



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:50 PM UTC

PDB ID : 5U07 / pdb_00005u07
EMDB ID : EMD-8477
Title : CRISPR RNA-guided surveillance complex
Authors : Xiao, Y.; Luo, M.; Hayes, R.P.; Kim, J.; Ng, S.; Ding, F.; Liao, M.; Ke, A.
Deposited on : 2016-11-23
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

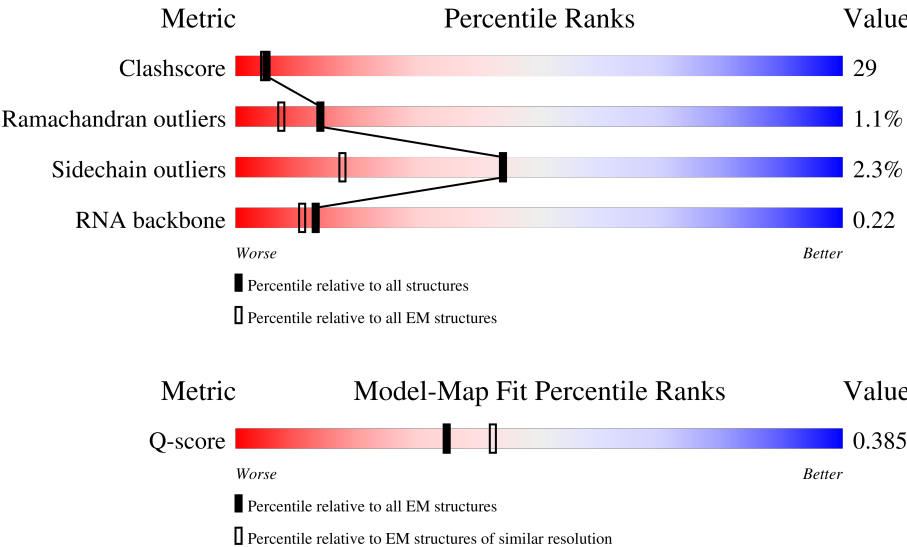
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	10198 (3.30 - 4.30)

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	A	232	82% 34% 44% 18%
2	B	244	66% 26% 36% 34%
2	J	244	69% 28% 35% 7% 30%

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Mol	Chain	Length	Quality of chain
3	C	549	
4	D	373	
4	E	373	
4	F	373	
4	G	373	
4	H	373	
4	I	373	
5	K	61	
6	M	21	
7	N	254	
8	O	13	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CRISPR-associated protein, Cse3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	190	Total	C	N	O	S	0	0
			1471	909	303	258	1		

- Molecule 2 is a protein called Cse2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	161	Total	C	N	O	S	0	0
			1285	811	256	216	2		
2	J	170	Total	C	N	O	S	0	0
			1319	831	261	225	2		

- Molecule 3 is a protein called CRISPR-associated protein, Cse1 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	493	Total	C	N	O	S	0	0
			3880	2466	709	696	9		

- Molecule 4 is a protein called CRISPR-associated protein, Cse4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	260	Total	C	N	O	S	0	0
			2017	1266	356	390	5		
4	E	367	Total	C	N	O	S	0	0
			2828	1775	507	541	5		
4	F	367	Total	C	N	O	S	0	0
			2834	1777	509	543	5		
4	G	366	Total	C	N	O	S	0	0
			2823	1769	505	544	5		
4	H	366	Total	C	N	O	S	0	0
			2829	1772	508	544	5		
4	I	329	Total	C	N	O	S	0	0
			2544	1595	459	487	3		

- Molecule 5 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	59	Total	C	N	O	P	0	0
			1267	565	235	409	58		

- Molecule 6 is a DNA chain called Target Strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	21	Total	C	N	O	P	0	0
			425	203	70	131	21		

- Molecule 7 is a protein called CRISPR-associated protein, Cas5e family.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	241	Total	C	N	O	S	0	0
			1891	1201	343	344	3		

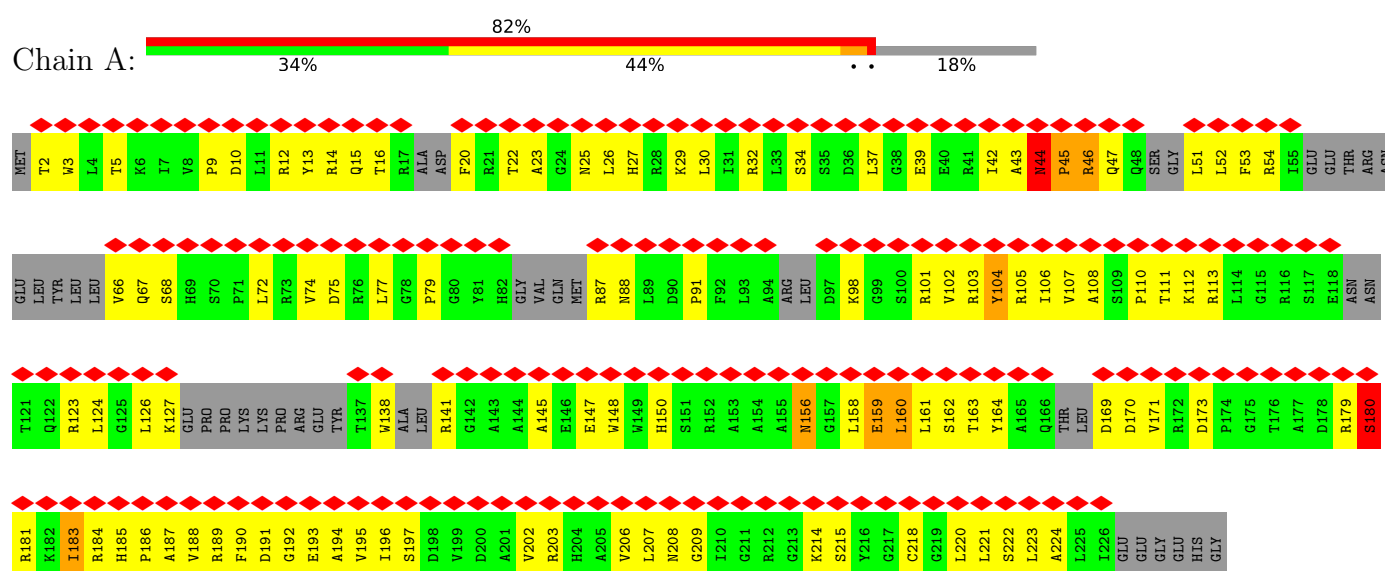
- Molecule 8 is a DNA chain called Nontarget Strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	13	Total	C	N	O	P	0	0
			268	125	55	75	13		

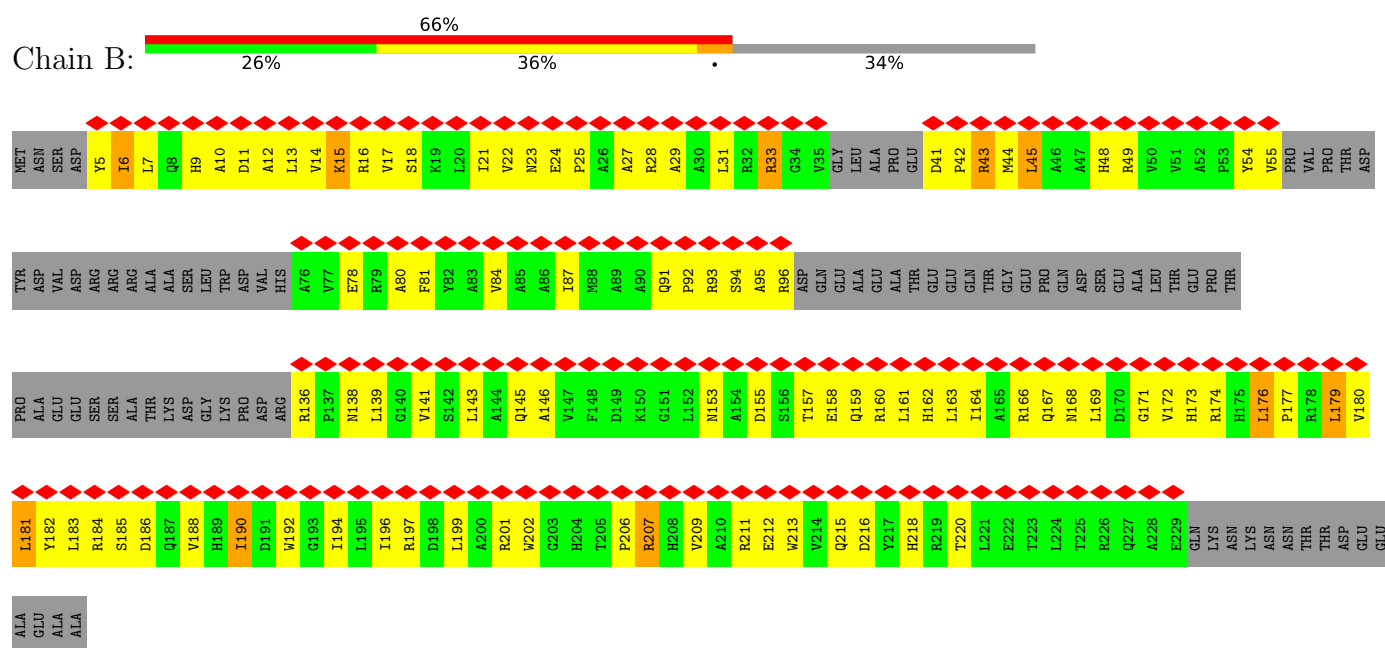
3 Residue-property plots

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.

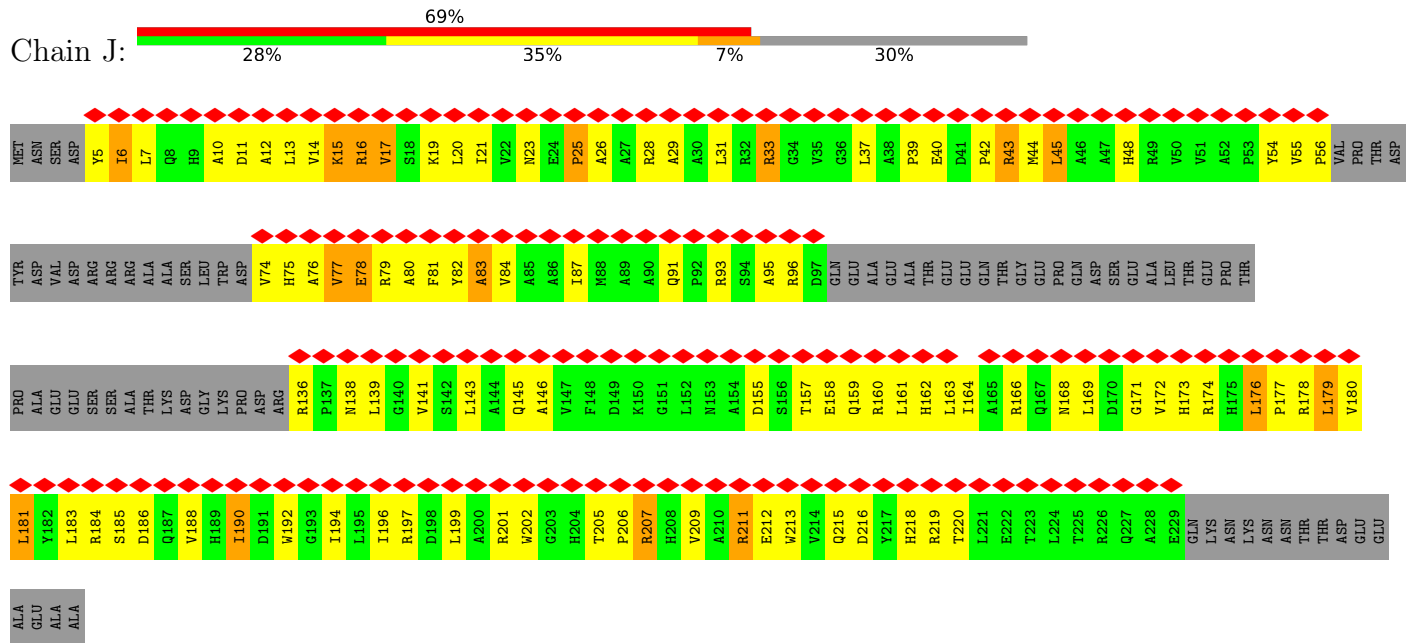
• Molecule 1: CRISPR-associated protein, Cse3 family



