Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:49 am GMT

PDB ID	:	6H25
EMDB ID	:	EMD-0128
Title	:	Human nuclear RNA exosome EXO-10-MPP6 complex
Authors	:	Gerlach, P.; Schuller, J.M.; Falk, S.; Basquin, J.; Conti, E.
Deposited on	:	2018-07-13
Resolution	:	3.80 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:

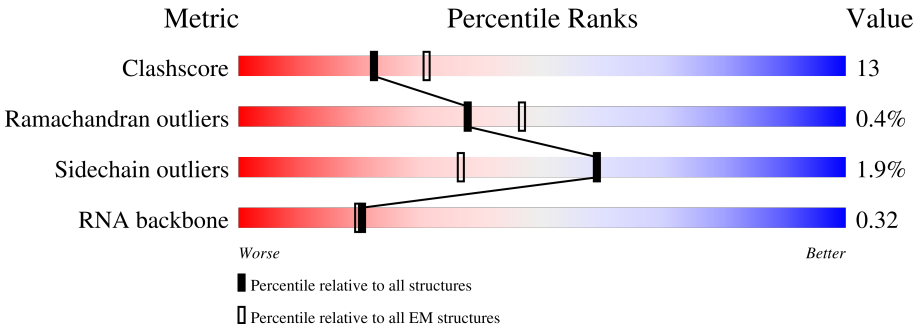
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	A	443	53% 12% 35%
2	B	249	79% 17%
3	C	278	81% 14% 5%
4	D	237	75% 14% 11%
5	E	295	80% 17%
6	F	276	82% 6% 12%
7	G	293	5% 63% 8% 28%

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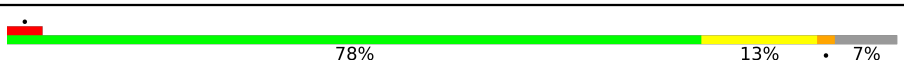
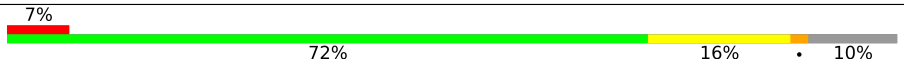
Mol	Chain	Length	Quality of chain
8	H	297	
9	I	199	
10	J	962	
11	K	166	
12	R	44	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22138 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 RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	287	Total	C	N	O	S	0	0
			2221	1400	394	410	17		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Exosome complex component RRP41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	239	Total	C	N	O	S	0	0
			1771	1096	332	334	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q9NPD3
B	-2	PRO	-	expression tag	UNP Q9NPD3
B	-1	ASP	-	expression tag	UNP Q9NPD3
B	0	SER	-	expression tag	UNP Q9NPD3

- Molecule 3 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	264	Total	C	N	O	S	0	0
			1923	1209	315	385	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ARG	-	expression tag	UNP Q96B26
C	0	SER	-	expression tag	UNP Q96B26

- Molecule 4 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	210	Total	C	N	O	S	0	0
			1570	982	280	297	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ARG	-	expression tag	UNP Q9NQT4
D	0	SER	-	expression tag	UNP Q9NQT4

- Molecule 5 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	287	Total	C	N	O	S	0	0
			2144	1345	364	420	15		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	244	Total	C	N	O	S	0	0
			1752	1097	326	322	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP Q5RKV6
F	-2	PRO	-	expression tag	UNP Q5RKV6
F	-1	ASP	-	expression tag	UNP Q5RKV6
F	0	SER	-	expression tag	UNP Q5RKV6

- Molecule 7 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	210	Total	C	N	O	S	0	0
			1527	979	272	267	9		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-17	GLY	-	expression tag	UNP Q9NQT5
G	-16	SER	-	expression tag	UNP Q9NQT5
G	-15	GLY	-	expression tag	UNP Q9NQT5
G	-14	SER	-	expression tag	UNP Q9NQT5
G	-13	GLY	-	expression tag	UNP Q9NQT5
G	-12	SER	-	expression tag	UNP Q9NQT5
G	-11	GLY	-	expression tag	UNP Q9NQT5
G	-10	SER	-	expression tag	UNP Q9NQT5
G	-9	GLY	-	expression tag	UNP Q9NQT5
G	-8	SER	-	expression tag	UNP Q9NQT5
G	-7	GLY	-	expression tag	UNP Q9NQT5
G	-6	SER	-	expression tag	UNP Q9NQT5
G	-5	GLY	-	expression tag	UNP Q9NQT5
G	-4	SER	-	expression tag	UNP Q9NQT5
G	-3	GLY	-	expression tag	UNP Q9NQT5
G	-2	SER	-	expression tag	UNP Q9NQT5
G	-1	GLY	-	expression tag	UNP Q9NQT5
G	0	SER	-	expression tag	UNP Q9NQT5

- Molecule 8 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	275	Total	C	N	O	S	0	0
			2066	1306	364	384	12		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 9 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	50	Total	C	N	O	S	0	0
			373	233	66	70	4		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 10 is a protein called Exosome complex exonuclease RRP44.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	868	Total	C	N	O	S	0	0
			6488	4100	1176	1184	28		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP Q9Y2L1
J	-2	PRO	-	expression tag	UNP Q9Y2L1
J	-1	ASP	-	expression tag	UNP Q9Y2L1
J	0	SER	-	expression tag	UNP Q9Y2L1
J	146	ASN	ASP	engineered mutation	UNP Q9Y2L1
J	487	ASN	ASP	engineered mutation	UNP Q9Y2L1

- Molecule 11 is a protein called M-phase phosphoprotein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			183	109	37	37		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	GLY	-	expression tag	UNP Q99547
K	-4	PRO	-	expression tag	UNP Q99547
K	-3	ASP	-	expression tag	UNP Q99547
K	-2	SER	-	expression tag	UNP Q99547
K	-1	ALA	-	expression tag	UNP Q99547
K	0	SER	-	expression tag	UNP Q99547

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Chain	Residue	Modelled	Actual	Comment	Reference
K	8	LYS	ARG	conflict	UNP Q99547

- Molecule 12 is a RNA chain called U44 ssRNA.

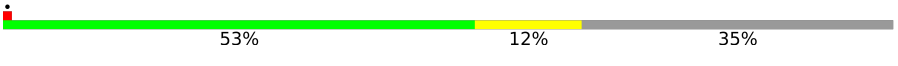
Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

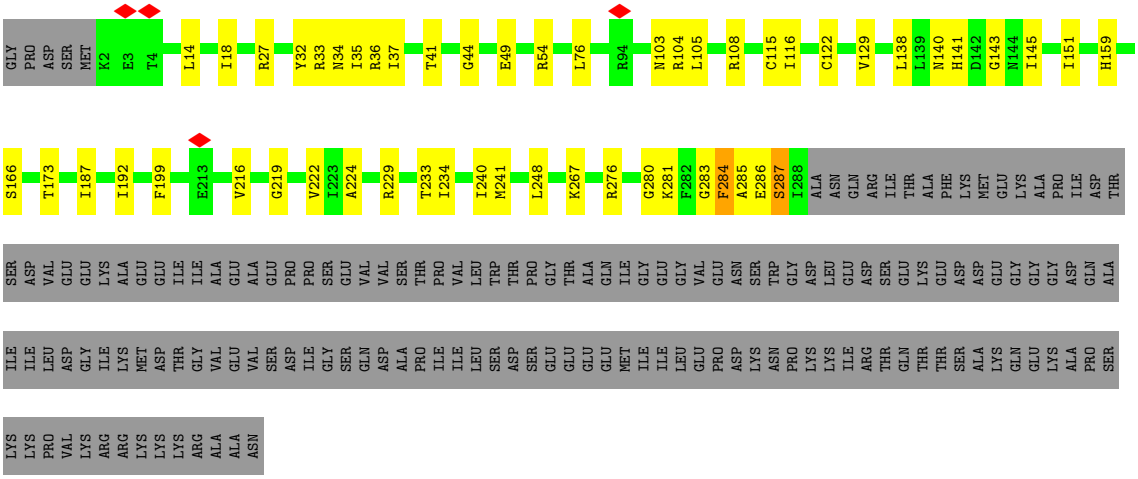
3 Residue-property plots (i)

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 RRP45

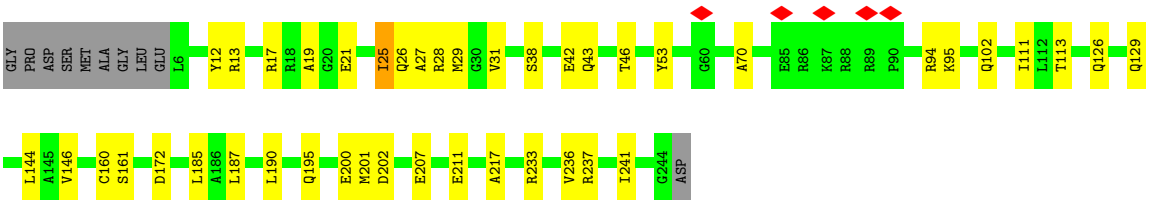
Chain A:





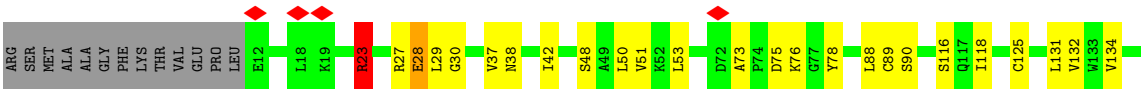
• Molecule 2: Exosome complex component RRP41

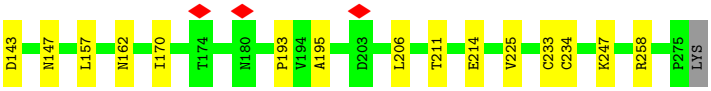
Chain B:



• Molecule 3: Exosome complex component RRP43

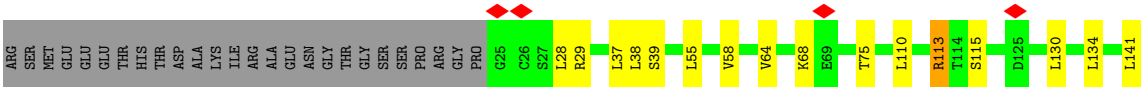
Chain C:

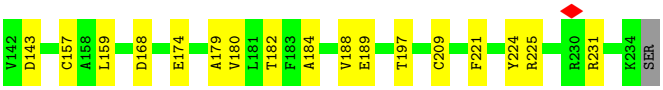




• Molecule 4: Exosome complex component RRP46

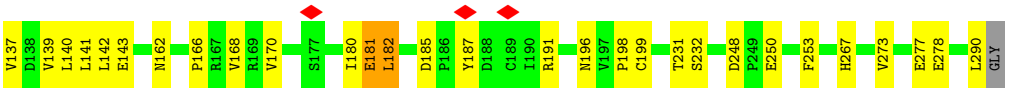
Chain D:





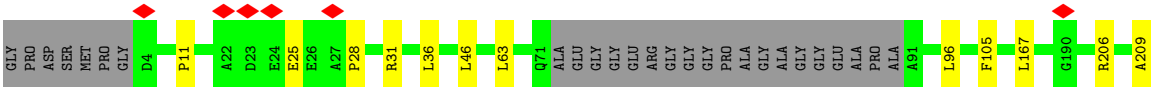
• Molecule 5: Exosome complex component RRP42

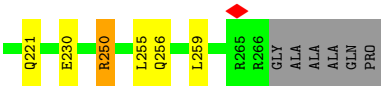
Chain E:



• Molecule 6: Exosome complex component MTR3

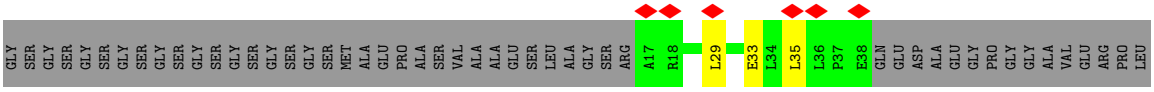
Chain F:

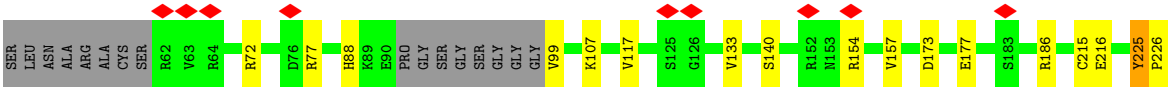


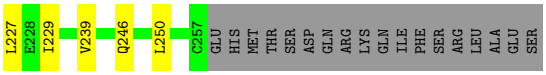


• Molecule 7: Exosome complex component RRP40

Chain G:

