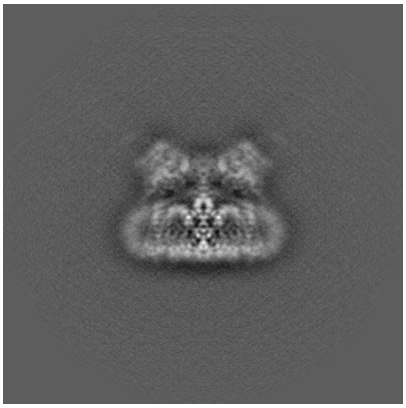


Y

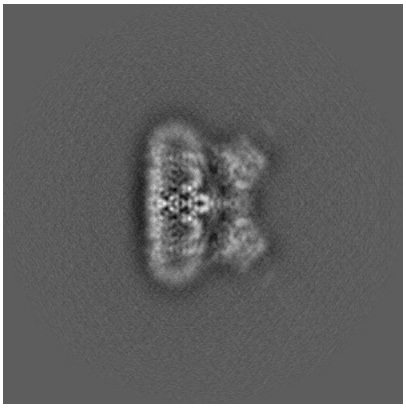


Z

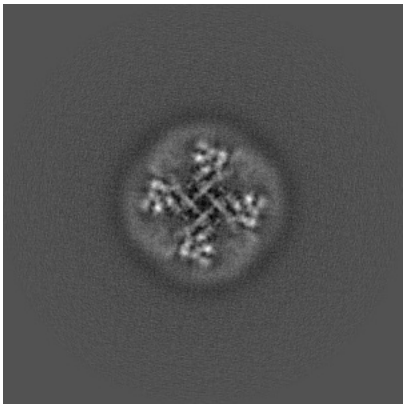
6.1.2 Raw map



X



Y

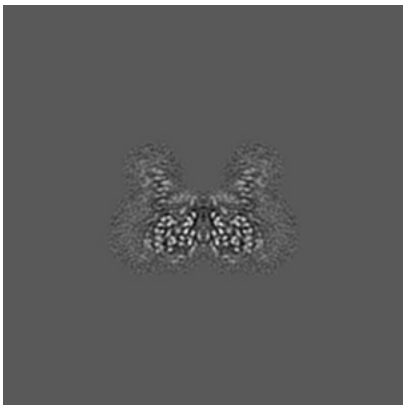


Z

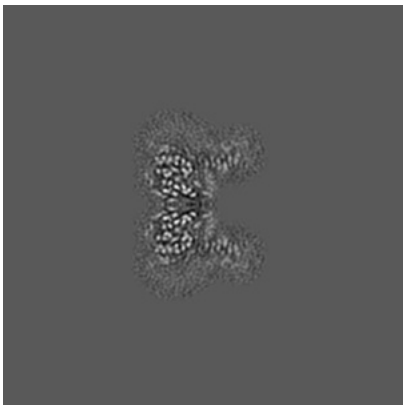
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

