



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:14 AM UTC

PDB ID : 9DEI / pdb_00009dei
EMDB ID : EMD-46791
Title : Trypanosoma brucei mitochondrial RNA-editing catalytic complex 1, U-deletion (RECC1)
Authors : Liu, Y.T.; Jih, J.; Zhou, Z.H.; Aphasizhev, R.
Deposited on : 2024-08-29
Resolution : 2.99 Å(reported)

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

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A user guide is available at

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

The types of validation reports are described at

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

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

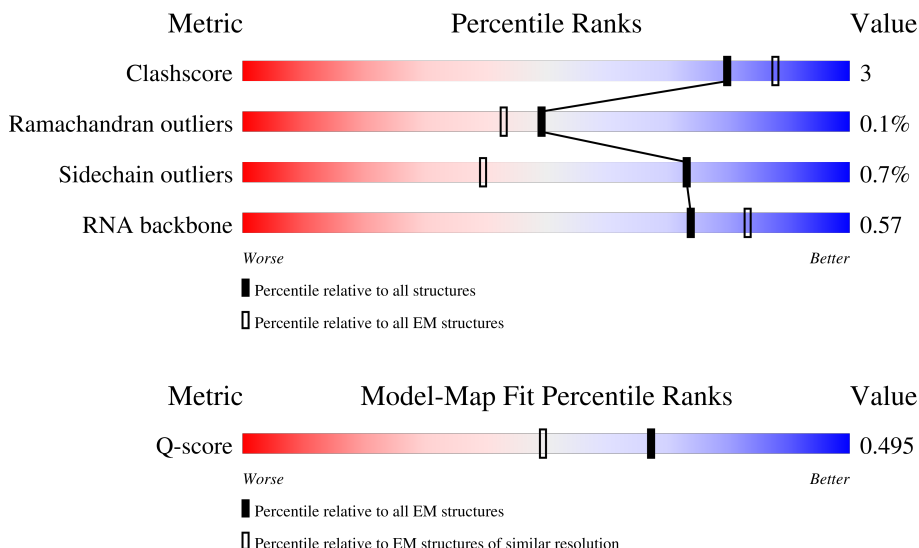
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13287 (2.49 - 3.49)

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	384	
2	B	368	
3	C	818	

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Mol	Chain	Length	Quality of chain
4	D	414	
5	E	164	
5	H	164	
5	J	164	
5	M	164	
5	P	164	
6	F	393	
6	N	393	
7	G	587	
7	K	587	
8	I	218	
9	L	169	
10	O	762	
11	R	76	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28120 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 KREPB5; RNA-editing catalytic complex core protein, B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			2991	1887	546	539	19		

- Molecule 2 is a protein called KREPB8; RNA editing catalytic complex core protein, B8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	302	Total	C	N	O	S	0	0
			2466	1568	442	436	20		

- Molecule 3 is a protein called MP90.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	521	Total	C	N	O	S	0	0
			4135	2618	732	765	20		

- Molecule 4 is a protein called RNA editing complex protein MP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	365	Total	C	N	O	S	0	0
			2890	1808	530	536	16		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	207	PHE	LEU	conflict	UNP Q86MV9
D	228	ASP	GLY	conflict	UNP Q86MV9
D	324	ALA	VAL	conflict	UNP Q86MV9

- Molecule 5 is a protein called MP18 RNA editing complex protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	114	Total	C	N	O	S	0	0
			895	567	155	170	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	118	Total	C	N	O	S	0	0
			931	588	165	175	3		
5	J	119	Total	C	N	O	S	0	0
			936	589	166	176	5		
5	M	133	Total	C	N	O	S	0	0
			1034	651	182	196	5		
5	P	116	Total	C	N	O	S	0	0
			907	573	157	172	5		

- Molecule 6 is a protein called RNA-editing complex protein MP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	129	Total	C	N	O	S	0	0
			1040	663	179	192	6		
6	N	142	Total	C	N	O	S	0	0
			1148	731	197	214	6		

- Molecule 7 is a protein called KREPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	159	Total	C	N	O	S	0	0
			1195	747	208	233	7		
7	K	184	Total	C	N	O	S	0	0
			1393	872	244	270	7		

- Molecule 8 is a protein called RNA editing complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	190	Total	C	N	O	S	0	0
			1453	896	266	279	12		

- Molecule 9 is a protein called KREPA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	143	Total	C	N	O	S	0	0
			1141	718	206	210	7		

- Molecule 10 is a protein called RNA-editing complex protein MP81.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	196	Total	C	N	O	S	0	0
			1545	971	275	290	9		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	9	ASP	GLY	conflict	UNP Q95W15
O	12	CYS	SER	conflict	UNP Q95W15
O	35	SER	ALA	conflict	UNP Q95W15
O	76	GLY	GLU	conflict	UNP Q95W15
O	244	GLY	GLU	conflict	UNP Q95W15
O	293	SER	PRO	conflict	UNP Q95W15
O	594	SER	ASN	conflict	UNP Q95W15

- Molecule 11 is a RNA chain called tRNA-valine (anticodon AAC).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	76	Total	C	N	O	P	0	0
			1621	722	285	538	76		

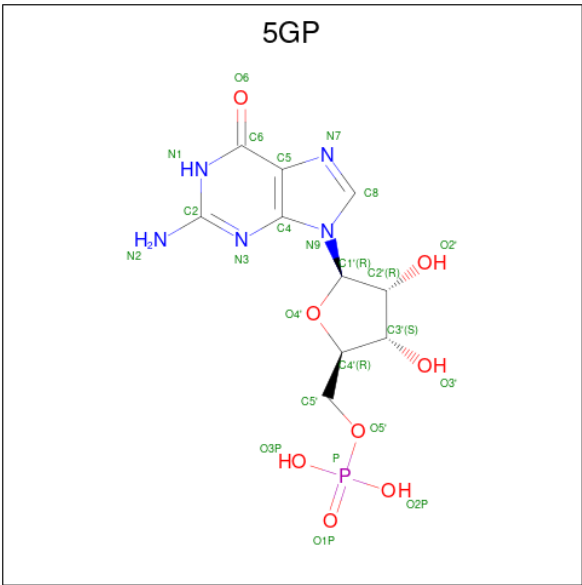
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total	Zn	0
			1	1	
12	C	1	Total	Zn	0
			1	1	
12	D	1	Total	Zn	0
			1	1	
12	K	1	Total	Zn	0
			1	1	
12	O	1	Total	Zn	0
			1	1	

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	C	3	Total	Mg	0
			3	3	

- Molecule 14 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms					AltConf
14	R	1	Total	C	N	O	P	0
			24	10	5	8	1	

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	62	Total	O	0
			62	62	
15	B	56	Total	O	0
			56	56	
15	C	67	Total	O	0
			67	67	
15	D	16	Total	O	0
			16	16	
15	E	14	Total	O	0
			14	14	
15	F	15	Total	O	0
			15	15	
15	G	8	Total	O	0
			8	8	
15	H	9	Total	O	0
			9	9	
15	K	2	Total	O	0
			2	2	
15	M	16	Total	O	0
			16	16	
15	N	17	Total	O	0
			17	17	

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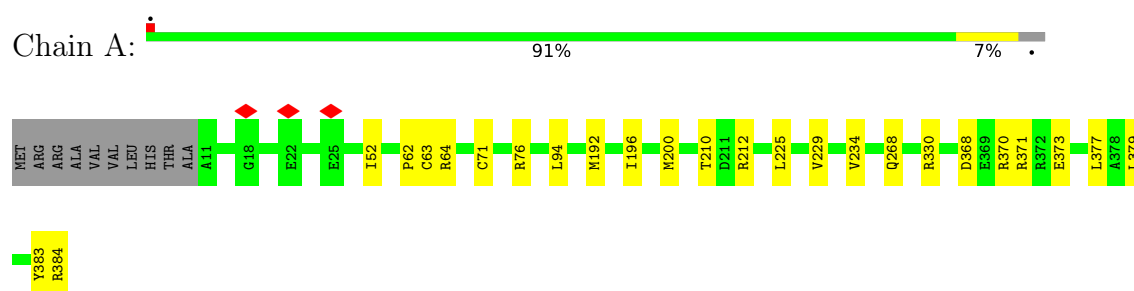
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Mol	Chain	Residues	Atoms		AltConf
15	O	13	Total 13	O 13	0
15	P	5	Total 5	O 5	0
15	R	67	Total 67	O 67	0

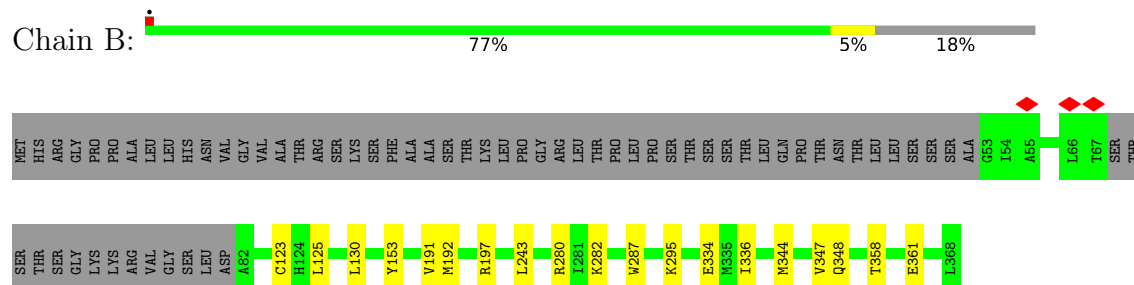
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

