



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 05:53 PM UTC

PDB ID : 9FQ0 / pdb_00009fq0
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

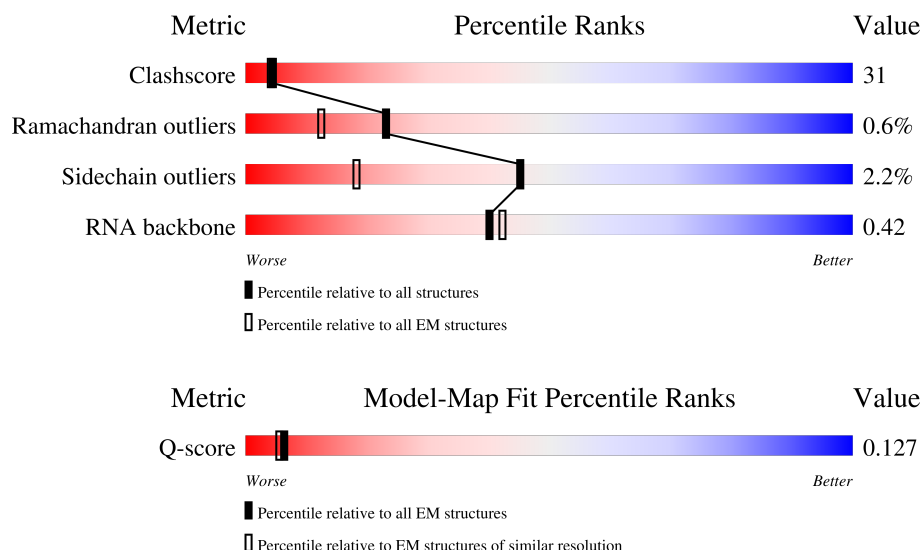
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



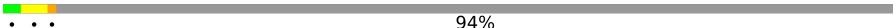
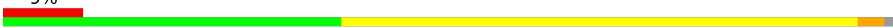
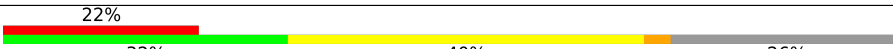
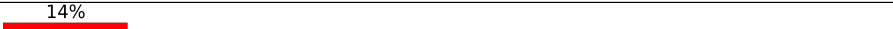
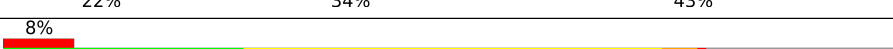
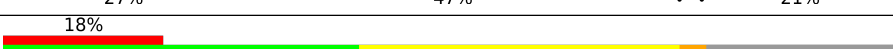
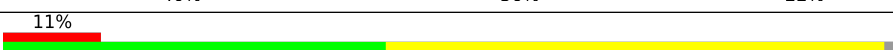
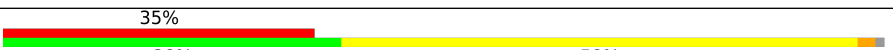
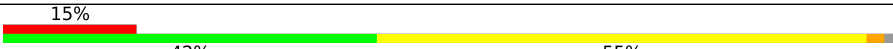
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2007 (4.17 - 5.16)

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	34% 53% 12%
2	E	392	8% 49% 31% 19%
3	D	206	33% 21% 34% 41%

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Mol	Chain	Length	Quality of chain
4	1	5070	 94%
5	LY	145	 10% 28% 61% 11%
6	Lh	123	 9% 38% 58% ..
7	LX	156	 22% 32% 40% 26%
8	A	221	 14% 22% 34% 43%
9	LU	128	 8% 27% 47% 21%
10	LR	196	 18% 40% 36% 22%
11	Lk	70	 11% 43% 56% .
12	2	171	 35% 38% 58% ..
13	B	840	 15% 42% 55% ..
14	LC	427	 21% 51% 34% 15%
15	LE	288	 5% 43% 31% 26%
16	Lr	137	 25% 52% 39% 9%

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
1	8	58	Total	C	N	O	P	0	0
			1237	554	224	401	58		

- Molecule 2 is a protein called Methionine aminopeptidase 1.

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

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
3	D	122	Total	C	N	O	S	0	0
			937	584	175	175	3		

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

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

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

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

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

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

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

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

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

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

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
9	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

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

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

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

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

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

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

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
13	B	834	Total	C	N	O	S	0	0
			6881	4379	1189	1272	41		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP Q9BXJ9

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

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

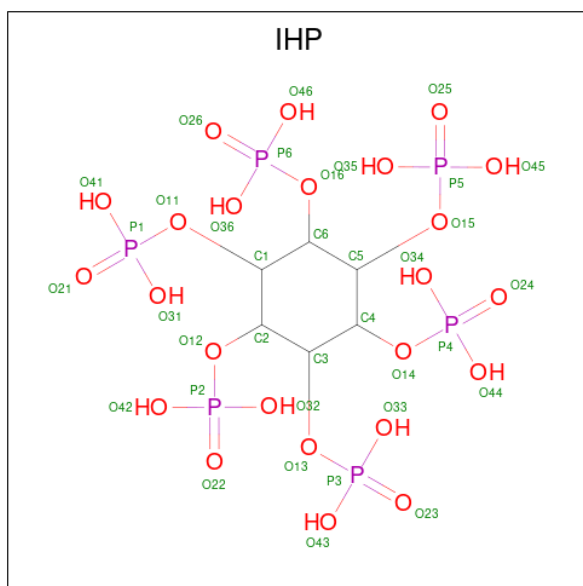
- Molecule 15 is a protein called Large ribosomal subunit protein eL6.

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

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

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

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

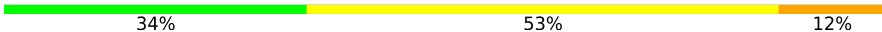


Mol	Chain	Residues	Atoms				AltConf
17	B	1	Total	C	O	P	0
			36	6	24	6	

3 Residue-property plots

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.

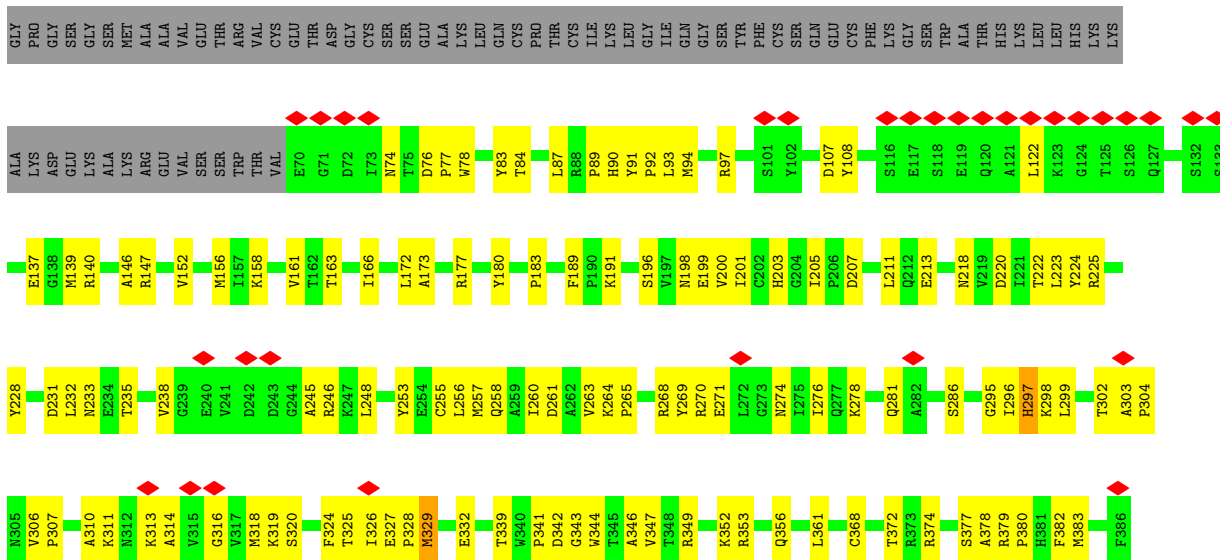
• Molecule 1: 5.8S rRNA

Chain 8: 



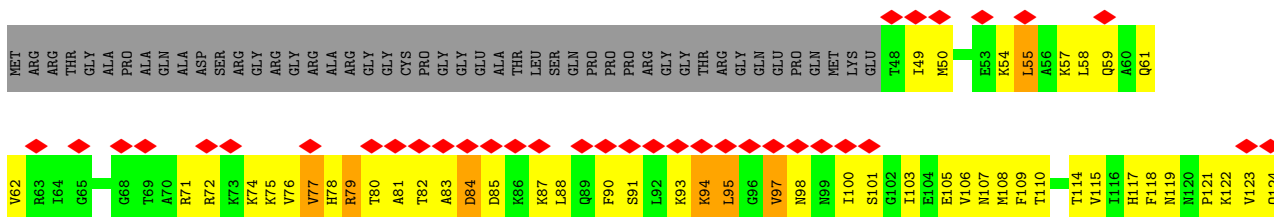
• Molecule 2: Methionine aminopeptidase 1

Chain E: 



• Molecule 3: Transcription factor BTF3

Chain D: 



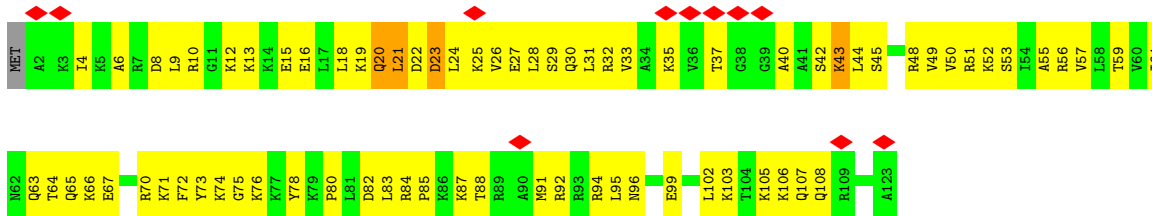




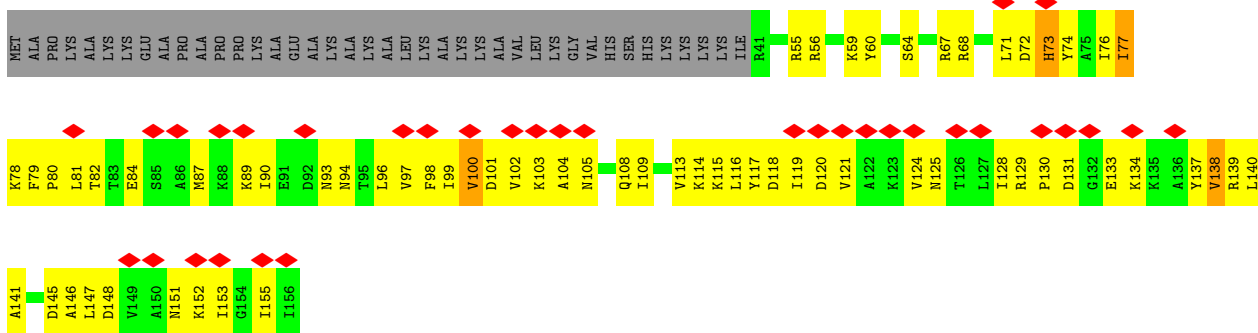
- Molecule 5: Large ribosomal subunit protein uL24

M1	K2	F3	N4	F5	F6	V7	T8	S9	D10	R11	S12	K13	M14	R17	H18	F19	N20	A21	P22	S23	H24	I25	R26	R27	K28	I29	M30	S31	S32	S33	P33	L34	S35	K36	E37	L38	R39	Q40	K41	Y42	R45	S46	M47	P48	I49	R50	D51	K52	D53	E54	V55	Q56	V57	F58	R59	G60	H61	V62
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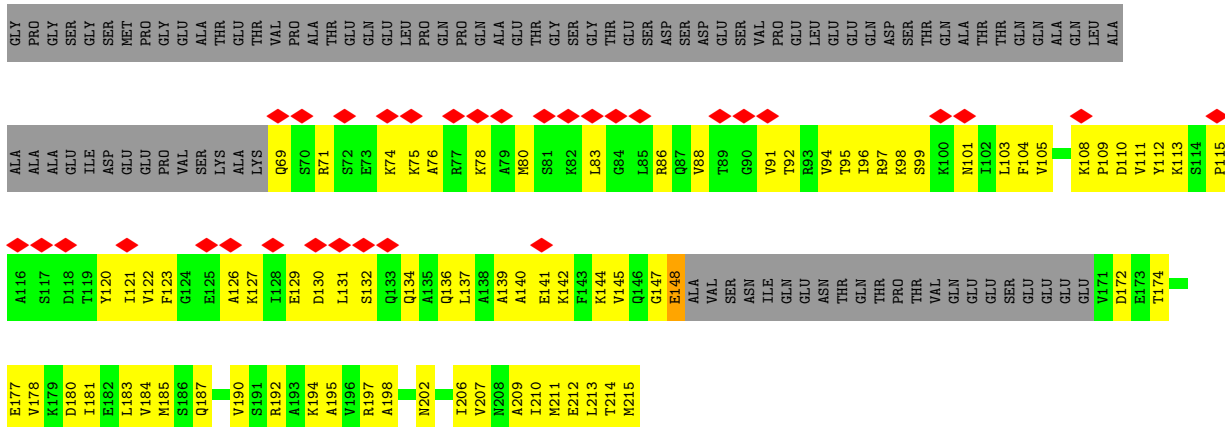
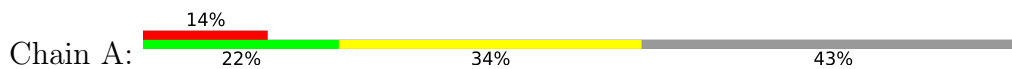
- Molecule 6: 60S ribosomal protein L35



