Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 01:12 PM EDT

PDB ID	:	6ULG / pdb_00006ulg
EMDB ID	:	EMD-20814
Title	:	Cryo-EM structure of the FLCN-FNIP2-Rag-Ragulator complex
Authors	:	Shen, K.; Rogala, K.B.; Yu, Z.H.; Sabatini, D.M.
Deposited on	:	2019-10-08
Resolution	:	3.31 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:

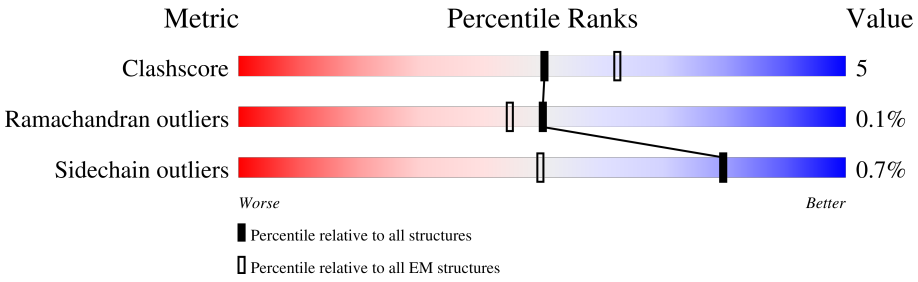
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.31 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	L	579	66% 13% 21%
2	A	124	84% 14% •
3	B	125	86% 13% •
4	C	91	85% 15%
5	D	99	78% 8% 14%
6	E	161	57% 8% • 34%
7	F	313	77% 10% 13%
8	G	399	65% 12% • 22%

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Mol	Chain	Length	Quality of chain
9	N	1114	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16351 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 Folliculin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	458	Total	C	N	O	S	0	0
			3632	2325	631	651	25		

- Molecule 2 is a protein called Ragulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	121	Total	C	N	O	S	0	0
			939	604	158	176	1		

- Molecule 3 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	125	Total	C	N	O	S	1	0
			950	596	163	183	8		

- Molecule 4 is a protein called Ragulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	91	Total	C	N	O	S	1	0
			672	409	116	139	8		

- Molecule 5 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	85	Total	C	N	O	S	0	0
			647	407	116	123	1		

- Molecule 6 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	106	Total	C	N	O	S	0	0
			829	524	142	161	2		

- Molecule 7 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	273	Total	C	N	O	S	0	0
			2246	1431	387	412	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	21	ASN	THR	engineered mutation	UNP Q7L523

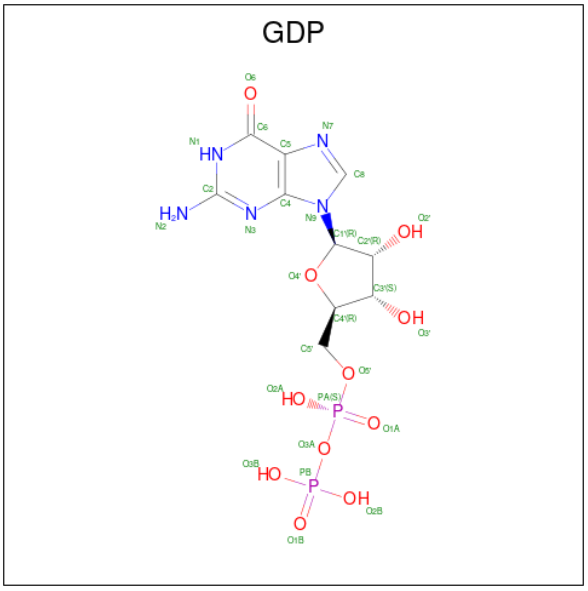
- Molecule 8 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	310	Total	C	N	O	S	0	0
			2506	1614	403	475	14		

- Molecule 9 is a protein called Folliculin-interacting protein 2.

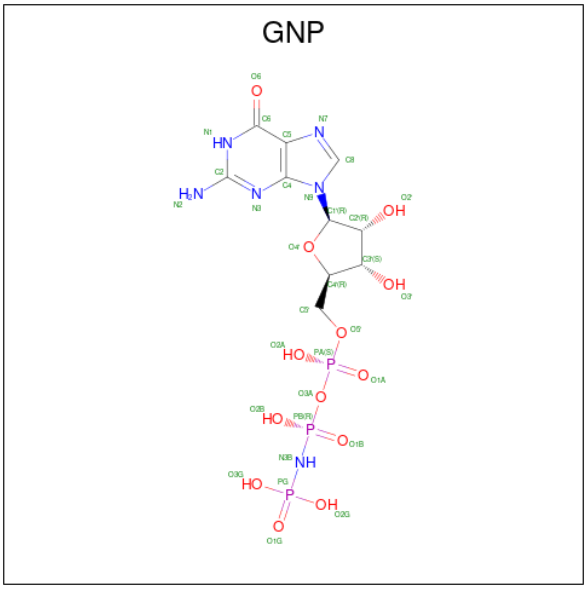
Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	483	Total	C	N	O	S	0	0
			3869	2481	659	703	26		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
10	F	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
11	G	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

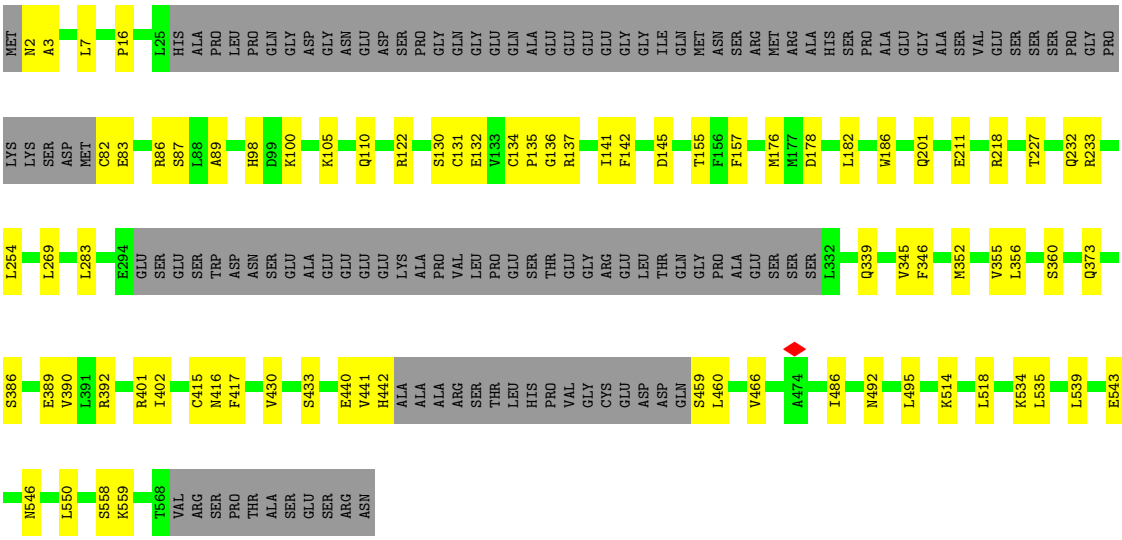
Mol	Chain	Residues	Atoms		AltConf
12	G	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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.

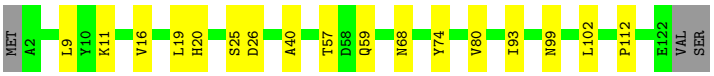
• Molecule 1: Folliculin

Chain L:



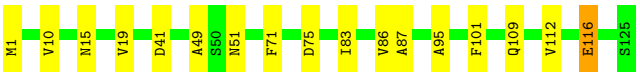
• Molecule 2: Ragulator complex protein LAMTOR3

Chain A:



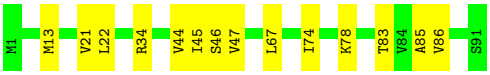
• Molecule 3: Ragulator complex protein LAMTOR2

Chain B:



• Molecule 4: Ragulator complex protein LAMTOR5

Chain C:



• Molecule 5: Ragulator complex protein LAMTOR4

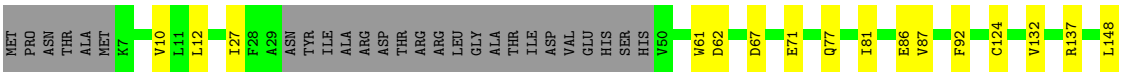
Chain D:

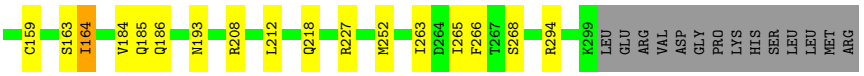
• Molecule 6: Ragulator complex protein LAMTOR1

Chain E:

• Molecule 7: Ras-related GTP-binding protein A

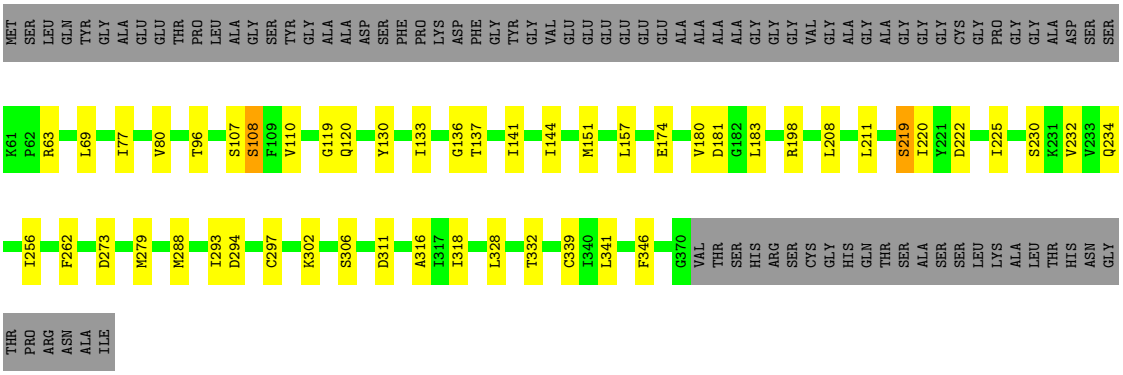
Chain F:





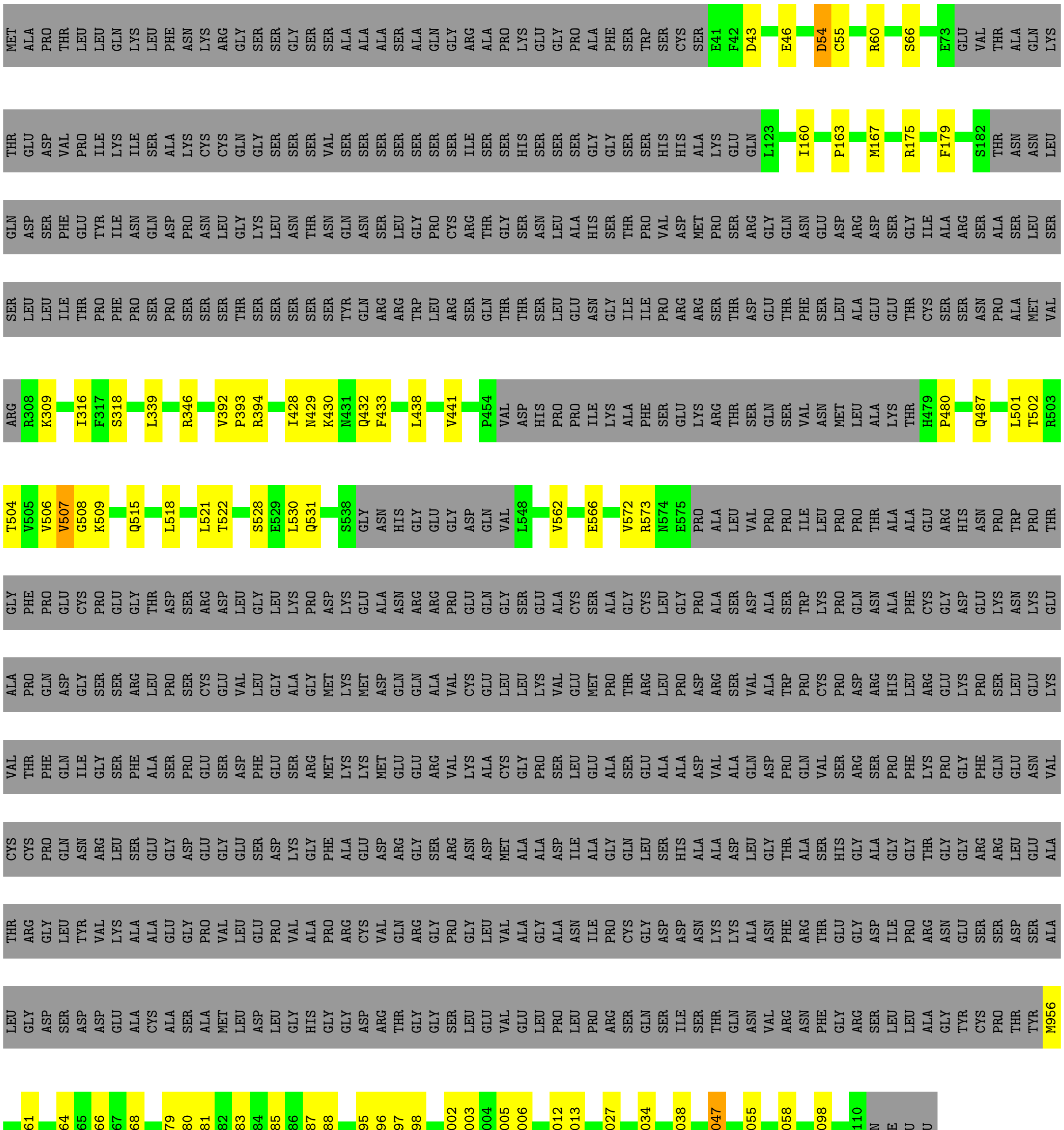
• Molecule 8: Ras-related GTP-binding protein C

Chain G:



• Molecule 9: Folliculin-interacting protein 2

Chain N:


MET ALA PRO THR LEU LEU GLN LYS LEU PHE ASN LYS ARG GLY SER SER GLY SER SER ALA ALA ALA SER ALA GLN GLY ARG ALA PRO LYS GLU GLY PRO ALA PHE SER TRP SER CYS SER E41 F42 D43 E46 D54 C55 R60 S66 E73 GLU VAL THR ALA GLN LYS
THR GLU ASP VAL PRO ILE LYS ILE SER ALA LYS CYS CYS GLN GLY SER SER SER VAL SER SER SER SER SER SER SER ILE SER SER HIS SER SER SER GLY GLY SER SER HIS HIS ALA LYS GLU GLN L123 I160 P163 M167 R175 F179 S182 THR ASN ASN LEU
GLN ASP SER PHE GLU TYR ILE ASN GLN ASP PRO ASN LEU GLY LYS LEU ASN THR ASN GLN ASN SER LEU GLY PRO CYS ARG THR GLY SER ASN LEU ALA HIS SER THR PRO VAL ASP MET PRO SER ARG GLY GLN ASN GLU ASP ARG ASP SER GLY ILE ALA ARG SER ALA SER LEU SER
SER LEU LEU ILE THR PRO PHE PRO SER PRO SER SER SER THR SER SER SER SER SER TYR GLN ARG ARG TRP LEU ARG SER GLN THR THR SER LEU GLU ASN GLY ILE ILE PRO ARG ARG SER THR ASP GLU THR PHE SER LEU ALA GLU GLU THR CYS SER SER ASN PRO ALA MET VAL
ARG R308 K309 I316 F317 S318 L339 R346 V392 P393 R394 I428 N429 K430 N431 Q432 F433 L438 V441 P454 VAL ASP HIS PRO PRO ILE LYS ALA PHE SER GLU LYS ARG THR SER GLN SER VAL ASN MET LEU ALA LYS THR H479 P480 Q487 L501 T502 R503
T504 V505 V506 V507 G508 K509 Q515 L518 L521 T522 S528 E529 L530 Q531 S538 GLY ASN HIS GLY GLU GLY ASP GLN VAL L548 V562 E566 V572 R573 N574 E575 PRO ALA LEU VAL PRO PRO ILE LEU PRO PRO THR ALA ALA GLU ARG HIS ASN PRO TRP PRO THR
GLY PHE PRO GLU CYS PRO GLU GLY THR ASP SER ARG ASP LEU GLY LEU LYS PRO ASP LYS GLU ALA ASN ARG ARG PRO GLU GLN GLY SER GLU ALA CYS SER ALA GLY CYS LEU GLY PRO ALA SER ASP ALA SER TRP LYS PRO GLN ASN ALA PHE CYS GLY ASP GLU LYS ASN LYS GLU
ALA PRO GLN ASP GLY SER SER ARG LEU PRO SER CYS GLU VAL LEU GLY ALA GLY MET LYS MET ASP GLN GLN ALA VAL CYS GLU LEU LEU LYS VAL GLU MET PRO THR ARG LEU PRO ASP ARG SER VAL ALA TRP PRO CYS PRO ASP ARG HIS LEU ARG GLU LYS PRO SER LEU GLU LYS
VAL THR PHE GLN ILE GLY SER PHE ALA SER PRO GLU SER ASP PHE GLU SER ARG MET LYS LYS MET GLU GLU ARG VAL LYS ALA CYS GLY PRO SER LEU GLU ALA SER GLU ALA ALA ASP VAL ALA GLN ASP PRO GLN VAL SER ARG SER PRO PHE LYS PRO GLY PHE GLN GLU ASN VAL
CYS CYS PRO GLN ASN ARG LEU SER GLU GLY ASP GLU GLY GLU SER ASP LYS GLY PHE ALA GLU ASP ARG GLY SER ARG ASN ASP MET ALA ALA ASP ILE ALA GLY GLN LEU SER HIS ALA ALA ASP LEU GLY THR ALA SER HIS GLY ALA GLY GLY THR GLY GLY ARG ARG LEU GLU ALA
THR ARG GLY LEU TYR VAL LYS ALA ALA GLU GLY PRO VAL LEU GLU PRO VAL ALA PRO ARG CYS VAL GLN ARG GLY PRO GLY LEU VAL ALA GLY ALA ASN ILE PRO CYS GLY ASP ASP ASN LYS LYS ALA ASN PHE ARG THR GLU GLY ASP ILE PRO ARG ASN GLU SER SER ASP SER ALA
LEU GLY ASP SER ASP ASP GLU ALA CYS ALA SER ALA MET LEU ASP LEU GLY HIS GLY GLY ASP ARG THR GLY GLY SER LEU GLU VAL GLU LEU PRO LEU PRO ARG SER GLN SER ILE SER THR GLN ASN VAL ARG ASN PHE GLY ARG SER LEU LEU ALA GLY TYR CYS PRO THR TYR M956
L961 T964 G965 S966 D967 E968 V979 H980 T981 V982 H983 H984 P985 V986 L987 D988 V995 C996 I997 I998 D1002 K1003 W1004 S1005 V1006 Q1012 R1013 V1027 L1034 I1038 P1047 L1055 R1058 L1098 A1110 GLN ILE LEU LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	126984	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 ($e^-/Å^2$)	59.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, GNP

