



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 9G8N / pdb_00009g8n
EMDB ID : EMD-51133
Title : 80S-bound human Ski2-exosome complex
Authors : Koegel, A.; Keidel, A.; Loukeri, M.J.; Kuhn, C.C.; Langer, L.M.; Schaefer, I.B.; Conti, E.
Deposited on : 2024-07-23
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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

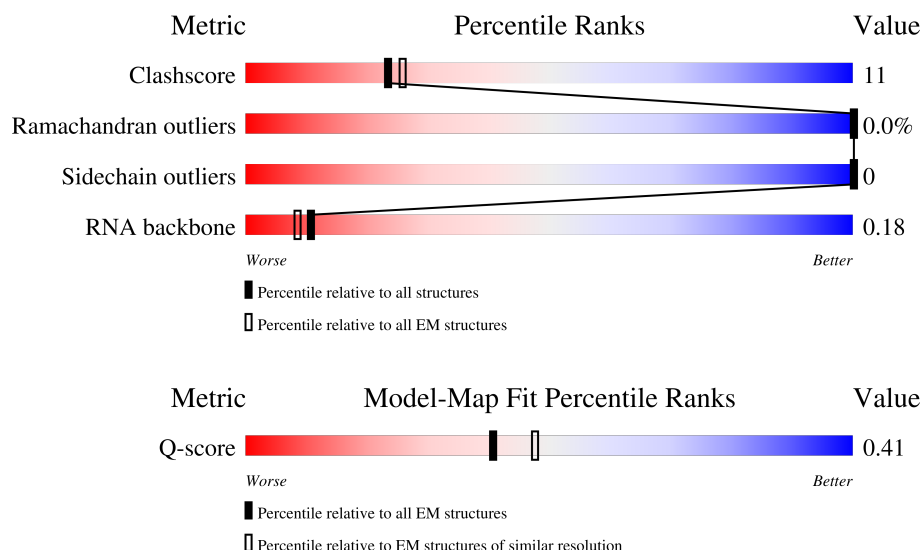
1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	L	245	
2	N	280	
3	O	239	

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Mol	Chain	Length	Quality of chain
4	F	295	
5	H	279	
6	J	199	
7	X	44	
8	A	1246	
9	G	272	
10	I	297	
11	E	274	
12	K	443	
13	M	1056	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34405 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Exosome complex component RRP41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	241	Total	C	N	O	S	0	0
			1819	1123	343	344	9		

- Molecule 2 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	265	Total	C	N	O	S	0	0
			2020	1272	337	397	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	GLY	-	expression tag	UNP Q96B26
N	-2	PRO	-	expression tag	UNP Q96B26
N	-1	ASP	-	expression tag	UNP Q96B26
N	0	SER	-	expression tag	UNP Q96B26

- Molecule 3 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	208	Total	C	N	O	S	0	0
			1566	979	278	297	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-3	GLY	-	expression tag	UNP Q9NQT4
O	-2	PRO	-	expression tag	UNP Q9NQT4
O	-1	ASP	-	expression tag	UNP Q9NQT4
O	0	SER	-	expression tag	UNP Q9NQT4

- Molecule 4 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	286	Total	C	N	O	S	0	0
			2194	1373	374	432	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP Q15024
F	-2	PRO	-	expression tag	UNP Q15024
F	-1	ASP	-	expression tag	UNP Q15024
F	0	SER	-	expression tag	UNP Q15024

- Molecule 5 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	237	Total	C	N	O	S	0	0
			1806	1136	329	329	12		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP Q9NQT5
H	-2	PRO	-	expression tag	UNP Q9NQT5
H	-1	ASP	-	expression tag	UNP Q9NQT5
H	0	SER	-	expression tag	UNP Q9NQT5
H	225	HIS	TYR	variant	UNP Q9NQT5

- Molecule 6 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	184	Total	C	N	O	S	0	0
			1414	889	248	267	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP Q9Y3B2
J	-2	PRO	-	expression tag	UNP Q9Y3B2
J	-1	ASP	-	expression tag	UNP Q9Y3B2
J	0	SER	-	expression tag	UNP Q9Y3B2

- Molecule 7 is a RNA chain called CrPV-IRES RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	44	Total	C	N	O	P	0	0
			841	376	82	339	44		

- Molecule 8 is a protein called Helicase SKI2W.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	949	Total	C	N	O	S	0	0
			7438	4710	1316	1370	42		

- Molecule 9 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	251	Total	C	N	O	S	0	0
			1852	1149	352	344	7		

- Molecule 10 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	289	Total	C	N	O	S	0	0
			2263	1424	405	419	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	GLY	-	expression tag	UNP Q13868
I	-2	PRO	-	expression tag	UNP Q13868
I	-1	ASP	-	expression tag	UNP Q13868
I	0	SER	-	expression tag	UNP Q13868

- Molecule 11 is a protein called Isoform 2 of HBS1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	66	Total	C	N	O	S	0	0
			525	340	89	95	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	365	GLY	-	expression tag	UNP Q9Y450
E	366	PRO	-	expression tag	UNP Q9Y450
E	367	ASP	-	expression tag	UNP Q9Y450
E	368	SER	-	expression tag	UNP Q9Y450

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Chain	Residue	Modelled	Actual	Comment	Reference
E	633	LEU	-	expression tag	UNP Q9Y450
E	634	GLU	-	expression tag	UNP Q9Y450
E	635	VAL	-	expression tag	UNP Q9Y450
E	636	LEU	-	expression tag	UNP Q9Y450
E	637	PHE	-	expression tag	UNP Q9Y450
E	638	GLN	-	expression tag	UNP Q9Y450

- Molecule 12 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	353	Total	C	N	O	S	0	0
			2764	1734	482	529	19		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	GLY	-	expression tag	UNP Q06265
K	-2	PRO	-	expression tag	UNP Q06265
K	-1	ASP	-	expression tag	UNP Q06265
K	0	SER	-	expression tag	UNP Q06265

- Molecule 13 is a protein called DIS3-like exonuclease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	975	Total	C	N	O	S	0	0
			7903	4986	1405	1471	41		

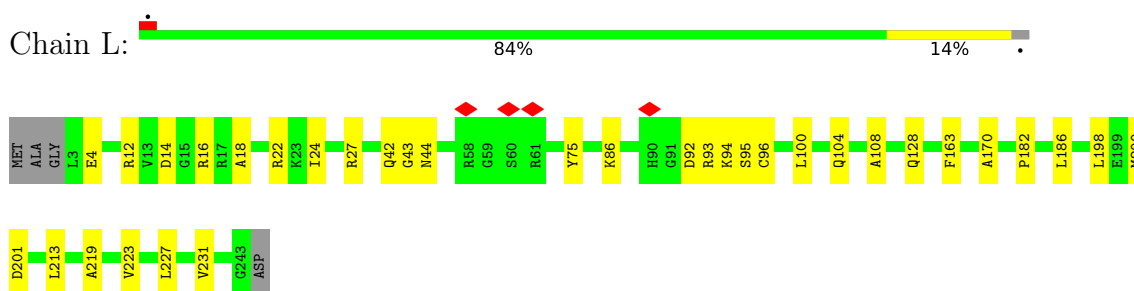
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	GLY	-	expression tag	UNP Q8TF46
M	0	PRO	-	expression tag	UNP Q8TF46
M	486	ASN	ASP	conflict	UNP Q8TF46

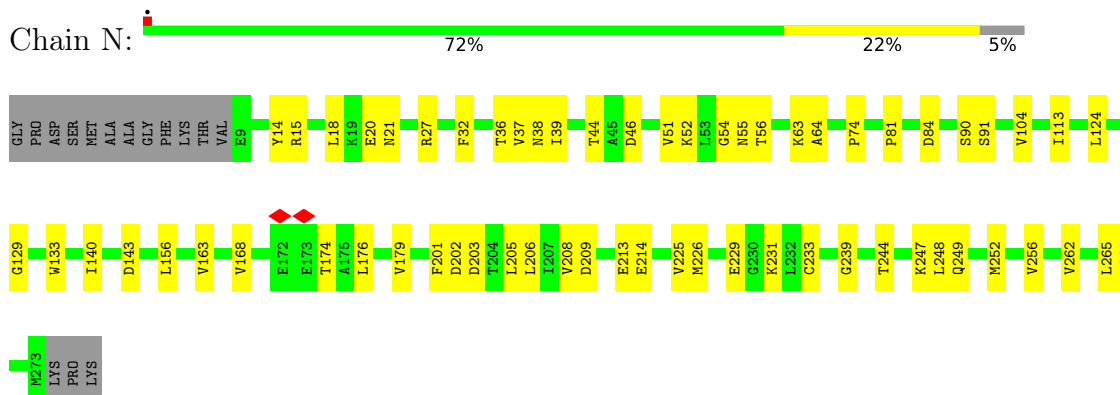
3 Residue-property plots [i](#)

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.

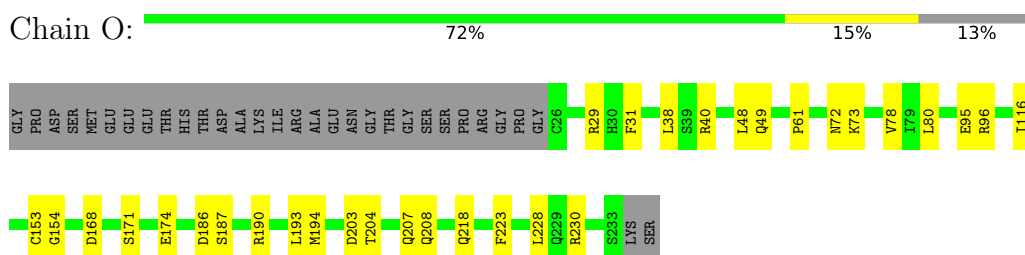
- Molecule 1: Exosome complex component RRP41



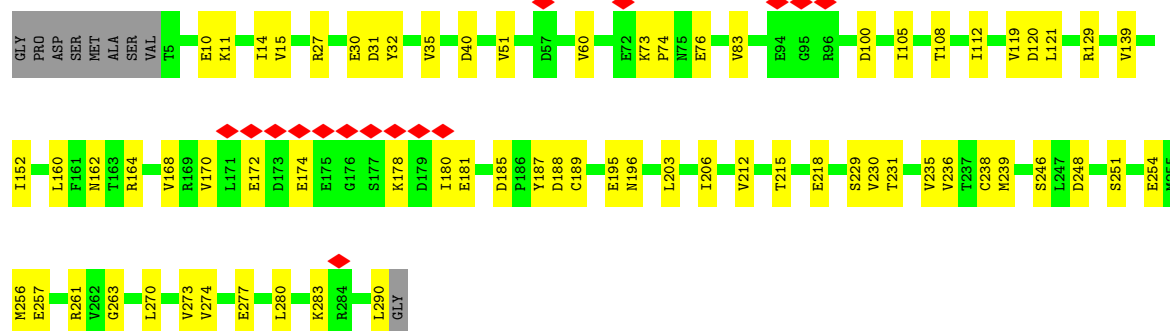
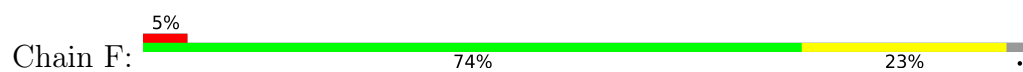
- Molecule 2: Exosome complex component RRP43



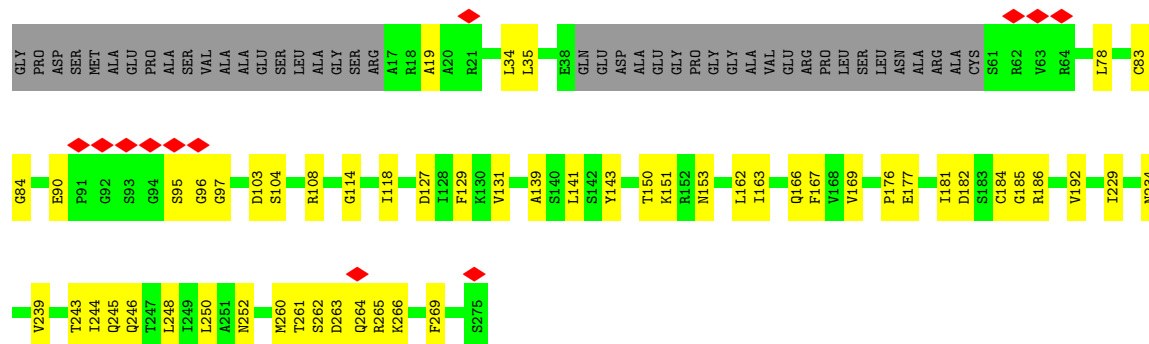
- Molecule 3: Exosome complex component RRP46



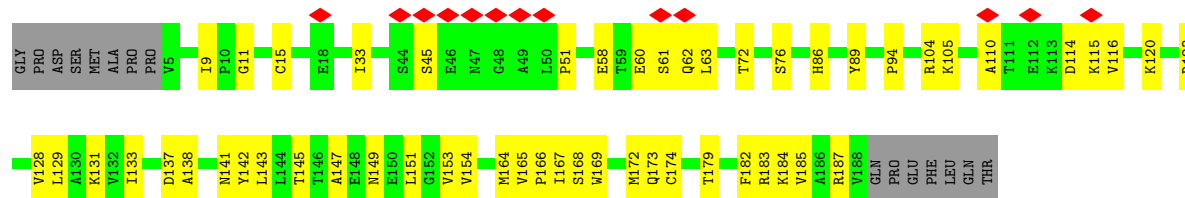
- Molecule 4: Exosome complex component RRP42



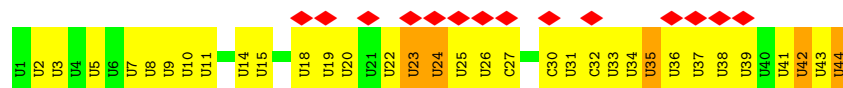
• Molecule 5: Exosome complex component RRP40



• Molecule 6: Exosome complex component CSL4



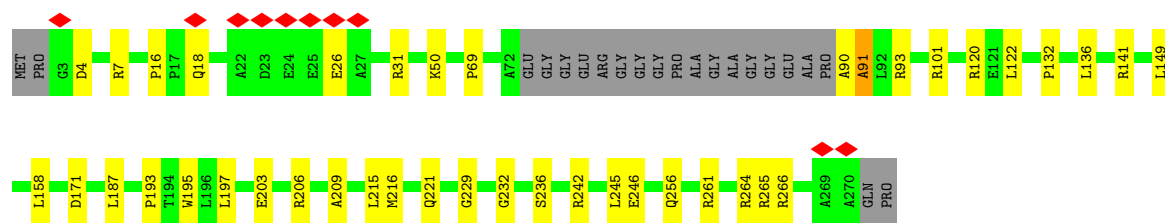
• Molecule 7: CrPV-IRES RNA



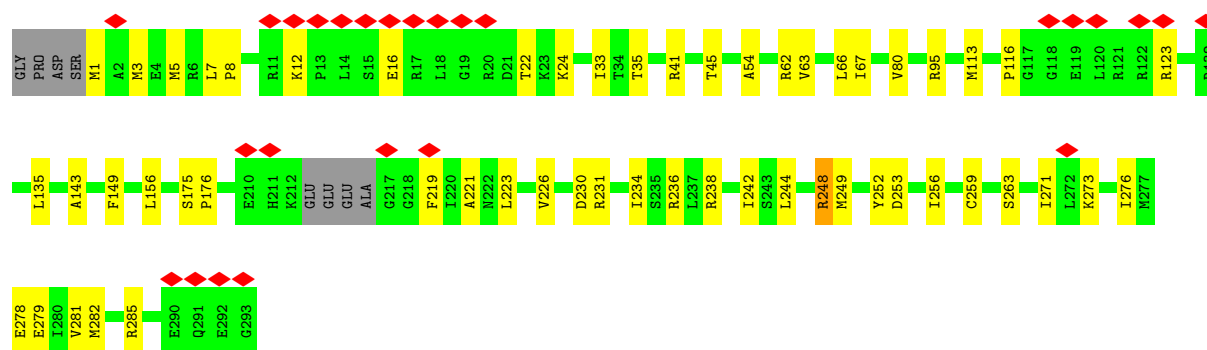
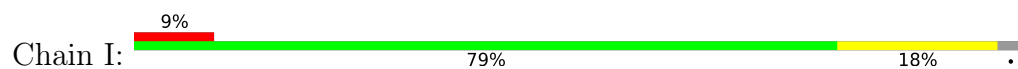
• Molecule 8: Helicase SKI2W