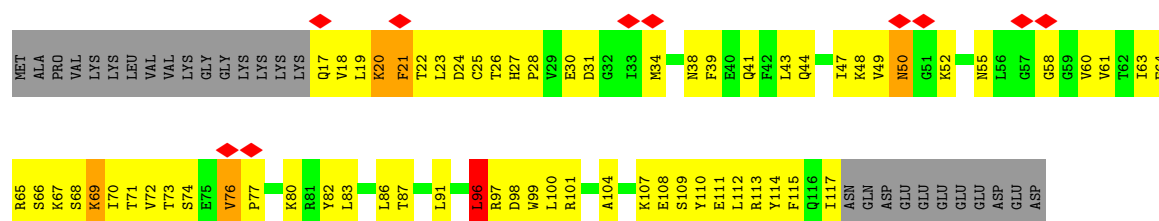
- Molecule 7: 60S ribosomal protein L23a



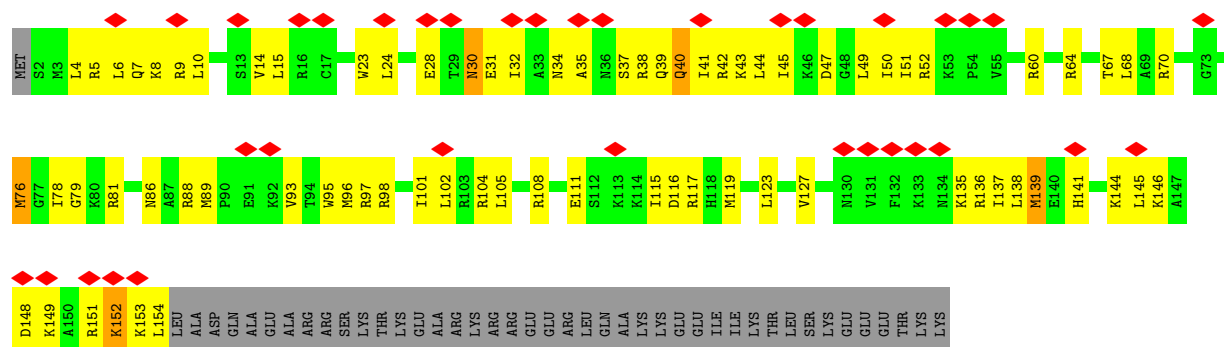
- Molecule 8: Nascent polypeptide-associated complex subunit alpha



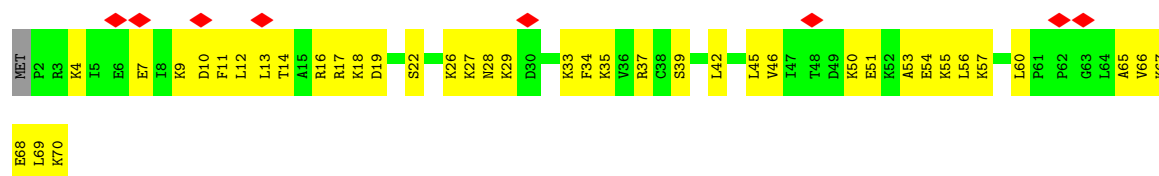
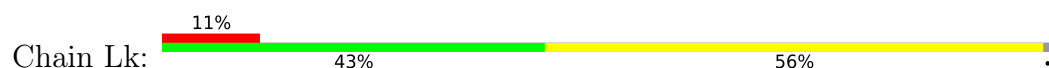
- Molecule 9: 60S ribosomal protein L22



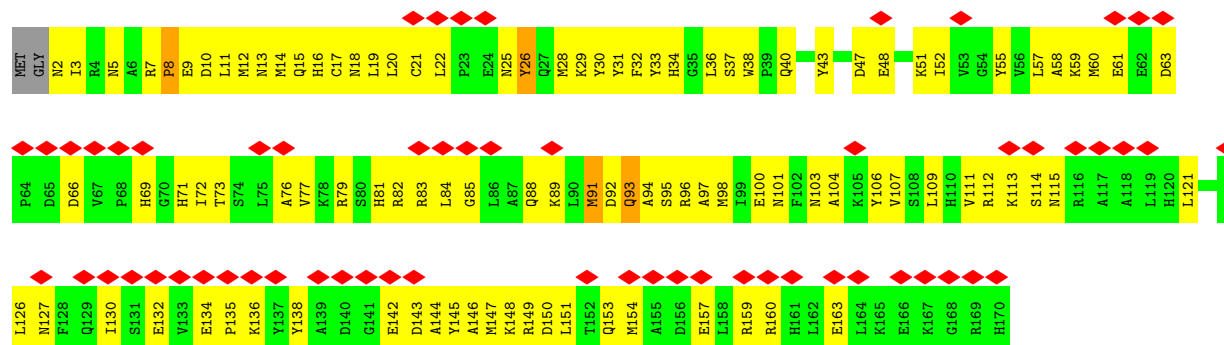
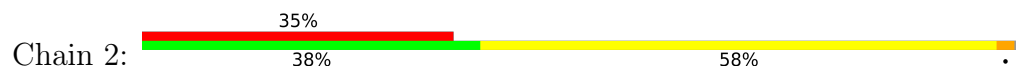
• Molecule 10: 60S ribosomal protein L19



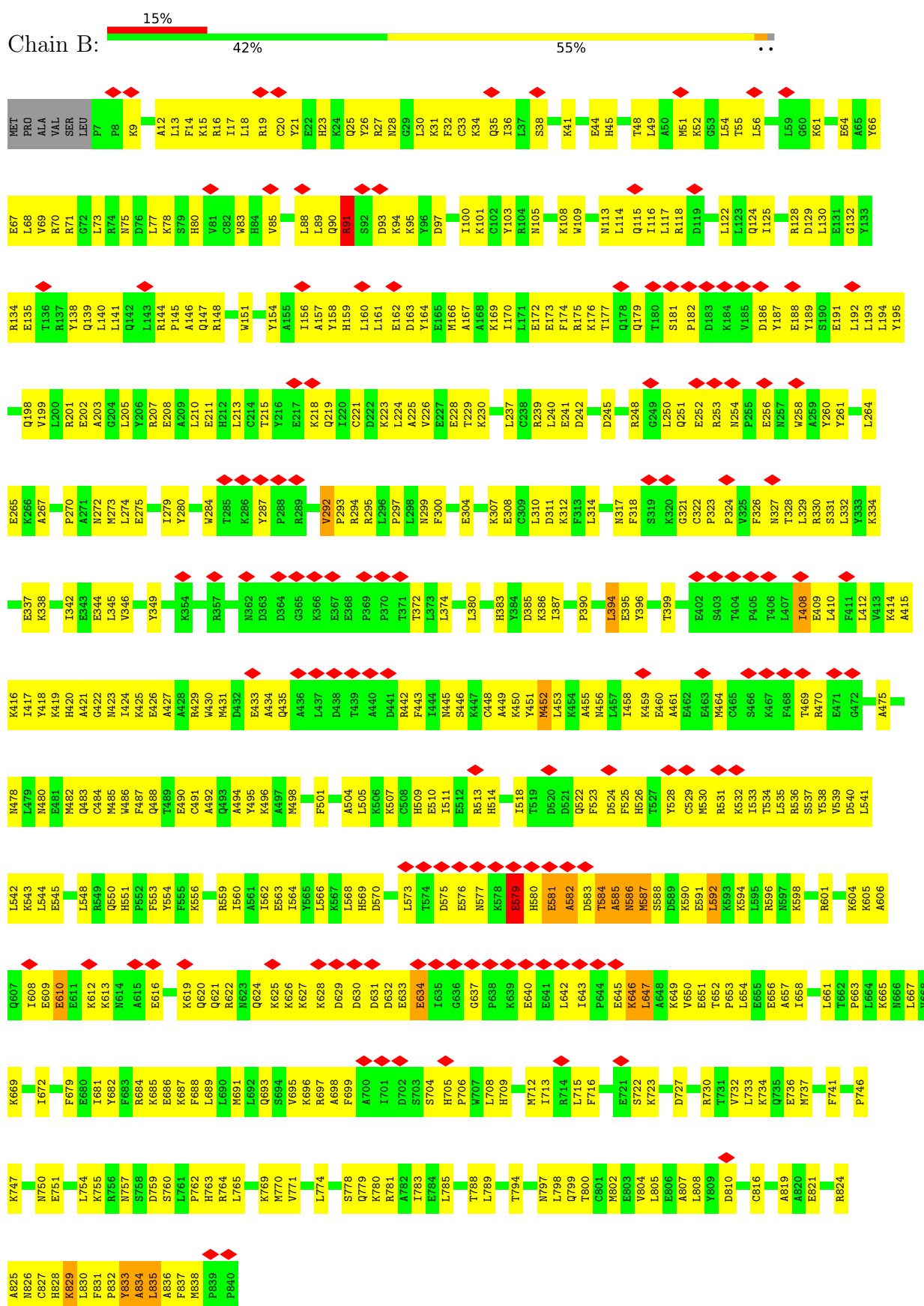
• Molecule 11: 60S ribosomal protein L38



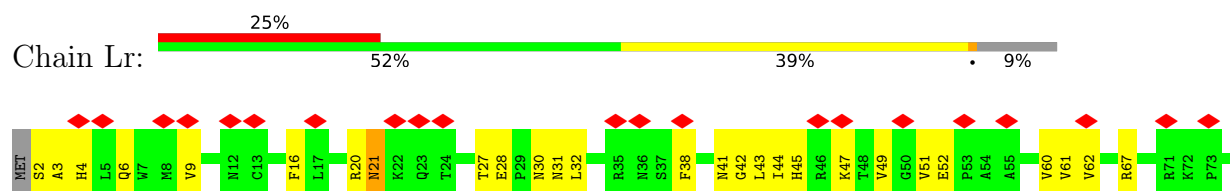
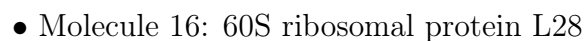
• Molecule 12: N-alpha-acetyltransferase 10



• Molecule 13: N-alpha-acetyltransferase 15, NatA auxiliary subunit



- Molecule 14: 60S ribosomal protein L4



R79	T80	T81	I82	N85	A86	R87	A88	T89	L90	S91	S92	I93	R94	H95	M96	I97	R98	K99	N100	K101	Y102	R103	P104	D105	L106	R107	M108	A109	A110	I111	R112	R113	A114	S115	A116	I117	L118	R119	S120	V124	M125	V126	LYS	ARG	LYS	LYS	ARG	THR	ARG	ARG	PRO	THR	LYS	SER	SER
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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 (Å)	782.72003, 782.72003, 782.72003	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.223, 1.223, 1.223	Depositor

5 Model quality

5.1 Standard geometry

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	0.22	0/1384	0.44	0/2154
2	E	0.23	0/2562	0.50	1/3479 (0.0%)
3	D	0.45	0/945	0.95	1/1269 (0.1%)
4	1	0.22	0/7128	0.43	3/11100 (0.0%)
5	LY	0.28	0/1092	0.78	0/1454
6	Lh	0.26	0/1023	0.71	1/1351 (0.1%)
7	LX	0.29	0/967	0.72	0/1301
8	A	0.25	0/972	0.67	0/1300
9	LU	0.25	0/839	0.76	2/1126 (0.2%)
10	LR	0.26	0/1297	0.74	1/1716 (0.1%)
11	Lk	0.22	0/575	0.65	0/761
12	2	0.25	0/1418	0.63	1/1909 (0.1%)
13	B	0.27	0/7019	0.65	7/9441 (0.1%)
14	LC	0.22	0/2962	0.57	0/3977
15	LE	0.23	0/1758	0.58	0/2359
16	Lr	0.21	0/1017	0.60	0/1364
All	All	0.25	0/32958	0.60	17/46061 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2
13	B	0	1
All	All	0	3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	79	ARG	N-CA-C	-7.93	101.44	111.90
13	B	835	LEU	CA-CB-CG	7.70	143.24	116.30
10	LR	139	MET	CA-CB-CG	6.75	127.59	114.10
13	B	829	LYS	CA-CB-CG	6.64	127.39	114.10
4	1	456	C	P-O3'-C3'	-6.32	110.72	120.20
13	B	829	LYS	CB-CG-CD	6.23	125.62	111.30
9	LU	69	LYS	CA-CB-CG	6.19	126.49	114.10
4	1	455	C	P-O3'-C3'	-6.17	110.95	120.20
2	E	329	MET	CB-CG-SD	5.85	130.26	112.70
6	Lh	21	LEU	CA-CB-CG	5.64	136.05	116.30
13	B	91	ARG	CB-CG-CD	5.61	124.20	111.30
13	B	835	LEU	CB-CA-C	-5.38	100.35	110.67
9	LU	96	LEU	CA-CB-CG	5.31	134.88	116.30
13	B	394	LEU	CA-CB-CG	5.25	134.68	116.30
13	B	834	ALA	N-CA-C	5.22	117.23	109.25
12	2	91	MET	CB-CG-SD	5.13	128.08	112.70
4	1	457	G	P-O3'-C3'	-5.12	112.53	120.20

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	44	0
2	E	2498	0	2425	110	0
3	D	937	0	989	137	0
4	1	6383	0	3239	282	0
5	LY	1075	0	1157	138	0
6	Lh	1015	0	1148	91	0
7	LX	950	0	1016	75	0
8	A	967	0	1017	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	LU	825	0	850	78	0
10	LR	1281	0	1418	100	0
11	Lk	569	0	637	40	0
12	2	1388	0	1356	142	0
13	B	6881	0	6924	565	0
14	LC	2908	0	3082	131	0
15	LE	1724	0	1874	78	0
16	Lr	1002	0	1068	47	0
17	B	36	0	6	1	0
All	All	31676	0	28831	1878	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 31.

