Full wwPDB EM Validation Report (i)

Dec 12, 2022 – 09:55 AM EST

PDB ID	:	1YSH
EMDB ID	:	EMD-1125
Title	:	Localization and dynamic behavior of ribosomal protein L30e
Authors	:	Halic, M.; Becker, T.; Frank, J.; Spahn, C.M.; Beckmann, R.
Deposited on	:	2005-02-08
Resolution	:	9.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

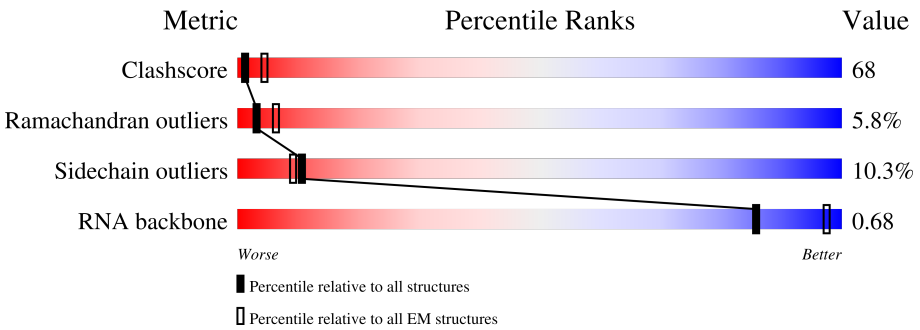
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.50 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	28	43% 50% 7%
2	F	34	47% 38% 15%
3	B	101	46% 46% 7% •
4	C	104	• 18% 54% 19% 9%
5	D	73	• 30% 55% 15%
6	E	84	• 29% 50% 19% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	28	611	272	121	190	28	0	0

- Molecule 2 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	F	34	717	320	139	225	33	0	1

- Molecule 3 is a RNA chain called RNA (101-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B	101	2189	973	417	698	101	0	0

- Molecule 4 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	104	803	509	140	148	6	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	LYS	GLU	SEE REMARK 999	UNP Q5I7K9
C	57	TYR	CYS	SEE REMARK 999	UNP Q5I7K9
C	101	SER	ASN	SEE REMARK 999	UNP Q5I7K9

- Molecule 5 is a protein called ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	73	557	353	102	96	6	0	0

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S13.

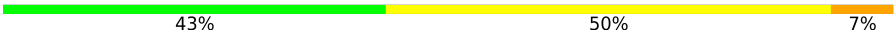
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	E	84	699	451	131	117	0	0

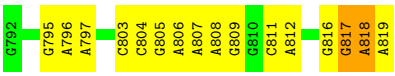
3 Residue-property plots (i)

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: RNA (28-MER)

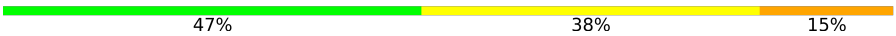
Chain A:

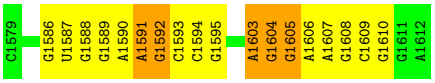




- Molecule 2: RNA (34-MER)

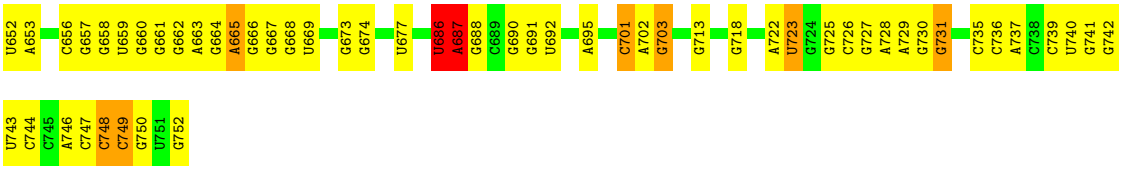
Chain F:





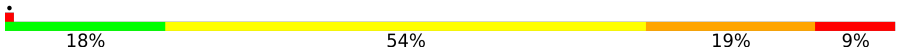
- Molecule 3: RNA (101-MER)

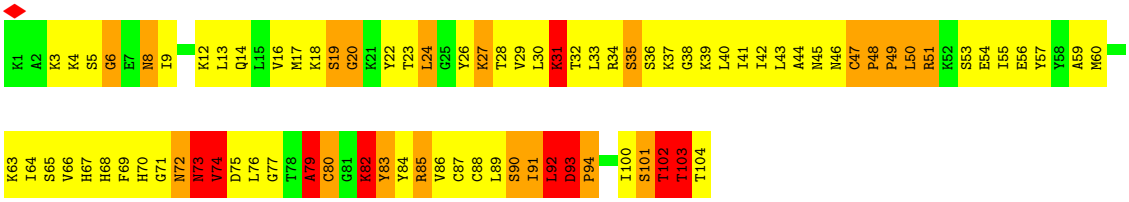
Chain B:



- Molecule 4: ribosomal protein L30

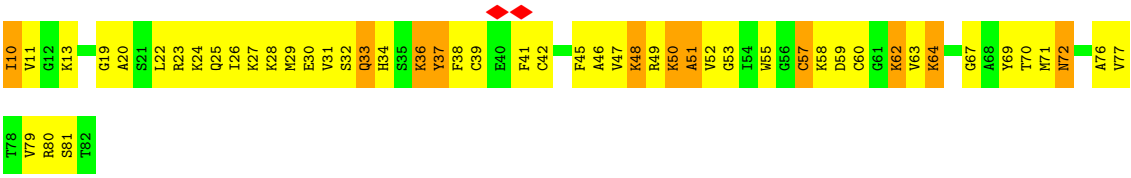
Chain C:





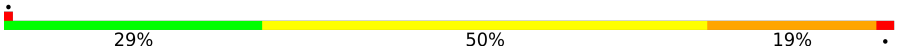
- Molecule 5: ribosomal protein L37a

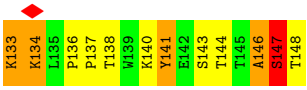
Chain D:



- Molecule 6: 40S RIBOSOMAL PROTEIN S13

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	7000.00	Depositor
Maximum defocus (nm)	45000.00	Depositor
Magnification	38300	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.002	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000155	Depositor
Map size (Å)	453.05, 453.05, 453.05	wwPDB
Map dimensions	221, 221, 221	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.05, 2.05, 2.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.46	0/686	0.66	0/1070
2	F	0.40	0/803	0.69	0/1252
3	B	0.51	0/2454	0.72	2/3832 (0.1%)
4	C	2.54	15/809 (1.9%)	2.58	34/1077 (3.2%)
5	D	1.05	2/566 (0.4%)	1.10	2/752 (0.3%)
6	E	2.50	7/710 (1.0%)	1.75	20/946 (2.1%)
All	All	1.36	24/6028 (0.4%)	1.25	58/8929 (0.6%)

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	B	0	1
4	C	0	8
5	D	0	2
6	E	0	5
All	All	0	16

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	133	LYS	CB-CG	46.84	2.79	1.52
4	C	93	ASP	CB-CG	46.73	2.49	1.51
4	C	19	SER	C-N	31.59	1.90	1.33
6	E	134	LYS	CB-CG	27.23	2.26	1.52
4	C	79	ALA	C-N	-19.82	0.88	1.34
4	C	8	ASN	CB-CG	18.22	1.93	1.51
4	C	103	THR	C-N	-16.04	0.97	1.34
6	E	132	THR	C-N	14.52	1.67	1.34
4	C	90	SER	CB-OG	-11.89	1.26	1.42
4	C	20	GLY	N-CA	9.72	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	82	PRO	C-N	9.52	1.55	1.34
4	C	49	PRO	N-CD	8.91	1.60	1.47
4	C	91	ILE	C-N	-8.29	1.15	1.34
4	C	94	PRO	N-CD	8.03	1.59	1.47
4	C	82	LYS	C-N	7.93	1.52	1.34
4	C	93	ASP	C-N	-7.43	1.20	1.34
6	E	84	ILE	N-CA	7.18	1.60	1.46
4	C	31	LYS	CD-CE	-6.65	1.34	1.51
5	D	64	LYS	CE-NZ	-6.15	1.33	1.49
5	D	57	CYS	CA-CB	-5.90	1.41	1.53
4	C	31	LYS	CE-NZ	5.73	1.63	1.49
6	E	133	LYS	C-O	5.39	1.33	1.23
6	E	104	ARG	CZ-NH2	5.38	1.40	1.33
4	C	35	SER	CA-CB	-5.31	1.45	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	102	THR	O-C-N	-34.43	67.61	122.70
4	C	93	ASP	CB-CG-OD2	-27.76	93.32	118.30
4	C	93	ASP	CA-CB-CG	-24.62	59.23	113.40
4	C	93	ASP	CB-CG-OD1	23.86	139.77	118.30
4	C	103	THR	O-C-N	-18.35	93.34	122.70
4	C	82	LYS	O-C-N	-17.27	95.06	122.70
4	C	103	THR	C-N-CA	17.00	164.20	121.70
4	C	79	ALA	O-C-N	-14.88	98.90	122.70
4	C	82	LYS	C-N-CA	14.86	158.86	121.70
4	C	93	ASP	O-C-N	-14.62	93.32	121.10
6	E	133	LYS	CA-CB-CG	-13.22	84.32	113.40
4	C	103	THR	CA-C-N	12.77	145.29	117.20
4	C	92	LEU	CB-CG-CD2	-12.41	89.91	111.00
4	C	82	LYS	CA-C-N	12.21	144.06	117.20
6	E	104	ARG	NE-CZ-NH2	-10.67	114.97	120.30
5	D	51	ALA	O-C-N	-9.96	106.76	122.70
4	C	92	LEU	CB-CG-CD1	9.48	127.12	111.00
6	E	83	GLU	O-C-N	-9.31	107.81	122.70
4	C	93	ASP	CA-C-N	8.63	141.26	117.10
4	C	83	TYR	N-CA-C	8.39	133.66	111.00
4	C	49	PRO	CA-N-CD	-8.38	99.77	111.50
4	C	83	TYR	CB-CA-C	-8.33	93.73	110.40
6	E	83	GLU	CA-C-N	8.09	135.00	117.20
6	E	133	LYS	CA-C-N	8.07	134.94	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	8	ASN	CB-CG-OD1	8.06	137.72	121.60
6	E	77	ALA	CB-CA-C	-7.87	98.30	110.10
6	E	134	LYS	CA-CB-CG	-7.68	96.50	113.40
4	C	74	VAL	CB-CA-C	7.53	125.71	111.40
4	C	94	PRO	CA-N-CD	-7.48	101.03	111.50
6	E	90	PHE	CB-CG-CD1	7.44	126.01	120.80
4	C	92	LEU	CA-CB-CG	7.40	132.33	115.30
4	C	73	ASN	C-N-CA	-7.23	103.63	121.70
3	B	687	A	C2'-C3'-O3'	7.20	125.35	109.50
4	C	8	ASN	CA-CB-CG	-7.14	97.69	113.40
4	C	8	ASN	CB-CG-ND2	-7.11	99.63	116.70
6	E	104	ARG	NE-CZ-NH1	7.11	123.86	120.30
4	C	35	SER	CA-CB-OG	-6.93	92.49	111.20
4	C	17	MET	CG-SD-CE	-6.80	89.31	100.20
6	E	147	SER	N-CA-C	-6.70	92.92	111.00
6	E	147	SER	N-CA-CB	6.68	120.52	110.50
5	D	51	ALA	CB-CA-C	6.65	120.07	110.10
6	E	89	TYR	CB-CG-CD2	-6.42	117.15	121.00
4	C	73	ASN	CA-C-N	-6.41	103.10	117.20
4	C	79	ALA	CA-C-N	6.32	131.10	117.20
6	E	146	ALA	N-CA-CB	6.16	118.73	110.10
4	C	19	SER	C-N-CA	-6.12	109.44	122.30
6	E	133	LYS	CA-C-O	-5.89	107.74	120.10
4	C	6	GLY	CA-C-N	-5.78	104.49	117.20
6	E	90	PHE	CB-CG-CD2	-5.34	117.06	120.80
4	C	6	GLY	O-C-N	5.22	131.05	122.70
4	C	31	LYS	CD-CE-NZ	-5.17	99.80	111.70
6	E	66	VAL	N-CA-C	-5.17	97.04	111.00
4	C	74	VAL	N-CA-C	-5.15	97.10	111.00
6	E	77	ALA	N-CA-CB	5.13	117.29	110.10
6	E	83	GLU	CB-CA-C	-5.12	100.16	110.40
3	B	686	U	C5'-C4'-C3'	-5.10	107.83	116.00
6	E	82	PRO	C-N-CA	-5.09	108.98	121.70
6	E	108	ASP	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	727	G	Sidechain
4	C	102	THR	Mainchain
4	C	103	THR	Peptide

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Mol	Chain	Res	Type	Group
4	C	73	ASN	Mainchain
4	C	79	ALA	Peptide,Mainchain
4	C	82	LYS	Peptide
4	C	93	ASP	Peptide,Mainchain
5	D	37	TYR	Sidechain
5	D	51	ALA	Mainchain
6	E	128	TYR	Sidechain
6	E	131	ARG	Sidechain
6	E	141	TYR	Sidechain
6	E	89	TYR	Sidechain
6	E	90	PHE	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	611	0	306	76	0
2	F	717	0	359	46	0
3	B	2189	0	1098	126	0
4	C	803	0	825	272	0
5	D	557	0	577	94	0
6	E	699	0	750	249	0
All	All	5576	0	3915	647	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 68.

