



## Full wwPDB EM Validation Report ⓘ

Oct 29, 2022 – 10:30 am BST

PDB ID : 7R4H  
EMDB ID : EMD-14312  
Title : phospho-STING binding to adaptor protein complex-1  
Authors : Xu, P.; Ablasser, A.  
Deposited on : 2022-02-08  
Resolution : 2.34 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

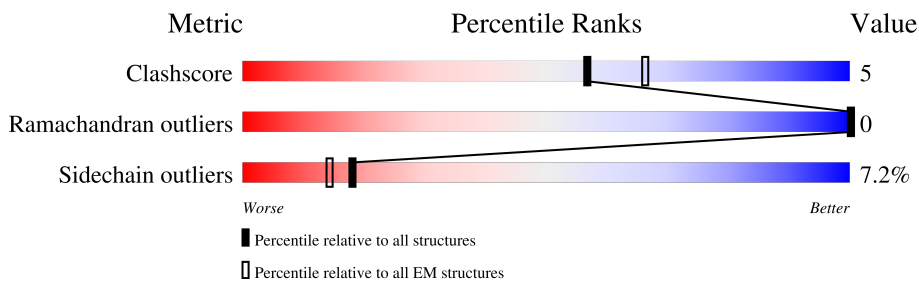
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.34 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	584	
2	C	165	
2	H	165	
3	G	595	
4	L	9	
5	M	423	
6	S	154	

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 16485 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 AP-1 complex subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	570	4513	2883	741	862	27	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	359	ARG	LYS	engineered mutation	UNP Q10567
B	476	LYS	GLU	engineered mutation	UNP Q10567

- Molecule 2 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	165	1330	842	233	249	6	0	0
2	H	163	1312	831	229	246	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	71	LEU	GLN	engineered mutation	UNP P84077
H	71	LEU	GLN	engineered mutation	UNP P84077

- Molecule 3 is a protein called AP-1 complex subunit gamma-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	585	4633	2914	815	865	39	0	0

- Molecule 4 is a protein called Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L	9	72	43	10	18	1	0	0

- Molecule 5 is a protein called AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	415	3362	2161	566	621	14	0	0

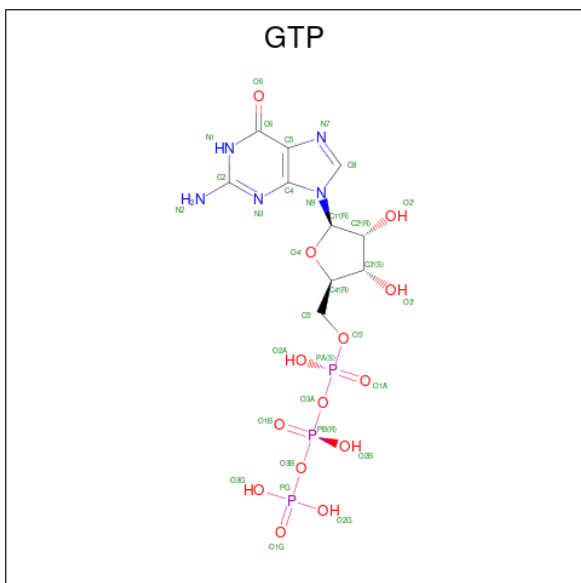
- Molecule 6 is a protein called AP-1 complex subunit sigma-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S	142	1197	782	197	213	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	148	CYS	SER	conflict	UNP Q96PC3

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

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

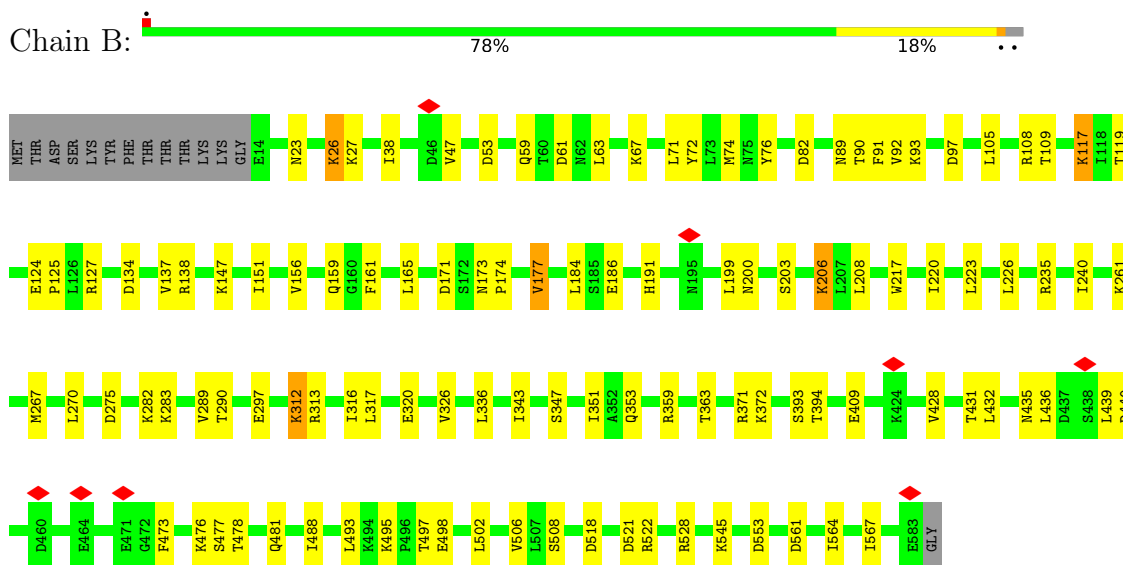
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	C	1	1	1	0
8	H	1	1	1	0

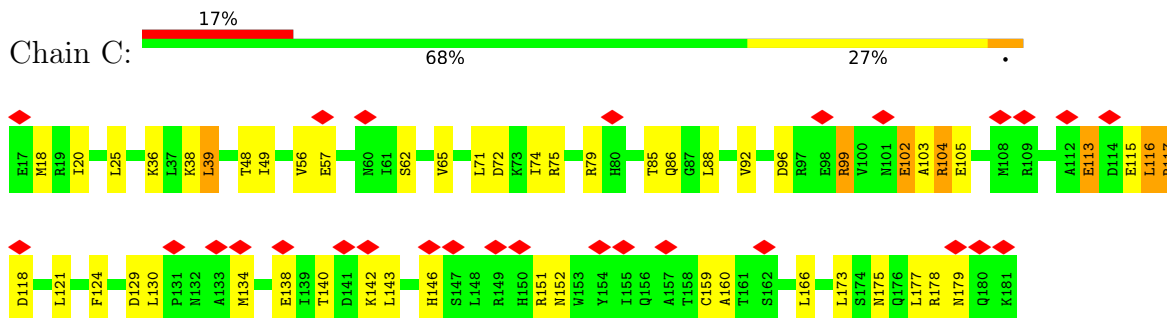
### 3 Residue-property plots

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.

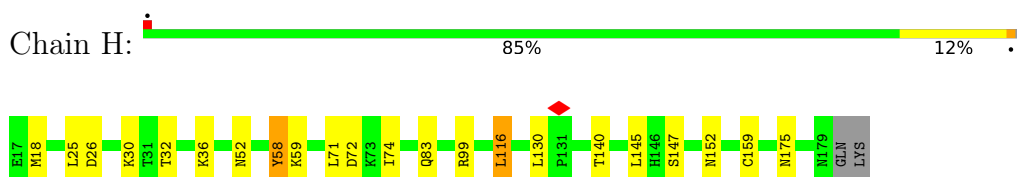
- Molecule 1: AP-1 complex subunit beta-1



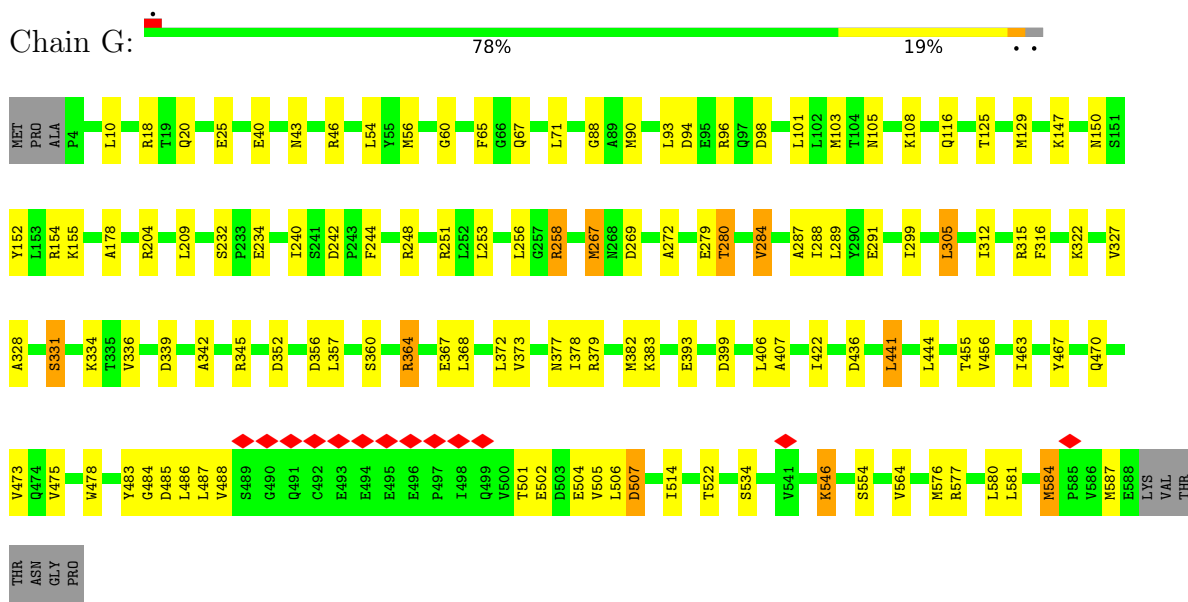
- Molecule 2: ADP-ribosylation factor 1



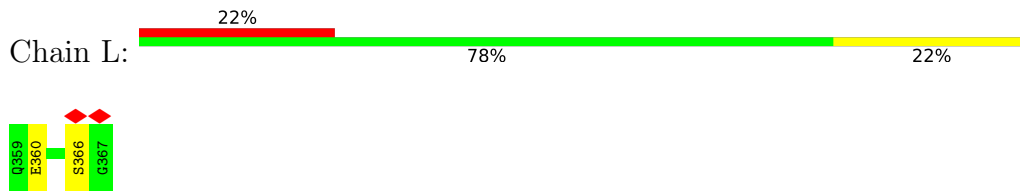
- Molecule 2: ADP-ribosylation factor 1



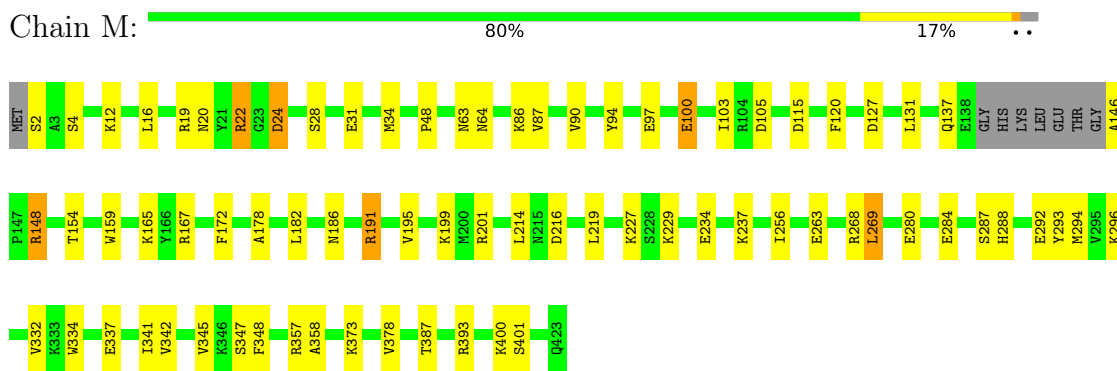
• Molecule 3: AP-1 complex subunit gamma-1



