



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 8QFS / pdb_00008qfs
EMDB ID : EMD-18383
Title : Cryo-EM structure of SidH from Legionella pneumophila
Authors : Sharma, R.; Weis, F.; Bhogaraju, S.
Deposited on : 2023-09-04
Resolution : 2.70 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

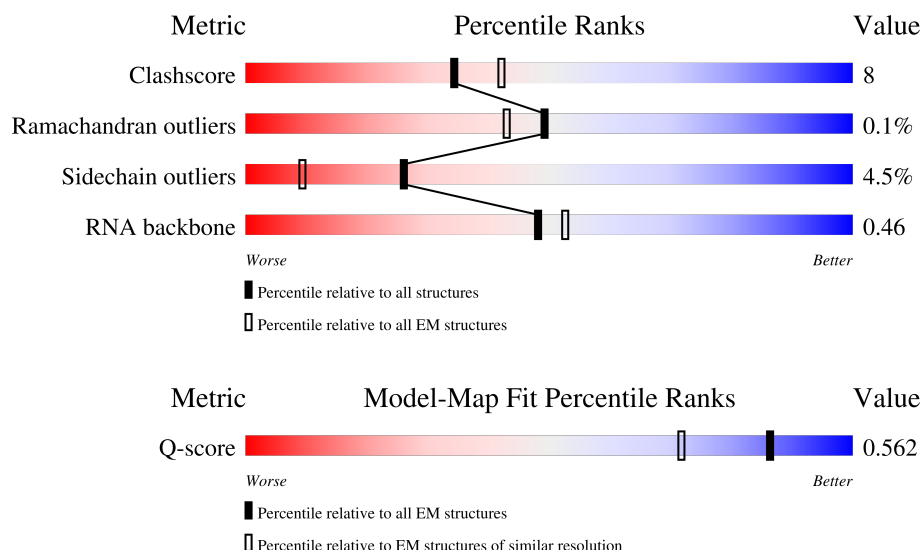
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	C	394	 76% 23%
2	B	76	 41% 25% 14% 20%
3	A	2248	 42% 10% 47%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13294 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 Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	393	Total	C	N	O	S	0	0
			2937	1864	513	547	13		

- Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	61	Total	C	N	O	P S	0	0
			1309	584	231	432	61 1		

- Molecule 3 is a protein called Protein SidH.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1183	Total	C	N	O	S	0	0
			9015	5746	1516	1730	23		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q6RCQ4
A	-21	LYS	-	expression tag	UNP Q6RCQ4
A	-20	HIS	-	expression tag	UNP Q6RCQ4
A	-19	HIS	-	expression tag	UNP Q6RCQ4
A	-18	HIS	-	expression tag	UNP Q6RCQ4
A	-17	HIS	-	expression tag	UNP Q6RCQ4
A	-16	HIS	-	expression tag	UNP Q6RCQ4
A	-15	HIS	-	expression tag	UNP Q6RCQ4
A	-14	HIS	-	expression tag	UNP Q6RCQ4
A	-13	HIS	-	expression tag	UNP Q6RCQ4
A	-12	HIS	-	expression tag	UNP Q6RCQ4
A	-11	HIS	-	expression tag	UNP Q6RCQ4
A	-10	SER	-	expression tag	UNP Q6RCQ4
A	-9	ALA	-	expression tag	UNP Q6RCQ4
A	-8	GLY	-	expression tag	UNP Q6RCQ4

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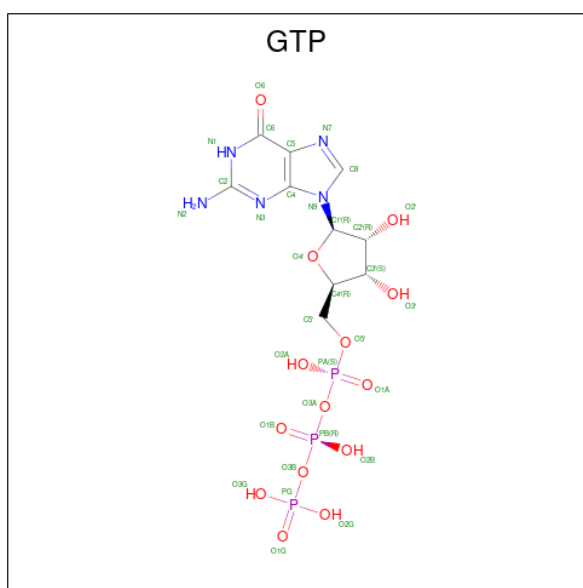
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP Q6RCQ4
A	-6	GLU	-	expression tag	UNP Q6RCQ4
A	-5	VAL	-	expression tag	UNP Q6RCQ4
A	-4	LEU	-	expression tag	UNP Q6RCQ4
A	-3	PHE	-	expression tag	UNP Q6RCQ4
A	-2	GLN	-	expression tag	UNP Q6RCQ4
A	-1	GLY	-	expression tag	UNP Q6RCQ4
A	0	PRO	-	expression tag	UNP Q6RCQ4

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total Mg 1 1	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			32	10	5	14	3	



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	367741	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.93	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.609	Depositor
Minimum map value	-0.197	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0459	Depositor
Map size (Å)	390.09598, 390.09598, 390.09598	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8127, 0.8127, 0.8127	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: MG, 4SU, GTP, PSU, 3AU, H2U, 5MU

