



Full wwPDB EM Validation Report ⓘ

Jul 9, 2024 – 10:06 pm BST

PDB ID : 9FQ0
EMDB ID : EMD-50642
Title : Human NatA-NAC-MAP1 80S ribosome complex
Authors : Klein, M.A.; Wild, K.; Sinning, I.
Deposited on : 2024-06-14
Resolution : 4.67 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

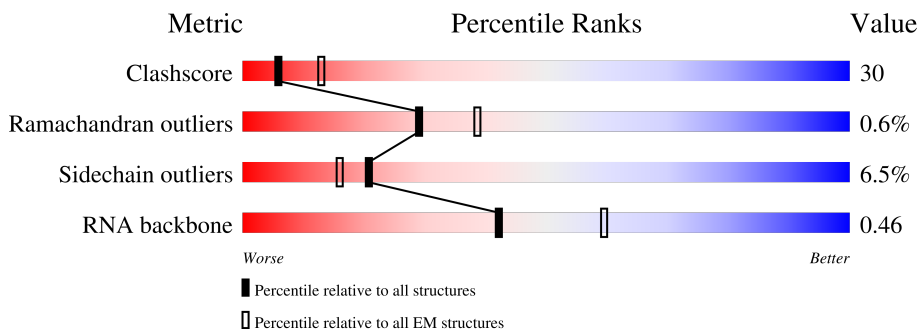
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.67 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	8	58	38% (green), 50% (yellow), 12% (orange)
2	E	392	8% (red), 49% (green), 29% (yellow), 19% (grey)
3	D	206	33% (red), 21% (green), 34% (yellow), 41% (grey)
4	1	5070	94% (grey)
5	LY	145	10% (red), 28% (green), 55% (yellow), 6% (orange), 11% (grey)
6	Lh	123	9% (red), 91% (green), 7% (yellow), 2% (orange)
7	LX	156	22% (red), 35% (green), 36% (yellow), 26% (grey)

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Mol	Chain	Length	Quality of chain
8	A	221	
9	LU	128	
10	LR	196	
11	Lk	70	
12	2	171	
13	B	840	
14	LC	427	
15	LE	288	
16	Lr	137	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31676 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 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	8	58	1237	554	224	401	58	0	0

- Molecule 2 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	317	2498	1569	445	466	18	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	GLY	-	expression tag	UNP P53582
E	-4	PRO	-	expression tag	UNP P53582
E	-3	GLY	-	expression tag	UNP P53582
E	-2	SER	-	expression tag	UNP P53582
E	-1	GLY	-	expression tag	UNP P53582
E	0	SER	-	expression tag	UNP P53582

- Molecule 3 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	122	937	584	175	175	3	0	0

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	1	298	6383	2840	1162	2083	298	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LY	129	1075	675	218	179	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Lh	122	1015	641	205	168	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LX	116	950	606	178	165	1	0	0

- Molecule 8 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	125	967	602	173	188	4	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q13765
A	-4	PRO	-	expression tag	UNP Q13765
A	-3	GLY	-	expression tag	UNP Q13765
A	-2	SER	-	expression tag	UNP Q13765
A	-1	GLY	-	expression tag	UNP Q13765
A	0	SER	-	expression tag	UNP Q13765

- Molecule 9 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LU	101	825	529	144	150	2	0	0

- Molecule 10 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LR	153	1281	799	276	197	9	0	0

- Molecule 11 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Lk	69	569	366	103	99	1	0	0

- Molecule 12 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	2	169	1388	869	253	256	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	0	MET	-	initiating methionine	UNP P41227
2	1	GLY	-	expression tag	UNP P41227

- Molecule 13 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B	834	6881	4379	1189	1272	41	0	0

- Molecule 14 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LC	365	2908	1829	580	486	13	0	0

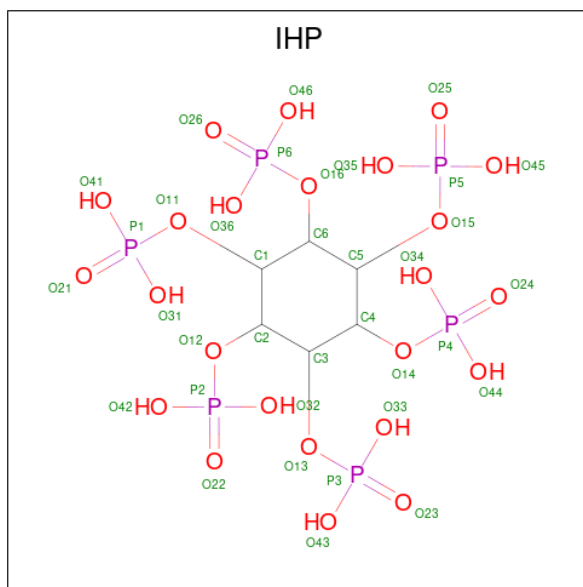
- Molecule 15 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LE	214	1724	1111	327	282	4	0	0

- Molecule 16 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Lr	125	1002	622	207	168	5	0	0

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	B	1	36	6	24	6	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.

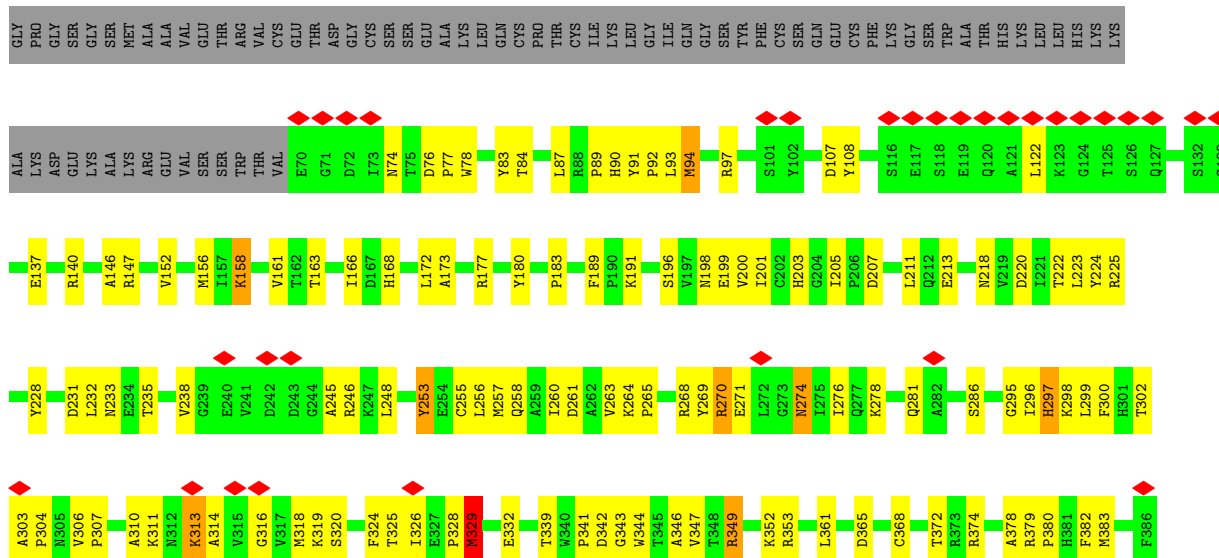
- Molecule 1: 5.8S rRNA

Chain 8: 




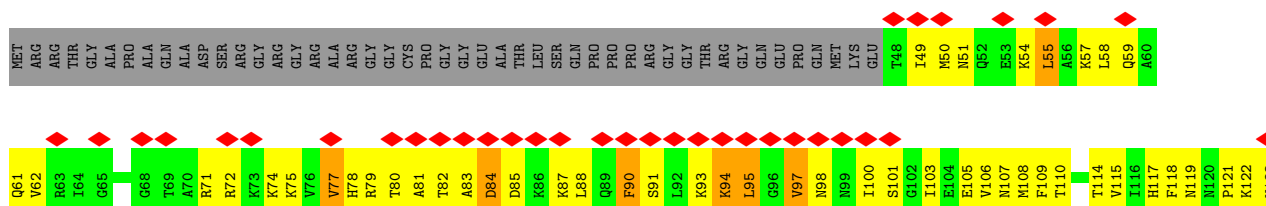
- Molecule 2: Methionine aminopeptidase 1

Chain E: 

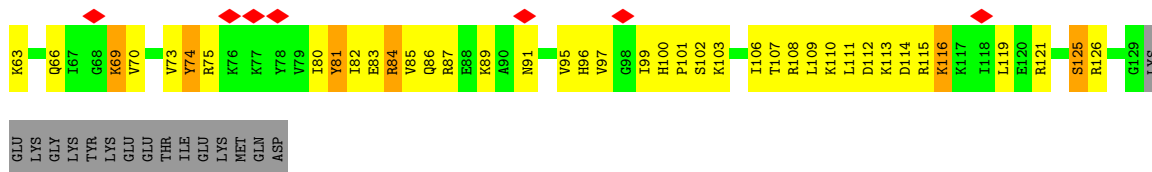


- Molecule 3: Transcription factor BTF3

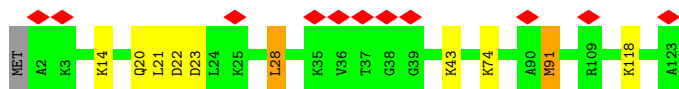
Chain D: 



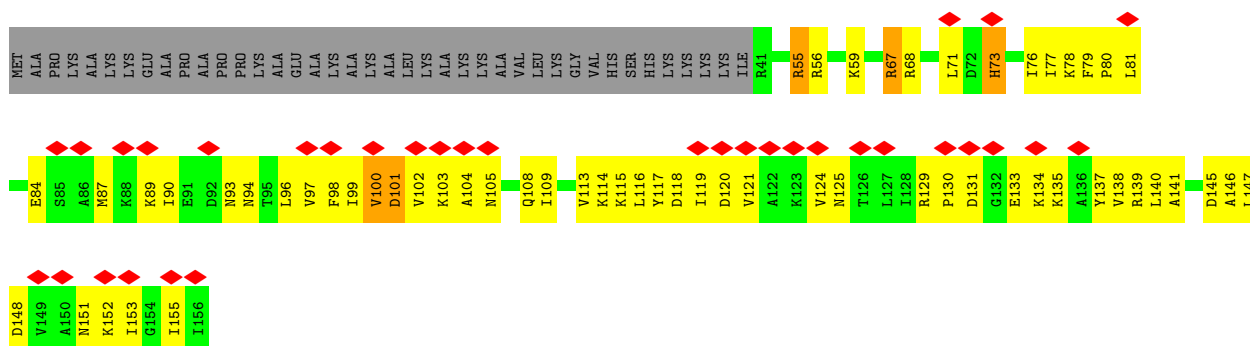
D C C C C C C D D C C C G G G G C C C A C C C C C G G G G G A A D C C C C C G G G G D D C C C C G G G G
G G G C C C G C C G G C C G D C D D C C D G G G G G G C C G G G C C A C C C D C C A C G C G G G A C G C G D C
D C C C A C C C C D C D C C C C C G G C C C C C C C G G C C G A C C G G G C C C G G G C C C G G G C C G G C C G
G G G G G C G G G C C G G A C D U G C C C C C C C C C C C C C G G C
A G G U D C D C C G C G G G C C C A C
G G G U C C G G C C G G C A C G G U C
A A C A A C G U G C C G C G G A G U C C G G G C
C G G C
A C C G G C
G A A A A A U G G G U G C A A C C U G C
U A C C G G U C
A A C C A A U C U A G U G C G A C C G G G C
C C C G G A A C
C C G A A A C C G A C
U G G A A G C C G G G C
U G C C G G A U G G A A C C C G G A A A C
A A A A G U U U G G A C
A G U G U A A C A A A C
C G G G C C C A U A C
G C C C G C
G G U D C
C C G G C
C C U U G A A A G C C G G C
U A G C C A A U U A U2371 U2372 C2373 A2374 A2375 A2376 C2377 G2380 U2385 U2386 G2387 A2388 A2389
G C
U G A A C A U G G G C



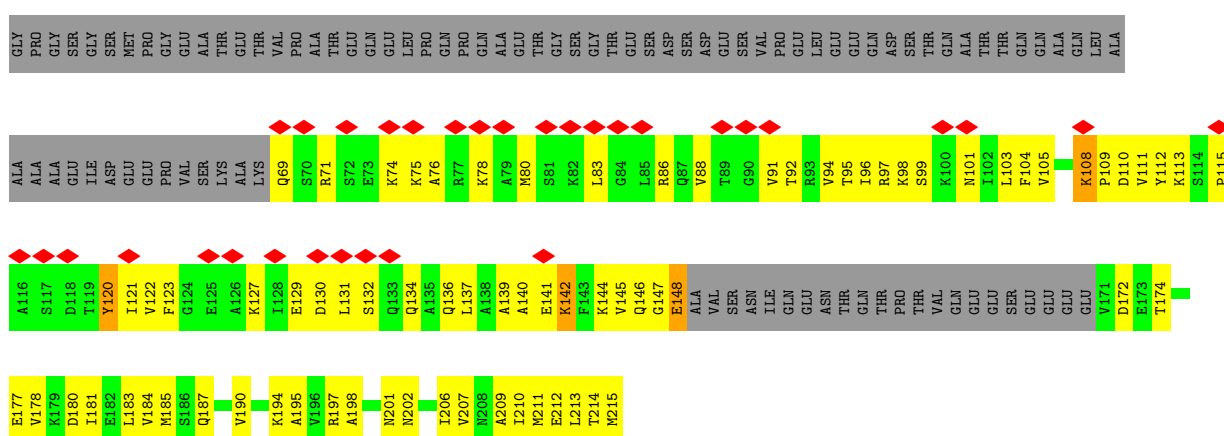
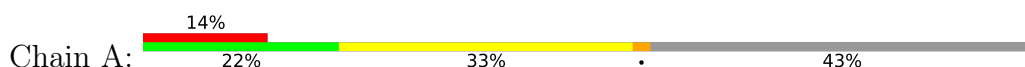
• Molecule 6: 60S ribosomal protein L35



• Molecule 7: 60S ribosomal protein L23a

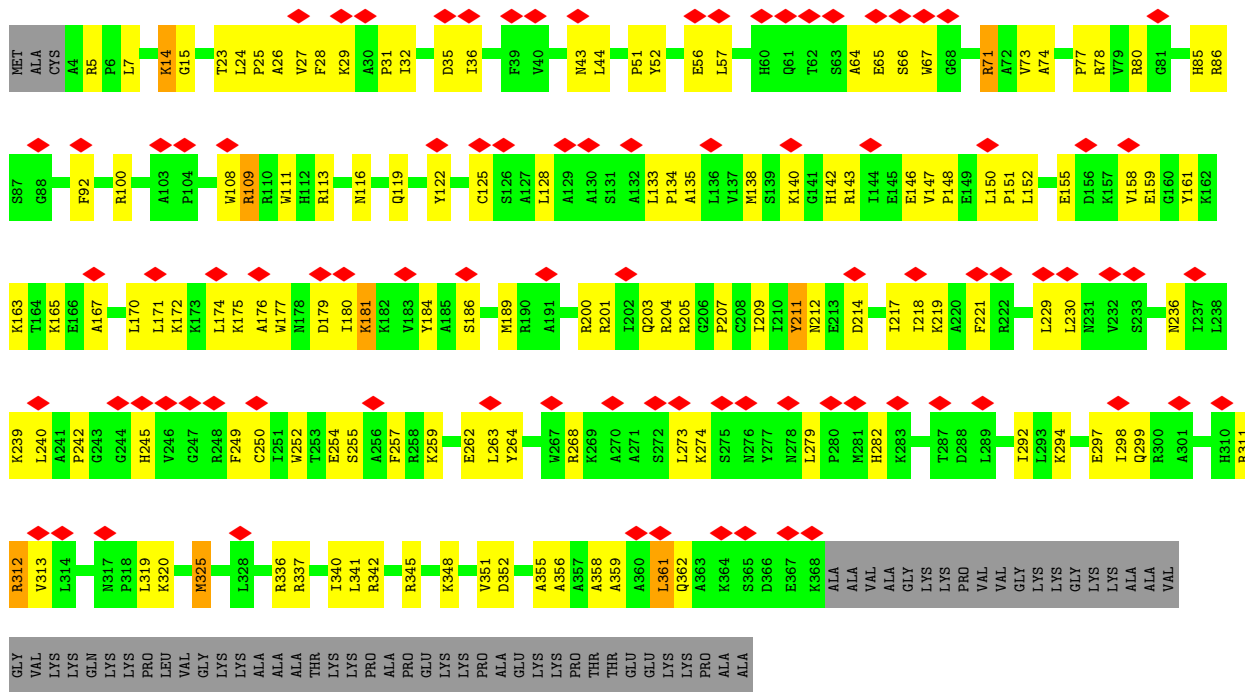


• Molecule 8: Nascent polypeptide-associated complex subunit alpha

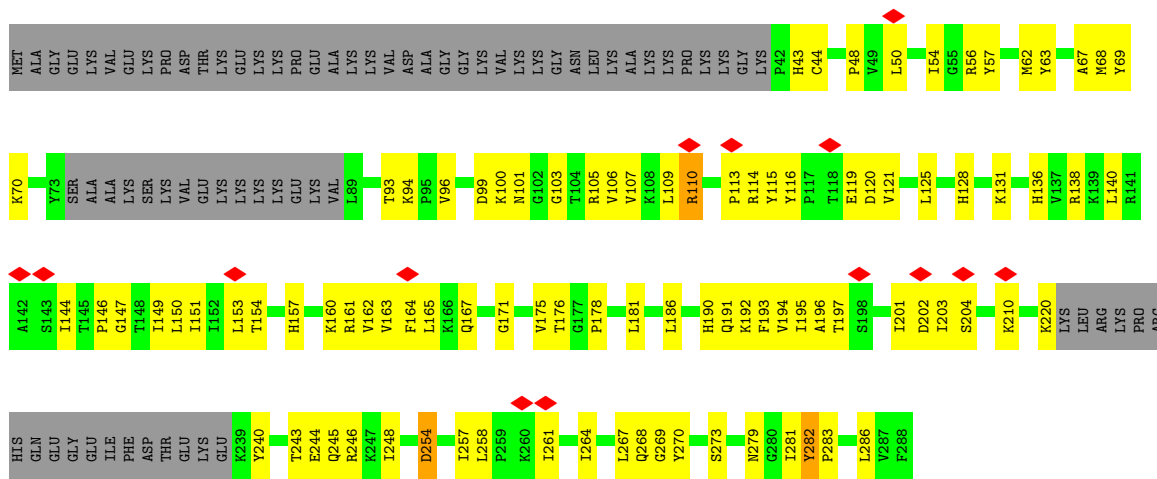


• Molecule 9: 60S ribosomal protein L22

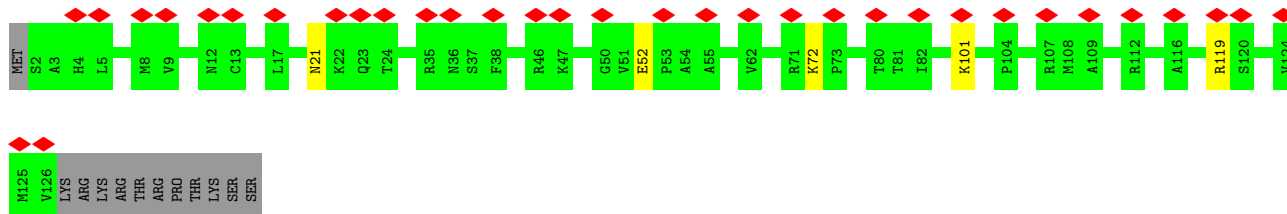
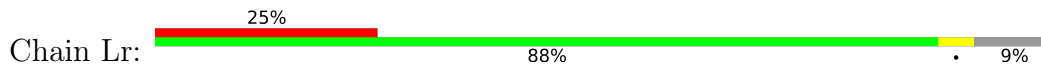




• Molecule 15: Large ribosomal subunit protein eL6



• Molecule 16: 60S ribosomal protein L28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24116	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.97	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.318	Depositor
Minimum map value	-1.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	782.72003, 782.72003, 782.72003	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.223, 1.223, 1.223	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

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	8	0.34	0/1384	0.82	0/2154
2	E	0.29	0/2562	0.59	2/3479 (0.1%)
3	D	0.40	0/945	0.85	2/1269 (0.2%)
4	1	0.38	0/7128	0.91	6/11100 (0.1%)
5	LY	0.34	0/1092	0.83	1/1454 (0.1%)
6	Lh	0.33	0/1023	0.81	3/1351 (0.2%)
7	LX	0.35	0/967	0.80	0/1301
8	A	0.32	0/972	0.73	0/1300
9	LU	0.33	0/839	0.84	2/1126 (0.2%)
10	LR	0.30	0/1297	0.85	2/1716 (0.1%)
11	Lk	0.33	0/575	0.75	0/761
12	2	0.32	0/1418	0.69	1/1909 (0.1%)
13	B	0.34	0/7019	0.71	12/9441 (0.1%)
14	LC	0.30	0/2962	0.70	1/3977 (0.0%)
15	LE	0.31	0/1758	0.69	0/2359
16	Lr	0.29	0/1017	0.70	0/1364
All	All	0.34	0/32958	0.78	32/46061 (0.1%)

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	D	0	2
13	B	0	1
All	All	0	3

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	835	LEU	CA-CB-CG	12.15	143.24	115.30
6	Lh	21	LEU	CA-CB-CG	9.02	136.05	115.30
4	1	485	C	C2-N1-C1'	8.59	128.25	118.80
9	LU	96	LEU	CA-CB-CG	8.51	134.88	115.30
13	B	394	LEU	CA-CB-CG	8.43	134.68	115.30
10	LR	139	MET	CA-CB-CG	8.41	127.59	113.30
4	1	456	C	P-O3'-C3'	-7.49	110.72	119.70
4	1	455	C	P-O3'-C3'	-7.29	110.95	119.70
6	Lh	28	LEU	CA-CB-CG	7.14	131.72	115.30
13	B	661	LEU	CA-CB-CG	6.57	130.42	115.30
13	B	829	LYS	CA-CB-CG	6.36	127.39	113.40
4	1	485	C	C6-N1-C1'	-6.30	113.24	120.80
4	1	457	G	P-O3'-C3'	-5.98	112.53	119.70
14	LC	361	LEU	CA-CB-CG	5.97	129.03	115.30
2	E	329	MET	CB-CG-SD	5.95	130.26	112.40
9	LU	69	LYS	CA-CB-CG	5.95	126.49	113.40
4	1	485	C	N1-C2-O2	5.94	122.46	118.90
10	LR	89	MET	CA-CB-CG	5.93	123.37	113.30
13	B	54	LEU	CA-CB-CG	5.88	128.82	115.30
13	B	274	LEU	CA-CB-CG	5.86	128.77	115.30
2	E	329	MET	CA-CB-CG	5.72	123.02	113.30
13	B	88	LEU	CA-CB-CG	5.69	128.39	115.30
13	B	18	LEU	CA-CB-CG	5.67	128.34	115.30
13	B	829	LYS	CB-CG-CD	5.39	125.62	111.60
3	D	55	LEU	CA-CB-CG	5.36	127.62	115.30
5	LY	81	TYR	CB-CG-CD1	5.33	124.19	121.00
6	Lh	91	MET	CA-CB-CG	5.29	122.29	113.30
13	B	161	LEU	CA-CB-CG	5.24	127.35	115.30
12	2	91	MET	CB-CG-SD	5.23	128.08	112.40
13	B	835	LEU	CB-CA-C	-5.18	100.35	110.20
3	D	143	LEU	CA-CB-CG	5.10	127.03	115.30
13	B	595	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	B	833	TYR	Mainchain
3	D	147	LEU	Peptide
3	D	77	VAL	Mainchain

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	8	1237	0	625	34	0
2	E	2498	0	2425	104	0
3	D	937	0	989	129	0
4	1	6383	0	3239	270	0
5	LY	1075	0	1157	133	0
6	Lh	1015	0	1148	0	0
7	LX	950	0	1016	68	0
8	A	967	0	1017	92	0
9	LU	825	0	850	74	0
10	LR	1281	0	1418	94	0
11	Lk	569	0	637	0	0
12	2	1388	0	1356	131	0
13	B	6881	0	6924	538	0
14	LC	2908	0	3082	112	0
15	LE	1724	0	1874	75	0
16	Lr	1002	0	1068	0	0
17	B	36	0	6	1	0
All	All	31676	0	28831	1625	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 30.