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	L	0.26	0/3718	0.57	4/5031 (0.1%)
2	A	0.22	0/956	0.49	0/1297
3	B	0.31	0/961	0.63	2/1301 (0.2%)
4	C	0.19	0/678	0.41	0/919
5	D	0.20	0/654	0.52	0/883
6	E	0.26	0/844	0.40	0/1146
7	F	0.25	0/2287	0.56	1/3076 (0.0%)
8	G	0.26	0/2559	0.55	3/3455 (0.1%)
9	N	0.28	0/3943	0.71	5/5325 (0.1%)
All	All	0.26	0/16600	0.59	15/22433 (0.1%)

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
8	G	0	2
9	N	0	2
All	All	0	4

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	1005	SER	CA-C-N	8.58	130.55	121.97
9	N	1005	SER	C-N-CA	8.58	130.55	121.97
9	N	1047	PRO	N-CA-CB	7.79	111.43	103.25
9	N	430	LYS	CA-C-N	6.35	133.67	121.54
9	N	430	LYS	C-N-CA	6.35	133.67	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	100	LYS	CA-C-N	5.69	132.42	121.54
1	L	100	LYS	C-N-CA	5.69	132.42	121.54
8	G	219	SER	CA-C-N	-5.59	111.91	121.97
8	G	219	SER	C-N-CA	-5.59	111.91	121.97
3	B	116	GLU	CA-C-N	-5.52	113.70	119.83
3	B	116	GLU	C-N-CA	-5.52	113.70	119.83
8	G	108	SER	N-CA-C	5.51	118.94	111.17
7	F	164	ILE	N-CA-C	-5.22	107.74	113.43
1	L	136	GLY	CA-C-N	5.01	131.11	121.54
1	L	136	GLY	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	G	107	SER	Peptide
8	G	119	GLY	Peptide
9	N	163	PRO	Peptide
9	N	54	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3632	0	3629	45	0
2	A	939	0	963	13	0
3	B	950	0	959	14	0
4	C	672	0	670	11	0
5	D	647	0	657	6	0
6	E	829	0	832	12	0
7	F	2246	0	2243	20	0
8	G	2506	0	2474	30	0
9	N	3869	0	3928	42	0
10	F	28	0	12	0	0
11	G	32	0	12	1	0
12	G	1	0	0	0	0
All	All	16351	0	16379	175	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 (175) 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)
6:E:99:LEU:HD11	6:E:102:TRP:HB2	1.54	0.90
3:B:112:VAL:O	3:B:116:GLU:HB2	1.90	0.71
8:G:230:SER:O	8:G:234:GLN:HB2	1.94	0.68
9:N:339:LEU:HD22	9:N:961:LEU:HD11	1.79	0.64
9:N:346:ARG:HH22	9:N:987:LEU:HB2	1.63	0.64
9:N:175:ARG:HB3	9:N:179:PHE:HB2	1.81	0.61
4:C:78:LYS:HB3	4:C:83:THR:HG22	1.81	0.61
7:F:252:MET:HG3	8:G:318:ILE:HG12	1.83	0.61
9:N:432:GLN:HB3	9:N:1027:VAL:HG21	1.83	0.60
6:E:112:THR:HG22	6:E:114:GLN:H	1.67	0.60
1:L:131:CYS:SG	1:L:132:GLU:N	2.75	0.60
9:N:956:MET:SD	9:N:956:MET:N	2.75	0.60
8:G:80:VAL:HG21	8:G:220:ILE:HD12	1.82	0.60
1:L:178:ASP:HB2	9:N:480:PRO:HG2	1.84	0.59
7:F:86:GLU:HG3	7:F:87:VAL:HG23	1.84	0.59
2:A:102:LEU:HD22	4:C:47:VAL:HG21	1.84	0.59
9:N:531:GLN:HG2	9:N:562:VAL:HG22	1.85	0.58
4:C:44:VAL:HG11	5:D:53:PHE:HB2	1.85	0.58
1:L:16:PRO:O	1:L:122:ARG:NH1	2.36	0.58
6:E:99:LEU:CD1	6:E:102:TRP:HB2	2.32	0.58
1:L:339:GLN:NE2	1:L:459:SER:O	2.37	0.58
2:A:80:VAL:HG12	2:A:93:ILE:HG12	1.86	0.58
9:N:392:VAL:HG23	9:N:394:ARG:HE	1.69	0.57
9:N:981:THR:HG22	9:N:1012:GLN:HB3	1.86	0.57
5:D:65:ARG:HH22	6:E:121:SER:HB2	1.70	0.57
8:G:151:MET:SD	8:G:198:ARG:NH1	2.79	0.56
1:L:518:LEU:HD22	1:L:550:LEU:HD13	1.89	0.55
3:B:86:VAL:HG22	3:B:112:VAL:HG23	1.88	0.55
8:G:141:ILE:HD11	8:G:232:VAL:HG11	1.89	0.55
7:F:218:GLN:OE1	7:F:227:ARG:NH1	2.39	0.55
9:N:506:VAL:HA	9:N:1002:ASP:HB3	1.88	0.55
1:L:339:GLN:HE22	1:L:460:LEU:HA	1.72	0.55
1:L:233:ARG:NH2	8:G:297:CYS:SG	2.80	0.55
9:N:996:CYS:SG	9:N:1013:ARG:NH1	2.80	0.54
1:L:346:PHE:HB2	1:L:390:VAL:HG21	1.89	0.54
1:L:373:GLN:NE2	1:L:415:CYS:SG	2.80	0.54
4:C:22:LEU:HB3	4:C:85:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:25:SER:OG	2:A:26:ASP:N	2.40	0.54
9:N:507:VAL:HG22	9:N:1003:LYS:HA	1.89	0.54
1:L:98:HIS:HA	1:L:105:LYS:HA	1.90	0.54
4:C:67:LEU:HB2	4:C:74:ILE:HB	1.90	0.53
1:L:233:ARG:NH1	8:G:294:ASP:OD1	2.41	0.53
1:L:227:THR:OG1	1:L:232:GLN:OE1	2.27	0.53
7:F:208:ARG:NH1	7:F:268:SER:O	2.42	0.53
9:N:393:PRO:HA	9:N:572:VAL:HG22	1.90	0.53
1:L:233:ARG:HH22	8:G:293:ILE:HG22	1.74	0.53
9:N:988:ASP:OD1	9:N:988:ASP:N	2.42	0.53
2:A:20:HIS:HB3	2:A:40:ALA:HB2	1.91	0.53
1:L:137:ARG:O	1:L:155:THR:OG1	2.27	0.52
2:A:99:ASN:ND2	4:C:46:SER:OG	2.42	0.52
8:G:256:ILE:HG23	8:G:341:LEU:HB3	1.91	0.52
3:B:87:ALA:HB2	3:B:116:GLU:HG3	1.91	0.52
2:A:57:THR:HG23	2:A:68:ASN:HB3	1.90	0.52
8:G:77:ILE:HG23	8:G:225:ILE:HD11	1.92	0.52
7:F:266:PHE:HA	7:F:294:ARG:HD3	1.91	0.51
7:F:265:ILE:O	7:F:294:ARG:NH2	2.43	0.51
8:G:302:LYS:NZ	8:G:306:SER:OG	2.43	0.51
8:G:273:ASP:OD1	8:G:273:ASP:N	2.40	0.51
9:N:997:ILE:H	9:N:1012:GLN:HG2	1.75	0.51
9:N:429:ASN:HA	9:N:433:PHE:HB3	1.93	0.51
1:L:176:MET:HG3	1:L:182:LEU:HD13	1.93	0.51
8:G:69:LEU:HD12	8:G:120:GLN:HB3	1.92	0.50
7:F:132:VAL:HG23	7:F:137:ARG:HG2	1.93	0.50
1:L:514:LYS:HD2	1:L:539:LEU:HG	1.94	0.50
6:E:159:GLY:O	7:F:193:ASN:ND2	2.44	0.50
3:B:75:ASP:HB2	3:B:101:PHE:HZ	1.76	0.50
9:N:55:CYS:HB3	9:N:309:LYS:HA	1.93	0.50
1:L:176:MET:HB2	1:L:182:LEU:HD22	1.93	0.50
1:L:543:GLU:OE1	1:L:546:ASN:ND2	2.45	0.49
2:A:11:LYS:HB3	6:E:105:LEU:HD11	1.95	0.49
1:L:345:VAL:HG13	1:L:386:SER:HB2	1.94	0.49
3:B:49:ALA:HB1	3:B:83:ILE:HD11	1.95	0.49
9:N:1038:ILE:HG13	9:N:1055:LEU:HD12	1.93	0.49
8:G:144:ILE:HD11	8:G:157:LEU:HD22	1.93	0.49
8:G:63:ARG:HB2	8:G:137:THR:HG22	1.95	0.49
3:B:41:ASP:N	3:B:41:ASP:OD1	2.46	0.49
7:F:27:ILE:HG23	7:F:212:LEU:HD21	1.94	0.49
2:A:112:PRO:HG2	6:E:102:TRP:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:401:ARG:O	1:L:416:ASN:N	2.46	0.48
9:N:509:LYS:H	9:N:968:GLU:HB3	1.78	0.48
7:F:62:ASP:OD1	7:F:62:ASP:N	2.43	0.48
