



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:28 AM UTC

PDB ID : 6NZD / pdb_00006nzd
EMDB ID : EMD-0554
Title : Cryo-EM Structure of the Lysosomal Folliculin Complex (FLCN-FNIP2-RagA-RagC-Ragulator)
Authors : Fromm, S.A.; Young, L.N.; Hurley, J.H.
Deposited on : 2019-02-13
Resolution : 3.60 Å (reported)
Based on initial models : 6B9X, 3V42, 6CES, 6EHR, 3LLU

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

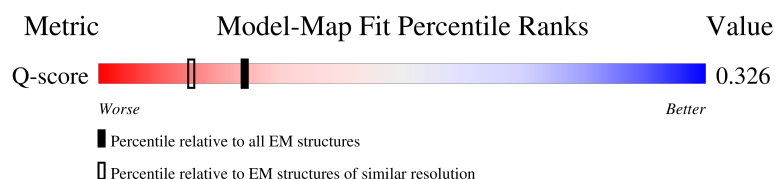
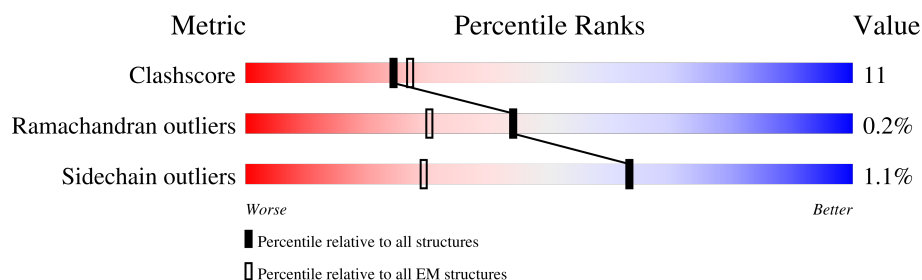
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	166	36% 43% 5% 51%
2	B	127	18% 93% 6%
3	C	124	25% 81% 15% ...
4	D	99	48% 82% 8% 9%

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Mol	Chain	Length	Quality of chain
5	E	173	17%49%47%
6	F	313	9%67%6%27%
7	G	404	5%56%17%26%
8	H	622	18%40%20%38%
9	I	1117	5%31%65%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13633 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 Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	81	622	397	103	122	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP Q6IAA8
A	-3	ASN	-	expression tag	UNP Q6IAA8
A	-2	ALA	-	expression tag	UNP Q6IAA8
A	-1	GLU	-	expression tag	UNP Q6IAA8
A	0	PHE	-	expression tag	UNP Q6IAA8
A	1	MET	-	expression tag	UNP Q6IAA8
A	2	ALA	-	expression tag	UNP Q6IAA8
A	3	CYS	-	expression tag	UNP Q6IAA8
A	4	CYS	-	expression tag	UNP Q6IAA8

- Molecule 2 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	126	949	596	163	183	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q9Y2Q5
B	0	ALA	-	expression tag	UNP Q9Y2Q5

- Molecule 3 is a protein called Regulator complex protein LAMTOR3.

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

- Molecule 4 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	90	Total	C	N	O	S	0	0
			684	427	125	130	2		

- Molecule 5 is a protein called Hepatitis B virus x interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	91	Total	C	N	O	S	0	0
			666	406	115	138	7		

- Molecule 6 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	227	Total	C	N	O	S	0	0
			1830	1169	310	338	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	299	Total	C	N	O	S	0	0
			2429	1570	391	454	14		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	GLY	-	expression tag	UNP Q9HB90
G	-3	ALA	-	expression tag	UNP Q9HB90
G	-2	ASP	-	expression tag	UNP Q9HB90
G	-1	SER	-	expression tag	UNP Q9HB90
G	0	ARG	-	expression tag	UNP Q9HB90
G	181	ASN	ASP	engineered mutation	UNP Q9HB90

- Molecule 8 is a protein called Folliculin.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	387	Total	C	N	O	S	0	0
			2934	1896	510	508	20		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-42	MET	-	initiating methionine	UNP Q8NFG4
H	-41	ALA	-	expression tag	UNP Q8NFG4
H	-40	SER	-	expression tag	UNP Q8NFG4
H	-39	TRP	-	expression tag	UNP Q8NFG4
H	-38	SER	-	expression tag	UNP Q8NFG4
H	-37	HIS	-	expression tag	UNP Q8NFG4
H	-36	PRO	-	expression tag	UNP Q8NFG4
H	-35	GLN	-	expression tag	UNP Q8NFG4
H	-34	PHE	-	expression tag	UNP Q8NFG4
H	-33	GLU	-	expression tag	UNP Q8NFG4
H	-32	LYS	-	expression tag	UNP Q8NFG4
H	-31	GLY	-	expression tag	UNP Q8NFG4
H	-30	GLY	-	expression tag	UNP Q8NFG4
H	-29	GLY	-	expression tag	UNP Q8NFG4
H	-28	ALA	-	expression tag	UNP Q8NFG4
H	-27	ARG	-	expression tag	UNP Q8NFG4
H	-26	GLY	-	expression tag	UNP Q8NFG4
H	-25	GLY	-	expression tag	UNP Q8NFG4
H	-24	SER	-	expression tag	UNP Q8NFG4
H	-23	GLY	-	expression tag	UNP Q8NFG4
H	-22	GLY	-	expression tag	UNP Q8NFG4
H	-21	GLY	-	expression tag	UNP Q8NFG4
H	-20	SER	-	expression tag	UNP Q8NFG4
H	-19	TRP	-	expression tag	UNP Q8NFG4
H	-18	SER	-	expression tag	UNP Q8NFG4
H	-17	HIS	-	expression tag	UNP Q8NFG4
H	-16	PRO	-	expression tag	UNP Q8NFG4
H	-15	GLN	-	expression tag	UNP Q8NFG4
H	-14	PHE	-	expression tag	UNP Q8NFG4
H	-13	GLU	-	expression tag	UNP Q8NFG4
H	-12	LYS	-	expression tag	UNP Q8NFG4
H	-11	GLY	-	expression tag	UNP Q8NFG4
H	-10	PHE	-	expression tag	UNP Q8NFG4
H	-9	ASP	-	expression tag	UNP Q8NFG4
H	-8	TYR	-	expression tag	UNP Q8NFG4
H	-7	LYS	-	expression tag	UNP Q8NFG4
H	-6	ASP	-	expression tag	UNP Q8NFG4
H	-5	ASP	-	expression tag	UNP Q8NFG4
H	-4	ASP	-	expression tag	UNP Q8NFG4
H	-3	ASP	-	expression tag	UNP Q8NFG4
H	-2	LYS	-	expression tag	UNP Q8NFG4
H	-1	GLY	-	expression tag	UNP Q8NFG4
H	0	THR	-	expression tag	UNP Q8NFG4

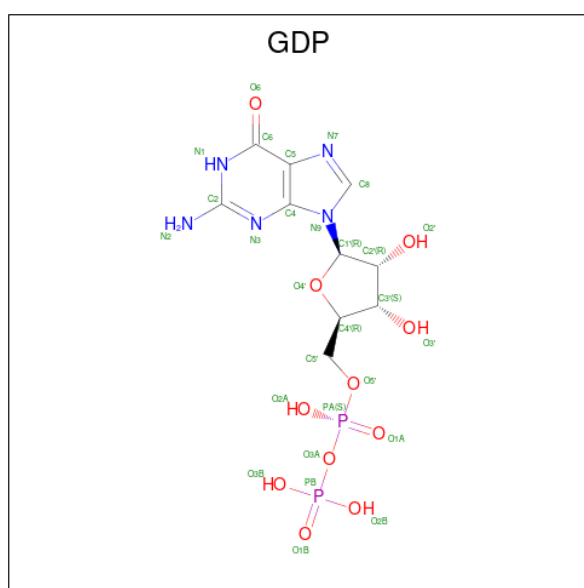
- Molecule 9 is a protein called Folliculin-interacting protein 2.

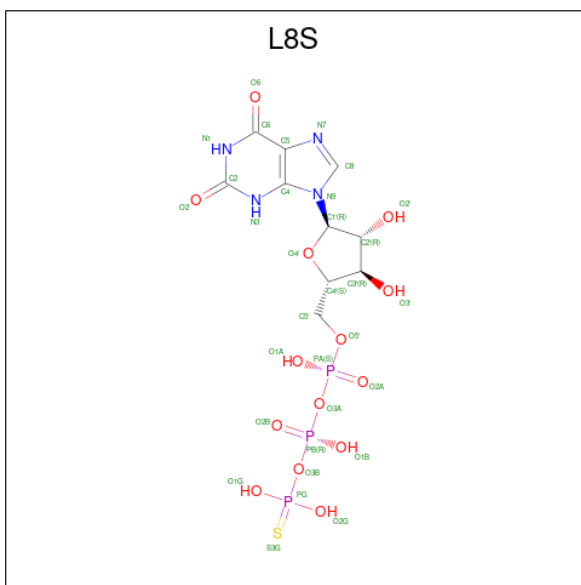
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	388	2520	1598	459	454	9	0	0

There are 3 discrepancies between the modelled and reference sequences:

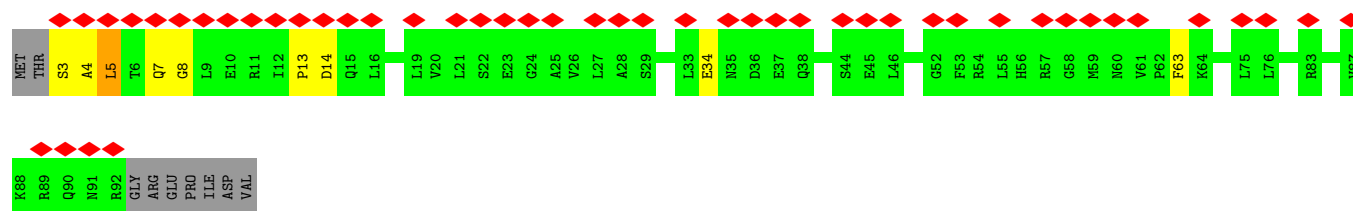
Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	expression tag	UNP Q9P278
I	-1	GLY	-	expression tag	UNP Q9P278
I	0	THR	-	expression tag	UNP Q9P278

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

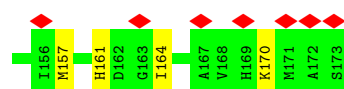
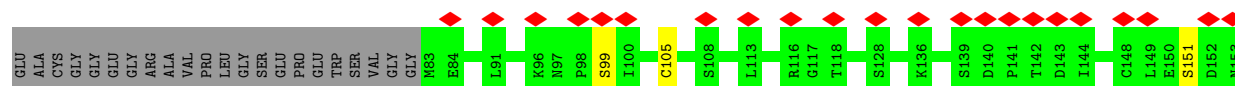




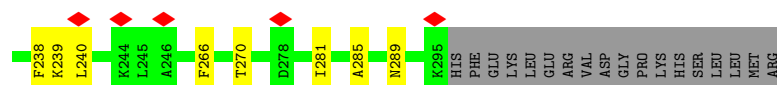
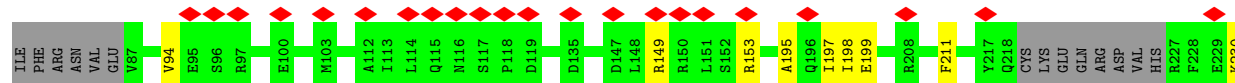
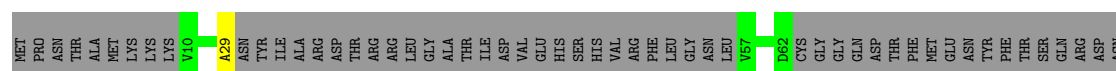
Mol	Chain	Residues	Atoms						AltConf
11	G	1	Total	C	N	O	P	S	0
			32	10	4	14	3	1	