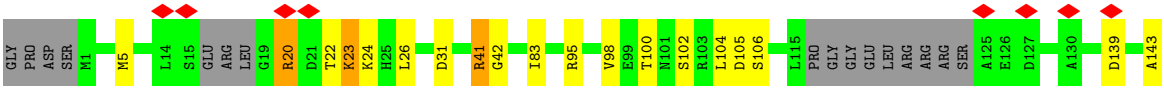


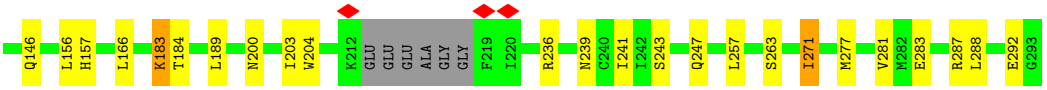




• Molecule 8: Exosome complex component RRP4

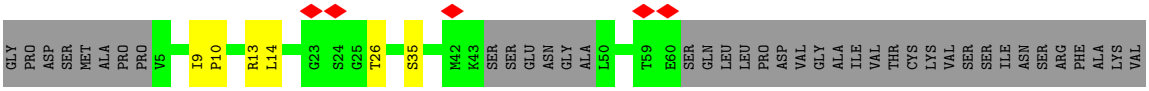
Chain H:





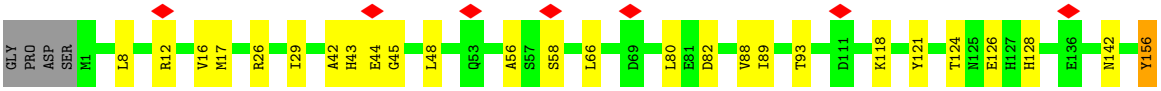
• Molecule 9: Exosome complex component CSL4

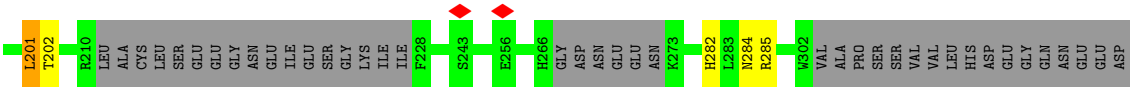
Chain I:

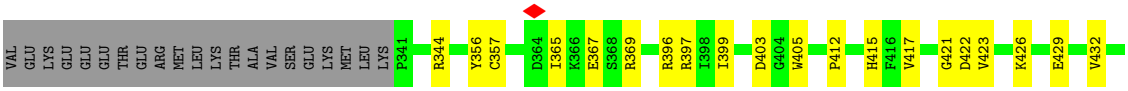


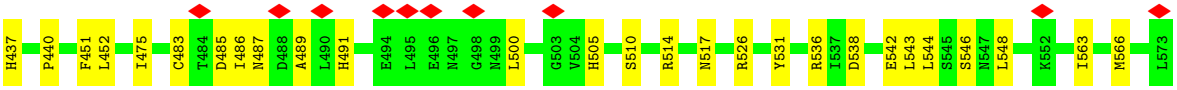
• Molecule 10: Exosome complex exonuclease RRP44

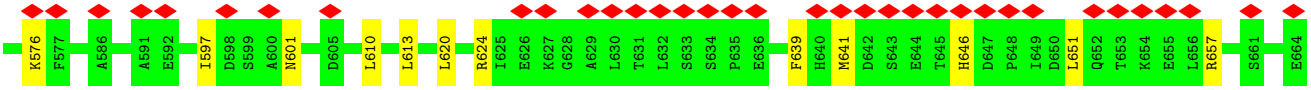
Chain J:

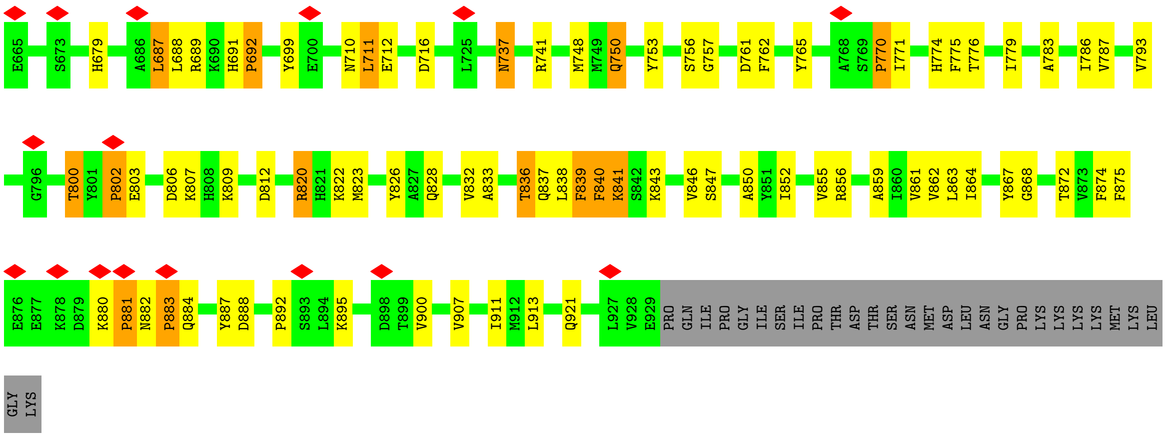




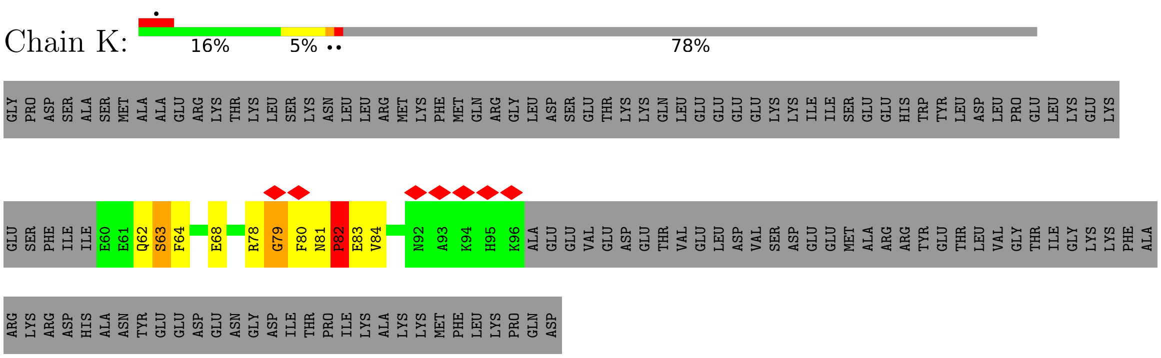




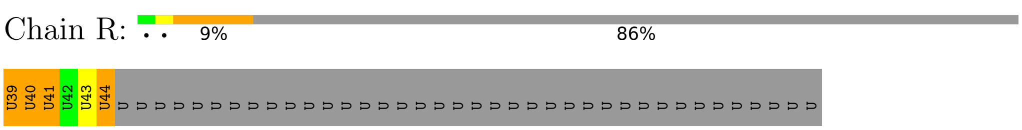




• Molecule 11: M-phase phosphoprotein 6



• Molecule 12: U44 ssRNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110958	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 ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.241	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	337.5, 337.5, 337.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	A	0.37	0/2254	0.57	0/3043
2	B	0.40	0/1795	0.60	1/2431 (0.0%)
3	C	0.36	0/1953	0.59	1/2662 (0.0%)
4	D	0.35	0/1590	0.58	0/2151
5	E	0.37	0/2175	0.60	1/2950 (0.0%)
6	F	0.33	0/1781	0.58	1/2425 (0.0%)
7	G	0.28	0/1549	0.53	0/2100
8	H	0.32	0/2094	0.57	0/2832
9	I	0.29	0/378	0.62	0/509
10	J	0.33	0/6621	0.61	7/9018 (0.1%)
11	K	0.62	0/182	0.64	1/252 (0.4%)
12	R	0.38	0/131	0.68	0/200
All	All	0.35	0/22503	0.59	12/30573 (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
3	C	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	802	PRO	CA-N-CD	-9.44	98.29	111.50
10	J	883	PRO	CA-N-CD	-9.42	98.31	111.50
10	J	881	PRO	CA-N-CD	-9.32	98.46	111.50
10	J	770	PRO	CA-N-CD	-9.20	98.62	111.50
10	J	692	PRO	CA-N-CD	-8.93	99.00	111.50
5	E	181	GLU	N-CA-C	5.85	126.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	53	LEU	CA-CB-CG	5.77	128.58	115.30
11	K	82	PRO	N-CA-CB	5.40	109.78	103.30
6	F	96	LEU	CA-CB-CG	5.29	127.46	115.30
10	J	716	ASP	CB-CG-OD2	5.23	123.01	118.30
10	J	812	ASP	CB-CG-OD2	5.22	122.99	118.30
2	B	190	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	23	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2221	0	2240	78	0
2	B	1771	0	1751	70	0
3	C	1923	0	1877	32	0
4	D	1570	0	1603	40	0
5	E	2144	0	2110	56	0
6	F	1752	0	1752	18	0
7	G	1527	0	1530	22	0
8	H	2066	0	2069	55	0
9	I	373	0	368	8	0
10	J	6488	0	6153	253	0
11	K	183	0	76	10	0
12	R	120	0	61	12	0
All	All	22138	0	21590	556	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 13.

