Full wwPDB EM Validation Report

Jul 10, 2023 – 10:29 AM EDT

PDB ID	:	8FNI
EMDB ID	:	EMD-29314
Title	:	Cryo-EM structure of RNase-treated RESC-B 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	:	3.40 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 (i) 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 (i)) were used in the production of this report:

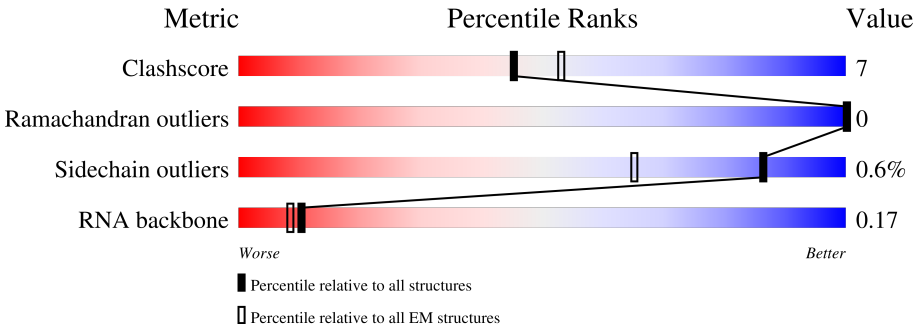
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.40 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 <=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	m	21	10% 43% 57%
2	g	16	12% 62% 38%
3	5	402	65% 9% 26%
4	6	516	74% 14% 12%
5	7	174	32% 5% 63%
6	8	545	78% 15% 6%
7	9	872	25% 78% 20%

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Mol	Chain	Length	Quality of chain
8	10	543	
9	11	934	
10	13	320	
11	14	366	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28858 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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	21	Total	C	N	O	P	0	0
			453	204	87	141	21		

- Molecule 2 is a RNA chain called gRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	g	16	Total	C	N	O	P	0	0
			320	144	32	128	16		

- Molecule 3 is a protein called RNA-editing substrate-binding complex protein 5 (RESC5).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	296	Total	C	N	O	S	0	0
			2318	1464	409	428	17		

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 4 is a protein called RNA-editing substrate-binding complex protein 6 (RESC6).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	453	Total	C	N	O	S	0	0
			3591	2288	636	650	17		

- Molecule 5 is a protein called RNA-editing substrate-binding complex protein 7 (RESC7).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	64	Total	C	N	O	S	0	0
			518	330	93	94	1		

- Molecule 6 is a protein called RNA-editing substrate-binding complex protein 8 (RESC8).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	513	Total	C	N	O	S	0	0
			4056	2569	692	756	39		

- Molecule 7 is a protein called RNA-editing substrate-binding complex protein 9 (RESC9).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	858	Total	C	N	O	S	0	0
			6662	4193	1172	1253	44		

- Molecule 8 is a protein called RNA-editing substrate-binding complex protein 10 (RESC10).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	10	416	Total	C	N	O	S	0	0
			3290	2060	583	620	27		

- Molecule 9 is a protein called RNA-editing substrate-binding complex protein 11 (RESC11).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	11	614	Total	C	N	O	S	0	0
			4918	3144	878	869	27		

- Molecule 10 is a protein called RNA-editing substrate-binding complex protein 13 (RESC13).

Mol	Chain	Residues	Atoms				AltConf	Trace
10	13	30	Total	C	N	O	0	0
			227	133	56	38		

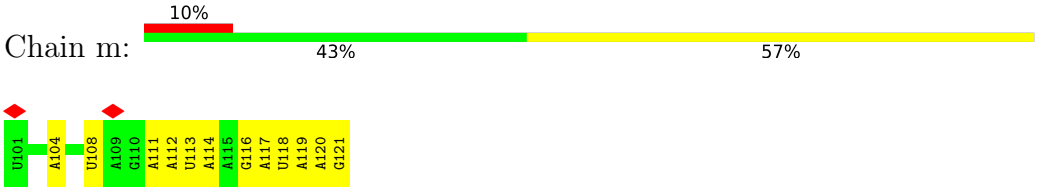
- Molecule 11 is a protein called RNA-editing substrate-binding complex protein 14 (RESC14).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	14	315	Total	C	N	O	S	0	0
			2505	1607	428	455	15		

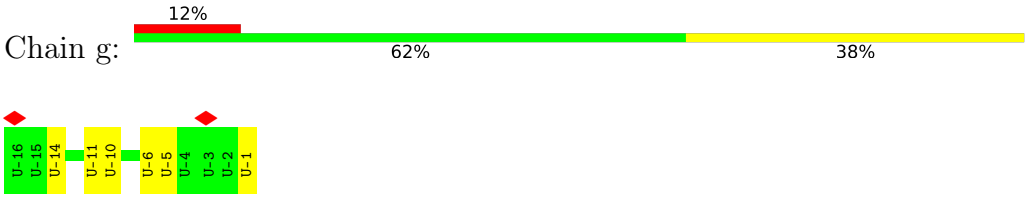
3 Residue-property plots (i)

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.

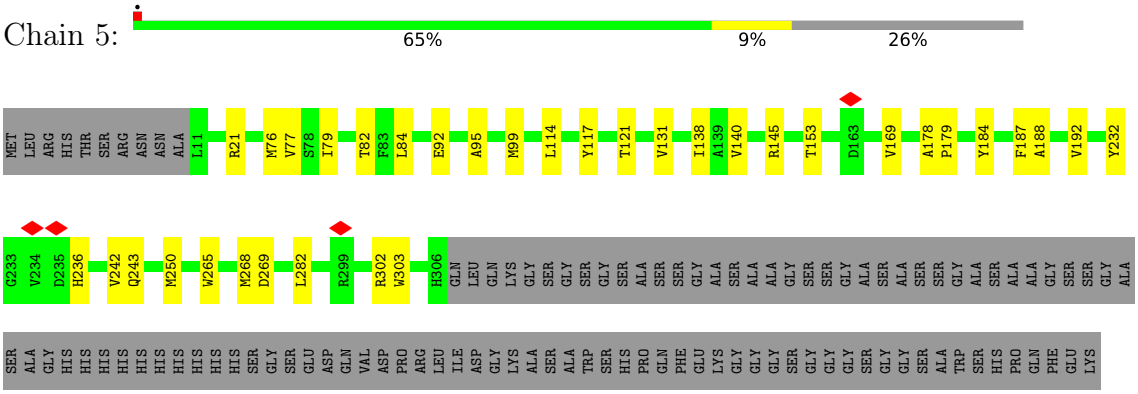
• Molecule 1: mRNA



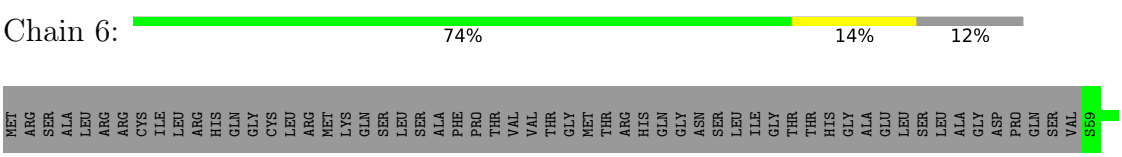
• Molecule 2: gRNA



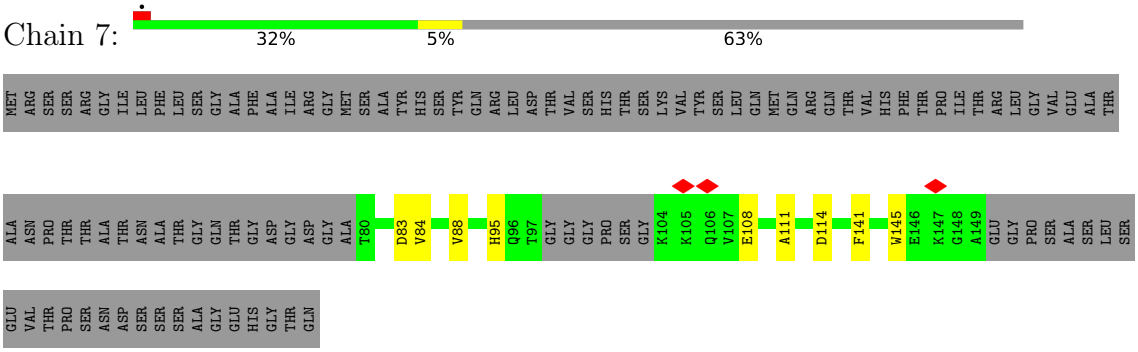
• Molecule 3: RNA-editing substrate-binding complex protein 5 (RESC5)



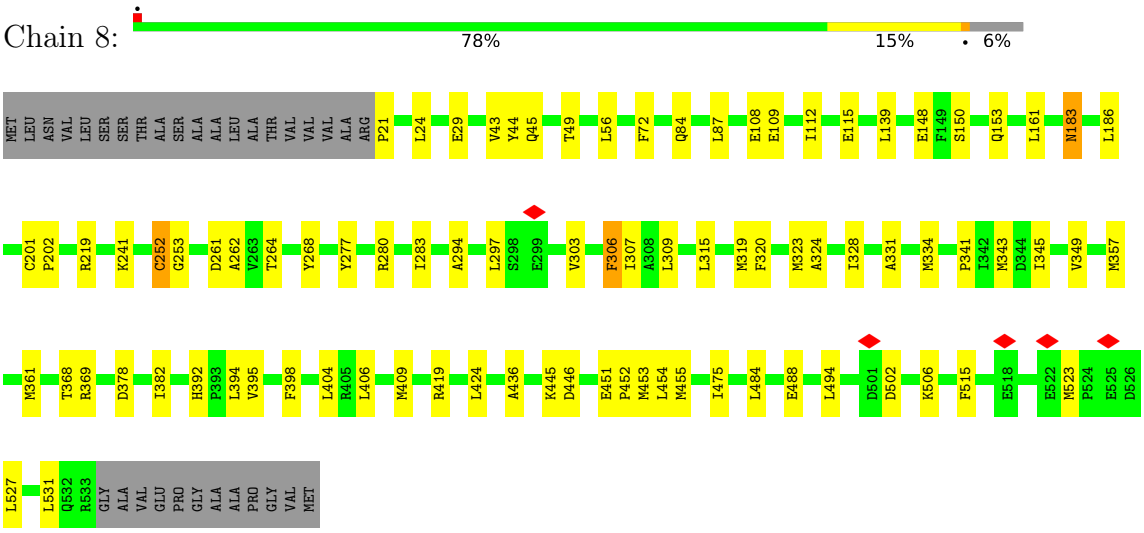
• Molecule 4: RNA-editing substrate-binding complex protein 6 (RESC6)



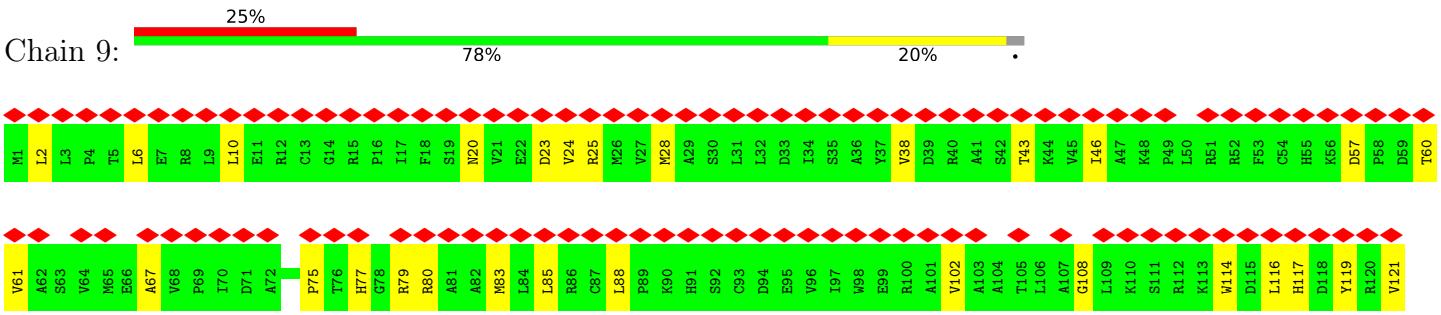
• Molecule 5: RNA-editing substrate-binding complex protein 7 (RESC7)