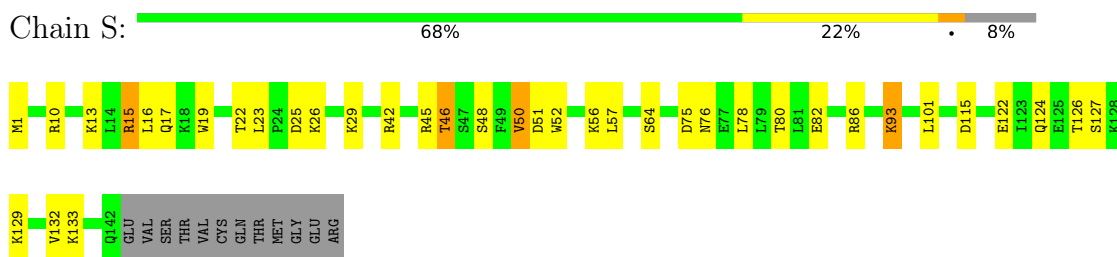
• Molecule 4: Stimulator of interferon genes protein



• Molecule 5: AP-1 complex subunit mu-1



• Molecule 6: AP-1 complex subunit sigma-3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	322238	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.489	Depositor
Minimum map value	-0.188	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	270.0, 270.0, 270.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	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: SEP, GTP, MG

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	B	0.32	0/4583	0.68	8/6216 (0.1%)
2	C	0.40	0/1353	0.87	7/1831 (0.4%)
2	H	0.35	0/1335	0.74	2/1808 (0.1%)
3	G	0.34	0/4697	0.78	16/6338 (0.3%)
4	L	0.40	0/61	0.75	0/80
5	M	0.32	0/3439	0.60	0/4648
6	S	0.32	0/1220	0.69	1/1639 (0.1%)
All	All	0.34	0/16688	0.72	34/22560 (0.2%)

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	B	0	1
2	C	0	2
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	507	ASP	CB-CG-OD2	9.82	127.14	118.30
3	G	406	LEU	CA-CB-CG	9.69	137.59	115.30
1	B	436	LEU	CA-CB-CG	8.98	135.96	115.30
2	C	116	LEU	CA-CB-CG	8.20	134.15	115.30
1	B	493	LEU	CA-CB-CG	8.01	133.73	115.30
2	H	130	LEU	CA-CB-CG	7.65	132.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	357	LEU	CA-CB-CG	7.55	132.66	115.30
3	G	101	LEU	CA-CB-CG	7.41	132.34	115.30
3	G	256	LEU	CA-CB-CG	6.39	130.00	115.30
2	H	116	LEU	CA-CB-CG	6.19	129.54	115.30
3	G	305	LEU	CA-CB-CG	6.06	129.25	115.30
3	G	514	ILE	CG1-CB-CG2	-6.00	98.20	111.40
3	G	444	LEU	CA-CB-CG	5.90	128.88	115.30
3	G	377	ASN	CB-CA-C	5.89	122.18	110.40
3	G	267	MET	CA-CB-CG	5.82	123.19	113.30
1	B	502	LEU	CA-CB-CG	5.78	128.60	115.30
3	G	546	LYS	CA-CB-CG	5.75	126.04	113.40
3	G	393	GLU	CA-CB-CG	5.73	126.01	113.40
1	B	26	LYS	CB-CG-CD	5.69	126.39	111.60
3	G	383	LYS	CA-CB-CG	5.68	125.89	113.40
6	S	23	LEU	CA-CB-CG	5.66	128.32	115.30
2	C	18	MET	CA-CB-CG	5.60	122.81	113.30
3	G	576	MET	CA-CB-CG	5.58	122.78	113.30
2	C	105	GLU	CA-CB-CG	5.56	125.63	113.40
3	G	441	LEU	CA-CB-CG	5.50	127.96	115.30
2	C	39	LEU	CA-CB-CG	5.46	127.85	115.30
2	C	121	LEU	CA-CB-CG	5.40	127.72	115.30
1	B	199	LEU	CA-CB-CG	5.38	127.67	115.30
2	C	88	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	493	LEU	CB-CG-CD2	5.28	119.97	111.00
1	B	26	LYS	CA-CB-CG	5.25	124.95	113.40
1	B	493	LEU	CB-CG-CD1	-5.21	102.13	111.00
3	G	98	ASP	CB-CG-OD1	5.03	122.83	118.30
2	C	117	ARG	CG-CD-NE	5.00	122.30	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	26	LYS	Peptide
2	C	104	ARG	Sidechain
2	C	175	ASN	Peptide
2	H	58	TYR	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	B	4513	0	4647	58	0
2	C	1330	0	1326	16	0
2	H	1312	0	1306	6	0
3	G	4633	0	4756	56	0
4	L	72	0	65	0	0
5	M	3362	0	3373	38	0
6	S	1197	0	1229	22	0
7	C	32	0	12	0	0
7	H	32	0	12	0	0
8	C	1	0	0	0	0
8	H	1	0	0	0	0
All	All	16485	0	16726	170	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 5.

