



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:32 AM UTC

PDB ID : 9FXM / pdb_00009fxm
EMDB ID : EMD-50851
Title : TRPC4 in complex with Z-AzPico
Authors : Vinayagam, D.; Raunser, S.
Deposited on : 2024-07-01
Resolution : 3.10 Å(reported)
Based on initial model : 6G1K

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

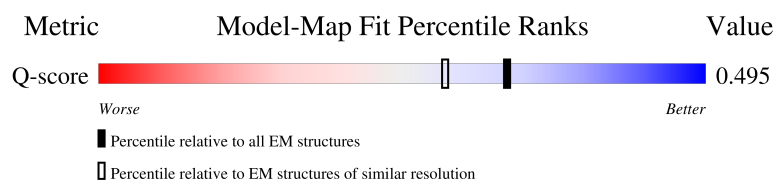
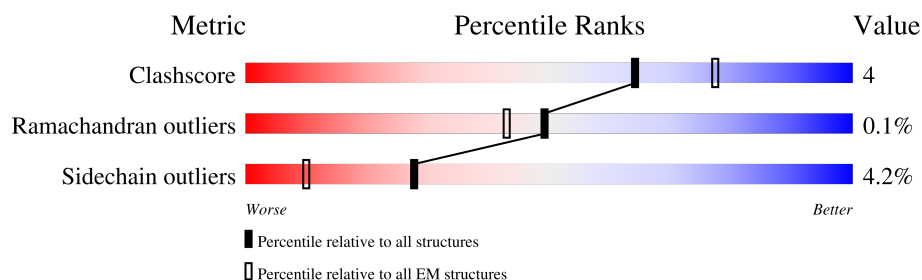
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	941	6% 59% 9% 32%
1	B	941	9% 59% 9% 31%
1	C	941	18% 59% 9% 32%
1	D	941	10% 58% 9% 32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21256 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 c member 4a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	644	Total	C	N	O	S	1	0
			5266	3439	868	932	27		
1	B	645	Total	C	N	O	S	1	0
			5274	3443	869	935	27		
1	C	644	Total	C	N	O	S	1	0
			5266	3439	868	932	27		
1	D	644	Total	C	N	O	S	2	0
			5274	3445	869	933	27		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP U3N7D8
A	-18	GLY	-	expression tag	UNP U3N7D8
A	-17	HIS	-	expression tag	UNP U3N7D8
A	-16	HIS	-	expression tag	UNP U3N7D8
A	-15	HIS	-	expression tag	UNP U3N7D8
A	-14	HIS	-	expression tag	UNP U3N7D8
A	-13	HIS	-	expression tag	UNP U3N7D8
A	-12	HIS	-	expression tag	UNP U3N7D8
A	-11	HIS	-	expression tag	UNP U3N7D8
A	-10	HIS	-	expression tag	UNP U3N7D8
A	-9	GLY	-	expression tag	UNP U3N7D8
A	-8	GLY	-	expression tag	UNP U3N7D8
A	-7	SER	-	expression tag	UNP U3N7D8
A	-6	GLU	-	expression tag	UNP U3N7D8
A	-5	ASN	-	expression tag	UNP U3N7D8
A	-4	LEU	-	expression tag	UNP U3N7D8
A	-3	TYR	-	expression tag	UNP U3N7D8
A	-2	PHE	-	expression tag	UNP U3N7D8
A	-1	GLN	-	expression tag	UNP U3N7D8
A	0	GLY	-	expression tag	UNP U3N7D8
A	1	GLY	-	expression tag	UNP U3N7D8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	916	LEU	-	expression tag	UNP U3N7D8
A	917	GLU	-	expression tag	UNP U3N7D8
A	918	VAL	-	expression tag	UNP U3N7D8
A	919	LEU	-	expression tag	UNP U3N7D8
A	920	PHE	-	expression tag	UNP U3N7D8
A	921	GLN	-	expression tag	UNP U3N7D8
B	-19	MET	-	initiating methionine	UNP U3N7D8
B	-18	GLY	-	expression tag	UNP U3N7D8
B	-17	HIS	-	expression tag	UNP U3N7D8
B	-16	HIS	-	expression tag	UNP U3N7D8
B	-15	HIS	-	expression tag	UNP U3N7D8
B	-14	HIS	-	expression tag	UNP U3N7D8
B	-13	HIS	-	expression tag	UNP U3N7D8
B	-12	HIS	-	expression tag	UNP U3N7D8
B	-11	HIS	-	expression tag	UNP U3N7D8
B	-10	HIS	-	expression tag	UNP U3N7D8
B	-9	GLY	-	expression tag	UNP U3N7D8
B	-8	GLY	-	expression tag	UNP U3N7D8
B	-7	SER	-	expression tag	UNP U3N7D8
B	-6	GLU	-	expression tag	UNP U3N7D8
B	-5	ASN	-	expression tag	UNP U3N7D8
B	-4	LEU	-	expression tag	UNP U3N7D8
B	-3	TYR	-	expression tag	UNP U3N7D8
B	-2	PHE	-	expression tag	UNP U3N7D8
B	-1	GLN	-	expression tag	UNP U3N7D8
B	0	GLY	-	expression tag	UNP U3N7D8
B	1	GLY	-	expression tag	UNP U3N7D8
B	916	LEU	-	expression tag	UNP U3N7D8
B	917	GLU	-	expression tag	UNP U3N7D8
B	918	VAL	-	expression tag	UNP U3N7D8
B	919	LEU	-	expression tag	UNP U3N7D8
B	920	PHE	-	expression tag	UNP U3N7D8
B	921	GLN	-	expression tag	UNP U3N7D8
C	-19	MET	-	initiating methionine	UNP U3N7D8
C	-18	GLY	-	expression tag	UNP U3N7D8
C	-17	HIS	-	expression tag	UNP U3N7D8
C	-16	HIS	-	expression tag	UNP U3N7D8
C	-15	HIS	-	expression tag	UNP U3N7D8
C	-14	HIS	-	expression tag	UNP U3N7D8
C	-13	HIS	-	expression tag	UNP U3N7D8
C	-12	HIS	-	expression tag	UNP U3N7D8
C	-11	HIS	-	expression tag	UNP U3N7D8

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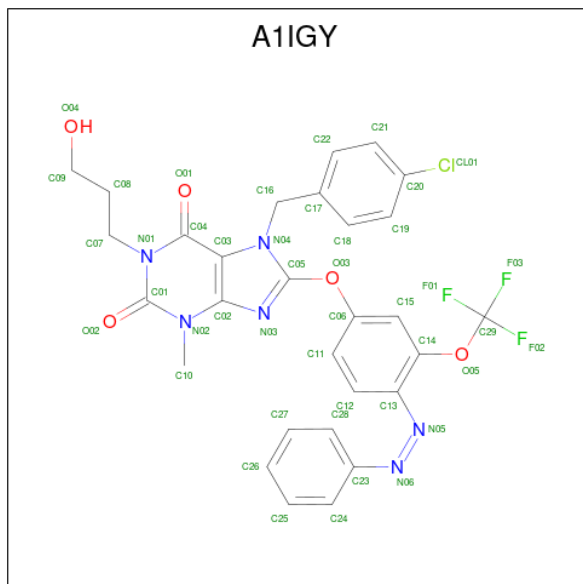
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C	-10	HIS	-	expression tag	UNP U3N7D8
C	-9	GLY	-	expression tag	UNP U3N7D8
C	-8	GLY	-	expression tag	UNP U3N7D8
C	-7	SER	-	expression tag	UNP U3N7D8
C	-6	GLU	-	expression tag	UNP U3N7D8
C	-5	ASN	-	expression tag	UNP U3N7D8
C	-4	LEU	-	expression tag	UNP U3N7D8
C	-3	TYR	-	expression tag	UNP U3N7D8
C	-2	PHE	-	expression tag	UNP U3N7D8
C	-1	GLN	-	expression tag	UNP U3N7D8
C	0	GLY	-	expression tag	UNP U3N7D8
C	1	GLY	-	expression tag	UNP U3N7D8
C	916	LEU	-	expression tag	UNP U3N7D8
C	917	GLU	-	expression tag	UNP U3N7D8
C	918	VAL	-	expression tag	UNP U3N7D8
C	919	LEU	-	expression tag	UNP U3N7D8
C	920	PHE	-	expression tag	UNP U3N7D8
C	921	GLN	-	expression tag	UNP U3N7D8
D	-19	MET	-	initiating methionine	UNP U3N7D8
D	-18	GLY	-	expression tag	UNP U3N7D8
D	-17	HIS	-	expression tag	UNP U3N7D8
D	-16	HIS	-	expression tag	UNP U3N7D8
D	-15	HIS	-	expression tag	UNP U3N7D8
D	-14	HIS	-	expression tag	UNP U3N7D8
D	-13	HIS	-	expression tag	UNP U3N7D8
D	-12	HIS	-	expression tag	UNP U3N7D8
D	-11	HIS	-	expression tag	UNP U3N7D8
D	-10	HIS	-	expression tag	UNP U3N7D8
D	-9	GLY	-	expression tag	UNP U3N7D8
D	-8	GLY	-	expression tag	UNP U3N7D8
D	-7	SER	-	expression tag	UNP U3N7D8
D	-6	GLU	-	expression tag	UNP U3N7D8
D	-5	ASN	-	expression tag	UNP U3N7D8
D	-4	LEU	-	expression tag	UNP U3N7D8
D	-3	TYR	-	expression tag	UNP U3N7D8
D	-2	PHE	-	expression tag	UNP U3N7D8
D	-1	GLN	-	expression tag	UNP U3N7D8
D	0	GLY	-	expression tag	UNP U3N7D8
D	1	GLY	-	expression tag	UNP U3N7D8
D	916	LEU	-	expression tag	UNP U3N7D8
D	917	GLU	-	expression tag	UNP U3N7D8
D	918	VAL	-	expression tag	UNP U3N7D8

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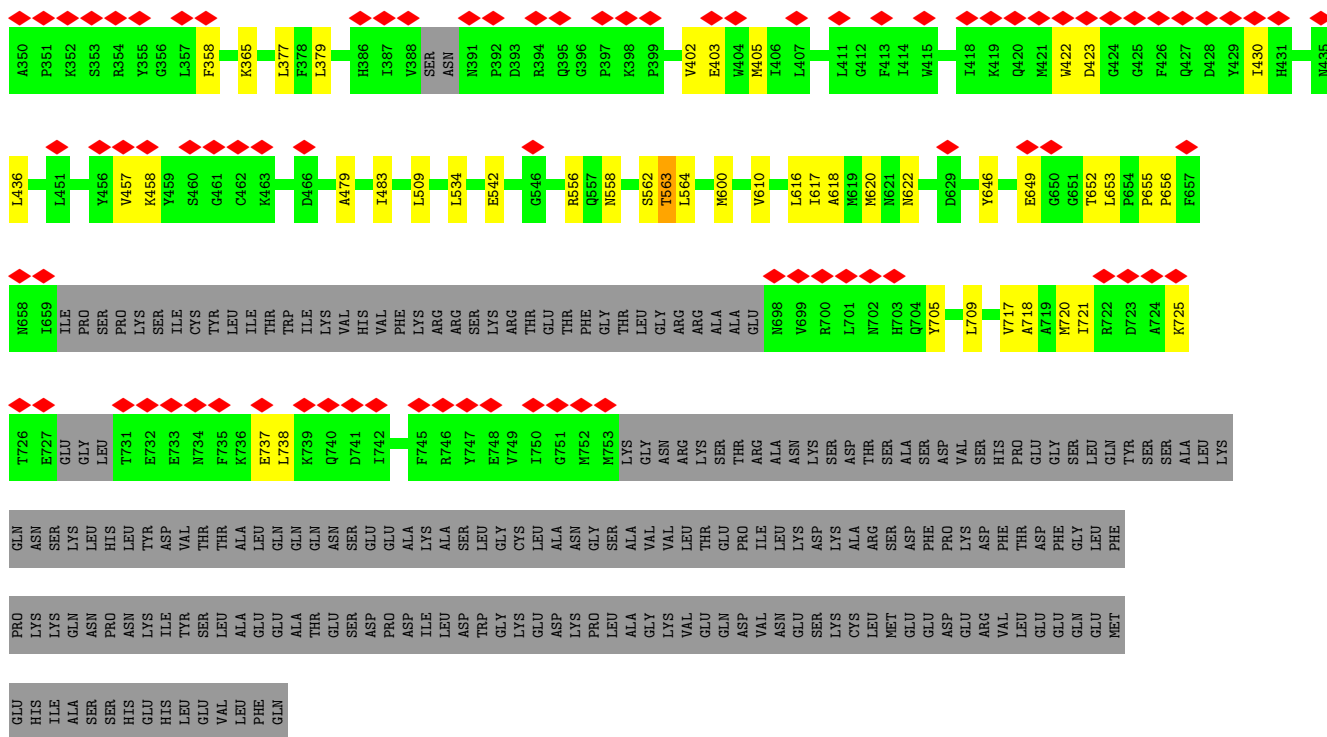
Chain	Residue	Modelled	Actual	Comment	Reference
D	919	LEU	-	expression tag	UNP U3N7D8
D	920	PHE	-	expression tag	UNP U3N7D8
D	921	GLN	-	expression tag	UNP U3N7D8

- Molecule 2 is (Z)-7-(4-chlorobenzyl)-1-(3-hydroxypropyl)-3-methyl-8-(4-(phenyldiazenyl)-3-(trifluoromethoxy)phenoxy)-3,7-dihydro-1H-purine-2,6-dione (CCD ID: A1IGY) (formula: $C_{29}H_{24}ClF_3N_6O_5$) (labeled as "Ligand of Interest" by depositor).

