



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 8YCP / pdb_00008ycp
EMDB ID : EMD-39151
Title : structure of human trpv1 in complex with BC5
Authors : Ke, B.W.; Hu, S.L.
Deposited on : 2024-02-18
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

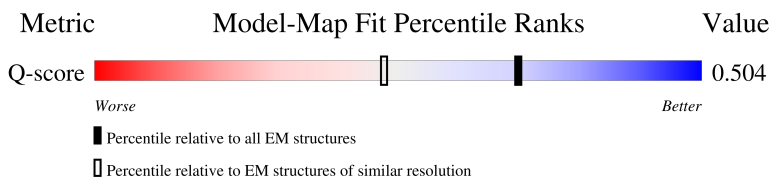
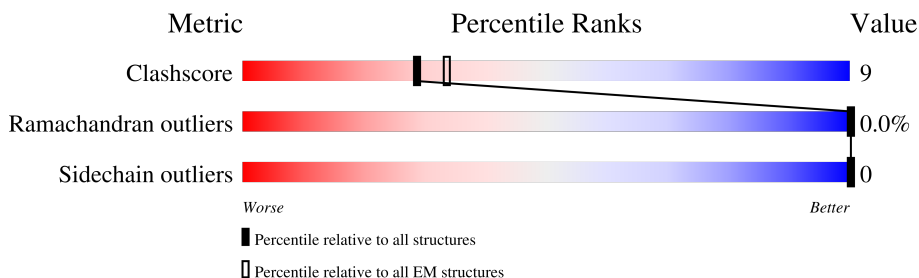
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	656	67% 72% 22% 5%
1	B	656	59% 74% 22%
1	C	656	64% 72% 22% 6%
1	D	656	48% 71% 24% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20462 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	620	Total	C	N	O	S	0	0
			5019	3266	816	904	33		
1	B	632	Total	C	N	O	S	0	0
			5110	3321	832	924	33		
1	C	615	Total	C	N	O	S	0	0
			4964	3230	805	896	33		
1	D	619	Total	C	N	O	S	0	0
			5008	3258	815	902	33		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	MET	-	initiating methionine	UNP Q8NER1
B	110	MET	-	initiating methionine	UNP Q8NER1
C	110	MET	-	initiating methionine	UNP Q8NER1
D	110	MET	-	initiating methionine	UNP Q8NER1

- Molecule 2 is (1 {R},2 {S})-1-butyl- {N}-(2,6-dimethylphenyl)-1-[5-[(2 {S})-2-[(2,6-dimethylphenyl)carbamoyl]piperidin-1-yl]pentyl]piperidin-1-ium-2-carboxamide (CCD ID: A1LZ2) (formula: C₃₇H₅₇N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 43	C 37	N 4	O 2	0
2	B	1	Total 43	C 37	N 4	O 2	0
2	C	1	Total 43	C 37	N 4	O 2	0
2	D	1	Total 43	C 37	N 4	O 2	0

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



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			46	37	8	1	
3	B	1	Total	C	O	P	0
			48	39	8	1	
3	B	1	Total	C	O	P	0
			48	39	8	1	
3	D	1	Total	C	O	P	0
			46	37	8	1	

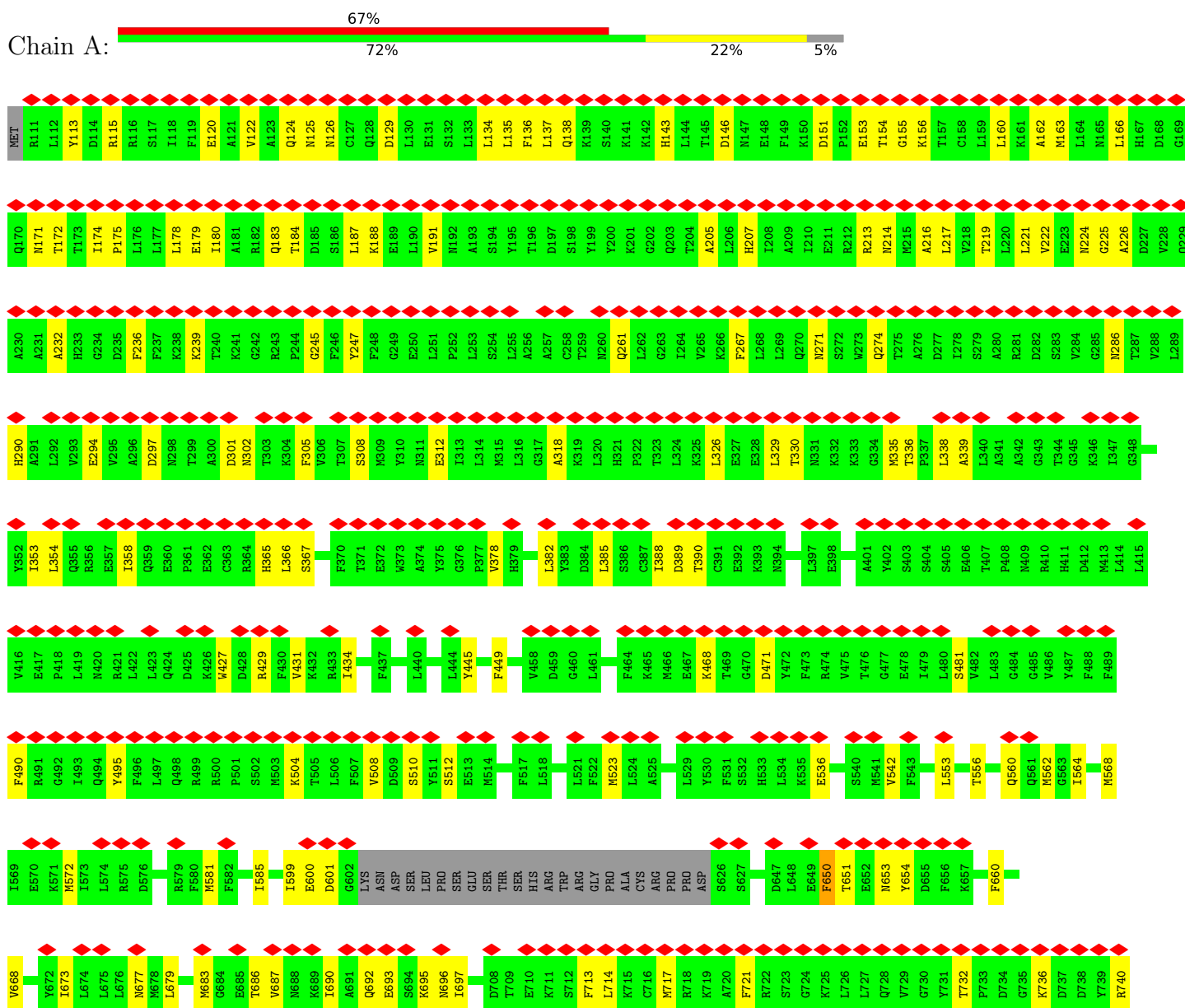
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

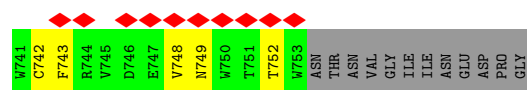
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Na	0
			1	1	

3 Residue-property plots

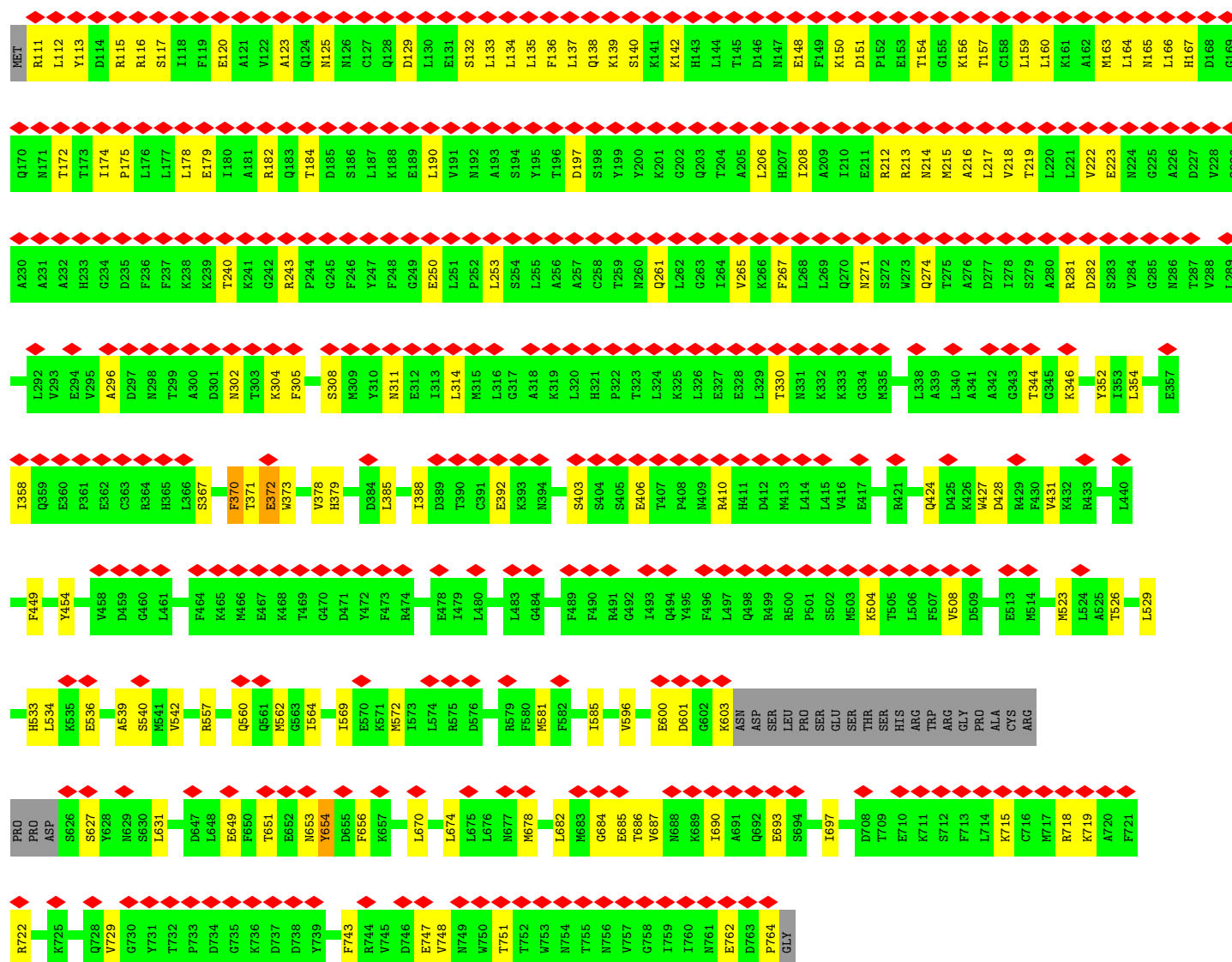
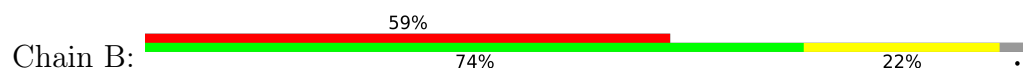
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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