All (170) 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)
5:M:127:ASP:O	5:M:131:LEU:HB2	1.83	0.79
1:B:347:SER:O	1:B:351:ILE:HB	1.88	0.73
5:M:234:GLU:HG3	5:M:269:LEU:HA	1.82	0.62
5:M:16:LEU:HD21	5:M:100:GLU:HG2	1.80	0.62
3:G:25:GLU:HB3	5:M:337:GLU:HB3	1.81	0.61
3:G:422:ILE:HD11	3:G:441:LEU:HD22	1.84	0.60
3:G:456:VAL:HG21	3:G:483:TYR:HB2	1.86	0.57
3:G:378:ILE:O	3:G:382:MET:HB2	2.03	0.57
5:M:4:SER:HA	5:M:22:ARG:HG3	1.85	0.57
1:B:71:LEU:HA	1:B:74:MET:HE2	1.87	0.56
1:B:528:ARG:HH22	3:G:584:MET:HG3	1.71	0.56
2:C:96:ASP:OD1	2:C:96:ASP:N	2.37	0.56
3:G:105:ASN:ND2	2:H:52:ASN:OD1	2.39	0.56
3:G:291:GLU:OE2	6:S:76:ASN:ND2	2.39	0.56
6:S:93:LYS:HB3	6:S:132:VAL:HG21	1.89	0.55
2:C:159:CYS:SG	2:C:160:ALA:N	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:42:ARG:NH1	6:S:46:THR:O	2.40	0.55
1:B:312:LYS:HD2	1:B:564:ILE:HG13	1.88	0.54
3:G:463:ILE:HG23	3:G:467:TYR:HB3	1.89	0.54
5:M:19:ARG:NH1	5:M:20:ASN:O	2.40	0.54
5:M:293:TYR:HB2	5:M:358:ALA:HB3	1.90	0.54
5:M:284:GLU:HB3	5:M:292:GLU:HB2	1.88	0.54
2:C:113:GLU:HG2	2:C:115:GLU:H	1.73	0.54
1:B:63:LEU:HD23	5:M:146:ALA:HB3	1.89	0.53
1:B:371:ARG:HB3	1:B:409:GLU:HG3	1.90	0.53
5:M:16:LEU:HD23	5:M:103:ILE:HG13	1.90	0.53
6:S:86:ARG:NH1	6:S:126:THR:O	2.41	0.53
3:G:43:ASN:OD1	3:G:46:ARG:NH2	2.42	0.53
2:C:36:LYS:NZ	2:C:160:ALA:O	2.42	0.53
2:C:99:ARG:NH1	2:C:102:GLU:OE1	2.42	0.53
3:G:364:ARG:NH2	3:G:367:GLU:OE1	2.42	0.53
1:B:290:THR:HB	5:M:268:ARG:HH21	1.74	0.52
1:B:473:PHE:O	1:B:481:GLN:NE2	2.42	0.52
6:S:10:ARG:HH11	6:S:64:SER:HA	1.75	0.52
1:B:217:TRP:HA	1:B:220:ILE:HD12	1.92	0.52
1:B:165:LEU:HD23	1:B:184:LEU:HD13	1.92	0.51
5:M:214:LEU:O	5:M:393:ARG:NH1	2.44	0.51
3:G:327:VAL:O	3:G:331:SER:OG	2.28	0.51
5:M:24:ASP:OD1	5:M:24:ASP:N	2.43	0.51
1:B:127:ARG:NH2	1:B:159:GLN:OE1	2.43	0.51
2:H:26:ASP:O	2:H:99:ARG:NH2	2.43	0.51
2:C:38:LYS:HB3	2:C:39:LEU:HD12	1.92	0.51
3:G:253:LEU:HD13	3:G:267:MET:HG3	1.93	0.51
3:G:504:GLU:HA	3:G:507:ASP:HB3	1.92	0.51
1:B:267:MET:HA	1:B:270:LEU:HD12	1.93	0.51
3:G:360:SER:OG	6:S:42:ARG:NH2	2.44	0.51
5:M:280:GLU:HB2	5:M:296:LYS:HG3	1.93	0.51
1:B:38:ILE:HD12	1:B:71:LEU:HD23	1.92	0.50
1:B:134:ASP:HB3	1:B:137:VAL:HG12	1.92	0.50
3:G:248:ARG:NH2	6:S:122:GLU:OE1	2.44	0.50
1:B:312:LYS:HG2	1:B:313:ARG:HG2	1.93	0.50
5:M:182:LEU:HB3	5:M:191:ARG:HB3	1.94	0.50
3:G:534:SER:OG	3:G:577:ARG:NH1	2.45	0.50
1:B:72:TYR:O	1:B:76:TYR:HB2	2.12	0.50
3:G:94:ASP:N	3:G:94:ASP:OD1	2.45	0.49
3:G:251:ARG:NH1	6:S:75:ASP:OD2	2.45	0.49
1:B:203:SER:HA	1:B:206:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:LEU:O	2:C:177:LEU:HB2	2.12	0.49
2:C:129:ASP:N	2:C:129:ASP:OD1	2.45	0.49
3:G:339:ASP:HB2	3:G:342:ALA:HB3	1.93	0.49
6:S:115:ASP:O	6:S:124:GLN:NE2	2.46	0.49
1:B:359:ARG:HD3	1:B:394:THR:HG23	1.94	0.49
1:B:124:GLU:OE1	1:B:127:ARG:NH1	2.46	0.49
2:H:83:GLN:NE2	5:M:288:HIS:O	2.46	0.49
2:C:25:LEU:HD11	2:C:103:ALA:HB2	1.93	0.48
2:H:140:THR:HG23	2:H:145:LEU:HD12	1.94	0.48
5:M:159:TRP:NE1	5:M:256:ILE:O	2.46	0.48
3:G:322:LYS:NZ	3:G:356:ASP:OD1	2.47	0.48
1:B:97:ASP:OD1	1:B:97:ASP:N	2.46	0.48
5:M:63:ASN:ND2	5:M:97:GLU:OE2	2.44	0.48
3:G:284:VAL:HG13	6:S:82:GLU:HG3	1.96	0.48
2:C:116:LEU:O	2:C:151:ARG:NH2	2.43	0.48
3:G:280:THR:HG21	3:G:315:ARG:HH12	1.78	0.48
1:B:119:THR:HG21	1:B:151:ILE:HG21	1.94	0.47
2:C:104:ARG:HE	2:C:143:LEU:HA	1.79	0.47
1:B:431:THR:O	1:B:435:ASN:ND2	2.47	0.47
1:B:59:GLN:HE21	1:B:90:THR:HG22	1.80	0.47
3:G:316:PHE:HB3	3:G:328:ALA:HB2	1.96	0.47
2:C:138:GLU:O	2:C:142:LYS:HB2	2.15	0.47
5:M:28:SER:O	5:M:28:SER:OG	2.32	0.47
3:G:485:ASP:OD1	3:G:485:ASP:N	2.45	0.46
2:C:71:LEU:HB2	2:C:74:ILE:HD12	1.97	0.46
5:M:165:LYS:HB3	5:M:165:LYS:HE3	1.71	0.46
5:M:105:ASP:OD1	5:M:105:ASP:N	2.45	0.46
2:C:20:ILE:HD11	2:C:65:VAL:HG22	1.97	0.46
6:S:50:VAL:HG22	6:S:57:LEU:HB2	1.97	0.46
1:B:174:PRO:HA	1:B:177:VAL:HG13	1.97	0.46
3:G:54:LEU:HD21	3:G:88:GLY:HA2	1.97	0.46
6:S:13:LYS:HB2	6:S:15:ARG:HH12	1.80	0.46
3:G:71:LEU:HD22	3:G:103:MET:HB3	1.97	0.45
5:M:178:ALA:HB3	5:M:195:VAL:HG23	1.98	0.45
1:B:223:LEU:HD23	1:B:226:LEU:HD12	1.98	0.45
1:B:528:ARG:HD3	3:G:580:LEU:HA	1.98	0.45
3:G:258:ARG:HA	3:G:299:ILE:HA	1.98	0.45
1:B:428:VAL:O	1:B:432:LEU:HB2	2.17	0.45
1:B:553:ASP:OD1	1:B:553:ASP:N	2.46	0.45
6:S:52:TRP:HB3	6:S:57:LEU:HD13	1.99	0.45
1:B:208:LEU:HD11	1:B:240:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:HD3	1:B:567:ILE:H	1.82	0.45
3:G:240:ILE:HD11	3:G:284:VAL:HB	1.99	0.45
1:B:138:ARG:NH1	1:B:171:ASP:OD2	2.50	0.45
1:B:297:GLU:HG3	5:M:48:PRO:HB3	1.99	0.45
5:M:12:LYS:HA	5:M:12:LYS:HD3	1.87	0.45
3:G:287:ALA:HB2	6:S:78:LEU:HB2	1.99	0.44
1:B:92:VAL:HG12	1:B:125:PRO:HG3	1.98	0.44
3:G:577:ARG:O	3:G:581:LEU:HB2	2.17	0.44
1:B:497:THR:OG1	1:B:498:GLU:OE1	2.36	0.44
5:M:216:ASP:HB3	5:M:219:LEU:HB3	2.00	0.44
1:B:343:ILE:HD13	1:B:343:ILE:HA	1.87	0.44
1:B:363:THR:OG1	5:M:373:LYS:NZ	2.50	0.44
3:G:67:GLN:HB3	3:G:93:LEU:HD21	2.00	0.44
1:B:173:ASN:OD1	5:M:154:THR:OG1	2.33	0.43
3:G:441:LEU:HD12	3:G:475:VAL:HG21	1.99	0.43
1:B:488:ILE:HG21	1:B:506:VAL:HG21	2.00	0.43
1:B:518:ASP:N	1:B:518:ASP:OD1	2.52	0.43
3:G:368:LEU:O	3:G:372:LEU:HB2	2.18	0.43
2:H:71:LEU:H	2:H:74:ILE:HD12	1.84	0.43
1:B:521:ASP:OD2	3:G:478:TRP:NE1	2.50	0.43
5:M:334:TRP:HA	5:M:341:ILE:HG22	2.00	0.43
1:B:147:LYS:HE3	5:M:120:PHE:HB2	1.99	0.43
5:M:31:GLU:H	5:M:31:GLU:HG3	1.61	0.43
3:G:234:GLU:HG2	6:S:127:SER:HB2	2.01	0.43
3:G:60:GLY:O	6:S:29:LYS:NZ	2.47	0.43
3:G:147:LYS:HD3	3:G:178:ALA:HA	2.00	0.43
3:G:272:ALA:HB2	3:G:305:LEU:HD22	2.00	0.43
1:B:67:LYS:HG3	1:B:105:LEU:HD21	2.01	0.42
5:M:199:LYS:HD3	5:M:263:GLU:HG3	2.01	0.42
1:B:108:ARG:NH1	5:M:115:ASP:OD2	2.45	0.42
3:G:364:ARG:NH1	6:S:51:ASP:OD2	2.52	0.42
3:G:436:ASP:OD1	3:G:436:ASP:N	2.48	0.42
1:B:117:LYS:H	1:B:117:LYS:HG3	1.60	0.42
5:M:227:LYS:HE3	5:M:227:LYS:HB3	1.83	0.42
3:G:484:GLY:HA2	3:G:487:LEU:HB3	2.00	0.42
6:S:129:LYS:H	6:S:129:LYS:HG2	1.73	0.42
1:B:289:VAL:HG21	1:B:320:GLU:HG2	2.00	0.42
1:B:545:LYS:HG2	3:G:564:VAL:HG21	2.01	0.42
1:B:89:ASN:HB2	2:C:49:ILE:H	1.85	0.42
3:G:116:GLN:OE1	3:G:150:ASN:ND2	2.47	0.42
5:M:19:ARG:HH21	5:M:115:ASP:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:289:LEU:HD13	3:G:312:ILE:HD11	2.01	0.41
3:G:373:VAL:HG11	3:G:407:ALA:HB1	2.01	0.41
3:G:90:MET:HG3	3:G:125:THR:HG23	2.02	0.41
3:G:488:VAL:HG11	3:G:502:GLU:HG3	2.02	0.41
5:M:86:LYS:HB2	5:M:86:LYS:HE3	1.94	0.41
3:G:108:LYS:HE3	3:G:108:LYS:HB2	1.80	0.41
3:G:501:THR:O	3:G:501:THR:OG1	2.34	0.41
1:B:82:ASP:OD1	1:B:82:ASP:N	2.46	0.41
3:G:94:ASP:HB2	6:S:22:THR:HG23	2.02	0.41
1:B:477:SER:OG	1:B:478:THR:N	2.53	0.41
2:H:25:LEU:O	2:H:30:LYS:NZ	2.54	0.41
5:M:172:PHE:HB2	5:M:201:ARG:HB3	2.02	0.41
1:B:353:GLN:H	1:B:353:GLN:HG3	1.61	0.41
3:G:240:ILE:HD12	3:G:288:ILE:HD12	2.03	0.41
3:G:152:TYR:HA	3:G:155:LYS:HE3	2.03	0.41
3:G:244:PHE:HD2	6:S:126:THR:HG23	1.85	0.41
6:S:17:GLN:HB2	6:S:19:TRP:HE1	1.86	0.41
1:B:47:VAL:O	1:B:72:TYR:OH	2.39	0.41
1:B:316:ILE:HG22	1:B:317:LEU:HG	2.02	0.41
2:C:72:ASP:OD2	2:C:72:ASP:N	2.44	0.41
3:G:470:GLN:HA	3:G:473:VAL:HG12	2.03	0.41
5:M:148:ARG:H	5:M:148:ARG:HG2	1.54	0.41
1:B:336:LEU:HD22	1:B:372:LYS:HD3	2.03	0.40
5:M:87:VAL:HA	5:M:90:VAL:HB	2.02	0.40
1:B:74:MET:HG3	1:B:109:THR:HG23	2.03	0.40
3:G:150:ASN:O	3:G:154:ARG:HB2	2.21	0.40
1:B:23:ASN:ND2	1:B:53:ASP:OD2	2.43	0.40
1:B:27:LYS:HA	1:B:27:LYS:HD3	1.86	0.40
1:B:156:VAL:HG13	1:B:161:PHE:HB2	2.02	0.40
1:B:336:LEU:O	1:B:372:LYS:NZ	2.54	0.40
6:S:76:ASN:O	6:S:80:THR:OG1	2.33	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	B	568/584 (97%)	544 (96%)	24 (4%)	0	100	100
2	C	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
2	H	161/165 (98%)	154 (96%)	7 (4%)	0	100	100
3	G	583/595 (98%)	567 (97%)	16 (3%)	0	100	100
4	L	6/9 (67%)	6 (100%)	0	0	100	100
5	M	411/423 (97%)	399 (97%)	12 (3%)	0	100	100
6	S	140/154 (91%)	132 (94%)	8 (6%)	0	100	100
All	All	2032/2095 (97%)	1957 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	510/522 (98%)	487 (96%)	23 (4%)	27	34
2	C	143/143 (100%)	120 (84%)	23 (16%)	2	1
2	H	141/143 (99%)	130 (92%)	11 (8%)	12	12
3	G	520/528 (98%)	486 (94%)	34 (6%)	17	19
4	L	7/7 (100%)	6 (86%)	1 (14%)	3	2
5	M	377/383 (98%)	350 (93%)	27 (7%)	14	14
6	S	132/143 (92%)	119 (90%)	13 (10%)	8	6
All	All	1830/1869 (98%)	1698 (93%)	132 (7%)	18	14