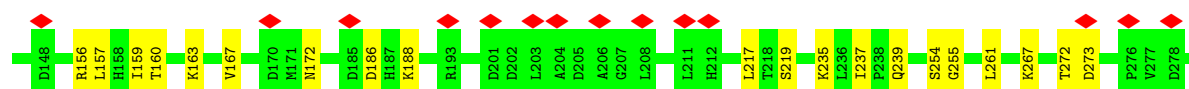
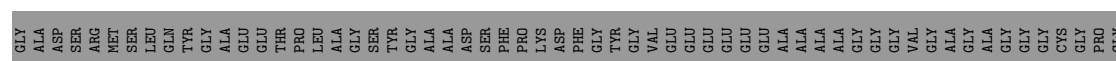
• Molecule 5: Hepatitis B virus x interacting protein

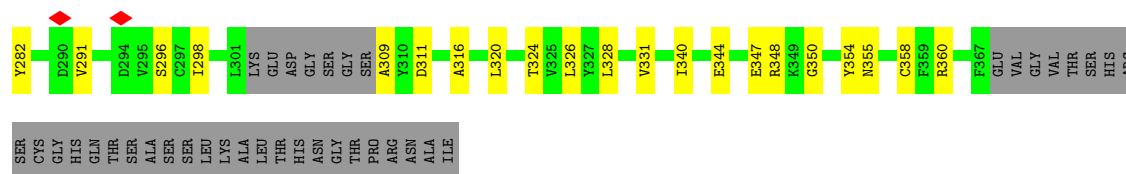


• Molecule 6: Ras-related GTP-binding protein A

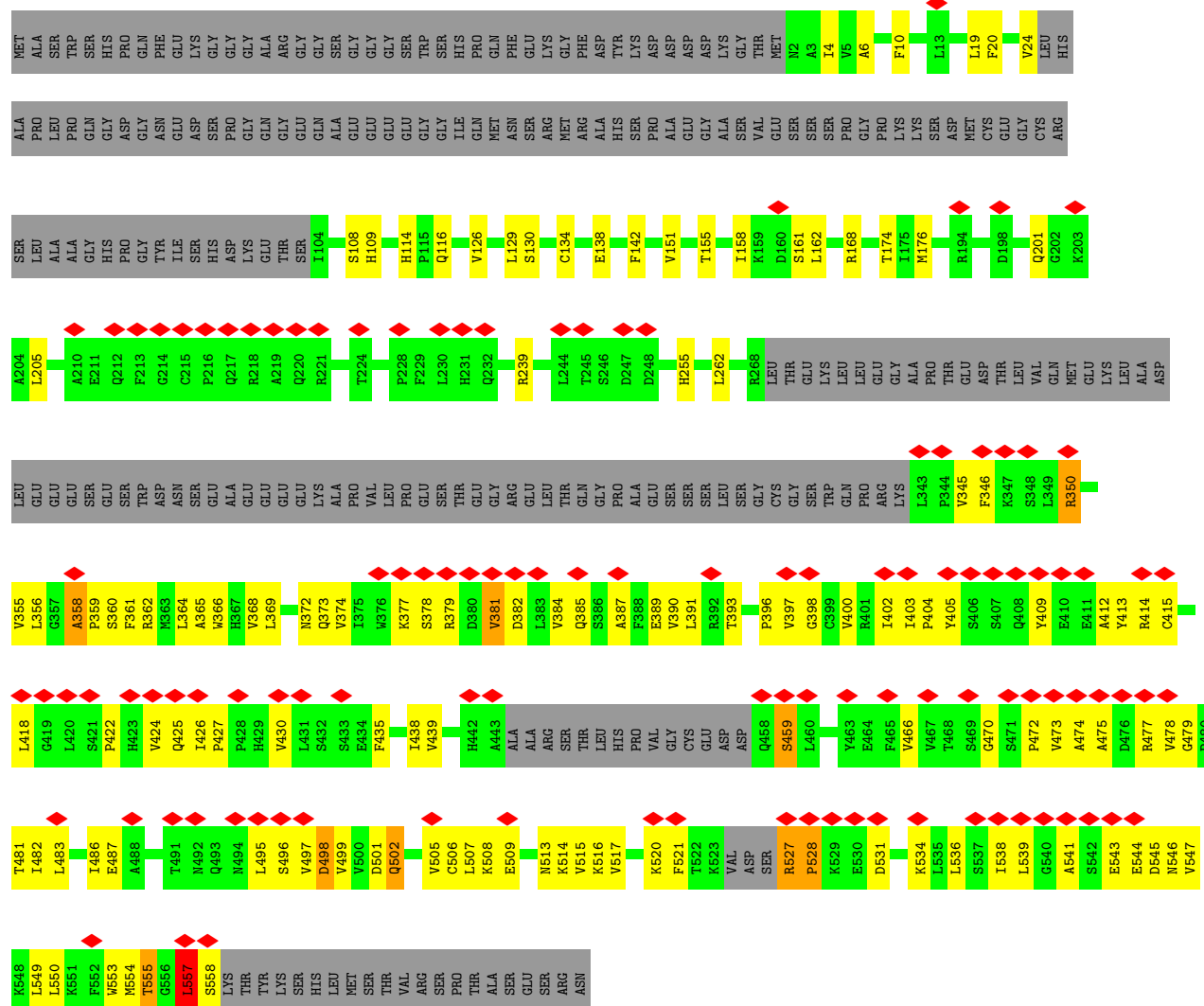


• Molecule 7: Ras-related GTP-binding protein C

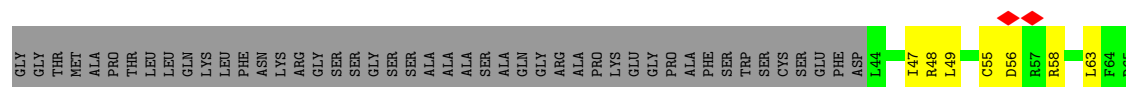


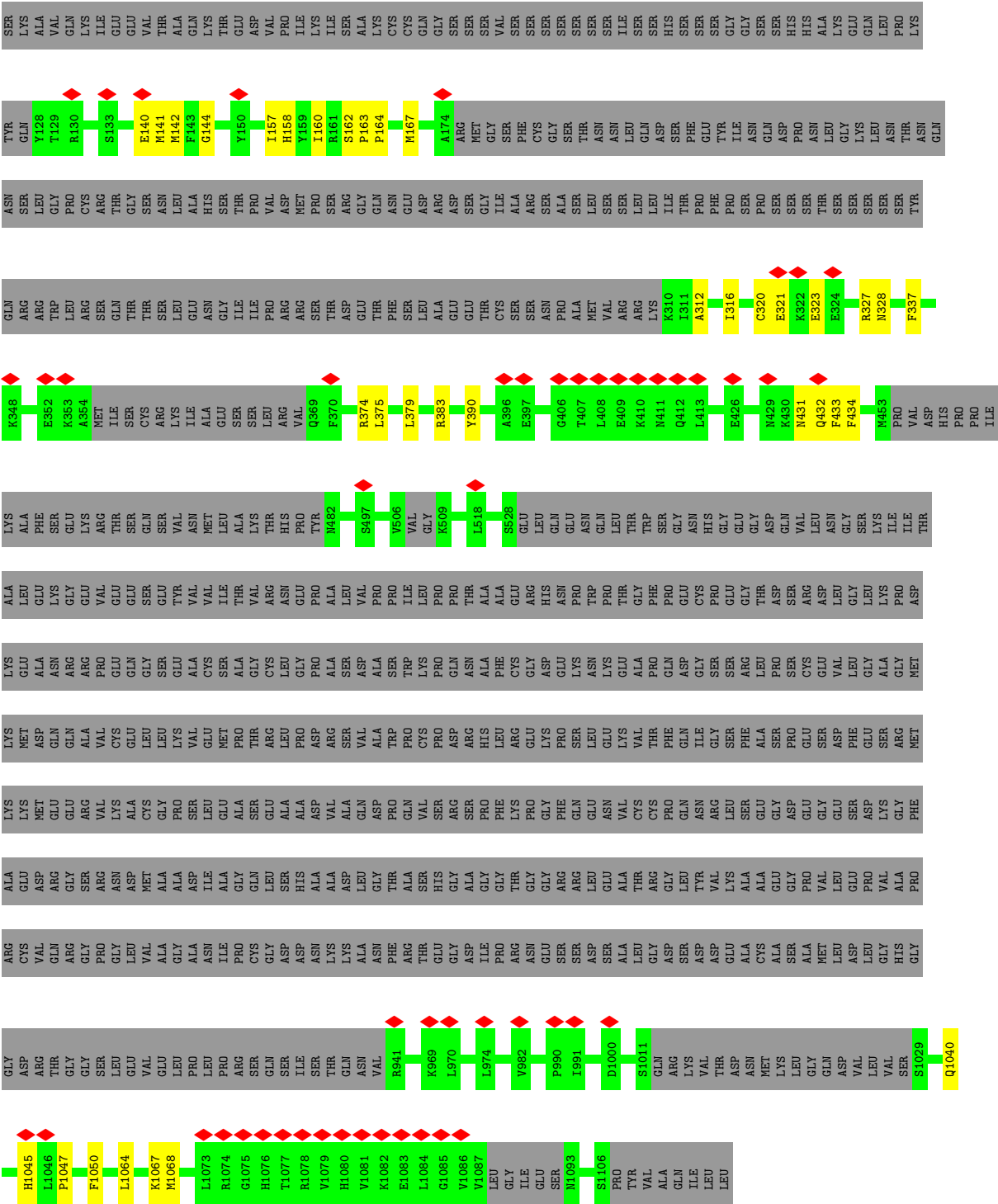


• Molecule 8: Folliculin



• Molecule 9: Folliculin-interacting protein 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	163376	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 ($e^-/\text{\AA}^2$)	65.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.791	Depositor
Minimum map value	-0.361	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.16	Depositor
Map size ($\text{\AA}$)	413.64, 413.64, 413.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.149, 1.149, 1.149	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: L8S, GDP

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	0.27	0/633	0.42	0/864
2	B	0.38	1/960 (0.1%)	0.52	0/1300
3	C	0.43	1/956 (0.1%)	0.64	4/1297 (0.3%)
4	D	0.42	1/692 (0.1%)	0.59	0/934
5	E	0.34	0/672	0.52	0/911
6	F	0.19	0/1859	0.51	0/2502
7	G	0.30	0/2481	0.57	0/3350
8	H	1.56	64/3005 (2.1%)	0.99	18/4085 (0.4%)
9	I	0.20	0/2571	0.57	4/3518 (0.1%)
All	All	0.78	67/13829 (0.5%)	0.67	26/18761 (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
9	I	0	2