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	C	0.11	0/2993	0.26	0/4067
2	B	0.19	0/1318	0.35	0/2048
3	A	0.15	1/9167 (0.0%)	0.32	3/12409 (0.0%)
All	All	0.14	1/13478 (0.0%)	0.31	3/18524 (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
3	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1295	PRO	CG-CD	-6.58	1.28	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1295	PRO	CA-N-CD	-12.49	94.51	112.00
3	A	1295	PRO	N-CD-CG	-9.20	89.39	103.20
3	A	1295	PRO	CA-CB-CG	-5.01	94.99	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	125	SER	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	C	2937	0	2899	52	0
2	B	1309	0	672	18	0
3	A	9015	0	8710	143	0
4	C	1	0	0	0	0
5	C	32	0	12	2	0
All	All	13294	0	12293	208	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (208) 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)
2:B:51:U:H3	2:B:63:G:H1	0.85	0.81
3:A:1529:ASP:O	3:A:1535:ASN:ND2	2.19	0.74
3:A:767:PHE:HA	3:A:770:ILE:HG12	1.68	0.74
1:C:53:ALA:HB3	1:C:56:GLU:HG3	1.70	0.72
1:C:16:GLY:HA3	1:C:99:MET:HE2	1.72	0.71
3:A:857:ASP:HA	3:A:860:LYS:HG2	1.73	0.71
3:A:972:LEU:HB2	3:A:994:ILE:HG21	1.73	0.70
3:A:403:ASN:ND2	3:A:584:ASN:OD1	2.26	0.68
1:C:91:ASN:ND2	2:B:2:C:OP1	2.21	0.66
3:A:1344:ASN:OD1	3:A:1403:ARG:NH2	2.27	0.66
3:A:1295:PRO:HD2	3:A:1296:GLY:N	2.10	0.65
1:C:98:GLN:NE2	1:C:216:GLU:OE1	2.29	0.65
1:C:213:LEU:HD12	1:C:232:VAL:HG22	1.80	0.64
3:A:253:SER:O	3:A:256:SER:OG	2.15	0.63
1:C:309:VAL:HG21	1:C:359:MET:HE2	1.79	0.63
3:A:387:ASP:OD1	3:A:387:ASP:N	2.30	0.62
3:A:1365:GLU:HG3	3:A:1366:LYS:HE2	1.82	0.61
3:A:425:ILE:HD12	3:A:506:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:191:LEU:H	3:A:191:LEU:HD23	1.65	0.60
1:C:104:LEU:HD11	1:C:116:THR:HG23	1.84	0.60
3:A:257:ILE:HD12	3:A:257:ILE:H	1.66	0.59
3:A:910:GLN:NE2	3:A:953:SER:O	2.35	0.59
3:A:971:LYS:HD3	3:A:994:ILE:HG12	1.85	0.59
1:C:25:LYS:N	5:C:402:GTP:O1B	2.30	0.58
3:A:623:GLU:OE2	3:A:626:ARG:NH1	2.36	0.58
3:A:936:SER:OG	3:A:940:LYS:NZ	2.37	0.58
3:A:267:ASP:OD1	3:A:267:ASP:N	2.37	0.57
1:C:302:HIS:HB2	1:C:369:MET:HE2	1.86	0.57
3:A:325:ASN:O	3:A:329:THR:OG1	2.20	0.57
1:C:115:GLN:NE2	1:C:118:GLU:OE1	2.36	0.57
3:A:15:ASP:OD2	3:A:1564:ARG:NH1	2.32	0.57
3:A:547:ASN:HB3	3:A:549:THR:HG22	1.87	0.57
1:C:100:ASP:OD2	1:C:205:ARG:NH2	2.38	0.56
3:A:287:LEU:HD21	3:A:331:LEU:HD22	1.87	0.56
1:C:306:GLU:HG2	1:C:360:VAL:HG22	1.86	0.56
3:A:127:SER:HA	3:A:130:GLN:HB2	1.88	0.56
1:C:14:ASN:ND2	1:C:272:GLY:O	2.39	0.56
1:C:118:GLU:OE2	1:C:378:ARG:NH1	2.39	0.55
3:A:1295:PRO:HD2	3:A:1296:GLY:H	1.71	0.55
3:A:1010:GLU:OE1	3:A:1020:TYR:N	2.34	0.54
1:C:90:LYS:HG3	1:C:332:TYR:HE2	1.73	0.54
1:C:295:LYS:O	1:C:298:THR:OG1	2.24	0.54
3:A:320:ALA:O	3:A:324:MET:HG2	2.08	0.53
3:A:126:ASN:O	3:A:128:ASP:N	2.41	0.53
1:C:206:ALA:HB1	1:C:209:LYS:HG3	1.91	0.53
3:A:628:ALA:O	3:A:631:THR:OG1	2.27	0.53
3:A:130:GLN:HB3	3:A:866:PRO:HG2	1.90	0.53
3:A:1595:ASP:OD1	3:A:1598:ARG:NH2	2.42	0.53
3:A:909:ASP:OD2	3:A:909:ASP:N	2.39	0.52
3:A:254:TYR:O	3:A:258:VAL:HG13	2.09	0.52
3:A:291:LYS:NZ	3:A:382:LEU:O	2.42	0.52
1:C:59:ARG:NH2	1:C:88:TYR:OH	2.35	0.52
3:A:751:SER:HA	3:A:1352:LYS:HG3	1.90	0.52
3:A:553:THR:HG22	3:A:555:ARG:H	1.75	0.52
3:A:1346:GLU:OE2	3:A:1357:SER:N	2.40	0.52
3:A:1552:LYS:HD3	3:A:1589:LEU:HD11	1.91	0.52
3:A:1355:THR:OG1	3:A:1356:TYR:N	2.41	0.52
3:A:754:VAL:HG21	3:A:1350:GLY:HA3	1.92	0.51
3:A:1425:HIS:NE2	3:A:1583:GLU:OE2	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:253:SER:OG	3:A:256:SER:OG	2.21	0.51
2:B:23:A:H2'	2:B:24:G:H8	1.76	0.51
3:A:302:LEU:HG	3:A:316:LEU:HD12	1.93	0.51
3:A:938:ARG:O	3:A:941:ILE:HG13	2.10	0.51
1:C:75:ARG:NH2	1:C:200:ILE:O	2.37	0.51
3:A:558:PRO:HB3	3:A:637:LEU:HB3	1.92	0.51
1:C:77:TYR:OH	1:C:197:ASP:OD1	2.27	0.51
1:C:14:ASN:O	1:C:100:ASP:N	2.43	0.50
1:C:17:THR:HG23	1:C:79:HIS:CE1	2.46	0.50
3:A:327:TYR:O	3:A:330:GLN:HG3	2.11	0.50
2:B:23:A:H2'	2:B:24:G:C8	2.46	0.50
3:A:746:LEU:O	3:A:750:LEU:HB2	2.12	0.50
3:A:921:GLN:NE2	3:A:925:ASP:OD2	2.45	0.50
3:A:64:THR:O	3:A:68:VAL:HG23	2.12	0.50
3:A:478:THR:HG21	3:A:709:LEU:HB3	1.94	0.50
3:A:314:GLY:HA2	3:A:317:THR:HG22	1.92	0.49
3:A:30:LEU:O	3:A:34:THR:OG1	2.22	0.49
3:A:1609:GLY:O	3:A:1612:ILE:HG13	2.13	0.49
2:B:51:U:O4	2:B:63:G:O6	2.30	0.49
3:A:779:SER:HB3	3:A:1596:THR:HG23	1.94	0.49
2:B:63:G:H2'	2:B:64:A:C8	2.48	0.49
1:C:254:SER:HB2	1:C:282:ILE:HD11	1.94	0.48
3:A:970:THR:O	3:A:973:GLU:HG3	2.13	0.48
1:C:122:LEU:O	1:C:126:VAL:HG22	2.12	0.48
2:B:13:C:O2'	2:B:14:A:OP1	2.28	0.48
3:A:726:SER:HA	3:A:803:GLU:HG2	1.94	0.48
1:C:245:ILE:O	1:C:251:THR:HA	2.13	0.47
2:B:63:G:H2'	2:B:64:A:H8	1.78	0.47
3:A:296:PRO:HG3	3:A:390:PHE:CD1	2.49	0.47
3:A:971:LYS:NZ	3:A:993:ASP:OD2	2.47	0.47
1:C:164:PRO:HB2	1:C:167:ASP:HB2	1.95	0.47
3:A:1291:LEU:HD12	3:A:1341:ALA:HB1	1.96	0.47
3:A:39:PHE:HA	3:A:311:LEU:HA	1.97	0.47
3:A:847:GLY:HA3	3:A:1351:LEU:HD11	1.95	0.47
3:A:975:GLN:HG2	3:A:990:LYS:HE2	1.97	0.47
3:A:549:THR:OG1	3:A:623:GLU:OE2	2.33	0.47
1:C:17:THR:HG23	1:C:79:HIS:HE1	1.80	0.47
3:A:291:LYS:HD3	3:A:328:TYR:CZ	2.50	0.47
3:A:1245:TYR:HE1	3:A:1298:VAL:HG13	1.78	0.47
1:C:33:THR:HG21	1:C:45:ARG:H	1.80	0.46
2:B:8:4SU:O2'	2:B:21:A:N1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1602:LYS:O	3:A:1605:GLU:HG2	2.14	0.46
3:A:724:GLN:HA	3:A:727:LYS:HE3	1.97	0.46
3:A:303:GLU:OE2	3:A:394:ARG:NH2	2.44	0.46
3:A:191:LEU:HD12	3:A:316:LEU:HD22	1.97	0.46
3:A:950:LYS:HE3	3:A:950:LYS:HB3	1.80	0.46
3:A:251:ILE:HG22	3:A:301:GLU:HB3	1.96	0.46
3:A:629:TYR:HA	3:A:632:PHE:CE2	2.51	0.46
3:A:919:LYS:O	3:A:922:GLU:HG3	2.16	0.46
1:C:15:VAL:O	1:C:79:HIS:HA	2.16	0.46
3:A:972:LEU:HA	3:A:994:ILE:HD13	1.98	0.46
3:A:843:GLY:HA3	3:A:852:VAL:HG11	1.98	0.45
3:A:1535:ASN:OD1	3:A:1535:ASN:N	2.27	0.45
3:A:311:LEU:HD13	3:A:315:LEU:HD23	1.98	0.45
3:A:1018:GLY:O	3:A:1022:ASN:ND2	2.49	0.45
3:A:1366:LYS:HD3	3:A:1366:LYS:HA	1.71	0.45
3:A:1354:GLY:O	3:A:1358:ARG:HB3	2.16	0.45
3:A:257:ILE:HG23	3:A:294:ILE:HG22	1.99	0.45
1:C:20:HIS:ND1	1:C:115:GLN:HB2	2.32	0.45
3:A:191:LEU:HA	3:A:248:LEU:HD12	1.99	0.45
1:C:152:MET:HG3	1:C:153:GLU:N	2.31	0.45
3:A:468:ASP:OD1	3:A:468:ASP:N	2.46	0.45
1:C:284:ARG:HH12	2:B:74:C:H42	1.64	0.45
3:A:26:LYS:HE3	3:A:26:LYS:HB3	1.67	0.44
3:A:1295:PRO:CD	3:A:1296:GLY:N	2.79	0.44
3:A:1543:TYR:OH	3:A:1558:ASP:O	2.28	0.44
3:A:600:PHE:HE1	3:A:668:VAL:HA	1.83	0.44
3:A:1253:LEU:HD22	3:A:1253:LEU:HA	1.84	0.44
2:B:68:C:H2'	2:B:69:G:C8	2.52	0.44
3:A:892:GLN:O	3:A:895:VAL:HG12	2.18	0.44
1:C:216:GLU:HG3	1:C:217:ASP:N	2.32	0.44
3:A:328:TYR:HE2	3:A:383:GLY:HA2	1.82	0.44
3:A:689:LYS:HE2	3:A:693:LEU:HD11	2.00	0.44
2:B:69:G:C2'	2:B:70:G:H5'	2.47	0.44
3:A:731:SER:OG	3:A:803:GLU:OE1	2.26	0.44
3:A:860:LYS:HA	3:A:860:LYS:HD3	1.72	0.44
3:A:1255:GLN:HA	3:A:1258:VAL:HG12	2.00	0.44
3:A:663:ARG:HG3	3:A:665:THR:H	1.83	0.43
3:A:564:PHE:CE2	3:A:578:ARG:HG2	2.53	0.43
3:A:706:LYS:HD3	3:A:706:LYS:HA	1.67	0.43
2:B:1:G:O2'	2:B:2:C:OP1	2.33	0.43
2:B:4:C:H2'	2:B:5:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:585:GLN:HG2	3:A:685:LEU:HD11	2.00	0.43
3:A:784:MET:HE3	3:A:784:MET:HB3	1.84	0.43
3:A:1016:LYS:HB3	3:A:1016:LYS:HE3	1.82	0.43
3:A:1422:GLY:H	3:A:1516:SER:HB3	1.82	0.43
3:A:566:LEU:HD12	3:A:575:TYR:HE1	1.84	0.43
3:A:680:GLU:HG3	3:A:681:LYS:N	2.34	0.43
3:A:985:GLU:O	3:A:988:LEU:HG	2.18	0.43
3:A:1295:PRO:CD	3:A:1296:GLY:H	2.32	0.43
3:A:1396:ARG:O	3:A:1400:GLU:HG2	2.19	0.43
3:A:284:VAL:O	3:A:288:GLU:HG2	2.19	0.42
3:A:321:LEU:HD21	3:A:386:MET:HE1	2.00	0.42
3:A:397:ASN:O	3:A:401:ARG:HG3	2.18	0.42
3:A:1342:ALA:HB2	3:A:1360:VAL:HG11	2.00	0.42
3:A:1423:THR:O	3:A:1423:THR:OG1	2.32	0.42
3:A:1516:SER:OG	3:A:1519:ASP:OD2	2.36	0.42
1:C:33:THR:CG2	1:C:45:ARG:H	2.32	0.42
3:A:426:GLY:HA2	3:A:507:LEU:HD11	2.02	0.42
3:A:552:LEU:HG	3:A:626:ARG:HG2	2.01	0.42
3:A:792:MET:HB3	3:A:792:MET:HE3	1.69	0.42
1:C:306:GLU:HG3	1:C:393:LEU:HD11	2.02	0.42
3:A:533:LYS:HD2	3:A:533:LYS:HA	1.86	0.42
1:C:65:THR:HA	1:C:81:ASP:O	2.20	0.42
3:A:81:LYS:HE3	3:A:81:LYS:HB2	1.84	0.42
3:A:198:TYR:CD1	3:A:242:LEU:HD13	2.55	0.42
3:A:424:LYS:HE3	3:A:424:LYS:HB2	1.93	0.42
3:A:1526:LEU:HD23	3:A:1526:LEU:HA	1.88	0.42
1:C:339:THR:HB	1:C:364:ILE:HD13	2.01	0.42
3:A:123:ASN:OD1	3:A:721:LEU:HB2	2.20	0.42
1:C:114:PRO:HG3	3:A:496:GLN:HG3	2.02	0.41
1:C:182:ASP:O	1:C:186:GLU:HG3	2.20	0.41
3:A:747:LYS:HD3	3:A:763:GLU:HA	2.03	0.41
1:C:92:MET:HE2	1:C:96:ALA:HB2	2.01	0.41
1:C:333:PHE:O	1:C:334:ARG:C	2.63	0.41
3:A:57:LYS:HZ2	3:A:57:LYS:HG3	1.58	0.41
3:A:727:LYS:HE2	3:A:727:LYS:HB3	1.79	0.41
3:A:1401:MET:HA	3:A:1608:ILE:HD11	2.02	0.41
3:A:1293:PHE:O	3:A:1297:SER:HB2	2.19	0.41
3:A:1580:ILE:HD13	3:A:1580:ILE:HA	1.89	0.41
1:C:37:ALA:HA	1:C:42:GLY:HA3	2.01	0.41
3:A:686:ASN:O	3:A:690:THR:HG23	2.19	0.41
1:C:133:VAL:HB	1:C:170:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:HG2	1:C:271:ALA:O	2.21	0.41
1:C:62:THR:HB	5:C:402:GTP:O1G	2.21	0.41
1:C:135:LEU:HD21	1:C:150:VAL:HG11	2.03	0.41
3:A:1432:TYR:HE1	3:A:1526:LEU:HG	1.85	0.41
1:C:332:TYR:CE1	1:C:378:ARG:HB2	2.56	0.41
2:B:1:G:HO2'	2:B:2:C:P	2.44	0.41
3:A:83:PHE:O	3:A:87:GLU:HG2	2.20	0.41
3:A:199:PHE:CE2	3:A:324:MET:HB3	2.56	0.41
3:A:1414:ILE:HD12	3:A:1414:ILE:HA	1.94	0.41
1:C:22:ASP:OD1	3:A:437:LYS:NZ	2.40	0.41
1:C:90:LYS:HE2	1:C:90:LYS:HB3	1.75	0.41
3:A:948:PHE:O	3:A:952:ILE:HG12	2.21	0.41
1:C:357:ILE:HG13	1:C:358:LYS:N	2.36	0.40
2:B:69:G:H2'	2:B:70:G:H5'	2.03	0.40
3:A:927:PHE:CE2	3:A:979:LEU:HB2	2.56	0.40
1:C:260:GLU:HB2	2:B:76:A:N3	2.36	0.40
3:A:264:HIS:HB3	3:A:290:ILE:HD11	2.04	0.40
3:A:796:LYS:HE2	3:A:796:LYS:HB3	1.89	0.40
3:A:1508:ARG:NH2	3:A:1523:ASP:OD1	2.55	0.40
3:A:1249:ILE:HG23	3:A:1334:PHE:CE1	2.56	0.40
1:C:12:HIS:HE1	1:C:78:ALA:HB2	1.87	0.40
2:B:68:C:H2'	2:B:69:G:H8	1.86	0.40
3:A:115:ILE:HD13	3:A:115:ILE:HA	1.93	0.40
3:A:629:TYR:OH	3:A:645:ASN:OD1	2.26	0.40
3:A:663:ARG:HA	3:A:663:ARG:HD2	1.91	0.40
3:A:750:LEU:HD11	3:A:785:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	391/394 (99%)	382 (98%)	9 (2%)	0	100	100
3	A	1153/2248 (51%)	1113 (96%)	39 (3%)	1 (0%)	48	73
All	All	1544/2642 (58%)	1495 (97%)	48 (3%)	1 (0%)	49	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	127	SER

