



Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 02:34 AM EDT

PDB ID : 8FN6
EMDB ID : EMD-29306
Title : Cryo-EM structure of RNase-untreated RESC-A in trypanosomal RNA editing
Authors : Liu, S.; Wang, H.; Li, X.; Zhang, F.; Lee, J.K.J.; Li, Z.; Yu, C.; Zhao, X.;
Hu, J.J.; Suematsu, T.; Alvarez-Cabrera, A.L.; Liu, Q.; Zhang, L.; Huang, L.;
Aphasizheva, I.; Aphasizhev, R.; Zhou, Z.H.
Deposited on : 2022-12-27
Resolution : 3.70 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

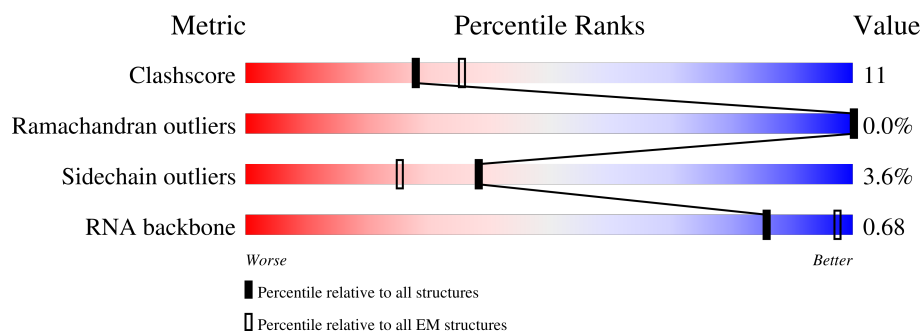
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	g	46	<div> <div>91%</div> <div>70% 30%</div> </div>
2	1	473	<div> <div>6%</div> <div>57% 17% 26%</div> </div>
3	2	492	<div> <div>16%</div> <div>62% 24% 13%</div> </div>
4	3	482	<div> <div>26%</div> <div>73% 26%</div> </div>
5	4	1087	<div> <div>53% 14% 32%</div> </div>
6	5	402	<div> <div>47% 20% 31%</div> </div>
7	6	516	<div> <div>5%</div> <div>66% 20% 12%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22421 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 RNA chain called gRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	46	Total	C	N	O	P	0	0
			960	434	152	328	46		

- Molecule 2 is a protein called RNA-editing substrate-binding complex protein 1 (RESC1).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	352	Total	C	N	O	S	0	0
			2768	1750	486	521	11		

- Molecule 3 is a protein called RNA-editing substrate-binding complex protein 2 (RESC2).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	428	Total	C	N	O	S	0	0
			3421	2165	597	638	21		

- Molecule 4 is a protein called RNA-editing substrate-binding complex protein 3 (RESC3).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	480	Total	C	N	O	S	0	0
			3705	2334	672	676	23		

- Molecule 5 is a protein called RNA-editing substrate-binding complex protein 4 (RESC4).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	741	Total	C	N	O	S	0	0
			5790	3647	1004	1103	36		

- Molecule 6 is a protein called RNA-editing substrate-binding complex protein 5 (RESC5).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	276	Total	C	N	O	S	0	0
			2163	1372	373	402	16		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	311	GLY	-	expression tag	UNP Q389F5
5	312	SER	-	expression tag	UNP Q389F5
5	313	GLY	-	expression tag	UNP Q389F5
5	314	SER	-	expression tag	UNP Q389F5
5	315	GLY	-	expression tag	UNP Q389F5
5	316	SER	-	expression tag	UNP Q389F5
5	317	ALA	-	expression tag	UNP Q389F5
5	318	SER	-	expression tag	UNP Q389F5
5	319	SER	-	expression tag	UNP Q389F5
5	320	GLY	-	expression tag	UNP Q389F5
5	321	ALA	-	expression tag	UNP Q389F5
5	322	SER	-	expression tag	UNP Q389F5
5	323	ALA	-	expression tag	UNP Q389F5
5	324	ALA	-	expression tag	UNP Q389F5
5	325	GLY	-	expression tag	UNP Q389F5
5	326	SER	-	expression tag	UNP Q389F5
5	327	SER	-	expression tag	UNP Q389F5
5	328	GLY	-	expression tag	UNP Q389F5
5	329	ALA	-	expression tag	UNP Q389F5
5	330	SER	-	expression tag	UNP Q389F5
5	331	ALA	-	expression tag	UNP Q389F5
5	332	SER	-	expression tag	UNP Q389F5
5	333	SER	-	expression tag	UNP Q389F5
5	334	GLY	-	expression tag	UNP Q389F5
5	335	ALA	-	expression tag	UNP Q389F5
5	336	SER	-	expression tag	UNP Q389F5
5	337	ALA	-	expression tag	UNP Q389F5
5	338	ALA	-	expression tag	UNP Q389F5
5	339	GLY	-	expression tag	UNP Q389F5
5	340	SER	-	expression tag	UNP Q389F5
5	341	SER	-	expression tag	UNP Q389F5
5	342	GLY	-	expression tag	UNP Q389F5
5	343	ALA	-	expression tag	UNP Q389F5
5	344	SER	-	expression tag	UNP Q389F5
5	345	ALA	-	expression tag	UNP Q389F5
5	346	GLY	-	expression tag	UNP Q389F5
5	347	HIS	-	expression tag	UNP Q389F5
5	348	HIS	-	expression tag	UNP Q389F5
5	349	HIS	-	expression tag	UNP Q389F5
5	350	HIS	-	expression tag	UNP Q389F5
5	351	HIS	-	expression tag	UNP Q389F5
5	352	HIS	-	expression tag	UNP Q389F5

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Chain	Residue	Modelled	Actual	Comment	Reference
5	353	HIS	-	expression tag	UNP Q389F5
5	354	HIS	-	expression tag	UNP Q389F5
5	355	HIS	-	expression tag	UNP Q389F5
5	356	HIS	-	expression tag	UNP Q389F5
5	357	SER	-	expression tag	UNP Q389F5
5	358	GLY	-	expression tag	UNP Q389F5
5	359	SER	-	expression tag	UNP Q389F5
5	360	GLU	-	expression tag	UNP Q389F5
5	361	ASP	-	expression tag	UNP Q389F5
5	362	GLN	-	expression tag	UNP Q389F5
5	363	VAL	-	expression tag	UNP Q389F5
5	364	ASP	-	expression tag	UNP Q389F5
5	365	PRO	-	expression tag	UNP Q389F5
5	366	ARG	-	expression tag	UNP Q389F5
5	367	LEU	-	expression tag	UNP Q389F5
5	368	ILE	-	expression tag	UNP Q389F5
5	369	ASP	-	expression tag	UNP Q389F5
5	370	GLY	-	expression tag	UNP Q389F5
5	371	LYS	-	expression tag	UNP Q389F5
5	372	ALA	-	expression tag	UNP Q389F5
5	373	SER	-	expression tag	UNP Q389F5
5	374	ALA	-	expression tag	UNP Q389F5
5	375	TRP	-	expression tag	UNP Q389F5
5	376	SER	-	expression tag	UNP Q389F5
5	377	HIS	-	expression tag	UNP Q389F5
5	378	PRO	-	expression tag	UNP Q389F5
5	379	GLN	-	expression tag	UNP Q389F5
5	380	PHE	-	expression tag	UNP Q389F5
5	381	GLU	-	expression tag	UNP Q389F5
5	382	LYS	-	expression tag	UNP Q389F5
5	383	GLY	-	expression tag	UNP Q389F5
5	384	GLY	-	expression tag	UNP Q389F5
5	385	GLY	-	expression tag	UNP Q389F5
5	386	SER	-	expression tag	UNP Q389F5
5	387	GLY	-	expression tag	UNP Q389F5
5	388	GLY	-	expression tag	UNP Q389F5
5	389	GLY	-	expression tag	UNP Q389F5
5	390	SER	-	expression tag	UNP Q389F5
5	391	GLY	-	expression tag	UNP Q389F5
5	392	GLY	-	expression tag	UNP Q389F5
5	393	SER	-	expression tag	UNP Q389F5
5	394	ALA	-	expression tag	UNP Q389F5

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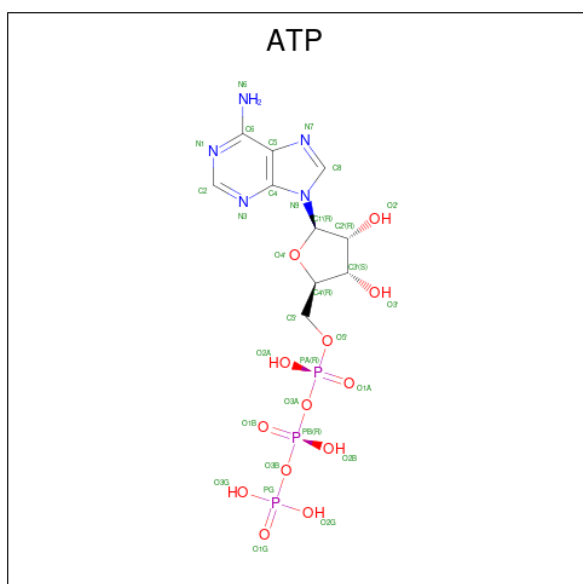
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Chain	Residue	Modelled	Actual	Comment	Reference
5	395	TRP	-	expression tag	UNP Q389F5
5	396	SER	-	expression tag	UNP Q389F5
5	397	HIS	-	expression tag	UNP Q389F5
5	398	PRO	-	expression tag	UNP Q389F5
5	399	GLN	-	expression tag	UNP Q389F5
5	400	PHE	-	expression tag	UNP Q389F5
5	401	GLU	-	expression tag	UNP Q389F5
5	402	LYS	-	expression tag	UNP Q389F5

- Molecule 7 is a protein called RNA-editing substrate-binding complex protein 6 (RESC6).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	452	Total	C	N	O	S	0	0
			3583	2285	632	649	17		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

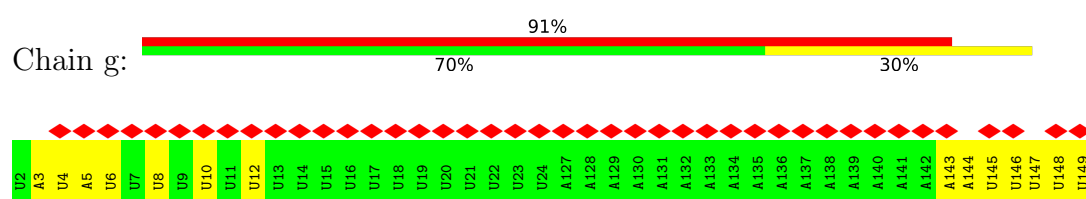


Mol	Chain	Residues	Atoms					AltConf
8	g	1	Total	C	N	O	P	0
			31	10	5	13	3	

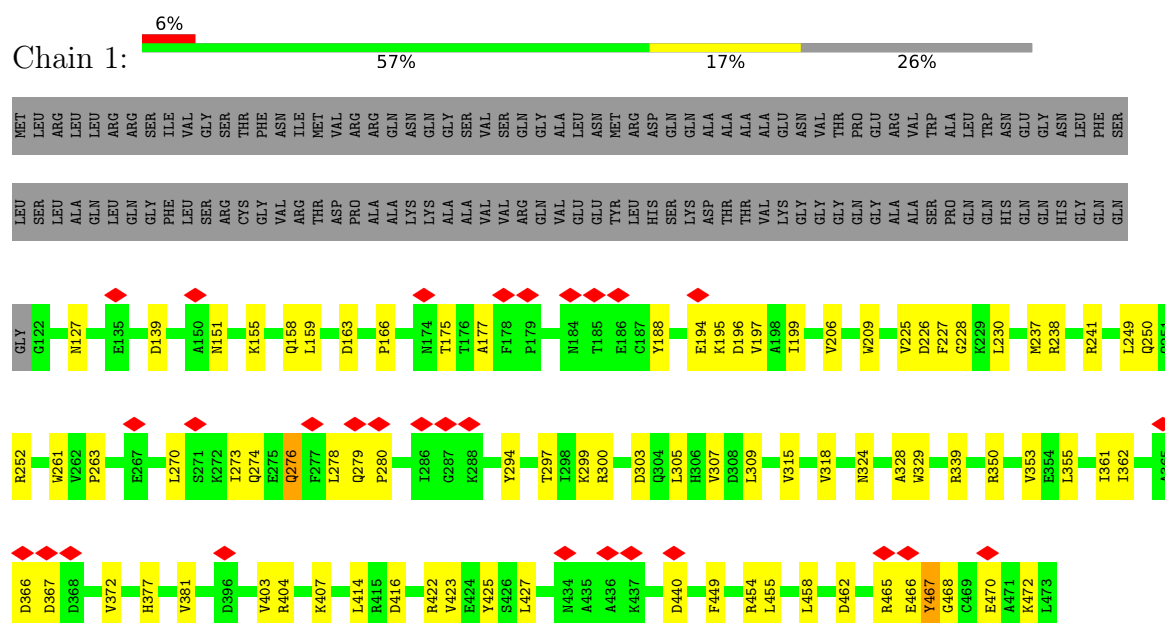
3 Residue-property plots [i](#)

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.