All (556) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ILE:CD1	8:H:20:ARG:HB3	1.34	1.52
2:B:126:GLN:NE2	5:E:140:LEU:HD21	1.18	1.47
10:J:639:PHE:CE1	10:J:651:LEU:HD21	1.57	1.40
11:K:78:ARG:O	11:K:80:PHE:N	1.58	1.36
1:A:267:LYS:CD	1:A:286:GLU:OE2	1.81	1.29
10:J:855:VAL:HG12	10:J:887:TYR:OH	1.15	1.28
10:J:839:PHE:CZ	10:J:867:TYR:CE1	2.20	1.28
4:D:28:LEU:HD12	4:D:168:ASP:OD2	1.10	1.27
10:J:839:PHE:CZ	10:J:867:TYR:HE1	1.51	1.26
10:J:837:GLN:NE2	10:J:921:GLN:O	1.64	1.26
10:J:822:LYS:CD	10:J:826:TYR:CE2	2.18	1.25
3:C:28:GLU:CG	3:C:29:LEU:H	1.40	1.25
10:J:822:LYS:CD	10:J:826:TYR:HE2	1.50	1.24
10:J:822:LYS:O	10:J:826:TYR:CD2	1.91	1.23
10:J:58:SER:OG	10:J:202:THR:CG2	1.87	1.22
10:J:58:SER:OG	10:J:202:THR:HG21	1.36	1.21
1:A:267:LYS:HD3	1:A:286:GLU:OE2	1.08	1.21
10:J:201:LEU:O	10:J:202:THR:HG23	1.42	1.18
8:H:146:GLN:CB	8:H:157:HIS:HD2	1.57	1.17
2:B:241:ILE:CD1	8:H:20:ARG:CB	2.21	1.16
10:J:855:VAL:CG1	10:J:887:TYR:OH	1.92	1.15
10:J:822:LYS:O	10:J:826:TYR:HD2	1.26	1.15
2:B:126:GLN:NE2	5:E:140:LEU:CD2	2.10	1.13
10:J:806:ASP:HB3	10:J:809:LYS:HE2	1.24	1.13
4:D:28:LEU:CD1	4:D:168:ASP:OD2	1.97	1.12
5:E:248:ASP:OD1	6:F:221:GLN:HG2	1.46	1.12
10:J:687:LEU:HD23	10:J:786:ILE:HD11	1.23	1.12
3:C:28:GLU:HG2	3:C:29:LEU:H	1.13	1.12
10:J:639:PHE:CD1	10:J:651:LEU:HD21	1.85	1.12
10:J:483:CYS:SG	10:J:486:ILE:HD11	1.90	1.11
1:A:103:ASN:HD21	2:B:94:ARG:NH1	1.48	1.11
10:J:687:LEU:CD2	10:J:786:ILE:HD11	1.79	1.11
10:J:651:LEU:HD12	10:J:867:TYR:HD1	1.10	1.11
5:E:182:LEU:HD21	10:J:16:VAL:CG2	1.80	1.11
1:A:103:ASN:ND2	2:B:94:ARG:CZ	2.14	1.10
5:E:182:LEU:HD11	10:J:8:LEU:HD23	1.33	1.09
10:J:822:LYS:HD2	10:J:826:TYR:CE2	1.85	1.09
10:J:56:ALA:HB1	10:J:202:THR:OG1	1.50	1.09
10:J:440:PRO:HD3	10:J:820:ARG:HH21	1.15	1.08
10:J:639:PHE:CD1	10:J:651:LEU:CD2	2.36	1.08
2:B:241:ILE:HD13	8:H:20:ARG:CB	1.84	1.07
1:A:36:ARG:HG2	1:A:287:SER:HB3	1.36	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:146:GLN:HB2	8:H:157:HIS:HD2	1.17	1.05
10:J:639:PHE:CE1	10:J:651:LEU:CD2	2.40	1.05
10:J:822:LYS:HD3	10:J:826:TYR:CZ	1.91	1.05
3:C:23:ARG:HB2	3:C:27:ARG:O	1.55	1.04
3:C:28:GLU:HG3	3:C:29:LEU:H	1.18	1.04
10:J:48:LEU:HD21	10:J:121:TYR:HB3	1.38	1.04
10:J:822:LYS:HD3	10:J:826:TYR:CE2	1.90	1.04
8:H:146:GLN:HB2	8:H:157:HIS:CD2	1.93	1.03
10:J:881:PRO:C	10:J:883:PRO:HD3	1.77	1.03
5:E:182:LEU:CD2	10:J:16:VAL:HG21	1.88	1.02
10:J:531:TYR:O	10:J:828:GLN:HG2	1.59	1.02
10:J:839:PHE:HZ	10:J:867:TYR:CE1	1.66	1.02
2:B:126:GLN:HE21	5:E:140:LEU:CD2	1.69	1.02
8:H:146:GLN:CA	8:H:157:HIS:HD2	1.73	1.02
7:G:225:TYR:HB2	7:G:226:PRO:HD2	1.41	1.01
10:J:837:GLN:HE22	10:J:921:GLN:C	1.63	1.01
10:J:856:ARG:HB2	10:J:859:ALA:O	1.60	1.01
1:A:103:ASN:ND2	2:B:94:ARG:NH1	2.08	1.01
10:J:651:LEU:HD12	10:J:867:TYR:CD1	1.95	1.00
10:J:833:ALA:O	10:J:836:THR:HG23	1.60	1.00
1:A:35:ILE:O	1:A:287:SER:HA	1.61	1.00
3:C:28:GLU:CG	3:C:29:LEU:N	2.13	0.99
10:J:48:LEU:HD21	10:J:121:TYR:CB	1.92	0.99
10:J:770:PRO:HD2	10:J:771:ILE:H	1.28	0.98
10:J:822:LYS:HD3	10:J:826:TYR:OH	1.60	0.98
10:J:832:VAL:O	10:J:836:THR:HG22	1.62	0.98
10:J:802:PRO:HD2	10:J:803:GLU:H	1.27	0.98
5:E:182:LEU:HD21	10:J:16:VAL:HG21	0.98	0.98
10:J:793:VAL:CB	10:J:800:THR:CG2	2.41	0.98
10:J:793:VAL:CB	10:J:800:THR:HG22	1.93	0.97
5:E:248:ASP:OD1	6:F:221:GLN:CG	2.13	0.97
8:H:146:GLN:CB	8:H:157:HIS:CD2	2.48	0.97
1:A:54:ARG:NH1	4:D:37:LEU:HB3	1.79	0.97
10:J:437:HIS:HB3	10:J:823:MET:HE3	1.48	0.96
3:C:28:GLU:HG3	3:C:29:LEU:N	1.80	0.95
2:B:241:ILE:CG1	8:H:20:ARG:HB3	1.97	0.94
1:A:54:ARG:NH1	4:D:37:LEU:HD23	1.83	0.94
8:H:146:GLN:CA	8:H:157:HIS:CD2	2.51	0.93
10:J:840:PHE:CZ	10:J:911:ILE:HG13	2.02	0.93
5:E:57:ASP:OD2	5:E:142:LEU:HD12	1.68	0.93
10:J:483:CYS:SG	10:J:486:ILE:CD1	2.57	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ILE:HD13	8:H:20:ARG:HB3	0.93	0.92
8:H:20:ARG:HH11	8:H:20:ARG:HG2	1.34	0.91
10:J:852:ILE:HD11	10:J:907:VAL:HG11	1.51	0.91
8:H:146:GLN:HA	8:H:157:HIS:CD2	2.06	0.89
2:B:126:GLN:HE22	5:E:140:LEU:HD21	1.34	0.89
1:A:54:ARG:HH12	4:D:37:LEU:HB3	1.35	0.89
10:J:855:VAL:HG12	10:J:887:TYR:HH	1.09	0.88
10:J:80:LEU:O	10:J:118:LYS:NZ	2.06	0.88
1:A:36:ARG:CG	1:A:287:SER:HB3	2.03	0.87
1:A:103:ASN:HD21	2:B:94:ARG:CZ	1.83	0.87
7:G:225:TYR:CE1	7:G:227:LEU:HD23	2.08	0.87
10:J:881:PRO:O	10:J:883:PRO:CD	2.21	0.87
10:J:56:ALA:CB	10:J:202:THR:OG1	2.22	0.86
10:J:639:PHE:HE1	10:J:651:LEU:HD21	1.39	0.86
10:J:822:LYS:CG	10:J:826:TYR:HE2	1.88	0.85
1:A:54:ARG:HH12	4:D:37:LEU:CD2	1.89	0.85
10:J:753:TYR:HH	10:J:774:HIS:HD1	1.23	0.84
10:J:880:LYS:CB	10:J:881:PRO:HD3	2.06	0.84
5:E:170:VAL:HG22	5:E:180:ILE:HG22	1.58	0.84
11:K:78:ARG:C	11:K:80:PHE:N	2.28	0.84
10:J:483:CYS:SG	10:J:486:ILE:CG1	2.65	0.84
10:J:833:ALA:O	10:J:836:THR:CG2	2.26	0.84
1:A:34:ASN:OD1	1:A:34:ASN:O	1.95	0.83
2:B:241:ILE:HD11	8:H:20:ARG:CB	2.08	0.83
2:B:12:TYR:CD2	10:J:124:THR:HG21	2.13	0.83
4:D:159:LEU:HD21	4:D:209:CYS:SG	2.18	0.82
10:J:840:PHE:HZ	10:J:911:ILE:HG13	1.42	0.82
2:B:241:ILE:HD11	8:H:20:ARG:HB3	1.55	0.82
10:J:620:LEU:O	10:J:624:ARG:HB2	1.80	0.82
5:E:39:THR:HG21	5:E:277:GLU:HG2	1.60	0.82
1:A:36:ARG:HH21	1:A:284:PHE:HZ	1.28	0.81
1:A:54:ARG:HH12	4:D:37:LEU:HD23	1.44	0.81
9:I:9:ILE:HG23	9:I:10:PRO:HD2	1.59	0.81
5:E:182:LEU:CD2	10:J:16:VAL:CG2	2.52	0.81
10:J:839:PHE:CE1	10:J:867:TYR:CE1	2.68	0.81
10:J:687:LEU:HD12	10:J:688:LEU:N	1.95	0.80
10:J:687:LEU:HD23	10:J:786:ILE:CD1	2.10	0.80
11:K:62:GLN:O	11:K:63:SER:O	2.00	0.80
10:J:881:PRO:C	10:J:883:PRO:CD	2.50	0.80
10:J:856:ARG:HB2	10:J:859:ALA:C	2.01	0.79
10:J:833:ALA:HA	10:J:836:THR:CG2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:483:CYS:SG	10:J:486:ILE:HG13	2.23	0.79
7:G:225:TYR:HE1	7:G:227:LEU:HD23	1.45	0.79
10:J:770:PRO:HD2	10:J:771:ILE:N	1.97	0.79
10:J:775:PHE:HD1	10:J:787:VAL:CG1	1.94	0.79
10:J:201:LEU:O	10:J:202:THR:CG2	2.30	0.78
5:E:248:ASP:OD1	6:F:221:GLN:CD	2.22	0.78
10:J:822:LYS:O	10:J:826:TYR:CE2	2.36	0.78
10:J:639:PHE:CD1	10:J:651:LEU:HD23	2.18	0.78
10:J:802:PRO:HD2	10:J:803:GLU:N	1.97	0.77
1:A:103:ASN:HD21	2:B:94:ARG:HH12	1.30	0.77
1:A:54:ARG:CZ	4:D:37:LEU:HB3	2.15	0.77
10:J:881:PRO:O	10:J:883:PRO:HD2	1.84	0.77
10:J:850:ALA:HB1	10:J:863:LEU:O	1.85	0.77
1:A:36:ARG:NH2	1:A:284:PHE:HZ	1.82	0.76
10:J:883:PRO:HD2	10:J:884:GLN:H	1.50	0.76
1:A:54:ARG:HH12	4:D:37:LEU:CB	1.98	0.76
1:A:36:ARG:HE	1:A:284:PHE:HZ	1.34	0.76
10:J:750:GLN:NE2	12:R:39:U:O2	2.18	0.76
10:J:850:ALA:HB2	10:J:864:ILE:HG12	1.68	0.76
10:J:58:SER:HG	10:J:202:THR:CG2	1.94	0.75
10:J:440:PRO:CD	10:J:820:ARG:HH21	1.95	0.75
10:J:856:ARG:CB	10:J:859:ALA:O	2.33	0.75
10:J:58:SER:OG	10:J:202:THR:HG23	1.83	0.75
10:J:852:ILE:CD1	10:J:907:VAL:HG11	2.16	0.75
11:K:78:ARG:O	11:K:79:GLY:C	2.23	0.75
3:C:28:GLU:HG2	3:C:29:LEU:N	1.86	0.74
10:J:803:GLU:HA	10:J:809:LYS:NZ	2.02	0.74
10:J:852:ILE:HG12	10:J:862:VAL:HG12	1.66	0.74
10:J:880:LYS:CB	10:J:881:PRO:CD	2.66	0.74
5:E:39:THR:CG2	5:E:277:GLU:HG2	2.17	0.73
10:J:687:LEU:HD22	10:J:786:ILE:HD11	1.70	0.73
1:A:104:ARG:NH2	2:B:95:LYS:HE2	2.03	0.73
1:A:103:ASN:ND2	2:B:94:ARG:NH2	2.37	0.73
5:E:248:ASP:OD1	6:F:221:GLN:NE2	2.22	0.73
10:J:783:ALA:O	10:J:787:VAL:HG23	1.89	0.73
10:J:806:ASP:CB	10:J:809:LYS:HE2	2.13	0.73
8:H:20:ARG:HG2	8:H:20:ARG:NH1	1.96	0.72
1:A:283:GLY:O	1:A:284:PHE:O	2.08	0.72
10:J:531:TYR:H	10:J:828:GLN:HE21	1.36	0.72
2:B:12:TYR:HD2	10:J:124:THR:HG21	1.55	0.72
4:D:157:CYS:SG	4:D:209:CYS:HB3	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:500:LEU:HB2	10:J:566:MET:O	1.91	0.71
10:J:531:TYR:HB2	10:J:828:GLN:NE2	2.05	0.70
2:B:241:ILE:HG12	8:H:20:ARG:CB	2.22	0.70
1:A:36:ARG:NH2	1:A:284:PHE:CZ	2.57	0.70
12:R:40:U:H4'	12:R:40:U:OP1	1.91	0.70
3:C:23:ARG:NE	3:C:214:GLU:OE2	2.24	0.70
5:E:115:ASN:HD22	5:E:118:SER:HB2	1.56	0.70
10:J:833:ALA:HA	10:J:836:THR:HG21	1.73	0.70
10:J:440:PRO:HD3	10:J:820:ARG:NH2	1.99	0.70
10:J:651:LEU:CD1	10:J:867:TYR:HD1	1.98	0.70
10:J:775:PHE:HD1	10:J:787:VAL:HG11	1.55	0.69
10:J:48:LEU:HD21	10:J:121:TYR:HB2	1.75	0.69
1:A:36:ARG:NE	1:A:284:PHE:HZ	1.89	0.69
2:B:126:GLN:HE22	5:E:140:LEU:HD11	1.57	0.68
10:J:840:PHE:CZ	10:J:911:ILE:CG1	2.75	0.68
1:A:35:ILE:O	1:A:287:SER:CA	2.40	0.68
1:A:54:ARG:HH22	4:D:37:LEU:CG	2.06	0.67
5:E:166:PRO:HB3	10:J:8:LEU:HD21	1.75	0.67
12:R:39:U:H4'	12:R:40:U:OP2	1.93	0.67
2:B:12:TYR:CE2	10:J:124:THR:HG21	2.30	0.67
10:J:841:LYS:O	10:J:841:LYS:HD3	1.93	0.67
2:B:126:GLN:HE22	5:E:140:LEU:CG	2.08	0.66
3:C:38:ASN:HD22	3:C:50:LEU:HD23	1.60	0.66
