



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 12:17 PM EST

PDB ID : 7UX2
EMDB ID : EMD-26846
Title : cryo-EM structure of the Raptor-TFEB-Rag-Ragulator complex
Authors : Cui, Z.; Hurley, J.
Deposited on : 2022-05-04
Resolution : 2.90 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

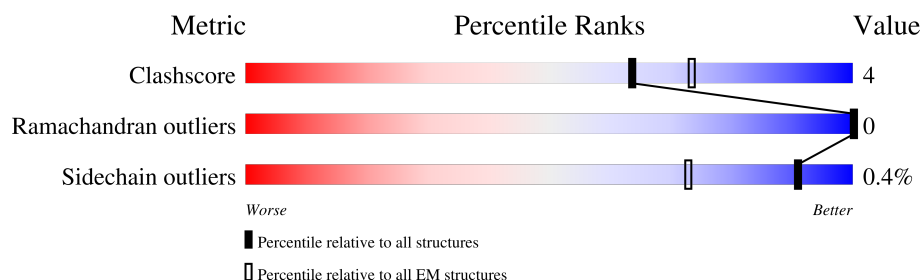
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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









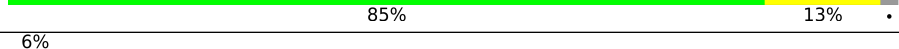
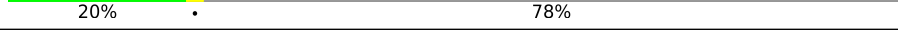
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1335	
2	B	313	
2	I	313	
3	C	399	
3	J	399	
4	D	161	
4	K	161	
5	E	125	

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Mol	Chain	Length	Quality of chain
5	L	125	
6	F	124	
6	M	124	
7	G	99	
7	N	99	
8	H	91	
8	O	91	
9	P	476	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 54436 atoms, of which 27187 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 Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1103	Total	C	H	N	O	S	0	0
			17564	5610	8770	1530	1595	59		

- Molecule 2 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	298	Total	C	H	N	O	S	0	0
			4882	1553	2438	427	447	17		
2	I	298	Total	C	H	N	O	S	0	0
			4882	1553	2438	427	447	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	LEU	GLN	conflict	UNP Q7L523
I	66	LEU	GLN	conflict	UNP Q7L523

- Molecule 3 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	281	Total	C	H	N	O	S	0	0
			4523	1459	2258	370	424	12		
3	J	277	Total	C	H	N	O	S	0	0
			4447	1430	2221	365	419	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	75	ASN	SER	engineered mutation	UNP Q9HB90
J	75	ASN	SER	engineered mutation	UNP Q9HB90

- Molecule 4 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	111	Total	C	H	N	O	S	0	0
			1738	547	870	150	170	1		
4	K	115	Total	C	H	N	O	S	0	0
			1791	562	896	155	176	2		

- Molecule 5 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	124	Total	C	H	N	O	S	0	0
			1888	590	950	161	180	7		
5	L	124	Total	C	H	N	O	S	0	0
			1888	590	950	161	180	7		

- Molecule 6 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	120	Total	C	H	N	O	S	0	0
			1892	601	958	157	175	1		
6	M	120	Total	C	H	N	O	S	0	0
			1892	601	958	157	175	1		

- Molecule 7 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	84	Total	C	H	N	O	S	0	0
			1294	404	652	115	122	1		
7	N	84	Total	C	H	N	O	S	0	0
			1294	404	652	115	122	1		

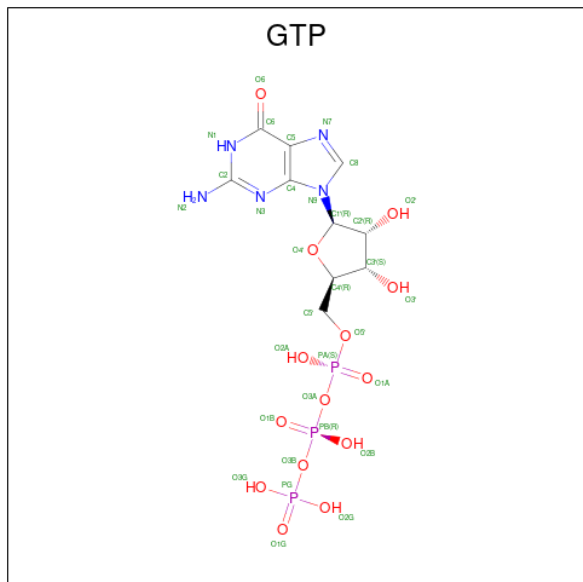
- Molecule 8 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		
8	O	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		

- Molecule 9 is a protein called Transcription factor EB.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	P	104	Total	C	H	N	O	S	0	0
			1677	526	824	160	162	5		

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

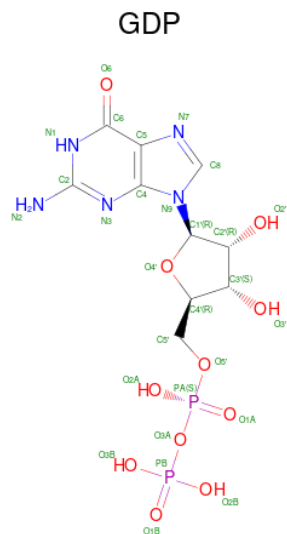


Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	H	N	O	P
			42	10	10	5	14	3
10	I	1	Total	C	H	N	O	P
			42	10	10	5	14	3

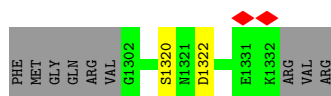
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Mg	0
			1	1	
11	I	1	Total	Mg	0
			1	1	

- Molecule 12 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

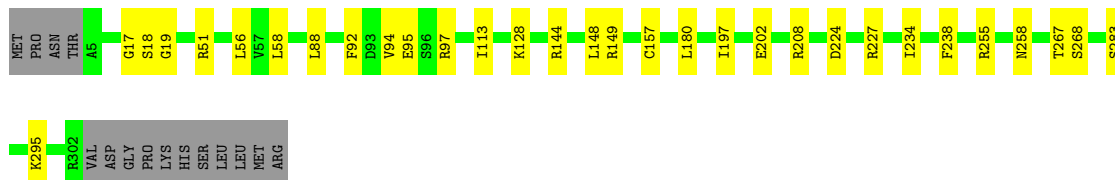


Mol	Chain	Residues	Atoms						AltConf
12	C	1	Total 38	C 10	H 10	N 5	O 11	P 2	0
12	J	1	Total 38	C 10	H 10	N 5	O 11	P 2	0



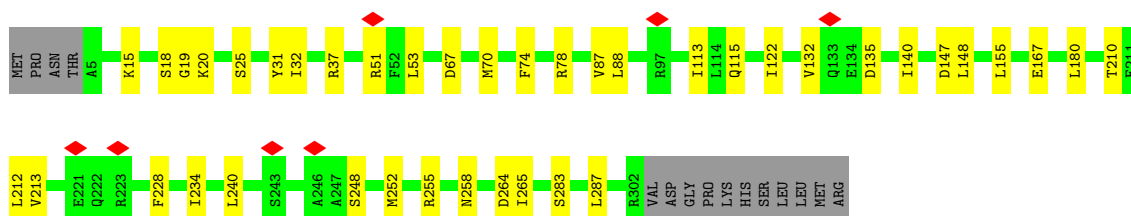
• Molecule 2: Ras-related GTP-binding protein A

Chain B: 85% 10% 5%



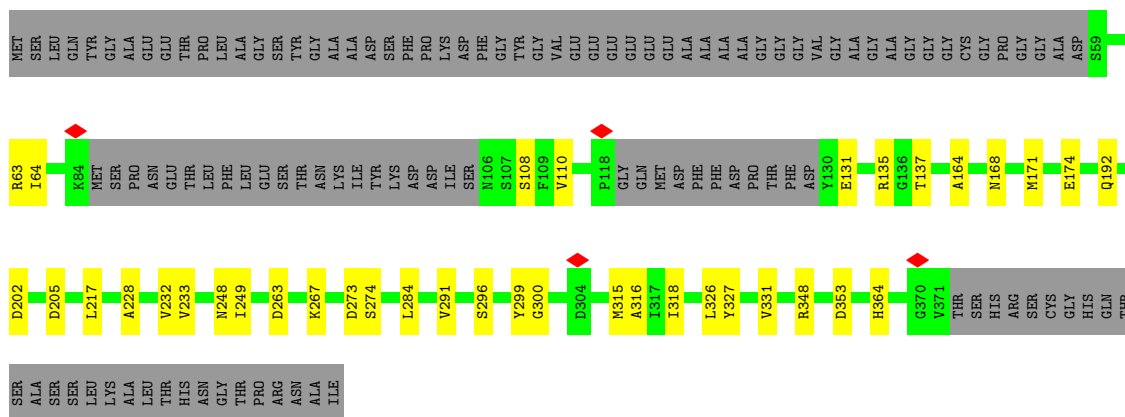
• Molecule 2: Ras-related GTP-binding protein A

Chain I: 82% 13% 5%



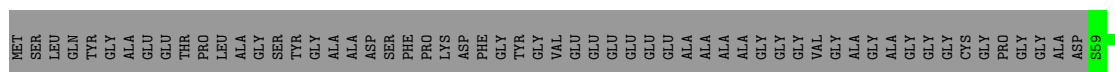
• Molecule 3: Ras-related GTP-binding protein C