All (1878) 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:LX:68:ARG:HH22	1.21	1.04
7:LX:94:ASN:HD21	7:LX:145:ASP:HA	1.21	1.02
6:Lh:21:LEU:HD23	6:Lh:57:VAL:CG1	1.89	1.01
3:D:79:ARG:HG3	4:1:2707:U:H2''	1.43	1.01
13:B:194:LEU:HB3	13:B:536:ARG:HD3	1.45	0.97
4:1:2533:C:H5''	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
13:B:423:ASN:HB2	13:B:833:TYR:O	1.68	0.92
13:B:798:LEU:HD12	13:B:802:MET:HE1	1.54	0.90
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
6:Lh:21:LEU:CD2	6:Lh:57:VAL:HG13	2.04	0.88
2:E:298:LYS:H	2:E:298:LYS:HD2	1.39	0.88
8:A:181:ILE:HG22	8:A:185:MET:HE1	1.55	0.87
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
6:Lh:87:LYS:HE2	6:Lh:91:MET:HE1	1.55	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:493:G:O6	4:1:660:A:N1	2.10	0.85
6:Lh:21:LEU:HD23	6:Lh:57:VAL:HG11	1.54	0.85
16:Lr:3:ALA:HB1	16:Lr:44:ILE:HD13	1.56	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
7:LX:76:ILE:O	7:LX:78:LYS:NZ	2.10	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
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
7:LX:84:GLU:HA	7:LX:87:MET:HE1	1.60	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
6:Lh:22:ASP:HA	6:Lh:25:LYS:HE3	1.64	0.80
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
6:Lh:21:LEU:CD2	6:Lh:57:VAL:CG1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Lk:7:GLU:OE2	11:Lk:9:LYS:HB3	1.83	0.79
8:A:185:MET:HE3	8:A:192:ARG:HG2	1.64	0.78
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
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
10:LR:116:ASP:HB3	10:LR:119:MET:HE3	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:76:MET:HE2	10:LR:88:ARG:HH21	1.51	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
4:1:686:A:OP1	13:B:594:LYS:NZ	2.19	0.74
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
13:B:609:GLU:HA	13:B:612:LYS:HZ3	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:625:LYS:HA	13:B:628:LYS:HD2	1.68	0.73
2:E:156:MET:HE1	2:E:166:ILE:HA	1.69	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
8:A:211:MET:SD	13:B:101:LYS:NZ	2.62	0.72
11:Lk:10:ASP:HA	11:Lk:13:LEU:HD23	1.70	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
6:Lh:4:ILE:HD11	6:Lh:9:LEU:HD21	1.70	0.71
5:LY:82:ILE:HB	5:LY:85:VAL:HG12	1.71	0.71
6:Lh:22:ASP:O	6:Lh:26:VAL:HG23	1.90	0.71
11:Lk:11:PHE:HB2	11:Lk:45:LEU:HD12	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
6:Lh:21:LEU:HD11	6:Lh:61:ILE:CD1	2.20	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
6:Lh:37:THR:HG22	7:LX:82:THR:HG21	1.72	0.70
9:LU:100:LEU:HD12	9:LU:112:LEU:HG	1.73	0.70
11:Lk:26:LYS:NZ	11:Lk:28:ASN:OD1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:256:LEU:HD23	2:E:257:MET:HE1	1.75	0.69
13:B:415:ALA:HB2	13:B:431:MET:HE3	1.73	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
16:Lr:90:LEU:HD22	16:Lr:111:ILE:HG13	1.75	0.69
4:1:2536:A:H5''	11:Lk:42:LEU:HD13	1.73	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
13:B:414:LYS:HZ3	13:B:418:TYR:HE2	1.40	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
6:Lh:29:SER:O	6:Lh:33:VAL:HG23	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:65:A:OP1	6:Lh:56:ARG:NH1	2.27	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
4:1:458:C:H5''	16:Lr:87:ARG:NH2	2.09	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
13:B:449:ALA:HB2	13:B:464:MET:HE1	1.75	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
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
1:8:90:C:O2'	5:LY:24:HIS:ND1	2.27	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
16:Lr:28:GLU:HG2	16:Lr:31:ASN:HB2	1.75	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
8:A:139:ALA:HB2	13:B:176:LYS:HZ1	1.60	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:587:MET:HE3	13:B:591:GLU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:824:ARG:CG	13:B:837:PHE:HA	2.26	0.66
4:1:237:G:HO2'	5:LY:45:ARG:HH22	1.41	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
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
16:Lr:92:SER:O	16:Lr:96:MET:HE2	1.95	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
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
4:1:237:G:HO2'	5:LY:45:ARG:NH2	1.94	0.66
4:1:662:C:H2'	4:1:663:G:H8	1.61	0.66
5:LY:30:MET:HE1	5:LY:75:ARG:HG2	1.76	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
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
12:2:91:MET:HE2	12:2:126:LEU:HD22	1.78	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
16:Lr:32:LEU:HA	16:Lr:113:ARG:HD2	1.77	0.65
4:1:227:A:H1'	5:LY:2:LYS:HB2	1.78	0.65
8:A:211:MET:HE1	13:B:83:TRP:CH2	2.32	0.65
14:LC:288:ASP:HA	16:Lr:4:HIS:HE2	1.62	0.65
2:E:158:LYS:HZ3	2:E:161:VAL:HG21	1.61	0.65
14:LC:289:LEU:H	16:Lr:4:HIS:CE1	2.15	0.65
4:1:218:A:H1'	4:1:219:G:C8	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:467:U:H4'	13:B:601:ARG:HD2	1.77	0.64
13:B:166:MET:HE3	13:B:166:MET:H	1.62	0.64
13:B:453:LEU:O	13:B:494:ALA:HB2	1.96	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
15:LE:112:MET:O	16:Lr:87:ARG:NE	2.16	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
6:Lh:4:ILE:HG23	6:Lh:56:ARG:HH21	1.63	0.63
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
1:8:61:A:H3'	6:Lh:51:ARG:HH21	1.63	0.63
6:Lh:23:ASP:OD2	6:Lh:23:ASP:N	2.29	0.63
6:Lh:99:GLU:OE1	6:Lh:99:GLU:N	2.31	0.63
15:LE:264:ILE:HD11	15:LE:267:LEU:HB2	1.81	0.63
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
16:Lr:2:SER:O	16:Lr:6:GLN:HG3	1.99	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
6:Lh:67:GLU:O	6:Lh:71:LYS:NZ	2.30	0.63
6:Lh:73:TYR:CD2	6:Lh:80:PRO:HD3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:222:C:OP2	14:LC:165:LYS:NZ	2.23	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
11:Lk:13:LEU:HD13	11:Lk:16:ARG:HE	1.61	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
4:1:2537:A:OP2	11:Lk:37:ARG:NH1	2.28	0.62
6:Lh:15:GLU:OE1	6:Lh:15:GLU:N	2.24	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
3:D:72:ARG:HH22	9:LU:117:ILE:C	2.07	0.62
4:1:493:G:N1	4:1:660:A:C2	2.61	0.62
6:Lh:52:LYS:HE3	6:Lh:56:ARG:HH12	1.64	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
11:Lk:29:LYS:HD3	11:Lk:29:LYS:N	2.15	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:115:VAL:HB	3:D:146:MET:HE1	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:215:C:O4'	13:B:626:LYS:NZ	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
16:Lr:86:ALA:O	16:Lr:89:THR:OG1	2.17	0.62
4:1:238:C:HO2'	5:LY:33:PRO:HD3	1.63	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
11:Lk:13:LEU:HD13	11:Lk:16:ARG:HH21	1.65	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
12:2:130:ILE:HG12	12:2:147:MET:HE1	1.82	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
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
6:Lh:40:ALA:HB3	6:Lh:43:LYS:HG2	1.82	0.61
7:LX:81:LEU:HG	7:LX:99:ILE:HD11	1.81	0.61
8:A:142:LYS:HZ1	13:B:173:GLU:HB3	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:394:LEU:HG	13:B:833:TYR:CZ	2.36	0.60
16:Lr:96:MET:O	16:Lr:100:ASN:HB2	2.01	0.60
1:8:49:G:OP1	6:Lh:48:ARG:NH2	2.33	0.60
6:Lh:21:LEU:CD2	6:Lh:57:VAL:CG2	2.79	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
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
11:Lk:19:ASP:HB2	11:Lk:39:SER:HB2	1.83	0.60
3:D:78:HIS:CG	4:1:2707:U:C5	2.90	0.60
6:Lh:13:LYS:HB3	6:Lh:15:GLU:OE1	2.01	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
4:1:2695:A:OP1	11:Lk:35:LYS:NZ	2.34	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
3:D:83:ALA:C	3:D:85:ASP:H	2.09	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
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
3:D:83:ALA:C	3:D:85:ASP:N	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:59:GLN:HG2	9:LU:99:TRP:NE1	2.18	0.59
3:D:91:SER:HA	3:D:94:LYS:HZ2	1.67	0.59
4:1:3604:A:H2'	4:1:3605:C:O4'	2.02	0.59
9:LU:20:LYS:HZ1	9:LU:73:THR:HA	1.66	0.59
13:B:31:LYS:O	13:B:34:LYS:NZ	2.34	0.59
16:Lr:108:MET:O	16:Lr:112:ARG:HG2	2.02	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
1:8:90:C:HO2'	5:LY:24:HIS:HD1	1.48	0.59
2:E:263:VAL:HG13	2:E:318:MET:SD	2.42	0.59
4:1:2696:A:H5'	11:Lk:70:LYS:NZ	2.17	0.59
6:Lh:20:GLN:O	6:Lh:24:LEU:HG	2.02	0.59
6:Lh:21:LEU:CD2	6:Lh:57:VAL:HG22	2.32	0.59
14:LC:288:ASP:HA	16:Lr:4:HIS:NE2	2.17	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
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
14:LC:177:TRP:CG	14:LC:181:LYS:HZ1	2.21	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
11:Lk:66:VAL:HG12	11:Lk:68:GLU:OE1	2.03	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
6:Lh:21:LEU:HD23	6:Lh:57:VAL:CG2	2.33	0.59
14:LC:336:ARG:O	14:LC:340:ILE:HG12	2.02	0.59
6:Lh:6:ALA:HA	6:Lh:9:LEU:HD12	1.85	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
13:B:770:MET:HA	13:B:770:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:Lr:106:LEU:O	16:Lr:110:ALA:N	2.29	0.58
4:1:679:C:H2'	4:1:680:G:C8	2.36	0.58
6:Lh:21:LEU:HD21	6:Lh:57:VAL:HG22	1.83	0.58
7:LX:78:LYS:HZ1	7:LX:101:ASP:N	2.01	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
12:2:94:ALA:C	12:2:98:MET:HE3	2.29	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
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
13:B:496:LYS:HZ1	13:B:563:GLU:HB2	1.67	0.58
5:LY:108:ARG:HG2	5:LY:108:ARG:HH11	1.69	0.58
6:Lh:8:ASP:O	6:Lh:12:LYS:NZ	2.37	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:78:HIS:C	3:D:80:THR:N	2.57	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:91:SER:HB2	8:A:80:MET:HE1	1.85	0.57
4:1:208:A:H4'	5:LY:60:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:8:64:U:OP1	6:Lh:52:LYS:NZ	2.33	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
4:1:458:C:H5''	16:Lr:87:ARG:HH21	1.69	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
10:LR:95:TRP:HZ3	10:LR:96:MET:HE2	1.69	0.57
13:B:420:HIS:C	13:B:798:LEU:HD13	2.29	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
6:Lh:57:VAL:O	6:Lh:61:ILE:HG13	2.04	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
4:1:197:A:N1	4:1:225:G:O2'	2.36	0.57
5:LY:34:LEU:HB3	5:LY:38:LEU:HB2	1.86	0.57
9:LU:20:LYS:C	9:LU:21:PHE:HD1	2.13	0.57
15:LE:116:TYR:CD1	16:Lr:90:LEU:HD11	2.40	0.57
5:LY:26:ARG:HB3	5:LY:30:MET:HE2	1.86	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
13:B:17:ILE:HG22	13:B:51:MET:HE3	1.86	0.57
14:LC:200:ARG:HG3	14:LC:201:ARG:HG3	1.86	0.57
14:LC:287:THR:O	16:Lr:4:HIS:NE2	2.36	0.57
16:Lr:60:VAL:HG22	16:Lr:117:ILE:HG21	1.87	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:Lh:21:LEU:HD11	6:Lh:61:ILE:HD12	1.87	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
3:D:80:THR:O	3:D:81:ALA:C	2.49	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
6:Lh:94:ARG:HD2	6:Lh:95:LEU:O	2.05	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
4:1:467: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
4:1:685:C:H3'	13:B:594:LYS:HZ2	1.71	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
4:1:232:G:H22	5:LY:61:HIS:CE1	2.24	0.56
7:LX:89:LYS:N	7:LX:89:LYS:HD3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:2:147:MET:HA	12:2:147:MET:HE3	1.88	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
1:8:78:G:O2'	6:Lh:42:SER:HA	2.06	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
10:LR:95:TRP:CG	10:LR:98:ARG:HH21	2.24	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
2:E:253:TYR:CD2	2:E:257:MET:HE3	2.41	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
12:2:37:SER:HB3	13:B:532:LYS:HZ2	1.70	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
8:A:99:SER:OG	8:A:101:ASN:OD1	2.21	0.55
13:B:835:LEU:HA	13:B:838:MET:CG	2.36	0.55
16:Lr:96:MET:N	16:Lr:96:MET:SD	2.79	0.55
11:Lk:65:ALA:CB	11:Lk:67:LYS:HZ1	2.20	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
9:LU:20:LYS:HZ3	9:LU:73:THR:HG23	1.70	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
5:LY:83:GLU:CD	5:LY:84:ARG:HB2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
8:A:215:MET:HA	8:A:215:MET:HE3	1.89	0.54
11:Lk:12:LEU:O	11:Lk:16:ARG:HG3	2.07	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
14:LC:155:GLU:HA	14:LC:254:GLU:CD	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:D:78:HIS:O	3:D:79:ARG:C	2.49	0.54
6:Lh:32:ARG:NH1	7:LX:80:PRO:HD3	2.23	0.54
8:A:215:MET:HE1	13:B:97:ASP:O	2.07	0.54
12:2:15:GLN:HE21	13:B:482:MET:HE3	1.73	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
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:101:MET:HE3	14:LC:102:PHE:N	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:47:C:O2'	1:8:62:A:OP2	2.20	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
4:1:691:C:H2'	4:1:692:A:H8	1.73	0.53
6:Lh:44:LEU:HD12	6:Lh:45:SER:N	2.23	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
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
14:LC:332:ALA:HA	14:LC:335:MET:HE3	1.91	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:115:GLN:H	13:B:115:GLN:CD	2.16	0.53
13:B:192:LEU:HB2	13:B:533:ILE:HG22	1.89	0.53
13:B:621:GLN:HG3	13:B:625:LYS:NZ	2.23	0.53
6:Lh:67:GLU:O	6:Lh:71:LYS:HG2	2.09	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
1:8:61:A:H3'	6:Lh:51:ARG:NH2	2.24	0.53
3:D:80:THR:C	3:D:82:THR:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:LYS:HZ1	5:LY:7:VAL:HB	1.74	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
6:Lh:27:GLU:OE2	6:Lh:50:VAL:HG21	2.09	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
14:LC:297:GLU:OE1	14:LC:297:GLU:N	2.25	0.52
5:LY:2:LYS:HZ3	5:LY:4:ASN:HB3	1.74	0.52
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
11:Lk:26:LYS:HD3	11:Lk:69:LEU:HD23	1.91	0.52
12:2:19:LEU:HG	13:B:482:MET:HE2	1.90	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
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
14:LC:177:TRP:CD1	14:LC:181:LYS:HZ1	2.27	0.52
14:LC:288:ASP:HA	16:Lr:4:HIS:CE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:ASP:C	13:B:94:LYS:HE2	2.34	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:93:LYS:HD2	3:D:97:VAL:HG11	1.92	0.52
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
6:Lh:10:ARG:NH1	6:Lh:63:GLN:OE1	2.43	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:253:TYR:O	2:E:257:MET:HE2	2.09	0.51
2:E:319:LYS:HD2	2:E:320:SER:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:492:U:H3'	4:1:493:G:H8	1.75	0.51
6:Lh:26:VAL:O	6:Lh:30:GLN:NE2	2.42	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
3:D:54:LYS:HZ2	3:D:61:GLN:HE22	1.59	0.51
4:1:2708:U:O2	10:LR:40:GLN:NE2	2.44	0.51
8:A:211:MET:HE1	13:B:83:TRP:HH2	1.74	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
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
16:Lr:41:ASN:OD1	16:Lr:44:ILE:HG13	2.11	0.51
4:1:485:C:O2	4:1:485:C:H2'	2.11	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
14:LC:321:ASN:C	14:LC:325:MET:HE3	2.36	0.51
15:LE:120:ASP:OD2	15:LE:121:VAL:N	2.44	0.51
1:8:64:U:H5''	6:Lh:52:LYS:HD3	1.92	0.51
3:D:115:VAL:CG1	3:D:146:MET:HE1	2.41	0.51
3:D:123:VAL:HA	3:D:133:THR:O	2.10	0.51
4:1:197:A:N3	4:1:222:C:O2'	2.32	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
14:LC:189:MET:HE2	14:LC:189:MET: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Lh:27:GLU:OE2	6:Lh:28:LEU:N	2.44	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
6:Lh:105:LYS:HA	6:Lh:108:GLN:NE2	2.27	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
15:LE:47:ASN:ND2	15:LE:62:MET:HE2	2.26	0.50
2:E:77:PRO:HG2	2:E:78:TRP:CD2	2.46	0.50
3:D:94:LYS:HB3	8:A:75:LYS:HZ2	1.75	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
6:Lh:35:LYS:HE2	6:Lh:43:LYS:NZ	2.26	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
6:Lh:25:LYS:HD2	7:LX:74:TYR:CG	2.47	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
13:B:130:LEU:HD21	13:B:160:LEU:C	2.37	0.50
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
8:A:96:ILE:HB	8:A:104:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:449:ALA:HA	13:B:452:MET:CG	2.42	0.50
13:B:821:GLU:CD	13:B:824:ARG:HE	2.19	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
6:Lh:27:GLU:HA	6:Lh:30:GLN:OE1	2.11	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: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
11:Lk:22:SER:OG	11:Lk:67:LYS:NZ	2.41	0.50
13:B:385:ASP:CG	13:B:417:ILE:HA	2.36	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
3:D:115:VAL:CB	3:D:146:MET:HE1	2.41	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
10:LR:7:GLN:H	10:LR:7:GLN:CD	2.20	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:292:ILE:O	14:LC:298:ILE:HD13	2.11	0.50
2:E:260:ILE:HG12	2:E:361:LEU:HD11	1.93	0.50
4:1:2696:A:H5'	11:Lk:70:LYS:HZ1	1.77	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
16:Lr:90:LEU:HA	16:Lr:93:ILE:HG12	1.94	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:253:TYR:CE2	2:E:257:MET:HE3	2.47	0.49
4:1:214:G:H2'	4:1:215:C:C6	2.47	0.49
10:LR:76:MET:HE2	10:LR:88:ARG:NH2	2.25	0.49
13:B:390:PRO:HB3	13:B:833:TYR:CD2	2.47	0.49