5:E:168:VAL:HG22	5:E:182:LEU:HD22	1.76	0.66
1:A:280:GLY:O	1:A:281:LYS:HG3	1.95	0.66
5:E:39:THR:HG21	5:E:277:GLU:CG	2.24	0.66
3:C:48:SER:H	3:C:162:ASN:HD22	1.44	0.66
10:J:775:PHE:CD1	10:J:787:VAL:HG12	2.29	0.66
11:K:78:ARG:O	11:K:80:PHE:CA	2.43	0.66
5:E:166:PRO:CB	10:J:8:LEU:HD21	2.26	0.66
6:F:36:LEU:HD11	6:F:250:ARG:HG2	1.78	0.66
10:J:687:LEU:HD12	10:J:687:LEU:C	2.16	0.65
10:J:775:PHE:CD1	10:J:787:VAL:CG1	2.78	0.65
2:B:241:ILE:CG1	8:H:20:ARG:CB	2.65	0.65
10:J:536:ARG:NH1	12:R:44:U:O3'	2.30	0.65
10:J:883:PRO:HD2	10:J:884:GLN:N	2.10	0.65
1:A:36:ARG:CZ	1:A:284:PHE:HZ	2.10	0.64
10:J:756:SER:HB3	10:J:762:PHE:HE2	1.62	0.64
10:J:856:ARG:HB2	10:J:859:ALA:CA	2.27	0.64
9:I:9:ILE:CG2	9:I:10:PRO:HD2	2.28	0.64
7:G:226:PRO:HA	11:K:78:ARG:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:689:ARG:NH2	12:R:41:U:OP2	2.31	0.64
7:G:225:TYR:HB2	7:G:226:PRO:CD	2.20	0.64
10:J:802:PRO:CD	10:J:803:GLU:H	2.08	0.64
8:H:283:GLU:OE2	8:H:287:ARG:NH2	2.31	0.63
10:J:856:ARG:N	10:J:859:ALA:O	2.29	0.63
1:A:54:ARG:HH22	4:D:37:LEU:HG	1.62	0.63
10:J:691:HIS:HD2	10:J:692:PRO:HD3	1.64	0.63
1:A:14:LEU:HD22	1:A:216:VAL:HG21	1.81	0.63
1:A:54:ARG:HH22	4:D:37:LEU:CB	2.12	0.62
5:E:170:VAL:HG22	5:E:180:ILE:CG2	2.28	0.62
7:G:225:TYR:CZ	7:G:246:GLN:HB3	2.34	0.62
1:A:54:ARG:NH2	4:D:37:LEU:HB3	2.15	0.62
3:C:157:LEU:HD21	3:C:193:PRO:HD2	1.81	0.62
12:R:39:U:H2'	12:R:39:U:OP2	2.00	0.62
3:C:30:GLY:O	3:C:258:ARG:NH2	2.32	0.61
5:E:39:THR:OG1	5:E:162:ASN:ND2	2.33	0.61
10:J:833:ALA:CA	10:J:836:THR:CG2	2.79	0.61
10:J:48:LEU:CD2	10:J:121:TYR:HB2	2.30	0.61
10:J:437:HIS:CB	10:J:823:MET:HE3	2.26	0.61
10:J:881:PRO:O	10:J:881:PRO:HD2	2.00	0.61
10:J:839:PHE:HZ	10:J:867:TYR:CZ	2.18	0.60
10:J:882:ASN:N	10:J:883:PRO:HD3	2.16	0.60
2:B:160:CYS:SG	2:B:161:SER:N	2.73	0.60
2:B:126:GLN:HE22	5:E:140:LEU:CD1	2.14	0.60
10:J:822:LYS:HD3	10:J:826:TYR:HH	1.63	0.60
1:A:108:ARG:NH1	2:B:200:GLU:OE1	2.32	0.60
2:B:237:ARG:HD3	8:H:20:ARG:NH1	2.17	0.60
8:H:236:ARG:NH2	8:H:263:SER:O	2.34	0.60
1:A:122:CYS:HA	1:A:129:VAL:HG23	1.84	0.59
2:B:28:ARG:CZ	5:E:290:LEU:HD13	2.33	0.59
5:E:182:LEU:HD12	5:E:182:LEU:O	2.03	0.59
10:J:452:LEU:HD13	10:J:543:LEU:HD22	1.83	0.59
10:J:856:ARG:HB2	10:J:859:ALA:N	2.16	0.59
1:A:44:GLY:H	1:A:159:HIS:HD2	1.49	0.59
3:C:78:TYR:HB2	3:C:134:VAL:HG22	1.85	0.59
10:J:58:SER:HG	10:J:202:THR:HG23	1.61	0.59
10:J:770:PRO:CD	10:J:771:ILE:N	2.66	0.59
10:J:802:PRO:CD	10:J:803:GLU:N	2.65	0.59
12:R:40:U:H2'	12:R:41:U:H5'	1.85	0.59
2:B:237:ARG:HD3	8:H:20:ARG:CZ	2.32	0.58
8:H:243:SER:HB2	8:H:277:MET:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:833:ALA:C	10:J:836:THR:CG2	2.71	0.58
7:G:140:SER:HB3	7:G:177:GLU:HG2	1.86	0.58
8:H:24:LYS:O	8:H:26:LEU:HD12	2.03	0.58
8:H:143:ALA:HB3	8:H:156:LEU:HD12	1.86	0.58
2:B:241:ILE:HG12	8:H:20:ARG:HB2	1.85	0.58
6:F:167:LEU:HD11	6:F:255:LEU:HD22	1.86	0.58
10:J:832:VAL:O	10:J:836:THR:CG2	2.47	0.58
2:B:126:GLN:HE22	5:E:140:LEU:CD2	1.97	0.58
10:J:437:HIS:HB3	10:J:823:MET:CE	2.27	0.58
4:D:113:ARG:NH2	7:G:173:ASP:O	2.38	0.57
9:I:9:ILE:HG23	9:I:10:PRO:CD	2.33	0.57
10:J:846:VAL:HG12	10:J:847:SER:N	2.19	0.57
10:J:16:VAL:O	10:J:16:VAL:HG13	2.04	0.57
1:A:103:ASN:HD22	2:B:94:ARG:CZ	2.09	0.57
1:A:267:LYS:CD	1:A:286:GLU:CD	2.67	0.57
10:J:803:GLU:HA	10:J:809:LYS:HZ1	1.70	0.57
10:J:12:ARG:HH21	10:J:369:ARG:HH11	1.51	0.57
10:J:437:HIS:CA	10:J:823:MET:CE	2.82	0.57
10:J:770:PRO:CD	10:J:771:ILE:H	2.09	0.57
5:E:83:VAL:HG22	5:E:139:VAL:HB	1.87	0.57
1:A:267:LYS:HD3	1:A:286:GLU:CD	2.11	0.57
3:C:37:VAL:HG12	3:C:51:VAL:HG22	1.87	0.56
4:D:159:LEU:CD2	4:D:209:CYS:SG	2.93	0.56
1:A:248:LEU:HD11	2:B:211:GLU:HB2	1.87	0.56
10:J:756:SER:CB	10:J:762:PHE:HE2	2.18	0.56
3:C:125:CYS:HA	3:C:132:VAL:HG23	1.86	0.56
10:J:803:GLU:CA	10:J:809:LYS:HZ1	2.18	0.56
10:J:793:VAL:CB	10:J:800:THR:HG21	2.33	0.56
10:J:856:ARG:HB2	10:J:859:ALA:H	1.69	0.56
1:A:115:CYS:SG	1:A:116:ILE:N	2.79	0.56
2:B:27:ALA:HB1	2:B:144:LEU:HD13	1.86	0.56
2:B:241:ILE:HD11	8:H:20:ARG:CG	2.35	0.56
6:F:25:GLU:O	6:F:206:ARG:NH2	2.38	0.56
10:J:396:ARG:HH21	10:J:421:GLY:HA2	1.69	0.56
10:J:822:LYS:HD2	10:J:826:TYR:HE2	1.28	0.56
2:B:21:GLU:OE2	10:J:26:ARG:NH1	2.39	0.56
5:E:112:ILE:HG23	5:E:198:PRO:HG2	1.88	0.56
4:D:188:VAL:HG12	4:D:189:GLU:HG3	1.86	0.56
10:J:437:HIS:O	10:J:823:MET:CE	2.54	0.56
10:J:822:LYS:CG	10:J:826:TYR:CE2	2.77	0.56
10:J:437:HIS:HA	10:J:823:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:803:GLU:CA	10:J:809:LYS:NZ	2.69	0.55
10:J:12:ARG:NH2	10:J:369:ARG:HH11	2.04	0.55
1:A:267:LYS:CE	1:A:286:GLU:OE2	2.53	0.55
2:B:126:GLN:HE21	5:E:140:LEU:HD21	0.76	0.55
10:J:43:HIS:O	10:J:45:GLY:N	2.40	0.55
10:J:833:ALA:C	10:J:836:THR:HG22	2.27	0.55
2:B:236:VAL:HG13	8:H:26:LEU:HD23	1.87	0.55
3:C:116:SER:OG	3:C:118:ILE:HG23	2.06	0.55
1:A:54:ARG:CZ	4:D:37:LEU:HD23	2.37	0.54
2:B:233:ARG:NH2	8:H:31:ASP:OD2	2.40	0.54
10:J:803:GLU:HA	10:J:809:LYS:HZ3	1.71	0.54
10:J:833:ALA:CA	10:J:836:THR:HG22	2.38	0.54
4:D:39:SER:O	7:G:107:LYS:NZ	2.40	0.54
4:D:159:LEU:HB2	4:D:179:ALA:HB3	1.90	0.54
11:K:62:GLN:C	11:K:63:SER:O	2.44	0.54
2:B:102:GLN:NE2	2:B:200:GLU:OE2	2.40	0.54
10:J:12:ARG:HH21	10:J:369:ARG:NH1	2.05	0.54
10:J:58:SER:CB	10:J:202:THR:HG21	2.33	0.53
10:J:839:PHE:CZ	10:J:843:LYS:HD2	2.43	0.53
10:J:856:ARG:HG3	10:J:859:ALA:HB3	1.90	0.53
10:J:855:VAL:CG1	10:J:887:TYR:CZ	2.89	0.53
10:J:89:ILE:HG21	10:J:156:TYR:HE2	1.73	0.53
12:R:39:U:C4'	12:R:40:U:OP2	2.56	0.53
1:A:241:MET:HB3	2:B:195:GLN:HB3	1.90	0.53
5:E:39:THR:OG1	5:E:162:ASN:OD1	2.27	0.53
10:J:542:GLU:O	10:J:546:SER:CB	2.57	0.53
10:J:489:ALA:HB3	10:J:505:HIS:HB2	1.89	0.53
1:A:166:SER:OG	1:A:173:THR:OG1	2.27	0.53
2:B:185:LEU:HD12	2:B:201:MET:HG3	1.90	0.53
2:B:241:ILE:CD1	8:H:20:ARG:CG	2.87	0.53
2:B:241:ILE:HG23	8:H:20:ARG:HA	1.90	0.53
2:B:46:THR:HA	2:B:129:GLN:O	2.09	0.53
10:J:510:SER:O	10:J:514:ARG:NH2	2.42	0.53
10:J:852:ILE:HG12	10:J:862:VAL:CG1	2.36	0.52
1:A:140:ASN:HD21	4:D:39:SER:H	1.58	0.52
6:F:28:PRO:HB2	6:F:31:ARG:HH12	1.74	0.52
10:J:437:HIS:CB	10:J:823:MET:CE	2.87	0.52
5:E:117:SER:O	5:E:196:ASN:ND2	2.43	0.52
5:E:191:ARG:NH2	5:E:278:GLU:OE2	2.42	0.52
10:J:451:PHE:HB3	10:J:517:ASN:HD21	1.75	0.52
8:H:288:LEU:O	8:H:292:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:531:TYR:HB2	10:J:828:GLN:HE21	1.74	0.52
2:B:25:ILE:HB	2:B:43:GLN:HG2	1.92	0.51
10:J:793:VAL:CB	10:J:800:THR:HB	2.40	0.51
7:G:33:GLU:OE1	7:G:77:ARG:NH1	2.42	0.51
10:J:793:VAL:CB	10:J:800:THR:CB	2.89	0.51
3:C:23:ARG:CB	3:C:27:ARG:O	2.44	0.51
8:H:102:SER:OG	8:H:104:LEU:O	2.29	0.51
8:H:203:ILE:HG21	8:H:241:ILE:HD13	1.91	0.51
10:J:437:HIS:O	10:J:823:MET:HE3	2.11	0.51
4:D:174:GLU:HG3	4:D:180:VAL:HG21	1.91	0.51
5:E:23:ARG:NH1	5:E:28:GLY:O	2.43	0.51
10:J:699:TYR:OH	10:J:748:MET:CE	2.59	0.51
2:B:25:ILE:HA	2:B:42:GLU:O	2.10	0.51
6:F:259:LEU:HD22	9:I:9:ILE:HG12	1.92	0.51
10:J:58:SER:HG	10:J:202:THR:HG21	1.58	0.51
10:J:692:PRO:HD2	10:J:692:PRO:O	2.11	0.51
10:J:822:LYS:HG2	10:J:826:TYR:HE2	1.67	0.50
10:J:850:ALA:HB2	10:J:864:ILE:CG1	2.40	0.50
10:J:756:SER:HB2	10:J:762:PHE:CZ	2.46	0.50
1:A:54:ARG:NH2	4:D:37:LEU:CB	2.74	0.50
8:H:146:GLN:HA	8:H:157:HIS:NE2	2.26	0.50
10:J:542:GLU:O	10:J:546:SER:HB2	2.10	0.50
10:J:756:SER:CB	10:J:762:PHE:CE2	2.95	0.50
4:D:143:ASP:OD1	4:D:231:ARG:NH1	2.44	0.50
10:J:66:LEU:HB2	10:J:88:VAL:HG22	1.93	0.50
10:J:485:ASP:O	10:J:486:ILE:HG13	2.11	0.50
10:J:689:ARG:NE	12:R:41:U:OP2	2.44	0.50
8:H:20:ARG:HH11	8:H:20:ARG:CG	2.13	0.50
10:J:82:ASP:O	10:J:118:LYS:HE2	2.11	0.50
10:J:822:LYS:HG2	10:J:826:TYR:CE2	2.43	0.50
1:A:267:LYS:HD2	1:A:286:GLU:OE2	1.98	0.50
5:E:182:LEU:CD1	10:J:8:LEU:HD23	2.24	0.50
7:G:227:LEU:HD22	7:G:250:LEU:HD22	1.94	0.50
8:H:98:VAL:O	8:H:106:SER:N	2.45	0.50
5:E:36:GLU:HB2	5:E:52:LYS:HB3	1.93	0.50
8:H:24:LYS:O	8:H:26:LEU:CD1	2.60	0.50
10:J:29:ILE:HB	10:J:128:HIS:HD2	1.76	0.50
1:A:116:ILE:HG22	1:A:187:ILE:HG12	1.94	0.49
10:J:526:ARG:NH1	10:J:538:ASP:O	2.45	0.49
10:J:531:TYR:N	10:J:828:GLN:HE21	2.08	0.49
1:A:103:ASN:HD22	2:B:94:ARG:NH2	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:O	1:A:234:ILE:HA	2.12	0.49
10:J:688:LEU:CD1	10:J:762:PHE:CD2	2.95	0.49
10:J:42:ALA:O	10:J:43:HIS:C	2.50	0.49
10:J:397:ARG:NE	10:J:429:GLU:OE2	2.46	0.49
10:J:426:LYS:NZ	10:J:646:HIS:O	2.44	0.49
10:J:756:SER:HB2	10:J:762:PHE:CE2	2.48	0.49
11:K:82:PRO:C	11:K:84:VAL:N	2.63	0.49
5:E:232:SER:HA	5:E:267:HIS:ND1	2.27	0.49
4:D:157:CYS:HG	4:D:209:CYS:CB	2.24	0.49