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	ASP
1	B	91	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	93	LYS
1	B	117	LYS
1	B	177	VAL
1	B	186	GLU
1	B	191	HIS
1	B	200	ASN
1	B	206	LYS
1	B	235	ARG
1	B	275	ASP
1	B	282	LYS
1	B	283	LYS
1	B	312	LYS
1	B	326	VAL
1	B	393	SER
1	B	439	LEU
1	B	440	ASP
1	B	476	LYS
1	B	495	LYS
1	B	508	SER
1	B	522	ARG
1	B	561	ASP
2	C	48	THR
2	C	56	VAL
2	C	57	GLU
2	C	62	SER
2	C	75	ARG
2	C	79	ARG
2	C	85	THR
2	C	86	GLN
2	C	92	VAL
2	C	99	ARG
2	C	102	GLU
2	C	113	GLU
2	C	117	ARG
2	C	118	ASP
2	C	124	PHE
2	C	130	LEU
2	C	134	MET
2	C	140	THR
2	C	146	HIS
2	C	152	ASN
2	C	166	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	178	ARG
2	C	179	ASN
3	G	10	LEU
3	G	18	ARG
3	G	20	GLN
3	G	40	GLU
3	G	56	MET
3	G	65	PHE
3	G	96	ARG
3	G	129	MET
3	G	204	ARG
3	G	209	LEU
3	G	232	SER
3	G	242	ASP
3	G	258	ARG
3	G	269	ASP
3	G	279	GLU
3	G	280	THR
3	G	284	VAL
3	G	331	SER
3	G	334	LYS
3	G	336	VAL
3	G	345	ARG
3	G	352	ASP
3	G	364	ARG
3	G	379	ARG
3	G	399	ASP
3	G	455	THR
3	G	486	LEU
3	G	505	VAL
3	G	506	LEU
3	G	522	THR
3	G	546	LYS
3	G	554	SER
3	G	584	MET
3	G	587	MET
2	H	18	MET
2	H	32	THR
2	H	36	LYS
2	H	58	TYR
2	H	59	LYS
2	H	72	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	116	LEU
2	H	147	SER
2	H	152	ASN
2	H	159	CYS
2	H	175	ASN
4	L	360	GLU
5	M	2	SER
5	M	22	ARG
5	M	24	ASP
5	M	34	MET
5	M	64	ASN
5	M	94	TYR
5	M	100	GLU
5	M	137	GLN
5	M	148	ARG
5	M	167	ARG
5	M	186	ASN
5	M	191	ARG
5	M	229	LYS
5	M	237	LYS
5	M	269	LEU
5	M	287	SER
5	M	294	MET
5	M	332	VAL
5	M	342	VAL
5	M	345	VAL
5	M	347	SER
5	M	348	PHE
5	M	357	ARG
5	M	378	VAL
5	M	387	THR
5	M	400	LYS
5	M	401	SER
6	S	1	MET
6	S	15	ARG
6	S	16	LEU
6	S	25	ASP
6	S	26	LYS
6	S	45	ARG
6	S	46	THR
6	S	48	SER
6	S	50	VAL

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Mol	Chain	Res	Type
6	S	56	LYS
6	S	93	LYS
6	S	101	LEU
6	S	133	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
4	SEP	L	366	4	8,9,10	1.56	1 (12%)	8,12,14	1.38	2 (25%)

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
4	SEP	L	366	4	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	366	SEP	P-O1P	3.38	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	366	SEP	P-OG-CB	-2.39	111.70	118.30
4	L	366	SEP	OG-CB-CA	2.36	110.44	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	366	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
7	GTP	H	1001	8	26,34,34	1.14	2 (7%)	32,54,54	1.59	6 (18%)
7	GTP	C	1001	8	26,34,34	1.07	2 (7%)	32,54,54	1.58	7 (21%)

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
7	GTP	H	1001	8	-	5/18/38/38	0/3/3/3
7	GTP	C	1001	8	-	5/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	1001	GTP	C5-C6	-3.95	1.39	1.47
7	C	1001	GTP	C5-C6	-3.68	1.39	1.47
7	C	1001	GTP	C2-N3	2.21	1.38	1.33
7	H	1001	GTP	C2-N3	2.13	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1001	GTP	PB-O3B-PG	-3.56	120.60	132.83
7	C	1001	GTP	C5-C6-N1	3.49	120.12	113.95
7	H	1001	GTP	PB-O3B-PG	-3.49	120.84	132.83
7	H	1001	GTP	PA-O3A-PB	-3.42	121.09	132.83
7	H	1001	GTP	C5-C6-N1	3.33	119.83	113.95
7	C	1001	GTP	PA-O3A-PB	-3.26	121.62	132.83
7	C	1001	GTP	C2-N1-C6	-3.20	119.21	125.10
7	H	1001	GTP	C8-N7-C5	3.08	108.85	102.99
7	C	1001	GTP	C8-N7-C5	2.96	108.63	102.99
7	H	1001	GTP	C3'-C2'-C1'	2.92	105.37	100.98
7	H	1001	GTP	C2-N1-C6	-2.87	119.81	125.10
7	C	1001	GTP	C3'-C2'-C1'	2.72	105.08	100.98
7	C	1001	GTP	O6-C6-C5	-2.20	120.07	124.37

There are no chirality outliers.

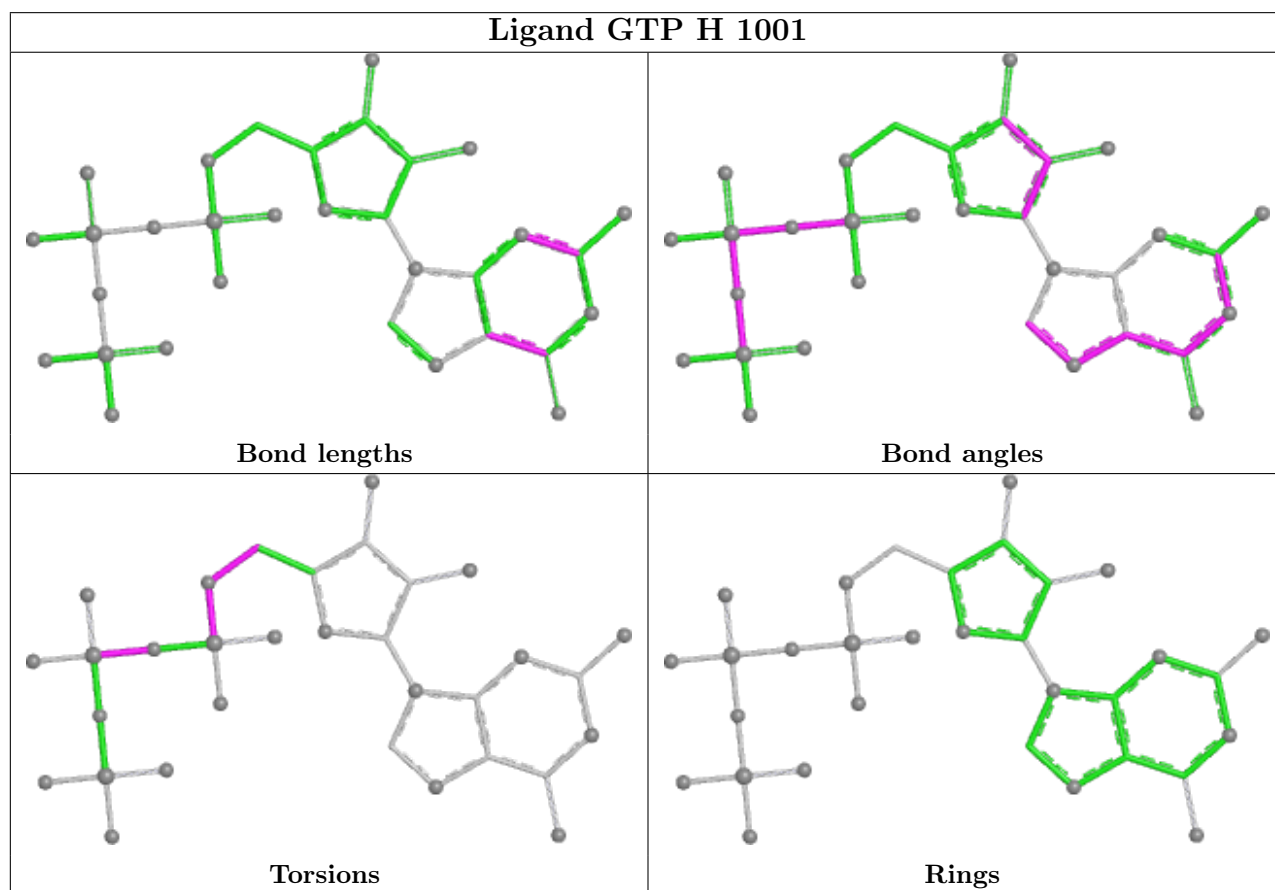
All (10) torsion outliers are listed below:

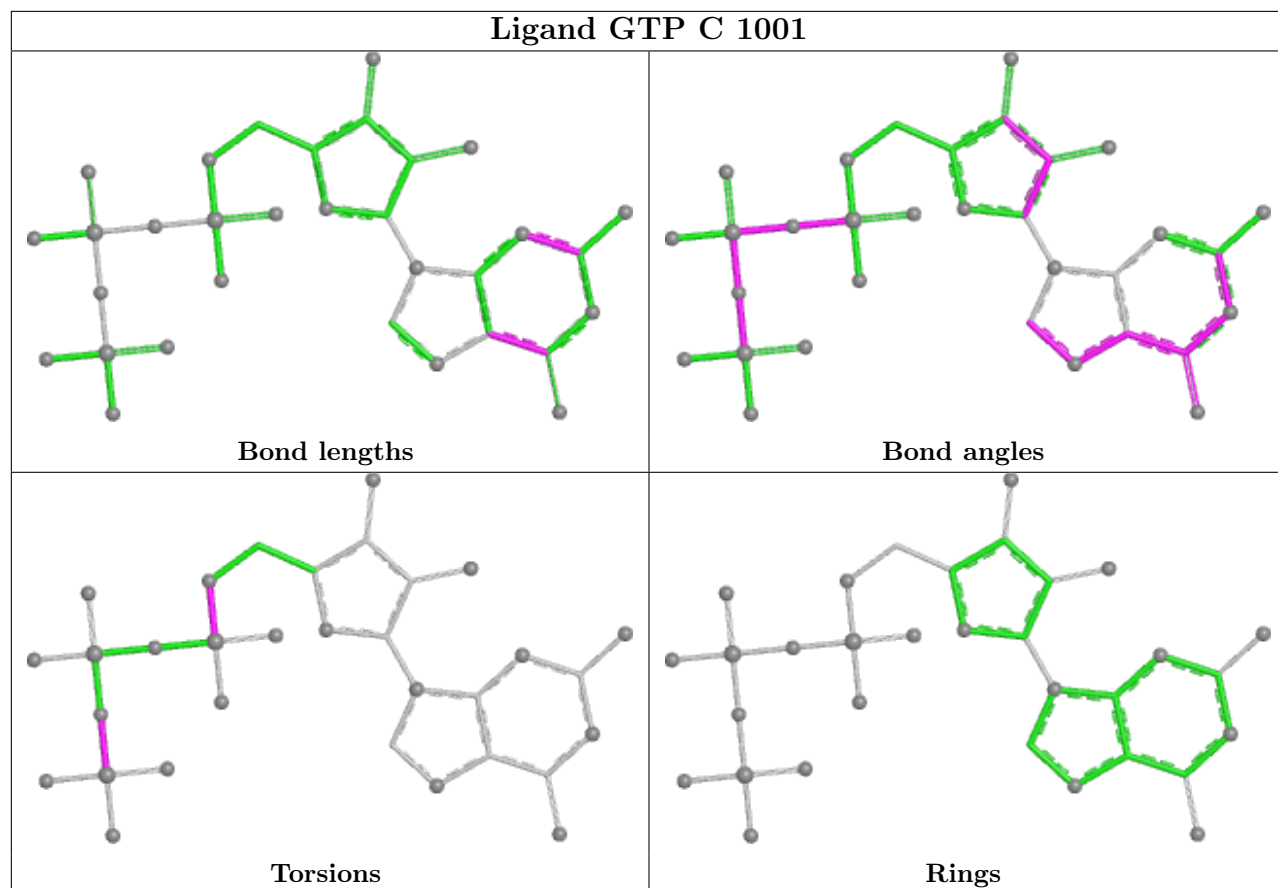
Mol	Chain	Res	Type	Atoms
7	C	1001	GTP	PB-O3B-PG-O3G
7	C	1001	GTP	C5'-O5'-PA-O2A
7	H	1001	GTP	C5'-O5'-PA-O2A
7	H	1001	GTP	C4'-C5'-O5'-PA
7	C	1001	GTP	C5'-O5'-PA-O3A
7	H	1001	GTP	C5'-O5'-PA-O3A
7	C	1001	GTP	C5'-O5'-PA-O1A
7	H	1001	GTP	C5'-O5'-PA-O1A
7	H	1001	GTP	PA-O3A-PB-O2B
7	C	1001	GTP	PB-O3B-PG-O1G

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



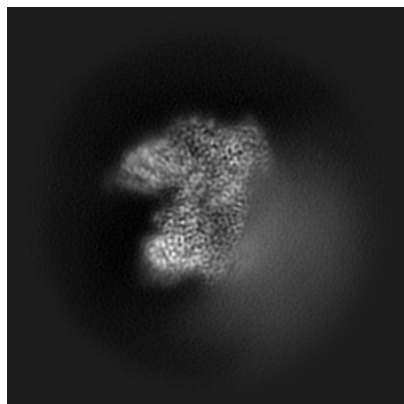
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14312. These allow visual inspection of the internal detail of the map and identification of artifacts.

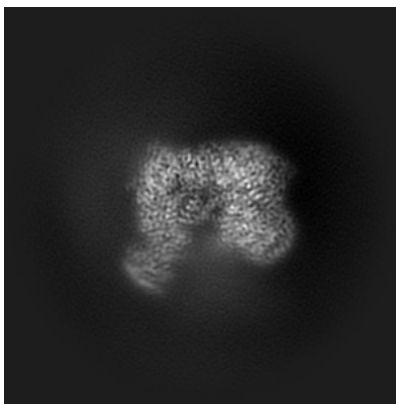
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

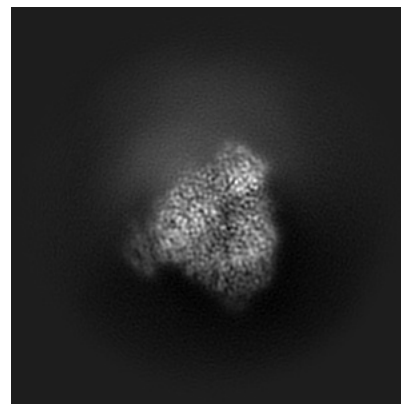
#### 6.1.1 Primary map



X

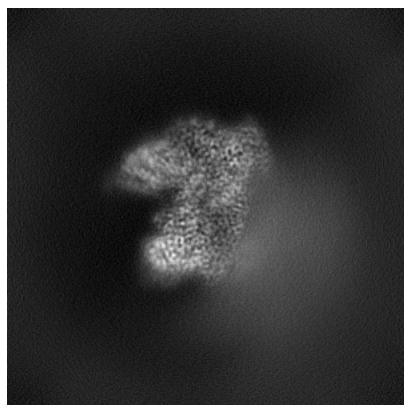


Y

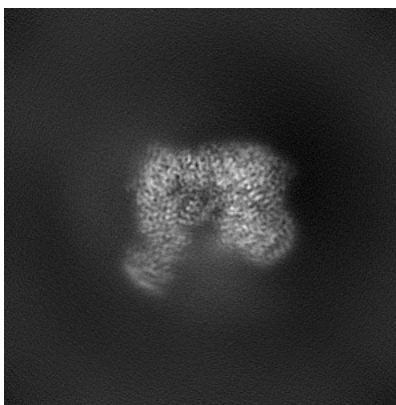


Z

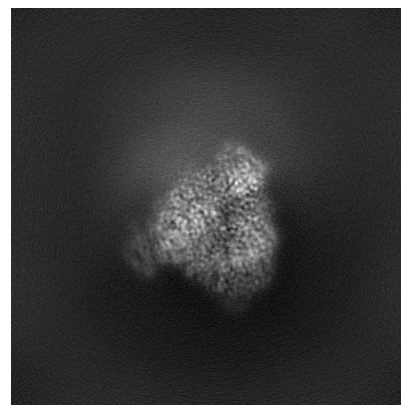
#### 6.1.2 Raw map



X



Y

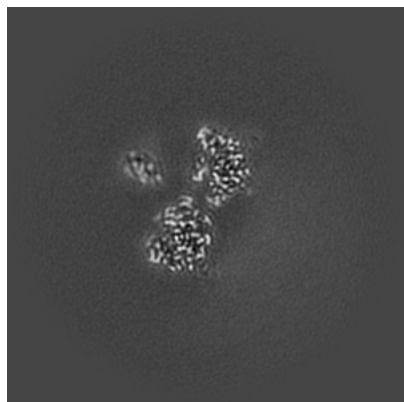


Z

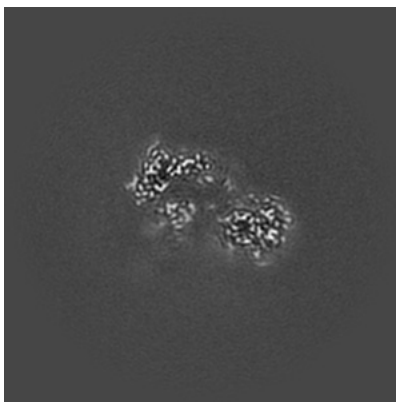
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

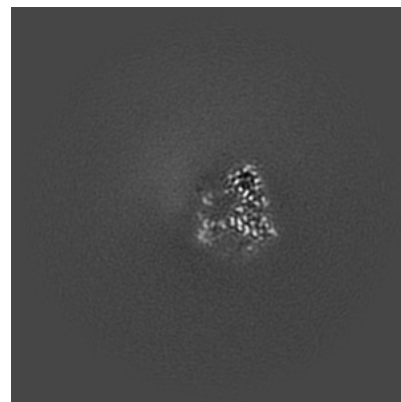
### 6.2.1 Primary map



X Index: 150

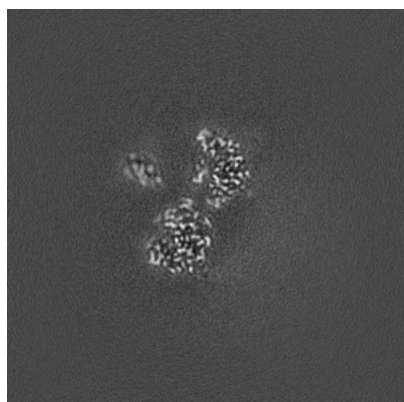


Y Index: 150

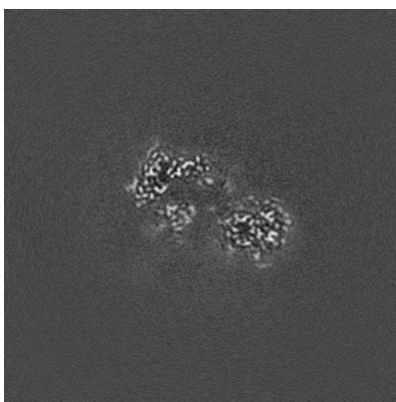


Z Index: 150

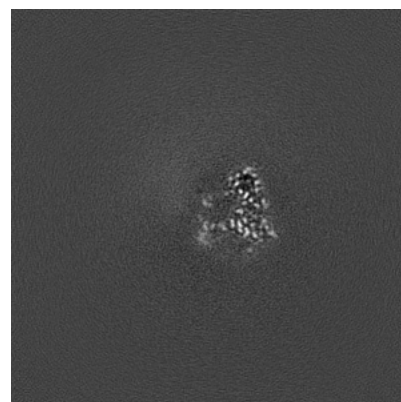
### 6.2.2 Raw map



X Index: 150



Y Index: 150

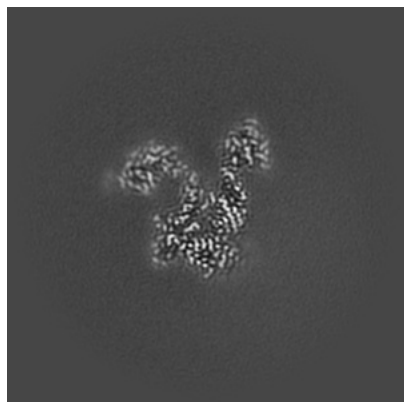


Z Index: 150

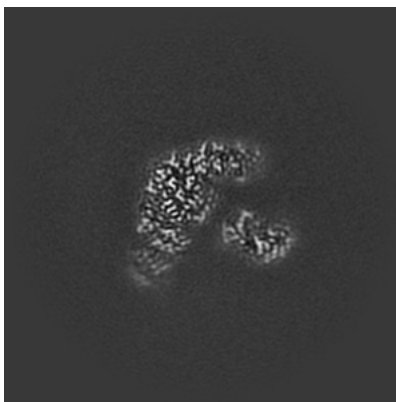
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