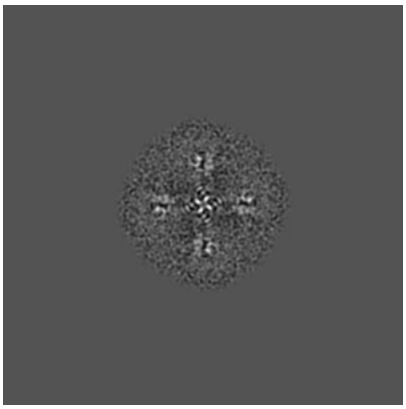
6.2.1 Primary map



X Index: 192

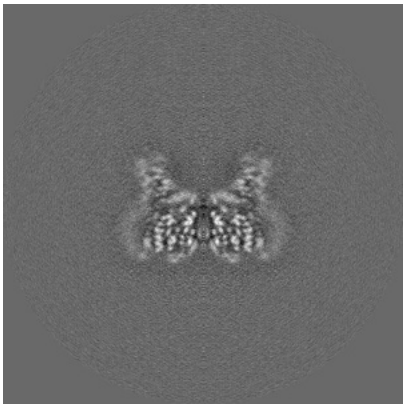


Y Index: 192

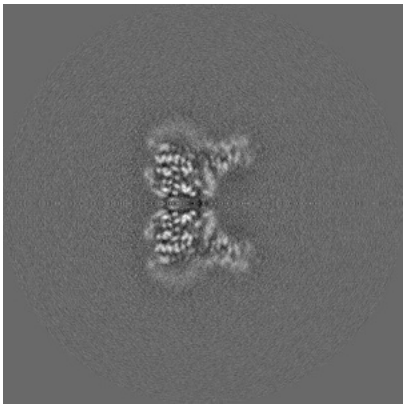


Z Index: 192

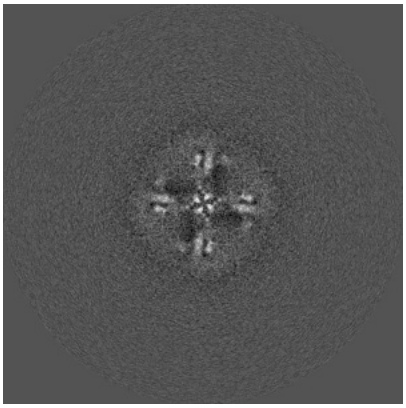
6.2.2 Raw map



X Index: 192



Y Index: 192

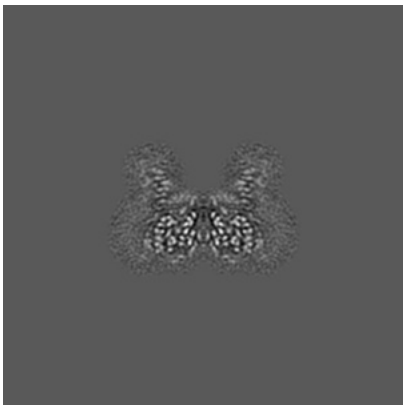


Z Index: 192

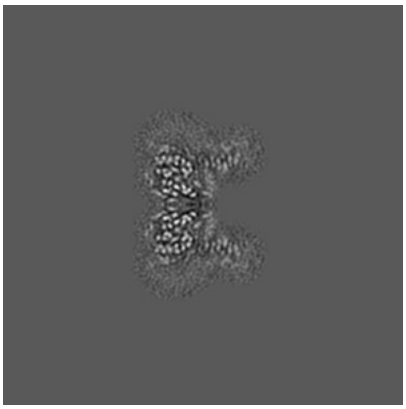
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