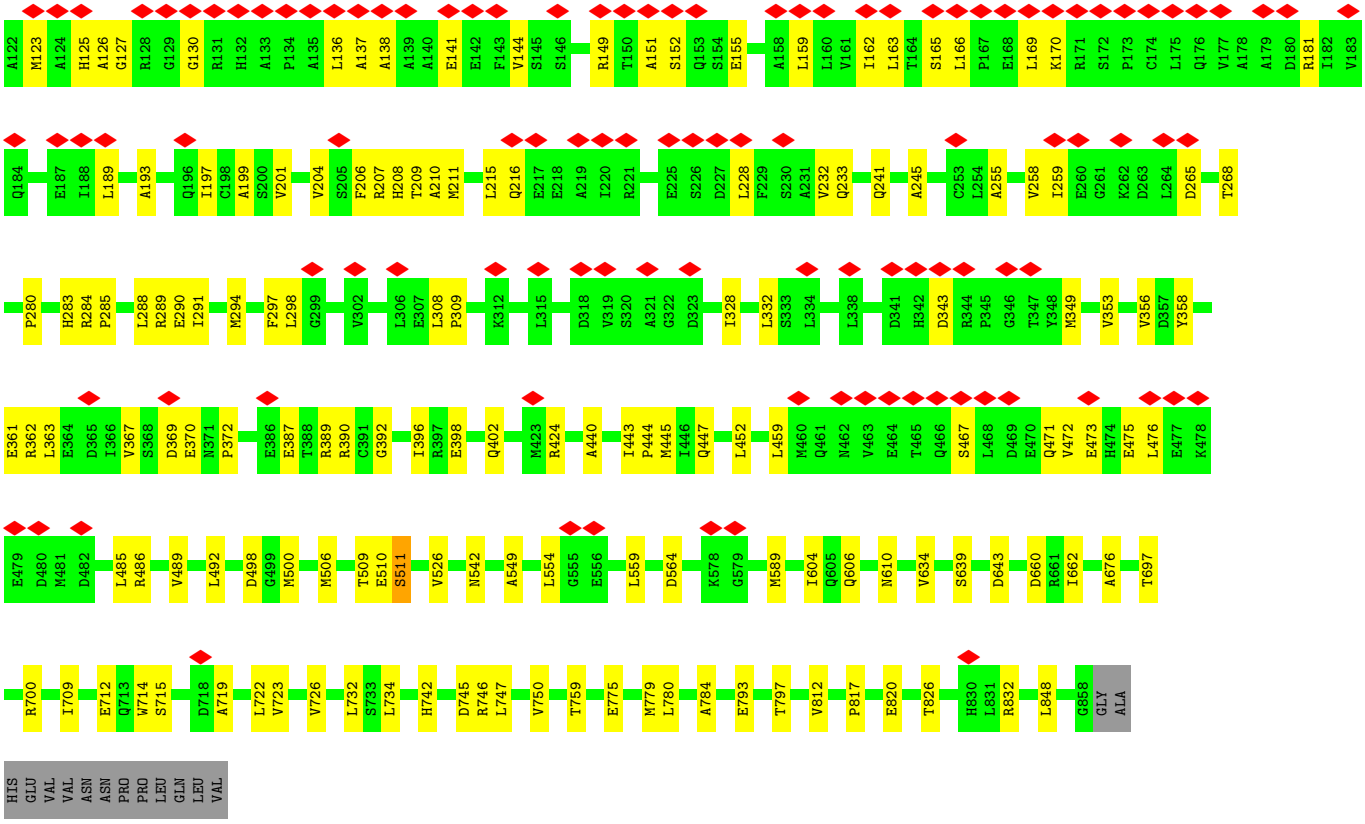


• Molecule 6: RNA-editing substrate-binding complex protein 8 (RESC8)



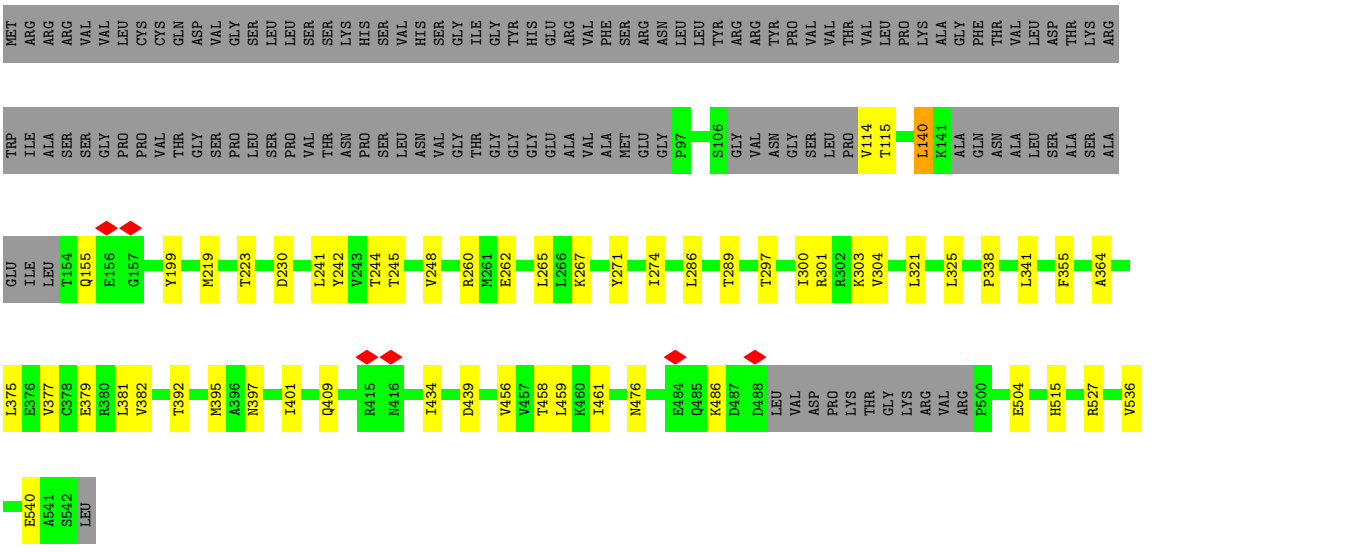
• Molecule 7: RNA-editing substrate-binding complex protein 9 (RESC9)





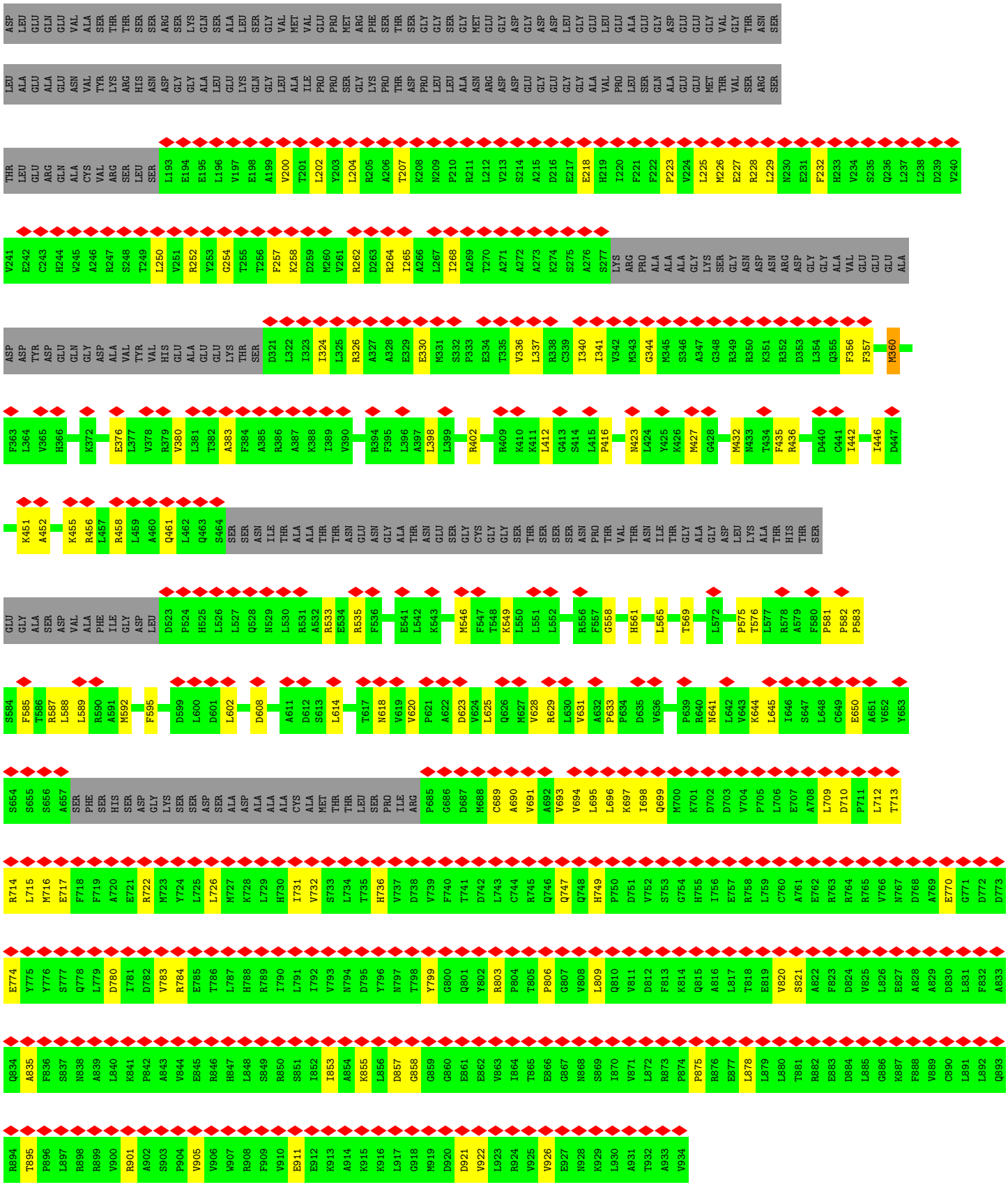
• Molecule 8: RNA-editing substrate-binding complex protein 10 (RESC10)

Chain 10:



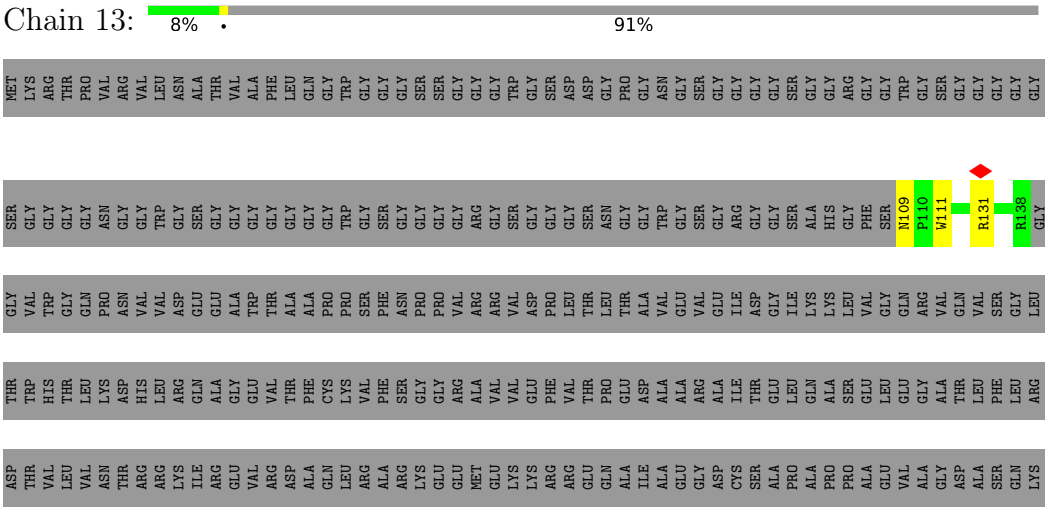
• Molecule 9: RNA-editing substrate-binding complex protein 11 (RESC11)

Chain 11:



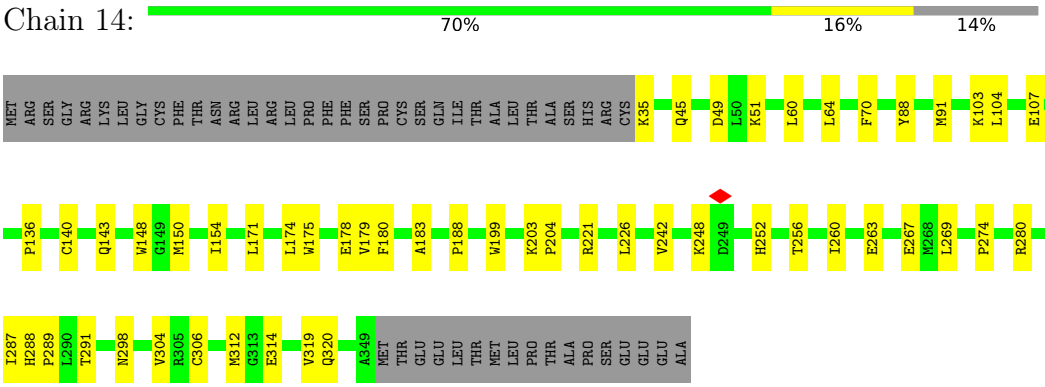
• Molecule 10: RNA-editing substrate-binding complex protein 13 (RESC13)

Chain 13:



• Molecule 11: RNA-editing substrate-binding complex protein 14 (RESC14)

Chain 14:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266942	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	271.872, 271.872, 271.872	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.062, 1.062, 1.062	Depositor

5 Model quality

5.1 Standard geometry

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	m	0.18	0/509	0.71	0/791
2	g	0.18	0/351	0.77	0/540
3	5	0.24	0/2375	0.47	0/3218
4	6	0.25	0/3655	0.47	0/4936
5	7	0.24	0/526	0.43	0/708
6	8	0.24	0/4129	0.46	0/5589
7	9	0.24	0/6774	0.48	0/9167
8	10	0.24	0/3341	0.47	0/4516
9	11	0.24	0/5010	0.49	0/6780
10	13	0.25	0/232	0.63	0/309
11	14	0.25	0/2579	0.48	0/3522
All	All	0.24	0/29481	0.49	0/40076

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

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	m	453	0	226	0	0
2	g	320	0	161	0	0
3	5	2318	0	2257	21	0
4	6	3591	0	3628	46	0
5	7	518	0	524	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	8	4056	0	4094	54	0
7	9	6662	0	6745	108	0
8	10	3290	0	3320	33	0
9	11	4918	0	5091	89	0
10	13	227	0	208	3	0
11	14	2505	0	2442	32	0
All	All	28858	0	28696	376	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 7.