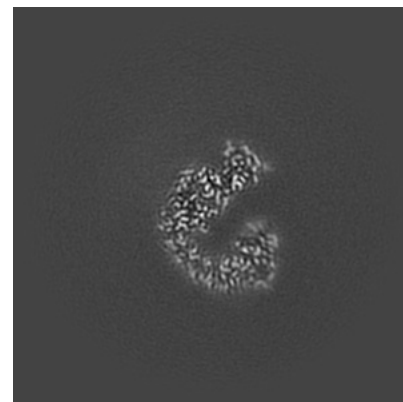
### 6.3.1 Primary map



X Index: 172

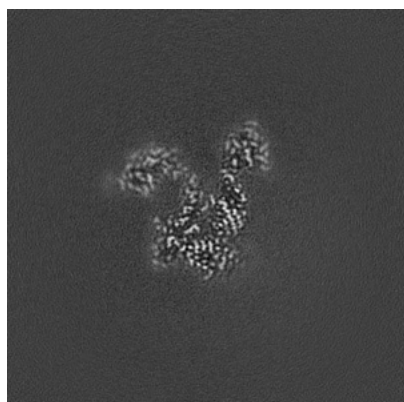


Y Index: 131

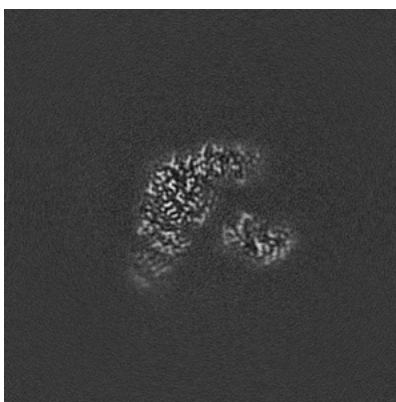


Z Index: 184

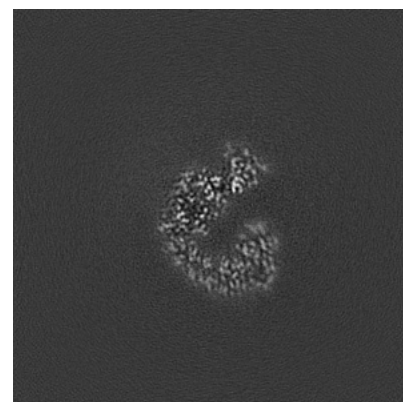
### 6.3.2 Raw map



X Index: 172



Y Index: 131

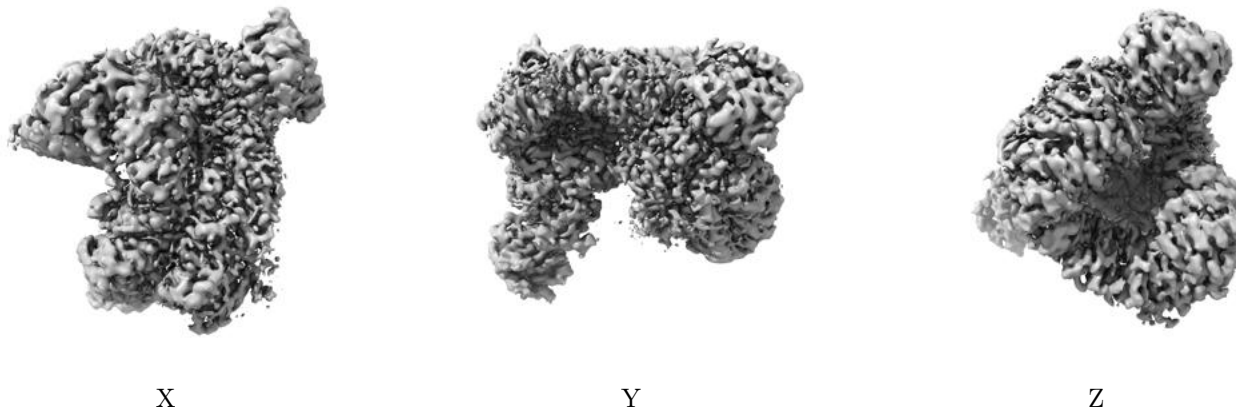


Z Index: 183

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

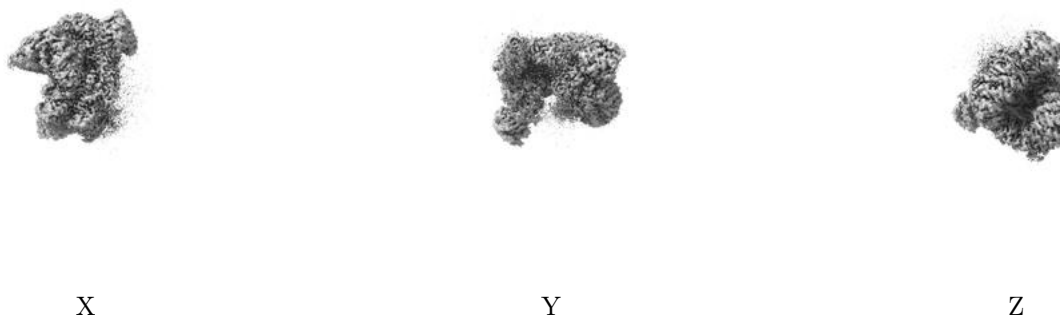
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

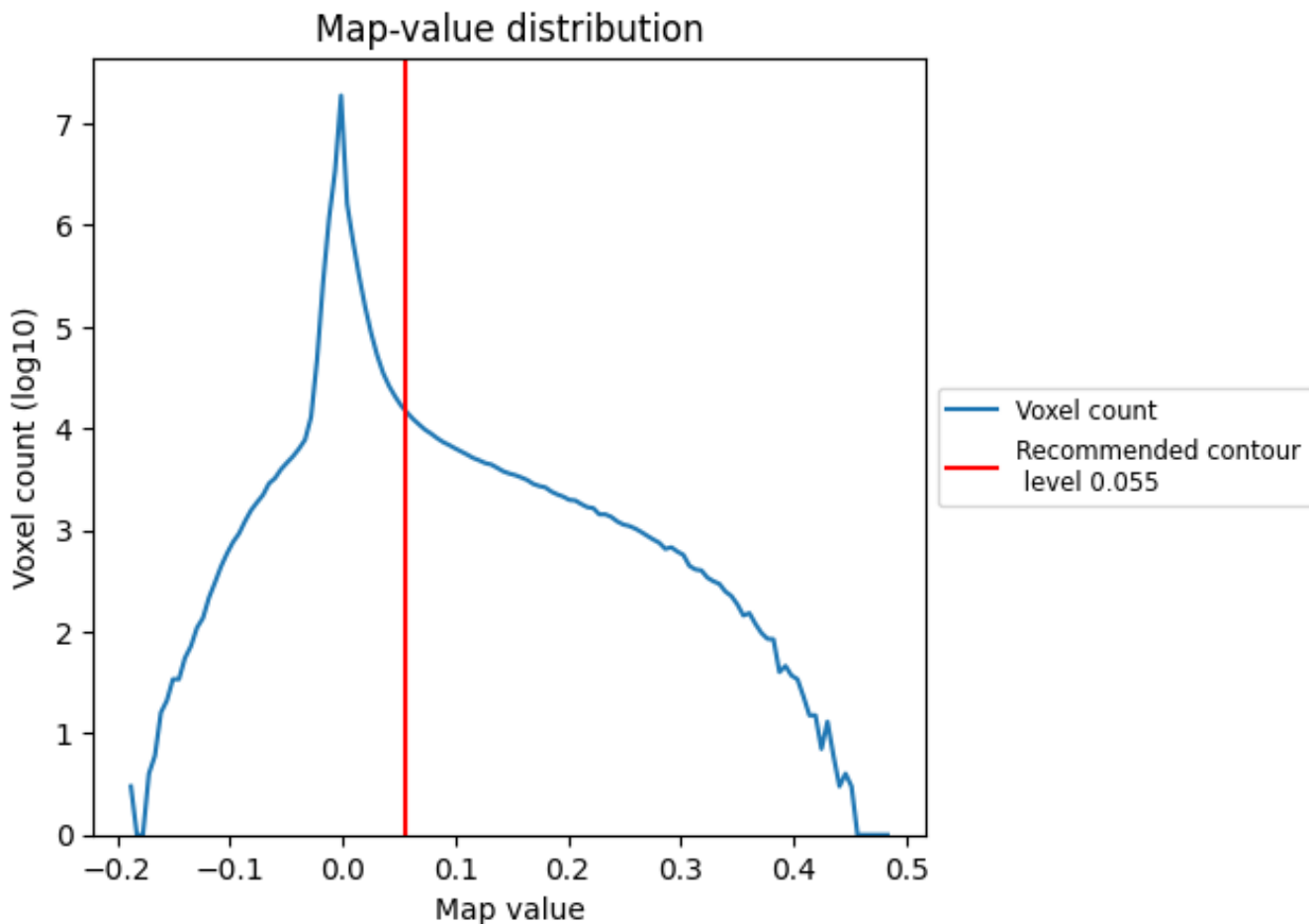
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