14:LC:135:ALA:O	14:LC:138:MET:HE3	2.12	0.49
2:E:94:MET:SD	2:E:191:LYS:NZ	2.86	0.49
4:1:2537:A:P	11:Lk:37:ARG:HH12	2.36	0.49
10:LR:9:ARG:HD2	10:LR:9:ARG:C	2.37	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
13:B:426:GLU:CD	13:B:429:ARG:HH21	2.19	0.49
16:Lr:3:ALA:CB	16:Lr:44:ILE:HD13	2.36	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
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
10:LR:95:TRP:CD1	10:LR:98:ARG:HH21	2.30	0.49
13:B:41:LYS:O	13:B:41:LYS:NZ	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:Lh:29:SER:HB2	6:Lh:32:ARG:NH2	2.28	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
6:Lh:88:THR:O	6:Lh:92:ARG:HG3	2.12	0.49
11:Lk:14:THR:HA	11:Lk:17:ARG:HG3	1.95	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
14:LC:34:PRO:HG3	16:Lr:9:VAL:HG13	1.94	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
11:Lk:57:LYS:HA	11:Lk:60:LEU:HD13	1.95	0.48
13:B:186:ASP:CG	13:B:189:TYR:H	2.21	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
3:D:87:LYS:HB3	8:A:83:LEU:HD22	1.94	0.48
4:1:2696:A:H62	11:Lk:35:LYS:HZ2	1.61	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
16:Lr:97:ILE:HD13	16:Lr:107:ARG:HA	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:Lh:80:PRO:O	6:Lh:84:ARG:HG3	2.13	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:422:GLY:C	13:B:834:ALA:HA	2.37	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
4:1:407:A:O2'	4:1:410:A:OP1	2.28	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
16:Lr:105:ASP:OD1	16:Lr:105:ASP:N	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:Lh:72:PHE:HD2	6:Lh:73:TYR:CE1	2.32	0.48
9:LU:50:ASN:HB2	9:LU:52:LYS:HZ3	1.79	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
4:1:2899:C:H2'	4:1:2900:U:C6	2.49	0.47
6:Lh:4:ILE:HG21	6:Lh:53:SER:HB3	1.95	0.47
6:Lh:96:ASN:HB2	6:Lh:99:GLU:OE1	2.14	0.47
8:A:187:GLN:HB2	13:B:108:LYS:HE2	1.96	0.47
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: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
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
3:D:88:LEU:O	8:A:80:MET:HE1	2.15	0.47
5:LY:81:TYR:C	5:LY:82:ILE:HD12	2.40	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
16:Lr:3:ALA:HA	16:Lr:44:ILE:HB	1.96	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: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:580:HIS:O	13:B:581:GLU:C	2.57	0.47
13:B:765:LEU:HG	13:B:769:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LE:190:HIS:CE1	15:LE:192:LYS:HE3	2.39	0.47
2:E:380:PRO:CD	2:E:383:MET:HE3	2.44	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
7:LX:118:ASP:C	7:LX:119:ILE:HD13	2.40	0.47
8:A:130:ASP:H	8:A:134:GLN:NE2	2.12	0.47
13:B:754:LEU:HB3	13:B:755:LYS:HZ2	1.78	0.47
14:LC:133:LEU:HD21	16:Lr:6:GLN:OE1	2.14	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
3:D:50:MET:HG2	3:D:54:LYS:HG3	1.95	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
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
13:B:83:TRP:NE1	13:B:109:TRP:HE1	2.13	0.47
13:B:631:ASP:OD1	13:B:631:ASP:C	2.58	0.47
13:B:679:PHE:O	13:B:691:MET:HE1	2.14	0.47
14:LC:7:LEU:HD12	14:LC:23:THR:HA	1.96	0.47
14:LC:259:LYS:HA	14:LC:262:GLU:CD	2.40	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
11:Lk:26:LYS:HB2	11:Lk:69:LEU:HD22	1.96	0.47
13:B:56:LEU:HD12	13:B:64:GLU:CD	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:B:579:GLU:O	13:B:580:HIS:C	2.58	0.47
14:LC:355:ALA:O	14:LC:359:ALA:N	2.39	0.47
16:Lr:16:PHE:HB3	16:Lr:27:THR:H	1.79	0.47
2:E:327:GLU:O	2:E:329:MET:HE2	2.14	0.46
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: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
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:78:LYS:HZ1	7:LX:101:ASP:H	1.63	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
11:Lk:65:ALA:HB3	11:Lk:67:LYS:HZ1	1.80	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
15:LE:94:LYS:HE2	15:LE:107:VAL:HG21	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Lh:29:SER:HA	6:Lh:32:ARG:HE	1.81	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
13:B:584:THR:O	13:B:585:ALA:C	2.57	0.46
16:Lr:30:ASN:O	16:Lr:42:GLY:HA3	2.16	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
6:Lh:65:GLN:NE2	6:Lh:66:LYS:HG2	2.31	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:621:GLN:C	13:B:625:LYS:HZ2	2.23	0.46
13:B:645:GLU:HG2	13:B:646:LYS:H	1.80	0.46
15:LE:116:TYR:CD2	16:Lr:115:SER:HA	2.50	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
6:Lh:32:ARG:HH11	7:LX:80:PRO:HD3	1.79	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: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
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: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
12:2:15:GLN:NE2	13:B:482:MET:HE3	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:Lk:53:ALA:O	11:Lk:57:LYS:NZ	2.49	0.46
12:2:130:ILE:HA	12:2:147:MET:HE1	1.98	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
8:A:207:VAL:O	8:A:211:MET:HE3	2.15	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:OP1	16:Lr:67:ARG:HD3	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Lh:82:ASP:OD1	7:LX:64:SER:HB3	2.16	0.45
9:LU:64:GLU:O	9:LU:70:ILE:HG13	2.17	0.45
11:Lk:27:LYS:HD2	11:Lk:28:ASN:O	2.16	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
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
6:Lh:102:LEU:O	6:Lh:103:LYS:HD3	2.17	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:332:LEU:HD13	13:B:338:LYS:HD3	1.96	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
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: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
6:Lh:16:GLU:O	6:Lh:20:GLN:HG2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:23:HIS:CG	13:B:23:HIS:O	2.69	0.45
13:B:83:TRP:CD1	13:B:109:TRP:HE1	2.35	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
5:LY:32:SER:OG	5:LY:101:PRO:O	2.27	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
6:Lh:13:LYS:N	6:Lh:16:GLU:OE2	2.45	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
14:LC:297:GLU:H	14:LC:297:GLU:CD	2.19	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:154:LEU:HD23	10:LR:154:LEU:C	2.42	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
6:Lh:74:LYS:HE2	6:Lh:74:LYS:HB2	1.53	0.45
8:A:112:TYR:HB2	8:A:121:ILE:HG12	1.99	0.45
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
13:B:708:LEU:HG	13:B:712:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LE:119:GLU:N	15:LE:119:GLU:OE1	2.50	0.45
2:E:156:MET:CE	2:E:166:ILE:HA	2.42	0.44
4:1:2373:C:H2'	4:1:2374:A:C8	2.52	0.44
6:Lh:35:LYS:HE2	6:Lh:43:LYS:HZ3	1.82	0.44
6:Lh:78:TYR:HB3	7:LX:60:TYR:HB3	2.00	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
13:B:430:TRP:HB3	13:B:431:MET:HE2	1.99	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
12:2:130:ILE:CG1	12:2:147:MET:HE1	2.45	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
16:Lr:82:ILE:CG2	16:Lr:89:THR:HG22	2.47	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: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
13:B:585:ALA:O	13:B:586:ASN:C	2.60	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
16:Lr:28:GLU:OE1	16:Lr:28:GLU:N	2.27	0.44
2:E:78:TRP:CZ3	2:E:89:PRO:HG3	2.52	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:64:ALA:HB1	14:LC:78:ARG:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:Lk:12:LEU:HB2	11:Lk:16:ARG:NH2	2.33	0.44
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
16:Lr:38:PHE:O	16:Lr:45:HIS:NE2	2.48	0.44
16:Lr:51:VAL:HG12	16:Lr:62:VAL:HG22	1.99	0.44
2:E:87:LEU:HB2	2:E:199:GLU:OE2	2.18	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
6:Lh:49:VAL:O	6:Lh:53:SER:OG	2.21	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: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
6:Lh:29:SER:HB2	6:Lh:32:ARG:HH21	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
11:Lk:53:ALA:O	11:Lk:57:LYS:HG2	2.17	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
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
6:Lh:19:LYS:HA	6:Lh:22:ASP:OD2	2.18	0.44
6:Lh:25:LYS:O	6:Lh:28:LEU:HD12	2.17	0.44
6:Lh:80:PRO:HD2	6:Lh:83:LEU:HD12	2.00	0.44
7:LX:55:ARG:HE	7:LX:56:ARG:N	2.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:380:PRO:CG	2:E:383:MET:HE3	2.47	0.44
3:D:108:MET:HE2	8:A:94:VAL:HG22	1.99	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
11:Lk:17:ARG:HA	11:Lk:18:LYS:HZ2	1.83	0.44
13:B:691:MET:HG3	13:B:715:LEU:HD23	1.99	0.44
14:LC:289:LEU:N	16:Lr:4:HIS:CE1	2.84	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
8:A:211:MET:HE2	8:A:211:MET:N	2.32	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
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
11:Lk:12:LEU:H	11:Lk:12:LEU:HD12	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:458:ILE:HD12	13:B:495:TYR:CE1	2.53	0.43
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
6:Lh:74:LYS:HG3	6:Lh:75:GLY:N	2.33	0.43
6:Lh:106:LYS:HB3	6:Lh:107:GLN:OE1	2.18	0.43
7:LX:72:ASP:C	7:LX:72:ASP:OD2	2.61	0.43
7:LX:94:ASN:ND2	7:LX:145:ASP:HA	2.07	0.43
10:LR:119:MET:HB3	10:LR:119:MET:HE2	1.83	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
16:Lr:85:ASN:OD1	16:Lr:86:ALA:N	2.52	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
16:Lr:79:ARG:HH22	16:Lr:81:THR:HB	1.84	0.43
3:D:151:LEU:CD1	3:D:162:LEU:HD13	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:Lh:85:PRO:O	6:Lh:87:LYS:NZ	2.51	0.43
11:Lk:51:GLU:C	11:Lk:55:LYS:HZ1	2.26	0.43
11:Lk:70:LYS:HA	11:Lk:70:LYS:HE3	2.01	0.43
12:2:91:MET:HE3	12:2:92:ASP:N	2.33	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
3:D:115:VAL:HG11	3:D:146:MET:HE1	2.01	0.43
4:1:460:C:H2'	4:1:461:G:H8	1.83	0.43
6:Lh:30:GLN:CD	6:Lh:30:GLN:H	2.27	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:85:VAL:HG22	5:LY:97:VAL:HB	2.00	0.43
6:Lh:16:GLU:OE1	6:Lh:16:GLU:N	2.43	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
11:Lk:9:LYS:HE2	11:Lk:12:LEU:HD13	2.01	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
14:LC:138:MET:SD	14:LC:138:MET:C	3.02	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
5:LY:47:MET:HE2	5:LY:47:MET:HA	2.00	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
13:B:626:LYS:HD2	13:B:626:LYS:C	2.43	0.42
14:LC:101:MET:HE3	14:LC:102:PHE:H	1.84	0.42
15:LE:99:ASP:C	15:LE:99:ASP:OD1	2.62	0.42
16:Lr:28:GLU:HB2	16:Lr:43:LEU:HD23	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:239:C:H2'	4:1:240:G:C8	2.54	0.42
5:LY:2:LYS:NZ	5:LY:4:ASN:HB3	2.33	0.42
13:B:693:GLN:O	13:B:696:LYS:HE3	2.19	0.42
16:Lr:95:HIS:O	16:Lr:99:LYS:HB2	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
5:LY:100:HIS:CD2	5:LY:102:SER:HB3	2.54	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:415:ALA:CB	13:B:431:MET:HE3	2.47	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
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
3:D:81:ALA:O	3:D:82:THR:C	2.62	0.42
4:1:224:U:OP1	14:LC:163:LYS:NZ	2.50	0.42
4:1:2385:U:H4'	10:LR:5:ARG:NH2	2.35	0.42
4:1:2696:A:H62	11:Lk:35:LYS:NZ	2.17	0.42
6:Lh:15:GLU:HA	6:Lh:18:LEU:HG	2.00	0.42
6:Lh:55:ALA:O	6:Lh:59:THR:OG1	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
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
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
16:Lr:20:ARG:HG2	16:Lr:21:ASN:CG	2.45	0.42
1:8:45:C:H2'	1:8:46:G:H8	1.84	0.42
3:D:124:GLN:N	3:D:124:GLN:CD	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LY:37:GLU:OE1	5:LY:41:LYS:HD2	2.19	0.42
6:Lh:21:LEU:HD21	6:Lh:57:VAL:HG13	1.94	0.42
6:Lh:73:TYR:CD1	6:Lh:76:LYS:HD2	2.55	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
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:164:TYR:CE1	13:B:202:GLU:HB2	2.54	0.42
13:B:485:MET:HE3	13:B:485:MET:HB2	1.82	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
16:Lr:103:ARG:NH2	16:Lr:105:ASP:OD2	2.34	0.42
2:E:297:HIS:CG	2:E:298:LYS:N	2.86	0.42
3:D:147:LEU:HD13	3:D:151:LEU:HD21	2.02	0.42
6:Lh:70:ARG:HB2	6:Lh:71:LYS:NZ	2.34	0.42
6:Lh:103:LYS:HD3	6:Lh:103:LYS:HA	1.79	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:456:ASN:HB3	13:B:498:MET:HE1	2.01	0.42
13:B:732:VAL:O	13:B:736:GLU:HG2	2.20	0.42
14:LC:101:MET:HE3	14:LC:102:PHE:HB3	2.02	0.42
1:8:65:A:OP2	6:Lh:52:LYS:NZ	2.53	0.42
4:1:381:U:H2'	4:1:382:G:O4'	2.20	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
9:LU:38:ASN:HA	9:LU:41:GLN:CD	2.45	0.42
10:LR:123:LEU:O	10:LR:127:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
6:Lh:85:PRO:HB2	6:Lh:87:LYS:HD3	2.01	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:113:ASN:CG	13:B:116:ILE:HG13	2.45	0.42
13:B:672:ILE:HD11	13:B:698:ALA:HB1	2.02	0.42
14:LC:174:LEU:C	14:LC:175:LYS:HZ3	2.28	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
12:2:28:MET:HG2	12:2:32:PHE:HE1	1.84	0.42
12:2:28:MET:HE2	13:B:483:GLN:CD	2.45	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
5:LY:124:LYS:C	5:LY:124:LYS:HD3	2.45	0.41
6:Lh:13:LYS:HB3	6:Lh:13:LYS:HE3	1.85	0.41
7:LX:87:MET:HA	7:LX:90:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:2:147:MET:N	12:2:147:MET:SD	2.93	0.41
13:B:430:TRP:HD1	13:B:431:MET:HE1	1.85	0.41
15:LE:57:TYR:HB2	15:LE:62:MET:SD	2.60	0.41
1:8:65:A:P	6:Lh:52:LYS:HZ2	2.43	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
13:B:691:MET:HA	13:B:691:MET:HE2	2.01	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
2:E:329:MET:HE1	2:E:356:GLN:OE1	2.20	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
16:Lr:49:VAL:HB	16:Lr:106:LEU:HD12	2.02	0.41
1:8:90:C:H2'	1:8:91:A:H8	1.84	0.41
3:D:75:LYS:HZ2	9:LU:117:ILE:C	2.28	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:174:PHE:O	13:B:177:THR:OG1	2.21	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:606:ALA:HA	13:B:609:GLU:CD	2.46	0.41
13:B:632:ASP:OD2	13:B:632:ASP:C	2.63	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
6:Lh:72:PHE:CD2	6:Lh:73:TYR:CE1	3.08	0.41
7:LX:77:ILE:HD12	7:LX:78:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Lk:54:GLU:H	11:Lk:54:GLU:CD	2.29	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
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
12:2:51:LYS:HZ1	13:B:551:HIS:HE1	1.69	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
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
11:Lk:34:PHE:CE2	11:Lk:56:LEU:HD22	2.56	0.41
11:Lk:50:LYS:N	11:Lk:50:LYS:HD3	2.35	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
16:Lr:47:LYS:HB2	16:Lr:102:TYR:CZ	2.55	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
13:B:646:LYS:C	13:B:646:LYS:HD3	2.46	0.41
13:B:709:HIS:HA	13:B:712:MET:HE3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:Lh:64:THR:O	6:Lh:67:GLU:HG3	2.21	0.41
6:Lh:95:LEU:HB3	6:Lh:99:GLU:HB2	2.02	0.41
8:A:126:ALA:C	8:A:127:LYS:HG3	2.45	0.41
8:A:177:GLU:CG	8:A:180:ASP:HB2	2.47	0.41
11:Lk:27:LYS:H	11:Lk:70:LYS:HD3	1.85	0.41
11:Lk:33:LYS:HG2	11:Lk:46:VAL:HG22	2.03	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:176:LYS:HD2	13:B:176:LYS:C	2.46	0.41
13:B:195:TYR:CD1	13:B:535:LEU:HG	2.56	0.41
13:B:294:ARG:C	13:B:297:PRO:HD2	2.46	0.41
13:B:311:ASP:OD1	13:B:349:TYR:OH	2.25	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:46:SER:O	5:LY:47:MET:HE2	2.21	0.41
5:LY:113:LYS:HA	5:LY:116:LYS:HE3	2.03	0.41
6:Lh:25:LYS:HE3	6:Lh:25:LYS:HB3	1.97	0.41
6:Lh:31:LEU:HB3	6:Lh:35:LYS:HE3	2.02	0.41
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
9:LU:66:SER:C	9:LU:68:SER:H	2.29	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
15:LE:220:LYS:HD2	15:LE:220:LYS:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:B:734:LYS:HA	13:B:737:MET:HE2	2.03	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
16:Lr:52:GLU:OE2	16:Lr:61:VAL:HB	2.21	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:163:ASP:HB3	13:B:166:MET:HE1	2.03	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
6:Lh:32:ARG:H	6:Lh:32:ARG:HG3	1.74	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: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
1:8:90:C:HO2'	5:LY:24:HIS:CE1	2.39	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
4:1:2692:U:H5'	11:Lk:4:LYS:HD2	2.03	0.40
5:LY:84:ARG:CZ	5:LY:86:GLN:OE1	2.69	0.40
6:Lh:88:THR:O	6:Lh:91:MET:SD	2.80	0.40
9:LU:21:PHE:HD1	9:LU:21:PHE:N	2.20	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:139:MET:HE1	2:E:228:TYR:HB3	2.04	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:245:ASP:HA	13:B:248:ARG:HG2	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%)	36	71
3	D	120/206 (58%)	104 (87%)	12 (10%)	4 (3%)	3	21
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%)	7	35
9	LU	99/128 (77%)	94 (95%)	5 (5%)	0	100	100
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%)	21	58
13	B	832/840 (99%)	779 (94%)	43 (5%)	10 (1%)	10	42
14	LC	363/427 (85%)	346 (95%)	17 (5%)	0	100	100
15	LE	208/288 (72%)	195 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
All	All	2927/3500 (84%)	2778 (95%)	131 (4%)	18 (1%)	23	58