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	C	301/327 (92%)	287 (95%)	14 (5%)	23	51
3	A	932/2019 (46%)	890 (96%)	42 (4%)	24	52
All	All	1233/2346 (53%)	1177 (96%)	56 (4%)	26	52

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	17	THR
1	C	66	SER
1	C	135	LEU
1	C	160	GLN
1	C	231	ARG
1	C	233	GLU
1	C	251	THR
1	C	255	THR
1	C	287	ILE
1	C	292	VAL
1	C	315	ASP
1	C	338	VAL
1	C	362	THR
1	C	391	LYS
3	A	61	THR

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Mol	Chain	Res	Type
3	A	82	SER
3	A	129	ILE
3	A	133	VAL
3	A	148	SER
3	A	195	LEU
3	A	267	ASP
3	A	284	VAL
3	A	294	ILE
3	A	302	LEU
3	A	317	THR
3	A	329	THR
3	A	384	VAL
3	A	387	ASP
3	A	389	VAL
3	A	425	ILE
3	A	481	THR
3	A	486	VAL
3	A	492	SER
3	A	512	SER
3	A	515	SER
3	A	591	ARG
3	A	603	ILE
3	A	625	LEU
3	A	631	THR
3	A	649	VAL
3	A	687	GLN
3	A	706	LYS
3	A	746	LEU
3	A	779	SER
3	A	804	SER
3	A	851	ILE
3	A	962	VAL
3	A	1012	HIS
3	A	1253	LEU
3	A	1254	TYR
3	A	1258	VAL
3	A	1406	SER
3	A	1421	PHE
3	A	1423	THR
3	A	1535	ASN
3	A	1604	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	323	GLN
3	A	419	ASN
3	A	461	HIS
3	A	523	GLN
3	A	910	GLN
3	A	1001	GLN
3	A	1618	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	60/76 (78%)	15 (25%)	4 (6%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	14	A
2	B	16	H2U
2	B	18	G
2	B	19	G
2	B	20	H2U
2	B	21	A
2	B	45	U
2	B	47	3AU
2	B	52	G
2	B	70	G
2	B	71	G
2	B	73	A
2	B	74	C
2	B	75	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	G
2	B	13	C
2	B	17	C
2	B	70	G

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

6 non-standard protein/DNA/RNA residues 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	3AU	B	47	2	24,28,29	2.76	9 (37%)	30,40,43	1.46	5 (16%)
2	H2U	B	16	2	18,21,22	0.47	0	19,30,33	0.99	1 (5%)
2	4SU	B	8	2	18,21,22	3.77	7 (38%)	25,30,33	2.34	5 (20%)
2	H2U	B	20	2	18,21,22	0.53	0	19,30,33	1.40	3 (15%)
2	5MU	B	54	2	19,22,23	0.42	0	27,32,35	0.55	0
2	PSU	B	55	2	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)