2:A:74:TYR:HB2	3:B:71:PHE:HB3	1.94	0.48
7:F:266:PHE:HB2	7:F:294:ARG:HB2	1.95	0.48
2:A:59:GLN:OE1	3:B:51:ASN:ND2	2.47	0.48
8:G:208:LEU:HB3	8:G:211:LEU:HD12	1.96	0.48
8:G:341:LEU:HD11	8:G:346:PHE:HD1	1.79	0.48
1:L:492:ASN:HB3	1:L:495:LEU:HD12	1.96	0.47
8:G:288:MET:HG3	8:G:318:ILE:HD12	1.96	0.47
1:L:135:PRO:HG2	9:N:160:ILE:HG23	1.96	0.47
9:N:506:VAL:H	9:N:966:SER:HB2	1.80	0.47
9:N:979:VAL:O	9:N:983:HIS:ND1	2.48	0.47
1:L:157:PHE:O	1:L:201:GLN:NE2	2.48	0.47
7:F:92:PHE:HZ	7:F:148:LEU:HD11	1.79	0.47
6:E:99:LEU:HD11	6:E:102:TRP:CB	2.36	0.47
2:A:16:VAL:HG13	2:A:102:LEU:HD23	1.96	0.47
3:B:10:VAL:HG13	6:E:148:VAL:HG21	1.96	0.47
8:G:256:ILE:HG21	8:G:339:CYS:HB3	1.97	0.46
9:N:502:THR:HG23	9:N:998:ILE:HB	1.98	0.46
1:L:145:ASP:N	1:L:145:ASP:OD1	2.48	0.46
3:B:19:VAL:HA	3:B:95:ALA:HA	1.98	0.46
5:D:55:LEU:HB2	5:D:62:PRO:HG3	1.98	0.46
7:F:67:ASP:O	7:F:71:GLU:HB3	2.16	0.46
8:G:63:ARG:NE	8:G:136:GLY:O	2.46	0.45
9:N:54:ASP:OD2	9:N:60:ARG:NE	2.47	0.45
1:L:518:LEU:HA	1:L:535:LEU:HD21	1.98	0.45
4:C:21:VAL:HG23	4:C:86:VAL:HG12	1.98	0.45
1:L:211:GLU:HG3	1:L:218:ARG:HH21	1.82	0.45
1:L:440:GLU:HB2	1:L:466:VAL:HG23	1.98	0.45
9:N:985:PRO:HG3	9:N:997:ILE:HG12	1.99	0.45
9:N:501:LEU:HB3	9:N:997:ILE:HD12	1.99	0.45
8:G:219:SER:OG	8:G:222:ASP:OD1	2.35	0.45
9:N:515:GLN:HG2	9:N:573:ARG:HH11	1.81	0.45
8:G:180:VAL:HA	8:G:183:LEU:HD13	1.99	0.45
9:N:46:GLU:HG2	9:N:318:SER:HB3	1.98	0.45
1:L:7:LEU:HD13	1:L:254:LEU:HD21	1.98	0.45
8:G:108:SER:O	8:G:108:SER:OG	2.30	0.44
8:G:130:TYR:HA	8:G:133:ILE:HG12	1.99	0.44
7:F:252:MET:HE2	7:F:263:ILE:HD12	1.99	0.44
8:G:174:GLU:HG2	8:G:232:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:181:ASP:OD1	8:G:181:ASP:N	2.37	0.44
9:N:441:VAL:HG11	9:N:521:LEU:HD21	1.98	0.44
9:N:1034:LEU:HD13	9:N:1058:ARG:HG2	1.98	0.44
7:F:184:VAL:HG23	7:F:186:GLN:HG2	2.00	0.44
8:G:311:ASP:OD1	8:G:311:ASP:N	2.50	0.44
3:B:109:GLN:HA	3:B:112:VAL:HG12	2.00	0.44
1:L:269:LEU:HD22	9:N:530:LEU:HD23	1.99	0.44
1:L:402:ILE:HG22	1:L:417:PHE:HB2	2.00	0.43
3:B:112:VAL:O	3:B:116:GLU:CB	2.64	0.43
1:L:82:CYS:SG	1:L:83:GLU:N	2.90	0.43
4:C:78:LYS:HA	4:C:83:THR:HA	2.00	0.43
1:L:142:PHE:HB2	1:L:186:TRP:HZ3	1.84	0.43
9:N:438:LEU:HA	9:N:441:VAL:HG22	2.00	0.43
4:C:13:MET:HE3	4:C:13:MET:HB3	1.92	0.43
5:D:61:VAL:HA	5:D:62:PRO:HD3	1.96	0.43
1:L:389:GLU:HA	1:L:392:ARG:HD2	2.00	0.42
2:A:16:VAL:HB	2:A:19:LEU:HB2	2.01	0.42
6:E:76:MET:HE2	6:E:81:TYR:HB2	2.01	0.42
4:C:21:VAL:HG12	4:C:34:ARG:HB2	2.02	0.42
7:F:12:LEU:HB3	7:F:62:ASP:HB3	2.01	0.42
1:L:486:ILE:HD12	1:L:486:ILE:HA	1.86	0.42
9:N:167:MET:HG3	9:N:316:ILE:HG13	2.02	0.42
1:L:352:MET:HA	1:L:355:VAL:HG12	2.02	0.42
9:N:980:HIS:HA	9:N:983:HIS:CE1	2.55	0.42
1:L:356:LEU:O	1:L:360:SER:OG	2.35	0.42
1:L:283:LEU:HB3	1:L:558:SER:HB2	2.02	0.42
9:N:66:SER:O	9:N:66:SER:OG	2.35	0.42
9:N:518:LEU:O	9:N:522:THR:OG1	2.35	0.42
3:B:1:MET:HE2	3:B:1:MET:HB3	1.95	0.41
3:B:15:ASN:HA	3:B:19:VAL:HG23	2.01	0.41
7:F:124:CYS:HB2	7:F:159:CYS:HB3	2.02	0.41
1:L:87:SER:OG	1:L:89:ALA:O	2.36	0.41
5:D:65:ARG:NH2	6:E:118:VAL:O	2.51	0.41
7:F:61:TRP:HH2	7:F:81:ILE:HA	1.84	0.41
1:L:534:LYS:HD3	1:L:534:LYS:HA	1.71	0.41
5:D:17:GLY:HA2	5:D:31:GLY:HA3	2.01	0.41
1:L:430:VAL:O	1:L:433:SER:OG	2.33	0.41
1:L:441:VAL:O	1:L:442:HIS:ND1	2.53	0.41
2:A:9:LEU:HD12	2:A:9:LEU:HA	1.91	0.41
9:N:438:LEU:HA	9:N:438:LEU:HD23	1.82	0.41
8:G:279:MET:HE3	8:G:279:MET:HB3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:96:THR:N	11:G:401:GNP:O1G	2.53	0.41
9:N:530:LEU:HB2	9:N:566:GLU:HG2	2.02	0.41
1:L:130:SER:OG	1:L:131:CYS:N	2.53	0.41
9:N:508:GLY:HA3	9:N:968:GLU:HG2	2.01	0.41
1:L:86:ARG:O	1:L:110:GLN:NE2	2.53	0.41
1:L:134:CYS:HB2	1:L:141:ILE:HD11	2.02	0.41
7:F:77:GLN:HA	7:F:81:ILE:HB	2.03	0.41
7:F:163:SER:OG	7:F:164:ILE:N	2.53	0.41
4:C:45:ILE:HG21	4:C:85:ALA:HB2	2.03	0.40
9:N:995:VAL:HG12	9:N:996:CYS:H	1.86	0.40
6:E:135:ILE:HD13	6:E:135:ILE:HA	1.92	0.40
9:N:487:GLN:NE2	9:N:528:SER:O	2.54	0.40
8:G:316:ALA:HB3	8:G:328:LEU:HB3	2.03	0.40
9:N:504:THR:HB	9:N:964:THR:HG22	2.03	0.40
1:L:2:ASN:HB3	1:L:3:ALA:H	1.61	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	L	450/579 (78%)	410 (91%)	39 (9%)	1 (0%)	44 72
2	A	119/124 (96%)	112 (94%)	7 (6%)	0	100 100
3	B	124/125 (99%)	114 (92%)	10 (8%)	0	100 100
4	C	90/91 (99%)	87 (97%)	3 (3%)	0	100 100
5	D	81/99 (82%)	77 (95%)	4 (5%)	0	100 100
6	E	102/161 (63%)	98 (96%)	4 (4%)	0	100 100
7	F	269/313 (86%)	256 (95%)	12 (4%)	1 (0%)	30 61
8	G	308/399 (77%)	283 (92%)	25 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	N	471/1114 (42%)	403 (86%)	67 (14%)	1 (0%)	44 72
All	All	2014/3005 (67%)	1840 (91%)	171 (8%)	3 (0%)	50 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	1047	PRO
1	L	559	LYS
7	F	185	GLN

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	L	403/503 (80%)	403 (100%)	0	100 100
2	A	105/108 (97%)	105 (100%)	0	100 100
3	B	99/98 (101%)	99 (100%)	0	100 100
4	C	78/77 (101%)	78 (100%)	0	100 100
5	D	71/83 (86%)	70 (99%)	1 (1%)	62 78
6	E	93/141 (66%)	90 (97%)	3 (3%)	34 61
7	F	252/287 (88%)	251 (100%)	1 (0%)	89 93
8	G	283/340 (83%)	280 (99%)	3 (1%)	70 82
9	N	433/955 (45%)	428 (99%)	5 (1%)	67 81
All	All	1817/2592 (70%)	1804 (99%)	13 (1%)	80 88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	77	VAL
6	E	97	SER
6	E	98	SER
6	E	148	VAL