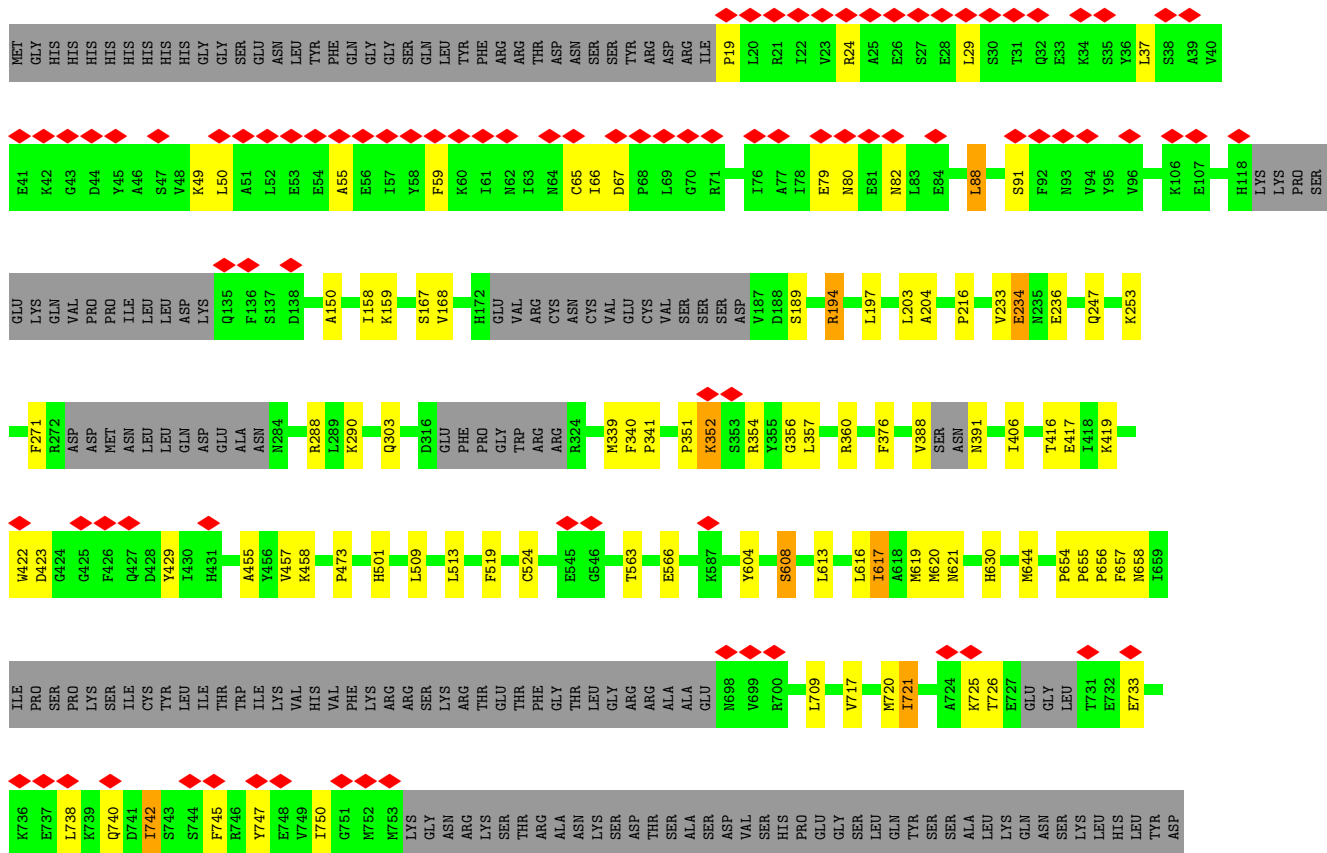


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	Cl	F	N	O	0
			44	29	1	3	6	5	
2	B	1	Total	C	Cl	F	N	O	0
			44	29	1	3	6	5	
2	C	1	Total	C	Cl	F	N	O	0
			44	29	1	3	6	5	
2	D	1	Total	C	Cl	F	N	O	0
			44	29	1	3	6	5	





• Molecule 1: Transient receptor potential cation channel subfamily c member 4a



LEU	TTR	VAL
GLU	SER	THR
VAL	LEU	ALA
LEU	GLU	LEU
PHE	GLU	GLN
GLN	THR	GLN
	SER	ASN
	ASP	GLU
	PRO	GLY
	ASP	ALA
	ILE	LYS
	LEU	ALA
	ASP	SER
	THR	GLY
	LYS	CYS
	GLU	LEU
	ASP	ALA
	LYS	ASN
	PRO	GLY
	LEU	SER
	ALA	ALA
	GLY	VAL
	VAL	LEU
	GLU	THR
	GLN	GLU
	ASP	PRO
	VAL	ILE
	ASN	LEU
	GLU	LYS
	SER	ASP
	LYS	LYS
	CYS	ALA
	LEU	ARG
	MET	SER
	GLU	ASP
	GLU	PHE
	ASP	PRO
	GLU	LYS
	ARG	ASP
	VAL	PHE
	LEU	THR
	GLU	ASP
	GLU	PHE
	GLN	GLY
	MET	LEU
	GLU	PRO
	HIS	LYS
	ILE	LYS
	ALA	GLN
	SER	ASN
	SER	PRO
	HIS	ASN
	GLU	LYS
	HIS	ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	490	Depositor
Maximum defocus (nm)	3070	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.986	Depositor
Minimum map value	-2.476	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.36	Depositor
Map size ($\text{\AA}$)	273.0, 273.0, 273.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.91, 0.91, 0.91	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: A1IGY

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	0.10	0/5391	0.26	0/7300
1	B	0.11	0/5399	0.33	0/7311
1	C	0.11	0/5391	0.31	0/7300
1	D	0.11	0/5399	0.34	0/7311
All	All	0.11	0/21580	0.31	0/29222

There are no bond length outliers.

There are no bond angle outliers.

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	5266	0	5298	44	0
1	B	5274	0	5302	46	0
1	C	5266	0	5298	51	0
1	D	5274	0	5308	53	0
2	A	44	0	0	3	0
2	B	44	0	0	1	0
2	C	44	0	0	0	0
2	D	44	0	0	2	0
All	All	21256	0	21206	173	0