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	369	LEU	C-O	-7.86	1.15	1.24
8	H	505	VAL	C-O	-7.57	1.15	1.24
8	H	466	VAL	C-O	-7.50	1.16	1.24
8	H	550	LEU	C-O	-6.80	1.16	1.24
8	H	362	ARG	C-O	-6.72	1.16	1.24
8	H	365	ALA	C-O	-6.61	1.16	1.24
8	H	553	TRP	C-O	-6.45	1.15	1.24
8	H	364	LEU	C-O	-6.39	1.16	1.24
8	H	487	GLU	C-O	-6.31	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	482	ILE	C-O	-6.25	1.16	1.24
8	H	555	THR	C-O	-6.18	1.16	1.24
3	C	87	PRO	C-O	-6.14	1.16	1.24
8	H	385	GLN	C-O	-6.03	1.17	1.24
8	H	360	SER	C-O	-5.97	1.17	1.24
8	H	400	VAL	C-O	-5.97	1.17	1.24
8	H	346	PHE	C-O	-5.93	1.16	1.23
8	H	397	VAL	C-O	-5.88	1.17	1.24
8	H	547	VAL	C-O	-5.87	1.17	1.24
8	H	486	ILE	C-O	-5.82	1.17	1.24
4	D	34	GLU	C-O	-5.79	1.17	1.24
8	H	356	LEU	C-O	-5.76	1.16	1.24
8	H	418	LEU	C-O	-5.72	1.17	1.24
8	H	384	VAL	C-O	-5.70	1.17	1.24
8	H	404	PRO	C-O	-5.69	1.17	1.24
8	H	513	ASN	C-O	-5.69	1.17	1.24
8	H	390	VAL	C-O	-5.64	1.17	1.24
8	H	413	TYR	C-O	-5.61	1.17	1.24
8	H	545	ASP	C-O	-5.59	1.17	1.24
2	B	36	GLY	C-O	-5.56	1.18	1.24
8	H	387	ALA	C-O	-5.56	1.17	1.24
8	H	544	GLU	C-O	-5.52	1.17	1.24
8	H	470	GLY	C-O	-5.48	1.18	1.24
8	H	393	THR	C-O	-5.48	1.17	1.24
8	H	368	VAL	C-O	-5.47	1.18	1.24
8	H	361	PHE	C-O	-5.46	1.17	1.24
8	H	516	LYS	C-O	-5.45	1.17	1.24
8	H	502	GLN	C-O	-5.42	1.17	1.24
8	H	382	ASP	C-O	-5.40	1.17	1.24
8	H	536	LEU	C-O	-5.39	1.17	1.24
8	H	358	ALA	C-O	-5.38	1.19	1.24
8	H	350	ARG	C-O	-5.38	1.17	1.24
8	H	345	VAL	C-O	-5.37	1.18	1.23
8	H	478	VAL	C-O	-5.36	1.17	1.24
8	H	409	TYR	C-O	-5.34	1.17	1.23
8	H	391	LEU	C-O	-5.34	1.17	1.24
8	H	472	PRO	C-O	-5.32	1.17	1.23
8	H	546	ASN	C-O	-5.31	1.18	1.24
8	H	426	ILE	C-O	-5.28	1.18	1.24
8	H	438	ILE	C-O	-5.26	1.18	1.24
8	H	483	LEU	C-O	-5.26	1.18	1.24
8	H	374	VAL	C-O	-5.25	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	501	ASP	C-O	-5.23	1.18	1.24
8	H	507	LEU	C-O	-5.20	1.18	1.24
8	H	541	ALA	CA-CB	-5.20	1.45	1.53
8	H	439	VAL	C-O	-5.18	1.18	1.24
8	H	481	THR	C-O	-5.18	1.18	1.24
8	H	373	GLN	C-O	-5.17	1.17	1.23
8	H	412	ALA	C-O	-5.17	1.17	1.24
8	H	479	GLY	C-O	-5.14	1.17	1.24
8	H	508	LYS	C-O	-5.10	1.18	1.24
8	H	534	LYS	C-O	-5.10	1.18	1.24
8	H	517	VAL	C-O	-5.09	1.18	1.24
8	H	366	TRP	C-O	-5.09	1.18	1.24
8	H	398	GLY	C-O	-5.08	1.18	1.24
8	H	475	ALA	C-O	-5.04	1.17	1.24
8	H	396	PRO	C-O	-5.02	1.18	1.23
8	H	549	LEU	C-O	-5.01	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	477	ARG	N-CA-C	10.83	124.38	111.82
8	H	430	VAL	N-CA-C	7.83	118.54	111.81
8	H	528	PRO	N-CA-C	-7.04	100.14	111.19
8	H	355	VAL	N-CA-C	7.02	117.13	110.53
3	C	87	PRO	CA-C-N	6.85	131.29	121.50
3	C	87	PRO	C-N-CA	6.85	131.29	121.50
8	H	389	GLU	CA-C-O	-6.53	113.97	120.82
3	C	86	LEU	CA-CB-CG	6.47	138.94	116.30
9	I	144	GLY	CA-C-N	6.38	130.39	120.82
9	I	144	GLY	C-N-CA	6.38	130.39	120.82
8	H	427	PRO	N-CA-C	6.28	118.36	110.70
8	H	389	GLU	N-CA-C	-6.12	104.52	111.07
8	H	414	ARG	N-CA-C	5.88	117.77	111.36
8	H	402	ILE	N-CA-C	5.87	116.32	108.11
9	I	431	ASN	CA-C-N	5.77	132.57	121.54
9	I	431	ASN	C-N-CA	5.77	132.57	121.54
8	H	381	VAL	N-CA-C	5.58	115.78	110.42
8	H	499	VAL	N-CA-C	-5.54	104.97	110.62
8	H	378	SER	N-CA-C	5.26	117.08	108.76
8	H	390	VAL	N-CA-C	5.25	115.46	110.53
8	H	544	GLU	N-CA-C	5.21	116.96	111.28
8	H	459	SER	N-CA-C	5.14	117.49	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	426	ILE	CA-C-N	5.12	125.65	120.38
8	H	426	ILE	C-N-CA	5.12	125.65	120.38
8	H	557	LEU	N-CA-C	-5.11	106.88	114.64
3	C	86	LEU	CB-CG-CD2	5.06	125.89	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	162	SER	Peptide
9	I	337	PHE	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	622	0	637	17	0
2	B	949	0	960	27	0
3	C	939	0	962	47	0
4	D	684	0	694	9	0
5	E	666	0	663	8	0
6	F	1830	0	1827	30	0
7	G	2429	0	2404	103	0
8	H	2934	0	2817	71	0
9	I	2520	0	1865	47	0
10	F	28	0	12	0	0
11	G	32	0	0	0	0
All	All	13633	0	12841	284	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 11.