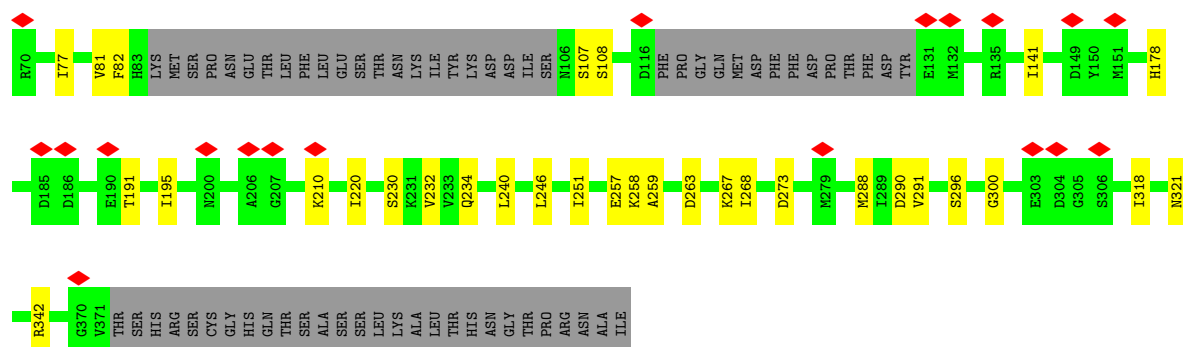
Chain C: 61% 10% 30%



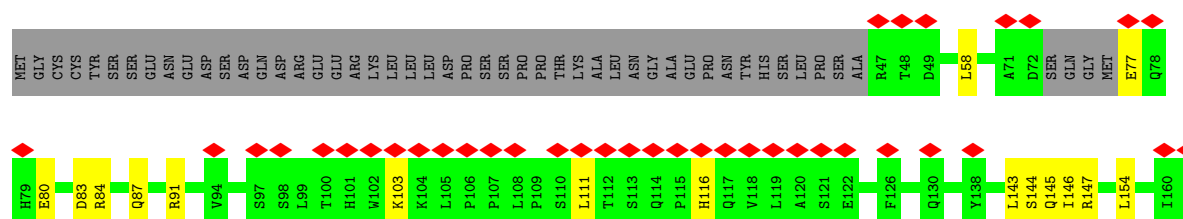
• Molecule 3: Ras-related GTP-binding protein C

Chain J: 5% 61% 8% 31%

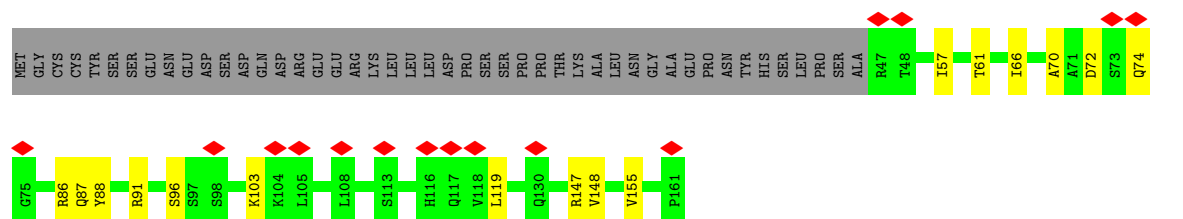




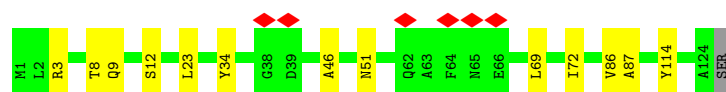
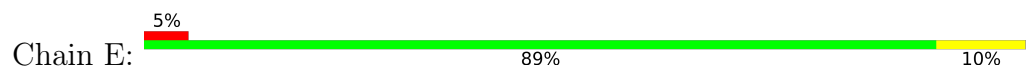
• Molecule 4: Regulator complex protein LAMTOR1



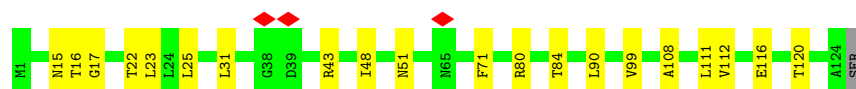
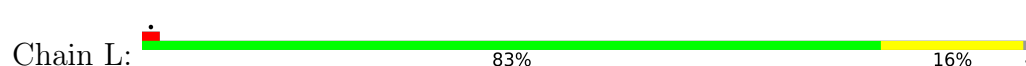
• Molecule 4: Regulator complex protein LAMTOR1




• Molecule 5: Regulator complex protein LAMTOR2

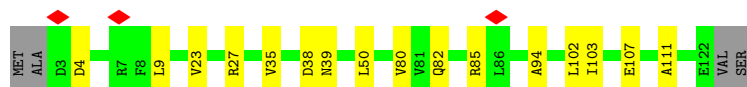


• Molecule 5: Regulator complex protein LAMTOR2




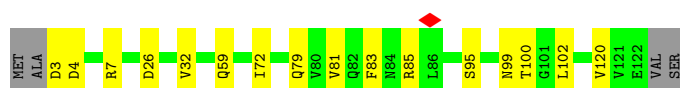
• Molecule 6: Regulator complex protein LAMTOR3

Chain F:  84% 13%



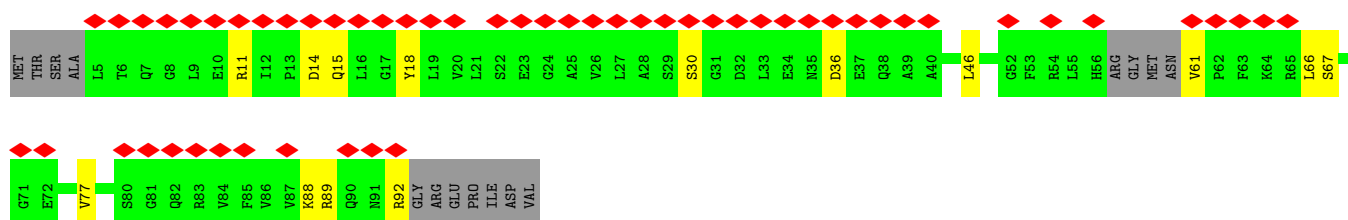
- Molecule 6: Regulator complex protein LAMTOR3

Chain M:  84% 13%




- Molecule 7: Regulator complex protein LAMTOR4

Chain G:  56% 71% 14% 15%




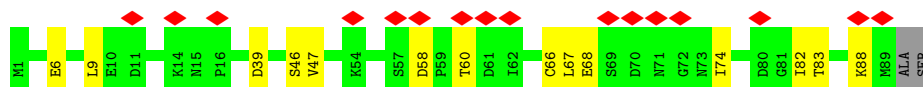
- Molecule 7: Regulator complex protein LAMTOR4

Chain N:  17% 76% 9% 15%




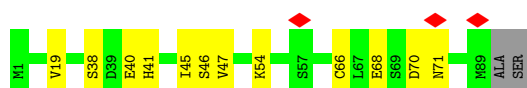
- Molecule 8: Regulator complex protein LAMTOR5