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

All (173) 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:D:351:PRO:HA	1:D:356:GLY:HA3	1.61	0.83
1:D:49:LYS:HD3	1:D:88:LEU:HD11	1.72	0.72
1:C:33:GLU:HG3	1:C:61:ILE:HG23	1.73	0.70
1:A:216:PRO:HD2	1:A:709:LEU:HD21	1.74	0.70
1:D:216:PRO:HD2	1:D:709:LEU:HD21	1.74	0.68
1:D:654:PRO:O	1:D:658:ASN:ND2	2.27	0.68
1:C:365:LYS:HE2	1:C:652:THR:HG23	1.77	0.66
1:B:227:LEU:HD13	1:B:244:LEU:HB3	1.76	0.66
1:B:204:ALA:O	1:B:247:GLN:NE2	2.28	0.66
1:C:52:LEU:HD11	1:C:89:LEU:HD23	1.77	0.66
1:C:534:LEU:HD23	1:C:600:MET:HE3	1.78	0.66
1:D:457:VAL:HG23	1:D:458:LYS:HG3	1.79	0.65
1:B:216:PRO:HD2	1:B:709:LEU:HD21	1.78	0.64
1:B:353:SER:HA	1:B:357:LEU:HB2	1.79	0.64
1:C:618:ALA:O	1:C:622:ASN:ND2	2.27	0.62
1:D:717:VAL:HA	1:D:720:MET:HG2	1.82	0.62
1:C:725:LYS:NZ	1:D:79:GLU:OE2	2.32	0.61
1:A:493:ILE:HG13	1:B:525:LEU:HD23	1.80	0.61
1:A:204:ALA:O	1:A:247:GLN:NE2	2.33	0.61
1:B:29:LEU:HD13	1:B:30:SER:H	1.65	0.60
1:D:617:ILE:O	1:D:621:ASN:ND2	2.35	0.60
1:C:365:LYS:HD2	1:C:646:TYR:HD1	1.67	0.58
1:D:455:ALA:HB2	1:D:473:PRO:HB2	1.86	0.58
1:B:343:LEU:HA	1:B:346:CYS:HB2	1.86	0.57
1:B:698:ASN:O	1:B:702:ASN:ND2	2.35	0.56
1:B:98:ASP:O	1:B:102:HIS:ND1	2.36	0.56
1:B:188:ASP:OD2	1:B:191:ARG:NH1	2.38	0.56
1:B:394:ARG:HG3	1:B:397:PRO:HB3	1.86	0.56
1:A:170:GLN:HG3	1:B:19:PRO:HD3	1.88	0.56
1:B:260:ARG:O	1:C:194:ARG:NH2	2.38	0.56
1:C:72:THR:H	1:C:75[A]:LEU:HD12	1.71	0.55
1:B:168:VAL:HG11	1:B:203:LEU:HD21	1.88	0.55
1:A:738:LEU:HD22	1:D:738:LEU:HD21	1.89	0.55
1:C:29:LEU:HD23	1:C:29:LEU:H	1.71	0.55
1:D:417:GLU:OE1	1:D:429:TYR:OH	2.24	0.55
1:B:380:LEU:HD21	1:B:485:ASN:HB2	1.89	0.55
1:C:67:ASP:OD1	1:C:71:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ARG:HE	1:A:701:LEU:HG	1.72	0.54
1:C:33:GLU:N	1:C:33:GLU:OE1	2.39	0.54
1:C:457:VAL:HG23	1:C:458:LYS:HG3	1.90	0.54
1:D:524:CYS:SG	2:D:1001:A1IGY:F01	2.57	0.53
1:C:738:LEU:HD21	1:D:738:LEU:HD23	1.90	0.53
1:D:290:LYS:HG2	1:D:644:MET:HE1	1.90	0.53
1:C:216:PRO:HD2	1:C:709:LEU:HD11	1.90	0.53
1:C:257:ASP:OD1	1:C:303:GLN:NE2	2.33	0.53
1:D:357:LEU:HA	1:D:360:ARG:HG3	1.91	0.53
1:D:194:ARG:HH21	1:D:197:LEU:HD23	1.75	0.52
1:D:55:ALA:HA	1:D:59:PHE:HB2	1.92	0.52
1:B:740:GLN:NE2	1:C:41:GLU:O	2.42	0.52
1:A:518:LYS:HE3	1:D:501:HIS:HB3	1.92	0.52
1:B:30:SER:O	1:B:34:LYS:NZ	2.41	0.51
1:B:417:GLU:OE1	1:B:429:TYR:OH	2.26	0.51
1:A:270:ASN:ND2	1:A:285:GLU:OE1	2.44	0.51
1:C:288:ARG:NH1	1:C:705:TYR:OH	2.44	0.51
1:C:422:TRP:HD1	1:C:423:ASP:N	2.09	0.51
1:D:616:LEU:HG	1:D:620:MET:HE3	1.93	0.50
1:B:722:ARG:HG2	1:B:725:LYS:HZ3	1.76	0.50
1:C:308:GLN:OE1	1:D:189:SER:OG	2.28	0.50
1:D:233:VAL:O	1:D:234:GLU:HB2	2.10	0.50
1:B:617:ILE:HD11	1:C:617:ILE:HG21	1.94	0.49
1:B:630:HIS:ND1	1:B:630:HIS:O	2.45	0.49
1:A:746:ARG:HD2	1:D:745:PHE:HB2	1.93	0.49
1:D:253:LYS:HE3	1:D:303:GLN:HG2	1.95	0.49
1:A:340:PHE:CD2	1:A:341:PRO:HD3	2.48	0.49
1:C:655:PRO:N	1:C:656:PRO:HD2	2.28	0.48
1:C:140:THR:HG22	1:C:141:PRO:HD2	1.94	0.48
1:C:717:VAL:HA	1:C:720:MET:HG2	1.95	0.48
1:C:563:THR:OG1	1:C:564:LEU:N	2.44	0.48
1:D:747:TYR:HD1	1:D:750:ILE:HD11	1.78	0.48
1:A:455:ALA:HB2	1:A:473:PRO:HB2	1.95	0.48
1:B:409:TRP:H	1:B:409:TRP:CD1	2.30	0.48
1:A:698:ASN:HA	1:A:700:ARG:HH21	1.79	0.48
1:C:308:GLN:HB2	1:D:236:GLU:HG3	1.96	0.47
1:A:655:PRO:N	1:A:656:PRO:HD2	2.30	0.47
1:B:261:SER:OG	1:B:264:GLU:OE1	2.26	0.47
1:C:75[B]:LEU:HD23	1:C:78:ILE:HD11	1.97	0.47
1:C:108:VAL:HG22	1:C:111:ALA:H	1.80	0.47
1:D:563:THR:HG23	1:D:566:GLU:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:654:PRO:HB2	1:D:656:PRO:HD2	1.97	0.47
1:A:69:LEU:HD22	1:D:721:ILE:HG21	1.96	0.47
1:B:655:PRO:N	1:B:656:PRO:HD2	2.30	0.46
1:B:351:PRO:HA	1:B:356:GLY:HA3	1.98	0.46
1:C:210:ALA:O	1:D:24:ARG:NH2	2.46	0.46
1:B:140:THR:HG22	1:B:141:PRO:HD2	1.98	0.46
1:B:438:ASP:CG	1:B:491:ARG:HE	2.23	0.46
1:C:430:ILE:HD11	1:C:436:LEU:HD13	1.97	0.46
1:D:655:PRO:N	1:D:656:PRO:HD2	2.30	0.46
1:C:402:VAL:HA	1:C:405:MET:HE3	1.97	0.46
2:A:1001:A1IGY:C25	1:B:610:VAL:HG11	2.46	0.46
1:C:616:LEU:HG	1:C:620:MET:HE2	1.98	0.46
1:B:722:ARG:HA	1:B:725:LYS:HG2	1.98	0.45
1:A:52:LEU:HD11	1:A:89:LEU:HD23	1.97	0.45
1:C:116:LEU:HB3	1:C:164:LYS:NZ	2.31	0.45
1:D:604:TYR:O	1:D:608:SER:HB3	2.17	0.45
1:A:201:LYS:HA	1:A:244:LEU:HD21	1.98	0.45
1:C:303:GLN:HG2	1:C:304:PRO:HD2	1.98	0.45
1:C:479:ALA:O	1:C:483:ILE:HG13	2.17	0.45
1:D:88:LEU:O	1:D:91:SER:OG	2.27	0.45
1:A:88:LEU:O	1:A:91:SER:OG	2.23	0.45
1:C:340:PHE:CD2	1:C:341:PRO:HD3	2.52	0.45
1:A:303:GLN:HG2	1:A:304:PRO:HD2	1.98	0.45
1:D:630:HIS:O	1:D:630:HIS:ND1	2.49	0.45
1:B:721:ILE:HD11	1:C:69:LEU:HD23	1.98	0.45
1:A:196:ARG:NH2	1:A:234:GLU:OE2	2.50	0.44
1:A:417:GLU:OE1	1:A:429:TYR:OH	2.33	0.44
1:A:376:PHE:HE1	1:A:406:ILE:HG23	1.82	0.44
1:A:520:LEU:HD11	2:A:1001:A1IGY:N05	2.32	0.44
1:B:260:ARG:HH21	1:C:140:THR:HA	1.82	0.44
1:D:654:PRO:HG2	1:D:657:PHE:HD2	1.81	0.44
1:D:416:THR:HA	1:D:419:LYS:HG2	2.00	0.44
1:B:298:LYS:NZ	1:B:634:GLU:OE1	2.43	0.44
1:A:566:GLU:HA	1:A:569:GLN:HG2	1.99	0.44
1:A:615:MET:SD	1:D:509:LEU:HG	2.58	0.44
1:D:616:LEU:HD12	1:D:619:MET:HE2	1.99	0.44
1:A:736:LYS:HD2	1:A:739:LYS:HZ1	1.81	0.44
1:C:150:ALA:HA	1:C:158:ILE:HD11	1.99	0.44
1:A:310:LEU:HD12	1:A:310:LEU:HA	1.86	0.43
1:B:391:ASN:HB2	1:B:394:ARG:HE	1.83	0.43
1:C:71:ARG:HH21	1:C:76:ILE:HG12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ALA:HA	1:D:158:ILE:HD11	2.00	0.43
1:A:432:ASP:N	1:A:432:ASP:OD1	2.51	0.43
1:B:740:GLN:HG2	1:C:80:ASN:HB3	2.00	0.43
1:C:348:LEU:HD21	1:C:653:LEU:HD11	2.00	0.43
1:D:376:PHE:HE1	1:D:406:ILE:HG23	1.82	0.43
1:A:81:GLU:HB3	1:A:108:VAL:HG11	2.01	0.43
1:A:742:ILE:HD13	1:D:742:ILE:HG22	2.00	0.43
1:B:534:LEU:HD23	1:B:600:MET:HE3	2.01	0.43
1:C:167:SER:OG	1:D:19:PRO:O	2.31	0.43
1:C:718:ALA:O	1:C:721:ILE:HG13	2.18	0.43
1:D:271:PHE:HD2	1:D:288:ARG:HH21	1.66	0.43
1:A:373:TYR:OH	1:A:488:SER:O	2.31	0.43
1:A:523:TYR:OH	1:A:575:ILE:HD11	2.18	0.42
1:B:457:VAL:HG23	1:B:458:LYS:HG2	2.01	0.42
1:D:29:LEU:HD13	1:D:66:ILE:HG22	2.00	0.42
1:A:608:SER:O	1:A:613:LEU:HB2	2.20	0.42
1:D:422:TRP:HD1	1:D:423:ASP:N	2.18	0.42
1:A:520:LEU:HD13	1:A:520:LEU:HA	1.90	0.42
1:B:303:GLN:HG2	1:B:304:PRO:HD2	2.01	0.42
1:C:59:PHE:O	1:C:60:LYS:HG2	2.19	0.42
1:D:66:ILE:HD12	1:D:66:ILE:HA	1.92	0.42
1:A:168:VAL:HG23	1:B:21:ARG:HD2	2.02	0.42
1:A:308:GLN:OE1	1:B:189:SER:OG	2.37	0.42
2:A:1001:A1IGY:C28	2:A:1001:A1IGY:C12	2.98	0.42
1:A:150:ALA:HA	1:A:158:ILE:HD11	2.01	0.41
1:A:20:LEU:HD23	1:D:167:SER:HB2	2.02	0.41
1:A:507:ILE:O	1:A:511:ARG:HG3	2.20	0.41
1:B:54:GLU:CD	1:B:54:GLU:H	2.28	0.41
1:C:69:LEU:HD22	1:C:71:ARG:NH1	2.35	0.41
1:A:405:MET:O	1:A:408:PRO:HD2	2.20	0.41
1:A:496:PHE:HB2	1:A:506:GLN:OE1	2.21	0.41
1:C:556:ARG:O	1:C:558:ASN:ND2	2.53	0.41
2:D:1001:A1IGY:C12	2:D:1001:A1IGY:C24	2.99	0.41
1:A:354:ARG:HG3	1:A:355:TYR:H	1.86	0.41
1:B:391:ASN:HD22	1:B:391:ASN:N	2.19	0.41
1:C:213:SER:OG	1:C:214:GLU:N	2.54	0.41
1:D:37:LEU:HD21	1:D:65:CYS:HB2	2.02	0.41
1:D:204:ALA:O	1:D:247:GLN:NE2	2.54	0.41
1:D:340:PHE:CD2	1:D:341:PRO:HD3	2.55	0.41
1:D:388:VAL:O	1:D:391:ASN:ND2	2.54	0.41
1:D:725:LYS:HE2	1:D:725:LYS:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:A1IGY:C25	1:C:610:VAL:HG21	2.50	0.41
1:C:71:ARG:HB3	1:C:75[B]:LEU:HB3	2.02	0.41
1:A:253:LYS:HD2	1:A:299:GLU:HB3	2.02	0.40
1:B:698:ASN:HB3	1:B:701:LEU:HB2	2.03	0.40
1:A:343:LEU:HD11	1:A:368:CYS:SG	2.62	0.40
1:A:516:ILE:HD11	1:A:620:MET:HE3	2.02	0.40
1:B:201:LYS:HA	1:B:244:LEU:HD21	2.04	0.40
1:C:542:GLU:HG3	1:C:562:SER:HB3	2.03	0.40
1:D:352:LYS:HE2	1:D:352:LYS:HB2	1.90	0.40
1:B:210:ALA:HB1	1:B:713:VAL:HG13	2.02	0.40
1:B:472:HIS:CG	1:B:473:PRO:HD2	2.57	0.40
1:B:360:ARG:HH22	1:B:649:GLU:HB2	1.86	0.40
1:D:726:THR:HG23	1:D:733:GLU:HB3	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	629/941 (67%)	603 (96%)	26 (4%)	0	100	100
1	B	630/941 (67%)	601 (95%)	27 (4%)	2 (0%)	36	67
1	C	629/941 (67%)	600 (95%)	29 (5%)	0	100	100
1	D	630/941 (67%)	595 (94%)	34 (5%)	1 (0%)	43	73
All	All	2518/3764 (67%)	2399 (95%)	116 (5%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	PRO
1	D	234	GLU

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Mol	Chain	Res	Type
1	B	187	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/839 (69%)	552 (96%)	24 (4%)	26	58
1	B	577/839 (69%)	545 (94%)	32 (6%)	19	50
1	C	576/839 (69%)	556 (96%)	20 (4%)	32	62
1	D	577/839 (69%)	557 (96%)	20 (4%)	32	62
All	All	2306/3356 (69%)	2210 (96%)	96 (4%)	28	58

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	211	LEU
1	A	233	VAL
1	A	234	GLU
1	A	303	GLN
1	A	310	LEU
1	A	426	PHE
1	A	437	MET
1	A	467	THR
1	A	493	ILE
1	A	505	LEU
1	A	519	PHE
1	A	520	LEU
1	A	540	TYR
1	A	549	CYS
1	A	552	ILE
1	A	554	CYS
1	A	617	ILE
1	A	649	GLU
1	A	657	PHE

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Mol	Chain	Res	Type
1	A	700	ARG
1	A	702	ASN
1	A	720	MET
1	A	738	LEU
1	B	20	LEU
1	B	26	GLU
1	B	28	GLU
1	B	29	LEU
1	B	31	THR
1	B	81	GLU
1	B	108	VAL
1	B	117	ASN
1	B	140	THR
1	B	168	VAL
1	B	170	GLN
1	B	244	LEU
1	B	267	LEU
1	B	303	GLN
1	B	339	MET
1	B	343	LEU
1	B	379	LEU
1	B	382	LEU
1	B	391	ASN
1	B	435	ASN
1	B	454	VAL
1	B	492	LEU
1	B	513	LEU
1	B	519	PHE
1	B	520	LEU
1	B	522	ILE
1	B	540	TYR
1	B	554	CYS
1	B	617	ILE
1	B	621	ASN
1	B	632	ASP
1	B	715	ARG
1	C	20	LEU
1	C	21	ARG
1	C	50	LEU
1	C	59	PHE
1	C	72	THR
1	C	74	LEU

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Mol	Chain	Res	Type
1	C	88	LEU
1	C	108	VAL
1	C	138	ASP
1	C	140	THR
1	C	240	GLU
1	C	244	LEU
1	C	358	PHE
1	C	377	LEU
1	C	379	LEU
1	C	403	GLU
1	C	509	LEU
1	C	563	THR
1	C	649	GLU
1	C	737	GLU
1	D	50	LEU
1	D	67	ASP
1	D	80	ASN
1	D	82	ASN
1	D	88	LEU
1	D	159	LYS
1	D	168	VAL
1	D	194	ARG
1	D	203	LEU
1	D	339	MET
1	D	352	LYS
1	D	354	ARG
1	D	513	LEU
1	D	519	PHE
1	D	608	SER
1	D	613	LEU
1	D	617	ILE
1	D	721	ILE
1	D	740	GLN
1	D	742	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	102	HIS
1	A	154	ASN
1	A	246	HIS

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Mol	Chain	Res	Type
1	A	305	ASN
1	A	391	ASN
1	A	395	GLN
1	A	472	HIS
1	A	501	HIS
1	B	80	ASN
1	B	82	ASN
1	B	170	GLN
1	B	391	ASN
1	B	558	ASN
1	B	569	GLN
1	B	625	GLN
1	B	626	HIS
1	C	135	GLN
1	C	385	GLN
1	C	391	ASN
1	D	153	ASN
1	D	228	GLN
1	D	391	ASN
1	D	431	HIS
1	D	536	GLN
1	D	558	ASN
1	D	559	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1IGY	C	1001	-	48,48,48	1.75	10 (20%)	66,69,69	3.13	15 (22%)
2	A1IGY	A	1001	-	48,48,48	1.73	10 (20%)	66,69,69	3.24	16 (24%)
2	A1IGY	D	1001	-	48,48,48	1.74	10 (20%)	66,69,69	3.14	14 (21%)
2	A1IGY	B	1001	-	48,48,48	1.75	10 (20%)	66,69,69	3.09	16 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IGY	C	1001	-	-	6/22/22/22	0/5/5/5
2	A1IGY	A	1001	-	-	6/22/22/22	0/5/5/5
2	A1IGY	D	1001	-	-	8/22/22/22	0/5/5/5
2	A1IGY	B	1001	-	-	5/22/22/22	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	A1IGY	C02-N02	6.82	1.49	1.38
2	D	1001	A1IGY	C02-N02	6.81	1.49	1.38
2	C	1001	A1IGY	C02-N02	6.81	1.49	1.38
2	B	1001	A1IGY	C02-N02	6.73	1.49	1.38
2	C	1001	A1IGY	C03-C04	4.33	1.53	1.43
2	B	1001	A1IGY	C03-C04	4.26	1.53	1.43
2	D	1001	A1IGY	C03-C04	4.25	1.53	1.43
2	A	1001	A1IGY	C03-C04	4.20	1.53	1.43
2	C	1001	A1IGY	O03-C05	3.76	1.40	1.34
2	A	1001	A1IGY	O03-C05	3.74	1.40	1.34
2	B	1001	A1IGY	O03-C05	3.73	1.40	1.34
2	D	1001	A1IGY	C01-N02	3.66	1.46	1.39
2	D	1001	A1IGY	O03-C05	3.62	1.40	1.34
2	C	1001	A1IGY	C01-N02	3.61	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	A1IGY	C01-N02	3.56	1.46	1.39
2	A	1001	A1IGY	C01-N02	3.49	1.45	1.39
2	C	1001	A1IGY	C01-N01	3.14	1.44	1.38
2	B	1001	A1IGY	C01-N01	3.05	1.44	1.38
2	D	1001	A1IGY	C01-N01	3.04	1.44	1.38
2	A	1001	A1IGY	C01-N01	2.97	1.43	1.38
2	B	1001	A1IGY	C05-N03	2.46	1.36	1.31
2	D	1001	A1IGY	C05-N03	2.41	1.35	1.31
2	D	1001	A1IGY	C03-N04	-2.37	1.34	1.39
2	A	1001	A1IGY	C05-N03	2.36	1.35	1.31
2	C	1001	A1IGY	C03-N04	-2.34	1.34	1.39
2	C	1001	A1IGY	C05-N03	2.34	1.35	1.31
2	B	1001	A1IGY	C03-N04	-2.31	1.34	1.39
2	A	1001	A1IGY	C03-N04	-2.27	1.34	1.39
2	A	1001	A1IGY	O01-C04	-2.26	1.18	1.23
2	B	1001	A1IGY	O01-C04	-2.26	1.18	1.23
2	D	1001	A1IGY	C13-N05	2.21	1.47	1.42
2	C	1001	A1IGY	C13-N05	2.20	1.47	1.42
2	D	1001	A1IGY	O01-C04	-2.17	1.18	1.23
2	B	1001	A1IGY	C13-N05	2.16	1.47	1.42
2	A	1001	A1IGY	C13-N05	2.11	1.46	1.42
2	C	1001	A1IGY	O01-C04	-2.10	1.18	1.23
2	B	1001	A1IGY	O02-C01	-2.04	1.18	1.22
2	D	1001	A1IGY	O02-C01	-2.02	1.18	1.22
2	C	1001	A1IGY	O02-C01	-2.01	1.18	1.22
2	A	1001	A1IGY	O02-C01	-2.01	1.18	1.22