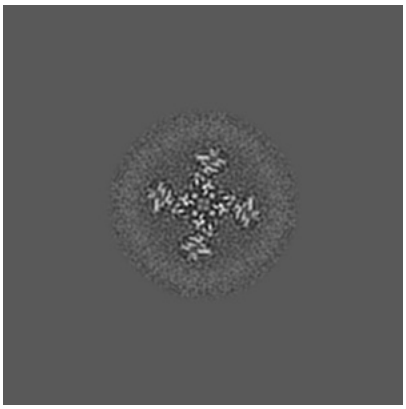
6.3.1 Primary map



X Index: 192

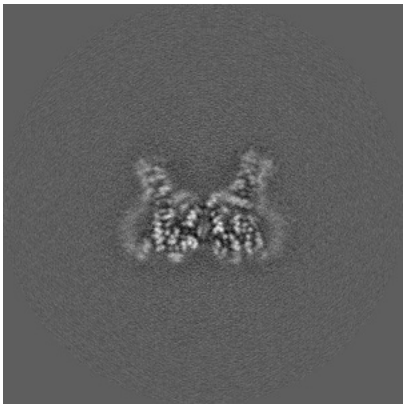


Y Index: 192

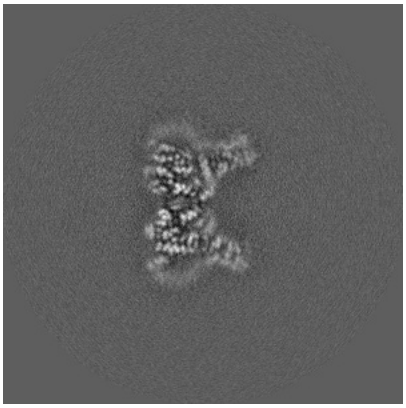


Z Index: 167

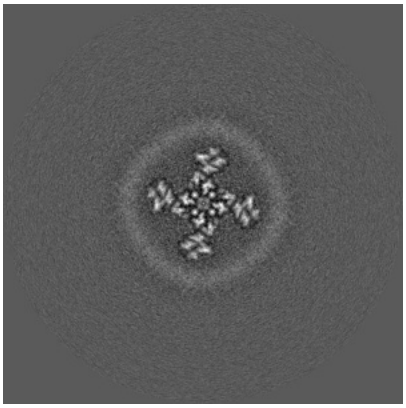
6.3.2 Raw map



X Index: 194



Y Index: 190

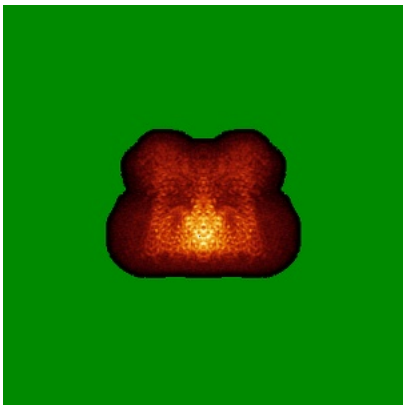


Z Index: 167

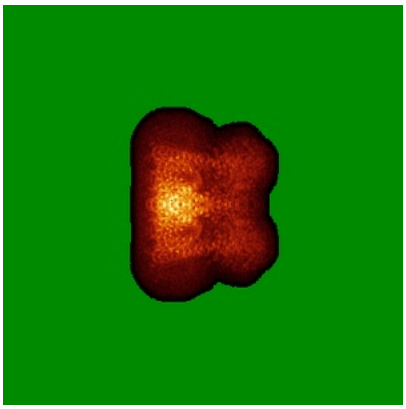
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

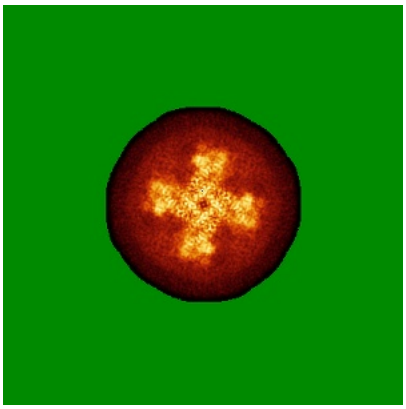
6.4.1 Primary map



X

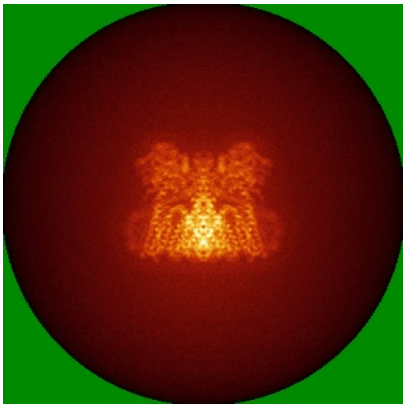


Y

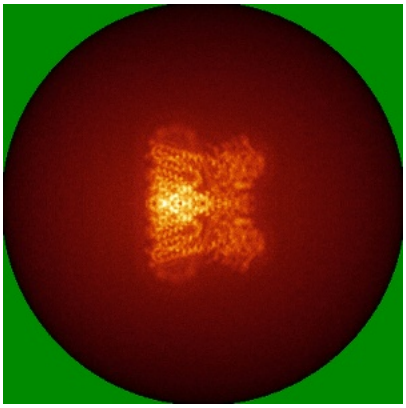


Z

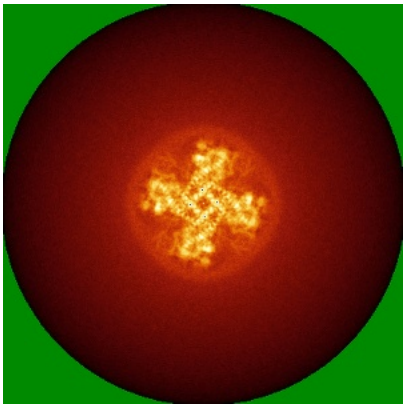
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