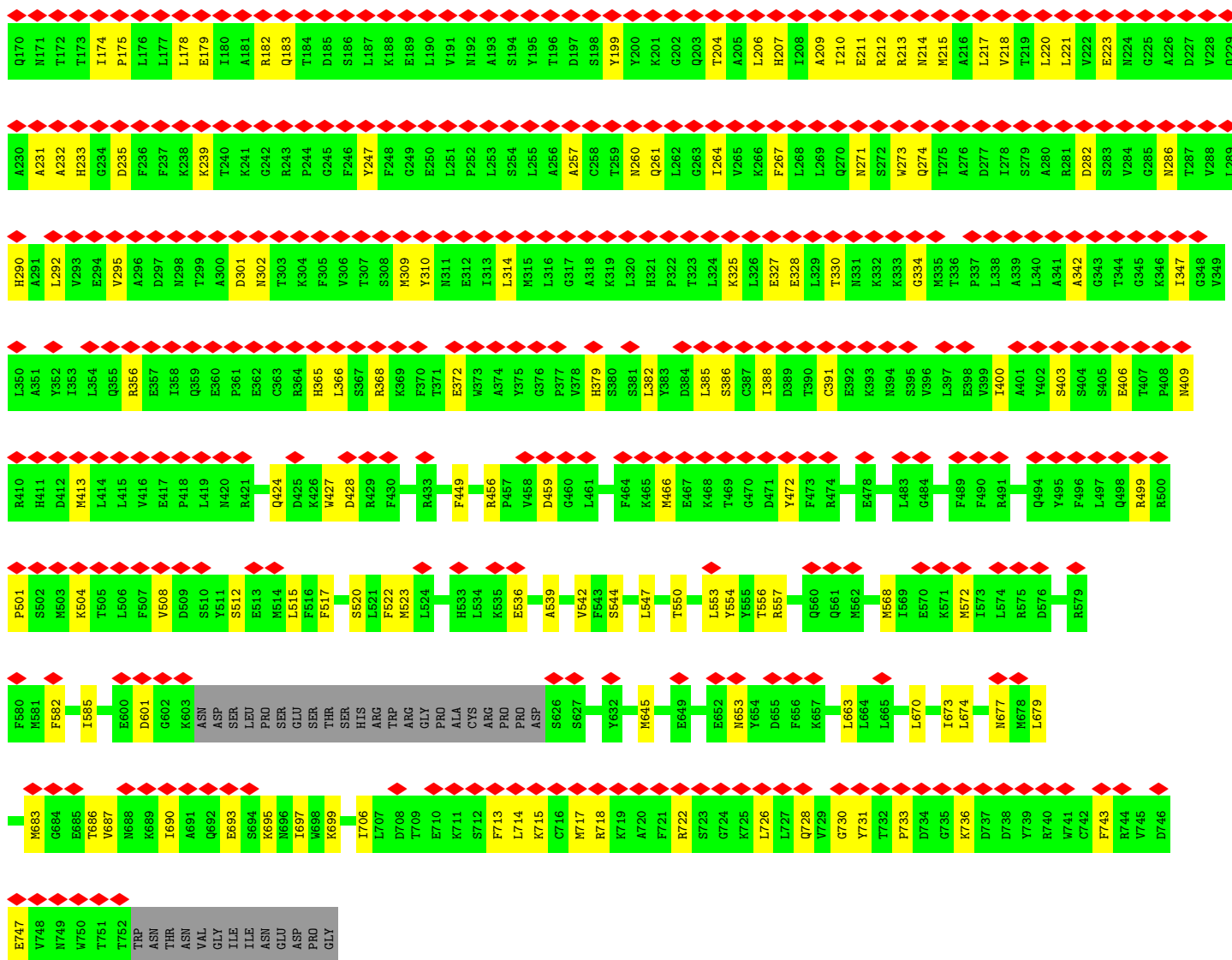


- Molecule 1: Transient receptor potential cation channel subfamily V member 1

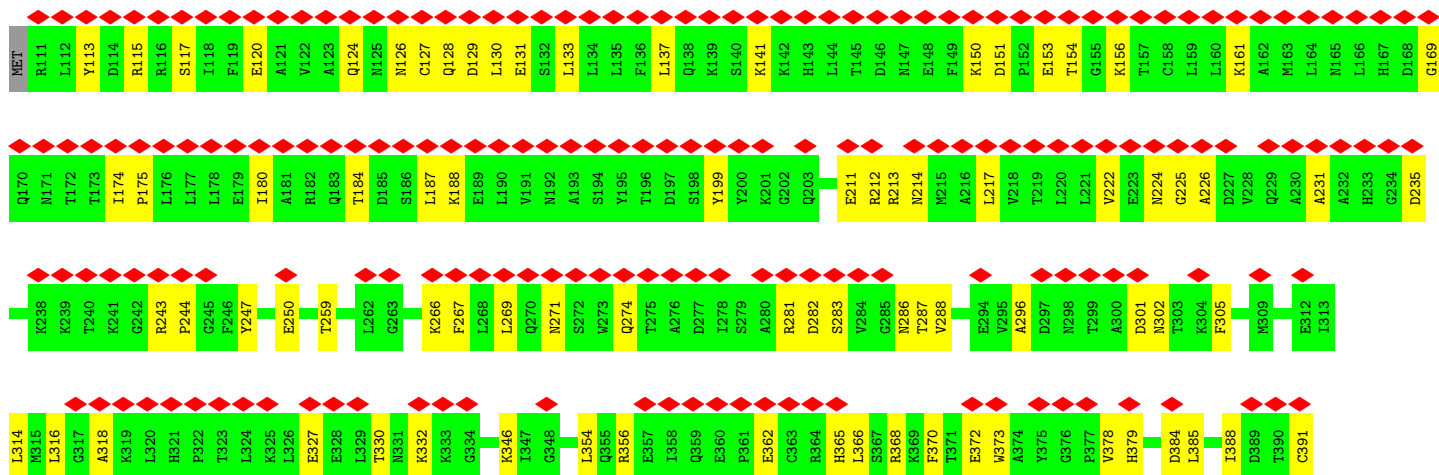


- Molecule 1: Transient receptor potential cation channel subfamily V member 1





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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	729166	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.402	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.172	Depositor
Map size ($\text{\AA}$)	294.84, 294.84, 294.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.819, 0.819, 0.819	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1LZ2, 6OU, NA

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	0/5131	0.41	0/6939
1	B	0.33	0/5223	0.44	2/7065 (0.0%)
1	C	0.30	0/5073	0.40	0/6859
1	D	0.34	0/5118	0.42	0/6919
All	All	0.32	0/20545	0.42	2/27782 (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	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	PHE	CA-C-N	-5.16	111.68	121.54
1	B	370	PHE	C-N-CA	-5.16	111.68	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	650	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	654	TYR	Peptide
1	D	650	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5019	0	5059	95	0
1	B	5110	0	5148	104	0
1	C	4964	0	5012	97	0
1	D	5008	0	5057	102	0
2	A	43	0	0	1	0
2	B	43	0	0	2	0
2	C	43	0	0	1	0
2	D	43	0	0	0	0
3	A	46	0	0	0	0
3	B	96	0	0	0	0
3	D	46	0	0	0	0
4	A	1	0	0	0	0
All	All	20462	0	20276	383	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 9.