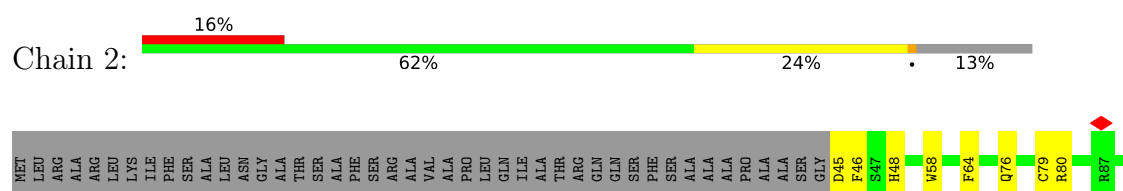
- Molecule 1: gRNA

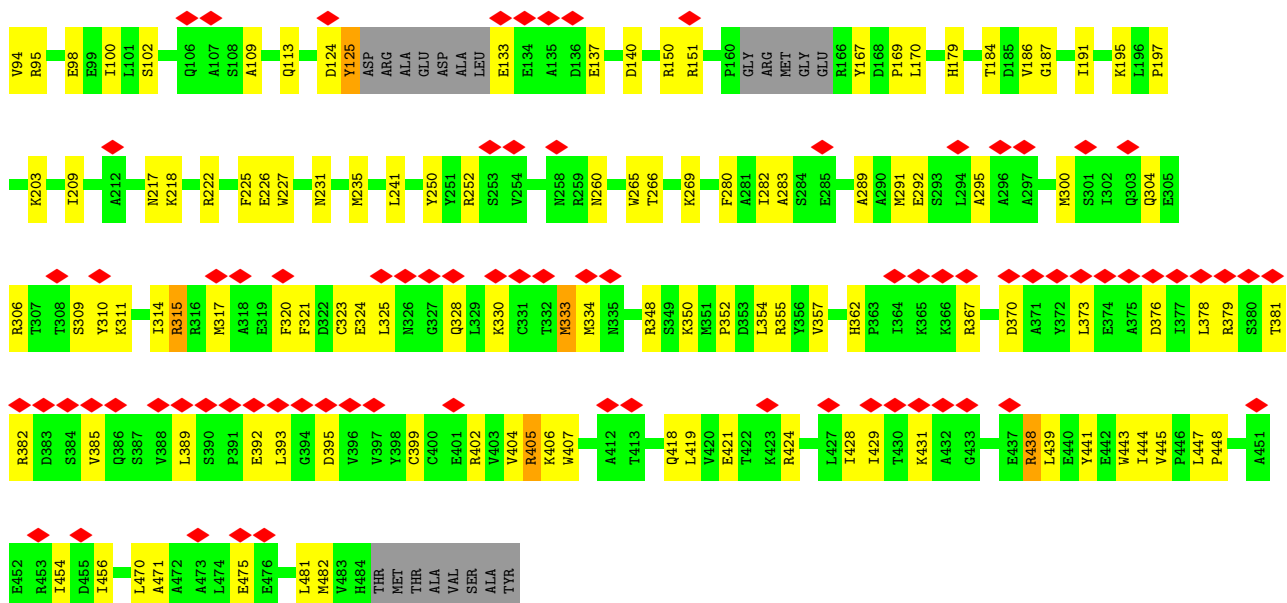


- Molecule 2: RNA-editing substrate-binding complex protein 1 (RESC1)

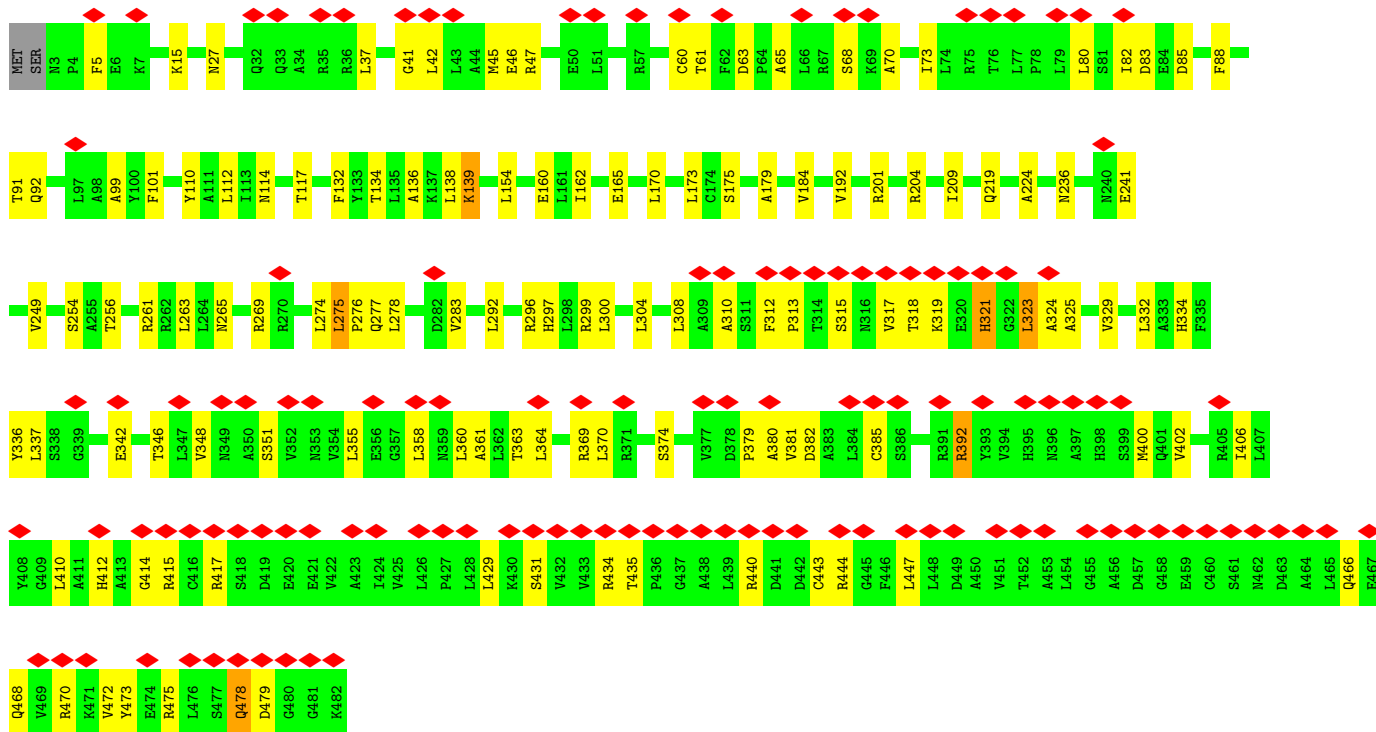


- Molecule 3: RNA-editing substrate-binding complex protein 2 (RESC2)



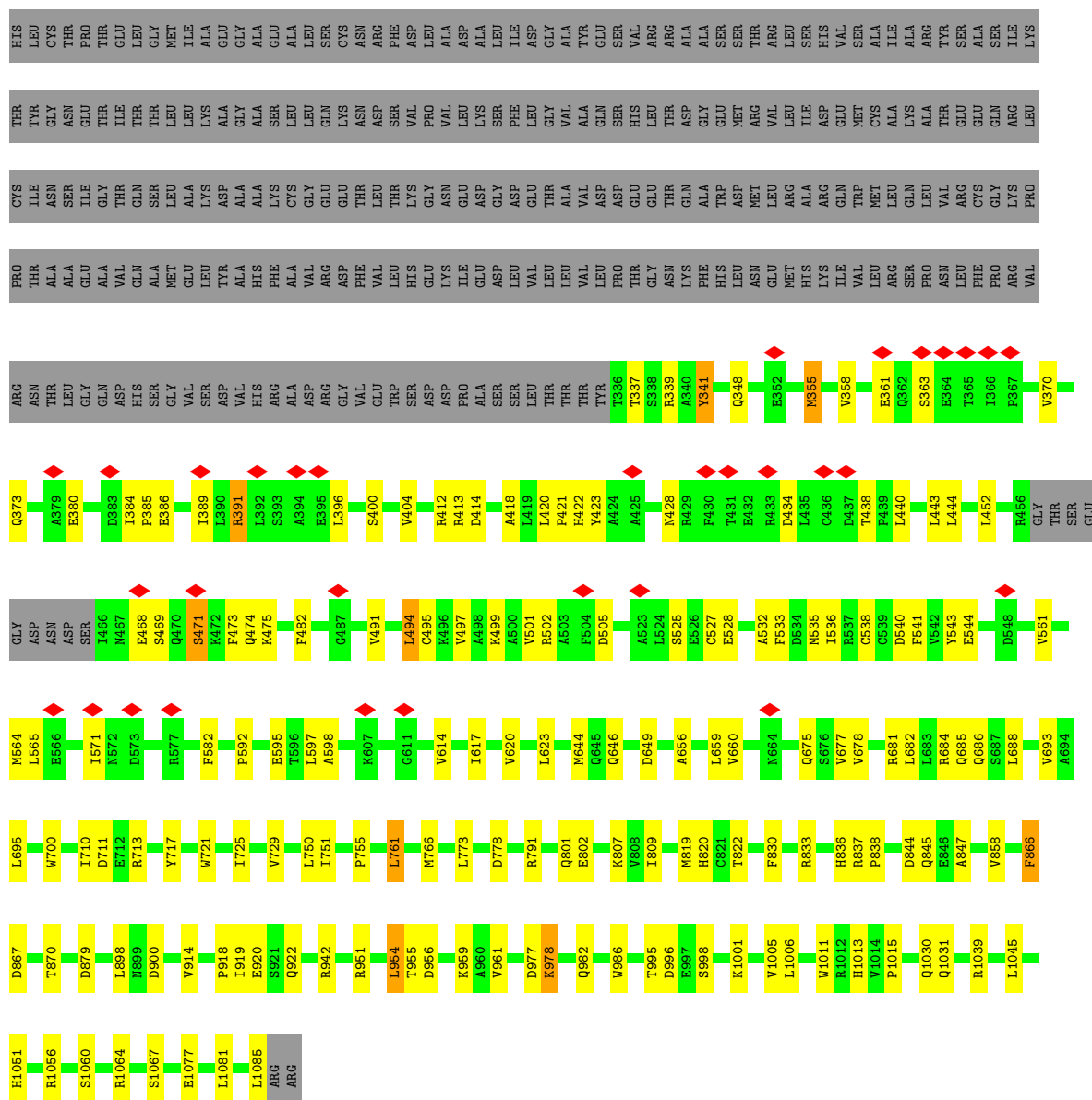


• Molecule 4: RNA-editing substrate-binding complex protein 3 (RESC3)



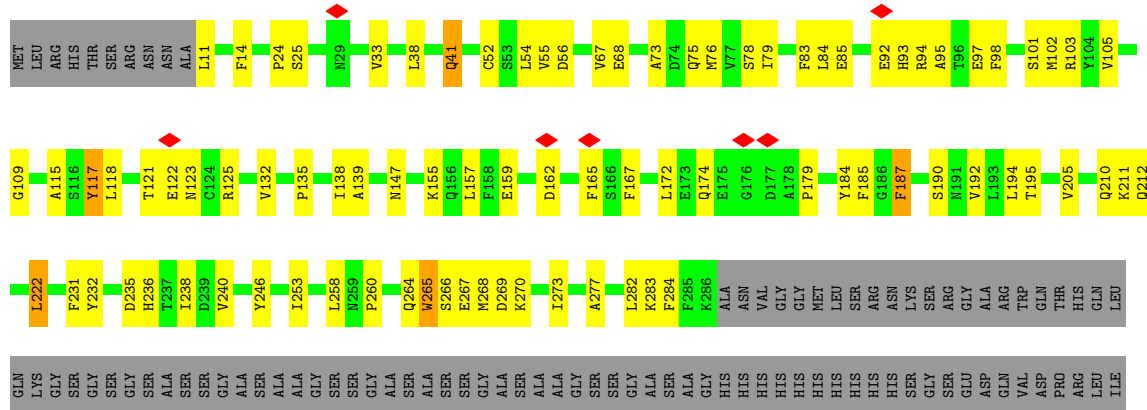
• Molecule 5: RNA-editing substrate-binding complex protein 4 (RESC4)

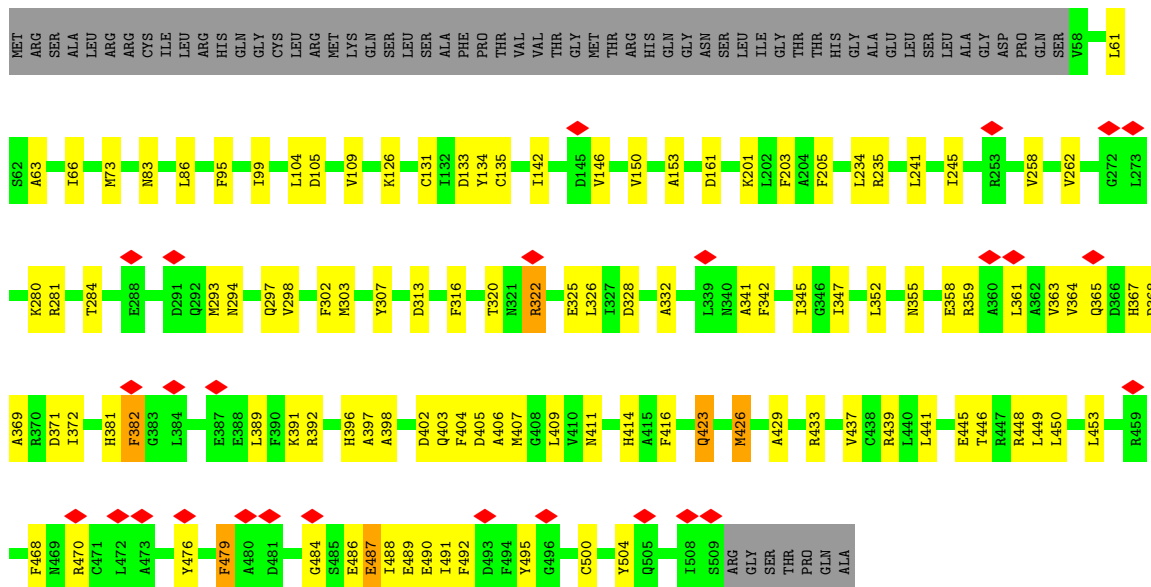




• Molecule 6: RNA-editing substrate-binding complex protein 5 (RESC5)

Chain 5: 47% 20% 31%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.207	Depositor
Minimum map value	-2.211	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.45	Depositor
Map size (\AA)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	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: ATP

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	g	0.18	0/1070	0.78	0/1656
2	1	0.24	0/2824	0.52	0/3837
3	2	0.24	0/3498	0.52	0/4744
4	3	0.24	0/3764	0.53	0/5106
5	4	0.25	0/5879	0.51	0/7961
6	5	0.25	0/2217	0.50	0/3007
7	6	0.26	0/3647	0.52	0/4927
All	All	0.25	0/22899	0.53	0/31238