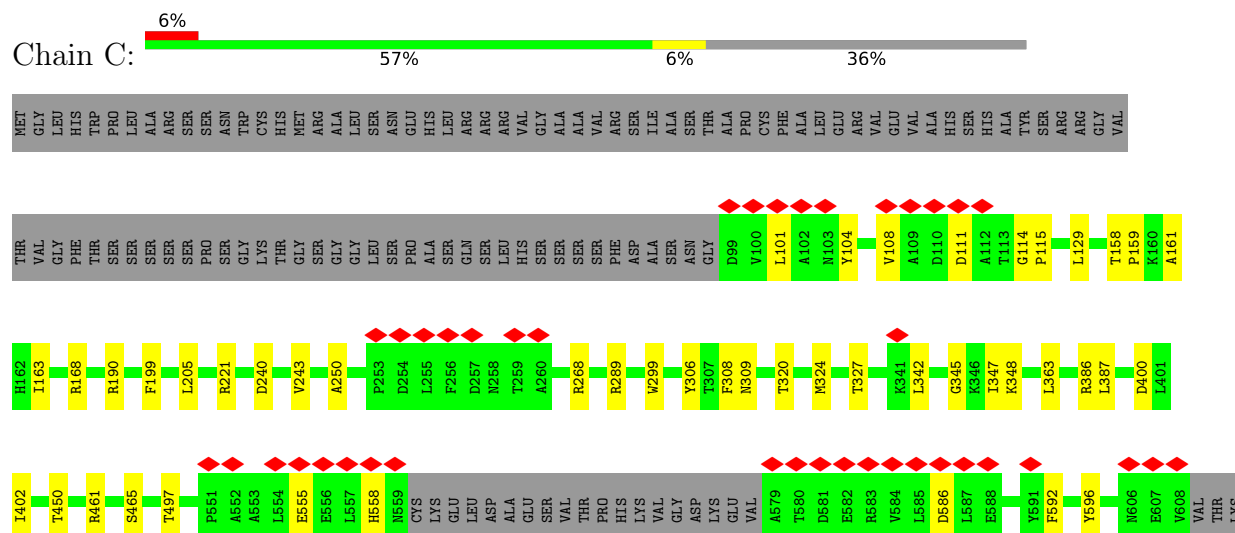
- Molecule 1: KREPB5; RNA-editing catalytic complex core protein, B5

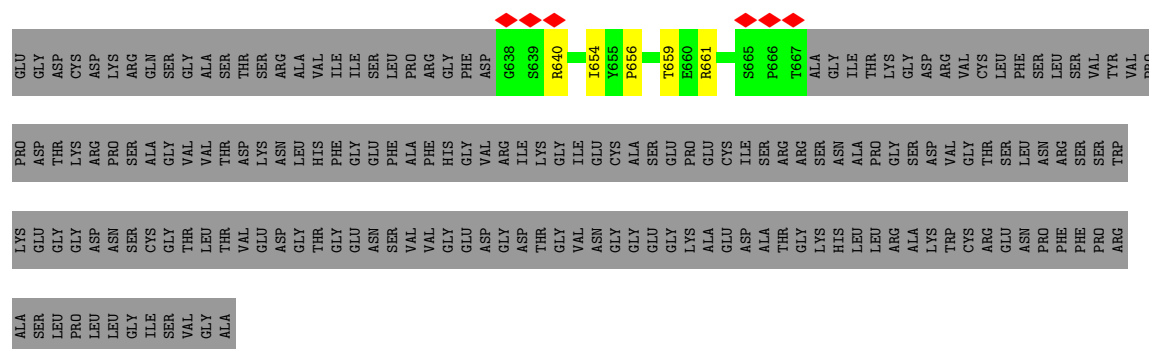


- Molecule 2: KREPB8; RNA editing catalytic complex core protein, B8

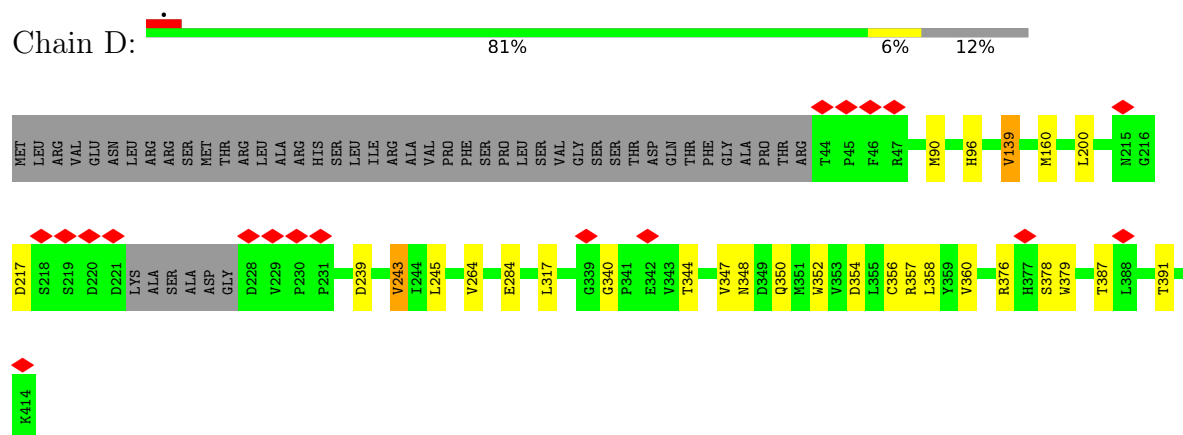


- Molecule 3: MP90

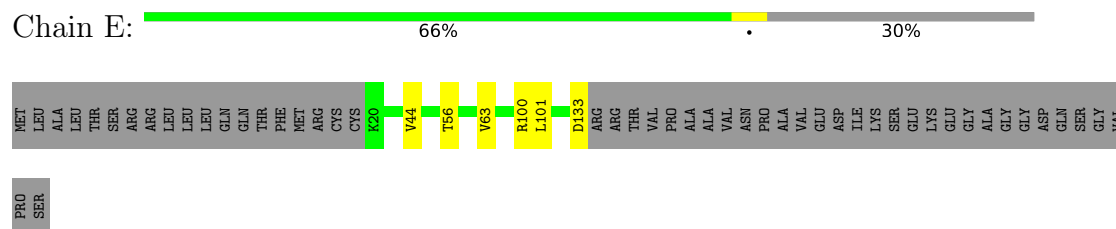




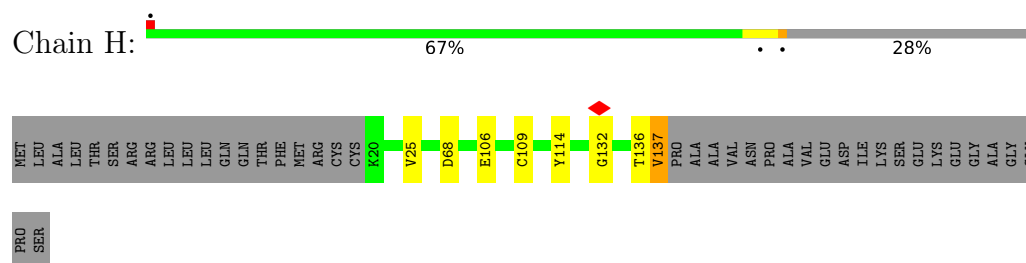
- Molecule 4: RNA editing complex protein MP46



- Molecule 5: MP18 RNA editing complex protein, putative



- Molecule 5: MP18 RNA editing complex protein, putative



- Molecule 5: MP18 RNA editing complex protein, putative



THR	GLU	GLU	GLU	THR	GLY	ARG	SER	ALA	MET	GLY	T262	E269	V272	V311	S324	P325	G326	D327	L357	R373	L391	K392	V393
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- Molecule 7: KREPA2



ALA	ALA	VAL	SER	GLN	ALA	ALA	ASN	PRO	ASN	GLU	VAL	SER	SER	PHE	ALA	ALA	VAL	SER	SER	PRO	PHE	VAL	GLY	GLN	VAL	ALA	SER	PRO	PHE	ALA	ASP	VAL	ALA	GLY	SER	PRO	PHE	GLJ	ALA	SER	CYS	ALA	ALA	SER	SER	PRO	PHE	THR	ALA
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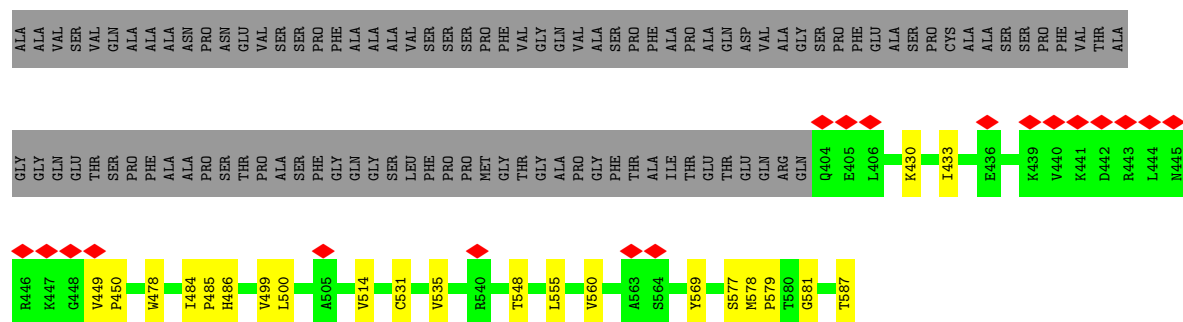
GLY	GLN	GLU	THR	SER	PRO	PHE	ALA	PRO	SER	THR	PRO	ALA	PHE	GLY	GLN	GLY	SER	LEU	PHE	PRO	PRO	MET	GLY	THR	GLY	ALA	PRO	PRO	ALA	PHE	THR	ALA	ILE	THR	GLU	THR	GLU	GLN	ARG	GLN	GLN	GLU	GLU	L406	E407	H408	G409	C410	P411	T412	T413	G414	K415	K416	F417	S418	T419	E420
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E421	G422	A423	A424	M425	H426	S427	K428	S429	K430	H431	G432	I433	V434	L435	E436	S437	K438	LYS	VAL	LYS	ASP	ARG	LEU	ASN	ARG	LYS	GLY	VAL	PRO	ASP	LEU	PRO	ALA	TYR	VAL	PRO	SER	PRO	VAL	ASP	L462	S463	R471	S491	V499	L543	R556
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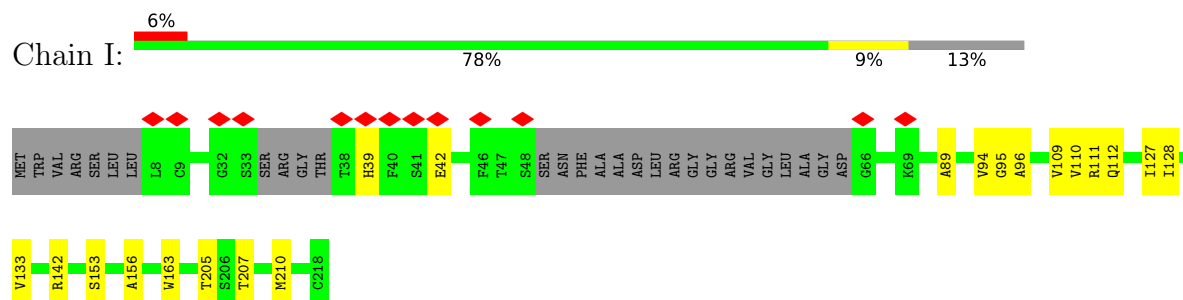
- Molecule 7: KREPA2