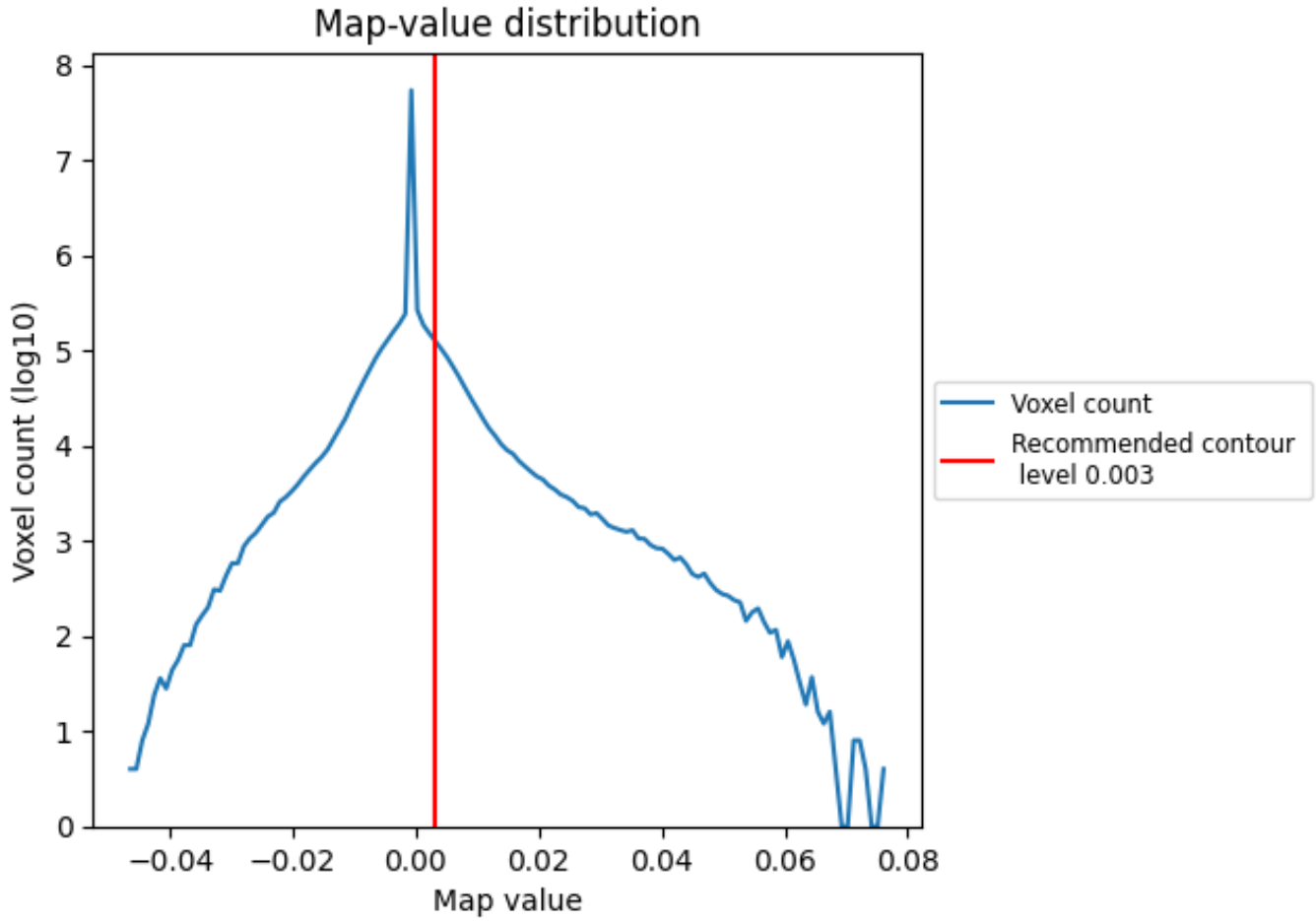
6.6 Mask visualisation (i)

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

7 Map analysis

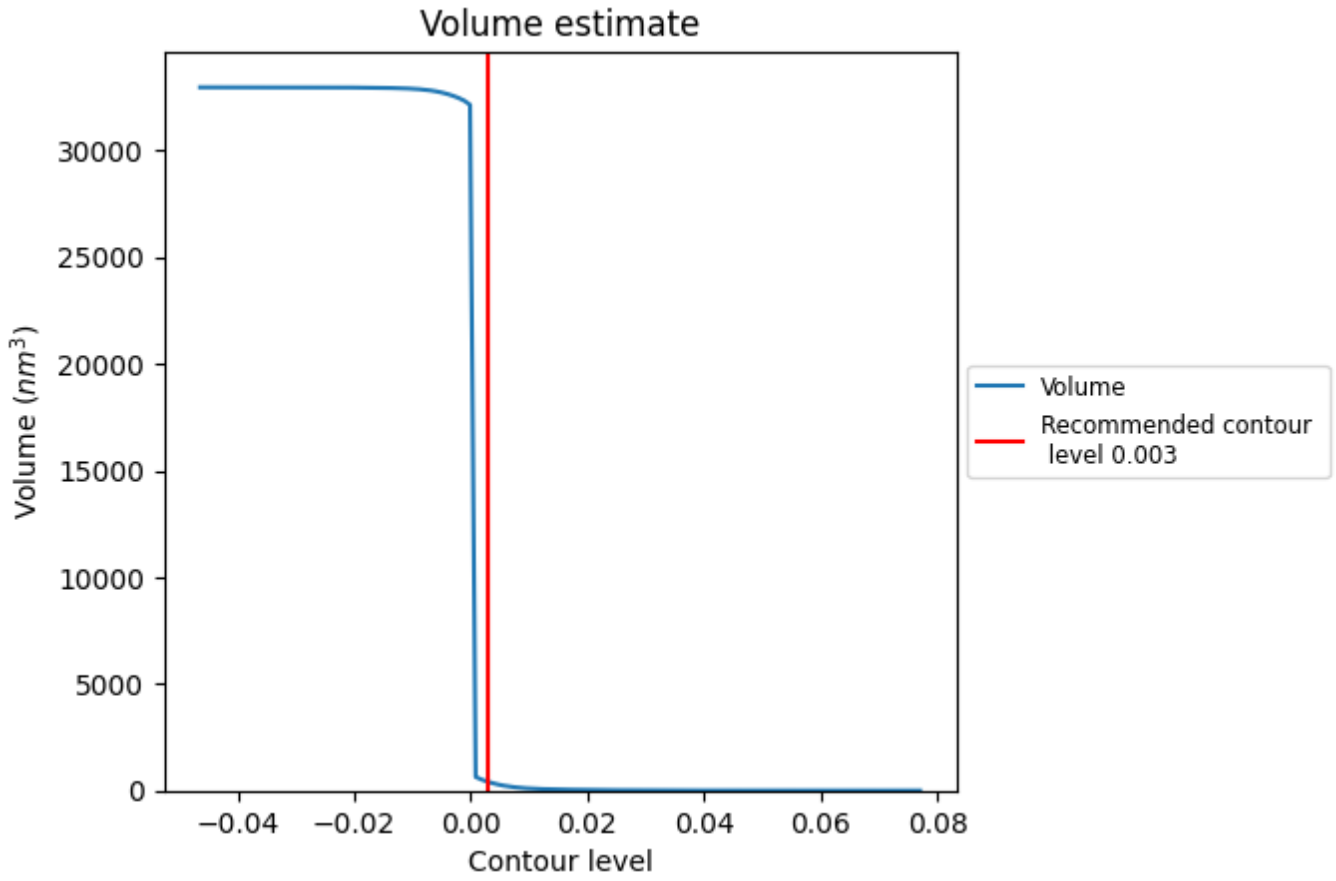
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