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	g	960	0	482	0	0
2	1	2768	0	2779	55	0
3	2	3421	0	3357	91	0
4	3	3705	0	3819	80	0
5	4	5790	0	5831	112	0
6	5	2163	0	2103	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	6	3583	0	3621	86	0
8	g	31	0	11	0	0
All	All	22421	0	22003	453	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 (453) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:337:THR:HG22	5:4:358:VAL:HG23	1.29	1.15
4:3:275:LEU:HD23	4:3:276:PRO:HD3	1.42	1.01
3:2:418:GLN:HB2	3:2:444:ILE:HG22	1.44	0.96
6:5:84:LEU:HA	6:5:115:ALA:HB2	1.52	0.90
3:2:418:GLN:HB2	3:2:444:ILE:CG2	2.04	0.87
5:4:337:THR:HG22	5:4:358:VAL:CG2	2.08	0.84
7:6:398:ALA:HB2	7:6:426:MET:HG3	1.69	0.73
3:2:424:ARG:HB2	3:2:438:ARG:HG3	1.69	0.72
5:4:755:PRO:HB3	5:4:791:ARG:HD2	1.71	0.72
2:1:361:ILE:HG22	2:1:362:ILE:HG23	1.72	0.71
3:2:124:ASP:OD2	7:6:235:ARG:NH2	2.25	0.69
7:6:489:GLU:HA	7:6:492:PHE:CE2	2.28	0.69
3:2:350:LYS:HG3	3:2:352:PRO:HD2	1.74	0.69
5:4:363:SER:O	5:4:391:ARG:NH1	2.26	0.68
7:6:201:LYS:HG2	7:6:205:PHE:CE2	2.29	0.68
2:1:470:GLU:HA	3:2:191:ILE:HD11	1.77	0.66
4:3:466:GLN:OE1	4:3:470:ARG:NH1	2.27	0.66
5:4:614:VAL:HG11	5:4:646:GLN:HG3	1.78	0.66
5:4:428:ASN:ND2	5:4:469:SER:O	2.29	0.66
3:2:45:ASP:CG	3:2:46:PHE:H	2.00	0.65
5:4:660:VAL:HG21	5:4:695:LEU:HD22	1.78	0.65
3:2:226:GLU:HG2	3:2:456:ILE:HD12	1.78	0.65
2:1:163:ASP:OD1	2:1:195:LYS:NZ	2.29	0.65
2:1:299:LYS:NZ	4:3:83:ASP:OD2	2.29	0.65
4:3:321:HIS:O	4:3:321:HIS:ND1	2.29	0.65
4:3:276:PRO:HB2	4:3:277:GLN:NE2	2.12	0.64
3:2:421:GLU:HG3	3:2:439:LEU:HD11	1.80	0.62
5:4:678:VAL:O	5:4:682:LEU:HG	2.00	0.62
7:6:486:GLU:O	7:6:489:GLU:HB2	1.99	0.62
2:1:225:VAL:HB	2:1:427:LEU:HB2	1.80	0.62
4:3:261:ARG:NH2	5:4:540:ASP:OD1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:187:PHE:HE2	6:5:232:TYR:HB2	1.63	0.62
2:1:227:PHE:HE2	2:1:455:LEU:HD13	1.65	0.62
5:4:951:ARG:NH1	5:4:982:GLN:OE1	2.30	0.62
6:5:25:SER:HA	6:5:33:VAL:HG22	1.82	0.61
4:3:132:PHE:HE2	4:3:154:LEU:HD21	1.65	0.61
3:2:295:ALA:HA	3:2:300:MET:HG2	1.82	0.61
6:5:192:VAL:HG21	6:5:258:LEU:HD11	1.80	0.61
5:4:801:GLN:OE1	5:4:833:ARG:NH1	2.34	0.61
7:6:63:ALA:HB3	7:6:104:LEU:HD11	1.83	0.61
4:3:410:LEU:HD12	4:3:415:ARG:HB2	1.83	0.61
2:1:307:VAL:HG12	2:1:318:VAL:HG22	1.81	0.61
4:3:468:GLN:O	4:3:472:VAL:HG23	2.00	0.61
6:5:54:LEU:HD23	6:5:55:VAL:HG13	1.82	0.61
6:5:11:LEU:N	6:5:282:LEU:O	2.34	0.61
7:6:332:ALA:HB3	7:6:363:VAL:CG1	2.30	0.61
4:3:392:ARG:O	4:3:392:ARG:NH1	2.33	0.60
3:2:186:VAL:HG12	3:2:187:GLY:N	2.16	0.60
3:2:348:ARG:HH21	3:2:352:PRO:HB2	1.65	0.60
5:4:681:ARG:HD2	5:4:684:ARG:HH21	1.67	0.60
3:2:46:PHE:HD2	3:2:48:HIS:HE1	1.48	0.60
3:2:309:SER:HB2	3:2:402:ARG:HG3	1.83	0.60
5:4:525:SER:OG	5:4:528:GLU:OE1	2.20	0.60
6:5:117:TYR:HD2	6:5:157:LEU:HD12	1.66	0.60
4:3:478:GLN:NE2	4:3:479:ASP:OD1	2.35	0.60
5:4:386:GLU:HA	5:4:389:ILE:HD12	1.83	0.60
4:3:429:LEU:HD22	4:3:472:VAL:HG21	1.83	0.60
5:4:499:LYS:HE2	5:4:535:MET:HA	1.84	0.60
5:4:497:VAL:O	5:4:501:VAL:HG12	2.02	0.60
2:1:454:ARG:HH22	2:1:458:LEU:HD21	1.67	0.59
4:3:5:PHE:CE2	7:6:403:GLN:HG2	2.37	0.59
2:1:276:GLN:HE21	2:1:278:LEU:HD23	1.68	0.59
4:3:342:GLU:O	4:3:346:THR:HG23	2.03	0.59
5:4:532:ALA:O	5:4:535:MET:HG2	2.03	0.59
4:3:361:ALA:HA	4:3:364:LEU:HD12	1.84	0.58
3:2:241:LEU:HB3	3:2:445:VAL:O	2.03	0.58
6:5:132:VAL:HG13	6:5:139:ALA:HB3	1.84	0.58
7:6:488:ILE:O	7:6:491:ILE:HG12	2.04	0.58
6:5:253:ILE:HD11	6:5:260:PRO:HB3	1.84	0.58
7:6:441:LEU:HB2	7:6:446:THR:HG23	1.85	0.58
2:1:472:LYS:HE3	3:2:209:ILE:HD12	1.84	0.58
5:4:474:GLN:NE2	5:4:505:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:845:GLN:NE2	5:4:879:ASP:O	2.36	0.58
5:4:428:ASN:HB2	5:4:473:PHE:CD2	2.39	0.58
4:3:160:GLU:O	5:4:837:ARG:NH1	2.33	0.57
4:3:325:ALA:O	4:3:329:VAL:HG22	2.04	0.57
7:6:364:VAL:HG22	7:6:396:HIS:CD2	2.39	0.57
4:3:313:PRO:HD2	4:3:317:VAL:HB	1.84	0.57
3:2:109:ALA:O	4:3:15:LYS:NZ	2.37	0.57
3:2:370:ASP:HA	3:2:373:LEU:HG	1.85	0.57
4:3:414:GLY:O	4:3:417:ARG:NE	2.38	0.57
7:6:429:ALA:O	7:6:433:ARG:HG2	2.05	0.57
5:4:384:ILE:HG23	5:4:389:ILE:HD11	1.86	0.56
4:3:42:LEU:O	4:3:46:GLU:HG2	2.03	0.56
4:3:321:HIS:HA	4:3:324:ALA:HB3	1.86	0.56
4:3:370:LEU:O	4:3:374:SER:OG	2.20	0.56
5:4:684:ARG:NH1	5:4:685:GLN:O	2.38	0.56
6:5:94:ARG:O	6:5:97:GLU:HG2	2.06	0.56
3:2:419:LEU:HB2	3:2:443:TRP:CZ3	2.40	0.56
7:6:426:MET:HE2	7:6:426:MET:H	1.70	0.56
2:1:155:LYS:NZ	2:1:324:ASN:O	2.37	0.56
3:2:283:ALA:N	3:2:439:LEU:O	2.38	0.56
7:6:361:LEU:HG	7:6:389:LEU:HD13	1.87	0.56
3:2:381:THR:HG22	3:2:382:ARG:N	2.21	0.56
2:1:163:ASP:HA	2:1:195:LYS:HD2	1.88	0.55
6:5:139:ALA:HB1	6:5:172:LEU:HD11	1.87	0.55
7:6:361:LEU:HG	7:6:389:LEU:CD1	2.36	0.55
2:1:194:GLU:OE2	2:1:196:ASP:N	2.39	0.55
5:4:914:VAL:HG11	5:4:942:ARG:HG3	1.88	0.55
3:2:150:ARG:NH2	7:6:161:ASP:OD1	2.40	0.55
4:3:91:THR:HG23	4:3:112:LEU:HD22	1.88	0.55
4:3:296:ARG:NH1	5:4:544:GLU:OE2	2.40	0.55
5:4:644:MET:HG3	5:4:677:VAL:HG21	1.89	0.55
5:4:1013:HIS:CE1	5:4:1015:PRO:HD2	2.42	0.55
7:6:302:PHE:HE2	7:6:341:ALA:HB3	1.72	0.55
3:2:79:CYS:HB3	3:2:100:ILE:HG21	1.88	0.54
4:3:219:GLN:HG2	4:3:256:THR:HG21	1.87	0.54
5:4:1056:ARG:O	5:4:1060:SER:OG	2.24	0.54
3:2:424:ARG:HB2	3:2:438:ARG:CG	2.37	0.54
3:2:76:GLN:O	3:2:80:ARG:NH1	2.40	0.54
4:3:297:HIS:HB3	4:3:300:LEU:HB3	1.89	0.54
2:1:294:TYR:HB2	2:1:309:LEU:HB2	1.90	0.54
5:4:468:GLU:OE1	5:4:468:GLU:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:235:ASP:OD1	6:5:236:HIS:N	2.41	0.53
2:1:188:TYR:HD2	3:2:250:TYR:HB2	1.74	0.53
3:2:310:TYR:HB2	3:2:325:LEU:HB2	1.91	0.53
7:6:382:PHE:CG	7:6:382:PHE:O	2.62	0.53
2:1:159:LEU:HD21	2:1:249:LEU:HD23	1.89	0.53
5:4:412:ARG:NH2	5:4:452:LEU:O	2.41	0.53
6:5:174:GLN:OE1	6:5:184:TYR:OH	2.25	0.53
7:6:313:ASP:N	7:6:313:ASP:OD1	2.42	0.53
3:2:315:ARG:NH1	3:2:321:PHE:O	2.42	0.53
4:3:283:VAL:HG13	4:3:304:LEU:HD22	1.91	0.53
6:5:78:SER:HB3	6:5:282:LEU:HD23	1.90	0.53
2:1:465:ARG:NE	2:1:466:GLU:OE1	2.33	0.53
3:2:227:TRP:O	3:2:231:ASN:ND2	2.32	0.53
7:6:201:LYS:HG2	7:6:205:PHE:CZ	2.45	0.52
4:3:63:ASP:OD1	4:3:63:ASP:N	2.42	0.52
5:4:751:ILE:HB	5:4:773:LEU:HD13	1.92	0.52
7:6:258:VAL:O	7:6:262:VAL:HG23	2.09	0.52
3:2:429:ILE:HD11	3:2:431:LYS:HG2	1.90	0.52
4:3:406:ILE:HG23	4:3:410:LEU:HD23	1.90	0.52
5:4:822:THR:HG22	5:4:858:VAL:HG12	1.92	0.52
7:6:73:MET:HG2	7:6:86:LEU:HD12	1.91	0.52
4:3:60:CYS:SG	4:3:61:THR:N	2.82	0.52
6:5:265:TRP:O	6:5:269:ASP:HB2	2.10	0.52
2:1:177:ALA:HB3	3:2:481:LEU:HD13	1.92	0.52
3:2:389:LEU:HD22	3:2:393:LEU:HD11	1.91	0.52
3:2:418:GLN:CB	3:2:444:ILE:CG2	2.85	0.52
6:5:85:GLU:H	6:5:115:ALA:CB	2.23	0.52
4:3:381:VAL:O	4:3:385:CYS:N	2.42	0.52
5:4:807:LYS:HA	5:4:847:ALA:HB2	1.90	0.52
5:4:900:ASP:OD1	5:4:900:ASP:N	2.36	0.52
3:2:399:CYS:N	3:2:428:ILE:O	2.39	0.52
3:2:328:GLN:HE22	3:2:330:LYS:HB3	1.76	0.51
4:3:41:GLY:O	4:3:45:MET:HG2	2.11	0.51
3:2:354:LEU:HD11	3:2:471:ALA:HB2	1.92	0.51
4:3:192:VAL:HG23	4:3:224:ALA:HB2	1.93	0.51
3:2:292:GLU:O	3:2:295:ALA:HB3	2.10	0.51
3:2:352:PRO:HG2	3:2:475:GLU:HA	1.92	0.51
6:5:155:LYS:NZ	6:5:159:GLU:HG3	2.24	0.51
7:6:409:LEU:HD12	7:6:437:VAL:HG21	1.92	0.51
7:6:441:LEU:O	7:6:470:ARG:NH1	2.44	0.51
4:3:334:HIS:HA	4:3:369:ARG:HH22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:951:ARG:HD2	5:4:986:TRP:CG	2.46	0.51
5:4:396:LEU:HD13	5:4:422:HIS:CE1	2.46	0.51
2:1:237:MET:SD	2:1:238:ARG:N	2.83	0.51
4:3:332:LEU:HD22	4:3:337:LEU:HD21	1.93	0.51
3:2:481:LEU:H	3:2:481:LEU:HD23	1.75	0.51
5:4:711:ASP:OD2	5:4:713:ARG:NE	2.44	0.51
3:2:186:VAL:CG1	3:2:187:GLY:N	2.74	0.51
5:4:495:CYS:O	5:4:499:LYS:HG2	2.11	0.51
3:2:389:LEU:HB3	3:2:393:LEU:HD11	1.92	0.50
5:4:1064:ARG:NE	6:5:235:ASP:OD2	2.40	0.50
2:1:226:ASP:OD1	2:1:226:ASP:N	2.44	0.50
5:4:380:GLU:OE2	5:4:413:ARG:NH1	2.45	0.50
7:6:203:PHE:CZ	7:6:234:LEU:HD21	2.46	0.50
2:1:250:GLN:NE2	3:2:140:ASP:OD1	2.41	0.50
3:2:314:ILE:HG13	3:2:321:PHE:HB2	1.94	0.50
5:4:440:LEU:HA	5:4:443:LEU:HD12	1.92	0.50
5:4:597:LEU:HD12	5:4:597:LEU:H	1.77	0.50
7:6:369:ALA:HB1	7:6:404:PHE:CD1	2.46	0.50
6:5:109:GLY:HA3	6:5:284:PHE:CE1	2.47	0.50
7:6:441:LEU:HD11	7:6:449:LEU:HD13	1.92	0.50
4:3:308:LEU:HD23	4:3:310:ALA:H	1.77	0.50
2:1:227:PHE:C	2:1:339:ARG:HH22	2.15	0.50
6:5:14:PHE:HE2	6:5:105:VAL:HG22	1.76	0.50
5:4:561:VAL:O	5:4:564:MET:HB3	2.12	0.49
4:3:435:THR:O	4:3:475:ARG:NH2	2.44	0.49
5:4:700:TRP:CG	5:4:710:ILE:HD13	2.46	0.49
7:6:368:ASP:CG	7:6:369:ALA:H	2.14	0.49
5:4:598:ALA:HB1	5:4:623:LEU:HD21	1.93	0.49
6:5:24:PRO:HD3	6:5:67:VAL:HG21	1.95	0.49
2:1:166:PRO:HA	3:2:184:THR:HG22	1.95	0.49
4:3:431:SER:HA	4:3:434:ARG:HG2	1.95	0.49
5:4:361:GLU:O	5:4:361:GLU:OE1	2.30	0.49
6:5:195:THR:HG21	6:5:205:VAL:HG23	1.95	0.49
5:4:471:SER:O	5:4:475:LYS:HG3	2.13	0.49
5:4:649:ASP:OD1	5:4:684:ARG:NH2	2.46	0.49
4:3:297:HIS:CD2	5:4:592:PRO:HB3	2.47	0.49
4:3:299:ARG:HH21	5:4:595:GLU:HG3	1.78	0.49
7:6:126:LYS:HD2	7:6:126:LYS:O	2.13	0.49
7:6:484:GLY:O	7:6:488:ILE:HD12	2.13	0.49
6:5:76:MET:HE1	6:5:83:PHE:HD1	1.78	0.49
3:2:448:PRO:HB3	3:2:454:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:348:VAL:HG11	4:3:380:ALA:HB1	1.95	0.49
4:3:443:CYS:O	4:3:447:LEU:HD23	2.12	0.49
6:5:240:VAL:HG21	6:5:253:ILE:HD12	1.94	0.49
2:1:158:GLN:HB2	2:1:328:ALA:HA	1.95	0.49
7:6:404:PHE:CD2	7:6:409:LEU:HD23	2.48	0.49
7:6:341:ALA:O	7:6:345:ILE:HG12	2.13	0.48
3:2:300:MET:HE3	3:2:300:MET:HA	1.95	0.48
3:2:151:ARG:HH11	3:2:151:ARG:HG3	1.77	0.48
6:5:268:MET:HG3	6:5:273:ILE:HB	1.96	0.48
3:2:376:ASP:OD1	3:2:376:ASP:N	2.37	0.48
5:4:761:LEU:HD21	5:4:766:MET:HE2	1.95	0.48
5:4:1039:ARG:HD3	5:4:1067:SER:HB3	1.94	0.48
4:3:379:PRO:O	4:3:382:ASP:HB2	2.14	0.48
5:4:778:ASP:OD1	5:4:820:HIS:NE2	2.47	0.48
7:6:342:PHE:CZ	7:6:352:LEU:HD21	2.49	0.48
7:6:365:GLN:HA	7:6:396:HIS:NE2	2.28	0.48
2:1:403:VAL:HG22	2:1:427:LEU:HD22	1.94	0.48
3:2:348:ARG:NH2	3:2:352:PRO:O	2.47	0.48
7:6:293:MET:HE2	7:6:298:VAL:HG22	1.95	0.48
2:1:297:THR:HG23	2:1:381:VAL:HG23	1.96	0.47
3:2:113:GLN:HE21	7:6:153:ALA:HA	1.79	0.47
5:4:339:ARG:H	5:4:339:ARG:HD2	1.80	0.47
5:4:495:CYS:HA	5:4:535:MET:HE3	1.96	0.47
5:4:725:ILE:HG23	5:4:729:VAL:HB	1.96	0.47
6:5:267:GLU:H	6:5:267:GLU:CD	2.15	0.47
2:1:468:GLY:HA2	3:2:195:LYS:HD2	1.96	0.47
3:2:45:ASP:CG	3:2:46:PHE:N	2.65	0.47
5:4:491:VAL:O	5:4:494:LEU:HG	2.13	0.47
2:1:175:THR:O	2:1:175:THR:OG1	2.29	0.47
5:4:656:ALA:O	5:4:660:VAL:HG23	2.14	0.47
7:6:316:PHE:O	7:6:320:THR:HG23	2.15	0.47
4:3:265:ASN:O	4:3:269:ARG:HG2	2.14	0.47