All (383) 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:C:260:ASN:HA	1:C:309:MET:HE1	1.58	0.84
1:A:601:ASP:O	1:A:653:ASN:ND2	2.13	0.81
1:A:651:THR:HB	1:A:654:TYR:HE1	1.48	0.79
1:D:601:ASP:O	1:D:653:ASN:ND2	2.17	0.78
1:A:151:ASP:HB3	1:A:155:GLY:H	1.49	0.76
1:D:485:GLY:O	1:D:520:SER:OG	2.03	0.75
1:B:378:VAL:HG12	1:B:748:VAL:HG22	1.68	0.74
1:D:133:LEU:HD11	1:D:180:ILE:HD13	1.68	0.74
1:C:715:LYS:HA	1:C:718:ARG:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD23	1:A:184:THR:HG21	1.70	0.73
1:D:327:GLU:OE1	1:D:356:ARG:NH2	2.18	0.72
1:C:379:HIS:ND1	1:C:747:GLU:OE2	2.21	0.71
1:C:695:LYS:HE2	1:C:699:LYS:HE2	1.72	0.70
1:C:163:MET:HE2	1:C:209:ALA:HA	1.72	0.70
1:B:569:ILE:HG12	1:D:678:MET:HE1	1.72	0.70
1:D:372:GLU:OE1	1:D:744:ARG:NH1	2.26	0.69
1:B:601:ASP:OD1	1:B:653:ASN:ND2	2.26	0.69
1:C:179:GLU:O	1:C:183:GLN:NE2	2.27	0.67
1:D:188:LYS:NZ	1:D:225:GLY:O	2.28	0.67
1:D:281:ARG:NH1	1:D:330:THR:O	2.28	0.67
1:D:187:LEU:HD21	1:D:224:ASN:HB3	1.77	0.66
1:D:354:LEU:HD22	1:D:388:ILE:HD11	1.77	0.66
1:B:354:LEU:HD22	1:B:388:ILE:HD11	1.76	0.66
1:C:213:ARG:NH1	1:C:261:GLN:OE1	2.29	0.66
1:A:378:VAL:HG12	1:A:748:VAL:HG12	1.76	0.66
1:C:553:LEU:O	1:C:556:THR:OG1	2.11	0.66
1:B:424:GLN:NE2	1:B:428:ASP:OD2	2.29	0.66
1:A:222:VAL:HG11	1:A:267:PHE:HE2	1.61	0.66
1:C:211:GLU:OE2	1:C:212:ARG:NH1	2.29	0.65
1:A:126:ASN:ND2	1:A:129:ASP:OD2	2.30	0.65
1:D:728:GLN:NE2	1:D:737:ASP:OD1	2.30	0.65
1:D:378:VAL:HG12	1:D:748:VAL:HG22	1.79	0.65
1:A:365:HIS:O	1:A:740:ARG:NH2	2.28	0.64
1:A:553:LEU:O	1:A:556:THR:OG1	2.13	0.64
1:A:163:MET:HE3	1:A:205:ALA:HB1	1.80	0.64
1:D:392:GLU:OE1	1:D:392:GLU:N	2.31	0.64
1:A:153:GLU:HG3	1:A:154:THR:HG23	1.80	0.64
1:C:601:ASP:O	1:C:653:ASN:ND2	2.30	0.64
1:C:728:GLN:NE2	1:C:730:GLY:O	2.30	0.63
1:B:216:ALA:O	1:B:219:THR:OG1	2.14	0.63
1:B:111:ARG:NH1	1:B:129:ASP:OD1	2.31	0.63
1:C:368:ARG:NH2	1:C:386:SER:O	2.32	0.63
1:D:153:GLU:HG2	1:D:154:THR:HG23	1.80	0.63
1:D:379:HIS:ND1	1:D:747:GLU:OE2	2.24	0.62
1:B:115:ARG:NH2	1:B:148:GLU:O	2.31	0.62
1:B:219:THR:O	1:B:223:GLU:HG2	2.00	0.61
1:B:371:THR:O	1:B:372:GLU:HB2	2.00	0.61
1:C:247:TYR:OH	1:C:286:ASN:OD1	2.19	0.61
1:D:126:ASN:ND2	1:D:129:ASP:OD2	2.34	0.61
1:B:526:THR:HG1	1:B:540:SER:HG	1.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TYR:OH	1:A:129:ASP:O	2.15	0.61
1:A:382:LEU:HB3	1:A:742:CYS:HB3	1.83	0.60
1:C:169:GLY:O	1:C:214:ASN:ND2	2.35	0.60
1:D:554:TYR:O	1:D:557:ARG:HG2	2.02	0.60
1:B:600:GLU:HG2	1:C:456:ARG:HH22	1.67	0.59
1:D:213:ARG:NH2	1:D:259:THR:O	2.34	0.59
1:D:301:ASP:OD1	1:D:302:ASN:N	2.34	0.59
1:B:137:LEU:HD23	1:B:184:THR:HG21	1.83	0.59
1:B:715:LYS:HG2	1:B:718:ARG:HH21	1.68	0.59
1:A:302:ASN:HA	1:A:305:PHE:CE1	2.36	0.59
1:A:354:LEU:HD22	1:A:388:ILE:HD11	1.85	0.59
1:B:693:GLU:O	1:B:697:ILE:HG12	2.03	0.58
1:C:424:GLN:NE2	1:C:428:ASP:OD2	2.37	0.58
1:B:572:MET:HE1	1:B:687:VAL:CG2	2.34	0.58
1:B:358:ILE:H	1:B:367:SER:HB3	1.67	0.58
1:C:282:ASP:OD1	1:C:286:ASN:N	2.35	0.58
1:A:330:THR:HG22	1:A:336:THR:HG22	1.86	0.58
1:C:119:PHE:HB3	1:C:161:LYS:HG2	1.86	0.58
1:D:269:LEU:HD12	1:D:316:LEU:HD23	1.86	0.58
1:B:572:MET:HE1	1:B:687:VAL:HG23	1.85	0.57
1:D:417:GLU:OE1	1:D:421:ARG:NH1	2.37	0.57
1:A:271:ASN:ND2	1:A:274:GLN:O	2.37	0.57
1:B:163:MET:HE1	1:B:217:LEU:HD13	1.86	0.57
1:D:287:THR:HG22	1:D:288:VAL:H	1.70	0.57
1:A:120:GLU:O	1:A:124:GLN:NE2	2.38	0.57
1:C:547:LEU:HA	1:C:550:THR:HG22	1.86	0.57
1:C:153:GLU:HG2	1:C:154:THR:HG23	1.86	0.57
1:B:115:ARG:HH12	1:B:150:LYS:C	2.13	0.57
1:A:560:GLN:O	1:A:564:ILE:HG12	2.04	0.56
1:C:175:PRO:HA	1:C:178:LEU:HD12	1.87	0.56
1:A:468:LYS:N	1:A:471:ASP:OD1	2.35	0.56
1:B:682:LEU:O	1:B:685:GLU:HG3	2.05	0.56
1:D:651:THR:HG22	1:D:660:PHE:CE1	2.40	0.56
1:C:239:LYS:HE2	1:C:247:TYR:HB3	1.87	0.56
1:C:673:ILE:O	1:C:677:ASN:ND2	2.39	0.55
1:D:365:HIS:O	1:D:740:ARG:NH2	2.36	0.55
1:A:679:LEU:HD11	1:A:683:MET:HE3	1.88	0.55
1:B:678:MET:HG3	1:C:572:MET:HE3	1.86	0.55
1:B:154:THR:HG23	1:B:156:LYS:H	1.71	0.55
1:C:231:ALA:O	1:C:233:HIS:ND1	2.35	0.55
1:A:222:VAL:HG11	1:A:267:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:GLU:HA	1:B:651:THR:HG23	1.89	0.55
1:A:163:MET:HE1	1:A:221:LEU:HD21	1.88	0.54
1:B:379:HIS:NE2	1:B:747:GLU:OE1	2.35	0.54
1:A:650:PHE:N	1:A:651:THR:HG23	2.23	0.54
1:C:207:HIS:CE1	1:C:232:ALA:HB2	2.42	0.54
1:A:115:ARG:NH1	1:A:151:ASP:OD1	2.35	0.54
1:D:282:ASP:OD1	1:D:286:ASN:N	2.41	0.54
1:B:601:ASP:OD2	1:B:627:SER:OG	2.19	0.54
1:D:266:LYS:HG2	1:D:316:LEU:HD21	1.89	0.54
1:A:504:LYS:O	1:A:508:VAL:HG22	2.08	0.53
1:B:197:ASP:OD1	1:B:197:ASP:N	2.40	0.53
1:B:684:GLY:HA2	1:D:681:ALA:HB1	1.90	0.53
1:D:385:LEU:HD11	1:D:743:PHE:HB2	1.90	0.53
1:A:187:LEU:HD21	1:A:224:ASN:HB3	1.91	0.53
1:C:199:TYR:HA	1:C:235:ASP:HB3	1.91	0.53
1:D:113:TYR:OH	1:D:129:ASP:O	2.26	0.53
1:A:581:MET:O	1:A:585:ILE:HG12	2.08	0.53
1:B:654:TYR:HB3	1:B:656:PHE:H	1.73	0.53
1:A:166:LEU:HD13	1:A:171:ASN:HB2	1.89	0.53
1:A:714:LEU:HD12	1:A:717:MET:HE1	1.90	0.53
1:A:135:LEU:HA	1:A:138:GLN:NE2	2.24	0.53
1:B:581:MET:O	1:B:585:ILE:HG12	2.08	0.53
1:D:404:SER:OG	1:D:406:GLU:OE1	2.17	0.53
1:A:562:MET:HE2	1:C:582:PHE:CD2	2.45	0.52
1:D:243:ARG:HH11	1:D:244:PRO:HD2	1.74	0.52
1:A:188:LYS:NZ	1:A:225:GLY:HA3	2.24	0.52
1:A:326:LEU:HD12	1:A:329:LEU:HD12	1.90	0.52
1:D:717:MET:O	1:D:721:PHE:N	2.43	0.52
1:A:143:HIS:N	1:A:146:ASP:OD2	2.36	0.52
1:A:651:THR:HB	1:A:654:TYR:CE1	2.36	0.52
1:D:131:GLU:N	1:D:131:GLU:OE1	2.43	0.52
1:A:673:ILE:O	1:A:677:ASN:ND2	2.43	0.52
1:D:243:ARG:HD2	1:D:244:PRO:HD2	1.91	0.52
1:B:115:ARG:HD2	1:B:116:ARG:NH1	2.25	0.52
1:B:271:ASN:ND2	1:B:274:GLN:O	2.39	0.52
1:C:301:ASP:OD1	1:C:302:ASN:N	2.42	0.52
1:C:427:TRP:HB2	1:C:706:ILE:HD11	1.91	0.52
1:D:283:SER:O	1:D:332:LYS:NZ	2.35	0.52
1:B:539:ALA:O	1:B:542:VAL:HG22	2.09	0.52
1:D:499:ARG:HB3	1:D:501:PRO:HD3	1.91	0.52
1:B:179:GLU:OE1	1:B:182:ARG:NH2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:GLU:O	1:A:697:ILE:HG13	2.10	0.51
1:C:178:LEU:HD11	1:C:220:LEU:HD21	1.92	0.51
1:D:302:ASN:HA	1:D:305:PHE:CE1	2.45	0.51
1:B:115:ARG:NH1	1:B:151:ASP:HA	2.24	0.51
1:B:557:ARG:HH22	2:B:801:A1LZ2:C35	2.24	0.51
1:C:568:MET:O	1:C:572:MET:HG2	2.10	0.51
1:C:572:MET:HE1	1:C:687:VAL:HG23	1.90	0.51
1:A:562:MET:HE2	1:C:582:PHE:HD2	1.75	0.51
1:D:127:CYS:HA	1:D:130:LEU:HD13	1.93	0.51
1:D:271:ASN:ND2	1:D:274:GLN:O	2.42	0.51
1:A:134:LEU:HB3	1:A:180:ILE:HG12	1.92	0.51
1:C:391:CYS:SG	1:C:722:ARG:NH1	2.84	0.51
1:B:392:GLU:N	1:B:392:GLU:OE1	2.44	0.51
1:D:247:TYR:OH	1:D:286:ASN:ND2	2.32	0.51
1:D:126:ASN:HD21	1:D:128:GLN:HE21	1.59	0.50
1:D:391:CYS:SG	1:D:722:ARG:NH2	2.85	0.50
1:B:526:THR:OG1	1:B:540:SER:OG	2.16	0.50
1:D:120:GLU:OE1	1:D:124:GLN:NE2	2.40	0.50
1:B:296:ALA:O	1:B:346:LYS:NZ	2.26	0.50
1:D:539:ALA:O	1:D:542:VAL:HG22	2.12	0.50
1:B:302:ASN:HA	1:B:305:PHE:CE1	2.45	0.50
1:D:174:ILE:HG13	1:D:175:PRO:HD3	1.94	0.50
1:D:318:ALA:HB2	1:D:366:LEU:HD11	1.94	0.50
1:A:385:LEU:HD11	1:A:743:PHE:HB2	1.94	0.50
1:C:400:ILE:O	1:C:403:SER:OG	2.29	0.50
1:A:191:VAL:HG13	1:A:221:LEU:HD12	1.94	0.49
1:C:286:ASN:HB3	1:C:290:HIS:HB2	1.94	0.49
1:B:715:LYS:HD3	1:B:719:LYS:HZ1	1.78	0.49
1:D:169:GLY:O	1:D:214:ASN:ND2	2.32	0.49
1:D:725:LYS:HD2	1:D:744:ARG:HH21	1.76	0.49
1:A:214:ASN:HB3	1:A:217:LEU:CD2	2.43	0.49
1:A:564:ILE:HD12	1:A:695:LYS:HA	1.94	0.49
1:B:403:SER:O	1:B:410:ARG:NE	2.46	0.49
1:A:217:LEU:O	1:A:221:LEU:HD23	2.13	0.49
1:D:368:ARG:HD2	1:D:384:ASP:HB3	1.95	0.49
1:D:373:TRP:HZ3	1:D:378:VAL:HG23	1.76	0.49
1:D:726:LEU:HD11	1:D:739:TYR:HB3	1.94	0.49
1:C:449:PHE:CZ	1:C:523:MET:HE1	2.47	0.49
1:C:713:PHE:HE2	1:C:717:MET:HB2	1.78	0.49
1:C:179:GLU:HG3	1:C:182:ARG:HH12	1.77	0.49
1:D:641:PHE:HA	1:D:646:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:O	1:B:164:LEU:HG	2.13	0.48
1:C:645:MET:O	1:C:645:MET:HG3	2.13	0.48
1:D:427:TRP:HA	1:D:431:VAL:HB	1.95	0.48
1:B:529:LEU:HD22	1:B:534:LEU:HD12	1.95	0.48
1:A:429:ARG:HH22	1:A:721:PHE:C	2.21	0.48
1:D:211:GLU:OE2	1:D:212:ARG:NH2	2.36	0.48
1:A:134:LEU:HD12	1:A:135:LEU:N	2.29	0.48
1:B:751:THR:HG23	1:D:301:ASP:OD2	2.14	0.48
1:C:679:LEU:HD11	1:C:683:MET:HE3	1.96	0.48
1:A:495:TYR:OH	1:A:510:SER:OG	2.24	0.48
1:C:459:ASP:N	1:C:459:ASP:OD1	2.46	0.48
1:A:178:LEU:HD21	1:A:224:ASN:OD1	2.14	0.48
1:C:310:TYR:O	1:C:314:LEU:HD23	2.14	0.48
1:A:179:GLU:OE1	1:A:183:GLN:NE2	2.47	0.48
1:D:180:ILE:O	1:D:184:THR:HG23	2.14	0.48
1:A:239:LYS:HB2	1:A:247:TYR:HB2	1.96	0.48
1:D:126:ASN:HD21	1:D:128:GLN:NE2	2.12	0.48
1:A:216:ALA:O	1:A:219:THR:HG22	2.14	0.47
1:A:335:MET:HE3	1:A:339:ALA:C	2.39	0.47
1:C:292:LEU:O	1:C:295:VAL:HG12	2.14	0.47
1:C:686:THR:O	1:C:690:ILE:HG12	2.14	0.47
1:B:135:LEU:HG	1:B:139:LYS:HD2	1.95	0.47
1:C:257:ALA:HA	1:C:309:MET:SD	2.54	0.47
1:C:327:GLU:OE1	1:C:356:ARG:NH2	2.45	0.47
1:D:370:PHE:CZ	1:D:729:VAL:HG11	2.50	0.47
1:A:717:MET:O	1:A:721:PHE:HD2	1.97	0.47
1:D:466:MET:HE1	1:D:472:TYR:CD1	2.50	0.47
1:D:443:CYS:O	1:D:447:ILE:HG12	2.14	0.47
1:A:213:ARG:HA	1:A:261:GLN:OE1	2.15	0.47
1:B:133:LEU:HA	1:B:136:PHE:HB3	1.96	0.47
1:B:370:PHE:CZ	1:B:729:VAL:HG11	2.49	0.47
1:B:373:TRP:HB2	1:B:764:PRO:HA	1.96	0.47
1:A:692:GLN:OE1	1:A:696:ASN:ND2	2.47	0.47
1:A:318:ALA:HB2	1:A:366:LEU:HD11	1.96	0.47
1:A:358:ILE:H	1:A:367:SER:HB3	1.80	0.47
1:B:656:PHE:CZ	1:C:536:GLU:HA	2.50	0.47
1:B:115:ARG:HH12	1:B:151:ASP:HA	1.80	0.47
1:D:137:LEU:O	1:D:141:LYS:N	2.47	0.47
1:D:199:TYR:HA	1:D:235:ASP:HB2	1.97	0.47
1:A:542:VAL:CG1	1:C:663:LEU:HD11	2.45	0.46
1:B:140:SER:HB2	1:B:142:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:NH2	1:D:150:LYS:O	2.46	0.46
1:A:536:GLU:OE1	1:A:536:GLU:N	2.45	0.46
1:D:113:TYR:CE2	1:D:133:LEU:HB3	2.50	0.46
1:A:301:ASP:N	1:A:301:ASP:OD1	2.48	0.46
1:C:342:ALA:O	1:C:413:MET:HE1	2.15	0.46
1:C:365:HIS:CG	1:C:733:PRO:HD3	2.51	0.46
1:A:207:HIS:CE1	1:A:232:ALA:HB2	2.51	0.46
1:C:539:ALA:O	1:C:542:VAL:HG22	2.16	0.46
1:A:308:SER:O	1:A:312:GLU:HG2	2.16	0.46
1:A:427:TRP:HA	1:A:431:VAL:HB	1.97	0.46
1:C:156:LYS:HZ1	1:C:160:LEU:HB3	1.80	0.46
1:B:250:GLU:HB2	1:B:282:ASP:OD1	2.16	0.46
1:D:439:PHE:HE1	1:D:552:MET:SD	2.39	0.46
1:A:568:MET:O	1:A:572:MET:HG2	2.15	0.46
1:B:174:ILE:O	1:B:178:LEU:HD23	2.16	0.46
1:B:651:THR:HG22	1:B:654:TYR:OH	2.15	0.46
1:C:271:ASN:ND2	1:C:274:GLN:O	2.37	0.46
1:B:344:THR:HG21	1:B:346:LYS:HE2	1.98	0.46
1:C:406:GLU:OE1	1:C:406:GLU:N	2.45	0.46
1:B:449:PHE:CZ	1:B:523:MET:HE1	2.51	0.46
1:C:174:ILE:HB	1:C:175:PRO:HD3	1.96	0.46
1:A:122:VAL:HB	1:A:162:ALA:HB2	1.98	0.45
1:A:749:ASN:ND2	1:A:752:THR:OG1	2.49	0.45
1:C:273:TRP:H	1:C:273:TRP:HE3	1.64	0.45
1:A:290:HIS:O	1:A:294:GLU:HG3	2.16	0.45
1:B:253:LEU:HD11	1:B:265:VAL:HG13	1.99	0.45
1:A:188:LYS:HZ3	1:A:225:GLY:HA3	1.81	0.45
1:B:372:GLU:HG3	1:B:373:TRP:CD1	2.52	0.45
1:B:601:ASP:O	1:B:603:LYS:N	2.41	0.45
1:C:601:ASP:N	1:C:601:ASP:OD1	2.49	0.45
1:A:222:VAL:HA	1:A:226:ALA:HB3	1.99	0.45
1:B:304:LYS:NZ	1:B:308:SER:HB2	2.32	0.45
1:B:572:MET:HE2	1:B:686:THR:HG22	1.99	0.45
1:D:479:ILE:HG13	1:D:480:LEU:N	2.30	0.45
1:A:512:SER:HB3	2:A:801:A1LZ2:C37	2.47	0.45
1:B:112:LEU:HA	1:B:136:PHE:HE1	1.81	0.45
1:A:113:TYR:HB2	1:A:136:PHE:CE2	2.52	0.45
1:A:572:MET:CE	1:A:687:VAL:HG23	2.47	0.45
1:B:113:TYR:OH	1:B:132:SER:HB2	2.17	0.45
1:B:214:ASN:O	1:B:218:VAL:HG23	2.17	0.45
1:D:429:ARG:NH2	1:D:721:PHE:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:713:PHE:O	1:D:718:ARG:NE	2.49	0.45
1:A:271:ASN:ND2	1:A:274:GLN:H	2.15	0.45
1:B:134:LEU:O	1:B:138:GLN:NE2	2.44	0.45
1:C:385:LEU:HD11	1:C:743:PHE:HB2	1.99	0.45
1:D:368:ARG:CD	1:D:384:ASP:HB3	2.47	0.45
1:D:686:THR:O	1:D:690:ILE:HG12	2.17	0.45
1:A:156:LYS:HA	1:A:160:LEU:HD12	1.99	0.44
1:C:206:LEU:O	1:C:210:ILE:HG12	2.17	0.44
1:D:561:GLN:HG2	1:D:562:MET:N	2.32	0.44
1:A:668:VAL:HG11	1:D:643:ILE:HD11	1.99	0.44
1:C:504:LYS:O	1:C:508:VAL:HB	2.18	0.44
1:A:601:ASP:OD1	1:A:601:ASP:N	2.50	0.44
1:A:651:THR:HG22	1:A:660:PHE:CE1	2.52	0.44
1:B:670:LEU:O	1:B:674:LEU:HB3	2.17	0.44
1:C:330:THR:HB	1:C:334:GLY:HA2	1.99	0.44
1:D:593:THR:O	1:D:597:THR:HG23	2.17	0.44
1:B:123:ALA:HA	1:B:165:ASN:HD21	1.83	0.44
1:C:499:ARG:HB2	1:C:501:PRO:HD3	2.00	0.44
1:B:651:THR:HB	1:B:654:TYR:CE1	2.53	0.44
1:D:693:GLU:O	1:D:697:ILE:HG13	2.17	0.44
1:A:338:LEU:HD13	1:A:353:ILE:HG21	1.99	0.44
1:C:261:GLN:HG2	1:C:264:ILE:HD12	1.98	0.44
1:B:222:VAL:HG21	1:B:267:PHE:CE2	2.53	0.44
1:D:156:LYS:HE3	1:D:161:LYS:HD3	1.99	0.44
1:C:175:PRO:O	1:C:178:LEU:HB2	2.18	0.44
1:C:214:ASN:O	1:C:218:VAL:HG23	2.18	0.44
1:D:287:THR:HG22	1:D:288:VAL:N	2.33	0.44
1:A:389:ASP:OD1	1:A:390:THR:N	2.51	0.43
1:A:434:ILE:HD13	1:A:713:PHE:CE2	2.52	0.43
1:D:222:VAL:HA	1:D:226:ALA:HB3	2.00	0.43
1:B:215:MET:O	1:B:219:THR:HG23	2.19	0.43
1:C:223:GLU:HG2	1:C:273:TRP:CE2	2.53	0.43
1:C:466:MET:HE2	1:C:472:TYR:CD2	2.53	0.43
1:A:297:ASP:OD1	1:A:302:ASN:ND2	2.27	0.43
1:B:678:MET:HE2	1:B:678:MET:HB3	1.75	0.43
1:B:762:GLU:OE1	1:B:762:GLU:N	2.51	0.43
1:C:347:ILE:HD13	1:C:413:MET:HG2	2.01	0.43
1:D:296:ALA:O	1:D:346:LYS:NZ	2.42	0.43
1:A:236:PHE:CE1	1:A:245:GLY:HA2	2.53	0.43
1:B:596:VAL:HG21	1:B:631:LEU:HA	2.00	0.43
1:C:161:LYS:NZ	1:C:165:ASN:OD1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ILE:CG1	1:D:175:PRO:HD3	2.48	0.43
1:A:172:THR:O	1:A:175:PRO:HD2	2.18	0.43
1:A:286:ASN:ND2	1:A:294:GLU:OE2	2.52	0.43
1:A:732:THR:HG21	1:A:736:LYS:NZ	2.34	0.43
1:C:204:THR:HG22	1:C:206:LEU:H	1.83	0.43
1:C:372:GLU:HG3	1:C:382:LEU:HG	2.01	0.43
1:D:577:LEU:O	1:D:581:MET:HG2	2.19	0.43
1:D:599:ILE:HG22	1:D:600:GLU:O	2.19	0.43
1:A:523:MET:HB2	1:A:523:MET:HE2	1.68	0.43
1:C:517:PHE:O	1:C:520:SER:OG	2.31	0.43
1:D:673:ILE:O	1:D:677:ASN:ND2	2.51	0.43
1:D:188:LYS:HD2	1:D:188:LYS:HA	1.85	0.43
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.90	0.42
1:C:137:LEU:O	1:C:141:LYS:N	2.52	0.42
1:A:445:TYR:HE2	1:A:481:SER:HA	1.85	0.42
1:B:115:ARG:HH12	1:B:151:ASP:N	2.16	0.42
1:D:689:LYS:HB2	1:D:689:LYS:HE2	1.82	0.42
1:B:504:LYS:O	1:B:508:VAL:HB	2.19	0.42
1:C:693:GLU:O	1:C:697:ILE:HG13	2.19	0.42
1:D:585:ILE:HD13	1:D:585:ILE:HA	1.93	0.42
1:A:174:ILE:HB	1:A:175:PRO:HD3	2.02	0.42
1:B:427:TRP:HA	1:B:431:VAL:HB	2.01	0.42
1:C:215:MET:HE1	1:C:267:PHE:HB2	2.00	0.42
1:C:731:TYR:HA	1:C:736:LYS:O	2.18	0.42
1:B:208:ILE:O	1:B:212:ARG:HG2	2.20	0.42
1:C:554:TYR:O	1:C:557:ARG:HG3	2.20	0.42
1:D:271:ASN:ND2	1:D:274:GLN:H	2.18	0.42
1:C:466:MET:HE2	1:C:472:TYR:HD2	1.84	0.42
1:B:213:ARG:HG2	1:B:261:GLN:NE2	2.34	0.42
1:B:562:MET:HE2	1:D:582:PHE:CD1	2.54	0.42
1:D:222:VAL:HG11	1:D:267:PHE:CE1	2.55	0.42
1:D:362:GLU:OE1	1:D:362:GLU:N	2.47	0.42
1:D:425:ASP:O	1:D:429:ARG:HB2	2.20	0.42
1:A:125:ASN:C	1:A:125:ASN:HD22	2.28	0.41
1:B:159:LEU:HB2	1:B:190:LEU:HD11	2.02	0.41
1:B:172:THR:O	1:B:175:PRO:HD2	2.20	0.41
1:B:222:VAL:HG21	1:B:267:PHE:HE2	1.84	0.41
1:B:311:ASN:OD1	1:B:352:TYR:OH	2.33	0.41
1:B:560:GLN:O	1:B:564:ILE:HG13	2.19	0.41
1:D:117:SER:O	1:D:120:GLU:HG3	2.20	0.41
1:D:151:ASP:OD2	1:D:154:THR:OG1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:PHE:CZ	1:A:523:MET:HE1	2.56	0.41
1:B:117:SER:O	1:B:120:GLU:HG3	2.20	0.41
1:D:314:LEU:HG	1:D:366:LEU:HD13	2.02	0.41
1:B:150:LYS:HB3	1:B:157:THR:HG22	2.02	0.41
1:C:409:ASN:O	1:C:413:MET:HG3	2.21	0.41
1:C:670:LEU:O	1:C:674:LEU:HB3	2.21	0.41
1:D:397:LEU:HA	1:D:397:LEU:HD23	1.83	0.41
1:B:240:THR:HG21	1:B:243:ARG:NH1	2.35	0.41
1:B:557:ARG:HH22	2:B:801:A1LZ2:C36	2.34	0.41
1:C:522:PHE:HB3	1:C:544:SER:HB2	2.03	0.41
1:C:693:GLU:N	1:C:693:GLU:OE2	2.51	0.41
1:B:536:GLU:OE1	1:B:536:GLU:N	2.45	0.41
1:C:325:LYS:HD2	1:C:328:GLU:OE2	2.21	0.41
1:B:163:MET:HE3	1:B:166:LEU:HD21	2.01	0.41
1:B:206:LEU:HD11	1:B:218:VAL:HG13	2.03	0.41
1:B:385:LEU:HD11	1:B:743:PHE:HB2	2.03	0.41
1:B:454:TYR:CE2	1:D:596:VAL:HG11	2.55	0.41
1:C:714:LEU:HD11	1:C:717:MET:HE2	2.03	0.41
1:C:726:LEU:HD12	1:C:726:LEU:HA	1.92	0.41
1:D:217:LEU:HD23	1:D:217:LEU:HA	1.79	0.41
1:D:642:THR:HG23	1:D:676:LEU:HD11	2.03	0.41
1:B:406:GLU:OE1	1:B:406:GLU:N	2.54	0.41
1:B:533:HIS:O	1:B:534:LEU:HD23	2.21	0.41
1:B:685:GLU:HG2	1:C:687:VAL:HG11	2.02	0.41
1:B:722:ARG:HE	1:B:722:ARG:HB3	1.61	0.41
1:C:217:LEU:O	1:C:221:LEU:HD23	2.21	0.41
1:C:512:SER:HB3	2:C:801:A1LZ2:C37	2.51	0.41
1:A:490:PHE:HD1	1:A:490:PHE:HA	1.77	0.40
1:B:686:THR:O	1:B:690:ILE:HG12	2.21	0.40
1:A:271:ASN:HD21	1:A:274:GLN:H	1.68	0.40
1:A:686:THR:O	1:A:690:ILE:HG12	2.22	0.40
1:B:542:VAL:HG12	1:D:597:THR:OG1	2.21	0.40
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.88	0.40
1:B:281:ARG:NH1	1:B:330:THR:O	2.55	0.40
1:B:600:GLU:CG	1:C:456:ARG:HH22	2.33	0.40
1:C:156:LYS:NZ	1:C:160:LEU:HB3	2.35	0.40
1:C:347:ILE:HD13	1:C:413:MET:HA	2.02	0.40
1:C:388:ILE:HD13	1:C:388:ILE:HA	1.89	0.40
1:D:504:LYS:O	1:D:508:VAL:HB	2.22	0.40
1:A:599:ILE:HG22	1:A:600:GLU:O	2.22	0.40
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:LEU:HD23	1:C:366:LEU:HA	1.89	0.40
1:B:125:ASN:HB2	1:B:167:HIS:CD2	2.57	0.40
1:C:585:ILE:HD13	1:C:585:ILE:HA	1.91	0.40
1:D:231:ALA:HA	1:D:250:GLU:O	2.22	0.40
1:D:714:LEU:HB2	1:D:717:MET:HE2	2.04	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	616/656 (94%)	597 (97%)	19 (3%)	0	100	100
1	B	628/656 (96%)	602 (96%)	25 (4%)	1 (0%)	43	70
1	C	611/656 (93%)	580 (95%)	31 (5%)	0	100	100
1	D	615/656 (94%)	599 (97%)	16 (3%)	0	100	100
All	All	2470/2624 (94%)	2378 (96%)	91 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	GLU