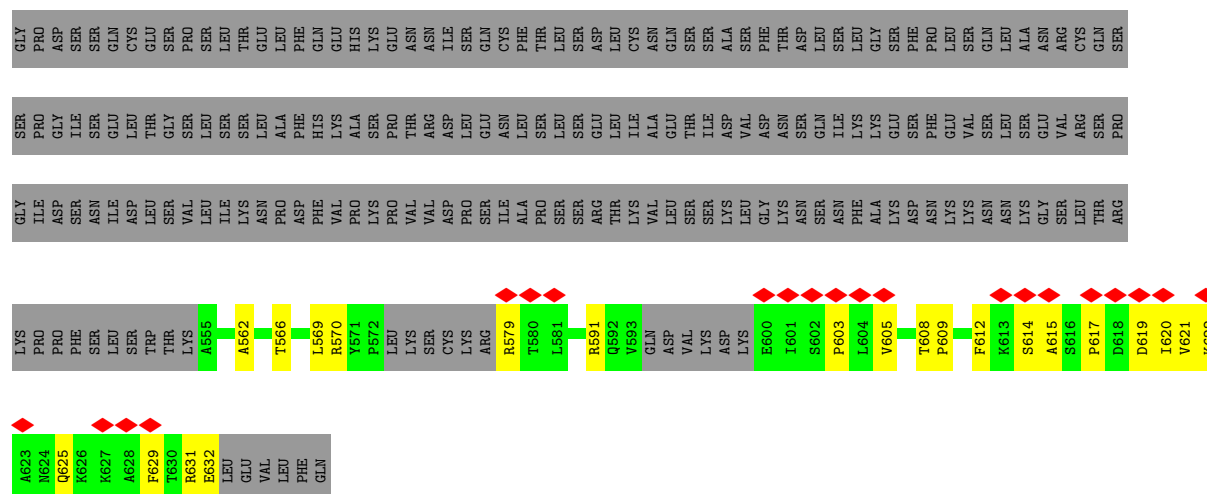




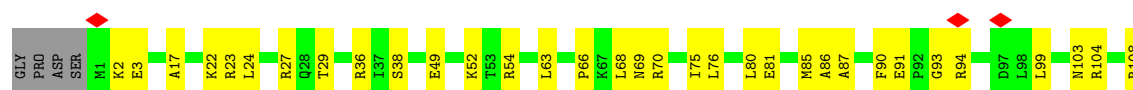
• Molecule 10: Exosome complex component RRP4

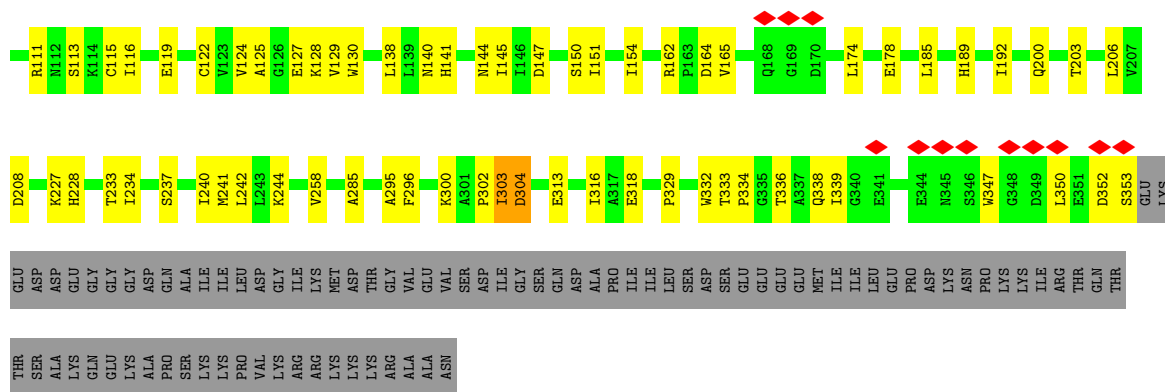


• Molecule 11: Isoform 2 of HBS1-like protein

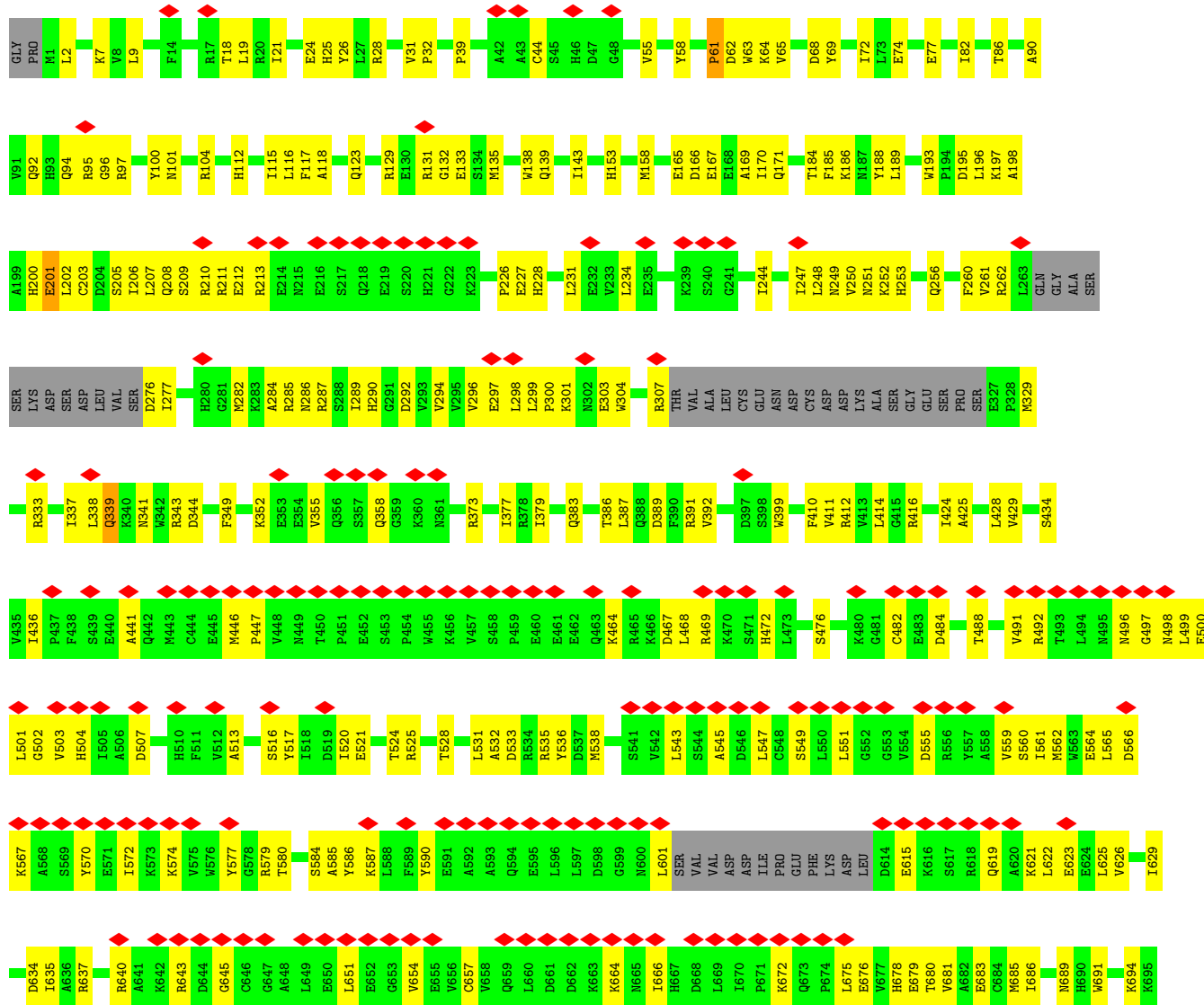


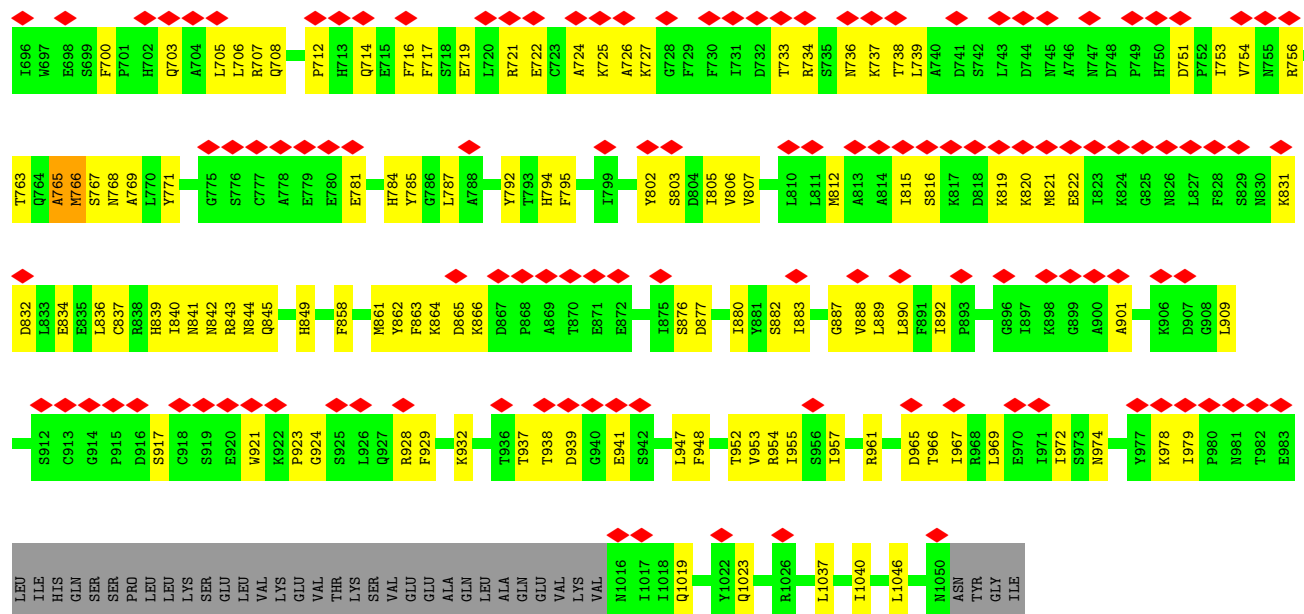
• Molecule 12: Exosome complex component RRP45





• Molecule 13: DIS3-like exonuclease 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79353	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 ($e^-/\text{\AA}^2$)	64.2	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	708.19836, 708.19836, 708.19836	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512, 0.8512, 0.8512	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	L	0.12	0/1843	0.35	0/2492
2	N	0.11	0/2053	0.33	0/2786
3	O	0.13	0/1586	0.36	0/2145
4	F	0.13	0/2225	0.41	0/3007
5	H	0.12	0/1832	0.43	0/2467
6	J	0.13	0/1438	0.48	0/1942
7	X	0.12	0/923	0.36	0/1424
8	A	0.13	0/7577	0.40	0/10257
9	G	0.13	0/1881	0.38	0/2551
10	I	0.13	0/2296	0.50	2/3092 (0.1%)
11	E	0.20	0/535	0.83	0/722
12	K	0.15	0/2807	0.57	4/3792 (0.1%)
13	M	0.15	0/8072	0.58	5/10916 (0.0%)
All	All	0.13	0/35068	0.47	11/47593 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	G	0	1
10	I	0	1
11	E	0	1
12	K	0	1
13	M	0	4
All	All	0	8

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	63	VAL	CA-C-N	10.39	141.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	63	VAL	C-N-CA	10.39	141.38	121.54
13	M	61	PRO	CA-C-N	-7.17	110.13	120.89
13	M	61	PRO	C-N-CA	-7.17	110.13	120.89
12	K	304	ASP	CA-C-N	-5.71	111.71	122.27
12	K	304	ASP	C-N-CA	-5.71	111.71	122.27
12	K	302	PRO	CA-C-N	-5.56	111.96	121.97
12	K	302	PRO	C-N-CA	-5.56	111.96	121.97
13	M	766	MET	CA-C-N	5.55	131.88	122.12
13	M	766	MET	C-N-CA	5.55	131.88	122.12
13	M	201	GLU	N-CA-CB	5.12	117.74	110.16