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	A1IGY	N04-C05-N03	-13.99	108.15	115.50
2	C	1001	A1IGY	N04-C05-N03	-13.98	108.16	115.50
2	B	1001	A1IGY	N04-C05-N03	-13.84	108.23	115.50
2	D	1001	A1IGY	N04-C05-N03	-13.74	108.29	115.50
2	A	1001	A1IGY	O03-C05-N04	12.98	127.50	116.83
2	D	1001	A1IGY	O03-C05-N04	12.34	126.97	116.83
2	C	1001	A1IGY	O03-C05-N04	12.32	126.96	116.83
2	B	1001	A1IGY	O03-C05-N04	11.61	126.37	116.83
2	C	1001	A1IGY	C13-N05-N06	9.99	136.50	114.51
2	B	1001	A1IGY	C13-N05-N06	9.91	136.33	114.51
2	D	1001	A1IGY	C13-N05-N06	9.80	136.07	114.51
2	A	1001	A1IGY	C13-N05-N06	9.65	135.74	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	A1IGY	C06-O03-C05	-7.49	102.22	118.03
2	D	1001	A1IGY	C06-O03-C05	-6.95	103.36	118.03
2	B	1001	A1IGY	C06-O03-C05	-6.13	105.08	118.03
2	C	1001	A1IGY	C06-O03-C05	-5.65	106.11	118.03
2	B	1001	A1IGY	C23-N06-N05	4.99	137.54	112.97
2	A	1001	A1IGY	C23-N06-N05	4.96	137.41	112.97
2	D	1001	A1IGY	C23-N06-N05	4.96	137.38	112.97
2	C	1001	A1IGY	C23-N06-N05	4.84	136.79	112.97
2	B	1001	A1IGY	C04-N01-C01	-4.57	120.00	125.62
2	C	1001	A1IGY	C04-N01-C01	-4.40	120.20	125.62
2	A	1001	A1IGY	C04-N01-C01	-4.38	120.23	125.62
2	D	1001	A1IGY	C04-N01-C01	-4.35	120.27	125.62
2	B	1001	A1IGY	C03-C04-N01	4.27	120.27	112.23
2	A	1001	A1IGY	C03-C04-N01	4.24	120.20	112.23
2	C	1001	A1IGY	C03-C04-N01	4.14	120.01	112.23
2	A	1001	A1IGY	C03-C02-N03	-4.13	107.71	112.77
2	D	1001	A1IGY	C03-C04-N01	4.12	119.98	112.23
2	D	1001	A1IGY	C03-C02-N03	-3.99	107.88	112.77
2	C	1001	A1IGY	C03-C02-N03	-3.97	107.90	112.77
2	B	1001	A1IGY	C03-C02-N03	-3.93	107.95	112.77
2	A	1001	A1IGY	C02-C03-N04	3.62	107.85	104.93
2	C	1001	A1IGY	N02-C02-N03	3.60	131.47	125.59
2	D	1001	A1IGY	N02-C02-N03	3.59	131.46	125.59
2	B	1001	A1IGY	N02-C02-N03	3.58	131.43	125.59
2	A	1001	A1IGY	N02-C02-N03	3.54	131.38	125.59
2	D	1001	A1IGY	C02-C03-N04	3.53	107.78	104.93
2	C	1001	A1IGY	C02-C03-N04	3.47	107.73	104.93
2	B	1001	A1IGY	C02-C03-N04	3.46	107.73	104.93
2	A	1001	A1IGY	C04-C03-C02	-3.15	118.95	122.92
2	B	1001	A1IGY	C04-C03-C02	-3.00	119.14	122.92
2	A	1001	A1IGY	O03-C05-N03	-2.94	124.34	128.41
2	B	1001	A1IGY	O01-C04-C03	-2.94	120.36	126.38
2	A	1001	A1IGY	O01-C04-C03	-2.93	120.38	126.38
2	C	1001	A1IGY	C04-C03-C02	-2.86	119.31	122.92
2	D	1001	A1IGY	O01-C04-C03	-2.85	120.54	126.38
2	D	1001	A1IGY	C04-C03-C02	-2.84	119.34	122.92
2	C	1001	A1IGY	O01-C04-C03	-2.77	120.71	126.38
2	D	1001	A1IGY	O03-C05-N03	-2.66	124.73	128.41
2	C	1001	A1IGY	O03-C05-N03	-2.55	124.88	128.41
2	D	1001	A1IGY	N01-C01-N02	2.49	119.79	116.72
2	A	1001	A1IGY	N01-C01-N02	2.47	119.76	116.72
2	B	1001	A1IGY	N01-C01-N02	2.46	119.75	116.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	A1IGY	C17-C16-N04	-2.46	108.98	113.09
2	C	1001	A1IGY	N01-C01-N02	2.44	119.73	116.72
2	B	1001	A1IGY	C17-C16-N04	-2.26	109.30	113.09
2	C	1001	A1IGY	C17-C16-N04	-2.19	109.43	113.09
2	B	1001	A1IGY	O03-C05-N03	-2.18	125.39	128.41
2	B	1001	A1IGY	C07-N01-C04	2.05	120.08	117.18
2	A	1001	A1IGY	C07-N01-C04	2.00	120.02	117.18

There are no chirality outliers.

All (25) torsion outliers are listed below:

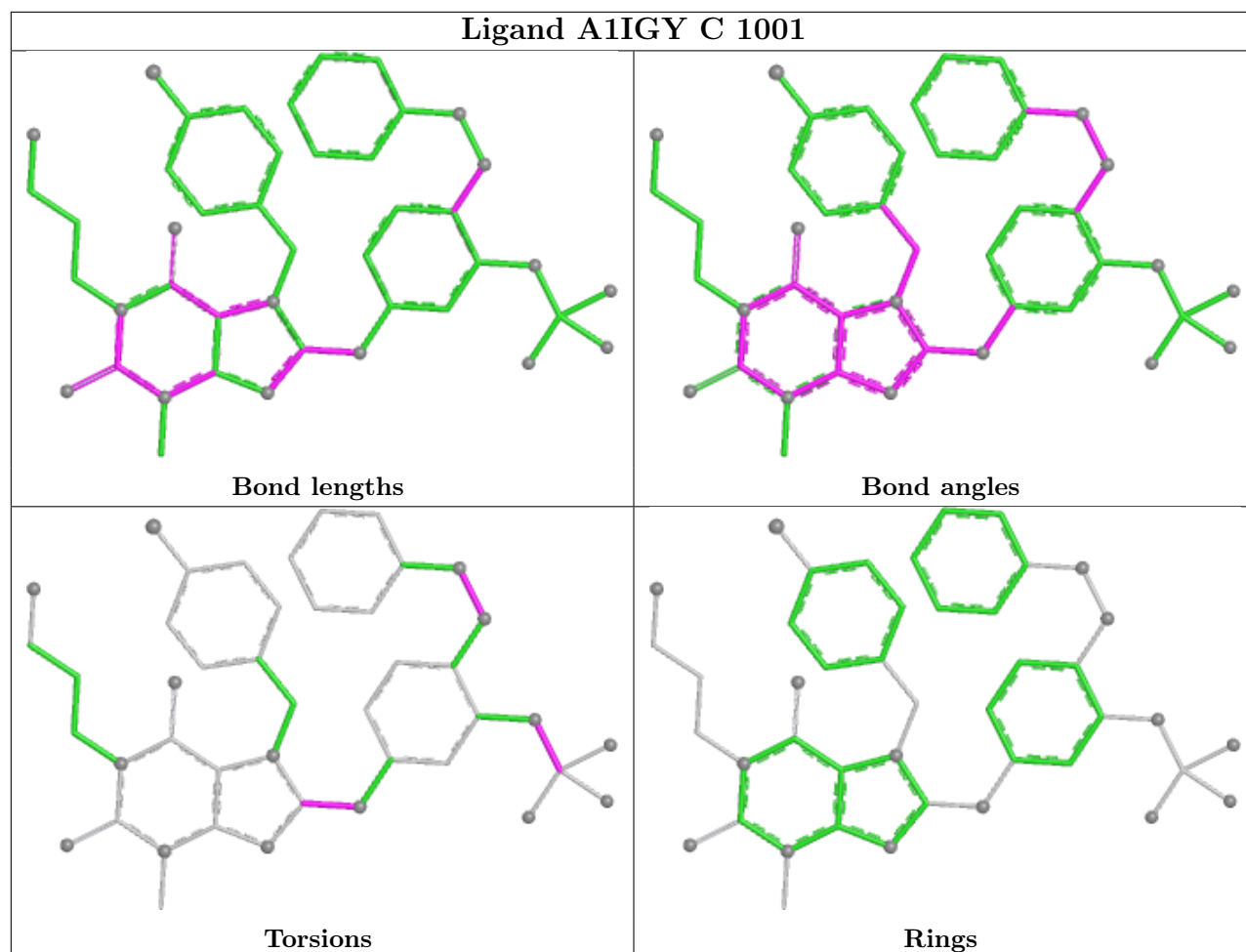
Mol	Chain	Res	Type	Atoms
2	C	1001	A1IGY	F03-C29-O05-C14
2	D	1001	A1IGY	N01-C07-C08-C09
2	D	1001	A1IGY	F02-C29-O05-C14
2	C	1001	A1IGY	F02-C29-O05-C14
2	D	1001	A1IGY	F03-C29-O05-C14
2	B	1001	A1IGY	N01-C07-C08-C09
2	C	1001	A1IGY	F01-C29-O05-C14
2	D	1001	A1IGY	F01-C29-O05-C14
2	D	1001	A1IGY	C07-C08-C09-O04
2	B	1001	A1IGY	C13-N05-N06-C23
2	A	1001	A1IGY	C13-N05-N06-C23
2	C	1001	A1IGY	C13-N05-N06-C23
2	D	1001	A1IGY	C13-N05-N06-C23
2	A	1001	A1IGY	F01-C29-O05-C14
2	A	1001	A1IGY	N01-C07-C08-C09
2	A	1001	A1IGY	F02-C29-O05-C14
2	A	1001	A1IGY	C07-C08-C09-O04
2	B	1001	A1IGY	C15-C14-O05-C29
2	A	1001	A1IGY	F03-C29-O05-C14
2	B	1001	A1IGY	N04-C05-O03-C06
2	C	1001	A1IGY	N04-C05-O03-C06
2	D	1001	A1IGY	N04-C05-O03-C06
2	C	1001	A1IGY	N03-C05-O03-C06
2	D	1001	A1IGY	N03-C05-O03-C06
2	B	1001	A1IGY	C13-C14-O05-C29

There are no ring outliers.