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	548/580 (94%)	548 (100%)	0	100	100
1	B	559/580 (96%)	559 (100%)	0	100	100
1	C	543/580 (94%)	543 (100%)	0	100	100
1	D	547/580 (94%)	547 (100%)	0	100	100
All	All	2197/2320 (95%)	2197 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	167	HIS
1	A	183	GLN
1	A	229	GLN
1	A	409	ASN
1	A	424	GLN
1	A	696	ASN
1	C	183	GLN
1	C	224	ASN
1	C	359	GLN
1	D	128	GLN
1	D	183	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	6OU	B	802	-	47,47,48	1.24	5 (10%)	50,52,53	0.91	2 (4%)
2	A1LZ2	B	801	-	45,46,46	2.82	12 (26%)	50,63,63	1.82	8 (16%)
2	A1LZ2	D	801	-	45,46,46	2.89	12 (26%)	50,63,63	1.53	11 (22%)
2	A1LZ2	C	801	-	45,46,46	2.79	10 (22%)	50,63,63	1.86	8 (16%)
3	6OU	A	802	-	45,45,48	1.27	4 (8%)	48,50,53	0.91	2 (4%)
3	6OU	B	803	-	47,47,48	1.23	4 (8%)	50,52,53	0.92	2 (4%)
3	6OU	D	802	-	45,45,48	1.26	5 (11%)	48,50,53	0.92	2 (4%)
2	A1LZ2	A	801	-	45,46,46	2.85	11 (24%)	50,63,63	2.24	18 (36%)

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	6OU	B	802	-	-	30/51/51/52	-
2	A1LZ2	B	801	-	-	8/30/55/55	0/4/4/4
2	A1LZ2	D	801	-	-	12/30/55/55	0/4/4/4
2	A1LZ2	C	801	-	-	10/30/55/55	0/4/4/4
3	6OU	A	802	-	-	26/49/49/52	-
3	6OU	B	803	-	-	26/51/51/52	-
3	6OU	D	802	-	-	24/49/49/52	-
2	A1LZ2	A	801	-	-	11/30/55/55	0/4/4/4

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	A1LZ2	C16-N17	-14.36	1.22	1.47
2	A	801	A1LZ2	C16-N17	-14.34	1.22	1.47
2	C	801	A1LZ2	C16-N17	-13.81	1.23	1.47
2	B	801	A1LZ2	C16-N17	-13.80	1.23	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	A1LZ2	C12-N07	-5.55	1.45	1.51
2	B	801	A1LZ2	C23-N24	5.47	1.48	1.35
2	C	801	A1LZ2	C23-N24	5.45	1.48	1.35
2	D	801	A1LZ2	C23-N24	5.38	1.47	1.35
2	A	801	A1LZ2	C05-N04	5.37	1.47	1.35
2	D	801	A1LZ2	C05-N04	5.31	1.47	1.35
2	A	801	A1LZ2	C23-N24	5.29	1.47	1.35
2	C	801	A1LZ2	C05-N04	5.17	1.47	1.35
2	B	801	A1LZ2	C05-N04	5.17	1.47	1.35
2	B	801	A1LZ2	C12-N07	-4.94	1.45	1.51
2	C	801	A1LZ2	C12-N07	-4.93	1.45	1.51
2	A	801	A1LZ2	C12-N07	-4.45	1.46	1.51
3	A	802	6OU	O30-C31	4.15	1.46	1.34
3	D	802	6OU	O30-C31	4.11	1.45	1.34
3	B	803	6OU	O30-C31	4.10	1.45	1.34
3	B	802	6OU	O30-C31	4.06	1.45	1.34
2	B	801	A1LZ2	C20-C21	-4.02	1.43	1.53
2	D	801	A1LZ2	C20-C21	-3.96	1.43	1.53
2	C	801	A1LZ2	C20-C21	-3.80	1.43	1.53
2	A	801	A1LZ2	C20-C21	-3.77	1.43	1.53
2	B	801	A1LZ2	C08-N07	-3.57	1.47	1.51
2	D	801	A1LZ2	C08-N07	-3.56	1.47	1.51
2	A	801	A1LZ2	C08-N07	-3.25	1.47	1.51
2	C	801	A1LZ2	C08-N07	-3.05	1.48	1.51
2	D	801	A1LZ2	O38-C05	-2.88	1.17	1.23
3	B	803	6OU	O18-C16	2.83	1.41	1.33
3	B	802	6OU	O18-C16	2.79	1.41	1.33
3	A	802	6OU	O18-C16	2.77	1.41	1.33
3	D	802	6OU	O18-C16	2.76	1.41	1.33
2	A	801	A1LZ2	O38-C05	-2.75	1.18	1.23
2	C	801	A1LZ2	O38-C05	-2.74	1.18	1.23
3	B	802	6OU	O30-C20	-2.73	1.40	1.46
3	D	802	6OU	O30-C20	-2.72	1.40	1.46
2	B	801	A1LZ2	O38-C05	-2.68	1.18	1.23
3	B	803	6OU	O30-C20	-2.67	1.40	1.46
3	A	802	6OU	O30-C20	-2.61	1.40	1.46
2	C	801	A1LZ2	O33-C23	-2.58	1.18	1.23
2	A	801	A1LZ2	O33-C23	-2.57	1.18	1.23
2	B	801	A1LZ2	C34-N07	-2.51	1.47	1.51
2	D	801	A1LZ2	O33-C23	-2.44	1.18	1.23
2	B	801	A1LZ2	O33-C23	-2.37	1.18	1.23
3	A	802	6OU	P23-O22	2.37	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	6OU	P23-O22	2.36	1.68	1.59
3	B	802	6OU	P23-O22	2.33	1.68	1.59
3	D	802	6OU	P23-O22	2.31	1.68	1.59
2	B	801	A1LZ2	C25-N24	2.22	1.47	1.43
2	D	801	A1LZ2	C25-N24	2.21	1.47	1.43
2	D	801	A1LZ2	C03-N04	2.19	1.47	1.43
2	B	801	A1LZ2	C19-C20	-2.18	1.43	1.51
2	A	801	A1LZ2	C03-N04	2.13	1.47	1.43
2	D	801	A1LZ2	C19-C20	-2.12	1.44	1.51
3	B	802	6OU	C33-C31	2.08	1.56	1.50
2	A	801	A1LZ2	C36-C37	-2.06	1.48	1.53
2	B	801	A1LZ2	C36-C37	-2.06	1.48	1.53
2	C	801	A1LZ2	C25-N24	2.05	1.47	1.43
3	D	802	6OU	P23-O26	2.02	1.67	1.59
2	A	801	A1LZ2	C18-N17	-2.01	1.43	1.47
2	C	801	A1LZ2	C03-N04	2.01	1.47	1.43
2	D	801	A1LZ2	C18-N17	-2.01	1.43	1.47

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	A1LZ2	C37-C06-C05	-8.90	98.08	109.21
2	A	801	A1LZ2	C06-C05-N04	8.28	127.26	114.11
2	B	801	A1LZ2	C37-C06-C05	-7.24	100.16	109.21
2	A	801	A1LZ2	C37-C06-C05	-6.22	101.44	109.21
2	B	801	A1LZ2	C21-C22-C23	-5.02	102.74	112.17
2	D	801	A1LZ2	C21-C22-C23	-4.72	103.31	112.17
2	C	801	A1LZ2	C21-C22-C23	-4.10	104.47	112.17
3	A	802	6OU	O30-C31-C33	3.99	120.12	111.48
3	B	802	6OU	O30-C31-C33	3.90	119.92	111.48
3	B	803	6OU	O30-C31-C33	3.83	119.78	111.48
2	D	801	A1LZ2	C03-N04-C05	3.83	130.56	123.12
2	A	801	A1LZ2	C34-C35-C36	3.74	118.86	111.07
2	B	801	A1LZ2	C35-C34-N07	-3.66	108.94	112.64
2	A	801	A1LZ2	C18-N17-C22	3.59	116.95	110.75
3	D	802	6OU	O30-C31-C33	3.58	119.24	111.48
2	A	801	A1LZ2	O38-C05-N04	-3.57	116.38	123.92
2	A	801	A1LZ2	C25-N24-C23	-3.29	116.73	123.12
2	A	801	A1LZ2	C22-C23-N24	3.27	121.82	114.03
2	C	801	A1LZ2	C02-C03-N04	3.06	123.54	118.99
2	A	801	A1LZ2	C35-C34-N07	2.91	115.58	112.64
3	B	802	6OU	O18-C16-C15	2.76	120.25	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	6OU	O18-C16-C15	2.75	120.23	111.83
3	A	802	6OU	O18-C16-C15	2.69	120.04	111.83
2	D	801	A1LZ2	C16-N17-C18	-2.64	105.76	111.20
2	D	801	A1LZ2	C43-C02-C03	2.62	121.40	117.76
2	B	801	A1LZ2	C30-C31-C25	2.54	121.29	117.76
3	B	803	6OU	O18-C16-C15	2.53	119.54	111.83
2	A	801	A1LZ2	C39-C03-N04	2.47	122.67	118.99
2	A	801	A1LZ2	O33-C23-N24	-2.47	118.71	123.92
2	A	801	A1LZ2	C21-C22-C23	-2.43	107.61	112.17
2	A	801	A1LZ2	C32-C31-C25	-2.42	118.48	121.42
2	D	801	A1LZ2	O33-C23-N24	-2.36	118.93	123.92
2	D	801	A1LZ2	C28-C26-C25	2.36	121.04	117.76
2	A	801	A1LZ2	C41-C39-C03	2.34	121.01	117.76
2	D	801	A1LZ2	C26-C25-N24	2.33	122.46	118.99
2	C	801	A1LZ2	O38-C05-N04	-2.32	119.03	123.92
2	B	801	A1LZ2	C02-C03-N04	2.25	122.34	118.99
2	C	801	A1LZ2	C22-C23-N24	2.25	119.39	114.03
2	A	801	A1LZ2	C30-C31-C25	2.24	120.87	117.76
2	C	801	A1LZ2	O33-C23-N24	-2.24	119.20	123.92
2	D	801	A1LZ2	C22-C23-N24	2.22	119.33	114.03
2	B	801	A1LZ2	C18-N17-C22	2.20	114.55	110.75
2	D	801	A1LZ2	C18-N17-C22	2.14	114.44	110.75
2	A	801	A1LZ2	C39-C03-C02	-2.13	118.52	121.55
2	A	801	A1LZ2	C20-C21-C22	2.13	115.92	110.97
2	C	801	A1LZ2	C41-C39-C03	2.12	120.71	117.76
2	A	801	A1LZ2	C03-N04-C05	-2.11	119.02	123.12
2	C	801	A1LZ2	C30-C31-C25	2.10	120.68	117.76
2	D	801	A1LZ2	C37-C06-C05	-2.08	106.61	109.21
2	B	801	A1LZ2	O38-C05-N04	-2.06	119.58	123.92
2	D	801	A1LZ2	C39-C03-C02	-2.05	118.63	121.55
2	B	801	A1LZ2	C20-C21-C22	2.04	115.71	110.97
2	A	801	A1LZ2	C26-C25-N24	2.02	121.99	118.99