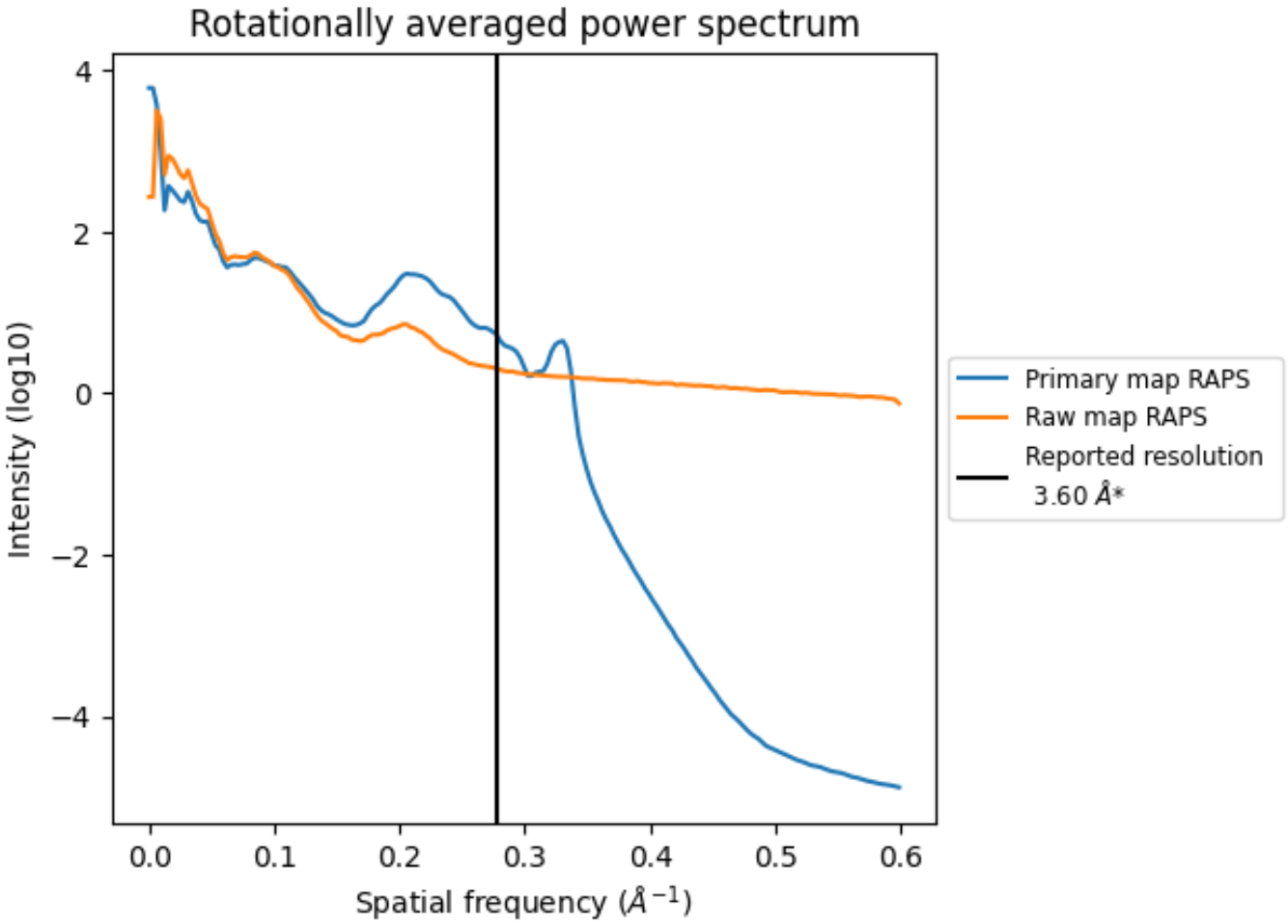
7.2 Volume estimate



The volume at the recommended contour level is 407 nm^3; this corresponds to an approximate mass of 368 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)