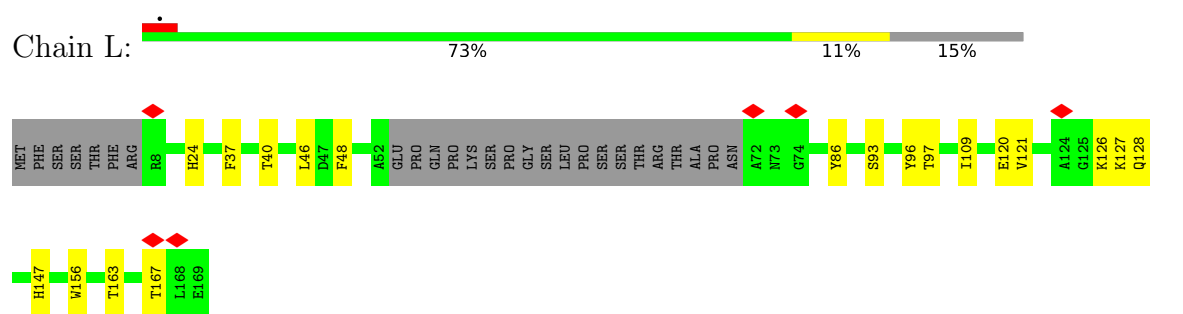
PRO	PHE	ARG	ALA	GLY	LYS	VAL	ARG	ASN	PRO	PHE	THR	THR	GLN	ARG	GLU	VAL	VAL	LYS	PRO	PRO	PRO	PRO	GLN	PRO	LYS	LYS	ALA	PRO	VAL	THR	THR	PHE	GLN	GLN	LEU	PRO	PRO	MET	PHE	GLY	GLN	THR	ARG	GLU	PRO	SER	ALA	ALA	PHE	ALA
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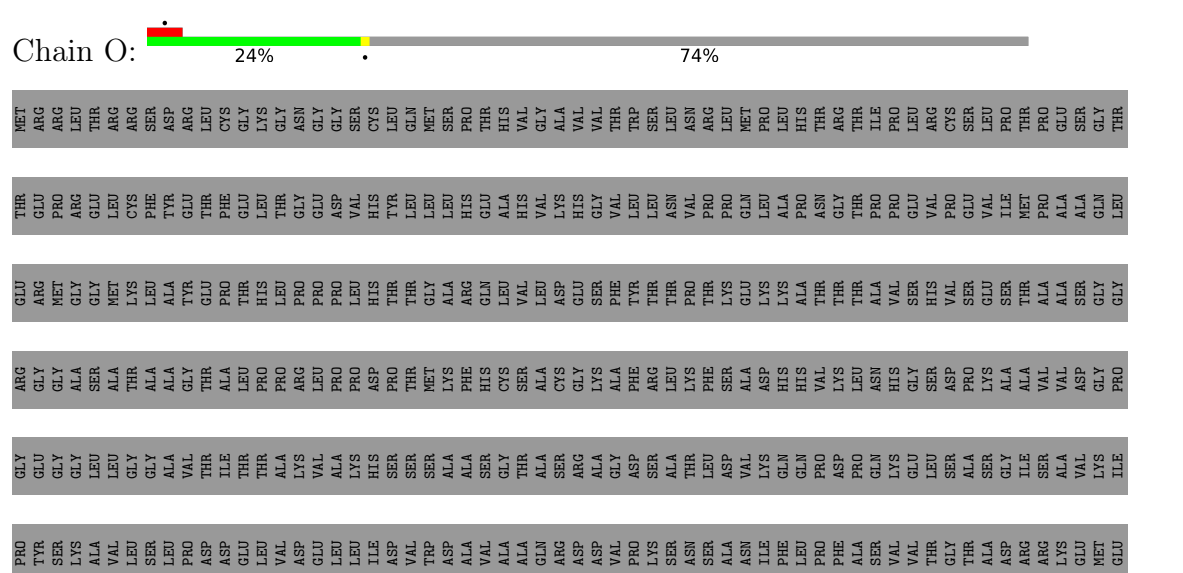
• Molecule 8: RNA editing complex protein

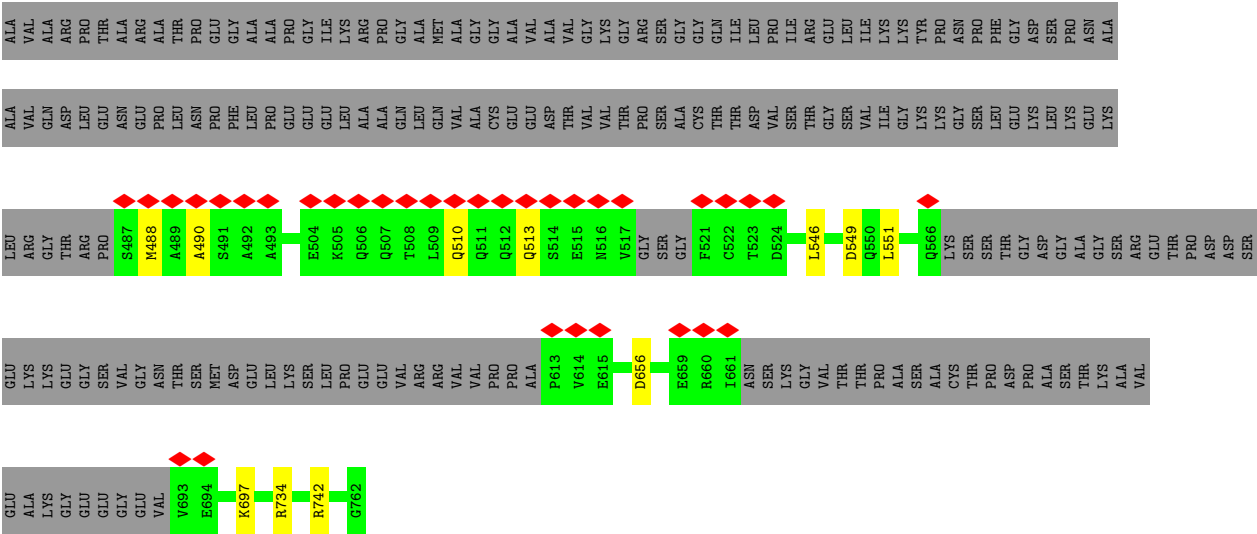


• Molecule 9: KREPA5

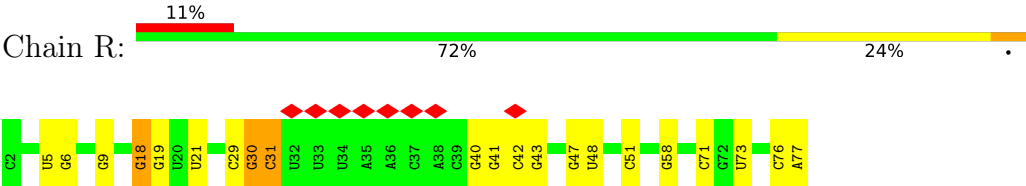


• Molecule 10: RNA-editing complex protein MP81





● Molecule 11: tRNA-valine (anticodon AAC)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	452724	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS, TFS KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45, 45	Depositor
Minimum defocus (nm)	1000, 600	Depositor
Maximum defocus (nm)	3000, 2800	Depositor
Magnification	81000, 130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	71.537	Depositor
Minimum map value	-39.675	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.084	Depositor
Recommended contour level	3.5	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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: 5GP, ZN, 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	0.14	0/3054	0.35	0/4132
2	B	0.15	0/2530	0.34	0/3421
3	C	0.13	0/4226	0.34	0/5746
4	D	0.16	0/2951	0.34	0/3998
5	E	0.13	0/916	0.35	0/1248
5	H	0.13	0/952	0.34	0/1296
5	J	0.11	0/957	0.31	0/1302
5	M	0.13	0/1057	0.33	0/1441
5	P	0.16	0/928	0.36	0/1264
6	F	0.13	0/1071	0.31	0/1455
6	N	0.12	0/1182	0.30	0/1608
7	G	0.12	0/1217	0.33	0/1647
7	K	0.11	0/1421	0.32	0/1927
8	I	0.11	0/1474	0.32	1/1986 (0.1%)
9	L	0.10	0/1157	0.26	0/1561
10	O	0.10	0/1568	0.30	0/2115
11	R	0.13	0/1810	0.35	0/2820
All	All	0.13	0/28471	0.33	1/38967 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	96	ALA	CB-CA-C	-5.47	110.28	116.63

There are no chirality outliers.

There are no planarity outliers.

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	2991	0	3052	16	0
2	B	2466	0	2417	11	0
3	C	4135	0	4124	34	0
4	D	2890	0	2871	19	0
5	E	895	0	877	3	0
5	H	931	0	919	4	0
5	J	936	0	920	9	0
5	M	1034	0	1021	3	0
5	P	907	0	887	4	0
6	F	1040	0	988	4	0
6	N	1148	0	1091	5	0
7	G	1195	0	1188	3	0
7	K	1393	0	1392	14	0
8	I	1453	0	1441	15	0
9	L	1141	0	1163	11	0
10	O	1545	0	1550	7	0
11	R	1621	0	818	14	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
12	K	1	0	0	0	0
12	O	1	0	0	0	0
13	C	3	0	0	0	0
14	R	24	0	11	0	0
15	A	62	0	0	0	0
15	B	56	0	0	0	0
15	C	67	0	0	0	0
15	D	16	0	0	1	0
15	E	14	0	0	0	0
15	F	15	0	0	0	0
15	G	8	0	0	0	0
15	H	9	0	0	0	0
15	K	2	0	0	0	0
15	M	16	0	0	0	0
15	N	17	0	0	1	0
15	O	13	0	0	0	0
15	P	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	R	67	0	0	0	0
All	All	28120	0	26730	145	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 3.