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	A1LZ2	C21-C22-C23-N24
2	B	801	A1LZ2	C15-C16-N17-C18
2	C	801	A1LZ2	C21-C22-C23-N24
2	C	801	A1LZ2	C21-C22-C23-O33
2	C	801	A1LZ2	C15-C16-N17-C18

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Mol	Chain	Res	Type	Atoms
2	D	801	A1LZ2	C21-C22-C23-N24
2	D	801	A1LZ2	C21-C22-C23-O33
2	D	801	A1LZ2	N04-C05-C06-C37
2	D	801	A1LZ2	O38-C05-C06-C37
2	D	801	A1LZ2	C09-C08-N07-C34
3	A	802	6OU	O30-C20-C21-O22
3	A	802	6OU	C21-O22-P23-O25
3	A	802	6OU	C21-O22-P23-O26
3	B	803	6OU	O32-C31-O30-C20
3	B	803	6OU	C33-C31-O30-C20
3	D	802	6OU	C21-O22-P23-O25
3	D	802	6OU	C21-O22-P23-O26
3	B	803	6OU	O17-C16-O18-C19
3	B	803	6OU	C15-C16-O18-C19
3	D	802	6OU	C33-C31-O30-C20
2	D	801	A1LZ2	C13-C14-C15-C16
3	D	802	6OU	O32-C31-O30-C20
2	A	801	A1LZ2	C13-C14-C15-C16
3	B	802	6OU	C15-C16-O18-C19
3	B	802	6OU	C33-C31-O30-C20
3	D	802	6OU	C34-C35-C36-C37
3	B	802	6OU	O17-C16-O18-C19
3	B	803	6OU	C34-C35-C36-C37
3	B	803	6OU	C36-C37-C38-C39
3	A	802	6OU	C36-C37-C38-C39
3	A	802	6OU	C34-C35-C36-C37
3	B	802	6OU	C13-C14-C15-C16
3	A	802	6OU	C33-C31-O30-C20
3	B	802	6OU	C43-C44-C45-C46
3	B	802	6OU	O32-C31-O30-C20
2	A	801	A1LZ2	N07-C08-C09-C10
2	B	801	A1LZ2	N07-C08-C09-C10
2	D	801	A1LZ2	N07-C12-C13-C14
3	A	802	6OU	O32-C31-O30-C20
3	A	802	6OU	C07-C08-C09-C10
2	C	801	A1LZ2	C14-C15-C16-N17
2	A	801	A1LZ2	C13-C12-N07-C34
2	C	801	A1LZ2	C09-C08-N07-C34
2	D	801	A1LZ2	N07-C08-C09-C10
3	D	802	6OU	C10-C11-C12-C13
3	D	802	6OU	C12-C13-C14-C15
3	A	802	6OU	C31-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	A	802	6OU	C09-C10-C11-C12
3	B	803	6OU	C12-C13-C14-C15
3	B	803	6OU	C04-C05-C06-C07
2	A	801	A1LZ2	C13-C12-N07-C06
2	D	801	A1LZ2	C09-C08-N07-C06
3	B	803	6OU	C06-C07-C08-C09
3	A	802	6OU	C04-C05-C06-C07
3	D	802	6OU	C09-C10-C11-C12
3	B	802	6OU	C11-C12-C13-C14
2	B	801	A1LZ2	C21-C22-C23-O33
3	D	802	6OU	C06-C07-C08-C09
3	A	802	6OU	C46-C47-C48-C49
3	B	802	6OU	C07-C08-C09-C10
3	B	803	6OU	C33-C34-C35-C36
3	B	802	6OU	C12-C13-C14-C15
2	A	801	A1LZ2	C08-C09-C10-C11
3	B	802	6OU	C33-C34-C35-C36
3	B	803	6OU	C37-C38-C39-C40
3	B	803	6OU	C41-C42-C43-C44
3	B	802	6OU	C10-C11-C12-C13
2	C	801	A1LZ2	C13-C14-C15-C16
3	B	802	6OU	C35-C36-C37-C38
3	B	802	6OU	C06-C07-C08-C09
3	A	802	6OU	C43-C44-C45-C46
3	B	802	6OU	C09-C10-C11-C12
3	A	802	6OU	C33-C34-C35-C36
3	D	802	6OU	C35-C36-C37-C38
2	A	801	A1LZ2	C09-C08-N07-C34
3	D	802	6OU	C08-C09-C10-C11
2	D	801	A1LZ2	C14-C15-C16-N17
3	A	802	6OU	O18-C19-C20-C21
3	A	802	6OU	C37-C38-C39-C40
3	A	802	6OU	C06-C07-C08-C09
3	A	802	6OU	C41-C42-C43-C44
3	D	802	6OU	C41-C42-C43-C44
3	D	802	6OU	C43-C44-C45-C46
3	B	802	6OU	O30-C20-C21-O22
3	D	802	6OU	C36-C37-C38-C39
3	D	802	6OU	C03-C04-C05-C06
3	B	803	6OU	C01-C02-C03-C04
3	B	803	6OU	C08-C09-C10-C11
2	B	801	A1LZ2	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	D	802	6OU	C01-C02-C03-C04
3	B	803	6OU	C10-C11-C12-C13
3	A	802	6OU	C19-C20-C21-O22
2	B	801	A1LZ2	N04-C05-C06-C37
3	B	802	6OU	C37-C38-C39-C40
2	D	801	A1LZ2	C08-C09-C10-C11
2	A	801	A1LZ2	C09-C08-N07-C06
3	D	802	6OU	O18-C19-C20-C21
3	A	802	6OU	O18-C19-C20-O30
3	B	803	6OU	O18-C19-C20-O30
2	A	801	A1LZ2	C13-C12-N07-C08
2	D	801	A1LZ2	C09-C08-N07-C12
3	D	802	6OU	C05-C06-C07-C08
3	B	802	6OU	C41-C42-C43-C44
3	B	802	6OU	C36-C37-C38-C39
3	A	802	6OU	C08-C09-C10-C11
3	B	803	6OU	C09-C10-C11-C12
3	D	802	6OU	C31-C33-C34-C35
3	A	802	6OU	C12-C13-C14-C15
2	A	801	A1LZ2	C12-C13-C14-C15
3	B	802	6OU	C34-C35-C36-C37
3	B	802	6OU	C42-C43-C44-C45
3	A	802	6OU	C10-C11-C12-C13
3	B	803	6OU	C11-C12-C13-C14
2	B	801	A1LZ2	O38-C05-C06-C37
3	B	803	6OU	C02-C03-C04-C05
2	A	801	A1LZ2	C09-C08-N07-C12
2	C	801	A1LZ2	C09-C08-N07-C12
3	B	802	6OU	C03-C04-C05-C06
3	D	802	6OU	O18-C19-C20-O30
2	C	801	A1LZ2	C09-C08-N07-C06
3	B	803	6OU	O18-C19-C20-C21
3	B	802	6OU	C21-O22-P23-O24
3	B	802	6OU	C21-O22-P23-O25
3	B	802	6OU	C21-O22-P23-O26
3	B	803	6OU	C43-C44-C45-C46
3	A	802	6OU	C20-C21-O22-P23
2	A	801	A1LZ2	C21-C22-C23-N24
3	B	802	6OU	C19-C20-C21-O22
2	C	801	A1LZ2	C13-C12-N07-C34
3	B	803	6OU	C20-C21-O22-P23
3	B	802	6OU	C05-C06-C07-C08

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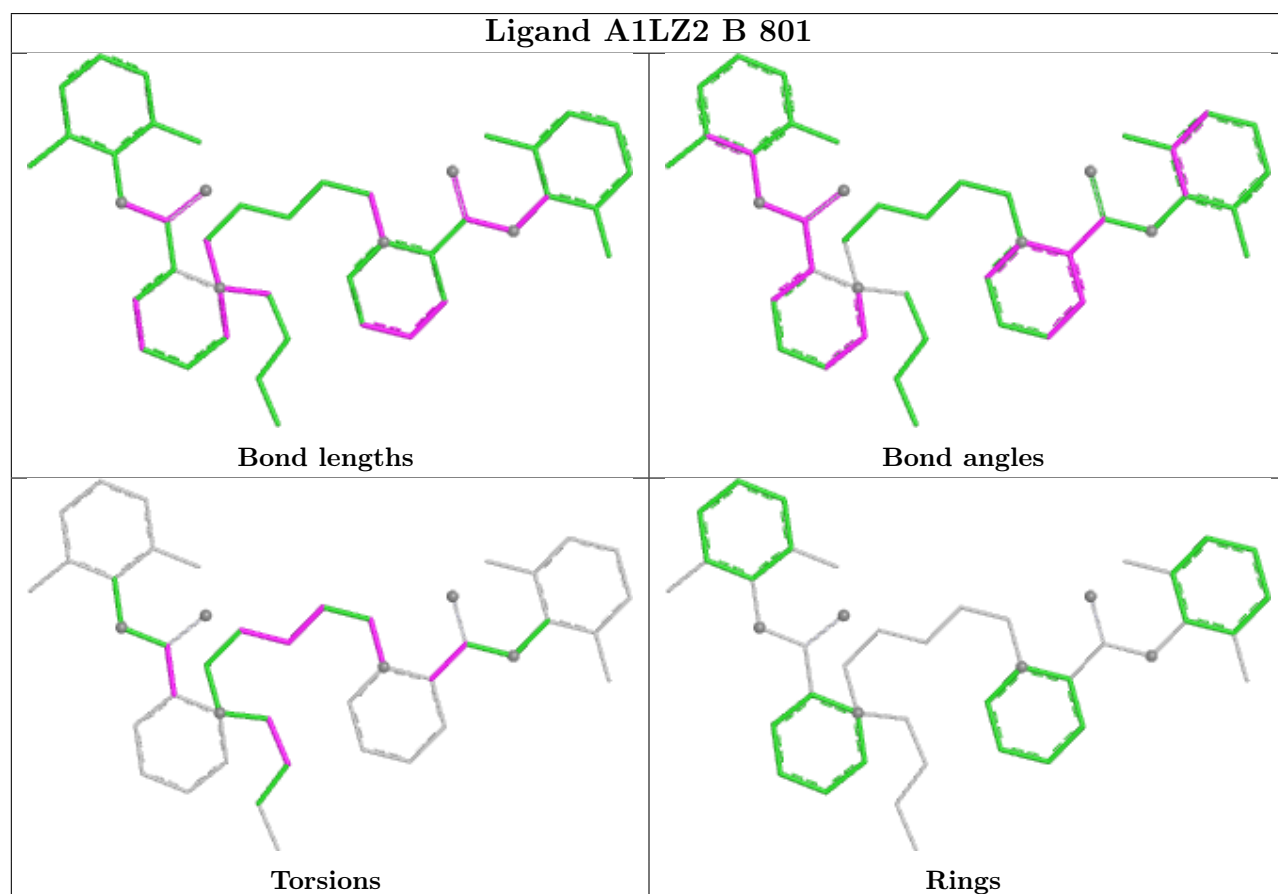
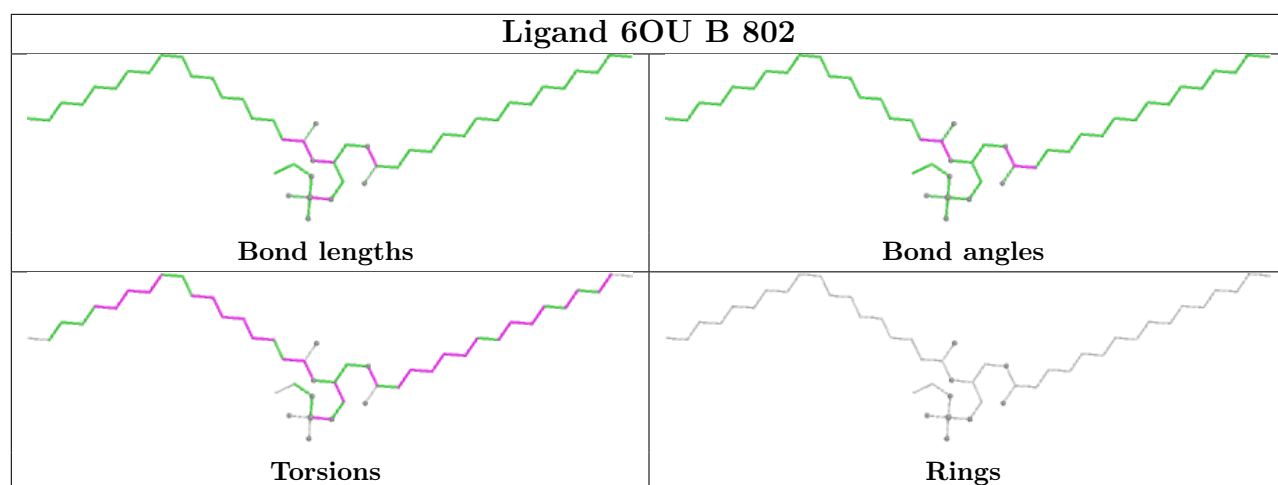
Mol	Chain	Res	Type	Atoms
3	B	802	6OU	C01-C02-C03-C04
3	B	803	6OU	C42-C43-C44-C45
3	D	802	6OU	C19-C20-C21-O22
2	B	801	A1LZ2	C12-C13-C14-C15
3	D	802	6OU	O30-C20-C21-O22
3	B	803	6OU	C40-C41-C42-C43
3	B	802	6OU	C40-C41-C42-C43
3	D	802	6OU	C07-C08-C09-C10
3	B	803	6OU	C03-C04-C05-C06
3	A	802	6OU	C40-C41-C42-C43
2	C	801	A1LZ2	C12-C13-C14-C15
3	B	802	6OU	O30-C31-C33-C34
3	D	802	6OU	C33-C34-C35-C36
3	A	802	6OU	C03-C04-C05-C06
3	B	803	6OU	C07-C08-C09-C10
3	B	802	6OU	O32-C31-C33-C34

There are no ring outliers.