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	E	614	SER	Peptide
9	G	91	ALA	Peptide
10	I	248	ARG	Peptide
12	K	303	ILE	Peptide
13	M	339	GLN	Peptide
13	M	532	ALA	Peptide
13	M	545	ALA	Peptide
13	M	765	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1819	0	1818	30	0
2	N	2020	0	2035	40	0
3	O	1566	0	1605	26	0
4	F	2194	0	2205	51	0
5	H	1806	0	1865	45	0
6	J	1414	0	1441	46	0
7	X	841	0	425	13	0
8	A	7438	0	7568	150	0
9	G	1852	0	1881	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	2263	0	2337	37	0
11	E	525	0	536	27	0
12	K	2764	0	2790	77	0
13	M	7903	0	7833	266	0
All	All	34405	0	34339	754	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 (754) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:164:MET:HE3	6:J:165:VAL:H	1.31	0.95
11:E:615:ALA:HB1	11:E:620:ILE:HD11	1.48	0.93
3:O:119:VAL:HG21	12:K:85:MET:HB3	1.57	0.86
8:A:621:VAL:HG23	8:A:643:LEU:HD11	1.57	0.85
8:A:1034:GLN:HA	8:A:1037:MET:SD	2.21	0.81
12:K:332:TRP:HB3	12:K:347:TRP:HE1	1.46	0.81
3:O:49:GLN:NE2	3:O:168:ASP:OD1	2.14	0.80
6:J:72:THR:HB	6:J:89:TYR:HB2	1.64	0.79
13:M:248:LEU:HD11	13:M:294:VAL:HG22	1.63	0.78
13:M:784:HIS:HD2	13:M:787:LEU:HB2	1.48	0.78
8:A:347:ALA:HA	11:E:631:ARG:HH11	1.48	0.78
1:L:93:ARG:HB2	12:K:104:ARG:HH22	1.48	0.77
3:O:230:ARG:NH1	12:K:295:ALA:O	2.18	0.76
13:M:260:PHE:HE2	13:M:307:ARG:HH21	1.34	0.75
13:M:864:LYS:HG2	13:M:866:LYS:HZ2	1.49	0.75
9:G:91:ALA:HA	9:G:93:ARG:H	1.52	0.75
8:A:1017:SER:HB2	8:A:1018:PRO:HD2	1.68	0.75
13:M:251:ASN:OD1	13:M:252:LYS:N	2.18	0.75
13:M:64:LYS:HD2	13:M:165:GLU:HB3	1.69	0.74
13:M:700:PHE:HD1	13:M:703:GLN:HE21	1.33	0.74
8:A:444:LEU:HD12	8:A:445:PRO:HD2	1.70	0.73
13:M:68:ASP:OD2	13:M:210:ARG:NH2	2.21	0.73
8:A:473:ARG:HH11	8:A:474:GLN:H	1.36	0.73
3:O:29:ARG:HA	12:K:300:LYS:HG2	1.70	0.73
6:J:164:MET:HG3	6:J:172:MET:HE2	1.68	0.73
13:M:61:PRO:HB3	13:M:65:VAL:HB	1.71	0.72
13:M:727:LYS:HG2	13:M:947:LEU:HD23	1.70	0.72
13:M:953:VAL:HG11	13:M:969:LEU:HB3	1.70	0.72
13:M:816:SER:O	13:M:819:LYS:NZ	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:201:PHE:HB2	2:N:205:LEU:HB3	1.73	0.71
10:I:143:ALA:HB3	10:I:156:LEU:HD12	1.73	0.71
4:F:239:MET:HE1	4:F:256:MET:HE2	1.72	0.71
8:A:494:GLY:O	8:A:525:LYS:NZ	2.22	0.70
13:M:784:HIS:CD2	13:M:787:LEU:HB2	2.26	0.70
2:N:36:THR:HB	12:K:338:GLN:HG3	1.72	0.70
5:H:269:PHE:HZ	13:M:1040:ILE:HG23	1.57	0.70
8:A:350:GLN:HG2	11:E:631:ARG:NH1	2.06	0.70
6:J:62:GLN:HB2	9:G:50:LYS:HE2	1.72	0.70
9:G:31:ARG:NH2	9:G:197:LEU:O	2.25	0.70
13:M:488:THR:OG1	13:M:504:HIS:O	2.09	0.69
13:M:657:CYS:HB3	13:M:672:LYS:HE2	1.75	0.69
8:A:624:MET:HE2	8:A:643:LEU:HD12	1.74	0.69
13:M:637:ARG:HE	13:M:640:ARG:HH21	1.41	0.69
8:A:347:ALA:HA	11:E:631:ARG:NH1	2.07	0.68
8:A:1069:ASP:OD1	8:A:1070:GLU:N	2.25	0.68
13:M:2:LEU:HD23	13:M:26:TYR:HB3	1.75	0.68
8:A:404:ARG:HD2	8:A:436:VAL:HG13	1.75	0.68
13:M:864:LYS:HZ3	13:M:866:LYS:HD3	1.59	0.68
13:M:500:GLU:HA	13:M:564:GLU:HA	1.75	0.68
6:J:164:MET:HE1	6:J:173:GLN:O	1.93	0.68
1:L:213:LEU:HB3	12:K:244:LYS:HZ3	1.59	0.68
13:M:86:THR:HG22	13:M:139:GLN:HE22	1.58	0.67
8:A:852:HIS:HE1	8:A:877:CYS:HB3	1.59	0.67
9:G:215:LEU:HD22	9:G:245:LEU:HG	1.77	0.67
13:M:339:GLN:NE2	13:M:341:ASN:OD1	2.24	0.67
2:N:84:ASP:HB3	2:N:140:ILE:HD13	1.76	0.67
13:M:428:LEU:HD11	13:M:536:TYR:HE2	1.58	0.67
13:M:947:LEU:HG	13:M:948:PHE:HD1	1.60	0.67
5:H:265:ARG:NH2	13:M:1046:LEU:HB3	2.10	0.66
6:J:138:ALA:HA	9:G:141:ARG:HH22	1.61	0.66
8:A:800:ASP:OD2	8:A:1019:ARG:NH2	2.29	0.66
8:A:459:ASN:HD21	8:A:740:LEU:H	1.44	0.66
2:N:20:GLU:OE2	11:E:579:ARG:NH2	2.29	0.65
4:F:195:GLU:OE2	4:F:196:ASN:ND2	2.29	0.65
3:O:186:ASP:OD1	3:O:187:SER:N	2.27	0.65
8:A:641:PRO:HA	8:A:644:LYS:HB2	1.78	0.65
2:N:168:VAL:HG12	2:N:179:VAL:HG12	1.77	0.65
13:M:565:LEU:HA	13:M:572:ILE:HA	1.78	0.65
9:G:261:ARG:NH1	12:K:352:ASP:OD1	2.30	0.65
13:M:909:LEU:HB3	13:M:921:TRP:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:12:ARG:NH2	1:L:18:ALA:O	2.31	0.64
13:M:208:GLN:HA	13:M:211:ARG:HE	1.62	0.64
13:M:531:LEU:HD12	13:M:533:ASP:H	1.62	0.64
13:M:845:GLN:O	13:M:849:HIS:ND1	2.26	0.64
4:F:35:VAL:HG12	10:I:5:MET:HG2	1.78	0.64
4:F:74:PRO:HB3	4:F:129:ARG:HG3	1.79	0.64
13:M:294:VAL:HG12	13:M:337:ILE:HG12	1.77	0.64
5:H:153:ASN:ND2	8:A:1236:ASP:OD1	2.30	0.64
8:A:1215:ARG:NH1	10:I:149:PHE:O	2.31	0.63
12:K:113:SER:HB3	12:K:189:HIS:HE1	1.63	0.63
8:A:627:LEU:HD12	8:A:632:LEU:HD12	1.81	0.63
8:A:1128:PRO:HD2	8:A:1131:LEU:HD12	1.79	0.63
10:I:113:MET:HE2	10:I:135:LEU:HD11	1.80	0.63
7:X:7:U:N3	8:A:406:MET:HE1	2.13	0.63
13:M:705:LEU:HD12	13:M:806:VAL:HG11	1.79	0.63
13:M:751:ASP:OD2	13:M:753:ILE:HG22	1.98	0.63
12:K:227:LYS:HG3	12:K:228:HIS:H	1.63	0.62
4:F:251:SER:HA	4:F:254:GLU:HG2	1.81	0.62
13:M:193:TRP:HE3	13:M:196:LEU:HD22	1.63	0.62
13:M:954:ARG:HG3	13:M:955:ILE:H	1.64	0.62
4:F:230:VAL:HG11	4:F:263:GLY:HA3	1.81	0.62
12:K:76:LEU:HD21	12:K:116:ILE:HD13	1.80	0.62
11:E:608:THR:HB	11:E:609:PRO:HD3	1.80	0.62
13:M:763:THR:HA	13:M:766:MET:HE1	1.81	0.62
13:M:74:GLU:O	13:M:112:HIS:NE2	2.32	0.62
13:M:77:GLU:OE1	13:M:77:GLU:N	2.33	0.62
13:M:209:SER:O	13:M:213:ARG:HG2	2.00	0.62
8:A:1099:ALA:HA	8:A:1137:ARG:HH21	1.64	0.62
12:K:164:ASP:OD1	12:K:165:VAL:N	2.33	0.62
3:O:61:PRO:HD2	5:H:108:ARG:HG2	1.81	0.61
13:M:261:VAL:HB	13:M:277:ILE:HB	1.82	0.61
2:N:21:ASN:O	2:N:21:ASN:ND2	2.33	0.61
6:J:164:MET:HE2	6:J:172:MET:HB3	1.82	0.61
13:M:62:ASP:OD1	13:M:63:TRP:N	2.27	0.61
13:M:643:ARG:NH1	13:M:787:LEU:O	2.32	0.61
13:M:284:ALA:HA	13:M:333:ARG:HH12	1.64	0.61
3:O:38:LEU:HD22	12:K:140:ASN:HB2	1.81	0.61
5:H:248:LEU:HD22	12:K:24:LEU:HA	1.83	0.61
8:A:618:LEU:HD23	8:A:620:GLN:H	1.65	0.61
9:G:31:ARG:NH1	9:G:203:GLU:OE1	2.34	0.61
8:A:1069:ASP:HB3	8:A:1075:LYS:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:69:ASN:OD1	12:K:70:ARG:N	2.33	0.60
5:H:129:PHE:HB2	5:H:141:LEU:HB2	1.83	0.60
13:M:615:GLU:O	13:M:619:GLN:NE2	2.34	0.60
4:F:174:GLU:HG3	4:F:178:LYS:HZ1	1.66	0.60
11:E:619:ASP:HA	11:E:622:LYS:HZ3	1.66	0.60
12:K:144:ASN:ND2	12:K:208:ASP:OD1	2.33	0.60
13:M:343:ARG:HG2	13:M:344:ASP:H	1.66	0.60
8:A:748:TYR:OH	8:A:1149:GLN:OE1	2.20	0.60
13:M:700:PHE:HD1	13:M:703:GLN:NE2	2.00	0.60
7:X:23:U:H4'	7:X:24:U:OP2	1.99	0.60
8:A:1146:GLY:HA3	8:A:1158:VAL:HG23	1.82	0.60
8:A:426:HIS:NE2	8:A:667:MET:HE1	2.17	0.59
5:H:163:ILE:HG12	5:H:192:VAL:HG22	1.84	0.59
8:A:870:VAL:HG13	8:A:919:LYS:HG3	1.84	0.59
7:X:27:C:H42	13:M:96:GLY:HA2	1.67	0.59
4:F:235:VAL:HB	9:G:232:GLY:HA3	1.83	0.59
12:K:29:THR:HG23	12:K:206:LEU:HD23	1.83	0.59
13:M:208:GLN:O	13:M:211:ARG:HG2	2.03	0.59
13:M:244:ILE:HD11	13:M:277:ILE:HD11	1.85	0.59
10:I:236:ARG:NH1	10:I:263:SER:OG	2.36	0.59
13:M:685:MET:O	13:M:689:ASN:ND2	2.36	0.59
13:M:691:TRP:HA	13:M:694:LYS:HD3	1.85	0.59
2:N:27:ARG:HH12	2:N:209:ASP:HB3	1.66	0.59
13:M:469:ARG:NE	13:M:555:ASP:OD1	2.36	0.58
8:A:457:VAL:HG23	8:A:460:ALA:HB2	1.85	0.58
8:A:1038:GLU:HA	8:A:1041:ARG:HG2	1.84	0.58
8:A:328:VAL:HB	8:A:451:ILE:HG23	1.84	0.58
13:M:352:LYS:HA	13:M:355:VAL:HG12	1.84	0.58
5:H:261:THR:HG23	5:H:264:GLN:HE22	1.67	0.58
9:G:16:PRO:HB2	9:G:18:GLN:OE1	2.04	0.58
12:K:52:LYS:O	12:K:140:ASN:ND2	2.35	0.58
8:A:567:LEU:HD21	8:A:591:LEU:HD22	1.85	0.58
13:M:446:MET:HE3	13:M:447:PRO:HD2	1.86	0.58
13:M:467:ASP:OD1	13:M:468:LEU:N	2.36	0.58
13:M:231:LEU:HD13	13:M:234:LEU:HD12	1.86	0.58
8:A:1119:SER:O	8:A:1166:ASN:ND2	2.36	0.57
3:O:40:ARG:HH21	12:K:87:ALA:HB1	1.69	0.57
12:K:76:LEU:O	12:K:111:ARG:NH2	2.37	0.57
2:N:262:VAL:HG12	2:N:266:MET:HE2	1.85	0.57
13:M:864:LYS:HG2	13:M:866:LYS:NZ	2.19	0.57
9:G:265:ARG:HB3	11:E:570:ARG:HH22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:22:THR:HG22	10:I:24:LYS:H	1.70	0.57
5:H:260:MET:O	5:H:260:MET:HG2	2.03	0.57
13:M:957:ILE:HG22	13:M:967:ILE:HG22	1.86	0.57
1:L:14:ASP:OD2	1:L:16:ARG:NH1	2.37	0.57
4:F:119:VAL:HG23	4:F:120:ASP:H	1.70	0.57
13:M:721:ARG:O	13:M:725:LYS:N	2.36	0.57
1:L:94:LYS:HE3	12:K:104:ARG:HH21	1.70	0.57
13:M:625:LEU:O	13:M:629:ILE:HG13	2.05	0.57
4:F:229:SER:HB3	4:F:238:CYS:H	1.70	0.57
8:A:800:ASP:O	8:A:801:MET:HE2	2.05	0.57
13:M:227:GLU:N	13:M:227:GLU:OE1	2.37	0.57
4:F:274:VAL:O	4:F:277:GLU:HG2	2.05	0.56
13:M:771:TYR:HB2	13:M:837:CYS:HB2	1.87	0.56
1:L:219:ALA:O	1:L:223:VAL:HG23	2.05	0.56
7:X:7:U:C2	8:A:406:MET:HE1	2.39	0.56
2:N:52:LYS:HE2	11:E:569:LEU:HB2	1.87	0.56
2:N:226:MET:HE1	2:N:256:VAL:HA	1.87	0.56
5:H:229:ILE:HD12	5:H:239:VAL:HG12	1.87	0.56
8:A:610:ARG:NH1	8:A:1243:LEU:O	2.38	0.56
8:A:706:ARG:HG3	8:A:709:LEU:HD13	1.87	0.56
13:M:491:VAL:HG22	13:M:501:LEU:HA	1.87	0.56
13:M:883:ILE:HA	13:M:888:VAL:HG12	1.86	0.56
6:J:164:MET:HE1	6:J:173:GLN:C	2.31	0.56
2:N:38:ASN:OD1	2:N:39:ILE:N	2.39	0.56
6:J:164:MET:HG3	6:J:172:MET:CE	2.36	0.56
13:M:812:MET:HA	13:M:815:ILE:HG12	1.87	0.56
12:K:165:VAL:HG12	12:K:174:LEU:HD13	1.88	0.56
13:M:496:ASN:OD1	13:M:497:GLY:N	2.38	0.56
9:G:264:ARG:HH21	12:K:352:ASP:HB2	1.70	0.56
13:M:9:LEU:HB2	13:M:21:ILE:HG23	1.88	0.56
13:M:186:LYS:HE2	13:M:207:LEU:HD13	1.87	0.56
6:J:165:VAL:C	6:J:172:MET:HE3	2.31	0.56
10:I:116:PRO:HA	10:I:219:PHE:HE1	1.69	0.56
13:M:32:PRO:HG3	13:M:44:CYS:HB3	1.88	0.56
8:A:857:GLY:HA3	8:A:875:VAL:HG22	1.88	0.55
12:K:63:LEU:HG	12:K:128:LYS:HB3	1.87	0.55
6:J:129:LEU:HD12	6:J:154:VAL:HG11	1.86	0.55
13:M:247:ILE:HG22	13:M:262:ARG:HB2	1.88	0.55
13:M:472:HIS:HE1	13:M:492:ARG:HB2	1.71	0.55
13:M:521:GLU:OE2	13:M:525:ARG:HD2	2.06	0.55
13:M:700:PHE:HB3	13:M:703:GLN:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:876:SER:O	13:M:952:THR:HG23	2.07	0.55
10:I:244:LEU:HB3	10:I:249:MET:HB2	1.88	0.55
7:X:43:U:O2'	13:M:590:TYR:OH	2.24	0.55
1:L:227:LEU:O	1:L:231:VAL:HG23	2.06	0.55
8:A:481:VAL:HG23	8:A:482:THR:HG23	1.89	0.55
8:A:639:ILE:HG13	8:A:644:LYS:HG3	1.87	0.55
13:M:184:THR:HG22	13:M:185:PHE:H	1.71	0.55
13:M:392:VAL:HB	13:M:410:PHE:HE1	1.72	0.55
13:M:645:GLY:O	13:M:737:LYS:NZ	2.39	0.55
13:M:842:ASN:O	13:M:845:GLN:HG3	2.07	0.55
13:M:947:LEU:HG	13:M:948:PHE:CD1	2.42	0.55
8:A:600:ILE:HG13	8:A:655:LEU:HD23	1.89	0.55
13:M:882:SER:HB3	13:M:889:LEU:HD12	1.89	0.55
13:M:706:LEU:HD11	13:M:792:TYR:H	1.72	0.54
13:M:706:LEU:HD12	13:M:707:ARG:H	1.72	0.54
2:N:90:SER:OG	2:N:91:SER:N	2.40	0.54
3:O:78:VAL:HG22	3:O:118:VAL:HB	1.88	0.54
4:F:170:VAL:HB	4:F:181:GLU:H	1.72	0.54
8:A:848:LYS:HB2	8:A:926:ALA:HB2	1.89	0.54
11:E:591:ARG:HB2	11:E:591:ARG:NH1	2.22	0.54
8:A:1134:GLY:HA2	8:A:1137:ARG:HD3	1.88	0.54
11:E:619:ASP:HA	11:E:622:LYS:NZ	2.22	0.54
13:M:507:ASP:HB2	13:M:559:VAL:HG23	1.89	0.54
13:M:965:ASP:OD1	13:M:966:THR:N	2.40	0.54
4:F:27:ARG:HB2	4:F:31:ASP:HB2	1.90	0.54
13:M:503:VAL:O	13:M:561:ILE:HG22	2.08	0.54
13:M:528:THR:HG23	13:M:536:TYR:O	2.07	0.54
13:M:689:ASN:OD1	13:M:795:PHE:N	2.41	0.54
6:J:114:ASP:CG	6:J:115:LYS:H	2.16	0.54
8:A:670:ASN:O	8:A:671:MET:HG3	2.08	0.54
13:M:61:PRO:CB	13:M:65:VAL:HB	2.38	0.54
13:M:282:MET:HE1	13:M:285:ARG:CZ	2.38	0.54
8:A:830:MET:HE3	8:A:830:MET:HA	1.90	0.54
13:M:736:ASN:HA	13:M:739:LEU:HD12	1.89	0.54
5:H:243:THR:HB	5:H:246:GLN:HG3	1.89	0.54
10:I:281:VAL:HG13	10:I:282:MET:HE3	1.90	0.54
13:M:300:PRO:HG2	13:M:303:GLU:HG2	1.90	0.54
13:M:428:LEU:HD11	13:M:536:TYR:CE2	2.40	0.53
8:A:336:ALA:HB3	8:A:706:ARG:NH1	2.23	0.53
8:A:814:TRP:CD1	8:A:1005:LEU:HD22	2.43	0.53
13:M:476:SER:OG	13:M:488:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:32:PHE:HE1	2:N:208:VAL:HB	1.73	0.53
10:I:273:LYS:HB2	10:I:276:ILE:HG12	1.90	0.53
13:M:717:PHE:HB2	13:M:721:ARG:HH21	1.72	0.53
8:A:376:THR:HG22	8:A:377:PHE:CD2	2.43	0.53
13:M:714:GLN:O	13:M:721:ARG:NH2	2.41	0.53
13:M:802:TYR:HD2	13:M:840:ILE:HD11	1.72	0.53
10:I:62:ARG:HA	10:I:66:LEU:O	2.09	0.53
10:I:236:ARG:NH1	10:I:263:SER:O	2.42	0.53
10:I:276:ILE:HA	10:I:279:GLU:HG2	1.91	0.53
8:A:1099:ALA:HB1	8:A:1137:ARG:HE	1.74	0.53
12:K:99:LEU:O	12:K:103:ASN:ND2	2.42	0.52
13:M:90:ALA:O	13:M:94:GLN:HB2	2.09	0.52
13:M:528:THR:OG1	13:M:538:MET:HB2	2.09	0.52
10:I:248:ARG:HH21	10:I:285:ARG:HH22	1.57	0.52
11:E:617:PRO:HA	11:E:620:ILE:HD12	1.91	0.52
13:M:256:GLN:O	13:M:282:MET:HE3	2.09	0.52
8:A:358:TYR:HB3	8:A:397:ILE:HG12	1.91	0.52
13:M:166:ASP:OD2	13:M:169:ALA:N	2.30	0.52
4:F:139:VAL:HG11	4:F:152:ILE:HD13	1.91	0.52
6:J:104:ARG:HH22	6:J:133:ILE:HD11	1.74	0.52