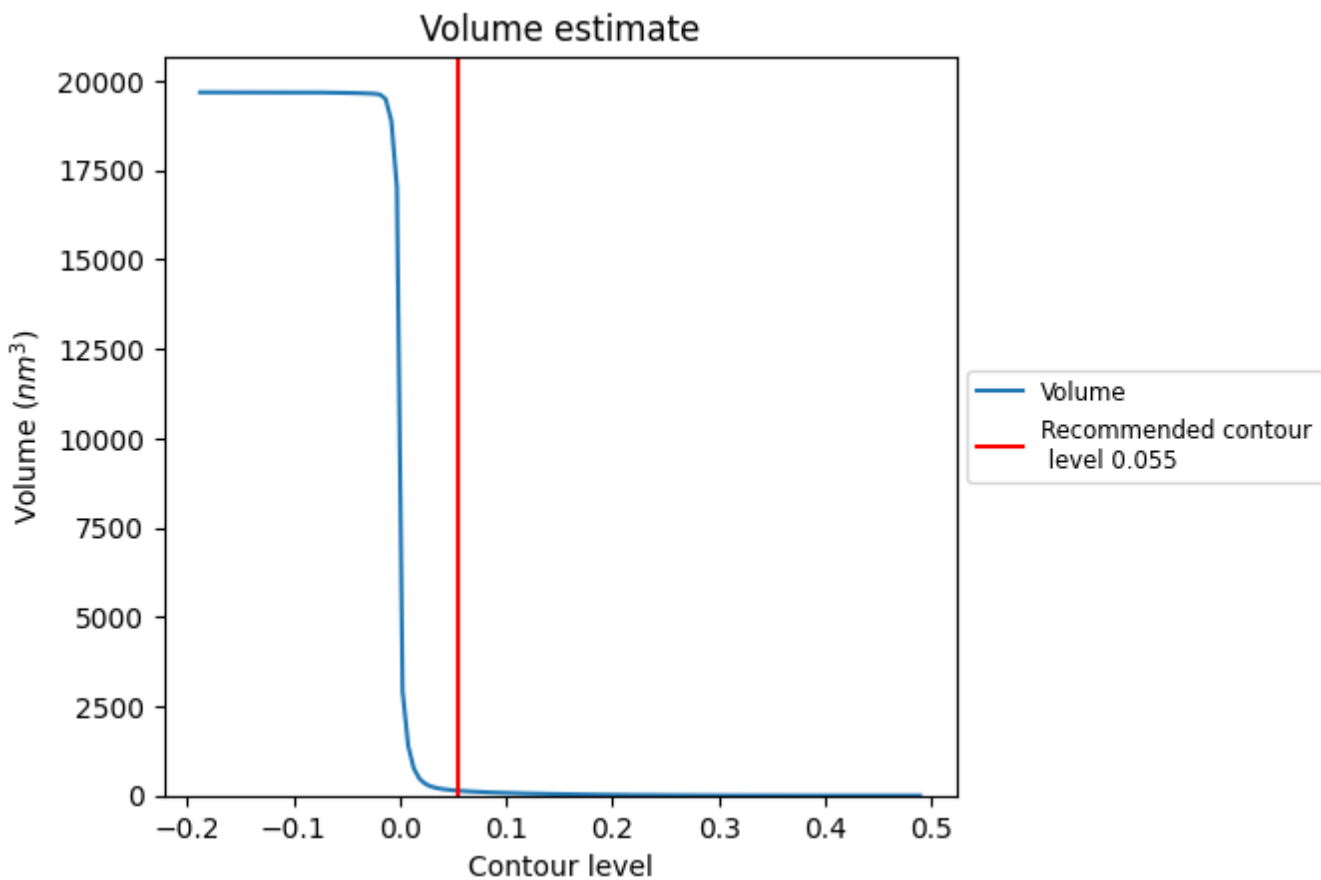
This section contains the results of statistical analysis of the map.

### 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.

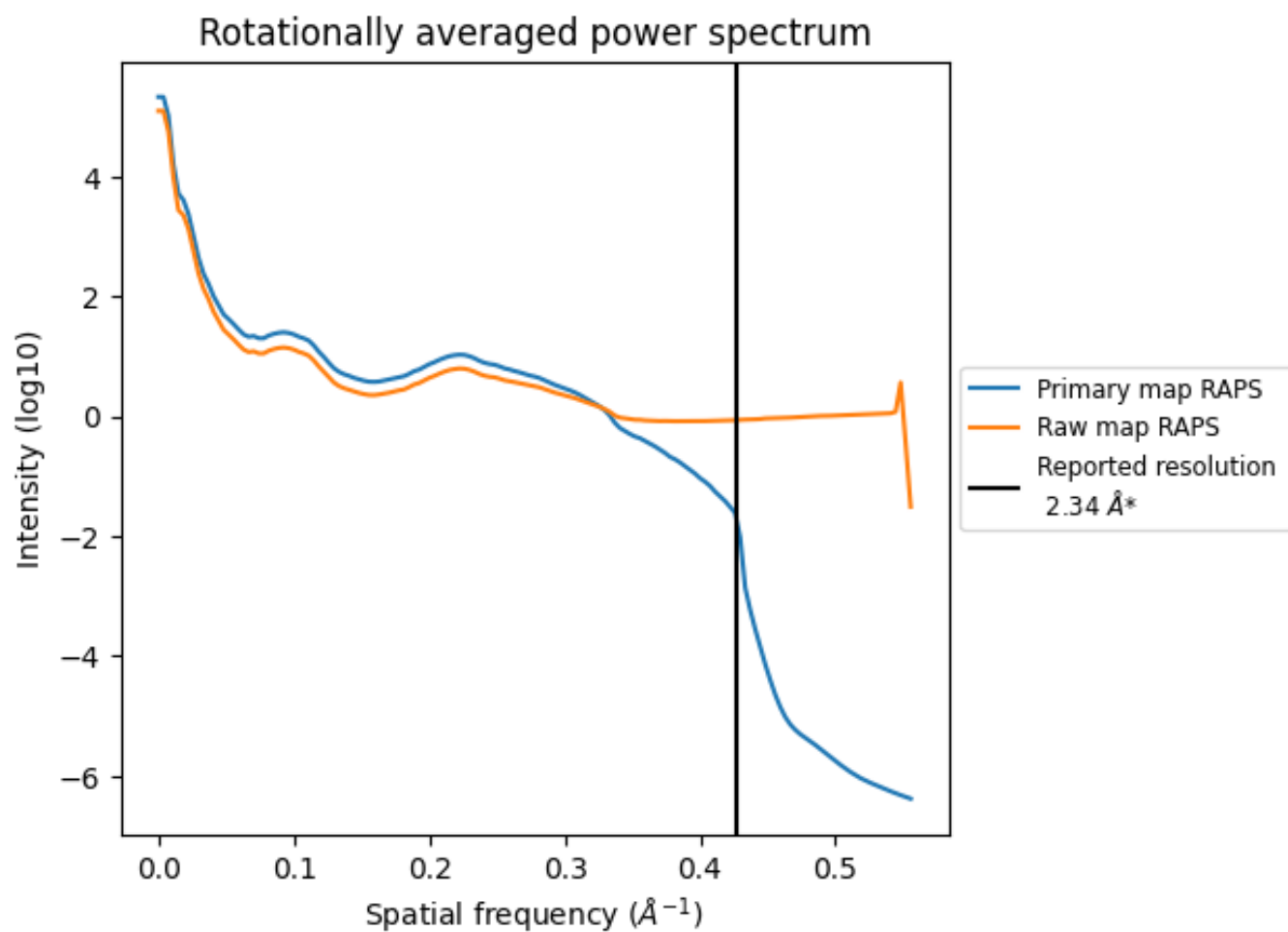
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm<sup>3</sup>; this corresponds to an approximate mass of 122 kDa.