7:6:322:ARG:NH1	7:6:326:LEU:HD13	2.29	0.47
6:5:155:LYS:HZ2	6:5:159:GLU:HG3	1.80	0.47
7:6:342:PHE:HZ	7:6:352:LEU:HD21	1.79	0.47
5:4:617:ILE:HA	5:4:620:VAL:HG22	1.96	0.47
5:4:700:TRP:CD1	5:4:710:ILE:HD13	2.50	0.47
5:4:1030:GLN:O	5:4:1031:GLN:HG3	2.14	0.47
6:5:92:GLU:OE1	6:5:92:GLU:N	2.47	0.47
6:5:117:TYR:CD2	6:5:157:LEU:HD12	2.48	0.47
7:6:83:ASN:OD1	7:6:83:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:133:ASP:O	7:6:134:TYR:HB3	2.15	0.47
7:6:280:LYS:HA	7:6:280:LYS:HE2	1.96	0.47
7:6:294:ASN:N	7:6:297:GLN:OE1	2.48	0.47
3:2:231:ASN:O	3:2:235:MET:HG2	2.14	0.47
3:2:421:GLU:HB2	3:2:441:TYR:CE2	2.50	0.47
5:4:502:ARG:NE	5:4:538:CYS:SG	2.86	0.47
6:5:38:LEU:O	6:5:41:GLN:HG3	2.15	0.47
2:1:300:ARG:HG3	2:1:305:LEU:HD13	1.97	0.47
3:2:378:LEU:H	3:2:379:ARG:NH2	2.12	0.47
7:6:322:ARG:HH22	7:6:326:LEU:HD22	1.79	0.47
3:2:125:TYR:HE2	7:6:303:MET:HG3	1.80	0.46
4:3:201:ARG:HA	4:3:204:ARG:HE	1.80	0.46
4:3:47:ARG:HD2	4:3:73:ILE:HG12	1.97	0.46
4:3:329:VAL:HG21	4:3:363:THR:HG23	1.98	0.46
7:6:109:VAL:HG13	7:6:131:CYS:SG	2.55	0.46
4:3:440:ARG:HB2	4:3:443:CYS:SG	2.56	0.46
7:6:61:LEU:HD23	7:6:66:ILE:HD11	1.98	0.46
7:6:322:ARG:HH12	7:6:326:LEU:HD13	1.81	0.46
5:4:384:ILE:HD12	5:4:385:PRO:HD2	1.98	0.46
6:5:109:GLY:HA3	6:5:284:PHE:CZ	2.51	0.46
7:6:133:ASP:C	7:6:135:CYS:H	2.19	0.46
2:1:127:ASN:HD21	5:4:918:PRO:HB2	1.80	0.46
2:1:270:LEU:HA	2:1:273:ILE:HB	1.98	0.46
4:3:70:ALA:HB1	4:3:101:PHE:HE2	1.80	0.46
5:4:836:HIS:HB3	5:4:838:PRO:HD2	1.96	0.46
2:1:151:ASN:OD1	4:3:27:ASN:ND2	2.48	0.46
2:1:366:ASP:OD1	2:1:367:ASP:N	2.48	0.46
3:2:179:HIS:O	3:2:217:ASN:ND2	2.44	0.46
2:1:355:LEU:HD11	2:1:377:HIS:CE1	2.50	0.46
4:3:274:LEU:O	4:3:278:LEU:HG	2.16	0.46
5:4:494:LEU:O	5:4:497:VAL:HG12	2.16	0.46
2:1:273:ILE:HG21	2:1:425:TYR:OH	2.16	0.45
4:3:318:THR:C	4:3:319:LYS:HD3	2.36	0.45
5:4:420:LEU:O	5:4:423:TYR:HB3	2.16	0.45
7:6:281:ARG:O	7:6:284:THR:OG1	2.24	0.45
7:6:332:ALA:HB3	7:6:363:VAL:HG11	1.97	0.45
7:6:426:MET:H	7:6:426:MET:CE	2.29	0.45
5:4:494:LEU:HA	5:4:497:VAL:HG12	1.98	0.45
5:4:1081:LEU:HD12	5:4:1081:LEU:HA	1.84	0.45
3:2:304:GLN:HB3	3:2:406:LYS:HG2	1.97	0.45
6:5:41:GLN:HG2	6:5:267:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:447:LEU:HD12	3:2:447:LEU:H	1.82	0.45
5:4:341:TYR:HD1	5:4:341:TYR:O	2.00	0.45
4:3:312:PHE:HB2	4:3:315:SER:HA	1.98	0.45
5:4:541:PHE:CE2	5:4:543:TYR:HB2	2.52	0.45
6:5:54:LEU:HD21	6:5:231:PHE:HD1	1.82	0.45
3:2:133:GLU:O	3:2:137:GLU:N	2.49	0.45
5:4:879:ASP:OD1	5:4:879:ASP:N	2.48	0.45
5:4:995:THR:OG1	5:4:996:ASP:N	2.49	0.45
7:6:302:PHE:CE2	7:6:341:ALA:HB3	2.52	0.45
3:2:323:CYS:SG	3:2:324:GLU:N	2.90	0.45
4:3:355:LEU:HD23	4:3:360:LEU:HG	1.97	0.45
6:5:11:LEU:HD23	6:5:283:LYS:HA	1.98	0.45
7:6:293:MET:O	7:6:322:ARG:NH2	2.40	0.45
2:1:350:ARG:HA	2:1:353:VAL:HB	1.98	0.45
4:3:134:THR:C	4:3:136:ALA:H	2.20	0.45
4:3:173:LEU:HD12	4:3:179:ALA:HA	1.98	0.45
2:1:230:LEU:HD21	2:1:329:TRP:CZ3	2.52	0.45
4:3:414:GLY:HA3	4:3:417:ARG:HH21	1.82	0.45
7:6:368:ASP:CG	7:6:369:ALA:N	2.70	0.45
5:4:533:PHE:HA	5:4:536:ILE:HG22	1.98	0.44
6:5:95:ALA:O	6:5:98:PHE:HB2	2.17	0.44
7:6:99:ILE:HD12	7:6:104:LEU:HD22	1.98	0.44
3:2:443:TRP:NE1	3:2:470:LEU:HD13	2.32	0.44
7:6:142:ILE:HD13	7:6:146:VAL:HG23	1.99	0.44
2:1:303:ASP:OD1	2:1:303:ASP:N	2.51	0.44
4:3:358:LEU:HD12	4:3:402:VAL:HG11	2.00	0.44
5:4:532:ALA:HA	5:4:535:MET:SD	2.57	0.44
6:5:73:ALA:HB3	6:5:277:ALA:HA	1.99	0.44
5:4:370:VAL:HA	5:4:373:GLN:HG2	2.00	0.44
6:5:194:LEU:HD12	6:5:222:LEU:HD11	2.00	0.44
2:1:238:ARG:HD3	2:1:252:ARG:NH2	2.33	0.44
4:3:80:LEU:HD23	4:3:82:ILE:HD11	1.98	0.44
6:5:266:SER:OG	6:5:267:GLU:OE1	2.35	0.44
3:2:405:ARG:CZ	3:2:407:TRP:HE1	2.31	0.44
5:4:954:LEU:HD12	5:4:959:LYS:HB2	2.00	0.44
6:5:115:ALA:HB1	6:5:118:LEU:HB3	1.99	0.44
3:2:306:ARG:HA	3:2:404:VAL:O	2.18	0.44
5:4:844:ASP:N	5:4:844:ASP:OD1	2.50	0.44
7:6:372:ILE:HG21	7:6:397:ALA:HB2	1.99	0.43
4:3:236:ASN:ND2	4:3:241:GLU:OE2	2.39	0.43
3:2:418:GLN:HG3	3:2:444:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:99:ALA:HA	4:3:138:LEU:HD21	1.98	0.43
4:3:276:PRO:HB2	4:3:277:GLN:HE22	1.81	0.43
5:4:434:ASP:O	5:4:438:THR:HG23	2.18	0.43
2:1:466:GLU:HG2	2:1:467:TYR:CD1	2.53	0.43
4:3:85:ASP:N	4:3:85:ASP:OD1	2.52	0.43
4:3:162:ILE:O	4:3:165:GLU:HG2	2.18	0.43
2:1:462:ASP:OD1	2:1:462:ASP:N	2.52	0.43
3:2:46:PHE:HB2	3:2:48:HIS:CE1	2.53	0.43
3:2:203:LYS:HA	3:2:203:LYS:HD3	1.69	0.43
6:5:162:ASP:HB3	6:5:165:PHE:HD1	1.83	0.43
4:3:37:LEU:HD12	4:3:41:GLY:HA3	2.00	0.43
5:4:348:GLN:HA	5:4:721:TRP:HA	2.00	0.43
5:4:675:GLN:HA	5:4:678:VAL:HG22	2.00	0.43
5:4:802:GLU:OE1	5:4:802:GLU:N	2.51	0.43
6:5:211:LYS:HB3	6:5:212:GLN:NE2	2.33	0.43
3:2:289:ALA:O	3:2:292:GLU:HB2	2.19	0.43
5:4:1051:HIS:ND1	6:5:135:PRO:HB3	2.33	0.43
3:2:58:TRP:NE1	3:2:98:GLU:OE1	2.52	0.43
6:5:179:PRO:HG2	6:5:184:TYR:CD1	2.54	0.43
4:3:88:PHE:O	4:3:92:GLN:HG2	2.19	0.43
6:5:11:LEU:HB2	6:5:56:ASP:HB2	2.00	0.43
2:1:228:GLY:N	2:1:339:ARG:HH22	2.17	0.42
3:2:324:GLU:HB2	3:2:333:MET:HE2	2.01	0.42
3:2:348:ARG:NH2	3:2:471:ALA:HB1	2.33	0.42
5:4:677:VAL:O	5:4:681:ARG:HG2	2.19	0.42
5:4:919:ILE:HA	5:4:922:GLN:NE2	2.34	0.42
6:5:68:GLU:OE2	6:5:93:HIS:NE2	2.51	0.42
7:6:468:PHE:HD2	7:6:500:CYS:HB2	1.84	0.42
2:1:194:GLU:OE2	2:1:197:VAL:HG23	2.19	0.42
7:6:332:ALA:HB3	7:6:363:VAL:HG12	1.99	0.42
3:2:424:ARG:HD2	3:2:438:ARG:HE	1.82	0.42
5:4:421:PRO:O	5:4:422:HIS:HB3	2.20	0.42
7:6:332:ALA:HB1	7:6:367:HIS:NE2	2.34	0.42
2:1:309:LEU:HD22	2:1:315:VAL:HG12	2.00	0.42
4:3:114:ASN:HA	4:3:117:THR:HG22	2.02	0.42
7:6:355:ASN:O	7:6:358:GLU:HG2	2.20	0.42
3:2:280:PHE:HE1	3:2:282:ILE:HB	1.83	0.42
3:2:311:LYS:HD2	3:2:424:ARG:HH21	1.84	0.42
5:4:501:VAL:HG22	5:4:501:VAL:O	2.19	0.42
5:4:898:LEU:HD23	5:4:898:LEU:HA	1.81	0.42
6:5:155:LYS:O	6:5:159:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:142:ILE:HD11	7:6:150:VAL:HG21	2.02	0.42
7:6:368:ASP:H	7:6:371:ASP:HB3	1.84	0.42
2:1:158:GLN:NE2	2:1:206:VAL:HG21	2.34	0.42
3:2:137:GLU:OE2	3:2:266:THR:OG1	2.37	0.42
3:2:218:LYS:O	3:2:222:ARG:HG2	2.20	0.42
4:3:440:ARG:O	4:3:444:ARG:N	2.33	0.42
5:4:1077:GLU:OE2	5:4:1077:GLU:HA	2.20	0.42
6:5:75:GLN:HE21	6:5:98:PHE:HB3	1.84	0.42
6:5:122:GLU:HG2	6:5:123:ASN:N	2.35	0.42
7:6:105:ASP:OD1	7:6:105:ASP:N	2.44	0.42
7:6:201:LYS:CG	7:6:205:PHE:CZ	3.03	0.42
5:4:440:LEU:O	5:4:444:LEU:HG	2.19	0.42
5:4:681:ARG:HB2	5:4:688:LEU:HD11	2.01	0.42
5:4:1001:LYS:O	5:4:1005:VAL:HG23	2.19	0.42
6:5:79:ILE:HG23	6:5:138:ILE:HD11	2.02	0.42
7:6:262:VAL:HG11	7:6:297:GLN:HB3	2.00	0.42
2:1:274:GLN:HA	2:1:278:LEU:HD12	2.01	0.42
3:2:167:TYR:HB2	3:2:362:HIS:HD2	1.85	0.42
5:4:337:THR:OG1	5:4:370:VAL:HG13	2.20	0.42
7:6:241:LEU:O	7:6:245:ILE:HG12	2.20	0.42
2:1:381:VAL:HB	2:1:414:LEU:HD22	2.01	0.42
3:2:265:TRP:O	3:2:269:LYS:HG2	2.19	0.42
5:4:866:PHE:O	5:4:870:THR:HG23	2.20	0.42
7:6:347:ILE:HD13	7:6:347:ILE:HA	1.90	0.42
3:2:315:ARG:HG3	3:2:320:PHE:CD1	2.54	0.42
5:4:961:VAL:HG11	5:4:998:SER:HB3	2.02	0.42
6:5:125:ARG:HD3	6:5:147:ASN:ND2	2.35	0.42
2:1:261:TRP:CZ2	2:1:263:PRO:HG3	2.55	0.41
3:2:317:MET:H	3:2:317:MET:HE3	1.85	0.41
4:3:170:LEU:HD11	4:3:184:VAL:HG22	2.01	0.41
4:3:323:LEU:H	4:3:323:LEU:HD12	1.85	0.41
5:4:920:GLU:OE1	5:4:920:GLU:N	2.52	0.41
7:6:407:MET:O	7:6:411:ASN:OD1	2.37	0.41
4:3:170:LEU:HB3	4:3:209:ILE:HD13	2.00	0.41
2:1:372:VAL:HG22	2:1:372:VAL:O	2.20	0.41
4:3:355:LEU:HD12	4:3:355:LEU:HA	1.90	0.41
5:4:685:GLN:HG3	5:4:686:GLN:H	1.85	0.41
7:6:367:HIS:HA	7:6:371:ASP:OD2	2.20	0.41
7:6:406:ALA:O	7:6:409:LEU:HB2	2.20	0.41
3:2:367:ARG:H	3:2:367:ARG:HD2	1.84	0.41
5:4:659:LEU:HA	5:4:659:LEU:HD23	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:488:ILE:HD12	7:6:488:ILE:H	1.85	0.41
3:2:169:PRO:HB2	3:2:170:LEU:HD12	2.03	0.41
3:2:355:ARG:HH11	3:2:357:VAL:HG21	1.86	0.41
7:6:445:GLU:OE1	7:6:448:ARG:NH2	2.53	0.41
2:1:440:ASP:OD2	7:6:433:ARG:NH1	2.53	0.41
3:2:395:ASP:OD1	3:2:395:ASP:N	2.54	0.41
5:4:355:MET:HA	5:4:358:VAL:HG12	2.01	0.41
5:4:693:VAL:HG21	5:4:717:TYR:CE2	2.55	0.41
5:4:996:ASP:N	5:4:996:ASP:OD1	2.54	0.41
6:5:54:LEU:HD21	6:5:231:PHE:CD1	2.56	0.41
7:6:479:PHE:HD1	7:6:479:PHE:HA	1.77	0.41
3:2:64:PHE:CZ	3:2:94:VAL:HG11	2.55	0.41
4:3:351:SER:O	4:3:355:LEU:HB2	2.19	0.41
5:4:1006:LEU:HD22	5:4:1011:TRP:HB3	2.01	0.41
2:1:273:ILE:HD13	2:1:273:ILE:HA	1.98	0.41
2:1:279:GLN:HB2	2:1:280:PRO:HD3	2.02	0.41
3:2:350:LYS:HE3	3:2:350:LYS:HB3	1.91	0.41
4:3:65:ALA:O	4:3:68:SER:OG	2.34	0.41
4:3:318:THR:OG1	4:3:319:LYS:N	2.54	0.41
5:4:809:ILE:HG23	5:4:830:PHE:HD2	1.85	0.41
5:4:955:THR:HG23	5:4:956:ASP:OD1	2.21	0.41
5:4:977:ASP:OD1	5:4:978:LYS:N	2.47	0.41
5:4:1060:SER:HB3	6:5:235:ASP:OD1	2.21	0.41
6:5:267:GLU:HA	6:5:270:LYS:NZ	2.36	0.41
7:6:86:LEU:HD13	7:6:86:LEU:HA	1.93	0.41
7:6:325:GLU:OE1	7:6:325:GLU:N	2.48	0.41
7:6:361:LEU:HD13	7:6:392:ARG:NH1	2.36	0.41
7:6:450:LEU:HA	7:6:453:LEU:HD12	2.03	0.41
7:6:484:GLY:O	7:6:487:GLU:HB2	2.21	0.41
2:1:407:LYS:HG2	2:1:423:VAL:HG23	2.03	0.41
5:4:571:ILE:HD13	5:4:571:ILE:HA	1.97	0.41
6:5:190:SER:O	6:5:192:VAL:HG23	2.21	0.41
3:2:125:TYR:CE2	7:6:303:MET:HG3	2.56	0.40
3:2:385:VAL:HB	3:2:428:ILE:HD13	2.02	0.40
5:4:400:SER:O	5:4:404:VAL:HG23	2.21	0.40
7:6:409:LEU:HD23	7:6:409:LEU:HA	1.95	0.40
3:2:421:GLU:HB2	3:2:441:TYR:CZ	2.57	0.40
4:3:355:LEU:HB3	4:3:360:LEU:HD12	2.04	0.40
5:4:1045:LEU:HD12	5:4:1045:LEU:HA	1.88	0.40
6:5:238:ILE:O	6:5:238:ILE:HG13	2.21	0.40
6:5:267:GLU:OE1	6:5:267:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:199:ILE:HD13	2:1:199:ILE:HA	1.90	0.40
2:1:422:ARG:HG2	3:2:197:PRO:HB2	2.04	0.40
4:3:249:VAL:HG21	4:3:263:LEU:HD21	2.03	0.40
5:4:414:ASP:OD2	5:4:418:ALA:N	2.51	0.40
4:3:299:ARG:NH2	5:4:595:GLU:HG3	2.37	0.40
5:4:750:LEU:HD12	5:4:750:LEU:HA	1.92	0.40
7:6:423:GLN:HB2	7:6:426:MET:CE	2.52	0.40
7:6:489:GLU:O	7:6:490:GLU:C	2.59	0.40
3:2:399:CYS:HB3	3:2:428:ILE:HB	2.04	0.40
4:3:139:LYS:H	4:3:139:LYS:HG2	1.64	0.40
6:5:85:GLU:H	6:5:115:ALA:HB2	1.87	0.40
7:6:328:ASP:HA	7:6:359:ARG:HH12	1.86	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	
2	1	350/473 (74%)	328 (94%)	22 (6%)	0	100	100
3	2	422/492 (86%)	401 (95%)	21 (5%)	0	100	100
4	3	478/482 (99%)	460 (96%)	18 (4%)	0	100	100
5	4	737/1087 (68%)	687 (93%)	49 (7%)	1 (0%)	51	83
6	5	274/402 (68%)	253 (92%)	21 (8%)	0	100	100
7	6	450/516 (87%)	417 (93%)	33 (7%)	0	100	100
All	All	2711/3452 (78%)	2546 (94%)	164 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	4	565	LEU