All (145) 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)
1:A:63:CYS:SG	7:G:471:ARG:NH1	2.59	0.76
8:I:110:VAL:HG22	8:I:128:ILE:HG22	1.70	0.74
3:C:289:ARG:NH1	3:C:400:ASP:OD1	2.28	0.67
5:P:33:ASP:O	5:P:34:ILE:HD13	1.95	0.66
3:C:320:THR:HG21	3:C:402:ILE:HG23	1.78	0.66
5:M:130:ILE:HG23	5:P:63:VAL:HG21	1.79	0.65
10:O:546:LEU:HD21	10:O:551:LEU:HD13	1.79	0.65
1:A:383:TYR:HB3	1:A:384:ARG:HD3	1.78	0.64
9:L:37:PHE:HD2	9:L:97:THR:HG23	1.62	0.64
1:A:330:ARG:NH1	6:F:281:GLU:OE2	2.29	0.64
2:B:295:LYS:NZ	3:C:111:ASP:OD2	2.25	0.63
7:K:499:VAL:HG22	7:K:514:VAL:HG22	1.81	0.62
10:O:510:GLN:HA	10:O:513:GLN:HG3	1.80	0.62
11:R:30:G:H2'	11:R:31:C:C6	2.34	0.62
7:G:499:VAL:HG21	7:G:543:LEU:HD21	1.82	0.61
10:O:488:MET:HG2	10:O:490:ALA:H	1.65	0.61
3:C:342:LEU:HB2	3:C:347:ILE:HG21	1.83	0.60
11:R:5:U:H2'	11:R:6:G:C8	2.37	0.59
3:C:324:MET:HA	3:C:327:THR:HG22	1.83	0.59
11:R:40:G:H2'	11:R:41:G:C8	2.37	0.59
3:C:250:ALA:O	3:C:268:ARG:NH1	2.34	0.58
4:D:379:TRP:HA	7:K:485:PRO:HG2	1.84	0.58
6:N:324:SER:OG	6:N:327:ASP:OD2	2.18	0.58
5:H:132:GLY:HA3	5:H:137:VAL:HA	1.86	0.57
2:B:197:ARG:NH1	2:B:334:GLU:OE2	2.33	0.57
3:C:654:ILE:HG22	3:C:656:PRO:HD2	1.88	0.55
3:C:240:ASP:OD2	4:D:96:HIS:NE2	2.32	0.55
1:A:370:ARG:NH1	1:A:373:GLU:OE2	2.37	0.55
4:D:354:ASP:OD2	4:D:357:ARG:NH1	2.40	0.54
1:A:373:GLU:O	1:A:377:LEU:HG	2.08	0.54
4:D:387:THR:O	4:D:391:THR:HG23	2.08	0.54
8:I:112:GLN:HB3	8:I:127:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:163:THR:O	9:L:167:THR:HG23	2.07	0.54
7:K:577:SER:O	7:K:581:GLY:N	2.40	0.54
5:J:48:THR:HG23	5:J:69:HIS:CE1	2.44	0.53
8:I:89:ALA:HB2	5:J:65:VAL:HG11	1.90	0.53
11:R:42:C:H2'	11:R:43:G:H8	1.74	0.53
3:C:243:VAL:HG21	3:C:387:LEU:HD11	1.92	0.52
3:C:158:THR:HG23	3:C:161:ALA:H	1.75	0.51
4:D:340:GLY:O	4:D:344:THR:HG23	2.11	0.51
5:P:60:THR:OG1	5:P:62:GLU:HG2	2.11	0.51
8:I:205:THR:HB	8:I:210:MET:HB2	1.93	0.50
8:I:153:SER:H	8:I:156:ALA:HB3	1.76	0.50
10:O:656:ASP:OD2	10:O:697:LYS:NZ	2.37	0.50
3:C:586:ASP:N	3:C:586:ASP:OD1	2.42	0.50
3:C:101:LEU:HD13	3:C:168:ARG:HG3	1.93	0.50
5:E:133:ASP:N	5:E:133:ASP:OD1	2.45	0.50
3:C:114:GLY:N	3:C:115:PRO:HD3	2.26	0.50
11:R:5:U:H2'	11:R:6:G:H8	1.77	0.50
6:F:324:SER:OG	6:F:327:ASP:OD2	2.21	0.49
5:H:136:THR:HG22	5:H:137:VAL:H	1.77	0.49
4:D:357:ARG:HG3	4:D:358:LEU:N	2.27	0.49
8:I:163:TRP:CH2	8:I:207:THR:HA	2.48	0.49
3:C:659:THR:HG22	3:C:661:ARG:H	1.77	0.49
7:G:556:ARG:NH1	5:H:68:ASP:OD2	2.45	0.49
3:C:640:ARG:H	3:C:640:ARG:HD3	1.78	0.49
4:D:352:TRP:CD1	4:D:356:CYS:HG	2.31	0.49
2:B:287:TRP:CE3	3:C:115:PRO:HG2	2.49	0.48
3:C:345:GLY:HA2	3:C:348:LYS:HG3	1.95	0.48
3:C:461:ARG:NH2	6:N:326:GLY:O	2.39	0.48
4:D:284:GLU:OE1	15:D:601:HOH:O	2.20	0.48
5:E:100:ARG:NH1	6:F:331:ASP:OD1	2.46	0.48
8:I:133:VAL:O	5:J:100:ARG:NH2	2.46	0.48
4:D:139:VAL:HG13	4:D:217:ASP:HB2	1.96	0.48
5:M:33:ASP:O	5:M:47:PHE:HA	2.14	0.47
3:C:596:TYR:OH	10:O:742:ARG:NH1	2.48	0.47
4:D:376:ARG:HD3	5:J:63:VAL:HG21	1.96	0.47
2:B:280:ARG:NH1	4:D:264:VAL:O	2.47	0.47
1:A:71:CYS:SG	1:A:76:ARG:HD2	2.55	0.47
8:I:111:ARG:HG3	8:I:111:ARG:HH11	1.80	0.47
2:B:191:VAL:HG22	2:B:192:MET:H	1.78	0.47
3:C:386:ARG:NH1	4:D:90:MET:SD	2.88	0.47
4:D:317:LEU:HD22	7:K:478:TRP:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:42:C:H2'	11:R:43:G:C8	2.50	0.46
8:I:94:VAL:HG11	5:J:54:ILE:HG13	1.96	0.46
6:N:357:LEU:HD23	6:N:391:LEU:HD21	1.96	0.46
7:K:579:PRO:HD2	9:L:48:PHE:CZ	2.51	0.46
7:K:531:CYS:HB3	7:K:535:VAL:HB	1.97	0.46
11:R:29:C:C2	11:R:30:G:H1'	2.50	0.46
11:R:48:U:O2'	11:R:51:C:OP1	2.33	0.46
3:C:299:TRP:CD1	3:C:308:PHE:HB2	2.51	0.45
11:R:30:G:H2'	11:R:31:C:H6	1.79	0.45
11:R:18:G:HO2'	11:R:58:G:H22	1.64	0.45
1:A:52:ILE:H	11:R:76:C:H5	1.65	0.45
9:L:93:SER:HB3	9:L:96:TYR:CD2	2.51	0.45
3:C:104:TYR:OH	3:C:306:TYR:O	2.34	0.45
9:L:120:GLU:HB2	9:L:127:LYS:HE3	1.98	0.45
1:A:192:MET:O	1:A:196:ILE:HG13	2.17	0.45
8:I:95:GLY:HA2	7:K:486:HIS:HB3	1.99	0.45
9:L:109:ILE:H	9:L:147:HIS:HB2	1.82	0.45
3:C:555:GLU:HA	3:C:558:HIS:CD2	2.52	0.44
5:P:33:ASP:C	5:P:34:ILE:HD13	2.42	0.44
4:D:200:LEU:HD22	4:D:245:LEU:HD23	1.99	0.44
3:C:190:ARG:NH1	3:C:497:THR:HG21	2.32	0.44
3:C:592:PHE:O	10:O:734:ARG:NH2	2.50	0.44
1:A:268:GLN:NE2	11:R:76:C:O2	2.50	0.44
5:J:48:THR:CG2	5:J:69:HIS:CE1	3.01	0.44
6:N:373:ARG:NH2	15:N:403:HOH:O	2.45	0.44
1:A:200:MET:HE1	1:A:234:VAL:HG11	2.00	0.44
4:D:347:VAL:HA	4:D:350:GLN:HG2	2.00	0.44
3:C:199:PHE:CD1	3:C:221:ARG:HA	2.53	0.43
3:C:465:SER:OG	6:N:259:GLU:O	2.29	0.43
11:R:41:G:H8	11:R:41:G:O5'	2.00	0.43
2:B:344:MET:HA	2:B:347:VAL:HG22	2.00	0.43
6:F:267:GLN:HG2	6:F:268:TYR:N	2.33	0.43
8:I:112:GLN:HG2	8:I:127:ILE:HD12	1.98	0.43
1:A:62:PRO:C	1:A:64:ARG:H	2.27	0.43
1:A:94:LEU:HD13	1:A:196:ILE:HD13	2.01	0.43
1:A:379:LEU:O	1:A:383:TYR:HB2	2.19	0.43
9:L:121:VAL:N	9:L:128:GLN:O	2.42	0.43
5:J:130:ILE:HG12	9:L:46:LEU:HD21	2.00	0.43
2:B:153:TYR:CE2	2:B:348:GLN:HA	2.54	0.43
3:C:363:LEU:HD23	3:C:363:LEU:HA	1.85	0.43
4:D:160:MET:SD	4:D:243:VAL:HG13	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:549:ASP:N	10:O:549:ASP:OD1	2.50	0.42
4:D:348:ASN:HB3	8:I:142:ARG:HD2	2.01	0.42
5:J:126:GLN:HB2	7:K:578:MET:HE3	2.02	0.42
2:B:358:THR:HG22	2:B:361:GLU:HG3	2.01	0.42
3:C:190:ARG:HH11	3:C:497:THR:HG21	1.85	0.42
2:B:123:CYS:HB2	2:B:130:LEU:HD13	2.02	0.42
2:B:243:LEU:HD23	2:B:336:ILE:HD12	2.00	0.42
7:K:548:THR:H	7:K:587:THR:HB	1.85	0.42
5:E:56:THR:HG22	5:E:63:VAL:HG23	2.02	0.42
7:K:430:LYS:NZ	11:R:73:U:OP1	2.45	0.42
7:K:555:LEU:HD23	9:L:86:TYR:CE1	2.55	0.42
3:C:450:THR:HG23	5:M:112:HIS:ND1	2.35	0.42
1:A:225:LEU:O	1:A:229:VAL:HG13	2.20	0.42
3:C:159:PRO:O	3:C:163:ILE:HG12	2.20	0.42
8:I:39:HIS:O	8:I:42:GLU:HG3	2.20	0.41
7:K:560:VAL:N	7:K:569:TYR:O	2.52	0.41
9:L:24:HIS:O	9:L:40:THR:OG1	2.34	0.41
3:C:205:LEU:HD22	3:C:289:ARG:HG2	2.02	0.41
9:L:126:LYS:HE2	9:L:126:LYS:HB2	1.91	0.41
7:K:449:VAL:N	7:K:450:PRO:HD2	2.35	0.41
2:B:282:LYS:HD2	2:B:287:TRP:CZ2	2.56	0.41
1:A:368:ASP:OD1	1:A:371:ARG:NH2	2.54	0.41
3:C:104:TYR:HE1	3:C:309:ASN:HD22	1.69	0.41
5:J:54:ILE:HG23	5:J:63:VAL:HG13	2.02	0.41
1:A:210:THR:C	1:A:212:ARG:H	2.29	0.40
8:I:142:ARG:HD2	8:I:142:ARG:O	2.20	0.40
4:D:378:SER:HB2	7:K:484:ILE:HA	2.02	0.40
8:I:109:VAL:HG11	8:I:111:ARG:HH21	1.86	0.40
4:D:356:CYS:O	4:D:360:VAL:HG23	2.22	0.40
3:C:101:LEU:HD22	3:C:168:ARG:NH1	2.37	0.40
5:H:106:GLU:HG3	5:H:109:CYS:H	1.87	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	372/384 (97%)	360 (97%)	12 (3%)	0	100	100
2	B	298/368 (81%)	294 (99%)	4 (1%)	0	100	100
3	C	515/818 (63%)	486 (94%)	29 (6%)	0	100	100
4	D	361/414 (87%)	352 (98%)	9 (2%)	0	100	100
5	E	112/164 (68%)	110 (98%)	2 (2%)	0	100	100
5	H	116/164 (71%)	112 (97%)	4 (3%)	0	100	100
5	J	117/164 (71%)	114 (97%)	3 (3%)	0	100	100
5	M	131/164 (80%)	129 (98%)	2 (2%)	0	100	100
5	P	114/164 (70%)	114 (100%)	0	0	100	100
6	F	127/393 (32%)	121 (95%)	5 (4%)	1 (1%)	16	50
6	N	140/393 (36%)	136 (97%)	4 (3%)	0	100	100
7	G	155/587 (26%)	145 (94%)	9 (6%)	1 (1%)	21	56
7	K	182/587 (31%)	177 (97%)	5 (3%)	0	100	100
8	I	184/218 (84%)	180 (98%)	4 (2%)	0	100	100
9	L	139/169 (82%)	137 (99%)	2 (1%)	0	100	100
10	O	188/762 (25%)	183 (97%)	5 (3%)	0	100	100
All	All	3251/5913 (55%)	3150 (97%)	99 (3%)	2 (0%)	49	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	491	SER
6	F	276	ALA