All (647) 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)
3:B:740:U:C1'	6:E:101:HIS:CE1	1.82	1.63
1:A:804:C:C6	6:E:148:THR:HG23	1.13	1.61
3:B:740:U:H1'	6:E:101:HIS:CE1	1.33	1.61
4:C:9:ILE:HG21	4:C:69:PHE:CE1	1.30	1.60
4:C:9:ILE:CG2	4:C:69:PHE:HE1	1.09	1.56
1:A:804:C:C6	6:E:148:THR:CG2	1.88	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:44:ALA:HA	4:C:70:HIS:C	1.31	1.48
1:A:797:A:H5'	5:D:10:ILE:CD1	1.43	1.47
3:B:658:G:OP1	6:E:90:PHE:CE2	1.68	1.46
6:E:130:LYS:HZ2	6:E:137:PRO:N	1.04	1.46
4:C:9:ILE:CG2	4:C:69:PHE:CE1	1.91	1.45
4:C:44:ALA:N	4:C:70:HIS:HB2	1.21	1.45
4:C:44:ALA:HA	4:C:70:HIS:CA	1.49	1.43
4:C:67:HIS:HA	4:C:104:THR:CG2	1.47	1.41
4:C:8:ASN:CB	4:C:8:ASN:CG	1.93	1.37
2:F:1605:G:N7	4:C:27:LYS:HB2	1.39	1.36
4:C:93:ASP:CG	4:C:93:ASP:HA	1.34	1.36
4:C:44:ALA:CA	4:C:70:HIS:HB2	1.52	1.35
6:E:79:GLY:HA2	6:E:80:LEU:N	1.34	1.35
1:A:804:C:H6	6:E:148:THR:CG2	1.28	1.35
3:B:740:U:O4'	6:E:101:HIS:CE1	1.78	1.34
2:F:1591:A:H62	4:C:24:LEU:CD2	1.38	1.32
4:C:76:LEU:HB3	6:E:92:ILE:CG2	1.58	1.31
2:F:1591:A:N6	4:C:24:LEU:CD2	1.93	1.30
1:A:804:C:O5'	6:E:148:THR:CG2	1.79	1.29
6:E:130:LYS:NZ	6:E:137:PRO:N	1.76	1.28
3:B:668:G:C5'	6:E:107:LYS:HG2	1.61	1.28
1:A:797:A:C5'	5:D:10:ILE:CD1	2.11	1.27
4:C:44:ALA:CA	4:C:70:HIS:CB	2.10	1.27
3:B:658:G:OP1	6:E:90:PHE:HE2	0.98	1.27
3:B:728:A:N1	6:E:113:PHE:HE2	1.29	1.27
3:B:668:G:H5"	6:E:107:LYS:CG	1.65	1.25
4:C:19:SER:C	4:C:20:GLY:N	1.89	1.25
4:C:71:GLY:O	4:C:72:ASN:CG	1.74	1.25
3:B:740:U:C4'	6:E:101:HIS:ND1	1.98	1.25
3:B:741:G:OP1	6:E:98:ILE:HD11	1.09	1.24
6:E:82:PRO:O	6:E:83:GLU:CG	1.85	1.23
6:E:82:PRO:O	6:E:83:GLU:HG3	1.33	1.23
1:A:797:A:C5'	5:D:10:ILE:HD12	1.67	1.23
3:B:728:A:N1	6:E:113:PHE:CE2	2.04	1.22
6:E:75:LEU:HA	6:E:80:LEU:CD2	1.67	1.22
6:E:75:LEU:CA	6:E:80:LEU:HD21	1.55	1.22
4:C:76:LEU:CD2	6:E:92:ILE:HG22	1.69	1.22
3:B:669:U:H5'	6:E:107:LYS:NZ	1.53	1.20
4:C:44:ALA:CA	4:C:70:HIS:C	2.07	1.20
4:C:73:ASN:N	4:C:83:TYR:CE2	2.02	1.20
4:C:42:ILE:HG22	4:C:70:HIS:CD2	1.76	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:130:LYS:HG2	6:E:141:TYR:CZ	1.74	1.19
1:A:804:C:C4'	6:E:148:THR:HG21	1.73	1.18
2:F:1591:A:N6	4:C:24:LEU:HD23	1.53	1.17
3:B:668:G:H5"	6:E:107:LYS:HG3	1.25	1.17
6:E:127:ARG:HH22	6:E:141:TYR:HA	1.09	1.16
3:B:740:U:O4'	6:E:101:HIS:ND1	1.80	1.15
1:A:797:A:C4'	5:D:10:ILE:HD12	1.76	1.15
3:B:741:G:O2'	6:E:114:ARG:HG2	1.45	1.14
1:A:806:A:OP2	6:E:147:SER:N	1.79	1.14
6:E:134:LYS:CG	6:E:134:LYS:CB	2.26	1.13
4:C:76:LEU:CB	6:E:92:ILE:HG21	1.79	1.13
4:C:48:PRO:HB3	5:D:42:CYS:SG	1.88	1.13
3:B:668:G:C5'	6:E:107:LYS:CG	2.25	1.12
4:C:44:ALA:HA	4:C:70:HIS:CB	1.76	1.12
4:C:71:GLY:O	4:C:72:ASN:OD1	1.67	1.12
4:C:93:ASP:CG	4:C:93:ASP:CA	2.16	1.12
5:D:57:CYS:HB2	5:D:62:LYS:HD3	1.21	1.11
6:E:130:LYS:HZ2	6:E:137:PRO:CA	1.62	1.11
1:A:797:A:C4'	5:D:10:ILE:CD1	2.27	1.11
3:B:740:U:H4'	6:E:101:HIS:ND1	1.65	1.11
2:F:1604:G:C4'	4:C:26:TYR:HD2	1.53	1.10
3:B:668:G:O2'	6:E:105:ASN:HA	1.52	1.09
6:E:130:LYS:HZ2	6:E:137:PRO:CD	1.64	1.09
3:B:741:G:OP1	6:E:98:ILE:CD1	2.00	1.08
4:C:44:ALA:HB2	4:C:70:HIS:HB3	1.21	1.08
1:A:804:C:C5'	6:E:148:THR:HG21	1.82	1.07
6:E:84:ILE:HB	6:E:86:GLU:OE2	1.54	1.07
2:F:1591:A:H62	4:C:24:LEU:HD21	1.12	1.07
3:B:668:G:C4'	6:E:107:LYS:HG2	1.83	1.07
4:C:39:LYS:O	4:C:40:LEU:HD12	1.51	1.07
5:D:57:CYS:CB	5:D:62:LYS:HD3	1.85	1.07
4:C:9:ILE:HG22	4:C:69:PHE:HE1	1.17	1.06
4:C:26:TYR:O	4:C:29:VAL:HG12	1.53	1.06
1:A:804:C:O5'	6:E:148:THR:HG21	1.50	1.06
3:B:741:G:P	6:E:98:ILE:HD11	1.94	1.06
3:B:668:G:HO2'	6:E:105:ASN:HA	1.00	1.06
3:B:741:G:C5'	6:E:98:ILE:HD12	1.85	1.06
2:F:1604:G:C4'	4:C:26:TYR:CD2	2.38	1.05
4:C:67:HIS:CD2	4:C:103:THR:O	2.08	1.05
3:B:669:U:C5'	6:E:107:LYS:NZ	2.19	1.05
4:C:44:ALA:N	4:C:70:HIS:CB	2.18	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:130:LYS:HG2	6:E:141:TYR:CE2	1.91	1.04
1:A:797:A:H5'	5:D:10:ILE:HD11	1.09	1.04
4:C:67:HIS:CA	4:C:104:THR:HG23	1.88	1.04
1:A:797:A:H4'	5:D:10:ILE:HD12	1.31	1.03
3:B:658:G:P	6:E:90:PHE:HE2	1.81	1.03
3:B:741:G:H5"	6:E:98:ILE:HD12	1.40	1.03
4:C:76:LEU:CB	6:E:92:ILE:CG2	2.36	1.02
6:E:133:LYS:HB3	6:E:136:PRO:HD2	1.37	1.02
2:F:1604:G:H4'	4:C:26:TYR:HD2	1.21	1.02
3:B:668:G:H4'	6:E:107:LYS:HG2	1.35	1.02
3:B:669:U:C5'	6:E:107:LYS:HZ2	1.71	1.02
3:B:742:G:H5'	6:E:114:ARG:HG2	1.42	1.01
6:E:79:GLY:CA	6:E:80:LEU:N	2.23	1.01
4:C:67:HIS:CA	4:C:104:THR:CG2	2.38	1.01
4:C:76:LEU:HD22	6:E:92:ILE:HG22	1.03	1.01
6:E:83:GLU:O	6:E:86:GLU:OE2	1.78	1.00
2:F:1605:G:N7	4:C:27:LYS:CB	2.23	1.00
1:A:805:G:OP2	6:E:147:SER:C	1.99	1.00
2:F:1591:A:H61	4:C:24:LEU:HD23	1.20	0.99
4:C:20:GLY:HA2	4:C:22:TYR:HE2	1.27	0.99
3:B:668:G:O2'	6:E:107:LYS:NZ	1.78	0.98
1:A:795:G:H2'	1:A:817:G:H22	1.25	0.98
6:E:83:GLU:O	6:E:84:ILE:CG1	2.12	0.98
2:F:1604:G:N2	5:D:60:CYS:SG	2.37	0.98
6:E:83:GLU:O	6:E:84:ILE:CB	2.12	0.98
6:E:130:LYS:CG	6:E:141:TYR:CZ	2.47	0.97
4:C:44:ALA:CB	4:C:70:HIS:HB3	1.94	0.97
3:B:740:U:C4'	6:E:101:HIS:CG	2.48	0.97
3:B:741:G:P	6:E:98:ILE:CD1	2.53	0.97
3:B:668:G:H4'	6:E:107:LYS:CG	1.85	0.96
4:C:44:ALA:CB	4:C:70:HIS:CB	2.42	0.96
3:B:728:A:C6	6:E:113:PHE:CD2	2.54	0.95
4:C:73:ASN:H	4:C:83:TYR:HE2	1.04	0.95
4:C:67:HIS:HA	4:C:104:THR:HG23	0.97	0.95
1:A:804:C:N1	6:E:148:THR:HG23	1.82	0.94
3:B:658:G:OP1	6:E:90:PHE:CZ	2.20	0.94
4:C:42:ILE:O	4:C:70:HIS:CD2	2.20	0.94
5:D:76:ALA:O	5:D:79:VAL:HG22	1.68	0.94
3:B:669:U:H5'	6:E:107:LYS:HZ2	1.14	0.94
4:C:73:ASN:OD1	4:C:84:TYR:O	1.86	0.94
4:C:76:LEU:HD22	6:E:92:ILE:CG2	1.96	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:67:HIS:HA	4:C:104:THR:HG21	1.48	0.93
4:C:44:ALA:HB2	4:C:70:HIS:CB	1.96	0.93
3:B:740:U:C1'	6:E:101:HIS:ND1	2.28	0.93
3:B:668:G:HO2'	6:E:105:ASN:CA	1.82	0.92
3:B:668:G:C4'	6:E:107:LYS:CG	2.39	0.92
3:B:664:G:H22	3:B:741:G:H1	1.15	0.92
1:A:797:A:H4'	5:D:10:ILE:HG23	1.50	0.92
6:E:83:GLU:O	6:E:84:ILE:HG13	1.67	0.92
4:C:69:PHE:CD2	4:C:70:HIS:HA	2.03	0.91
6:E:134:LYS:O	6:E:134:LYS:HD3	1.69	0.91
2:F:1604:G:H4'	4:C:26:TYR:CD2	2.03	0.90
5:D:11:VAL:HG11	5:D:23:ARG:O	1.71	0.90
4:C:83:TYR:C	4:C:84:TYR:HA	1.92	0.90
4:C:75:ASP:O	4:C:79:ALA:HB2	1.72	0.90
6:E:123:HIS:CD2	6:E:144:THR:HB	2.06	0.89
5:D:62:LYS:H	5:D:62:LYS:HD2	1.35	0.89
4:C:13:LEU:HD23	4:C:13:LEU:O	1.70	0.89
3:B:741:G:O2'	6:E:114:ARG:CG	2.21	0.89
4:C:76:LEU:HB3	6:E:92:ILE:HG21	0.89	0.89
6:E:127:ARG:NE	6:E:141:TYR:CE1	2.36	0.88
4:C:31:LYS:HE2	4:C:31:LYS:O	1.74	0.87
3:B:741:G:H5"	6:E:98:ILE:CD1	2.05	0.87
6:E:82:PRO:O	6:E:83:GLU:HG2	1.72	0.87
6:E:82:PRO:C	6:E:83:GLU:HG3	1.92	0.87
3:B:742:G:H5'	6:E:114:ARG:CG	2.05	0.87
6:E:83:GLU:C	6:E:84:ILE:HG13	1.94	0.87
3:B:740:U:O3'	6:E:98:ILE:HD13	1.75	0.87
1:A:804:C:O5'	6:E:148:THR:CB	2.22	0.86
3:B:728:A:C6	6:E:113:PHE:HD2	1.91	0.86
3:B:741:G:C5'	6:E:98:ILE:CD1	2.53	0.86
1:A:804:C:H6	6:E:148:THR:HG22	1.41	0.86