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 ⓘ

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%)	270 (100%)	1 (0%)	84	83
3	D	102/165 (62%)	99 (97%)	3 (3%)	37	58
5	LY	120/135 (89%)	119 (99%)	1 (1%)	73	78
6	Lh	109/110 (99%)	106 (97%)	3 (3%)	38	59
7	LX	104/133 (78%)	98 (94%)	6 (6%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A	107/186 (58%)	106 (99%)	1 (1%)	70	76
9	LU	91/115 (79%)	85 (93%)	6 (7%)	15	37
10	LR	137/175 (78%)	129 (94%)	8 (6%)	18	40
11	Lk	64/65 (98%)	64 (100%)	0	100	100
12	2	148/149 (99%)	145 (98%)	3 (2%)	48	66
13	B	744/749 (99%)	730 (98%)	14 (2%)	50	66
14	LC	304/348 (87%)	297 (98%)	7 (2%)	44	63
15	LE	190/252 (75%)	186 (98%)	4 (2%)	47	65
16	Lr	109/121 (90%)	108 (99%)	1 (1%)	70	76
All	All	2600/3036 (86%)	2542 (98%)	58 (2%)	45	64

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	377	SER
3	D	55	LEU
3	D	76	VAL
3	D	95	LEU
5	LY	35	SER
6	Lh	20	GLN
6	Lh	23	ASP
6	Lh	43	LYS
7	LX	73	HIS
7	LX	77	ILE
7	LX	100	VAL
7	LX	116	LEU
7	LX	128	ILE
7	LX	138	VAL
8	A	148	GLU
9	LU	20	LYS
9	LU	21	PHE
9	LU	50	ASN
9	LU	72	VAL
9	LU	76	VAL
9	LU	96	LEU
10	LR	30	ASN
10	LR	34	ASN
10	LR	40	GLN
10	LR	51	ILE

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Mol	Chain	Res	Type
10	LR	76	MET
10	LR	89	MET
10	LR	111	GLU
10	LR	152	LYS
12	2	26	TYR
12	2	93	GLN
12	2	103	ASN
13	B	91	ARG
13	B	408	ILE
13	B	452	MET
13	B	575	ASP
13	B	579	GLU
13	B	587	MET
13	B	592	LEU
13	B	610	GLU
13	B	630	ASP
13	B	634	GLU
13	B	646	LYS
13	B	647	LEU
13	B	650	VAL
13	B	810	ASP
14	LC	52	TYR
14	LC	55	SER
14	LC	118	THR
14	LC	211	TYR
14	LC	262	GLU
14	LC	274	LYS
14	LC	313	VAL
15	LE	116	TYR
15	LE	154	THR
15	LE	240	TYR
15	LE	282	TYR
16	Lr	21	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	74	ASN
2	E	178	ASN
2	E	188	ASN
2	E	218	ASN
2	E	258	GLN

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Mol	Chain	Res	Type
2	E	274	ASN
2	E	281	GLN
2	E	381	HIS
3	D	61	GLN
3	D	89	GLN
5	LY	40	GLN
5	LY	61	HIS
5	LY	96	HIS
5	LY	100	HIS
6	Lh	62	ASN
6	Lh	96	ASN
7	LX	93	ASN
7	LX	94	ASN
8	A	69	GLN
8	A	146	GLN
8	A	208	ASN
10	LR	30	ASN
10	LR	75	HIS
12	2	15	GLN
12	2	69	HIS
12	2	71	HIS
13	B	23	HIS
13	B	25	GLN
13	B	105	ASN
13	B	478	ASN
13	B	480	ASN
13	B	514	HIS
13	B	522	GLN
13	B	526	HIS
13	B	551	HIS
13	B	577	ASN
13	B	621	GLN
13	B	717	ASN
13	B	757	ASN
13	B	797	ASN
13	B	828	HIS
14	LC	245	HIS
14	LC	299	GLN
15	LE	190	HIS
15	LE	245	GLN

5.3.3 RNA ⓘ

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
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

Continued on next page...

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Mol	Chain	Res	Type
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
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

Continued on next page...