All (1625) 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)
13:B:425:LYS:HG2	13:B:835:LEU:HD21	1.22	1.19
1:8:97:A:H5 ⁷	7:LX:68:ARG:HH22	1.21	1.04
7:LX:94:ASN:HD21	7:LX:145:ASP:HA	1.21	1.02
3:D:79:ARG:HG3	4:1:2707:U:H2 ⁷	1.43	1.01
13:B:194:LEU:HB3	13:B:536:ARG:HD3	1.45	0.97
4:1:2533:C:H5 ⁷	7:LX:93:ASN:HD22	1.29	0.96
8:A:113:LYS:HA	8:A:120:TYR:HB3	1.48	0.95
13:B:425:LYS:HG2	13:B:835:LEU:CD2	1.96	0.94
14:LC:25:PRO:HG2	14:LC:28:PHE:HE1	1.32	0.93
13:B:93:ASP:HB2	13:B:95:LYS:HE2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:423:ASN:HB2	13:B:833:TYR:O	1.68	0.92
4:1:2527:A:OP2	10:LR:38:ARG:NH2	2.05	0.89
5:LY:53:ASP:HA	5:LY:108:ARG:HH12	1.36	0.89
2:E:298:LYS:H	2:E:298:LYS:HD2	1.39	0.88
10:LR:15:LEU:HD22	10:LR:52:ARG:HE	1.38	0.87
10:LR:105:LEU:HA	10:LR:108:ARG:HE	1.37	0.87
4:1:200:U:OP2	5:LY:39:ARG:NH1	2.07	0.87
3:D:151:LEU:HD12	3:D:162:LEU:HD13	1.58	0.86
12:2:96:ARG:HH21	13:B:224:LEU:HD23	1.40	0.85
4:1:493:G:O6	4:1:660:A:N1	2.10	0.85
1:8:90:C:HO2'	5:LY:24:HIS:HD1	1.22	0.85
4:1:512:U:H3	4:1:647:G:H1	1.23	0.85
4:1:493:G:H1	4:1:660:A:H2	1.22	0.84
13:B:550:GLN:HG3	13:B:667:LEU:HD23	1.56	0.84
14:LC:25:PRO:HG2	14:LC:28:PHE:CE1	2.12	0.84
5:LY:13:LYS:HB3	5:LY:17:ARG:HH21	1.40	0.84
13:B:421:ALA:HB3	13:B:833:TYR:HB2	1.59	0.84
9:LU:100:LEU:HB3	9:LU:112:LEU:HD11	1.59	0.84
5:LY:22:PRO:HG2	5:LY:25:ILE:HG12	1.60	0.84
8:A:202:ASN:ND2	8:A:212:GLU:OE1	2.11	0.84
4:1:2701:U:H3	4:1:2715:G:H1	0.83	0.83
7:LX:76:ILE:O	7:LX:78:LYS:NZ	2.10	0.83
4:1:215:C:O2'	13:B:627:LYS:NZ	2.09	0.83
4:1:2701:U:O2	4:1:2715:G:N2	2.11	0.83
3:D:87:LYS:NZ	10:LR:30:ASN:HB2	1.94	0.82
12:2:81:HIS:HA	13:B:324:PRO:HG3	1.59	0.82
12:2:85:GLY:HA2	12:2:88:GLN:HG2	1.61	0.82
4:1:455:C:O2	4:1:701:G:N1	2.12	0.82
13:B:496:LYS:HD2	13:B:560:ILE:HG23	1.62	0.82
7:LX:55:ARG:HE	7:LX:56:ARG:H	1.26	0.82
2:E:343:GLY:HA2	3:D:137:HIS:CE1	2.15	0.81
3:D:79:ARG:CG	4:1:2707:U:H2'	2.09	0.81
12:2:77:VAL:HG23	12:2:82:ARG:HG2	1.62	0.81
13:B:166:MET:HB2	13:B:169:LYS:HE3	1.63	0.81
4:1:664:G:N2	4:1:666:G:O6	2.14	0.81
15:LE:254:ASP:HA	15:LE:257:ILE:HG12	1.62	0.81
12:2:96:ARG:HH11	13:B:253:ARG:HG2	1.45	0.81
4:1:237:G:O2'	5:LY:45:ARG:NH2	2.13	0.81
12:2:19:LEU:HB2	13:B:486:TRP:HH2	1.46	0.81
13:B:704:SER:HB2	13:B:757:ASN:HD21	1.44	0.80
4:1:2532:C:OP1	7:LX:125:ASN:ND2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:2533:C:H5''	7:LX:93:ASN:ND2	1.97	0.80
4:1:239:C:H5''	5:LY:46:SER:HB3	1.62	0.80
4:1:404:U:O3'	5:LY:87:ARG:NH2	2.15	0.79
2:E:156:MET:O	2:E:158:LYS:NZ	2.14	0.79
12:2:96:ARG:NH1	13:B:253:ARG:HG2	1.98	0.79
13:B:148:ARG:HH21	13:B:174:PHE:HD1	1.31	0.78
7:LX:67:ARG:H	7:LX:67:ARG:HD3	1.48	0.78
1:8:97:A:H5''	7:LX:68:ARG:NH2	1.98	0.78
12:2:130:ILE:HA	12:2:147:MET:HE3	1.65	0.78
2:E:74:ASN:HD22	2:E:90:HIS:HD2	1.30	0.78
7:LX:115:LYS:HA	7:LX:115:LYS:HE3	1.66	0.78
15:LE:153:LEU:HD11	15:LE:195:ILE:HG22	1.66	0.78
3:D:143:LEU:HD21	3:D:165:LEU:HD12	1.66	0.78
13:B:824:ARG:HA	13:B:837:PHE:HD1	1.48	0.78
1:8:71:A:OP1	5:LY:27:ARG:NH1	2.16	0.77
9:LU:101:ARG:HB2	9:LU:115:PHE:HE2	1.48	0.77
12:2:109:LEU:HG	12:2:147:MET:HB2	1.65	0.77
3:D:79:ARG:NE	4:1:2707:U:H3'	1.99	0.77
12:2:30:TYR:HA	12:2:33:TYR:HB3	1.65	0.77
13:B:191:GLU:HG3	13:B:534:THR:HG22	1.66	0.77
15:LE:190:HIS:HE1	15:LE:192:LYS:HE3	1.49	0.77
5:LY:86:GLN:HA	5:LY:97:VAL:HG23	1.66	0.77
13:B:553:PHE:HD1	13:B:556:LYS:HD3	1.48	0.76
10:LR:151:ARG:NE	10:LR:151:ARG:O	2.17	0.76
13:B:446:SER:HA	13:B:487:PHE:HZ	1.50	0.76
13:B:778:SER:HB3	13:B:781:ARG:HE	1.50	0.76
10:LR:104:ARG:HH12	10:LR:108:ARG:HB3	1.50	0.76
13:B:164:TYR:HB2	13:B:203:ALA:HB2	1.66	0.76
13:B:682:TYR:HB3	13:B:687:LYS:HB2	1.66	0.76
14:LC:212:ASN:HD22	14:LC:255:SER:HB3	1.48	0.76
4:1:202:C:O2'	13:B:632:ASP:OD2	2.02	0.75
9:LU:17:GLN:HG3	9:LU:18:VAL:HG23	1.68	0.75
13:B:824:ARG:HA	13:B:837:PHE:CD1	2.21	0.75
10:LR:5:ARG:HH21	10:LR:8:LYS:HE3	1.51	0.75
12:2:3:ILE:HD11	13:B:256:GLU:HB2	1.69	0.75
5:LY:45:ARG:H	5:LY:126:ARG:HH21	1.35	0.74
4:1:232:G:H1	5:LY:61:HIS:CE1	2.04	0.74
9:LU:65:ARG:HE	9:LU:67:LYS:HD2	1.51	0.74
12:2:19:LEU:HD21	13:B:482:MET:HG2	1.69	0.74
14:LC:146:GLU:OE1	14:LC:146:GLU:N	2.20	0.74
13:B:556:LYS:HA	13:B:559:ARG:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:609:GLU:HA	13:B:612:LYS:HZ3	1.53	0.74
13:B:625:LYS:HA	13:B:628:LYS:HD2	1.68	0.73
13:B:709:HIS:NE2	13:B:750:ASN:HA	2.03	0.73
5:LY:2:LYS:NZ	5:LY:4:ASN:O	2.22	0.73
13:B:827:CYS:O	13:B:831:PHE:N	2.19	0.73
3:D:126:SER:HG	3:D:131:THR:HG1	1.27	0.72
4:1:512:U:O4	4:1:647:G:O6	2.07	0.72
13:B:631:ASP:HA	13:B:634:GLU:HB2	1.71	0.72
13:B:505:LEU:O	13:B:509:HIS:ND1	2.21	0.72
15:LE:258:LEU:HA	15:LE:261:ILE:HD12	1.71	0.72
2:E:256:LEU:HB3	2:E:257:MET:HE2	1.71	0.72
8:A:211:MET:SD	13:B:101:LYS:NZ	2.62	0.72
13:B:162:GLU:HA	13:B:164:TYR:CE2	2.24	0.72
10:LR:104:ARG:NH1	10:LR:104:ARG:O	2.21	0.72
8:A:214:THR:HG21	13:B:105:ASN:HD21	1.54	0.71
5:LY:82:ILE:HB	5:LY:85:VAL:HG12	1.71	0.71
13:B:318:PHE:HB3	13:B:372:THR:HG23	1.72	0.71
13:B:553:PHE:CD1	13:B:556:LYS:HD3	2.26	0.71
3:D:59:GLN:HG2	9:LU:99:TRP:HE1	1.53	0.71
5:LY:42:TYR:HB3	5:LY:119:LEU:HD11	1.72	0.71
9:LU:101:ARG:HB2	9:LU:115:PHE:CE2	2.25	0.71
5:LY:23:SER:HA	5:LY:26:ARG:HD2	1.73	0.71
8:A:110:ASP:HB3	8:A:123:PHE:HB2	1.73	0.71
13:B:654:LEU:HD22	13:B:681:ILE:HG12	1.73	0.71
8:A:194:LYS:HG2	8:A:213:LEU:HD22	1.73	0.71
13:B:49:LEU:HD13	13:B:71:ARG:HH12	1.56	0.71
13:B:825:ALA:O	13:B:829:LYS:HD3	1.91	0.71
14:LC:177:TRP:O	14:LC:181:LYS:NZ	2.24	0.70
4:1:496:G:H2'	4:1:498:C:H5''	1.72	0.70
9:LU:100:LEU:HD12	9:LU:112:LEU:HG	1.73	0.70
4:1:196:C:H5''	5:LY:126:ARG:HH11	1.57	0.70
4:1:405:U:H1'	4:1:410:A:H61	1.56	0.70
5:LY:81:TYR:HD1	5:LY:96:HIS:HB3	1.57	0.70
13:B:529:CYS:O	13:B:533:ILE:N	2.23	0.70
5:LY:8:THR:OG1	5:LY:10:ASP:OD2	2.09	0.70
2:E:91:TYR:HB3	2:E:92:PRO:HA	1.72	0.70
10:LR:41:ILE:HG22	10:LR:45:ILE:HD11	1.74	0.70
10:LR:137:ILE:HD12	10:LR:137:ILE:H	1.57	0.70
2:E:201:ILE:N	2:E:346:ALA:O	2.24	0.70
5:LY:37:GLU:O	5:LY:40:GLN:NE2	2.24	0.70
10:LR:146:LYS:HA	10:LR:149:LYS:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:421:ALA:CB	13:B:833:TYR:HB2	2.21	0.70
7:LX:119:ILE:HG21	7:LX:140:LEU:HD23	1.74	0.69
12:2:30:TYR:O	12:2:34:HIS:ND1	2.23	0.69
13:B:824:ARG:HG2	13:B:837:PHE:HA	1.74	0.69
10:LR:93:VAL:HG12	10:LR:97:ARG:HE	1.56	0.69
5:LY:54:GLU:HG2	5:LY:108:ARG:CZ	2.22	0.69
13:B:429:ARG:NH1	13:B:433:GLU:OE2	2.26	0.69
4:1:238:C:O2'	5:LY:33:PRO:HD3	1.92	0.69
8:A:111:VAL:HG22	8:A:122:VAL:HG22	1.75	0.69
13:B:587:MET:SD	13:B:588:SER:N	2.66	0.69
13:B:9:LYS:HD3	13:B:9:LYS:H	1.58	0.69
4:1:679:C:H2'	4:1:680:G:H8	1.57	0.69
5:LY:58:VAL:HG23	5:LY:59:ARG:HG2	1.72	0.69
8:A:105:VAL:HG23	8:A:127:LYS:HE2	1.75	0.69
13:B:629:ASP:HA	13:B:632:ASP:HB3	1.75	0.69
3:D:100:ILE:O	3:D:122:LYS:NZ	2.22	0.68
4:1:457:G:C5'	15:LE:115:TYR:HB3	2.24	0.68
3:D:88:LEU:HD22	8:A:83:LEU:HB3	1.75	0.68
8:A:177:GLU:HG2	8:A:180:ASP:HB2	1.74	0.68
8:A:195:ALA:HA	8:A:213:LEU:HD11	1.75	0.68
13:B:330:ARG:HH22	13:B:386:LYS:HD3	1.59	0.68
13:B:470:ARG:HH11	13:B:478:ASN:HD21	1.42	0.68
14:LC:294:LYS:HA	14:LC:299:GLN:HE21	1.58	0.68
8:A:214:THR:CG2	13:B:105:ASN:HD21	2.07	0.68
3:D:71:ARG:NH1	9:LU:97:ARG:HH21	1.92	0.68
10:LR:104:ARG:HG3	10:LR:108:ARG:NH2	2.09	0.68
12:2:134:GLU:OE1	12:2:134:GLU:N	2.27	0.68
13:B:261:TYR:HB3	13:B:280:TYR:HE1	1.58	0.68
4:1:2526:C:H4'	10:LR:9:ARG:HH22	1.58	0.68
3:D:72:ARG:HE	3:D:74:LYS:H	1.41	0.68
3:D:122:LYS:HG3	3:D:124:GLN:HE22	1.59	0.68
4:1:210:C:OP1	5:LY:59:ARG:NH1	2.26	0.68
4:1:457:G:H5'	15:LE:115:TYR:HB3	1.76	0.68
7:LX:100:VAL:HG21	7:LX:109:ILE:HD12	1.74	0.68
1:8:67:U:H2'	1:8:68:G:H8	1.58	0.68
13:B:576:GLU:O	13:B:577:ASN:ND2	2.26	0.68
14:LC:27:VAL:HG22	14:LC:128:LEU:HD11	1.75	0.68
2:E:228:TYR:HE1	2:E:298:LYS:HE3	1.58	0.67
4:1:196:C:OP2	5:LY:121:ARG:NH1	2.28	0.67
2:E:349:ARG:NH1	2:E:349:ARG:O	2.27	0.67
14:LC:66:SER:HA	14:LC:77:PRO:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:25:ASN:HB3	13:B:482:MET:SD	2.34	0.67
12:2:127:ASN:O	12:2:149:ARG:NH1	2.27	0.67
13:B:747:LYS:HD3	13:B:774:LEU:HD13	1.76	0.67
4:1:229:G:OP1	5:LY:11:ARG:NE	2.28	0.67
9:LU:19:LEU:HD11	9:LU:74:SER:HB3	1.74	0.67
9:LU:22:THR:HG22	9:LU:109:SER:HA	1.77	0.67
13:B:284:TRP:HB3	13:B:293:PRO:HB2	1.76	0.67
13:B:661:LEU:O	13:B:665:LYS:N	2.22	0.67
5:LY:100:HIS:CD2	5:LY:102:SER:H	2.13	0.67
12:2:113:LYS:HE2	12:2:145:TYR:CZ	2.30	0.67
4:1:404:U:O2'	5:LY:87:ARG:NH2	2.27	0.67
7:LX:94:ASN:O	7:LX:139:ARG:NH1	2.28	0.67
13:B:390:PRO:HB2	13:B:832:PRO:HD2	1.77	0.67
3:D:90:PHE:HA	3:D:93:LYS:HE2	1.77	0.67
13:B:426:GLU:OE2	13:B:429:ARG:NH2	2.25	0.67
13:B:448:CYS:HA	13:B:451:TYR:CD2	2.30	0.66
3:D:105:GLU:HB3	8:A:97:ARG:HH21	1.60	0.66
4:1:513:U:N3	4:1:516:C:OP2	2.28	0.66
13:B:513:ARG:HD3	13:B:642:LEU:HD11	1.76	0.66
14:LC:74:ALA:O	14:LC:78:ARG:NH2	2.28	0.66
15:LE:210:LYS:HE2	15:LE:210:LYS:N	2.11	0.66
3:D:100:ILE:HG23	3:D:123:VAL:HG13	1.76	0.66
13:B:824:ARG:CG	13:B:837:PHE:HA	2.26	0.66
2:E:264:LYS:HE2	2:E:265:PRO:HD2	1.76	0.66
3:D:54:LYS:HA	3:D:57:LYS:HG2	1.78	0.66
4:1:237:G:HO2'	5:LY:45:ARG:NH2	1.93	0.66
13:B:496:LYS:NZ	13:B:560:ILE:O	2.27	0.66
13:B:562:ILE:O	13:B:566:LEU:HD23	1.95	0.66
14:LC:325:MET:SD	14:LC:336:ARG:NH2	2.69	0.66
2:E:274:ASN:ND2	2:E:311:LYS:H	1.93	0.66
3:D:100:ILE:HD12	3:D:101:SER:H	1.60	0.66
8:A:207:VAL:O	8:A:211:MET:HE3	1.95	0.66
10:LR:93:VAL:O	10:LR:97:ARG:HG3	1.96	0.66
13:B:496:LYS:NZ	13:B:563:GLU:HB2	2.10	0.66
13:B:764:ARG:HE	13:B:788:THR:HG21	1.60	0.66
4:1:662:C:H2'	4:1:663:G:H8	1.61	0.66
4:1:458:C:O2'	15:LE:110:ARG:NH1	2.28	0.66
7:LX:78:LYS:N	7:LX:78:LYS:HD3	2.09	0.66
4:1:405:U:H5'	5:LY:87:ARG:HH22	1.60	0.65
4:1:493:G:C6	4:1:660:A:N1	2.64	0.65
12:2:96:ARG:NH1	13:B:254:ASN:HB2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:91:ARG:NE	13:B:91:ARG:O	2.26	0.65
9:LU:41:GLN:HA	9:LU:44:GLN:NE2	2.10	0.65
4:1:2386:U:H5''	10:LR:24:LEU:HD21	1.79	0.65
14:LC:337:ARG:O	14:LC:341:LEU:HG	1.96	0.65
2:E:198:ASN:HB3	2:E:353:ARG:HG2	1.77	0.65
13:B:570:ASP:HB3	13:B:684:ARG:HE	1.61	0.65
14:LC:5:ARG:HH21	14:LC:24:LEU:HG	1.61	0.65
3:D:115:VAL:HB	3:D:146:MET:HE1	1.78	0.65
4:1:227:A:H1'	5:LY:2:LYS:HB2	1.78	0.65
4:1:686:A:OP1	13:B:594:LYS:NZ	2.19	0.65
2:E:158:LYS:HZ3	2:E:161:VAL:HG21	1.61	0.65
4:1:218:A:H1'	4:1:219:G:C8	2.32	0.65
4:1:237:G:HO2'	5:LY:45:ARG:HH22	1.41	0.65
13:B:254:ASN:HB3	13:B:260:TYR:HE2	1.61	0.65
13:B:488:GLN:HA	13:B:507:LYS:HD2	1.79	0.65
9:LU:49:VAL:O	9:LU:52:LYS:HG2	1.97	0.65
13:B:559:ARG:HA	13:B:562:ILE:HG22	1.78	0.65
14:LC:263:LEU:HD23	14:LC:273:LEU:HD12	1.79	0.65
4:1:467:U:H4'	13:B:601:ARG:HD2	1.77	0.64
13:B:453:LEU:O	13:B:494:ALA:HB2	1.96	0.64
13:B:496:LYS:HZ1	13:B:563:GLU:HB2	1.62	0.64
3:D:78:HIS:HB3	4:1:2707:U:C4	2.32	0.64
10:LR:105:LEU:HA	10:LR:108:ARG:NE	2.11	0.64
13:B:128:ARG:HH12	13:B:522:GLN:HE22	1.44	0.64
13:B:523:PHE:HA	13:B:526:HIS:CD2	2.31	0.64
2:E:374:ARG:NH1	2:E:379:ARG:O	2.28	0.64
12:2:43:TYR:CE2	12:2:93:GLN:HG3	2.33	0.64
14:LC:147:VAL:HA	14:LC:175:LYS:HE2	1.80	0.64
5:LY:52:ASP:HA	5:LY:69:LYS:HZ3	1.63	0.64
14:LC:311:ARG:HE	14:LC:312:ARG:H	1.46	0.64
10:LR:149:LYS:HA	10:LR:152:LYS:HE2	1.79	0.64
14:LC:64:ALA:HB3	14:LC:92:PHE:CE2	2.33	0.64
3:D:87:LYS:HZ1	10:LR:30:ASN:HB2	1.61	0.64
4:1:199:G:O5'	5:LY:45:ARG:NH2	2.31	0.64
4:1:231:U:H4'	5:LY:100:HIS:CD2	2.32	0.64
2:E:297:HIS:CD2	2:E:302:THR:HG21	2.34	0.63
9:LU:69:LYS:NZ	9:LU:71:THR:HB	2.12	0.63
8:A:139:ALA:HB2	13:B:176:LYS:NZ	2.14	0.63
12:2:97:ALA:O	12:2:101:ASN:ND2	2.31	0.63
13:B:420:HIS:O	13:B:798:LEU:HD13	1.99	0.63
15:LE:264:ILE:HD11	15:LE:267:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:139:GLU:OE2	3:D:141:LYS:HE3	1.98	0.63
4:1:196:C:H5''	5:LY:126:ARG:NH1	2.14	0.63
5:LY:85:VAL:HG11	5:LY:99:ILE:HD11	1.81	0.63
13:B:619:LYS:HD2	13:B:620:GLN:N	2.13	0.63
2:E:380:PRO:HG2	2:E:383:MET:HG3	1.81	0.63
3:D:79:ARG:HE	4:1:2707:U:H3'	1.62	0.63
5:LY:66:GLN:OE1	5:LY:66:GLN:N	2.30	0.63
13:B:798:LEU:HG	13:B:799:GLN:N	2.13	0.63
4:1:388:A:N6	4:1:411:G:O2'	2.32	0.63
15:LE:128:HIS:ND1	15:LE:128:HIS:O	2.32	0.63
8:A:96:ILE:N	8:A:104:PHE:O	2.29	0.63
10:LR:30:ASN:ND2	10:LR:30:ASN:H	1.97	0.63
13:B:94:LYS:HE2	13:B:94:LYS:N	2.14	0.63
13:B:453:LEU:HD22	13:B:491:CYS:HA	1.81	0.63
13:B:620:GLN:OE1	13:B:624:GLN:NE2	2.32	0.63
2:E:218:ASN:HA	2:E:235:THR:HA	1.80	0.62
4:1:481:G:H1	4:1:673:C:H42	1.47	0.62
9:LU:22:THR:OG1	9:LU:69:LYS:HE2	1.99	0.62
10:LR:40:GLN:O	10:LR:44:LEU:HG	1.98	0.62
12:2:132:GLU:H	12:2:146:ALA:HB3	1.63	0.62
13:B:164:TYR:CD1	13:B:199:VAL:HG13	2.33	0.62
3:D:117:HIS:O	3:D:139:GLU:N	2.28	0.62
13:B:49:LEU:HD22	13:B:68:LEU:HD11	1.81	0.62
9:LU:49:VAL:HG12	9:LU:50:ASN:OD1	1.99	0.62
13:B:215:THR:O	13:B:218:LYS:NZ	2.32	0.62
13:B:483:GLN:HG2	13:B:514:HIS:CD2	2.34	0.62
13:B:722:SER:O	13:B:730:ARG:NH2	2.31	0.62
14:LC:5:ARG:CZ	14:LC:26:ALA:HA	2.29	0.62
2:E:310:ALA:O	2:E:311:LYS:HG2	1.99	0.62
4:1:493:G:N1	4:1:660:A:C2	2.61	0.62
12:2:14:MET:HG2	12:2:31:TYR:HE2	1.63	0.62
13:B:205:LEU:HG	13:B:208:GLU:HB2	1.79	0.62
2:E:74:ASN:HD22	2:E:90:HIS:CD2	2.16	0.62
2:E:205:ILE:HD12	2:E:342:ASP:HB2	1.81	0.62
12:2:19:LEU:HB2	13:B:486:TRP:CH2	2.32	0.62
13:B:54:LEU:CD1	13:B:88:LEU:HD11	2.30	0.62
3:D:148:PRO:HA	3:D:151:LEU:HD23	1.82	0.62
5:LY:41:LYS:HD3	5:LY:42:TYR:CZ	2.34	0.62
13:B:67:GLU:O	13:B:71:ARG:HG3	1.99	0.62
13:B:704:SER:HB2	13:B:757:ASN:ND2	2.12	0.62
14:LC:56:GLU:HG2	14:LC:57:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LE:157:HIS:HB3	15:LE:160:LYS:HG3	1.80	0.62
4:1:200:U:O2'	5:LY:59:ARG:NH2	2.33	0.62
12:2:20:LEU:O	13:B:443:PHE:HA	1.99	0.62
13:B:562:ILE:HG13	13:B:657:ALA:HB1	1.82	0.62
13:B:665:LYS:NZ	13:B:682:TYR:OH	2.33	0.62
13:B:770:MET:SD	13:B:774:LEU:HG	2.40	0.62
1:8:66:A:H2'	1:8:67:U:C6	2.35	0.62
4:1:691:C:H2'	4:1:692:A:C8	2.35	0.62
4:1:383:A:N1	5:LY:61:HIS:NE2	2.47	0.61
10:LR:30:ASN:ND2	10:LR:30:ASN:N	2.45	0.61
13:B:765:LEU:HD13	13:B:804:VAL:HG13	1.82	0.61
14:LC:209:ILE:HB	14:LC:229:LEU:HD13	1.81	0.61
4:1:240:G:H4'	5:LY:28:LYS:HG2	1.81	0.61
10:LR:101:ILE:HG13	10:LR:102:LEU:HD22	1.82	0.61
13:B:307:LYS:NZ	13:B:344:GLU:OE1	2.32	0.61
3:D:114:THR:HA	3:D:142:GLN:OE1	2.00	0.61
14:LC:218:ILE:HD12	14:LC:219:LYS:N	2.16	0.61
8:A:88:VAL:HG21	8:A:113:LYS:HD2	1.83	0.61
8:A:94:VAL:HG23	8:A:109:PRO:HG3	1.82	0.61
9:LU:20:LYS:HZ1	9:LU:73:THR:HA	1.65	0.61
12:2:57:LEU:O	12:2:73:THR:N	2.31	0.61
14:LC:264:TYR:HB3	14:LC:279:LEU:HD21	1.83	0.61
1:8:67:U:H2'	1:8:68:G:C8	2.36	0.61
10:LR:30:ASN:HD22	10:LR:31:GLU:H	1.47	0.61
13:B:310:LEU:HD21	13:B:342:ILE:HG22	1.81	0.61
13:B:608:ILE:HG22	13:B:612:LYS:HZ1	1.65	0.61
14:LC:340:ILE:HD12	15:LE:50:LEU:HD11	1.83	0.61
10:LR:39:GLN:OE1	10:LR:42:ARG:NH1	2.33	0.61
7:LX:76:ILE:HD11	7:LX:109:ILE:HD13	1.81	0.61
13:B:834:ALA:HB3	13:B:837:PHE:HB2	1.80	0.61
14:LC:320:LYS:HA	14:LC:320:LYS:HE3	1.83	0.61
7:LX:81:LEU:HG	7:LX:99:ILE:HD11	1.81	0.61
13:B:416:LYS:HD2	13:B:420:HIS:CE1	2.36	0.61
13:B:416:LYS:HD3	13:B:419:LYS:HD3	1.83	0.61
2:E:78:TRP:HD1	3:D:140:THR:HB	1.65	0.60
5:LY:82:ILE:HB	5:LY:85:VAL:CG1	2.31	0.60
8:A:69:GLN:HE22	8:A:74:LYS:HG3	1.64	0.60
13:B:394:LEU:HG	13:B:833:TYR:CZ	2.36	0.60
13:B:414:LYS:HZ3	13:B:418:TYR:HE2	1.49	0.60
4:1:2896:G:C8	4:1:2896:G:H5''	2.36	0.60
13:B:631:ASP:OD1	13:B:632:ASP:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:824:ARG:NH1	13:B:837:PHE:O	2.34	0.60
7:LX:81:LEU:HD13	7:LX:97:VAL:HG22	1.83	0.60
3:D:78:HIS:CG	4:1:2707:U:C5	2.90	0.60
7:LX:81:LEU:HG	7:LX:99:ILE:CD1	2.32	0.60
13:B:342:ILE:O	13:B:346:VAL:HG12	2.02	0.60
14:LC:161:TYR:HE2	14:LC:170:LEU:HD22	1.66	0.60
4:1:457:G:O2'	15:LE:113:PRO:HB3	2.01	0.60
13:B:693:GLN:O	13:B:697:ARG:HD3	2.01	0.60
2:E:274:ASN:O	2:E:278:LYS:HG2	2.01	0.60
3:D:82:THR:HG22	3:D:83:ALA:H	1.67	0.60
7:LX:96:LEU:HB2	7:LX:138:VAL:HG13	1.82	0.60
12:2:25:ASN:OD1	13:B:442:ARG:NH2	2.34	0.60
3:D:50:MET:HB3	9:LU:31:ASP:OD1	2.02	0.60
3:D:106:VAL:HB	3:D:118:PHE:HB2	1.83	0.60
3:D:160:THR:O	3:D:164:ARG:HG3	2.02	0.60
4:1:210:C:H5	5:LY:103:LYS:HZ1	1.47	0.60
4:1:222:C:OP2	14:LC:165:LYS:NZ	2.23	0.60
5:LY:37:GLU:HA	5:LY:40:GLN:HE21	1.66	0.60
8:A:211:MET:O	8:A:215:MET:HG2	2.02	0.60
7:LX:84:GLU:OE1	7:LX:84:GLU:N	2.34	0.60
12:2:7:ARG:O	12:2:9:GLU:N	2.35	0.60
10:LR:5:ARG:HG2	10:LR:5:ARG:HH11	1.67	0.60
13:B:210:LEU:HG	13:B:230:LYS:HZ3	1.67	0.59
13:B:609:GLU:HA	13:B:612:LYS:NZ	2.17	0.59
2:E:89:PRO:HB2	2:E:91:TYR:CE2	2.36	0.59
4:1:661:C:H2'	4:1:662:C:C6	2.37	0.59
5:LY:81:TYR:CD1	5:LY:96:HIS:HB3	2.38	0.59
13:B:69:VAL:HG11	13:B:89:LEU:HD22	1.83	0.59
13:B:124:GLN:O	13:B:129:ASP:N	2.35	0.59
13:B:169:LYS:HA	13:B:172:GLU:HG3	1.84	0.59
13:B:654:LEU:HD11	13:B:684:ARG:HB2	1.84	0.59
3:D:59:GLN:HG2	9:LU:99:TRP:NE1	2.18	0.59
4:1:3604:A:H2'	4:1:3605:C:O4'	2.02	0.59
13:B:31:LYS:O	13:B:34:LYS:NZ	2.34	0.59
2:E:270:ARG:NH2	2:E:316:GLY:O	2.34	0.59
14:LC:171:LEU:HB2	14:LC:176:ALA:HB3	1.83	0.59
2:E:263:VAL:HG13	2:E:318:MET:SD	2.42	0.59
2:E:78:TRP:CD1	3:D:140:THR:HB	2.38	0.59
3:D:94:LYS:HB3	8:A:75:LYS:NZ	2.17	0.59
4:1:457:G:H2'	4:1:458:C:C6	2.38	0.59
4:1:2535:G:H2'	4:1:2536:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:22:LEU:HD21	12:2:76:ALA:HB2	1.85	0.59
13:B:164:TYR:CB	13:B:203:ALA:HB2	2.32	0.59
13:B:770:MET:HA	13:B:770:MET:HE2	1.84	0.59
1:8:82:A:H5'	1:8:82:A:H8	1.66	0.59
4:1:662:C:H2'	4:1:663:G:C8	2.37	0.59
12:2:16:HIS:CE1	13:B:553:PHE:HD2	2.20	0.59
13:B:450:LYS:HG3	13:B:490:GLU:HG3	1.83	0.59
3:D:95:LEU:HB2	3:D:129:ALA:HB2	1.84	0.59
14:LC:336:ARG:O	14:LC:340:ILE:HG12	2.02	0.59
13:B:713:ILE:HG21	13:B:770:MET:SD	2.43	0.59
14:LC:35:ASP:OD1	14:LC:36:ILE:N	2.36	0.59
15:LE:164:PHE:HA	15:LE:175:VAL:HG23	1.85	0.59
4:1:499:G:H2'	4:1:504:G:N2	2.18	0.58
8:A:198:ALA:O	8:A:202:ASN:ND2	2.32	0.58
9:LU:111:GLU:OE2	9:LU:113:ARG:NE	2.25	0.58
13:B:16:ARG:HD3	13:B:19:ARG:HH22	1.67	0.58
13:B:28:ASN:HA	13:B:31:LYS:HG2	1.85	0.58
3:D:131:THR:HG22	8:A:123:PHE:CE1	2.38	0.58
3:D:158:SER:O	3:D:162:LEU:HG	2.03	0.58
3:D:159:LEU:HA	3:D:162:LEU:HD12	1.85	0.58
9:LU:28:PRO:HB2	9:LU:34:MET:SD	2.43	0.58
10:LR:102:LEU:HD12	10:LR:138:LEU:HD23	1.83	0.58
14:LC:211:TYR:CD1	14:LC:217:ILE:HG21	2.38	0.58
4:1:679:C:H2'	4:1:680:G:C8	2.36	0.58
8:A:142:LYS:HZ1	13:B:173:GLU:HB3	1.69	0.58
12:2:28:MET:HG2	12:2:32:PHE:CE1	2.39	0.58
12:2:36:LEU:HA	13:B:537:SER:HB3	1.85	0.58
12:2:159:ARG:O	12:2:163:GLU:HG2	2.03	0.58
13:B:80:HIS:HB3	13:B:109:TRP:HB2	1.85	0.58
13:B:385:ASP:HB2	13:B:417:ILE:HG12	1.85	0.58
4:1:455:C:H1'	4:1:701:G:H22	1.68	0.58
13:B:21:TYR:OH	13:B:55:THR:HA	2.03	0.58
14:LC:155:GLU:O	14:LC:158:VAL:HG22	2.03	0.58
4:1:239:C:H5''	5:LY:46:SER:CB	2.33	0.58
4:1:2707:U:O2	10:LR:43:LYS:NZ	2.34	0.58
4:1:2896:G:H5''	4:1:2896:G:H8	1.67	0.58
4:1:3600:G:H2'	4:1:3601:C:C6	2.39	0.58
13:B:23:HIS:CE1	13:B:25:GLN:HE22	2.20	0.58
4:1:386:A:H1'	5:LY:87:ARG:CZ	2.34	0.58
12:2:112:ARG:HD3	12:2:113:LYS:N	2.18	0.58
14:LC:352:ASP:O	14:LC:356:ALA:N	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LE:96:VAL:HG12	15:LE:103:GLY:HA2	1.85	0.58
2:E:228:TYR:CE1	2:E:298:LYS:HE3	2.37	0.58
3:D:83:ALA:O	3:D:85:ASP:N	2.30	0.58
12:2:36:LEU:HD11	13:B:541:LEU:HD22	1.86	0.58
5:LY:108:ARG:HG2	5:LY:108:ARG:HH11	1.69	0.58
12:2:16:HIS:ND1	13:B:553:PHE:HD2	2.01	0.58
13:B:14:PHE:HE2	13:B:36:ILE:HG13	1.69	0.58
2:E:232:LEU:HD13	2:E:372:THR:HB	1.85	0.58
2:E:281:GLN:HE22	2:E:286:SER:HA	1.69	0.58
3:D:103:ILE:HD12	3:D:123:VAL:CG1	2.34	0.58
13:B:422:GLY:O	13:B:835:LEU:N	2.26	0.58
3:D:72:ARG:HH22	9:LU:117:ILE:C	2.07	0.57
4:1:208:A:H4'	5:LY:60:GLY:HA2	1.86	0.57
4:1:467:U:O4'	13:B:604:LYS:HE3	2.04	0.57
7:LX:155:ILE:H	7:LX:155:ILE:HD12	1.68	0.57
13:B:90:GLN:HA	13:B:95:LYS:HE3	1.85	0.57
13:B:706:PRO:HG3	13:B:763:HIS:CG	2.39	0.57
14:LC:140:LYS:HE3	14:LC:245:HIS:HB2	1.85	0.57
3:D:153:GLN:HE21	8:A:103:LEU:HD13	1.70	0.57
4:1:3599:A:H2'	4:1:3600:G:C8	2.39	0.57
8:A:211:MET:HA	13:B:101:LYS:HD2	1.85	0.57
12:2:58:ALA:HA	12:2:72:ILE:HA	1.85	0.57
3:D:91:SER:HA	3:D:94:LYS:HZ2	1.70	0.57
9:LU:65:ARG:HG2	9:LU:67:LYS:H	1.70	0.57
12:2:93:GLN:HE22	12:2:96:ARG:NE	2.02	0.57
1:8:73:U:P	5:LY:75:ARG:HD2	2.44	0.57
7:LX:131:ASP:OD2	7:LX:133:GLU:HG3	2.04	0.57
13:B:56:LEU:HB3	13:B:61:LYS:HD2	1.85	0.57
3:D:145:GLU:OE2	3:D:146:MET:HG3	2.04	0.57
4:1:2533:C:H2'	4:1:2534:C:C6	2.39	0.57
12:2:19:LEU:HD11	13:B:482:MET:HG3	1.86	0.57
13:B:44:GLU:O	13:B:75:ASN:ND2	2.36	0.57
13:B:218:LYS:HE2	13:B:219:GLN:HG2	1.87	0.57
15:LE:161:ARG:NH1	15:LE:273:SER:OG	2.36	0.57
5:LY:34:LEU:HB3	5:LY:38:LEU:HB2	1.86	0.57
12:2:37:SER:HB3	13:B:532:LYS:HZ2	1.68	0.57
12:2:96:ARG:NH2	13:B:224:LEU:HD23	2.17	0.57
14:LC:14:LYS:H	14:LC:14:LYS:HD2	1.70	0.57
2:E:122:LEU:HD12	2:E:299:LEU:HD11	1.87	0.57
12:2:88:GLN:HE22	12:2:121:LEU:HD13	1.68	0.57
14:LC:200:ARG:HG3	14:LC:201:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:394:G:OP2	8:A:71:ARG:NH2	2.38	0.57
8:A:180:ASP:O	8:A:184:VAL:HG23	2.05	0.57
13:B:31:LYS:HA	13:B:34:LYS:HG3	1.86	0.57
13:B:709:HIS:CE1	13:B:750:ASN:HA	2.39	0.57
7:LX:73:HIS:O	7:LX:76:ILE:HG22	2.04	0.56
13:B:195:TYR:HE1	13:B:539:VAL:HG11	1.70	0.56
14:LC:67:TRP:O	14:LC:71:ARG:NH1	2.38	0.56
14:LC:140:LYS:HB3	14:LC:142:HIS:HD2	1.69	0.56
4:1:3599:A:H2'	4:1:3600:G:H8	1.70	0.56
10:LR:28:GLU:OE2	10:LR:31:GLU:HB2	2.05	0.56
13:B:117:LEU:HD11	13:B:140:LEU:HD13	1.87	0.56
13:B:164:TYR:HD1	13:B:199:VAL:HG13	1.68	0.56
13:B:449:ALA:HB3	13:B:487:PHE:CE1	2.39	0.56
2:E:319:LYS:HD2	2:E:320:SER:H	1.71	0.56
4:1:207:G:O2'	5:LY:61:HIS:CE1	2.58	0.56
4:1:457:G:H2'	4:1:458:C:H6	1.69	0.56
10:LR:30:ASN:N	10:LR:30:ASN:HD22	2.03	0.56
13:B:21:TYR:CE2	13:B:54:LEU:HD23	2.39	0.56
13:B:213:LEU:HD22	13:B:230:LYS:HE3	1.86	0.56
13:B:657:ALA:O	13:B:661:LEU:HD12	2.05	0.56
3:D:78:HIS:CG	4:1:2707:U:C4	2.94	0.56
8:A:140:ALA:O	8:A:144:LYS:HG3	2.06	0.56
13:B:592:LEU:HD22	13:B:596:ARG:HE	1.69	0.56
15:LE:151:ILE:HB	15:LE:195:ILE:HG23	1.87	0.56
4:1:207:G:H2'	4:1:208:A:C8	2.39	0.56
4:1:210:C:H41	4:1:231:U:H2'	1.71	0.56
4:1:215:C:O4'	13:B:626:LYS:NZ	2.33	0.56
4:1:467:U:H5'	13:B:601:ARG:NH1	2.20	0.56
10:LR:149:LYS:HA	10:LR:152:LYS:CE	2.35	0.56
13:B:704:SER:O	13:B:763:HIS:CD2	2.58	0.56
14:LC:92:PHE:O	14:LC:100:ARG:NH2	2.39	0.56
14:LC:143:ARG:HB2	14:LC:179:ASP:OD1	2.06	0.56
3:D:147:LEU:HA	3:D:151:LEU:HD21	1.88	0.56
5:LY:86:GLN:HG2	5:LY:96:HIS:HA	1.88	0.56
9:LU:55:ASN:OD1	9:LU:58:GLY:N	2.34	0.56
13:B:835:LEU:HA	13:B:838:MET:HG3	1.86	0.56
2:E:222:THR:OG1	2:E:231:ASP:OD1	2.24	0.56
12:2:8:PRO:HG2	13:B:540:ASP:OD1	2.05	0.56
3:D:87:LYS:HZ3	10:LR:30:ASN:HB2	1.68	0.56
3:D:88:LEU:O	8:A:80:MET:HE1	2.05	0.56
4:1:232:G:H22	5:LY:61:HIS:CE1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LX:89:LYS:N	7:LX:89:LYS:HD3	2.20	0.56
12:2:5:ASN:OD1	12:2:40:GLN:HA	2.06	0.56
12:2:10:ASP:HA	12:2:13:ASN:OD1	2.05	0.56
9:LU:26:THR:HG22	9:LU:68:SER:HB3	1.88	0.56
10:LR:97:ARG:O	10:LR:101:ILE:HG12	2.06	0.56
13:B:166:MET:HA	13:B:169:LYS:HG3	1.86	0.56
13:B:765:LEU:HD22	13:B:804:VAL:HG22	1.86	0.56
8:A:172:ASP:OD1	8:A:174:THR:HG22	2.05	0.56
8:A:184:VAL:HA	8:A:187:GLN:HE21	1.71	0.56
2:E:271:GLU:HA	2:E:274:ASN:OD1	2.06	0.55
13:B:9:LYS:O	13:B:13:LEU:HG	2.06	0.55
3:D:105:GLU:OE1	3:D:119:ASN:HA	2.06	0.55
4:1:230:G:H4'	5:LY:18:HIS:CE1	2.41	0.55
7:LX:90:ILE:H	7:LX:90:ILE:HD12	1.71	0.55
10:LR:15:LEU:HD22	10:LR:52:ARG:NE	2.15	0.55
13:B:213:LEU:HB3	13:B:230:LYS:HZ1	1.71	0.55
3:D:88:LEU:CD2	8:A:83:LEU:HB3	2.36	0.55
5:LY:86:GLN:HB3	5:LY:95:VAL:O	2.06	0.55
7:LX:93:ASN:OD1	7:LX:93:ASN:O	2.24	0.55
13:B:23:HIS:CE1	13:B:25:GLN:NE2	2.75	0.55
12:2:25:ASN:HB2	13:B:470:ARG:HH22	1.70	0.55
13:B:211:GLU:O	13:B:215:THR:HG23	2.06	0.55
3:D:83:ALA:C	3:D:85:ASP:N	2.60	0.55
8:A:99:SER:OG	8:A:101:ASN:OD1	2.21	0.55
10:LR:96:MET:N	10:LR:96:MET:SD	4.21	0.55
13:B:835:LEU:HA	13:B:838:MET:CG	2.36	0.55
13:B:130:LEU:HD11	13:B:157:ALA:O	2.07	0.55
13:B:716:PHE:HD2	13:B:746:PRO:HG3	1.72	0.55
3:D:122:LYS:HG3	3:D:124:GLN:NE2	2.22	0.55
3:D:153:GLN:NE2	8:A:103:LEU:HD13	2.22	0.55
4:1:2526:C:H4'	10:LR:9:ARG:NH2	2.22	0.55
13:B:114:LEU:H	13:B:114:LEU:HD12	1.70	0.55
3:D:62:VAL:HG21	9:LU:115:PHE:CD1	2.41	0.55
10:LR:86:ASN:OD1	10:LR:86:ASN:N	2.40	0.55
12:2:12:MET:SD	12:2:16:HIS:CE1	3.00	0.55
13:B:35:GLN:O	13:B:38:SER:OG	2.23	0.55
13:B:323:PRO:HB3	13:B:409:GLU:OE2	2.06	0.55
13:B:540:ASP:HA	13:B:543:LYS:HG2	1.88	0.55
14:LC:262:GLU:OE1	14:LC:262:GLU:N	2.29	0.55
15:LE:165:LEU:HD11	15:LE:176:THR:HG22	1.87	0.55
2:E:295:GLY:HA3	2:E:303:ALA:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:55:LEU:O	3:D:59:GLN:HG3	2.07	0.55