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

### 7.3 Rotationally averaged power spectrum i

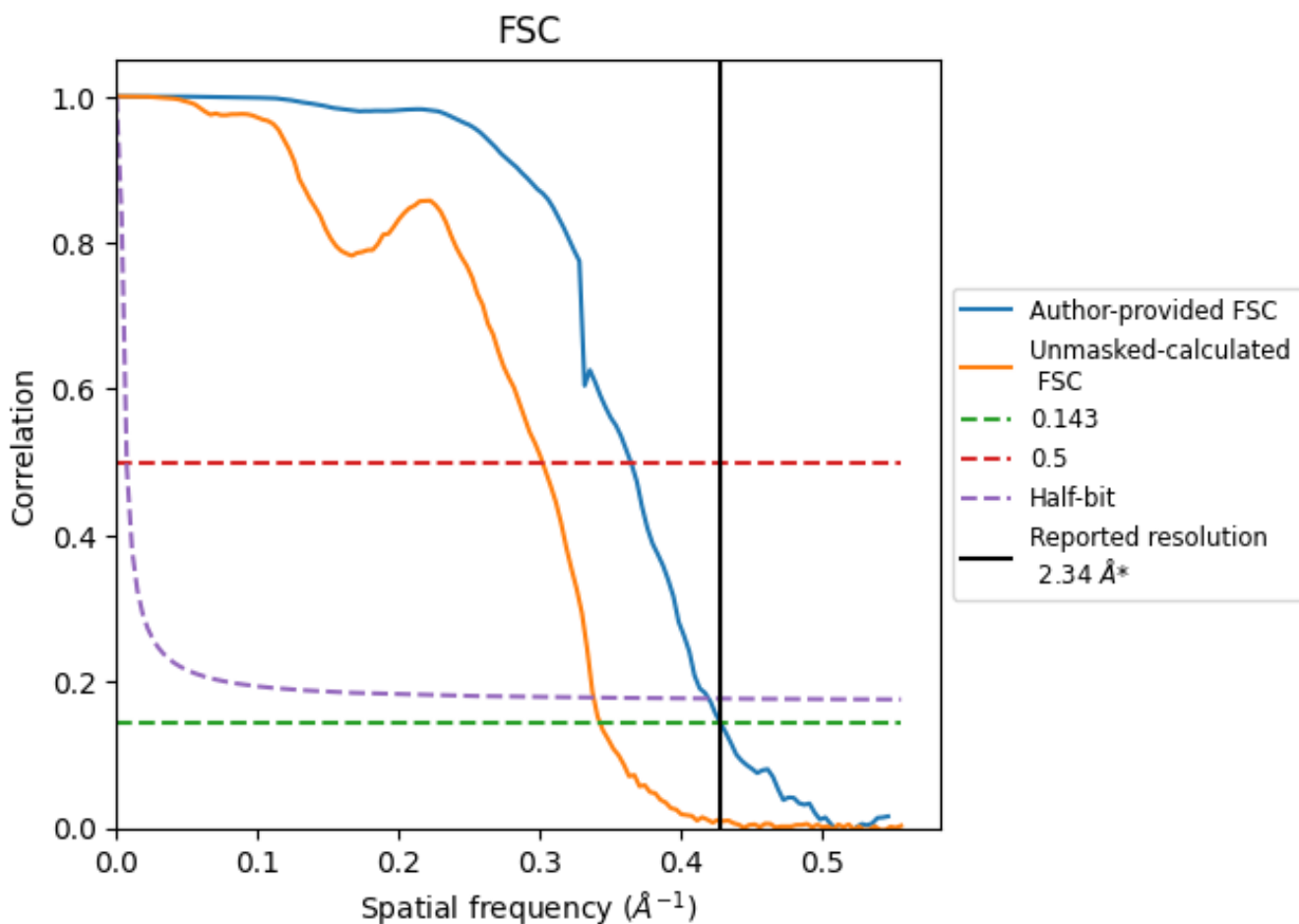


\*Reported resolution corresponds to spatial frequency of 0.427 Å<sup>-1</sup>

## 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 0.427 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

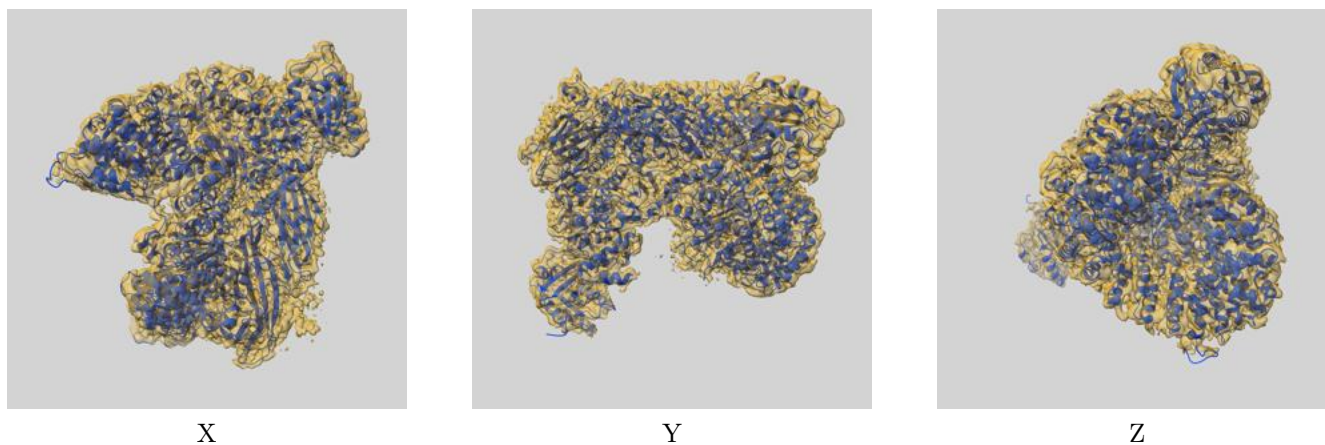
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.34	-	-
Author-provided FSC curve	2.34	2.75	2.38
Unmasked-calculated*	2.92	3.32	2.96

\*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 2.92 differs from the reported value 2.34 by more than 10 %

## 9 Map-model fit [i](#)

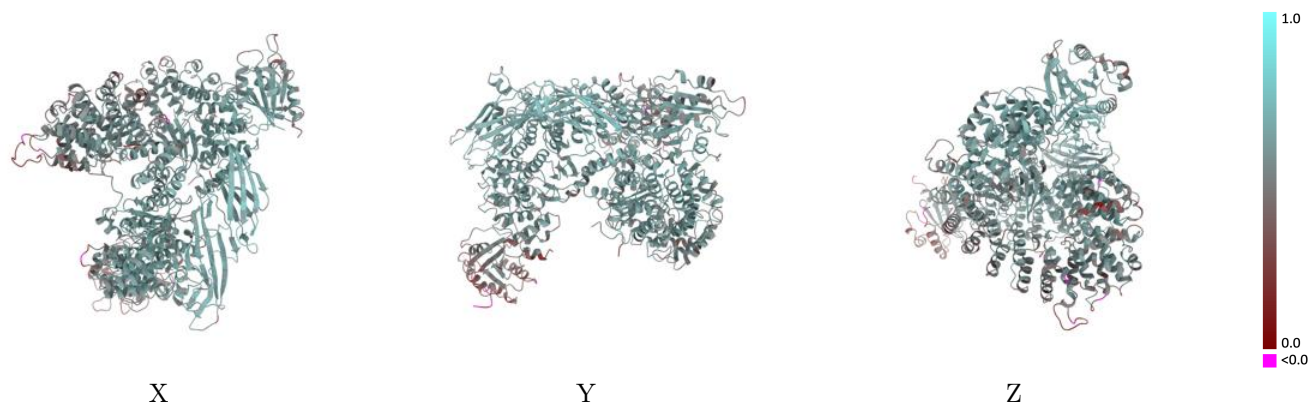
This section contains information regarding the fit between EMDB map EMD-14312 and PDB model 7R4H. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



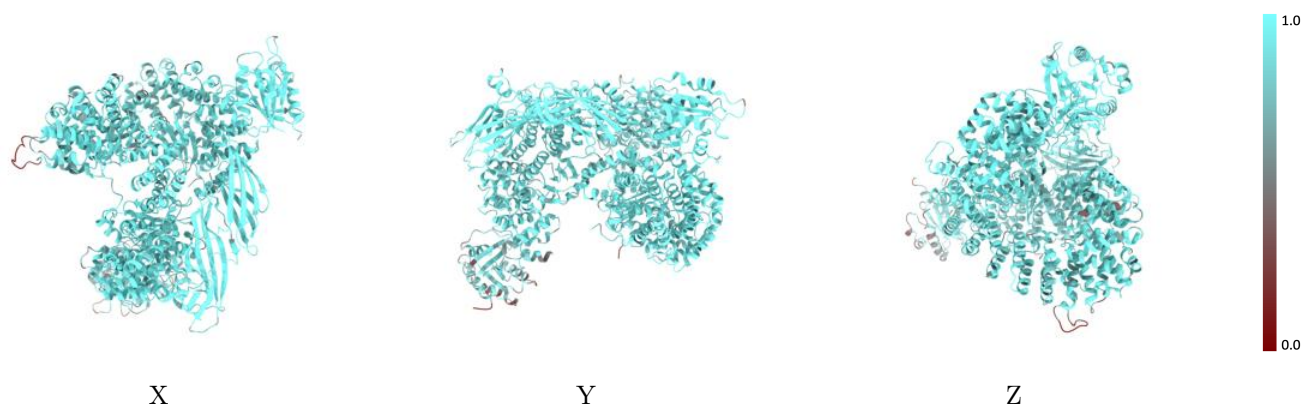
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



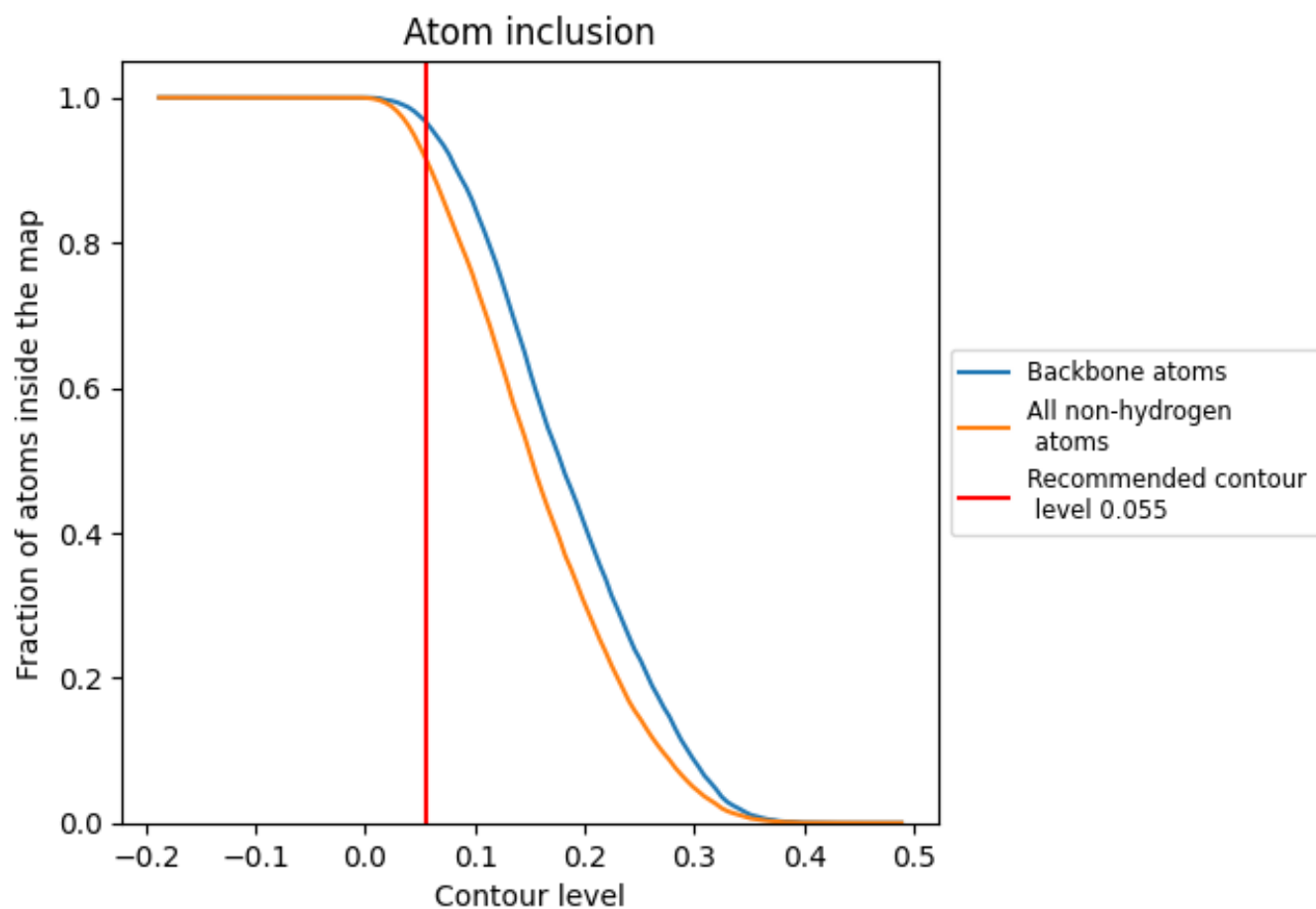
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9167	 0.5510
B	 0.9303	 0.5620
C	 0.7177	 0.3560
G	 0.9250	 0.5390
H	 0.9490	 0.5680
L	 0.6944	 0.4350
M	 0.9484	 0.6140
S	 0.9471	 0.5920