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Mol	Chain	Res	Type
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 oligosaccharides 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	0.80	0	60,60,60	0.50	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-C4-O14-P4
17	B	901	IHP	C3-C4-O14-P4
17	B	901	IHP	C5-O15-P5-O35
17	B	901	IHP	C1-O11-P1-O21
17	B	901	IHP	C2-O12-P2-O42

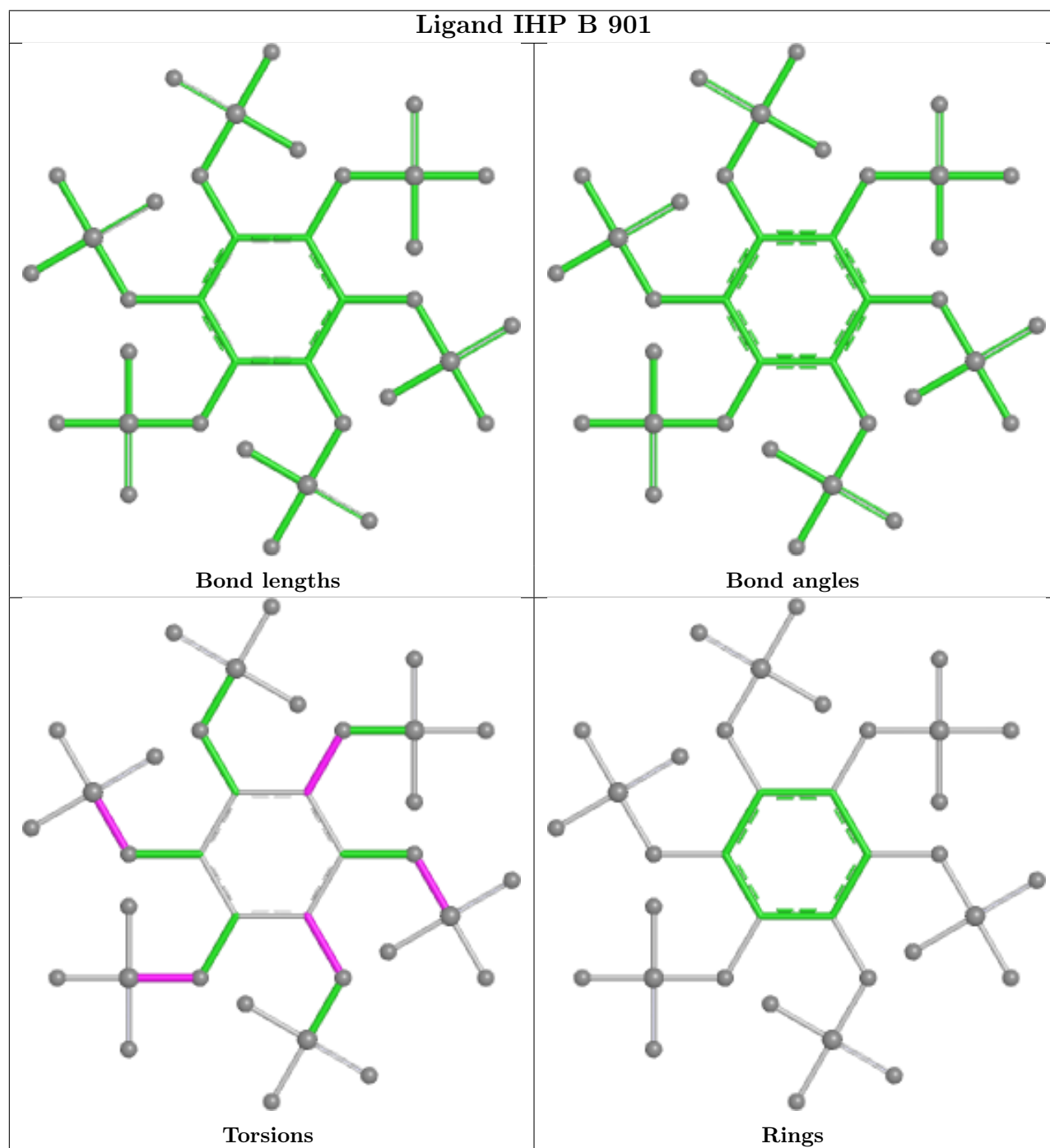
There are no ring outliers.

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 ⓘ

There are no chain breaks in this entry.

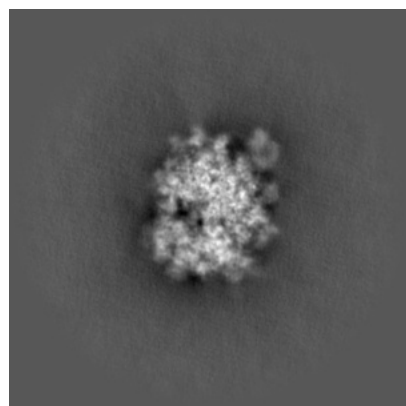
6 Map visualisation [i](#)

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.

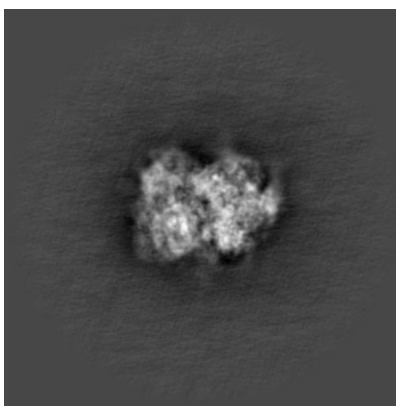
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

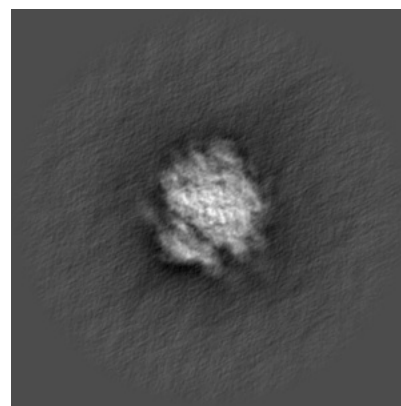
6.1.1 Primary map



X

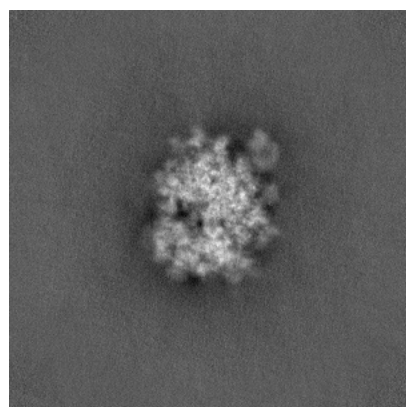


Y

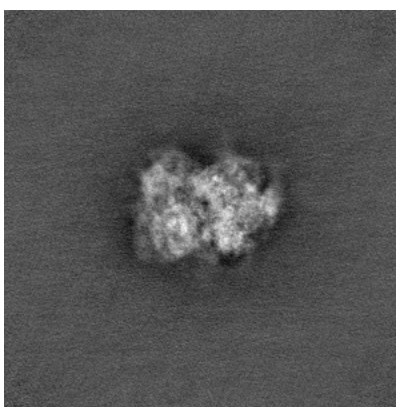


Z

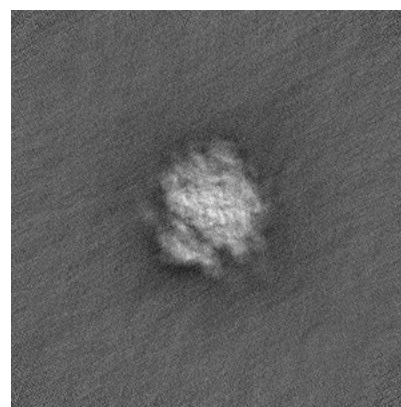
6.1.2 Raw map



X



Y

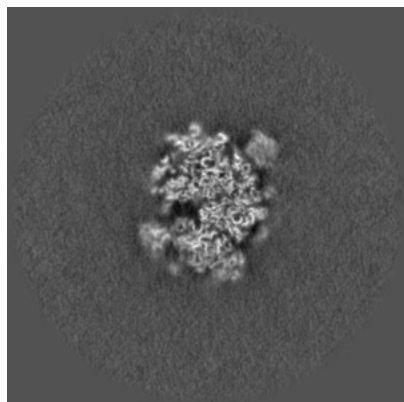


Z

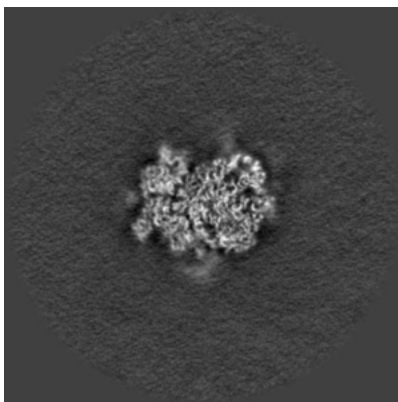
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

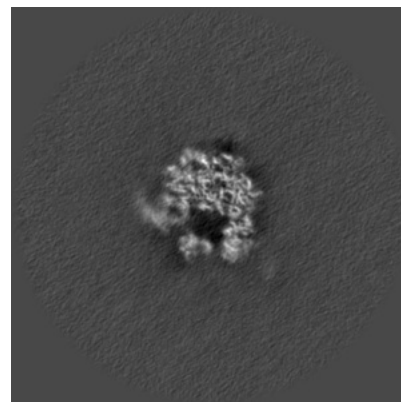
6.2.1 Primary map



X Index: 320

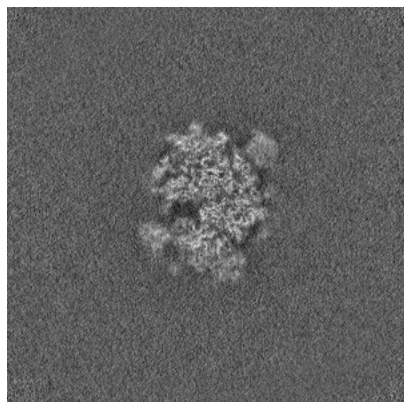


Y Index: 320

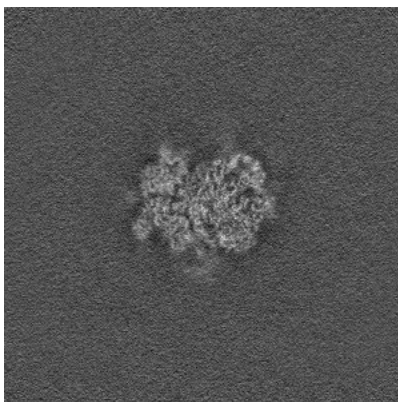


Z Index: 320

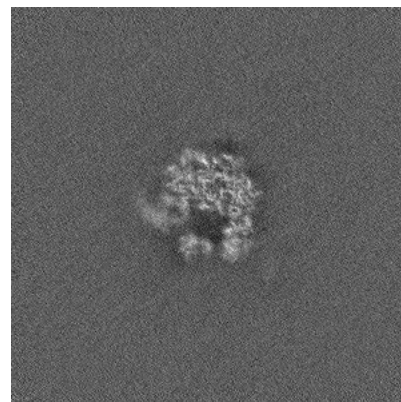
6.2.2 Raw map



X Index: 320



Y Index: 320

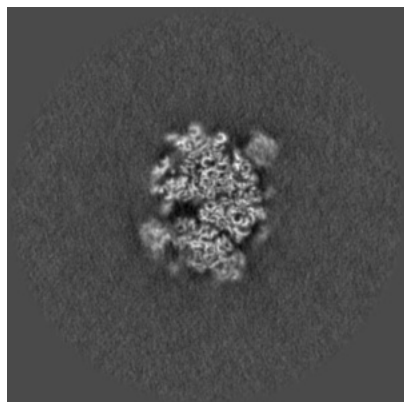


Z Index: 320

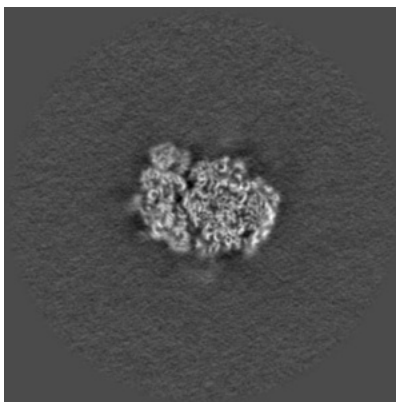
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