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	
2	1	304/400 (76%)	296 (97%)	8 (3%)	46	69
3	2	364/410 (89%)	350 (96%)	14 (4%)	33	61
4	3	405/407 (100%)	391 (96%)	14 (4%)	36	63
5	4	643/933 (69%)	628 (98%)	15 (2%)	50	71
6	5	236/322 (73%)	221 (94%)	15 (6%)	17	48
7	6	376/428 (88%)	358 (95%)	18 (5%)	25	56
All	All	2328/2900 (80%)	2244 (96%)	84 (4%)	38	63

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	139	ASP
2	1	209	TRP
2	1	241	ARG
2	1	276	GLN
2	1	404	ARG
2	1	416	ASP
2	1	449	PHE
2	1	467	TYR
3	2	95	ARG
3	2	102	SER
3	2	125	TYR
3	2	225	PHE
3	2	252	ARG
3	2	260	ASN
3	2	291	MET
3	2	315	ARG
3	2	333	MET
3	2	334	MET
3	2	392	GLU
3	2	405	ARG
3	2	438	ARG
3	2	482	MET

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Mol	Chain	Res	Type
4	3	110	TYR
4	3	139	LYS
4	3	175	SER
4	3	254	SER
4	3	275	LEU
4	3	292	LEU
4	3	321	HIS
4	3	323	LEU
4	3	336	TYR
4	3	392	ARG
4	3	400	MET
4	3	412	HIS
4	3	473	TYR
4	3	478	GLN
5	4	341	TYR
5	4	355	MET
5	4	391	ARG
5	4	471	SER
5	4	482	PHE
5	4	494	LEU
5	4	527	CYS
5	4	582	PHE
5	4	761	LEU
5	4	819	MET
5	4	866	PHE
5	4	867	ASP
5	4	954	LEU
5	4	978	LYS
5	4	1085	LEU
6	5	41	GLN
6	5	52	CYS
6	5	101	SER
6	5	102	MET
6	5	103	ARG
6	5	117	TYR
6	5	121	THR
6	5	167	PHE
6	5	185	PHE
6	5	187	PHE
6	5	210	GLN
6	5	222	LEU
6	5	246	TYR

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Mol	Chain	Res	Type
6	5	264	GLN
6	5	265	TRP
7	6	95	PHE
7	6	307	TYR
7	6	322	ARG
7	6	381	HIS
7	6	382	PHE
7	6	391	LYS
7	6	402	ASP
7	6	405	ASP
7	6	414	HIS
7	6	416	PHE
7	6	423	GLN
7	6	426	MET
7	6	439	ARG
7	6	476	TYR
7	6	479	PHE
7	6	487	GLU
7	6	495	TYR
7	6	504	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	276	GLN
3	2	113	GLN
3	2	362	HIS
5	4	428	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	g	44/46 (95%)	14 (31%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	g	3	A
1	g	4	U
1	g	5	A

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Mol	Chain	Res	Type
1	g	6	U
1	g	8	U
1	g	10	U
1	g	12	U
1	g	143	A
1	g	144	A
1	g	145	U
1	g	146	U
1	g	147	U
1	g	148	U
1	g	149	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ATP	g	201	1	26,33,33	0.95	1 (3%)	31,52,52	1.33	4 (12%)

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
8	ATP	g	201	1	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	g	201	ATP	C5-C4	2.40	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	201	ATP	PB-O3B-PG	-3.28	121.57	132.83
8	g	201	ATP	N3-C2-N1	-3.23	123.63	128.68
8	g	201	ATP	C4-C5-N7	-2.57	106.72	109.40
8	g	201	ATP	PA-O3A-PB	-2.50	124.25	132.83

There are no chirality outliers.

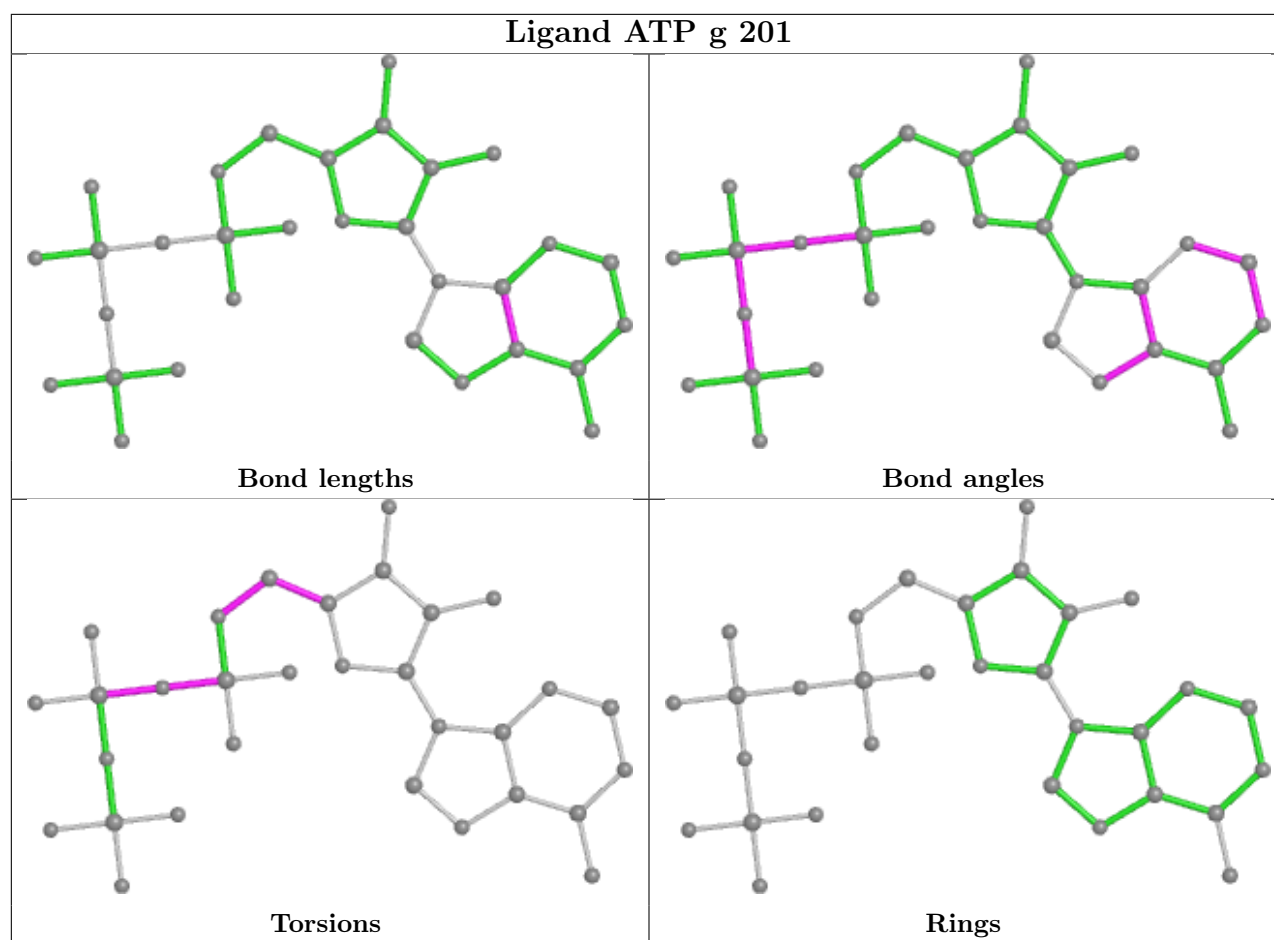
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	g	201	ATP	C4'-C5'-O5'-PA
8	g	201	ATP	O4'-C4'-C5'-O5'
8	g	201	ATP	C3'-C4'-C5'-O5'
8	g	201	ATP	PB-O3A-PA-O1A
8	g	201	ATP	PB-O3A-PA-O5'
8	g	201	ATP	PA-O3A-PB-O2B