All (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:CE	6:F:198:ILE:HG23	1.33	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:LEU:CD2	3:C:118:ARG:HD2	1.06	1.50
3:C:86:LEU:HG	3:C:87:PRO:CD	1.41	1.49
3:C:86:LEU:CD2	3:C:118:ARG:CD	1.86	1.48
8:H:506:CYS:SG	9:I:1064:LEU:HB3	1.66	1.34
1:A:66:ILE:HG21	3:C:59:GLN:NE2	1.43	1.33
3:C:86:LEU:HD21	3:C:118:ARG:CG	1.57	1.32
3:C:86:LEU:CG	3:C:87:PRO:HD3	1.62	1.27
7:G:131:GLU:HG3	7:G:167:VAL:CG2	1.65	1.25
8:H:520:LYS:HE2	9:I:1050:PHE:CB	1.67	1.24
2:B:1:MET:CE	6:F:198:ILE:CG2	2.18	1.20
7:G:65:LEU:HD13	7:G:137:THR:CG2	1.72	1.20
7:G:123:PHE:CG	7:G:163:LYS:HE3	1.76	1.19
8:H:520:LYS:CE	9:I:1050:PHE:CB	2.20	1.18
3:C:86:LEU:HD21	3:C:118:ARG:CD	1.56	1.18
3:C:86:LEU:CG	3:C:87:PRO:CD	2.19	1.17
7:G:65:LEU:HD13	7:G:137:THR:HG21	1.24	1.12
7:G:131:GLU:HG3	7:G:167:VAL:HG21	1.14	1.12
7:G:74:LYS:NZ	7:G:118:PRO:O	1.82	1.11
2:B:1:MET:HE1	6:F:198:ILE:CG2	1.76	1.10
2:B:1:MET:HE3	6:F:198:ILE:HG23	1.21	1.10
2:B:47:ALA:HB2	7:G:350:GLY:O	1.52	1.09
2:B:1:MET:HE1	6:F:198:ILE:HG23	1.13	1.07
7:G:65:LEU:CD1	7:G:137:THR:CG2	2.32	1.07
8:H:527:ARG:HH12	9:I:1045:HIS:CB	1.69	1.06
2:B:1:MET:CE	6:F:197:ILE:HG22	1.85	1.04
2:B:1:MET:HE3	6:F:197:ILE:HG22	1.04	1.03
7:G:69:LEU:O	7:G:120:GLN:N	1.93	1.02
3:C:86:LEU:HD21	3:C:118:ARG:HG3	1.37	1.02
2:B:1:MET:HE3	6:F:197:ILE:CG2	1.88	1.01
3:C:86:LEU:HG	3:C:87:PRO:HD2	1.01	1.01
3:C:86:LEU:CB	3:C:87:PRO:HD3	1.91	1.01
1:A:66:ILE:HG21	3:C:59:GLN:HE22	1.02	0.98
7:G:140:LEU:HD23	7:G:141:ILE:N	1.78	0.98
7:G:65:LEU:CD1	7:G:137:THR:HG23	1.91	0.98
7:G:65:LEU:HD11	7:G:137:THR:OG1	1.63	0.98
8:H:520:LYS:HE2	9:I:1047:PRO:HD2	1.45	0.97
3:C:86:LEU:HG	3:C:87:PRO:HD3	1.27	0.97
8:H:520:LYS:CE	9:I:1047:PRO:HD2	1.95	0.97
7:G:69:LEU:O	7:G:119:GLY:C	2.08	0.95
7:G:123:PHE:HZ	7:G:160:THR:HG22	1.32	0.94
7:G:123:PHE:CD1	7:G:163:LYS:HE3	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:538:ILE:HD13	9:I:1040:GLN:CB	1.98	0.92
3:C:86:LEU:HD23	3:C:118:ARG:HD2	1.51	0.92
7:G:123:PHE:CZ	7:G:160:THR:HG22	2.06	0.90
7:G:118:PRO:HG2	7:G:121:MET:CE	2.04	0.88
7:G:121:MET:O	7:G:156:ARG:NH2	2.08	0.86
2:B:47:ALA:CB	7:G:350:GLY:O	2.22	0.86
3:C:86:LEU:HD22	3:C:118:ARG:HD2	0.87	0.86
2:B:1:MET:HE1	6:F:198:ILE:HG12	1.57	0.86
3:C:86:LEU:HD23	3:C:118:ARG:CD	2.00	0.85
2:B:1:MET:SD	6:F:289:ASN:OD1	2.34	0.85
8:H:520:LYS:CD	9:I:1050:PHE:CB	2.54	0.85
8:H:520:LYS:HZ1	9:I:1047:PRO:HG2	1.42	0.85
3:C:5:LEU:HD11	3:C:113:LEU:HD21	1.58	0.85
3:C:86:LEU:CB	3:C:87:PRO:CD	2.48	0.85
7:G:123:PHE:CD2	7:G:163:LYS:HE3	2.11	0.84
7:G:69:LEU:O	7:G:119:GLY:CA	2.26	0.84
7:G:131:GLU:HG3	7:G:167:VAL:HG23	1.56	0.83
2:B:1:MET:CE	6:F:197:ILE:CG2	2.53	0.83
3:C:86:LEU:CD1	3:C:87:PRO:HD3	2.09	0.82
3:C:86:LEU:CD2	3:C:118:ARG:HG3	2.08	0.80
8:H:527:ARG:NH1	9:I:1045:HIS:CB	2.44	0.80
8:H:509:GLU:OE1	9:I:1064:LEU:HD22	1.83	0.78
8:H:520:LYS:NZ	9:I:1047:PRO:HG2	1.99	0.78
7:G:131:GLU:CG	7:G:167:VAL:HG21	2.07	0.77
1:A:66:ILE:HG21	3:C:59:GLN:HE21	1.50	0.77
1:A:66:ILE:CG2	3:C:59:GLN:NE2	2.37	0.76
7:G:118:PRO:HD2	7:G:121:MET:SD	2.26	0.75
2:B:1:MET:SD	6:F:198:ILE:HG21	2.27	0.75
7:G:65:LEU:HD12	7:G:137:THR:HG23	1.70	0.74
7:G:67:MET:HE1	7:G:134:PHE:CZ	2.23	0.74
8:H:126:VAL:O	8:H:130:SER:HB3	1.87	0.74
2:B:1:MET:SD	6:F:198:ILE:CG2	2.76	0.73
8:H:506:CYS:SG	9:I:1064:LEU:CB	2.62	0.73
8:H:555:THR:HA	8:H:558:SER:HB2	1.73	0.71
8:H:502:GLN:NE2	9:I:1067:LYS:CB	2.53	0.71
6:F:195:ALA:O	6:F:199:GLU:HB3	1.90	0.71
8:H:509:GLU:OE1	9:I:1064:LEU:CD2	2.37	0.71
7:G:135:ARG:HG3	7:G:167:VAL:HG22	1.71	0.70
7:G:67:MET:HE1	7:G:134:PHE:HZ	1.55	0.70
7:G:123:PHE:CD2	7:G:163:LYS:CE	2.75	0.69
2:B:28:GLU:HB3	7:G:347:GLU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HE1	6:F:198:ILE:CG1	2.22	0.69
8:H:520:LYS:CE	9:I:1047:PRO:CD	2.68	0.69
8:H:520:LYS:NZ	9:I:1050:PHE:CB	2.54	0.69
7:G:74:LYS:CE	7:G:118:PRO:O	2.40	0.69
3:C:86:LEU:HD22	3:C:118:ARG:CD	1.82	0.68
8:H:502:GLN:HE22	9:I:1067:LYS:CB	2.07	0.67
7:G:65:LEU:CD1	7:G:137:THR:OG1	2.41	0.67
5:E:105:CYS:SG	5:E:164:ILE:HD11	2.34	0.67
8:H:377:LYS:CE	8:H:422:PRO:O	2.43	0.67
3:C:5:LEU:HD11	3:C:113:LEU:CD2	2.24	0.67
7:G:131:GLU:CG	7:G:167:VAL:CG2	2.60	0.66
1:A:66:ILE:HD13	3:C:59:GLN:HE22	1.61	0.65
7:G:74:LYS:HZ1	7:G:118:PRO:C	1.97	0.65
8:H:557:LEU:HD12	8:H:557:LEU:C	2.21	0.65
4:D:5:LEU:H	4:D:5:LEU:CD1	2.10	0.65
1:A:129:LEU:HD23	5:E:157:MET:HE3	1.79	0.64
6:F:230:LYS:HD2	7:G:298:ILE:HD11	1.79	0.64
3:C:6:LYS:HG2	3:C:35:VAL:HG22	1.80	0.64
7:G:120:GLN:HG3	7:G:156:ARG:NE	2.12	0.64
7:G:140:LEU:HD23	7:G:140:LEU:C	2.22	0.64
3:C:86:LEU:CD2	3:C:118:ARG:CG	2.37	0.63
3:C:86:LEU:HB2	3:C:87:PRO:HD3	1.77	0.63
3:C:86:LEU:HD12	3:C:87:PRO:HD3	1.81	0.63
2:B:1:MET:HE1	6:F:198:ILE:CB	2.28	0.63
8:H:514:LYS:HE2	8:H:539:LEU:O	2.00	0.62
2:B:47:ALA:HB2	7:G:350:GLY:C	2.23	0.62
1:A:143:LEU:HD11	5:E:164:ILE:HD12	1.81	0.62
5:E:161:HIS:O	5:E:164:ILE:HG22	1.98	0.62
7:G:67:MET:HE3	7:G:134:PHE:HE1	1.64	0.62
4:D:3:SER:O	4:D:7:GLN:HG2	2.01	0.61
7:G:100:TYR:HB3	7:G:116:ASP:HB3	1.83	0.60
7:G:118:PRO:HG2	7:G:121:MET:HE1	1.83	0.60
7:G:118:PRO:CG	7:G:121:MET:CE	2.77	0.60
4:D:5:LEU:H	4:D:5:LEU:HD12	1.66	0.60
8:H:520:LYS:HE3	9:I:1047:PRO:CD	2.31	0.60
7:G:118:PRO:CG	7:G:121:MET:HE2	2.31	0.60
8:H:350:ARG:HH22	8:H:495:LEU:HB2	1.67	0.60
1:A:64:ASN:ND2	7:G:358:CYS:SG	2.75	0.59
7:G:123:PHE:CG	7:G:163:LYS:CE	2.70	0.59
2:B:1:MET:SD	6:F:285:ALA:HB1	2.43	0.59
9:I:49:LEU:HD11	9:I:375:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:131:GLU:CG	7:G:167:VAL:HG23	2.32	0.58
8:H:520:LYS:HD2	9:I:1050:PHE:CB	2.32	0.58
6:F:149:ARG:HB3	6:F:153:ARG:HH21	1.67	0.58
7:G:118:PRO:CD	7:G:121:MET:SD	2.91	0.58
8:H:377:LYS:HE2	8:H:422:PRO:O	2.03	0.58
7:G:123:PHE:CD1	7:G:163:LYS:CE	2.81	0.58
8:H:201:GLN:O	8:H:205:LEU:HB2	2.03	0.58
7:G:123:PHE:CE2	7:G:163:LYS:NZ	2.72	0.57
7:G:188:LYS:HE2	7:G:217:LEU:HD13	1.87	0.57
1:A:64:ASN:ND2	3:C:62:LYS:NZ	2.53	0.57
7:G:69:LEU:O	7:G:119:GLY:HA2	2.03	0.56
7:G:123:PHE:CD2	7:G:163:LYS:NZ	2.73	0.56
7:G:135:ARG:HG3	7:G:167:VAL:CG2	2.37	0.55
7:G:99:ILE:HD11	7:G:128:PHE:CE1	2.42	0.55
7:G:326:LEU:HG	7:G:340:ILE:HG12	1.89	0.55
7:G:67:MET:CE	7:G:134:PHE:CE1	2.89	0.55
6:F:266:PHE:HB3	6:F:270:THR:HG23	1.89	0.55
6:F:29:ALA:HB1	6:F:240:LEU:HD11	1.89	0.54
8:H:557:LEU:C	8:H:557:LEU:CD1	2.80	0.54
9:I:320:CYS:SG	9:I:321:GLU:N	2.80	0.54
8:H:538:ILE:CD1	9:I:1040:GLN:CB	2.81	0.54
8:H:521:PHE:CZ	8:H:527:ARG:HG2	2.43	0.54
7:G:123:PHE:CE2	7:G:163:LYS:CE	2.91	0.54
8:H:520:LYS:HE3	9:I:1047:PRO:HD2	1.83	0.53
1:A:116:HIS:HD2	4:D:8:GLY:C	2.15	0.53
7:G:121:MET:C	7:G:156:ARG:NH2	2.66	0.53
9:I:47:ILE:HD13	9:I:383:ARG:HG3	1.89	0.53
3:C:115:GLU:OE1	3:C:118:ARG:NE	2.39	0.53
9:I:167:MET:HB3	9:I:316:ILE:HG12	1.88	0.53
2:B:1:MET:HB2	6:F:197:ILE:HG21	1.90	0.53
7:G:115:TRP:CZ3	7:G:133:ILE:HG23	2.44	0.53
7:G:99:ILE:HD11	7:G:128:PHE:HE1	1.74	0.53
8:H:10:PHE:HB2	8:H:129:LEU:HD13	1.91	0.53
8:H:520:LYS:NZ	9:I:1047:PRO:CG	2.72	0.53
2:B:1:MET:HE3	6:F:198:ILE:CG2	2.13	0.52
2:B:1:MET:HE2	6:F:197:ILE:CG2	2.38	0.52
7:G:135:ARG:CG	7:G:167:VAL:HG22	2.40	0.52
2:B:47:ALA:CB	7:G:350:GLY:C	2.82	0.52
8:H:502:GLN:HG2	9:I:1068:MET:CB	2.40	0.52
8:H:403:ILE:HG13	8:H:415:CYS:HB3	1.92	0.52
9:I:55:CYS:SG	9:I:56:ASP:N	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:74:LYS:HE3	7:G:118:PRO:O	2.10	0.51
7:G:140:LEU:C	7:G:140:LEU:CD2	2.84	0.51
7:G:121:MET:C	7:G:156:ARG:HH22	2.18	0.51
9:I:63:LEU:HG	9:I:379:LEU:HD22	1.91	0.51
7:G:65:LEU:CD1	7:G:137:THR:CB	2.89	0.51
8:H:506:CYS:HA	9:I:1064:LEU:HD23	1.92	0.51
9:I:48:ARG:HG3	9:I:316:ILE:HB	1.93	0.51
7:G:122:ASP:O	7:G:130:TYR:OH	2.24	0.51
3:C:2:ALA:O	3:C:4:ASP:N	2.44	0.51
8:H:134:CYS:SG	8:H:155:THR:OG1	2.68	0.51
9:I:142:MET:HE2	9:I:312:ALA:HB1	1.92	0.51
8:H:520:LYS:CE	9:I:1047:PRO:HG2	2.41	0.50
8:H:498:ASP:C	8:H:498:ASP:OD1	2.53	0.50
7:G:118:PRO:HG2	7:G:121:MET:SD	2.52	0.49
8:H:24:VAL:HB	8:H:262:LEU:HD13	1.94	0.49
7:G:172:ASN:OD1	7:G:235:LYS:NZ	2.45	0.49
9:I:141:MET:HE1	9:I:160:ILE:HD11	1.92	0.49
7:G:186:ASP:OD1	7:G:186:ASP:N	2.44	0.49
5:E:99:SER:OG	5:E:170:LYS:HE3	2.13	0.48
8:H:377:LYS:HE3	8:H:422:PRO:O	2.12	0.48
8:H:509:GLU:OE1	9:I:1064:LEU:HD21	2.13	0.48
1:A:66:ILE:CG2	3:C:59:GLN:HE22	1.96	0.48
3:C:5:LEU:HD22	3:C:113:LEU:HD11	1.95	0.48
7:G:67:MET:CE	7:G:134:PHE:CZ	2.95	0.48
9:I:49:LEU:HD23	9:I:379:LEU:HD13	1.94	0.48
7:G:123:PHE:CE1	7:G:163:LYS:CE	2.96	0.48
7:G:67:MET:HE3	7:G:134:PHE:CE1	2.45	0.48
4:D:4:ALA:HA	4:D:7:GLN:CD	2.39	0.48
8:H:114:HIS:HD2	8:H:116:GLN:HB2	1.78	0.47
3:C:80:VAL:HG13	3:C:93:ILE:HD13	1.97	0.47
8:H:424:VAL:HG12	8:H:425:GLN:N	2.28	0.47
1:A:48:THR:OG1	1:A:49:ASP:N	2.47	0.47
2:B:31:LEU:O	6:F:281:ILE:HG13	2.14	0.47
6:F:195:ALA:O	6:F:199:GLU:CB	2.63	0.47
7:G:237:ILE:HG22	7:G:239:GLN:H	1.79	0.47
7:G:123:PHE:CE1	7:G:163:LYS:HE2	2.50	0.47
2:B:28:GLU:CB	7:G:347:GLU:O	2.63	0.47
7:G:78:GLN:NE2	7:G:102:ASP:OD2	2.48	0.47
7:G:254:SER:OG	7:G:255:GLY:N	2.48	0.47
8:H:502:GLN:HG2	9:I:1068:MET:CA	2.45	0.47
1:A:156:VAL:HG11	6:F:197:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:118:PRO:CD	7:G:121:MET:HE2	2.46	0.46
7:G:311:ASP:OD1	7:G:311:ASP:N	2.48	0.46
8:H:19:LEU:HD12	8:H:20:PHE:HB2	1.96	0.46
4:D:3:SER:O	4:D:3:SER:OG	2.24	0.46
8:H:557:LEU:HD12	8:H:558:SER:N	2.30	0.46
7:G:140:LEU:HD23	7:G:141:ILE:CA	2.46	0.46
8:H:521:PHE:CE2	8:H:527:ARG:HG2	2.50	0.46
8:H:176:MET:HE2	8:H:176:MET:HB3	1.85	0.46
8:H:381:VAL:HG22	8:H:405:TYR:CE2	2.50	0.46
9:I:328:ASN:ND2	9:I:390:TYR:OH	2.47	0.46
7:G:110:VAL:HG12	7:G:112:PHE:HB2	1.98	0.46
4:D:63:PHE:HA	5:E:151:SER:HB3	1.97	0.46
7:G:219:SER:O	7:G:219:SER:OG	2.34	0.46
9:I:158:HIS:HB2	9:I:167:MET:HG3	1.97	0.45
1:A:64:ASN:CG	3:C:62:LYS:NZ	2.75	0.45
8:H:520:LYS:CE	9:I:1047:PRO:CG	2.95	0.45
3:C:5:LEU:CD2	3:C:113:LEU:HD11	2.47	0.45
8:H:372:ASN:HB3	8:H:435:PHE:O	2.17	0.45
3:C:86:LEU:HD21	3:C:118:ARG:HD2	1.16	0.45
7:G:65:LEU:HD11	7:G:137:THR:CB	2.47	0.45
7:G:296:SER:OG	7:G:309:ALA:O	2.34	0.45
8:H:108:SER:O	8:H:109:HIS:ND1	2.49	0.45
6:F:195:ALA:O	6:F:199:GLU:CA	2.65	0.45
8:H:527:ARG:HD3	8:H:527:ARG:HA	1.32	0.44
6:F:211:PHE:HE2	6:F:239:LYS:HD3	1.81	0.44
8:H:108:SER:HB3	8:H:255:HIS:CD2	2.53	0.44
3:C:42:GLU:O	3:C:42:GLU:OE2	2.35	0.44
5:E:164:ILE:HD13	5:E:164:ILE:HG21	1.70	0.44
8:H:495:LEU:HD23	8:H:495:LEU:HA	1.60	0.44
8:H:142:PHE:HB3	9:I:157:ILE:HB	2.00	0.44
8:H:358:ALA:HB3	8:H:359:PRO:HD3	1.99	0.44
4:D:5:LEU:HD12	4:D:5:LEU:N	2.33	0.44
8:H:6:ALA:HA	8:H:20:PHE:O	2.18	0.44
9:I:323:GLU:HB3	9:I:327:ARG:HH21	1.82	0.44
7:G:272:THR:OG1	7:G:273:ASP:N	2.49	0.44
8:H:424:VAL:CG1	8:H:425:GLN:N	2.81	0.44
3:C:24:VAL:HG11	3:C:117:LEU:HD23	2.00	0.43
7:G:67:MET:CE	7:G:134:PHE:HE1	2.27	0.43
8:H:527:ARG:HH11	8:H:527:ARG:HD2	1.59	0.43
8:H:4:ILE:O	8:H:174:THR:HA	2.17	0.43
8:H:161:SER:OG	8:H:162:LEU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:58:ARG:NH1	9:I:140:GLU:OE2	2.51	0.43
9:I:432:GLN:O	9:I:434:PHE:N	2.52	0.43
3:C:62:LYS:HE2	7:G:354:TYR:HE2	1.68	0.43
7:G:254:SER:HB2	7:G:355:ASN:HD22	1.84	0.43
3:C:5:LEU:HD13	3:C:113:LEU:HD11	2.01	0.43
7:G:316:ALA:HB3	7:G:328:LEU:HB3	2.01	0.43
8:H:515:VAL:CG1	8:H:554:MET:HG3	2.49	0.43
1:A:66:ILE:HD13	3:C:59:GLN:NE2	2.32	0.43
6:F:238:PHE:HB2	7:G:291:VAL:HG21	2.00	0.42
7:G:331:VAL:O	7:G:360:ARG:NE	2.52	0.42
1:A:48:THR:N	1:A:51:GLN:OE1	2.53	0.42
4:D:13:PRO:O	4:D:14:ASP:OD1	2.37	0.42
7:G:118:PRO:HB2	7:G:119:GLY:H	1.57	0.42
7:G:267:LYS:O	7:G:282:TYR:OH	2.33	0.42
8:H:381:VAL:HG22	8:H:405:TYR:CZ	2.55	0.42
8:H:473:VAL:O	8:H:474:ALA:HB3	2.20	0.42
7:G:96:THR:O	7:G:118:PRO:HB3	2.19	0.41
3:C:5:LEU:CD1	3:C:113:LEU:HD11	2.50	0.41
8:H:158:ILE:HA	8:H:201:GLN:HE22	1.85	0.41
1:A:129:LEU:HD23	5:E:157:MET:CE	2.49	0.41
2:B:2:LEU:HD21	2:B:7:LEU:HB2	2.02	0.41
7:G:74:LYS:H	7:G:74:LYS:HG2	1.58	0.41
7:G:156:ARG:HD2	7:G:159:ILE:HD11	2.02	0.41
8:H:168:ARG:NH2	8:H:239:ARG:O	2.53	0.41
7:G:107:SER:O	7:G:107:SER:OG	2.32	0.41
3:C:34:LYS:HE3	3:C:34:LYS:HB2	1.79	0.41
7:G:144:ILE:HD11	7:G:157:LEU:HD13	2.03	0.41
3:C:42:GLU:OE2	3:C:45:LEU:HB2	2.20	0.41
3:C:115:GLU:O	3:C:118:ARG:HB3	2.21	0.41
7:G:344:GLU:O	7:G:348:ARG:NH1	2.53	0.41
7:G:140:LEU:HD23	7:G:141:ILE:C	2.45	0.41
7:G:320:LEU:HB2	7:G:324:THR:HG23	2.01	0.41
8:H:138:GLU:HA	8:H:155:THR:O	2.21	0.41
7:G:261:LEU:HD12	7:G:261:LEU:HA	1.91	0.41
9:I:163:PRO:HA	9:I:164:PRO:HD3	1.95	0.41
8:H:527:ARG:HG3	8:H:531:ASP:HB2	2.03	0.40
9:I:374:ARG:HD2	9:I:374:ARG:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	77/166 (46%)	76 (99%)	1 (1%)	0	100	100
2	B	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
3	C	119/124 (96%)	115 (97%)	3 (2%)	1 (1%)	16	49
4	D	88/99 (89%)	87 (99%)	1 (1%)	0	100	100
5	E	89/173 (51%)	88 (99%)	1 (1%)	0	100	100
6	F	219/313 (70%)	201 (92%)	18 (8%)	0	100	100
7	G	295/404 (73%)	270 (92%)	24 (8%)	1 (0%)	36	65
8	H	377/622 (61%)	356 (94%)	21 (6%)	0	100	100
9	I	370/1117 (33%)	334 (90%)	35 (10%)	1 (0%)	36	65
All	All	1758/3145 (56%)	1650 (94%)	105 (6%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	86	LEU
7	G	118	PRO
9	I	433	PHE