4:1:690:C:H2'	4:1:691:C:C6	2.42	0.55
4:1:2694:G:H5'	4:1:2695:A:C2	2.41	0.55
8:A:137:LEU:O	8:A:141:GLU:HG2	2.06	0.55
13:B:424:ILE:HG13	13:B:455:ALA:HB2	1.89	0.55
14:LC:361:LEU:HD12	14:LC:362:GLN:H	1.72	0.55
3:D:62:VAL:HG21	9:LU:115:PHE:HD1	1.71	0.55
8:A:75:LYS:HA	8:A:78:LYS:HD2	1.89	0.55
13:B:54:LEU:HD12	13:B:85:VAL:HG13	1.89	0.55
13:B:85:VAL:O	13:B:88:LEU:HD12	2.06	0.55
13:B:327:ASN:HA	13:B:330:ARG:HG2	1.88	0.55
15:LE:56:ARG:HG3	15:LE:57:TYR:CD1	2.41	0.55
1:8:90:C:HO2'	5:LY:24:HIS:CE1	2.25	0.54
2:E:255:CYS:HB3	2:E:276:ILE:HG23	1.90	0.54
3:D:78:HIS:ND1	3:D:79:ARG:N	2.52	0.54
5:LY:38:LEU:H	5:LY:38:LEU:HD12	1.72	0.54
5:LY:52:ASP:HA	5:LY:69:LYS:NZ	2.21	0.54
13:B:21:TYR:OH	13:B:54:LEU:O	2.22	0.54
13:B:54:LEU:HD12	13:B:88:LEU:HD11	1.88	0.54
13:B:310:LEU:O	13:B:314:LEU:HG	2.07	0.54
2:E:213:GLU:OE2	2:E:213:GLU:N	2.34	0.54
3:D:103:ILE:HD12	3:D:123:VAL:HG11	1.90	0.54
8:A:207:VAL:O	8:A:211:MET:HG2	2.07	0.54
13:B:421:ALA:O	13:B:834:ALA:HB2	2.08	0.54
13:B:431:MET:N	13:B:431:MET:SD	2.80	0.54
14:LC:161:TYR:CE2	14:LC:170:LEU:HD22	2.41	0.54
4:1:207:G:O2'	5:LY:61:HIS:HE1	1.90	0.54
13:B:166:MET:SD	13:B:167:ALA:N	2.80	0.54
13:B:606:ALA:O	13:B:610:GLU:HG2	2.08	0.54
14:LC:71:ARG:HG3	14:LC:73:VAL:HG22	1.89	0.54
14:LC:140:LYS:O	14:LC:204:ARG:NH2	2.33	0.54
3:D:154:LEU:HB2	3:D:162:LEU:HD11	1.88	0.54
7:LX:117:TYR:CZ	7:LX:153:ILE:HG12	2.42	0.54
13:B:427:ALA:O	13:B:431:MET:HG2	2.06	0.54
14:LC:134:PRO:HG3	14:LC:150:LEU:HG	1.88	0.54
2:E:298:LYS:H	2:E:298:LYS:CD	2.15	0.54
3:D:78:HIS:C	3:D:80:THR:N	2.57	0.54
3:D:108:MET:O	3:D:115:VAL:HA	2.07	0.54
4:1:2372:U:H2'	4:1:2373:C:C6	2.42	0.54
4:1:3606:U:H5'	10:LR:76:MET:SD	2.46	0.54
9:LU:20:LYS:O	9:LU:108:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LC:67:TRP:HE3	14:LC:71:ARG:HD3	1.71	0.54
3:D:78:HIS:ND1	4:1:2707:U:C5	2.76	0.54
4:1:470:A:H61	4:1:684:G:H1'	1.72	0.54
13:B:241:GLU:OE2	13:B:241:GLU:N	2.37	0.54
14:LC:5:ARG:NH1	14:LC:26:ALA:HA	2.22	0.54
13:B:297:PRO:HA	13:B:300:PHE:CE2	2.43	0.54
2:E:78:TRP:CE2	2:E:341:PRO:HB2	2.43	0.54
3:D:78:HIS:CB	4:1:2707:U:C4	2.91	0.54
3:D:79:ARG:CZ	4:1:2707:U:H3'	2.38	0.54
5:LY:34:LEU:HD22	5:LY:38:LEU:HD22	1.89	0.54
8:A:95:THR:HG23	8:A:97:ARG:NH1	2.23	0.54
2:E:91:TYR:CD1	2:E:93:LEU:HG	2.43	0.54
2:E:200:VAL:HA	2:E:347:VAL:HG12	1.89	0.54
2:E:211:LEU:HB3	2:E:238:VAL:HG11	1.90	0.54
2:E:263:VAL:HG12	2:E:368:CYS:HB3	1.89	0.54
3:D:83:ALA:C	3:D:85:ASP:H	2.09	0.54
4:1:678:C:H2'	4:1:679:C:C6	2.43	0.54
12:2:9:GLU:OE1	13:B:544:LEU:HA	2.07	0.54
13:B:394:LEU:HG	13:B:833:TYR:CE1	2.42	0.54
14:LC:148:PRO:HD3	14:LC:175:LYS:HE3	1.90	0.54
14:LC:362:GLN:OE1	14:LC:362:GLN:N	2.41	0.54
3:D:78:HIS:CB	4:1:2707:U:O4	2.56	0.54
13:B:461:ALA:HA	13:B:464:MET:SD	2.48	0.54
2:E:248:LEU:HD22	2:E:332:GLU:HG3	1.89	0.53
13:B:416:LYS:HA	13:B:419:LYS:HG2	1.89	0.53
15:LE:140:LEU:HD11	15:LE:144:ILE:HG21	1.90	0.53
3:D:152:ASN:ND2	8:A:129:GLU:OE2	2.41	0.53
5:LY:41:LYS:HA	12:2:136:LYS:HE3	1.89	0.53
13:B:12:ALA:HA	13:B:15:LYS:HE2	1.91	0.53
15:LE:125:LEU:HD23	15:LE:125:LEU:H	1.72	0.53
12:2:112:ARG:HG3	12:2:115:ASN:H	1.73	0.53
13:B:154:TYR:CZ	13:B:158:TYR:HE2	2.26	0.53
1:8:47:C:O2'	1:8:62:A:OP2	2.20	0.53
4:1:691:C:H2'	4:1:692:A:H8	1.73	0.53
9:LU:69:LYS:HZ3	9:LU:71:THR:HB	1.71	0.53
13:B:390:PRO:HB3	13:B:833:TYR:CE2	2.42	0.53
1:8:70:G:O2'	5:LY:114:ASP:OD2	2.26	0.53
4:1:678:C:H2'	4:1:679:C:H6	1.74	0.53
4:1:2898:G:H2'	4:1:2899:C:C6	2.44	0.53
5:LY:53:ASP:OD1	5:LY:110:LYS:N	2.42	0.53
8:A:145:VAL:HA	8:A:148:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:63:ASP:HB3	12:2:66:ASP:HB3	1.90	0.53
13:B:141:LEU:HD11	13:B:151:TRP:CE2	2.43	0.53
13:B:158:TYR:HB3	13:B:167:ALA:HB2	1.90	0.53
13:B:540:ASP:HA	13:B:543:LYS:HE3	1.90	0.53
14:LC:65:GLU:OE1	14:LC:80:ARG:HB3	2.09	0.53
14:LC:236:ASN:O	14:LC:240:LEU:HG	2.08	0.53
5:LY:26:ARG:O	5:LY:30:MET:HG2	2.09	0.53
13:B:541:LEU:O	13:B:544:LEU:HB3	2.09	0.53
15:LE:63:TYR:CE2	15:LE:68:MET:HG3	2.44	0.53
15:LE:176:THR:HB	15:LE:186:LEU:HD23	1.91	0.53
4:1:221:C:H2'	4:1:222:C:C6	2.44	0.53
4:1:2387:G:H2'	4:1:2388:A:C8	2.44	0.53
8:A:202:ASN:ND2	8:A:209:ALA:HA	2.24	0.53
9:LU:91:LEU:HD13	9:LU:96:LEU:HD23	1.91	0.53
12:2:72:ILE:HD12	12:2:72:ILE:O	2.09	0.53
12:2:95:SER:HA	12:2:98:MET:SD	2.49	0.53
13:B:192:LEU:HB2	13:B:533:ILE:HG22	1.89	0.53
13:B:420:HIS:C	13:B:798:LEU:HD13	2.29	0.53
13:B:621:GLN:HG3	13:B:625:LYS:NZ	2.23	0.53
12:2:69:HIS:HA	12:2:104:ALA:HB1	1.91	0.53
13:B:144:ARG:HH12	13:B:146:ALA:HB3	1.74	0.53
13:B:173:GLU:O	13:B:177:THR:HG23	2.09	0.53
13:B:530:MET:SD	13:B:531:ARG:N	2.82	0.53
3:D:117:HIS:HB2	3:D:141:LYS:HG2	1.89	0.53
4:1:456:C:H2'	4:1:457:G:C8	2.43	0.53
4:1:462:G:H2'	4:1:463:A:C8	2.44	0.53
4:1:685:C:H5''	4:1:686:A:OP1	2.09	0.53
13:B:816:CYS:HB3	13:B:819:ALA:HB3	1.90	0.53
4:1:196:C:O4'	5:LY:125:SER:HB3	2.09	0.52
5:LY:49:ILE:HD12	5:LY:80:ILE:HG21	1.90	0.52
12:2:2:ASN:HB2	13:B:258:TRP:CZ3	2.44	0.52
12:2:112:ARG:NE	12:2:142:GLU:OE2	2.41	0.52
14:LC:109:ARG:HA	14:LC:109:ARG:HE	1.74	0.52
3:D:87:LYS:HZ3	10:LR:30:ASN:CB	2.22	0.52
5:LY:30:MET:CE	5:LY:75:ARG:HG2	2.39	0.52
7:LX:78:LYS:HZ3	7:LX:101:ASP:N	2.07	0.52
2:E:76:ASP:OD1	2:E:83:TYR:OH	2.27	0.52
4:1:2709:C:H2'	10:LR:39:GLN:HG3	1.91	0.52
8:A:142:LYS:NZ	13:B:173:GLU:HB3	2.23	0.52
9:LU:20:LYS:C	9:LU:21:PHE:HD1	2.13	0.52
14:LC:297:GLU:OE1	14:LC:297:GLU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LX:119:ILE:HG22	7:LX:120:ASP:H	1.74	0.52
10:LR:5:ARG:HH21	10:LR:8:LYS:CE	2.21	0.52
12:2:138:TYR:CE2	12:2:144:ALA:HB2	2.45	0.52
13:B:164:TYR:OH	13:B:202:GLU:OE1	2.23	0.52
15:LE:153:LEU:HD13	15:LE:194:VAL:HA	1.90	0.52
15:LE:165:LEU:HD21	15:LE:176:THR:HG22	1.92	0.52
4:1:197:A:N3	4:1:222:C:O2'	2.32	0.52
13:B:213:LEU:HD21	13:B:226:VAL:HG13	1.92	0.52
13:B:251:GLN:HG3	13:B:264:LEU:HD11	1.91	0.52
14:LC:64:ALA:HB3	14:LC:92:PHE:HE2	1.75	0.52
15:LE:150:LEU:N	15:LE:162:VAL:O	2.24	0.52
4:1:227:A:N3	5:LY:2:LYS:HD3	2.24	0.52
4:1:390:C:H2'	4:1:391:U:H6	1.75	0.52
8:A:144:LYS:HE3	13:B:145:PRO:HG3	1.92	0.52
8:A:147:GLY:HA2	13:B:138:TYR:OH	2.09	0.52
9:LU:24:ASP:HB2	9:LU:111:GLU:HB2	1.90	0.52
13:B:706:PRO:HB3	13:B:763:HIS:HA	1.91	0.52
13:B:712:MET:HB3	13:B:741:PHE:CE2	2.44	0.52
2:E:158:LYS:NZ	2:E:161:VAL:HG21	2.25	0.52
4:1:239:C:H4'	5:LY:31:SER:HB2	1.92	0.52
4:1:2701:U:O4	4:1:2715:G:O6	2.27	0.52
5:LY:52:ASP:HB2	5:LY:110:LYS:HD2	1.90	0.52
5:LY:54:GLU:OE2	5:LY:108:ARG:NH2	2.42	0.52
8:A:140:ALA:HB1	13:B:145:PRO:HB2	1.92	0.52
13:B:169:LYS:HD2	13:B:170:ILE:N	2.24	0.52
13:B:654:LEU:HB3	13:B:681:ILE:HG23	1.92	0.52
2:E:177:ARG:O	2:E:225:ARG:NH1	2.43	0.52
8:A:180:ASP:OD2	8:A:206:ILE:HG12	2.10	0.52
10:LR:105:LEU:O	10:LR:108:ARG:HG2	2.10	0.52
10:LR:144:LYS:H	10:LR:144:LYS:HD3	1.73	0.52
12:2:113:LYS:HB2	12:2:142:GLU:OE1	2.10	0.52
12:2:135:PRO:O	12:2:136:LYS:HG2	2.10	0.52
12:2:150:ASP:O	12:2:153:GLN:NE2	2.41	0.52
13:B:210:LEU:HD13	13:B:237:LEU:HD12	1.92	0.52
13:B:395:GLU:O	13:B:399:THR:HG23	2.10	0.52
13:B:545:GLU:HA	13:B:548:LEU:HB2	1.91	0.52
13:B:652:THR:O	13:B:656:GLU:HG2	2.10	0.52
14:LC:361:LEU:HD12	14:LC:362:GLN:N	2.25	0.52
15:LE:190:HIS:CE1	15:LE:192:LYS:HG3	2.45	0.52
3:D:80:THR:O	3:D:81:ALA:C	2.49	0.52
3:D:93:LYS:HD2	3:D:97:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:140:ALA:CB	13:B:145:PRO:HB2	2.40	0.52
13:B:205:LEU:HA	13:B:207:ARG:NH2	2.24	0.52
13:B:258:TRP:CD1	13:B:292:VAL:HG13	2.45	0.52
13:B:482:MET:HG3	13:B:482:MET:O	2.10	0.52
4:1:699:C:H2'	4:1:700:G:C8	2.45	0.52
13:B:418:TYR:CD1	13:B:423:ASN:HB3	2.45	0.52
2:E:253:TYR:CE2	2:E:380:PRO:HG3	2.45	0.51
4:1:654:C:H5'	14:LC:268:ARG:HE	1.75	0.51
10:LR:10:LEU:HD21	10:LR:38:ARG:N	2.25	0.51
12:2:83:ARG:HH11	13:B:323:PRO:HD3	1.75	0.51
13:B:103:TYR:CG	13:B:116:ILE:HG23	2.44	0.51
4:1:685:C:P	15:LE:101:ASN:HD21	2.32	0.51
4:1:690:C:H2'	4:1:691:C:H6	1.74	0.51
10:LR:37:SER:O	10:LR:41:ILE:HG12	2.09	0.51
12:2:11:LEU:HD11	13:B:544:LEU:CD2	2.40	0.51
13:B:484:CYS:HG	13:B:487:PHE:HD2	1.58	0.51
13:B:708:LEU:O	13:B:712:MET:HG3	2.10	0.51
14:LC:133:LEU:HD12	14:LC:134:PRO:HD2	1.93	0.51
2:E:319:LYS:HD2	2:E:320:SER:N	2.25	0.51
4:1:492:U:H3'	4:1:493:G:H8	1.75	0.51
7:LX:113:VAL:HG21	7:LX:121:VAL:HG21	1.92	0.51
9:LU:20:LYS:NZ	9:LU:73:THR:HG23	2.26	0.51
10:LR:136:ARG:O	10:LR:139:MET:SD	2.68	0.51
13:B:274:LEU:HD12	13:B:275:GLU:H	1.76	0.51
13:B:418:TYR:CE1	13:B:833:TYR:HD1	2.29	0.51
13:B:643:ILE:HG13	13:B:646:LYS:HB3	1.93	0.51
15:LE:99:ASP:O	15:LE:100:LYS:HG2	2.10	0.51
7:LX:80:PRO:HG3	7:LX:98:PHE:CE2	2.45	0.51
13:B:224:LEU:H	13:B:224:LEU:HD12	1.75	0.51
13:B:705:HIS:HB3	13:B:708:LEU:HB3	1.92	0.51
4:1:2708:U:O2	10:LR:40:GLN:NE2	2.44	0.51
13:B:20:CYS:HB2	13:B:25:GLN:HB2	1.92	0.51
13:B:186:ASP:OD1	13:B:188:GLU:HB2	2.09	0.51
13:B:646:LYS:NZ	13:B:651:GLU:OE2	2.35	0.51
13:B:708:LEU:HG	13:B:712:MET:HE3	1.92	0.51
14:LC:259:LYS:O	14:LC:263:LEU:HG	2.09	0.51
9:LU:48:LYS:HB2	9:LU:82:TYR:OH	2.10	0.51
9:LU:111:GLU:HG3	9:LU:113:ARG:HG3	1.93	0.51
10:LR:64:ARG:O	10:LR:67:THR:HG22	2.10	0.51
13:B:501:PHE:HD2	13:B:568:LEU:HD21	1.76	0.51
4:1:485:C:O2	4:1:485:C:H2'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LX:78:LYS:HZ3	7:LX:100:VAL:C	2.14	0.51
9:LU:43:LEU:O	9:LU:47:ILE:HG12	2.10	0.51
10:LR:101:ILE:HB	10:LR:135:LYS:HE3	1.92	0.51
13:B:17:ILE:HG12	13:B:32:PHE:HB2	1.92	0.51
13:B:452:MET:HA	13:B:455:ALA:HB3	1.92	0.51
15:LE:120:ASP:OD2	15:LE:121:VAL:N	2.44	0.51
3:D:123:VAL:HA	3:D:133:THR:O	2.10	0.51
4:1:406:C:H2'	4:1:407:A:C8	2.45	0.51
5:LY:83:GLU:OE2	5:LY:84:ARG:HB2	2.11	0.51
13:B:240:LEU:HD12	13:B:267:ALA:HA	1.92	0.51
3:D:133:THR:HA	8:A:120:TYR:O	2.11	0.51
4:1:468:U:H5	4:1:688:U:H3	1.59	0.51
9:LU:28:PRO:HG3	9:LU:100:LEU:HD11	1.93	0.51
9:LU:96:LEU:HA	9:LU:99:TRP:CE3	2.46	0.51
10:LR:41:ILE:O	10:LR:45:ILE:HG12	2.11	0.51
12:2:29:LYS:NZ	13:B:524:ASP:OD1	2.36	0.51
12:2:47:ASP:OD1	12:2:51:LYS:N	2.42	0.51
14:LC:207:PRO:HA	14:LC:249:PHE:O	2.10	0.51
15:LE:191:GLN:OE1	15:LE:191:GLN:N	2.35	0.51
5:LY:35:SER:HB3	5:LY:38:LEU:CD1	2.42	0.50
9:LU:64:GLU:OE1	9:LU:71:THR:HG23	2.10	0.50
13:B:187:TYR:HE1	13:B:532:LYS:HE2	1.75	0.50
13:B:609:GLU:O	13:B:613:LYS:HG2	2.10	0.50
2:E:77:PRO:HG2	2:E:78:TRP:CD2	2.46	0.50
3:D:97:VAL:HG22	3:D:98:ASN:N	2.26	0.50
5:LY:30:MET:HB2	5:LY:101:PRO:HG2	1.92	0.50
12:2:79:ARG:HD3	13:B:408:ILE:HD13	1.93	0.50
13:B:460:GLU:O	13:B:464:MET:HG3	2.11	0.50
13:B:484:CYS:SG	13:B:487:PHE:HD2	2.35	0.50
14:LC:152:LEU:H	14:LC:252:TRP:HZ3	1.59	0.50
8:A:95:THR:OG1	8:A:103:LEU:HD21	2.12	0.50
8:A:190:VAL:HG21	8:A:213:LEU:HD13	1.93	0.50
10:LR:144:LYS:HD3	10:LR:144:LYS:N	2.26	0.50
13:B:409:GLU:HG3	13:B:412:LEU:HD21	1.92	0.50
13:B:505:LEU:HG	13:B:564:ILE:HG21	1.93	0.50
3:D:54:LYS:NZ	3:D:61:GLN:HE22	2.09	0.50
4:1:389:A:O4'	5:LY:91:ASN:HA	2.12	0.50
5:LY:83:GLU:O	5:LY:96:HIS:HE1	1.94	0.50
7:LX:101:ASP:OD1	7:LX:104:ALA:N	2.43	0.50
12:2:11:LEU:HD11	13:B:544:LEU:HD22	1.94	0.50
13:B:70:ARG:NH1	13:B:70:ARG:HB2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:390:PRO:HG2	13:B:830:LEU:O	2.11	0.50
13:B:592:LEU:HD22	13:B:596:ARG:HH21	1.76	0.50
3:D:137:HIS:HD1	3:D:138:ALA:H	1.58	0.50
4:1:223:G:N7	14:LC:165:LYS:HE3	2.27	0.50
5:LY:83:GLU:CD	5:LY:84:ARG:HB2	2.32	0.50
8:A:96:ILE:HB	8:A:104:PHE:HB2	1.93	0.50
13:B:449:ALA:HA	13:B:452:MET:CG	2.42	0.50
14:LC:337:ARG:O	14:LC:340:ILE:HG13	2.12	0.50
1:8:93:C:O2'	1:8:94:G:H8	1.94	0.50
4:1:683:C:H2'	4:1:684:G:O4'	2.12	0.50
4:1:2535:G:H2'	4:1:2536:A:H8	1.75	0.50
10:LR:153:LYS:HD2	10:LR:153:LYS:O	2.11	0.50
12:2:7:ARG:HG2	12:2:7:ARG:HH11	1.77	0.50
13:B:25:GLN:HB3	13:B:28:ASN:OD1	2.11	0.50
13:B:189:TYR:CE2	13:B:193:LEU:HD11	2.46	0.50
14:LC:218:ILE:HD12	14:LC:219:LYS:H	1.77	0.50
2:E:156:MET:HE1	2:E:166:ILE:HA	1.94	0.50
2:E:201:ILE:HG23	2:E:329:MET:HG3	1.94	0.50
4:1:2385:U:H5''	10:LR:5:ARG:CZ	2.41	0.50
4:1:2693:G:H2'	4:1:2694:G:N2	2.27	0.50
5:LY:38:LEU:HB3	5:LY:42:TYR:HE1	1.77	0.50
13:B:480:ASN:ND2	13:B:488:GLN:OE1	2.43	0.50
13:B:780:LYS:HA	13:B:783:ILE:HD12	1.92	0.50
15:LE:99:ASP:O	15:LE:101:ASN:ND2	2.44	0.50
2:E:180:TYR:HB3	2:E:224:TYR:HB3	1.94	0.50
9:LU:38:ASN:HA	9:LU:41:GLN:NE2	2.27	0.50
9:LU:39:PHE:HE2	9:LU:70:ILE:HG21	1.76	0.50
13:B:295:ARG:NH1	13:B:299:ASN:OD1	2.44	0.50
13:B:622:ARG:HA	13:B:625:LYS:HG2	1.94	0.50
14:LC:155:GLU:HA	14:LC:254:GLU:CD	2.32	0.50
14:LC:292:ILE:O	14:LC:298:ILE:HD13	2.11	0.50
2:E:156:MET:CE	2:E:166:ILE:HA	2.42	0.50
2:E:260:ILE:HG12	2:E:361:LEU:HD11	1.93	0.50
7:LX:84:GLU:O	7:LX:87:MET:HE2	2.12	0.50
8:A:109:PRO:HA	8:A:123:PHE:O	2.11	0.50
10:LR:141:HIS:CE1	10:LR:145:LEU:HD21	2.47	0.50
12:2:16:HIS:HA	13:B:486:TRP:HZ3	1.76	0.50
12:2:93:GLN:HE22	12:2:96:ARG:HE	1.59	0.50
13:B:250:LEU:HD22	13:B:260:TYR:CZ	2.47	0.50
13:B:261:TYR:OH	13:B:293:PRO:HG3	2.11	0.50
15:LE:150:LEU:HD23	15:LE:196:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:105:GLU:HB3	8:A:97:ARG:NH2	2.26	0.49
9:LU:91:LEU:HD13	9:LU:96:LEU:HB2	1.94	0.49
12:2:16:HIS:NE2	13:B:485:MET:SD	2.85	0.49
13:B:164:TYR:CD1	13:B:199:VAL:O	2.65	0.49
13:B:661:LEU:HD22	13:B:665:LYS:HE3	1.94	0.49
13:B:754:LEU:HB3	13:B:755:LYS:NZ	2.27	0.49
4:1:214:G:H2'	4:1:215:C:C6	2.47	0.49
13:B:390:PRO:HB3	13:B:833:TYR:CD2	2.47	0.49
2:E:94:MET:SD	2:E:191:LYS:NZ	2.86	0.49
13:B:54:LEU:HD13	13:B:85:VAL:HG22	1.94	0.49
13:B:97:ASP:HA	13:B:100:ILE:HD12	1.93	0.49
1:8:89:U:H2'	1:8:90:C:C6	2.47	0.49
2:E:94:MET:SD	2:E:97:ARG:NH2	2.85	0.49
2:E:324:PHE:HE2	2:E:326:ILE:HD11	1.76	0.49
4:1:202:C:H2'	4:1:203:U:C6	2.48	0.49
4:1:405:U:H1'	4:1:410:A:N6	2.26	0.49
14:LC:298:ILE:H	14:LC:298:ILE:HD12	1.77	0.49
14:LC:341:LEU:O	14:LC:345:ARG:HG3	2.13	0.49
3:D:78:HIS:O	3:D:79:ARG:C	2.49	0.49
13:B:261:TYR:HB3	13:B:280:TYR:CE1	2.44	0.49
14:LC:167:ALA:HB1	14:LC:221:PHE:HD2	1.77	0.49
15:LE:268:GLN:OE1	15:LE:268:GLN:N	2.34	0.49
15:LE:282:TYR:O	15:LE:286:LEU:HD22	2.12	0.49
4:1:220:C:H2'	4:1:221:C:C6	2.46	0.49
12:2:71:HIS:CE1	12:2:109:LEU:HA	2.48	0.49
12:2:157:GLU:HA	12:2:160:ARG:HB2	1.94	0.49
13:B:525:PHE:HD1	13:B:528:TYR:HD1	1.60	0.49
13:B:797:ASN:ND2	13:B:799:GLN:OE1	2.45	0.49
4:1:200:U:OP1	5:LY:36:LYS:HE2	2.13	0.49
4:1:518:G:H1	4:1:643:C:H2'	1.78	0.49
5:LY:27:ARG:NH2	5:LY:48:PRO:HG2	2.28	0.49
9:LU:38:ASN:O	9:LU:41:GLN:HG2	2.12	0.49
13:B:45:HIS:HB3	13:B:48:THR:HG22	1.94	0.49
13:B:128:ARG:NH1	13:B:522:GLN:HE22	2.10	0.49
13:B:132:GLY:O	13:B:135:GLU:HG3	2.13	0.49
4:1:232:G:H22	5:LY:61:HIS:HE1	1.61	0.49
4:1:2533:C:H2'	4:1:2534:C:H6	1.78	0.49
8:A:136:GLN:NE2	13:B:146:ALA:O	2.46	0.49
13:B:579:GLU:HG2	13:B:580:HIS:ND1	2.27	0.49
13:B:695:VAL:O	13:B:699:PHE:HB2	2.12	0.49
1:8:83:C:H6	1:8:83:C:H5''	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:ARG:HH12	2:E:382:PHE:HE2	1.61	0.49
2:E:257:MET:SD	2:E:257:MET:N	2.85	0.49
4:1:473:C:H2'	4:1:474:C:C6	2.47	0.49
5:LY:56:GLN:NE2	5:LY:66:GLN:O	2.46	0.49
5:LY:73:VAL:HA	5:LY:80:ILE:HG22	1.94	0.49
12:2:79:ARG:HD3	13:B:408:ILE:CD1	2.42	0.49
13:B:431:MET:HA	13:B:434:ALA:HB3	1.94	0.49
13:B:834:ALA:CB	13:B:837:PHE:HD2	2.26	0.49
2:E:199:GLU:HA	2:E:352:LYS:O	2.13	0.48
2:E:274:ASN:HD22	2:E:311:LYS:H	1.60	0.48
4:1:2894:A:H2'	4:1:2895:A:C8	2.48	0.48
9:LU:80:LYS:O	9:LU:83:LEU:HG	2.12	0.48
9:LU:98:ASP:O	9:LU:115:PHE:HE1	1.95	0.48
13:B:451:TYR:O	13:B:455:ALA:N	2.46	0.48
15:LE:93:THR:HG22	15:LE:106:VAL:HG13	1.95	0.48
10:LR:5:ARG:NH2	10:LR:8:LYS:HE3	2.22	0.48
12:2:36:LEU:HB3	13:B:529:CYS:SG	2.53	0.48
12:2:100:GLU:OE1	13:B:223:LYS:HG2	2.13	0.48
14:LC:159:GLU:HA	14:LC:217:ILE:HD13	1.95	0.48
15:LE:57:TYR:HD2	15:LE:62:MET:HE1	1.78	0.48
3:D:87:LYS:HB3	8:A:83:LEU:HD22	1.94	0.48
4:1:685:C:H3'	13:B:594:LYS:HZ2	1.79	0.48
8:A:181:ILE:HG22	8:A:185:MET:CE	2.43	0.48
9:LU:23:LEU:HD21	9:LU:83:LEU:HD13	1.94	0.48
13:B:492:ALA:HA	13:B:504:ALA:HA	1.96	0.48
14:LC:135:ALA:O	14:LC:138:MET:HE3	2.12	0.48
3:D:58:LEU:HA	3:D:61:GLN:NE2	2.29	0.48
3:D:142:GLN:O	3:D:145:GLU:HG3	2.12	0.48
4:1:675:C:H2'	4:1:676:C:C6	2.48	0.48
5:LY:54:GLU:HG2	5:LY:108:ARG:NH2	2.29	0.48
7:LX:96:LEU:HG	7:LX:140:LEU:HD11	1.94	0.48
12:2:61:GLU:HG3	12:2:69:HIS:CE1	2.49	0.48
13:B:201:ARG:HH21	13:B:229:THR:HG21	1.79	0.48
13:B:330:ARG:HH22	13:B:386:LYS:CD	2.25	0.48
13:B:330:ARG:HH12	13:B:386:LYS:HG2	1.77	0.48
13:B:604:LYS:O	13:B:608:ILE:HG12	2.13	0.48
10:LR:6:LEU:O	10:LR:9:ARG:HG3	2.13	0.48
10:LR:64:ARG:O	10:LR:68:LEU:HD22	2.13	0.48
12:2:9:GLU:HA	13:B:544:LEU:HD13	1.95	0.48
13:B:134:ARG:NH1	13:B:161:LEU:HD11	2.29	0.48
13:B:430:TRP:HB3	13:B:431:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LC:5:ARG:HH12	14:LC:29:LYS:HB2	1.79	0.48
2:E:298:LYS:HD2	2:E:298:LYS:N	2.17	0.48
4:1:228:C:O2'	5:LY:14:ASN:OD1	2.22	0.48
4:1:493:G:N1	4:1:660:A:H2	2.03	0.48
9:LU:100:LEU:HD12	9:LU:112:LEU:CG	2.43	0.48
12:2:19:LEU:HD13	13:B:484:CYS:HA	1.95	0.48
13:B:78:LYS:HA	13:B:109:TRP:CD2	2.48	0.48
13:B:553:PHE:O	13:B:556:LYS:HG2	2.13	0.48
2:E:269:TYR:CZ	2:E:304:PRO:HG3	2.49	0.48
4:1:228:C:H2'	4:1:229:G:H8	1.79	0.48
12:2:37:SER:HB2	12:2:38:TRP:CE3	2.49	0.48
12:2:88:GLN:NE2	12:2:121:LEU:HD13	2.29	0.48
12:2:135:PRO:HA	12:2:143:ASP:OD2	2.12	0.48
13:B:64:GLU:O	13:B:67:GLU:HG3	2.13	0.48
13:B:73:LEU:HD11	13:B:83:TRP:CE2	2.48	0.48
13:B:115:GLN:H	13:B:115:GLN:CD	2.16	0.48
13:B:759:ASP:O	13:B:794:THR:N	2.44	0.48
14:LC:319:LEU:O	14:LC:320:LYS:HD2	2.14	0.48
15:LE:163:VAL:HG21	15:LE:201:ILE:HD11	1.95	0.48
3:D:80:THR:C	3:D:82:THR:N	2.66	0.48
4:1:2716:C:O2'	9:LU:107:LYS:HG2	2.14	0.48
8:A:96:ILE:O	8:A:103:LEU:HG	2.13	0.48
10:LR:38:ARG:HA	10:LR:41:ILE:HG12	1.96	0.48
15:LE:167:GLN:NE2	15:LE:171:GLY:HA2	2.28	0.48
1:8:86:U:H6	1:8:86:U:H5''	1.79	0.48
2:E:152:VAL:HG21	2:E:177:ARG:HH22	1.79	0.48
4:1:228:C:H2'	4:1:229:G:C8	2.49	0.48
13:B:380:LEU:HD13	13:B:396:TYR:CE1	2.49	0.48
13:B:480:ASN:ND2	13:B:510:GLU:OE1	2.47	0.48
13:B:486:TRP:HB3	13:B:553:PHE:CZ	2.48	0.48
3:D:58:LEU:HA	3:D:61:GLN:HE21	1.78	0.48
3:D:107:ASN:HB2	8:A:95:THR:CG2	2.44	0.48
4:1:457:G:N1	4:1:700:G:C6	2.82	0.48
5:LY:112:ASP:O	5:LY:116:LYS:HG3	2.14	0.48
9:LU:91:LEU:CD1	9:LU:96:LEU:HB2	2.43	0.48
13:B:13:LEU:O	13:B:17:ILE:HG13	2.14	0.48
13:B:414:LYS:HD3	13:B:430:TRP:NE1	2.28	0.48
13:B:779:GLN:HB3	13:B:780:LYS:HE2	1.96	0.48
2:E:263:VAL:HG22	2:E:318:MET:HE1	1.96	0.47
4:1:2899:C:H2'	4:1:2900:U:C6	2.49	0.47
8:A:187:GLN:HB2	13:B:108:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:81:HIS:HA	13:B:324:PRO:CG	2.38	0.47
13:B:608:ILE:HG22	13:B:612:LYS:NZ	2.27	0.47
13:B:679:PHE:O	13:B:691:MET:HE1	2.14	0.47
13:B:682:TYR:HA	13:B:685:LYS:HB2	1.96	0.47
4:1:216:C:OP2	4:1:219:G:O2'	2.32	0.47
8:A:111:VAL:HG11	8:A:113:LYS:HZ3	1.78	0.47
13:B:275:GLU:O	13:B:279:ILE:HG13	2.14	0.47
13:B:295:ARG:NH2	13:B:331:SER:OG	2.47	0.47
13:B:374:LEU:HD11	13:B:410:LEU:HD11	1.96	0.47
14:LC:43:ASN:ND2	14:LC:113:ARG:HB3	2.28	0.47
12:2:37:SER:HB3	13:B:532:LYS:NZ	2.28	0.47
12:2:79:ARG:HB2	12:2:82:ARG:NH2	2.29	0.47
13:B:195:TYR:CE1	13:B:535:LEU:HG	2.50	0.47
13:B:326:PHE:CE2	13:B:330:ARG:HD3	2.49	0.47
4:1:458:C:OP1	15:LE:114:ARG:HG2	2.14	0.47
4:1:654:C:H5'	14:LC:268:ARG:NE	2.29	0.47
4:1:2376:A:H2'	4:1:2377:C:C6	2.50	0.47
7:LX:71:LEU:HD22	7:LX:103:LYS:NZ	2.30	0.47
9:LU:83:LEU:O	9:LU:87:THR:HG23	2.13	0.47
13:B:93:ASP:C	13:B:94:LYS:HE2	2.34	0.47
13:B:205:LEU:HD12	13:B:207:ARG:HH21	1.79	0.47
13:B:408:ILE:HD12	13:B:409:GLU:N	2.30	0.47
3:D:91:SER:HA	3:D:94:LYS:HG2	1.95	0.47
7:LX:139:ARG:NH1	7:LX:140:LEU:O	2.47	0.47
13:B:28:ASN:HA	13:B:31:LYS:CE	2.45	0.47
13:B:765:LEU:HG	13:B:769:LYS:HE3	1.97	0.47
15:LE:190:HIS:CE1	15:LE:192:LYS:HE3	2.39	0.47
3:D:108:MET:CE	8:A:94:VAL:HG22	2.44	0.47
5:LY:69:LYS:NZ	5:LY:70:VAL:O	2.45	0.47
7:LX:90:ILE:HG22	7:LX:147:LEU:HD23	1.97	0.47
8:A:130:ASP:H	8:A:134:GLN:NE2	2.12	0.47
14:LC:140:LYS:HB3	14:LC:142:HIS:CD2	2.49	0.47
1:8:90:C:H2'	1:8:91:A:C8	2.50	0.47
2:E:74:ASN:HA	2:E:91:TYR:O	2.14	0.47
2:E:183:PRO:HD3	2:E:222:THR:HB	1.96	0.47
2:E:203:HIS:HB2	2:E:344:TRP:O	2.15	0.47
2:E:253:TYR:CD2	2:E:257:MET:HE3	2.50	0.47
3:D:50:MET:HG2	3:D:54:LYS:HG3	1.95	0.47
4:1:197:A:N1	4:1:225:G:O2'	2.36	0.47
4:1:208:A:OP2	13:B:27:ARG:NH2	2.47	0.47
4:1:456:C:C2	4:1:700:G:N1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:2374:A:H2'	4:1:2375:A:H8	1.80	0.47
4:1:2523:G:C2	4:1:2533:C:C2	3.03	0.47
5:LY:53:ASP:HA	5:LY:108:ARG:NH1	2.17	0.47
7:LX:81:LEU:HD13	7:LX:97:VAL:HG13	1.97	0.47
8:A:197:ARG:HG2	8:A:197:ARG:HH11	1.78	0.47
9:LU:20:LYS:HZ3	9:LU:73:THR:HG23	1.78	0.47
13:B:311:ASP:OD1	13:B:349:TYR:OH	2.25	0.47
14:LC:7:LEU:HD12	14:LC:23:THR:HA	1.96	0.47
1:8:57:C:O2	1:8:61:A:O2'	2.29	0.47
3:D:161:SER:HA	3:D:164:ARG:HD2	1.96	0.47
9:LU:104:ALA:HB2	9:LU:110:TYR:CE1	2.50	0.47
13:B:248:ARG:O	13:B:252:GLU:HG2	2.15	0.47
13:B:592:LEU:HD13	13:B:596:ARG:HH21	1.80	0.47
13:B:626:LYS:HA	13:B:632:ASP:HB2	1.96	0.47
13:B:698:ALA:HB3	13:B:708:LEU:HD13	1.96	0.47
2:E:137:GLU:OE2	2:E:140:ARG:NH1	2.46	0.47
3:D:59:GLN:CG	9:LU:99:TRP:HE1	2.23	0.47
4:1:202:C:O3'	13:B:633:GLU:HG2	2.15	0.47
5:LY:32:SER:HB2	5:LY:106:ILE:HD11	1.96	0.47
7:LX:79:PHE:CE1	7:LX:99:ILE:HD13	2.50	0.47
13:B:27:ARG:HG3	13:B:28:ASN:N	2.29	0.47
13:B:764:ARG:NE	13:B:788:THR:HG21	2.28	0.47
14:LC:294:LYS:HD3	14:LC:299:GLN:NE2	2.30	0.47
2:E:231:ASP:HB2	2:E:296:ILE:HD12	1.97	0.47
2:E:263:VAL:CG1	2:E:368:CYS:HB3	2.45	0.47
3:D:78:HIS:HB3	4:1:2707:U:O4	2.15	0.47
3:D:82:THR:HG22	3:D:83:ALA:N	2.29	0.47
4:1:467:U:OP1	13:B:604:LYS:HE2	2.15	0.47
7:LX:152:LYS:HD3	7:LX:152:LYS:N	2.30	0.47
12:2:51:LYS:NZ	13:B:551:HIS:HE1	2.12	0.47
14:LC:355:ALA:O	14:LC:359:ALA:N	2.39	0.47
4:1:499:G:N2	4:1:656:C:H1'	2.30	0.46
4:1:677:G:H2'	4:1:678:C:C6	2.50	0.46
5:LY:26:ARG:HB3	5:LY:30:MET:HE2	1.98	0.46
5:LY:30:MET:HE3	5:LY:75:ARG:HG2	1.97	0.46
5:LY:38:LEU:HD23	5:LY:109:LEU:HG	1.98	0.46
8:A:144:LYS:CE	13:B:145:PRO:HG3	2.45	0.46
15:LE:283:PRO:HA	15:LE:286:LEU:HD23	1.97	0.46
1:8:66:A:H2'	1:8:67:U:H6	1.80	0.46
1:8:97:A:C5'	7:LX:68:ARG:HH22	2.08	0.46
2:E:107:ASP:OD1	2:E:108:TYR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:657:C:H2'	4:1:658:C:O4'	2.15	0.46
12:2:13:ASN:O	12:2:16:HIS:HB2	2.15	0.46
12:2:18:ASN:O	12:2:22:LEU:N	2.45	0.46
13:B:66:TYR:O	13:B:70:ARG:HG3	2.15	0.46
13:B:159:HIS:CD2	13:B:164:TYR:CE1	3.03	0.46
2:E:147:ARG:HA	2:E:232:LEU:HD11	1.98	0.46
2:E:313:LYS:O	2:E:313:LYS:HD2	2.16	0.46
5:LY:62:TYR:CD2	5:LY:85:VAL:HG23	2.50	0.46
7:LX:101:ASP:OD2	7:LX:104:ALA:HB2	2.14	0.46
8:A:194:LYS:HG2	8:A:213:LEU:CD2	2.43	0.46
12:2:34:HIS:CD2	12:2:59:LYS:HB3	2.49	0.46
12:2:38:TRP:CZ2	12:2:60:MET:HB2	2.50	0.46
13:B:33:CYS:SG	13:B:52:LYS:HB2	2.54	0.46
13:B:176:LYS:HZ1	13:B:177:THR:HG22	1.80	0.46
15:LE:94:LYS:HE2	15:LE:107:VAL:HG21	1.97	0.46
15:LE:149:ILE:O	15:LE:197:THR:OG1	2.27	0.46
4:1:202:C:H4'	13:B:632:ASP:OD2	2.15	0.46
4:1:650:C:H2'	4:1:651:C:C6	2.50	0.46
5:LY:35:SER:OG	5:LY:36:LYS:N	2.49	0.46
10:LR:105:LEU:HD22	10:LR:138:LEU:HD21	1.98	0.46
10:LR:141:HIS:CE1	10:LR:145:LEU:HD11	2.50	0.46
13:B:272:ASN:OD1	13:B:273:MET:N	2.48	0.46
13:B:535:LEU:HA	13:B:538:TYR:HB2	1.98	0.46
3:D:93:LYS:CD	3:D:97:VAL:HG11	2.45	0.46
4:1:408:A:H4'	4:1:409:G:H3'	1.97	0.46
4:1:512:U:C4	4:1:647:G:O6	2.67	0.46
5:LY:14:ASN:O	5:LY:17:ARG:HG2	2.16	0.46
5:LY:41:LYS:HA	12:2:136:LYS:CE	2.45	0.46
8:A:88:VAL:CG2	8:A:113:LYS:HD2	2.44	0.46
8:A:103:LEU:HD23	8:A:104:PHE:N	2.31	0.46
13:B:73:LEU:HG	13:B:77:LEU:HD23	1.97	0.46
13:B:645:GLU:HG2	13:B:646:LYS:H	1.80	0.46
15:LE:150:LEU:HD13	15:LE:194:VAL:HG11	1.98	0.46
4:1:388:A:H1'	4:1:403:G:N2	2.29	0.46
4:1:470:A:N6	4:1:684:G:H1'	2.30	0.46
7:LX:59:LYS:H	7:LX:59:LYS:HD2	1.79	0.46
7:LX:73:HIS:ND1	7:LX:73:HIS:N	2.63	0.46
9:LU:39:PHE:CE2	9:LU:70:ILE:HG21	2.50	0.46
13:B:449:ALA:HB2	13:B:464:MET:CE	2.45	0.46
13:B:492:ALA:HB1	13:B:560:ILE:HG21	1.98	0.46
13:B:686:GLU:OE1	13:B:686:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LC:15:GLY:HA2	14:LC:174:LEU:HD13	1.96	0.46
15:LE:43:HIS:CD2	15:LE:44:CYS:H	2.33	0.46
15:LE:48:PRO:HD2	15:LE:57:TYR:CE2	2.50	0.46
15:LE:268:GLN:HG2	15:LE:269:GLY:N	2.31	0.46
5:LY:2:LYS:HZ1	5:LY:4:ASN:HB3	1.81	0.46
5:LY:2:LYS:HZ1	5:LY:7:VAL:HB	1.79	0.46
5:LY:85:VAL:HG21	5:LY:99:ILE:HD11	1.98	0.46
7:LX:145:ASP:OD2	7:LX:146:ALA:N	2.49	0.46
9:LU:107:LYS:O	9:LU:108:GLU:HB3	2.16	0.46
12:2:21:CYS:SG	12:2:22:LEU:HG	2.56	0.46
2:E:307:PRO:HD2	2:E:314:ALA:HB2	1.98	0.46
4:1:499:G:H2'	4:1:504:G:H22	1.81	0.46
4:1:2695:A:H1'	4:1:2697:A:N7	2.31	0.46
4:1:3599:A:O5'	4:1:3599:A:H8	1.99	0.46
4:1:3600:G:H2'	4:1:3601:C:H6	1.78	0.46
8:A:92:THR:O	8:A:109:PRO:HD2	2.16	0.46
13:B:118:ARG:O	13:B:122:LEU:HG	2.16	0.46