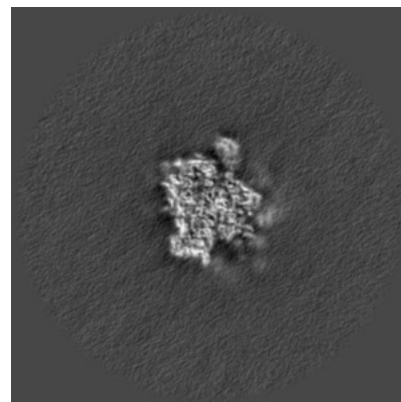
6.3.1 Primary map



X Index: 318

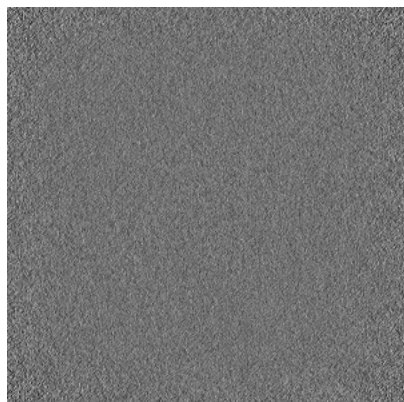


Y Index: 336

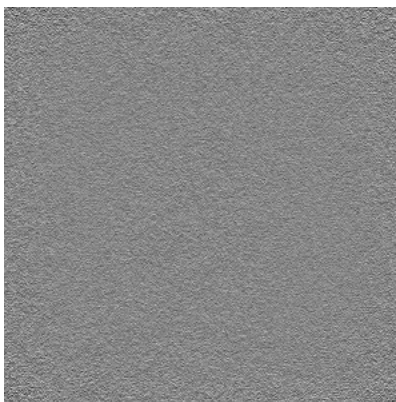


Z Index: 355

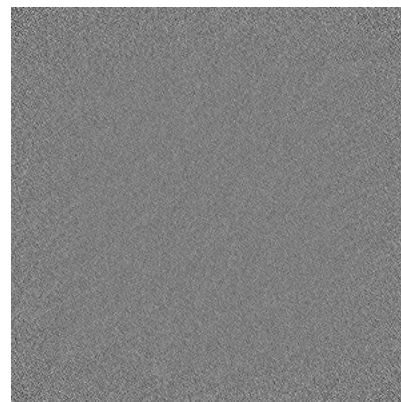
6.3.2 Raw map



X Index: 0



Y Index: 0

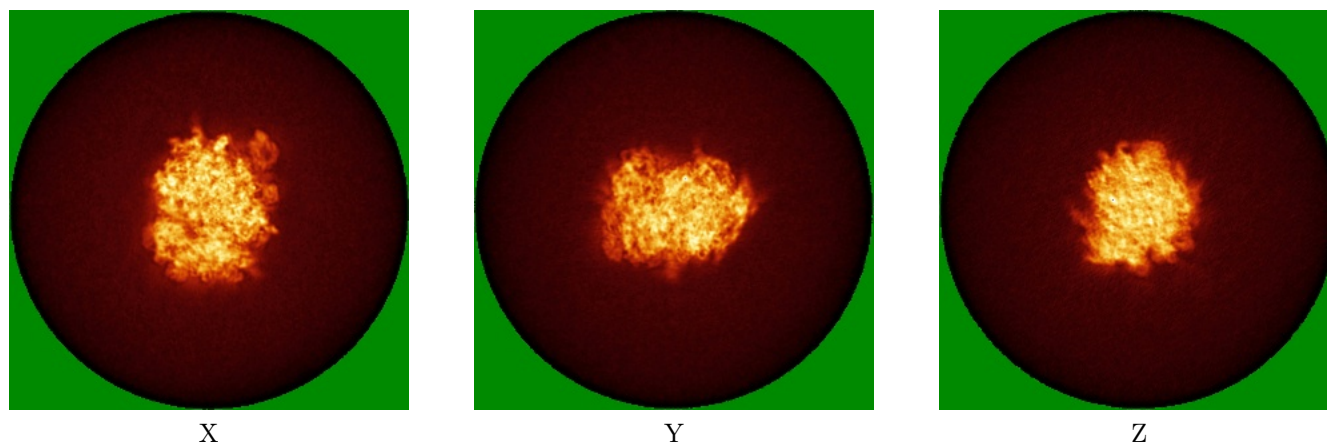


Z Index: 639

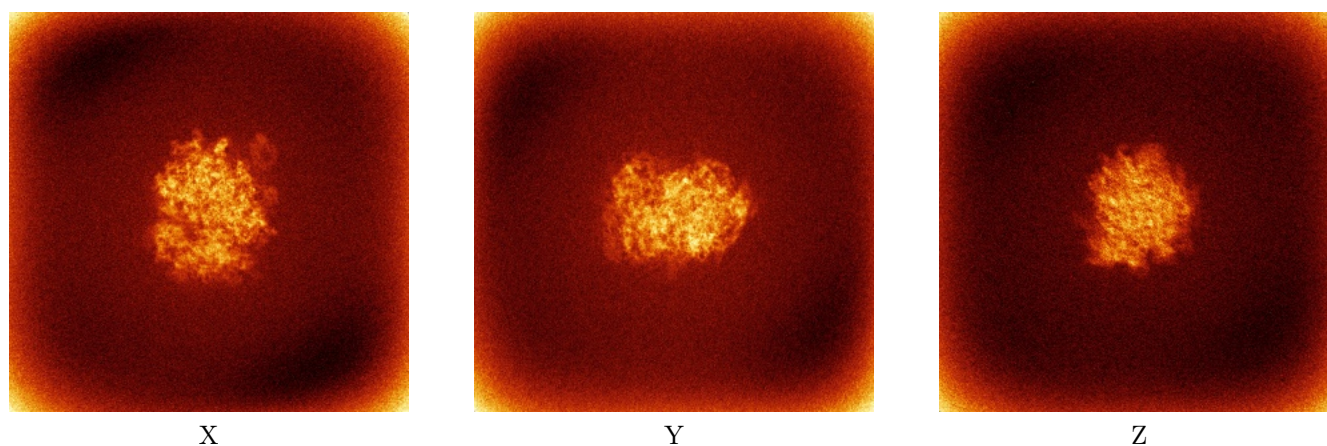
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

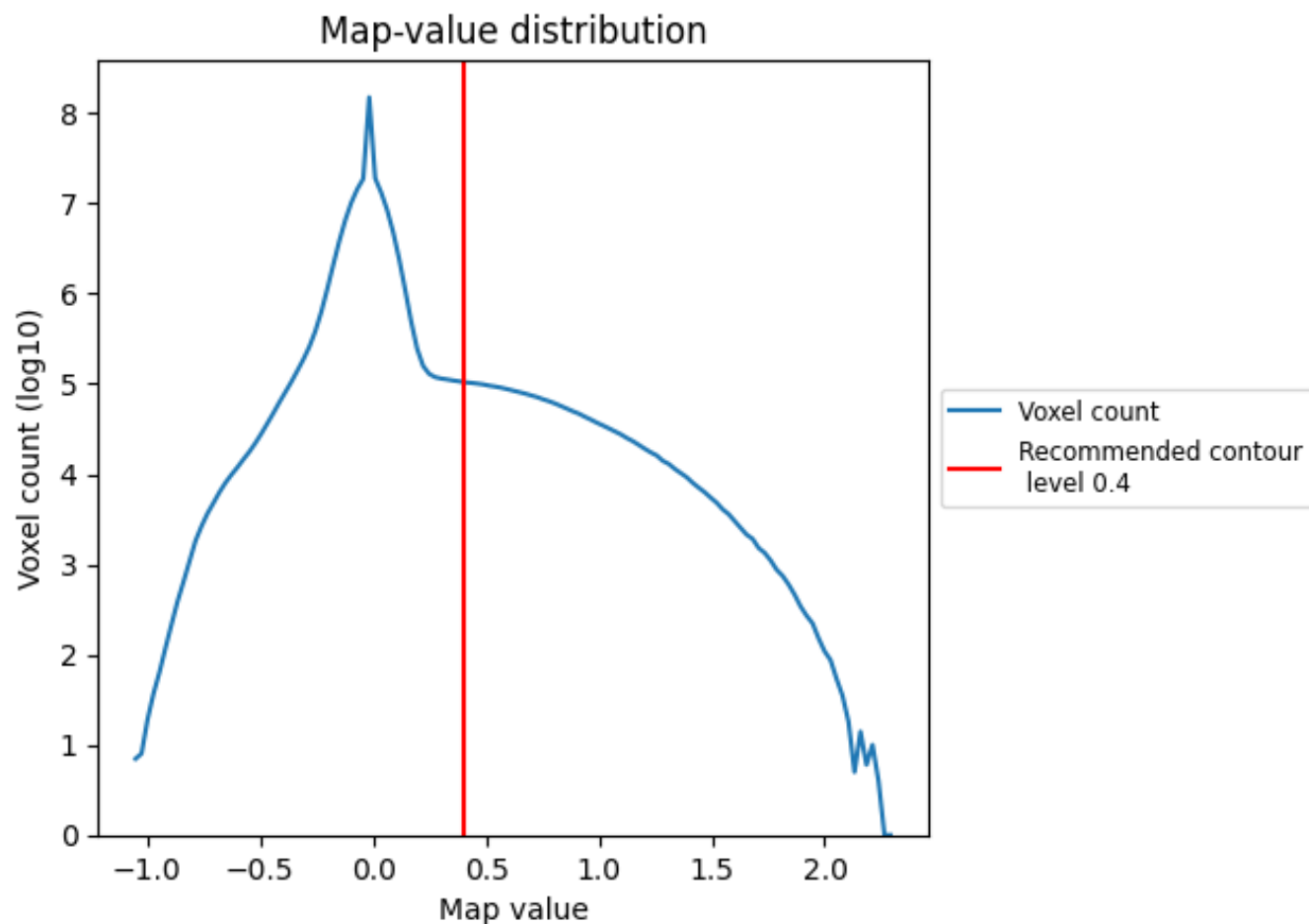
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

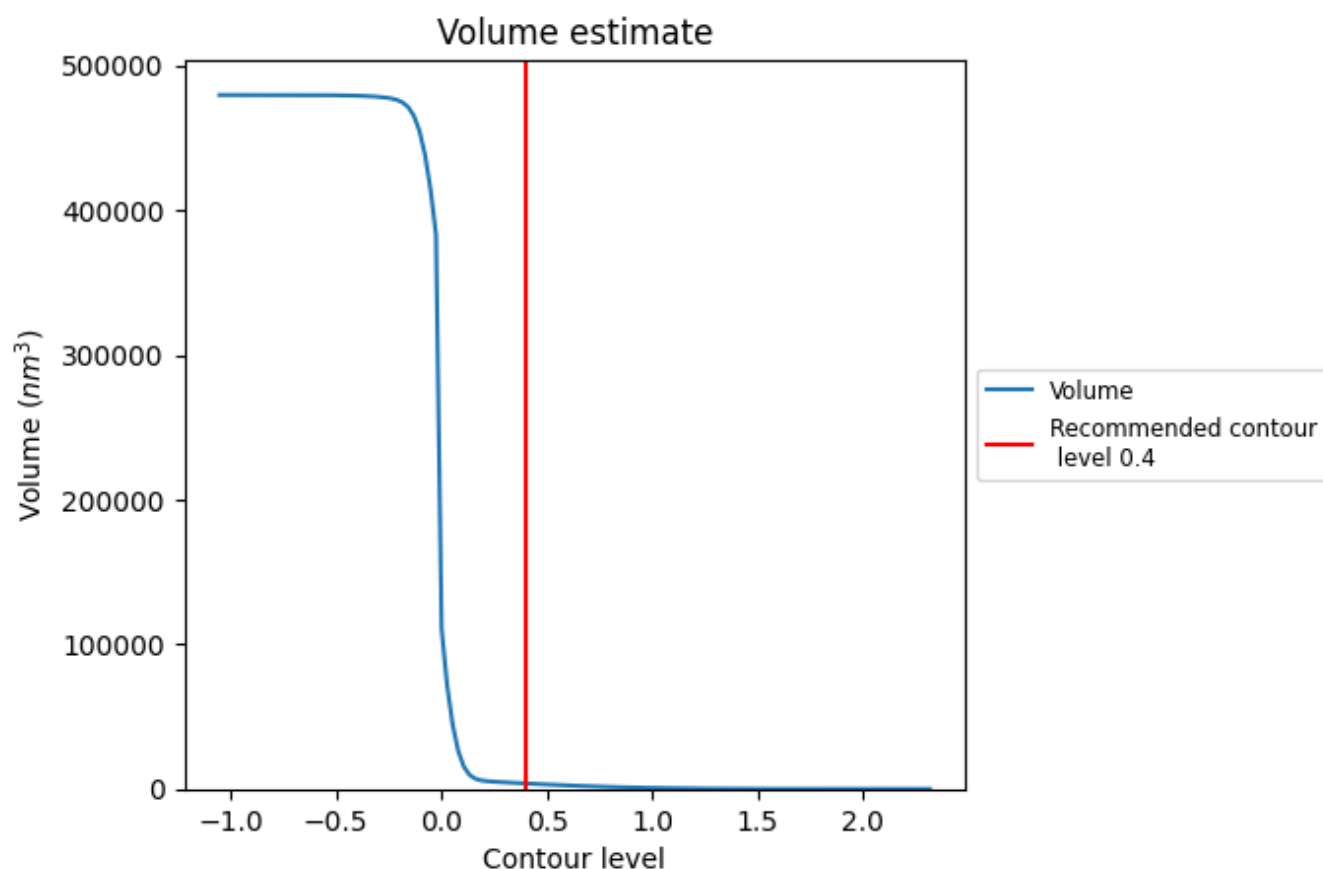
This section contains the results of statistical analysis of the map.

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.

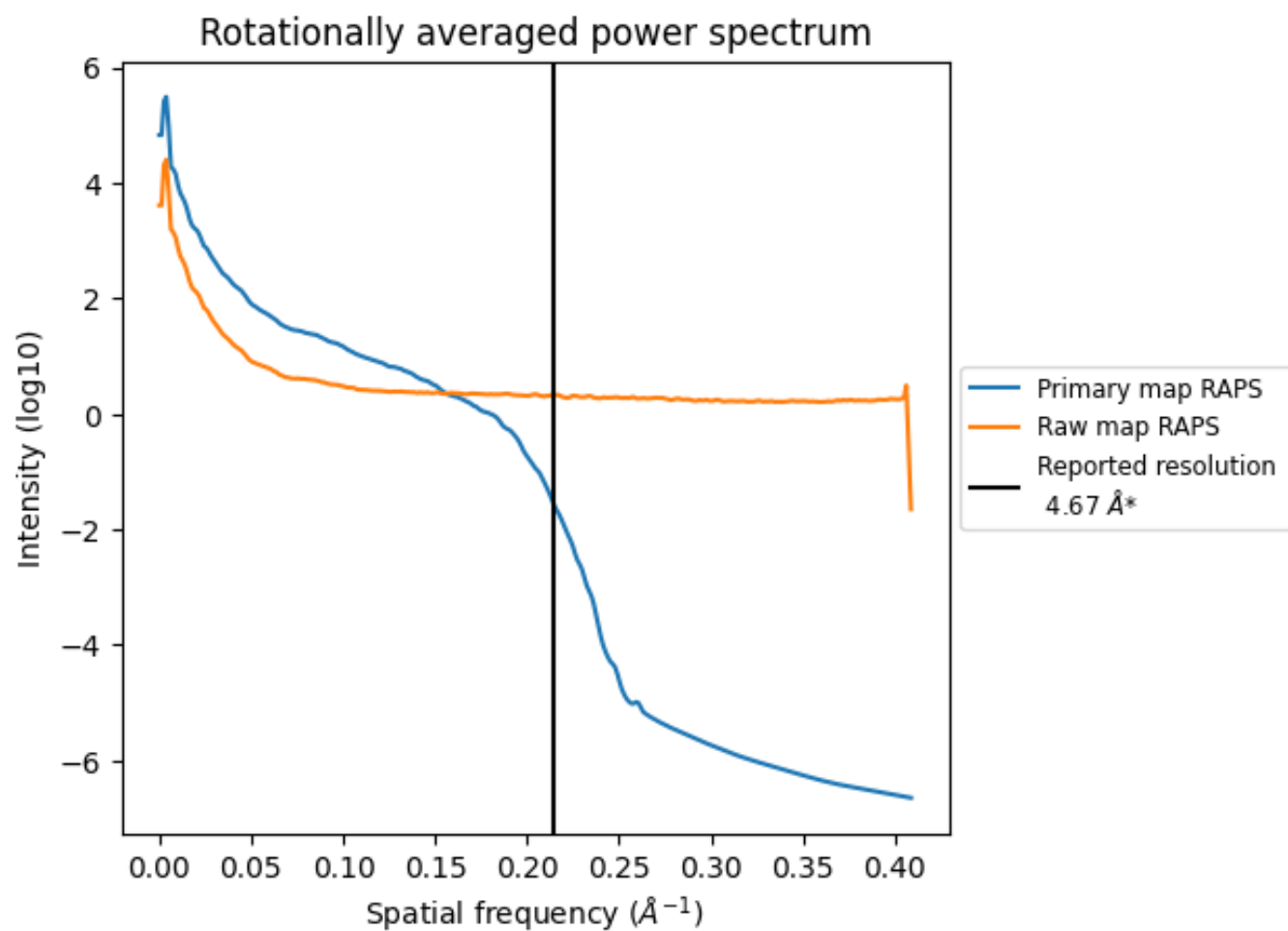
7.2 Volume estimate [i](#)