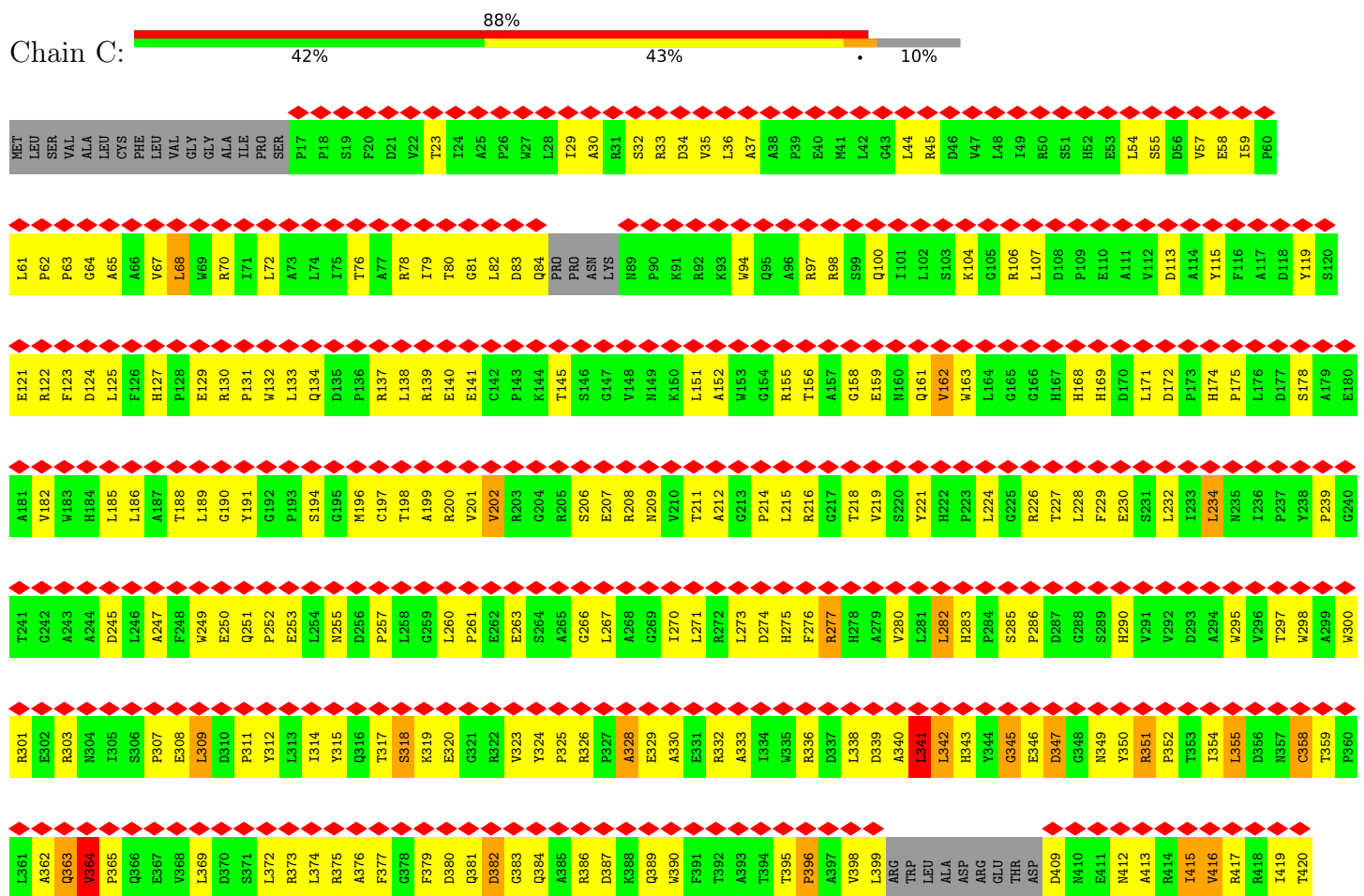
• Molecule 2: Cse2

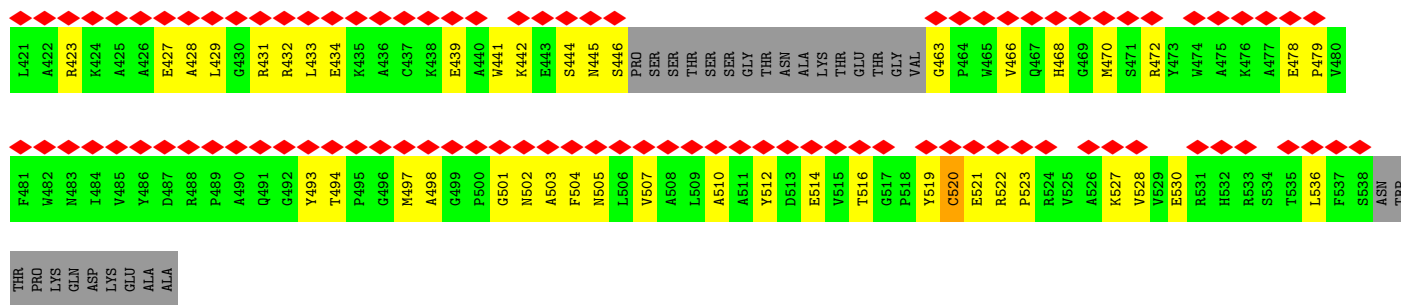


- Molecule 2: Cse2

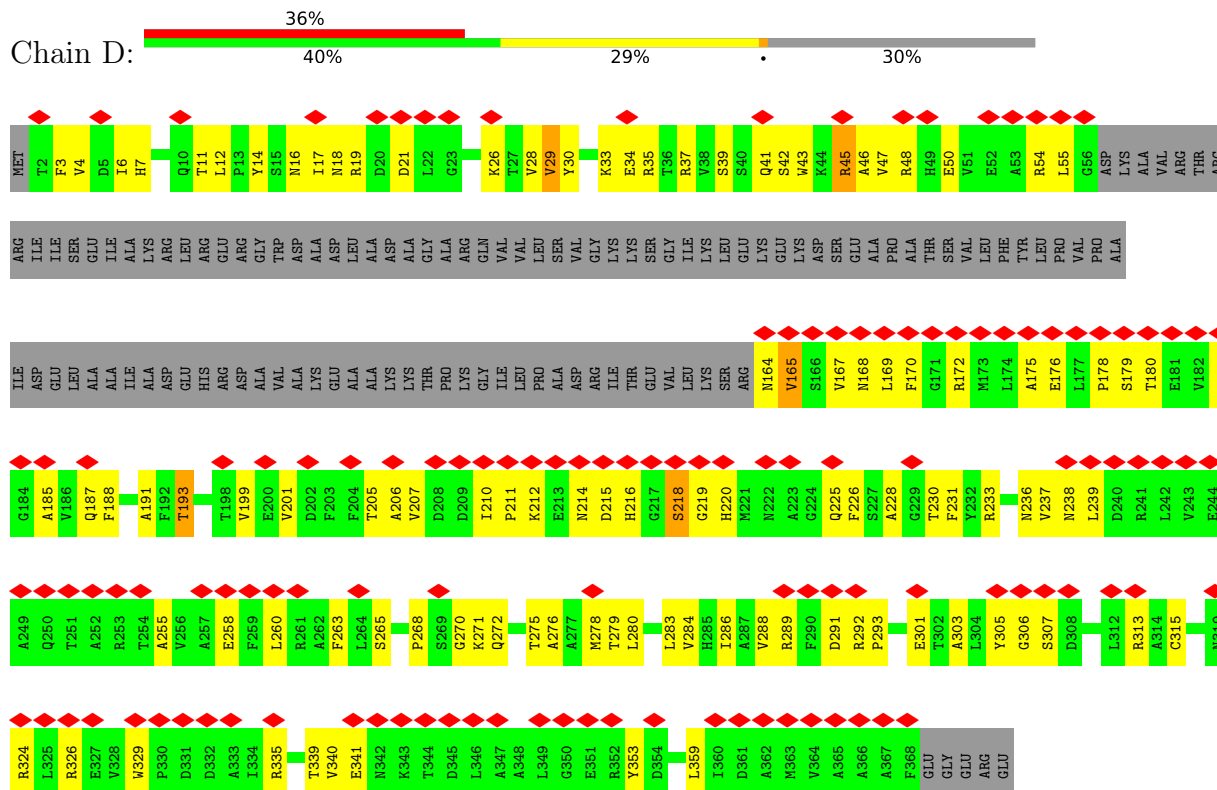


- Molecule 3: CRISPR-associated protein, Cse1 family

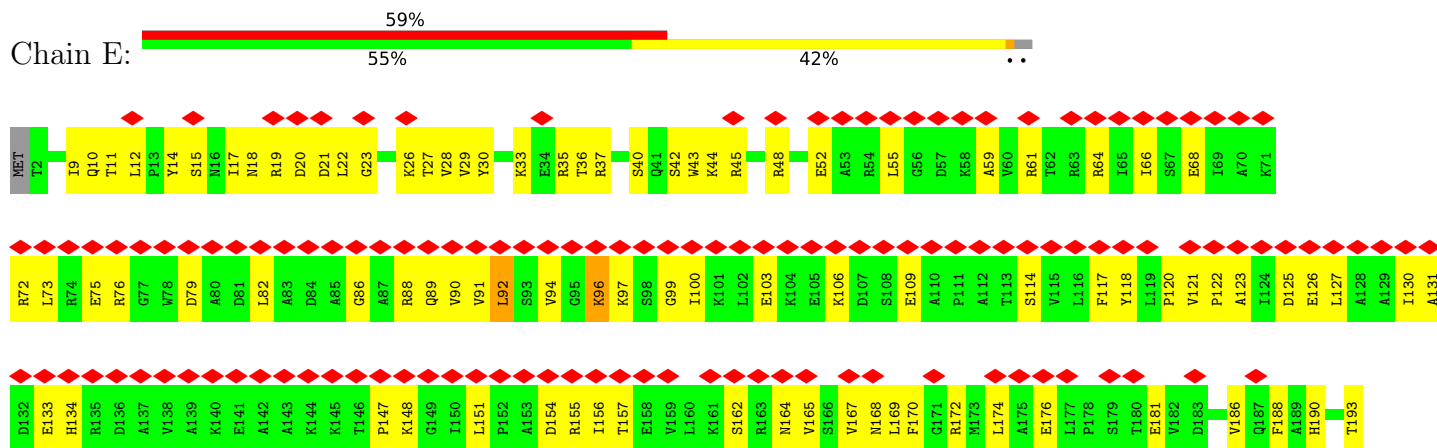


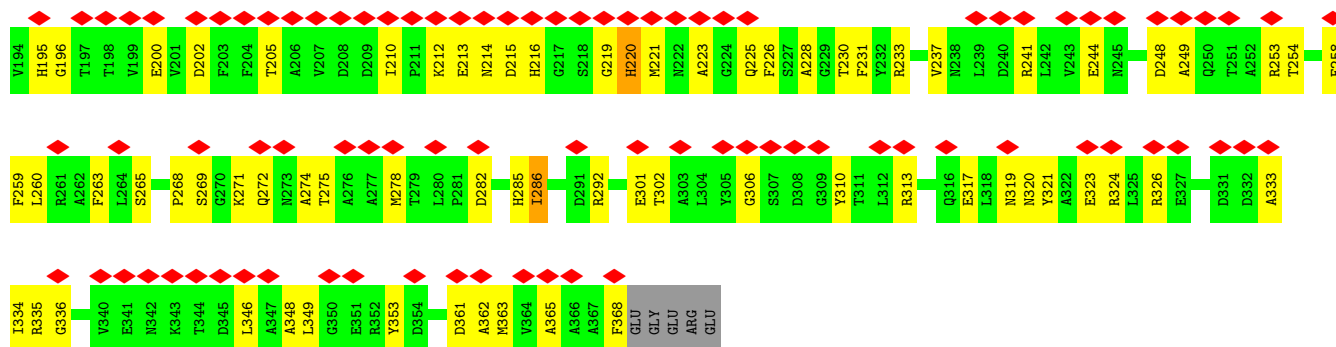


• Molecule 4: CRISPR-associated protein, Cse4 family

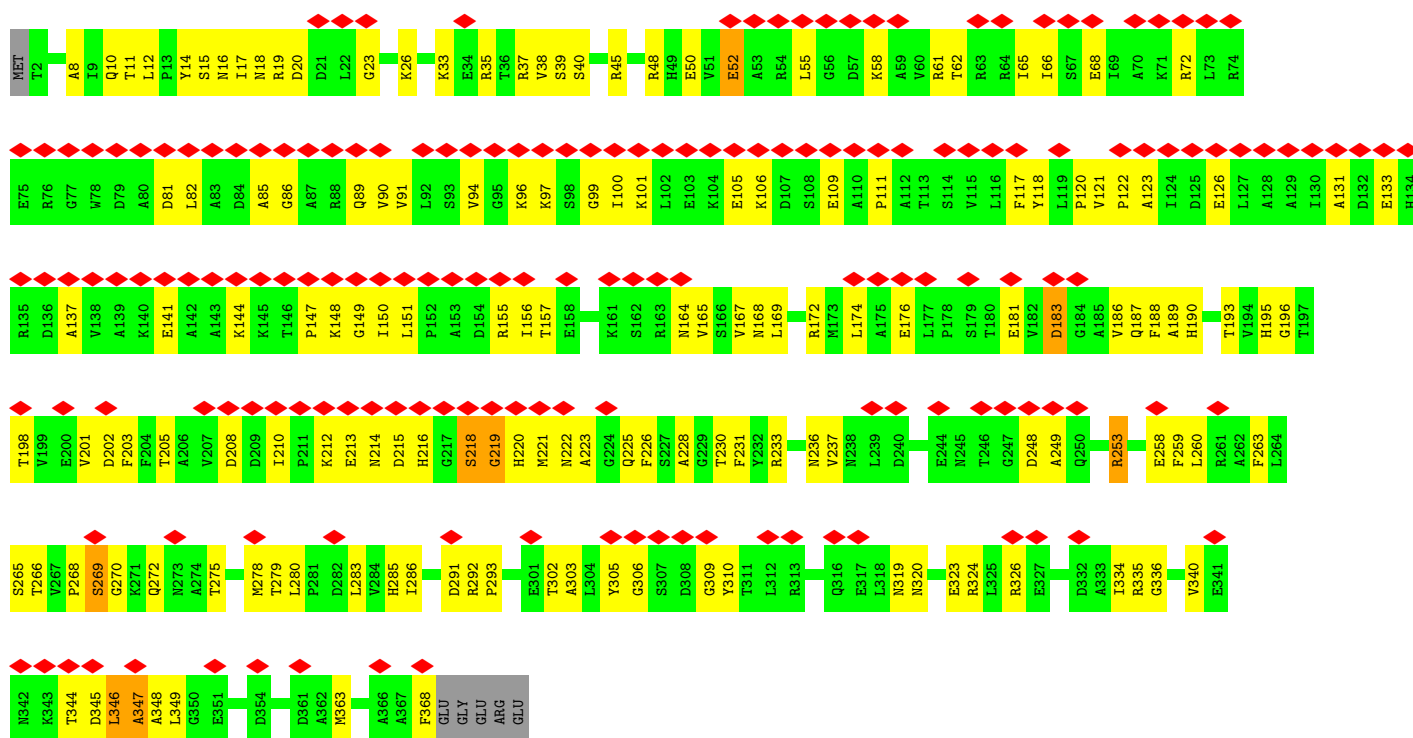


• Molecule 4: CRISPR-associated protein, Cse4 family

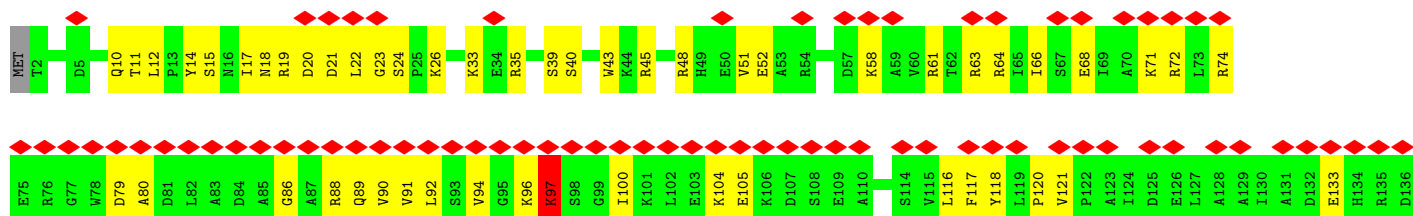


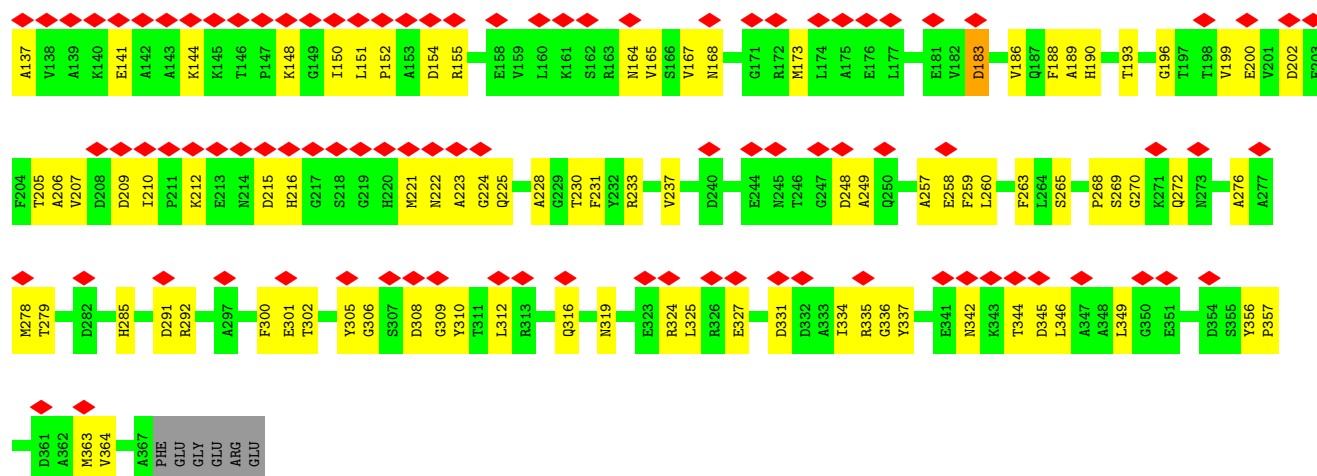


• Molecule 4: CRISPR-associated protein, Cse4 family

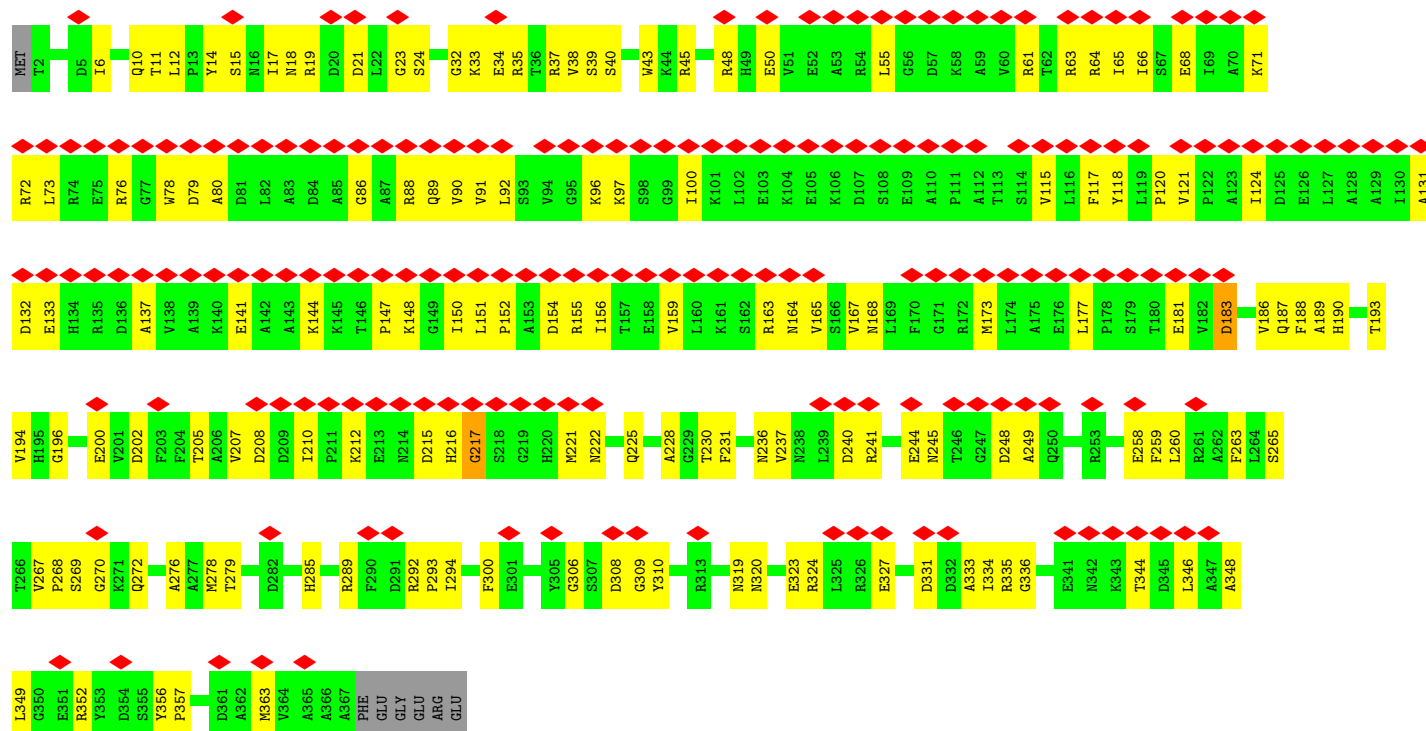


• Molecule 4: CRISPR-associated protein, Cse4 family

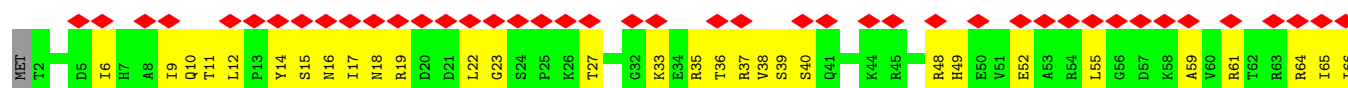


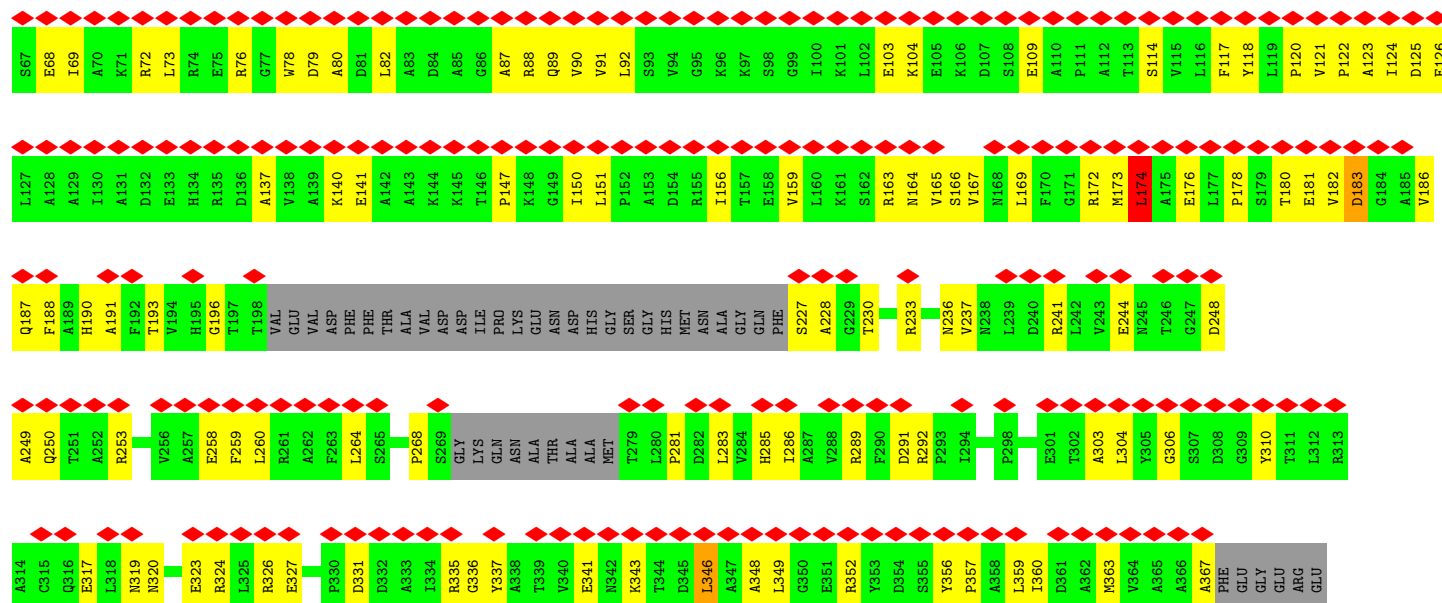


- Molecule 4: CRISPR-associated protein, Cse4 family

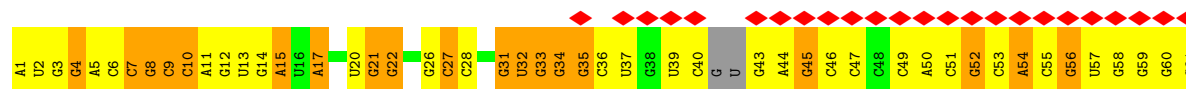
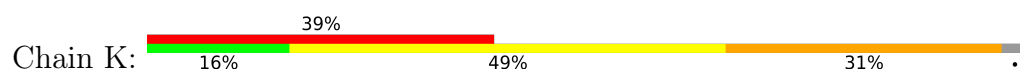


- Molecule 4: CRISPR-associated protein, Cse4 family

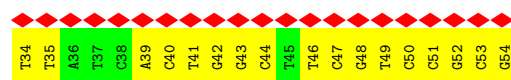




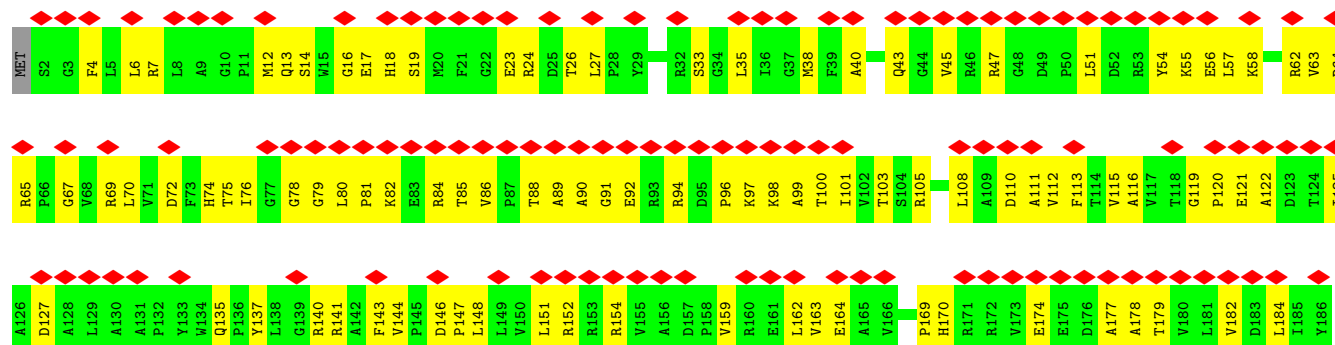
- Molecule 5: crRNA

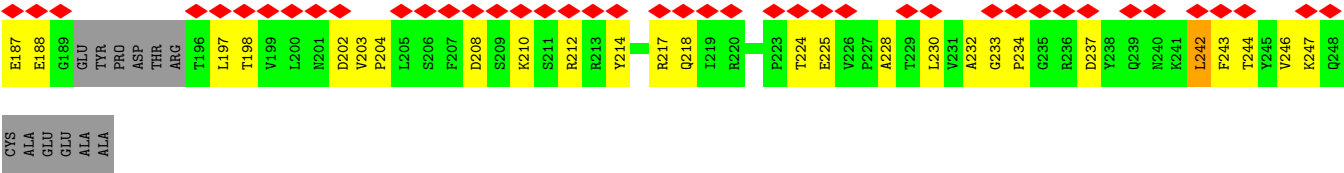


- Molecule 6: Target Strand



- Molecule 7: CRISPR-associated protein, Cas5e family





● Molecule 8: Nontarget Strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70222	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/1489	1.04	6/1995 (0.3%)
2	B	0.39	0/1310	0.87	1/1777 (0.1%)
2	J	0.41	0/1348	0.89	1/1836 (0.1%)
3	C	0.40	0/3991	0.87	4/5445 (0.1%)
4	D	0.52	0/2060	0.80	0/2802
4	E	0.50	0/2881	0.79	2/3910 (0.1%)
4	F	0.54	1/2888 (0.0%)	0.81	1/3919 (0.0%)