10:J:688:LEU:CD1	10:J:762:PHE:HD2	2.26	0.49
2:B:241:ILE:HD11	8:H:20:ARG:HG2	1.93	0.49
10:J:440:PRO:HG2	10:J:526:ARG:HG2	1.94	0.49
3:C:206:LEU:HD22	3:C:247:LYS:HD2	1.95	0.49
1:A:283:GLY:C	1:A:284:PHE:O	2.48	0.49
3:C:131:LEU:HD12	3:C:170:ILE:HD11	1.95	0.49
10:J:806:ASP:HB3	10:J:809:LYS:CE	2.18	0.49
10:J:856:ARG:O	10:J:887:TYR:CZ	2.66	0.49
6:F:256:GLN:HG3	9:I:9:ILE:HD12	1.94	0.49
10:J:883:PRO:CD	10:J:884:GLN:N	2.76	0.49
8:H:105:ASP:OD1	8:H:105:ASP:N	2.46	0.48
10:J:365:ILE:HG22	10:J:367:GLU:H	1.77	0.48
10:J:563:ILE:HB	10:J:576:LYS:HB3	1.95	0.48
1:A:151:ILE:HG12	1:A:192:ILE:HD11	1.93	0.48
9:I:9:ILE:CG2	9:I:10:PRO:CD	2.91	0.48
10:J:403:ASP:OD2	10:J:415:HIS:ND1	2.45	0.48
4:D:130:LEU:HB2	4:D:182:THR:HG21	1.94	0.48
7:G:117:VAL:HG11	7:G:133:VAL:HG13	1.94	0.48
10:J:82:ASP:O	10:J:118:LYS:CE	2.62	0.48
1:A:37:ILE:O	1:A:285:ALA:HB3	2.13	0.48
1:A:138:LEU:HD13	1:A:145:ILE:HG23	1.95	0.48
3:C:73:ALA:HB1	3:C:76:LYS:HB2	1.96	0.48
3:C:89:CYS:SG	3:C:90:SER:N	2.87	0.48
7:G:215:CYS:SG	7:G:216:GLU:N	2.87	0.48
10:J:688:LEU:HD12	10:J:762:PHE:CD2	2.49	0.48
10:J:750:GLN:O	10:J:750:GLN:HG2	2.13	0.48
8:H:239:ASN:HB3	8:H:271:ILE:HD11	1.95	0.48
10:J:855:VAL:HG11	10:J:887:TYR:OH	2.03	0.48
8:H:183:LYS:HG2	8:H:184:THR:HG23	1.96	0.48
8:H:100:THR:HB	8:H:200:ASN:HD22	1.78	0.48
10:J:846:VAL:CG1	10:J:847:SER:N	2.76	0.48
10:J:895:LYS:HA	10:J:900:VAL:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLY:O	1:A:284:PHE:C	2.49	0.47
3:C:88:LEU:HD21	6:F:63:LEU:HD22	1.96	0.47
10:J:544:LEU:HD22	10:J:548:LEU:HB2	1.95	0.47
10:J:776:THR:OG1	12:R:43:U:OP1	2.24	0.47
5:E:182:LEU:HD23	10:J:16:VAL:HB	1.96	0.47
10:J:397:ARG:HG3	10:J:423:VAL:HG22	1.96	0.47
10:J:399:ILE:HG13	10:J:417:VAL:HG23	1.96	0.47
10:J:691:HIS:CD2	10:J:692:PRO:CD	2.98	0.47
10:J:475:ILE:HG12	10:J:491:HIS:HB3	1.96	0.47
10:J:839:PHE:CD1	10:J:839:PHE:C	2.85	0.47
4:D:28:LEU:HD12	4:D:168:ASP:CG	2.14	0.47
9:I:26:THR:HG22	9:I:35:SER:HA	1.95	0.47
1:A:36:ARG:NE	1:A:284:PHE:CZ	2.71	0.47
4:D:225:ARG:HB2	7:G:29:LEU:HD11	1.96	0.47
5:E:185:ASP:O	5:E:187:TYR:N	2.46	0.47
2:B:28:ARG:HD2	2:B:29:MET:N	2.30	0.47
4:D:64:VAL:HG22	4:D:115:SER:HB3	1.97	0.47
8:H:23:LYS:HD3	8:H:23:LYS:C	2.34	0.47
2:B:241:ILE:CG2	8:H:20:ARG:HA	2.45	0.47
10:J:356:TYR:O	10:J:399:ILE:HA	2.15	0.47
10:J:93:THR:OG1	10:J:126:GLU:OE2	2.31	0.47
8:H:41:ARG:NH1	8:H:42:GLY:O	2.48	0.46
10:J:657:ARG:HD3	10:J:657:ARG:N	2.29	0.46
10:J:775:PHE:CD1	10:J:787:VAL:HG11	2.44	0.46
1:A:224:ALA:HB3	1:A:233:THR:H	1.80	0.46
2:B:70:ALA:H	2:B:113:THR:HB	1.79	0.46
2:B:126:GLN:NE2	5:E:140:LEU:HD11	2.27	0.46
4:D:68:LYS:HB3	4:D:75:THR:HG21	1.98	0.46
8:H:166:LEU:HD23	8:H:204:TRP:CE2	2.50	0.46
5:E:12:VAL:HA	5:E:15:VAL:HG22	1.97	0.46
10:J:451:PHE:CB	10:J:517:ASN:HD21	2.29	0.46
10:J:699:TYR:OH	10:J:748:MET:HE2	2.16	0.46
1:A:103:ASN:HD21	2:B:94:ARG:NH2	2.08	0.46
10:J:397:ARG:HD3	10:J:432:VAL:HG21	1.97	0.46
12:R:39:U:H2'	12:R:39:U:P	2.55	0.46
1:A:44:GLY:H	1:A:159:HIS:CD2	2.30	0.46
1:A:219:GLY:HA3	1:A:240:ILE:HD13	1.96	0.46
10:J:610:LEU:HD23	10:J:613:LEU:HD12	1.98	0.46
11:K:82:PRO:O	11:K:84:VAL:N	2.49	0.46
2:B:17:ARG:NH1	2:B:172:ASP:O	2.45	0.45
2:B:13:ARG:HH21	2:B:19:ALA:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:THR:OG1	5:E:162:ASN:CG	2.55	0.45
3:C:23:ARG:CD	3:C:214:GLU:OE2	2.64	0.45
7:G:225:TYR:CD1	7:G:225:TYR:C	2.90	0.45
10:J:285:ARG:HB2	10:J:405:TRP:CD2	2.51	0.45
12:R:39:U:H2'	12:R:39:U:O5'	2.16	0.45
10:J:803:GLU:C	10:J:809:LYS:HZ1	2.20	0.45
10:J:43:HIS:C	10:J:45:GLY:N	2.69	0.45
2:B:187:LEU:HD22	2:B:217:ALA:HB1	1.99	0.45
3:C:225:VAL:HB	3:C:233:CYS:HB2	1.99	0.45
2:B:27:ALA:HB1	2:B:144:LEU:CD1	2.46	0.45
6:F:46:LEU:HD11	6:F:63:LEU:HD21	1.98	0.45
1:A:76:LEU:HD11	1:A:116:ILE:HD11	1.99	0.45
4:D:38:LEU:HD11	4:D:55:LEU:HD21	1.97	0.45
1:A:233:THR:HG22	2:B:202:ASP:HA	1.98	0.44
2:B:31:VAL:N	2:B:38:SER:OG	2.49	0.44
5:E:7:SER:HB2	8:H:139:ASP:HA	2.00	0.44
5:E:56:THR:HA	5:E:143:GLU:O	2.17	0.44
7:G:225:TYR:HE1	7:G:227:LEU:CD2	2.23	0.44
10:J:679:HIS:CD2	10:J:771:ILE:CD1	3.00	0.44
2:B:25:ILE:O	2:B:25:ILE:HG12	2.18	0.44
5:E:168:VAL:CG2	5:E:182:LEU:HD22	2.46	0.44
6:F:36:LEU:HD11	6:F:250:ARG:CG	2.45	0.44
10:J:864:ILE:O	10:J:868:GLY:HA2	2.17	0.44
10:J:864:ILE:O	10:J:868:GLY:CA	2.65	0.44
10:J:839:PHE:CD1	10:J:840:PHE:N	2.85	0.44
4:D:134:LEU:HD13	4:D:184:ALA:HB2	2.00	0.44
3:C:143:ASP:HB2	6:F:46:LEU:HD22	1.99	0.44
1:A:140:ASN:ND2	4:D:39:SER:H	2.16	0.44
8:H:247:GLN:HG3	8:H:281:VAL:HG21	1.99	0.44
4:D:110:LEU:HD21	7:G:72:ARG:HH21	1.83	0.44
10:J:437:HIS:O	10:J:823:MET:HE2	2.17	0.44
4:D:28:LEU:CD1	4:D:168:ASP:CG	2.80	0.43
5:E:250:GLU:HA	5:E:253:PHE:HD2	1.84	0.43
1:A:192:ILE:O	1:A:224:ALA:HA	2.18	0.43
10:J:282:HIS:HA	10:J:344:ARG:HG3	2.00	0.43
1:A:105:LEU:HD21	1:A:222:VAL:HG11	2.00	0.43
1:A:49:GLU:HG2	1:A:54:ARG:HG2	2.00	0.43
10:J:775:PHE:CE1	10:J:787:VAL:HG12	2.54	0.43
2:B:241:ILE:HD11	8:H:20:ARG:HH11	1.83	0.43
5:E:39:THR:CG2	5:E:277:GLU:CG	2.90	0.43
8:H:189:LEU:HD22	8:H:257:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:ALA:HB2	3:C:225:VAL:HG22	2.01	0.43
1:A:229:ARG:NH2	2:B:207:GLU:OE1	2.47	0.42
10:J:737:ASN:O	10:J:741:ARG:HG2	2.19	0.42
1:A:199:PHE:HE2	1:A:216:VAL:HG23	1.82	0.42
6:F:209:ALA:HB2	6:F:230:GLU:H	1.84	0.42
10:J:861:VAL:HA	10:J:872:THR:HA	2.01	0.42
3:C:38:ASN:HB2	3:C:50:LEU:HB3	2.00	0.42
8:H:83:ILE:H	8:H:83:ILE:HG13	1.64	0.42
11:K:82:PRO:O	11:K:83:GLU:C	2.56	0.42
1:A:267:LYS:HD2	1:A:286:GLU:CD	2.39	0.42
10:J:487:ASN:HB3	10:J:779:ILE:HD12	2.00	0.42
1:A:41:THR:O	1:A:276:ARG:NH2	2.52	0.41
2:B:26:GLN:HG3	2:B:42:GLU:CG	2.50	0.41
2:B:53:TYR:OH	5:E:89:ALA:O	2.28	0.41
2:B:233:ARG:HA	2:B:236:VAL:HG12	2.01	0.41
7:G:229:ILE:HG22	7:G:239:VAL:HG12	2.01	0.41
10:J:405:TRP:CZ3	10:J:412:PRO:HG3	2.55	0.41
10:J:396:ARG:HA	10:J:422:ASP:HA	2.03	0.41
10:J:859:ALA:CB	10:J:874:PHE:HA	2.51	0.41
2:B:95:LYS:HE3	2:B:95:LYS:HB2	1.88	0.41
2:B:111:ILE:HD11	2:B:146:VAL:HG11	2.02	0.41
1:A:141:HIS:CE1	1:A:145:ILE:HD11	2.55	0.41
1:A:280:GLY:O	1:A:281:LYS:CG	2.66	0.41
4:D:157:CYS:SG	4:D:209:CYS:CB	3.04	0.41
8:H:146:GLN:N	8:H:157:HIS:CD2	2.87	0.41
5:E:199:CYS:HG	5:E:267:HIS:HE2	1.67	0.41
10:J:691:HIS:HB3	10:J:765:TYR:H	1.84	0.41
10:J:838:LEU:HD23	10:J:838:LEU:HA	1.84	0.41
3:C:134:VAL:HG21	6:F:11:PRO:HG3	2.03	0.41
3:C:211:THR:H	3:C:214:GLU:HB3	1.85	0.41
5:E:231:THR:C	5:E:267:HIS:CE1	2.94	0.41
10:J:357:CYS:HA	10:J:399:ILE:HG22	2.03	0.41
1:A:37:ILE:HB	1:A:285:ALA:HB3	2.03	0.41
7:G:154:ARG:HH12	7:G:157:VAL:H	1.67	0.41
9:I:14:LEU:HD11	9:I:35:SER:HB2	2.02	0.41
10:J:841:LYS:HE3	10:J:913:LEU:HD11	2.03	0.41
10:J:883:PRO:CD	10:J:884:GLN:H	2.24	0.41
3:C:42:ILE:HD13	6:F:105:PHE:HE2	1.86	0.41
6:F:28:PRO:HB2	6:F:31:ARG:HH22	1.86	0.41
7:G:88:HIS:ND1	7:G:99:VAL:O	2.54	0.41
10:J:48:LEU:CD2	10:J:121:TYR:CB	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:225:TYR:OH	7:G:246:GLN:HB3	2.20	0.41
8:H:22:THR:O	8:H:22:THR:HG23	2.21	0.41
10:J:757:GLY:HA3	10:J:807:LYS:HG2	2.02	0.41
10:J:809:LYS:HE3	10:J:809:LYS:HB2	1.85	0.41
10:J:856:ARG:CA	10:J:859:ALA:O	2.68	0.41
3:C:234:CYS:HA	4:D:197:THR:HG21	2.03	0.40
10:J:881:PRO:HB2	10:J:883:PRO:HD3	2.03	0.40
5:E:62:VAL:HG22	5:E:137:VAL:HG22	2.02	0.40
1:A:33:ARG:HH22	1:A:143:GLY:HA3	1.86	0.40
5:E:85:CYS:HA	5:E:141:LEU:HD21	2.03	0.40
10:J:597:ILE:HD11	10:J:610:LEU:HB3	2.03	0.40
10:J:856:ARG:HA	10:J:856:ARG:NE	2.36	0.40
10:J:888:ASP:O	10:J:892:PRO:HA	2.21	0.40
1:A:27:ARG:NH1	1:A:33:ARG:HG3	2.36	0.40
3:C:75:ASP:OD1	3:C:75:ASP:N	2.52	0.40
10:J:43:HIS:C	10:J:45:GLY:H	2.25	0.40
1:A:14:LEU:O	1:A:18:ILE:HG12	2.22	0.40
4:D:58:VAL:HG21	4:D:141:LEU:HD22	2.03	0.40
4:D:221:PHE:HA	4:D:224:TYR:HD2	1.87	0.40
5:E:273:VAL:HG21	8:H:5:MET:HB2	2.03	0.40
7:G:35:LEU:HB3	7:G:77:ARG:HG2	2.02	0.40
10:J:710:ASN:O	10:J:711:LEU:HD23	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
1	A	285/443 (64%)	275 (96%)	9 (3%)	1 (0%)	34 70
2	B	237/249 (95%)	223 (94%)	14 (6%)	0	100 100
3	C	262/278 (94%)	249 (95%)	12 (5%)	1 (0%)	34 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	208/237 (88%)	202 (97%)	6 (3%)	0	100 100
5	E	285/295 (97%)	253 (89%)	31 (11%)	1 (0%)	34 70
6	F	240/276 (87%)	232 (97%)	8 (3%)	0	100 100
7	G	204/293 (70%)	196 (96%)	8 (4%)	0	100 100
8	H	267/297 (90%)	254 (95%)	13 (5%)	0	100 100
9	I	46/199 (23%)	44 (96%)	2 (4%)	0	100 100
10	J	860/962 (89%)	800 (93%)	57 (7%)	3 (0%)	41 74
11	K	35/166 (21%)	23 (66%)	6 (17%)	6 (17%)	0 3
All	All	2929/3695 (79%)	2751 (94%)	166 (6%)	12 (0%)	38 70