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	331/339 (98%)	331 (100%)	0	100	100
2	B	262/318 (82%)	261 (100%)	1 (0%)	84	90
3	C	455/693 (66%)	453 (100%)	2 (0%)	84	90
4	D	321/362 (89%)	318 (99%)	3 (1%)	70	85
5	E	104/145 (72%)	102 (98%)	2 (2%)	50	76
5	H	108/145 (74%)	105 (97%)	3 (3%)	38	70
5	J	109/145 (75%)	107 (98%)	2 (2%)	51	77
5	M	120/145 (83%)	120 (100%)	0	100	100
5	P	106/145 (73%)	105 (99%)	1 (1%)	70	85
6	F	114/327 (35%)	114 (100%)	0	100	100
6	N	127/327 (39%)	125 (98%)	2 (2%)	55	79
7	G	135/486 (28%)	134 (99%)	1 (1%)	76	86
7	K	158/486 (32%)	156 (99%)	2 (1%)	61	81
8	I	158/178 (89%)	158 (100%)	0	100	100
9	L	127/151 (84%)	126 (99%)	1 (1%)	73	86
10	O	171/623 (27%)	171 (100%)	0	100	100
All	All	2906/5015 (58%)	2886 (99%)	20 (1%)	73	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	125	LEU
3	C	108	VAL
3	C	129	LEU
4	D	139	VAL
4	D	239	ASP
4	D	243	VAL
5	E	44	VAL
5	E	101	LEU
7	G	418	SER
5	H	25	VAL
5	H	114	TYR
5	H	137	VAL
5	J	51	THR
5	J	69	HIS
7	K	433	ILE
7	K	500	LEU

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Mol	Chain	Res	Type
9	L	156	TRP
6	N	272	VAL
6	N	311	VAL
5	P	110	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	127	HIS
2	B	124	HIS
2	B	246	GLN
2	B	268	ASN
2	B	339	GLN
2	B	348	GLN
3	C	285	HIS
3	C	544	GLN
4	D	86	HIS
4	D	92	GLN
4	D	125	HIS
4	D	127	GLN
4	D	169	GLN
4	D	309	HIS
4	D	364	ASN
5	E	58	HIS
5	E	69	HIS
6	F	382	GLN
5	H	112	HIS
5	J	32	HIS
5	J	69	HIS
5	J	112	HIS
7	K	508	ASN
7	K	546	ASN
7	K	558	HIS
9	L	147	HIS
5	M	46	GLN
5	M	69	HIS
6	N	299	GLN
6	N	367	GLN
6	N	377	HIS
10	O	744	HIS
5	P	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	75/76 (98%)	9 (12%)	1 (1%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	9	G
11	R	18	G
11	R	19	G
11	R	21	U
11	R	30	G
11	R	31	C
11	R	47	G
11	R	71	C
11	R	77	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	R	30	G

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 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	5GP	R	101	11	26,26,26	3.45	10 (38%)	39,40,40	1.51	7 (17%)

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
14	5GP	R	101	11	-	4/10/26/26	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	101	5GP	O3'-C3'	-9.55	1.19	1.43
14	R	101	5GP	O6-C6	8.89	1.40	1.23
14	R	101	5GP	C5-N7	5.39	1.49	1.39
14	R	101	5GP	C2-N2	5.19	1.46	1.34
14	R	101	5GP	C2-N3	3.75	1.42	1.33
14	R	101	5GP	C2-N1	3.66	1.46	1.37
14	R	101	5GP	C4-N3	3.06	1.41	1.34
14	R	101	5GP	P-O3P	2.95	1.65	1.54
14	R	101	5GP	C8-N9	-2.40	1.32	1.37
14	R	101	5GP	P-O2P	-2.23	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	101	5GP	C8-N9-C4	4.26	114.01	106.03
14	R	101	5GP	C2-N1-C6	-3.32	119.08	125.11
14	R	101	5GP	C5-C6-N1	2.57	119.80	113.25
14	R	101	5GP	O6-C6-C5	-2.46	120.04	126.53
14	R	101	5GP	O2P-P-O1P	-2.42	101.40	110.83
14	R	101	5GP	C6-C5-N7	2.02	133.97	130.29
14	R	101	5GP	N9-C4-N3	2.00	129.96	125.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	R	101	5GP	C5'-O5'-P-O1P
14	R	101	5GP	C5'-O5'-P-O2P

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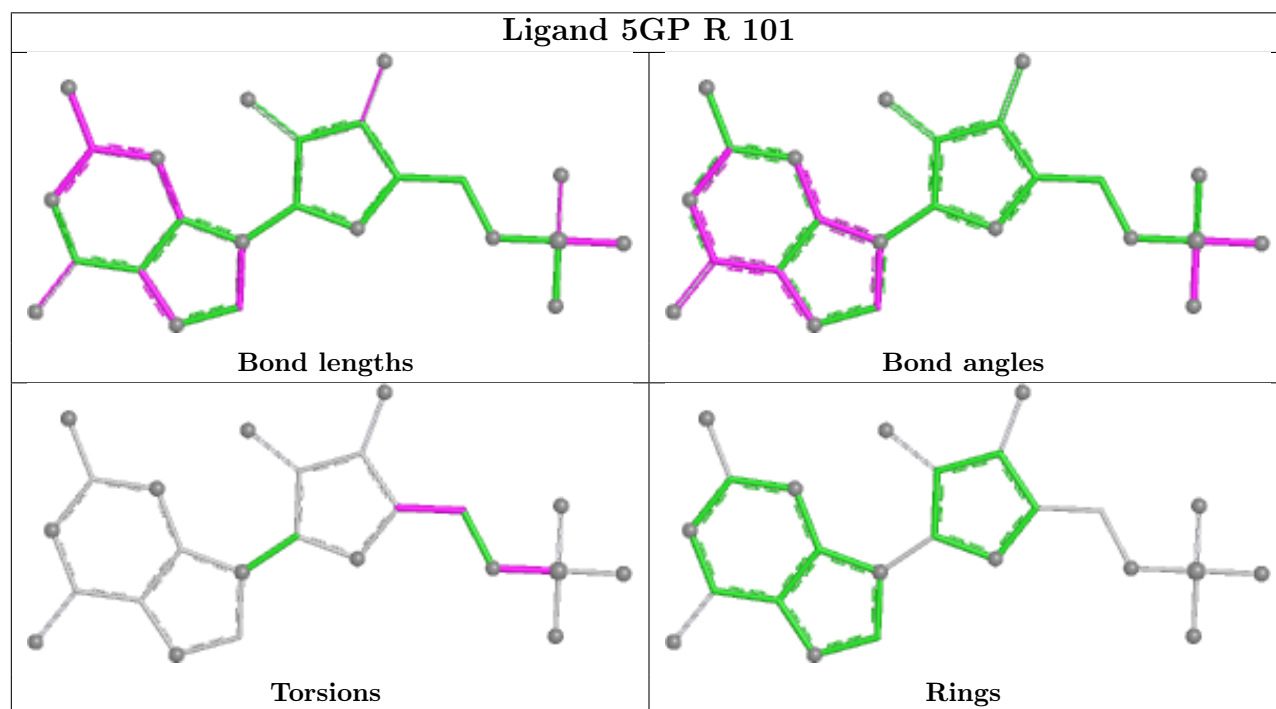
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Mol	Chain	Res	Type	Atoms
14	R	101	5GP	C5'-O5'-P-O3P
14	R	101	5GP	O4'-C4'-C5'-O5'

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 ⓘ

There are no chain breaks in this entry.