13:B:747:LYS:H	13:B:747:LYS:HE2	1.81	0.46
1:8:78:G:H2'	1:8:79:G:C8	2.50	0.46
2:E:268:ARG:NH1	2:E:270:ARG:HD2	2.31	0.46
3:D:91:SER:O	3:D:94:LYS:HG2	2.16	0.46
4:1:413:G:OP2	4:1:413:G:N2	2.25	0.46
10:LR:4:LEU:H	10:LR:5:ARG:HH12	1.63	0.46
12:2:16:HIS:HA	13:B:486:TRP:CZ3	2.51	0.46
13:B:49:LEU:HD13	13:B:71:ARG:NH1	2.27	0.46
13:B:78:LYS:HE3	13:B:78:LYS:HB3	1.74	0.46
13:B:128:ARG:HH12	13:B:522:GLN:NE2	2.13	0.46
13:B:583:ASP:OD2	13:B:592:LEU:HD21	2.16	0.46
3:D:72:ARG:HE	3:D:74:LYS:N	2.11	0.46
4:1:480:C:H2'	4:1:481:G:H8	1.82	0.46
8:A:98:LYS:HB2	8:A:104:PHE:HE2	1.81	0.46
8:A:178:VAL:HA	8:A:181:ILE:HD12	1.97	0.46
10:LR:47:ASP:HB2	10:LR:49:LEU:HD13	1.98	0.46
12:2:5:ASN:HB3	12:2:7:ARG:NH1	2.31	0.46
13:B:135:GLU:O	13:B:139:GLN:HG2	2.16	0.46
13:B:304:GLU:O	13:B:308:GLU:HG2	2.16	0.46
13:B:418:TYR:O	13:B:422:GLY:N	2.49	0.46
2:E:258:GLN:HA	2:E:261:ASP:OD2	2.15	0.45
2:E:268:ARG:NH2	7:LX:147:LEU:HD12	2.31	0.45
3:D:110:THR:HG22	3:D:114:THR:O	2.16	0.45
4:1:211:G:H1'	4:1:233:U:O4	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LX:78:LYS:NZ	7:LX:101:ASP:N	2.64	0.45
8:A:183:LEU:HD21	13:B:77:LEU:HD12	1.97	0.45
13:B:148:ARG:HE	13:B:174:PHE:HE1	1.62	0.45
13:B:307:LYS:HD2	13:B:345:LEU:HD11	1.97	0.45
13:B:485:MET:SD	13:B:553:PHE:HB3	2.56	0.45
13:B:789:LEU:HD11	13:B:827:CYS:SG	2.56	0.45
1:8:86:U:H5'	1:8:87:G:OP1	2.16	0.45
3:D:79:ARG:HH21	4:1:2707:U:H5'	1.81	0.45
4:1:384:A:H2	5:LY:87:ARG:NH1	2.13	0.45
5:LY:112:ASP:H	5:LY:115:ARG:HB2	1.81	0.45
9:LU:64:GLU:O	9:LU:70:ILE:HG13	2.17	0.45
13:B:23:HIS:CG	13:B:23:HIS:O	2.69	0.45
13:B:176:LYS:HA	13:B:179:GLN:HG2	1.99	0.45
13:B:737:MET:HA	13:B:741:PHE:HD1	1.81	0.45
13:B:821:GLU:CD	13:B:824:ARG:HE	2.19	0.45
15:LE:178:PRO:HG2	15:LE:181:LEU:HD12	1.98	0.45
2:E:78:TRP:CD2	2:E:341:PRO:HB2	2.52	0.45
3:D:157:ASP:O	3:D:160:THR:OG1	2.33	0.45
4:1:481:G:H1	4:1:673:C:N4	2.12	0.45
4:1:684:G:H5''	15:LE:100:LYS:HE2	1.98	0.45
12:2:14:MET:HG2	12:2:31:TYR:CE2	2.47	0.45
12:2:100:GLU:HG3	13:B:221:CYS:O	2.16	0.45
13:B:708:LEU:HG	13:B:712:MET:CE	2.47	0.45
13:B:826:ASN:HA	13:B:829:LYS:HG2	1.97	0.45
2:E:89:PRO:HB2	2:E:91:TYR:HE2	1.81	0.45
4:1:244:G:H8	4:1:244:G:O5'	1.99	0.45
4:1:385:A:N3	4:1:387:G:H5''	2.31	0.45
4:1:685:C:N4	13:B:598:LYS:HE2	2.32	0.45
4:1:685:C:OP1	15:LE:101:ASN:ND2	2.41	0.45
4:1:3603:G:H2'	4:1:3604:A:N3	2.31	0.45
9:LU:100:LEU:HD21	9:LU:114:TYR:CE2	2.52	0.45
10:LR:38:ARG:O	10:LR:42:ARG:HG3	2.16	0.45
13:B:130:LEU:HD21	13:B:160:LEU:C	2.37	0.45
13:B:332:LEU:HD13	13:B:338:LYS:HD3	1.96	0.45
13:B:385:ASP:CG	13:B:417:ILE:HA	2.36	0.45
13:B:418:TYR:HB3	13:B:423:ASN:O	2.16	0.45
13:B:769:LYS:HE2	13:B:807:ALA:HB1	1.99	0.45
14:LC:109:ARG:HA	14:LC:109:ARG:NE	2.31	0.45
15:LE:146:PRO:HB3	15:LE:203:ILE:HD11	1.98	0.45
3:D:143:LEU:HD13	3:D:162:LEU:HD23	1.98	0.45
4:1:2373:C:H2'	4:1:2374:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:2387:G:H2'	4:1:2388:A:H8	1.81	0.45
8:A:110:ASP:O	8:A:122:VAL:HA	2.17	0.45
10:LR:7:GLN:H	10:LR:7:GLN:CD	2.20	0.45
10:LR:9:ARG:NH2	10:LR:10:LEU:HD22	2.32	0.45
14:LC:44:LEU:O	14:LC:44:LEU:HD12	2.16	0.45
2:E:189:PHE:HD1	2:E:344:TRP:CD2	2.35	0.45
3:D:154:LEU:CB	3:D:162:LEU:HD11	2.47	0.45
4:1:2374:A:H2'	4:1:2375:A:C8	2.52	0.45
4:1:2525:U:OP2	10:LR:38:ARG:HD2	2.17	0.45
7:LX:118:ASP:O	7:LX:119:ILE:HD13	2.17	0.45
10:LR:67:THR:OG1	10:LR:70:ARG:NH2	2.32	0.45
13:B:156:ILE:O	13:B:160:LEU:HG	2.17	0.45
13:B:159:HIS:ND1	13:B:539:VAL:HG11	2.31	0.45
13:B:186:ASP:OD2	13:B:188:GLU:N	2.49	0.45
13:B:588:SER:O	13:B:592:LEU:N	2.41	0.45
14:LC:36:ILE:HD11	14:LC:122:TYR:CE1	2.51	0.45
4:1:219:G:N7	14:LC:172:LYS:HD3	2.32	0.45
4:1:2385:U:O2'	10:LR:4:LEU:HD13	2.17	0.45
10:LR:38:ARG:HG3	10:LR:42:ARG:NH2	2.31	0.45
13:B:18:LEU:HD12	13:B:19:ARG:N	2.32	0.45
13:B:21:TYR:CE1	13:B:26:TYR:CE1	3.04	0.45
13:B:591:GLU:O	13:B:594:LYS:HB2	2.17	0.45
13:B:727:ASP:HA	13:B:730:ARG:HB2	1.98	0.45
2:E:270:ARG:HE	2:E:270:ARG:H	1.65	0.45
4:1:2375:A:H2'	4:1:2376:A:H8	1.82	0.45
5:LY:109:LEU:O	5:LY:111:LEU:HD22	2.17	0.45
13:B:270:PRO:CB	13:B:275:GLU:HB3	2.47	0.45
13:B:424:ILE:HD11	13:B:451:TYR:HB3	1.98	0.45
4:1:473:C:H2'	4:1:474:C:H6	1.82	0.45
7:LX:77:ILE:CD1	7:LX:98:PHE:HD2	2.29	0.45
7:LX:102:VAL:HA	7:LX:134:LYS:HE3	1.99	0.45
8:A:136:GLN:HG3	13:B:148:ARG:HH11	1.82	0.45
9:LU:101:ARG:O	9:LU:113:ARG:N	2.36	0.45
10:LR:9:ARG:HD2	10:LR:9:ARG:C	2.37	0.45
12:2:14:MET:SD	12:2:14:MET:N	2.89	0.45
13:B:56:LEU:HD12	13:B:64:GLU:OE1	2.17	0.45
13:B:181:SER:N	13:B:182:PRO:HD3	2.32	0.45
13:B:762:PRO:HG3	13:B:800:THR:HG22	1.98	0.45
15:LE:244:GLU:OE2	15:LE:248:ILE:HG12	2.17	0.45
4:1:482:G:H2'	4:1:485:C:C5	2.52	0.45
8:A:112:TYR:HB2	8:A:121:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LU:24:ASP:OD2	9:LU:111:GLU:HB3	2.17	0.45
13:B:496:LYS:NZ	13:B:564:ILE:HG13	2.32	0.45
14:LC:217:ILE:HD12	14:LC:221:PHE:CE1	2.52	0.45
15:LE:56:ARG:NH1	15:LE:57:TYR:HD1	2.13	0.45
15:LE:119:GLU:N	15:LE:119:GLU:OE1	2.50	0.45
4:1:2373:C:H2'	4:1:2374:A:C8	2.52	0.44
10:LR:60:ARG:HH21	10:LR:64:ARG:NE	2.15	0.44
12:2:5:ASN:HB3	12:2:7:ARG:HH12	1.81	0.44
12:2:19:LEU:CB	13:B:486:TRP:CH2	2.99	0.44
13:B:213:LEU:HB3	13:B:230:LYS:NZ	2.31	0.44
2:E:297:HIS:NE2	2:E:302:THR:HG21	2.32	0.44
4:1:517:C:N4	4:1:646:G:H4'	2.33	0.44
5:LY:86:GLN:HG2	5:LY:96:HIS:ND1	2.32	0.44
9:LU:27:HIS:HA	9:LU:30:GLU:OE1	2.17	0.44
10:LR:115:ILE:HB	10:LR:119:MET:CG	2.48	0.44
12:2:18:ASN:OD1	12:2:25:ASN:ND2	2.42	0.44
13:B:689:LEU:HD23	13:B:689:LEU:H	1.83	0.44
15:LE:261:ILE:HG23	15:LE:267:LEU:HG	1.98	0.44
1:8:75:G:H2'	1:8:76:C:C6	2.52	0.44
3:D:77:VAL:O	3:D:80:THR:HB	2.17	0.44
4:1:219:G:H2'	4:1:219:G:N3	2.31	0.44
4:1:387:G:O5'	5:LY:89:LYS:NZ	2.49	0.44
10:LR:28:GLU:OE1	10:LR:28:GLU:N	4.62	0.44
10:LR:35:ALA:HB1	10:LR:41:ILE:HD13	1.98	0.44
12:2:36:LEU:HD21	13:B:541:LEU:HB2	1.99	0.44
14:LC:5:ARG:NH2	14:LC:25:PRO:O	2.51	0.44
14:LC:342:ARG:HA	14:LC:345:ARG:CZ	2.47	0.44
2:E:78:TRP:CZ3	2:E:89:PRO:HG3	2.52	0.44
3:D:54:LYS:HZ2	3:D:61:GLN:HE22	1.64	0.44
8:A:215:MET:HE3	13:B:101:LYS:HB2	1.99	0.44
10:LR:45:ILE:CD1	10:LR:50:ILE:HB	2.47	0.44
13:B:105:ASN:HA	13:B:108:LYS:HE3	1.98	0.44
13:B:651:GLU:O	13:B:653:PRO:HD3	2.17	0.44
14:LC:167:ALA:HB1	14:LC:221:PHE:CD2	2.53	0.44
14:LC:186:SER:O	14:LC:203:GLN:HA	2.18	0.44
2:E:264:LYS:HD3	2:E:265:PRO:O	2.18	0.44
3:D:117:HIS:HB3	3:D:139:GLU:O	2.18	0.44
4:1:197:A:O5'	4:1:197:A:H8	1.99	0.44
5:LY:1:MET:HG3	5:LY:3:PHE:CZ	2.53	0.44
5:LY:26:ARG:HA	5:LY:29:ILE:HG22	1.98	0.44
5:LY:50:ARG:NH1	5:LY:110:LYS:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:28:MET:O	12:2:31:TYR:HB2	2.17	0.44
13:B:67:GLU:HA	13:B:70:ARG:NH2	2.31	0.44
13:B:334:LYS:HA	13:B:334:LYS:HD3	1.81	0.44
2:E:87:LEU:HB2	2:E:199:GLU:OE2	2.18	0.44
2:E:297:HIS:CG	2:E:298:LYS:N	2.86	0.44
2:E:326:ILE:HG22	2:E:328:PRO:HD3	2.00	0.44
4:1:382:G:H1'	4:1:386:A:H61	1.82	0.44
4:1:2901:G:C6	4:1:3599:A:C6	3.05	0.44
9:LU:25:CYS:O	9:LU:28:PRO:HD2	2.17	0.44
10:LR:123:LEU:HA	10:LR:123:LEU:HD23	1.76	0.44
13:B:186:ASP:CG	13:B:189:TYR:H	2.21	0.44
13:B:230:LYS:HE2	13:B:230:LYS:HA	2.00	0.44
13:B:423:ASN:CB	13:B:833:TYR:O	2.54	0.44
13:B:688:PHE:HA	13:B:691:MET:HB2	1.99	0.44
13:B:805:LEU:HD23	13:B:836:ALA:HB1	1.99	0.44
13:B:825:ALA:HB1	13:B:829:LYS:NZ	2.33	0.44
14:LC:214:ASP:HA	14:LC:217:ILE:HG22	1.99	0.44
2:E:146:ALA:HA	2:E:223:LEU:HD13	1.99	0.44
3:D:94:LYS:HB2	3:D:95:LEU:HD12	1.99	0.44
4:1:229:G:H2'	4:1:230:G:H8	1.83	0.44
4:1:229:G:H4'	5:LY:14:ASN:HB3	1.99	0.44
8:A:139:ALA:HB2	13:B:176:LYS:HZ3	1.82	0.44
8:A:198:ALA:HB2	8:A:213:LEU:HD21	1.99	0.44
10:LR:23:TRP:O	10:LR:50:ILE:HA	2.18	0.44
12:2:11:LEU:HA	12:2:14:MET:SD	2.58	0.44
12:2:28:MET:H	12:2:28:MET:CE	2.30	0.44
15:LE:131:LYS:O	15:LE:136:HIS:NE2	2.46	0.44
2:E:325:THR:O	2:E:326:ILE:HD13	2.18	0.44
3:D:94:LYS:HB3	8:A:75:LYS:HZ3	1.83	0.44
4:1:196:C:C4'	5:LY:125:SER:HB3	2.47	0.44
4:1:202:C:H2'	4:1:203:U:H6	1.82	0.44
4:1:516:C:O2	4:1:645:G:N1	2.36	0.44
4:1:2385:U:H2'	4:1:2386:U:C6	2.53	0.44
7:LX:55:ARG:HE	7:LX:56:ARG:N	2.06	0.44
7:LX:148:ASP:HA	7:LX:151:ASN:OD1	2.18	0.44
9:LU:23:LEU:HD13	9:LU:110:TYR:HB3	1.98	0.44
10:LR:45:ILE:HD12	10:LR:50:ILE:HB	1.99	0.44
10:LR:81:ARG:O	10:LR:81:ARG:HD2	2.17	0.44
10:LR:151:ARG:HH12	10:LR:154:LEU:HD22	1.83	0.44
13:B:141:LEU:HD12	13:B:145:PRO:HA	2.00	0.44
13:B:195:TYR:HA	13:B:536:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:256:GLU:OE2	13:B:287:TYR:HE2	2.00	0.44
13:B:453:LEU:HB3	13:B:490:GLU:HB3	2.00	0.44
13:B:581:GLU:CG	13:B:582:ALA:H	2.31	0.44
13:B:581:GLU:HG3	13:B:582:ALA:H	1.83	0.44
3:D:154:LEU:O	3:D:159:LEU:HG	2.17	0.44
4:1:3603:G:H2'	4:1:3604:A:C2	2.53	0.44
7:LX:139:ARG:HH11	7:LX:140:LEU:H	1.66	0.44
13:B:452:MET:HE2	13:B:452:MET:HB3	1.79	0.44
13:B:691:MET:HG3	13:B:715:LEU:HD23	1.99	0.44
13:B:754:LEU:HB3	13:B:755:LYS:HZ2	1.82	0.44
2:E:163:THR:HA	2:E:166:ILE:HD12	1.99	0.43
3:D:87:LYS:NZ	10:LR:30:ASN:CB	2.71	0.43
5:LY:10:ASP:OD2	5:LY:13:LYS:HD2	2.17	0.43
13:B:312:LYS:HB3	13:B:312:LYS:HE3	1.78	0.43
13:B:416:LYS:HD2	13:B:420:HIS:NE2	2.33	0.43
13:B:430:TRP:CD1	13:B:431:MET:HE1	2.53	0.43
14:LC:31:PRO:HG3	14:LC:282:HIS:ND1	2.33	0.43
14:LC:32:ILE:HD12	14:LC:32:ILE:O	2.18	0.43
4:1:385:A:H4'	4:1:386:A:OP1	2.17	0.43
4:1:460:C:H2'	4:1:461:G:C8	2.53	0.43
12:2:112:ARG:HD3	12:2:113:LYS:H	1.81	0.43
13:B:239:ARG:NE	13:B:242:ASP:OD2	2.51	0.43
3:D:78:HIS:CE1	4:1:2707:U:C5	3.06	0.43
4:1:223:G:H4'	4:1:225:G:N7	2.33	0.43
4:1:389:A:C1'	5:LY:91:ASN:HA	2.47	0.43
5:LY:2:LYS:NZ	5:LY:4:ASN:HB3	2.33	0.43
12:2:7:ARG:O	12:2:10:ASP:N	2.41	0.43
13:B:265:GLU:HA	13:B:279:ILE:HD13	2.00	0.43
13:B:510:GLU:HG2	13:B:513:ARG:NH2	2.34	0.43
13:B:542:LEU:HA	13:B:545:GLU:OE1	2.18	0.43
13:B:751:GLU:O	13:B:755:LYS:HG2	2.18	0.43
13:B:798:LEU:HD23	13:B:798:LEU:H	1.83	0.43
2:E:84:THR:HG21	2:E:349:ARG:HA	1.99	0.43
3:D:84:ASP:O	3:D:88:LEU:HD23	2.18	0.43
4:1:479:G:H2'	4:1:480:C:C6	2.53	0.43
4:1:496:G:N1	4:1:658:C:O2	2.49	0.43
5:LY:82:ILE:CG2	5:LY:83:GLU:N	2.82	0.43
12:2:106:TYR:HA	12:2:151:LEU:HG	1.99	0.43
13:B:54:LEU:HD11	13:B:88:LEU:HD11	2.00	0.43
13:B:422:GLY:C	13:B:834:ALA:HA	2.37	0.43
13:B:458:ILE:HD12	13:B:495:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:488:GLN:HB3	13:B:511:ILE:HD11	2.00	0.43
13:B:654:LEU:O	13:B:658:ILE:HG12	2.18	0.43
13:B:750:ASN:ND2	13:B:771:VAL:HG23	2.34	0.43
14:LC:279:LEU:HD23	14:LC:279:LEU:HA	1.89	0.43
3:D:108:MET:O	3:D:115:VAL:HG13	2.19	0.43
4:1:3597:G:H2'	4:1:3598:C:O4'	2.18	0.43
8:A:214:THR:HG21	13:B:105:ASN:ND2	2.28	0.43
12:2:19:LEU:HA	13:B:442:ARG:NH2	2.33	0.43
13:B:430:TRP:HB3	13:B:431:MET:CE	2.49	0.43
13:B:569:HIS:ND1	13:B:654:LEU:HG	2.33	0.43
7:LX:94:ASN:ND2	7:LX:145:ASP:HA	2.07	0.43
12:2:48:GLU:O	12:2:48:GLU:HG2	2.18	0.43
12:2:159:ARG:NE	12:2:163:GLU:OE1	2.52	0.43
13:B:390:PRO:CB	13:B:832:PRO:HD2	2.46	0.43
13:B:733:LEU:O	13:B:737:MET:SD	2.76	0.43
13:B:828:HIS:CE1	13:B:832:PRO:O	2.72	0.43
15:LE:96:VAL:HB	15:LE:105:ARG:HG2	2.00	0.43
3:D:124:GLN:N	3:D:133:THR:O	2.41	0.43
4:1:215:C:H2'	4:1:220:C:H5'	2.01	0.43
4:1:467:U:O2	13:B:605:LYS:HE2	2.19	0.43
4:1:677:G:H2'	4:1:678:C:H6	1.83	0.43
9:LU:43:LEU:H	9:LU:43:LEU:HG	1.70	0.43
10:LR:8:LYS:HG3	10:LR:9:ARG:N	2.34	0.43
12:2:18:ASN:HA	12:2:21:CYS:SG	2.59	0.43
14:LC:108:TRP:CE3	14:LC:108:TRP:O	2.71	0.43
15:LE:281:ILE:HD12	15:LE:281:ILE:O	2.19	0.43
3:D:151:LEU:CD1	3:D:162:LEU:HD13	2.38	0.43
5:LY:36:LYS:O	5:LY:40:GLN:HG3	2.18	0.43
5:LY:54:GLU:HG2	5:LY:108:ARG:NE	2.34	0.43
13:B:317:ASN:O	13:B:321:GLY:N	2.50	0.43
13:B:418:TYR:O	13:B:423:ASN:N	2.35	0.43
4:1:460:C:H2'	4:1:461:G:H8	1.83	0.43
8:A:177:GLU:HG3	8:A:180:ASP:H	1.83	0.43
9:LU:19:LEU:HB2	9:LU:21:PHE:HE1	1.84	0.43
10:LR:24:LEU:H	10:LR:24:LEU:HD23	1.84	0.43
13:B:52:LYS:O	13:B:56:LEU:HG	2.19	0.43
1:8:75:G:OP2	5:LY:74:TYR:OH	2.24	0.43
2:E:339:THR:HG21	3:D:137:HIS:NE2	2.33	0.43
4:1:644:G:C2	4:1:645:G:H1'	2.54	0.43
4:1:2898:G:H2'	4:1:2899:C:H6	1.82	0.43
5:LY:81:TYR:C	5:LY:82:ILE:HD12	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LY:85:VAL:HG22	5:LY:97:VAL:HB	2.00	0.43
9:LU:60:VAL:HG13	9:LU:61:VAL:H	1.84	0.43
9:LU:76:VAL:HG23	9:LU:77:PRO:HD2	2.01	0.43
10:LR:6:LEU:HD12	10:LR:9:ARG:NH2	2.33	0.43
10:LR:30:ASN:HD22	10:LR:31:GLU:N	2.14	0.43
13:B:144:ARG:HA	13:B:144:ARG:HH11	1.84	0.43
13:B:825:ALA:HB1	13:B:829:LYS:HZ2	1.83	0.43
2:E:378:ALA:O	2:E:379:ARG:NH1	2.51	0.42
4:1:698:G:H2'	4:1:699:C:C6	2.53	0.42
4:1:2380:G:OP2	4:1:2380:G:H8	2.01	0.42
13:B:459:LYS:HE3	13:B:459:LYS:HB3	1.74	0.42
13:B:509:HIS:O	13:B:513:ARG:HG3	2.19	0.42
3:D:151:LEU:HD22	3:D:151:LEU:N	2.34	0.42
4:1:197:A:H2'	4:1:198:A:C8	2.54	0.42
4:1:239:C:H2'	4:1:240:G:C8	2.54	0.42
13:B:580:HIS:O	13:B:581:GLU:C	2.57	0.42
13:B:693:GLN:O	13:B:696:LYS:HE3	2.19	0.42
2:E:196:SER:HB2	2:E:218:ASN:HB3	2.02	0.42
4:1:387:G:C8	4:1:412:G:C6	3.06	0.42
4:1:390:C:H2'	4:1:391:U:C6	2.53	0.42
4:1:499:G:HO2'	4:1:504:G:H1	1.67	0.42
5:LY:100:HIS:CD2	5:LY:102:SER:HB3	2.54	0.42
7:LX:118:ASP:C	7:LX:119:ILE:HD13	2.40	0.42
7:LX:120:ASP:HB3	7:LX:141:ALA:HB2	2.01	0.42
8:A:91:VAL:HG12	8:A:109:PRO:HG2	2.00	0.42
8:A:210:ILE:O	8:A:214:THR:OG1	2.31	0.42
10:LR:10:LEU:O	10:LR:14:VAL:HG22	2.19	0.42
12:2:36:LEU:HD21	13:B:541:LEU:HD22	2.01	0.42
12:2:84:LEU:HD21	13:B:322:CYS:HB2	2.00	0.42
13:B:175:ARG:NH2	13:B:176:LYS:HB2	2.33	0.42
13:B:272:ASN:OD1	13:B:274:LEU:HG	2.19	0.42
13:B:423:ASN:N	13:B:833:TYR:O	2.52	0.42
13:B:430:TRP:O	13:B:433:GLU:HB2	2.19	0.42
14:LC:259:LYS:HA	14:LC:262:GLU:CD	2.40	0.42
1:8:82:A:H5'	1:8:82:A:C8	2.51	0.42
3:D:72:ARG:HH21	3:D:74:LYS:N	2.17	0.42
3:D:78:HIS:CG	3:D:79:ARG:H	2.37	0.42
4:1:2385:U:H4'	10:LR:5:ARG:NH2	2.35	0.42
9:LU:101:ARG:N	9:LU:113:ARG:O	2.53	0.42
12:2:26:TYR:O	13:B:482:MET:SD	2.77	0.42
13:B:469:THR:HG21	13:B:475:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:483:GLN:HG2	13:B:514:HIS:CG	2.54	0.42
13:B:484:CYS:SG	13:B:487:PHE:CD2	3.12	0.42
13:B:559:ARG:O	13:B:563:GLU:HG2	2.20	0.42
13:B:631:ASP:OD1	13:B:631:ASP:C	2.58	0.42
14:LC:67:TRP:CE3	14:LC:71:ARG:HD3	2.53	0.42
15:LE:167:GLN:HE21	15:LE:171:GLY:HA2	1.84	0.42
1:8:45:C:H2'	1:8:46:G:H8	1.84	0.42
4:1:220:C:H2'	4:1:221:C:H6	1.83	0.42
4:1:2703:G:C6	4:1:2714:G:C6	3.07	0.42
5:LY:37:GLU:OE1	5:LY:41:LYS:HD2	2.19	0.42
10:LR:104:ARG:HH12	10:LR:108:ARG:CB	2.27	0.42
13:B:154:TYR:CZ	13:B:158:TYR:CE2	3.07	0.42
13:B:581:GLU:OE1	13:B:584:THR:HG23	2.19	0.42
13:B:798:LEU:HD12	13:B:802:MET:CE	2.50	0.42
15:LE:67:ALA:HB1	15:LE:70:LYS:HE2	2.01	0.42
1:8:70:G:C2	1:8:87:G:N3	2.88	0.42
2:E:93:LEU:HD21	2:E:207:ASP:HB2	2.01	0.42
2:E:220:ASP:HA	2:E:233:ASN:HB3	2.00	0.42
3:D:121:PRO:HB3	3:D:136:GLY:HA3	2.01	0.42
4:1:659:G:H3'	4:1:660:A:H8	1.85	0.42
8:A:76:ALA:O	8:A:80:MET:HG2	2.18	0.42
8:A:183:LEU:O	8:A:187:GLN:HG3	2.19	0.42
13:B:56:LEU:HD12	13:B:64:GLU:CD	2.39	0.42
13:B:164:TYR:CE1	13:B:202:GLU:HB2	2.54	0.42
13:B:591:GLU:HA	13:B:594:LYS:HG3	2.01	0.42
13:B:612:LYS:HG3	13:B:613:LYS:HD3	2.02	0.42
13:B:706:PRO:HG2	13:B:762:PRO:HB2	2.01	0.42
13:B:808:LEU:HD12	13:B:808:LEU:HA	1.85	0.42
14:LC:51:PRO:HB3	14:LC:111:TRP:HE1	1.84	0.42
3:D:147:LEU:HD13	3:D:151:LEU:HD21	2.02	0.42
7:LX:105:ASN:OD1	7:LX:108:GLN:HG2	2.20	0.42
12:2:14:MET:HA	12:2:17:CYS:HB3	2.01	0.42
13:B:21:TYR:CZ	13:B:54:LEU:HD23	2.55	0.42
13:B:33:CYS:HA	13:B:36:ILE:HG12	2.02	0.42
13:B:732:VAL:O	13:B:736:GLU:HG2	2.20	0.42
4:1:381:U:H2'	4:1:382:G:O4'	2.20	0.42
4:1:385:A:HO2'	4:1:387:G:H8	1.64	0.42
4:1:469:C:O2	15:LE:105:ARG:NE	2.51	0.42
5:LY:100:HIS:ND1	5:LY:101:PRO:HD2	2.35	0.42
7:LX:109:ILE:O	7:LX:113:VAL:HG13	2.19	0.42
9:LU:19:LEU:CD1	9:LU:74:SER:HB3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LR:123:LEU:O	10:LR:127:VAL:HG22	2.20	0.42
12:2:38:TRP:NE1	12:2:60:MET:HG2	2.35	0.42
12:2:91:MET:HG3	12:2:126:LEU:HD13	2.02	0.42
13:B:144:ARG:NH2	13:B:147:GLN:HG3	2.35	0.42
13:B:192:LEU:HB2	13:B:533:ILE:CG2	2.50	0.42
13:B:198:GLN:HA	13:B:201:ARG:HG2	2.02	0.42
13:B:584:THR:O	13:B:585:ALA:C	2.57	0.42
13:B:640:GLU:OE1	13:B:640:GLU:N	2.53	0.42
14:LC:340:ILE:HD12	15:LE:50:LEU:CD1	2.47	0.42
15:LE:153:LEU:HD13	15:LE:193:PHE:O	2.20	0.42
1:8:82:A:H4'	1:8:83:C:OP1	2.20	0.42
2:E:77:PRO:HG2	2:E:78:TRP:CE2	2.55	0.42
2:E:172:LEU:HD12	2:E:173:ALA:N	2.35	0.42
3:D:62:VAL:HG11	9:LU:115:PHE:CE1	2.54	0.42
3:D:106:VAL:O	3:D:118:PHE:N	2.41	0.42
4:1:238:C:O2	5:LY:102:SER:OG	2.30	0.42
4:1:518:G:H1'	4:1:644:G:C2	2.55	0.42
7:LX:129:ARG:CD	7:LX:130:PRO:HD2	2.49	0.42
7:LX:139:ARG:HH11	7:LX:140:LEU:N	2.16	0.42
8:A:108:LYS:HD2	8:A:108:LYS:O	2.19	0.42
8:A:136:GLN:HG3	13:B:148:ARG:NH1	2.35	0.42
9:LU:44:GLN:OE1	9:LU:63:ILE:HD11	2.20	0.42
10:LR:78:ILE:HG13	10:LR:79:GLY:N	2.34	0.42
12:2:52:ILE:HD11	12:2:55:TYR:HB3	2.02	0.42
13:B:113:ASN:HB3	13:B:116:ILE:HD12	2.02	0.42
13:B:579:GLU:O	13:B:580:HIS:C	2.58	0.42
13:B:672:ILE:HD11	13:B:698:ALA:HB1	2.02	0.42
1:8:73:U:OP1	5:LY:75:ARG:HD2	2.19	0.42
3:D:72:ARG:NH1	3:D:75:LYS:HD3	2.35	0.42
3:D:75:LYS:HZ3	9:LU:117:ILE:HG22	1.84	0.42
3:D:137:HIS:HD1	3:D:138:ALA:N	2.17	0.42
4:1:217:C:H3'	4:1:218:A:C5'	2.50	0.42
5:LY:30:MET:HE1	5:LY:75:ARG:HG2	2.02	0.42
12:2:28:MET:HG2	12:2:32:PHE:HE1	1.84	0.42
13:B:103:TYR:HB3	13:B:116:ILE:HG23	2.02	0.42
14:LC:116:ASN:HB2	14:LC:119:GLN:HG3	2.01	0.42
15:LE:150:LEU:HD23	15:LE:150:LEU:HA	1.80	0.42
4:1:2528:G:C5	4:1:2529:A:C6	3.08	0.41
7:LX:87:MET:HA	7:LX:90:ILE:CD1	2.49	0.41
7:LX:114:LYS:HB3	7:LX:114:LYS:NZ	2.34	0.41
12:2:107:VAL:O	12:2:148:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:147:MET:N	12:2:147:MET:SD	2.93	0.41
15:LE:57:TYR:HB2	15:LE:62:MET:SD	2.60	0.41
2:E:304:PRO:O	2:E:306:VAL:HG23	2.20	0.41
3:D:108:MET:SD	3:D:109:PHE:N	2.93	0.41
4:1:2520:C:H2'	4:1:2521:G:H8	1.86	0.41
4:1:2523:G:N2	4:1:2533:C:C2	2.88	0.41
12:2:112:ARG:HD3	12:2:114:SER:H	1.85	0.41
13:B:21:TYR:CZ	13:B:55:THR:HA	2.54	0.41
13:B:78:LYS:HA	13:B:109:TRP:CE2	2.55	0.41
13:B:210:LEU:HA	13:B:230:LYS:NZ	2.35	0.41
14:LC:85:HIS:CE1	14:LC:86:ARG:HE	2.37	0.41
14:LC:294:LYS:HA	14:LC:299:GLN:NE2	2.32	0.41
2:E:245:ALA:HB2	2:E:353:ARG:NH1	2.35	0.41
10:LR:116:ASP:OD1	10:LR:117:ARG:N	2.52	0.41
12:2:89:LYS:HA	12:2:92:ASP:OD2	2.19	0.41
14:LC:230:LEU:HD21	14:LC:239:LYS:HD2	2.01	0.41
1:8:90:C:H2'	1:8:91:A:H8	1.84	0.41
4:1:478:G:C6	4:1:677:G:C6	3.08	0.41
9:LU:83:LEU:HA	9:LU:86:LEU:HG	2.01	0.41
12:2:111:VAL:HG22	12:2:112:ARG:O	2.20	0.41
13:B:297:PRO:HA	13:B:300:PHE:CZ	2.54	0.41
13:B:456:ASN:HB3	13:B:498:MET:CE	2.51	0.41
13:B:550:GLN:CG	13:B:667:LEU:HD23	2.41	0.41
13:B:828:HIS:CE1	13:B:832:PRO:HA	2.54	0.41
14:LC:358:ALA:O	14:LC:361:LEU:HG	2.20	0.41
4:1:394:G:N2	4:1:396:A:H3'	2.35	0.41
4:1:475:G:H2'	4:1:476:G:C8	2.56	0.41
4:1:676:C:H2'	4:1:677:G:H8	1.85	0.41
7:LX:77:ILE:HD12	7:LX:78:LYS:N	2.35	0.41
12:2:32:PHE:HZ	13:B:518:ILE:HG23	1.84	0.41
12:2:132:GLU:N	12:2:146:ALA:HB3	2.32	0.41
13:B:66:TYR:O	13:B:69:VAL:HG12	2.20	0.41
13:B:122:LEU:O	13:B:125:ILE:HG13	2.20	0.41
13:B:256:GLU:OE2	13:B:287:TYR:CE2	2.74	0.41
13:B:470:ARG:HD3	13:B:478:ASN:OD1	2.20	0.41
15:LE:67:ALA:HA	15:LE:69:TYR:CE2	2.55	0.41
3:D:133:THR:OG1	8:A:121:ILE:HG22	2.20	0.41
4:1:206:U:N3	4:1:209:U:OP2	2.30	0.41
4:1:209:U:OP1	5:LY:63:LYS:HE3	2.21	0.41
4:1:475:G:H2'	4:1:476:G:H8	1.86	0.41
4:1:2520:C:H2'	4:1:2521:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LY:54:GLU:O	5:LY:107:THR:N	2.43	0.41
5:LY:81:TYR:HD1	5:LY:96:HIS:CB	2.29	0.41
13:B:416:LYS:NZ	17:B:901:IHP:O25	2.52	0.41
13:B:505:LEU:CB	13:B:647:LEU:HG	2.49	0.41
14:LC:311:ARG:NE	14:LC:311:ARG:HA	2.35	0.41
15:LE:202:ASP:OD1	15:LE:204:SER:OG	2.24	0.41
4:1:198:A:N7	5:LY:45:ARG:NH1	2.68	0.41
4:1:685:C:O5'	4:1:685:C:H6	2.03	0.41
7:LX:115:LYS:HE3	7:LX:115:LYS:CA	2.44	0.41
13:B:621:GLN:C	13:B:625:LYS:HZ2	2.23	0.41
13:B:665:LYS:HA	13:B:669:LYS:NZ	2.36	0.41
15:LE:54:ILE:HD13	15:LE:54:ILE:HA	1.93	0.41
15:LE:147:GLY:HA3	15:LE:201:ILE:O	2.21	0.41
15:LE:261:ILE:HA	15:LE:267:LEU:HD23	2.03	0.41
3:D:103:ILE:HD12	3:D:123:VAL:HG12	2.02	0.41
3:D:106:VAL:HG13	8:A:95:THR:O	2.21	0.41
4:1:2385:U:H4'	10:LR:5:ARG:HH22	1.86	0.41
9:LU:50:ASN:O	9:LU:52:LYS:NZ	2.53	0.41
12:2:96:ARG:HE	13:B:224:LEU:CD2	2.33	0.41
13:B:383:HIS:O	13:B:387:ILE:HG12	2.21	0.41
13:B:453:LEU:HD23	13:B:453:LEU:HA	1.82	0.41
14:LC:180:ILE:HG22	14:LC:184:TYR:CD2	2.55	0.41
1:8:47:C:H1'	1:8:61:A:H2'	2.02	0.41
2:E:246:ARG:HD2	2:E:246:ARG:HA	1.74	0.41
4:1:224:U:OP1	14:LC:163:LYS:NZ	2.50	0.41
4:1:393:U:H2'	4:1:394:G:C8	2.56	0.41
4:1:680:G:H2'	4:1:681:G:H8	1.86	0.41
8:A:177:GLU:CG	8:A:180:ASP:HB2	2.47	0.41
12:2:32:PHE:HB2	13:B:525:PHE:CE2	2.56	0.41
12:2:96:ARG:HD2	13:B:253:ARG:HG2	2.03	0.41
12:2:153:GLN:HG2	12:2:154:MET:N	2.36	0.41
13:B:103:TYR:HB3	13:B:116:ILE:CG2	2.51	0.41
13:B:195:TYR:CD1	13:B:535:LEU:HG	2.56	0.41
13:B:554:TYR:OH	13:B:663:PRO:HG2	2.21	0.41
13:B:616:GLU:HA	13:B:619:LYS:HG3	2.02	0.41
13:B:696:LYS:HE3	13:B:696:LYS:HB3	1.89	0.41
15:LE:136:HIS:HB2	15:LE:138:ARG:NH1	2.35	0.41
2:E:220:ASP:HA	2:E:233:ASN:CB	2.51	0.41
4:1:2386:U:H2'	4:1:2387:G:C8	2.56	0.41
4:1:2708:U:H4'	4:1:2709:C:OP1	2.21	0.41
5:LY:113:LYS:HA	5:LY:116:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LX:120:ASP:HB3	7:LX:141:ALA:CB	2.51	0.41
7:LX:140:LEU:H	7:LX:140:LEU:HD12	1.86	0.41
8:A:91:VAL:HG11	8:A:111:VAL:HG23	2.03	0.41
12:2:154:MET:HA	12:2:157:GLU:OE2	2.20	0.41
13:B:723:LYS:HD3	13:B:723:LYS:H	1.86	0.41
14:LC:348:LYS:O	14:LC:351:VAL:HG22	2.20	0.41
1:8:49:G:H2'	1:8:50:C:C6	2.56	0.40
3:D:155:GLY:HA2	3:D:159:LEU:HG	2.03	0.40
10:LR:28:GLU:O	10:LR:32:ILE:HG13	2.21	0.40
10:LR:145:LEU:HA	10:LR:148:ASP:OD1	2.20	0.40
12:2:36:LEU:HD21	13:B:541:LEU:CB	2.51	0.40
13:B:27:ARG:O	13:B:30:LEU:HG	2.21	0.40
13:B:225:ALA:HA	13:B:228:GLU:HG3	2.03	0.40
13:B:337:GLU:OE2	13:B:338:LYS:HG3	2.21	0.40
13:B:435:GLN:HG3	13:B:445:ASN:HA	2.02	0.40
13:B:645:GLU:O	13:B:649:LYS:HG2	2.20	0.40
14:LC:172:LYS:HG3	14:LC:177:TRP:CD1	2.57	0.40
14:LC:205:ARG:CD	14:LC:242:PRO:HB3	2.51	0.40
4:1:207:G:OP2	13:B:31:LYS:NZ	2.49	0.40
7:LX:124:VAL:HA	7:LX:137:TYR:O	2.21	0.40
13:B:541:LEU:HD12	13:B:544:LEU:HD23	2.02	0.40
14:LC:125:CYS:O	14:LC:128:LEU:HG	2.22	0.40
14:LC:211:TYR:H	14:LC:211:TYR:HD2	1.69	0.40
1:8:70:G:N2	1:8:87:G:H1'	2.37	0.40
1:8:81:C:O2'	1:8:84:A:N1	2.55	0.40
4:1:221:C:H2'	4:1:222:C:H6	1.86	0.40
4:1:383:A:H2'	4:1:384:A:C8	2.56	0.40
4:1:457:G:H5''	4:1:457:G:H8	1.85	0.40
4:1:2386:U:H2'	4:1:2387:G:H8	1.86	0.40
5:LY:85:VAL:O	5:LY:85:VAL:HG13	2.21	0.40
8:A:86:ARG:NH1	8:A:115:PRO:HA	2.36	0.40
13:B:416:LYS:HD3	13:B:416:LYS:HA	1.65	0.40
13:B:417:ILE:HG22	13:B:833:TYR:CE2	2.55	0.40
13:B:781:ARG:O	13:B:785:LEU:HG	2.21	0.40
14:LC:64:ALA:HB1	14:LC:78:ARG:C	2.41	0.40
14:LC:150:LEU:HB3	14:LC:151:PRO:HD3	2.04	0.40
14:LC:298:ILE:HD12	14:LC:298:ILE:N	2.36	0.40
4:1:481:G:C6	4:1:674:G:C6	3.10	0.40
4:1:513:U:H5''	4:1:514:U:H4'	2.02	0.40
5:LY:84:ARG:CZ	5:LY:86:GLN:OE1	2.69	0.40
9:LU:21:PHE:HD1	9:LU:21:PHE:N	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LU:21:PHE:N	9:LU:21:PHE:CD1	2.89	0.40
12:2:19:LEU:HD22	13:B:484:CYS:SG	2.61	0.40
13:B:188:GLU:HG2	13:B:532:LYS:O	2.22	0.40
13:B:292:VAL:HB	13:B:293:PRO:HD3	2.03	0.40
13:B:328:THR:OG1	13:B:329:LEU:HD22	2.22	0.40
13:B:760:SER:O	13:B:764:ARG:HG3	2.22	0.40
15:LE:109:LEU:HD13	15:LE:109:LEU:HA	1.97	0.40
15:LE:243:THR:OG1	15:LE:246:ARG:HG2	2.21	0.40
4:1:2700:G:H2'	4:1:2701:U:O4'	2.22	0.40
13:B:21:TYR:CE2	13:B:55:THR:HA	2.55	0.40
13:B:159:HIS:CG	13:B:195:TYR:HH	2.34	0.40
13:B:245:ASP:HA	13:B:248:ARG:HG2	2.03	0.40
13:B:456:ASN:HB3	13:B:498:MET:HE1	2.03	0.40
13:B:456:ASN:HA	13:B:494:ALA:HB1	2.03	0.40
13:B:625:LYS:O	13:B:628:LYS:HB2	2.22	0.40
15:LE:96:VAL:HG11	15:LE:101:ASN:HB3	2.03	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	
2	E	315/392 (80%)	301 (96%)	13 (4%)	1 (0%)	41	76
3	D	120/206 (58%)	104 (87%)	12 (10%)	4 (3%)	4	29
5	LY	127/145 (88%)	121 (95%)	6 (5%)	0	100	100
6	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
7	LX	114/156 (73%)	112 (98%)	2 (2%)	0	100	100
8	A	121/221 (55%)	116 (96%)	3 (2%)	2 (2%)	9	43
9	LU	99/128 (77%)	94 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	LR	151/196 (77%)	150 (99%)	1 (1%)	0	100	100
11	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
12	2	167/171 (98%)	161 (96%)	5 (3%)	1 (1%)	25	65
13	B	832/840 (99%)	779 (94%)	43 (5%)	10 (1%)	13	50
14	LC	363/427 (85%)	346 (95%)	17 (5%)	0	100	100
15	LE	208/288 (72%)	195 (94%)	13 (6%)	0	100	100
16	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
All	All	2927/3500 (84%)	2778 (95%)	131 (4%)	18 (1%)	29	65