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	PHE
10	J	761	ASP
11	K	63	SER
11	K	79	GLY
11	K	81	ASN
11	K	82	PRO
10	J	44	GLU
3	C	28	GLU
11	K	64	PHE
10	J	201	LEU
11	K	68	GLU
5	E	69	PRO

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
1	A	242/384 (63%)	240 (99%)	2 (1%)	81 89
2	B	174/189 (92%)	173 (99%)	1 (1%)	86 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	208/237 (88%)	206 (99%)	2 (1%)	76 86
4	D	170/195 (87%)	168 (99%)	2 (1%)	71 84
5	E	236/255 (92%)	229 (97%)	7 (3%)	41 66
6	F	164/191 (86%)	163 (99%)	1 (1%)	86 92
7	G	150/230 (65%)	148 (99%)	2 (1%)	69 82
8	H	218/257 (85%)	212 (97%)	6 (3%)	43 68
9	I	41/173 (24%)	40 (98%)	1 (2%)	49 71
10	J	645/856 (75%)	627 (97%)	18 (3%)	43 68
All	All	2248/2967 (76%)	2206 (98%)	42 (2%)	59 76

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	287	SER
2	B	25	ILE
3	C	23	ARG
3	C	147	ASN
4	D	29	ARG
4	D	113	ARG
5	E	33	ARG
5	E	44	ASN
5	E	50	ARG
5	E	112	ILE
5	E	114	ASN
5	E	181	GLU
5	E	182	LEU
6	F	250	ARG
7	G	186	ARG
7	G	225	TYR
8	H	20	ARG
8	H	23	LYS
8	H	41	ARG
8	H	95	ARG
8	H	183	LYS
8	H	271	ILE
9	I	13	ARG
10	J	17	MET
10	J	142	ASN

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Mol	Chain	Res	Type
10	J	156	TYR
10	J	284	ASN
10	J	601	ASN
10	J	641	MET
10	J	687	LEU
10	J	711	LEU
10	J	712	GLU
10	J	737	ASN
10	J	750	GLN
10	J	800	THR
10	J	820	ARG
10	J	836	THR
10	J	839	PHE
10	J	840	PHE
10	J	841	LYS
10	J	875	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	103	ASN
1	A	159	HIS
2	B	43	GLN
2	B	126	GLN
3	C	38	ASN
3	C	147	ASN
3	C	162	ASN
3	C	192	HIS
4	D	173	GLN
5	E	44	ASN
5	E	114	ASN
5	E	115	ASN
8	H	157	HIS
10	J	43	HIS
10	J	127	HIS
10	J	142	ASN
10	J	146	ASN
10	J	282	HIS
10	J	288	HIS
10	J	437	HIS
10	J	517	ASN

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Mol	Chain	Res	Type
10	J	567	ASN
10	J	679	HIS
10	J	737	ASN
10	J	750	GLN
10	J	828	GLN
10	J	835	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	6/44 (13%)	3 (50%)	1 (16%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	40	U
12	R	41	U
12	R	44	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	R	39	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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.

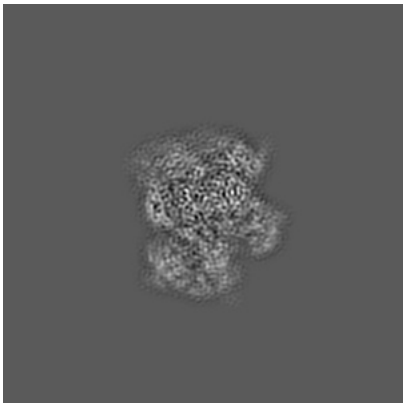
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0128. These allow visual inspection of the internal detail of the map and identification of artifacts.