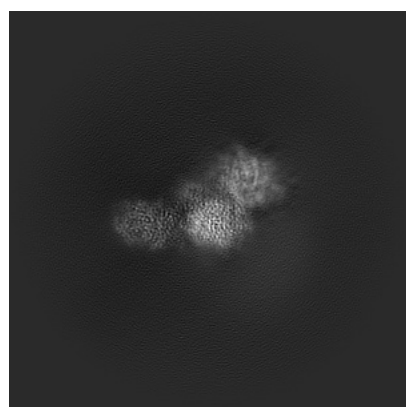
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46791. These allow visual inspection of the internal detail of the map and identification of artifacts.

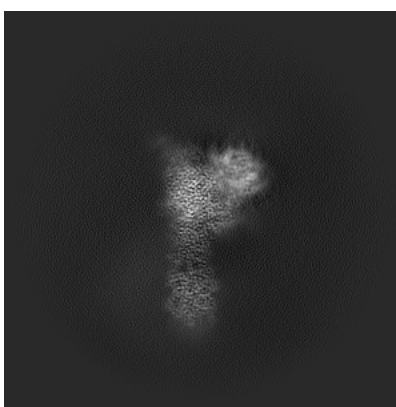
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

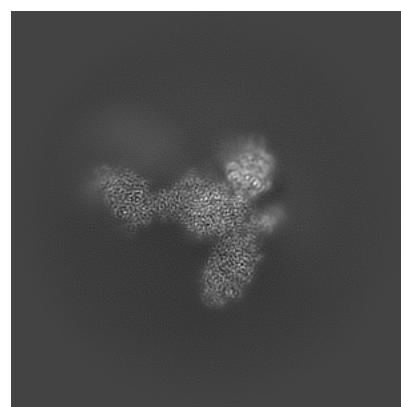
6.1.1 Primary map



X



Y

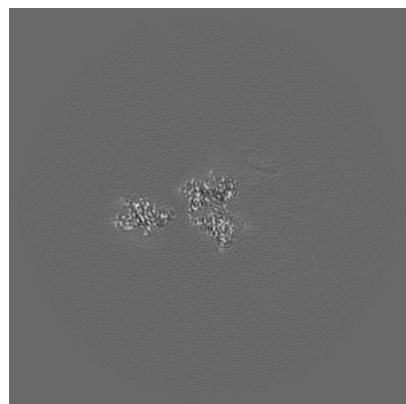


Z

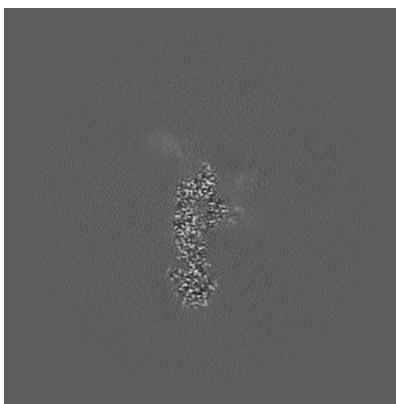
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

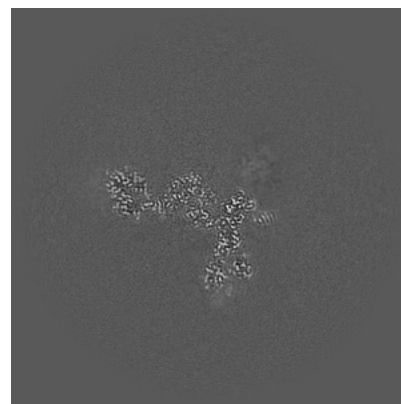
6.2.1 Primary map



X Index: 192



Y Index: 192

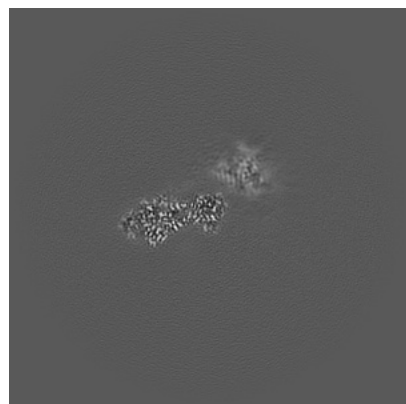


Z Index: 192

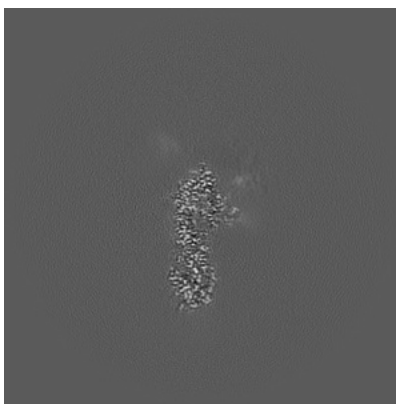
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

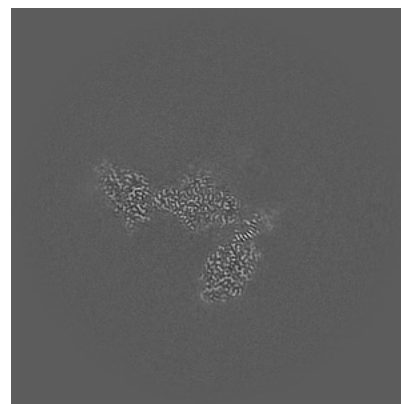
6.3.1 Primary map



X Index: 217



Y Index: 196

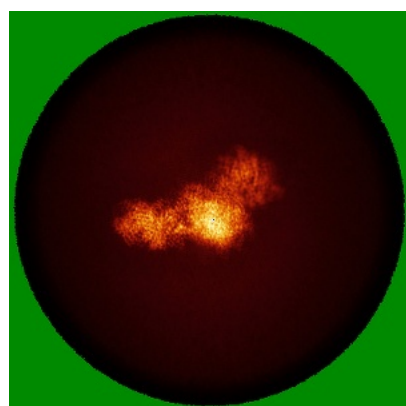


Z Index: 176

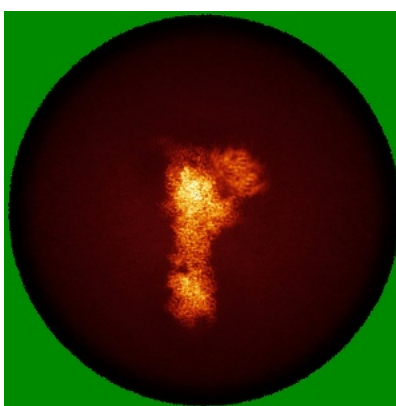
The images above show the largest variance slices of the map in three orthogonal directions.

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

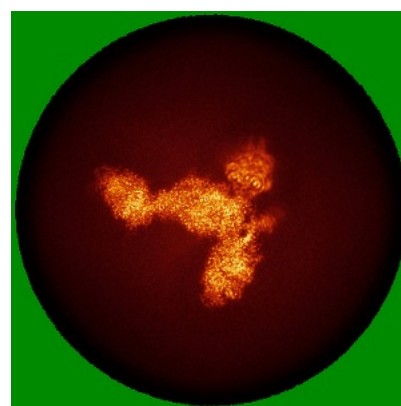
6.4.1 Primary map



X



Y

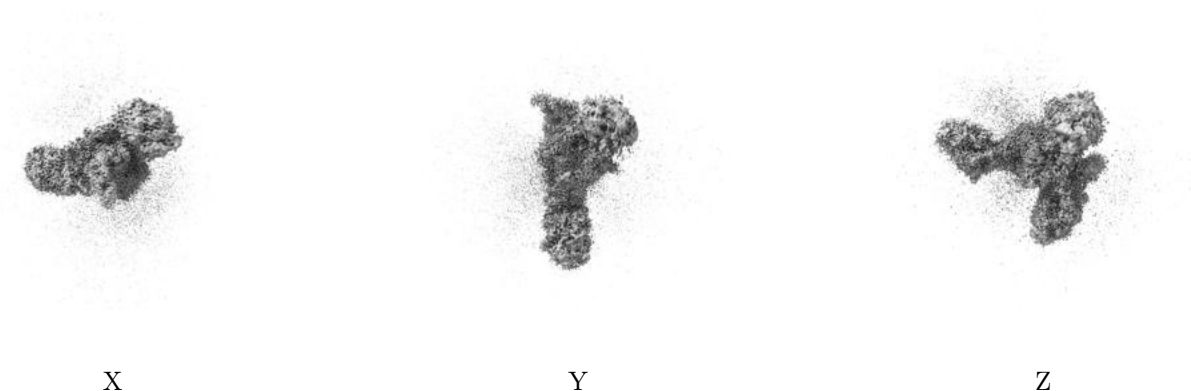


Z

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 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