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	A	132	SER
13	B	579	GLU
2	E	297	HIS
3	D	84	ASP
3	D	97	VAL
8	A	131	LEU
13	B	581	GLU
13	B	582	ALA
13	B	584	THR
13	B	586	ASN
3	D	94	LYS
13	B	292	VAL
3	D	49	ILE
13	B	585	ALA
12	2	8	PRO
13	B	573	LEU
13	B	590	LYS
13	B	637	GLY

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	
2	E	271/333 (81%)	260 (96%)	11 (4%)	30	56
3	D	102/165 (62%)	99 (97%)	3 (3%)	42	64
5	LY	120/135 (89%)	110 (92%)	10 (8%)	11	36
6	Lh	109/110 (99%)	100 (92%)	9 (8%)	11	36
7	LX	104/133 (78%)	97 (93%)	7 (7%)	16	43
8	A	107/186 (58%)	101 (94%)	6 (6%)	21	48
9	LU	91/115 (79%)	81 (89%)	10 (11%)	6	25
10	LR	137/175 (78%)	123 (90%)	14 (10%)	7	27
11	Lk	64/65 (98%)	63 (98%)	1 (2%)	62	79
12	2	148/149 (99%)	131 (88%)	17 (12%)	5	23
13	B	744/749 (99%)	692 (93%)	52 (7%)	15	41
14	LC	304/348 (87%)	291 (96%)	13 (4%)	29	55
15	LE	190/252 (75%)	180 (95%)	10 (5%)	22	49
16	Lr	109/121 (90%)	104 (95%)	5 (5%)	27	53
All	All	2600/3036 (86%)	2432 (94%)	168 (6%)	21	44