Chain H:  18% 82% 15%



- Molecule 8: Regulator complex protein LAMTOR5

Chain O:  85% 13%



- Molecule 9: Transcription factor EB

Chain P:  6% 20% 78%

MET	GLU	GLU	GLY	ASP	VAL	LEU	PRO	PRO	GLY	GLY	TYR	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	377569	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	79.717	Depositor
Minimum map value	-45.300	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.412	Depositor
Recommended contour level	6.0	Depositor
Map size (\AA)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP, 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	A	0.26	0/9001	0.54	0/12230
2	B	0.28	0/2489	0.56	0/3350
2	I	0.27	0/2489	0.58	0/3350
3	C	0.27	0/2309	0.49	0/3114
3	J	0.27	0/2267	0.52	0/3057
4	D	0.26	0/884	0.54	0/1201
4	K	0.26	0/912	0.56	1/1239 (0.1%)
5	E	0.26	0/949	0.54	0/1285
5	L	0.27	0/949	0.53	0/1285
6	F	0.28	0/951	0.54	0/1290
6	M	0.27	0/951	0.53	0/1290
7	G	0.24	0/649	0.55	0/876
7	N	0.26	0/649	0.56	0/876
8	H	0.28	0/661	0.52	0/896
8	O	0.25	0/661	0.49	0/896
9	P	0.26	0/872	0.50	0/1178
All	All	0.27	0/27643	0.54	1/37413 (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
6	M	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	72	ASP	CB-CG-OD1	5.40	123.16	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	M	85	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8794	8770	8769	58	0
2	B	2444	2438	2438	22	0
2	I	2444	2438	2438	28	0
3	C	2265	2258	2258	27	0
3	J	2226	2221	2220	24	0
4	D	868	870	870	12	0
4	K	895	896	896	12	0
5	E	938	950	950	9	0
5	L	938	950	950	14	0
6	F	934	958	958	12	0
6	M	934	958	958	10	0
7	G	642	652	652	9	0
7	N	642	652	652	8	0
8	H	655	656	656	10	0
8	O	655	656	656	9	0
9	P	853	824	824	7	0
10	B	32	10	12	3	0
10	I	32	10	12	2	0
11	B	1	0	0	0	0
11	I	1	0	0	0	0
12	C	28	10	12	0	0
12	J	28	10	12	0	0
All	All	27249	27187	27193	235	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 (235) 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:I:51:ARG:NH1	2:I:53:LEU:O	2.07	0.88
2:B:58:LEU:HD22	2:B:180:LEU:HD13	1.65	0.79
6:M:4:ASP:OD2	6:M:7:ARG:NH1	2.18	0.77
5:L:15:ASN:OD1	5:L:22:THR:OG1	2.02	0.77
7:G:67:SER:OG	8:H:66:CYS:SG	2.42	0.76
7:N:38:GLN:NE2	8:O:54:LYS:O	2.19	0.75
1:A:1175:ASP:OD2	1:A:1178:ARG:NH1	2.18	0.75
1:A:1209:GLU:OE1	1:A:1237:ARG:NH2	2.22	0.72
1:A:1210:HIS:ND1	1:A:1231:SER:OG	2.21	0.72
1:A:810:GLN:OE1	1:A:813:ARG:NH1	2.22	0.72
2:B:202:GLU:OE1	2:B:227:ARG:NH1	2.23	0.71
4:D:77:GLU:N	4:D:80:GLU:OE2	2.24	0.71
1:A:1283:SER:OG	1:A:1285:GLU:OE1	2.09	0.70
4:D:103:LYS:NZ	6:F:4:ASP:OD2	2.25	0.70
9:P:21:GLN:OE1	9:P:24:ARG:NH2	2.25	0.70
4:D:143:LEU:HD13	4:D:146:ILE:HD12	1.72	0.69
5:L:116:GLU:O	5:L:120:THR:OG1	2.07	0.69
1:A:1132:GLU:OE2	1:A:1135:THR:OG1	2.10	0.68
1:A:325:TRP:O	1:A:330:ARG:NH2	2.26	0.68
7:N:65:ARG:NE	8:O:68:GLU:OE1	2.27	0.68
1:A:788:ARG:O	1:A:794:SER:OG	2.09	0.67
2:B:208:ARG:NH2	2:B:267:THR:O	2.28	0.67
1:A:257:ASP:O	1:A:276:ARG:NH2	2.28	0.66
4:D:87:GLN:OE1	4:D:91:ARG:NH2	2.28	0.66
2:I:132:VAL:HG21	2:I:140:ILE:CD1	2.25	0.66
2:I:78:ARG:NE	2:I:115:GLN:OE1	2.29	0.66
7:N:72:GLU:OE2	7:N:73:HIS:ND1	2.28	0.66
2:B:18:SER:N	10:B:401:GTP:O1B	2.29	0.66
3:C:202:ASP:OD1	4:K:86:ARG:NH1	2.28	0.65
3:J:108:SER:OG	3:J:263:ASP:OD2	2.14	0.65
3:J:251:ILE:HD11	3:J:259:ALA:CB	2.27	0.64
8:H:46:SER:HA	8:H:83:THR:HG21	1.79	0.64
7:G:14:ASP:OD2	7:G:89:ARG:NH2	2.30	0.63
2:I:213:VAL:HG21	2:I:228:PHE:HB3	1.79	0.63
3:J:141:ILE:HD11	3:J:232:VAL:HG11	1.80	0.62
8:O:41:HIS:O	8:O:45:ILE:HD12	1.99	0.62
1:A:558:LEU:HD21	1:A:580:CYS:SG	2.39	0.62
1:A:558:LEU:HD23	1:A:584:ILE:HD12	1.82	0.62
5:L:16:THR:HG22	5:L:17:GLY:H	1.65	0.62
7:G:14:ASP:OD1	7:G:15:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:258:LYS:NZ	3:J:273:ASP:OD1	2.31	0.61
3:J:246:LEU:CD2	4:K:61:THR:HG21	2.32	0.60
6:M:102:LEU:HD22	8:O:47:VAL:HG11	1.82	0.60
1:A:267:LEU:O	1:A:349:ASN:ND2	2.34	0.59
3:J:251:ILE:HD11	3:J:259:ALA:HB2	1.84	0.59
5:E:86:VAL:HG12	5:E:87:ALA:H	1.68	0.59
1:A:437:LEU:HD11	1:A:470:VAL:HG22	1.85	0.58
1:A:1016:GLN:NE2	1:A:1018:PHE:O	2.37	0.58
1:A:547:HIS:NE2	1:A:551:GLU:OE2	2.37	0.58
3:C:205:ASP:OD2	4:K:86:ARG:NH2	2.37	0.57
7:N:16:LEU:O	7:N:32:ASP:N	2.38	0.57
2:B:224:ASP:O	2:B:227:ARG:NE	2.38	0.57
6:F:102:LEU:CD1	8:H:47:VAL:HG11	2.36	0.56
1:A:331:ASP:OD1	1:A:332:LEU:N	2.38	0.56
7:N:15:GLN:N	7:N:15:GLN:OE1	2.38	0.56
6:F:85:ARG:NH2	6:F:107:GLU:OE2	2.38	0.55
2:I:248:SER:N	3:J:321:ASN:OD1	2.38	0.55
6:F:38:ASP:OD1	6:F:39:ASN:N	2.40	0.55
8:H:67:LEU:HD12	8:H:74:ILE:HD11	1.89	0.55
4:D:145:GLN:N	4:D:145:GLN:OE1	2.40	0.54
1:A:1071:THR:OG1	1:A:1089:ASP:OD1	2.25	0.54
5:E:69:LEU:HD21	5:E:72:ILE:HD11	1.90	0.54
3:C:192:GLN:HB2	3:C:217:LEU:HD21	1.89	0.54
4:K:87:GLN:OE1	4:K:91:ARG:NH2	2.41	0.53
4:K:96:SER:OG	4:K:103:LYS:NZ	2.37	0.53
1:A:1251:GLN:NE2	1:A:1252:ILE:O	2.41	0.53
9:P:99:THR:HG22	9:P:100:TYR:CD1	2.43	0.53
5:L:84:THR:HG21	5:L:112:VAL:HG21	1.91	0.53
4:D:144:SER:OG	4:D:145:GLN:OE1	2.21	0.53
9:P:27:GLN:HA	9:P:30:VAL:HG12	1.91	0.53
2:I:32:ILE:CD1	2:I:240:LEU:HD13	2.38	0.53
7:G:18:TYR:O	7:G:30:SER:OG	2.16	0.53
3:J:263:ASP:O	3:J:267:LYS:N	2.40	0.53
2:B:19:GLY:HA2	10:B:401:GTP:H5'	1.90	0.53
3:C:64:ILE:HD12	3:C:110:VAL:HG21	1.91	0.53
4:K:119:LEU:O	7:N:65:ARG:NH1	2.42	0.53
2:B:197:ILE:O	5:E:3:ARG:NH2	2.42	0.53
5:L:25:LEU:O	5:L:90:LEU:N	2.41	0.52
3:C:348:ARG:NH2	5:E:51:ASN:OD1	2.42	0.52
1:A:301:ARG:NH2	1:A:304:ASP:OD1	2.43	0.52
1:A:458:ASP:OD1	1:A:497:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:99:THR:HG22	9:P:100:TYR:CE1	2.44	0.52
3:J:251:ILE:HD11	3:J:259:ALA:HB3	1.93	0.51
6:M:79:GLN:NE2	6:M:95:SER:O	2.42	0.51
6:M:99:ASN:ND2	8:O:46:SER:OG	2.40	0.51
2:B:238:PHE:CE2	3:C:318:ILE:HG21	2.45	0.51
1:A:191:ILE:HD11	1:A:343:VAL:HG22	1.93	0.51
1:A:304:ASP:O	1:A:306:ARG:NH1	2.44	0.51
6:F:94:ALA:CB	6:F:103:ILE:HD11	2.42	0.50
5:L:80:ARG:NH1	5:L:99:VAL:O	2.43	0.50
2:B:267:THR:HG22	2:B:268:SER:H	1.77	0.50
1:A:522:LEU:O	1:A:565:GLN:NE2	2.45	0.50
4:D:154:LEU:HD11	5:E:114:TYR:HE1	1.77	0.50
3:J:290:ASP:OD2	9:P:8:ARG:NH2	2.45	0.50
5:L:71:PHE:HD1	5:L:84:THR:HG1	1.59	0.50
1:A:1190:ILE:HD11	1:A:1214:VAL:HG21	1.94	0.49
6:F:9:LEU:HD23	6:F:35:VAL:HG21	1.95	0.49
4:K:88:TYR:OH	6:M:26:ASP:OD2	2.29	0.49
1:A:796:LEU:HD12	1:A:796:LEU:O	2.13	0.49
2:B:17:GLY:O	2:B:128:LYS:NZ	2.41	0.48
8:H:39:ASP:OD2	8:H:39:ASP:N	2.46	0.48
8:O:38:SER:OG	8:O:40:GLU:OE2	2.30	0.48
2:B:94:VAL:O	2:B:144:ARG:NH2	2.47	0.48
5:E:23:LEU:CD2	5:E:46:ALA:HB2	2.44	0.48
1:A:667:LEU:O	1:A:671:VAL:HG23	2.13	0.48
2:I:37:ARG:NH2	9:P:19:GLU:OE2	2.46	0.48
2:I:135:ASP:N	2:I:135:ASP:OD1	2.46	0.48
5:L:51:ASN:ND2	6:M:59:GLN:OE1	2.47	0.48
1:A:592:ARG:NH2	1:A:641:ASP:OD1	2.47	0.47
4:K:148:VAL:HG11	5:L:111:LEU:HD23	1.95	0.47
6:M:81:VAL:HG12	6:M:83:PHE:CE1	2.49	0.47
1:A:1219:LEU:HD13	1:A:1227:ILE:HG13	1.94	0.47
1:A:1064:ASN:ND2	1:A:1068:THR:O	2.47	0.47
7:G:36:ASP:OD1	7:G:36:ASP:N	2.45	0.47
7:G:66:LEU:HD23	7:G:77:VAL:CG2	2.44	0.47
2:I:234:ILE:CG2	3:J:291:VAL:HG23	2.44	0.47
1:A:164:VAL:O	1:A:177:LEU:N	2.47	0.47
1:A:635:ASP:OD1	1:A:636:HIS:N	2.48	0.47
2:B:95:GLU:O	2:B:97:ARG:NH1	2.48	0.47
2:I:210:THR:HG22	2:I:212:LEU:HG	1.96	0.47
3:C:296:SER:O	3:C:300:GLY:N	2.44	0.47
1:A:1170:THR:OG1	1:A:1214:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:LEU:HD21	2:B:58:LEU:HD21	1.97	0.46
1:A:667:LEU:HD22	1:A:811:ILE:HD12	1.97	0.46
3:C:327:TYR:OH	3:C:353:ASP:OD1	2.25	0.46
2:I:147:ASP:OD1	2:I:148:LEU:N	2.48	0.46
2:I:32:ILE:HD12	2:I:240:LEU:HD13	1.95	0.46
5:L:16:THR:HG22	5:L:17:GLY:N	2.31	0.46
1:A:1050:ASP:O	1:A:1054:GLY:N	2.48	0.46
1:A:138:ARG:NH2	1:A:141:ALA:O	2.45	0.46
4:D:83:ASP:OD1	4:D:84:ARG:N	2.48	0.46
7:N:67:SER:O	8:O:66:CYS:N	2.47	0.46
1:A:1320:SER:OG	1:A:1322:ASP:OD1	2.19	0.46
3:C:263:ASP:O	3:C:267:LYS:N	2.47	0.46
8:H:68:GLU:N	8:H:68:GLU:OE1	2.49	0.46
6:F:102:LEU:HD12	8:H:47:VAL:HG11	1.97	0.46
6:M:72:ILE:HD13	6:M:100:THR:HG21	1.97	0.46
3:J:296:SER:O	3:J:300:GLY:N	2.45	0.46
2:B:258:ASN:ND2	3:C:300:GLY:O	2.49	0.46
2:I:252:MET:HE1	3:J:291:VAL:HG21	1.98	0.45
2:B:255:ARG:NH2	2:B:283:SER:OG	2.46	0.45
3:C:64:ILE:HD11	3:C:233:VAL:HG22	1.98	0.45
3:C:228:ALA:O	3:C:232:VAL:HG23	2.16	0.45
2:I:67:ASP:O	2:I:70:MET:N	2.49	0.45
3:C:108:SER:OG	3:C:263:ASP:OD2	2.33	0.45
2:I:255:ARG:NH2	2:I:283:SER:OG	2.49	0.45
3:C:137:THR:HG23	3:C:171:MET:SD	2.56	0.45
3:J:257:GLU:OE2	3:J:342:ARG:NE	2.50	0.45
5:E:9:GLN:O	5:E:12:SER:OG	2.23	0.45
3:J:107:SER:O	3:J:107:SER:OG	2.35	0.45
4:D:143:LEU:HG	8:H:82:ILE:HD11	1.97	0.45
8:O:70:ASP:OD1	8:O:71:ASN:N	2.49	0.45
1:A:652:VAL:HG11	1:A:796:LEU:HD21	2.00	0.44
9:P:70:LEU:O	9:P:70:LEU:HD23	2.18	0.44
1:A:1237:ARG:HH12	1:A:1249:VAL:HG22	1.82	0.44
4:K:57:ILE:O	4:K:61:THR:HG22	2.17	0.44
2:B:88:LEU:HD22	2:B:113:ILE:HG13	1.99	0.44
2:I:87:VAL:HG21	2:I:180:LEU:HD11	2.00	0.44
2:I:234:ILE:HG22	3:J:291:VAL:HG23	2.00	0.44
2:B:202:GLU:OE2	3:C:299:TYR:OH	2.27	0.44
3:C:284:LEU:CD2	3:C:326:LEU:HD21	2.48	0.44
6:F:23:VAL:HG11	6:F:50:LEU:HD13	2.00	0.44
3:C:315:MET:SD	3:C:316:ALA:N	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:70:ALA:O	4:K:74:GLN:NE2	2.50	0.44
3:C:273:ASP:OD1	3:C:273:ASP:N	2.49	0.43
3:J:178:HIS:CE1	3:J:220:ILE:HG23	2.53	0.43
1:A:199:ALA:CB	1:A:244:ALA:HB1	2.49	0.43
3:C:284:LEU:HD23	3:C:326:LEU:HD21	1.99	0.43
2:I:15:LYS:O	2:I:20:LYS:NZ	2.52	0.43
3:C:249:ILE:HD12	4:D:58:LEU:HD11	2.00	0.43
1:A:394:PRO:HA	1:A:397:ILE:HG22	1.99	0.43
5:E:86:VAL:HG12	5:E:87:ALA:N	2.31	0.43
6:M:32:VAL:HG13	6:M:120:VAL:HG11	2.00	0.43
1:A:610:ASP:OD2	1:A:615:VAL:HG11	2.19	0.43
4:D:116:HIS:O	7:G:11:ARG:NH2	2.51	0.43
8:H:58:ASP:OD2	8:H:60:THR:OG1	2.27	0.43
2:I:88:LEU:HD22	2:I:113:ILE:HG13	2.00	0.43
2:I:264:ASP:OD1	2:I:265:ILE:N	2.52	0.43
3:J:77:ILE:O	3:J:81:VAL:HG22	2.18	0.43
1:A:778:ILE:HD12	1:A:778:ILE:H	1.83	0.43
1:A:437:LEU:CD1	1:A:470:VAL:HG22	2.48	0.43
2:B:234:ILE:CG2	3:C:291:VAL:HG23	2.49	0.43
1:A:328:LEU:HD21	1:A:370:LEU:HD22	2.01	0.43
1:A:1174:CYS:SG	1:A:1181:ILE:HG23	2.59	0.43
2:I:18:SER:N	10:I:401:GTP:O1B	2.52	0.43
1:A:439:VAL:HG22	1:A:445:HIS:HB2	1.99	0.43
6:F:23:VAL:HG11	6:F:50:LEU:CD1	2.49	0.43
3:J:230:SER:HA	3:J:268:ILE:HG23	2.01	0.43
8:H:6:GLU:O	8:H:9:LEU:N	2.52	0.42
4:K:155:VAL:HG22	4:K:155:VAL:O	2.19	0.42
2:I:258:ASN:ND2	3:J:300:GLY:O	2.48	0.42
5:L:108:ALA:O	5:L:112:VAL:HG23	2.19	0.42
7:N:36:ASP:OD1	7:N:36:ASP:N	2.52	0.42
6:F:80:VAL:HG12	6:F:82:GLN:HG3	2.01	0.42
1:A:147:LEU:HD11	1:A:346:LEU:HD11	2.01	0.42
1:A:191:ILE:HD11	1:A:343:VAL:CG2	2.50	0.42
4:D:111:LEU:HD13	7:G:61:VAL:HG21	2.02	0.42
5:L:23:LEU:HD12	5:L:31:LEU:HD22	2.02	0.42
2:B:92:PHE:CZ	2:B:148:LEU:HD21	2.54	0.42
3:C:164:ALA:HB1	3:C:171:MET:CE	2.50	0.42
3:J:288:MET:HG3	3:J:318:ILE:HD12	2.01	0.42
3:C:331:VAL:O	3:C:364:HIS:NE2	2.51	0.42
1:A:412:GLN:CB	1:A:435:ILE:HG21	2.50	0.41
1:A:1187:ASP:OD1	1:A:1188:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:ARG:NH2	1:A:1166:ASP:OD1	2.52	0.41
3:J:191:THR:O	3:J:195:ILE:HD12	2.19	0.41
2:I:283:SER:O	2:I:287:LEU:HD23	2.20	0.41
3:J:81:VAL:HG23	3:J:82:PHE:CD2	2.55	0.41
2:B:149:ARG:NH1	2:B:157:CYS:O	2.54	0.41
3:C:137:THR:O	3:C:168:ASN:ND2	2.53	0.41
3:C:174:GLU:HG3	3:C:232:VAL:HG13	2.01	0.41
6:F:27:ARG:NH1	6:F:85:ARG:O	2.50	0.41
2:I:74:PHE:O	2:I:78:ARG:NH1	2.48	0.41
1:A:114:GLN:HG3	1:A:117:ALA:HB2	2.02	0.41
1:A:564:GLU:OE2	2:B:51:ARG:NH1	2.49	0.41
3:C:131:GLU:OE2	3:C:135:ARG:NH1	2.50	0.41
5:L:31:LEU:HD12	5:L:43:ARG:NH1	2.34	0.41
6:M:3:ASP:N	6:M:3:ASP:OD1	2.52	0.41
2:I:19:GLY:HA2	10:I:401:GTP:H5'	2.03	0.41
8:O:19:VAL:O	8:O:19:VAL:HG13	2.20	0.41
1:A:88:ILE:HD13	1:A:101:THR:HG22	2.03	0.41
2:B:19:GLY:N	10:B:401:GTP:O1B	2.50	0.41
2:I:167:GLU:OE1	2:I:167:GLU:N	2.47	0.41
1:A:319:ILE:HD13	1:A:382:TRP:HB2	2.02	0.41
3:C:248:ASN:OD1	3:C:274:SER:N	2.47	0.41
3:J:234:GLN:CG	3:J:240:LEU:HD11	2.51	0.41
4:K:66:ILE:CD1	5:L:48:ILE:HD12	2.51	0.41
1:A:26:LEU:O	1:A:1079:GLN:NE2	2.54	0.40
7:G:46:LEU:HD22	7:G:66:LEU:HD21	2.03	0.40
2:I:122:ILE:HD13	2:I:155:LEU:HG	2.02	0.40
1:A:1090:ASP:O	1:A:1113:GLN:NE2	2.53	0.40
5:E:8:THR:HG23	5:E:34:TYR:O	2.22	0.40
2:I:25:SER:HB3	2:I:31:TYR:CD2	2.56	0.40
1:A:1069:ARG:NH1	1:A:1089:ASP:OD1	2.54	0.40
6:F:107:GLU:O	6:F:111:ALA:N	2.54	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	1087/1335 (81%)	1044 (96%)	43 (4%)	0	100	100
2	B	296/313 (95%)	281 (95%)	15 (5%)	0	100	100
2	I	296/313 (95%)	280 (95%)	16 (5%)	0	100	100
3	C	275/399 (69%)	264 (96%)	11 (4%)	0	100	100
3	J	271/399 (68%)	254 (94%)	17 (6%)	0	100	100
4	D	107/161 (66%)	104 (97%)	3 (3%)	0	100	100
4	K	113/161 (70%)	106 (94%)	7 (6%)	0	100	100
5	E	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
5	L	122/125 (98%)	115 (94%)	7 (6%)	0	100	100
6	F	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
6	M	118/124 (95%)	115 (98%)	3 (2%)	0	100	100
7	G	80/99 (81%)	76 (95%)	4 (5%)	0	100	100
7	N	80/99 (81%)	68 (85%)	12 (15%)	0	100	100
8	H	87/91 (96%)	83 (95%)	4 (5%)	0	100	100
8	O	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
9	P	102/476 (21%)	92 (90%)	10 (10%)	0	100	100
All	All	3361/4435 (76%)	3190 (95%)	171 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	972/1163 (84%)	968 (100%)	4 (0%)	91	97
2	B	271/287 (94%)	270 (100%)	1 (0%)	91	97
2	I	271/287 (94%)	271 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	255/340 (75%)	254 (100%)	1 (0%)	91	97
3	J	251/340 (74%)	250 (100%)	1 (0%)	91	97
4	D	97/141 (69%)	96 (99%)	1 (1%)	76	92
4	K	100/141 (71%)	99 (99%)	1 (1%)	76	92
5	E	97/98 (99%)	97 (100%)	0	100	100
5	L	97/98 (99%)	97 (100%)	0	100	100
6	F	105/108 (97%)	105 (100%)	0	100	100
6	M	105/108 (97%)	105 (100%)	0	100	100
7	G	71/83 (86%)	69 (97%)	2 (3%)	43	76
7	N	71/83 (86%)	71 (100%)	0	100	100
8	H	76/77 (99%)	75 (99%)	1 (1%)	69	90
8	O	76/77 (99%)	76 (100%)	0	100	100
9	P	94/419 (22%)	94 (100%)	0	100	100
All	All	3009/3850 (78%)	2997 (100%)	12 (0%)	91	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	83	ARG
1	A	1123	ARG
1	A	1178	ARG
2	B	295	LYS
3	C	63	ARG
4	D	147	ARG
7	G	88	LYS
7	G	92	ARG
8	H	88	LYS
3	J	210	LYS
4	K	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1016	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
10	GTP	B	401	11	26,34,34	1.16	2 (7%)	32,54,54	1.60	6 (18%)
10	GTP	I	401	11	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
12	GDP	C	401	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
12	GDP	J	401	-	24,30,30	0.93	1 (4%)	30,47,47	1.27	4 (13%)