4:C:44:ALA:CA	4:C:70:HIS:CA	2.38	0.86
4:C:89:LEU:HD23	4:C:90:SER:N	1.90	0.85
2:F:1604:G:N1	5:D:42:CYS:SG	2.44	0.85
3:B:656:C:O2'	6:E:121:ARG:NH2	2.09	0.85
4:C:42:ILE:HG22	4:C:70:HIS:NE2	1.92	0.85
4:C:73:ASN:OD1	4:C:84:TYR:C	2.15	0.85
1:A:804:C:O5'	6:E:148:THR:HG22	1.77	0.84
6:E:123:HIS:CD2	6:E:146:ALA:HB2	2.11	0.84
1:A:806:A:OP2	6:E:147:SER:CA	2.26	0.84
6:E:130:LYS:CB	6:E:141:TYR:CZ	2.61	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:728:A:N6	6:E:113:PHE:CD2	2.46	0.84
6:E:83:GLU:O	6:E:84:ILE:HB	1.76	0.84
6:E:85:PRO:HG3	6:E:129:TYR:CE1	2.12	0.84
4:C:24:LEU:HD22	4:C:24:LEU:O	1.78	0.83
1:A:797:A:C4'	5:D:10:ILE:HD13	2.07	0.83
4:C:49:PRO:C	5:D:41:PHE:CZ	2.50	0.83
4:C:70:HIS:HB3	4:C:71:GLY:N	1.92	0.83
3:B:740:U:H4'	6:E:101:HIS:CG	2.08	0.83
4:C:93:ASP:HA	4:C:93:ASP:OD1	1.77	0.83
6:E:130:LYS:H	6:E:140:LYS:NZ	1.77	0.82
1:A:795:G:H2'	1:A:817:G:N2	1.94	0.82
1:A:804:C:C5	6:E:148:THR:HG23	2.08	0.82
4:C:49:PRO:C	5:D:41:PHE:HZ	1.83	0.82
6:E:130:LYS:O	6:E:133:LYS:O	1.98	0.82
3:B:728:A:N6	6:E:110:ASP:HA	1.94	0.82
4:C:24:LEU:H	4:C:24:LEU:HD13	1.43	0.82
4:C:42:ILE:C	4:C:70:HIS:HD2	1.83	0.81
4:C:69:PHE:CD2	4:C:70:HIS:CA	2.62	0.81
4:C:23:THR:HG22	4:C:90:SER:OG	1.78	0.81
4:C:66:VAL:O	4:C:104:THR:HG21	1.79	0.81
4:C:43:LEU:C	4:C:70:HIS:HB2	2.00	0.81
1:A:795:G:N2	1:A:817:G:H2'	1.94	0.81
4:C:42:ILE:O	4:C:70:HIS:HD2	1.63	0.81
4:C:40:LEU:HG	4:C:65:SER:OG	1.81	0.80
4:C:42:ILE:C	4:C:70:HIS:CD2	2.55	0.80
4:C:83:TYR:C	4:C:84:TYR:N	2.33	0.80
1:A:817:G:H4'	1:A:818:A:OP1	1.80	0.80
4:C:101:SER:O	4:C:103:THR:N	2.13	0.80
1:A:797:A:H4'	5:D:10:ILE:CD1	2.01	0.80
4:C:75:ASP:HA	4:C:83:TYR:CZ	2.17	0.80
3:B:728:A:C6	6:E:113:PHE:CE2	2.70	0.80
1:A:804:C:O4'	6:E:148:THR:HG21	1.82	0.80
2:F:1605:G:C8	4:C:27:LYS:HG3	2.16	0.80
4:C:83:TYR:C	4:C:84:TYR:CA	2.51	0.79
4:C:4:LYS:C	4:C:5:SER:C	2.40	0.79
4:C:9:ILE:HG22	4:C:69:PHE:CE1	1.96	0.79
2:F:1591:A:N6	4:C:24:LEU:CG	2.46	0.79
3:B:728:A:N1	6:E:113:PHE:CD2	2.50	0.79
3:B:673:G:H2'	3:B:674:G:C8	2.17	0.79
3:B:740:U:C5'	6:E:101:HIS:HB2	2.13	0.79
5:D:39:CYS:HB3	5:D:62:LYS:HZ2	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:57:CYS:SG	5:D:62:LYS:HD3	2.23	0.79
1:A:804:C:C4'	6:E:148:THR:CG2	2.58	0.79
3:B:661:G:OP2	4:C:3:LYS:NZ	2.15	0.79
3:B:741:G:H5'	6:E:98:ILE:HD12	1.64	0.79
6:E:88:LEU:HD11	6:E:122:ILE:HG23	1.65	0.78
4:C:83:TYR:O	4:C:84:TYR:HD1	1.66	0.78
2:F:1591:A:H62	4:C:24:LEU:CG	1.96	0.78
2:F:1590:A:N6	2:F:1605:G:H1'	1.99	0.78
4:C:45:ASN:H	4:C:70:HIS:C	1.86	0.78
4:C:75:ASP:O	4:C:79:ALA:CB	2.32	0.78
6:E:130:LYS:H	6:E:140:LYS:HZ1	1.28	0.78
4:C:23:THR:CG2	4:C:90:SER:OG	2.32	0.77
2:F:1604:G:C4	4:C:51:ARG:HG3	2.19	0.77
6:E:73:ARG:NH2	6:E:77:ALA:HB2	2.00	0.77
6:E:75:LEU:HA	6:E:80:LEU:HD21	0.81	0.77
6:E:81:ALA:N	6:E:82:PRO:HD3	2.00	0.77
4:C:76:LEU:CG	6:E:92:ILE:HG22	2.15	0.77
4:C:30:LEU:HD23	4:C:30:LEU:O	1.85	0.76
6:E:127:ARG:NH2	6:E:141:TYR:HA	1.84	0.76
4:C:31:LYS:HZ1	4:C:35:SER:CB	1.99	0.76
1:A:797:A:O4'	5:D:10:ILE:HD13	1.85	0.76
3:B:740:U:H1'	6:E:101:HIS:HE1	0.65	0.75
5:D:53:GLY:HA2	5:D:67:GLY:O	1.87	0.75
4:C:71:GLY:HA3	4:C:86:VAL:O	1.86	0.75
4:C:49:PRO:O	5:D:41:PHE:CZ	2.39	0.75
4:C:9:ILE:HG21	4:C:69:PHE:CD1	2.15	0.75
1:A:804:C:C6	6:E:148:THR:HG22	2.13	0.74
4:C:39:LYS:C	4:C:40:LEU:HD12	2.06	0.74
1:A:796:A:N6	1:A:817:G:H1'	2.01	0.74
3:B:750:G:H1'	6:E:83:GLU:OE1	1.87	0.74
3:B:740:U:O4'	6:E:101:HIS:CG	2.38	0.74
3:B:750:G:C1'	6:E:83:GLU:OE1	2.36	0.73
4:C:42:ILE:CG2	4:C:70:HIS:NE2	2.51	0.73
3:B:667:G:H22	6:E:101:HIS:HE2	1.37	0.73
2:F:1589:G:N2	2:F:1605:G:H2'	2.05	0.72
6:E:130:LYS:HZ2	6:E:137:PRO:CG	2.01	0.72
3:B:669:U:C5'	6:E:107:LYS:HZ1	1.99	0.72
6:E:130:LYS:HZ3	6:E:137:PRO:N	1.88	0.72
4:C:70:HIS:CB	4:C:71:GLY:N	2.52	0.72
3:B:748:C:H1'	3:B:749:C:H5	1.53	0.72
4:C:8:ASN:CB	4:C:8:ASN:ND2	2.52	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:24:LEU:HD22	4:C:24:LEU:C	2.10	0.71
6:E:84:ILE:N	6:E:86:GLU:CB	2.54	0.71
4:C:8:ASN:O	4:C:12:LYS:HB2	1.90	0.71
2:F:1604:G:O5'	4:C:51:ARG:NH2	2.21	0.71
3:B:740:U:H5'	6:E:101:HIS:HB2	1.70	0.71
3:B:740:U:H4'	6:E:101:HIS:CB	2.20	0.70
3:B:668:G:H5'	6:E:107:LYS:HG2	1.70	0.70
4:C:20:GLY:HA2	4:C:22:TYR:CE2	2.19	0.70
4:C:48:PRO:CB	5:D:42:CYS:SG	2.75	0.70
4:C:45:ASN:N	4:C:70:HIS:C	2.45	0.70
4:C:73:ASN:C	4:C:75:ASP:N	2.44	0.70
6:E:125:LEU:O	6:E:140:LYS:HE3	1.91	0.70
4:C:44:ALA:CB	4:C:70:HIS:C	2.60	0.70
4:C:49:PRO:O	5:D:41:PHE:HZ	1.74	0.70
4:C:70:HIS:CA	4:C:71:GLY:N	2.54	0.70
6:E:81:ALA:N	6:E:82:PRO:CD	2.55	0.70
6:E:73:ARG:HH22	6:E:77:ALA:HB2	1.55	0.70
4:C:49:PRO:HG2	5:D:41:PHE:CG	1.55	0.70
6:E:123:HIS:NE2	6:E:144:THR:HB	2.06	0.70
3:B:740:U:O3'	6:E:98:ILE:CD1	2.39	0.70
3:B:667:G:N2	6:E:101:HIS:HE2	1.89	0.69
1:A:805:G:OP2	6:E:148:THR:N	2.24	0.69
3:B:686:U:HO2'	3:B:687:A:H8	1.39	0.69
1:A:804:C:O5'	6:E:148:THR:HB	1.91	0.69
3:B:701:C:H5'	3:B:703:G:O4'	1.92	0.69
5:D:57:CYS:HB2	5:D:62:LYS:CD	2.12	0.69
3:B:740:U:C1'	6:E:101:HIS:HE1	1.54	0.69
4:C:8:ASN:CG	4:C:8:ASN:CA	2.61	0.69
4:C:9:ILE:HG23	4:C:69:PHE:HE1	1.45	0.69
4:C:26:TYR:OH	4:C:54:GLU:CB	2.41	0.69
4:C:40:LEU:HD23	4:C:67:HIS:CE1	2.28	0.69
4:C:20:GLY:CA	4:C:22:TYR:HE2	2.02	0.68
2:F:1605:G:C8	4:C:27:LYS:CG	2.76	0.68
2:F:1605:G:O6	4:C:28:THR:N	2.23	0.68
5:D:20:ALA:O	5:D:24:LYS:HG2	1.94	0.68
4:C:91:ILE:CG2	4:C:94:PRO:HD3	2.23	0.68
4:C:31:LYS:NZ	4:C:35:SER:CB	2.57	0.67
4:C:31:LYS:CE	4:C:35:SER:OG	2.42	0.67
4:C:76:LEU:HD22	6:E:92:ILE:C	2.14	0.67
5:D:57:CYS:HB3	5:D:59:ASP:OD1	1.95	0.67
2:F:1590:A:H61	2:F:1605:G:H1'	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:27:LYS:HA	4:C:27:LYS:NZ	2.10	0.67
4:C:70:HIS:HA	4:C:71:GLY:N	2.09	0.67
4:C:85:ARG:O	4:C:85:ARG:NE	2.28	0.67
1:A:806:A:O3'	6:E:144:THR:O	2.11	0.67
1:A:804:C:H6	6:E:148:THR:HG21	1.48	0.67
2:F:1591:A:N3	4:C:84:TYR:HD2	1.92	0.67
3:B:662:G:H2'	3:B:663:A:C8	2.30	0.66
6:E:85:PRO:HG3	6:E:129:TYR:HE1	1.57	0.66
3:B:667:G:O2'	6:E:108:ASP:HA	1.95	0.66
4:C:29:VAL:CG2	4:C:41:ILE:HD12	2.26	0.66
6:E:134:LYS:O	6:E:134:LYS:CD	2.43	0.66
2:F:1591:A:N6	4:C:24:LEU:HG	2.11	0.66
4:C:50:LEU:O	4:C:54:GLU:HG2	1.95	0.66
3:B:750:G:O2'	6:E:84:ILE:HG12	1.96	0.66
4:C:24:LEU:CD2	4:C:24:LEU:C	2.64	0.66
3:B:668:G:O2'	6:E:105:ASN:CA	2.36	0.66
4:C:73:ASN:O	4:C:75:ASP:N	2.29	0.66
6:E:127:ARG:HA	6:E:141:TYR:HE1	1.60	0.66
4:C:32:THR:HG22	4:C:38:GLY:N	2.11	0.66
4:C:76:LEU:CB	6:E:92:ILE:HG22	2.15	0.66
4:C:32:THR:HG22	4:C:38:GLY:H	1.61	0.65
4:C:76:LEU:HD13	6:E:92:ILE:HB	1.77	0.65
6:E:130:LYS:HB3	6:E:141:TYR:CZ	2.31	0.65
6:E:123:HIS:CD2	6:E:144:THR:CB	2.80	0.65
5:D:62:LYS:HG3	5:D:64:LYS:HZ2	1.61	0.65
4:C:73:ASN:N	4:C:83:TYR:HE2	1.67	0.64
6:E:82:PRO:C	6:E:83:GLU:CG	2.60	0.64
6:E:130:LYS:HZ2	6:E:137:PRO:CB	2.10	0.64
3:B:748:C:H1'	3:B:749:C:C5	2.30	0.64
6:E:91:LEU:HD11	6:E:121:ARG:NH1	2.13	0.64
6:E:133:LYS:HB2	6:E:136:PRO:HG2	1.79	0.64