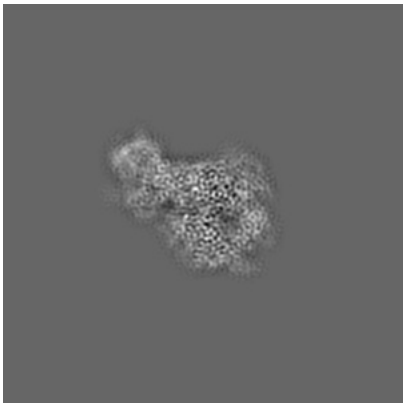
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

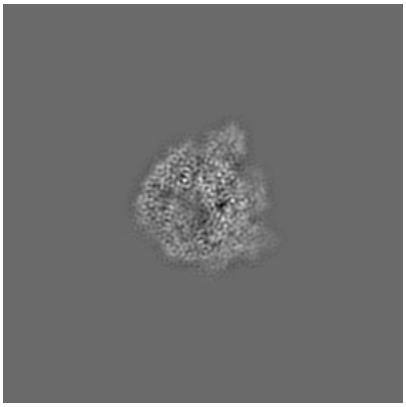
6.1.1 Primary map



X



Y

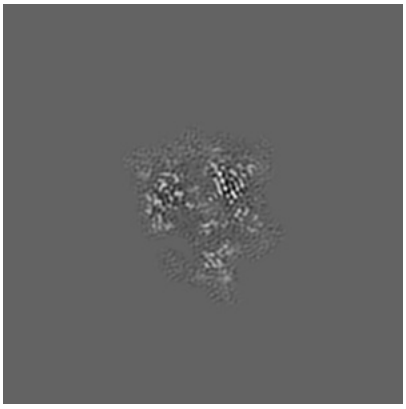


Z

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

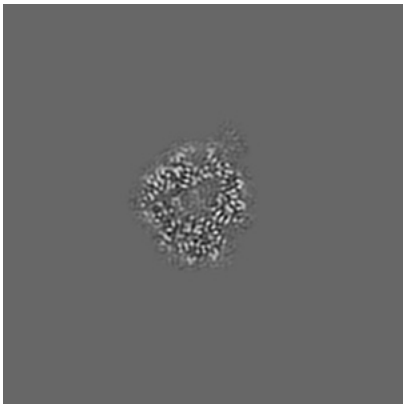
6.2 Central slices

6.2.1 Primary map



X Index: 125

Y Index: 125

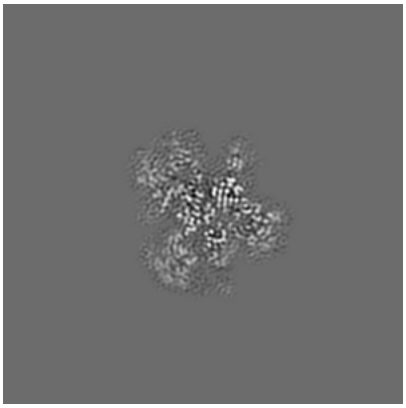


Z Index: 125

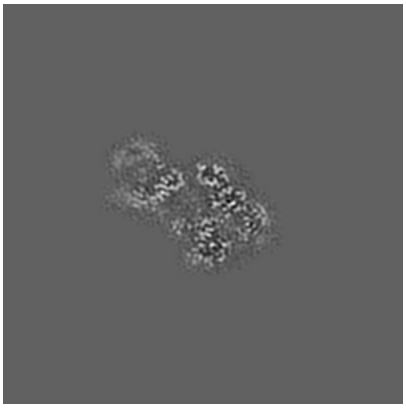
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

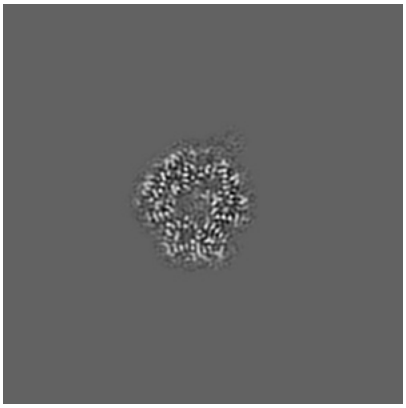
6.3.1 Primary map



X Index: 138



Y Index: 135

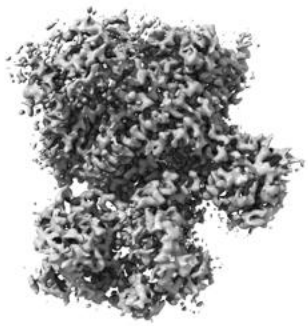


Z Index: 127

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

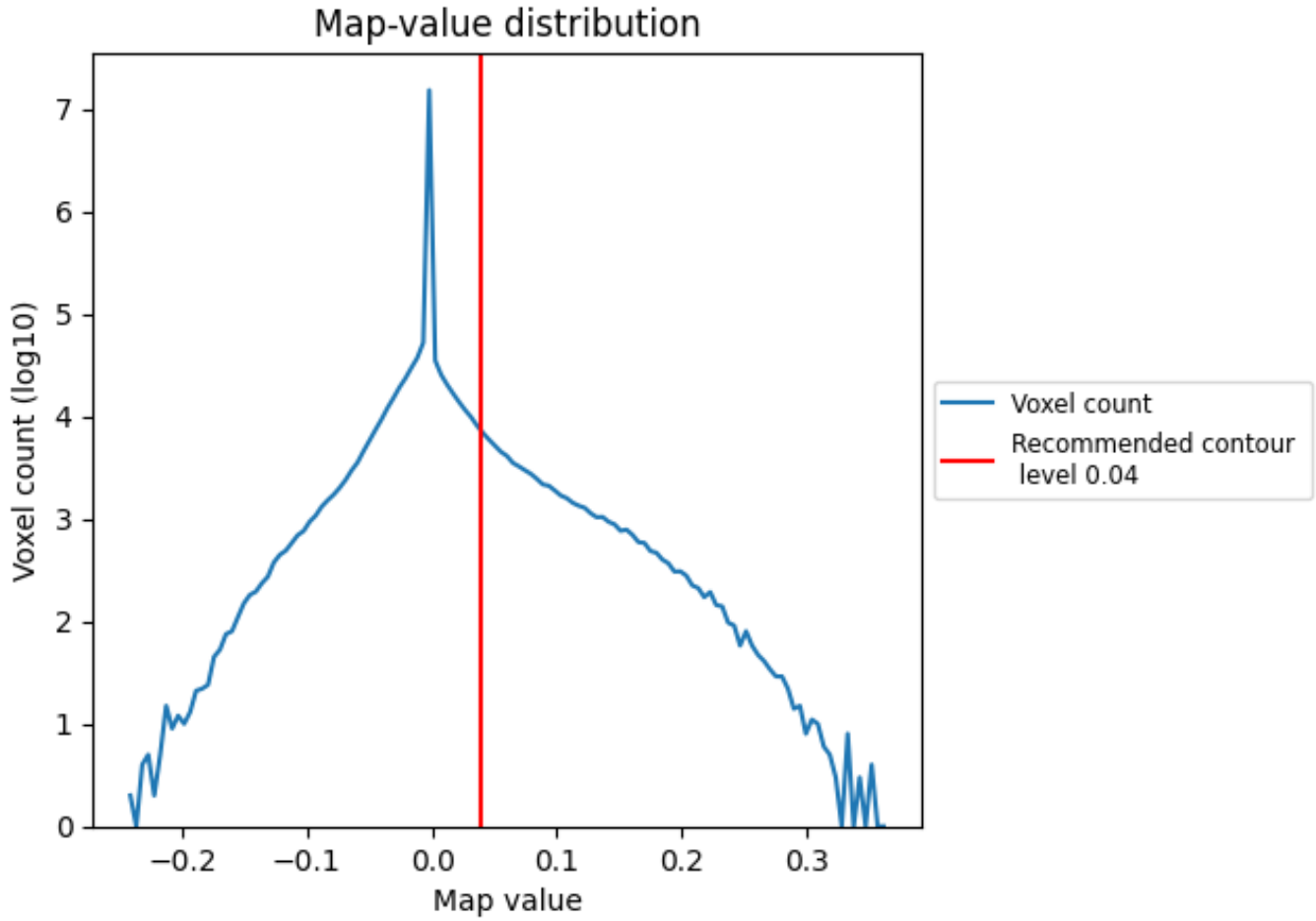
6.5 Mask visualisation (i)

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

7 Map analysis

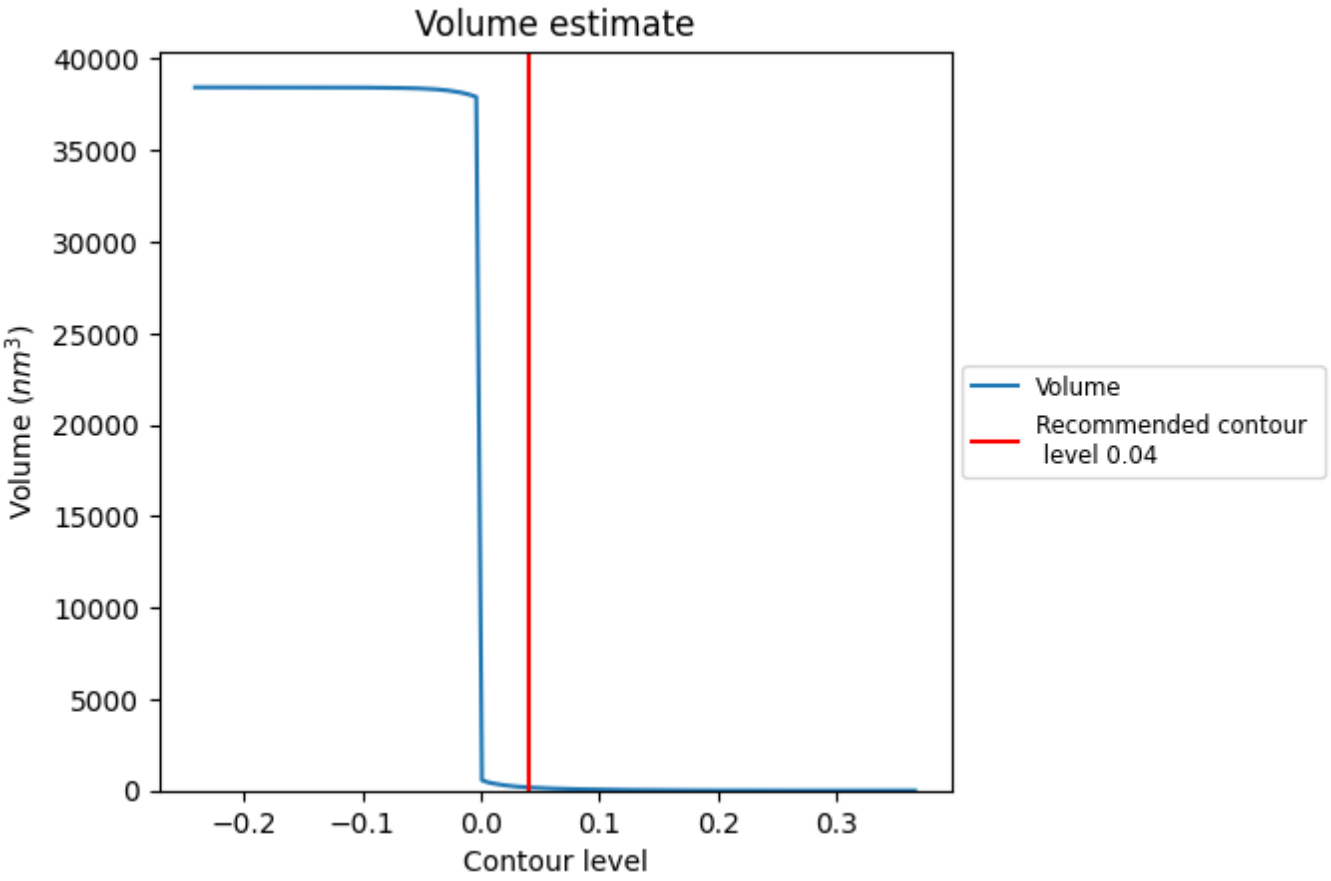
This section contains the results of statistical analysis of the map.

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.