All (376) 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)
9:11:710:ASP:O	9:11:713:THR:HG22	1.40	1.20
9:11:710:ASP:O	9:11:713:THR:CG2	2.31	0.74
9:11:911:GLU:HB2	9:11:926:VAL:HG11	1.70	0.74
6:8:309:LEU:HD13	6:8:319:MET:CE	2.18	0.73
11:14:319:VAL:HG12	11:14:320:GLN:HG3	1.70	0.72
9:11:344:GLY:HA3	9:11:383:ALA:HB1	1.72	0.70
4:6:331:ASN:H	4:6:334:TYR:HD2	1.40	0.70
7:9:398:GLU:OE1	7:9:402:GLN:NE2	2.25	0.69
9:11:582:PRO:HB2	9:11:799:TYR:HB3	1.74	0.69
7:9:732:LEU:HB3	7:9:734:LEU:HD23	1.74	0.69
6:8:331:ALA:HA	6:8:334:MET:HG3	1.75	0.68
3:5:92:GLU:HG2	8:10:515:HIS:HB2	1.76	0.67
9:11:713:THR:OG1	9:11:749:HIS:CE1	2.47	0.67
8:10:271:TYR:HB3	8:10:274:ILE:HD11	1.76	0.66
7:9:38:VAL:O	7:9:79:ARG:NH1	2.28	0.66
7:9:10:LEU:HD21	7:9:46:ILE:HD13	1.77	0.66
4:6:372:ILE:O	4:6:376:VAL:HG22	1.96	0.65
4:6:70:ALA:HB1	4:6:115:THR:HG21	1.80	0.64
5:7:111:ALA:HA	5:7:114:ASP:HB2	1.81	0.63
7:9:349:MET:O	7:9:353:VAL:HG23	1.97	0.63
4:6:320:THR:HG23	4:6:352:LEU:HD22	1.80	0.63
9:11:689:CYS:O	9:11:693:VAL:HG23	1.99	0.63
4:6:142:ILE:O	4:6:172:LYS:NZ	2.29	0.62
11:14:60:LEU:HD11	11:14:104:LEU:HD21	1.80	0.62
7:9:424:ARG:NH1	7:9:459:LEU:O	2.32	0.62
7:9:24:VAL:O	7:9:28:MET:HG2	2.00	0.62
8:10:289:THR:HG23	8:10:301:ARG:HH22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:131:VAL:HG22	3:5:140:VAL:HG12	1.83	0.61
7:9:506:MET:HE1	7:9:542:ASN:HB3	1.81	0.61
9:11:691:VAL:O	9:11:695:LEU:HG	2.00	0.61
9:11:722:ARG:NH2	9:11:835:ALA:O	2.30	0.61
6:8:309:LEU:HD13	6:8:319:MET:HE2	1.83	0.60
7:9:387:GLU:OE1	7:9:390:ARG:NH1	2.33	0.60
4:6:144:VAL:HG11	4:6:180:LEU:HD22	1.83	0.60
4:6:246:ALA:O	4:6:250:MET:HG2	2.00	0.60
3:5:188:ALA:O	3:5:192:VAL:HB	2.01	0.60
7:9:369:ASP:OD1	7:9:370:GLU:N	2.34	0.60
4:6:180:LEU:HB2	4:6:185:VAL:HG23	1.84	0.59
8:10:392:THR:HG22	8:10:395:MET:HG3	1.82	0.59
7:9:445:MET:HG3	7:9:500:MET:HE2	1.84	0.59
7:9:2:LEU:HB3	7:9:6:LEU:HD23	1.84	0.59
7:9:75:PRO:HA	7:9:114:TRP:HD1	1.66	0.59
8:10:476:ASN:OD1	8:10:527:ARG:NH1	2.34	0.59
11:14:280:ARG:H	11:14:283:GLU:HG3	1.68	0.59
9:11:356:PHE:O	9:11:360:MET:HG2	2.02	0.59
9:11:250:LEU:HD12	9:11:254:GLY:HA3	1.84	0.59
4:6:311:ARG:HD2	4:6:347:ILE:HD11	1.85	0.59
7:9:288:LEU:HA	7:9:291:ILE:HD12	1.86	0.58
7:9:489:VAL:HA	7:9:492:LEU:HB2	1.86	0.58
9:11:535:ARG:NH2	9:11:576:THR:OG1	2.37	0.58
6:8:306:PHE:HD1	6:8:345:ILE:HG21	1.69	0.58
7:9:209:THR:HB	7:9:245:ALA:HB2	1.86	0.57
6:8:21:PRO:HB2	6:8:24:LEU:HB3	1.87	0.57
7:9:144:VAL:HA	7:9:159:LEU:HD11	1.87	0.57
4:6:442:ASP:OD1	4:6:443:ALA:N	2.38	0.57
9:11:546:MET:HA	9:11:549:LYS:HE3	1.87	0.57
11:14:91:MET:HG3	11:14:284:ALA:HB3	1.86	0.57
6:8:109:GLU:OE2	6:8:109:GLU:N	2.35	0.56
7:9:444:PRO:HB2	7:9:447:GLN:HG2	1.87	0.56
3:5:138:ILE:HG12	3:5:169:VAL:HG12	1.86	0.56
4:6:492:PHE:HZ	4:6:503:LEU:HB3	1.71	0.56
11:14:103:LYS:O	11:14:107:GLU:HG3	2.05	0.56
4:6:257:THR:HG22	4:6:258:VAL:H	1.70	0.56
4:6:290:VAL:HG11	4:6:318:VAL:HG12	1.88	0.56
6:8:406:LEU:HA	6:8:409:MET:HG3	1.88	0.56
7:9:826:THR:O	7:9:832:ARG:NH1	2.39	0.56
4:6:345:ILE:HG23	4:6:347:ILE:H	1.70	0.56
6:8:395:VAL:HG12	6:8:424:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:261:ASP:OD1	6:8:262:ALA:N	2.38	0.55
4:6:208:ARG:O	4:6:212:THR:HG23	2.07	0.55
7:9:137:ALA:O	7:9:141:GLU:N	2.36	0.55
3:5:243:GLN:NE2	3:5:269:ASP:OD2	2.35	0.55
6:8:43:VAL:HG11	6:8:72:PHE:HB2	1.88	0.55
8:10:321:LEU:HD12	8:10:355:PHE:CZ	2.42	0.55
7:9:363:LEU:HG	7:9:398:GLU:HG2	1.89	0.55
7:9:719:ALA:O	7:9:723:VAL:HG13	2.06	0.55
9:11:218:GLU:OE2	9:11:252:ARG:NE	2.38	0.55
4:6:63:ALA:HB3	4:6:104:LEU:HD21	1.88	0.55
4:6:386:ASP:HB3	4:6:389:LEU:HB3	1.89	0.55
8:10:230:ASP:HB3	8:10:260:ARG:HH21	1.70	0.55
6:8:392:HIS:HB3	6:8:394:LEU:HD22	1.89	0.55
6:8:523:MET:HB2	6:8:527:LEU:HD12	1.88	0.55
7:9:440:ALA:HA	7:9:443:ILE:HD11	1.89	0.54
6:8:252:CYS:SG	6:8:253:GLY:N	2.80	0.54
7:9:476:LEU:HD22	9:11:451:LYS:HG3	1.88	0.54
4:6:425:ASP:OD1	4:6:426:MET:N	2.39	0.54
7:9:121:VAL:O	7:9:125:HIS:ND1	2.40	0.54
8:10:248:VAL:HB	8:10:297:THR:HG23	1.90	0.54
9:11:895:THR:O	9:11:901:ARG:NH2	2.40	0.54
6:8:139:LEU:HD11	6:8:161:LEU:HD21	1.88	0.54
4:6:253:ARG:O	4:6:254:GLU:HG2	2.08	0.54
7:9:138:ALA:O	7:9:141:GLU:HB2	2.08	0.54
3:5:95:ALA:O	3:5:99:MET:HG3	2.07	0.53
7:9:473:GLU:HA	7:9:476:LEU:HD12	1.90	0.53
9:11:436:ARG:NH2	10:13:111:TRP:O	2.41	0.53
3:5:82:THR:HG22	6:8:241:LYS:HE3	1.91	0.53
7:9:127:GLY:HA3	7:9:165:SER:HB3	1.91	0.53
7:9:812:VAL:HG23	7:9:848:LEU:HD22	1.91	0.53
11:14:120:LYS:HB3	11:14:123:ARG:HG3	1.91	0.53
7:9:358:TYR:OH	7:9:362:ARG:NH1	2.43	0.52
7:9:676:ALA:HB1	7:9:709:ILE:HG22	1.91	0.52
7:9:151:ALA:O	7:9:181:ARG:NE	2.26	0.52
11:14:203:LYS:HB3	11:14:204:PRO:HD3	1.92	0.52
7:9:467:SER:HA	7:9:471:GLN:HG2	1.92	0.52
6:8:303:VAL:O	6:8:307:ILE:HG12	2.10	0.52
7:9:208:HIS:HB3	7:9:211:MET:HE2	1.92	0.52
7:9:604:ILE:HG21	7:9:639:SER:HB2	1.90	0.52
6:8:306:PHE:CE2	6:8:323:MET:HB3	2.45	0.52
7:9:353:VAL:HA	7:9:356:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:85:LEU:HD13	7:9:126:ALA:HB2	1.91	0.52
9:11:336:VAL:O	9:11:340:ILE:HG13	2.09	0.52
11:14:64:LEU:HD12	11:14:70:PHE:HZ	1.75	0.52
7:9:817:PRO:HA	7:9:820:GLU:HG2	1.92	0.52
8:10:375:LEU:O	8:10:379:GLU:HG3	2.09	0.52
9:11:337:LEU:O	9:11:341:ILE:HG12	2.10	0.52
4:6:464:LEU:HD12	4:6:468:PHE:HE2	1.75	0.51
7:9:207:ARG:HG2	7:9:241:GLN:HA	1.92	0.51
7:9:509:THR:HG21	7:9:526:VAL:HG11	1.90	0.51
7:9:211:MET:O	7:9:215:LEU:HG	2.11	0.51
3:5:76:MET:HE2	3:5:114:LEU:HD11	1.92	0.51
4:6:117:VAL:O	11:14:45:GLN:NE2	2.38	0.51
4:6:435:VAL:HG23	4:6:466:PRO:HG2	1.92	0.51
11:14:263:GLU:O	11:14:267:GLU:HG2	2.10	0.51
7:9:130:GLY:HA3	7:9:166:LEU:HD11	1.93	0.51
9:11:254:GLY:O	9:11:258:LYS:HG2	2.11	0.51
11:14:171:LEU:HB3	11:14:314:GLU:HB2	1.91	0.51
6:8:357:MET:O	6:8:361:MET:HG3	2.10	0.51
7:9:123:MET:HG3	7:9:162:ILE:HG23	1.92	0.51
9:11:340:ILE:HG21	9:11:380:VAL:HG13	1.92	0.51
6:8:343:MET:HB3	6:8:382:ILE:HG21	1.92	0.51
3:5:302:ARG:HB3	3:5:303:TRP:CD1	2.46	0.51
7:9:152:SER:H	7:9:155:GLU:HB2	1.74	0.50
7:9:75:PRO:HA	7:9:114:TRP:CD1	2.47	0.50
9:11:699:GLN:HG2	9:11:709:LEU:HD22	1.94	0.50
5:7:95:HIS:NE2	5:7:108:GLU:OE1	2.44	0.50
7:9:747:LEU:HD23	7:9:780:LEU:HD11	1.93	0.50
7:9:308:LEU:HD12	7:9:309:PRO:HD2	1.93	0.50
9:11:693:VAL:O	9:11:697:LYS:HG2	2.11	0.50
4:6:504:TYR:O	4:6:508:ILE:HG12	2.12	0.50
9:11:857:ASP:HA	9:11:905:VAL:HG11	1.94	0.50
9:11:432:MET:HA	9:11:435:PHE:HD2	1.76	0.50
4:6:163:ARG:NH2	8:10:262:GLU:OE1	2.36	0.50
6:8:454:LEU:HD11	6:8:475:ILE:HD11	1.94	0.50
8:10:364:ALA:HB2	8:10:381:LEU:HD23	1.94	0.49
9:11:696:LEU:HD13	9:11:747:GLN:HG2	1.94	0.49
11:14:154:ILE:HG21	11:14:174:LEU:HD22	1.94	0.49
6:8:108:GLU:O	6:8:112:ILE:HG13	2.12	0.49
7:9:265:ASP:O	7:9:268:THR:HG22	2.11	0.49
7:9:634:VAL:HG11	7:9:662:ILE:HG23	1.93	0.49
9:11:561:HIS:HB3	9:11:595:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:452:LEU:HB3	7:9:511:SER:OG	2.11	0.49
6:8:378:ASP:O	6:8:382:ILE:HG12	2.12	0.49
7:9:57:ASP:OD2	7:9:60:THR:OG1	2.29	0.49
7:9:144:VAL:HG21	7:9:163:LEU:HD21	1.93	0.49
6:8:341:PRO:O	6:8:345:ILE:HG12	2.12	0.49
9:11:546:MET:HA	9:11:549:LYS:HG2	1.95	0.49
4:6:67:ALA:HB2	4:6:112:LEU:HG	1.95	0.49
4:6:193:SER:HA	4:6:234:LEU:HD21	1.94	0.49
7:9:216:GLN:NE2	7:9:245:ALA:O	2.46	0.49
9:11:608:ASP:OD1	9:11:641:ASN:ND2	2.46	0.49
4:6:71:LEU:HD13	4:6:111:LEU:HD22	1.94	0.49
7:9:289:ARG:NH2	7:9:290:GLU:OE2	2.46	0.49
9:11:533:ARG:HH21	9:11:581:PRO:HD3	1.78	0.49
11:14:183:ALA:O	11:14:298:ASN:ND2	2.46	0.49
9:11:690:ALA:O	9:11:694:VAL:HG12	2.12	0.49
4:6:144:VAL:HG13	4:6:188:ILE:HD11	1.95	0.48
9:11:631:VAL:HG23	9:11:698:ILE:HD11	1.93	0.48
9:11:726:LEU:HD23	9:11:732:VAL:HB	1.95	0.48
9:11:731:ILE:O	9:11:784:ARG:NH1	2.45	0.48
11:14:49:ASP:OD1	11:14:123:ARG:HD3	2.13	0.48
9:11:200:VAL:HG11	9:11:225:LEU:HD22	1.95	0.48
7:9:284:ARG:O	7:9:288:LEU:HD12	2.14	0.48
7:9:486:ARG:HA	7:9:489:VAL:HG22	1.95	0.48
7:9:606:GLN:NE2	7:9:610:ASN:OD1	2.46	0.48
7:9:20:ASN:HB3	7:9:23:ASP:HB2	1.96	0.48
6:8:186:LEU:O	6:8:219:ARG:NH2	2.47	0.47
8:10:300:ILE:O	8:10:304:VAL:HG23	2.14	0.47
8:10:458:THR:HG22	8:10:459:LEU:HD12	1.96	0.47
11:14:226:LEU:HD12	11:14:291:THR:HG21	1.96	0.47
6:8:183:ASN:C	6:8:183:ASN:HD22	2.15	0.47
7:9:25:ARG:HH12	7:9:67:ALA:HB2	1.79	0.47
9:11:806:PRO:HD2	9:11:809:LEU:HD12	1.96	0.47
7:9:328:ILE:O	7:9:332:LEU:HG	2.14	0.47
6:8:394:LEU:HD12	6:8:398:PHE:CE2	2.49	0.47
8:10:114:VAL:HG22	8:10:115:THR:HG23	1.97	0.47
3:5:242:VAL:HG11	3:5:250:MET:HG2	1.97	0.47
8:10:397:ASN:O	8:10:401:ILE:HG12	2.14	0.47
11:14:143:GLN:HE22	11:14:179:VAL:HG13	1.78	0.47
3:5:265:TRP:CZ2	3:5:268:MET:HG3	2.50	0.47
6:8:294:ALA:HA	6:8:297:LEU:HD13	1.97	0.47
6:8:445:LYS:HG3	6:8:446:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:10:199:TYR:HB2	8:10:242:TYR:OH	2.15	0.47
9:11:569:THR:HG23	9:11:602:LEU:HD13	1.96	0.47
9:11:858:GLY:HA2	9:11:875:PRO:HG3	1.96	0.47
6:8:29:GLU:OE2	11:14:280:ARG:NH2	2.47	0.47
6:8:261:ASP:HB3	6:8:264:THR:HG22	1.96	0.47
7:9:510:GLU:OE2	7:9:549:ALA:HB3	2.15	0.47
7:9:746:ARG:O	7:9:750:VAL:HG22	2.15	0.47
9:11:423:ASN:O	9:11:427:MET:HG3	2.15	0.47