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Mol	Chain	Res	Type
7	F	10	VAL
8	G	110	VAL
8	G	262	PHE
8	G	332	THR
9	N	43	ASP
9	N	428	ILE
9	N	507	VAL
9	N	1006	VAL
9	N	1098	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	110	GLN
1	L	111	HIS
1	L	123	GLN
1	L	147	GLN
1	L	255	HIS
1	L	285	GLN
1	L	339	GLN
1	L	373	GLN
1	L	416	ASN
1	L	429	HIS
1	L	494	ASN
1	L	502	GLN
1	L	513	ASN
1	L	533	GLN
2	A	20	HIS
2	A	59	GLN
3	B	51	ASN
4	C	30	ASN
4	C	77	GLN
4	C	79	HIS
6	E	114	GLN
7	F	72	ASN
7	F	107	GLN
7	F	115	GLN
7	F	116	ASN
7	F	179	GLN
7	F	222	GLN
7	F	237	GLN
8	G	357	HIS

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Mol	Chain	Res	Type
9	N	70	GLN
9	N	549	ASN
9	N	980	HIS
9	N	983	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
10	GDP	F	500	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)
11	GNP	G	401	12	29,34,34	1.84	8 (27%)	33,54,54	2.28	5 (15%)

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	GDP	F	500	-	-	2/12/32/32	0/3/3/3
11	GNP	G	401	12	-	9/14/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	401	GNP	C6-N1	4.38	1.40	1.33
11	G	401	GNP	PB-O3A	4.21	1.64	1.59
11	G	401	GNP	O6-C6	3.53	1.33	1.24
11	G	401	GNP	PG-N3B	2.82	1.70	1.63
11	G	401	GNP	PB-O1B	2.78	1.50	1.46
11	G	401	GNP	PG-O1G	2.66	1.50	1.46
11	G	401	GNP	C5-C6	2.44	1.45	1.41
10	F	500	GDP	C6-N1	-2.34	1.34	1.37
11	G	401	GNP	PB-O2B	-2.20	1.51	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	401	GNP	C5-C6-N1	-9.30	110.99	123.42
11	G	401	GNP	C2-N1-C6	6.26	124.67	115.96
10	F	500	GDP	C8-N7-C5	2.74	107.21	102.55
11	G	401	GNP	N3-C2-N1	-2.64	123.85	127.21
11	G	401	GNP	C2-N3-C4	-2.22	113.09	115.48
11	G	401	GNP	O1B-PB-N3B	-2.22	108.51	111.77
10	F	500	GDP	O6-C6-C5	-2.06	120.24	124.32

There are no chirality outliers.

All (11) torsion outliers are listed below:

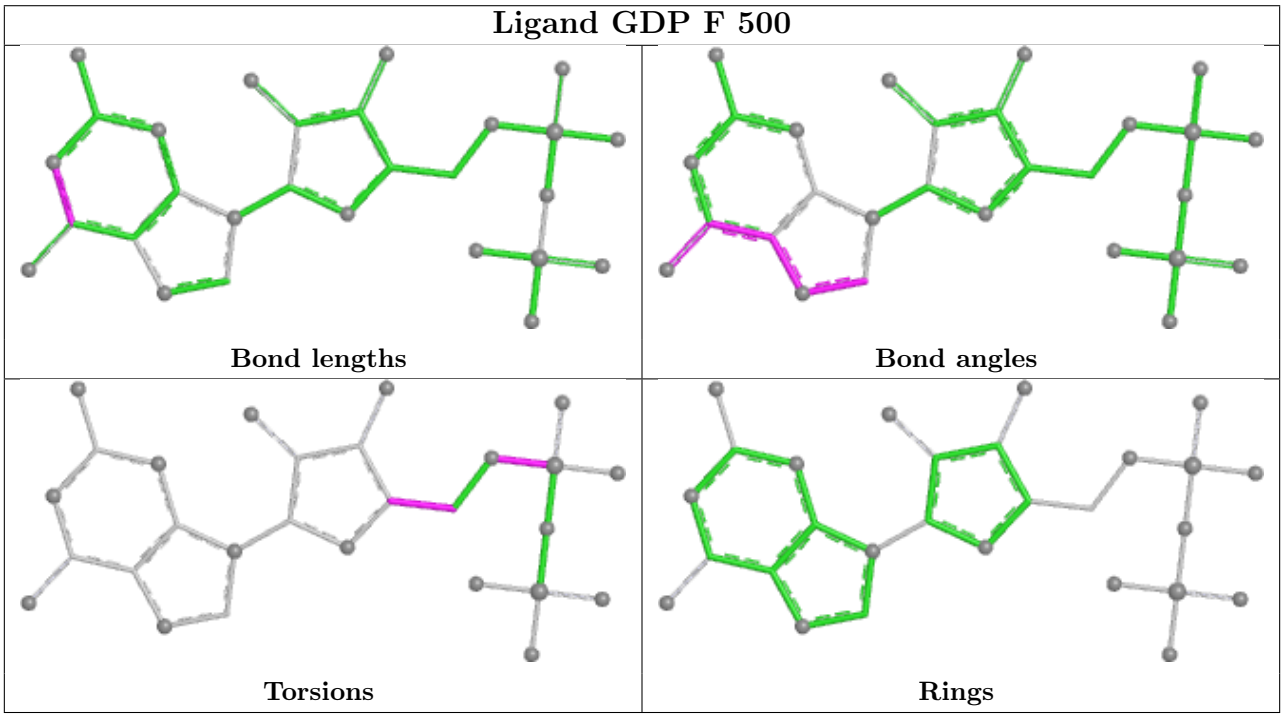
Mol	Chain	Res	Type	Atoms
11	G	401	GNP	PB-N3B-PG-O1G
11	G	401	GNP	PG-N3B-PB-O1B
11	G	401	GNP	PG-N3B-PB-O3A
11	G	401	GNP	PA-O3A-PB-O2B
11	G	401	GNP	C5'-O5'-PA-O3A
11	G	401	GNP	C5'-O5'-PA-O2A
11	G	401	GNP	C3'-C4'-C5'-O5'
11	G	401	GNP	O4'-C4'-C5'-O5'
10	F	500	GDP	C5'-O5'-PA-O3A
10	F	500	GDP	C3'-C4'-C5'-O5'
11	G	401	GNP	PA-O3A-PB-O1B

There are no ring outliers.

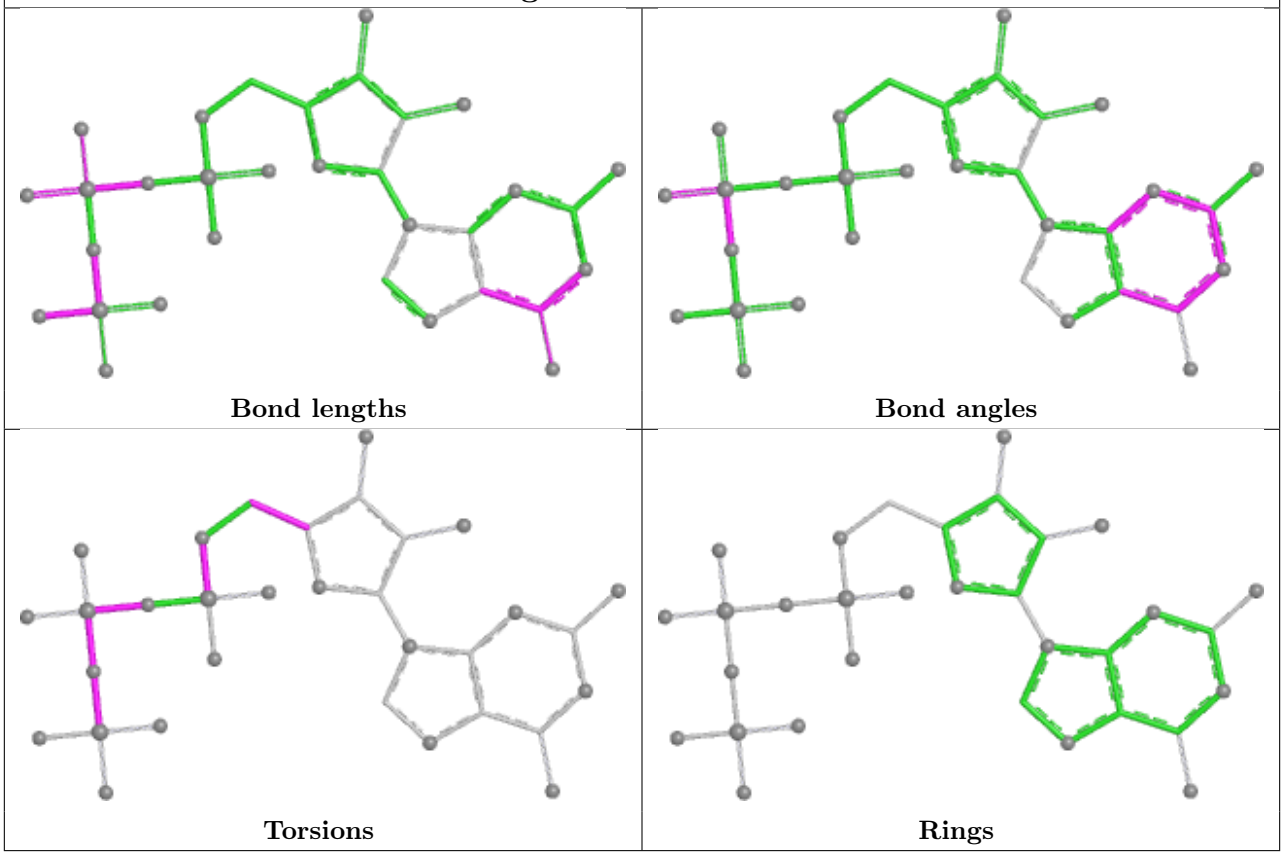
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	401	GNP	1	0

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



Ligand GNP G 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

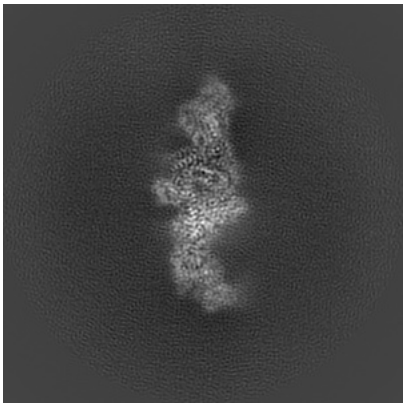
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20814. These allow visual inspection of the internal detail of the map and identification of artifacts.