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	94	MET
2	E	158	LYS
2	E	168	HIS
2	E	253	TYR
2	E	270	ARG
2	E	274	ASN
2	E	300	PHE
2	E	313	LYS
2	E	329	MET
2	E	349	ARG
2	E	365	ASP
3	D	51	ASN
3	D	90	PHE
3	D	95	LEU
5	LY	11	ARG
5	LY	12	SER
5	LY	19	PHE
5	LY	35	SER
5	LY	42	TYR

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Mol	Chain	Res	Type
5	LY	69	LYS
5	LY	74	TYR
5	LY	84	ARG
5	LY	116	LYS
5	LY	125	SER
6	Lh	14	LYS
6	Lh	20	GLN
6	Lh	22	ASP
6	Lh	23	ASP
6	Lh	28	LEU
6	Lh	43	LYS
6	Lh	74	LYS
6	Lh	91	MET
6	Lh	118	LYS
7	LX	55	ARG
7	LX	67	ARG
7	LX	73	HIS
7	LX	100	VAL
7	LX	101	ASP
7	LX	116	LEU
7	LX	135	LYS
8	A	108	LYS
8	A	120	TYR
8	A	142	LYS
8	A	146	GLN
8	A	148	GLU
8	A	201	ASN
9	LU	19	LEU
9	LU	21	PHE
9	LU	27	HIS
9	LU	30	GLU
9	LU	50	ASN
9	LU	52	LYS
9	LU	79	SER
9	LU	95	ASN
9	LU	96	LEU
9	LU	110	TYR
10	LR	30	ASN
10	LR	34	ASN
10	LR	40	GLN
10	LR	52	ARG
10	LR	76	MET