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	3AU	B	47	2	-	5/16/34/35	0/2/2/2
2	H2U	B	16	2	-	3/7/38/39	0/2/2/2
2	4SU	B	8	2	-	0/7/25/26	0/2/2/2
2	H2U	B	20	2	-	7/7/38/39	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	4SU	C2-N3	7.23	1.50	1.38
2	B	8	4SU	C2-N1	7.19	1.49	1.38
2	B	8	4SU	C4-N3	6.95	1.44	1.37
2	B	47	3AU	C2-N1	6.88	1.48	1.38
2	B	47	3AU	C2-N3	6.20	1.49	1.38
2	B	8	4SU	C5-C4	6.16	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	47	3AU	C6-C5	6.11	1.49	1.35
2	B	8	4SU	C6-C5	5.52	1.47	1.35
2	B	8	4SU	C4-S4	-4.86	1.60	1.68
2	B	55	PSU	C6-C5	3.60	1.39	1.35
2	B	47	3AU	C6-N1	3.57	1.46	1.38
2	B	47	3AU	O2-C2	-3.49	1.16	1.22
2	B	47	3AU	C4-N3	3.32	1.46	1.40
2	B	8	4SU	C6-N1	2.77	1.44	1.38
2	B	47	3AU	O4-C4	-2.42	1.18	1.23
2	B	47	3AU	O30-C13	2.35	1.29	1.22
2	B	47	3AU	C11-C10	2.08	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	4SU	C4-N3-C2	-7.99	119.65	127.31
2	B	8	4SU	C5-C4-N3	5.68	120.03	114.75
2	B	55	PSU	C4-N3-C2	-4.94	119.57	126.37
2	B	55	PSU	N1-C2-N3	4.81	120.24	115.17
2	B	8	4SU	C5-C4-S4	-3.96	119.79	124.31
2	B	20	H2U	C5-C4-N3	-3.89	112.55	116.69
2	B	47	3AU	C4-N3-C2	-3.81	120.18	124.66
2	B	8	4SU	N3-C2-N1	3.75	119.77	114.89
2	B	16	H2U	C5-C4-N3	-3.28	113.20	116.69
2	B	20	H2U	O2-C2-N1	3.18	126.93	123.10
2	B	47	3AU	C6-N1-C2	-2.99	119.36	121.80
2	B	47	3AU	C5-C4-N3	2.90	119.64	115.64
2	B	47	3AU	O2-C2-N3	-2.84	118.16	121.98
2	B	47	3AU	C1'-N1-C2	2.83	121.67	117.04
2	B	55	PSU	O2-C2-N1	-2.66	120.04	122.79
2	B	55	PSU	C6-N1-C2	-2.26	120.59	122.69
2	B	20	H2U	O2-C2-N3	-2.18	117.47	121.49
2	B	8	4SU	O2-C2-N1	-2.03	120.16	122.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	20	H2U	O4'-C1'-N1-C6
2	B	47	3AU	C10-C11-C12-N40
2	B	16	H2U	C3'-C4'-C5'-O5'
2	B	47	3AU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	16	H2U	O4'-C4'-C5'-O5'
2	B	20	H2U	O4'-C4'-C5'-O5'
2	B	20	H2U	C3'-C4'-C5'-O5'
2	B	47	3AU	C10-C11-C12-C13
2	B	47	3AU	C3'-C4'-C5'-O5'
2	B	20	H2U	C2'-C1'-N1-C2
2	B	20	H2U	C2'-C1'-N1-C6
2	B	16	H2U	C4'-C5'-O5'-P
2	B	20	H2U	C4'-C5'-O5'-P
2	B	20	H2U	O4'-C1'-N1-C2
2	B	47	3AU	C2'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
5	GTP	C	402	4	33,34,34	0.89	1 (3%)	50,54,54	1.60	9 (18%)

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
5	GTP	C	402	4	-	3/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402	GTP	C2-N3	2.06	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	402	GTP	C5-C4-N3	-4.97	120.48	128.39
5	C	402	GTP	C2-N3-C4	4.66	120.33	112.30
5	C	402	GTP	N9-C4-N3	3.07	132.09	125.95
5	C	402	GTP	C2-N1-C6	-2.95	119.77	125.11
5	C	402	GTP	N9-C8-N7	-2.65	108.48	113.40
5	C	402	GTP	C5-C6-N1	2.54	119.73	113.25
5	C	402	GTP	C8-N7-C5	2.51	108.73	104.26
5	C	402	GTP	O6-C6-C5	-2.35	120.32	126.53
5	C	402	GTP	C3'-C2'-C1'	2.13	105.50	101.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	402	GTP	O4'-C4'-C5'-O5'
5	C	402	GTP	C3'-C4'-C5'-O5'
5	C	402	GTP	C5'-O5'-PA-O1A

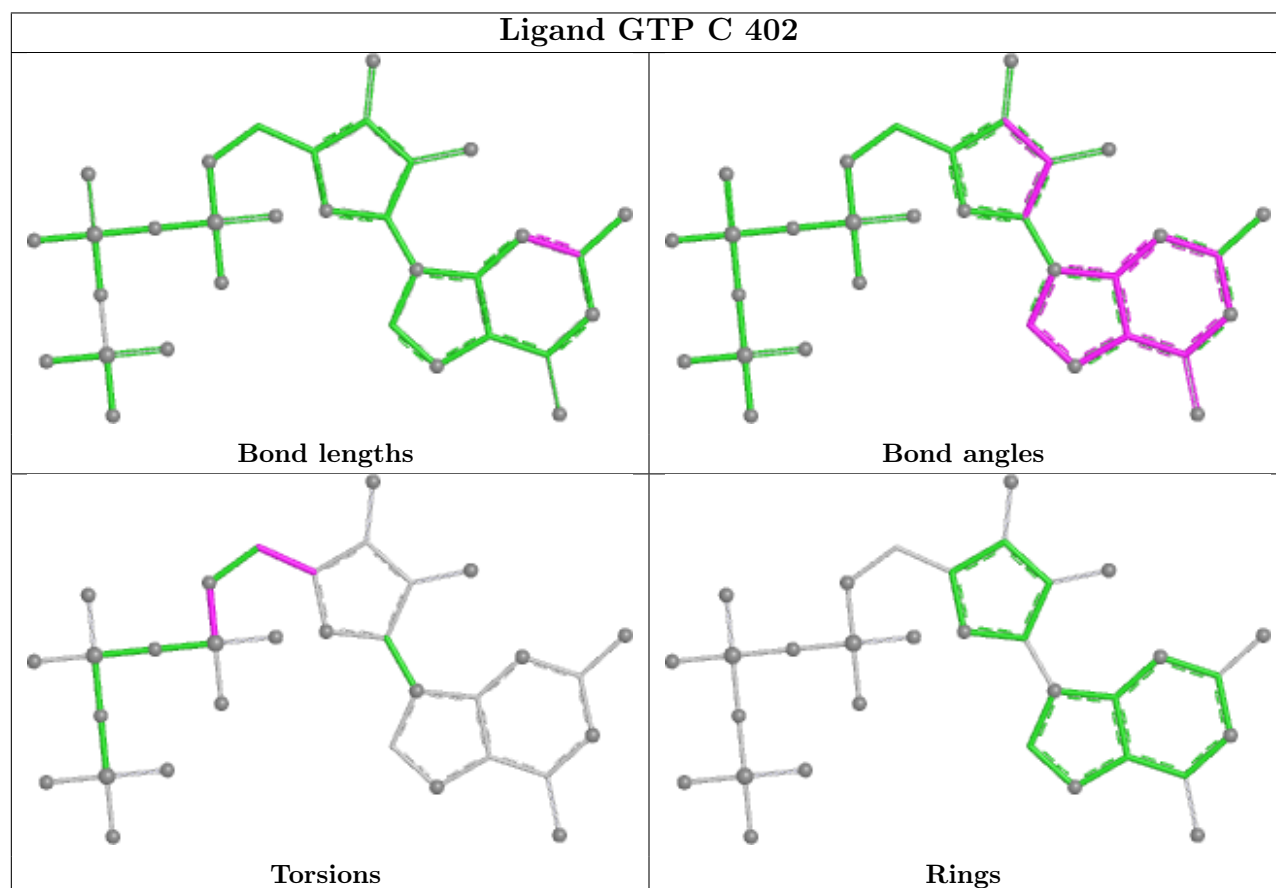
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	402	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18383. These allow visual inspection of the internal detail of the map and identification of artifacts.

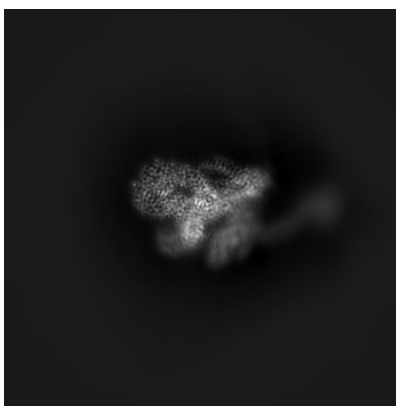
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

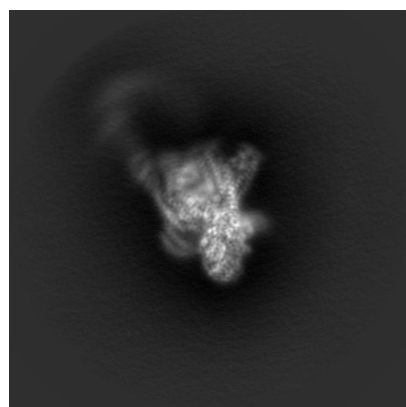


Y

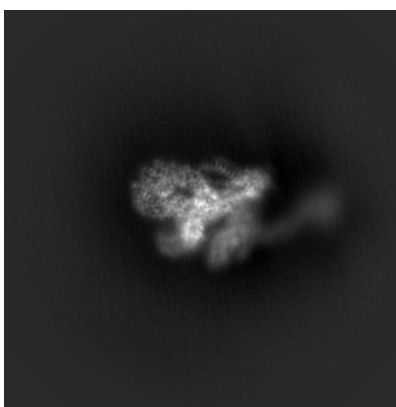


Z

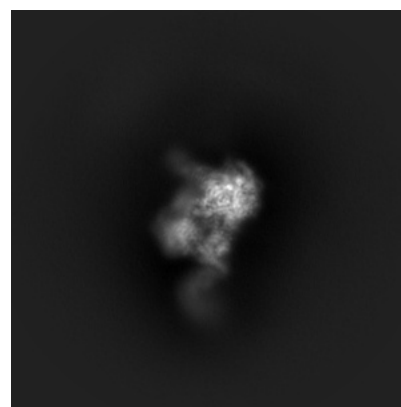
6.1.2 Raw map



X



Y

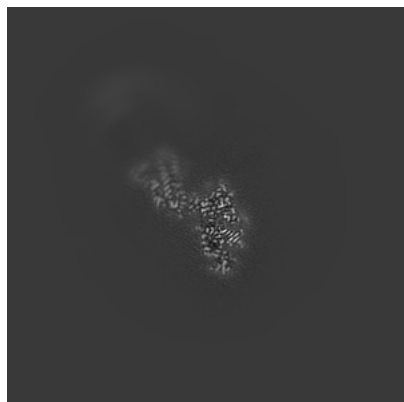


Z

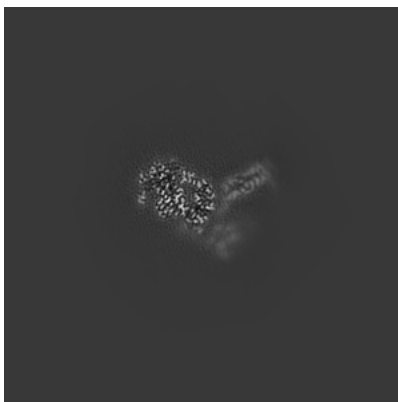
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