9:11:458:ARG:O	9:11:461:GLN:HG3	2.14	0.47
9:11:713:THR:O	9:11:717:GLU:HG2	2.13	0.47
3:5:131:VAL:HG13	3:5:138:ILE:HD12	1.96	0.46
6:8:506:LYS:HA	6:8:506:LYS:HD3	1.68	0.46
7:9:472:VAL:HG22	9:11:458:ARG:HG2	1.97	0.46
9:11:265:ILE:HA	9:11:268:ILE:HG22	1.97	0.46
11:14:252:HIS:O	11:14:256:THR:HG23	2.15	0.46
6:8:419:ARG:HE	6:8:452:PRO:HG3	1.80	0.46
9:11:535:ARG:NH2	9:11:575:PRO:HB2	2.30	0.46
7:9:712:GLU:O	7:9:715:SER:OG	2.33	0.46
8:10:267:LYS:HE3	8:10:267:LYS:HB3	1.79	0.46
4:6:351:GLU:OE2	4:6:355:ASN:ND2	2.48	0.46
9:11:821:SER:HB2	9:11:878:LEU:HD21	1.97	0.46
8:10:382:VAL:HG13	8:10:434:ILE:HD11	1.98	0.46
7:9:392:GLY:O	7:9:396:ILE:HG13	2.15	0.46
9:11:442:ILE:O	9:11:446:ILE:HG13	2.16	0.46
9:11:820:VAL:O	9:11:855:LYS:NZ	2.44	0.46
6:8:150:SER:H	6:8:153:GLN:NE2	2.14	0.45
7:9:61:VAL:HG11	7:9:88:LEU:HD21	1.98	0.45
7:9:564:ASP:OD1	7:9:564:ASP:N	2.49	0.45
8:10:325:LEU:HD13	8:10:325:LEU:HA	1.85	0.45
9:11:340:ILE:HG12	9:11:360:MET:HE3	1.98	0.45
7:9:199:ALA:HA	7:9:233:GLN:HE21	1.80	0.45
7:9:255:ALA:O	7:9:259:ILE:HG13	2.16	0.45
7:9:170:LYS:HD3	7:9:204:VAL:HG22	1.98	0.45
9:11:853:ILE:O	9:11:857:ASP:HB2	2.17	0.45
7:9:102:VAL:HG13	7:9:136:LEU:HD11	1.99	0.45
9:11:262:ARG:HG2	9:11:356:PHE:CE2	2.52	0.45
9:11:625:LEU:O	9:11:629:ARG:HG3	2.16	0.45
9:11:629:ARG:O	9:11:633:PRO:HD3	2.17	0.45
4:6:370:ARG:H	4:6:370:ARG:HG2	1.55	0.45
5:7:141:PHE:O	5:7:145:TRP:N	2.50	0.45
6:8:436:ALA:HA	6:8:453:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:44:TYR:HE1	6:8:87:LEU:HD23	1.82	0.45
6:8:484:LEU:HB2	6:8:515:PHE:HD2	1.82	0.45
8:10:219:MET:O	8:10:223:THR:HG23	2.17	0.45
9:11:357:PHE:HA	9:11:360:MET:HG3	1.99	0.45
4:6:462:LYS:HE2	4:6:462:LYS:HB2	1.70	0.44
7:9:201:VAL:HB	7:9:206:PHE:HE1	1.82	0.44
7:9:367:VAL:HA	7:9:372:PRO:HB3	1.98	0.44
7:9:447:GLN:NE2	7:9:589:MET:SD	2.87	0.44
9:11:337:LEU:HD11	9:11:376:GLU:HB3	1.99	0.44
11:14:143:GLN:NE2	11:14:179:VAL:HG13	2.33	0.44
9:11:398:LEU:O	9:11:402:ARG:HG2	2.16	0.44
7:9:255:ALA:O	7:9:258:VAL:HG12	2.18	0.44
9:11:227:GLU:HG3	9:11:228:ARG:HG3	1.99	0.44
11:14:221:ARG:O	11:14:304:VAL:HG11	2.18	0.44
6:8:277:TYR:HB3	6:8:283:ILE:HD11	1.99	0.44
6:8:368:THR:HG23	6:8:369:ARG:HD2	1.99	0.44
9:11:713:THR:HG23	9:11:714:ARG:N	2.32	0.44
11:14:285:LEU:HD23	11:14:287:ILE:HD11	1.99	0.44
6:8:324:ALA:O	6:8:328:ILE:HG12	2.16	0.44
6:8:484:LEU:O	6:8:488:GLU:HG3	2.17	0.44
7:9:149:ARG:O	7:9:181:ARG:NH1	2.51	0.44
8:10:241:LEU:O	8:10:245:THR:HG23	2.18	0.44
4:6:257:THR:HG22	4:6:258:VAL:N	2.31	0.44
9:11:614:LEU:O	9:11:618:ASN:ND2	2.41	0.44
3:5:121:THR:HG21	3:5:153:THR:HG21	1.99	0.44
7:9:367:VAL:HG21	7:9:398:GLU:HG3	1.99	0.44
9:11:340:ILE:HG12	9:11:360:MET:CE	2.47	0.44
4:6:189:ILE:HG21	4:6:227:LEU:HD12	1.99	0.44
7:9:775:GLU:O	7:9:779:MET:HG2	2.17	0.44
9:11:452:ALA:O	9:11:455:LYS:HG2	2.18	0.44
9:11:264:ARG:HH22	9:11:324:ILE:HG13	1.82	0.44
4:6:296:GLU:HG3	4:6:334:TYR:CE1	2.53	0.43
7:9:742:HIS:HA	7:9:745:ASP:OD2	2.18	0.43
9:11:452:ALA:O	9:11:456:ARG:HG3	2.18	0.43
9:11:585:PHE:O	9:11:589:LEU:HG	2.17	0.43
4:6:366:ASP:O	11:14:35:LYS:N	2.51	0.43
4:6:468:PHE:HD1	4:6:503:LEU:HD12	1.83	0.43
5:7:84:VAL:O	5:7:88:VAL:HG23	2.18	0.43
6:8:45:GLN:O	6:8:49:THR:HG22	2.18	0.43
7:9:208:HIS:NE2	7:9:210:ALA:HB3	2.33	0.43
4:6:113:LEU:HB2	4:6:131:CYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:115:GLU:HG2	6:8:153:GLN:OE1	2.18	0.43
7:9:709:ILE:HD11	7:9:714:TRP:CE2	2.53	0.43
7:9:793:GLU:O	7:9:797:THR:HG23	2.19	0.43
11:14:140:CYS:O	11:14:178:GLU:HA	2.17	0.43
7:9:117:HIS:O	7:9:121:VAL:HG23	2.19	0.43
7:9:475:GLU:HB3	9:11:458:ARG:HH12	1.82	0.43
9:11:770:GLU:HB2	9:11:774:GLU:HB3	2.00	0.43
11:14:175:TRP:HZ3	11:14:199:TRP:CG	2.36	0.43
4:6:458:VAL:HG23	4:6:464:LEU:HD21	2.00	0.43
7:9:280:PRO:HB2	7:9:283:HIS:HD2	1.83	0.43
7:9:660:ASP:OD2	7:9:697:THR:OG1	2.28	0.43
8:10:456:VAL:HG13	8:10:461:ILE:HB	2.01	0.43
9:11:223:PRO:HA	9:11:226:MET:HB3	2.01	0.43
6:8:315:LEU:HD12	6:8:320:PHE:HB2	1.99	0.43
7:9:108:GLY:HA3	7:9:114:TRP:CZ3	2.53	0.43
11:14:136:PRO:HB2	11:14:188:PRO:HD3	2.01	0.43
6:8:280:ARG:HE	6:8:280:ARG:HB3	1.66	0.43
8:10:338:PRO:HG2	8:10:341:LEU:HD13	2.00	0.43
7:9:343:ASP:OD1	7:9:343:ASP:N	2.45	0.42
6:8:24:LEU:HD11	6:8:56:LEU:HD13	2.01	0.42
8:10:262:GLU:HG3	8:10:303:LYS:HD2	2.01	0.42
9:11:204:LEU:O	9:11:207:THR:OG1	2.34	0.42
9:11:549:LYS:HE2	9:11:587:ARG:HH12	1.83	0.42
9:11:565:LEU:O	9:11:569:THR:OG1	2.29	0.42
6:8:494:LEU:HD23	6:8:494:LEU:HA	1.88	0.42
7:9:137:ALA:HB1	7:9:169:LEU:HG	2.01	0.42
8:10:244:THR:HG21	8:10:265:LEU:HD11	1.99	0.42
9:11:588:LEU:O	9:11:592:MET:HG3	2.19	0.42
8:10:377:VAL:HG22	8:10:381:LEU:HD13	2.00	0.42
8:10:486:LYS:HD3	8:10:536:VAL:HG23	2.01	0.42
9:11:770:GLU:OE1	9:11:770:GLU:N	2.45	0.42
6:8:320:PHE:CE1	6:8:349:VAL:HG11	2.54	0.42
7:9:722:LEU:O	7:9:726:VAL:HG13	2.20	0.42
3:5:145:ARG:NH2	3:5:178:ALA:O	2.31	0.42
4:6:385:LYS:HE3	4:6:385:LYS:HB2	1.86	0.42
8:10:439:ASP:OD1	8:10:439:ASP:N	2.47	0.42
9:11:921:ASP:OD1	9:11:922:VAL:N	2.53	0.42
11:14:180:PHE:HB2	11:14:306:CYS:SG	2.60	0.42
7:9:284:ARG:N	7:9:285:PRO:HD2	2.35	0.42
7:9:358:TYR:O	7:9:361:GLU:HG2	2.20	0.42
7:9:43:THR:HG23	7:9:83:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:350:PRO:HD2	4:6:351:GLU:H	1.85	0.42
9:11:582:PRO:N	9:11:583:PRO:HD2	2.35	0.42
11:14:148:TRP:O	11:14:150:MET:N	2.50	0.42
7:9:294:MET:HA	7:9:297:PHE:CE2	2.55	0.41
9:11:628:VAL:HG22	9:11:645:LEU:HD21	2.01	0.41
9:11:780:ASP:HB3	9:11:783:VAL:HG23	2.02	0.41
4:6:224:LEU:HD22	4:6:245:ILE:HG23	2.01	0.41
6:8:201:CYS:HA	6:8:202:PRO:HD3	1.94	0.41
6:8:404:LEU:HD23	6:8:404:LEU:HA	1.94	0.41
7:9:554:LEU:HB3	7:9:559:LEU:HD21	2.01	0.41
8:10:504:GLU:OE1	8:10:540:GLU:HB2	2.20	0.41
9:11:641:ASN:HB2	9:11:644:LYS:HD2	2.02	0.41
3:5:76:MET:SD	3:5:282:LEU:HD21	2.60	0.41
3:5:179:PRO:HG2	3:5:184:TYR:CD2	2.55	0.41
4:6:409:LEU:HD23	4:6:437:VAL:HG21	2.02	0.41
9:11:695:LEU:HD22	9:11:712:LEU:HD22	2.01	0.41
11:14:288:HIS:CG	11:14:289:PRO:HD2	2.55	0.41
7:9:723:VAL:HA	7:9:726:VAL:HG22	2.01	0.41
3:5:179:PRO:HG2	3:5:184:TYR:HD2	1.85	0.41
4:6:458:VAL:HG23	4:6:459:ARG:H	1.86	0.41
9:11:583:PRO:HG3	9:11:803:ARG:HE	1.84	0.41
4:6:468:PHE:CD1	4:6:503:LEU:HD12	2.56	0.41
8:10:140:LEU:HD11	8:10:155:GLN:HG3	2.02	0.41
9:11:326:ARG:NE	9:11:330:GLU:HG2	2.36	0.41
3:5:21:ARG:NH1	8:10:409:GLN:HA	2.36	0.41
4:6:290:VAL:HA	4:6:293:MET:SD	2.61	0.41
6:8:306:PHE:CD1	6:8:345:ILE:HG21	2.52	0.41
9:11:202:LEU:HD12	9:11:202:LEU:HA	1.95	0.41
3:5:77:VAL:HG22	3:5:79:ILE:HG13	2.02	0.41
3:5:84:LEU:HD11	3:5:117:TYR:HB2	2.03	0.41
4:6:123:SER:HB3	4:6:157:LEU:HG	2.03	0.41
7:9:77:HIS:O	7:9:80:ARG:HB3	2.19	0.41
7:9:259:ILE:HG12	7:9:297:PHE:CE2	2.56	0.41
7:9:298:LEU:HD23	7:9:298:LEU:HA	1.96	0.41
9:11:620:VAL:HB	9:11:623:ASP:OD1	2.21	0.41
9:11:716:MET:HE2	9:11:716:MET:HB2	1.92	0.41
11:14:88:TYR:CG	11:14:226:LEU:HD11	2.56	0.41
11:14:242:VAL:HA	11:14:260:ILE:HD13	2.02	0.41
7:9:228:LEU:O	7:9:232:VAL:HG13	2.20	0.41
8:10:244:THR:O	8:10:248:VAL:HG22	2.21	0.41
6:8:148:GLU:OE1	7:9:700:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:451:GLU:O	6:8:455:MET:HG2	2.20	0.40
8:10:286:LEU:HD22	8:10:301:ARG:HG2	2.03	0.40
7:9:485:LEU:O	7:9:489:VAL:HG13	2.20	0.40
9:11:412:LEU:HD11	9:11:416:PRO:HB2	2.03	0.40
9:11:650:GLU:HG3	9:11:715:LEU:HD21	2.02	0.40
11:14:49:ASP:HB3	11:14:51:LYS:HG2	2.03	0.40
6:8:527:LEU:O	6:8:531:LEU:HG	2.21	0.40
7:9:116:LEU:HA	7:9:119:TYR:HD2	1.86	0.40
7:9:123:MET:HB2	7:9:162:ILE:HG12	2.04	0.40
7:9:193:ALA:O	7:9:197:ILE:HG12	2.21	0.40
9:11:229:LEU:HA	9:11:232:PHE:CD1	2.57	0.40
9:11:229:LEU:HD11	9:11:257:PHE:CZ	2.56	0.40
9:11:436:ARG:HG2	10:13:111:TRP:CH2	2.56	0.40
9:11:558:GLY:HA3	10:13:109:ASN:HD21	1.85	0.40
7:9:152:SER:N	7:9:155:GLU:HB2	2.36	0.40
7:9:759:THR:HG21	7:9:784:ALA:HB2	2.04	0.40
11:14:269:LEU:HD21	11:14:274:PRO:HD3	2.04	0.40
3:5:187:PHE:HB3	3:5:232:TYR:CD1	2.57	0.40
6:8:44:TYR:CZ	6:8:84:GLN:HG2	2.57	0.40
7:9:201:VAL:HB	7:9:206:PHE:CE1	2.57	0.40
9:11:225:LEU:O	9:11:229:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	5	294/402 (73%)	286 (97%)	8 (3%)	0	100	100
4	6	451/516 (87%)	439 (97%)	12 (3%)	0	100	100
5	7	60/174 (34%)	57 (95%)	3 (5%)	0	100	100
6	8	511/545 (94%)	496 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	9	856/872 (98%)	838 (98%)	18 (2%)	0	100	100
8	10	408/543 (75%)	399 (98%)	9 (2%)	0	100	100
9	11	606/934 (65%)	598 (99%)	8 (1%)	0	100	100
10	13	28/320 (9%)	27 (96%)	1 (4%)	0	100	100
11	14	313/366 (86%)	305 (97%)	8 (3%)	0	100	100
All	All	3527/4672 (76%)	3445 (98%)	82 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	5	251/322 (78%)	250 (100%)	1 (0%)	91	95
4	6	376/428 (88%)	375 (100%)	1 (0%)	92	97
5	7	53/138 (38%)	52 (98%)	1 (2%)	57	78
6	8	449/470 (96%)	444 (99%)	5 (1%)	73	86
7	9	725/737 (98%)	720 (99%)	5 (1%)	84	92
8	10	365/470 (78%)	364 (100%)	1 (0%)	92	97
9	11	542/796 (68%)	540 (100%)	2 (0%)	91	95
10	13	17/212 (8%)	16 (94%)	1 (6%)	19	49
11	14	272/317 (86%)	270 (99%)	2 (1%)	84	92
All	All	3050/3890 (78%)	3031 (99%)	19 (1%)	86	94