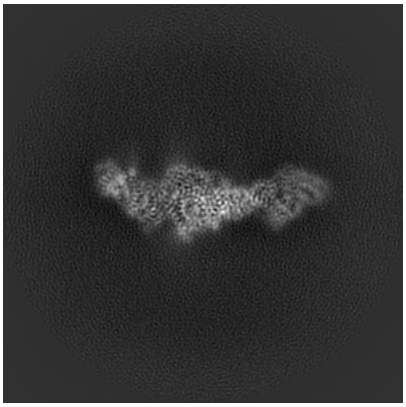
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

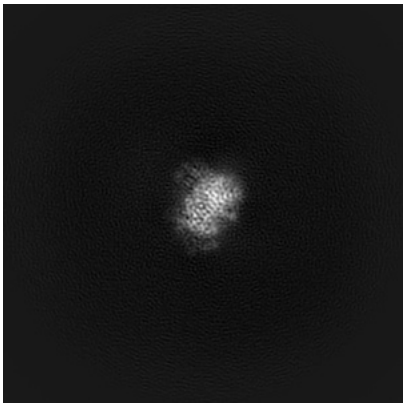
6.1.1 Primary map



X



Y

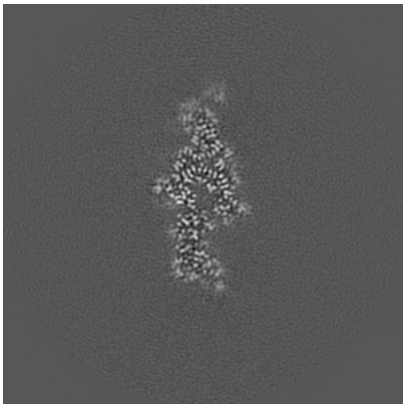


Z

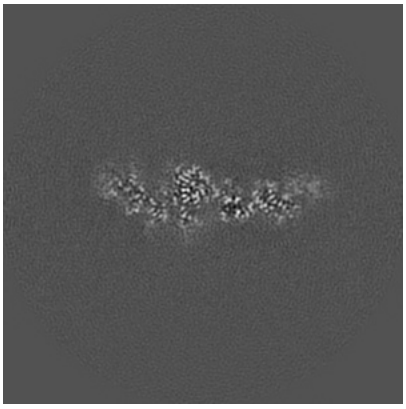
The images above show the map projected in three orthogonal directions.

6.2 Central slices

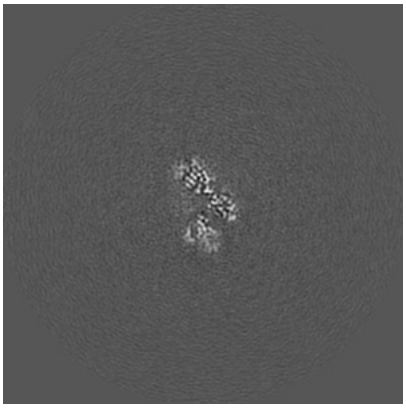
6.2.1 Primary map



X Index: 180



Y Index: 180

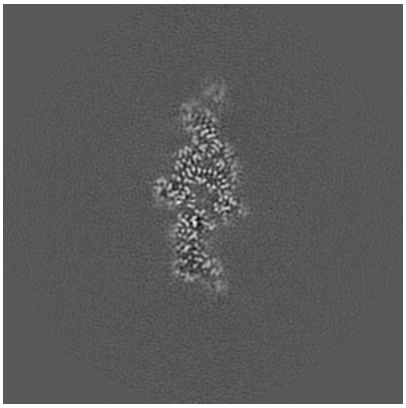


Z Index: 180

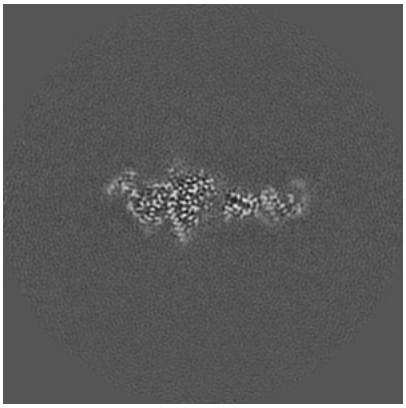
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

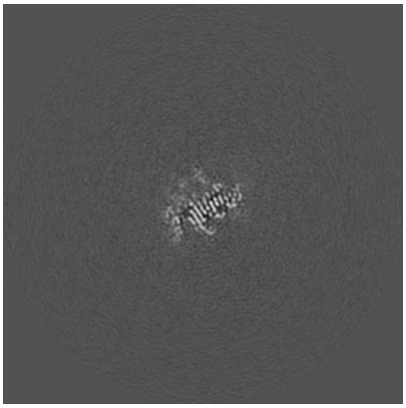
6.3.1 Primary map



X Index: 181



Y Index: 173

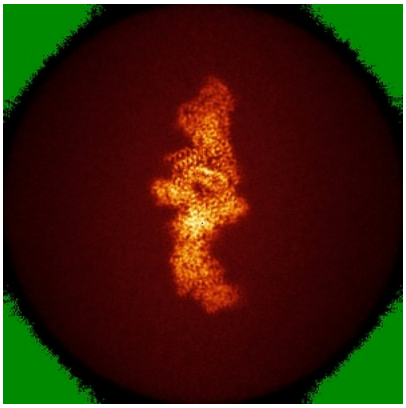


Z Index: 162

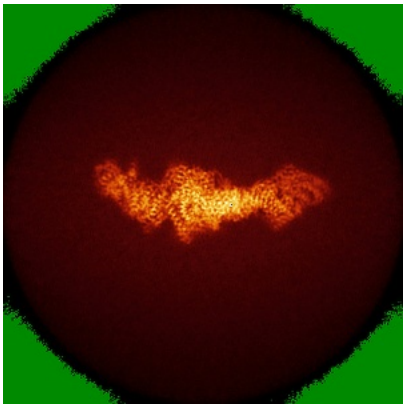
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

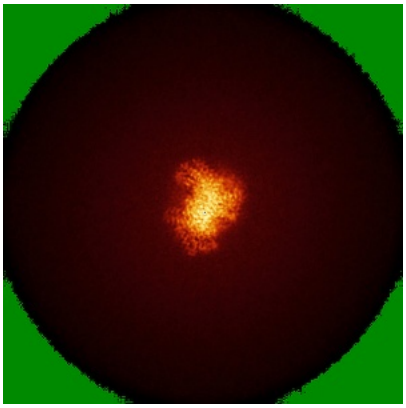
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.002. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