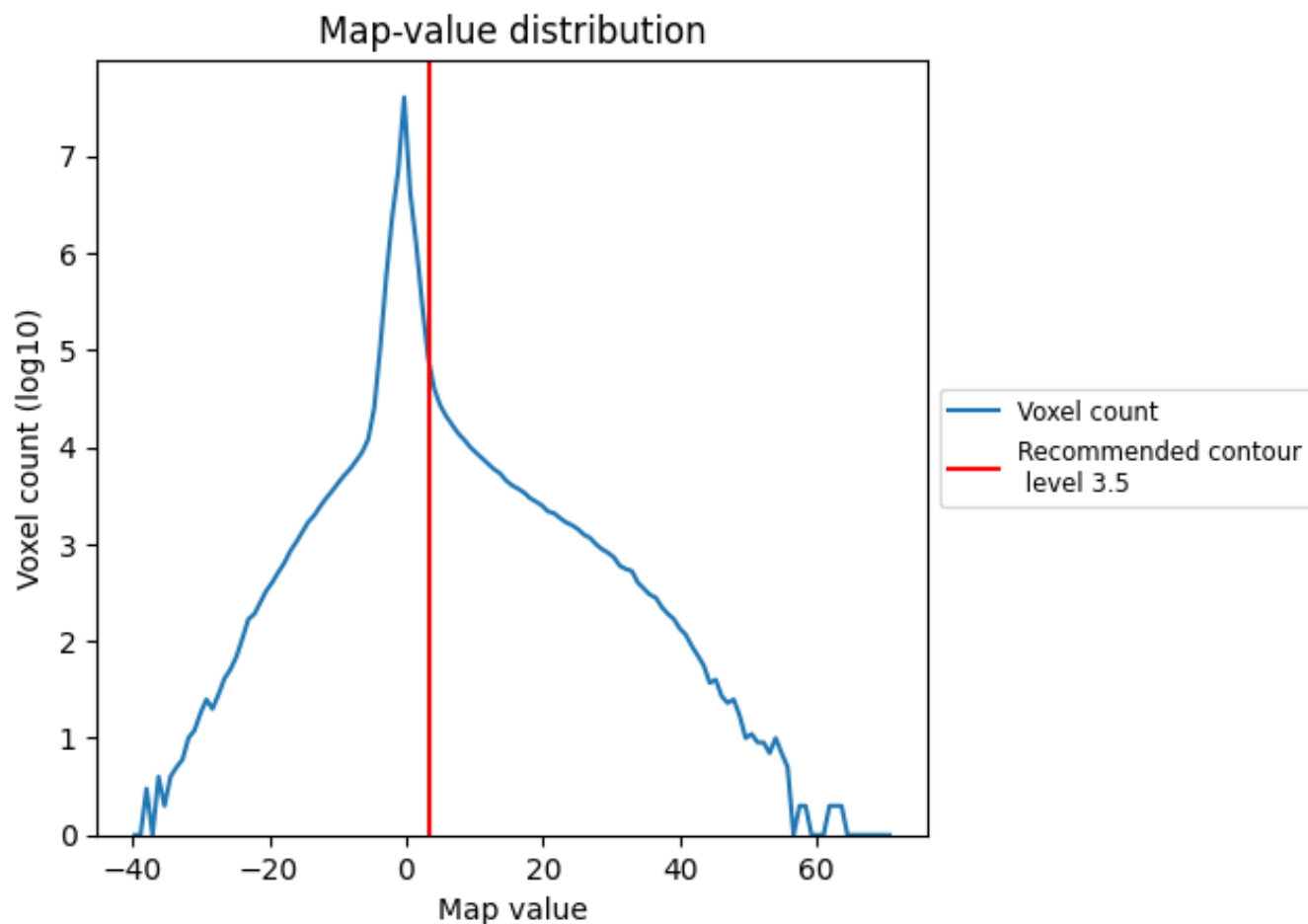
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

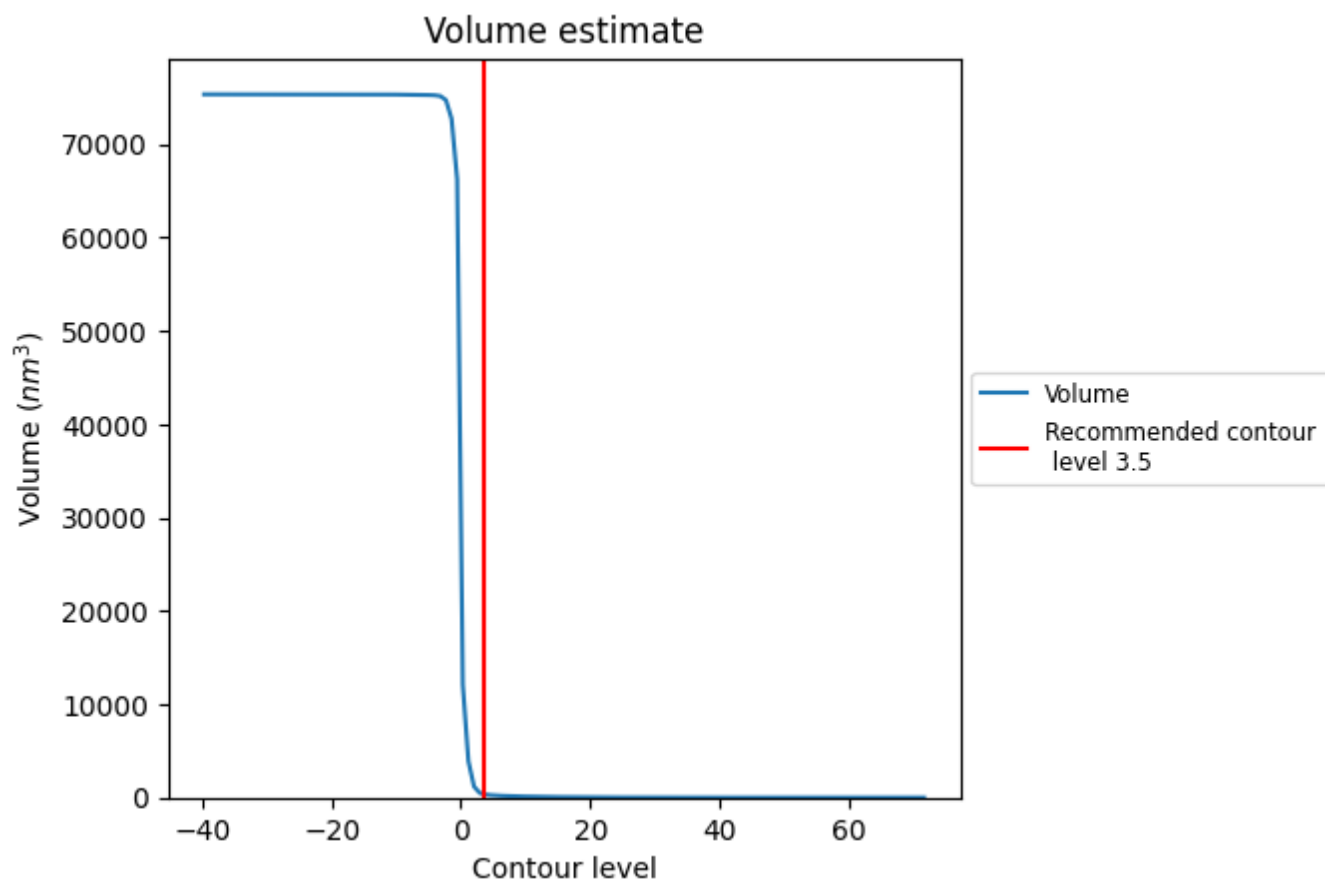
This section contains the results of statistical analysis of the map.

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.

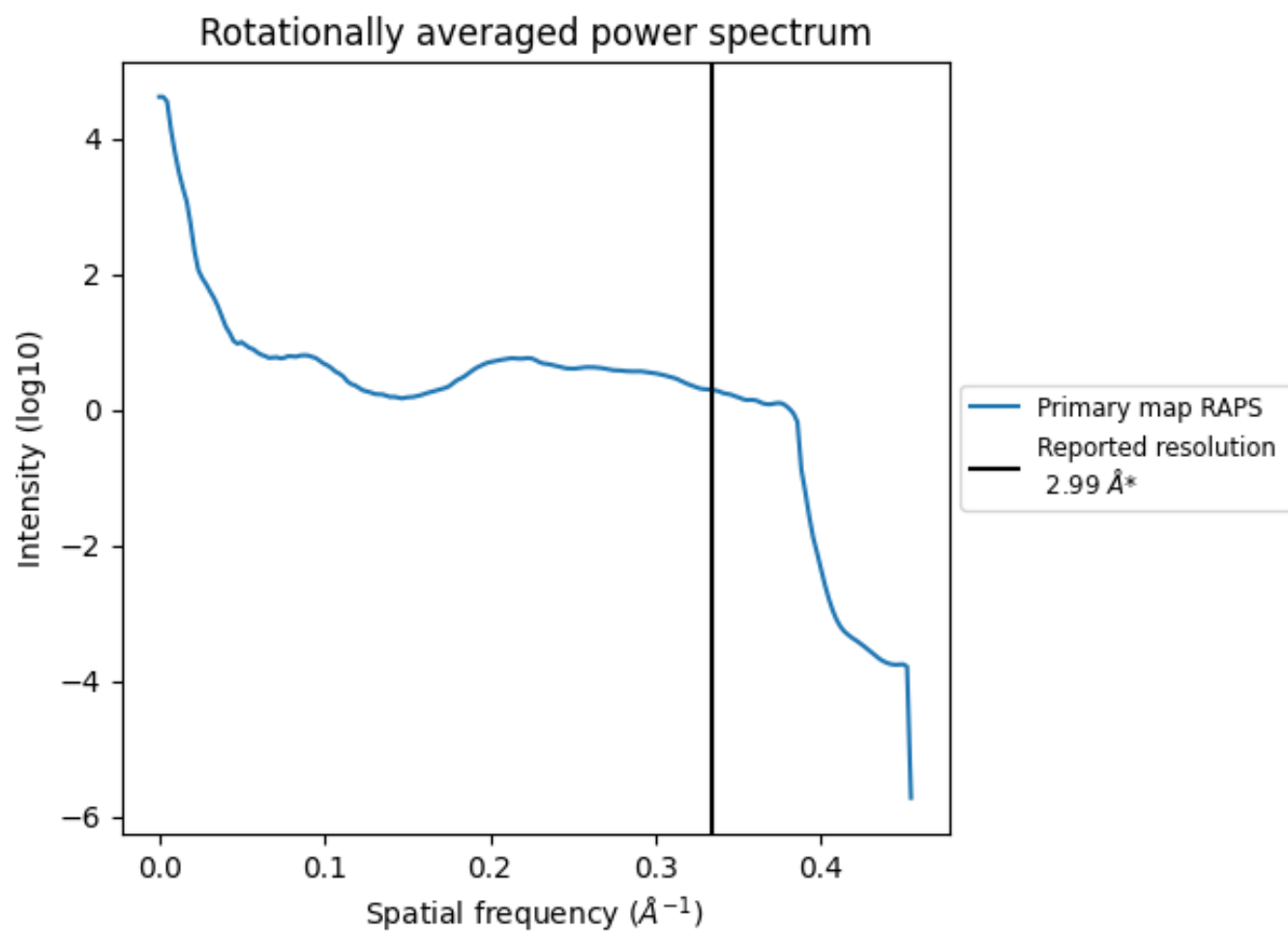
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 377 nm^3 ; this corresponds to an approximate mass of 341 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 0.334 Å⁻¹