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5	236	HIS
4	6	160	ARG
5	7	83	ASP
6	8	183	ASN

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Mol	Chain	Res	Type
6	8	252	CYS
6	8	268	TYR
6	8	306	PHE
6	8	502	ASP
7	9	189	LEU
7	9	389	ARG
7	9	498	ASP
7	9	511	SER
7	9	643	ASP
8	10	140	LEU
9	11	360	MET
9	11	736	HIS
10	13	131	ARG
11	14	248	LYS
11	14	312	MET

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

Mol	Chain	Res	Type
6	8	153	GLN
6	8	236	ASN
7	9	233	GLN
9	11	749	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	m	20/21 (95%)	12 (60%)	0
2	g	15/16 (93%)	6 (40%)	0
All	All	35/37 (94%)	18 (51%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	m	104	A
1	m	108	U
1	m	111	A
1	m	112	A
1	m	113	U
1	m	114	A

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Mol	Chain	Res	Type
1	m	116	G
1	m	117	A
1	m	118	U
1	m	119	A
1	m	120	A
1	m	121	G
2	g	-14	U
2	g	-11	U
2	g	-10	U
2	g	-6	U
2	g	-5	U
2	g	-1	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

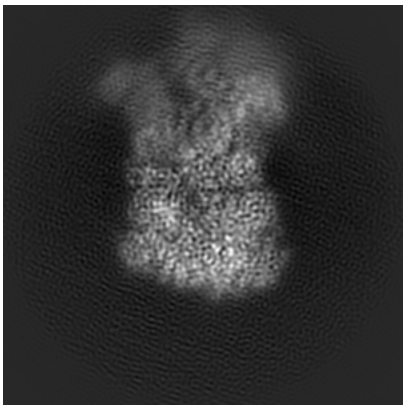
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29314. These allow visual inspection of the internal detail of the map and identification of artifacts.