5:D:39:CYS:HB3	5:D:62:LYS:NZ	2.12	0.64
4:C:26:TYR:O	4:C:29:VAL:CG1	2.39	0.64
4:C:76:LEU:HD21	6:E:93:LYS:HA	1.78	0.63
6:E:130:LYS:HB2	6:E:141:TYR:CE1	2.33	0.63
3:B:723:U:H2'	3:B:723:U:O2	1.98	0.63
1:A:795:G:H1'	1:A:818:A:N6	2.14	0.63
3:B:677:U:H3	3:B:713:G:H22	1.45	0.63
4:C:42:ILE:HB	4:C:70:HIS:HE2	1.63	0.63
2:F:1604:G:O4'	4:C:26:TYR:HD2	1.80	0.63
6:E:130:LYS:NZ	6:E:137:PRO:CD	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:56:GLU:O	4:C:60:MET:HG2	1.98	0.63
4:C:100:ILE:HG13	4:C:101:SER:N	2.12	0.63
4:C:43:LEU:HD21	4:C:55:ILE:HD13	1.80	0.63
4:C:69:PHE:HD2	4:C:70:HIS:CA	2.10	0.62
1:A:804:C:C6	6:E:148:THR:HG21	2.21	0.62
4:C:4:LYS:C	4:C:5:SER:O	2.36	0.62
2:F:1604:G:O4'	4:C:26:TYR:CD2	2.52	0.62
6:E:130:LYS:CB	6:E:141:TYR:CE1	2.82	0.62
5:D:62:LYS:HG2	5:D:64:LYS:NZ	2.15	0.62
3:B:686:U:O2'	3:B:687:A:H8	1.82	0.62
3:B:667:G:N2	6:E:101:HIS:NE2	2.48	0.62
4:C:49:PRO:CG	5:D:41:PHE:CG	2.50	0.62
4:C:19:SER:HG	4:C:20:GLY:N	1.97	0.62
2:F:1591:A:N6	4:C:24:LEU:HD21	1.88	0.62
6:E:80:LEU:C	6:E:82:PRO:HD3	2.20	0.62
4:C:67:HIS:NE2	4:C:103:THR:O	2.32	0.61
5:D:47:VAL:HG22	5:D:57:CYS:SG	2.40	0.61
6:E:91:LEU:HD11	6:E:121:ARG:HH11	1.65	0.61
6:E:127:ARG:HH22	6:E:141:TYR:CA	1.80	0.61
5:D:62:LYS:HG2	5:D:64:LYS:HZ3	1.63	0.61
3:B:728:A:H61	6:E:110:ASP:HA	1.65	0.61
4:C:31:LYS:NZ	4:C:35:SER:OG	2.33	0.61
4:C:8:ASN:CG	4:C:8:ASN:C	2.59	0.61
4:C:24:LEU:HD13	4:C:24:LEU:N	2.16	0.61
5:D:37:TYR:HB2	5:D:47:VAL:HB	1.82	0.61
4:C:32:THR:HG21	4:C:92:LEU:HD23	1.83	0.61
4:C:71:GLY:C	4:C:72:ASN:CG	2.58	0.60
4:C:53:SER:O	4:C:57:TYR:CD1	2.55	0.60
6:E:133:LYS:CG	6:E:133:LYS:CB	2.79	0.60
1:A:796:A:H62	1:A:817:G:H1'	1.64	0.60
2:F:1605:G:C5	4:C:27:LYS:HB2	2.31	0.60
4:C:94:PRO:HG3	4:C:100:ILE:CG2	2.31	0.60
4:C:31:LYS:HE2	4:C:31:LYS:C	2.21	0.60
3:B:750:G:O4'	6:E:83:GLU:OE1	2.20	0.60
4:C:20:GLY:C	4:C:22:TYR:CD2	2.74	0.60
5:D:50:LYS:HE3	5:D:50:LYS:HA	1.83	0.60
6:E:84:ILE:HB	6:E:86:GLU:CD	2.22	0.60
4:C:67:HIS:CA	4:C:104:THR:HG21	2.20	0.60
5:D:36:LYS:HA	5:D:36:LYS:NZ	2.17	0.60
3:B:740:U:O4'	6:E:101:HIS:NE2	2.33	0.60
4:C:71:GLY:O	4:C:72:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:75:ASP:CA	4:C:83:TYR:CZ	2.84	0.59
5:D:57:CYS:SG	5:D:62:LYS:CD	2.90	0.59
4:C:4:LYS:C	4:C:5:SER:HA	2.23	0.59
5:D:22:LEU:O	5:D:26:ILE:HG12	2.02	0.59
5:D:38:PHE:HB3	5:D:45:PHE:CE2	2.37	0.59
1:A:807:A:H2'	1:A:808:A:O4'	2.03	0.58
4:C:40:LEU:CD2	4:C:67:HIS:CE1	2.86	0.58
4:C:20:GLY:O	4:C:22:TYR:HD2	1.86	0.58
5:D:62:LYS:CG	5:D:64:LYS:NZ	2.66	0.58
1:A:806:A:OP2	6:E:147:SER:HA	2.03	0.58
4:C:49:PRO:C	4:C:51:ARG:H	2.07	0.58
3:B:736:C:H2'	3:B:737:A:C8	2.39	0.58
4:C:42:ILE:CG2	4:C:70:HIS:CD2	2.69	0.57
6:E:88:LEU:CD1	6:E:122:ILE:HG23	2.33	0.57
1:A:803:C:O2'	1:A:804:C:H5'	2.03	0.57
1:A:805:G:C8	6:E:147:SER:O	2.57	0.57
1:A:806:A:P	6:E:147:SER:H	2.25	0.57
4:C:69:PHE:HD2	4:C:70:HIS:HA	1.66	0.57
1:A:795:G:C2'	1:A:817:G:N2	2.64	0.57
2:F:1605:G:N7	4:C:27:LYS:CG	2.68	0.57
6:E:80:LEU:C	6:E:82:PRO:CD	2.73	0.57
4:C:49:PRO:HD2	5:D:41:PHE:O	2.04	0.57
4:C:72:ASN:HB3	4:C:83:TYR:CE2	2.39	0.57
4:C:29:VAL:HG23	4:C:41:ILE:HD12	1.87	0.57
5:D:69:TYR:CD1	5:D:70:THR:HG23	2.40	0.57
4:C:46:ASN:OD1	4:C:47:CYS:N	2.38	0.57
4:C:79:ALA:O	4:C:80:CYS:O	2.23	0.57
5:D:60:CYS:HB2	5:D:62:LYS:HE3	1.86	0.57
6:E:130:LYS:N	6:E:140:LYS:NZ	2.50	0.57
1:A:817:G:HO2'	1:A:818:A:H8	1.53	0.57
4:C:51:ARG:O	4:C:51:ARG:HD3	2.05	0.57
4:C:66:VAL:O	4:C:66:VAL:HG13	2.04	0.57
4:C:47:CYS:CB	4:C:87:CYS:SG	2.92	0.56
4:C:83:TYR:O	4:C:84:TYR:HA	2.05	0.56
5:D:60:CYS:HB2	5:D:62:LYS:CE	2.35	0.56
4:C:49:PRO:HG2	5:D:41:PHE:CD2	2.28	0.56
4:C:73:ASN:OD1	4:C:84:TYR:N	2.38	0.56
4:C:73:ASN:C	4:C:83:TYR:CE2	2.76	0.56
6:E:133:LYS:O	6:E:137:PRO:CG	2.52	0.56
6:E:83:GLU:CB	6:E:84:ILE:HG13	2.36	0.56
1:A:795:G:C2'	1:A:817:G:H22	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1586:G:O2'	2:F:1587:U:H5'	2.06	0.56
3:B:743:U:H2'	3:B:744:C:C6	2.42	0.55
1:A:817:G:O2'	1:A:818:A:H8	1.90	0.55
3:B:739:C:O2	6:E:101:HIS:NE2	2.39	0.55
4:C:26:TYR:OH	4:C:54:GLU:HB2	2.05	0.55
1:A:806:A:C8	6:E:123:HIS:ND1	2.71	0.55
4:C:4:LYS:C	4:C:5:SER:CA	2.75	0.55
4:C:66:VAL:C	4:C:104:THR:HG21	2.27	0.55
5:D:39:CYS:SG	5:D:47:VAL:HG23	2.47	0.55
4:C:20:GLY:CA	4:C:22:TYR:CE2	2.87	0.54
4:C:32:THR:CG2	4:C:38:GLY:N	2.70	0.54
6:E:133:LYS:HB3	6:E:136:PRO:CD	2.24	0.54
3:B:741:G:O2'	6:E:114:ARG:CD	2.55	0.54
1:A:819:A:C4'	5:D:13:LYS:HB2	2.38	0.54
2:F:1603:A:H5'	2:F:1605:G:O4'	2.07	0.54
6:E:130:LYS:NZ	6:E:137:PRO:CG	2.68	0.54
4:C:20:GLY:C	4:C:22:TYR:HD2	2.10	0.54
4:C:32:THR:HG22	4:C:38:GLY:CA	2.38	0.54
6:E:75:LEU:CA	6:E:80:LEU:CD2	2.45	0.54
1:A:805:G:O5'	6:E:147:SER:O	2.25	0.53
2:F:1588:G:C6	2:F:1589:G:N1	2.77	0.53
4:C:33:LEU:HD23	4:C:64:ILE:HG13	1.89	0.53
4:C:89:LEU:HD23	4:C:90:SER:H	1.73	0.53
1:A:817:G:O2'	1:A:818:A:C8	2.62	0.53
5:D:62:LYS:HD2	5:D:62:LYS:N	2.09	0.53
6:E:123:HIS:HD2	6:E:144:THR:CB	2.21	0.53
4:C:79:ALA:HB1	6:E:99:ARG:HH22	1.73	0.53
5:D:62:LYS:CG	5:D:64:LYS:HZ2	2.21	0.53
4:C:43:LEU:O	4:C:70:HIS:N	2.42	0.53
2:F:1591:A:H4'	2:F:1592:G:O5'	2.09	0.53
4:C:23:THR:HG22	4:C:90:SER:HG	1.73	0.53
4:C:32:THR:HG21	4:C:92:LEU:CD2	2.38	0.53
5:D:39:CYS:CB	5:D:62:LYS:HZ2	2.20	0.53
4:C:27:LYS:HA	4:C:27:LYS:HZ2	1.73	0.53
1:A:806:A:N3	6:E:119:GLU:CG	2.72	0.52
4:C:44:ALA:C	4:C:70:HIS:C	2.66	0.52
2:F:1589:G:H22	2:F:1605:G:H2'	1.73	0.52
5:D:46:ALA:HB1	5:D:58:LYS:HG2	1.90	0.52
3:B:740:U:H5'	6:E:101:HIS:CB	2.40	0.52
1:A:804:C:C5	6:E:148:THR:CG2	2.79	0.52
5:D:10:ILE:HB	5:D:27:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:42:ILE:O	4:C:88:CYS:HA	2.10	0.52
4:C:32:THR:CG2	4:C:92:LEU:CD2	2.88	0.52
4:C:35:SER:O	4:C:36:SER:HB2	2.09	0.52
1:A:805:G:H3'	6:E:147:SER:O	2.10	0.51
4:C:76:LEU:HD22	6:E:92:ILE:O	2.10	0.51
1:A:806:A:O2'	6:E:119:GLU:OE2	2.25	0.51
4:C:20:GLY:O	4:C:93:ASP:HB3	2.09	0.51
6:E:84:ILE:N	6:E:86:GLU:CG	2.74	0.51
3:B:728:A:N6	6:E:113:PHE:CE2	2.78	0.51
4:C:14:GLN:HE22	4:C:74:VAL:HG22	1.76	0.51
4:C:44:ALA:CB	4:C:70:HIS:HB2	2.20	0.51
3:B:740:U:C2'	6:E:101:HIS:ND1	2.73	0.51
3:B:746:A:O2'	3:B:747:C:H5'	2.10	0.51
4:C:26:TYR:C	4:C:29:VAL:HG12	2.25	0.51
3:B:658:G:P	6:E:90:PHE:CE2	2.73	0.50
4:C:91:ILE:HG23	4:C:93:ASP:O	2.11	0.50
5:D:28:LYS:O	5:D:31:VAL:HG12	2.11	0.50
6:E:130:LYS:HB3	6:E:141:TYR:OH	2.10	0.50
1:A:804:C:C1'	6:E:148:THR:CG2	2.89	0.50
6:E:84:ILE:H	6:E:86:GLU:CB	2.25	0.50
6:E:115:LEU:O	6:E:118:VAL:HG12	2.12	0.50
1:A:806:A:N3	6:E:119:GLU:HG2	2.26	0.50
4:C:44:ALA:HA	4:C:70:HIS:N	2.22	0.50
4:C:39:LYS:C	4:C:40:LEU:CD1	2.79	0.50
4:C:43:LEU:N	4:C:70:HIS:HD2	2.10	0.50
4:C:80:CYS:SG	6:E:143:SER:O	2.70	0.50
6:E:133:LYS:CB	6:E:136:PRO:HD2	2.26	0.50
6:E:84:ILE:CB	6:E:86:GLU:OE2	2.45	0.50
5:D:79:VAL:HG23	5:D:80:ARG:N	2.27	0.49
6:E:84:ILE:H	6:E:86:GLU:HB3	1.77	0.49
4:C:91:ILE:HG22	4:C:94:PRO:HD3	1.95	0.49
3:B:659:U:O2'	3:B:660:G:H5'	2.12	0.49