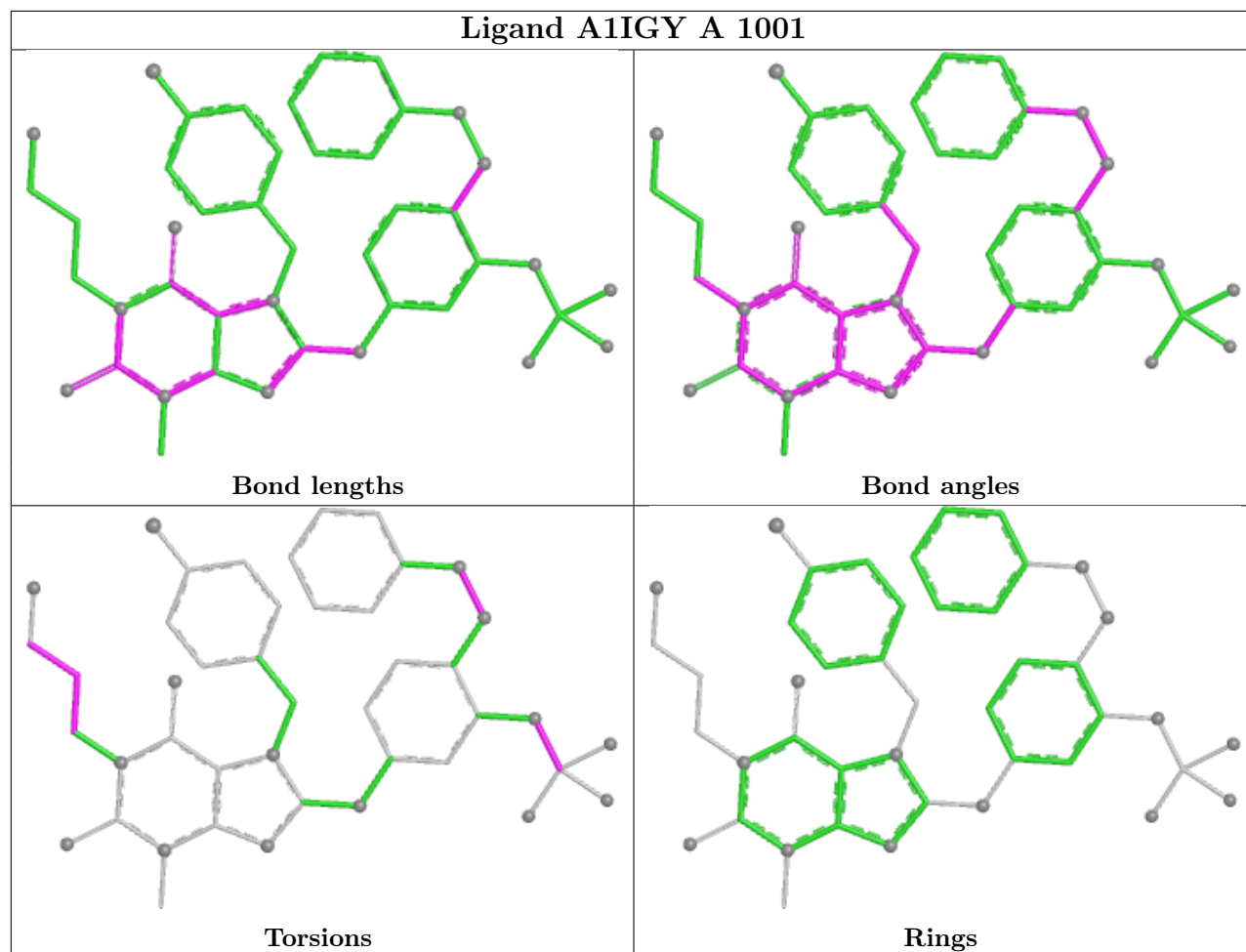
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	A1IGY	3	0
2	D	1001	A1IGY	2	0
2	B	1001	A1IGY	1	0

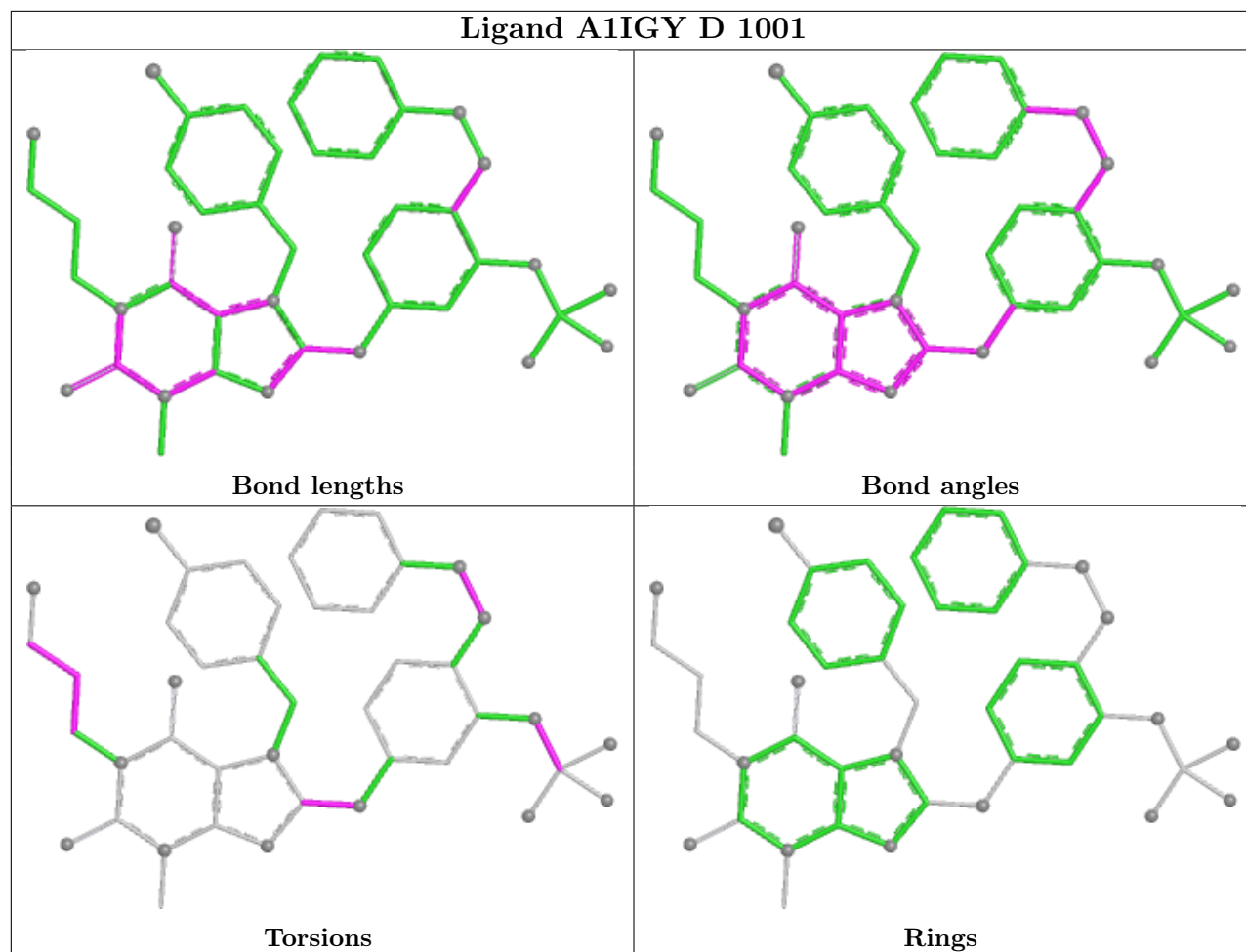
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

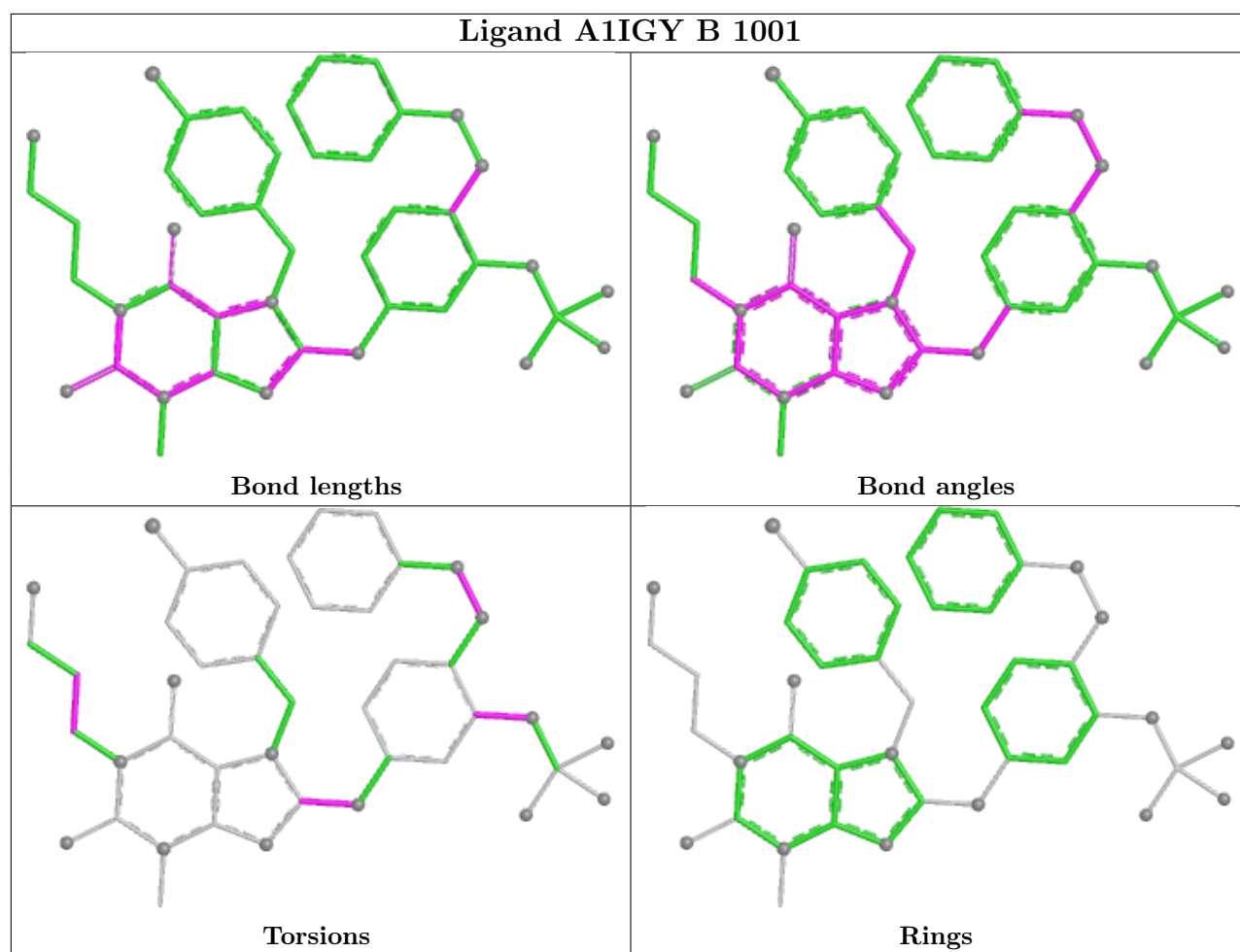


Ligand A1IGY A 1001



Ligand A1IGY D 1001





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.

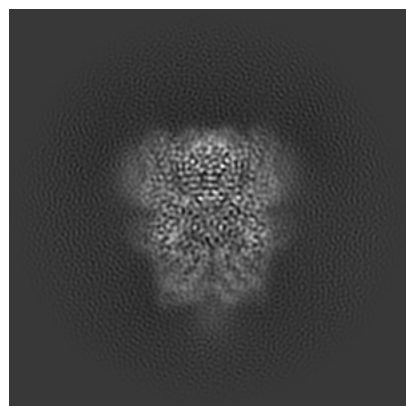
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50851. These allow visual inspection of the internal detail of the map and identification of artifacts.

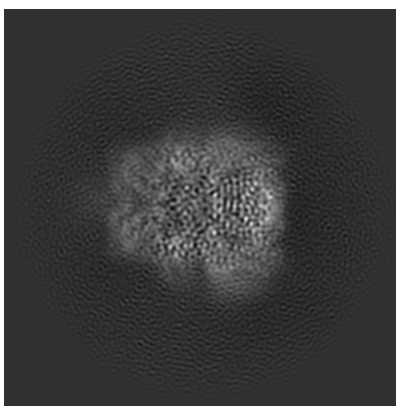
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

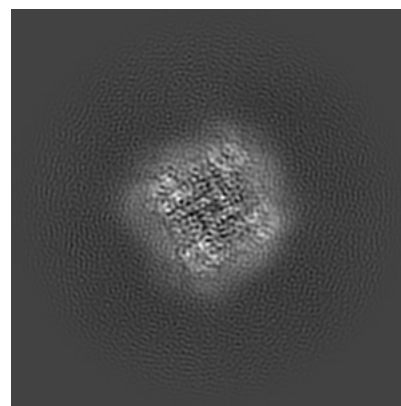
6.1.1 Primary map



X

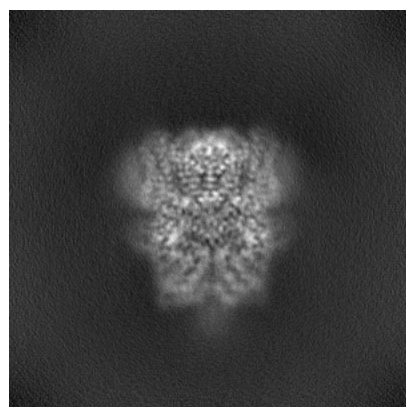


Y

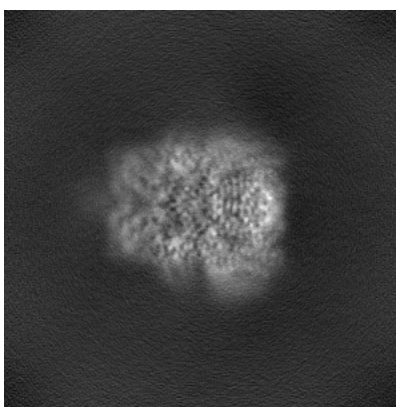


Z

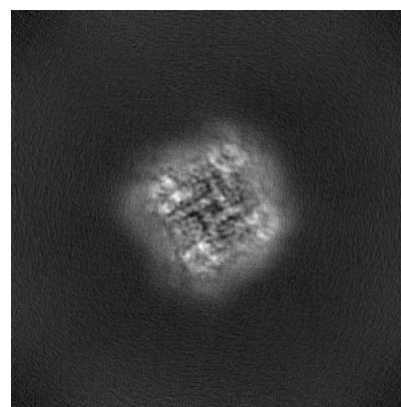
6.1.2 Raw map



X



Y

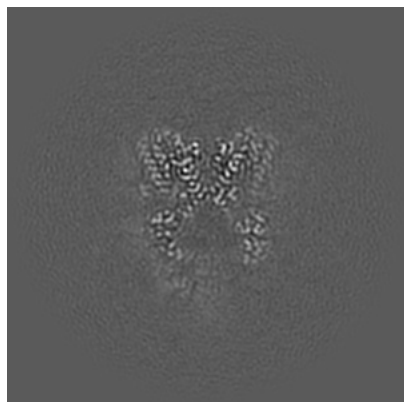


Z

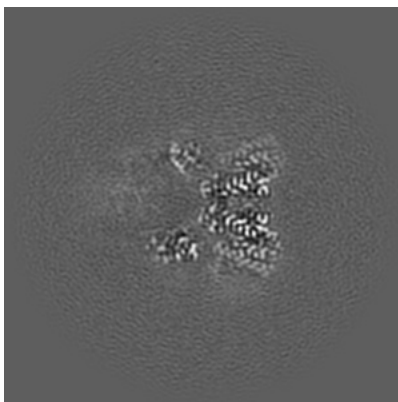
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