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
10	GTP	B	401	11	-	3/18/38/38	0/3/3/3
10	GTP	I	401	11	-	5/18/38/38	0/3/3/3
12	GDP	C	401	-	-	5/12/32/32	0/3/3/3
12	GDP	J	401	-	-	5/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	401	GTP	C5-C6	-4.18	1.38	1.47
10	I	401	GTP	C5-C6	-4.07	1.39	1.47
12	C	401	GDP	C6-N1	-2.46	1.34	1.37
12	J	401	GDP	C6-N1	-2.46	1.34	1.37
10	B	401	GTP	C2-N3	2.15	1.38	1.33
10	I	401	GTP	C2-N3	2.10	1.38	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	401	GDP	PA-O3A-PB	-3.78	119.85	132.83
10	B	401	GTP	PB-O3B-PG	-3.76	119.93	132.83
10	I	401	GTP	PB-O3B-PG	-3.68	120.21	132.83
10	I	401	GTP	C5-C6-N1	3.45	120.05	113.95
10	B	401	GTP	C5-C6-N1	3.31	119.79	113.95
10	B	401	GTP	C8-N7-C5	3.23	109.14	102.99
10	I	401	GTP	C2-N1-C6	-3.15	119.29	125.10
12	J	401	GDP	PA-O3A-PB	-3.09	122.22	132.83
10	B	401	GTP	C2-N1-C6	-3.00	119.57	125.10
10	I	401	GTP	C8-N7-C5	2.99	108.69	102.99
10	B	401	GTP	C3'-C2'-C1'	2.96	105.43	100.98
12	J	401	GDP	C3'-C2'-C1'	2.92	105.38	100.98
12	C	401	GDP	C3'-C2'-C1'	2.85	105.27	100.98
10	I	401	GTP	C3'-C2'-C1'	2.79	105.17	100.98
10	I	401	GTP	PA-O3A-PB	-2.76	123.34	132.83
12	C	401	GDP	C5-C6-N1	2.54	118.44	113.95
12	J	401	GDP	C8-N7-C5	2.53	107.81	102.99
12	J	401	GDP	C5-C6-N1	2.47	118.31	113.95
12	C	401	GDP	C8-N7-C5	2.46	107.68	102.99
10	I	401	GTP	O6-C6-C5	-2.13	120.22	124.37
10	B	401	GTP	O6-C6-C5	-2.08	120.31	124.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	401	GDP	C5'-O5'-PA-O1A
12	C	401	GDP	C5'-O5'-PA-O2A
12	J	401	GDP	PA-O3A-PB-O3B
12	J	401	GDP	C5'-O5'-PA-O1A
12	J	401	GDP	C5'-O5'-PA-O2A