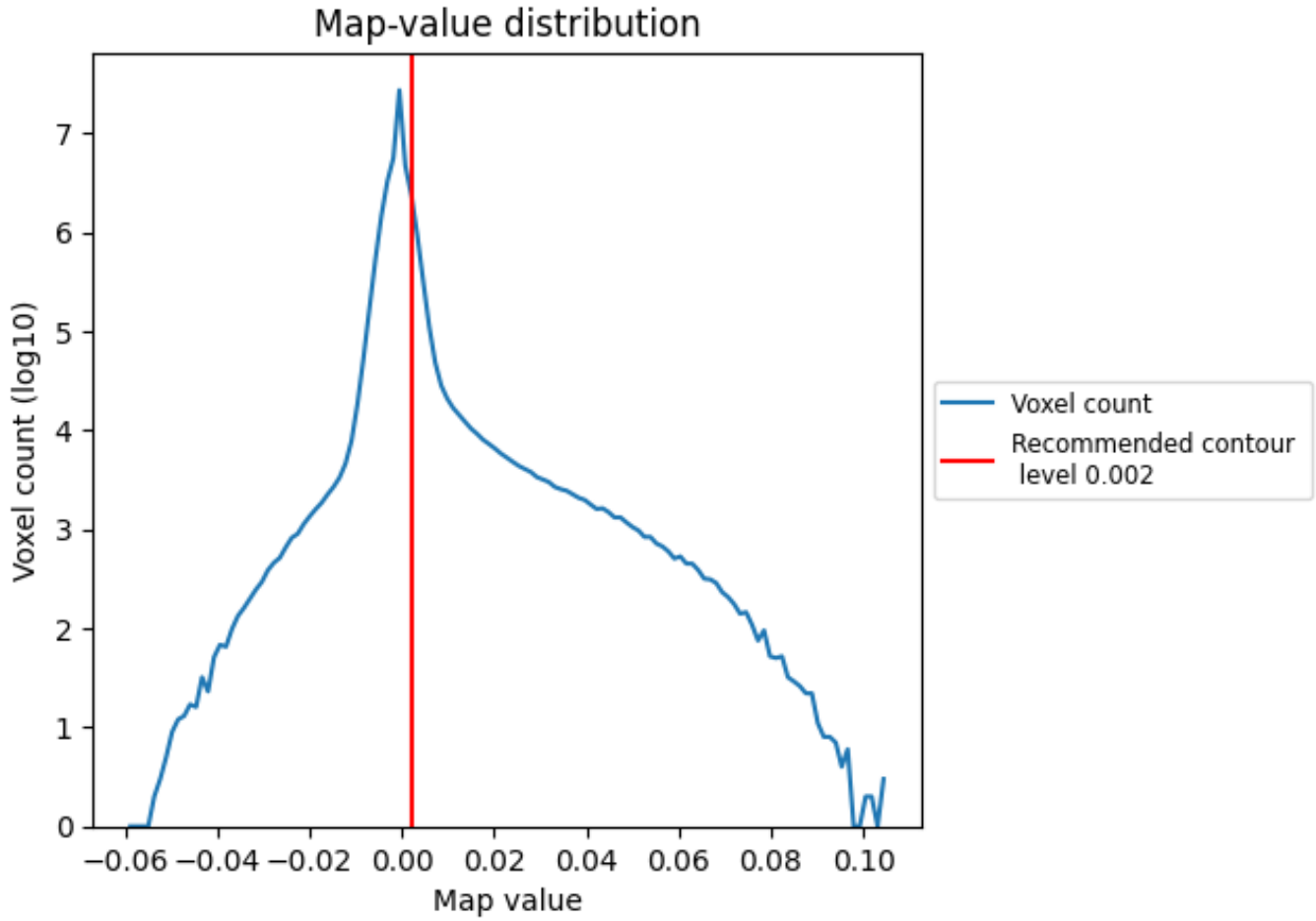
6.6 Mask visualisation (i)

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

7 Map analysis

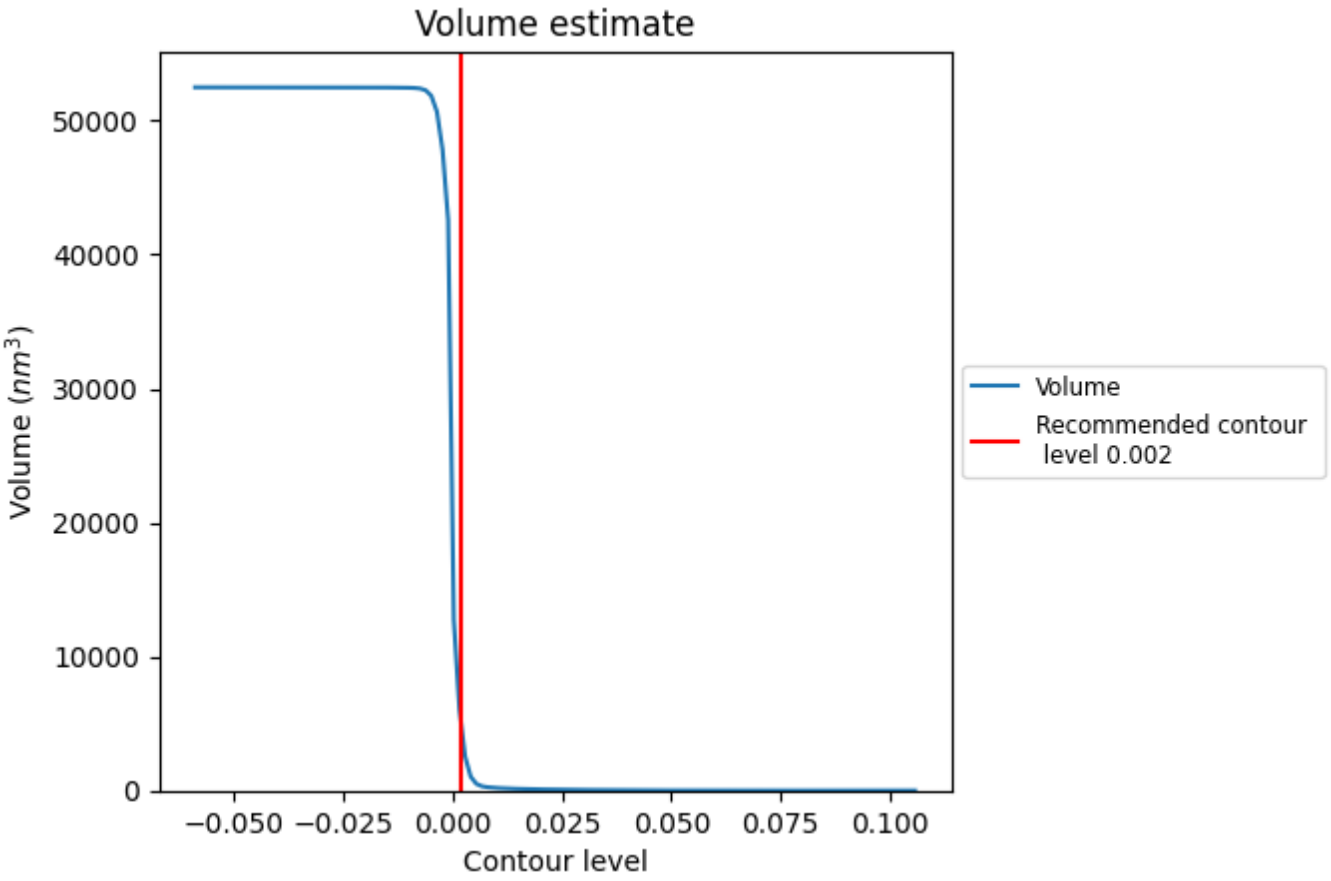
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

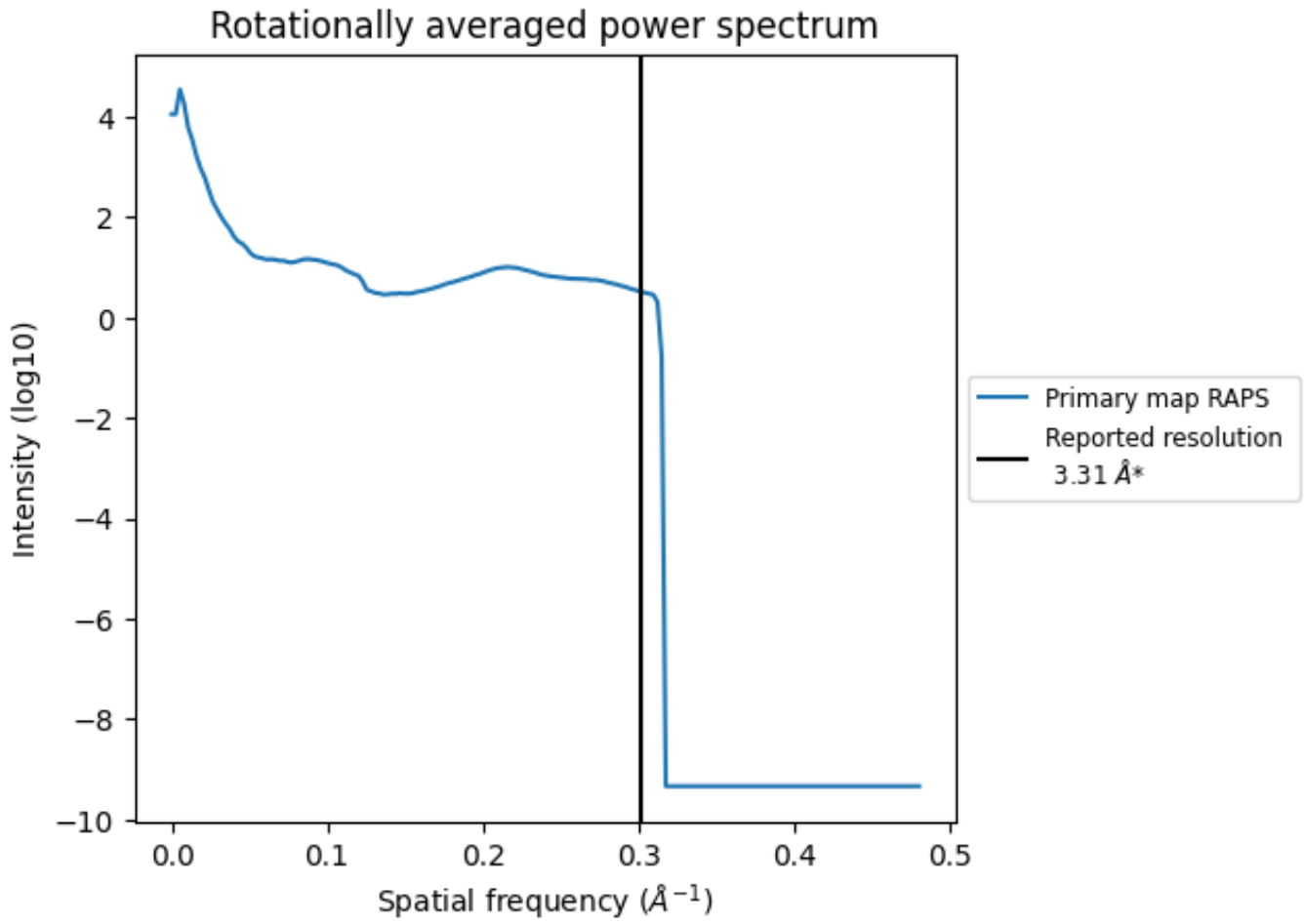
7.2 Volume estimate (i)