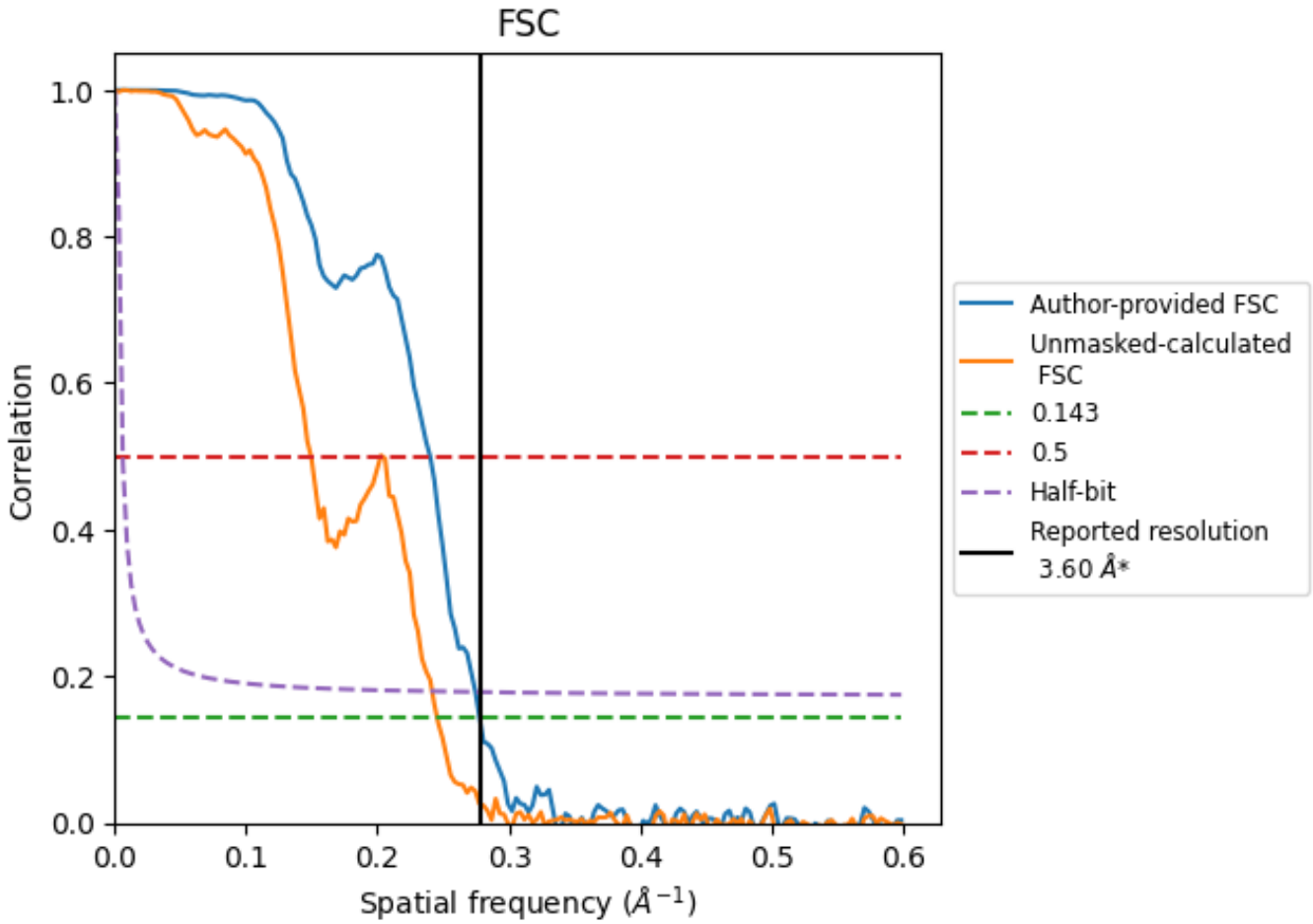


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

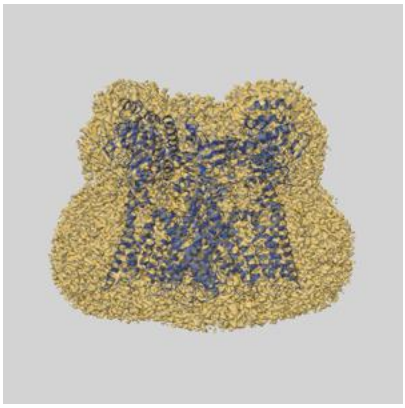
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.16	3.64
Unmasked-calculated*	4.07	6.69	4.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.6 by more than 10 %

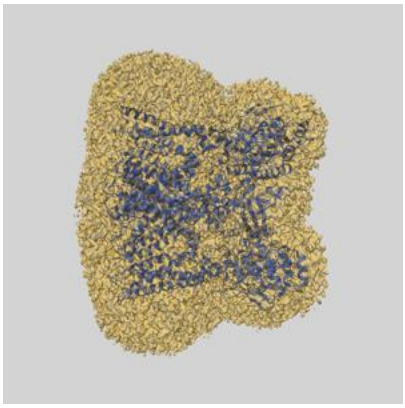