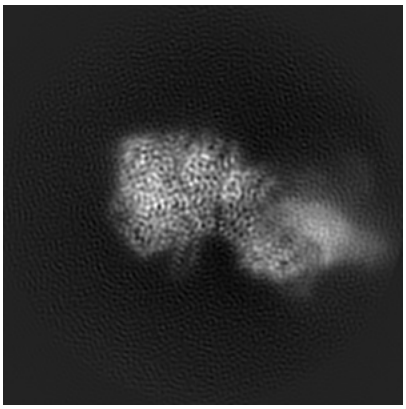
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

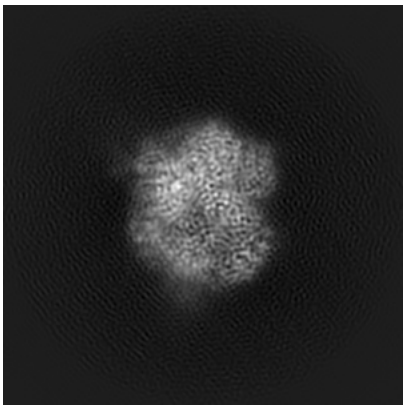
6.1.1 Primary map



X

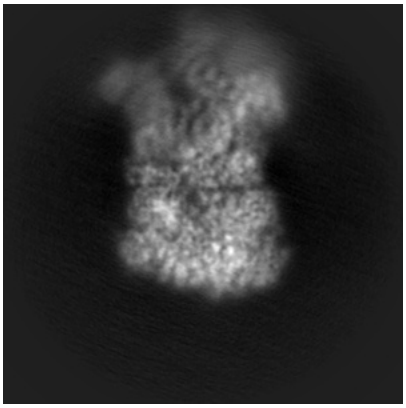


Y

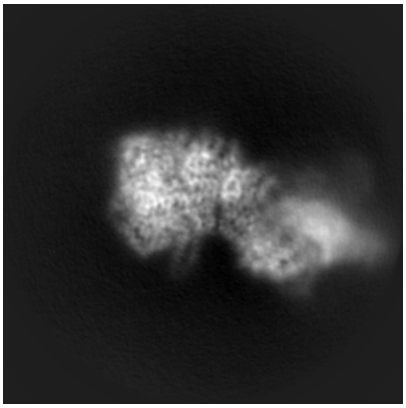


Z

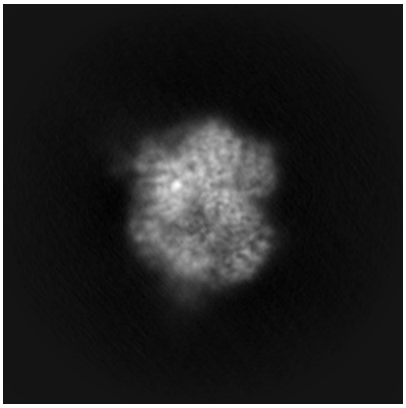
6.1.2 Raw map



X



Y

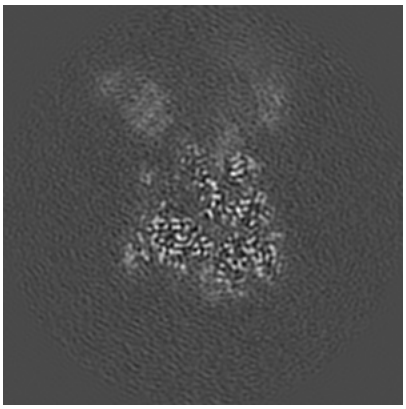


Z

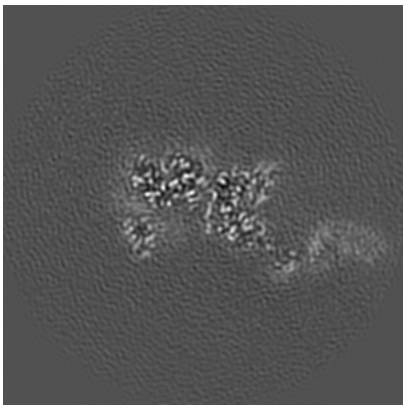
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

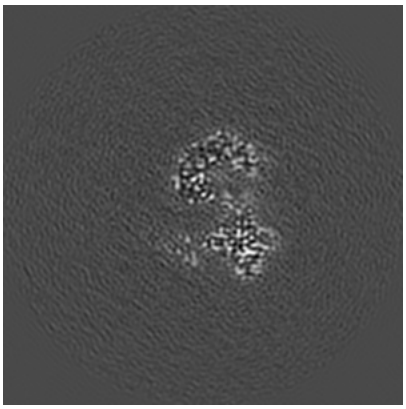
6.2.1 Primary map



X Index: 128

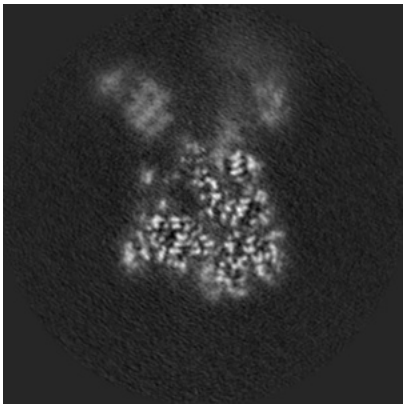


Y Index: 128

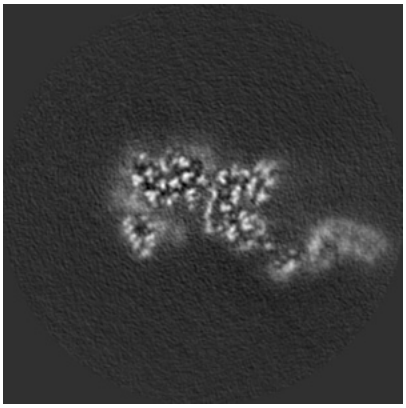


Z Index: 128

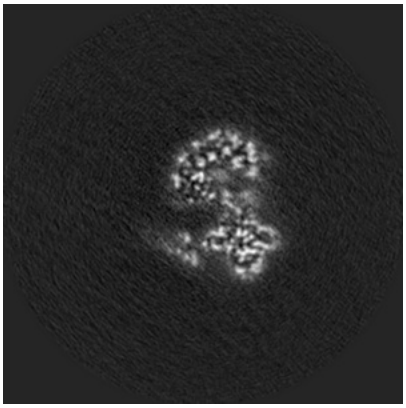
6.2.2 Raw map



X Index: 128



Y Index: 128

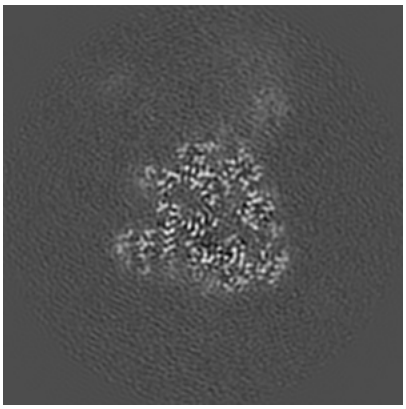


Z Index: 128

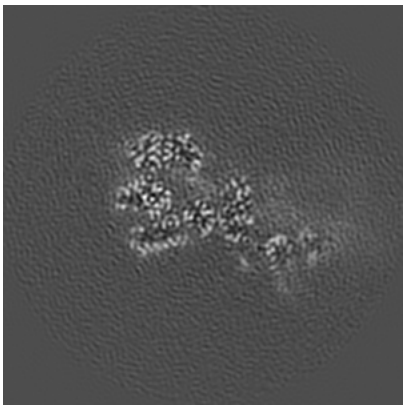
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

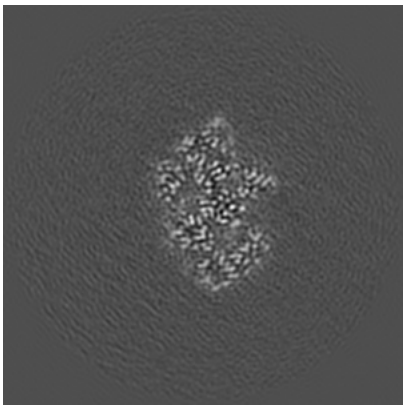
6.3.1 Primary map



X Index: 134

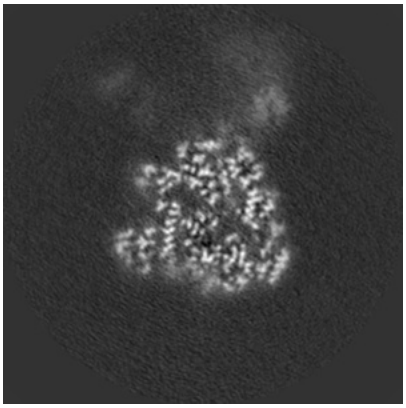


Y Index: 145

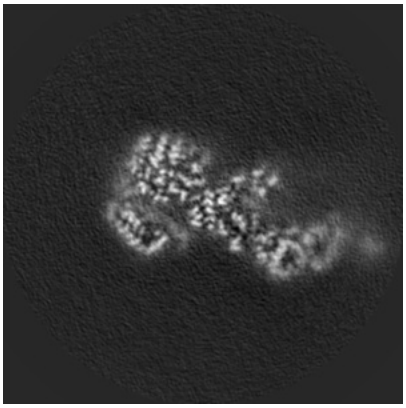


Z Index: 97

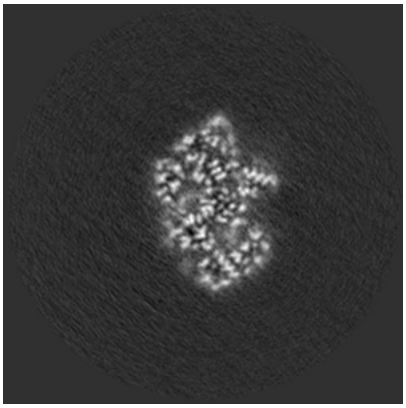
6.3.2 Raw map



X Index: 134



Y Index: 135

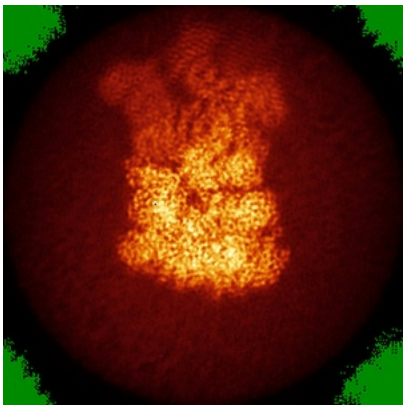


Z Index: 97

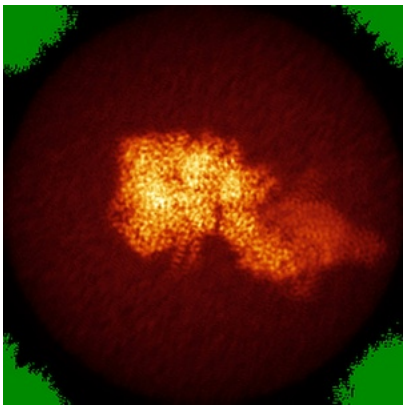
The images above show the largest variance slices of the map in three orthogonal directions.

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

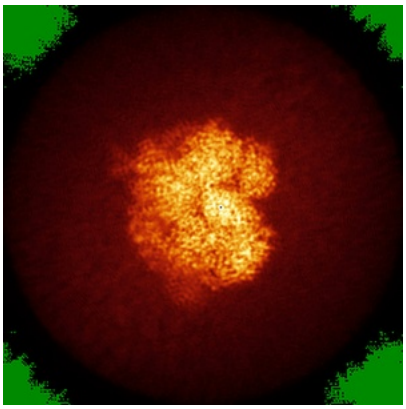
6.4.1 Primary map



X

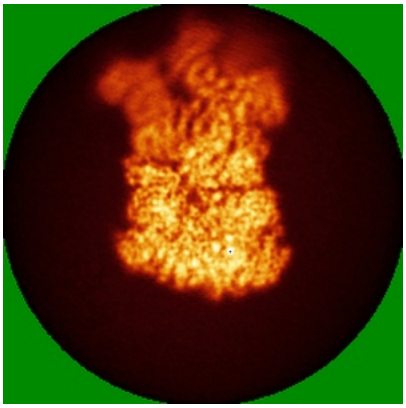


Y

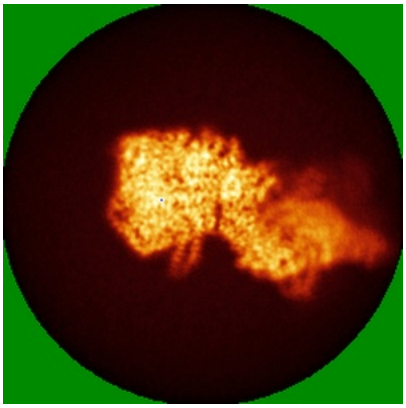


Z

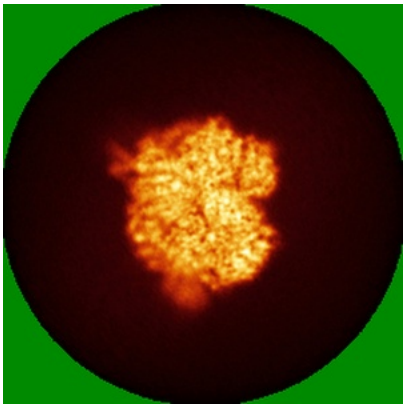
6.4.2 Raw map



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.