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Mol	Chain	Res	Type
10	LR	89	MET
10	LR	96	MET
10	LR	97	ARG
10	LR	116	ASP
10	LR	139	MET
10	LR	141	HIS
10	LR	144	LYS
10	LR	152	LYS
10	LR	153	LYS
11	Lk	31	ASN
12	2	4	ARG
12	2	11	LEU
12	2	14	MET
12	2	17	CYS
12	2	26	TYR
12	2	30	TYR
12	2	33	TYR
12	2	91	MET
12	2	93	GLN
12	2	103	ASN
12	2	105	LYS
12	2	122	TYR
12	2	149	ARG
12	2	154	MET
12	2	160	ARG
12	2	165	LYS
12	2	167	LYS
13	B	9	LYS
13	B	21	TYR
13	B	33	CYS
13	B	78	LYS
13	B	86	TYR
13	B	88	LEU
13	B	91	ARG
13	B	94	LYS
13	B	166	MET
13	B	169	LYS
13	B	175	ARG
13	B	176	LYS
13	B	184	LYS
13	B	216	TYR
13	B	218	LYS

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Mol	Chain	Res	Type
13	B	232	GLU
13	B	262	LYS
13	B	274	LEU
13	B	282	GLU
13	B	286	LYS
13	B	379	TYR
13	B	395	GLU
13	B	447	LYS
13	B	451	TYR
13	B	452	MET
13	B	459	LYS
13	B	464	MET
13	B	482	MET
13	B	498	MET
13	B	530	MET
13	B	538	TYR
13	B	575	ASP
13	B	587	MET
13	B	591	GLU
13	B	592	LEU
13	B	604	LYS
13	B	610	GLU
13	B	619	LYS
13	B	626	LYS
13	B	630	ASP
13	B	631	ASP
13	B	634	GLU
13	B	646	LYS
13	B	647	LEU
13	B	661	LEU
13	B	683	PHE
13	B	696	LYS
13	B	697	ARG
13	B	699	PHE
13	B	723	LYS
13	B	810	ASP
13	B	829	LYS
14	LC	14	LYS
14	LC	52	TYR
14	LC	71	ARG
14	LC	109	ARG
14	LC	181	LYS

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Mol	Chain	Res	Type
14	LC	189	MET
14	LC	211	TYR
14	LC	250	CYS
14	LC	257	PHE
14	LC	274	LYS
14	LC	312	ARG
14	LC	313	VAL
14	LC	325	MET
15	LE	110	ARG
15	LE	116	TYR
15	LE	154	THR
15	LE	220	LYS
15	LE	240	TYR
15	LE	245	GLN
15	LE	254	ASP
15	LE	270	TYR
15	LE	279	ASN
15	LE	282	TYR
16	Lr	21	ASN
16	Lr	52	GLU
16	Lr	72	LYS
16	Lr	101	LYS
16	Lr	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	90	HIS
2	E	274	ASN
3	D	61	GLN
5	LY	40	GLN
5	LY	61	HIS
5	LY	96	HIS
5	LY	100	HIS
7	LX	93	ASN
7	LX	94	ASN
8	A	69	GLN
8	A	146	GLN
8	A	208	ASN
10	LR	30	ASN
12	2	69	HIS
12	2	71	HIS

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Mol	Chain	Res	Type
13	B	23	HIS
13	B	25	GLN
13	B	105	ASN
13	B	478	ASN
13	B	514	HIS
13	B	522	GLN
13	B	526	HIS
13	B	551	HIS
13	B	577	ASN
13	B	750	ASN
13	B	757	ASN
13	B	795	ASN
13	B	828	HIS
14	LC	299	GLN
15	LE	190	HIS
15	LE	245	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	8	57/58 (98%)	13 (22%)	3 (5%)
4	1	289/5070 (5%)	73 (25%)	4 (1%)
All	All	346/5128 (6%)	86 (24%)	7 (2%)

All (86) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	8	51	U
1	8	59	A
1	8	62	A
1	8	63	U
1	8	80	A
1	8	81	C
1	8	82	A
1	8	83	C
1	8	84	A
1	8	85	U
1	8	86	U
1	8	87	G
1	8	88	A
4	1	200	U

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Mol	Chain	Res	Type
4	1	209	U
4	1	210	C
4	1	211	G
4	1	216	C
4	1	218	A
4	1	219	G
4	1	220	C
4	1	232	G
4	1	233	U
4	1	234	G
4	1	387	G
4	1	390	C
4	1	412	G
4	1	413	G
4	1	456	C
4	1	457	G
4	1	465	G
4	1	468	U
4	1	469	C
4	1	484	U
4	1	485	C
4	1	486	C
4	1	489	C
4	1	492	U
4	1	493	G
4	1	495	C
4	1	497	G
4	1	498	C
4	1	500	G
4	1	501	C
4	1	502	C
4	1	503	C
4	1	505	G
4	1	506	C
4	1	509	A
4	1	510	U
4	1	512	U
4	1	513	U
4	1	514	U
4	1	517	C
4	1	518	G
4	1	643	C

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Mol	Chain	Res	Type
4	1	644	G
4	1	646	G
4	1	654	C
4	1	657	C
4	1	665	C
4	1	666	G
4	1	667	A
4	1	668	C
4	1	672	C
4	1	673	C
4	1	675	C
4	1	686	A
4	1	687	U
4	1	697	G
4	1	2380	G
4	1	2693	G
4	1	2694	G
4	1	2695	A
4	1	2696	A
4	1	2697	A
4	1	2700	G
4	1	2701	U
4	1	2705	G
4	1	2707	U
4	1	2708	U
4	1	2709	C
4	1	2710	C
4	1	2711	G
4	1	2716	C
4	1	2897	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	8	81	C
1	8	82	A
1	8	84	A
4	1	385	A
4	1	685	C
4	1	2707	U
4	1	2896	G

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	IHP	B	901	-	36,36,36	0.78	0	54,60,60	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	IHP	B	901	-	-	7/30/54/54	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	901	IHP	C1-C6-O16-P6
17	B	901	IHP	C5-C6-O16-P6
17	B	901	IHP	C5-O15-P5-O35
17	B	901	IHP	C2-O12-P2-O42

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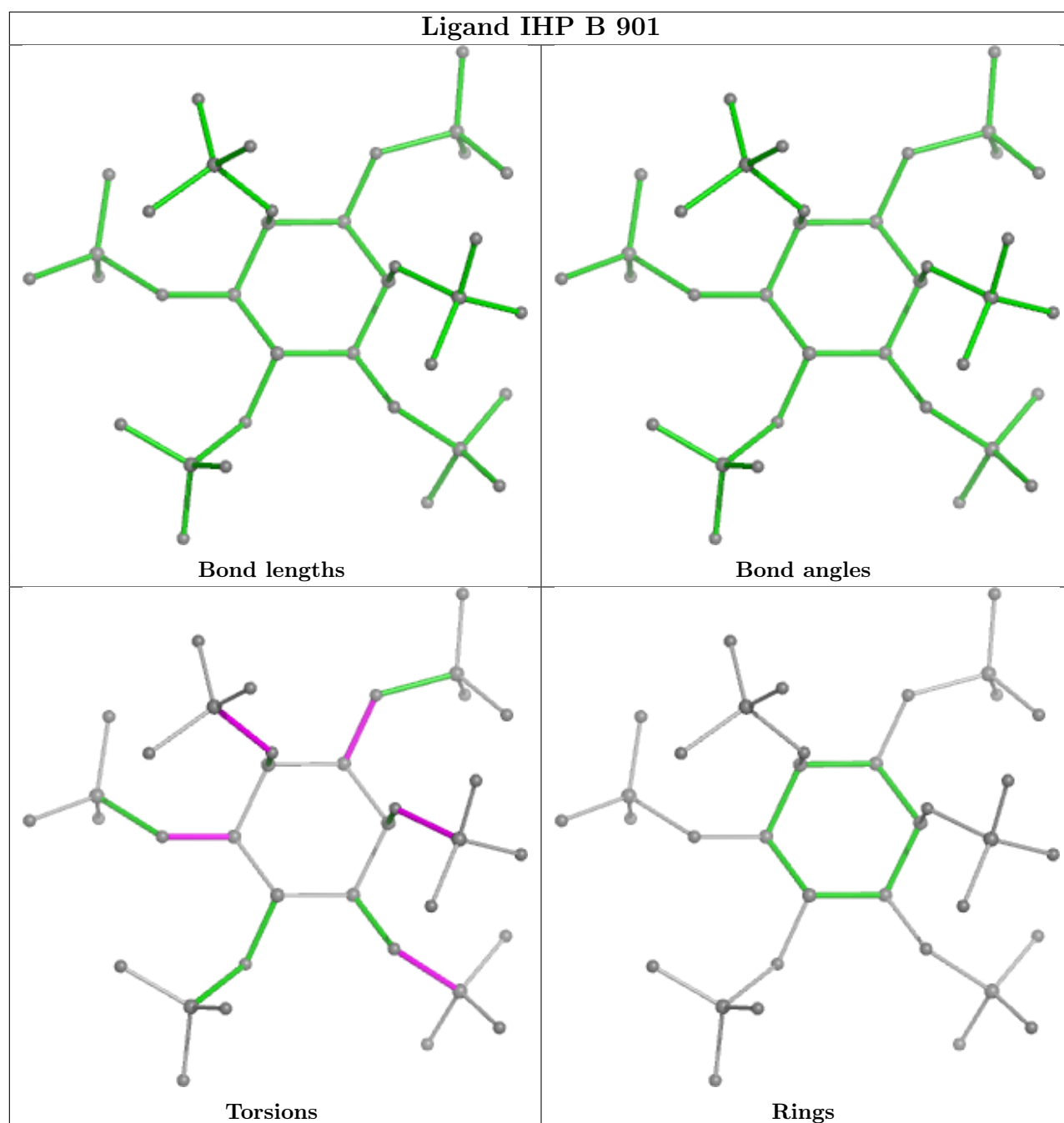
Mol	Chain	Res	Type	Atoms
17	B	901	IHP	C5-C4-O14-P4
17	B	901	IHP	C3-C4-O14-P4
17	B	901	IHP	C1-O11-P1-O21

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	901	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

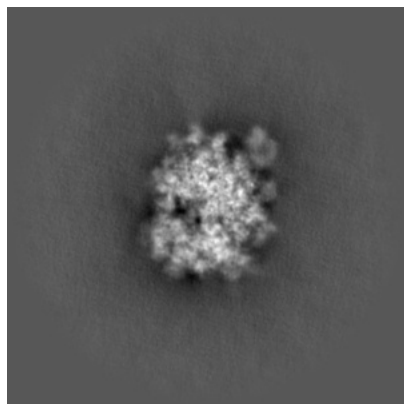
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50642. These allow visual inspection of the internal detail of the map and identification of artifacts.

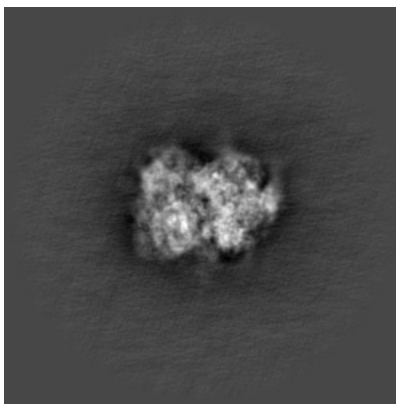
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

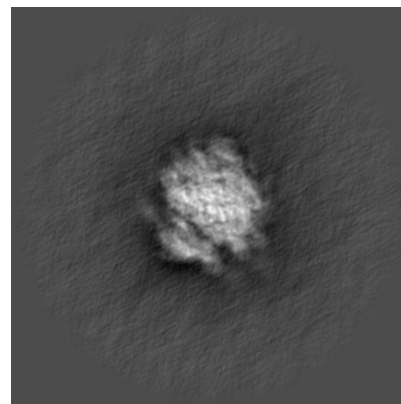
6.1.1 Primary map



X

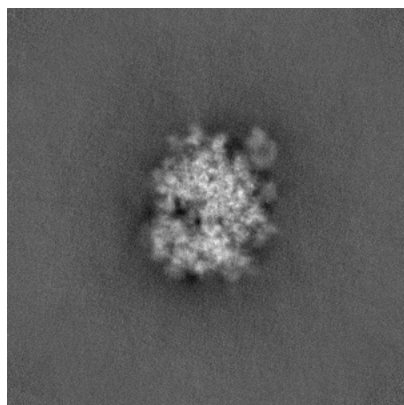


Y

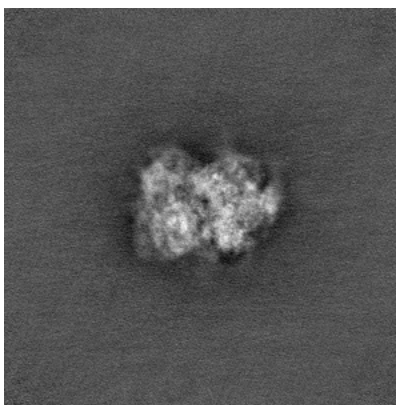


Z

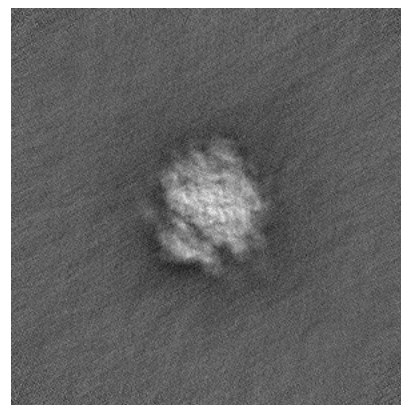
6.1.2 Raw map



X



Y

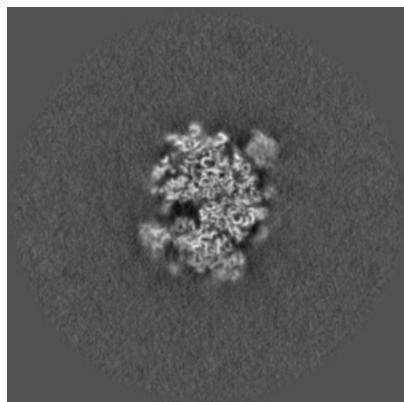


Z

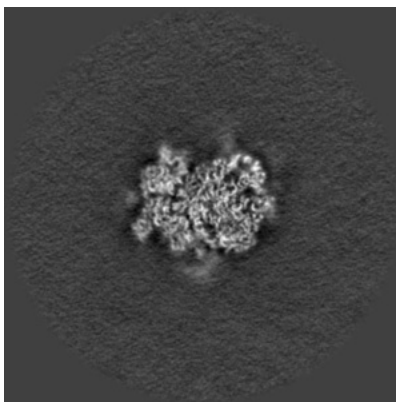
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

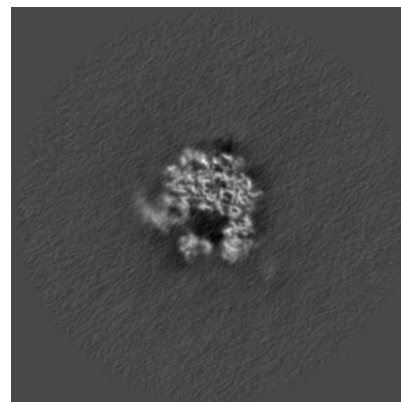
6.2.1 Primary map



X Index: 320

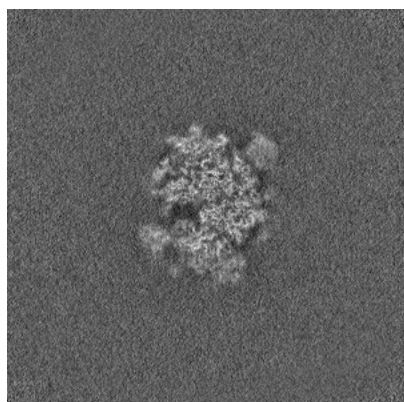


Y Index: 320

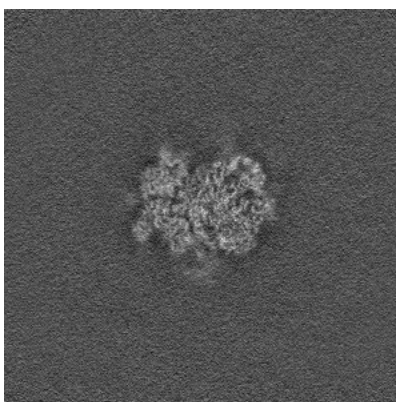


Z Index: 320

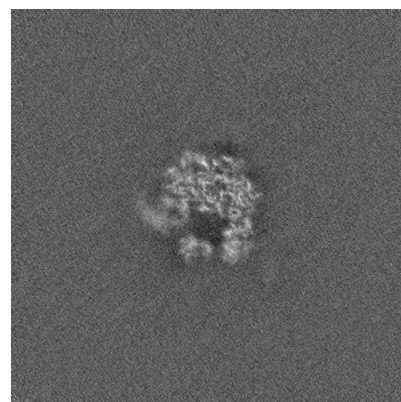
6.2.2 Raw map



X Index: 320



Y Index: 320

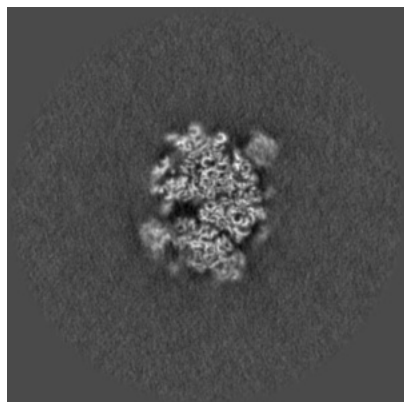


Z Index: 320

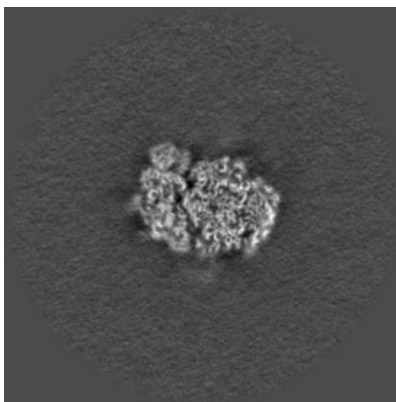
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

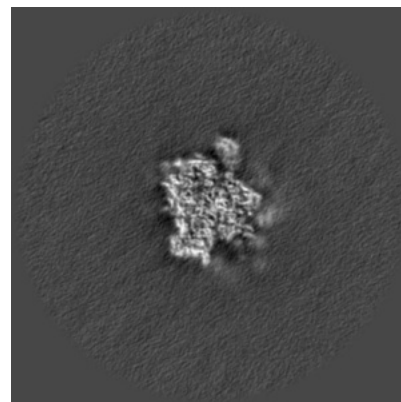
6.3.1 Primary map



X Index: 318

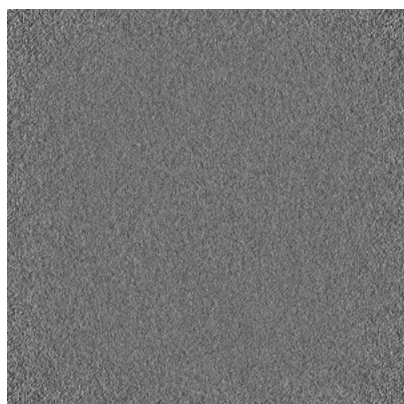


Y Index: 336

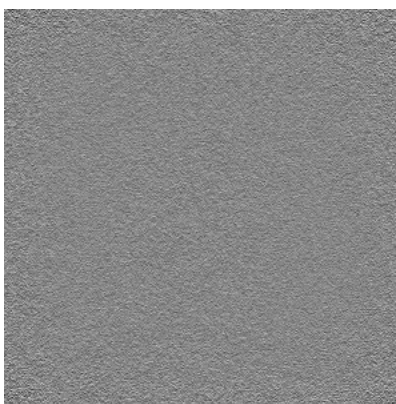


Z Index: 355

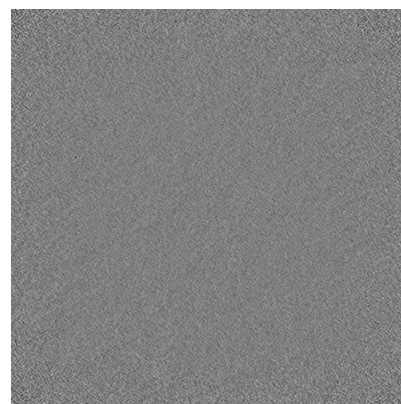
6.3.2 Raw map



X Index: 0



Y Index: 0

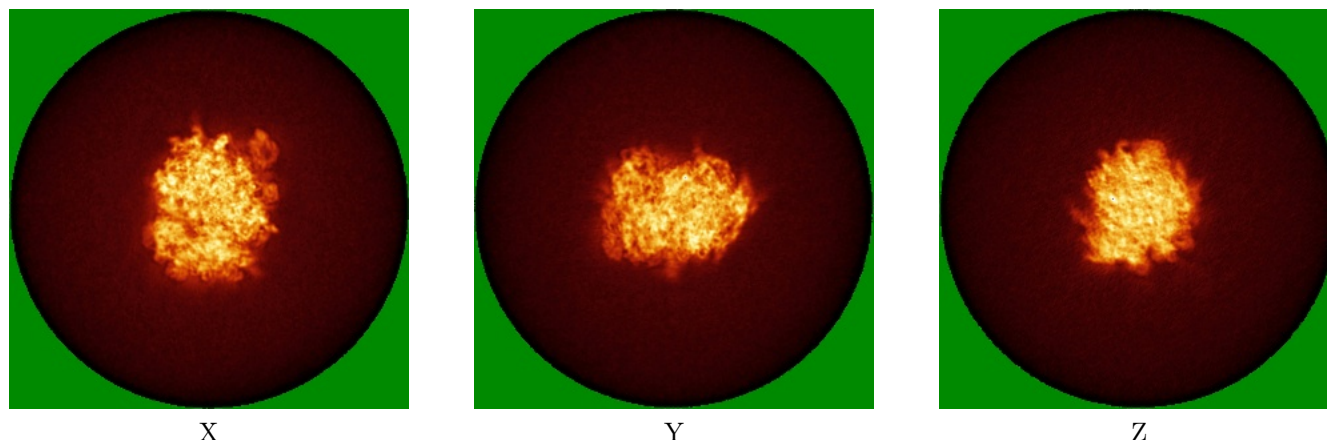


Z Index: 639

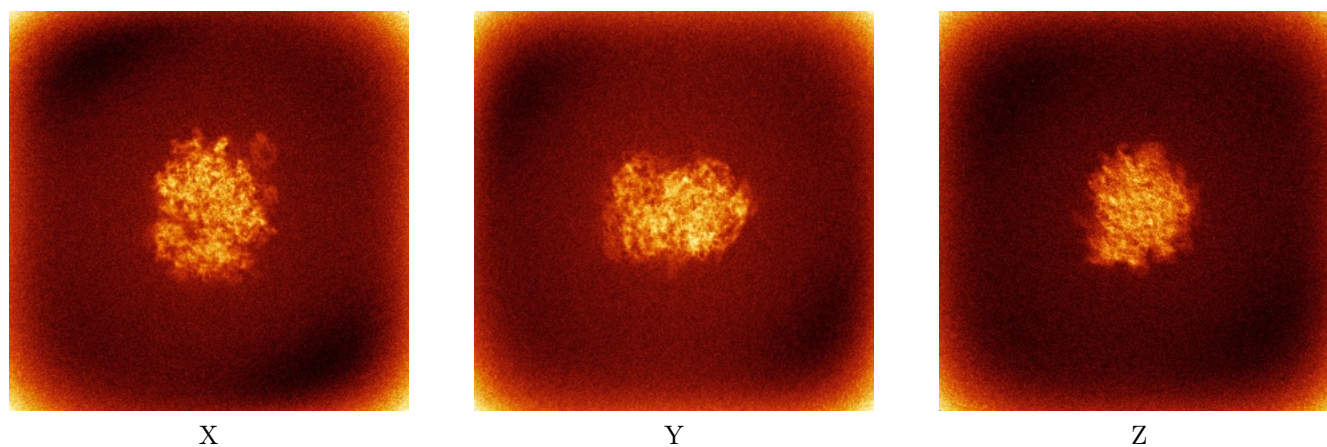
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