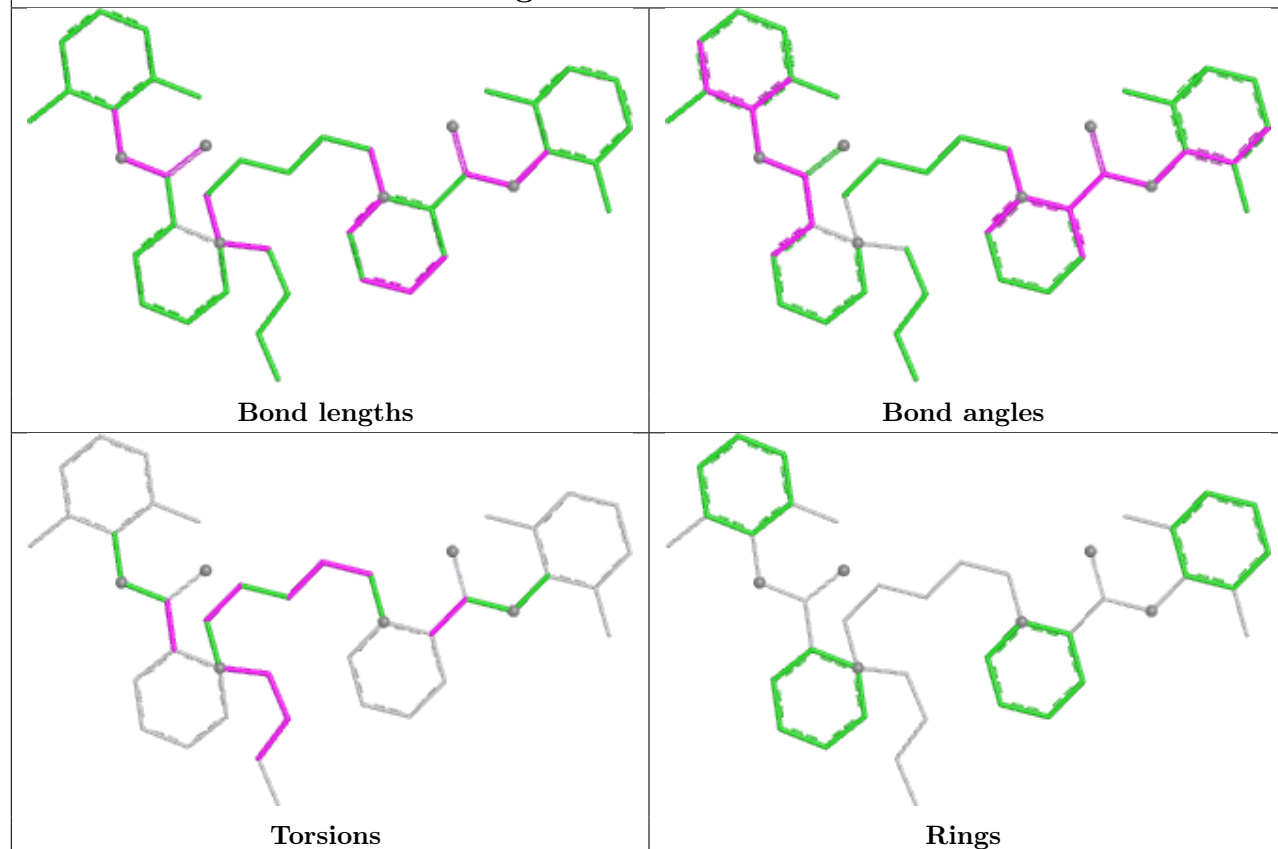
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	A1LZ2	2	0
2	C	801	A1LZ2	1	0
2	A	801	A1LZ2	1	0

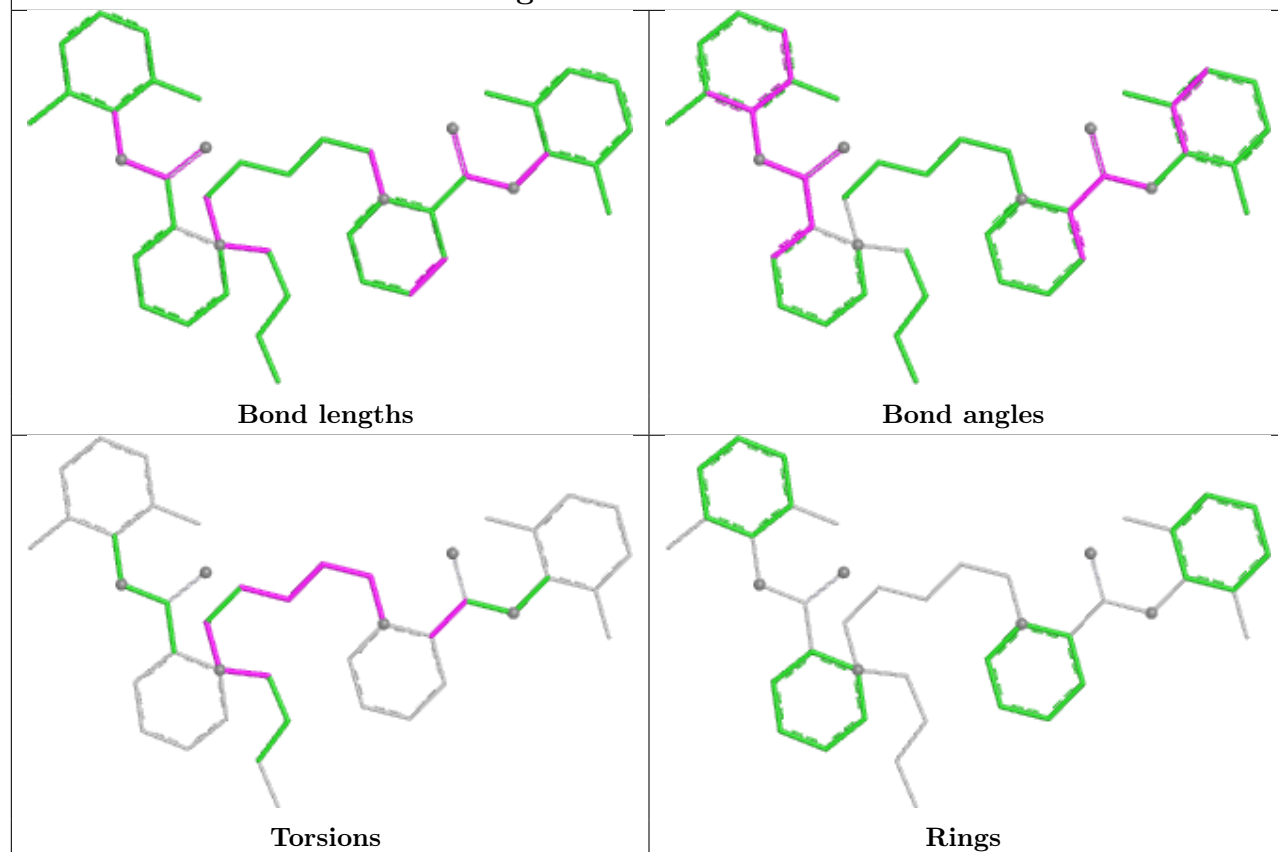
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

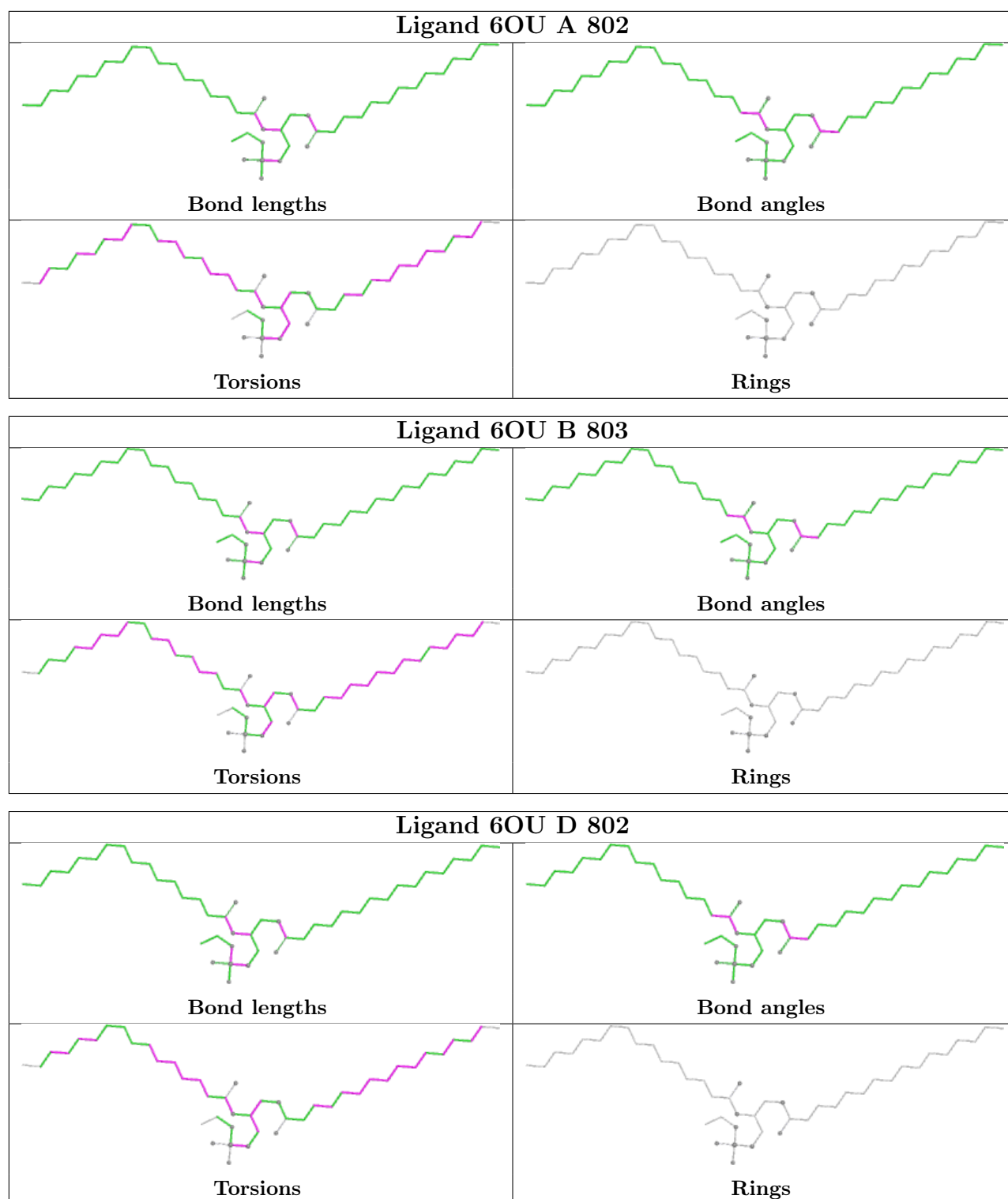


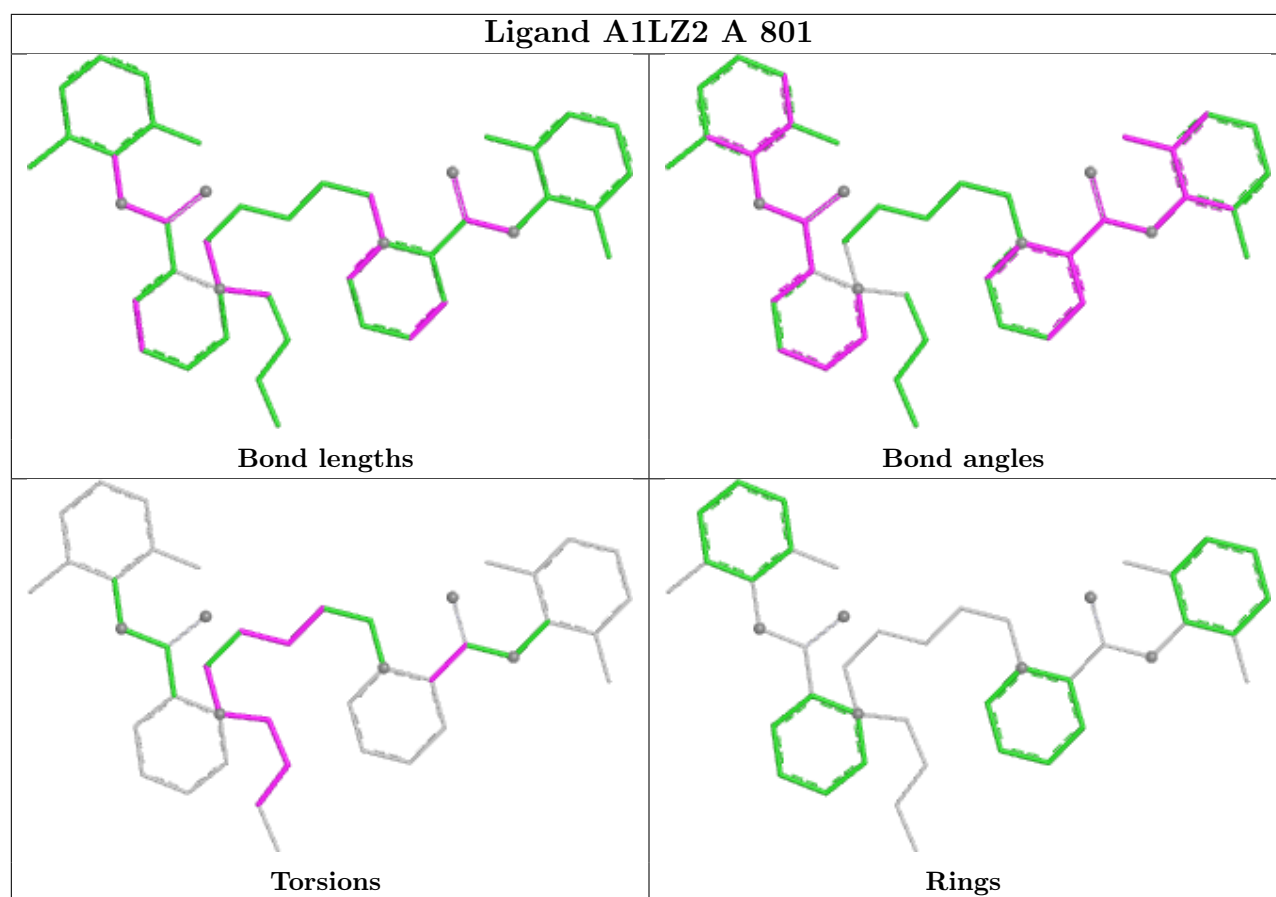
Ligand A1LZ2 D 801



Ligand A1LZ2 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.