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41847 and PDB model 8U2Z. Per-residue inclusion information can be found in section 3 on page 9.

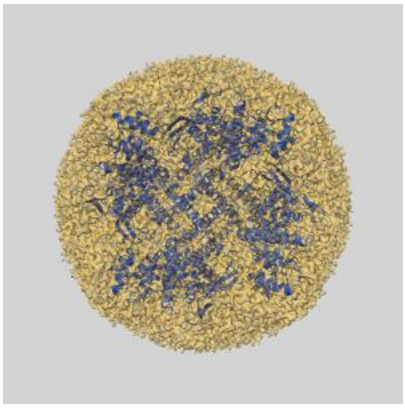
9.1 Map-model overlay



X



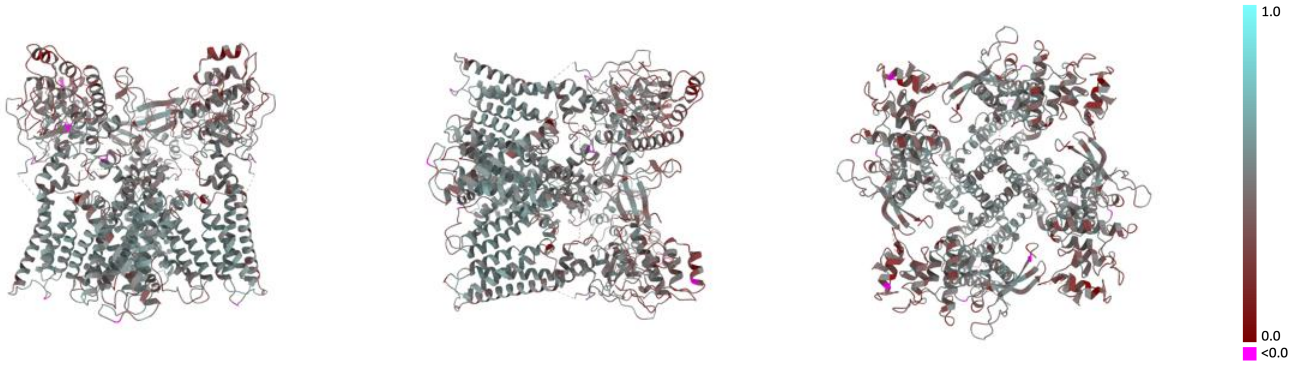
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 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.

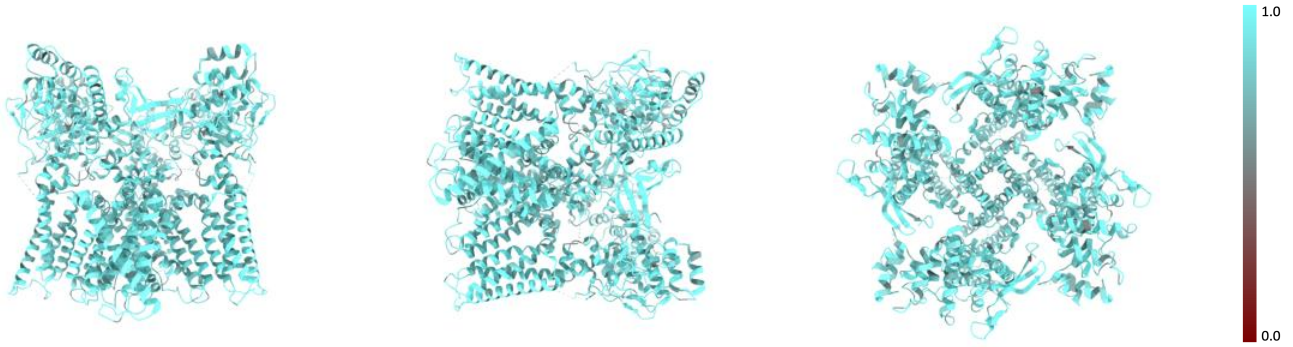
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