4	G	0.51	0/2876	0.77	1/3904 (0.0%)
4	H	0.49	0/2882	0.76	0/3911
4	I	0.43	0/2587	0.77	1/3508 (0.0%)
5	K	0.43	0/1417	0.52	0/2208
6	M	0.43	0/473	0.66	0/727
7	N	0.45	0/1934	0.78	0/2631
8	O	0.40	0/301	0.71	2/462 (0.4%)
All	All	0.46	1/28437 (0.0%)	0.81	19/39035 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	269	SER	C-N	7.44	1.37	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLU	N-CA-C	9.42	123.20	108.79
8	O	11	DG	O3'-P-O5'	7.96	115.93	104.00
1	A	106	ILE	N-CA-CB	6.65	122.36	111.45
1	A	104	TYR	N-CA-C	6.60	119.35	108.99
1	A	104	TYR	N-CA-CB	-5.93	100.48	111.52
3	C	520	CYS	N-CA-C	-5.65	106.19	112.57
3	C	359	THR	N-CA-C	5.61	122.22	109.81
2	J	159	GLN	N-CA-CB	5.58	118.93	110.28
8	O	11	DG	P-O3'-C3'	5.56	128.54	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	159	GLN	N-CA-CB	5.55	118.88	110.28
4	F	253	ARG	CA-CB-CG	-5.50	103.11	114.10
3	C	364	VAL	CA-C-N	-5.39	114.40	119.90
3	C	364	VAL	C-N-CA	-5.39	114.40	119.90
4	E	96	LYS	CA-CB-CG	5.24	124.57	114.10
4	G	305	TYR	CA-CB-CG	-5.23	104.49	113.90
4	E	220	HIS	N-CA-CB	-5.17	102.45	110.57
4	I	174	LEU	CA-CB-CG	5.11	134.19	116.30
1	A	159	GLU	CA-C-N	5.06	131.20	121.54
1	A	159	GLU	C-N-CA	5.06	131.20	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1471	0	1452	140	0
2	B	1285	0	1299	125	0
2	J	1319	0	1291	137	0
3	C	3880	0	3775	295	0
4	D	2017	0	1937	127	0
4	E	2828	0	2798	147	0
4	F	2834	0	2798	164	0
4	G	2823	0	2789	122	0
4	H	2829	0	2800	129	0
4	I	2544	0	2542	130	0
5	K	1267	0	642	94	0
6	M	425	0	239	28	0
7	N	1891	0	1914	127	0
8	O	268	0	144	15	0
All	All	27681	0	26420	1556	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 29.