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 ⓘ

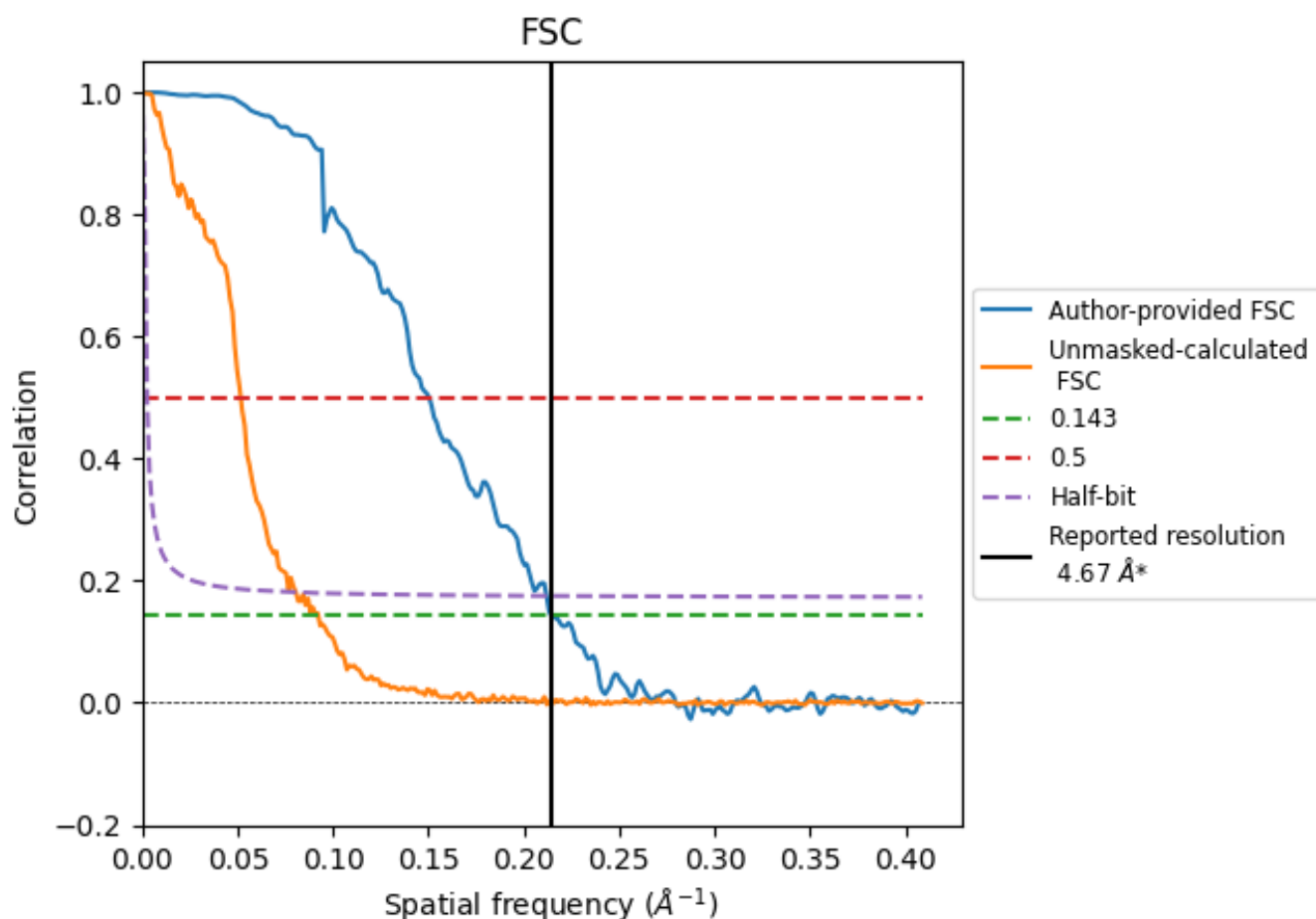


*Reported resolution corresponds to spatial frequency of 0.214 $\text{\AA}^{-1}$

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

8.2 Resolution estimates [i](#)

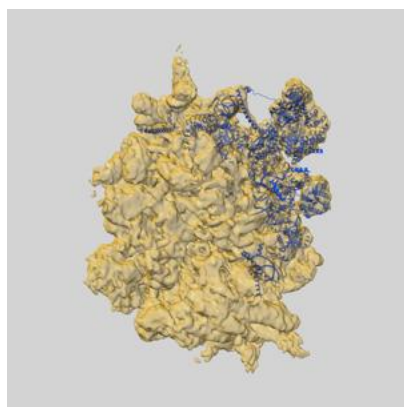
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.67	-	-
Author-provided FSC curve	4.67	6.65	4.72
Unmasked-calculated*	10.85	19.38	12.42

*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 %

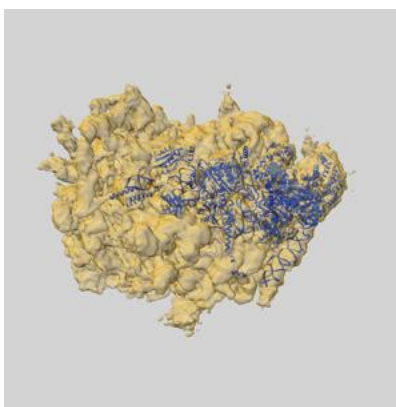
9 Map-model fit [i](#)

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](#).

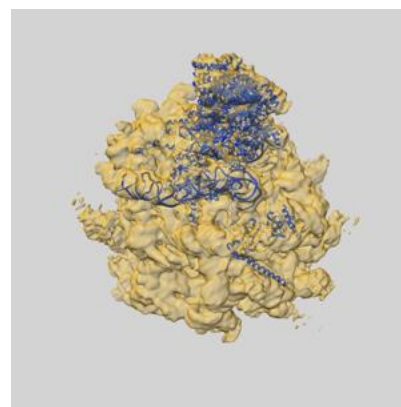
9.1 Map-model overlay [i](#)



X



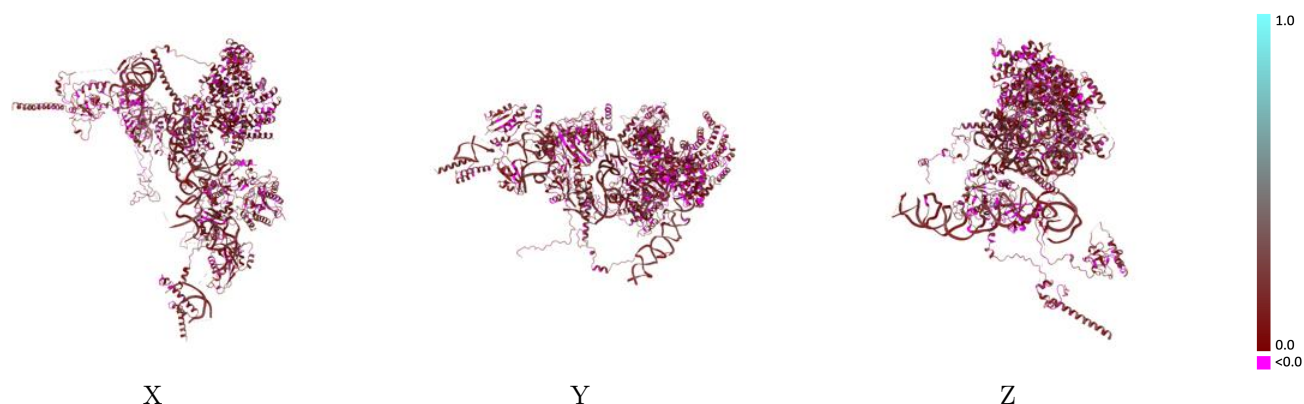
Y



Z

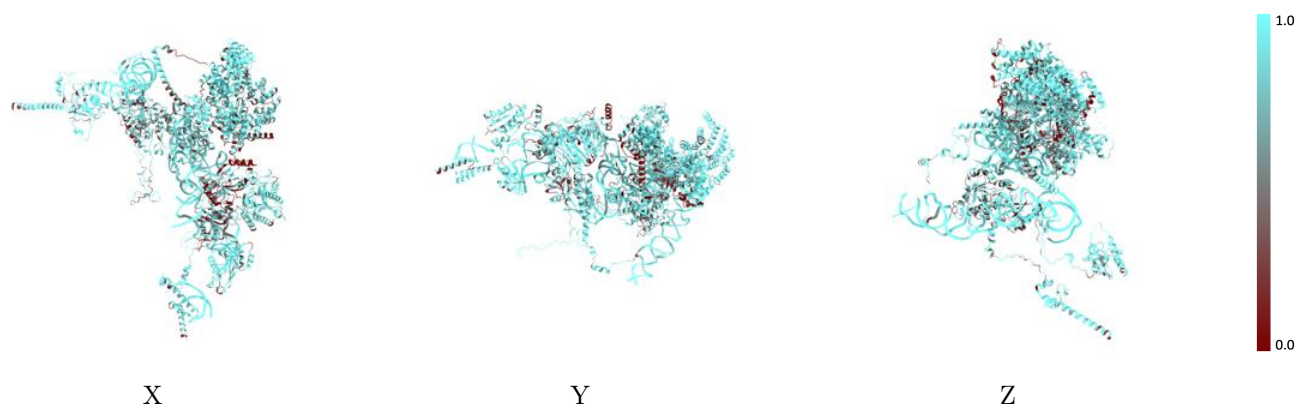
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



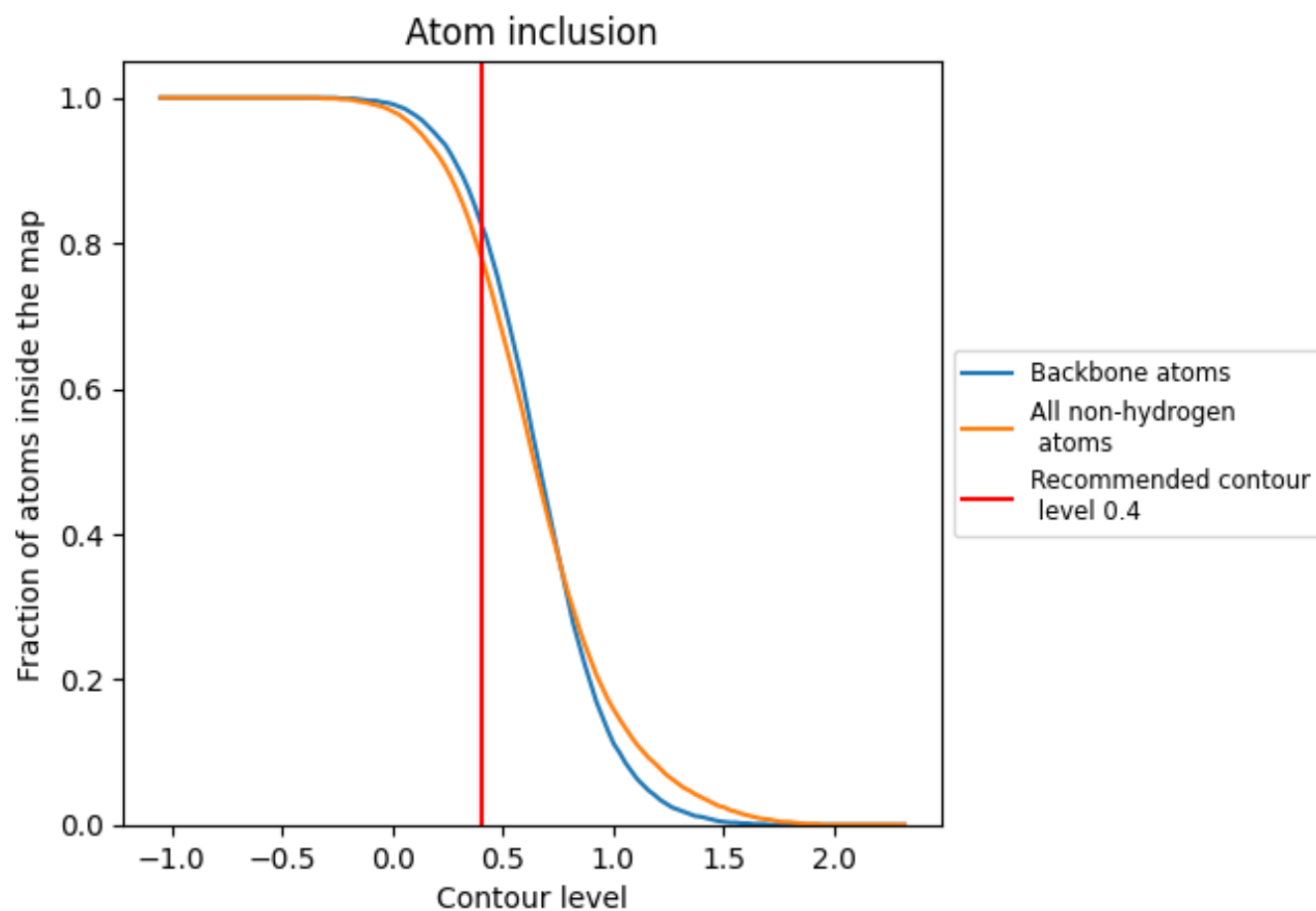
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