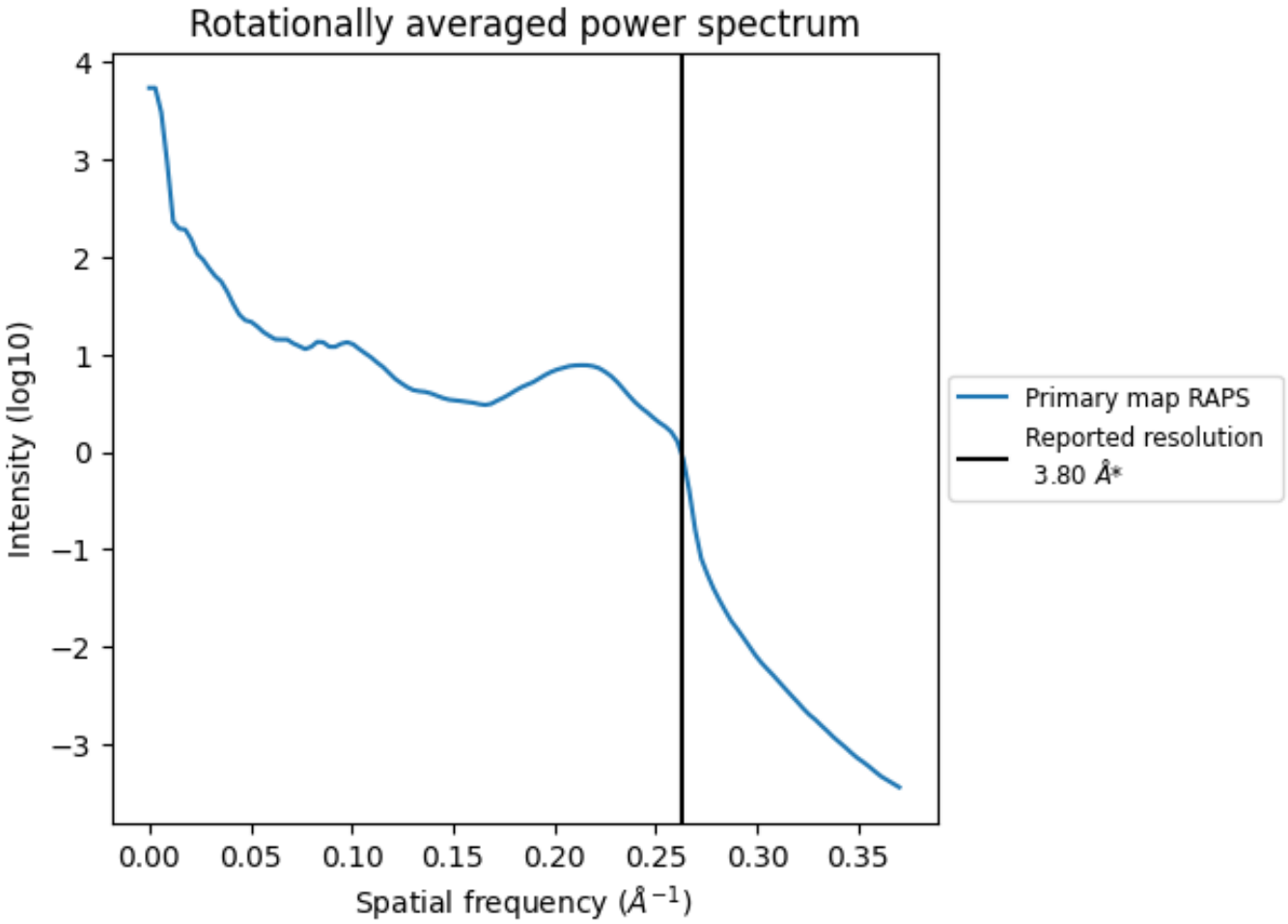
7.2 Volume estimate



The volume at the recommended contour level is 171 nm^3; this corresponds to an approximate mass of 154 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 0.263 Å^{-1}

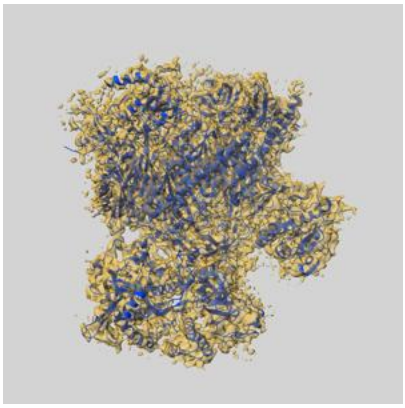
8 Fourier-Shell correlation (i)

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

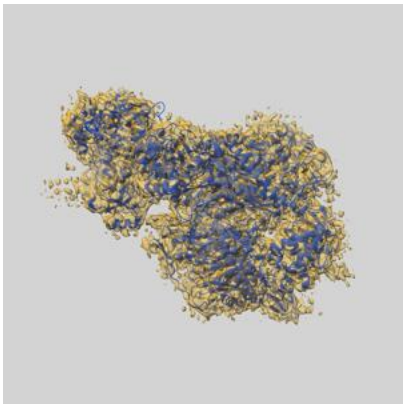
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0128 and PDB model 6H25. Per-residue inclusion information can be found in section 3 on page 9.

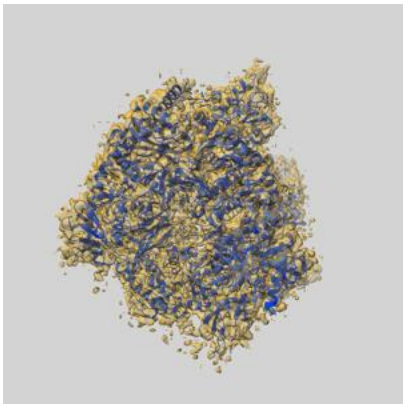
9.1 Map-model overlay



X



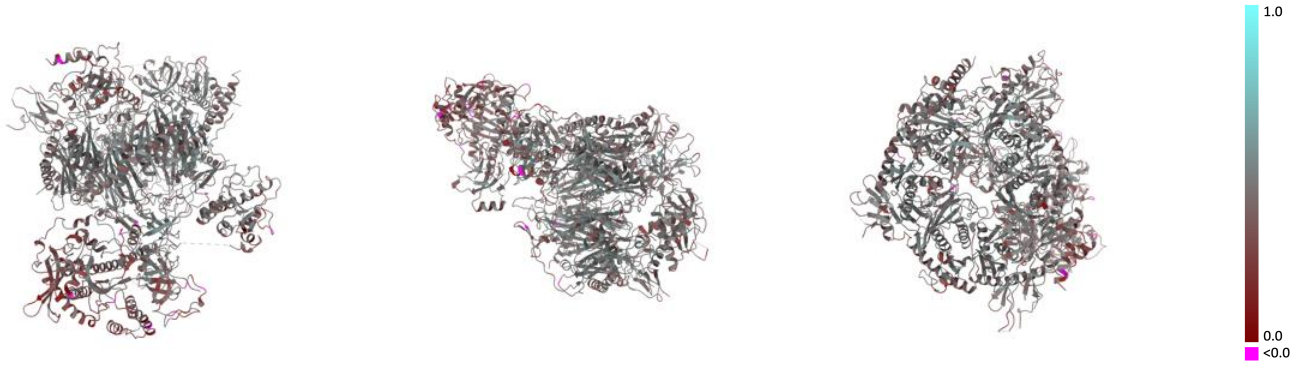
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

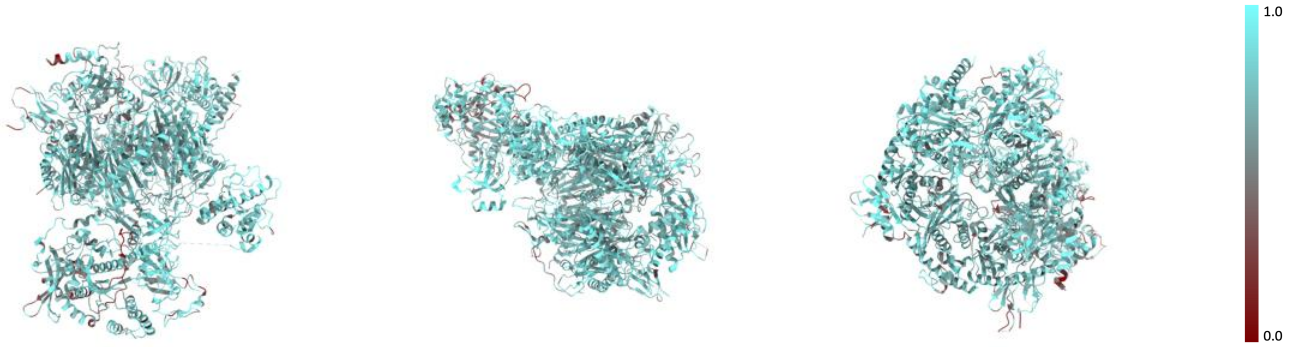
9.2 Q-score mapped to coordinate model (i)



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.

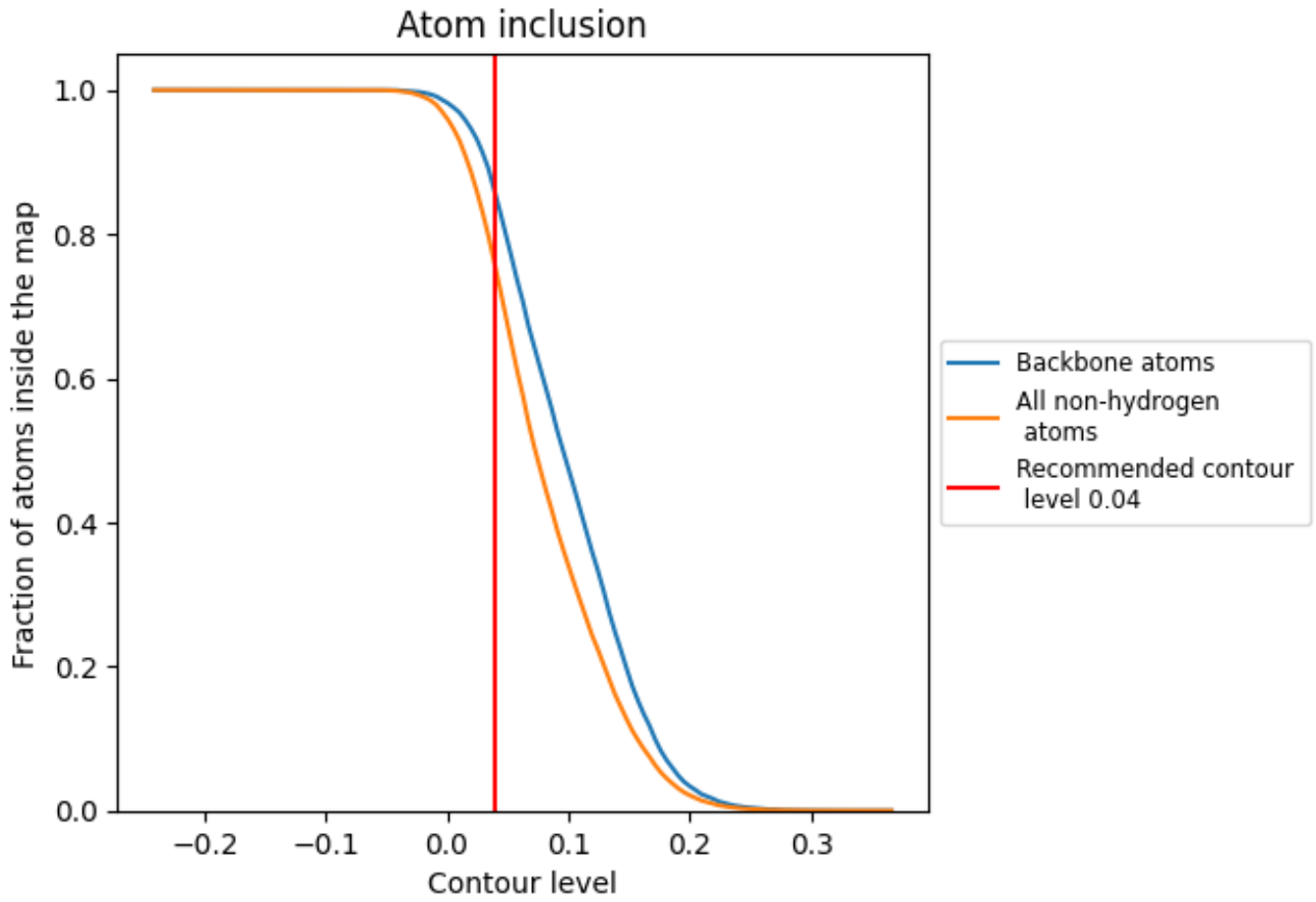
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7534	0.4270
A	0.7694	0.4540
B	0.7863	0.4630
C	0.7675	0.4330
D	0.7536	0.4540
E	0.7853	0.4540
F	0.7671	0.4550
G	0.6807	0.4220
H	0.7642	0.4320
I	0.7218	0.4170
J	0.7362	0.3830
K	0.6995	0.3840
R	0.8250	0.4740