All (1556) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ASN:HD21	4:F:220:HIS:CD2	1.41	1.37
2:B:153:ASN:ND2	4:F:220:HIS:HD2	1.32	1.27
1:A:107:VAL:HA	1:A:188:VAL:O	1.41	1.18
3:C:211:THR:HG21	3:C:277:ARG:HG2	1.25	1.18
3:C:341:LEU:CD1	3:C:374:LEU:HD21	1.76	1.14
3:C:211:THR:CG2	3:C:277:ARG:HG2	1.77	1.13
1:A:159:GLU:CB	1:A:194:ALA:HA	1.78	1.12
4:I:17:ILE:HG21	4:I:268:PRO:HB2	1.25	1.10
2:J:77:VAL:HG13	2:J:78:GLU:H	1.16	1.07
8:O:11:DG:H2''	8:O:12:DC:H5'	1.35	1.07
2:J:13:LEU:O	2:J:17:VAL:HG23	1.56	1.05
2:J:74:VAL:HG12	2:J:75:HIS:H	1.24	1.02
1:A:105:ARG:HA	1:A:190:PHE:O	1.59	1.00
3:C:341:LEU:HD12	3:C:374:LEU:HD21	1.42	1.00
3:C:341:LEU:HD12	3:C:374:LEU:CD2	1.91	0.99
1:A:102:VAL:O	1:A:193:GLU:HA	1.60	0.98
1:A:29:LYS:HD3	1:A:32:ARG:HE	1.29	0.98
1:A:103:ARG:O	1:A:223:LEU:HA	1.60	0.98
2:J:77:VAL:O	2:J:80:ALA:N	1.96	0.97
2:J:43:ARG:HG2	2:J:43:ARG:HH11	1.30	0.96
1:A:54:ARG:HG3	1:A:220:LEU:HB3	1.47	0.96
2:J:39:PRO:HB3	2:J:82:TYR:HD2	1.27	0.96
2:B:166:ARG:HG2	2:J:42:PRO:HB3	1.48	0.96
2:B:43:ARG:HG2	2:B:43:ARG:HH11	1.30	0.95
4:D:238:ASN:HB2	7:N:135:GLN:HE22	1.30	0.95
3:C:341:LEU:C	3:C:342:LEU:HD23	1.92	0.94
2:J:39:PRO:HB3	2:J:82:TYR:CD2	2.03	0.93
1:A:159:GLU:CB	1:A:194:ALA:CA	2.45	0.93
2:B:84:VAL:HG11	2:B:196:ILE:HG12	1.49	0.93
4:H:289:ARG:HH12	4:H:294:ILE:HD12	1.31	0.93
3:C:169:HIS:HE1	4:D:178:PRO:HD2	1.31	0.92
5:K:33:G:N2	5:K:34:G:C2	2.37	0.92
2:J:74:VAL:O	2:J:77:VAL:HG12	1.70	0.91
3:C:341:LEU:HD11	3:C:374:LEU:HD21	1.52	0.91
1:A:159:GLU:CB	1:A:194:ALA:CB	2.49	0.91
4:G:141:GLU:HG3	4:G:150:ILE:HD11	1.54	0.90
3:C:523:PRO:HB2	2:J:162:HIS:ND1	1.86	0.90
4:F:324:ARG:HH12	4:G:342:ASN:HB2	1.37	0.89
3:C:119:TYR:CE2	3:C:250:GLU:HG2	2.07	0.89
1:A:126:LEU:HD22	1:A:138:TRP:HB3	1.54	0.89
1:A:101:ARG:HA	1:A:194:ALA:O	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ARG:HB2	2:J:40:GLU:HG2	1.53	0.88
1:A:160:LEU:HB3	1:A:193:GLU:H	1.39	0.87
3:C:211:THR:HG21	3:C:277:ARG:CG	2.05	0.87
4:G:14:TYR:H	4:G:228:ALA:HB2	1.41	0.85
2:J:143:LEU:HD13	2:J:161:LEU:HD21	1.58	0.85
7:N:85:THR:HG21	7:N:99:ALA:HB1	1.57	0.85
2:J:91:GLN:HE21	2:J:184:ARG:HB3	1.40	0.85
4:D:3:PHE:HD2	4:D:293:PRO:HD3	1.41	0.84
4:D:3:PHE:CD2	4:D:293:PRO:HD3	2.12	0.84
6:M:54:DG:N2	8:O:1:DC:O2	2.10	0.84
2:B:91:GLN:HE21	2:B:184:ARG:HB3	1.40	0.84
4:I:141:GLU:HG3	4:I:150:ILE:HD11	1.58	0.84
3:C:502:ASN:HB2	3:C:505:ASN:HD22	1.43	0.83
1:A:98:LYS:HA	1:A:196:ILE:HB	1.59	0.83
4:F:141:GLU:HG2	4:F:150:ILE:HD11	1.61	0.83
4:E:353:TYR:HE2	4:E:363:MET:HE3	1.44	0.82
2:B:172:VAL:O	2:B:176:LEU:HB2	1.79	0.82
3:C:97:ARG:NH2	3:C:100:GLN:HE21	1.77	0.82
2:B:182:TYR:CD2	4:E:22:LEU:HB3	2.15	0.82
2:B:143:LEU:HD13	2:B:161:LEU:HD21	1.58	0.82
2:B:153:ASN:ND2	4:F:220:HIS:CD2	2.20	0.82
2:J:172:VAL:O	2:J:176:LEU:HB2	1.79	0.82
3:C:342:LEU:HD12	3:C:416:VAL:HG13	1.62	0.82
4:F:105:GLU:HG3	4:F:111:PRO:HB3	1.62	0.82
1:A:104:TYR:HA	1:A:222:SER:O	1.80	0.81
3:C:119:TYR:HE2	3:C:250:GLU:HG2	1.44	0.81
8:O:11:DG:H2''	8:O:12:DC:C5'	2.08	0.81
4:E:202:ASP:HB3	4:I:37:ARG:HH22	1.46	0.81
7:N:78:GLY:HA2	7:N:100:THR:HG22	1.63	0.81
4:D:238:ASN:HB2	7:N:135:GLN:NE2	1.96	0.80
4:F:14:TYR:H	4:F:228:ALA:HB2	1.45	0.80
4:G:96:LYS:HG2	4:G:97:LYS:H	1.46	0.80
4:H:17:ILE:O	4:H:270:GLY:HA3	1.82	0.80
3:C:379:PHE:HD1	3:C:390:TRP:HB3	1.45	0.80
2:B:87:ILE:HD11	2:B:177:PRO:HA	1.63	0.80
1:A:161:LEU:H	4:I:14:TYR:HE1	1.29	0.79
1:A:112:LYS:HE3	1:A:127:LYS:HA	1.63	0.79
3:C:494:THR:HB	3:C:497:MET:HG2	1.65	0.79
1:A:43:ALA:O	1:A:45:PRO:HD3	1.82	0.79
1:A:158:LEU:O	1:A:195:VAL:HG12	1.83	0.79
3:C:212:ALA:H	3:C:303:ARG:HH21	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:155:ASP:O	2:J:158:GLU:HB3	1.83	0.79
4:F:164:ASN:OD1	4:F:165:VAL:N	2.16	0.79
4:E:96:LYS:HD2	4:E:97:LYS:N	1.98	0.78
4:H:14:TYR:H	4:H:228:ALA:HB2	1.48	0.78
3:C:211:THR:HG23	3:C:277:ARG:HG2	1.65	0.78
2:J:87:ILE:HD11	2:J:177:PRO:HA	1.63	0.78
1:A:16:THR:HB	2:B:54:TYR:HE1	1.48	0.77
4:G:64:ARG:HG3	4:H:210:ILE:HD11	1.66	0.77
1:A:107:VAL:HG13	1:A:218:CYS:HA	1.64	0.77
2:J:77:VAL:HG13	2:J:78:GLU:N	1.96	0.77
7:N:202:ASP:OD1	7:N:203:VAL:N	2.17	0.77
2:B:155:ASP:O	2:B:158:GLU:HB3	1.85	0.76
3:C:104:LYS:HD2	3:C:106:ARG:H	1.50	0.76
3:C:191:TYR:CE1	3:C:215:LEU:O	2.38	0.76
3:C:169:HIS:CE1	4:D:178:PRO:HD2	2.18	0.76
4:G:18:ASN:HD21	4:G:39:SER:H	1.31	0.76
5:K:32:U:H2'	5:K:33:G:H4'	1.66	0.76
4:E:164:ASN:OD1	4:E:165:VAL:N	2.18	0.76
3:C:522:ARG:H	3:C:522:ARG:HD2	1.51	0.76
4:D:28:VAL:CG2	4:D:37:ARG:HD3	2.15	0.76
4:D:28:VAL:HG23	4:D:37:ARG:HD3	1.66	0.76
2:B:93:ARG:HD2	4:E:220:HIS:HA	1.68	0.75
3:C:44:LEU:HD11	3:C:72:LEU:HD21	1.68	0.75
4:I:72:ARG:HH22	4:I:121:VAL:HG13	1.50	0.75
2:B:91:GLN:HE22	2:B:181:LEU:HA	1.52	0.75
3:C:175:PRO:HB2	3:C:290:HIS:HB3	1.69	0.75
3:C:504:PHE:HA	3:C:507:VAL:HG12	1.68	0.75
3:C:382:ASP:HB2	3:C:386:ARG:HB2	1.69	0.75
2:J:56:PRO:HD2	2:J:81:PHE:CE2	2.22	0.75
2:J:91:GLN:HE22	2:J:181:LEU:HA	1.52	0.74
4:E:14:TYR:H	4:E:228:ALA:HB2	1.51	0.74
4:F:17:ILE:HD11	4:F:38:VAL:HG21	1.69	0.74
4:G:164:ASN:OD1	4:G:165:VAL:N	2.20	0.74
1:A:46:ARG:HA	5:K:59:G:H4'	1.70	0.74
1:A:104:TYR:O	1:A:191:ASP:HA	1.87	0.74
4:G:120:PRO:HG3	4:G:164:ASN:HB2	1.68	0.74
4:F:319:ASN:ND2	4:F:346:LEU:HA	2.01	0.74
3:C:106:ARG:NH1	3:C:107:LEU:O	2.20	0.74
4:I:164:ASN:OD1	4:I:165:VAL:N	2.20	0.74
1:A:42:ILE:O	1:A:45:PRO:HD2	1.88	0.74
4:H:163:ARG:NH1	4:H:245:ASN:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:H	4:I:16:ASN:HD22	1.37	0.73
3:C:341:LEU:O	3:C:342:LEU:HD23	1.87	0.73
7:N:198:THR:O	7:N:218:GLN:NE2	2.21	0.73
1:A:103:ARG:HB3	1:A:224:ALA:HB3	1.71	0.73
4:H:34:GLU:HB2	2:J:207:ARG:HH22	1.53	0.73
4:H:61:ARG:HA	4:H:117:PHE:O	1.89	0.73
2:B:138:ASN:HD21	2:B:213:TRP:HD1	1.37	0.73
4:E:35:ARG:HB3	4:E:193:THR:OG1	1.89	0.73
3:C:97:ARG:HH22	3:C:100:GLN:HE21	1.33	0.73
5:K:2:U:OP1	7:N:47:ARG:NH2	2.21	0.73
2:B:160:ARG:NH2	4:E:21:ASP:OD1	2.21	0.73
4:D:276:ALA:HB3	4:H:189:ALA:HB2	1.71	0.73
3:C:199:ALA:HB2	3:C:208:ARG:HB3	1.71	0.73
4:E:21:ASP:HA	5:K:33:G:N7	2.04	0.72
4:E:210:ILE:HD11	4:I:64:ARG:HG3	1.69	0.72
4:H:164:ASN:OD1	4:H:165:VAL:N	2.22	0.72
4:H:17:ILE:HD11	4:H:38:VAL:HG21	1.71	0.72
4:F:26:LYS:NZ	5:K:27:C:OP1	2.21	0.72
3:C:191:TYR:HD1	3:C:216:ARG:HA	1.54	0.72
4:I:289:ARG:NH1	4:I:331:ASP:OD2	2.21	0.72
6:M:39:DA:H2'	6:M:40:DC:C6	2.24	0.72
3:C:216:ARG:NH1	3:C:382:ASP:O	2.23	0.71
4:I:10:GLN:OE1	4:I:233:ARG:NH1	2.22	0.71
4:E:61:ARG:HA	4:E:117:PHE:O	1.90	0.71
4:D:265:SER:O	4:H:292:ARG:NH2	2.23	0.71
4:E:66:ILE:HD11	4:E:91:VAL:HG21	1.73	0.71
4:F:62:THR:HG21	4:G:210:ILE:HG13	1.71	0.71
2:J:138:ASN:HD21	2:J:213:TRP:HD1	1.37	0.71
3:C:363:GLN:O	3:C:364:VAL:HG13	1.90	0.71
4:G:154:ASP:OD1	4:G:155:ARG:N	2.24	0.71
3:C:211:THR:CG2	3:C:277:ARG:CG	2.65	0.71
4:F:72:ARG:HH22	4:F:121:VAL:HG13	1.55	0.71
3:C:274:ASP:OD1	3:C:275:HIS:ND1	2.23	0.71
1:A:123:ARG:NH2	5:K:59:G:O6	2.23	0.70
4:G:63:ARG:HG3	4:G:116:LEU:HG	1.73	0.70
3:C:98:ARG:HH12	3:C:234:LEU:HA	1.56	0.70
2:B:92:PRO:HG3	4:E:223:ALA:HB2	1.73	0.70
4:H:72:ARG:HH22	4:H:121:VAL:HG13	1.57	0.70
3:C:216:ARG:HH12	3:C:383:GLY:HA2	1.56	0.70
4:F:319:ASN:CG	4:F:346:LEU:CB	2.65	0.70
3:C:341:LEU:CD1	3:C:374:LEU:CD2	2.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:HIS:ND1	3:C:129:GLU:O	2.25	0.70
4:E:154:ASP:OD1	4:E:155:ARG:N	2.24	0.70
7:N:7:ARG:NH1	7:N:146:ASP:OD2	2.25	0.70
1:A:16:THR:HB	2:B:54:TYR:CE1	2.27	0.70
3:C:138:LEU:HD11	3:C:297:THR:HB	1.73	0.70
3:C:201:VAL:HG12	3:C:206:SER:HB3	1.73	0.69
3:C:381:GLN:HB2	3:C:387:ASP:HA	1.74	0.69
4:F:17:ILE:O	4:F:270:GLY:HA3	1.92	0.69
1:A:147:GLU:HA	1:A:150:HIS:CD2	2.27	0.69
2:B:162:HIS:ND1	2:J:45:LEU:HD13	2.06	0.69
3:C:161:GLN:HE21	7:N:94:ARG:CZ	2.05	0.69
4:D:28:VAL:HG21	7:N:12:MET:CE	2.22	0.69
3:C:382:ASP:OD1	3:C:383:GLY:N	2.26	0.69
4:G:173:MET:HE1	5:K:17:A:C4	2.27	0.69
4:H:154:ASP:OD1	4:H:155:ARG:N	2.25	0.69
3:C:158:GLY:O	7:N:90:ALA:N	2.24	0.69
4:H:141:GLU:HG3	4:H:144:LYS:HD3	1.73	0.69
4:I:61:ARG:HA	4:I:117:PHE:O	1.93	0.69
4:I:248:ASP:OD2	4:I:250:GLN:NE2	2.24	0.69
3:C:23:THR:HB	3:C:45:ARG:HB2	1.74	0.69
4:F:205:THR:HA	4:F:221:MET:HG2	1.75	0.69
4:H:183:ASP:OD1	4:H:183:ASP:N	2.25	0.69
4:I:173:MET:HA	4:I:181:GLU:OE1	1.93	0.69
4:G:133:GLU:OE2	4:G:155:ARG:NH2	2.25	0.69
4:G:183:ASP:OD1	4:G:183:ASP:N	2.24	0.69
2:J:93:ARG:HB3	2:J:96:ARG:HH21	1.57	0.69
7:N:76:ILE:HD11	7:N:101:ILE:HD12	1.74	0.69
3:C:32:SER:HA	3:C:55:SER:H	1.57	0.69
4:H:320:ASN:OD1	4:H:324:ARG:NH1	2.26	0.69
1:A:159:GLU:CB	1:A:194:ALA:HB2	2.23	0.69
1:A:170:ASP:H	2:B:23:ASN:HD21	1.41	0.69
2:B:167:GLN:HE22	4:F:198:THR:HB	1.58	0.69
3:C:34:ASP:O	3:C:36:LEU:N	2.23	0.69
3:C:119:TYR:CE2	3:C:250:GLU:CG	2.76	0.68
3:C:215:LEU:HD23	3:C:215:LEU:H	1.58	0.68
5:K:33:G:C2	5:K:34:G:N1	2.61	0.68
4:G:222:ASN:OD1	4:G:223:ALA:N	2.26	0.68
2:B:93:ARG:HB3	2:B:96:ARG:HH21	1.57	0.68
3:C:122:ARG:NH2	3:C:251:GLN:O	2.26	0.68
3:C:216:ARG:NH1	3:C:383:GLY:HA2	2.09	0.68
4:D:28:VAL:HG23	4:D:37:ARG:CD	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:TRP:CD1	4:D:268:PRO:HD3	2.29	0.68
4:I:15:SER:HB3	4:I:17:ILE:HG12	1.76	0.68
4:I:320:ASN:O	4:I:323:GLU:HG3	1.93	0.68
7:N:82:LYS:HD3	7:N:96:PRO:HD3	1.75	0.68
3:C:152:ALA:HB3	3:C:155:ARG:HD3	1.74	0.68
4:F:14:TYR:CE2	4:F:226:PHE:HD2	2.11	0.68
4:F:345:ASP:O	4:F:347:ALA:N	2.27	0.68