5:H:169:VAL:HB	5:H:177:GLU:HG2	1.90	0.52
8:A:575:SER:HB3	8:A:578:ARG:HE	1.72	0.52
8:A:668:GLY:HA2	8:A:703:ARG:NH1	2.25	0.52
12:K:68:LEU:O	12:K:69:ASN:HB3	2.09	0.52
13:M:186:LYS:NZ	13:M:203:CYS:SG	2.81	0.52
13:M:543:LEU:O	13:M:547:LEU:HB3	2.10	0.52
13:M:923:PRO:O	13:M:938:THR:N	2.43	0.52
1:L:108:ALA:HB1	12:K:241:MET:HE1	1.91	0.51
8:A:651:PHE:HD2	8:A:671:MET:HE1	1.75	0.51
10:I:41:ARG:NH2	10:I:45:THR:O	2.42	0.51
12:K:115:CYS:HB3	12:K:189:HIS:CE1	2.45	0.51
3:O:153:CYS:SG	3:O:154:GLY:N	2.83	0.51
8:A:288:ASP:OD1	8:A:289:ALA:N	2.43	0.51
13:M:231:LEU:O	13:M:234:LEU:N	2.43	0.51
5:H:181:ILE:HG13	5:H:182:ASP:N	2.24	0.51
8:A:844:VAL:O	8:A:929:THR:OG1	2.22	0.51
8:A:1221:VAL:O	8:A:1225:LYS:NZ	2.38	0.51
1:L:93:ARG:HB2	12:K:104:ARG:NH2	2.22	0.51
13:M:55:VAL:HG23	13:M:158:MET:HE2	1.92	0.51
2:N:46:ASP:HB3	2:N:163:VAL:HG23	1.92	0.51
3:O:203:ASP:OD1	3:O:203:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:138:LEU:HD13	12:K:145:ILE:HG23	1.93	0.51
13:M:472:HIS:CE1	13:M:492:ARG:HB2	2.45	0.51
3:O:171:SER:HA	3:O:174:GLU:HB2	1.91	0.51
4:F:187:TYR:HD2	13:M:131:ARG:HH11	1.58	0.51
4:F:270:LEU:HA	4:F:273:VAL:HG12	1.92	0.51
8:A:421:ILE:HG22	8:A:451:ILE:HB	1.93	0.51
8:A:383:LEU:HD12	8:A:398:MET:HE2	1.92	0.51
12:K:76:LEU:HD21	12:K:116:ILE:HG21	1.92	0.51
5:H:90:GLU:N	5:H:90:GLU:OE1	2.43	0.51
9:G:187:LEU:HD11	9:G:193:PRO:HB2	1.92	0.51
8:A:1108:ILE:HD12	8:A:1226:MET:CE	2.41	0.50
5:H:181:ILE:HG13	5:H:182:ASP:H	1.76	0.50
1:L:92:ASP:OD1	1:L:93:ARG:N	2.45	0.50
8:A:901:LEU:HD13	8:A:1009:ILE:HD13	1.93	0.50
13:M:289:ILE:HD11	13:M:399:TRP:HZ3	1.76	0.50
13:M:339:GLN:OE1	13:M:341:ASN:ND2	2.39	0.50
13:M:566:ASP:OD1	13:M:567:LYS:N	2.36	0.50
4:F:100:ASP:OD1	9:G:120:ARG:NH2	2.34	0.50
8:A:610:ARG:NH1	8:A:1242:SER:O	2.44	0.50
8:A:1041:ARG:O	8:A:1045:SER:OG	2.26	0.50
13:M:978:LYS:NZ	13:M:979:ILE:O	2.38	0.50
12:K:113:SER:HB3	12:K:189:HIS:CE1	2.45	0.50
13:M:876:SER:OG	13:M:877:ASP:N	2.45	0.50
2:N:14:TYR:OH	2:N:214:GLU:OE2	2.27	0.50
2:N:206:LEU:HD12	2:N:247:LYS:HE3	1.93	0.50
8:A:1107:GLU:CD	8:A:1131:LEU:HD21	2.36	0.50
13:M:208:GLN:O	13:M:212:GLU:HG3	2.12	0.50
8:A:838:SER:O	8:A:843:ARG:NE	2.32	0.50
12:K:80:LEU:HD12	12:K:81:GLU:H	1.77	0.50
13:M:82:ILE:HG22	13:M:115:ILE:HG12	1.93	0.50
13:M:231:LEU:HD11	13:M:338:LEU:HA	1.94	0.50
13:M:880:ILE:HD13	13:M:888:VAL:HG21	1.93	0.50
8:A:945:SER:O	8:A:948:GLN:HG3	2.11	0.50
13:M:434:SER:OG	13:M:436:ILE:HG12	2.11	0.50
13:M:666:ILE:HG21	13:M:862:TYR:HD1	1.76	0.50
3:O:204:THR:O	3:O:208:GLN:HG3	2.12	0.49
8:A:652:SER:HA	8:A:671:MET:HE2	1.94	0.49
8:A:801:MET:HE1	8:A:808:LEU:HD23	1.93	0.49
13:M:666:ILE:HG13	13:M:861:MET:HE3	1.94	0.49
13:M:681:VAL:HG22	13:M:685:MET:SD	2.52	0.49
7:X:36:U:OP1	13:M:251:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:124:VAL:HB	12:K:127:GLU:HB2	1.92	0.49
2:N:265:LEU:HD13	12:K:339:ILE:HG23	1.95	0.49
4:F:257:GLU:O	4:F:261:ARG:HG3	2.11	0.49
6:J:110:ALA:HA	6:J:147:ALA:HB1	1.93	0.49
6:J:187:ARG:HG3	11:E:612:PHE:CD2	2.47	0.49
8:A:303:PRO:HG2	11:E:629:PHE:HD2	1.76	0.49
8:A:724:PRO:HB2	8:A:729:LEU:HD11	1.93	0.49
8:A:939:LYS:HE3	8:A:958:LEU:HD23	1.95	0.49
8:A:1141:VAL:O	8:A:1145:ILE:HG12	2.12	0.49
13:M:31:VAL:CG1	13:M:118:ALA:HB3	2.42	0.49
13:M:287:ARG:HD2	13:M:399:TRP:CD1	2.46	0.49
13:M:841:ASN:HA	13:M:844:ASN:HD21	1.78	0.49
8:A:852:HIS:HB3	8:A:855:ALA:HB3	1.95	0.49
13:M:31:VAL:HG11	13:M:118:ALA:HB3	1.94	0.49
13:M:499:LEU:HD23	13:M:635:ILE:HD11	1.94	0.49
6:J:187:ARG:HA	11:E:612:PHE:CZ	2.48	0.49
8:A:464:ALA:HB1	8:A:475:ILE:HG21	1.95	0.49
13:M:877:ASP:N	13:M:877:ASP:OD1	2.45	0.49
2:N:74:PRO:HB2	2:N:129:GLY:HA2	1.94	0.49
5:H:262:SER:HA	5:H:266:LYS:HB2	1.94	0.49
8:A:706:ARG:CD	8:A:707:ARG:H	2.26	0.49
12:K:124:VAL:HG12	12:K:125:ALA:N	2.28	0.49
12:K:329:PRO:HA	12:K:339:ILE:HG22	1.93	0.49
13:M:284:ALA:O	13:M:333:ARG:NH2	2.46	0.49
1:L:200:MET:HG3	1:L:201:ASP:N	2.28	0.49
4:F:280:LEU:HB2	4:F:283:LYS:HD2	1.94	0.49
4:F:35:VAL:HG21	4:F:51:VAL:HG13	1.94	0.49
6:J:123:ARG:HD2	6:J:183:ARG:HH21	1.78	0.49
12:K:91:GLU:OE1	12:K:94:ARG:HB2	2.13	0.49
13:M:707:ARG:HB3	13:M:792:TYR:O	2.12	0.49
13:M:708:GLN:O	13:M:769:ALA:HA	2.12	0.49
8:A:1049:LEU:HD12	8:A:1052:LEU:HD13	1.95	0.49
13:M:841:ASN:HA	13:M:844:ASN:ND2	2.28	0.49
4:F:187:TYR:OH	13:M:132:GLY:N	2.42	0.48
4:F:215:THR:HG23	4:F:218:GLU:H	1.77	0.48
5:H:118:ILE:O	5:H:234:ASN:ND2	2.44	0.48
9:G:4:ASP:OD2	9:G:7:ARG:NH1	2.45	0.48
13:M:535:ARG:O	13:M:536:TYR:CD1	2.65	0.48
7:X:35:U:H2'	7:X:36:U:C6	2.48	0.48
8:A:1067:TYR:OH	8:A:1092:THR:OG1	2.24	0.48
13:M:297:GLU:CD	13:M:298:LEU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1117:CYS:HB2	8:A:1169:LEU:HB2	1.95	0.48
13:M:58:TYR:CE2	13:M:158:MET:HG2	2.49	0.48
6:J:168:SER:OG	6:J:169:TRP:N	2.46	0.48
13:M:637:ARG:NH2	13:M:640:ARG:HE	2.10	0.48
13:M:767:SER:OG	13:M:768:ASN:N	2.45	0.48
13:M:802:TYR:O	13:M:805:ILE:HG22	2.13	0.48
1:L:22:ARG:HD2	1:L:43:GLY:HA3	1.96	0.48
6:J:60:GLU:N	6:J:60:GLU:OE1	2.46	0.48
6:J:149:ASN:HD21	11:E:619:ASP:CG	2.21	0.48
4:F:170:VAL:HG11	4:F:180:ILE:HD13	1.95	0.48
8:A:758:ASP:OD1	8:A:758:ASP:N	2.46	0.48
5:H:167:PHE:CE1	5:H:176:PRO:HB2	2.48	0.48
8:A:362:ILE:HD11	8:A:664:THR:HA	1.95	0.48
13:M:135:MET:O	13:M:139:GLN:HB2	2.13	0.48
5:H:265:ARG:HH21	13:M:1046:LEU:HB3	1.77	0.48
6:J:169:TRP:CZ2	11:E:612:PHE:HB3	2.49	0.48
8:A:1227:GLU:O	8:A:1231:THR:HG23	2.14	0.48
12:K:36:ARG:NH2	12:K:38:SER:OG	2.46	0.48
13:M:924:GLY:HA3	13:M:937:THR:HA	1.94	0.48
6:J:137:ASP:C	9:G:141:ARG:HH12	2.22	0.48
13:M:62:ASP:HB2	13:M:143:ILE:HD13	1.96	0.48
2:N:38:ASN:HB2	12:K:336:THR:HG22	1.95	0.48
6:J:15:CYS:HB2	6:J:33:ILE:HD12	1.96	0.48
8:A:642:ILE:HG23	8:A:643:LEU:HD22	1.95	0.48
8:A:895:VAL:HG21	8:A:1021:PRO:HB3	1.96	0.48
8:A:906:LEU:HD11	8:A:979:PRO:HD3	1.95	0.48
10:I:12:LYS:HE2	10:I:16:GLU:HB2	1.95	0.48
13:M:858:PHE:HD1	13:M:861:MET:HE2	1.79	0.48
2:N:248:LEU:O	2:N:252:MET:HG3	2.14	0.47
8:A:1104:ARG:NH1	8:A:1106:GLU:OE2	2.37	0.47
12:K:313:GLU:O	12:K:316:ILE:HG22	2.14	0.47
13:M:189:LEU:HB3	13:M:200:HIS:CE1	2.49	0.47
13:M:712:PRO:HD3	13:M:785:TYR:CE2	2.49	0.47
13:M:714:GLN:HB3	13:M:721:ARG:HH22	1.79	0.47
2:N:104:VAL:HG21	3:O:96:ARG:HE	1.79	0.47
4:F:172:GLU:HG3	4:F:172:GLU:O	2.13	0.47
5:H:244:ILE:O	5:H:248:LEU:HG	2.14	0.47
6:J:151:LEU:O	6:J:184:LYS:NZ	2.45	0.47
8:A:1014:CYS:O	8:A:1020:PHE:HB2	2.14	0.47
6:J:60:GLU:HG2	6:J:63:LEU:HD11	1.95	0.47
2:N:81:PRO:HG3	2:N:113:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:LYS:HB2	4:F:76:GLU:OE1	2.13	0.47
4:F:119:VAL:HG23	4:F:120:ASP:N	2.28	0.47
4:F:246:SER:HB3	9:G:221:GLN:HB3	1.96	0.47
12:K:147:ASP:O	12:K:151:ILE:HG13	2.14	0.47
13:M:39:PRO:HD2	13:M:153:HIS:CE1	2.49	0.47
10:I:226:VAL:O	10:I:231:ARG:NH1	2.47	0.47
12:K:66:PRO:HB3	12:K:129:VAL:HG21	1.96	0.47
2:N:113:ILE:HD11	2:N:156:LEU:HD11	1.96	0.47
5:H:184:CYS:SG	5:H:186:ARG:HG2	2.54	0.47
9:G:26:GLU:O	9:G:206:ARG:NH2	2.43	0.47
13:M:201:GLU:HG2	13:M:202:LEU:HD22	1.95	0.47
13:M:208:GLN:HA	13:M:211:ARG:NE	2.29	0.47
13:M:226:PRO:HG2	13:M:286:ASN:ND2	2.29	0.47
13:M:468:LEU:HD13	13:M:580:THR:HG23	1.97	0.47
10:I:230:ASP:O	10:I:234:ILE:HG13	2.14	0.47
5:H:264:GLN:N	5:H:264:GLN:OE1	2.47	0.47
12:K:75:ILE:O	12:K:76:LEU:HD12	2.14	0.47
1:L:44:ASN:OD1	1:L:128:GLN:NE2	2.48	0.47
4:F:119:VAL:HG11	4:F:160:LEU:HD21	1.96	0.47
8:A:1018:PRO:HG2	8:A:1019:ARG:HH11	1.79	0.47
12:K:2:LYS:HG2	12:K:3:GLU:H	1.79	0.47
13:M:733:THR:HA	13:M:739:LEU:HD21	1.96	0.47
4:F:270:LEU:O	4:F:274:VAL:HG22	2.16	0.46
12:K:141:HIS:ND1	12:K:145:ILE:HD11	2.31	0.46
13:M:282:MET:HE1	13:M:285:ARG:NH2	2.29	0.46
13:M:954:ARG:HG3	13:M:955:ILE:N	2.28	0.46
1:L:94:LYS:CE	12:K:104:ARG:HH21	2.27	0.46
2:N:44:THR:O	2:N:63:LYS:NZ	2.42	0.46
4:F:31:ASP:OD1	10:I:1:MET:HE1	2.15	0.46
8:A:346:ILE:O	11:E:631:ARG:NH1	2.49	0.46
13:M:377:ILE:HG22	13:M:379:ILE:HG23	1.97	0.46
8:A:330:VAL:HG11	8:A:338:LYS:HG2	1.97	0.46
8:A:844:VAL:HG22	8:A:858:VAL:HB	1.96	0.46
12:K:200:GLN:HG3	12:K:203:THR:OG1	2.16	0.46
1:L:24:ILE:HG22	1:L:42:GLN:HG3	1.98	0.46
4:F:203:LEU:HD23	4:F:212:VAL:HG12	1.97	0.46
8:A:1157:THR:HB	8:A:1160:GLU:HG2	1.96	0.46
13:M:307:ARG:HG3	13:M:329:MET:HE1	1.97	0.46
4:F:40:ASP:CG	4:F:162:ASN:HD21	2.23	0.46
9:G:209:ALA:HB2	9:G:229:GLY:HA3	1.98	0.46
3:O:61:PRO:HG3	3:O:116:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:15:VAL:HG23	4:F:206:ILE:HG22	1.97	0.46
13:M:425:ALA:O	13:M:429:VAL:HG12	2.15	0.46
13:M:664:LYS:O	13:M:664:LYS:HG3	2.16	0.46
4:F:108:THR:O	4:F:112:ILE:HG12	2.15	0.46
8:A:350:GLN:HG2	11:E:631:ARG:HH12	1.80	0.46
8:A:401:GLU:O	8:A:404:ARG:HG2	2.15	0.46
8:A:1147:GLU:N	8:A:1147:GLU:OE1	2.49	0.46
13:M:736:ASN:HB3	13:M:785:TYR:CE1	2.51	0.46
6:J:9:ILE:HD13	9:G:256:GLN:OE1	2.16	0.45
8:A:779:SER:O	8:A:782:HIS:HB2	2.16	0.45
5:H:243:THR:HG22	5:H:245:GLN:H	1.81	0.45
10:I:33:ILE:HG21	10:I:67:ILE:HG21	1.97	0.45
11:E:591:ARG:HB2	11:E:591:ARG:HH11	1.81	0.45
13:M:821:MET:HG3	13:M:822:GLU:H	1.81	0.45
8:A:726:MET:HA	8:A:729:LEU:HD13	1.98	0.45
12:K:227:LYS:HG3	12:K:228:HIS:N	2.29	0.45
13:M:97:ARG:HG2	13:M:101:ASN:ND2	2.30	0.45
13:M:887:GLY:HA3	13:M:901:ALA:O	2.16	0.45
4:F:168:VAL:HG13	4:F:181:GLU:O	2.16	0.45
5:H:95:SER:O	5:H:97:GLY:HA3	2.16	0.45
5:H:261:THR:HG23	5:H:264:GLN:NE2	2.30	0.45
8:A:1069:ASP:OD1	8:A:1073:THR:HB	2.17	0.45
12:K:86:ALA:HB3	12:K:90:PHE:CD2	2.52	0.45
13:M:299:LEU:HD22	13:M:303:GLU:OE2	2.16	0.45
13:M:831:LYS:O	13:M:834:GLU:HG3	2.17	0.45
2:N:174:THR:HG22	2:N:176:LEU:HG	1.98	0.45
13:M:301:LYS:HG2	13:M:304:TRP:CZ3	2.52	0.45
13:M:464:LYS:HG3	13:M:579:ARG:NH2	2.32	0.45
2:N:225:VAL:HG13	2:N:233:CYS:HB2	1.98	0.45
5:H:131:VAL:HG13	5:H:139:ALA:HB3	1.98	0.45
6:J:166:PRO:HA	6:J:172:MET:HG2	1.98	0.45
8:A:819:THR:O	8:A:823:HIS:ND1	2.49	0.45
10:I:33:ILE:HD11	10:I:54:ALA:HB2	1.99	0.45
12:K:240:ILE:HG13	12:K:242:LEU:HG	1.97	0.45
8:A:415:ARG:HD2	10:I:123:ARG:NH1	2.32	0.45
9:G:242:ARG:O	9:G:246:GLU:HG3	2.17	0.45
12:K:162:ARG:HE	12:K:185:LEU:CD2	2.30	0.45
13:M:92:GLN:HB2	13:M:100:TYR:CE1	2.52	0.45
13:M:352:LYS:O	13:M:355:VAL:HG12	2.16	0.45
1:L:104:GLN:OE1	12:K:237:SER:HA	2.16	0.45
3:O:223:PHE:CE1	12:K:296:PHE:HD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:128:VAL:HG12	6:J:153:VAL:HA	1.99	0.45
8:A:303:PRO:O	11:E:629:PHE:HE2	1.99	0.45
8:A:992:ASP:O	8:A:996:VAL:HG23	2.17	0.45
13:M:972:ILE:HG22	13:M:972:ILE:O	2.17	0.45
1:L:96:CYS:O	1:L:100:LEU:HD23	2.17	0.45
2:N:213:GLU:HG2	2:N:214:GLU:N	2.32	0.45
3:O:190:ARG:HH22	3:O:218:GLN:HG3	1.82	0.45
4:F:30:GLU:OE2	4:F:261:ARG:NH2	2.50	0.45
5:H:83:CYS:SG	5:H:84:GLY:N	2.89	0.45
5:H:103:ASP:OD1	5:H:103:ASP:N	2.50	0.45
6:J:62:GLN:HE21	9:G:69:PRO:HD2	1.81	0.45
9:G:132:PRO:O	9:G:216:MET:HE1	2.17	0.45
13:M:601:LEU:HD11	13:M:622:LEU:HD13	1.99	0.45
13:M:844:ASN:OD1	13:M:845:GLN:N	2.50	0.45
1:L:12:ARG:HH22	1:L:170:ALA:H	1.65	0.45
5:H:269:PHE:CZ	13:M:1040:ILE:HG23	2.45	0.45
8:A:814:TRP:HB3	8:A:1009:ILE:HD11	1.99	0.45
13:M:560:SER:HB2	13:M:580:THR:OG1	2.17	0.45
13:M:839:HIS:O	13:M:843:ARG:HG2	2.17	0.45
3:O:80:LEU:N	3:O:95:GLU:OE2	2.41	0.44
5:H:162:LEU:HD23	5:H:162:LEU:H	1.82	0.44
13:M:249:ASN:HA	13:M:290:HIS:ND1	2.33	0.44
1:L:86:LYS:O	1:L:86:LYS:HG3	2.17	0.44
3:O:48:LEU:HD11	12:K:285:ALA:HA	2.00	0.44
8:A:459:ASN:HD21	8:A:740:LEU:N	2.13	0.44
13:M:566:ASP:CG	13:M:567:LYS:H	2.23	0.44
4:F:280:LEU:HD12	4:F:283:LYS:HG3	1.98	0.44
8:A:818:LEU:HD21	8:A:1005:LEU:HB2	1.99	0.44
13:M:18:THR:C	13:M:19:LEU:HD12	2.43	0.44
13:M:195:ASP:OD1	13:M:195:ASP:N	2.48	0.44
13:M:386:THR:O	13:M:387:LEU:HD23	2.18	0.44
13:M:517:TYR:HA	13:M:520:ILE:HG12	1.98	0.44
8:A:824:MET:O	8:A:828:ARG:HG3	2.18	0.44
8:A:1193:GLU:OE1	8:A:1193:GLU:N	2.49	0.44
12:K:119:GLU:OE1	13:M:383:GLN:NE2	2.50	0.44
13:M:129:ARG:HD2	13:M:133:GLU:CD	2.43	0.44
13:M:640:ARG:HD2	13:M:640:ARG:C	2.43	0.44
4:F:10:GLU:O	4:F:14:ILE:HG13	2.18	0.44
4:F:280:LEU:HD23	4:F:280:LEU:H	1.83	0.44
6:J:45:SER:HA	6:J:51:PRO:HB3	2.00	0.44
6:J:76:SER:OG	6:J:86:HIS:ND1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:589:LEU:HD23	8:A:589:LEU:HA	1.82	0.44
13:M:939:ASP:OD1	13:M:941:GLU:HG3	2.17	0.44
4:F:60:VAL:HG12	4:F:139:VAL:HA	2.00	0.44
4:F:164:ARG:O	4:F:189:CYS:HB3	2.17	0.44
8:A:784:GLN:O	8:A:788:GLU:HG2	2.18	0.44
12:K:141:HIS:HD1	12:K:145:ILE:HD11	1.81	0.44