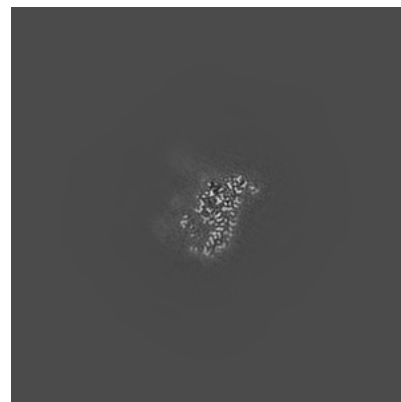
6.2.1 Primary map



X Index: 240

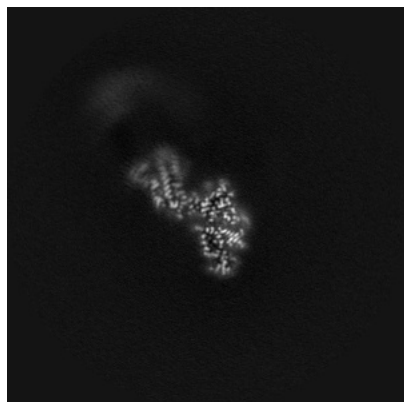


Y Index: 240

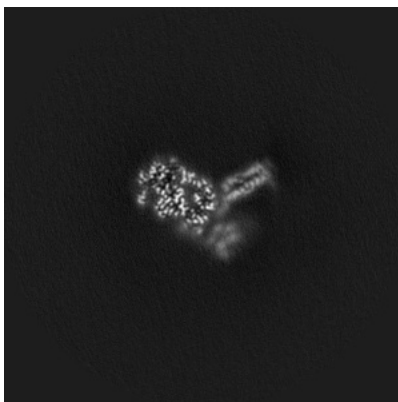


Z Index: 240

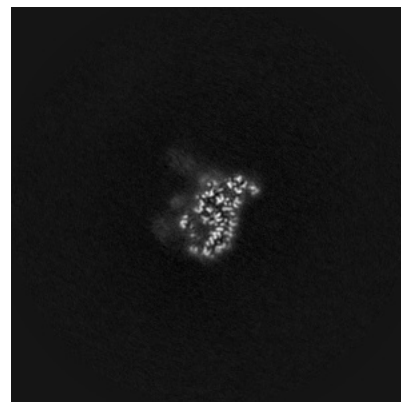
6.2.2 Raw map



X Index: 240



Y Index: 240

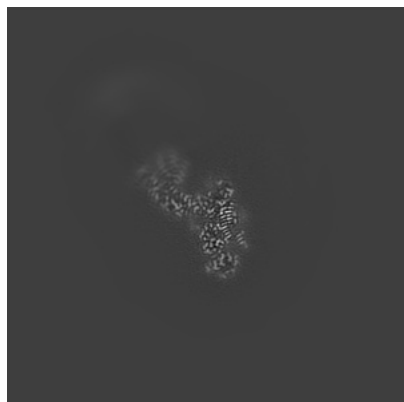


Z Index: 240

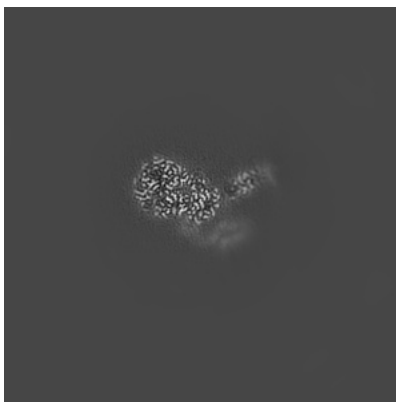
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

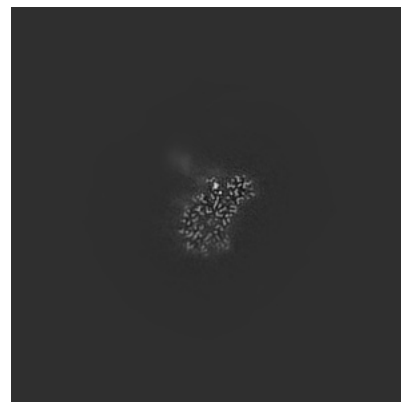
6.3.1 Primary map



X Index: 245

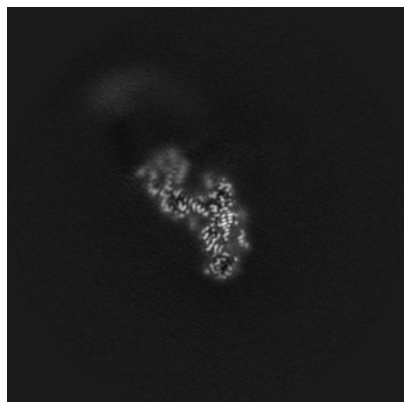


Y Index: 247

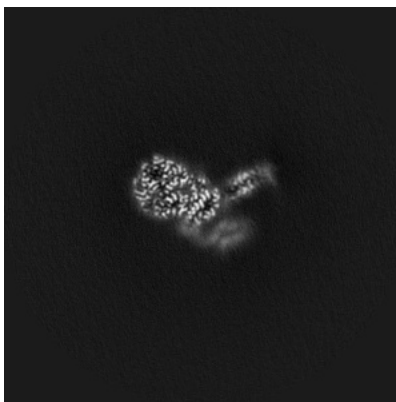


Z Index: 234

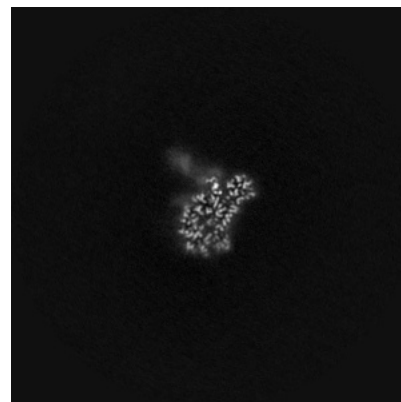
6.3.2 Raw map



X Index: 248



Y Index: 247

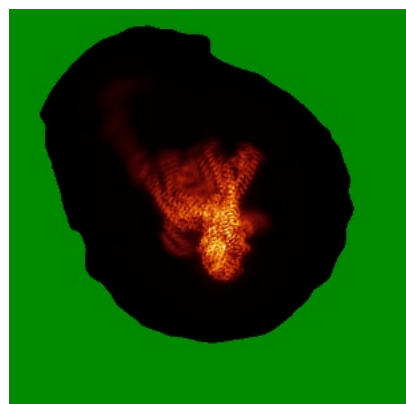


Z Index: 234

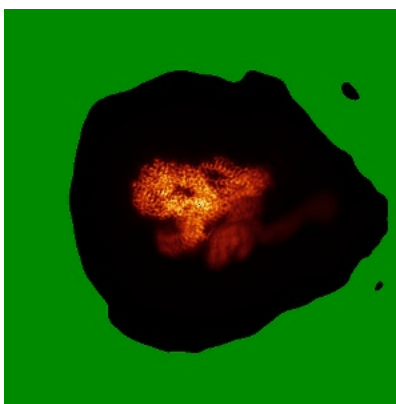
The images above show the largest variance slices of the map in three orthogonal directions.