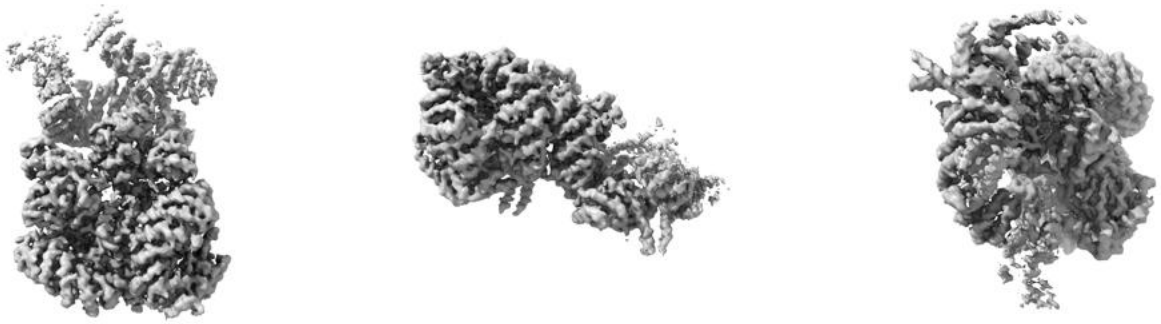
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



X Y Z

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.

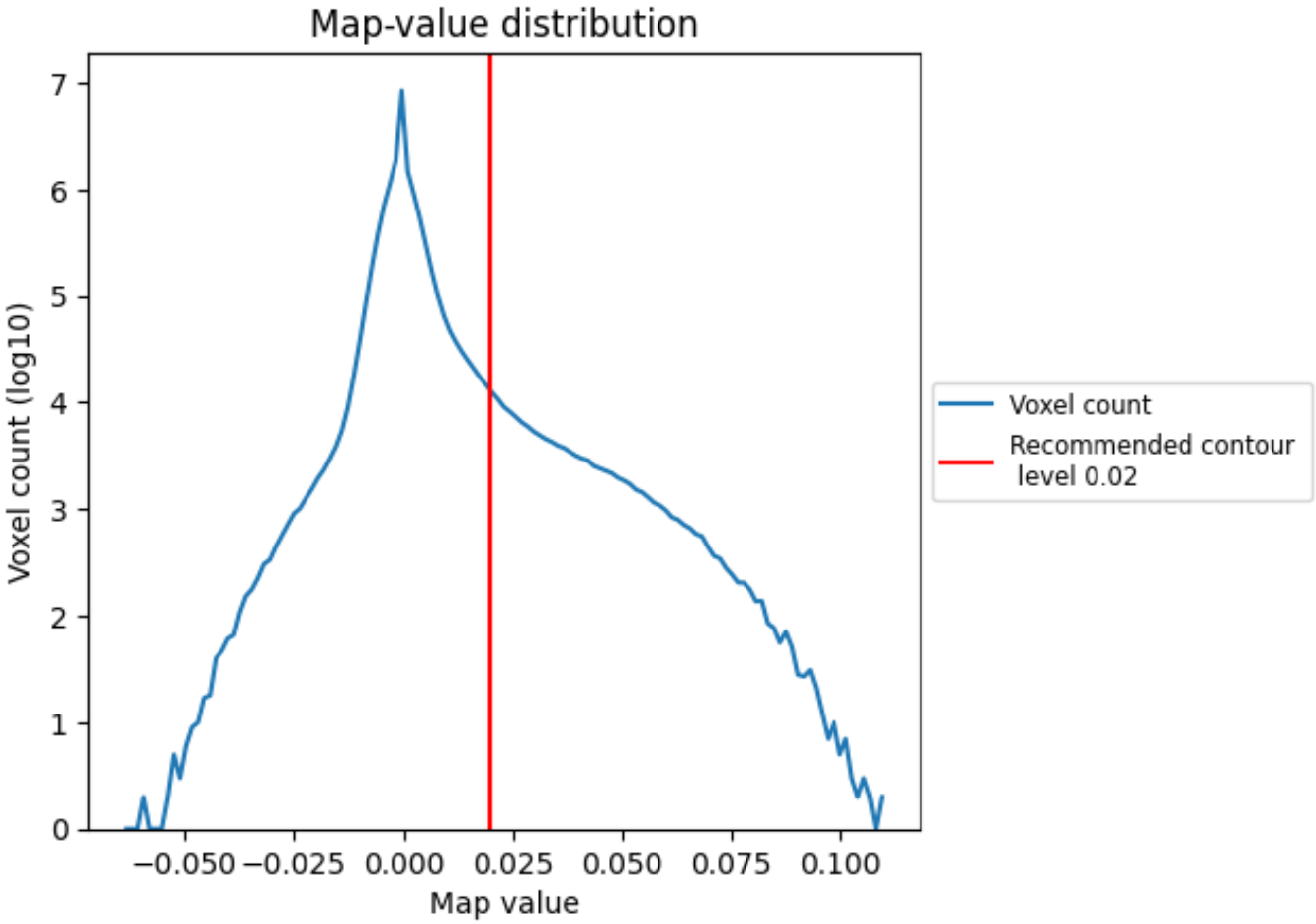
6.6 Mask visualisation (i)

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

7 Map analysis

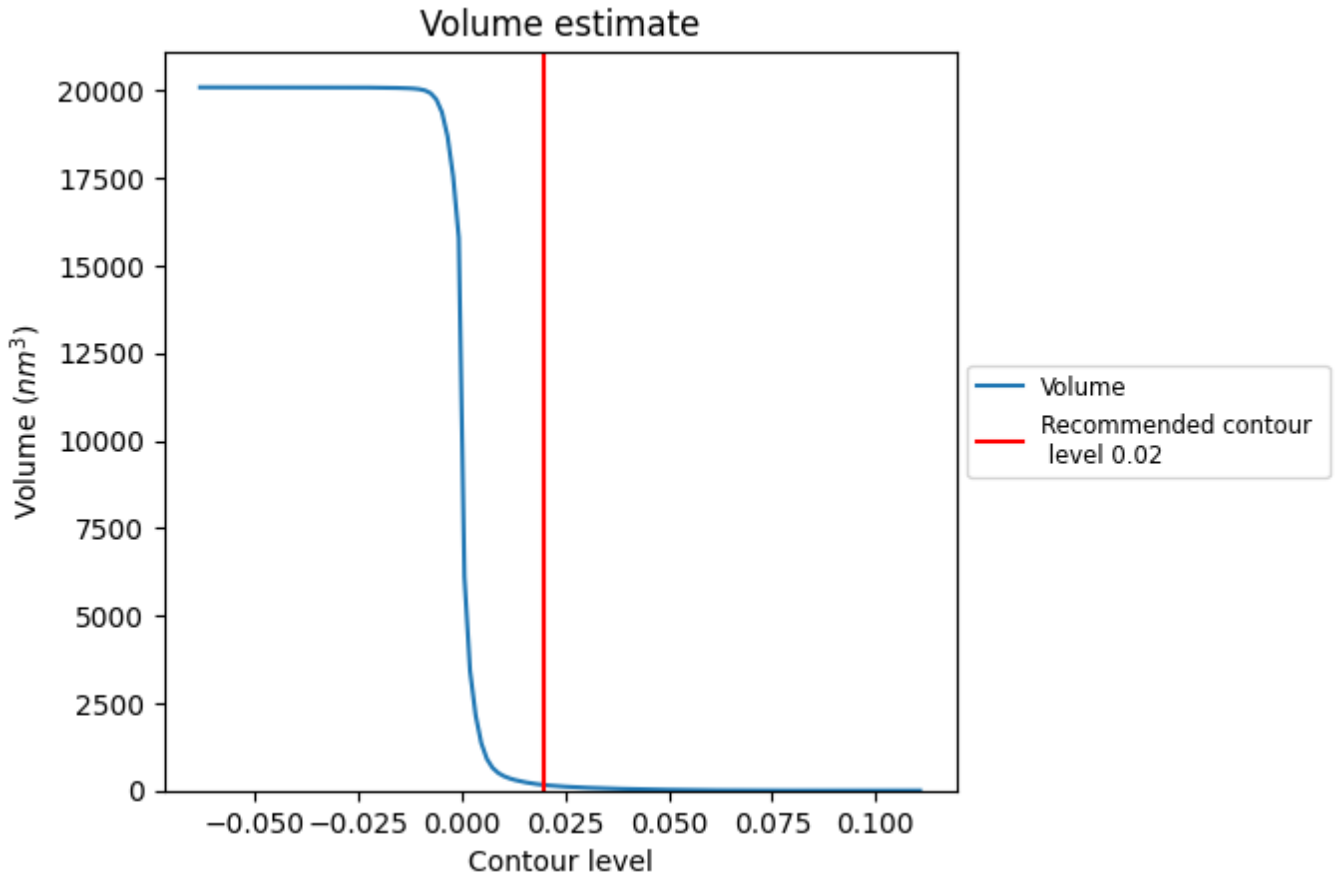
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

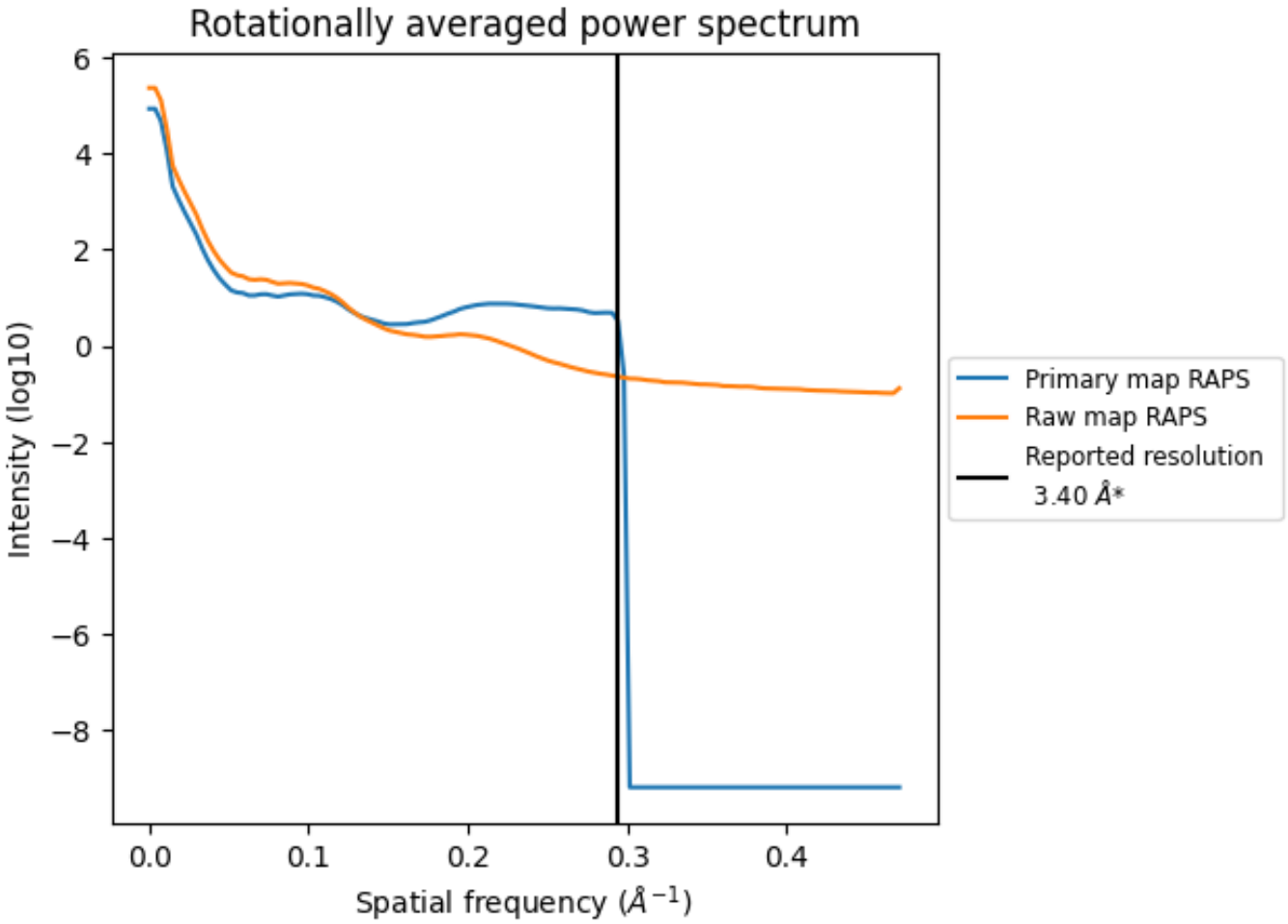
7.2 Volume estimate



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 143 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