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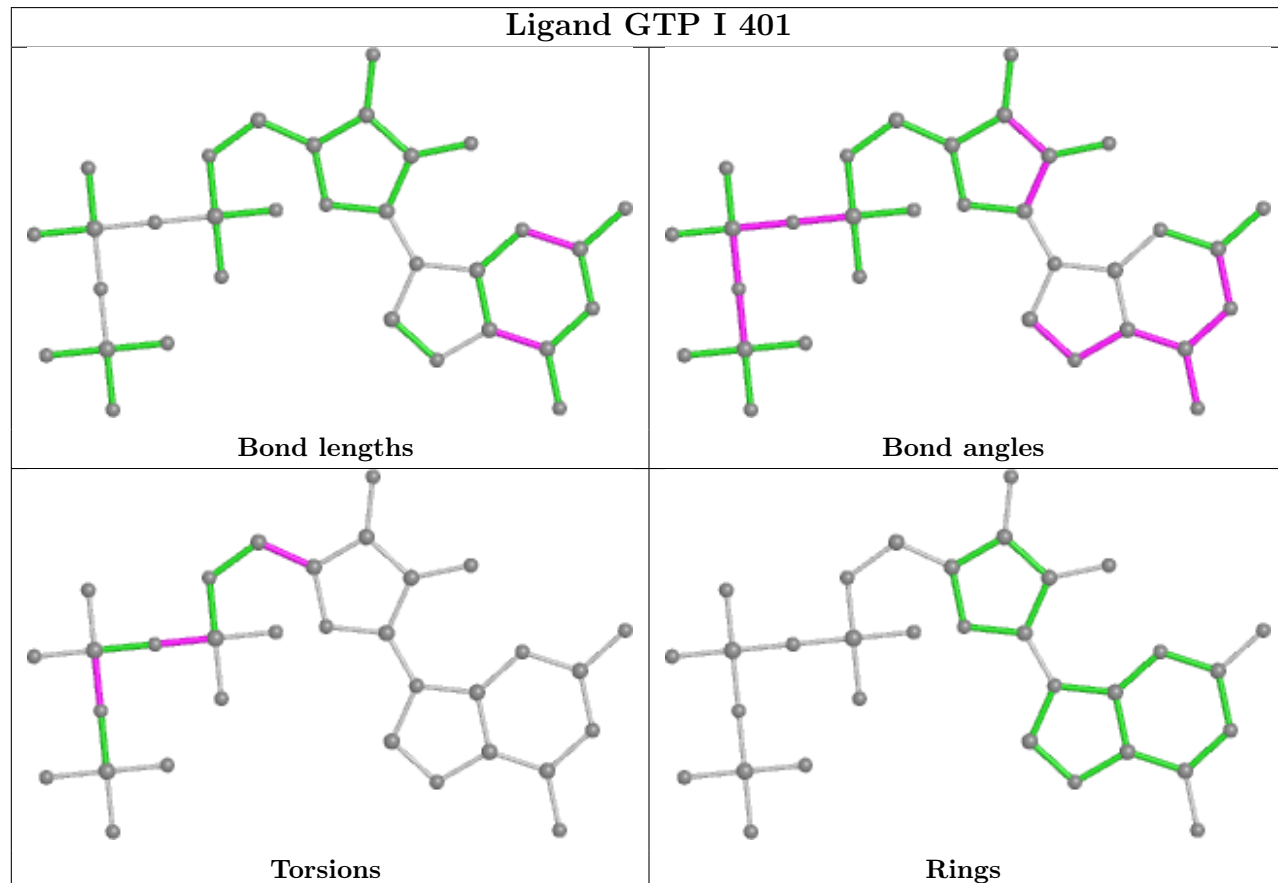
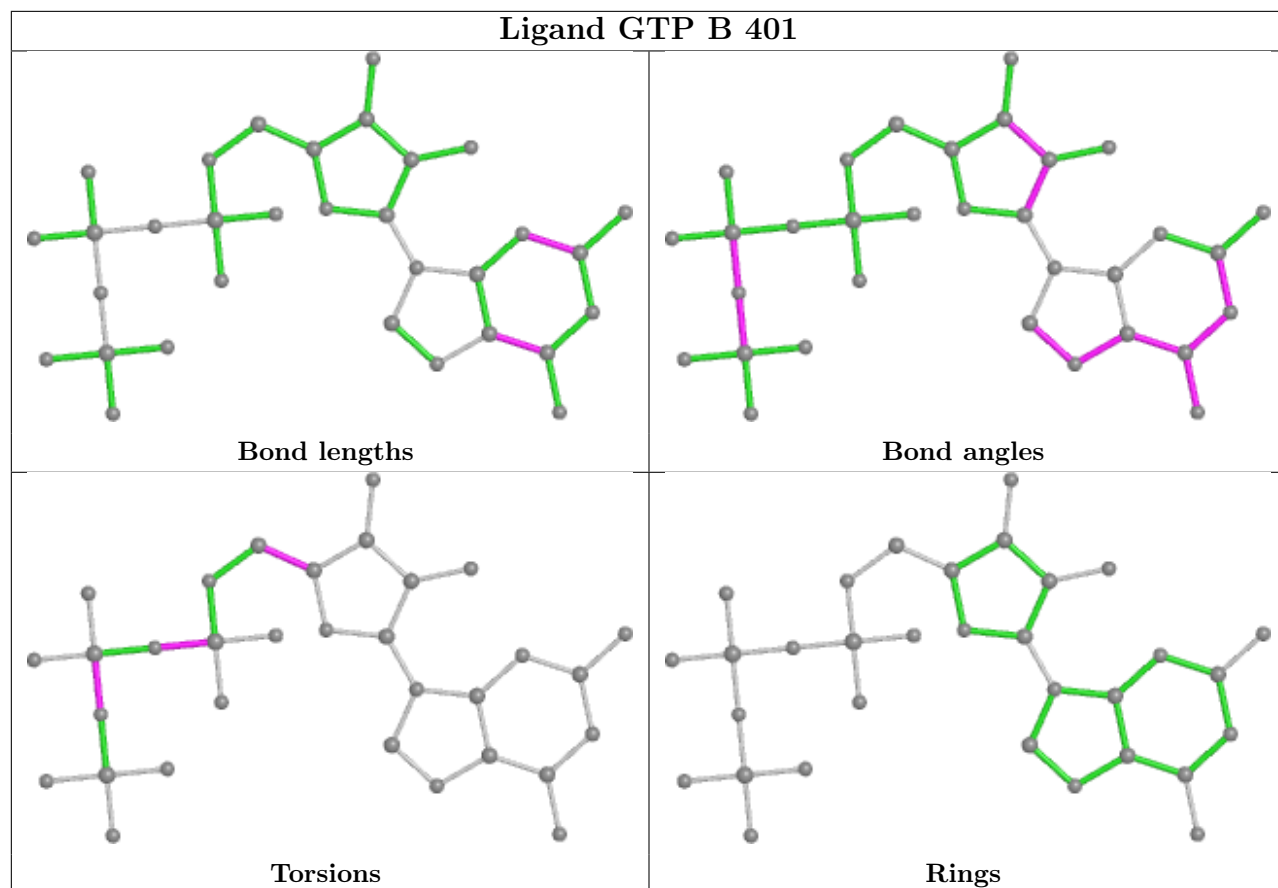
Mol	Chain	Res	Type	Atoms
12	C	401	GDP	O4'-C4'-C5'-O5'
12	C	401	GDP	C3'-C4'-C5'-O5'
10	B	401	GTP	PB-O3A-PA-O5'
10	I	401	GTP	PB-O3A-PA-O5'
12	C	401	GDP	C5'-O5'-PA-O3A
10	I	401	GTP	O4'-C4'-C5'-O5'
10	I	401	GTP	PB-O3A-PA-O1A
10	B	401	GTP	PG-O3B-PB-O2B
10	I	401	GTP	PG-O3B-PB-O1B
12	J	401	GDP	C5'-O5'-PA-O3A
12	J	401	GDP	PB-O3A-PA-O2A
10	B	401	GTP	O4'-C4'-C5'-O5'
10	I	401	GTP	C3'-C4'-C5'-O5'