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

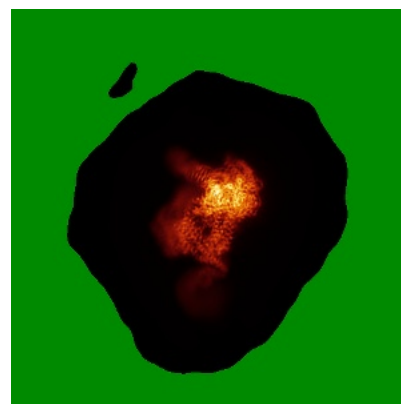
6.4.1 Primary map



X



Y

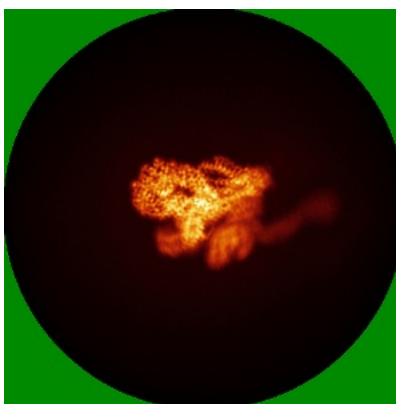


Z

6.4.2 Raw map



X



Y

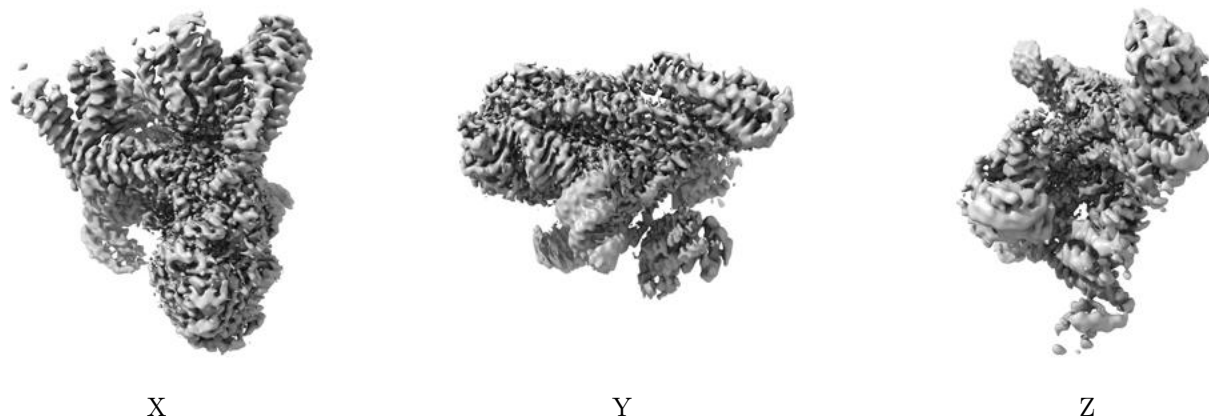


Z

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.

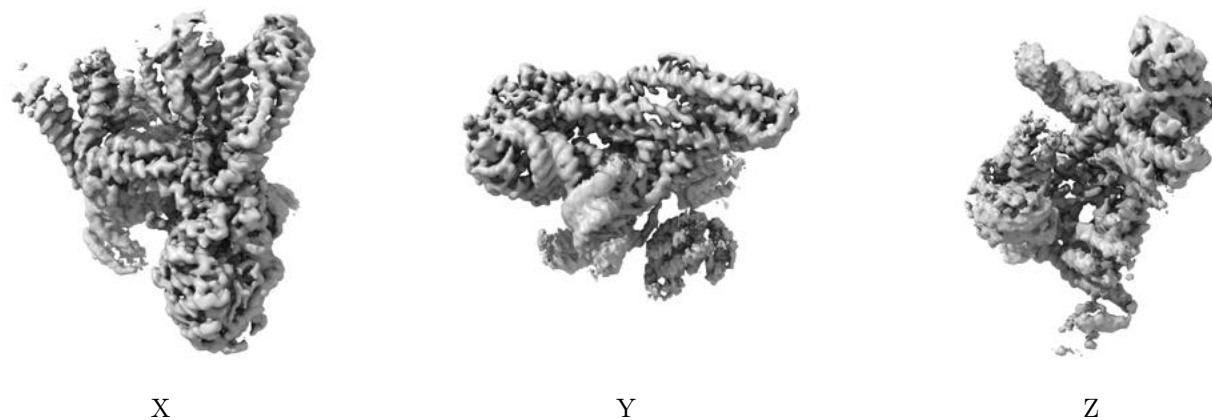
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0459. 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.

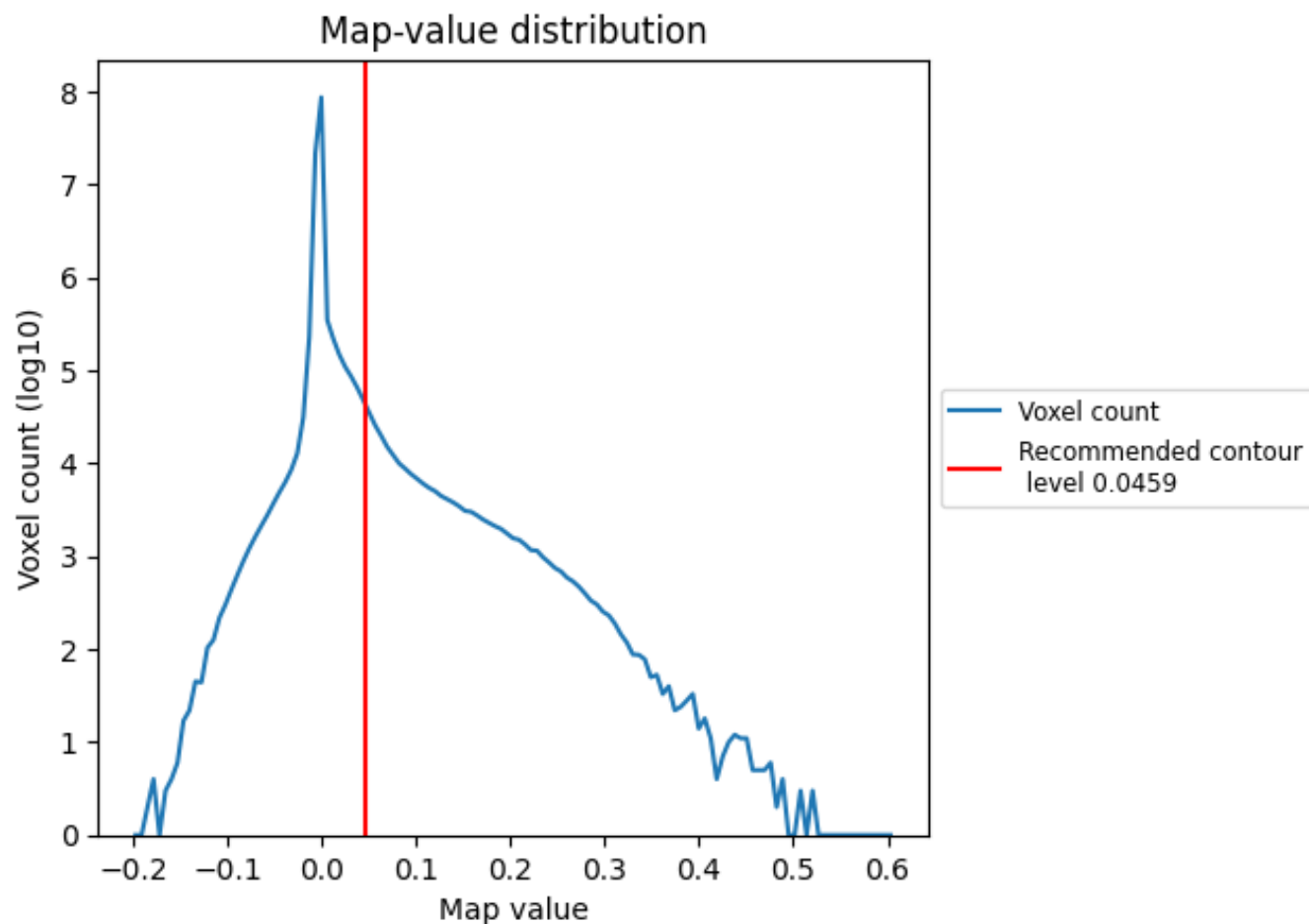
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

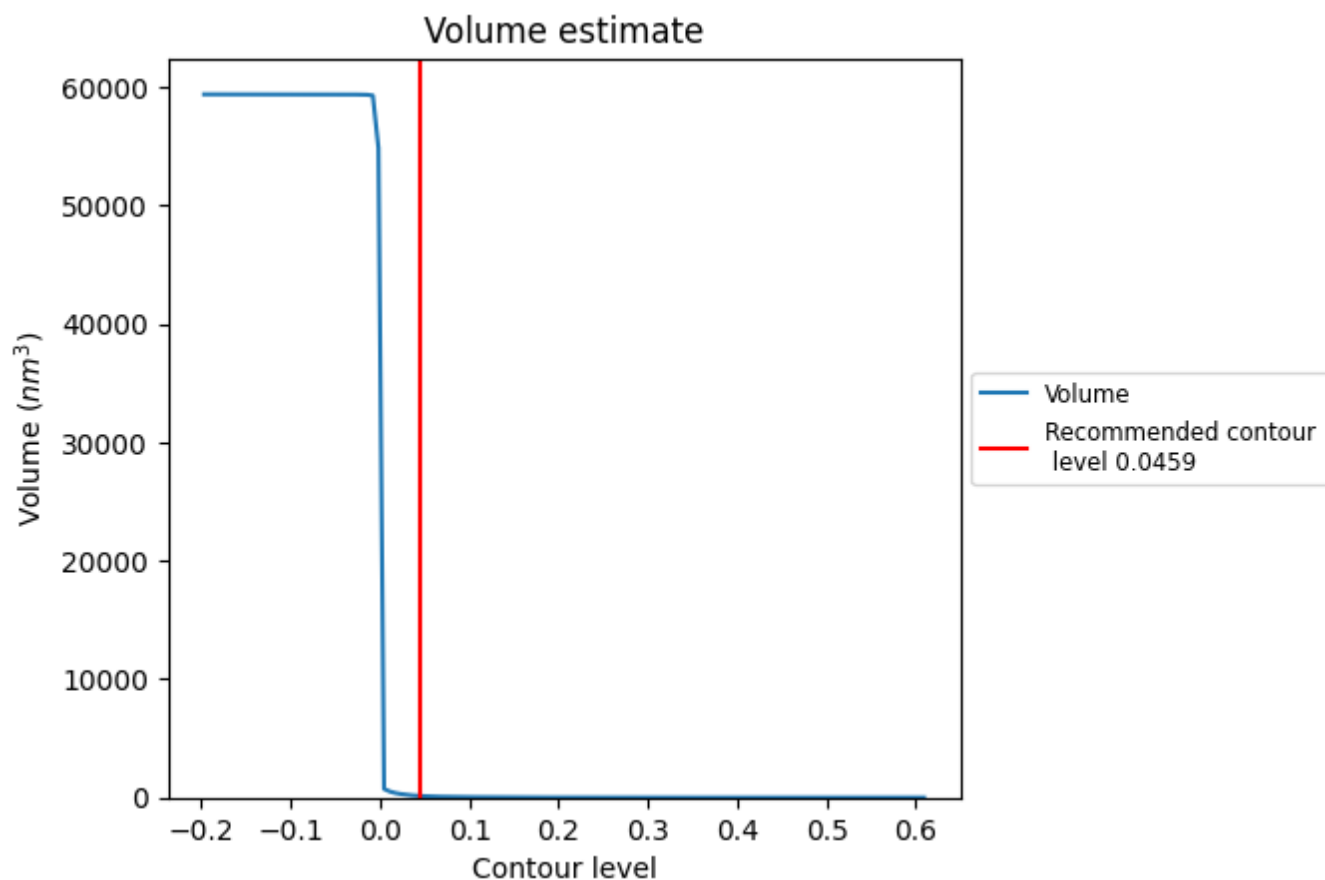
This section contains the results of statistical analysis of the map.