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	g	24:U	O3'	127:A	P	17.01

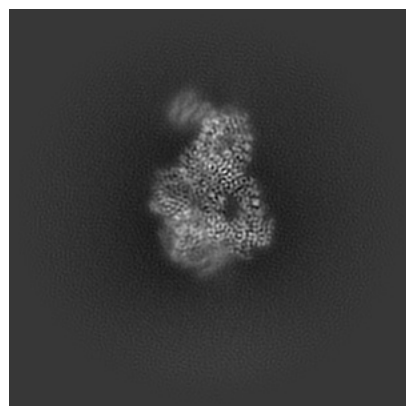
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29306. These allow visual inspection of the internal detail of the map and identification of artifacts.

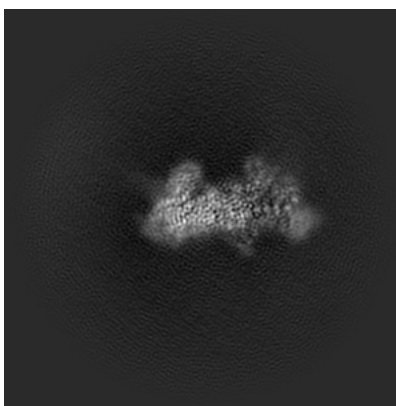
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

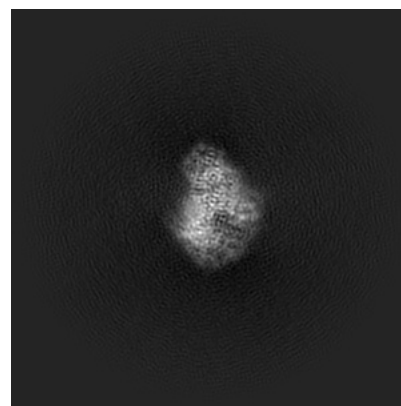
6.1.1 Primary map



X

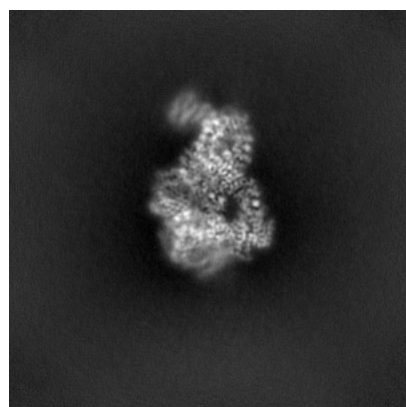


Y

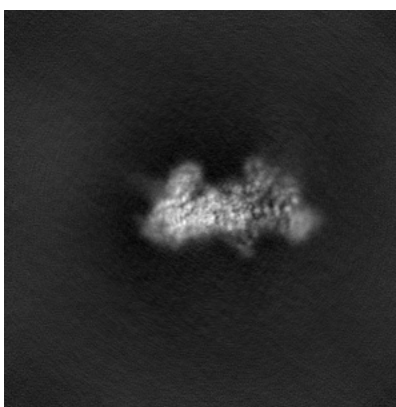


Z

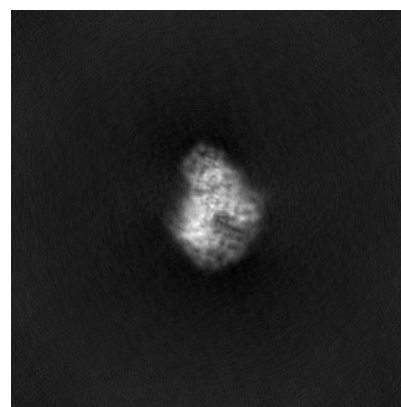
6.1.2 Raw map



X



Y

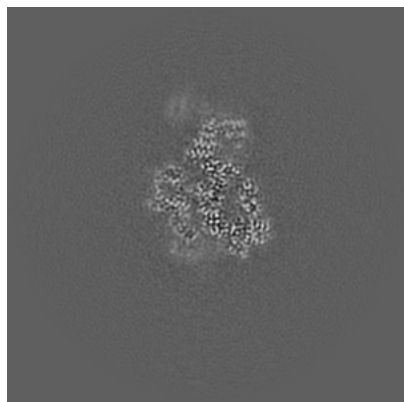


Z

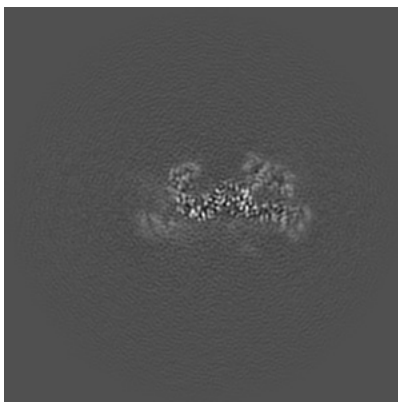
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

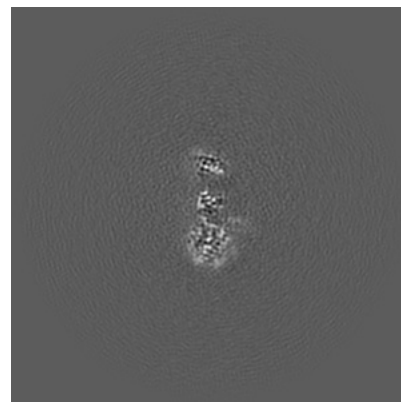
6.2.1 Primary map



X Index: 180

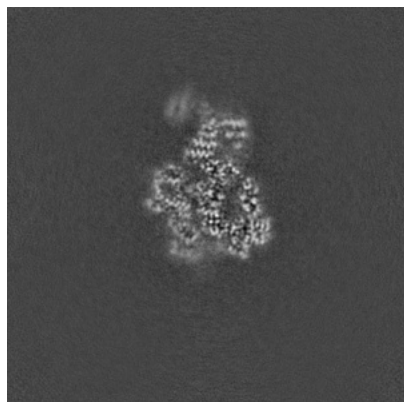


Y Index: 180

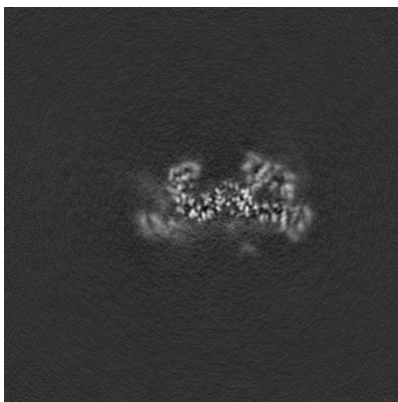


Z Index: 180

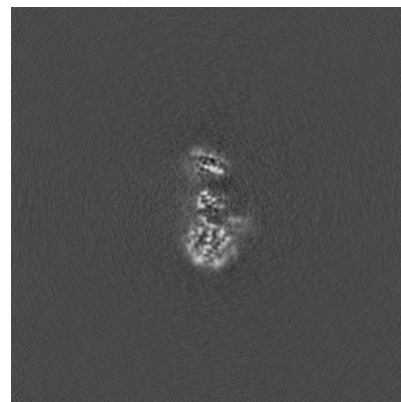
6.2.2 Raw map



X Index: 180



Y Index: 180

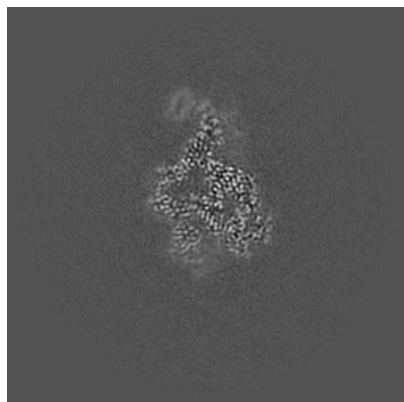


Z Index: 180

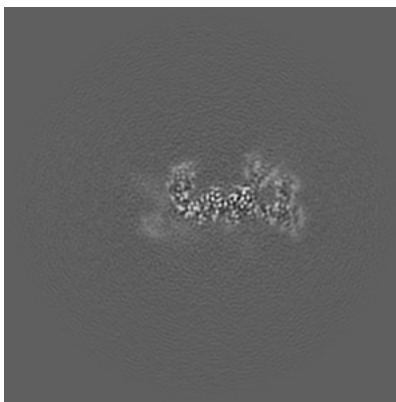
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

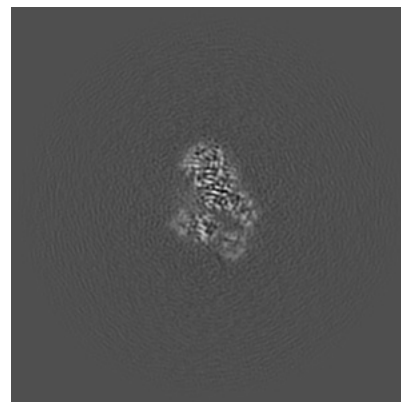
6.3.1 Primary map



X Index: 174

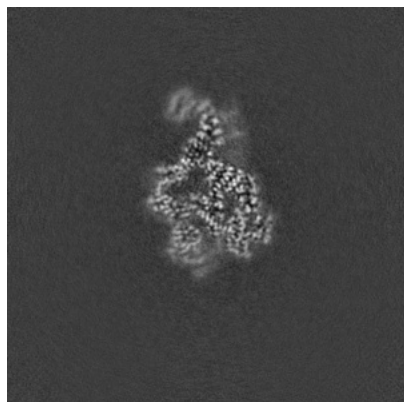


Y Index: 184

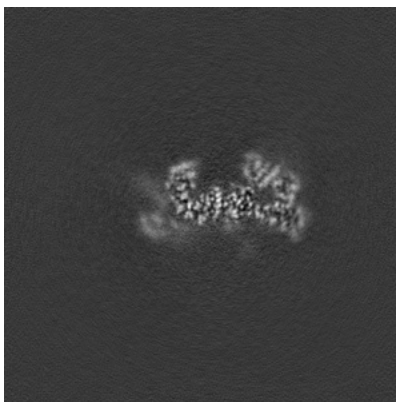


Z Index: 157

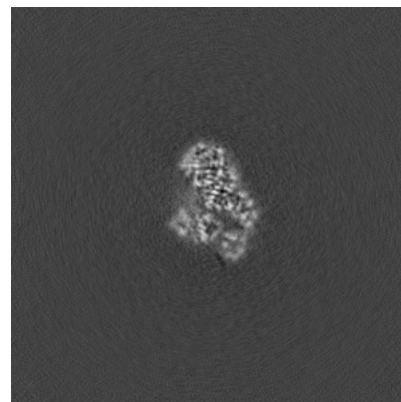
6.3.2 Raw map



X Index: 174



Y Index: 183

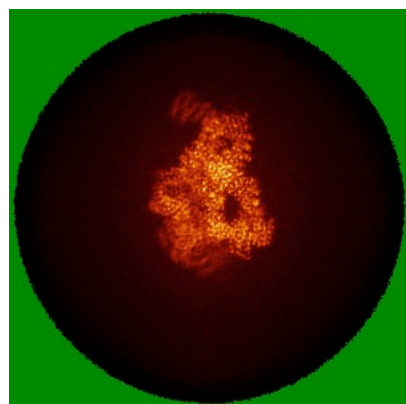


Z Index: 157

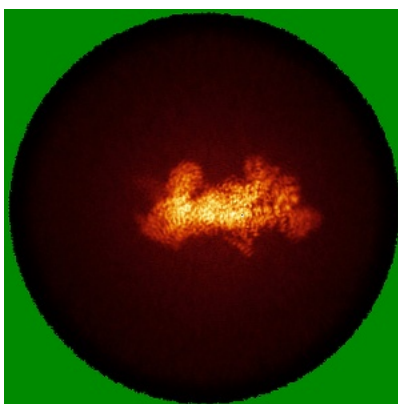
The images above show the largest variance slices of the map in three orthogonal directions.