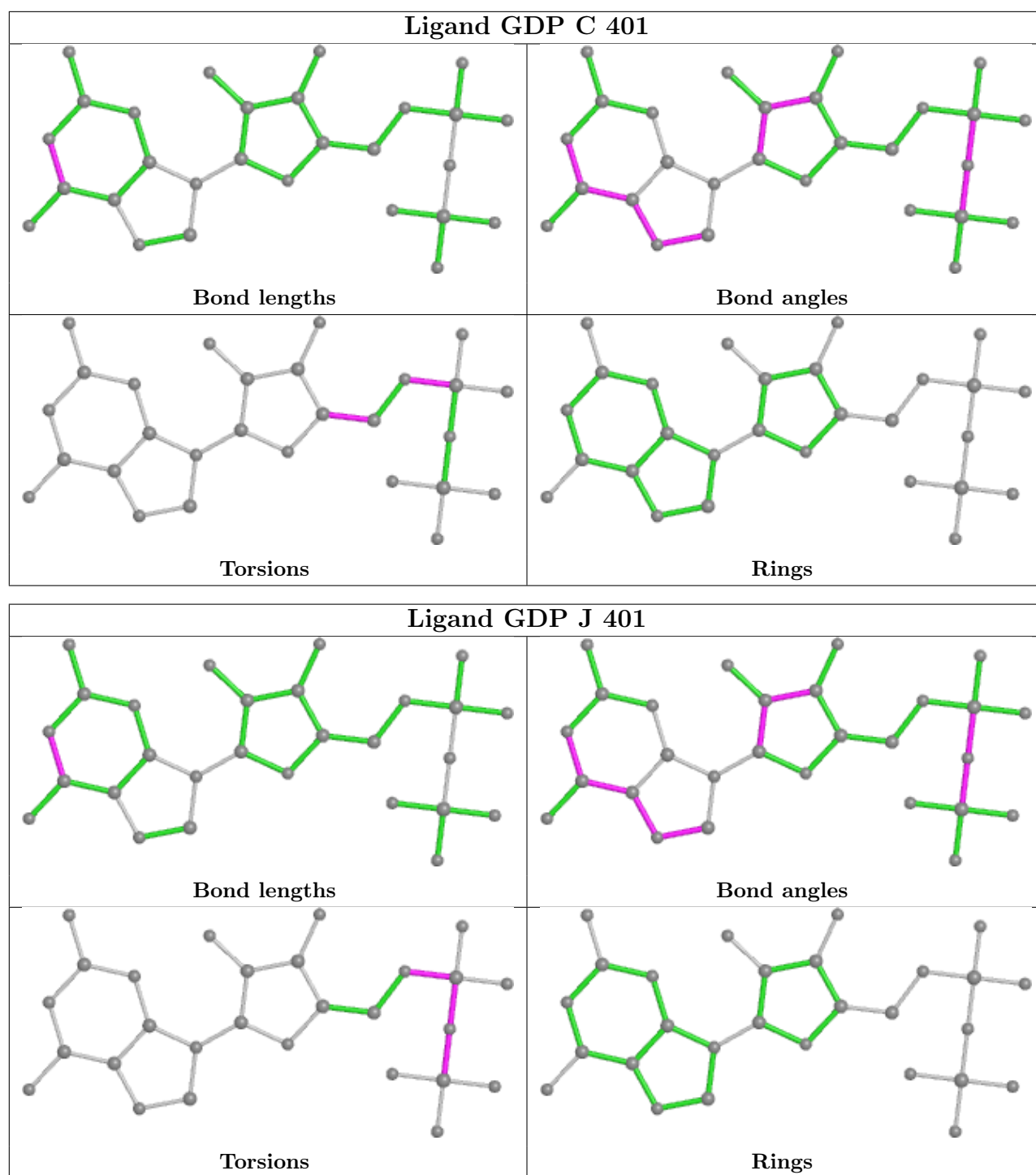
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	401	GTP	3	0
10	I	401	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.

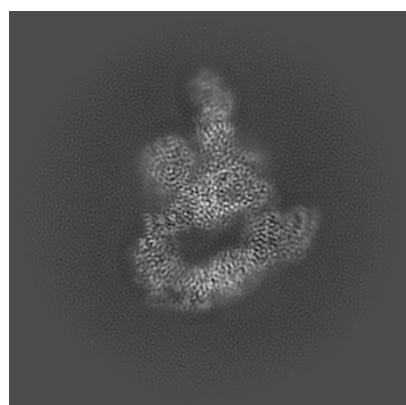
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26846. These allow visual inspection of the internal detail of the map and identification of artifacts.

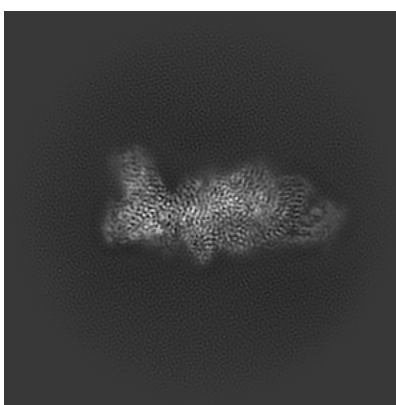
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

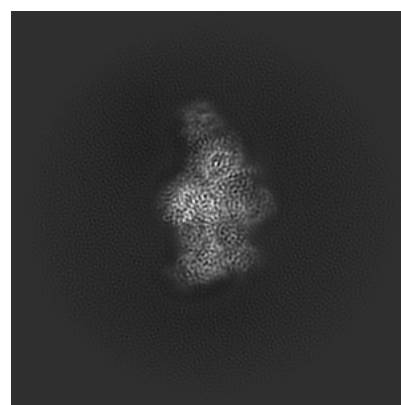
6.1.1 Primary map



X



Y

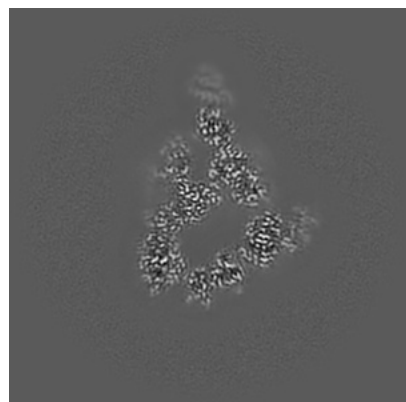


Z

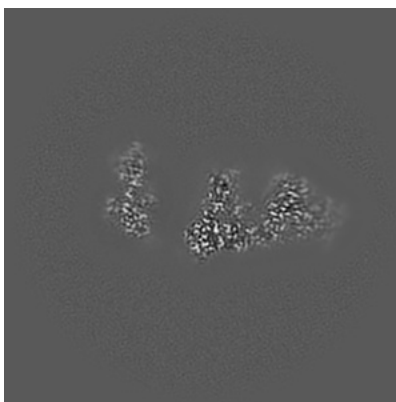
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

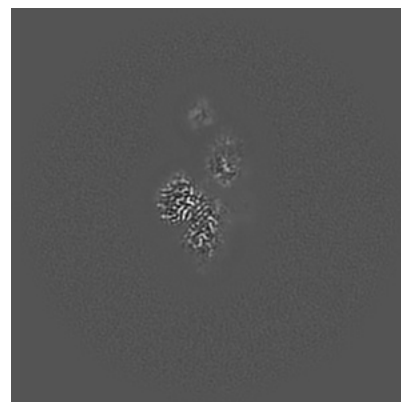
6.2.1 Primary map



X Index: 160



Y Index: 160

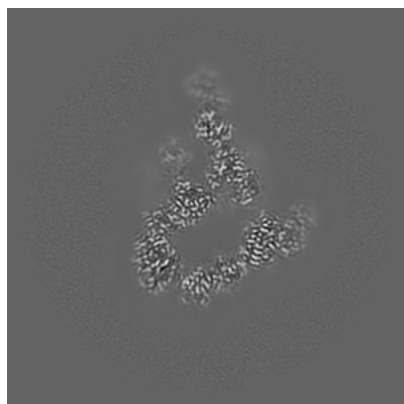


Z Index: 160

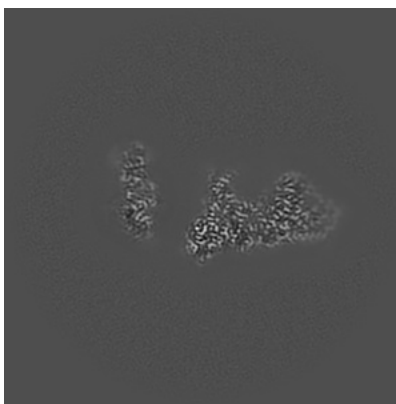
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

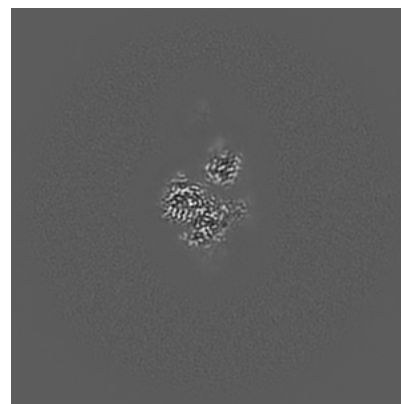
6.3.1 Primary map



X Index: 157



Y Index: 164



Z Index: 165

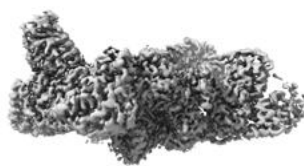
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