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.

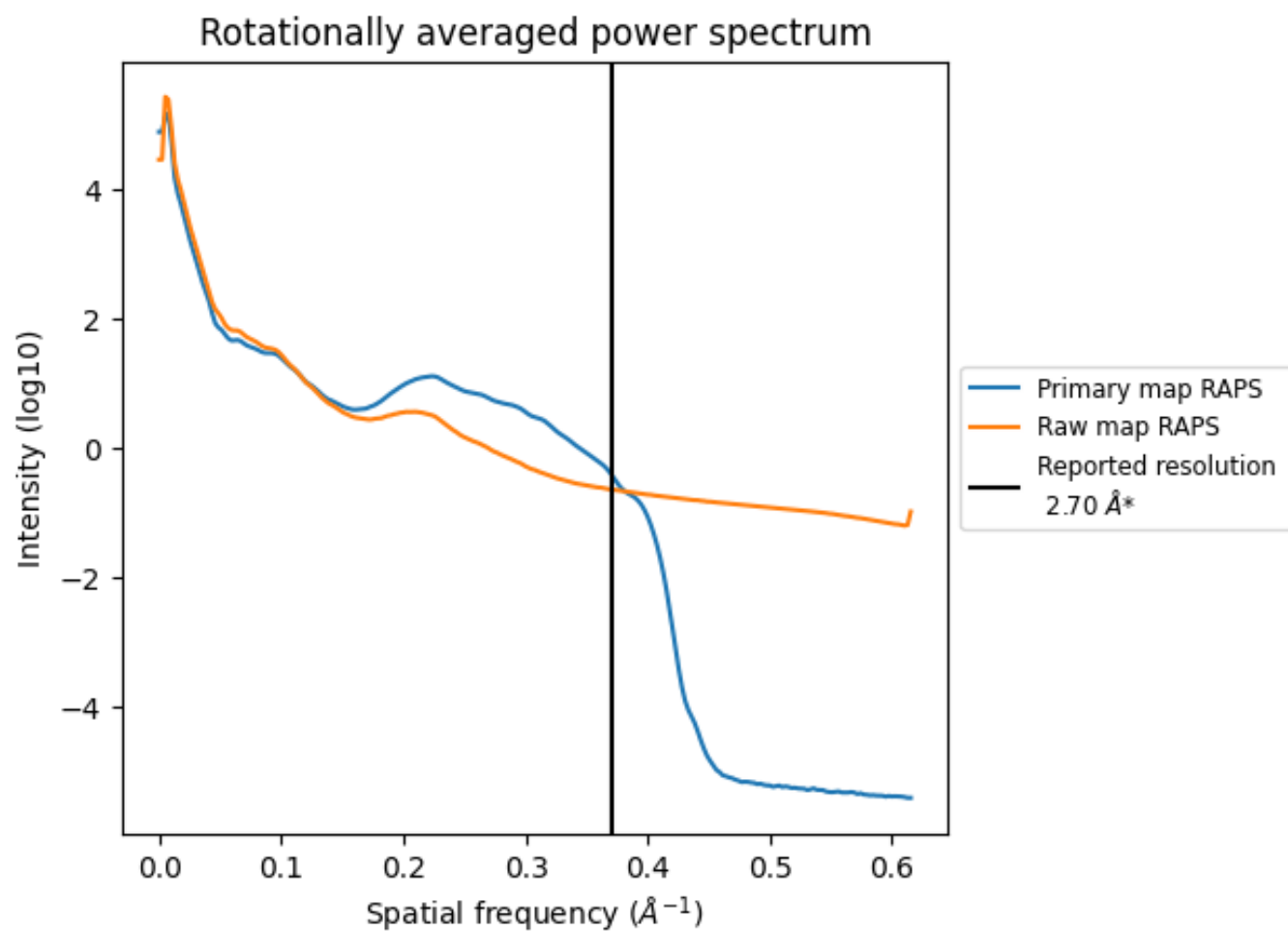
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm^3 ; this corresponds to an approximate mass of 118 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 ⓘ

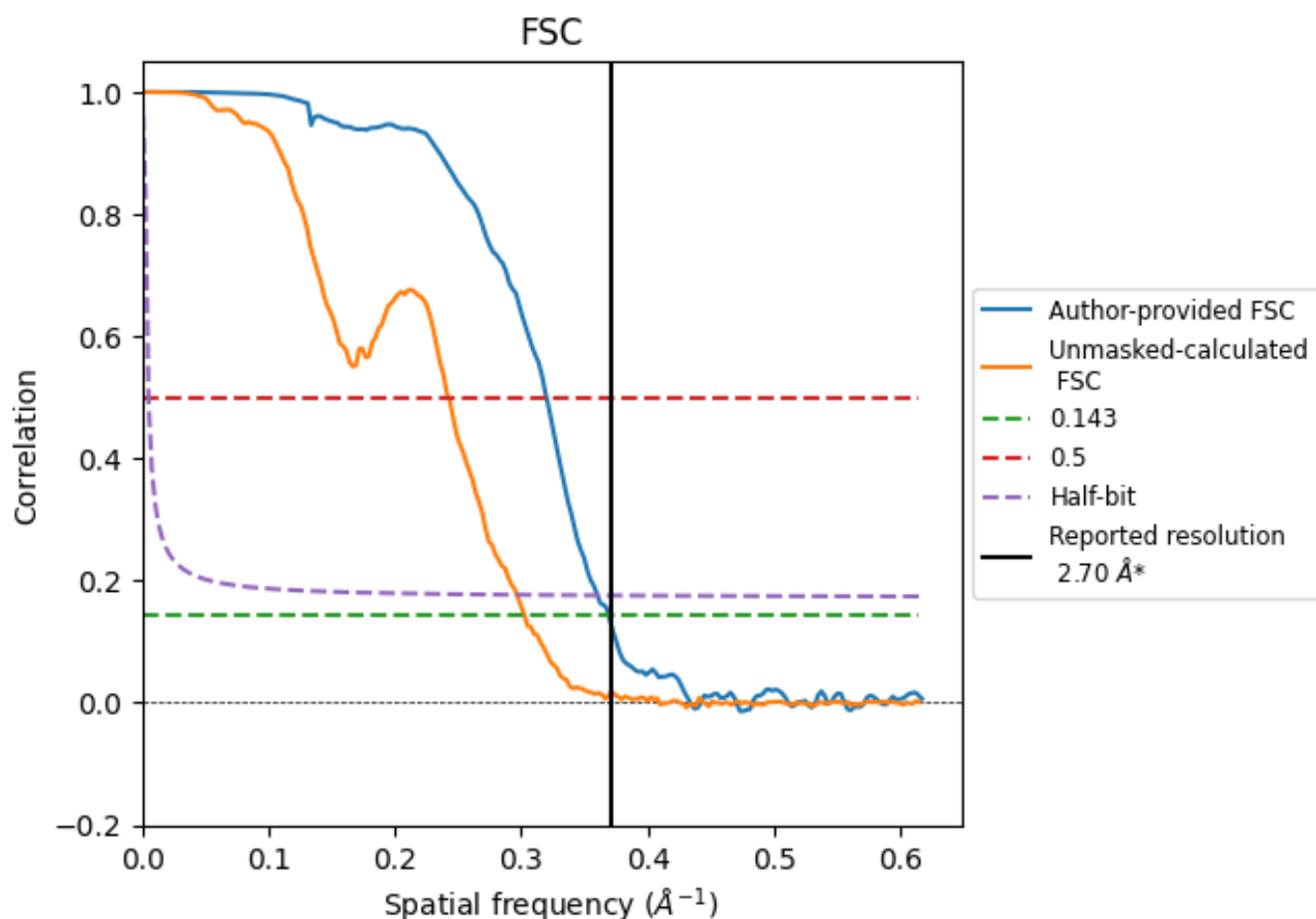


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

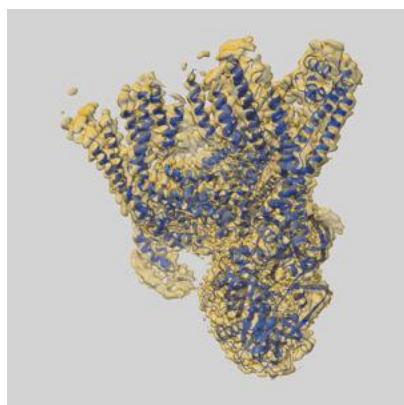
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.12	2.78
Unmasked-calculated*	3.31	4.13	3.37

*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 3.31 differs from the reported value 2.7 by more than 10 %

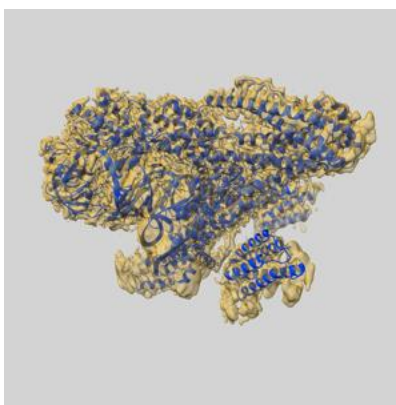
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18383 and PDB model 8QFS. Per-residue inclusion information can be found in section [3](#) on page [5](#).