3:B:728:A:H62	6:E:110:ASP:HA	1.75	0.49
5:D:11:VAL:HG22	5:D:27:LYS:HD3	1.95	0.49
6:E:109:LYS:H	6:E:109:LYS:HD2	1.77	0.49
2:F:1604:G:P	4:C:51:ARG:HH21	2.36	0.49
3:B:657:G:O2'	3:B:658:G:H5'	2.12	0.49
3:B:666:G:H5'	3:B:726:C:H1'	1.94	0.49
4:C:31:LYS:NZ	4:C:37:LYS:HE3	2.28	0.49
4:C:48:PRO:HB2	4:C:51:ARG:CB	2.42	0.49
5:D:11:VAL:HG13	5:D:27:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:134:LYS:CG	6:E:134:LYS:CA	2.90	0.49
2:F:1604:G:N3	4:C:51:ARG:HG3	2.26	0.49
5:D:11:VAL:HB	5:D:23:ARG:HB2	1.95	0.48
6:E:85:PRO:HG3	6:E:129:TYR:CZ	2.48	0.48
4:C:44:ALA:H	4:C:70:HIS:HB2	1.56	0.48
4:C:49:PRO:N	5:D:41:PHE:CE2	2.81	0.48
1:A:797:A:H4'	5:D:10:ILE:CG2	2.32	0.48
4:C:30:LEU:HD23	4:C:30:LEU:C	2.33	0.48
5:D:22:LEU:O	5:D:25:GLN:HG2	2.13	0.48
3:B:722:A:H4'	3:B:723:U:C5	2.49	0.48
4:C:23:THR:HG23	4:C:90:SER:OG	2.10	0.48
5:D:22:LEU:HD13	5:D:22:LEU:C	2.34	0.48
4:C:40:LEU:CD2	4:C:67:HIS:HE1	2.26	0.48
5:D:39:CYS:SG	5:D:47:VAL:CG2	3.01	0.48
6:E:83:GLU:HB2	6:E:84:ILE:HG13	1.95	0.48
4:C:48:PRO:HB2	4:C:51:ARG:HB3	1.94	0.48
3:B:728:A:N6	6:E:113:PHE:HD2	1.93	0.48
4:C:49:PRO:HD2	5:D:41:PHE:C	2.35	0.48
5:D:77:VAL:HA	5:D:80:ARG:HH11	1.79	0.48
3:B:659:U:H2'	3:B:660:G:O4'	2.14	0.47
3:B:740:U:H4'	6:E:101:HIS:HB2	1.95	0.47
4:C:30:LEU:CD2	4:C:34:ARG:NE	2.77	0.47
4:C:73:ASN:OD1	4:C:84:TYR:CA	2.62	0.47
3:B:743:U:H2'	3:B:744:C:H6	1.78	0.47
5:D:63:VAL:O	5:D:63:VAL:HG13	2.14	0.47
3:B:686:U:O4	3:B:703:G:H1'	2.14	0.47
2:F:1607:A:H2'	2:F:1608:G:O4'	2.15	0.47
3:B:740:U:C5'	6:E:101:HIS:CG	2.97	0.47
5:D:57:CYS:SG	5:D:62:LYS:CG	3.03	0.47
3:B:750:G:O2'	6:E:84:ILE:CG1	2.61	0.47
5:D:33:GLN:O	5:D:37:TYR:HE1	1.98	0.47
3:B:652:U:O4	3:B:752:G:O2'	2.29	0.46
5:D:48:LYS:HE2	5:D:48:LYS:HA	1.96	0.46
2:F:1605:G:C8	2:F:1605:G:H5"	2.50	0.46
4:C:9:ILE:CG2	4:C:69:PHE:CZ	2.80	0.46
4:C:29:VAL:HG23	4:C:41:ILE:CD1	2.44	0.46
4:C:29:VAL:HG13	4:C:30:LEU:N	2.30	0.46
4:C:94:PRO:CG	4:C:100:ILE:CG2	2.94	0.46
6:E:133:LYS:CG	6:E:133:LYS:HA	2.45	0.46
5:D:72:ASN:ND2	5:D:72:ASN:O	2.48	0.46
6:E:84:ILE:O	6:E:87:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:134:LYS:CG	6:E:134:LYS:O	2.63	0.46
3:B:740:U:C5'	6:E:101:HIS:CB	2.90	0.46
4:C:9:ILE:HG21	4:C:69:PHE:CZ	2.25	0.46
4:C:42:ILE:CB	4:C:70:HIS:NE2	2.79	0.46
6:E:127:ARG:HH12	6:E:146:ALA:HB3	1.80	0.46
2:F:1603:A:H4'	2:F:1604:G:OP2	2.14	0.46
4:C:43:LEU:CA	4:C:70:HIS:HD2	2.28	0.46
4:C:45:ASN:HA	4:C:68:HIS:CE1	2.50	0.46
1:A:796:A:O2'	5:D:10:ILE:CD1	2.64	0.46
4:C:32:THR:CG2	4:C:38:GLY:CA	2.93	0.46
1:A:795:G:H21	1:A:817:G:H2'	1.78	0.46
3:B:741:G:O4'	6:E:111:SER:HB2	2.16	0.46
5:D:47:VAL:HG11	5:D:71:MET:SD	2.57	0.45
1:A:804:C:P	6:E:148:THR:HG22	2.55	0.45
2:F:1586:G:H2'	2:F:1587:U:O4'	2.16	0.45
4:C:85:ARG:O	4:C:85:ARG:CZ	2.64	0.45
1:A:819:A:H5'	5:D:13:LYS:HB2	1.98	0.45
4:C:26:TYR:HB2	4:C:51:ARG:HH21	1.80	0.45
3:B:740:U:C2'	6:E:101:HIS:CE1	2.87	0.45
1:A:804:C:O4'	6:E:148:THR:CG2	2.61	0.45
4:C:42:ILE:HB	4:C:70:HIS:NE2	2.31	0.45
6:E:130:LYS:NZ	6:E:136:PRO:C	2.62	0.45
3:B:740:U:O4'	6:E:101:HIS:CD2	2.70	0.45
3:B:740:U:C4'	6:E:101:HIS:CB	2.88	0.45
4:C:83:TYR:O	4:C:84:TYR:CD1	2.58	0.45
1:A:816:G:C6	1:A:817:G:N1	2.85	0.45
6:E:130:LYS:N	6:E:140:LYS:HZ2	2.14	0.45
5:D:49:ARG:HD2	5:D:52:VAL:HA	1.98	0.45
1:A:796:A:O2'	5:D:10:ILE:HD11	2.17	0.45
5:D:19:GLY:O	5:D:23:ARG:HG2	2.17	0.45
1:A:806:A:H1'	6:E:119:GLU:HG3	1.98	0.45
3:B:735:C:O2'	3:B:736:C:H5'	2.17	0.44
4:C:40:LEU:CG	4:C:65:SER:OG	2.59	0.44
4:C:91:ILE:HG21	4:C:94:PRO:HG3	1.99	0.44
6:E:133:LYS:O	6:E:137:PRO:HG2	2.17	0.44
3:B:740:U:H5'	6:E:101:HIS:CG	2.53	0.44
4:C:100:ILE:HG13	4:C:101:SER:H	1.81	0.44
6:E:84:ILE:C	6:E:86:GLU:CD	2.76	0.44
3:B:652:U:H2'	3:B:752:G:N1	2.32	0.44
1:A:804:C:C1'	6:E:148:THR:HG23	2.47	0.44
2:F:1587:U:C4	2:F:1588:G:C6	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:690:G:H2'	3:B:691:G:O4'	2.18	0.44
4:C:4:LYS:O	4:C:5:SER:C	2.56	0.44
4:C:43:LEU:HD21	4:C:55:ILE:HG21	1.99	0.44
3:B:742:G:H5'	6:E:114:ARG:HG3	1.93	0.44
4:C:77:GLY:C	4:C:82:LYS:HD2	2.39	0.44
4:C:26:TYR:CE1	4:C:55:ILE:HG13	2.53	0.43
4:C:76:LEU:HD21	6:E:96:VAL:CG1	2.48	0.43
2:F:1594:C:O2'	2:F:1595:G:H5'	2.19	0.43
3:B:740:U:C4'	6:E:101:HIS:HB2	2.48	0.43
4:C:20:GLY:C	4:C:22:TYR:CE2	2.91	0.43
4:C:55:ILE:O	4:C:59:ALA:HB2	2.18	0.43
4:C:91:ILE:CG2	4:C:94:PRO:CD	2.94	0.43
6:E:127:ARG:NH2	6:E:141:TYR:CA	2.47	0.43
5:D:29:MET:O	5:D:33:GLN:HB2	2.19	0.43
5:D:11:VAL:CG1	5:D:27:LYS:HB2	2.49	0.43
6:E:84:ILE:O	6:E:85:PRO:O	2.35	0.43
4:C:91:ILE:HG23	4:C:94:PRO:CD	2.49	0.43
4:C:44:ALA:HB1	4:C:70:HIS:C	2.38	0.43
5:D:33:GLN:O	5:D:33:GLN:NE2	2.49	0.42
5:D:62:LYS:HG2	5:D:62:LYS:O	2.17	0.42
4:C:76:LEU:CA	6:E:92:ILE:HG21	2.44	0.42
5:D:57:CYS:SG	5:D:64:LYS:NZ	2.92	0.42
1:A:807:A:N1	1:A:808:A:C2	2.87	0.42
1:A:811:C:H2'	1:A:812:A:C8	2.55	0.42
3:B:730:G:C5	3:B:731:G:H1'	2.55	0.42
5:D:33:GLN:HE21	5:D:33:GLN:C	2.22	0.42
4:C:19:SER:C	4:C:20:GLY:CA	2.86	0.42
5:D:76:ALA:O	5:D:79:VAL:CG2	2.55	0.42
1:A:795:G:H22	1:A:817:G:H2'	1.82	0.42
3:B:665:A:H2'	3:B:725:G:N2	2.34	0.42
3:B:667:G:O2'	6:E:108:ASP:CB	2.67	0.42
4:C:76:LEU:CG	6:E:92:ILE:CG2	2.83	0.42
2:F:1609:C:H2'	2:F:1610:G:H8	1.83	0.42
3:B:667:G:N2	6:E:101:HIS:CE1	2.88	0.42
1:A:804:C:C5'	6:E:148:THR:CG2	2.63	0.42
2:F:1604:G:OP1	4:C:26:TYR:HB2	2.15	0.42
4:C:47:CYS:HB2	4:C:87:CYS:SG	2.60	0.42
4:C:49:PRO:O	4:C:51:ARG:N	2.53	0.42
4:C:49:PRO:C	4:C:51:ARG:N	2.72	0.42
6:E:106:ARG:H	6:E:106:ARG:HH11	1.67	0.42
2:F:1605:G:H8	4:C:27:LYS:HG3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:13:LEU:HD23	4:C:13:LEU:C	2.38	0.41
4:C:49:PRO:O	5:D:41:PHE:CE2	2.72	0.41
4:C:66:VAL:O	4:C:104:THR:CG2	2.60	0.41
5:D:41:PHE:HB3	5:D:62:LYS:HZ3	1.85	0.41
1:A:819:A:H4'	5:D:13:LYS:HB2	2.02	0.41
4:C:46:ASN:O	4:C:47:CYS:O	2.38	0.41
5:D:30:GLU:HA	5:D:33:GLN:CB	2.51	0.41
5:D:32:SER:O	5:D:37:TYR:OH	2.38	0.41
5:D:34:HIS:O	5:D:34:HIS:CG	2.74	0.41
4:C:57:TYR:O	4:C:60:MET:HB2	2.20	0.41
4:C:76:LEU:HD21	6:E:96:VAL:HG11	2.03	0.41
4:C:16:VAL:HA	4:C:19:SER:OG	2.21	0.41
3:B:723:U:O2	3:B:723:U:C2'	2.68	0.41
3:B:736:C:H2'	3:B:737:A:H8	1.83	0.41
3:B:741:G:HO2'	6:E:114:ARG:CG	2.31	0.41
4:C:76:LEU:CA	6:E:92:ILE:CG2	2.97	0.41
5:D:49:ARG:HB2	5:D:55:TRP:CZ3	2.56	0.41
3:B:692:U:H1'	3:B:695:A:N7	2.36	0.41
5:D:36:LYS:HA	5:D:36:LYS:HZ3	1.84	0.40
3:B:662:G:H2'	3:B:663:A:H8	1.78	0.40
3:B:728:A:H2'	3:B:729:A:C8	2.56	0.40
6:E:133:LYS:CB	6:E:136:PRO:HG2	2.49	0.40
4:C:26:TYR:OH	4:C:54:GLU:HB3	2.17	0.40
4:C:33:LEU:CD2	4:C:64:ILE:HG13	2.52	0.40
4:C:71:GLY:HA3	4:C:86:VAL:HG23	2.03	0.40
1:A:805:G:OP2	6:E:147:SER:CA	2.69	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
4	C	92/104 (88%)	70 (76%)	12 (13%)	10 (11%)	0 8
5	D	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	11 46
6	E	77/84 (92%)	71 (92%)	3 (4%)	3 (4%)	3 23
All	All	240/261 (92%)	206 (86%)	20 (8%)	14 (6%)	3 18