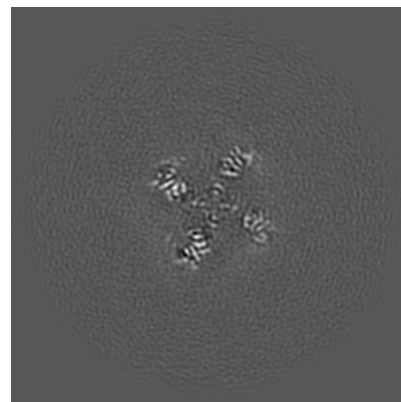
6.2.1 Primary map



X Index: 150

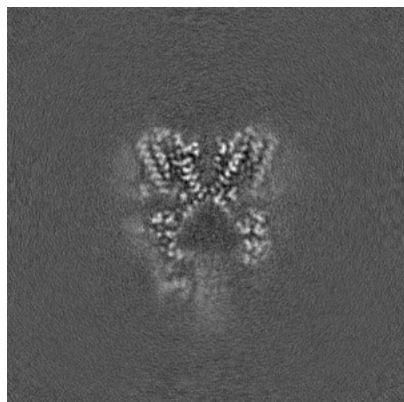


Y Index: 150

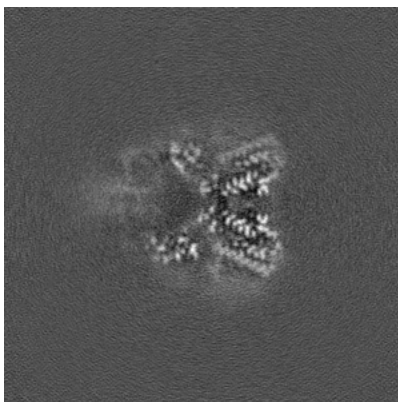


Z Index: 150

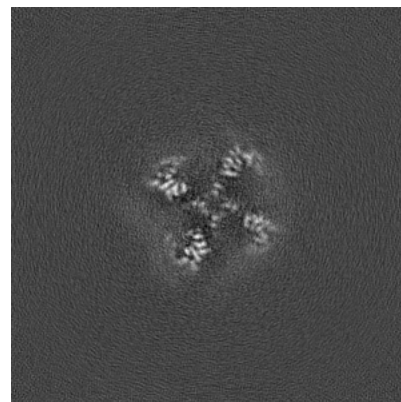
6.2.2 Raw map



X Index: 150



Y Index: 150

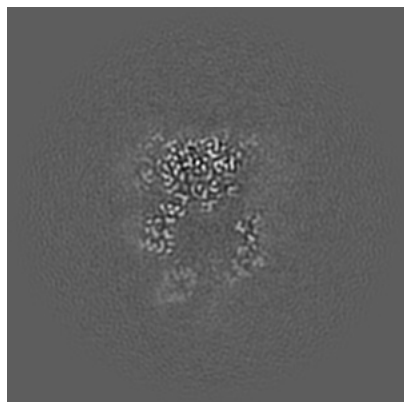


Z Index: 150

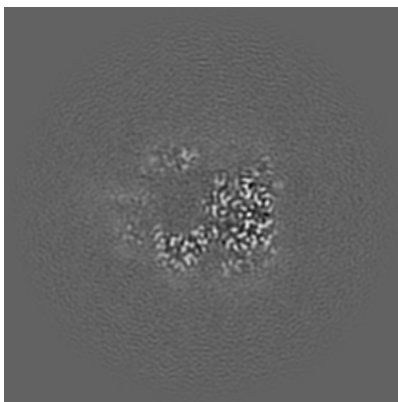
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

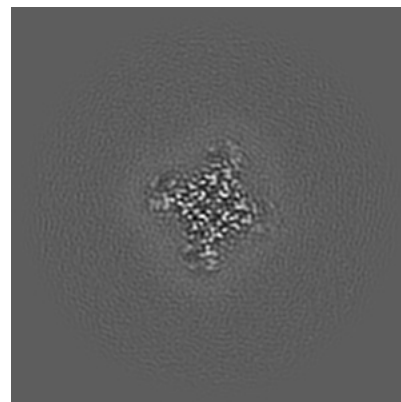
6.3.1 Primary map



X Index: 143

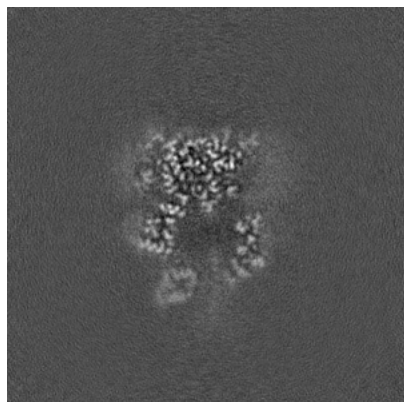


Y Index: 159

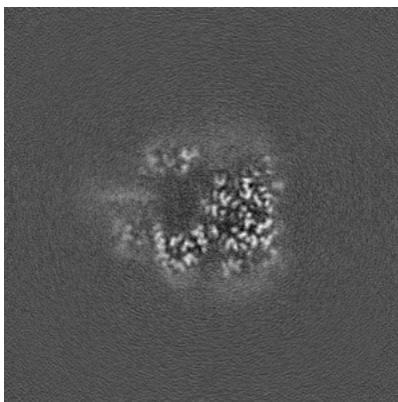


Z Index: 183

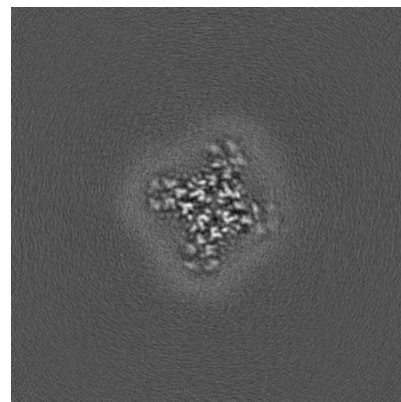
6.3.2 Raw map



X Index: 143



Y Index: 159

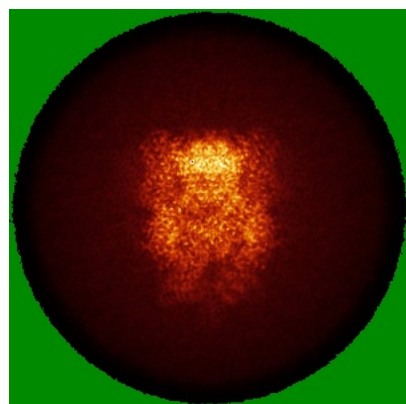


Z Index: 182

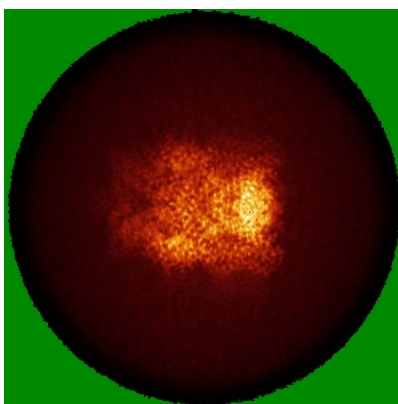
The images above show the largest variance slices of the map in three orthogonal directions.

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

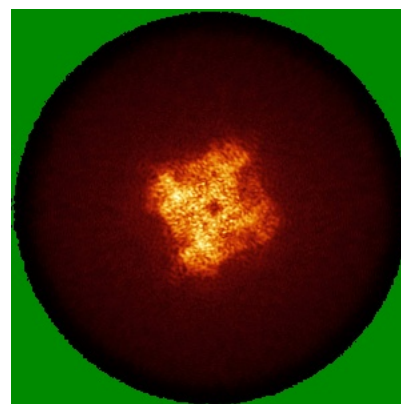
6.4.1 Primary map



X

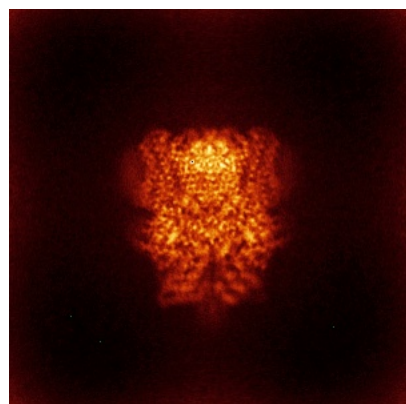


Y

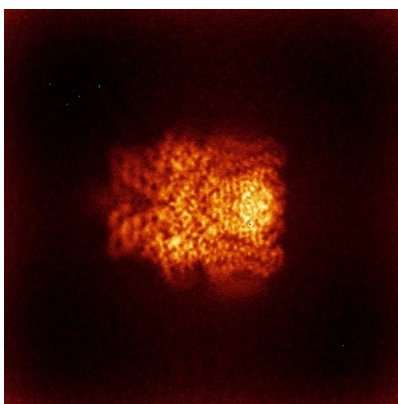


Z

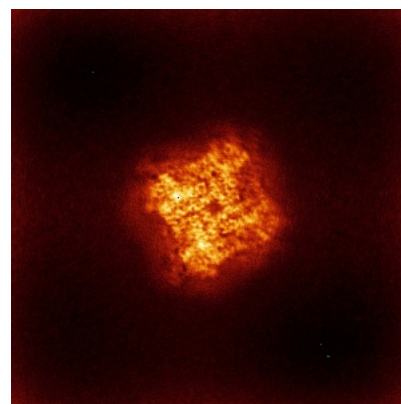
6.4.2 Raw map



X



Y

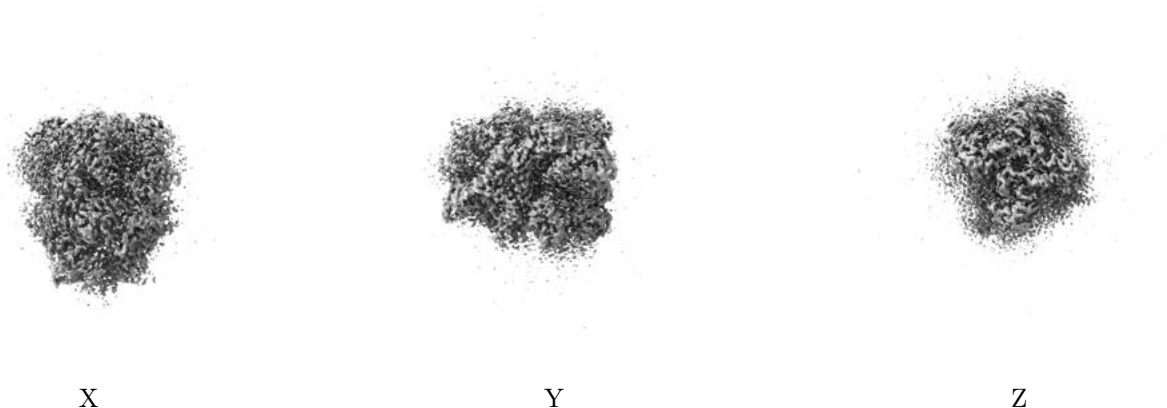


Z

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.

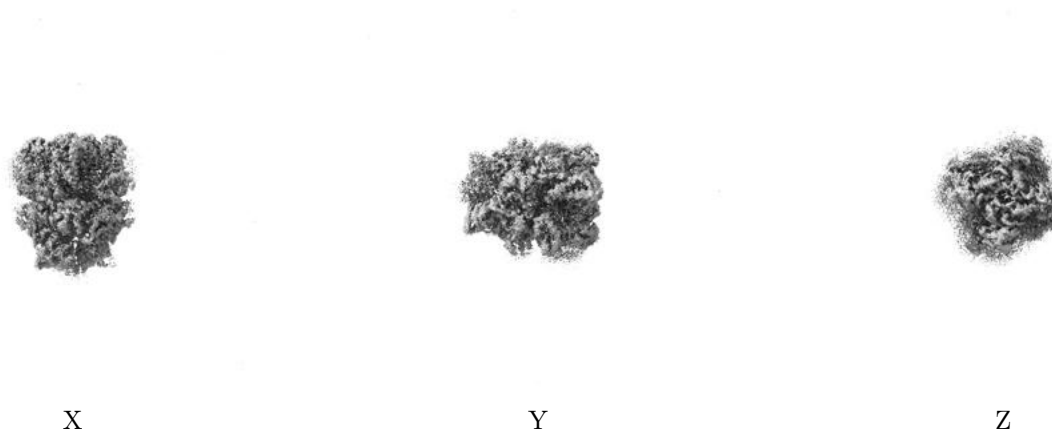
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. 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



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.