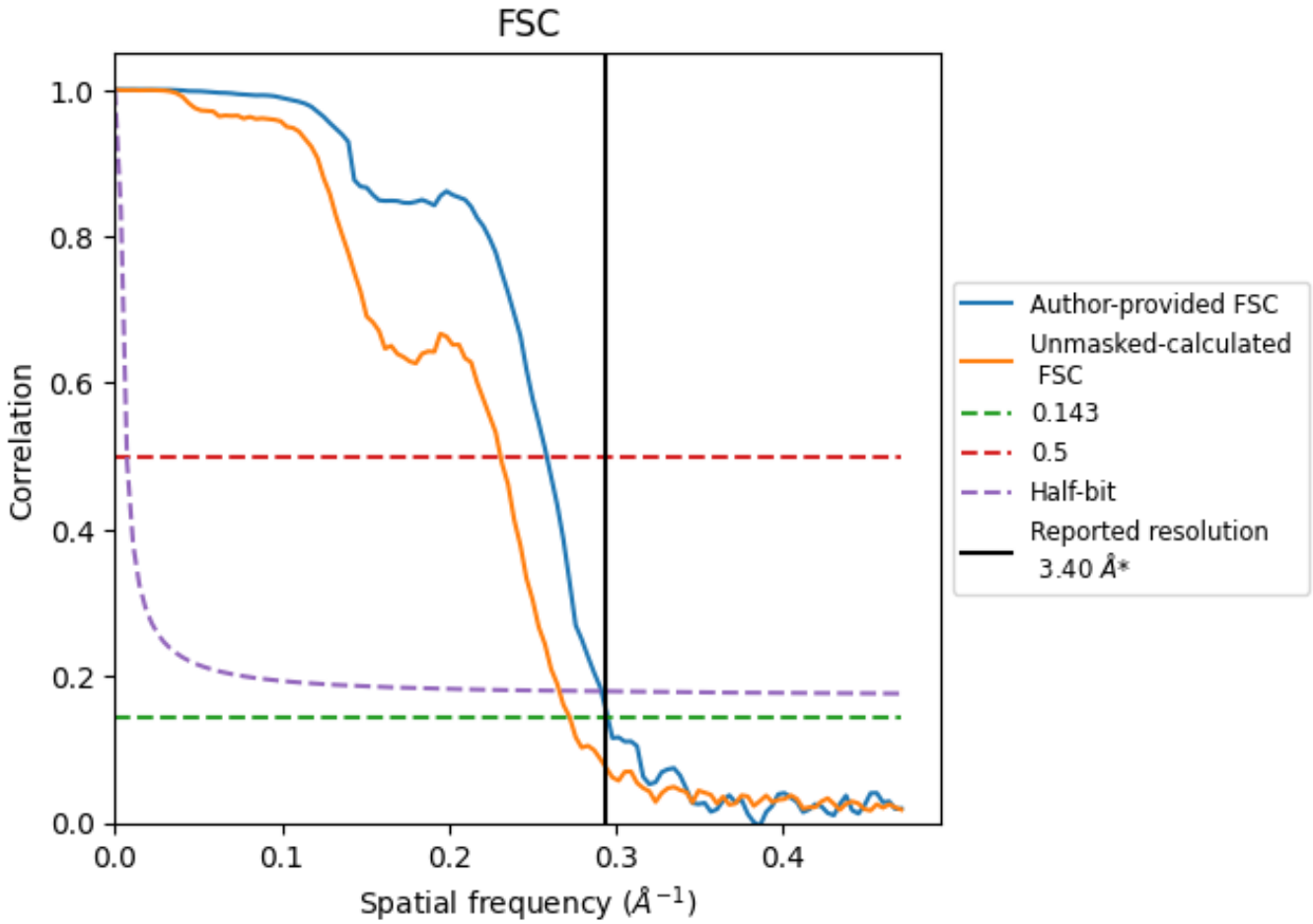


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

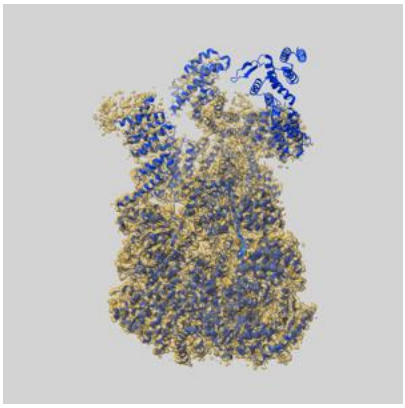
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.87	3.43
Unmasked-calculated*	3.67	4.33	3.76

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

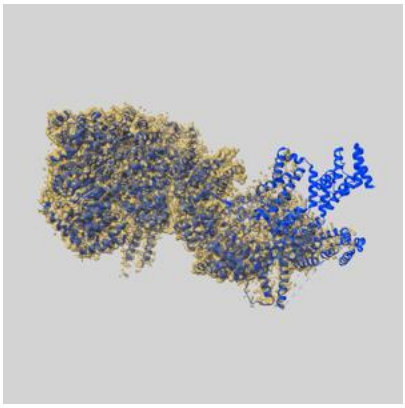
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29314 and PDB model 8FNI. Per-residue inclusion information can be found in section 3 on page 8.

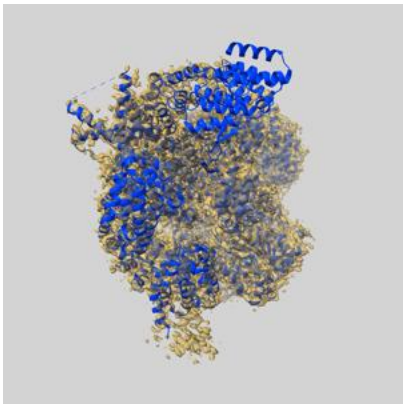
9.1 Map-model overlay



X



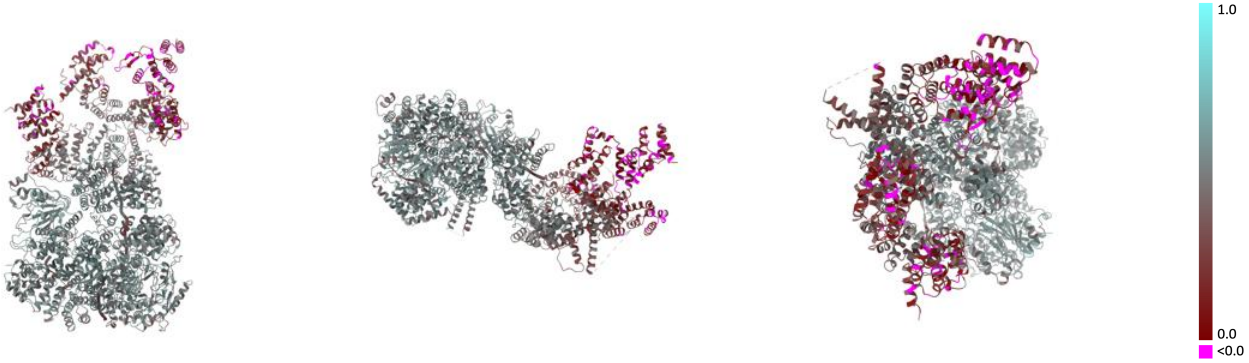
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

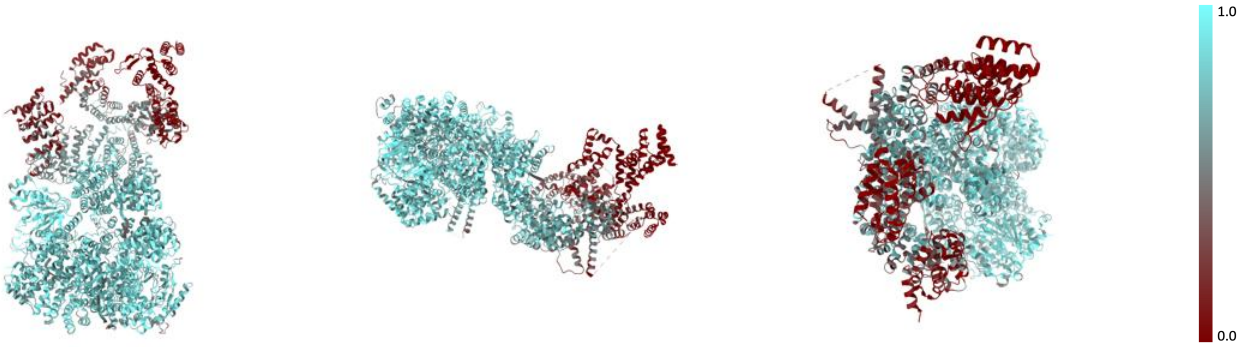
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

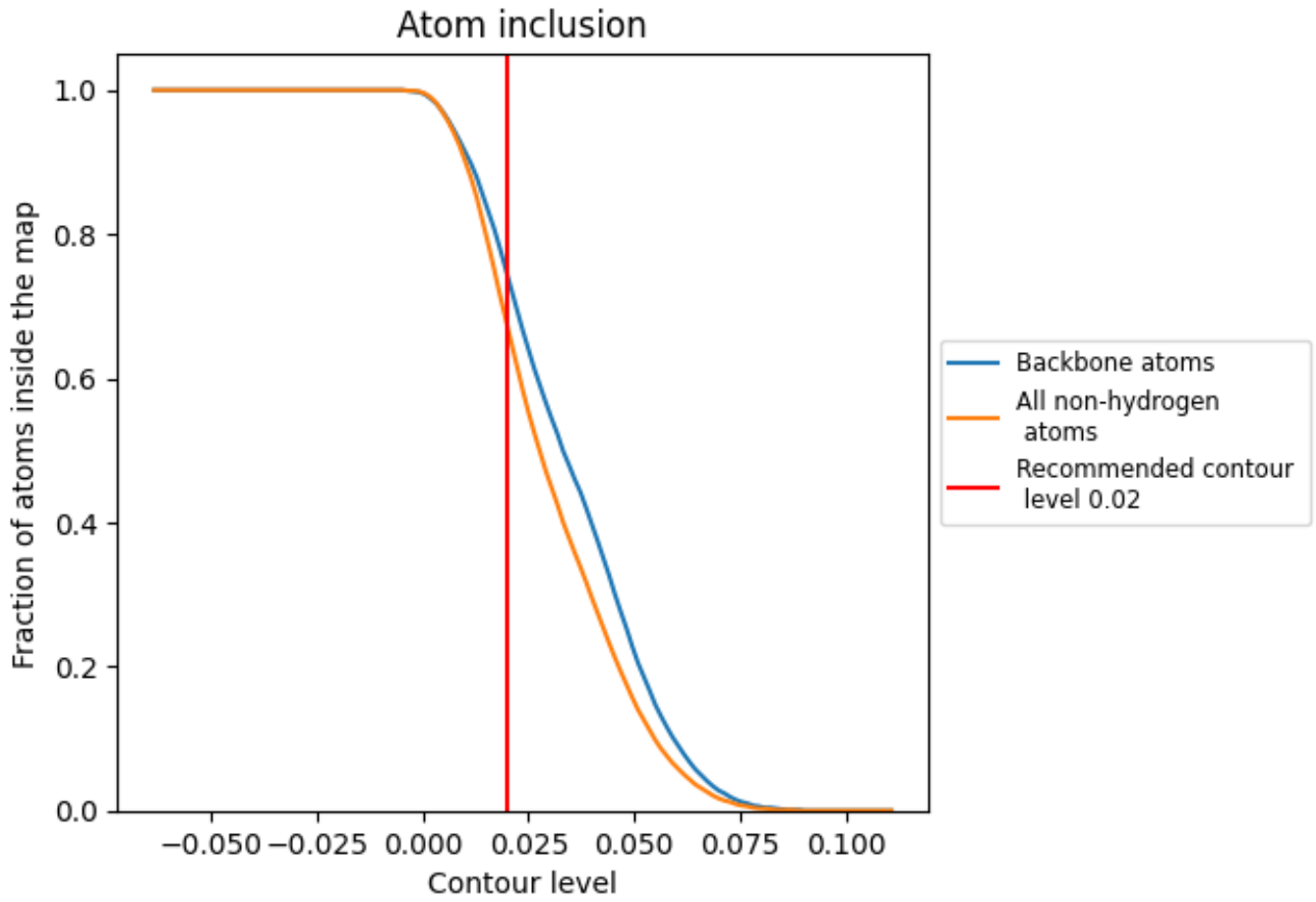
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 67% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6730	0.4430
10	0.8280	0.5200
11	0.2190	0.2150
13	0.8060	0.5190
14	0.8600	0.5410
5	0.8400	0.5350
6	0.8320	0.5250
7	0.7850	0.4860
8	0.8380	0.5240
9	0.6010	0.4080
g	0.6160	0.3790
m	0.7240	0.4440