13:M:129:ARG:HD2	13:M:133:GLU:OE2	2.17	0.44
6:J:114:ASP:O	6:J:116:VAL:HG23	2.17	0.44
8:A:1057:GLN:HG2	8:A:1153:GLY:HA3	1.98	0.44
11:E:621:VAL:O	11:E:625:GLN:HG3	2.17	0.44
12:K:122:CYS:HA	12:K:129:VAL:HG12	1.99	0.44
13:M:820:LYS:HA	13:M:820:LYS:HD3	1.74	0.44
2:N:249:GLN:OE1	3:O:207:GLN:NE2	2.48	0.44
10:I:238:ARG:O	10:I:242:ILE:HG12	2.17	0.44
13:M:389:ASP:OD2	13:M:416:ARG:NE	2.46	0.44
13:M:488:THR:OG1	13:M:504:HIS:HB2	2.18	0.44
5:H:96:GLY:HA2	5:H:97:GLY:C	2.41	0.44
8:A:612:ARG:HE	8:A:615:ASP:CG	2.24	0.44
13:M:355:VAL:HA	13:M:358:GLN:HG2	1.99	0.44
13:M:880:ILE:HG23	13:M:889:LEU:O	2.17	0.44
1:L:86:LYS:HE2	7:X:23:U:O2'	2.17	0.43
5:H:252:ASN:HD22	13:M:1037:LEU:HD13	1.82	0.43
8:A:895:VAL:HG13	8:A:1024:TYR:CD2	2.53	0.43
13:M:716:PHE:HB3	13:M:765:ALA:HA	2.00	0.43
1:L:163:PHE:HB3	1:L:182:PRO:HG2	2.00	0.43
5:H:19:ALA:HA	5:H:35:LEU:HB2	2.00	0.43
6:J:141:ASN:OD1	6:J:142:TYR:N	2.51	0.43
7:X:11:U:O2	10:I:95:ARG:NH2	2.50	0.43
8:A:756:ARG:NE	10:I:80:VAL:O	2.47	0.43
10:I:252:TYR:HD2	10:I:253:ASP:OD1	2.01	0.43
13:M:7:LYS:HE2	13:M:25:HIS:CG	2.53	0.43
2:N:46:ASP:OD2	2:N:64:ALA:N	2.51	0.43
8:A:1225:LYS:HA	8:A:1228:THR:OG1	2.18	0.43
13:M:95:ARG:HA	13:M:95:ARG:HD3	1.75	0.43
13:M:167:GLU:HA	13:M:170:ILE:HD12	2.00	0.43
8:A:604:LEU:HD21	8:A:608:LEU:HD12	1.99	0.43
8:A:1122:ASP:OD1	8:A:1122:ASP:N	2.49	0.43
13:M:502:GLY:HA3	13:M:562:MET:CE	2.48	0.43
13:M:651:LEU:HD23	13:M:763:THR:OG1	2.19	0.43
5:H:114:GLY:C	5:H:166:GLN:HE21	2.26	0.43
5:H:182:ASP:HB3	5:H:185:GLY:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:63:LEU:HB2	12:K:130:TRP:CZ3	2.54	0.43
13:M:261:VAL:N	13:M:276:ASP:OD1	2.49	0.43
13:M:676:GLU:O	13:M:680:THR:HG23	2.19	0.43
1:L:27:ARG:HD2	4:F:290:LEU:HA	1.99	0.43
6:J:166:PRO:HB3	6:J:185:VAL:HG11	1.99	0.43
6:J:167:ILE:HB	6:J:172:MET:HA	2.01	0.43
8:A:305:PHE:CE1	11:E:632:GLU:HB3	2.54	0.43
8:A:1211:ARG:HD2	8:A:1226:MET:HB2	2.00	0.43
11:E:608:THR:HB	11:E:609:PRO:CD	2.48	0.43
13:M:202:LEU:O	13:M:206:ILE:HG13	2.19	0.43
6:J:9:ILE:O	6:J:11:GLY:N	2.52	0.43
7:X:22:U:O2'	7:X:23:U:O4'	2.32	0.43
8:A:425:VAL:HG21	8:A:452:LEU:HB3	2.00	0.43
8:A:1001:ARG:O	8:A:1005:LEU:HG	2.19	0.43
12:K:49:GLU:OE2	12:K:54:ARG:NH1	2.52	0.43
13:M:69:TYR:HB3	13:M:72:ILE:HD12	2.00	0.43
13:M:228:HIS:CD2	13:M:287:ARG:HH21	2.36	0.43
13:M:250:VAL:HB	13:M:373:ARG:HG3	2.00	0.43
13:M:754:VAL:HG22	13:M:948:PHE:CE2	2.54	0.43
13:M:803:SER:O	13:M:807:VAL:HG23	2.19	0.43
13:M:876:SER:OG	13:M:892:ILE:HD12	2.18	0.43
1:L:16:ARG:HA	13:M:28:ARG:HH12	1.83	0.43
3:O:134:LEU:HD11	3:O:194:MET:HE1	2.01	0.43
4:F:185:ASP:HB3	4:F:188:ASP:HB2	2.00	0.43
5:H:244:ILE:H	5:H:244:ILE:HD12	1.83	0.43
5:H:260:MET:HA	5:H:265:ARG:NH1	2.33	0.43
8:A:529:MET:SD	8:A:529:MET:N	2.88	0.43
8:A:578:ARG:O	8:A:582:GLN:HG2	2.19	0.43
13:M:570:TYR:OH	13:M:634:ASP:OD2	2.32	0.43
2:N:239:GLY:HA2	3:O:193:LEU:O	2.19	0.43
13:M:184:THR:HG22	13:M:185:PHE:N	2.34	0.43
13:M:513:ALA:O	13:M:516:SER:OG	2.35	0.43
1:L:201:ASP:N	1:L:201:ASP:OD1	2.52	0.43
2:N:37:VAL:HG12	2:N:51:VAL:HG22	2.00	0.43
7:X:44:U:H5'	13:M:482:CYS:SG	2.59	0.43
9:G:101:ARG:O	9:G:149:LEU:HA	2.19	0.43
13:M:686:ILE:HA	13:M:792:TYR:HE1	1.84	0.43
4:F:11:LYS:O	4:F:15:VAL:HG12	2.19	0.42
4:F:231:THR:OG1	4:F:235:VAL:HG22	2.19	0.42
8:A:958:LEU:HD12	8:A:958:LEU:HA	1.91	0.42
8:A:1004:LYS:HE2	8:A:1008:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:350:LEU:O	12:K:350:LEU:HD23	2.19	0.42
13:M:551:LEU:HA	13:M:587:LYS:HE2	2.01	0.42
2:N:18:LEU:HD11	2:N:201:PHE:CE2	2.55	0.42
5:H:127:ASP:HB2	5:H:143:TYR:CE2	2.54	0.42
13:M:561:ILE:HD12	13:M:577:TYR:HA	2.01	0.42
5:H:34:LEU:HD11	5:H:78:LEU:HD12	2.01	0.42
6:J:131:LYS:O	6:J:145:THR:HG22	2.19	0.42
8:A:589:LEU:HD12	8:A:632:LEU:HD21	2.01	0.42
8:A:635:HIS:O	8:A:661:ALA:HA	2.20	0.42
10:I:278:GLU:HA	10:I:281:VAL:HG12	2.00	0.42
12:K:192:ILE:HB	12:K:258:VAL:HG13	2.01	0.42
13:M:185:PHE:O	13:M:188:TYR:HB3	2.18	0.42
13:M:679:GLU:O	13:M:683:GLU:HG2	2.19	0.42
13:M:863:PHE:O	13:M:957:ILE:HD13	2.18	0.42
2:N:124:LEU:HB3	2:N:133:TRP:HB2	2.01	0.42
4:F:235:VAL:HA	9:G:232:GLY:O	2.18	0.42
5:H:246:GLN:O	5:H:250:LEU:HD23	2.20	0.42
7:X:35:U:H5"	13:M:253:HIS:ND1	2.35	0.42
10:I:244:LEU:HD11	10:I:259:CYS:CB	2.50	0.42
11:E:562:ALA:O	11:E:566:THR:HG22	2.20	0.42
8:A:325:HIS:HA	8:A:419:TRP:HH2	1.85	0.42
8:A:430:ASP:OD2	8:A:433:ARG:N	2.50	0.42
5:H:83:CYS:O	5:H:104:SER:HB3	2.19	0.42
6:J:89:TYR:CD1	6:J:94:PRO:HA	2.55	0.42
8:A:917:VAL:HB	8:A:944:PHE:CE2	2.55	0.42
10:I:7:LEU:HG	10:I:8:PRO:HD2	2.00	0.42
13:M:198:ALA:HA	13:M:201:GLU:CD	2.45	0.42
13:M:734:ARG:HG2	13:M:738:THR:HG21	2.00	0.42
4:F:83:VAL:HG21	4:F:105:ILE:HG22	2.01	0.42
6:J:61:SER:HB2	9:G:50:LYS:NZ	2.35	0.42
12:K:150:SER:O	12:K:154:ILE:HG12	2.20	0.42
13:M:24:GLU:HG3	13:M:25:HIS:H	1.85	0.42
13:M:198:ALA:HA	13:M:201:GLU:OE2	2.18	0.42
13:M:498:ASN:HA	13:M:567:LYS:HD3	2.02	0.42
13:M:717:PHE:HB2	13:M:721:ARG:NH2	2.35	0.42
13:M:28:ARG:O	13:M:123:GLN:HB2	2.20	0.42
13:M:116:LEU:HD12	13:M:117:PHE:H	1.83	0.42
5:H:127:ASP:HB2	5:H:143:TYR:CD2	2.55	0.42
6:J:133:ILE:HG12	6:J:143:LEU:O	2.19	0.42
8:A:376:THR:HG22	8:A:377:PHE:HD2	1.83	0.42
8:A:463:PHE:CE1	8:A:467:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:670:ASN:C	8:A:671:MET:HG3	2.45	0.42
8:A:1219:GLU:OE2	8:A:1221:VAL:HB	2.19	0.42
9:G:93:ARG:HH21	9:G:136:LEU:HB2	1.83	0.42
11:E:603:PRO:HB2	11:E:605:VAL:CG2	2.49	0.42
8:A:316:LYS:O	8:A:320:LEU:HG	2.20	0.42
13:M:564:GLU:HB3	13:M:574:LYS:HG3	2.02	0.42
13:M:675:LEU:HB2	13:M:678:HIS:CE1	2.55	0.42
2:N:56:THR:HA	2:N:143:ASP:O	2.20	0.41
4:F:230:VAL:HA	4:F:235:VAL:O	2.20	0.41
8:A:702:GLY:C	8:A:703:ARG:HD2	2.45	0.41
8:A:766:MET:HE1	8:A:1051:LEU:HB2	2.02	0.41
13:M:197:LYS:O	13:M:201:GLU:OE1	2.38	0.41
13:M:292:ASP:OD2	13:M:337:ILE:HD13	2.20	0.41
13:M:391:ARG:O	13:M:414:LEU:HB2	2.20	0.41
1:L:200:MET:HB3	12:K:234:ILE:H	1.85	0.41
12:K:108:ARG:HG3	12:K:233:THR:HG21	2.02	0.41
12:K:318:GLU:O	12:K:318:GLU:HG2	2.21	0.41
13:M:586:TYR:OH	13:M:621:LYS:HD3	2.20	0.41
1:L:186:LEU:HD11	1:L:213:LEU:HD12	2.01	0.41
8:A:1242:SER:OG	8:A:1243:LEU:N	2.53	0.41
12:K:23:ARG:HD3	12:K:27:ARG:O	2.20	0.41
12:K:303:ILE:HG13	12:K:304:ASP:N	2.36	0.41
2:N:27:ARG:NH1	2:N:209:ASP:HB3	2.34	0.41
4:F:229:SER:O	4:F:236:VAL:HA	2.20	0.41
8:A:496:SER:HB3	8:A:500:GLN:OE1	2.20	0.41
9:G:195:TRP:HE1	9:G:236:SER:HB2	1.85	0.41
9:G:264:ARG:NH2	12:K:352:ASP:O	2.52	0.41
12:K:17:ALA:HB1	12:K:22:LYS:O	2.21	0.41
13:M:784:HIS:CG	13:M:792:TYR:HB3	2.55	0.41
13:M:890:LEU:HD13	13:M:953:VAL:HG21	2.02	0.41
1:L:4:GLU:OE2	13:M:104:ARG:NH1	2.53	0.41
2:N:54:GLY:O	2:N:55:ASN:HB2	2.21	0.41
2:N:229:GLU:HG3	2:N:231:LYS:HG3	2.02	0.41
10:I:221:ALA:HB1	10:I:223:LEU:HG	2.01	0.41
2:N:15:ARG:HA	2:N:18:LEU:HD12	2.02	0.41
3:O:31:PHE:CE1	3:O:49:GLN:HB2	2.55	0.41
4:F:76:GLU:HG3	4:F:121:LEU:HB3	2.02	0.41
8:A:694:PRO:HB3	8:A:732:MET:O	2.20	0.41
9:G:171:ASP:OD1	9:G:266:ARG:NH1	2.53	0.41
4:F:32:TYR:CD2	10:I:3:MET:HG3	2.56	0.41
5:H:150:THR:OG1	5:H:151:LYS:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:42:U:OP1	13:M:794:HIS:NE2	2.52	0.41
9:G:90:ALA:O	9:G:93:ARG:HB2	2.20	0.41
10:I:271:ILE:HG13	10:I:271:ILE:O	2.21	0.41
13:M:349:PHE:O	13:M:961:ARG:NH2	2.32	0.41
1:L:93:ARG:HD2	12:K:104:ARG:HH12	1.86	0.41
1:L:198:LEU:HD12	1:L:198:LEU:HA	1.95	0.41
6:J:120:LYS:HB2	6:J:182:PHE:HB2	2.03	0.41
8:A:416:ASP:OD2	10:I:123:ARG:HB2	2.21	0.41
8:A:636:HIS:O	8:A:639:ILE:HG12	2.21	0.41
9:G:261:ARG:HH11	12:K:352:ASP:CG	2.26	0.41
10:I:252:TYR:O	10:I:256:ILE:HG13	2.21	0.41
10:I:281:VAL:HG13	10:I:282:MET:CE	2.51	0.41
13:M:623:GLU:HA	13:M:626:VAL:HG12	2.03	0.41
3:O:228:LEU:HD23	5:H:83:CYS:SG	2.60	0.41
6:J:105:LYS:HE2	6:J:116:VAL:O	2.20	0.41
6:J:114:ASP:CG	6:J:115:LYS:N	2.78	0.41
8:A:601:HIS:O	8:A:605:GLN:HB2	2.20	0.41
8:A:624:MET:HE1	8:A:643:LEU:O	2.21	0.41
8:A:692:LEU:HD22	8:A:700:MET:HE1	2.03	0.41
8:A:723:VAL:HA	8:A:724:PRO:HD3	1.88	0.41
8:A:845:VAL:HG12	8:A:928:ILE:HA	2.02	0.41
8:A:1108:ILE:HD12	8:A:1226:MET:HE1	2.03	0.41
13:M:296:VAL:HG12	13:M:297:GLU:O	2.21	0.41
13:M:654:VAL:HG12	13:M:756:ARG:HH12	1.86	0.41
13:M:1019:GLN:NE2	13:M:1023:GLN:OE1	2.54	0.41
1:L:75:TYR:HD2	1:L:95:SER:HA	1.84	0.41
2:N:244:THR:O	2:N:248:LEU:HG	2.21	0.41
9:G:122:LEU:HD22	9:G:158:LEU:HD13	2.03	0.41
13:M:205:SER:HA	13:M:208:GLN:HE21	1.86	0.41
13:M:917:SER:HB2	13:M:974:ASN:H	1.86	0.41
10:I:175:SER:HA	10:I:176:PRO:HD3	1.94	0.40
12:K:178:GLU:HB2	13:M:441:ALA:HB3	2.02	0.40
13:M:520:ILE:O	13:M:524:THR:HG23	2.21	0.40
13:M:574:LYS:HE3	13:M:574:LYS:HB3	1.94	0.40
13:M:719:GLU:O	13:M:722:GLU:HB2	2.21	0.40
13:M:726:ALA:O	13:M:727:LYS:HD2	2.22	0.40
13:M:821:MET:CG	13:M:822:GLU:H	2.35	0.40
3:O:72:ASN:OD1	3:O:73:LYS:HG3	2.21	0.40
5:H:269:PHE:CZ	13:M:1040:ILE:HG12	2.56	0.40
6:J:149:ASN:ND2	11:E:619:ASP:OD2	2.54	0.40
6:J:174:CYS:HB2	6:J:179:THR:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:566:GLN:HB3	8:A:674:ARG:HG2	2.03	0.40
12:K:93:GLY:O	12:K:94:ARG:HD2	2.20	0.40
13:M:637:ARG:O	13:M:640:ARG:HB3	2.22	0.40
13:M:832:ASP:O	13:M:836:LEU:HG	2.21	0.40
13:M:865:ASP:O	13:M:866:LYS:C	2.64	0.40
8:A:587:THR:O	8:A:587:THR:HG22	2.22	0.40
13:M:167:GLU:O	13:M:171:GLN:HG3	2.21	0.40
13:M:411:VAL:HG12	13:M:412:ARG:HG2	2.02	0.40
13:M:424:ILE:O	13:M:428:LEU:HD23	2.20	0.40
13:M:484:ASP:HA	13:M:549:SER:OG	2.22	0.40
13:M:584:SER:OG	13:M:585:ALA:N	2.54	0.40
13:M:781:GLU:N	13:M:781:GLU:OE1	2.55	0.40
13:M:928:ARG:O	13:M:929:PHE:HD1	2.04	0.40
3:O:187:SER:O	3:O:187:SER:OG	2.33	0.40
8:A:570:VAL:HG12	8:A:659:LEU:HB3	2.04	0.40
8:A:946:LYS:HE2	8:A:952:PHE:CE2	2.56	0.40
9:G:261:ARG:HH12	12:K:353:SER:HB3	1.85	0.40
10:I:33:ILE:O	10:I:35:THR:HG23	2.21	0.40
12:K:333:THR:O	12:K:334:PRO:C	2.65	0.40
13:M:721:ARG:HA	13:M:724:ALA:HB3	2.04	0.40
2:N:202:ASP:OD1	2:N:203:ASP:N	2.50	0.40
6:J:58:GLU:O	6:J:58:GLU:HG3	2.21	0.40
8:A:572:PHE:HD2	8:A:678:PHE:CE1	2.40	0.40
12:K:2:LYS:HE2	12:K:2:LYS:HB3	1.90	0.40
13:M:97:ARG:NE	13:M:358:GLN:HA	2.36	0.40
13:M:133:GLU:OE2	13:M:138:TRP:HB2	2.21	0.40
13:M:707:ARG:NH1	13:M:769:ALA:O	2.52	0.40
13:M:929:PHE:HB2	13:M:932:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	239/245 (98%)	237 (99%)	2 (1%)	0	100	100
2	N	263/280 (94%)	260 (99%)	3 (1%)	0	100	100
3	O	206/239 (86%)	206 (100%)	0	0	100	100
4	F	284/295 (96%)	271 (95%)	12 (4%)	1 (0%)	30	60
5	H	233/279 (84%)	226 (97%)	6 (3%)	1 (0%)	30	60
6	J	182/199 (92%)	174 (96%)	8 (4%)	0	100	100
8	A	945/1246 (76%)	934 (99%)	11 (1%)	0	100	100
9	G	247/272 (91%)	246 (100%)	1 (0%)	0	100	100
10	I	285/297 (96%)	275 (96%)	10 (4%)	0	100	100
11	E	60/274 (22%)	50 (83%)	10 (17%)	0	100	100
12	K	351/443 (79%)	326 (93%)	25 (7%)	0	100	100
13	M	965/1056 (91%)	884 (92%)	81 (8%)	0	100	100
All	All	4260/5125 (83%)	4089 (96%)	169 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	263	ASP
4	F	248	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	183/186 (98%)	183 (100%)	0	100	100
2	N	227/238 (95%)	227 (100%)	0	100	100
3	O	172/196 (88%)	172 (100%)	0	100	100
4	F	249/255 (98%)	249 (100%)	0	100	100
5	H	196/224 (88%)	196 (100%)	0	100	100
6	J	160/173 (92%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A	813/1062 (77%)	813 (100%)	0	100	100
9	G	178/188 (95%)	178 (100%)	0	100	100
10	I	251/257 (98%)	251 (100%)	0	100	100
11	E	57/251 (23%)	57 (100%)	0	100	100
12	K	307/384 (80%)	307 (100%)	0	100	100
13	M	873/945 (92%)	873 (100%)	0	100	100
All	All	3666/4359 (84%)	3666 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	O	111	HIS
4	F	162	ASN
5	H	252	ASN
6	J	62	GLN
8	A	333	HIS
8	A	459	ASN
8	A	495	ASN
8	A	629	ASN
8	A	684	HIS
8	A	782	HIS
8	A	804	GLN
8	A	975	HIS
8	A	1156	GLN
12	K	140	ASN
13	M	208	GLN
13	M	228	HIS
13	M	280	HIS
13	M	383	GLN
13	M	619	GLN
13	M	665	ASN
13	M	714	GLN
13	M	808	HIS
13	M	841	ASN
13	M	950	HIS
13	M	1019	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	X	43/44 (97%)	25 (58%)	2 (4%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	X	2	U
7	X	3	U
7	X	5	U
7	X	9	U
7	X	10	U
7	X	14	U
7	X	15	U
7	X	18	U
7	X	19	U
7	X	20	U
7	X	23	U
7	X	24	U
7	X	25	U
7	X	26	U
7	X	30	C
7	X	31	U
7	X	32	C
7	X	33	U
7	X	34	U
7	X	35	U
7	X	37	U
7	X	39	U
7	X	41	U
7	X	42	U
7	X	44	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	X	8	U
7	X	38	U