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	47	CYS
4	C	72	ASN
4	C	79	ALA
4	C	80	CYS
4	C	102	THR
6	E	147	SER
4	C	74	VAL
4	C	101	SER
4	C	6	GLY
4	C	48	PRO
5	D	81	SER
6	E	138	THR
4	C	50	LEU
6	E	81	ALA

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
4	C	91/91 (100%)	82 (90%)	9 (10%)	8 26
5	D	57/57 (100%)	50 (88%)	7 (12%)	4 19
6	E	76/76 (100%)	69 (91%)	7 (9%)	9 29
All	All	224/224 (100%)	201 (90%)	23 (10%)	11 25

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	18	LYS
4	C	24	LEU
4	C	27	LYS
4	C	31	LYS
4	C	51	ARG
4	C	63	LYS
4	C	85	ARG
4	C	92	LEU
4	C	93	ASP
5	D	10	ILE
5	D	33	GLN
5	D	36	LYS
5	D	48	LYS
5	D	50	LYS
5	D	62	LYS
5	D	72	ASN
6	E	73	ARG
6	E	76	LYS
6	E	100	LYS
6	E	106	ARG
6	E	107	LYS
6	E	109	LYS
6	E	129	TYR

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

Mol	Chain	Res	Type
4	C	10	ASN
4	C	67	HIS
4	C	70	HIS
5	D	25	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	27/28 (96%)	3 (11%)	1 (3%)
2	F	32/34 (94%)	5 (15%)	3 (9%)
3	B	100/101 (99%)	11 (11%)	3 (3%)
All	All	159/163 (97%)	19 (11%)	7 (4%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	809	G
1	A	817	G
1	A	818	A
2	F	1592	G
2	F	1593	C
2	F	1604	G
2	F	1605	G
2	F	1606	A
3	B	653	A
3	B	665	A
3	B	686	U
3	B	687	A
3	B	688	G
3	B	702	A
3	B	703	G
3	B	718	G
3	B	723	U
3	B	731	G
3	B	749	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	817	G
2	F	1591	A
2	F	1603	A
2	F	1605	G
3	B	687	A
3	B	701	C
3	B	748	C

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	C	11
6	E	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	4:LYS	C	5:SER	N	3.64
1	C	20:GLY	C	21:LYS	N	3.56
1	E	79:GLY	C	80:LEU	N	3.26
1	E	84:ILE	C	85:PRO	N	3.14
1	C	69:PHE	C	70:HIS	N	3.02
1	C	1:LYS	C	2:ALA	N	2.92
1	C	70:HIS	C	71:GLY	N	2.89
1	C	83:TYR	C	84:TYR	N	2.33
1	E	85:PRO	C	86:GLU	N	2.23
1	C	19:SER	C	20:GLY	N	1.89
1	E	132:THR	C	133:LYS	N	1.67
1	C	93:ASP	C	94:PRO	N	1.20
1	C	91:ILE	C	92:LEU	N	1.15
1	C	103:THR	C	104:THR	N	0.97
1	C	79:ALA	C	80:CYS	N	0.88

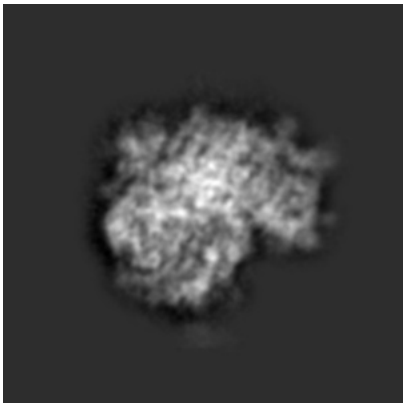
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1125. These allow visual inspection of the internal detail of the map and identification of artifacts.