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

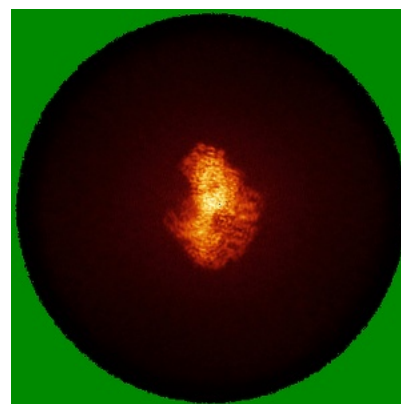
6.4.1 Primary map



X

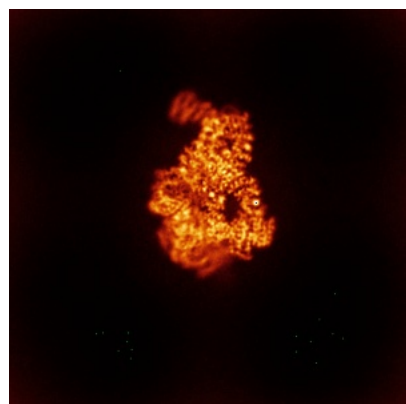


Y

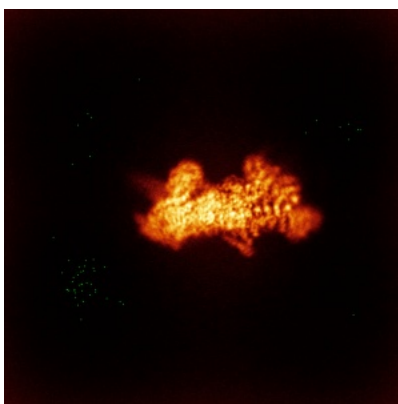


Z

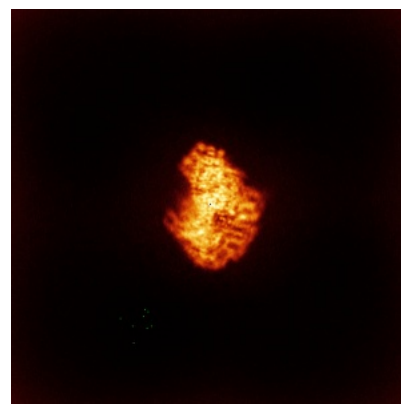
6.4.2 Raw map



X



Y

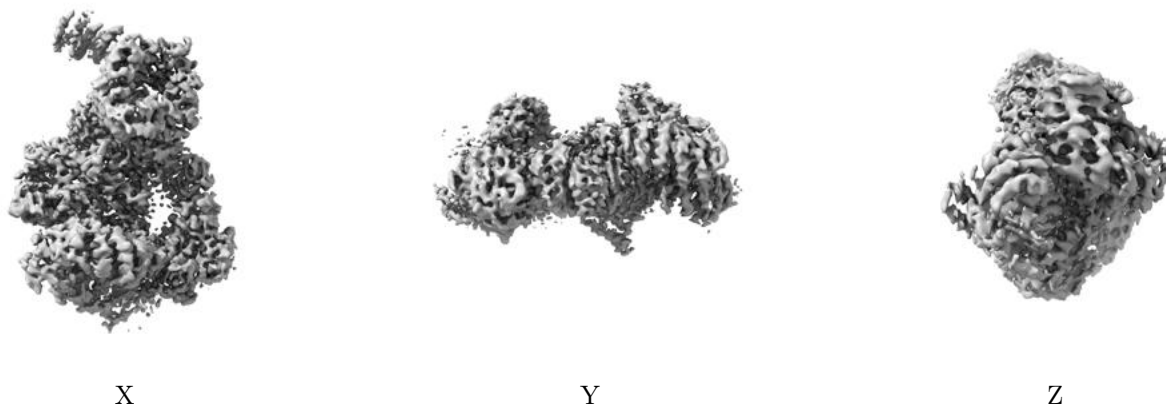


Z

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.

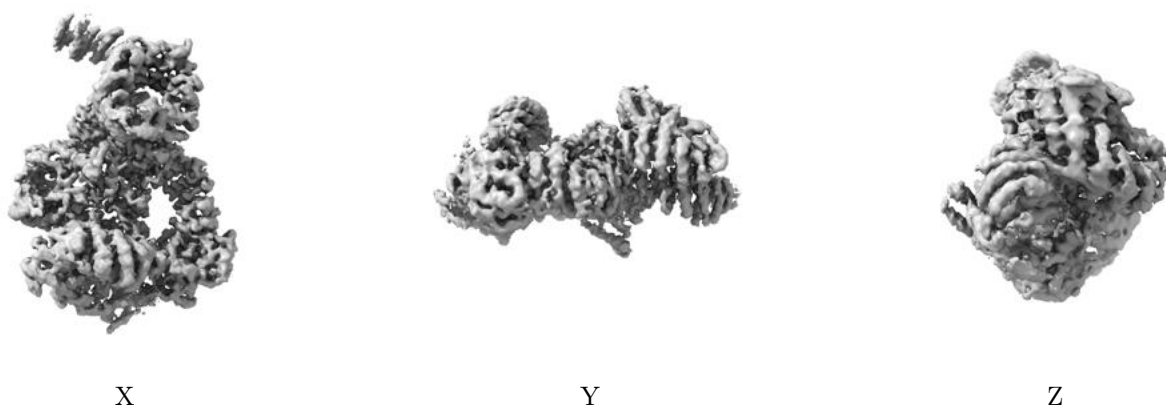
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

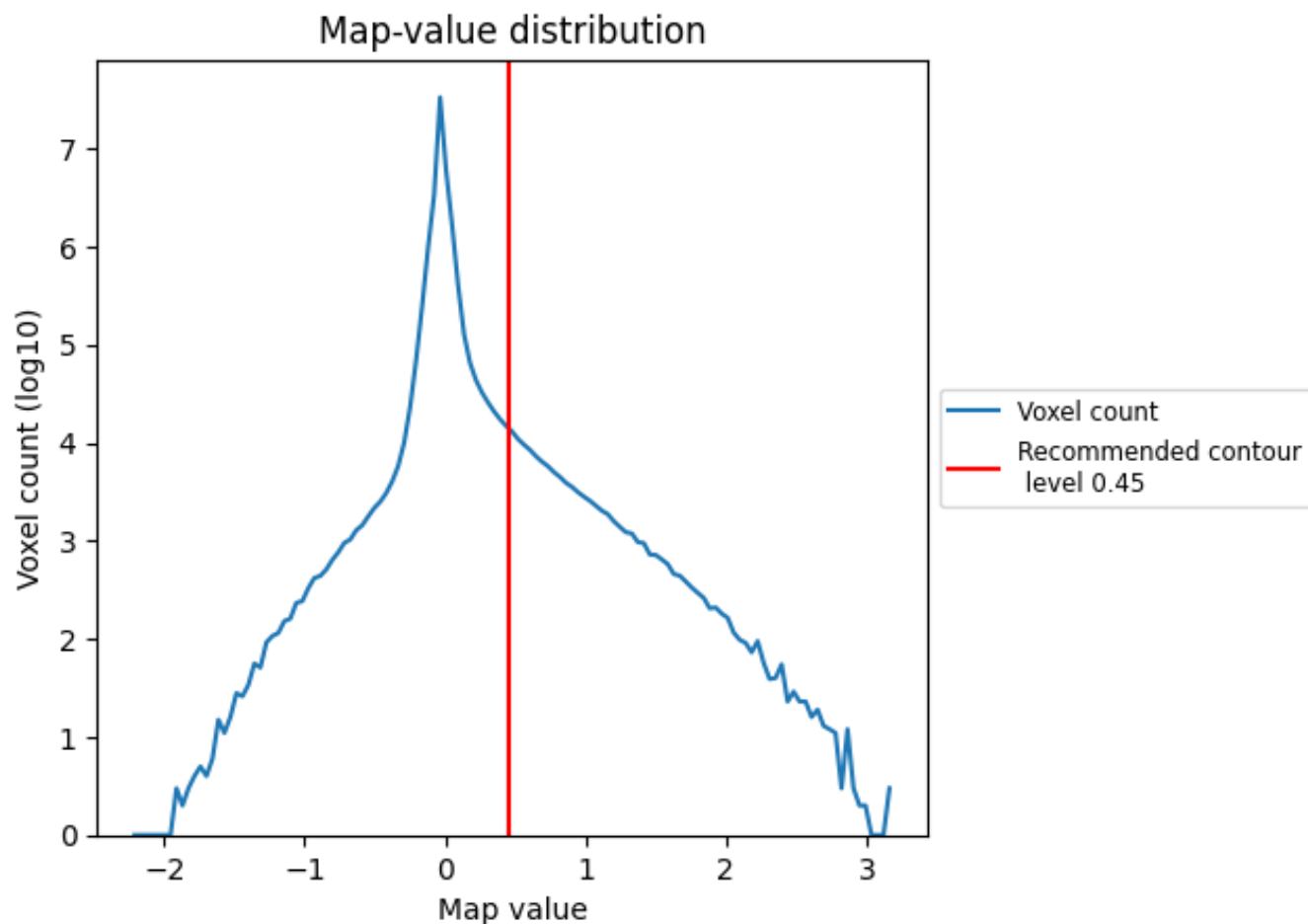
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

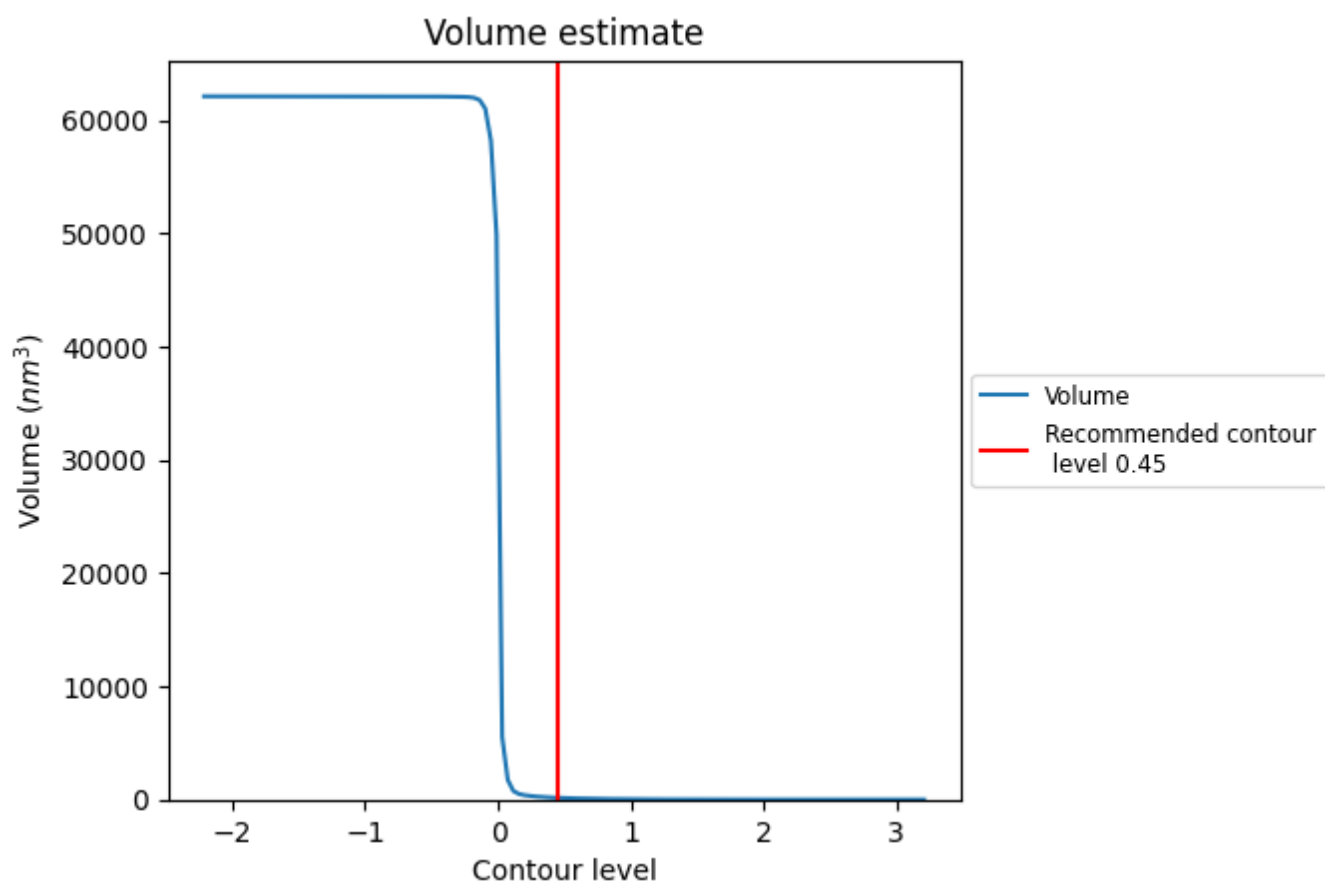
This section contains the results of statistical analysis of the map.

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.

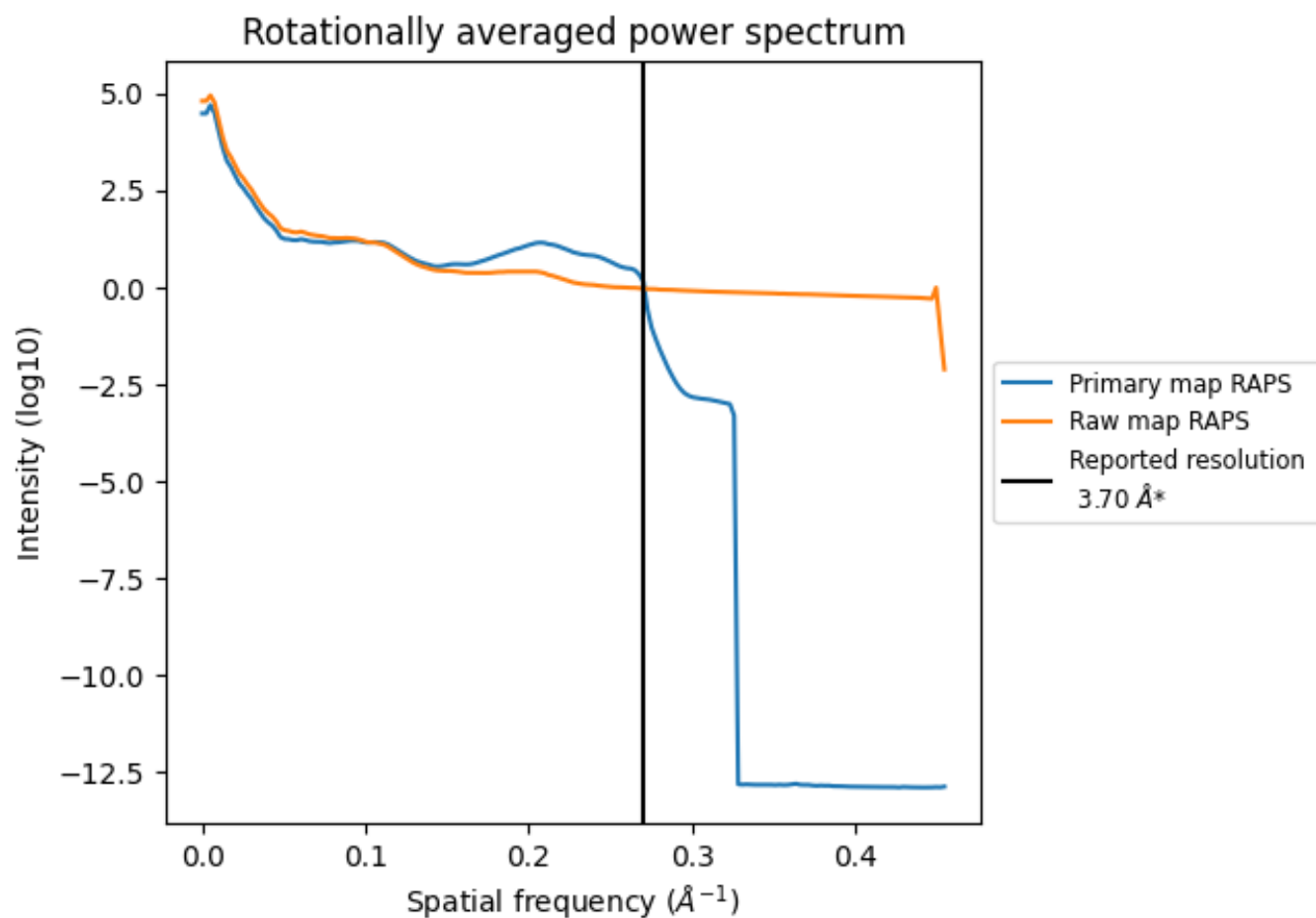
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 140 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 ⓘ