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

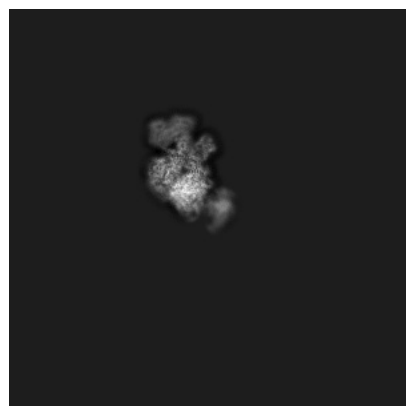
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51133. These allow visual inspection of the internal detail of the map and identification of artifacts.

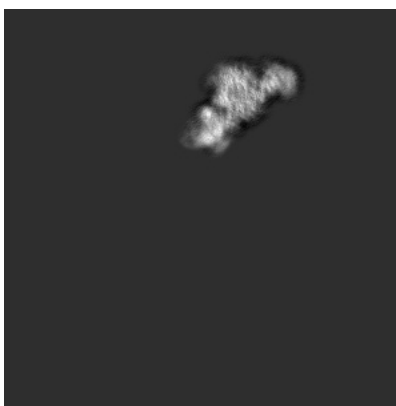
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

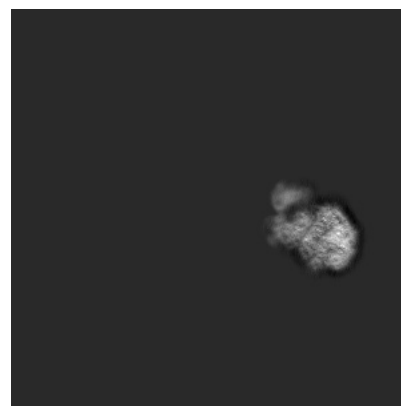
6.1.1 Primary map



X

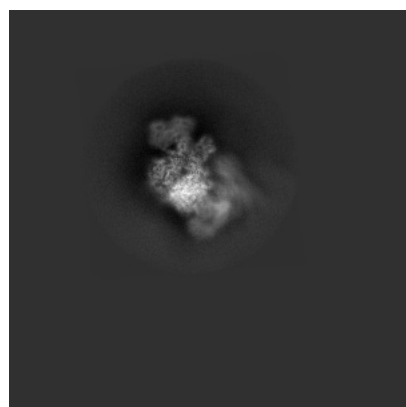


Y

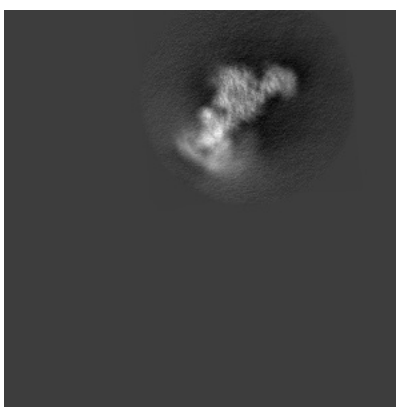


Z

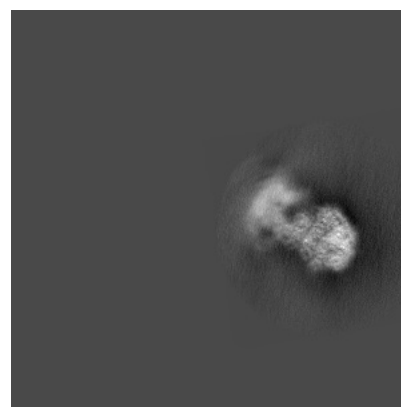
6.1.2 Raw map



X



Y

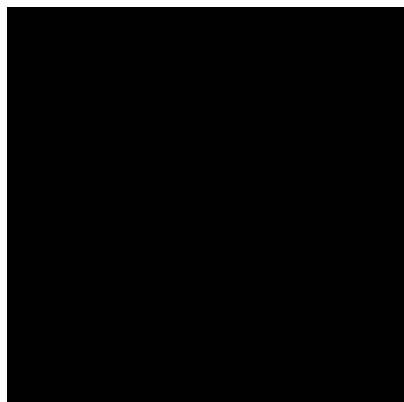


Z

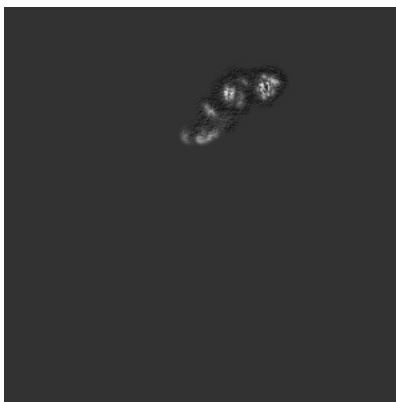
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

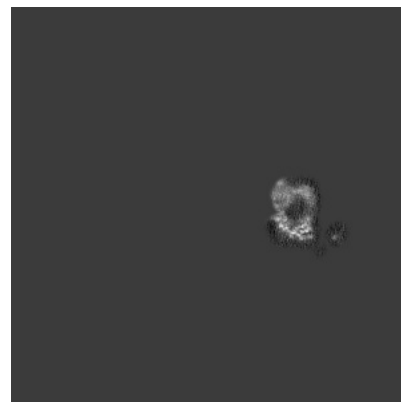
6.2.1 Primary map



X Index: 416



Y Index: 416

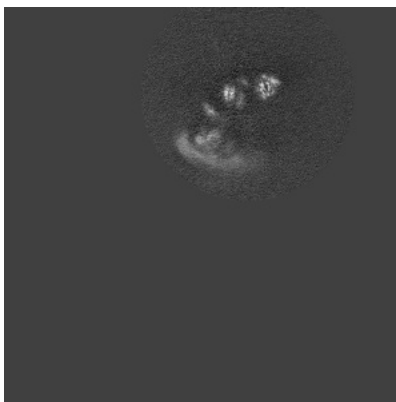


Z Index: 416

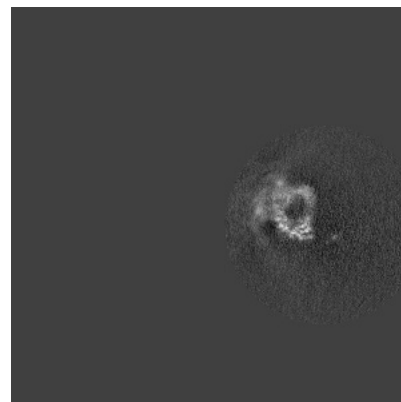
6.2.2 Raw map



X Index: 416



Y Index: 416

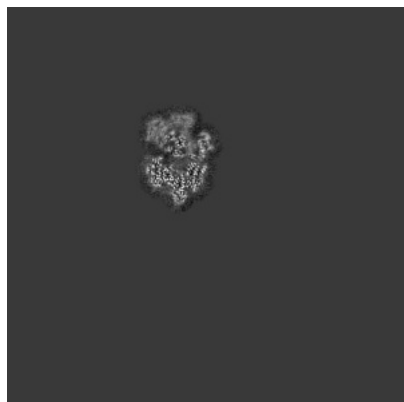


Z Index: 416

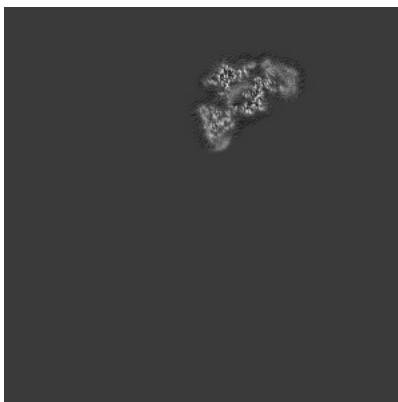
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