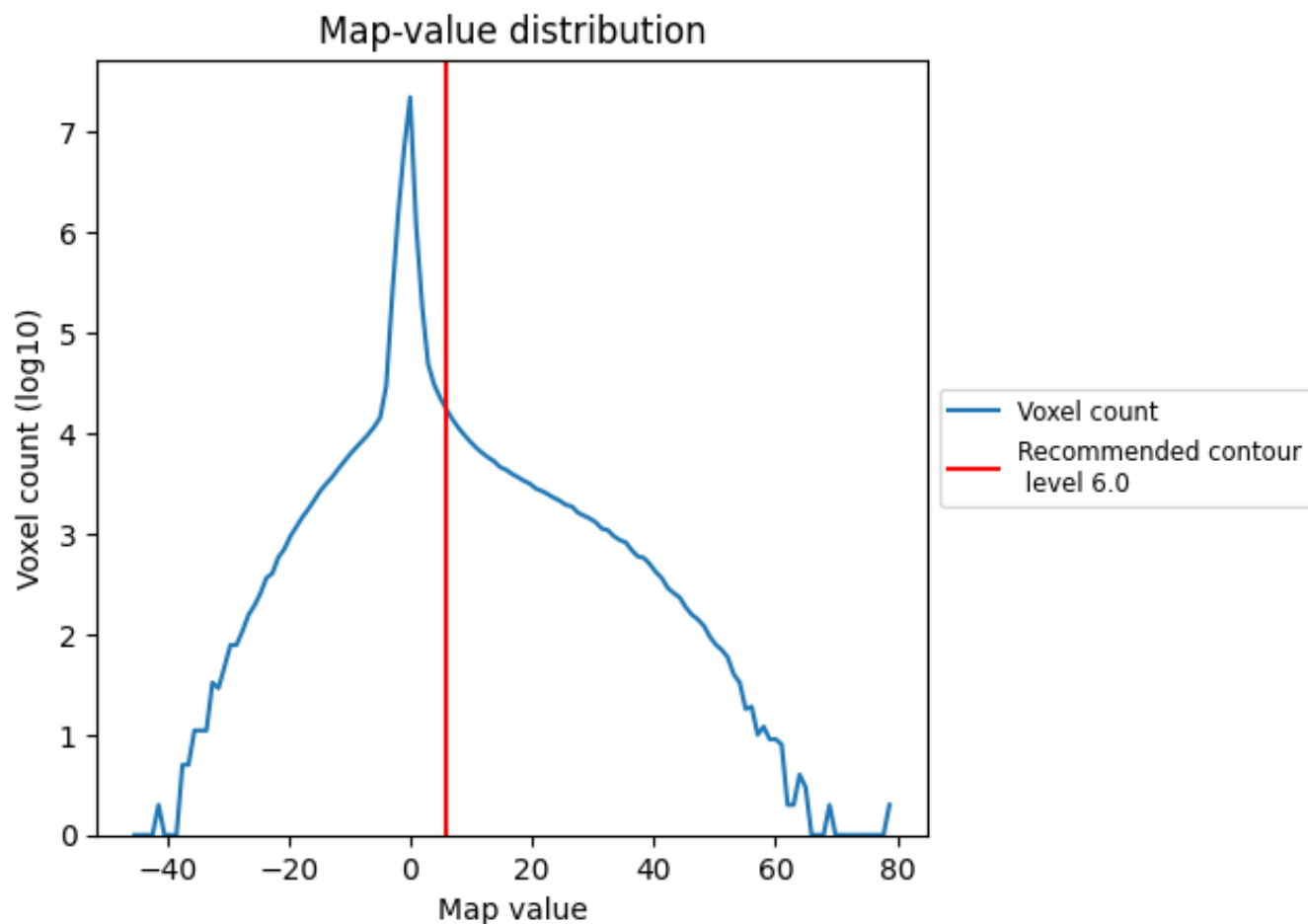
6.5 Mask visualisation

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

7 Map analysis [i](#)

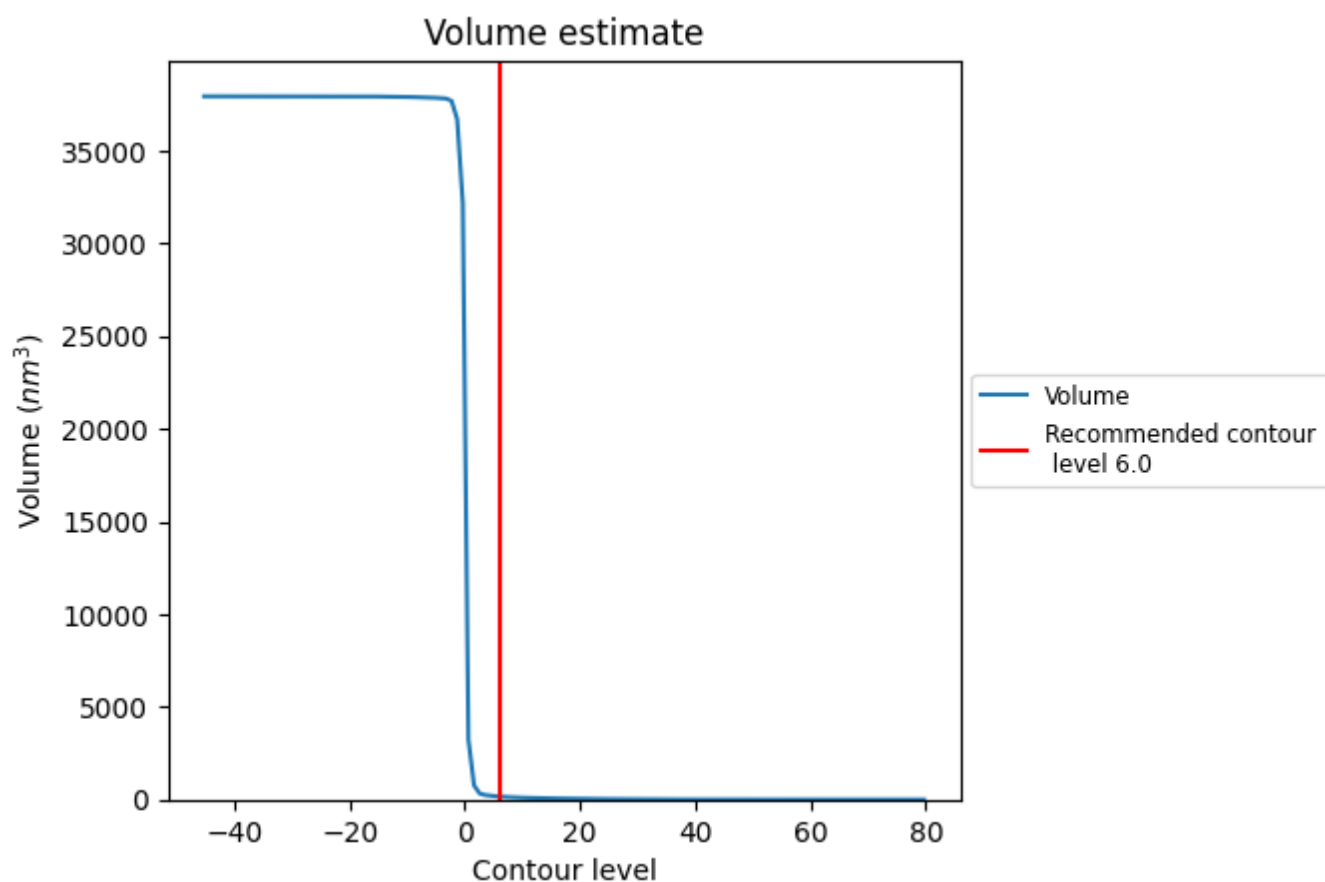
This section contains the results of statistical analysis of the map.

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.

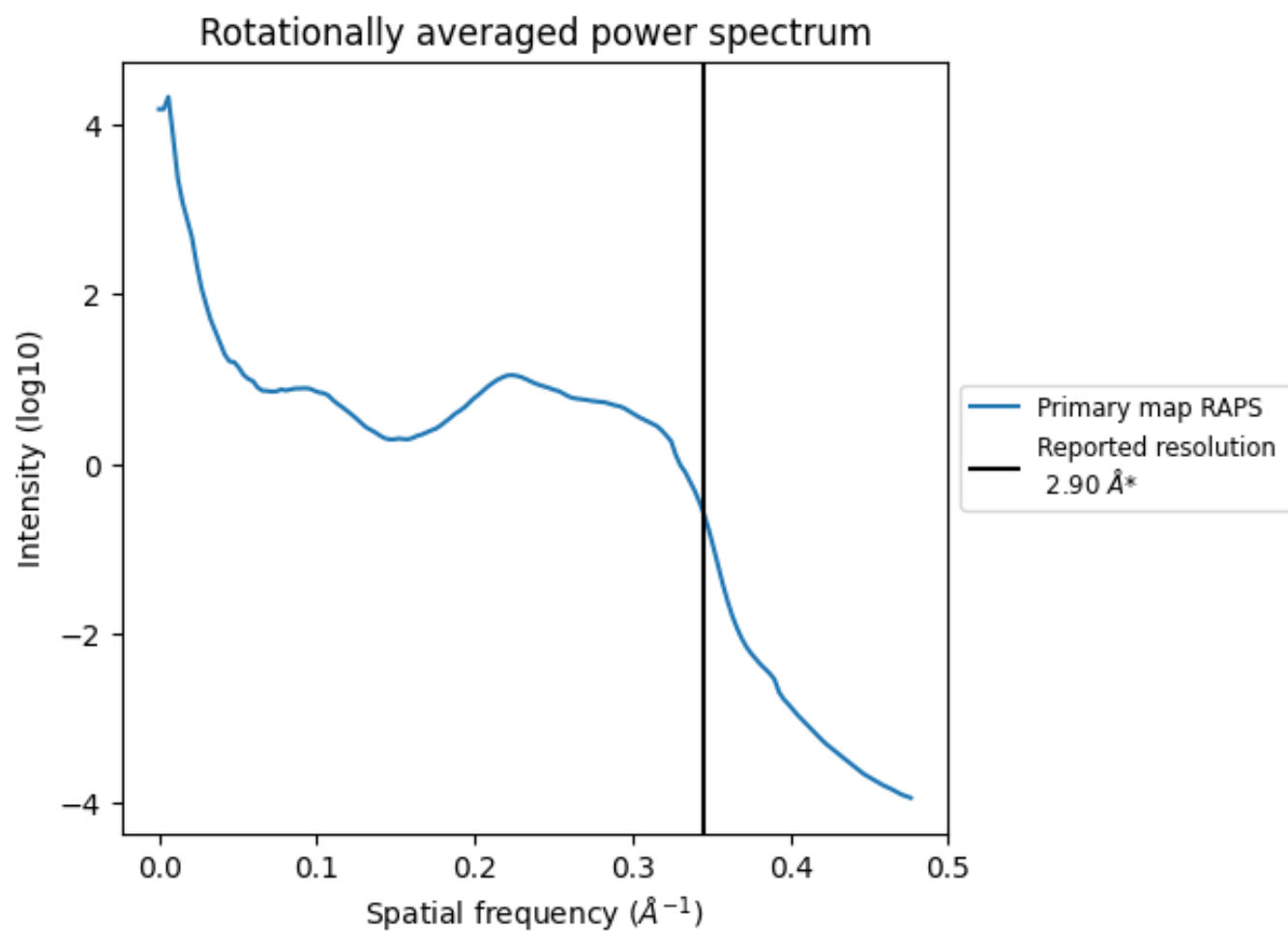
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm^3 ; this corresponds to an approximate mass of 146 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 0.345 Å⁻¹