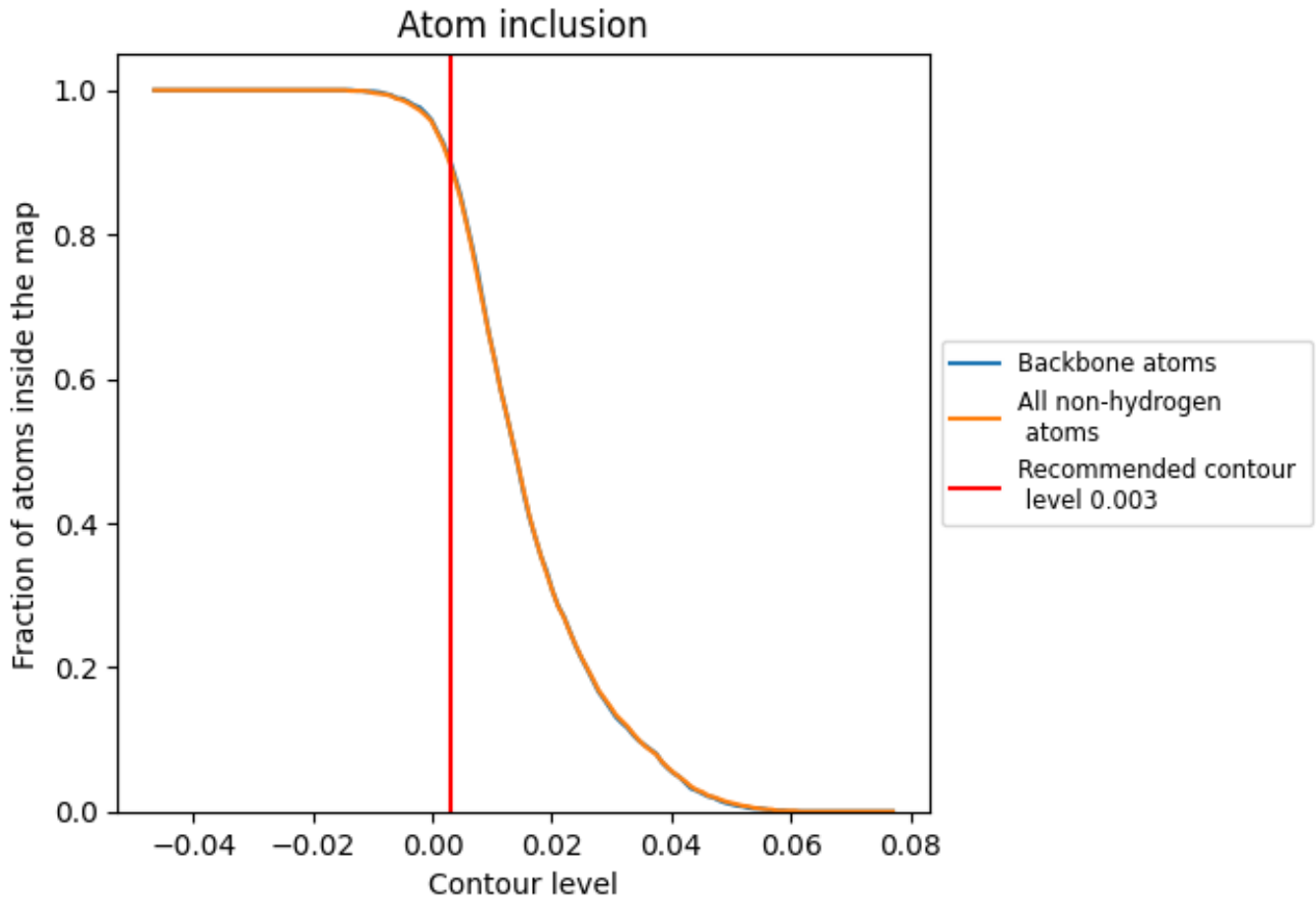
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.4470
A	0.9030	0.4500
B	0.8930	0.4450
C	0.8970	0.4460
D	0.9000	0.4470