4:F:253:ARG:NH2	4:F:368:PHE:O	2.24	0.68
4:I:17:ILE:CG2	4:I:268:PRO:HB2	2.13	0.68
4:G:96:LYS:CG	4:G:97:LYS:N	2.57	0.68
4:I:19:ARG:HB3	4:I:23:GLY:HA2	1.75	0.67
4:I:137:ALA:O	4:I:141:GLU:HB2	1.94	0.67
1:A:23:ALA:O	1:A:26:LEU:HG	1.95	0.67
3:C:137:ARG:NH1	3:C:255:ASN:O	2.27	0.67
4:D:43:TRP:HD1	4:D:268:PRO:HD3	1.60	0.67
4:F:302:THR:HG22	4:G:309:GLY:HA3	1.76	0.67
7:N:16:GLY:HA2	7:N:26:THR:HA	1.75	0.67
7:N:233:GLY:N	7:N:237:ASP:OD2	2.28	0.67
1:A:87:ARG:NH1	1:A:88:ASN:O	2.27	0.67
4:E:265:SER:O	4:I:292:ARG:NH2	2.28	0.67
4:D:29:VAL:HG12	7:N:70:LEU:HD11	1.77	0.67
4:H:66:ILE:HD11	4:H:91:VAL:HG11	1.76	0.67
2:B:25:PRO:HB3	4:I:22:LEU:HD22	1.76	0.67
6:M:34:DT:H2''	6:M:35:DT:H5'	1.76	0.67
3:C:303:ARG:HH12	8:O:12:DC:P	2.18	0.67
4:F:133:GLU:OE2	4:F:155:ARG:NH2	2.26	0.67
3:C:318:SER:OG	3:C:324:TYR:CE1	2.48	0.66
4:I:87:ALA:O	4:I:90:VAL:HG12	1.94	0.66
7:N:80:LEU:HD12	7:N:81:PRO:HD2	1.76	0.66
4:F:148:LYS:HD3	4:F:149:GLY:N	2.11	0.66
4:I:89:GLN:HE22	4:I:147:PRO:HB2	1.60	0.66
4:I:186:VAL:HG22	4:I:237:VAL:HG22	1.77	0.66
4:H:68:GLU:O	4:H:71:LYS:HG3	1.96	0.66
4:H:212:LYS:HB3	4:H:215:ASP:HB2	1.77	0.66
4:I:356:TYR:HB2	4:I:357:PRO:HD3	1.76	0.66
4:E:64:ARG:NH1	4:F:208:ASP:OD2	2.28	0.66
5:K:33:G:C2	5:K:34:G:C6	2.84	0.66
4:F:101:LYS:NZ	4:F:176:GLU:OE2	2.29	0.66
7:N:67:GLY:HA3	7:N:111:ALA:HB2	1.76	0.66
2:B:141:VAL:HG13	2:B:216:ASP:HB3	1.78	0.66
4:E:30:TYR:HD2	4:E:35:ARG:HH21	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:GLU:HG2	3:C:307:PRO:HG3	1.78	0.66
4:I:11:THR:HA	4:I:230:THR:HA	1.78	0.66
7:N:137:TYR:CG	7:N:141:ARG:HA	2.30	0.66
1:A:44:ASN:ND2	5:K:51:C:H4'	2.11	0.66
2:J:37:LEU:O	2:J:79:ARG:NH1	2.28	0.66
1:A:164:TYR:CE1	1:A:189:ARG:HG3	2.31	0.66
4:I:241:ARG:O	4:I:244:GLU:HG3	1.96	0.66
2:J:77:VAL:O	2:J:78:GLU:C	2.38	0.66
5:K:46:C:H6	5:K:46:C:O5'	1.78	0.66
2:B:199:LEU:HA	2:B:202:TRP:HD1	1.60	0.65
4:F:203:PHE:CD2	4:F:223:ALA:HB2	2.31	0.65
3:C:520:CYS:HB3	2:J:215:GLN:HE21	1.62	0.65
4:F:40:SER:H	4:F:190:HIS:CE1	2.13	0.65
4:F:96:LYS:NZ	4:F:176:GLU:OE1	2.25	0.65
2:J:84:VAL:HA	2:J:87:ILE:HG22	1.78	0.65
5:K:33:G:N2	5:K:34:G:N1	2.44	0.65
7:N:4:PHE:HB2	7:N:152:ARG:O	1.95	0.65
4:I:326:ARG:HH11	4:I:335:ARG:HH12	1.43	0.65
7:N:6:LEU:HB2	7:N:115:VAL:HG13	1.78	0.65
7:N:74:HIS:CD2	7:N:105:ARG:HE	2.15	0.65
4:E:35:ARG:HG3	4:E:196:GLY:HA2	1.78	0.65
4:G:64:ARG:NH1	4:H:208:ASP:OD2	2.30	0.65
2:J:91:GLN:NE2	2:J:184:ARG:HB3	2.12	0.65
3:C:347:ASP:OD1	3:C:347:ASP:N	2.29	0.65
4:D:353:TYR:CD2	4:D:359:LEU:HA	2.32	0.65
4:F:14:TYR:H	4:F:228:ALA:CB	2.09	0.65
4:G:302:THR:HG22	4:H:309:GLY:HA3	1.78	0.65
5:K:4:G:H21	7:N:47:ARG:NH2	1.95	0.65
1:A:39:GLU:OE2	1:A:47:GLN:NE2	2.29	0.65
1:A:164:TYR:HE1	1:A:189:ARG:HG3	1.60	0.65
2:B:91:GLN:NE2	2:B:184:ARG:HB3	2.12	0.65
2:B:94:SER:OG	4:E:221:MET:N	2.29	0.65
4:G:24:SER:HB3	4:G:225:GLN:NE2	2.11	0.65
4:G:72:ARG:HH22	4:G:121:VAL:HG13	1.60	0.65
4:I:324:ARG:NH1	4:I:327:GLU:OE1	2.30	0.65
2:B:160:ARG:HH22	4:E:21:ASP:CG	2.05	0.65
2:J:141:VAL:HG13	2:J:216:ASP:HB3	1.78	0.64
3:C:239:PRO:HB3	3:C:267:LEU:HB3	1.79	0.64
4:G:96:LYS:CG	4:G:97:LYS:H	2.09	0.64
2:J:176:LEU:O	2:J:180:VAL:HG22	1.97	0.64
2:J:199:LEU:HA	2:J:202:TRP:HD1	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:HB3	1:A:191:ASP:H	1.62	0.64
4:H:208:ASP:HB3	4:H:215:ASP:OD2	1.97	0.64
4:I:12:LEU:HB3	4:I:15:SER:OG	1.97	0.64
4:I:104:LYS:H	4:I:104:LYS:HD3	1.62	0.64
4:G:45:ARG:HE	4:H:207:VAL:HG11	1.61	0.64
3:C:211:THR:OG1	3:C:303:ARG:NE	2.28	0.64
1:A:44:ASN:ND2	5:K:51:C:C4'	2.61	0.64
4:D:305:TYR:CZ	2:J:205:THR:HG22	2.31	0.64
5:K:3:G:OP2	7:N:212:ARG:NH2	2.31	0.64
5:K:49:C:H2'	5:K:50:A:H8	1.62	0.64
3:C:119:TYR:HE2	3:C:250:GLU:CG	2.09	0.64
3:C:326:ARG:HH21	3:C:349:ASN:HD22	1.46	0.64
3:C:336:ARG:HG3	3:C:423:ARG:HG2	1.79	0.64
5:K:8:G:C5	5:K:10:C:H5''	2.32	0.64
1:A:113:ARG:HH22	1:A:123:ARG:HH21	1.45	0.64
2:B:5:TYR:O	2:B:7:LEU:N	2.31	0.64
2:B:176:LEU:O	2:B:180:VAL:HG22	1.97	0.64
2:B:158:GLU:OE1	2:B:158:GLU:HA	1.98	0.64
3:C:412:ASN:O	3:C:416:VAL:HG23	1.98	0.63
2:J:93:ARG:HA	2:J:96:ARG:HE	1.63	0.63
2:J:138:ASN:HD21	2:J:213:TRP:CD1	2.15	0.63
4:H:120:PRO:HG3	4:H:164:ASN:HB2	1.80	0.63
7:N:69:ARG:HB2	7:N:108:LEU:HD23	1.78	0.63
4:G:22:LEU:HD11	2:J:178:ARG:HD3	1.80	0.63
4:H:173:MET:HA	4:H:181:GLU:HG3	1.79	0.63
4:H:186:VAL:HG22	4:H:237:VAL:HG22	1.80	0.63
4:I:253:ARG:NH2	4:I:367:ALA:O	2.30	0.63
4:F:52:GLU:HG2	4:F:58:LYS:HA	1.81	0.63
2:B:138:ASN:HD21	2:B:213:TRP:CD1	2.15	0.63
2:J:158:GLU:HA	2:J:158:GLU:OE1	1.98	0.63
5:K:44:A:H4'	5:K:45:G:OP1	1.97	0.63
3:C:131:PRO:HB2	3:C:134:GLN:HB2	1.81	0.63
4:D:326:ARG:CZ	4:D:335:ARG:HH22	2.11	0.63
4:G:319:ASN:HB2	4:G:346:LEU:HD22	1.81	0.63
7:N:179:THR:CG2	7:N:225:GLU:HB3	2.28	0.63
4:G:35:ARG:NH2	4:G:301:GLU:O	2.31	0.62
7:N:212:ARG:NH2	7:N:214:TYR:OH	2.31	0.62
4:E:48:ARG:O	4:E:52:GLU:HG2	1.99	0.62
4:G:215:ASP:OD1	4:G:216:HIS:N	2.31	0.62
6:M:43:DG:N3	7:N:100:THR:OG1	2.31	0.62
1:A:163:THR:O	4:I:16:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:340:ALA:C	3:C:342:LEU:H	2.07	0.62
3:C:433:LEU:HD13	3:C:536:LEU:HD21	1.81	0.62
4:D:14:TYR:OH	4:H:37:ARG:NH2	2.32	0.62
4:F:292:ARG:NH2	4:G:265:SER:O	2.32	0.62
4:F:293:PRO:HG2	4:G:278:MET:HG3	1.80	0.62
2:J:5:TYR:O	2:J:7:LEU:N	2.31	0.62
2:J:197:ARG:O	2:J:201:ARG:HG3	2.00	0.62
1:A:44:ASN:HD21	5:K:51:C:C4'	2.13	0.62
1:A:203:ARG:NH1	1:A:207:LEU:HB2	2.15	0.62
4:D:48:ARG:NH1	5:K:7:C:OP1	2.31	0.62
4:D:187:GLN:HB3	4:D:236:ASN:OD1	1.99	0.62
4:E:214:ASN:OD1	4:E:215:ASP:N	2.32	0.62
4:H:306:GLY:HA2	4:H:310:TYR:CE1	2.34	0.62
1:A:12:ARG:HA	1:A:77:LEU:HD22	1.81	0.62
3:C:224:LEU:HB2	3:C:373:ARG:O	1.99	0.62
4:E:188:PHE:HE1	4:E:263:PHE:HE1	1.47	0.62
3:C:197:CYS:O	3:C:208:ARG:HB2	1.99	0.62
3:C:369:LEU:HA	3:C:372:LEU:HD23	1.81	0.62
4:E:259:PHE:HD2	4:E:260:LEU:HD12	1.65	0.62
4:I:248:ASP:OD1	4:I:249:ALA:N	2.33	0.62
4:I:323:GLU:HB3	4:I:348:ALA:HB2	1.80	0.62
3:C:247:ALA:O	3:C:251:GLN:HG2	1.99	0.62
7:N:62:ARG:HD3	7:N:182:VAL:HG11	1.81	0.62
4:E:320:ASN:O	4:E:323:GLU:HG2	2.00	0.62
4:F:55:LEU:HD23	4:F:165:VAL:HG21	1.82	0.62
4:H:68:GLU:OE2	4:H:72:ARG:NE	2.31	0.62
7:N:76:ILE:HG13	7:N:101:ILE:HB	1.81	0.62
4:E:302:THR:HG22	4:F:309:GLY:HA3	1.82	0.62
4:F:201:VAL:HG22	4:F:225:GLN:HG3	1.81	0.62
4:I:73:LEU:HD23	4:I:76:ARG:HD2	1.82	0.62
7:N:187:GLU:OE2	7:N:217:ARG:NH2	2.32	0.62
2:B:93:ARG:HA	2:B:96:ARG:HE	1.63	0.61
4:G:269:SER:HA	4:G:272:GLN:CD	2.25	0.61
4:I:336:GLY:HA3	4:I:363:MET:HE1	1.81	0.61
2:B:197:ARG:O	2:B:201:ARG:HG3	1.99	0.61
4:E:72:ARG:HH22	4:E:121:VAL:HG13	1.66	0.61
4:F:326:ARG:HH11	4:F:335:ARG:NH1	1.98	0.61
7:N:85:THR:HG22	7:N:86:VAL:H	1.65	0.61
1:A:163:THR:H	4:I:16:ASN:ND2	1.99	0.61
3:C:32:SER:HB3	3:C:54:LEU:HD23	1.81	0.61
4:I:9:ILE:HG22	4:I:283:LEU:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:186:VAL:HG22	4:G:237:VAL:HG22	1.81	0.61
7:N:62:ARG:NE	7:N:64:ASP:OD1	2.34	0.61
3:C:125:LEU:HA	3:C:132:TRP:HB3	1.81	0.61
3:C:137:ARG:HH12	3:C:257:PRO:HD3	1.64	0.61
3:C:340:ALA:O	3:C:342:LEU:N	2.33	0.61
4:F:94:VAL:HG23	4:F:100:ILE:HG12	1.82	0.61
4:I:183:ASP:OD1	4:I:183:ASP:N	2.30	0.61
1:A:46:ARG:HA	5:K:59:G:C5'	2.30	0.61
4:D:219:GLY:O	4:H:63:ARG:NH1	2.33	0.61
4:E:205:THR:HG23	4:E:221:MET:HB3	1.83	0.61
4:E:253:ARG:HE	4:E:368:PHE:HB3	1.65	0.61
4:G:68:GLU:OE2	4:G:72:ARG:NE	2.34	0.61
4:G:248:ASP:OD1	4:G:249:ALA:N	2.34	0.61
3:C:58:GLU:CD	3:C:375:ARG:HH22	2.08	0.61
3:C:230:GLU:O	3:C:234:LEU:HD23	2.01	0.61
4:I:306:GLY:HA2	4:I:310:TYR:CE1	2.36	0.61
4:E:253:ARG:NE	4:E:368:PHE:HB3	2.16	0.61
4:H:241:ARG:O	4:H:244:GLU:HG3	2.01	0.61
4:D:26:LYS:NZ	5:K:9:C:OP1	2.33	0.61
3:C:215:LEU:O	3:C:215:LEU:HG	2.01	0.60
7:N:64:ASP:HB2	7:N:112:VAL:HG23	1.83	0.60
1:A:126:LEU:HD12	5:K:43:G:H1'	1.82	0.60
1:A:138:TRP:O	1:A:141:ARG:HB2	2.02	0.60
3:C:58:GLU:OE2	3:C:375:ARG:NH1	2.30	0.60
3:C:345:GLY:O	3:C:346:GLU:CB	2.46	0.60
4:F:219:GLY:O	5:K:33:G:N2	2.34	0.60
2:J:202:TRP:O	2:J:206:PRO:HG3	2.02	0.60
7:N:17:GLU:O	7:N:18:HIS:ND1	2.35	0.60
4:G:141:GLU:OE2	4:G:148:LYS:N	2.33	0.60
4:D:41:GLN:HB2	5:K:7:C:H2'	1.83	0.60
4:E:33:LYS:O	4:E:35:ARG:HD3	2.00	0.60
4:F:326:ARG:HH11	4:F:335:ARG:HH12	1.47	0.60
4:G:292:ARG:NH2	4:H:265:SER:O	2.34	0.60
4:H:118:TYR:CE2	4:H:167:VAL:HG12	2.37	0.60
4:I:35:ARG:HB3	4:I:193:THR:OG1	2.01	0.60
2:B:136:ARG:HD2	2:B:194:ILE:HD11	1.82	0.60
2:B:202:TRP:O	2:B:206:PRO:HG3	2.01	0.60
3:C:364:VAL:H	3:C:365:PRO:HD2	1.65	0.60
1:A:162:SER:O	1:A:190:PHE:HA	2.01	0.60
3:C:227:THR:N	3:C:230:GLU:OE2	2.26	0.60
4:G:12:LEU:HD12	4:G:231:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:56:PRO:HD2	2:J:81:PHE:HE2	1.66	0.60
1:A:3:TRP:HZ2	1:A:72:LEU:H	1.50	0.60
3:C:79:ILE:HG12	3:C:115:TYR:CG	2.36	0.60
4:D:35:ARG:HB2	4:D:193:THR:OG1	2.01	0.60
4:E:11:THR:HA	4:E:230:THR:HA	1.82	0.60
7:N:55:LYS:O	7:N:56:GLU:HB2	2.01	0.60
4:E:94:VAL:HG23	4:E:100:ILE:HG12	1.83	0.60
1:A:196:ILE:HG23	1:A:202:VAL:HG21	1.84	0.60
4:G:285:HIS:CD2	4:G:349:LEU:HD22	2.37	0.60
1:A:43:ALA:C	1:A:45:PRO:HD3	2.26	0.59
4:F:259:PHE:HD2	4:F:260:LEU:HD12	1.67	0.59
4:G:18:ASN:HD21	4:G:39:SER:N	2.00	0.59
4:H:133:GLU:OE2	4:H:155:ARG:NH2	2.31	0.59
4:I:156:ILE:O	4:I:159:VAL:HG12	2.02	0.59
2:J:39:PRO:HA	2:J:44:MET:SD	2.42	0.59
2:J:136:ARG:HD2	2:J:194:ILE:HD11	1.82	0.59