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	72/145 (50%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	98/98 (100%)	97 (99%)	1 (1%)	68	75
3	C	105/108 (97%)	104 (99%)	1 (1%)	68	75
4	D	75/83 (90%)	74 (99%)	1 (1%)	61	72
5	E	77/140 (55%)	77 (100%)	0	100	100
6	F	203/287 (71%)	202 (100%)	1 (0%)	81	80
7	G	274/343 (80%)	273 (100%)	1 (0%)	84	81
8	H	298/534 (56%)	288 (97%)	10 (3%)	32	57
9	I	154/956 (16%)	154 (100%)	0	100	100
All	All	1356/2694 (50%)	1341 (99%)	15 (1%)	63	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	25	LEU
3	C	122	GLU
4	D	5	LEU
6	F	94	VAL
7	G	121	MET
8	H	151	VAL
8	H	379	ARG
8	H	459	SER
8	H	496	SER
8	H	497	VAL
8	H	498	ASP
8	H	527	ARG
8	H	528	PRO
8	H	543	GLU
8	H	557	LEU

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

Mol	Chain	Res	Type
1	A	64	ASN
1	A	116	HIS
1	A	130	GLN
2	B	51	ASN
2	B	109	GLN
3	C	59	GLN

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Mol	Chain	Res	Type
4	D	38	GLN
4	D	60	ASN
5	E	112	ASN
5	E	161	HIS
6	F	104	HIS
6	F	136	GLN
6	F	179	GLN
6	F	289	ASN
7	G	158	HIS
7	G	200	ASN
7	G	239	GLN
7	G	248	ASN
7	G	357	HIS
8	H	114	HIS
8	H	148	HIS
8	H	167	GLN
8	H	201	GLN
8	H	255	HIS
8	H	429	HIS
9	I	328	ASN
9	I	980	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GDP	F	500	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
11	L8S	G	500	-	33,34,34	0.71	0	42,54,54	1.06	2 (4%)

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	-	-	5/16/32/32	0/3/3/3
11	L8S	G	500	-	-	5/21/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	500	GDP	C5-C4	2.97	1.46	1.38
10	F	500	GDP	C6-N1	-2.48	1.34	1.38
10	F	500	GDP	C5-N7	-2.05	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	500	GDP	C5-C4-N3	-6.08	118.72	128.39
10	F	500	GDP	C2-N3-C4	5.08	121.05	112.30
11	G	500	L8S	C5-C4-N9	4.50	108.33	106.25
10	F	500	GDP	N9-C4-N3	4.44	134.82	125.95
10	F	500	GDP	C6-C5-N7	3.41	136.50	130.29
10	F	500	GDP	C4-C5-N7	-2.66	106.46	110.67
10	F	500	GDP	O6-C6-C5	-2.13	120.90	126.53
11	G	500	L8S	C8-N9-C4	-2.03	104.96	106.67
10	F	500	GDP	O4'-C1'-N9	2.01	112.90	108.36

There are no chirality outliers.

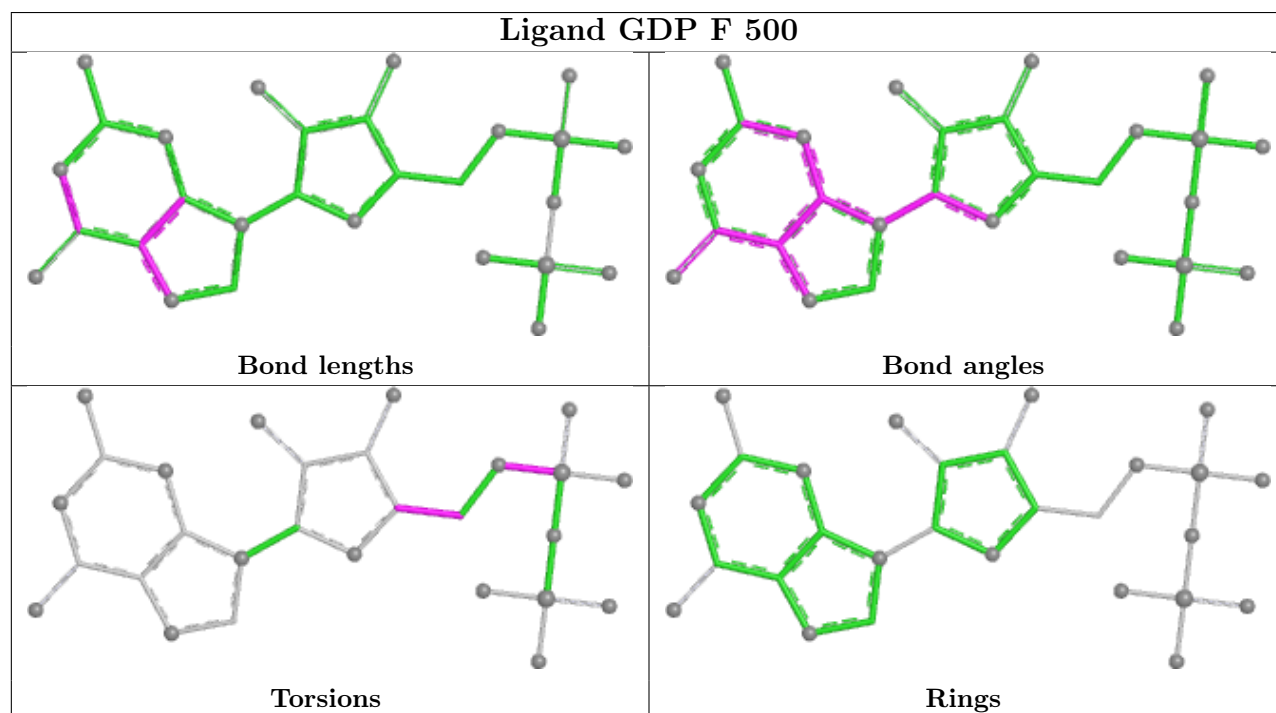
All (10) torsion outliers are listed below:

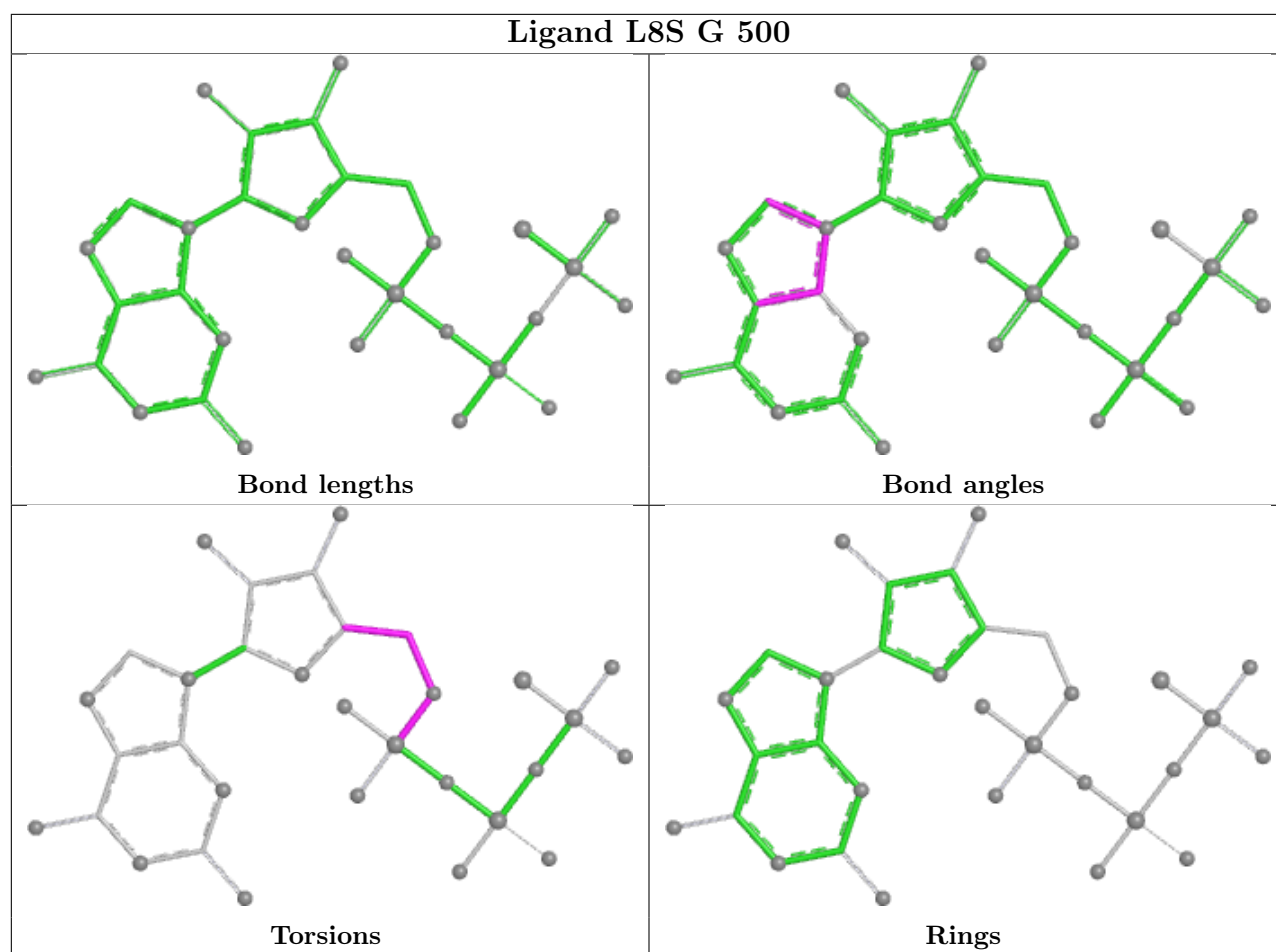
Mol	Chain	Res	Type	Atoms
10	F	500	GDP	C5'-O5'-PA-O3A
10	F	500	GDP	C5'-O5'-PA-O1A
10	F	500	GDP	C5'-O5'-PA-O2A
11	G	500	L8S	C4'-C5'-O5'-PA
11	G	500	L8S	C5'-O5'-PA-O1A
11	G	500	L8S	C5'-O5'-PA-O2A
11	G	500	L8S	C5'-O5'-PA-O3A
11	G	500	L8S	C3'-C4'-C5'-O5'
10	F	500	GDP	O4'-C4'-C5'-O5'
10	F	500	GDP	C3'-C4'-C5'-O5'

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.

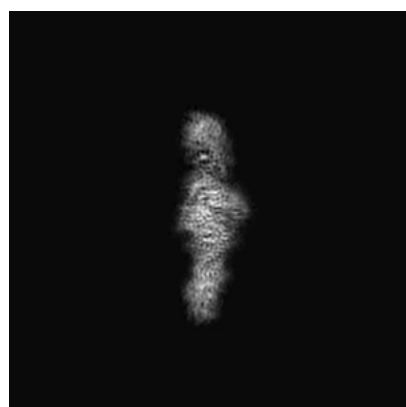
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0554. 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](#)

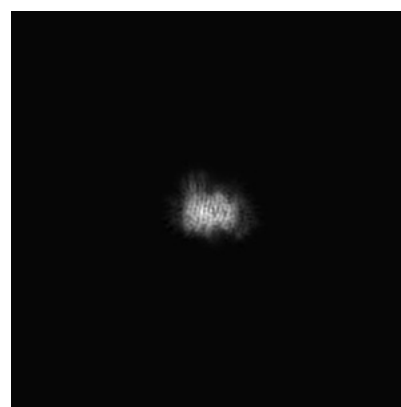
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

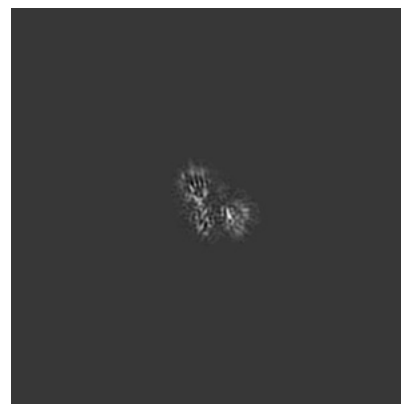
6.2.1 Primary map



X Index: 180



Y Index: 180

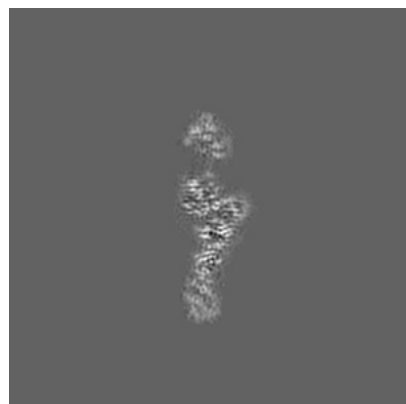


Z Index: 180

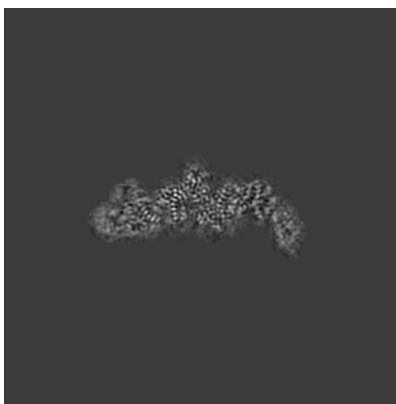
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

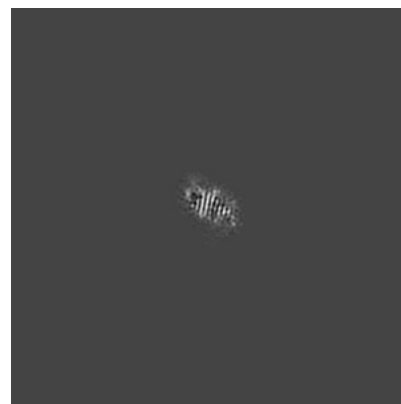
6.3.1 Primary map



X Index: 170



Y Index: 176

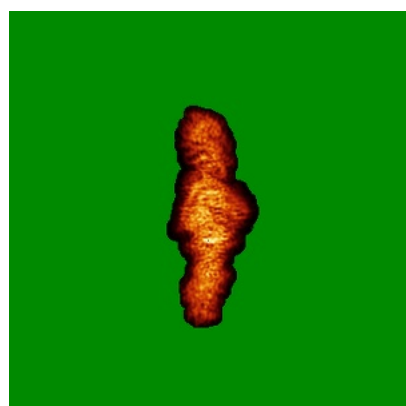


Z Index: 154

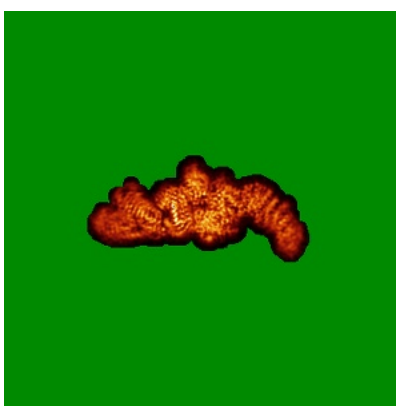
The images above show the largest variance slices of the map in three orthogonal directions.