The volume at the recommended contour level is 4938 nm^3; this corresponds to an approximate mass of 4460 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 0.302 Å^{-1}

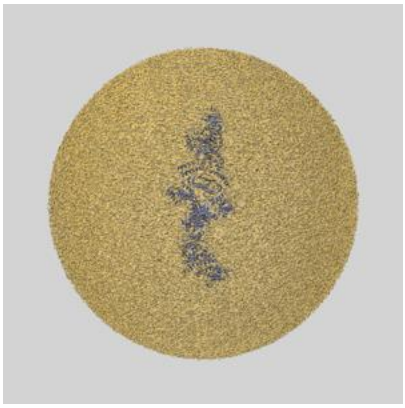
8 Fourier-Shell correlation (i)

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

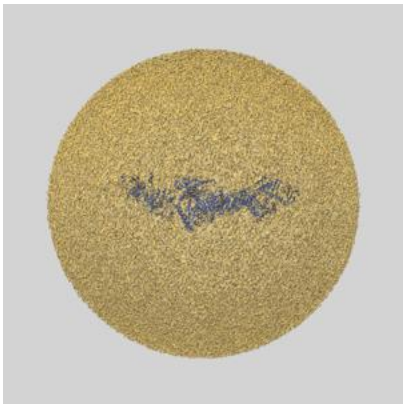
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20814 and PDB model 6ULG. Per-residue inclusion information can be found in section 3 on page 7.

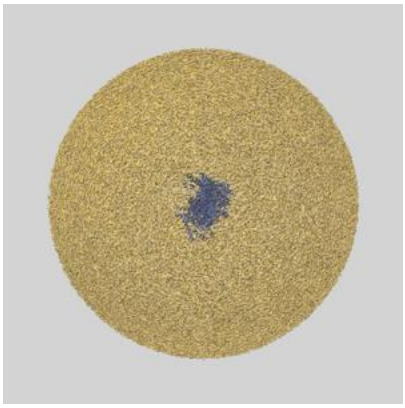
9.1 Map-model overlay



X



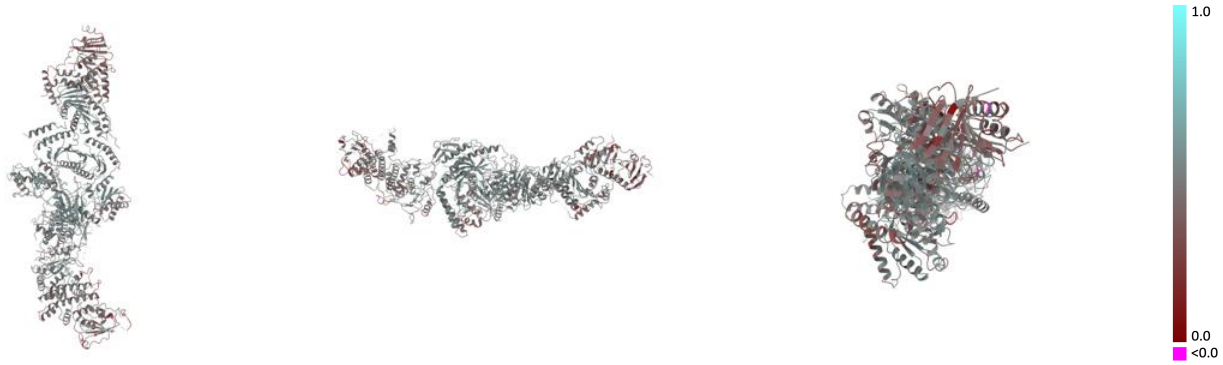
Y



Z

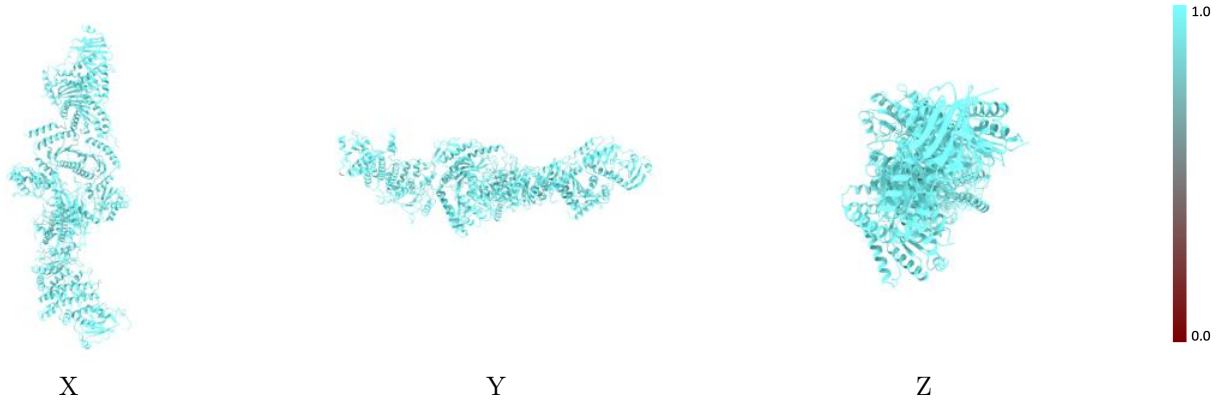
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



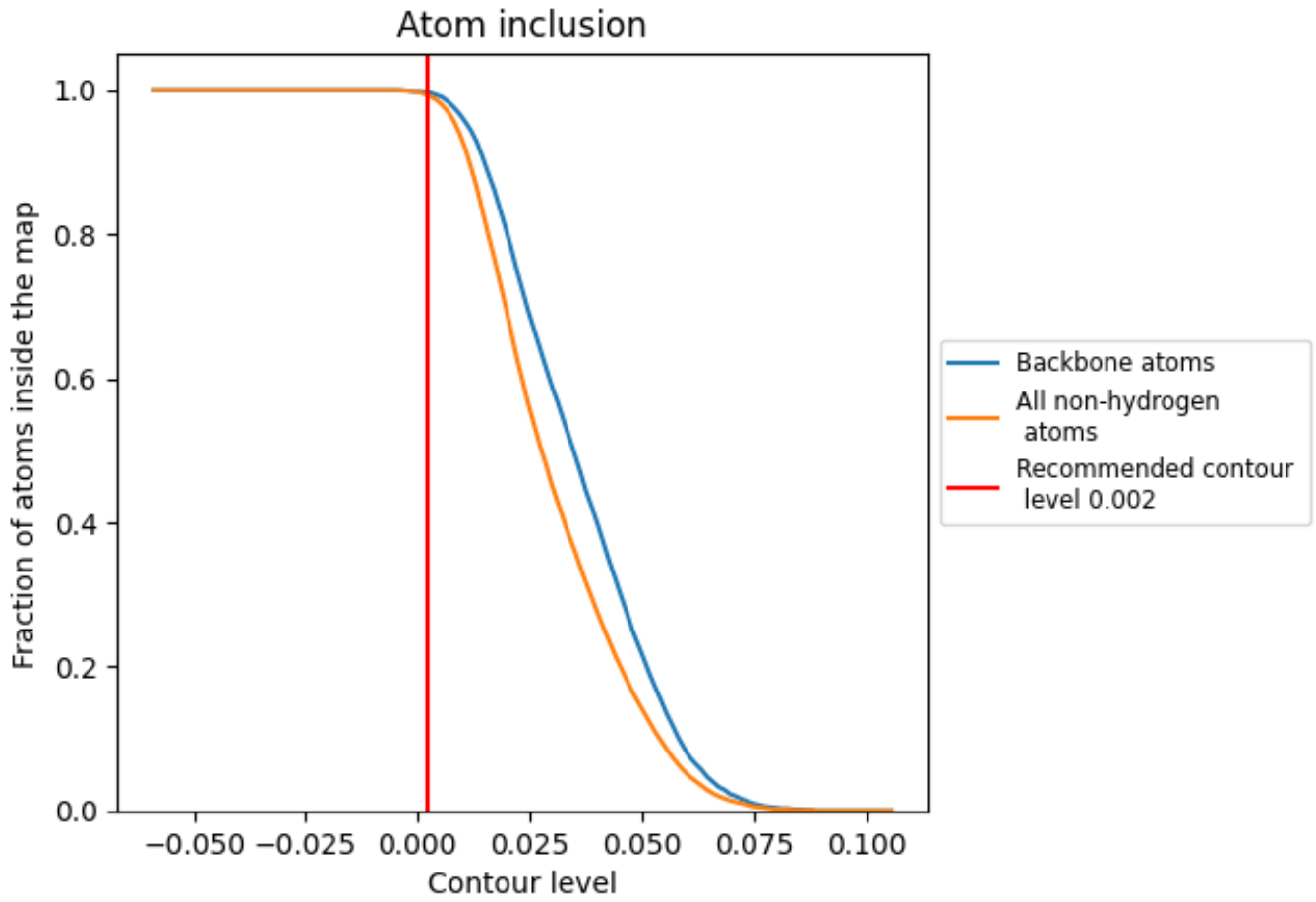
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.002).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9930	0.4670
A	0.9960	0.4760
B	0.9950	0.4880
C	0.9970	0.4410
D	0.9950	0.3670
E	1.0000	0.4100
F	0.9940	0.4860
G	0.9940	0.5010
L	0.9940	0.4630
N	0.9890	0.4630