6:M:43:DG:H1'	7:N:100:THR:O	2.02	0.59
3:C:185:LEU:HD12	3:C:282:LEU:HD11	1.84	0.59
3:C:317:THR:HG21	3:C:350:TYR:HE2	1.67	0.59
3:C:362:ALA:O	3:C:363:GLN:O	2.20	0.59
3:C:78:ARG:HA	3:C:82:LEU:HD23	1.84	0.59
3:C:311:PRO:O	3:C:354:ILE:HG22	2.02	0.59
3:C:354:ILE:O	3:C:358:CYS:HB2	2.01	0.59
4:E:186:VAL:HG22	4:E:237:VAL:HG22	1.84	0.59
2:J:25:PRO:HD2	2:J:26:ALA:H	1.67	0.59
2:B:43:ARG:HG2	2:B:43:ARG:NH1	2.07	0.59
4:D:55:LEU:HD12	4:D:258:GLU:CD	2.27	0.59
4:F:205:THR:O	5:K:31:G:O2'	2.21	0.59
1:A:108:ALA:O	1:A:188:VAL:HG22	2.03	0.59
3:C:174:HIS:CD2	7:N:210:LYS:HD3	2.38	0.59
3:C:309:LEU:HB3	3:C:315:TYR:CE2	2.37	0.59
3:C:527:LYS:HA	2:J:218:HIS:ND1	2.18	0.59
4:E:15:SER:HB2	4:E:17:ILE:HG12	1.85	0.59
4:E:133:GLU:OE2	4:E:134:HIS:NE2	2.34	0.59
1:A:27:HIS:HD2	1:A:215:SER:HB2	1.68	0.59
4:F:248:ASP:OD1	4:F:249:ALA:N	2.36	0.59
4:I:14:TYR:H	4:I:228:ALA:HB2	1.68	0.59
7:N:122:ALA:O	7:N:125:ILE:HG13	2.02	0.59
3:C:444:SER:OG	3:C:445:ASN:N	2.35	0.59
4:G:35:ARG:HB3	4:G:193:THR:OG1	2.01	0.59
4:I:66:ILE:HD11	4:I:91:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:13:LEU:O	2:J:17:VAL:CG2	2.42	0.59
2:J:74:VAL:HG12	2:J:75:HIS:N	2.04	0.59
2:B:80:ALA:O	2:B:84:VAL:HG12	2.03	0.59
3:C:369:LEU:O	3:C:399:LEU:HD21	2.02	0.59
4:E:361:ASP:OD1	4:E:362:ALA:N	2.36	0.59
4:H:319:ASN:HB2	4:H:346:LEU:HD22	1.84	0.59
1:A:164:TYR:HE1	1:A:189:ARG:H	1.50	0.59
4:E:45:ARG:HA	4:E:48:ARG:HG2	1.84	0.59
4:E:195:HIS:HE1	4:E:230:THR:H	1.51	0.59
4:G:335:ARG:C	4:G:363:MET:HE1	2.28	0.59
4:D:185:ALA:HB1	4:D:238:ASN:HB3	1.85	0.59
4:E:12:LEU:HD12	4:E:231:PHE:CE2	2.38	0.59
5:K:6:C:O2'	5:K:7:C:O4'	2.17	0.59
4:H:18:ASN:HD21	4:H:39:SER:H	1.51	0.58
1:A:10:ASP:HB2	1:A:77:LEU:HG	1.85	0.58
3:C:59:ILE:HD11	3:C:64:GLY:C	2.27	0.58
3:C:416:VAL:O	3:C:420:THR:HG23	2.04	0.58
4:E:336:GLY:HA3	4:E:363:MET:HE1	1.83	0.58
4:F:216:HIS:O	5:K:34:G:N2	2.35	0.58
4:H:156:ILE:O	4:H:159:VAL:HG12	2.03	0.58
4:H:216:HIS:HB2	5:K:22:G:H21	1.68	0.58
7:N:76:ILE:CG1	7:N:101:ILE:HB	2.32	0.58
4:D:172:ARG:NH2	4:D:176:GLU:O	2.35	0.58
1:A:23:ALA:CB	1:A:171:VAL:HG11	2.33	0.58
4:E:156:ILE:HD12	4:E:157:THR:N	2.18	0.58
4:E:248:ASP:OD1	4:E:249:ALA:N	2.37	0.58
4:I:167:VAL:HG11	4:I:172:ARG:HH11	1.67	0.58
2:J:139:LEU:HD12	2:J:190:ILE:HD11	1.86	0.58
4:H:319:ASN:ND2	4:H:346:LEU:HA	2.19	0.58
3:C:212:ALA:H	3:C:303:ARG:NH2	2.02	0.58
4:H:248:ASP:OD1	4:H:249:ALA:N	2.36	0.58
2:J:56:PRO:CD	2:J:81:PHE:CE2	2.86	0.58
8:O:4:DG:H2''	8:O:5:DG:C8	2.38	0.58
1:A:45:PRO:O	5:K:59:G:H5'	2.04	0.58
3:C:97:ARG:HH22	3:C:100:GLN:NE2	2.00	0.58
3:C:341:LEU:HD12	3:C:374:LEU:HD22	1.85	0.58
3:C:442:LYS:O	3:C:446:SER:N	2.37	0.58
4:H:285:HIS:CD2	4:H:349:LEU:HD22	2.38	0.58
4:D:42:SER:O	4:D:45:ARG:HG3	2.04	0.57
4:E:89:GLN:HE22	4:E:147:PRO:HB2	1.68	0.57
4:I:89:GLN:NE2	4:I:147:PRO:HB2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:286:ILE:HB	4:I:363:MET:SD	2.44	0.57
1:A:126:LEU:HD12	5:K:43:G:C1'	2.34	0.57
1:A:169:ASP:O	1:A:184:ARG:HG2	2.03	0.57
3:C:124:ASP:HB3	3:C:127:HIS:HB2	1.86	0.57
4:F:259:PHE:CD2	4:F:260:LEU:HD12	2.39	0.57
4:G:336:GLY:HA3	4:G:363:MET:HE3	1.87	0.57
2:B:139:LEU:HD12	2:B:190:ILE:HD11	1.86	0.57
4:E:202:ASP:HB3	4:I:37:ARG:NH2	2.18	0.57
4:F:156:ILE:HD12	4:F:157:THR:N	2.18	0.57
7:N:57:LEU:HD23	7:N:119:GLY:HA3	1.86	0.57
1:A:113:ARG:O	5:K:56:G:H5''	2.05	0.57
4:E:259:PHE:CD2	4:E:260:LEU:HD12	2.39	0.57
4:I:6:ILE:HG22	4:I:286:ILE:HG23	1.87	0.57
5:K:33:G:N2	5:K:34:G:N2	2.52	0.57
1:A:23:ALA:HB2	1:A:171:VAL:HG11	1.86	0.57
1:A:29:LYS:HD3	1:A:32:ARG:NE	2.10	0.57
4:E:174:LEU:H	4:E:181:GLU:HG2	1.69	0.57
4:F:324:ARG:NH1	4:G:342:ASN:HB2	2.14	0.57
4:G:202:ASP:HB3	4:G:224:GLY:O	2.05	0.57
4:H:336:GLY:HA3	4:H:363:MET:HE3	1.87	0.57
2:B:162:HIS:O	2:B:166:ARG:NH1	2.38	0.57
3:C:29:ILE:O	3:C:57:VAL:HA	2.03	0.57
3:C:191:TYR:CD1	3:C:216:ARG:HA	2.38	0.57
3:C:445:ASN:CG	4:D:201:VAL:HG11	2.30	0.57
4:F:10:GLN:OE1	4:F:233:ARG:NH1	2.38	0.57
4:F:35:ARG:HB2	4:F:193:THR:OG1	2.05	0.57
4:I:76:ARG:NH2	4:I:125:ASP:OD1	2.38	0.57
2:J:17:VAL:O	2:J:20:LEU:N	2.38	0.57
4:F:335:ARG:C	4:F:363:MET:HE1	2.28	0.57
4:I:118:TYR:CE2	4:I:167:VAL:HG22	2.40	0.57
4:D:207:VAL:HG11	4:H:45:ARG:HE	1.70	0.57
4:G:14:TYR:H	4:G:228:ALA:CB	2.17	0.57
1:A:14:ARG:HB3	2:B:9:HIS:CE1	2.40	0.57
1:A:156:ASN:O	1:A:197:SER:HB3	2.05	0.57
4:D:183:ASP:OD1	5:K:5:A:O2'	2.20	0.57
4:E:286:ILE:HD11	4:E:363:MET:CB	2.35	0.57
4:F:219:GLY:HA3	5:K:33:G:H22	1.69	0.57
5:K:46:C:O2'	5:K:47:C:H5'	2.05	0.57
1:A:2:THR:HG21	1:A:67:GLN:HB3	1.86	0.56
3:C:261:PRO:HG3	3:C:300:TRP:CD2	2.40	0.56
3:C:478:GLU:CG	3:C:479:PRO:HD3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:96:LYS:HG2	4:F:97:LYS:N	2.20	0.56
4:G:212:LYS:HB3	4:G:215:ASP:OD2	2.04	0.56
4:H:55:LEU:HD22	4:H:258:GLU:OE2	2.04	0.56
4:I:285:HIS:CD2	4:I:349:LEU:HD22	2.40	0.56
7:N:43:GLN:NE2	7:N:125:ILE:HG22	2.20	0.56
3:C:159:GLU:O	7:N:88:THR:HG23	2.04	0.56
3:C:191:TYR:HE1	3:C:215:LEU:O	1.85	0.56
4:H:89:GLN:HE22	4:H:147:PRO:HB2	1.70	0.56
3:C:207:GLU:HB2	3:C:301:ARG:CZ	2.36	0.56
4:D:43:TRP:CZ2	4:D:233:ARG:NH2	2.73	0.56
4:E:319:ASN:HB2	4:E:346:LEU:HD22	1.86	0.56
4:F:18:ASN:HD21	4:F:39:SER:H	1.53	0.56
4:G:96:LYS:HG2	4:G:97:LYS:N	2.16	0.56
4:H:12:LEU:HD12	4:H:231:PHE:CE2	2.40	0.56
2:J:43:ARG:HG2	2:J:43:ARG:NH1	2.07	0.56
4:G:66:ILE:HD11	4:G:91:VAL:HG21	1.86	0.56
4:G:259:PHE:HD2	4:G:260:LEU:HD12	1.71	0.56
2:J:11:ASP:HA	2:J:14:VAL:HG22	1.88	0.56
2:J:77:VAL:O	2:J:79:ARG:N	2.38	0.56
2:J:162:HIS:O	2:J:166:ARG:NH1	2.38	0.56
5:K:13:U:H3	6:M:39:DA:H62	1.54	0.56
2:B:55:VAL:HG11	2:B:78:GLU:HA	1.87	0.56
3:C:510:ALA:O	3:C:514:GLU:HG3	2.06	0.56
4:I:69:ILE:HG22	4:I:124:ILE:HG23	1.86	0.56
1:A:107:VAL:HG22	1:A:187:ALA:HB1	1.88	0.56
3:C:318:SER:OG	3:C:324:TYR:HE1	1.88	0.56
4:E:14:TYR:H	4:E:228:ALA:CB	2.17	0.56
4:F:253:ARG:NE	4:F:368:PHE:O	2.38	0.56
4:H:14:TYR:HD1	4:H:200:GLU:OE2	1.88	0.56
6:M:42:DG:H5"	7:N:98:LYS:HZ1	1.70	0.56
7:N:120:PRO:HG2	7:N:121:GLU:OE1	2.06	0.56
3:C:423:ARG:NH1	3:C:427:GLU:OE2	2.37	0.56
4:D:39:SER:OG	4:D:41:GLN:OE1	2.20	0.56
4:D:283:LEU:HD12	4:D:315:CYS:SG	2.46	0.56
4:F:12:LEU:HD12	4:F:231:PHE:CE2	2.41	0.56
5:K:52:G:H2'	5:K:54:A:C2	2.41	0.56
7:N:179:THR:HG22	7:N:225:GLU:HB3	1.86	0.56
4:D:55:LEU:HD12	4:D:258:GLU:OE2	2.06	0.56
7:N:197:LEU:HD12	7:N:218:GLN:NE2	2.20	0.56
4:D:283:LEU:HG	4:D:339:THR:HG22	1.87	0.56
4:E:323:GLU:O	4:E:326:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:40:SER:H	4:G:190:HIS:CE1	2.23	0.56
4:G:189:ALA:HB2	4:H:276:ALA:HB3	1.88	0.56
4:I:11:THR:HG22	4:I:230:THR:HG22	1.87	0.56
4:D:18:ASN:ND2	4:D:39:SER:H	2.04	0.55
2:B:158:GLU:OE2	2:B:218:HIS:NE2	2.39	0.55
3:C:412:ASN:O	3:C:415:ILE:HG22	2.06	0.55
3:C:497:MET:HE1	3:C:501:GLY:HA3	1.86	0.55
4:D:16:ASN:HB2	4:D:226:PHE:CD1	2.41	0.55
4:D:18:ASN:HD21	4:D:39:SER:H	1.53	0.55
4:I:78:TRP:HE3	4:I:82:LEU:HB3	1.70	0.55
3:C:502:ASN:HB2	3:C:505:ASN:ND2	2.19	0.55
1:A:215:SER:HB3	5:K:61:G:OP2	2.07	0.55
2:B:11:ASP:HA	2:B:14:VAL:HG22	1.88	0.55
2:B:176:LEU:HD13	2:B:180:VAL:HG21	1.89	0.55
3:C:530:GLU:OE2	2:J:219:ARG:NE	2.35	0.55
5:K:12:G:N2	6:M:39:DA:N7	2.54	0.55
2:B:171:GLY:HA2	2:B:174:ARG:HD3	1.88	0.55
2:J:171:GLY:HA2	2:J:174:ARG:HD3	1.88	0.55
7:N:17:GLU:HG2	7:N:27:LEU:HD11	1.89	0.55
3:C:132:TRP:NE1	3:C:133:LEU:HD23	2.22	0.55
4:D:179:SER:O	4:D:180:THR:HG22	2.07	0.55
4:E:188:PHE:HE1	4:E:263:PHE:CE1	2.25	0.55
4:F:11:THR:HA	4:F:230:THR:HA	1.87	0.55
4:G:61:ARG:HA	4:G:117:PHE:O	2.05	0.55
4:G:164:ASN:O	4:G:168:ASN:ND2	2.40	0.55
2:J:199:LEU:HA	2:J:202:TRP:CD1	2.41	0.55
1:A:173:ASP:OD2	1:A:180:SER:C	2.50	0.55
4:D:14:TYR:CE2	4:D:226:PHE:HD2	2.25	0.55
4:E:306:GLY:HA2	4:E:310:TYR:CE1	2.41	0.55
6:M:53:DC:H2"	6:M:54:DG:C8	2.42	0.55
2:B:215:GLN:NE2	2:J:78:GLU:OE2	2.40	0.55
4:D:268:PRO:O	4:D:272:GLN:NE2	2.40	0.55
4:E:188:PHE:CE1	4:E:263:PHE:HE1	2.25	0.55
4:F:216:HIS:CE1	5:K:34:G:N3	2.75	0.55
2:J:13:LEU:HD12	2:J:81:PHE:CD1	2.42	0.55
1:A:189:ARG:O	1:A:189:ARG:HD3	2.07	0.55
2:B:91:GLN:NE2	2:B:181:LEU:HA	2.21	0.55
3:C:229:PHE:O	3:C:232:LEU:HG	2.07	0.55
3:C:527:LYS:HB2	2:J:218:HIS:HE1	1.72	0.55
4:F:45:ARG:HE	4:G:207:VAL:HG11	1.72	0.55
4:F:120:PRO:HG3	4:F:164:ASN:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:72:ARG:O	4:E:75:GLU:HG3	2.06	0.55
4:F:106:LYS:HD2	4:F:109:GLU:OE2	2.07	0.55
7:N:14:SER:OG	7:N:140:ARG:HD3	2.07	0.55
1:A:20:PHE:HZ	2:B:49:ARG:NH1	2.04	0.54
2:B:7:LEU:HD21	2:B:136:ARG:NH1	2.23	0.54
2:B:209:VAL:O	2:B:212:GLU:HG2	2.08	0.54
4:D:260:LEU:HD13	4:D:286:ILE:HD13	1.89	0.54
4:F:285:HIS:CD2	4:F:349:LEU:HD22	2.42	0.54
2:J:209:VAL:O	2:J:212:GLU:HG2	2.08	0.54
2:B:22:VAL:HG22	2:B:96:ARG:HD2	1.88	0.54
2:B:84:VAL:HA	2:B:87:ILE:HG22	1.89	0.54
4:I:281:PRO:O	4:I:356:TYR:OH	2.26	0.54
7:N:179:THR:HG22	7:N:225:GLU:OE1	2.07	0.54
2:B:13:LEU:HD12	2:B:81:PHE:CD1	2.42	0.54
3:C:152:ALA:CB	3:C:155:ARG:HD3	2.38	0.54
3:C:219:VAL:HG13	3:C:221:TYR:HE2	1.72	0.54
4:F:320:ASN:O	4:F:323:GLU:HG2	2.06	0.54
4:G:15:SER:HB2	4:G:17:ILE:HG12	1.89	0.54
4:I:118:TYR:OH	4:I:166:SER:OG	2.21	0.54
2:B:199:LEU:HA	2:B:202:TRP:CD1	2.41	0.54
4:E:73:LEU:HD23	4:E:76:ARG:HD2	1.88	0.54
5:K:33:G:C2	5:K:34:G:C2	2.95	0.54
7:N:242:LEU:O	7:N:246:VAL:HG23	2.08	0.54
1:A:43:ALA:O	1:A:44:ASN:HB2	2.06	0.54
4:E:353:TYR:CE2	4:E:363:MET:HE3	2.34	0.54