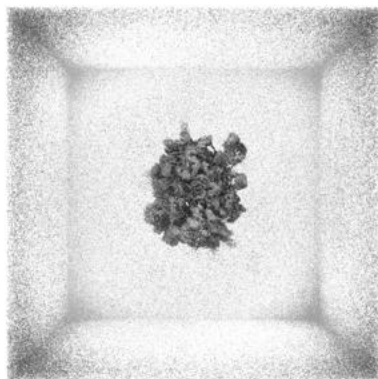
Y



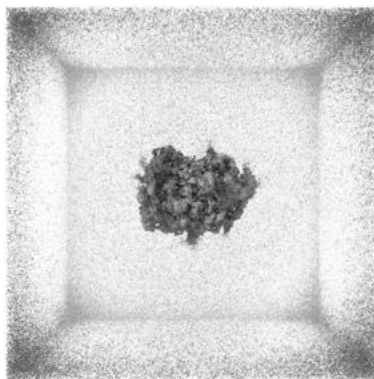
Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

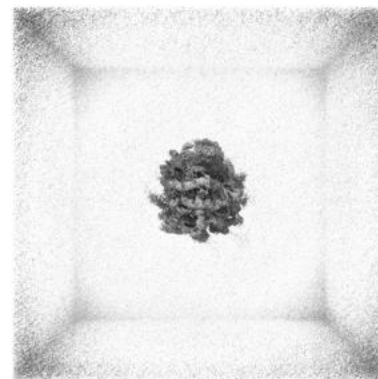
6.5.2 Raw map



X



Y



Z

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

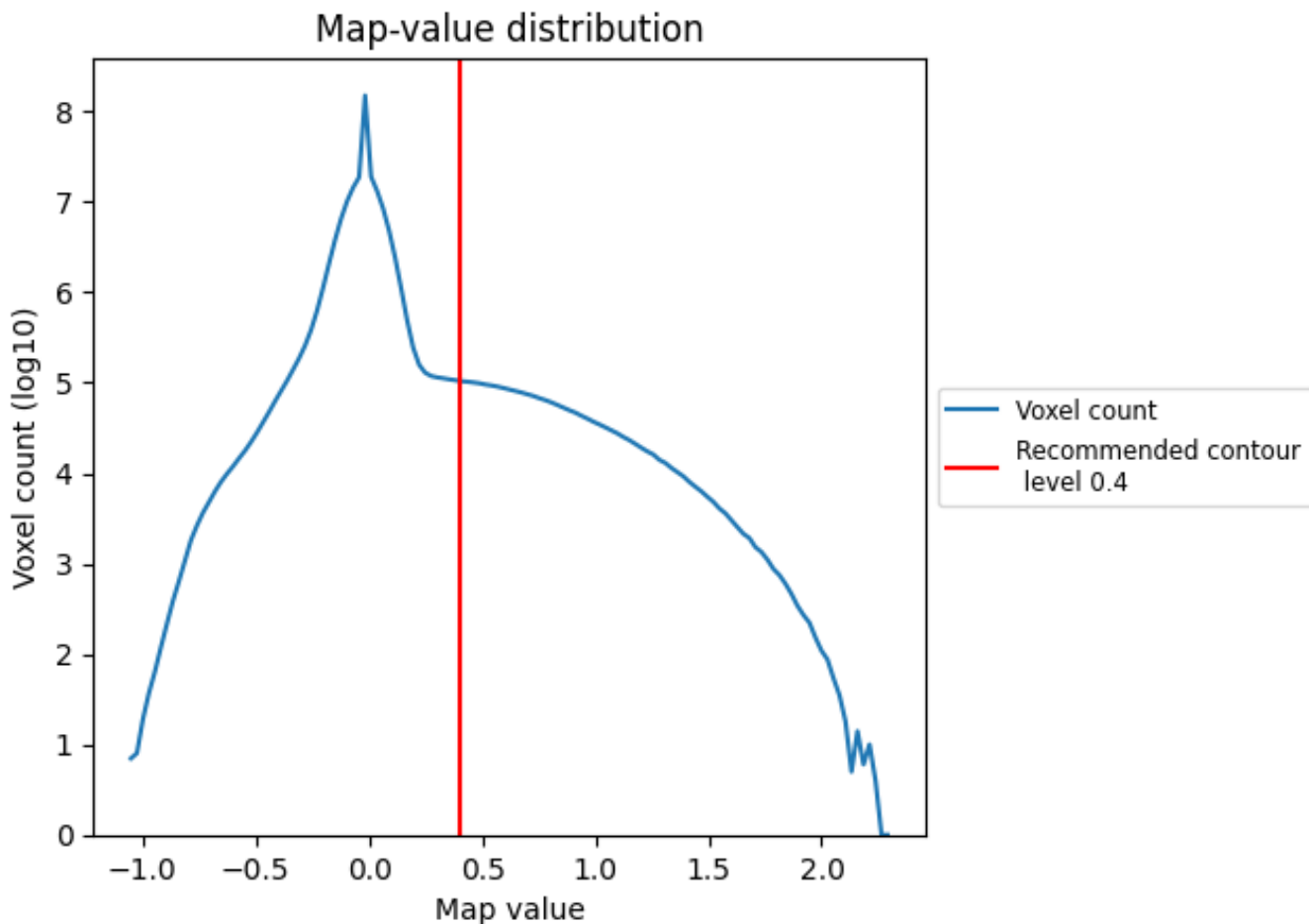
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

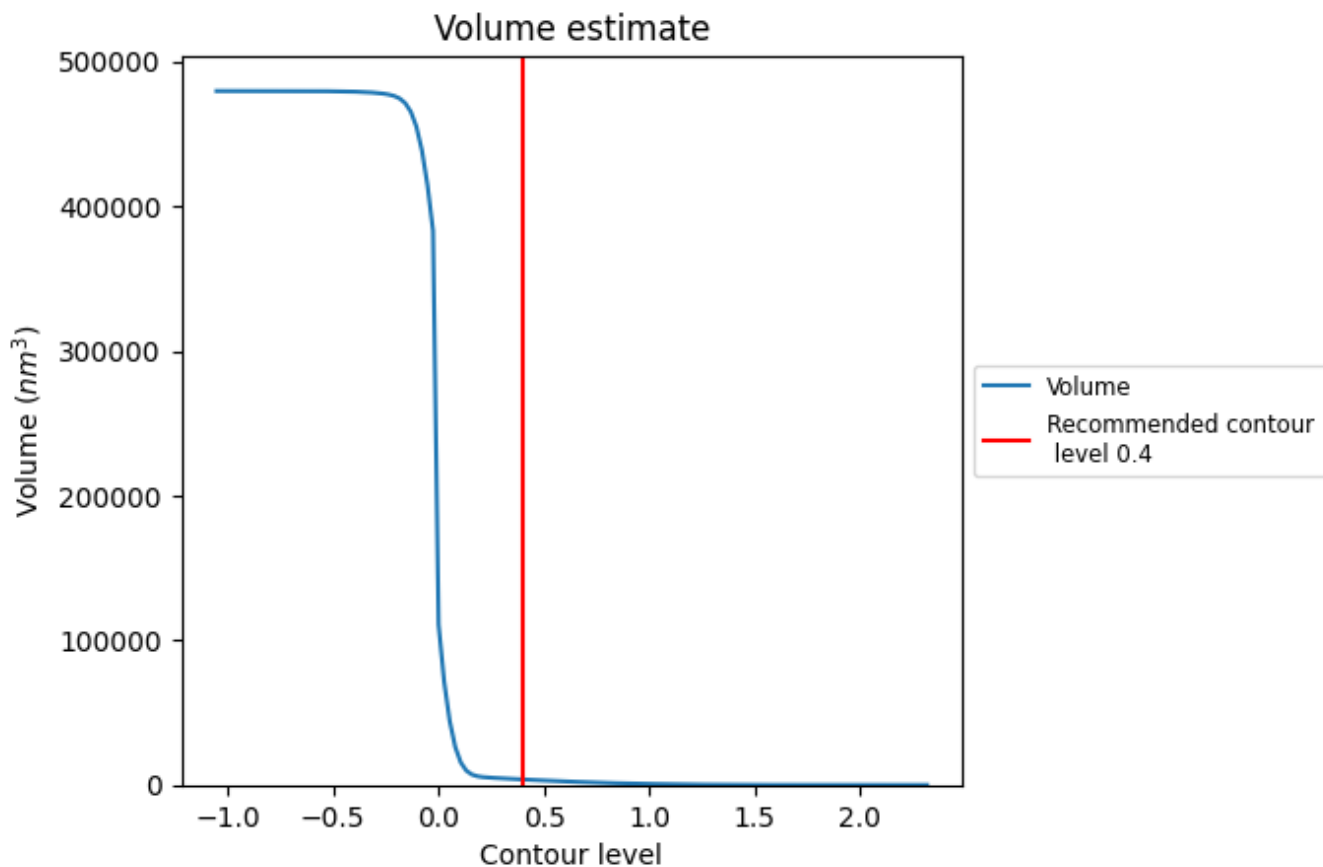
This section contains the results of statistical analysis of the map.

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.

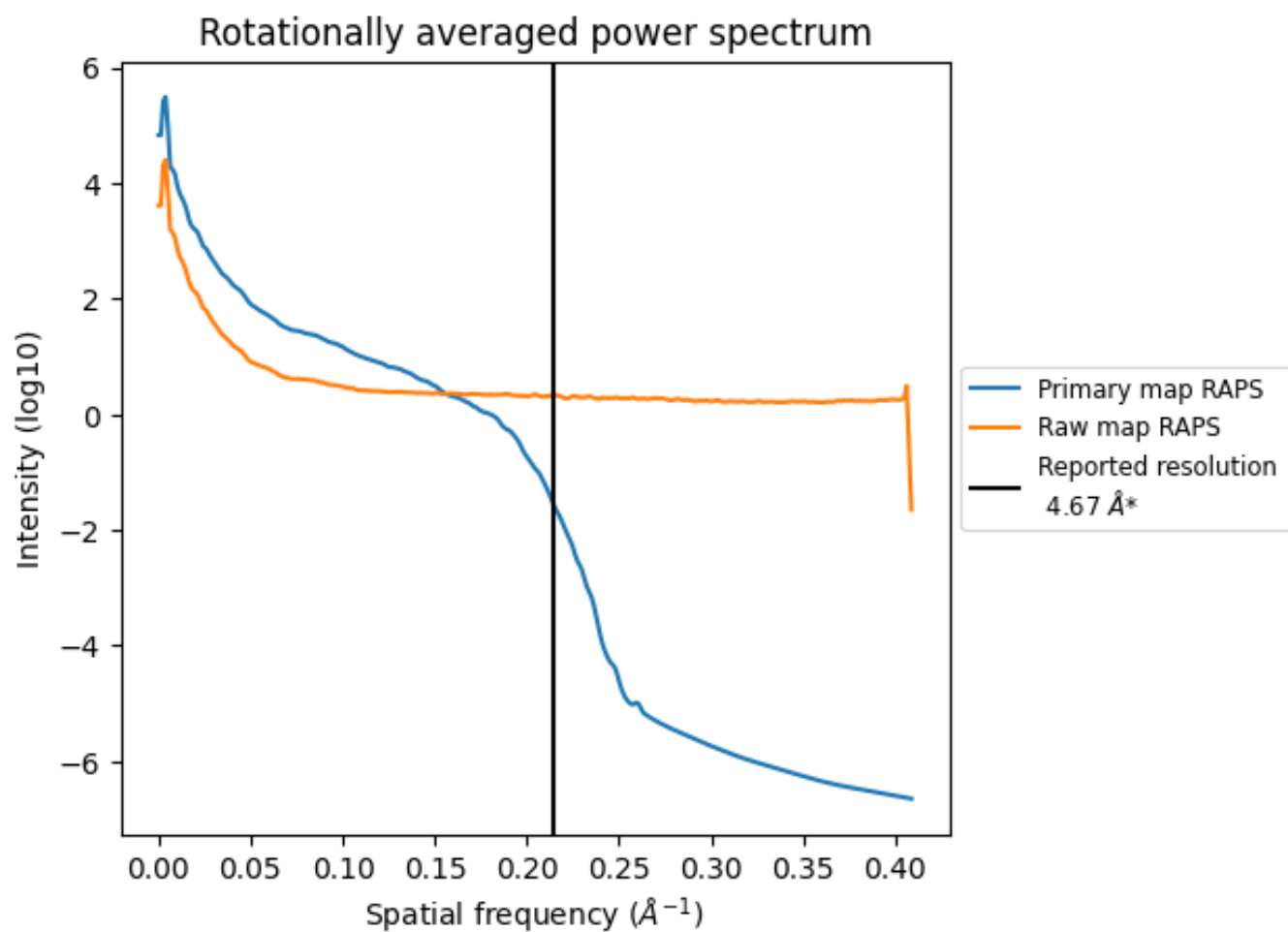
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3801 nm³; this corresponds to an approximate mass of 3433 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](#)

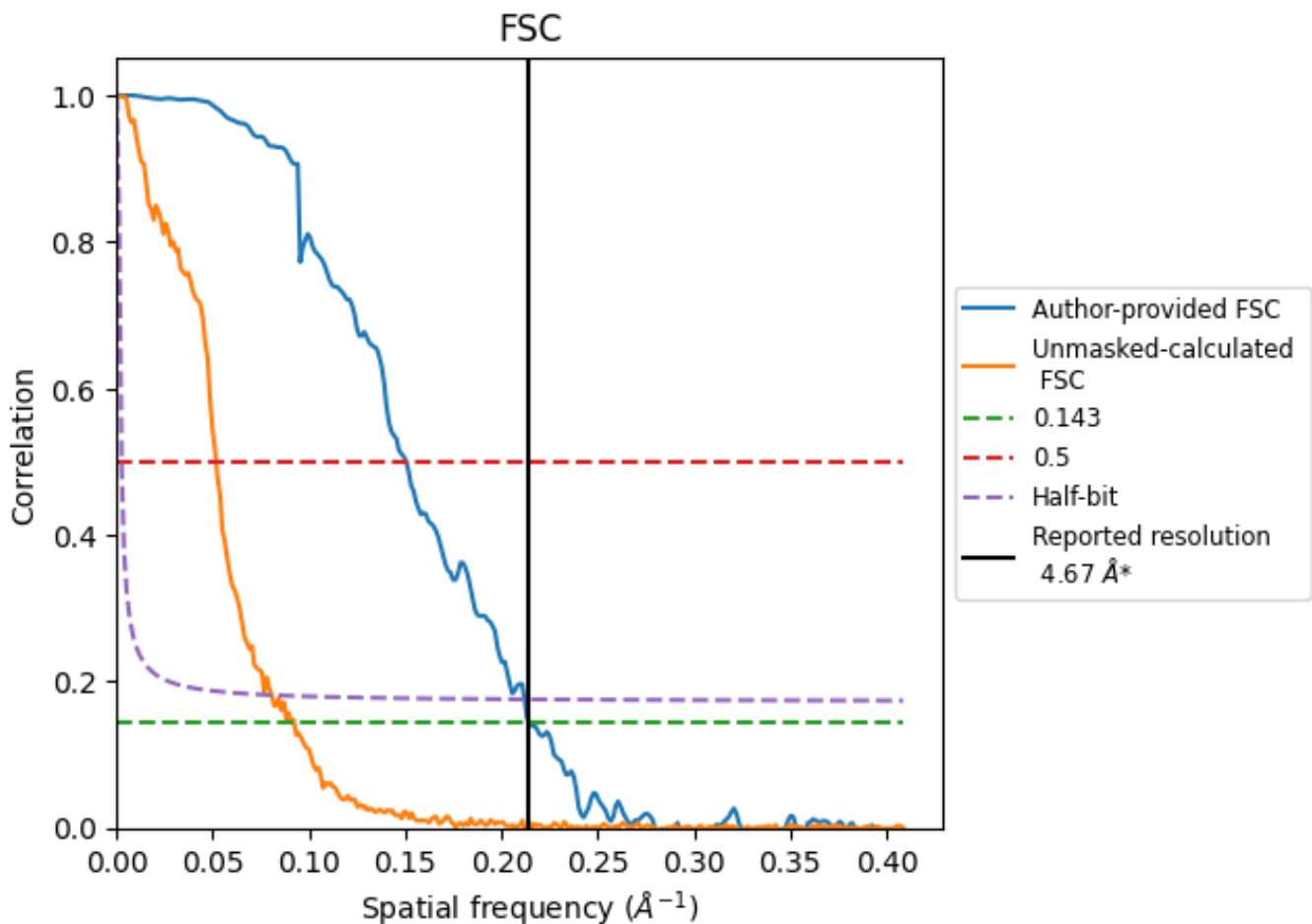


*Reported resolution corresponds to spatial frequency of 0.214 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.214 Å⁻¹

8.2 Resolution estimates [i](#)

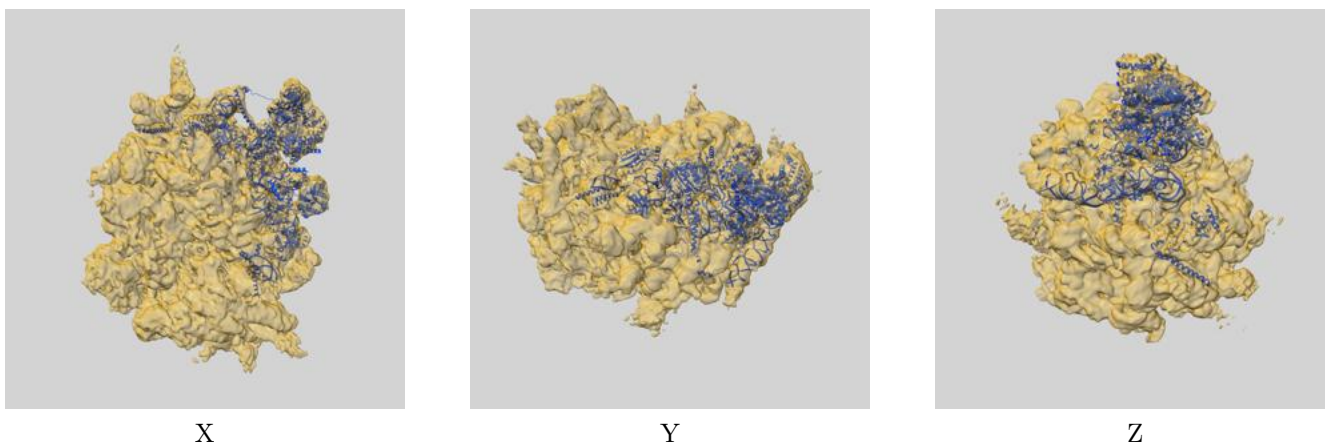
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.67	-	-
Author-provided FSC curve	4.67	6.65	4.72
Unmasked-calculated*	10.85	19.38	12.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.85 differs from the reported value 4.67 by more than 10 %

9 Map-model fit [i](#)

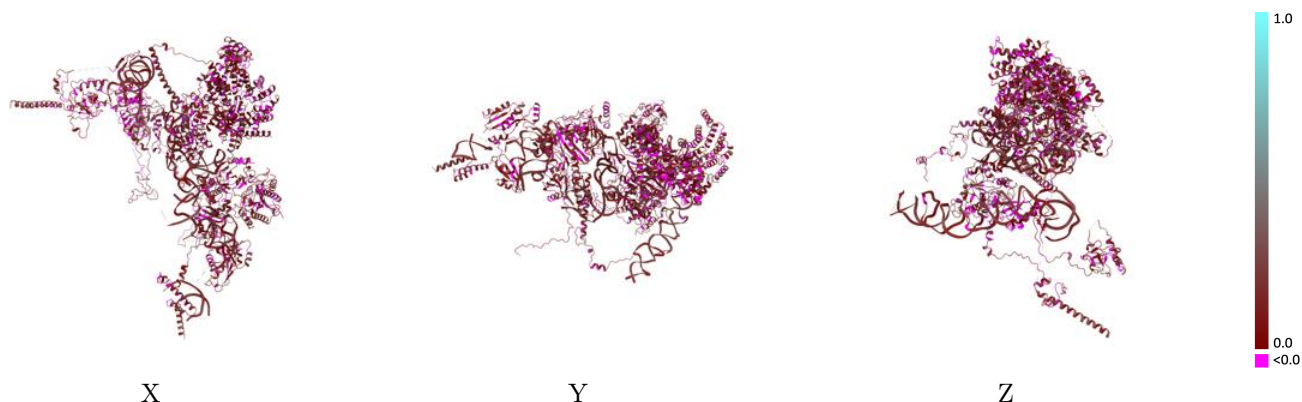
This section contains information regarding the fit between EMDB map EMD-50642 and PDB model 9FQ0. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



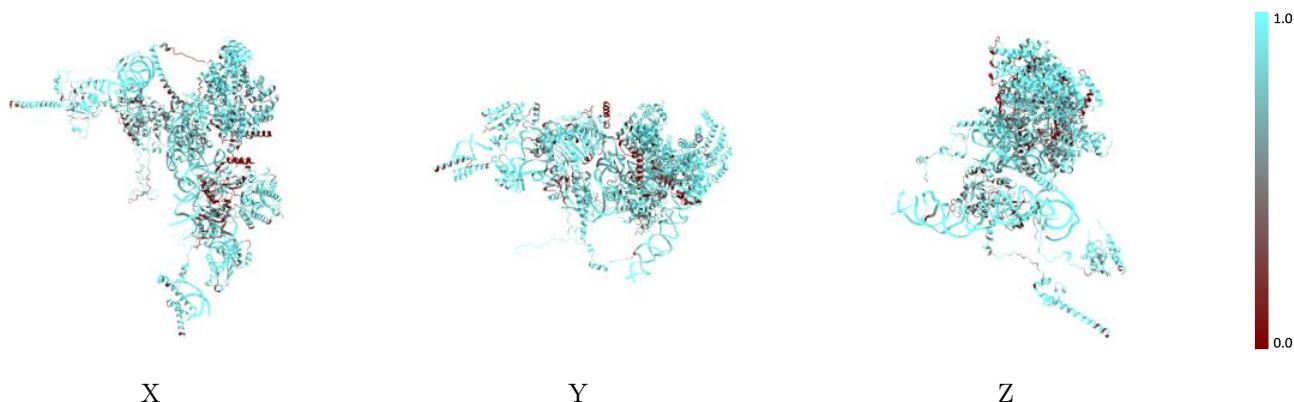
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



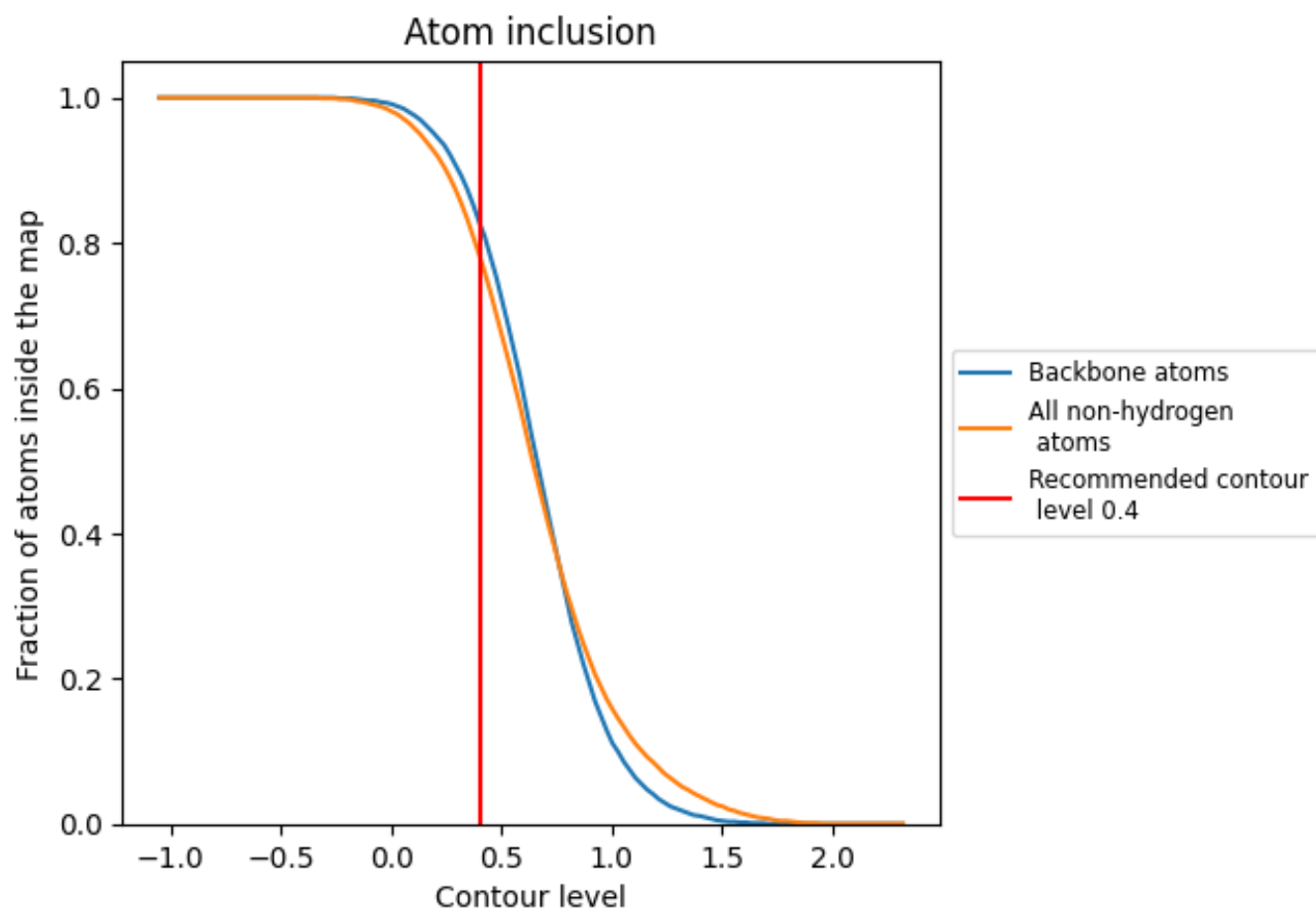
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.1270
1	 0.9280	 0.1720
2	 0.5980	 0.0950
8	 0.9200	 0.1910
A	 0.6490	 0.1250
B	 0.7710	 0.1000
D	 0.4140	 0.1000
E	 0.8370	 0.1380
LC	 0.6750	 0.1290
LE	 0.8580	 0.1300
LR	 0.6760	 0.1340
LU	 0.8230	 0.1220
LX	 0.6390	 0.1120
LY	 0.8070	 0.1080
Lh	 0.8040	 0.1350
Lk	 0.8400	 0.1150
Lr	 0.6400	 0.0050