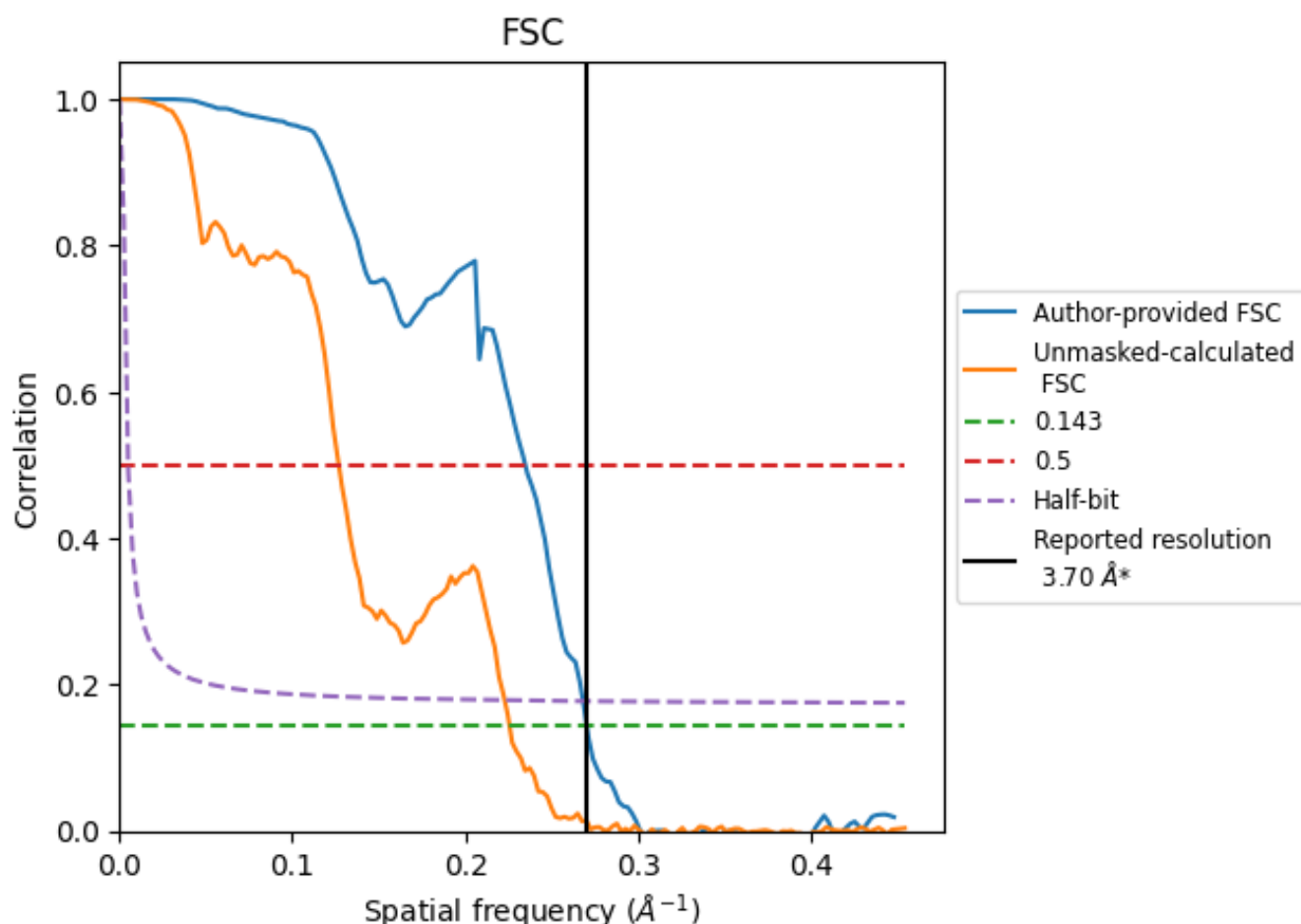


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

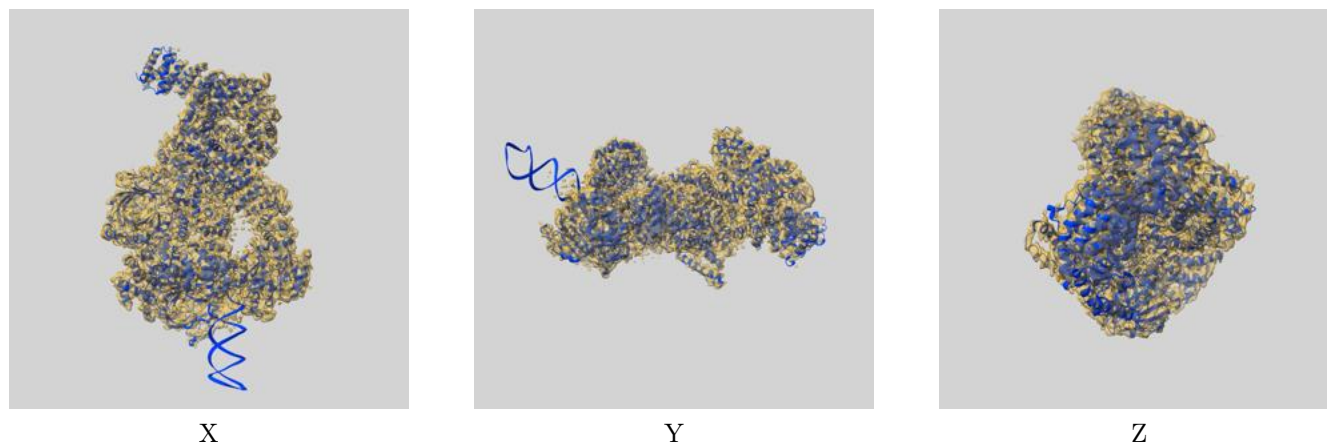
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.26	3.73
Unmasked-calculated*	4.43	7.89	4.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

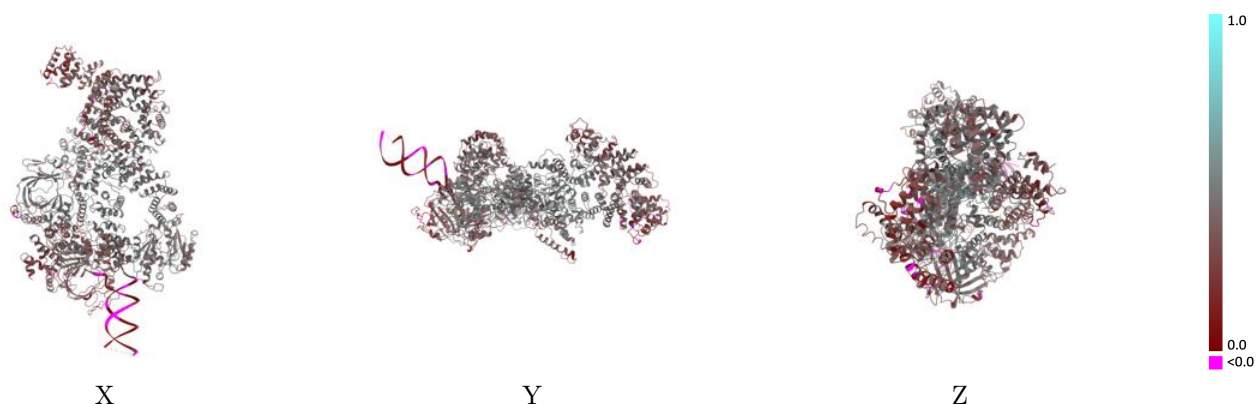
This section contains information regarding the fit between EMDB map EMD-29306 and PDB model 8FN6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



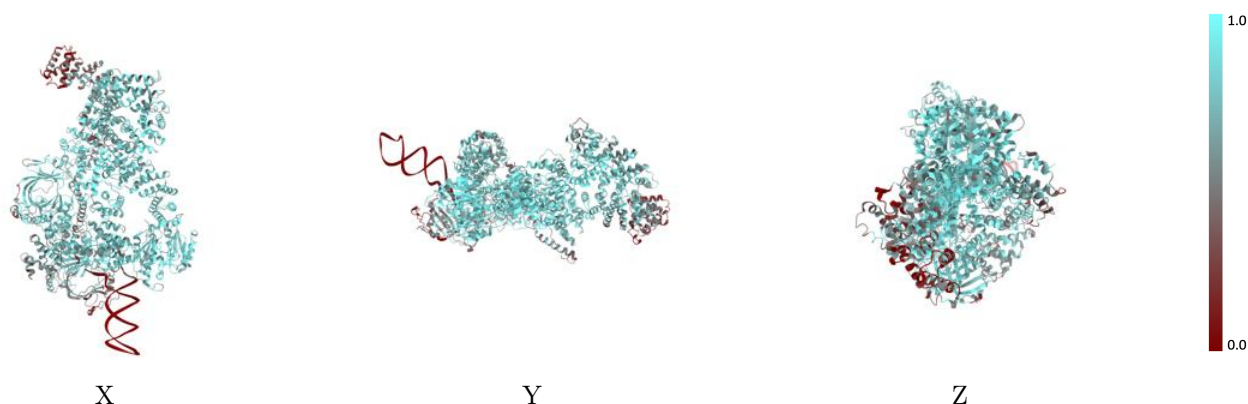
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



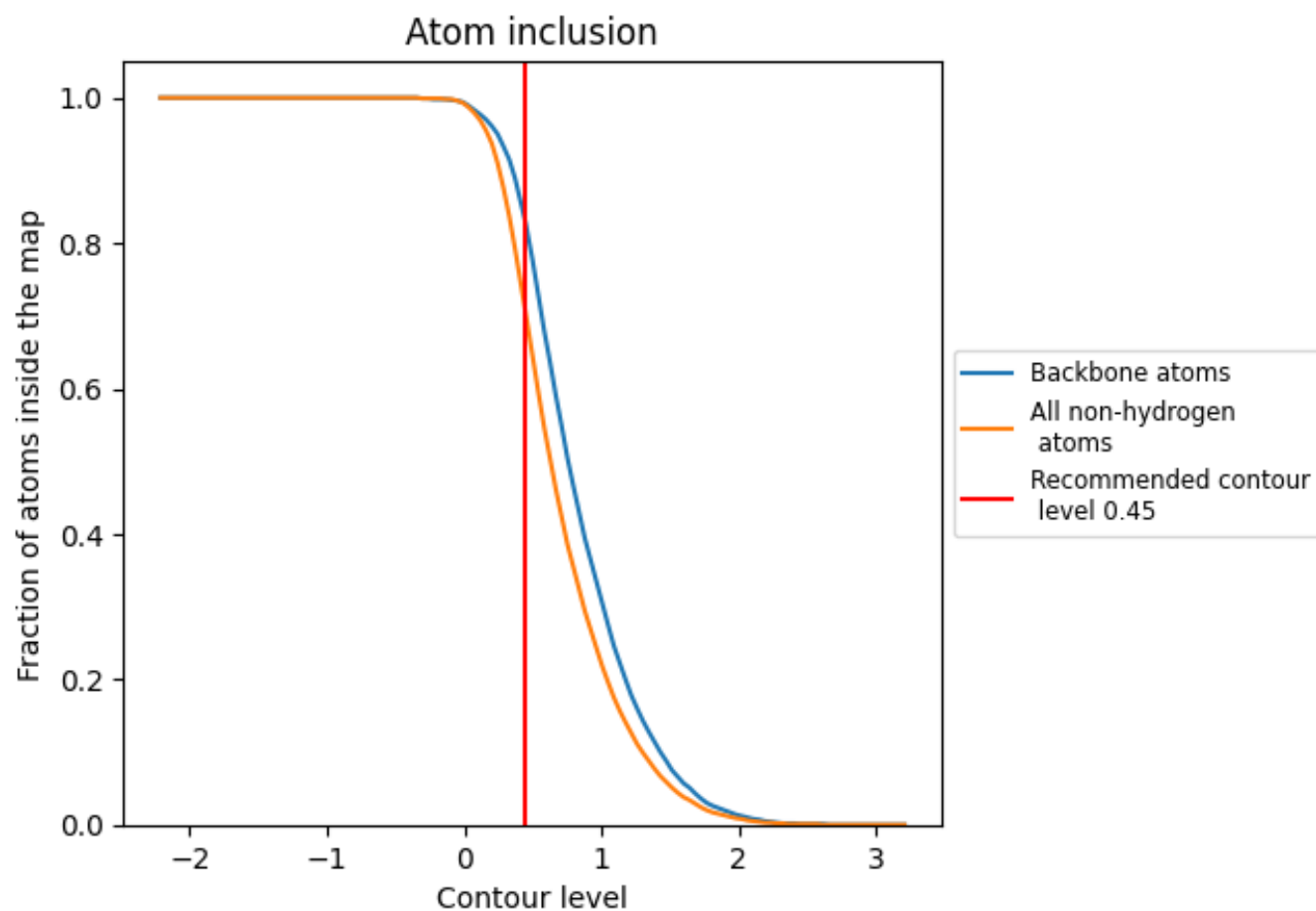
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7020</div>	<div><div></div>0.3860</div>
1	<div><div></div>0.7610</div>	<div><div></div>0.4240</div>
2	<div><div></div>0.6630</div>	<div><div></div>0.3750</div>
3	<div><div></div>0.5970</div>	<div><div></div>0.3530</div>
4	<div><div></div>0.7880</div>	<div><div></div>0.4170</div>
5	<div><div></div>0.8160</div>	<div><div></div>0.4240</div>
6	<div><div></div>0.7550</div>	<div><div></div>0.4060</div>
g	<div><div></div>0.1320</div>	<div><div></div>0.1060</div>

1.0

0.0

<0.0