4:F:218:SER:O	4:F:220:HIS:N	2.40	0.54
4:H:35:ARG:HB3	4:H:193:THR:OG1	2.07	0.54
4:I:319:ASN:HB2	4:I:346:LEU:HD22	1.90	0.54
2:J:176:LEU:HD13	2:J:180:VAL:HG21	1.89	0.54
4:D:45:ARG:HG2	4:D:45:ARG:HH11	1.73	0.54
3:C:30:ALA:HB1	3:C:54:LEU:HD13	1.88	0.54
3:C:521:GLU:OE2	2:J:207:ARG:HB2	2.08	0.54
2:B:42:PRO:O	2:B:45:LEU:HG	2.08	0.54
4:E:335:ARG:O	4:E:363:MET:HE1	2.08	0.54
4:F:14:TYR:N	4:F:228:ALA:HB2	2.20	0.54
2:B:172:VAL:O	2:B:176:LEU:CB	2.54	0.54
3:C:178:SER:O	3:C:182:VAL:HG23	2.08	0.54
4:H:323:GLU:HB2	4:H:348:ALA:HB2	1.89	0.54
7:N:208:ASP:OD2	7:N:210:LYS:HB3	2.08	0.54
3:C:339:ASP:OD2	3:C:420:THR:HA	2.08	0.53
4:D:33:LYS:HD2	4:D:303:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:195:HIS:HE1	4:F:230:THR:H	1.55	0.53
4:H:259:PHE:CD2	4:H:260:LEU:HD12	2.43	0.53
7:N:19:SER:OG	7:N:23:GLU:O	2.25	0.53
7:N:127:ASP:CG	7:N:154:ARG:HH22	2.16	0.53
1:A:206:VAL:HG22	1:A:221:LEU:HD23	1.88	0.53
4:I:104:LYS:HD3	4:I:104:LYS:N	2.23	0.53
3:C:478:GLU:HG3	3:C:479:PRO:HD3	1.89	0.53
4:F:269:SER:HA	4:F:272:GLN:CD	2.34	0.53
1:A:124:LEU:HD23	1:A:126:LEU:H	1.74	0.53
4:D:341:GLU:N	4:D:341:GLU:OE1	2.42	0.53
4:F:164:ASN:O	4:F:168:ASN:ND2	2.41	0.53
4:G:137:ALA:O	4:G:141:GLU:HB2	2.09	0.53
4:H:40:SER:HB2	4:H:188:PHE:HD2	1.74	0.53
1:A:107:VAL:CG2	1:A:187:ALA:HB1	2.39	0.53
1:A:169:ASP:HB3	1:A:185:HIS:O	2.08	0.53
2:B:182:TYR:HD2	4:E:22:LEU:HD13	1.74	0.53
3:C:221:TYR:CE1	3:C:376:ALA:HB2	2.44	0.53
4:E:190:HIS:CD2	4:F:275:THR:HG22	2.43	0.53
4:F:219:GLY:O	5:K:33:G:C2	2.61	0.53
4:G:11:THR:HA	4:G:230:THR:HA	1.89	0.53
4:H:336:GLY:HA3	4:H:363:MET:CE	2.38	0.53
4:I:40:SER:HB2	4:I:188:PHE:HD2	1.73	0.53
7:N:137:TYR:CD1	7:N:141:ARG:HA	2.43	0.53
2:J:42:PRO:O	2:J:45:LEU:HG	2.08	0.53
3:C:219:VAL:HA	3:C:377:PHE:O	2.08	0.53
4:E:176:GLU:OE1	4:E:176:GLU:N	2.41	0.53
4:F:336:GLY:HA3	4:F:363:MET:HE3	1.91	0.53
4:I:326:ARG:HH11	4:I:335:ARG:NH1	2.07	0.53
2:J:7:LEU:HD21	2:J:136:ARG:NH1	2.23	0.53
2:J:56:PRO:CD	2:J:81:PHE:HE2	2.21	0.53
1:A:44:ASN:HD21	5:K:51:C:C1'	2.22	0.53
4:D:289:ARG:NH1	4:D:291:ASP:OD2	2.38	0.53
4:I:359:LEU:O	4:I:363:MET:HG2	2.08	0.53
7:N:164:GLU:HA	7:N:230:LEU:HD11	1.89	0.53
3:C:429:LEU:HA	3:C:432:ARG:HG2	1.91	0.53
5:K:43:G:N2	5:K:44:A:N1	2.56	0.53
3:C:132:TRP:O	3:C:134:GLN:HG3	2.09	0.53
4:E:79:ASP:OD1	4:E:82:LEU:HB2	2.09	0.53
4:D:289:ARG:HH11	4:D:291:ASP:CG	2.16	0.52
4:F:253:ARG:HH21	4:F:368:PHE:C	2.17	0.52
4:I:169:LEU:HD21	4:I:259:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:HG23	1:A:25:ASN:H	1.74	0.52
2:B:202:TRP:HE3	2:B:206:PRO:HB3	1.74	0.52
4:E:68:GLU:OE2	4:E:72:ARG:NE	2.42	0.52
4:E:320:ASN:OD1	4:E:321:TYR:N	2.42	0.52
8:O:10:DA:H2"	8:O:11:DG:C8	2.44	0.52
4:H:11:THR:HA	4:H:230:THR:HA	1.91	0.52
4:H:40:SER:H	4:H:190:HIS:CE1	2.27	0.52
4:H:334:ILE:H	4:H:334:ILE:HD12	1.74	0.52
4:I:65:ILE:O	4:I:69:ILE:HG12	2.08	0.52
2:J:172:VAL:O	2:J:176:LEU:CB	2.54	0.52
4:H:15:SER:HB2	4:H:17:ILE:HG23	1.92	0.52
4:H:86:GLY:O	4:H:90:VAL:HG23	2.09	0.52
2:J:160:ARG:O	2:J:163:LEU:HG	2.09	0.52
2:B:167:GLN:HE22	4:F:198:THR:CB	2.22	0.52
4:G:79:ASP:OD1	4:G:80:ALA:N	2.43	0.52
4:G:259:PHE:CD2	4:G:260:LEU:HD12	2.44	0.52
4:H:131:ALA:HA	4:H:151:LEU:HD11	1.92	0.52
2:B:12:ALA:HA	2:B:15:LYS:NZ	2.25	0.52
2:B:169:LEU:HD23	2:B:202:TRP:HB2	1.92	0.52
3:C:104:LYS:HD3	3:C:106:ARG:O	2.10	0.52
3:C:512:TYR:O	3:C:516:THR:HG22	2.10	0.52
4:D:28:VAL:HG21	7:N:12:MET:HE2	1.90	0.52
4:G:285:HIS:HD2	4:G:349:LEU:HB3	1.74	0.52
2:J:172:VAL:HG11	2:J:202:TRP:CE2	2.45	0.52
2:J:202:TRP:HE3	2:J:206:PRO:HB3	1.75	0.52
3:C:122:ARG:NE	3:C:249:TRP:O	2.43	0.52
3:C:159:GLU:HG3	6:M:46:DT:OP2	2.09	0.52
4:E:301:GLU:OE2	4:F:310:TYR:N	2.41	0.52
4:G:10:GLN:NE2	4:G:279:THR:O	2.43	0.52
4:H:14:TYR:H	4:H:228:ALA:CB	2.20	0.52
4:H:19:ARG:HD2	4:H:23:GLY:HA2	1.92	0.52
7:N:74:HIS:O	7:N:103:THR:OG1	2.25	0.52
2:B:93:ARG:CB	2:B:96:ARG:HH21	2.23	0.52
2:B:172:VAL:HG11	2:B:202:TRP:CE2	2.45	0.52
4:E:14:TYR:CE2	4:E:226:PHE:HD2	2.28	0.52
4:E:202:ASP:CB	4:I:37:ARG:HH22	2.21	0.52
4:G:71:LYS:HA	4:G:74:ARG:HG2	1.92	0.52
4:E:14:TYR:OH	4:I:37:ARG:NH2	2.43	0.52
4:G:331:ASP:OD1	4:G:331:ASP:N	2.43	0.52
4:H:308:ASP:OD1	4:H:309:GLY:N	2.43	0.52
2:B:93:ARG:HD2	4:E:219:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:309:LEU:HD12	3:C:315:TYR:CG	2.45	0.52
3:C:317:THR:HG22	3:C:323:VAL:HA	1.92	0.52
4:D:193:THR:HG23	4:D:231:PHE:CE1	2.45	0.52
4:F:334:ILE:HD12	4:F:334:ILE:H	1.75	0.52
2:B:141:VAL:HG12	2:B:220:THR:OG1	2.10	0.51
2:B:160:ARG:O	2:B:163:LEU:HG	2.09	0.51
3:C:333:ALA:HB3	3:C:336:ARG:NH2	2.25	0.51
3:C:341:LEU:O	3:C:355:LEU:HD12	2.10	0.51
4:E:241:ARG:O	4:E:244:GLU:HG2	2.10	0.51
4:F:66:ILE:HD11	4:F:91:VAL:HG21	1.92	0.51
6:M:42:DG:H5'	7:N:97:LYS:NZ	2.25	0.51
6:M:43:DG:H5'	7:N:98:LYS:HG3	1.92	0.51
2:B:55:VAL:HG11	2:B:78:GLU:HG3	1.92	0.51
3:C:493:TYR:HB2	3:C:503:ALA:HB2	1.91	0.51
4:D:6:ILE:N	4:D:6:ILE:HD12	2.25	0.51
4:E:37:ARG:NH2	4:F:14:TYR:OH	2.44	0.51
2:B:182:TYR:HH	4:E:225:GLN:CD	2.14	0.51
3:C:68:LEU:HD23	3:C:186:LEU:HD21	1.93	0.51
3:C:429:LEU:HD21	3:C:504:PHE:HB2	1.92	0.51
3:C:520:CYS:O	2:J:211:ARG:HG3	2.09	0.51
4:E:285:HIS:HD2	4:E:349:LEU:HB3	1.74	0.51
2:J:12:ALA:HA	2:J:15:LYS:NZ	2.25	0.51
2:J:16:ARG:O	2:J:20:LEU:N	2.42	0.51
5:K:5:A:H5''	7:N:141:ARG:HG2	1.92	0.51
5:K:52:G:H1'	5:K:56:G:N2	2.26	0.51
6:M:40:DC:H2''	6:M:41:DT:H5'	1.92	0.51
1:A:46:ARG:HA	5:K:59:G:C4'	2.40	0.51
3:C:155:ARG:HH12	3:C:174:HIS:CE1	2.29	0.51
3:C:267:LEU:HA	3:C:270:ILE:HG12	1.93	0.51
3:C:274:ASP:OD1	3:C:275:HIS:N	2.42	0.51
3:C:434:GLU:OE2	3:C:470:MET:HG2	2.11	0.51
4:D:17:ILE:CG2	4:D:268:PRO:HB2	2.41	0.51
4:D:169:LEU:HD12	4:D:170:PHE:CE2	2.46	0.51
4:D:216:HIS:O	4:D:218:SER:N	2.38	0.51
4:G:337:TYR:OH	4:G:345:ASP:O	2.24	0.51
7:N:7:ARG:HD2	7:N:151:LEU:HD21	1.91	0.51
1:A:44:ASN:ND2	5:K:51:C:O4'	2.43	0.51
3:C:318:SER:O	3:C:319:LYS:C	2.54	0.51
7:N:4:PHE:CZ	7:N:125:ILE:HD11	2.45	0.51
3:C:409:ASP:O	3:C:413:ALA:N	2.40	0.51
3:C:527:LYS:HA	2:J:218:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:191:ALA:HB2	4:I:233:ARG:HG2	1.91	0.51
2:J:169:LEU:HD23	2:J:202:TRP:HB2	1.92	0.51
3:C:76:THR:HG21	3:C:232:LEU:HD13	1.93	0.51
4:D:164:ASN:HB3	4:D:167:VAL:HG12	1.93	0.51
4:D:167:VAL:HG23	4:D:172:ARG:HA	1.93	0.51
4:I:174:LEU:N	4:I:181:GLU:OE2	2.34	0.51
4:D:353:TYR:HD2	4:D:359:LEU:HA	1.76	0.51
4:F:89:GLN:HE22	4:F:147:PRO:HB2	1.76	0.51
4:G:141:GLU:HG2	4:G:144:LYS:HZ3	1.76	0.51
2:J:25:PRO:CD	2:J:26:ALA:H	2.23	0.51
1:A:180:SER:HB3	5:K:61:G:O2'	2.11	0.51
3:C:330:ALA:N	3:C:380:ASP:OD2	2.44	0.51
4:E:127:LEU:O	4:E:130:ILE:HG13	2.11	0.51
4:F:137:ALA:HB1	4:F:150:ILE:HG21	1.93	0.51
4:F:212:LYS:HE3	4:F:214:ASN:HB3	1.92	0.51
4:F:219:GLY:CA	5:K:33:G:H22	2.23	0.51
4:G:89:GLN:NE2	4:G:141:GLU:OE1	2.43	0.51
4:G:12:LEU:HB3	4:G:15:SER:HB3	1.92	0.51
4:G:141:GLU:HG3	4:G:150:ILE:CD1	2.35	0.51
4:I:36:THR:O	4:I:193:THR:HG23	2.10	0.51
4:I:137:ALA:HA	4:I:140:LYS:NZ	2.26	0.51
4:I:174:LEU:HD11	4:I:180:THR:OG1	2.11	0.51
2:J:176:LEU:N	2:J:177:PRO:HD2	2.26	0.51
6:M:39:DA:H2''	6:M:40:DC:O5'	2.11	0.51
4:D:329:TRP:HH2	7:N:148:LEU:HD13	1.75	0.50
4:F:306:GLY:HA2	4:F:310:TYR:CE1	2.46	0.50
6:M:51:DC:H2''	6:M:52:DG:C8	2.46	0.50
3:C:215:LEU:HD23	3:C:215:LEU:N	2.26	0.50
4:G:207:VAL:HG12	5:K:26:G:OP1	2.11	0.50
4:H:269:SER:HA	4:H:272:GLN:CD	2.36	0.50
4:I:33:LYS:HD3	4:I:303:ALA:CB	2.40	0.50
4:I:79:ASP:OD1	4:I:80:ALA:N	2.43	0.50
1:A:181:ARG:NH1	5:K:47:C:H1'	2.26	0.50
4:D:43:TRP:CZ3	4:D:47:VAL:HG21	2.46	0.50
4:D:46:ALA:O	4:D:50:GLU:OE1	2.29	0.50
4:H:18:ASN:HD21	4:H:39:SER:N	2.09	0.50
4:H:73:LEU:HD23	4:H:76:ARG:HD2	1.92	0.50
2:J:177:PRO:O	2:J:181:LEU:HB3	2.12	0.50
1:A:15:GLN:O	1:A:16:THR:HG22	2.12	0.50
2:B:163:LEU:HD22	4:F:201:VAL:HB	1.92	0.50
4:D:12:LEU:HD12	4:D:231:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:285:HIS:CD2	4:E:349:LEU:HD22	2.46	0.50
4:H:267:VAL:CG1	4:H:272:GLN:HE22	2.24	0.50
6:M:52:DG:H2"	6:M:53:DC:OP2	2.11	0.50
3:C:434:GLU:HG2	3:C:470:MET:HE3	1.93	0.50
4:E:20:ASP:OD1	4:E:26:LYS:HG2	2.11	0.50
2:J:141:VAL:HG12	2:J:220:THR:OG1	2.10	0.50
5:K:7:C:O2'	7:N:76:ILE:HG22	2.12	0.50
7:N:146:ASP:OD1	7:N:147:PRO:HD2	2.12	0.50
2:B:176:LEU:N	2:B:177:PRO:HD2	2.26	0.50
3:C:329:GLU:HB2	3:C:332:ARG:HG2	1.93	0.50
4:E:233:ARG:NH2	4:E:263:PHE:O	2.39	0.50
1:A:43:ALA:C	1:A:45:PRO:CD	2.85	0.50
2:B:177:PRO:O	2:B:181:LEU:HB3	2.12	0.50
4:D:292:ARG:NH1	7:N:147:PRO:O	2.40	0.50
4:I:141:GLU:HG3	4:I:150:ILE:CD1	2.35	0.50
7:N:65:ARG:NE	7:N:110:ASP:O	2.45	0.50
4:D:28:VAL:CG2	4:D:37:ARG:CD	2.87	0.50
4:E:292:ARG:NH2	4:F:265:SER:O	2.44	0.50
4:G:205:THR:HA	4:G:221:MET:HB3	1.94	0.50
4:H:335:ARG:O	4:H:363:MET:HE1	2.11	0.50
2:B:29:ALA:O	2:B:33:ARG:HG2	2.12	0.50
3:C:32:SER:HA	3:C:54:LEU:HA	1.93	0.50
4:D:275:THR:HG22	4:H:190:HIS:CD2	2.47	0.50
4:E:18:ASN:HA	5:K:34:G:OP2	2.11	0.50
5:K:3:G:N3	7:N:17:GLU:HA	2.27	0.50
7:N:116:ALA:HB2	7:N:162:LEU:HD23	1.94	0.50
3:C:122:ARG:O	3:C:122:ARG:HG2	2.11	0.49
4:G:306:GLY:HA2	4:G:310:TYR:CE1	2.47	0.49
3:C:79:ILE:HG12	3:C:115:TYR:CB	2.42	0.49
3:C:156:THR:HG21	3:C:162:VAL:HA	1.92	0.49
3:C:472:ARG:NH2	4:D:29:VAL:HG21	2.27	0.49
4:D:191:ALA:HB2	4:D:233:ARG:HG2	1.94	0.49
4:E:286:ILE:HD11	4:E:363:MET:HB3	1.94	0.49
4:H:148:LYS:HE2	4:H:148:LYS:HA	1.94	0.49
4:I:33:LYS:HE2	4:I:196:GLY:HA3	1.93	0.49