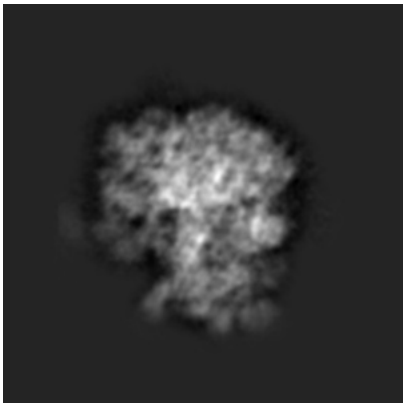
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

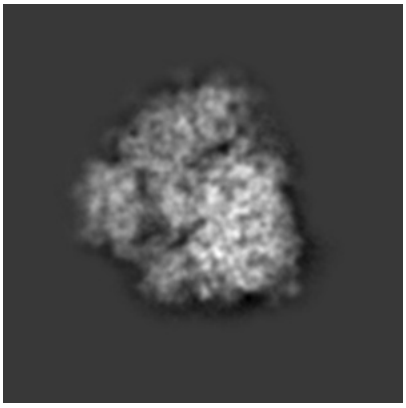
6.1.1 Primary map



X



Y

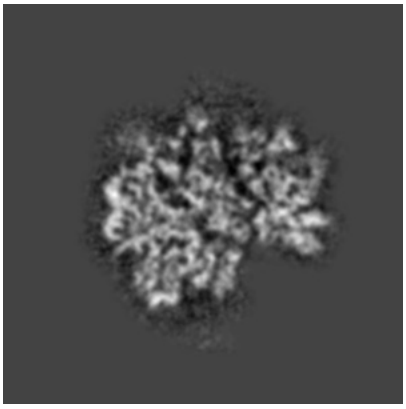


Z

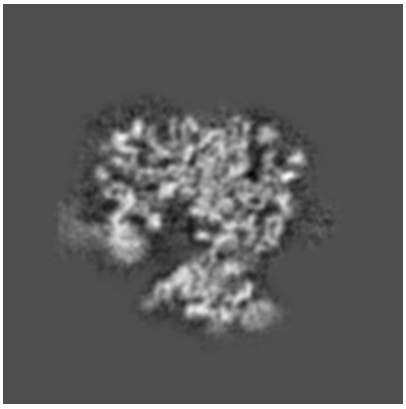
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

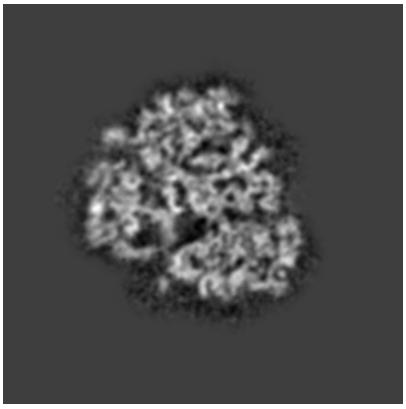
6.2.1 Primary map



X Index: 110



Y Index: 110

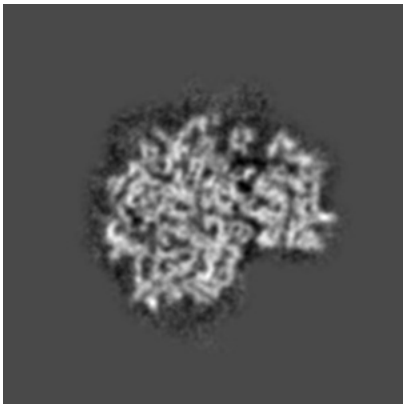


Z Index: 110

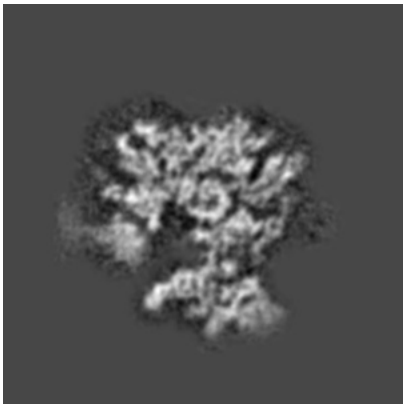
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

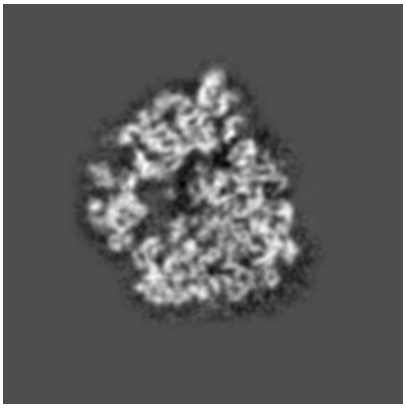
6.3.1 Primary map



X Index: 114



Y Index: 113



Z Index: 102

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 0.000155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

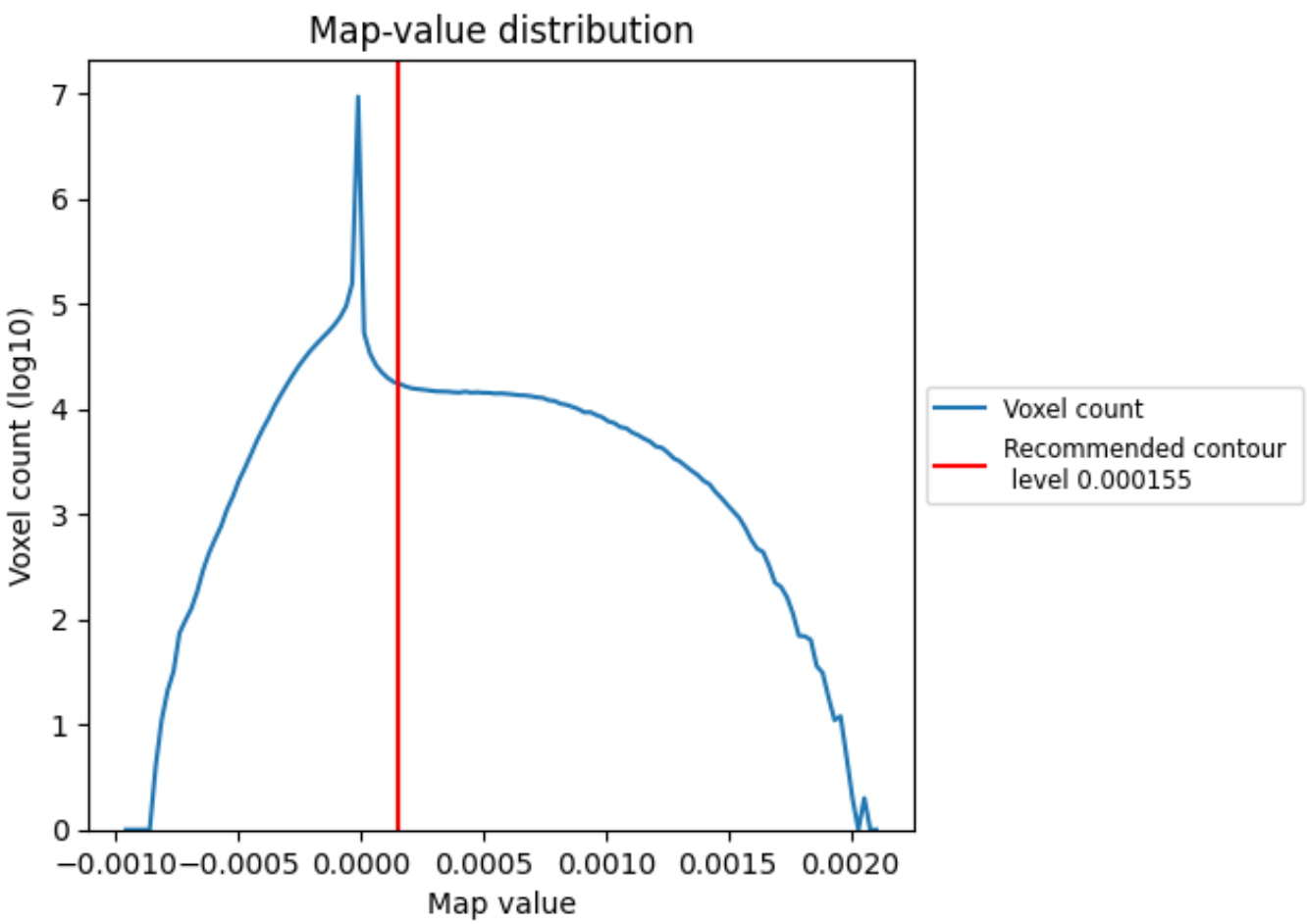
6.5 Mask visualisation (i)

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

7 Map analysis (i)

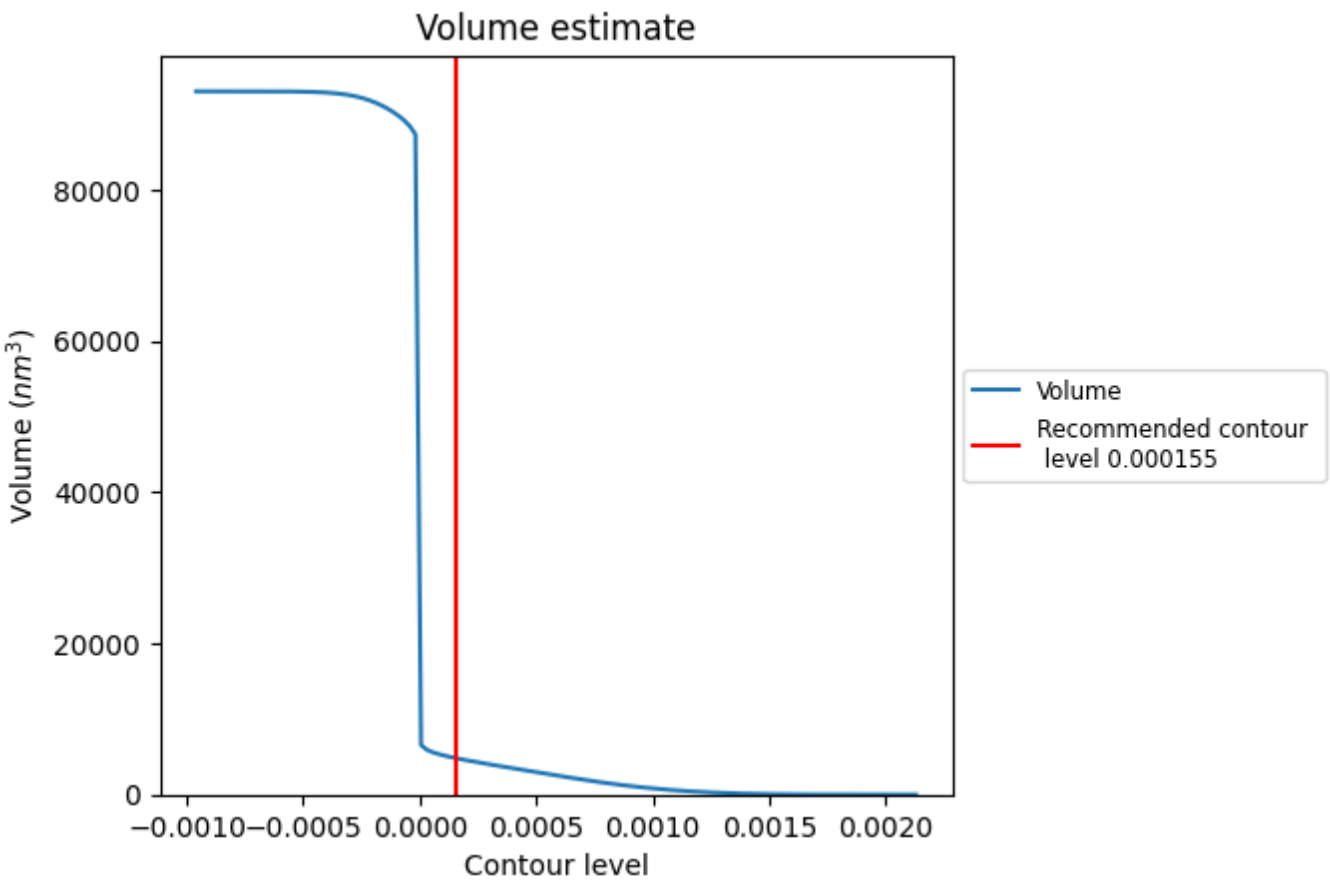
This section contains the results of statistical analysis of the map.