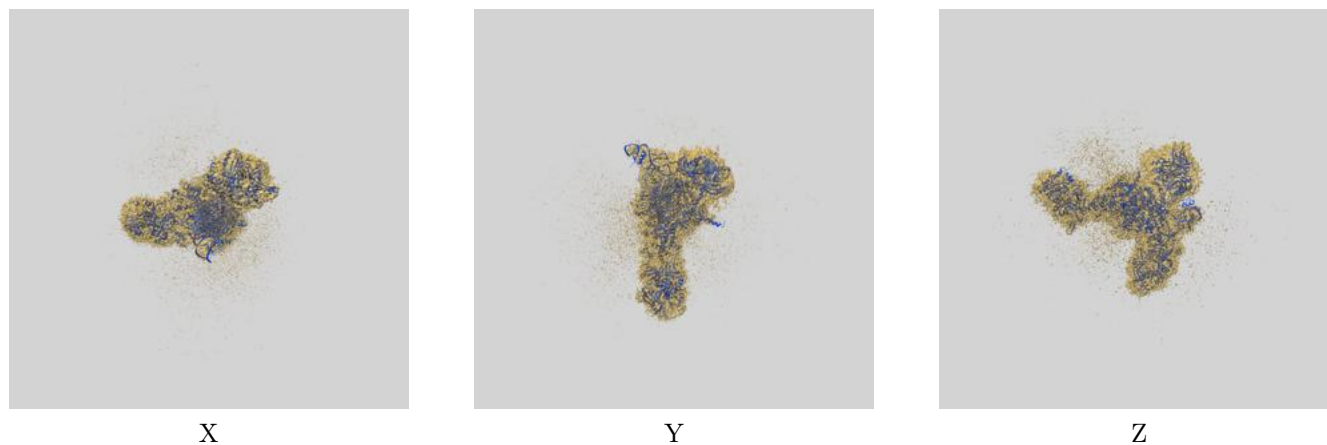
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

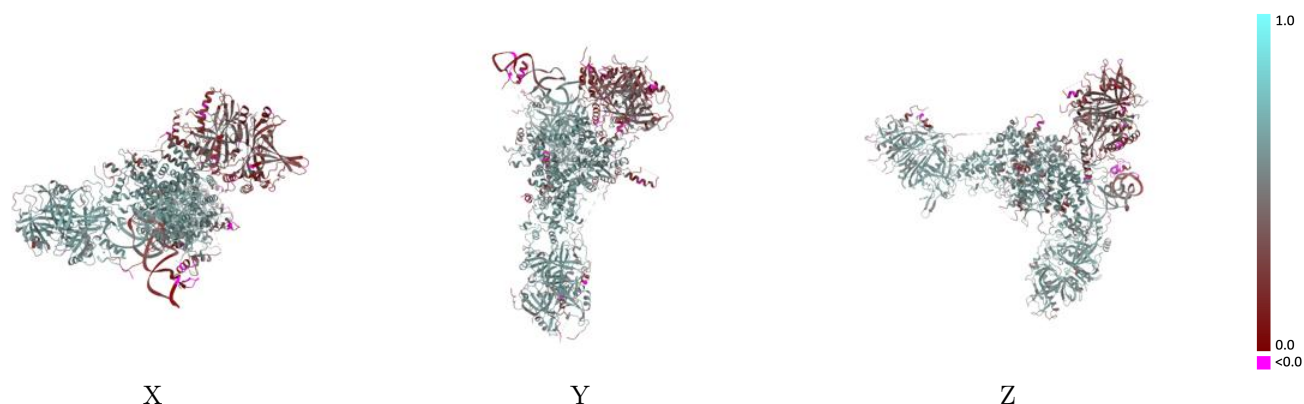
This section contains information regarding the fit between EMDB map EMD-46791 and PDB model 9DEI. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



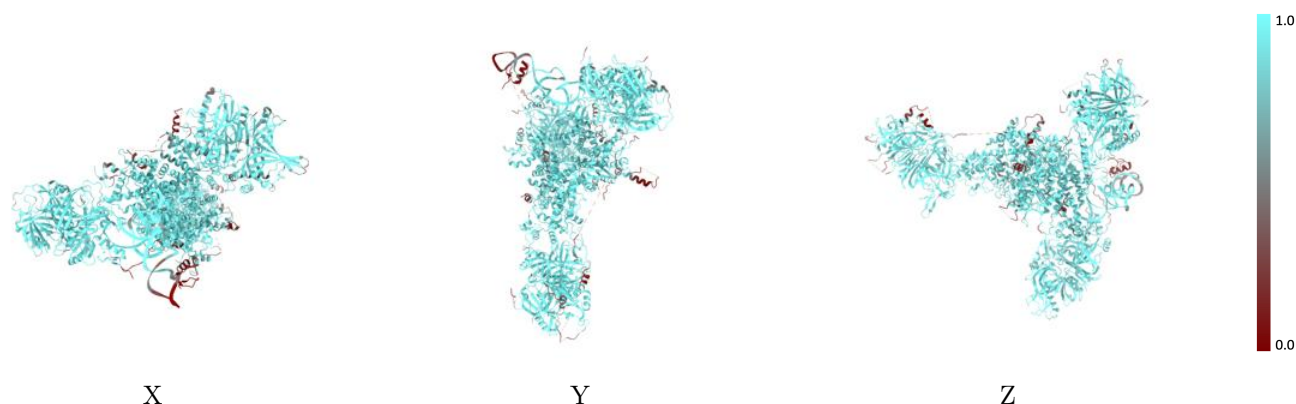
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



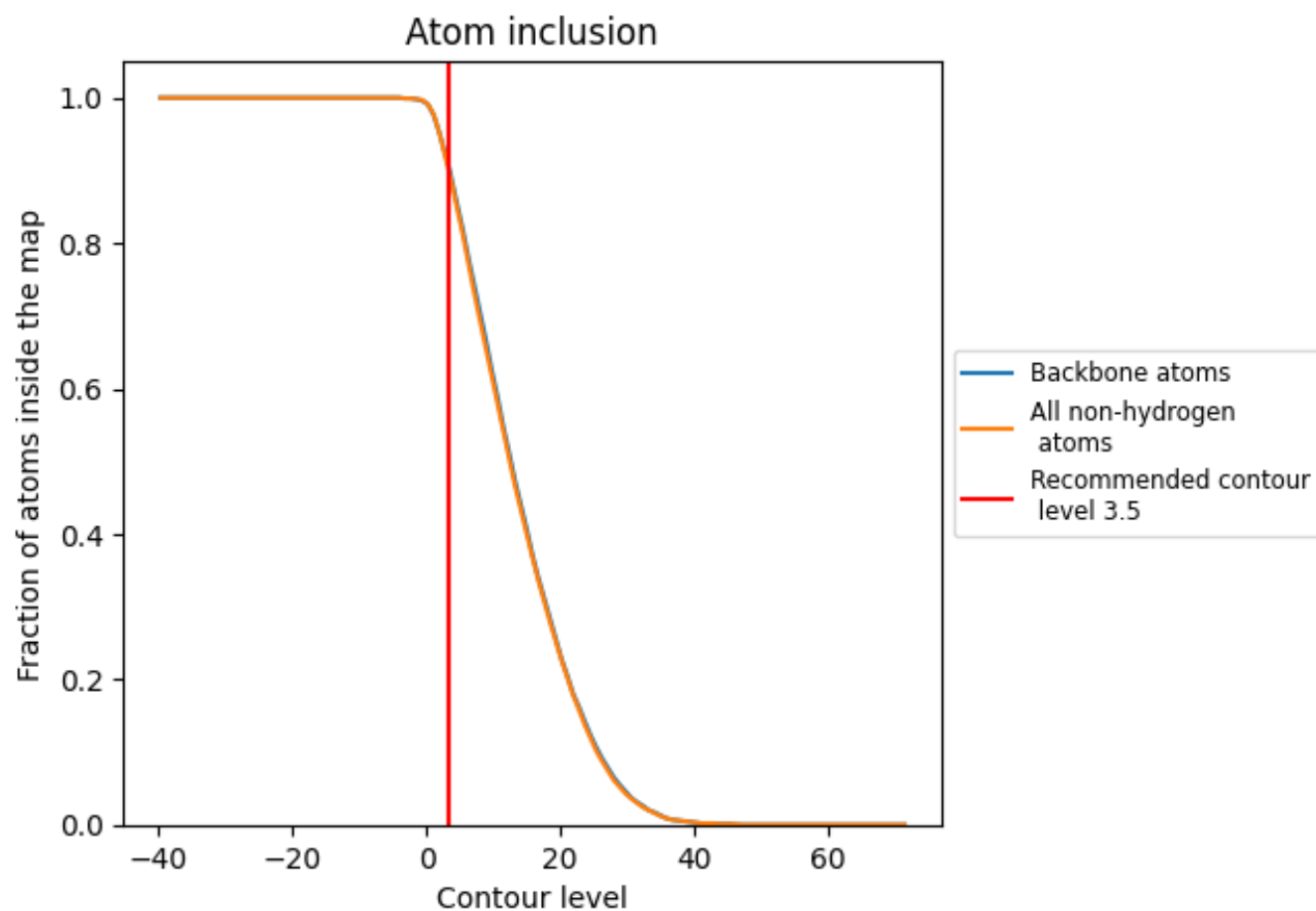
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.4950
A	 0.9500	 0.5730
B	 0.9510	 0.5800
C	 0.8600	 0.5170
D	 0.9010	 0.4740
E	 0.9800	 0.6060
F	 0.9450	 0.5850
G	 0.7570	 0.4500
H	 0.9580	 0.5580
I	 0.9010	 0.3520
J	 0.9580	 0.3580
K	 0.8330	 0.3530
L	 0.9130	 0.2780
M	 0.9430	 0.5770
N	 0.9680	 0.5930
O	 0.7830	 0.4760
P	 0.9490	 0.5630
R	 0.8280	 0.4170