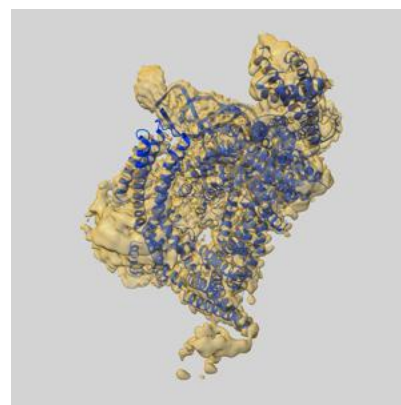
9.1 Map-model overlay [i](#)



X



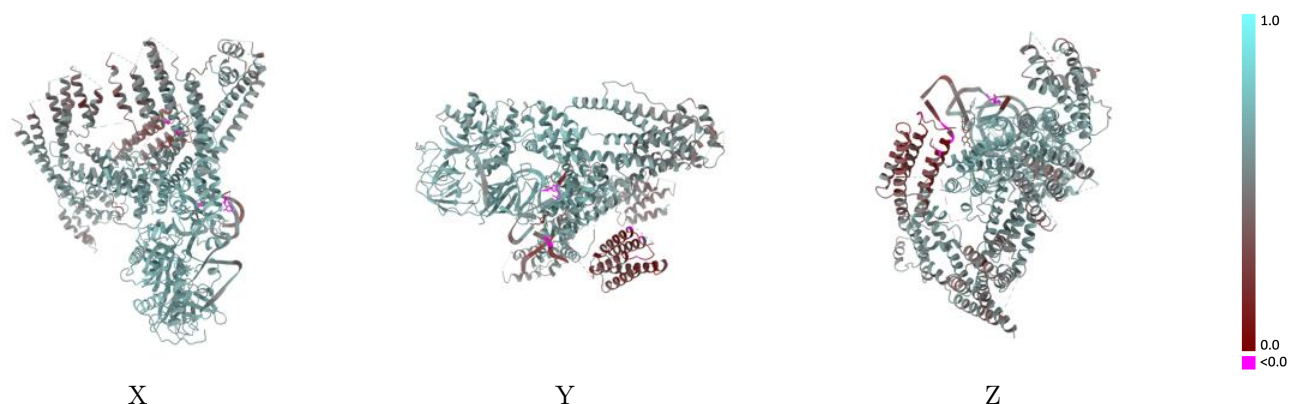
Y



Z

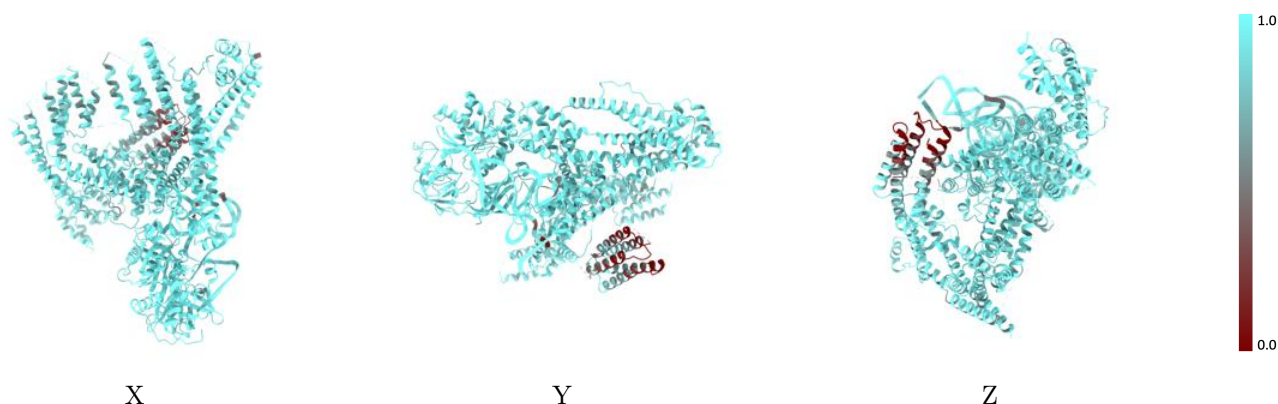
The images above show the 3D surface view of the map at the recommended contour level 0.0459 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



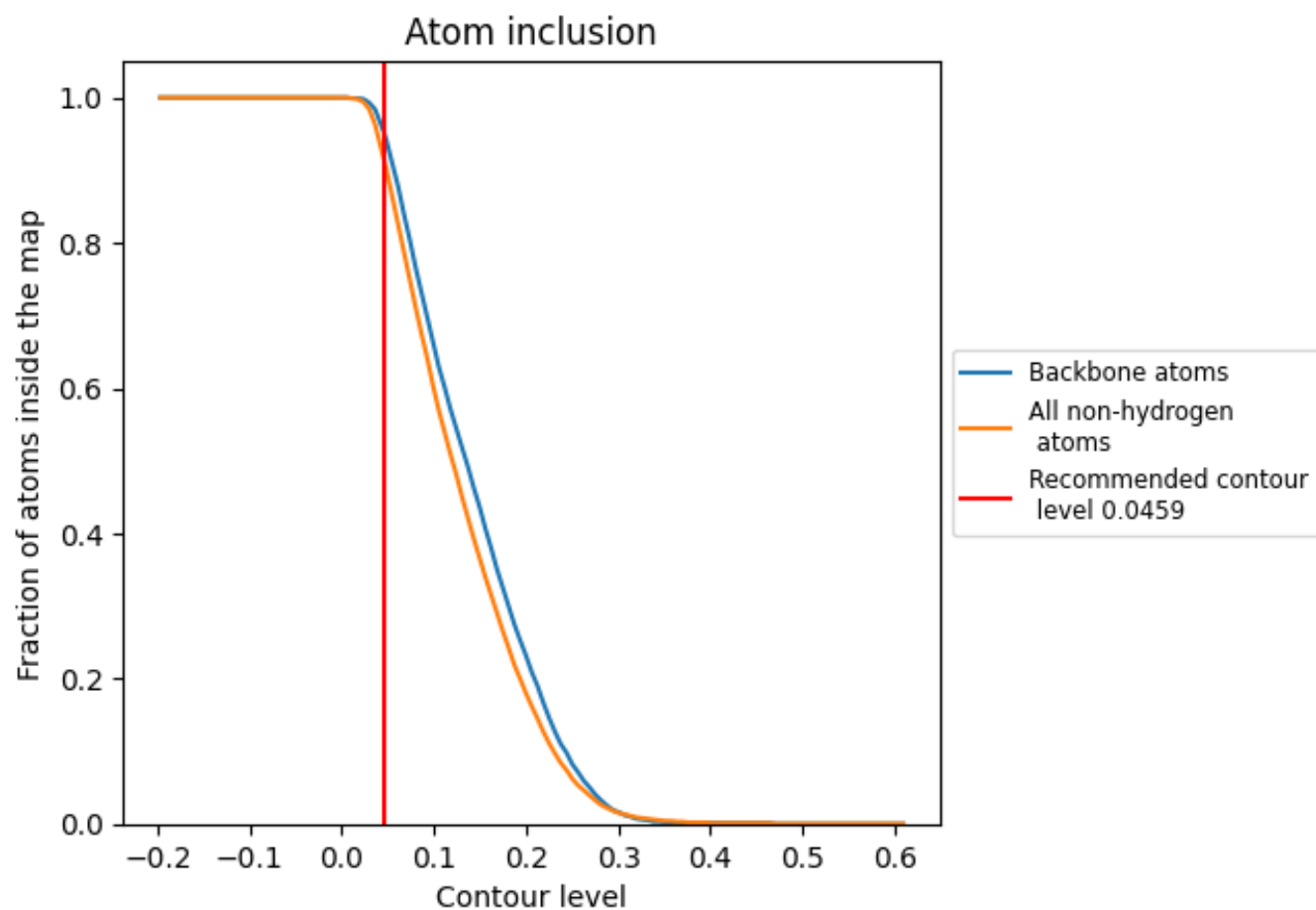
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0459).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0459) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.5620
A	0.8940	0.5400
B	0.9230	0.5180
C	0.9780	0.6480