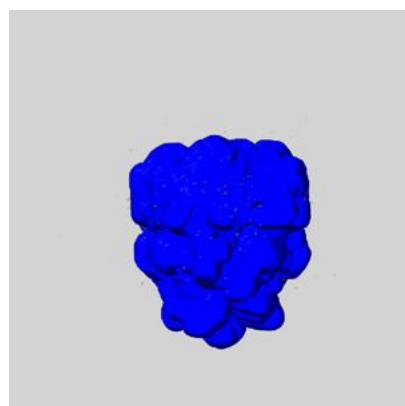
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

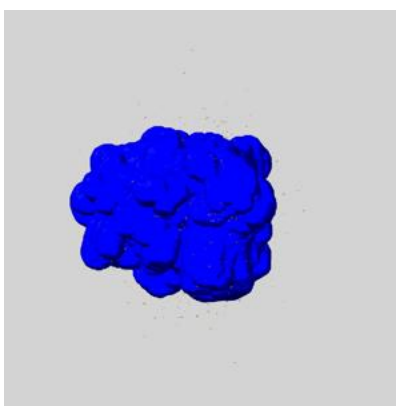
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

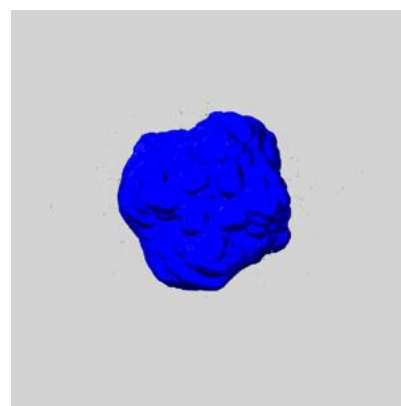
6.6.1 emd_50851_msk_1.map [i](#)



X



Y

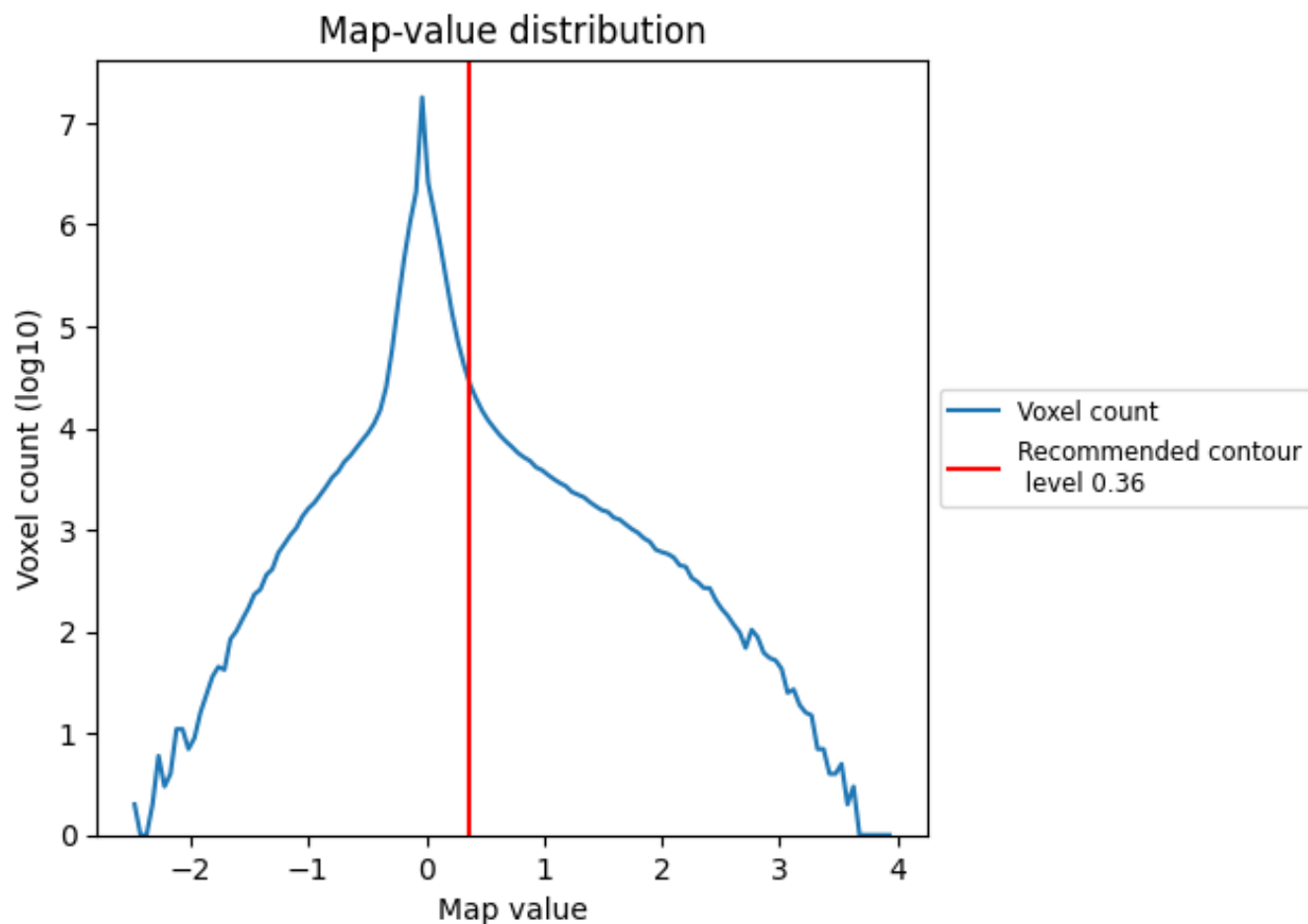


Z

7 Map analysis [i](#)

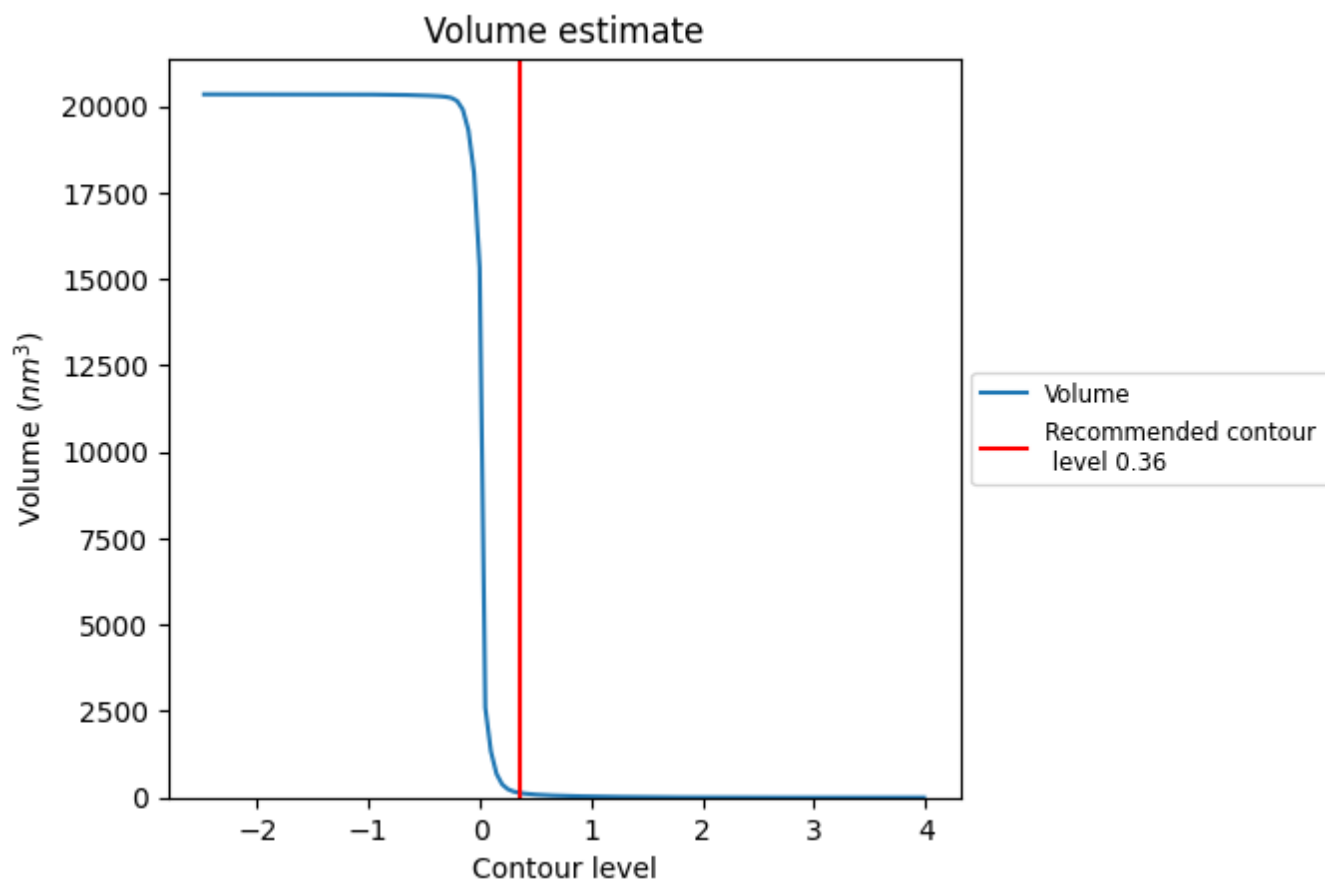
This section contains the results of statistical analysis of the map.

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.

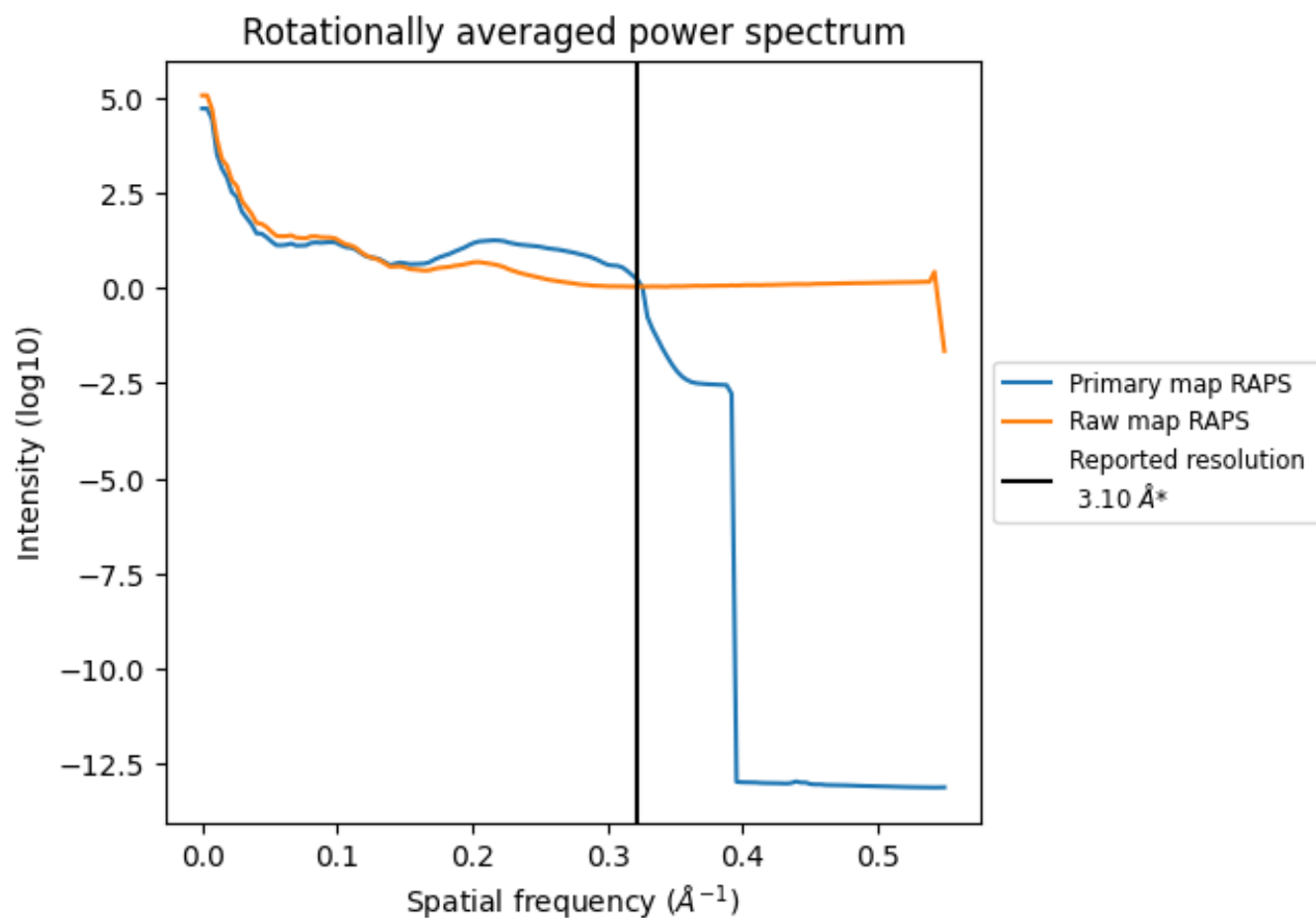
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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 ⓘ