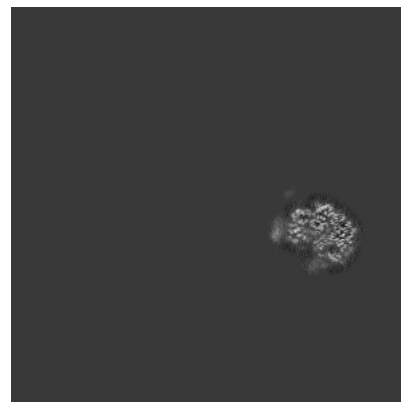
6.3.1 Primary map



X Index: 679

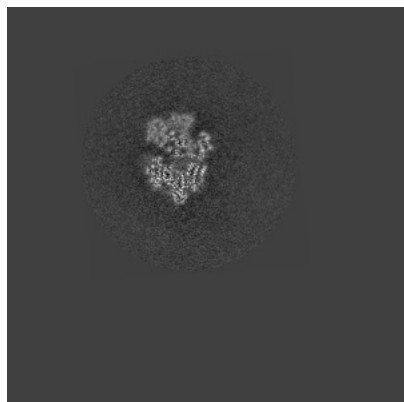


Y Index: 354

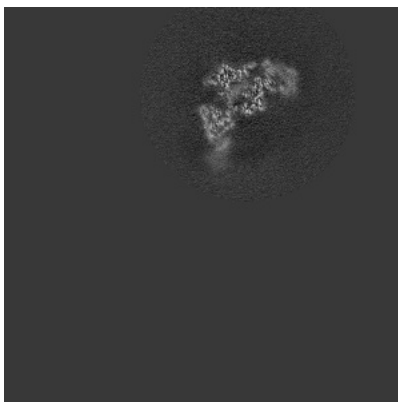


Z Index: 463

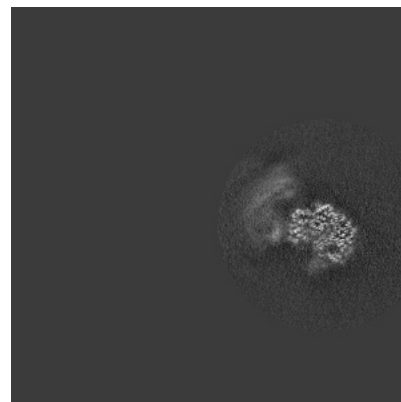
6.3.2 Raw map



X Index: 680



Y Index: 354

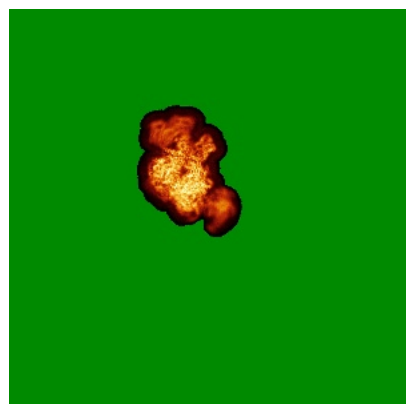


Z Index: 463

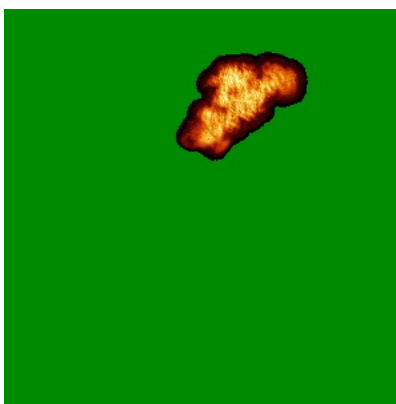
The images above show the largest variance slices of the map in three orthogonal directions.

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

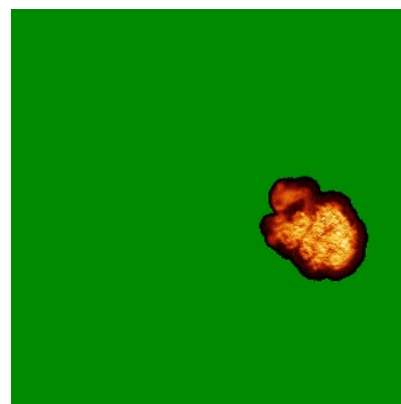
6.4.1 Primary map



X

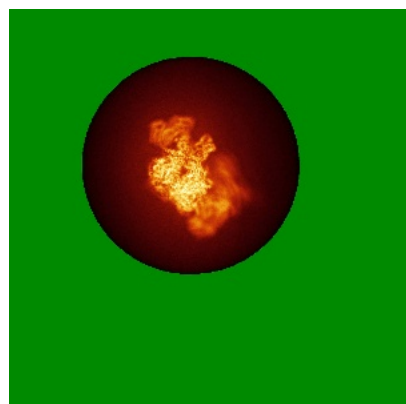


Y

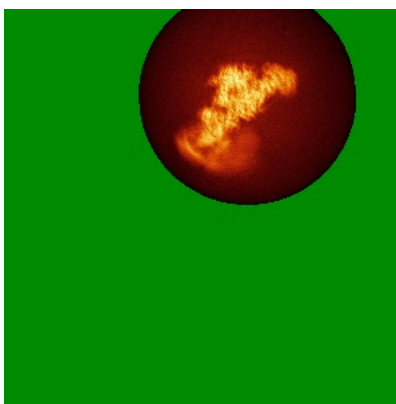


Z

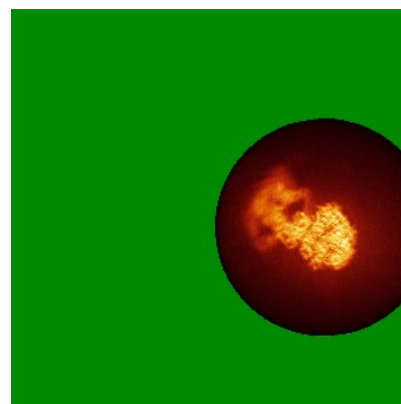
6.4.2 Raw map



X



Y

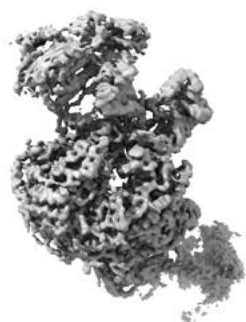


Z

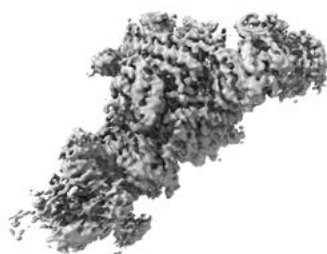
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

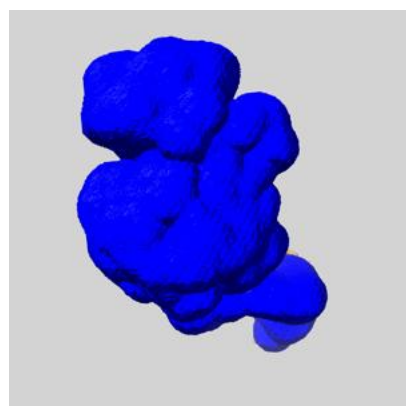
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

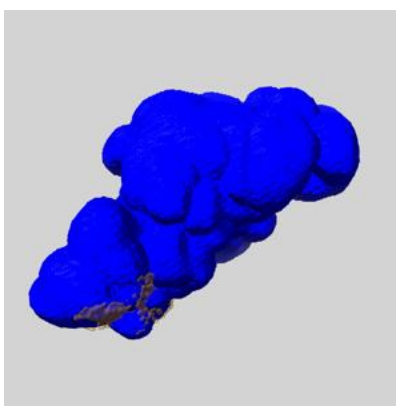
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

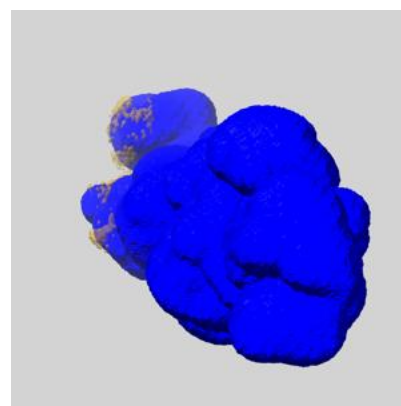
6.6.1 emd_51133_msk_1.map [i](#)



X



Y

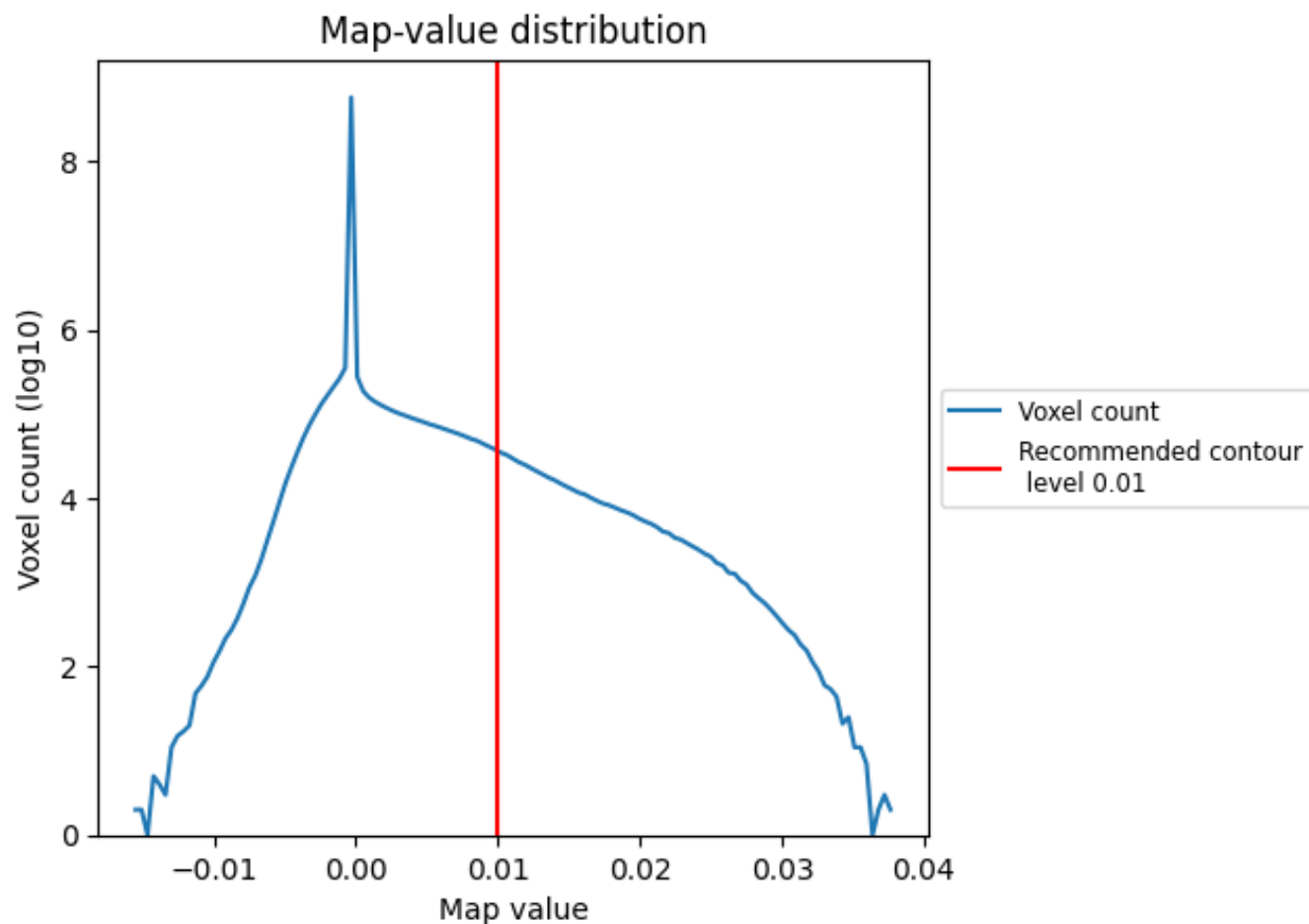


Z

7 Map analysis [i](#)

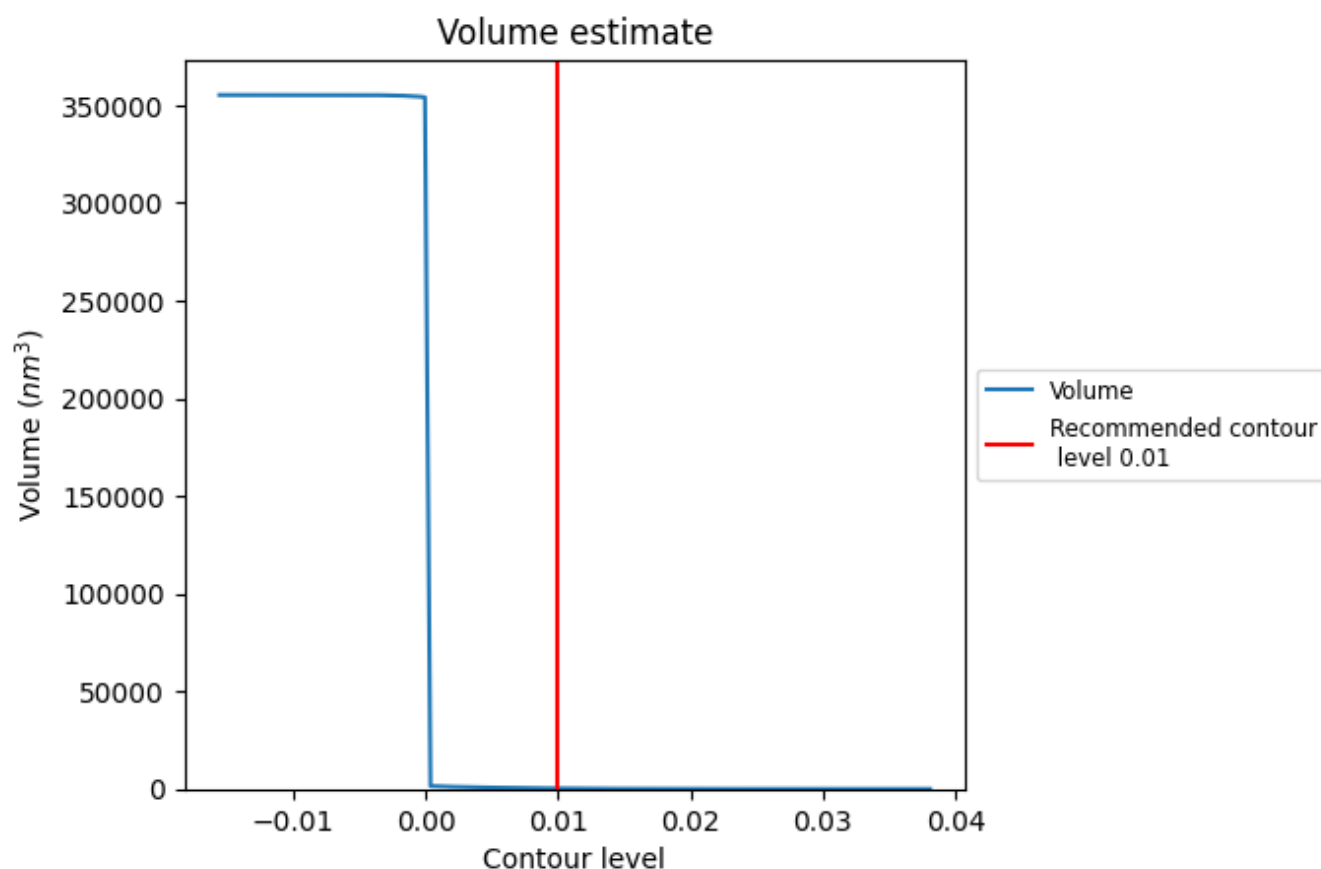
This section contains the results of statistical analysis of the map.

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.