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

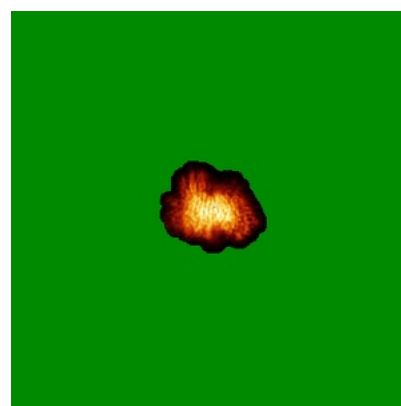
6.4.1 Primary map



X



Y

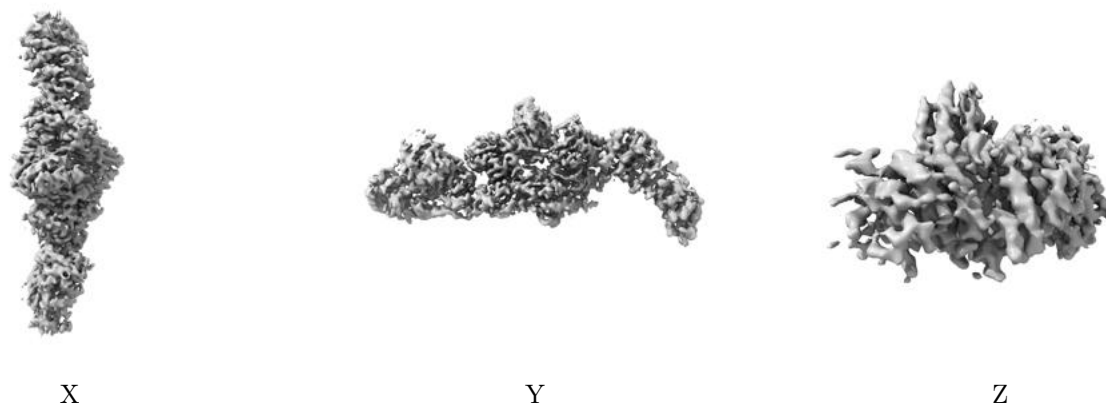


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

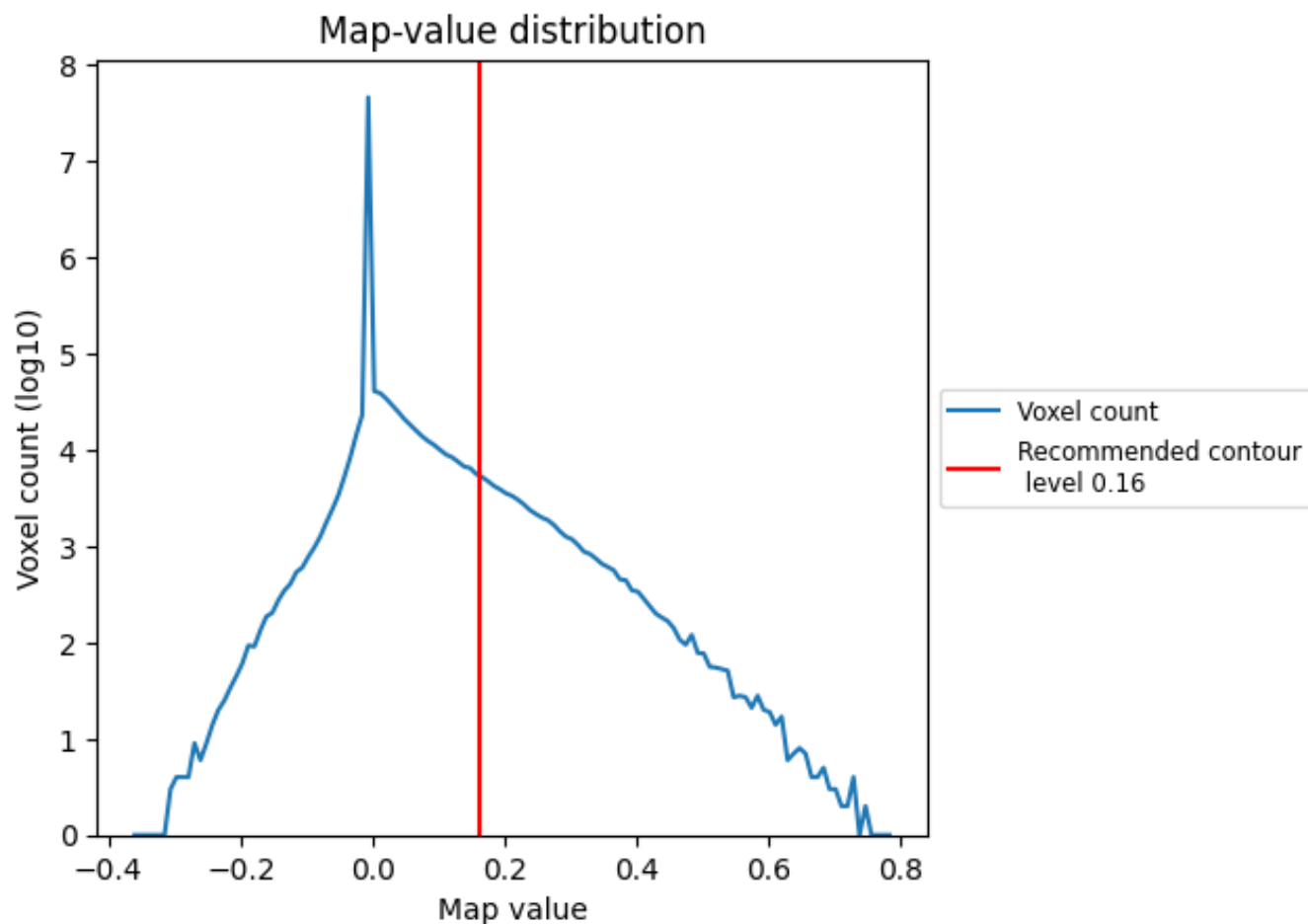
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

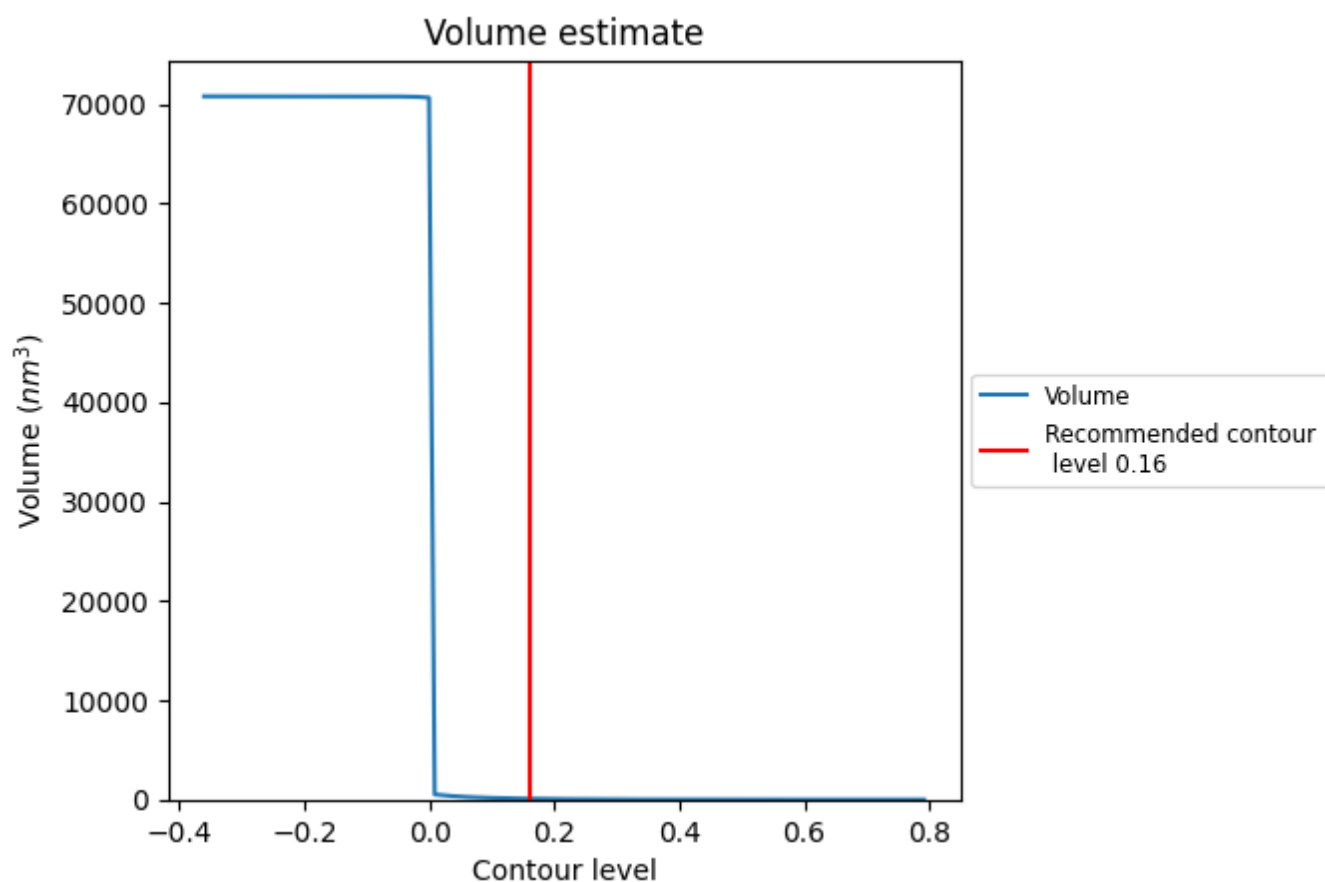
This section contains the results of statistical analysis of the map.

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.

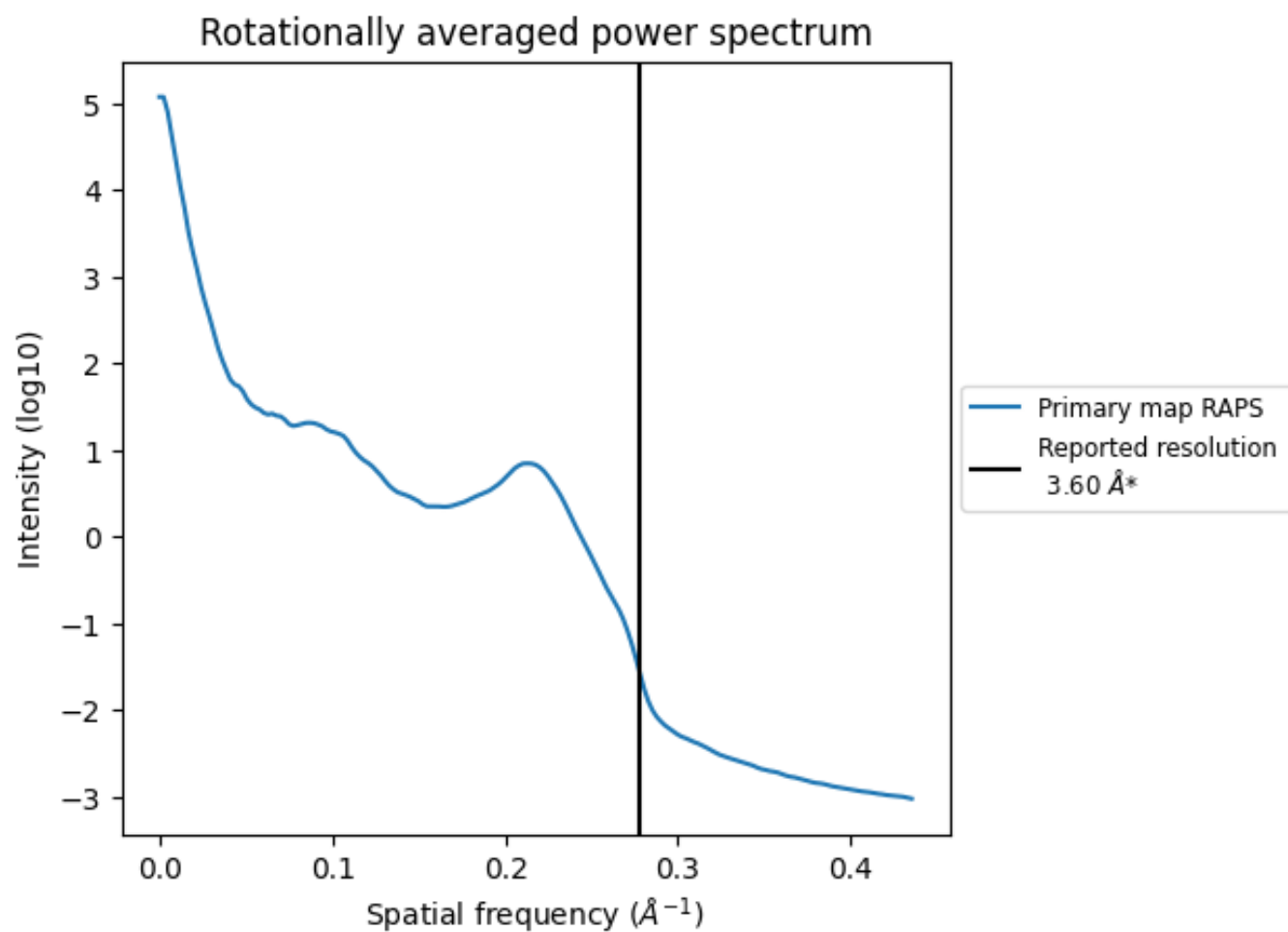
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm^3 ; this corresponds to an approximate mass of 78 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 ⓘ