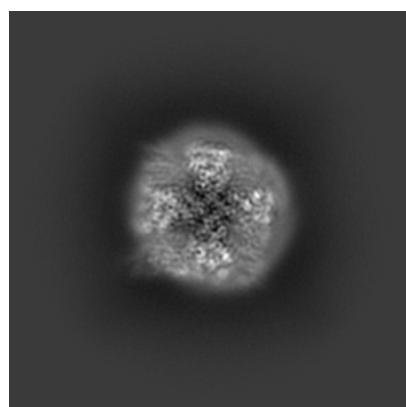
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39151. These allow visual inspection of the internal detail of the map and identification of artifacts.

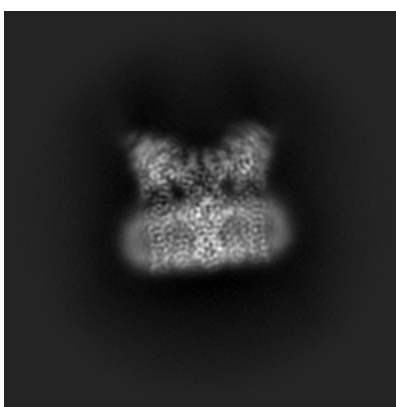
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

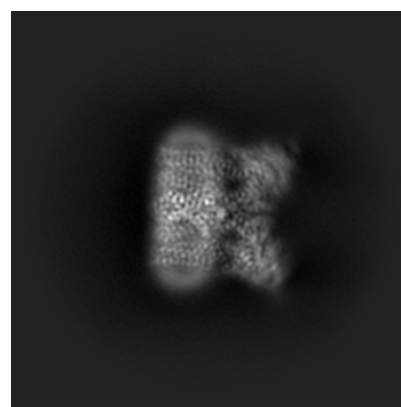
6.1.1 Primary map



X



Y

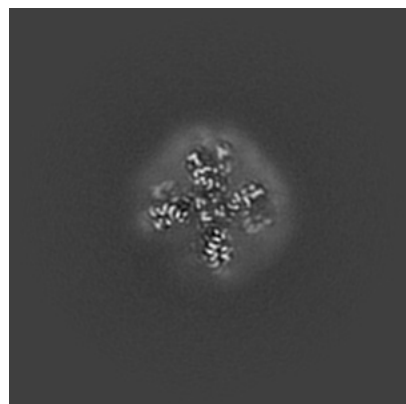


Z

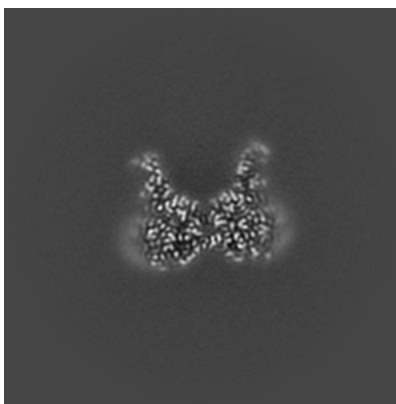
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

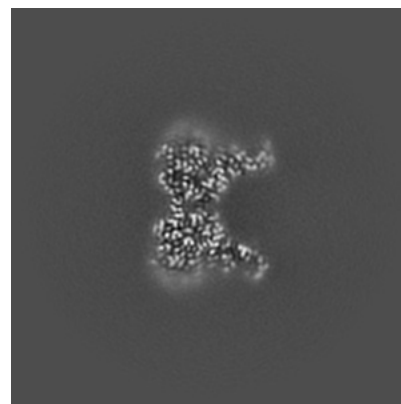
6.2.1 Primary map



X Index: 180



Y Index: 180

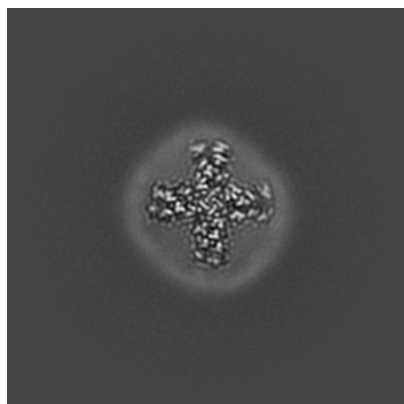


Z Index: 180

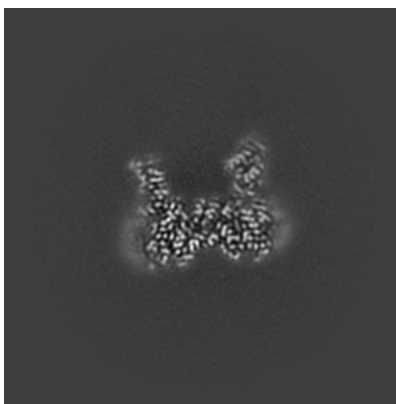
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

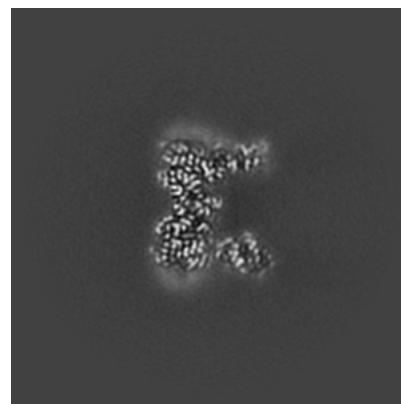
6.3.1 Primary map



X Index: 146



Y Index: 188

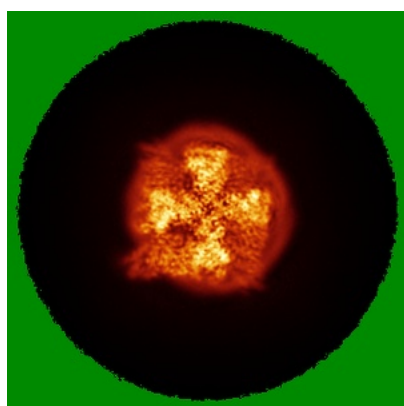


Z Index: 189

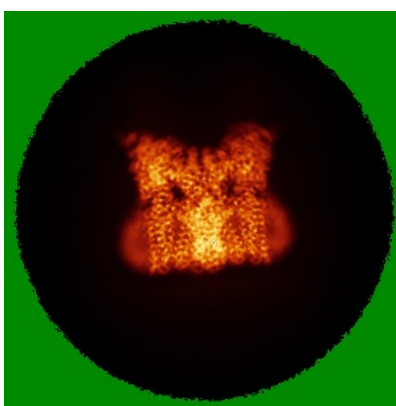
The images above show the largest variance slices of the map in three orthogonal directions.

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

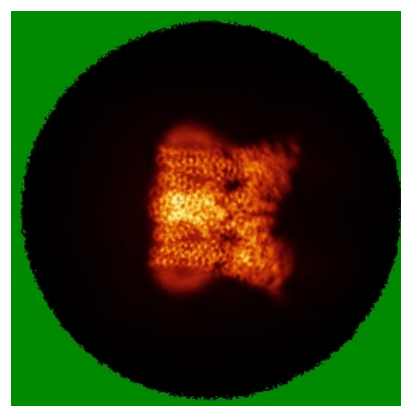
6.4.1 Primary map



X



Y

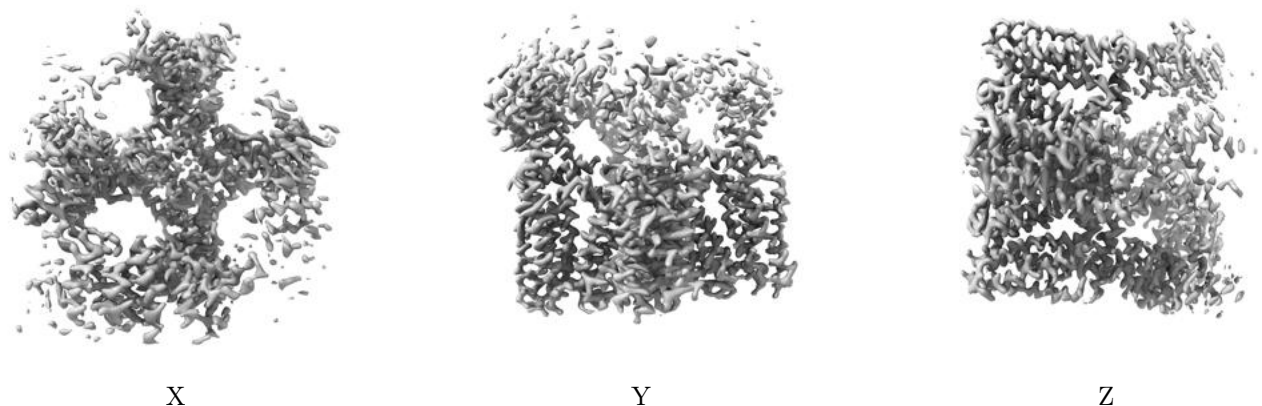


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

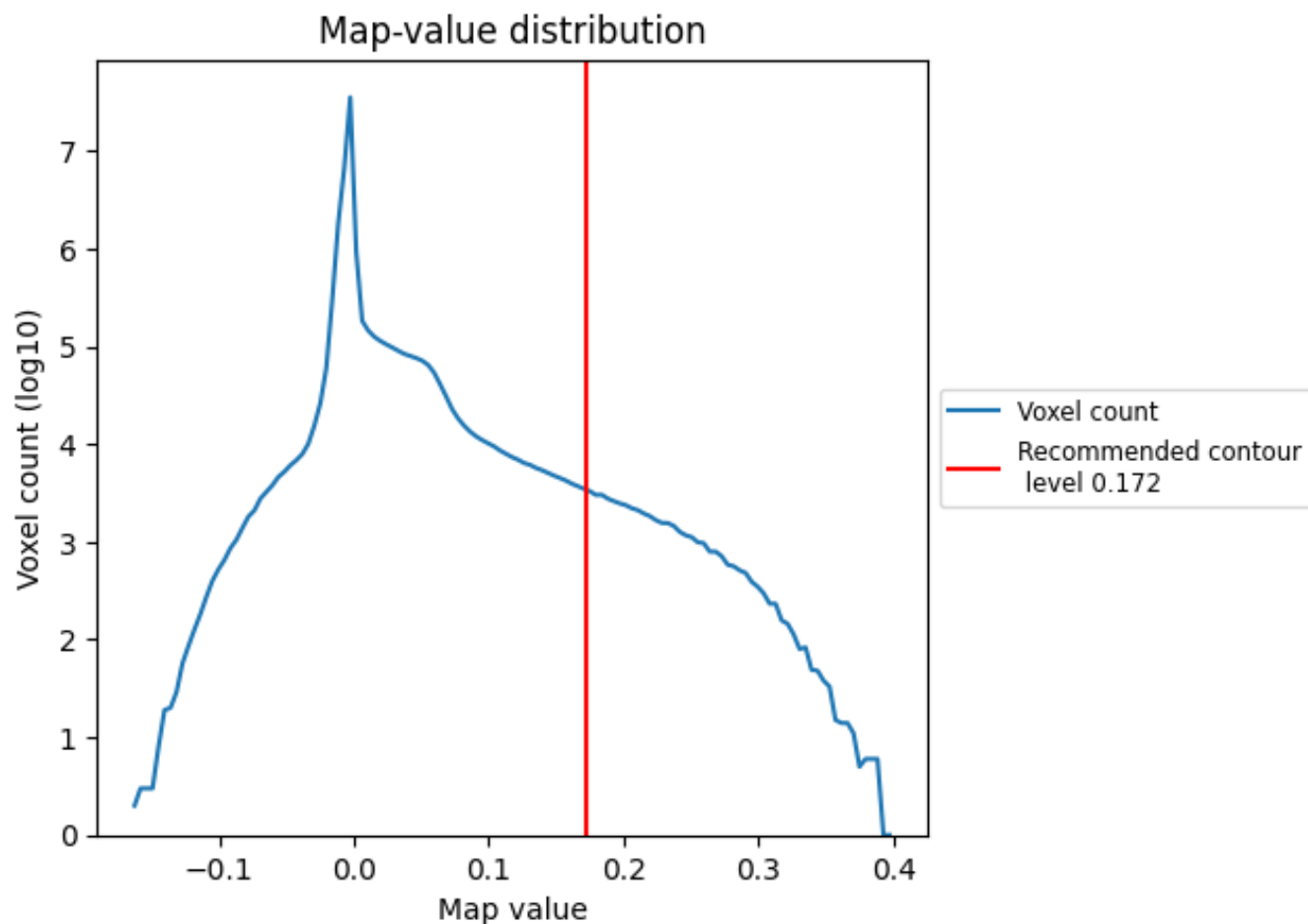
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

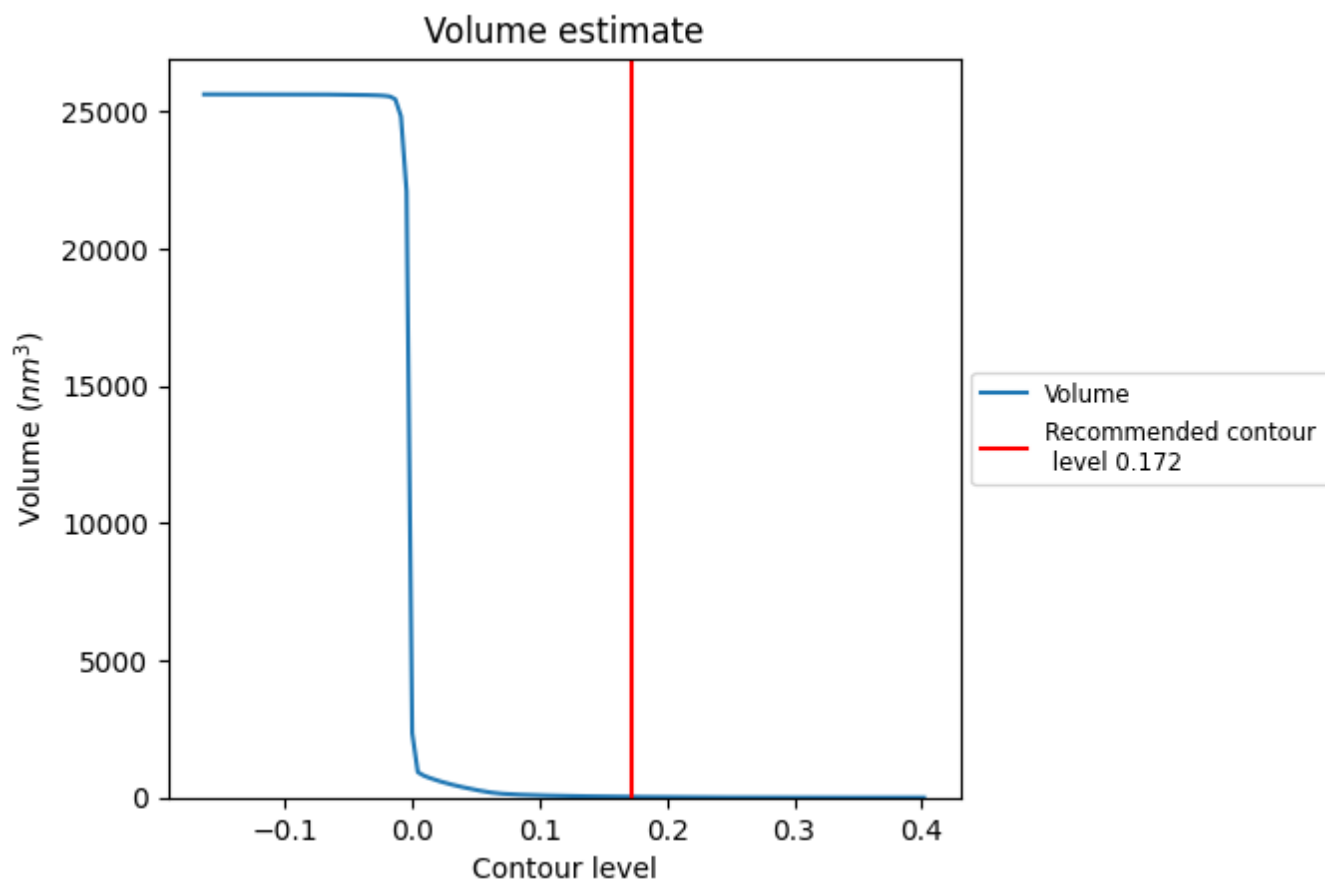
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