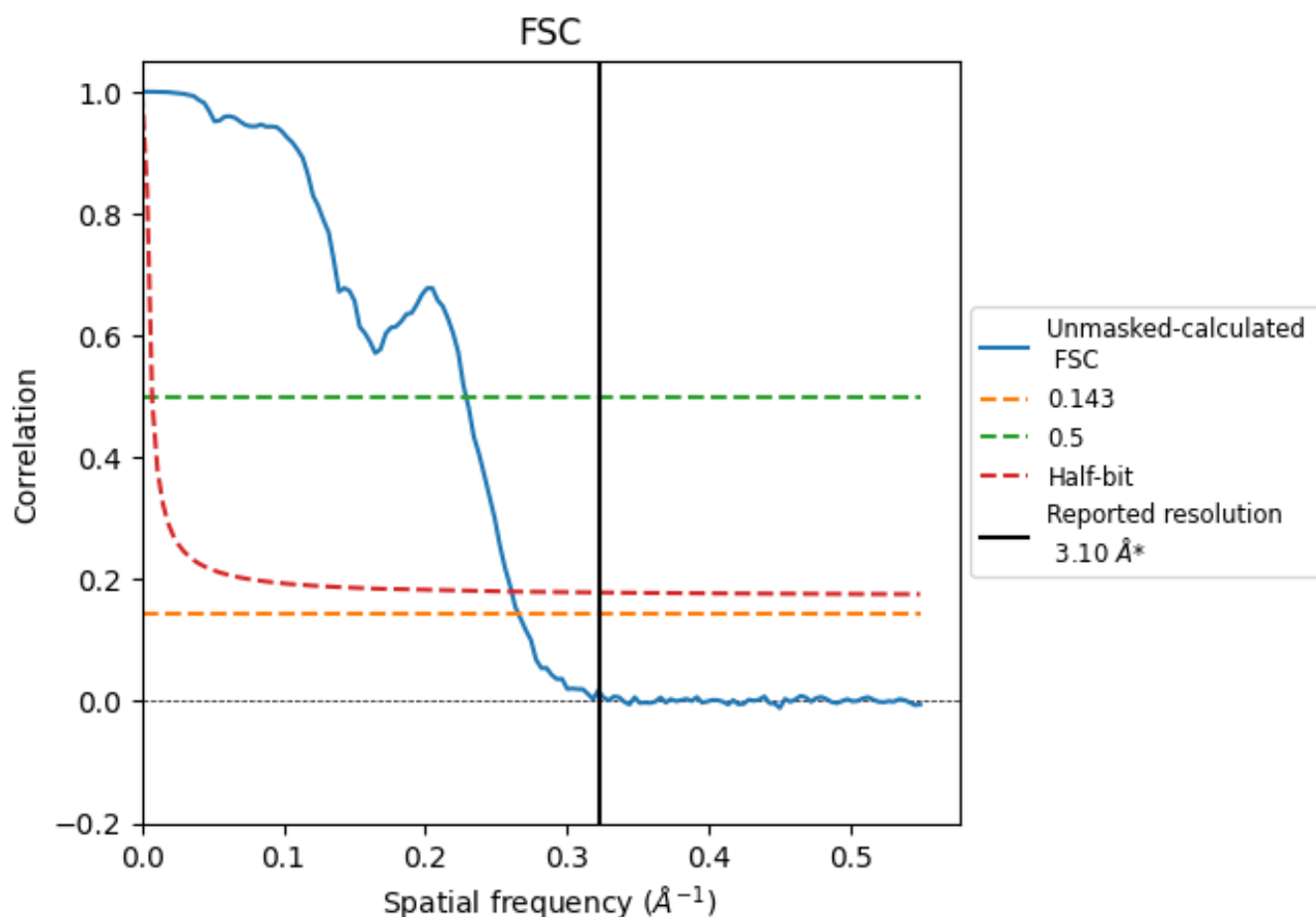


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

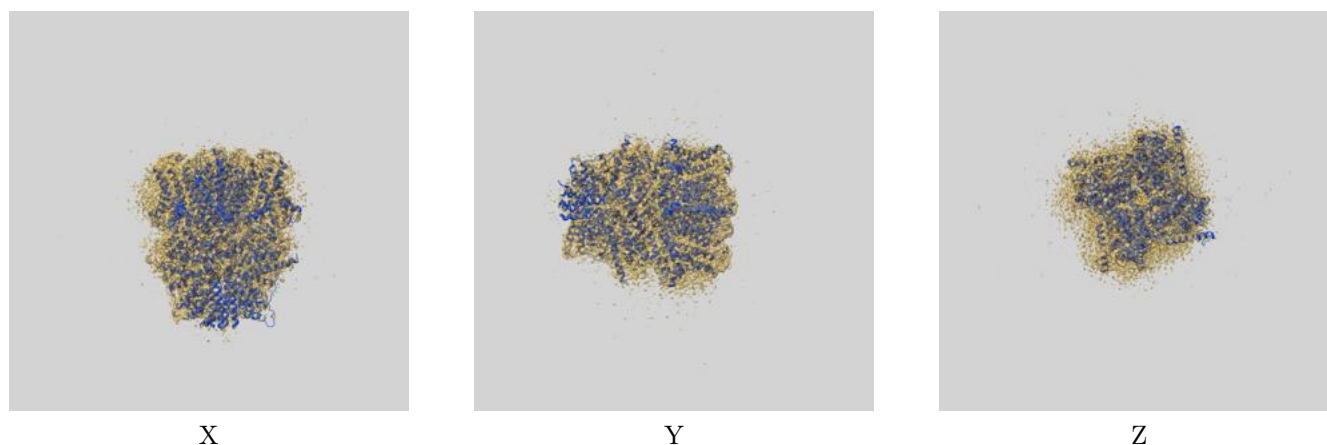
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.37	3.83

*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 3.76 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

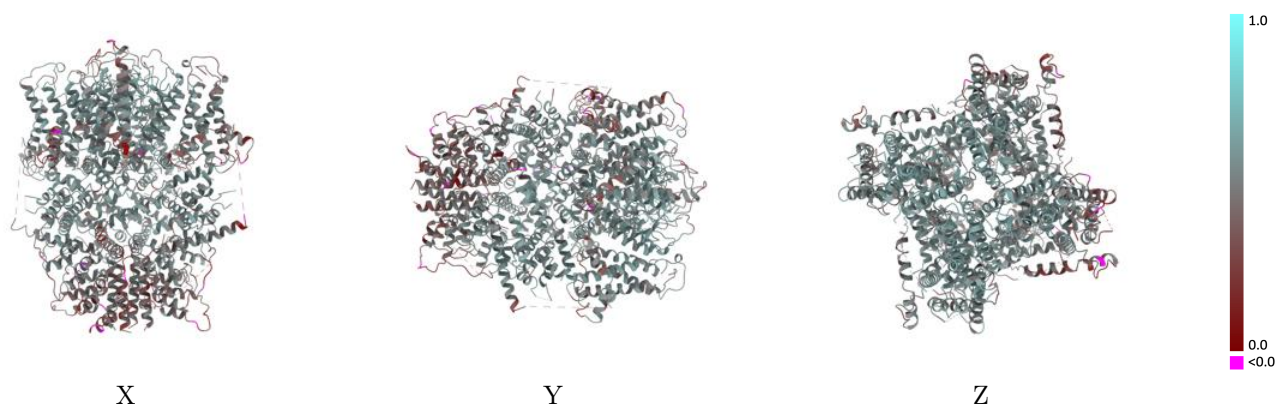
This section contains information regarding the fit between EMDB map EMD-50851 and PDB model 9FXM. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



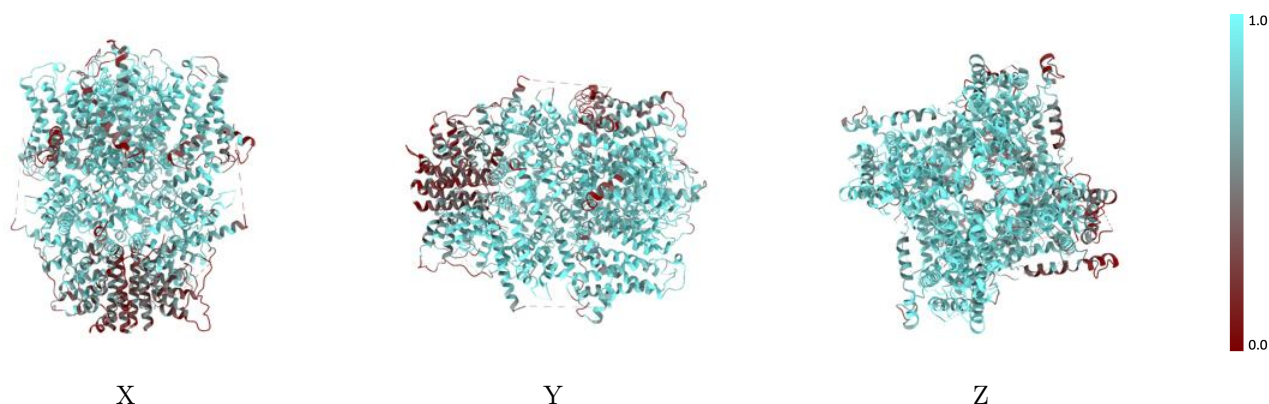
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



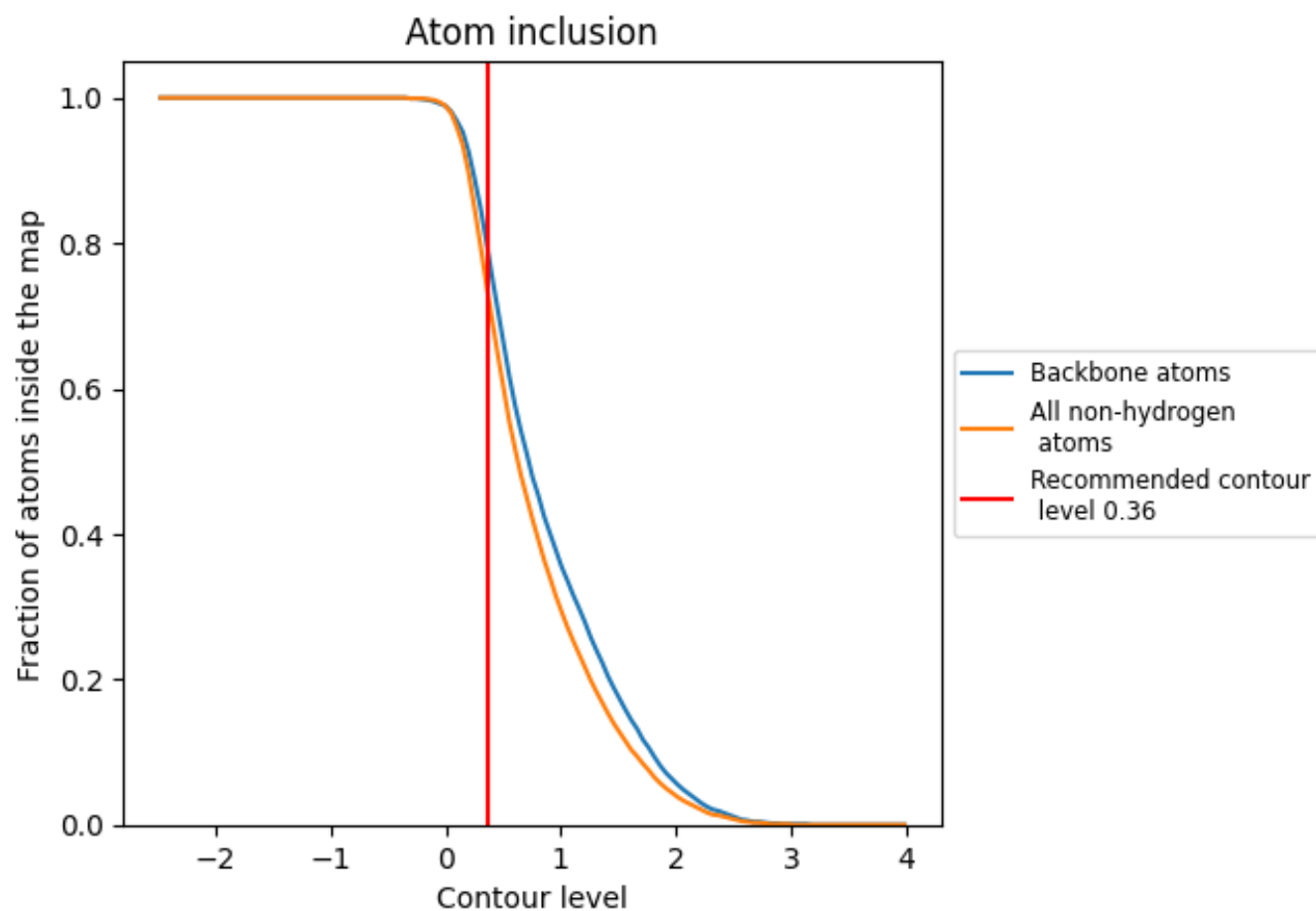
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7370	0.4950
A	0.8060	0.5150
B	0.7540	0.4920
C	0.6360	0.4700
D	0.7530	0.5040