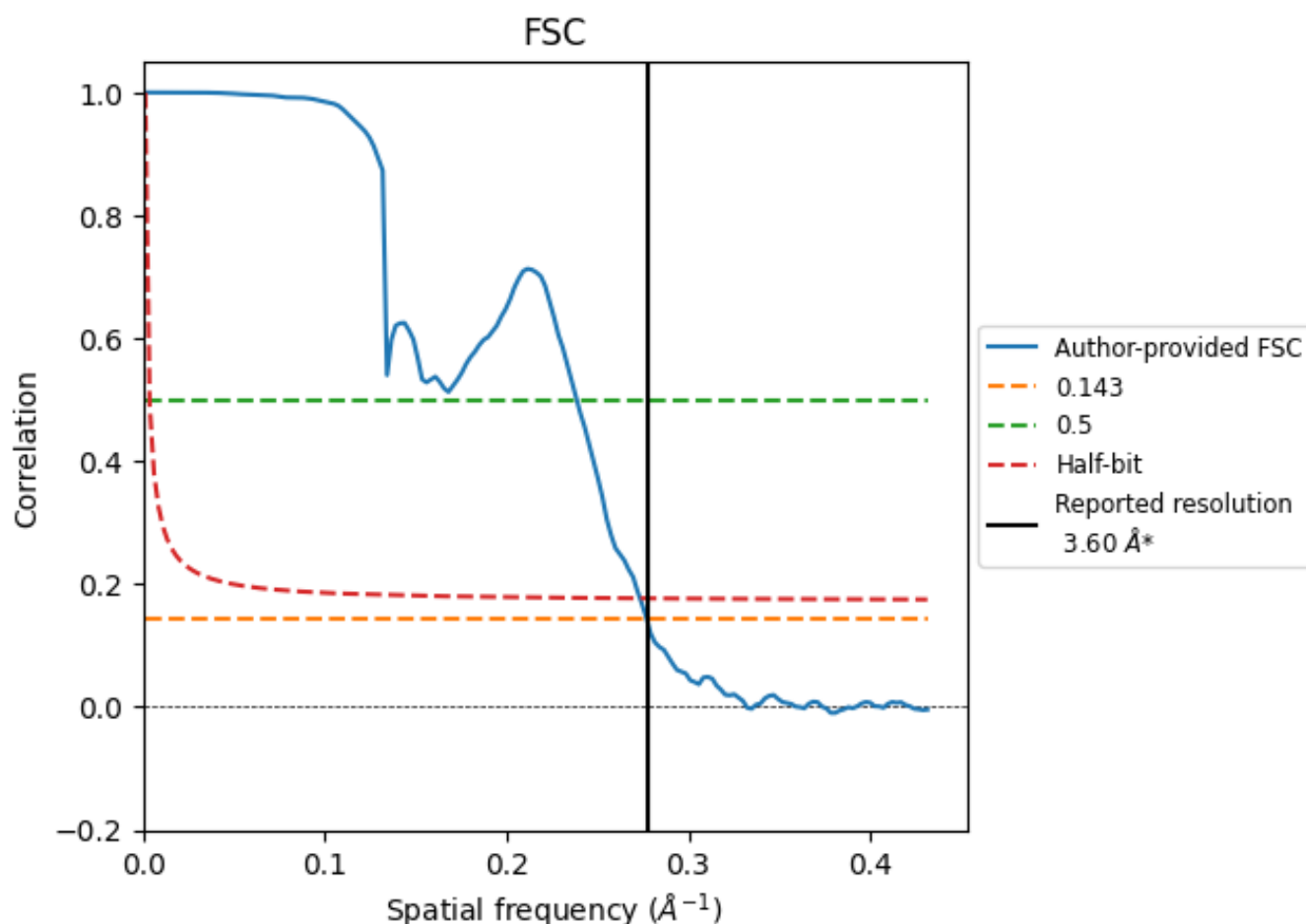


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

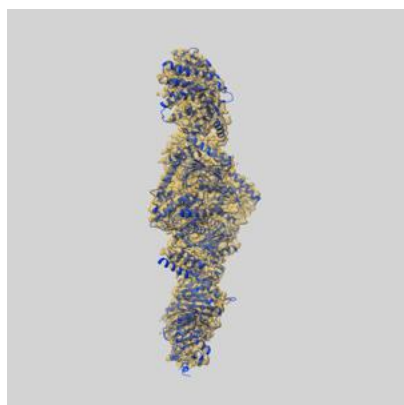
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.19	3.66
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

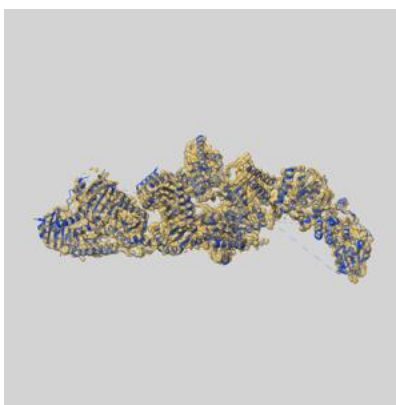
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0554 and PDB model 6NZD. Per-residue inclusion information can be found in section 3 on page 9.

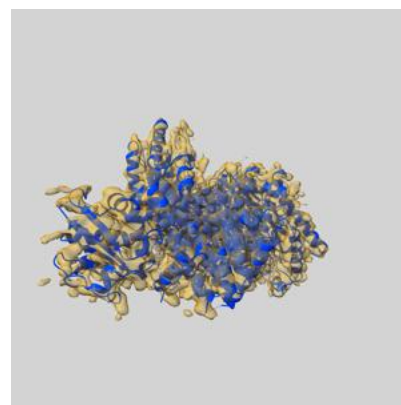
9.1 Map-model overlay [i](#)



X



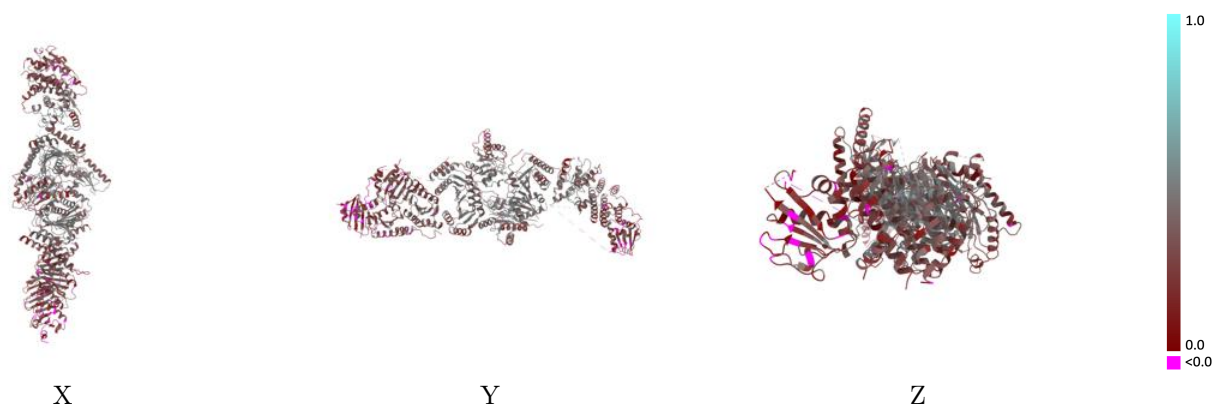
Y



Z

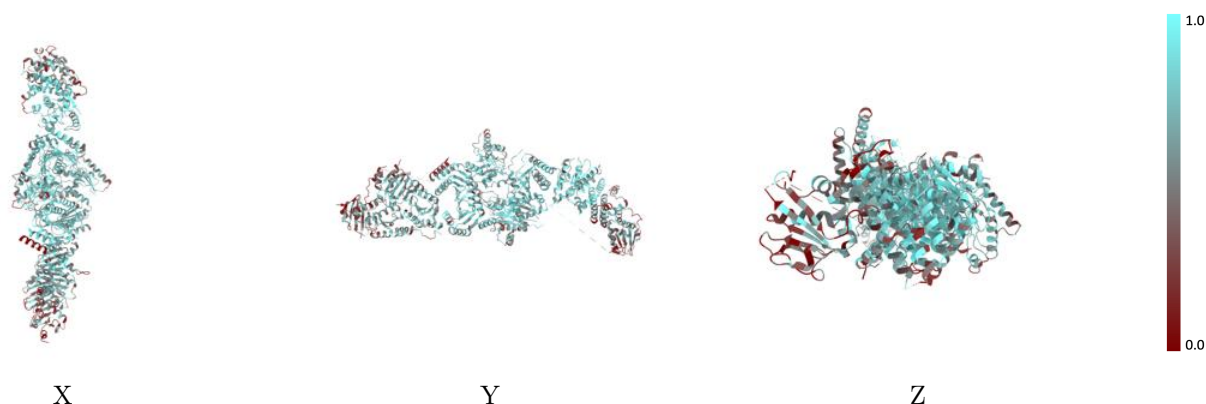
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



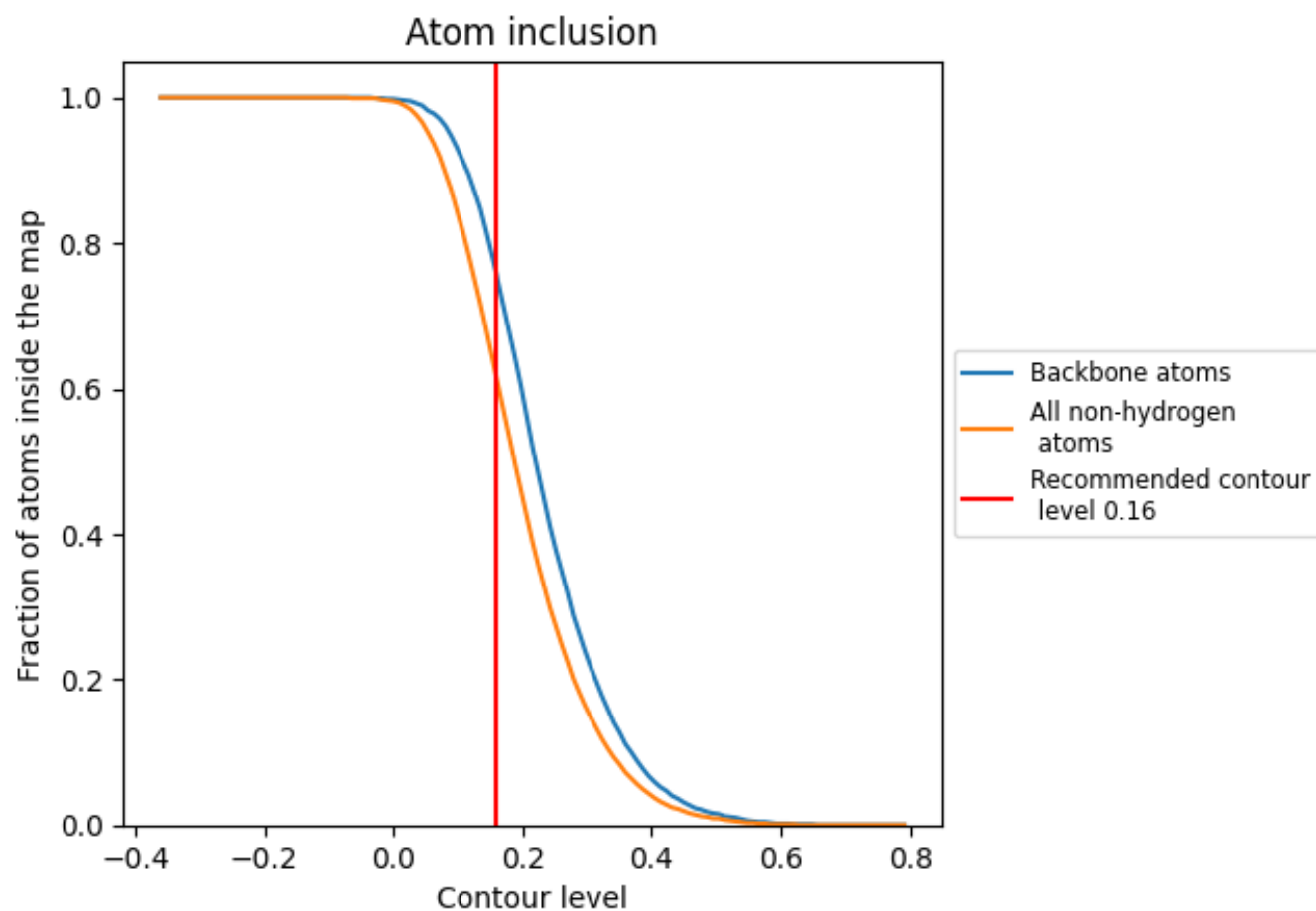
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 61% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.3260
A	0.2850	0.2010
B	0.6170	0.3040
C	0.5560	0.2540
D	0.3530	0.1280
E	0.5380	0.2340
F	0.6830	0.3810
G	0.7080	0.3860
H	0.5830	0.3120
I	0.6980	0.3860

1.0

0.0

<0.0