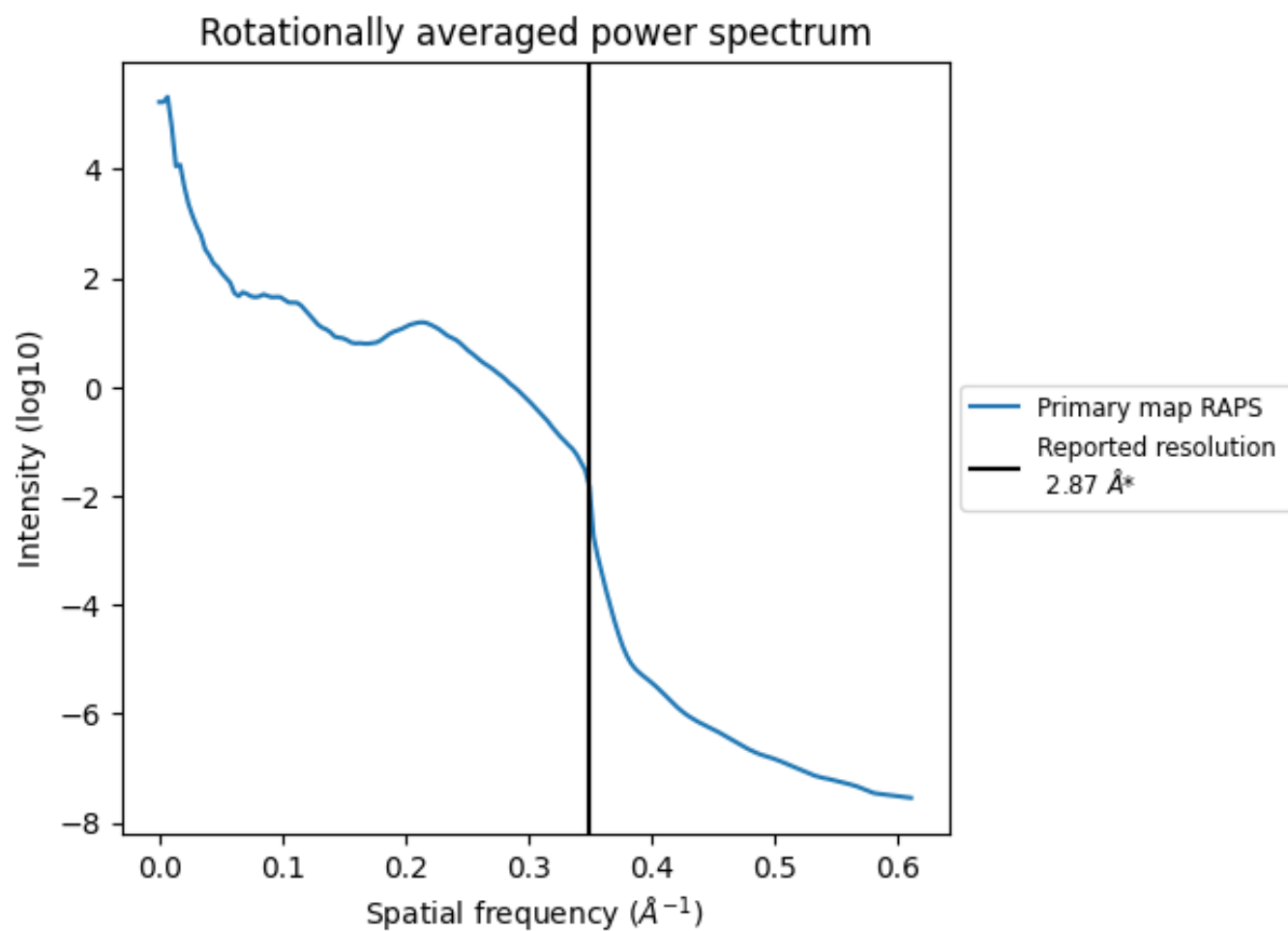
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27 nm³; this corresponds to an approximate mass of 24 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

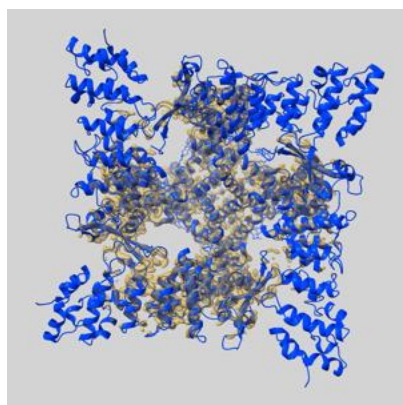
8 Fourier-Shell correlation

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

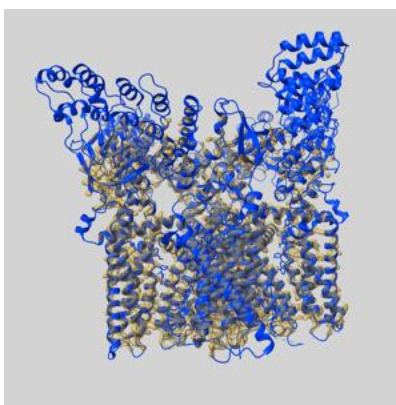
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39151 and PDB model 8YCP. Per-residue inclusion information can be found in section 3 on page 6.

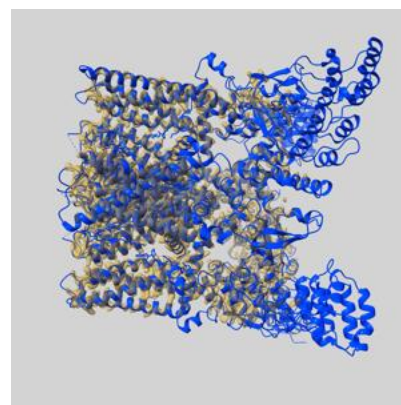
9.1 Map-model overlay [i](#)



X



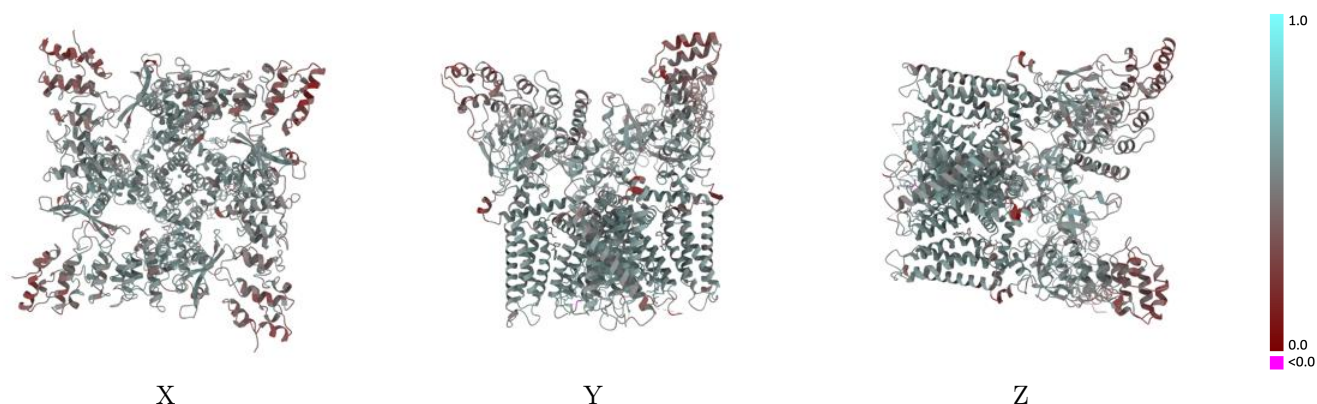
Y



Z

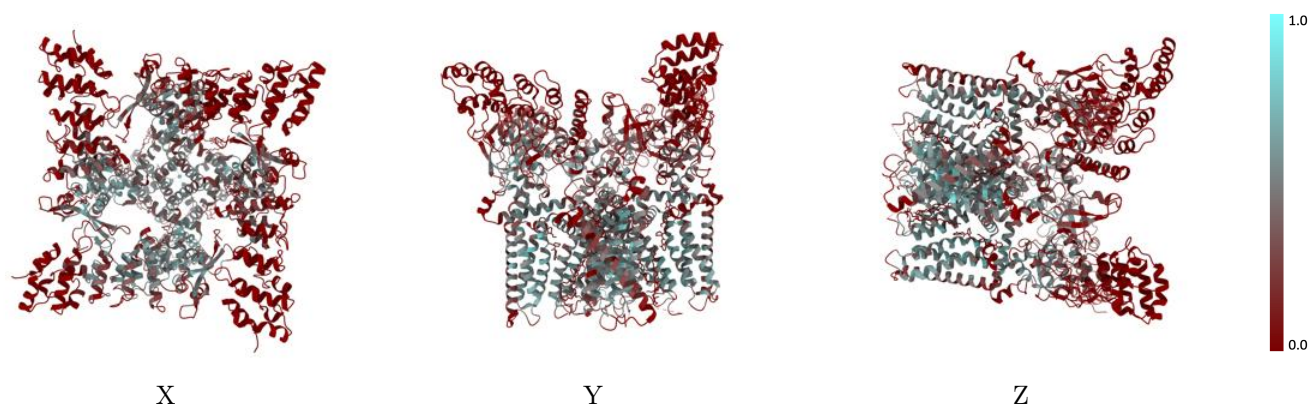
The images above show the 3D surface view of the map at the recommended contour level 0.172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



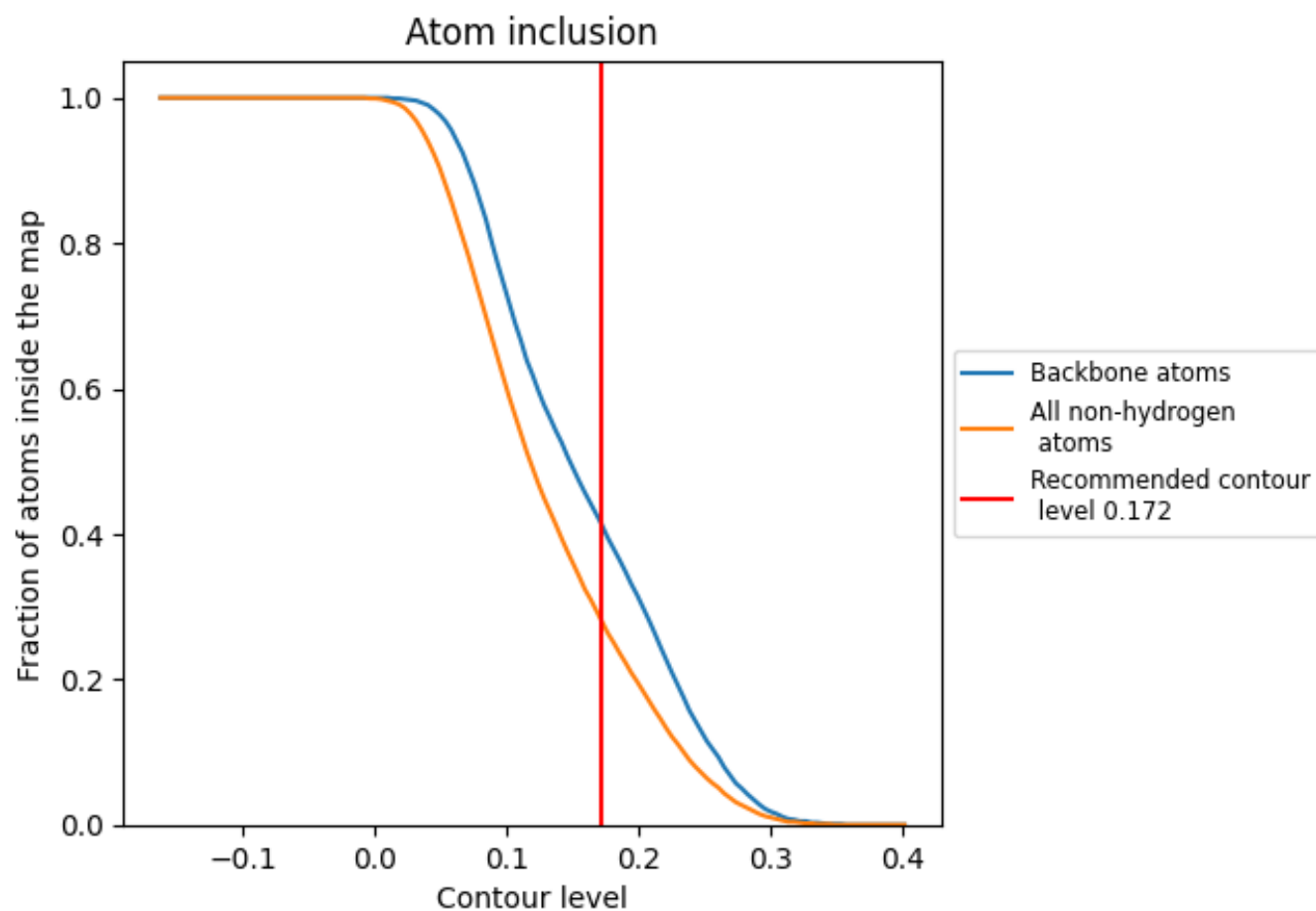
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.172).

9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 28% 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 (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2800	0.5040
A	0.2300	0.5000
B	0.2920	0.5030
C	0.2470	0.4970
D	0.3510	0.5170