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.

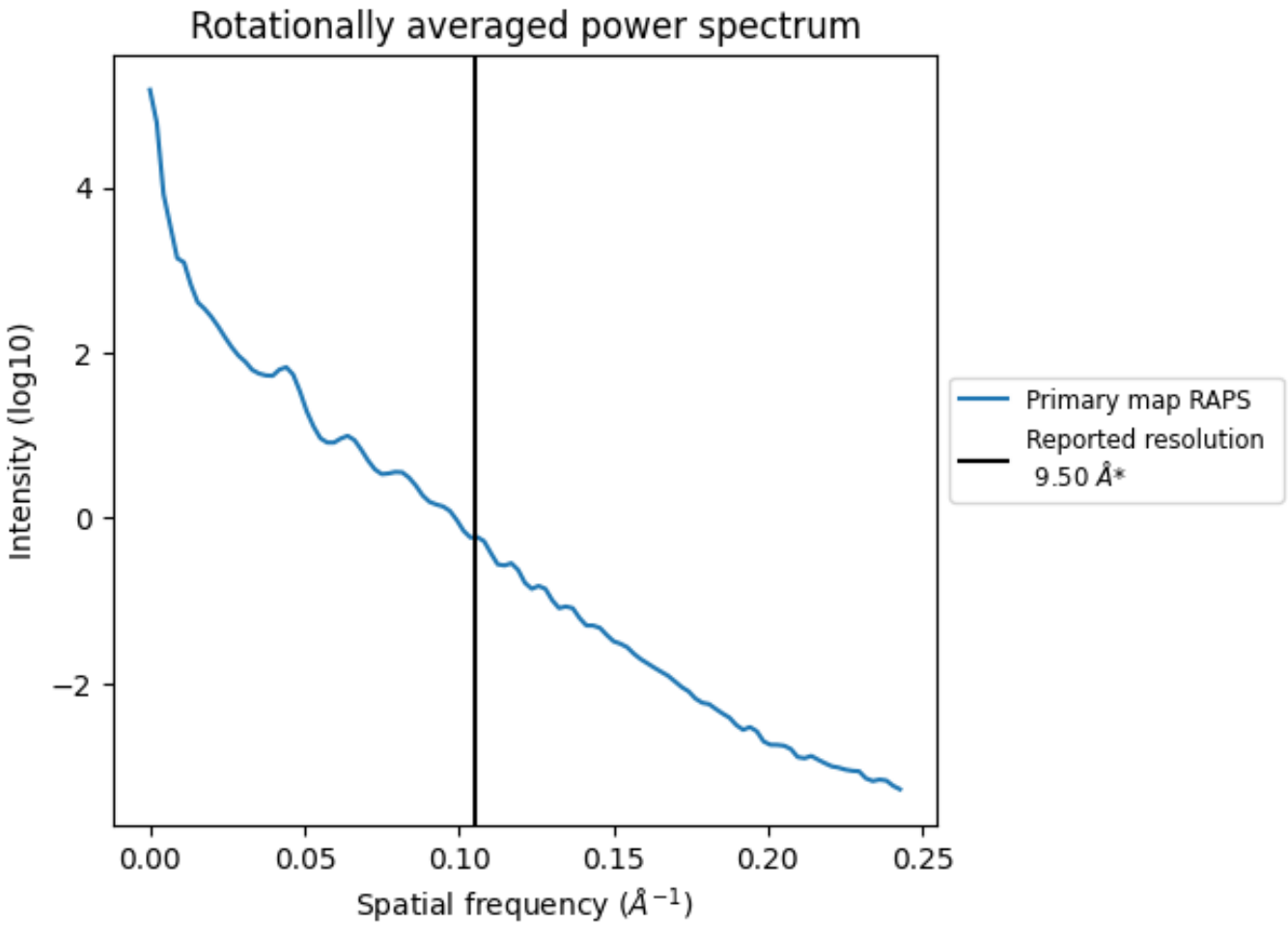
7.2 Volume estimate (i)



The volume at the recommended contour level is 4814 nm^3; this corresponds to an approximate mass of 4348 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 0.105 Å^{-1}

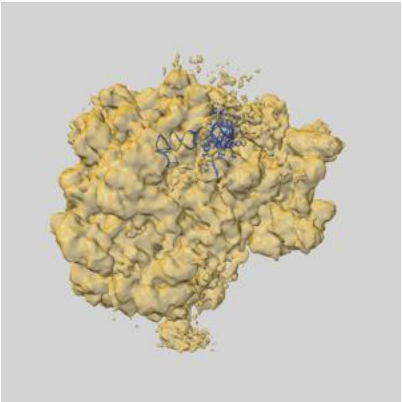
8 Fourier-Shell correlation (i)

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

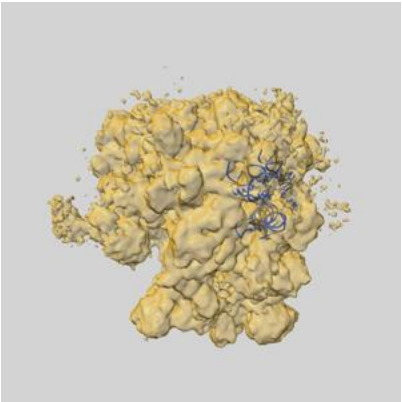
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1125 and PDB model 1YSH. Per-residue inclusion information can be found in section 3 on page 5.

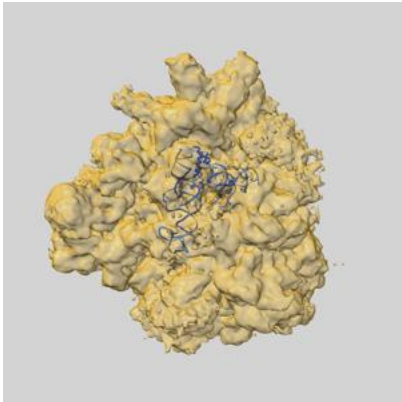
9.1 Map-model overlay (i)



X



Y



Z

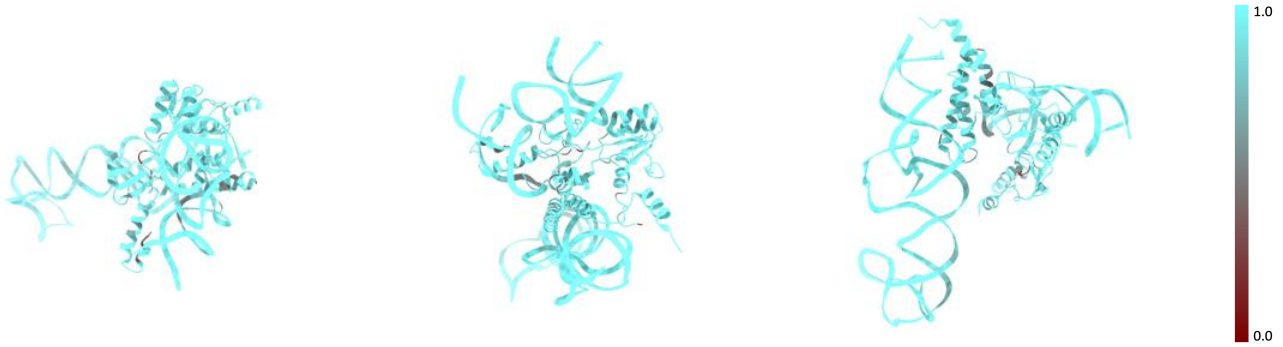
The images above show the 3D surface view of the map at the recommended contour level 0.000155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

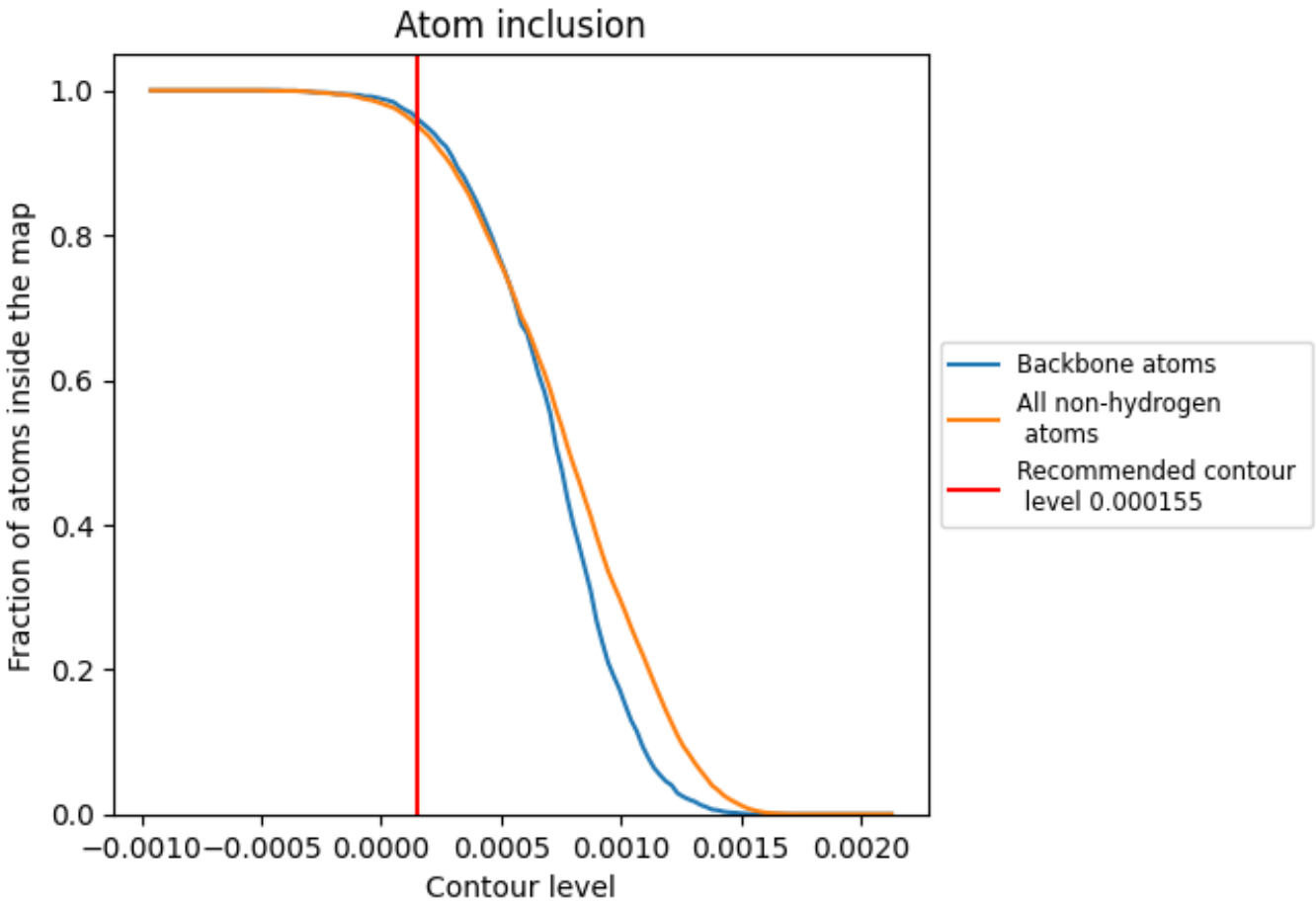
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.000155).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.000155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9506	0.1250
A	0.9280	0.1400
B	0.9616	0.1270
C	0.9558	0.1360
D	0.8971	0.0780
E	0.9364	0.1270
F	0.9847	0.1300