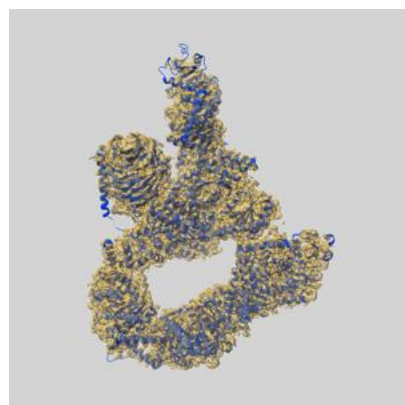
8 Fourier-Shell correlation

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

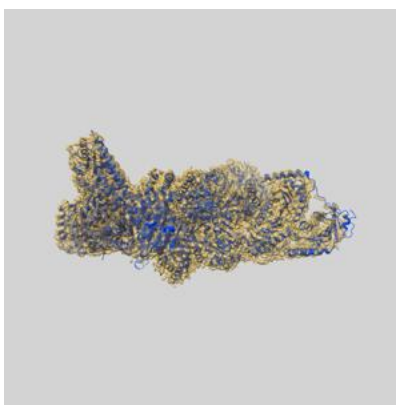
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26846 and PDB model 7UX2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

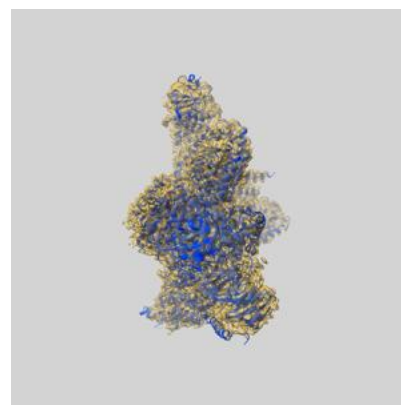
9.1 Map-model overlay [i](#)



X



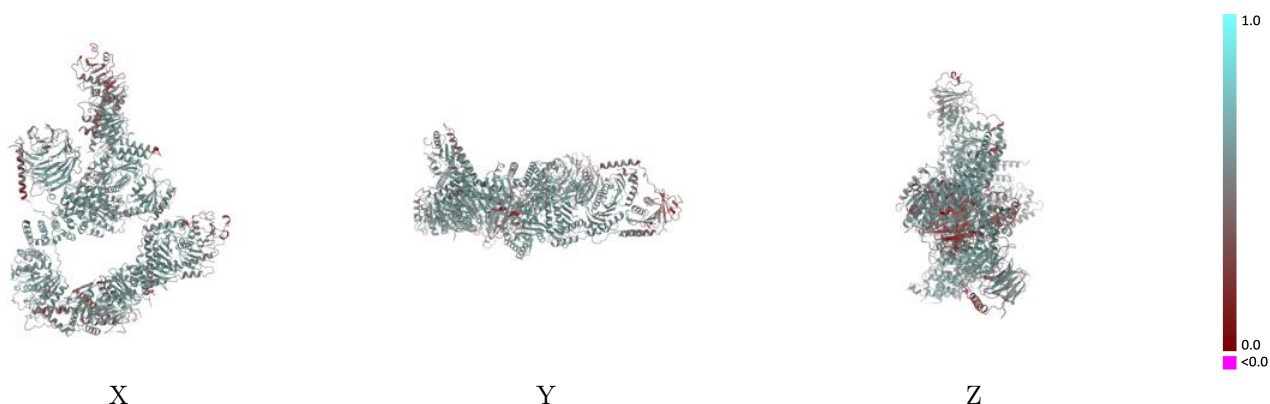
Y



Z

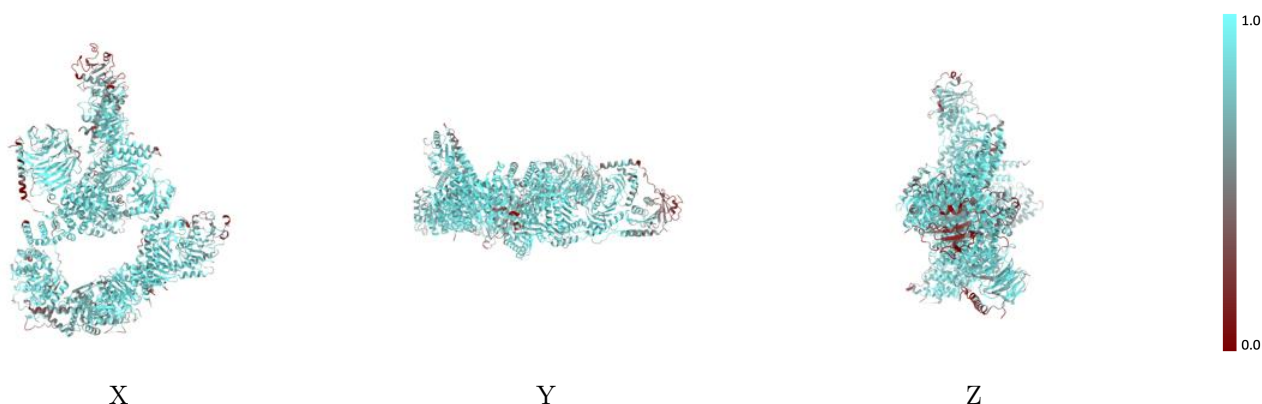
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



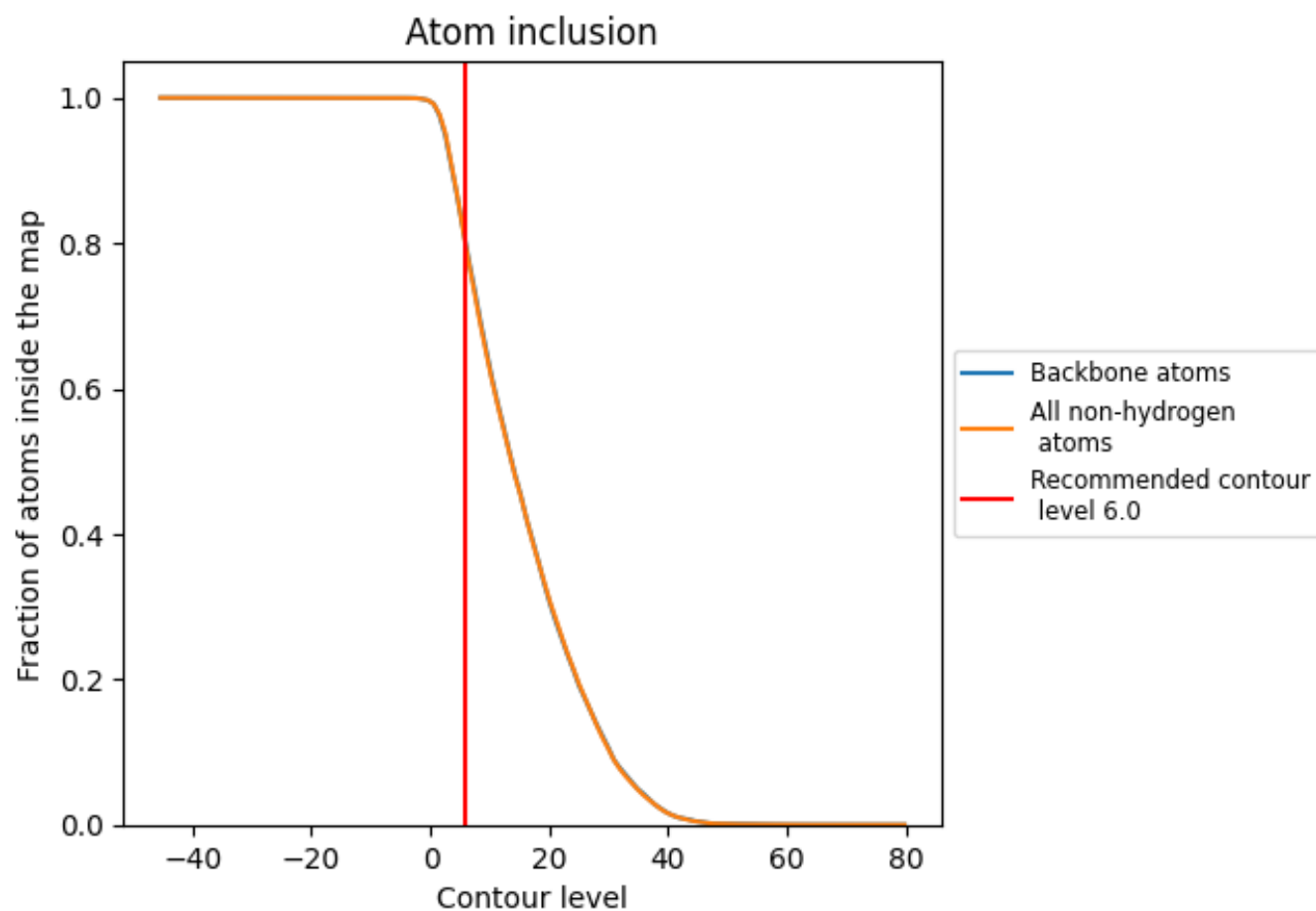
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.0).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7956	 0.5320
A	 0.8223	 0.5500
B	 0.9095	 0.5840
C	 0.8942	 0.5810
D	 0.5382	 0.3930
E	 0.8612	 0.5480
F	 0.8337	 0.5170
G	 0.2973	 0.3050
H	 0.6723	 0.4510
I	 0.8596	 0.5550
J	 0.8195	 0.5210
K	 0.6936	 0.4640
L	 0.8980	 0.5720
M	 0.9152	 0.5850
N	 0.6041	 0.4140
O	 0.8193	 0.5280
P	 0.5514	 0.4530