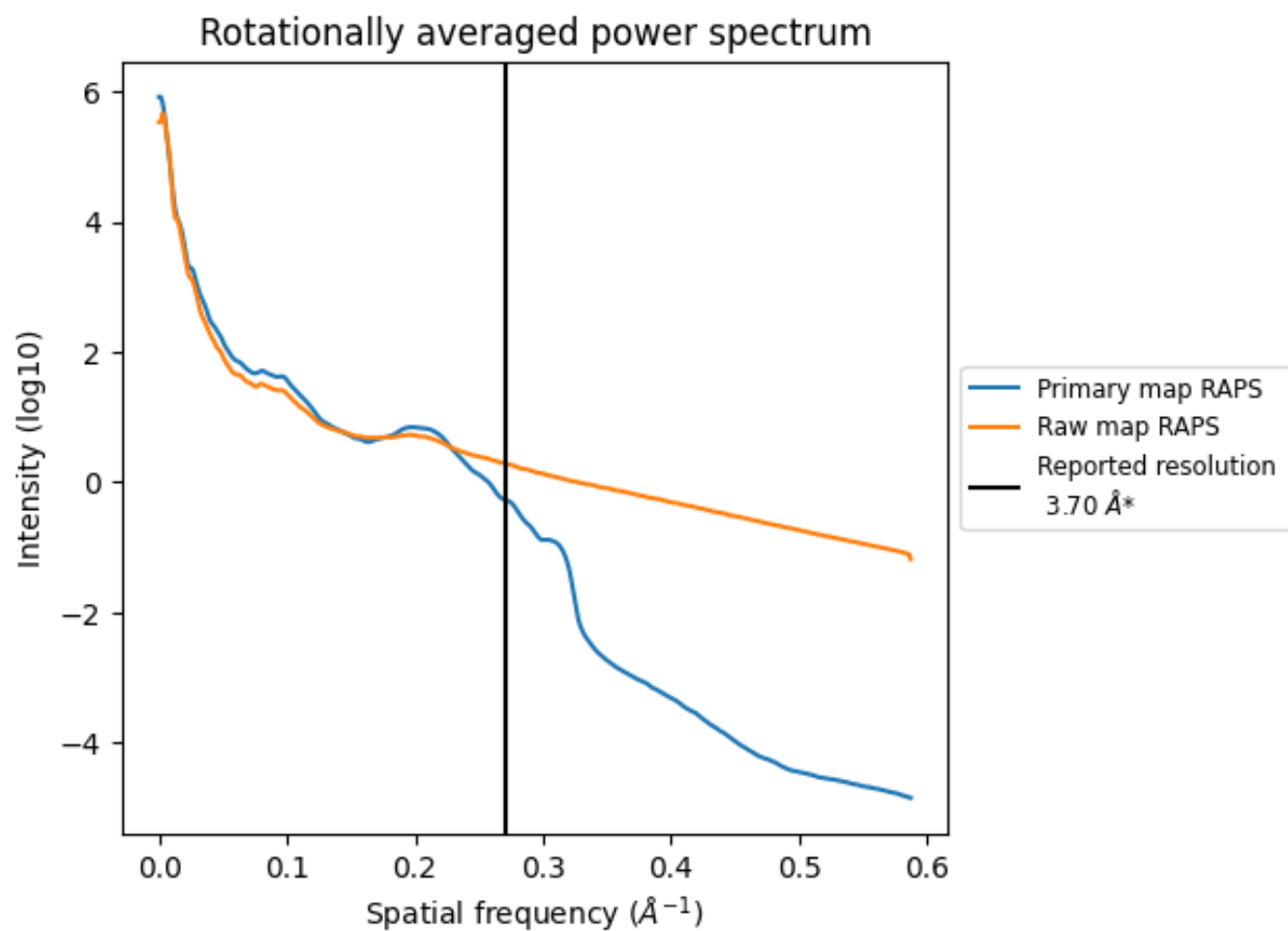
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278 nm^3 ; this corresponds to an approximate mass of 251 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](#)

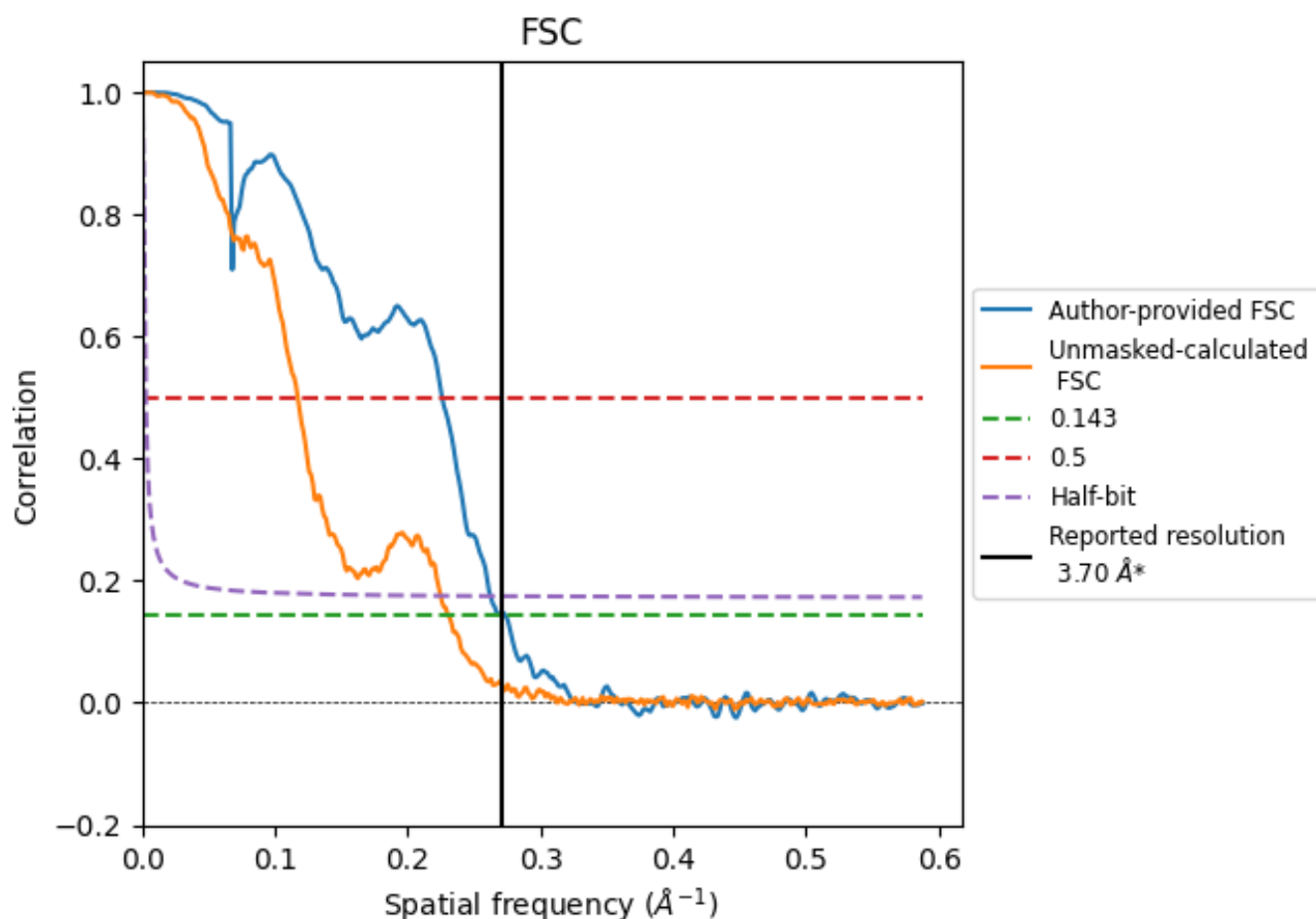


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

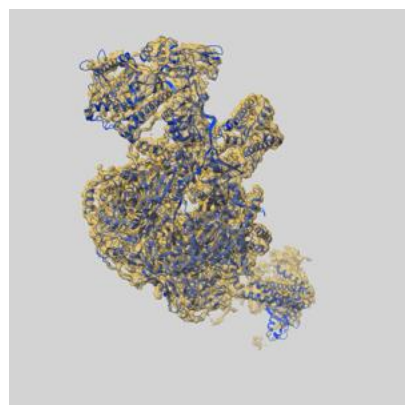
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.66	4.43	3.81
Unmasked-calculated*	4.35	8.54	4.45

*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 4.35 differs from the reported value 3.7 by more than 10 %

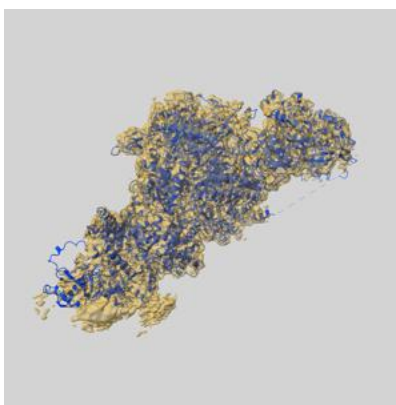
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51133 and PDB model 9G8N. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

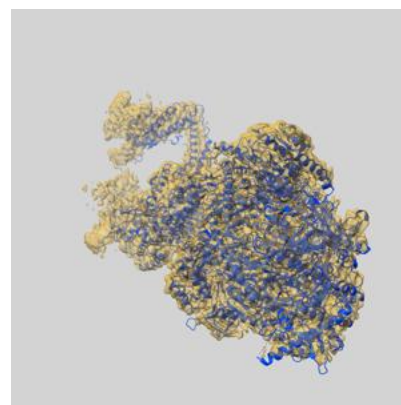
9.1 Map-model overlay [i](#)



X



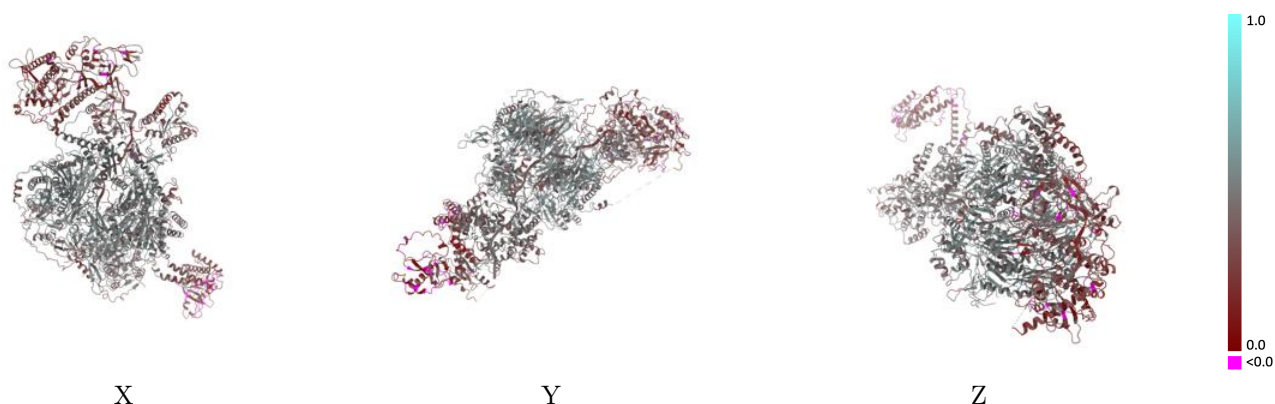
Y



Z

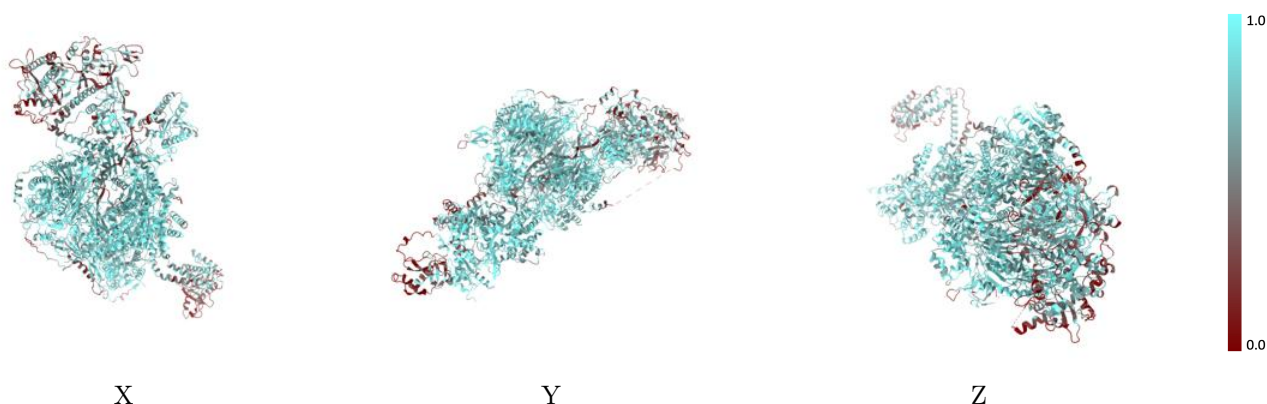
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



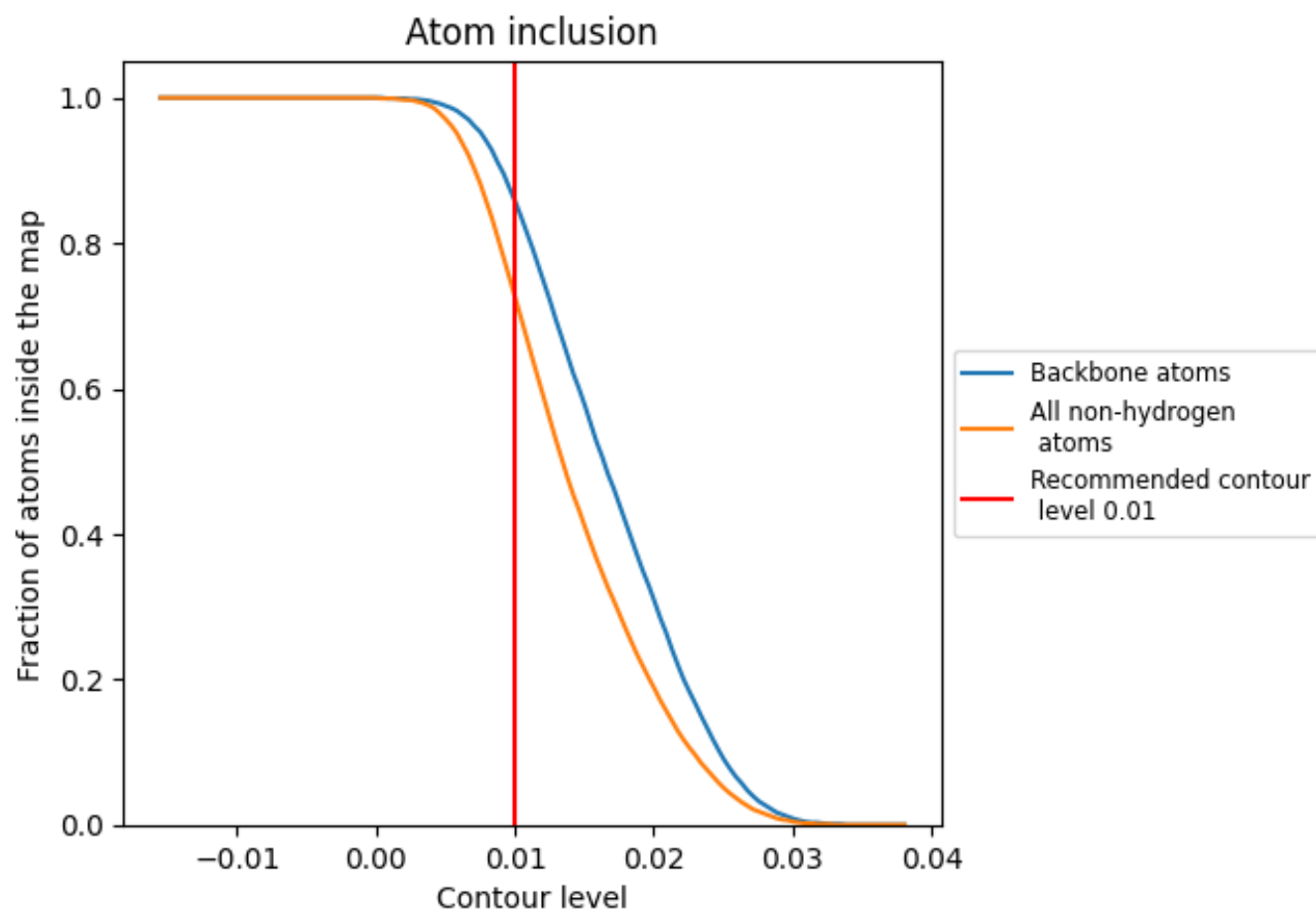
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.4100
A	0.7210	0.3520
E	0.5820	0.3870
F	0.7960	0.4600
G	0.8290	0.4890
H	0.8190	0.4760
I	0.7700	0.4590
J	0.7600	0.4590
K	0.7960	0.4800
L	0.8170	0.4970
M	0.5720	0.3210
N	0.8560	0.4820
O	0.8510	0.5060
X	0.6140	0.3410