2:J:29:ALA:O	2:J:33:ARG:HG2	2.12	0.49
2:B:55:VAL:CG1	2:B:78:GLU:HA	2.42	0.49
3:C:201:VAL:CG1	3:C:206:SER:HB3	2.42	0.49
3:C:338:LEU:O	3:C:341:LEU:HB2	2.12	0.49
4:E:88:ARG:O	4:E:92:LEU:HB2	2.12	0.49
4:F:68:GLU:OE2	4:F:72:ARG:NE	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:69:ILE:HD12	4:I:90:VAL:HG11	1.94	0.49
1:A:162:SER:CB	1:A:191:ASP:H	2.25	0.49
2:B:13:LEU:HD22	2:B:17:VAL:HG21	1.93	0.49
4:G:45:ARG:HA	4:G:48:ARG:HG2	1.94	0.49
4:H:96:LYS:HG3	4:H:97:LYS:H	1.78	0.49
6:M:49:DT:H2''	6:M:50:DC:C6	2.47	0.49
1:A:110:PRO:HB3	1:A:148:TRP:CD2	2.48	0.49
3:C:319:LYS:O	3:C:320:GLU:HB3	2.12	0.49
4:E:292:ARG:HH11	4:F:278:MET:HE3	1.76	0.49
4:G:137:ALA:HB1	4:G:150:ILE:HG21	1.95	0.49
2:J:45:LEU:HA	2:J:48:HIS:CD2	2.47	0.49
2:J:91:GLN:NE2	2:J:181:LEU:HA	2.21	0.49
5:K:20:U:H2'	5:K:21:G:H4'	1.93	0.49
7:N:187:GLU:HG2	7:N:217:ARG:HD3	1.94	0.49
1:A:160:LEU:HD11	4:I:227:SER:C	2.37	0.49
4:E:18:ASN:ND2	4:E:42:SER:OG	2.41	0.49
4:F:174:LEU:H	4:F:181:GLU:HG2	1.77	0.49
4:G:72:ARG:HH22	4:G:121:VAL:CG1	2.23	0.49
4:H:259:PHE:HD2	4:H:260:LEU:HD12	1.76	0.49
1:A:111:THR:O	1:A:127:LYS:HD2	2.13	0.49
3:C:134:GLN:NE2	3:C:282:LEU:HD13	2.28	0.49
4:E:334:ILE:HD12	4:E:334:ILE:H	1.78	0.49
4:G:148:LYS:HA	4:G:148:LYS:HE2	1.93	0.49
5:K:49:C:H2'	5:K:50:A:C8	2.44	0.49
7:N:40:ALA:HB1	7:N:45:VAL:HB	1.94	0.49
3:C:260:LEU:HD22	3:C:261:PRO:HD2	1.94	0.49
4:E:278:MET:HE3	4:I:292:ARG:HH11	1.78	0.49
4:G:141:GLU:CG	4:G:150:ILE:HD11	2.34	0.49
4:I:40:SER:H	4:I:190:HIS:CE1	2.31	0.49
6:M:50:DC:H2''	6:M:51:DC:C6	2.48	0.49
7:N:67:GLY:HA2	7:N:110:ASP:OD1	2.13	0.49
2:B:45:LEU:HA	2:B:48:HIS:CD2	2.47	0.49
3:C:168:HIS:HE1	3:C:174:HIS:HE1	1.59	0.49
4:H:79:ASP:OD1	4:H:80:ALA:N	2.45	0.49
4:H:289:ARG:HD2	4:H:333:ALA:CB	2.43	0.49
4:I:17:ILE:HG21	4:I:268:PRO:CB	2.18	0.49
6:M:52:DG:C2	8:O:4:DG:C2	3.01	0.49
3:C:190:GLY:O	3:C:214:PRO:HD2	2.13	0.49
3:C:381:GLN:CB	3:C:387:ASP:HA	2.42	0.49
3:C:398:VAL:O	3:C:399:LEU:HD23	2.12	0.49
4:F:131:ALA:HA	4:F:151:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ARG:CD	4:E:220:HIS:HA	2.41	0.48
3:C:151:LEU:HD12	3:C:188:THR:HG21	1.93	0.48
3:C:328:ALA:HB3	3:C:380:ASP:HB3	1.94	0.48
4:F:19:ARG:HB3	4:F:23:GLY:HA2	1.93	0.48
4:F:205:THR:O	5:K:32:U:H5''	2.13	0.48
4:F:336:GLY:HA3	4:F:363:MET:CE	2.43	0.48
4:I:38:VAL:HG12	4:I:191:ALA:HB3	1.95	0.48
4:D:43:TRP:HD1	4:D:268:PRO:CD	2.26	0.48
4:H:267:VAL:HG12	4:H:272:GLN:HE22	1.78	0.48
1:A:20:PHE:HZ	2:B:49:ARG:HH11	1.61	0.48
3:C:123:PHE:CZ	3:C:249:TRP:CZ3	3.02	0.48
4:E:76:ARG:NH2	4:E:125:ASP:OD1	2.47	0.48
4:H:68:GLU:OE2	4:H:71:LYS:HE3	2.13	0.48
2:J:37:LEU:O	2:J:44:MET:HE1	2.13	0.48
2:J:93:ARG:CB	2:J:96:ARG:HH21	2.23	0.48
5:K:1:A:C8	7:N:47:ARG:HG3	2.49	0.48
7:N:58:LYS:HZ1	7:N:188:GLU:H	1.61	0.48
4:F:37:ARG:NH2	4:G:202:ASP:OD1	2.37	0.48
4:G:199:VAL:O	2:J:43:ARG:NH2	2.47	0.48
2:J:145:GLN:HE22	2:J:188:VAL:HG13	1.79	0.48
7:N:208:ASP:O	7:N:212:ARG:HG3	2.12	0.48
1:A:164:TYR:CZ	1:A:188:VAL:HA	2.49	0.48
2:B:80:ALA:HA	2:B:173:HIS:HE1	1.79	0.48
4:E:215:ASP:OD2	4:I:64:ARG:NH2	2.46	0.48
2:J:84:VAL:HA	2:J:87:ILE:CG2	2.42	0.48
6:M:48:DG:C2	8:O:8:DG:C2	3.02	0.48
3:C:381:GLN:HB2	3:C:386:ARG:O	2.14	0.48
4:E:40:SER:H	4:E:190:HIS:CE1	2.31	0.48
4:F:141:GLU:HA	4:F:144:LYS:NZ	2.28	0.48
4:G:164:ASN:OD1	4:G:165:VAL:HG12	2.13	0.48
3:C:519:TYR:CE1	4:D:199:VAL:HG12	2.49	0.48
3:C:522:ARG:HD2	3:C:522:ARG:N	2.25	0.48
4:F:55:LEU:HD22	4:F:258:GLU:OE2	2.14	0.48
4:F:285:HIS:HD2	4:F:349:LEU:HB3	1.79	0.48
4:I:341:GLU:HG3	4:I:343:LYS:HZ3	1.79	0.48
2:J:77:VAL:CG1	2:J:78:GLU:H	2.00	0.48
2:J:83:ALA:CB	2:J:173:HIS:ND1	2.77	0.48
8:O:5:DG:H2''	8:O:6:DA:C8	2.48	0.48
1:A:113:ARG:HD2	5:K:57:U:H5	1.79	0.48
3:C:122:ARG:NH1	3:C:130:ARG:HD3	2.29	0.48
4:H:6:ILE:HD13	4:H:263:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:272:GLN:HA	4:E:275:THR:O	2.14	0.48
4:F:319:ASN:ND2	4:F:346:LEU:CA	2.75	0.48
4:H:72:ARG:HH22	4:H:121:VAL:CG1	2.25	0.48
4:H:331:ASP:OD1	4:H:331:ASP:N	2.43	0.48
3:C:298:TRP:CE2	3:C:301:ARG:NH2	2.81	0.47
4:D:279:THR:HG22	4:D:280:LEU:N	2.29	0.47
4:I:163:ARG:HE	4:I:182:VAL:CG2	2.27	0.47
2:J:84:VAL:CA	2:J:87:ILE:HG22	2.43	0.47
5:K:52:G:C2	5:K:56:G:C6	3.02	0.47
7:N:64:ASP:HB3	7:N:169:PRO:HD2	1.97	0.47
1:A:91:PRO:HG3	1:A:203:ARG:HD3	1.95	0.47
2:B:145:GLN:HE22	2:B:188:VAL:HG13	1.79	0.47
3:C:379:PHE:CE1	3:C:390:TRP:HE3	2.32	0.47
3:C:468:HIS:CD2	7:N:70:LEU:HD21	2.49	0.47
4:D:307:SER:H	4:H:32:GLY:HA3	1.79	0.47
4:E:103:GLU:OE1	4:E:114:SER:HA	2.14	0.47
4:E:365:ALA:HA	4:E:368:PHE:CE1	2.48	0.47
4:F:15:SER:HB2	4:F:17:ILE:HG23	1.95	0.47
4:F:346:LEU:O	4:F:347:ALA:C	2.56	0.47
4:I:341:GLU:HG3	4:I:343:LYS:HD3	1.95	0.47
2:J:163:LEU:HA	2:J:166:ARG:NH2	2.29	0.47
6:M:53:DC:H2"	6:M:54:DG:H8	1.78	0.47
1:A:29:LYS:O	1:A:32:ARG:HG2	2.13	0.47
1:A:113:ARG:NH2	1:A:123:ARG:HE	2.12	0.47
1:A:170:ASP:H	2:B:23:ASN:ND2	2.11	0.47
2:B:209:VAL:HA	2:B:212:GLU:HG2	1.96	0.47
3:C:98:ARG:NH1	3:C:358:CYS:SG	2.88	0.47
3:C:382:ASP:CB	3:C:386:ARG:HB2	2.41	0.47
4:D:206:ALA:O	4:D:218:SER:OG	2.32	0.47
4:D:324:ARG:HD2	7:N:243:PHE:CE2	2.50	0.47
4:F:81:ASP:OD1	4:F:82:LEU:N	2.48	0.47
3:C:182:VAL:O	3:C:186:LEU:HD13	2.14	0.47
4:E:292:ARG:HD3	4:F:280:LEU:HD11	1.96	0.47
2:J:209:VAL:HA	2:J:212:GLU:HG2	1.96	0.47
7:N:76:ILE:HG13	7:N:76:ILE:O	2.14	0.47
3:C:132:TRP:CE2	3:C:133:LEU:HD23	2.49	0.47
3:C:468:HIS:HD2	7:N:70:LEU:HD21	1.78	0.47
4:D:11:THR:HA	4:D:230:THR:HA	1.95	0.47
4:D:326:ARG:NH1	4:D:335:ARG:HH22	2.12	0.47
4:H:324:ARG:O	4:H:327:GLU:HG2	2.15	0.47
4:I:363:MET:HB3	4:I:363:MET:HE2	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:85:THR:HG22	7:N:86:VAL:N	2.30	0.47
1:A:162:SER:O	1:A:190:PHE:CD1	2.68	0.47
3:C:340:ALA:C	3:C:342:LEU:N	2.69	0.47
4:E:72:ARG:HA	4:E:75:GLU:HG3	1.96	0.47
4:G:141:GLU:HG2	4:G:144:LYS:NZ	2.30	0.47
4:G:334:ILE:HD12	4:G:334:ILE:H	1.79	0.47
4:H:89:GLN:NE2	4:H:147:PRO:HB2	2.29	0.47
4:H:205:THR:HG23	4:H:221:MET:HB2	1.97	0.47
4:H:335:ARG:C	4:H:363:MET:HE1	2.39	0.47
4:I:163:ARG:HE	4:I:182:VAL:HG22	1.80	0.47
4:I:285:HIS:HD2	4:I:349:LEU:HB3	1.80	0.47
2:J:76:ALA:O	2:J:79:ARG:HB3	2.14	0.47
1:A:23:ALA:HA	1:A:26:LEU:HD23	1.97	0.47
2:B:92:PRO:HG3	4:E:223:ALA:CB	2.44	0.47
2:B:153:ASN:CG	4:F:220:HIS:CD2	2.91	0.47
3:C:207:GLU:HB2	3:C:301:ARG:NH2	2.30	0.47
3:C:311:PRO:HB2	3:C:354:ILE:HB	1.95	0.47
3:C:342:LEU:HD23	3:C:342:LEU:N	2.25	0.47
3:C:439:GLU:HA	3:C:442:LYS:HG2	1.95	0.47
3:C:445:ASN:OD1	4:D:201:VAL:HG11	2.15	0.47
4:D:43:TRP:CZ3	4:D:188:PHE:CE2	3.03	0.47
4:E:106:LYS:HB2	4:E:109:GLU:HG2	1.95	0.47
4:F:253:ARG:HD3	4:F:253:ARG:HA	1.51	0.47
2:J:80:ALA:HA	2:J:173:HIS:HE1	1.79	0.47
4:D:29:VAL:HA	4:D:34:GLU:HA	1.97	0.47
7:N:162:LEU:CD1	7:N:184:LEU:HD11	2.45	0.47
8:O:7:DC:H2''	8:O:8:DG:C8	2.50	0.47
1:A:160:LEU:HD12	4:I:14:TYR:HD1	1.80	0.47
4:E:225:GLN:O	4:E:226:PHE:HD1	1.98	0.47
4:G:324:ARG:NH2	4:H:352:ARG:HH21	2.13	0.47
2:J:138:ASN:CG	2:J:139:LEU:H	2.23	0.47
1:A:102:VAL:HA	1:A:224:ALA:O	2.15	0.47
3:C:104:LYS:HB3	3:C:104:LYS:HE3	1.44	0.47
3:C:395:THR:HB	3:C:396:PRO:HD2	1.97	0.47
4:I:10:GLN:OE1	4:I:281:PRO:HG3	2.14	0.47
1:A:170:ASP:O	1:A:171:VAL:HG13	2.15	0.46
3:C:98:ARG:NH1	3:C:234:LEU:HD13	2.30	0.46
4:G:86:GLY:O	4:G:90:VAL:HG23	2.15	0.46
6:M:39:DA:H2'	6:M:40:DC:C5	2.49	0.46
3:C:141:GLU:HG3	3:C:200:ARG:HG3	1.98	0.46
3:C:303:ARG:NH2	8:O:11:DG:O3'	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:314:ILE:HG21	3:C:326:ARG:HE	1.81	0.46
3:C:317:THR:CG2	3:C:323:VAL:HG22	2.45	0.46
3:C:350:TYR:O	3:C:351:ARG:CB	2.63	0.46
3:C:463:GLY:O	3:C:466:VAL:HG22	2.15	0.46
3:C:472:ARG:NH1	3:C:514:GLU:HB3	2.30	0.46
4:D:43:TRP:CE3	4:D:188:PHE:CE2	3.04	0.46
4:D:165:VAL:HG11	4:D:255:ALA:HB2	1.97	0.46
4:D:175:ALA:HB2	7:N:84:ARG:O	2.15	0.46
4:E:28:VAL:CG2	4:E:37:ARG:HD3	2.45	0.46
4:E:269:SER:HA	4:E:272:GLN:CD	2.40	0.46
4:F:18:ASN:HA	5:K:28:C:OP2	2.15	0.46
4:F:97:LYS:CD	4:F:97:LYS:H	2.28	0.46
4:G:52:GLU:OE1	4:G:58:LYS:HG2	2.15	0.46
4:I:88:ARG:O	4:I:92:LEU:HB2	2.15	0.46
2:J:17:VAL:C	2:J:19:LYS:N	2.73	0.46
7:N:7:ARG:HG2	7:N:148:LEU:O	2.15	0.46
7:N:58:LYS:NZ	7:N:187:GLU:HB2	2.30	0.46
1:A:44:ASN:HD21	5:K:51:C:H4'	1.77	0.46
3:C:168:HIS:CE1	3:C:174:HIS:HE1	2.32	0.46
3:C:444:SER:HB3	3:C:528:VAL:HG11	1.98	0.46
4:F:86:GLY:O	4:F:90:VAL:HG23	2.14	0.46
4:I:55:LEU:HD23	4:I:165:VAL:HG21	1.97	0.46
3:C:98:ARG:NH1	3:C:234:LEU:HA	2.29	0.46
3:C:139:ARG:HH12	3:C:283:HIS:HD2	1.63	0.46
3:C:139:ARG:HH11	3:C:295:TRP:HH2	1.63	0.46
4:H:344:THR:HG22	4:H:346:LEU:H	1.80	0.46
5:K:14:G:N2	5:K:15:A:N3	2.63	0.46
5:K:33:G:H1'	5:K:34:G:C8	2.51	0.46
7:N:159:VAL:O	7:N:163:VAL:HG23	2.15	0.46
1:A:124:LEU:HD11	5:K:43:G:H2'	1.96	0.46
2:B:138:ASN:CG	2:B:139:LEU:H	2.23	0.46
2:B:163:LEU:HA	2:B:166:ARG:NH2	2.30	0.46
4:D:14:TYR:HA	4:D:228:ALA:HB2	1.96	0.46
4:F:335:ARG:O	4:F:363:MET:HE1	2.16	0.46
4:H:45:ARG:HA	4:H:48:ARG:HG2	1.96	0.46
4:H:164:ASN:O	4:H:168:ASN:ND2	2.49	0.46
5:K:52:G:O3'	5:K:53:C:H6	1.99	0.46
7:N:244:THR:HA	7:N:247:LYS:NZ	2.31	0.46
3:C:194:SER:HB2	3:C:212:ALA:HB2	1.96	0.46
3:C:494:THR:H	3:C:497:MET:HE2	1.81	0.46
4:E:72:ARG:HH22	4:E:121:VAL:CG1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:16:ASN:HD22	4:F:226:PHE:HD1	1.64	0.46
4:F:121:VAL:N	4:F:122:PRO:HD2	2.31	0.46
4:F:202:ASP:OD1	4:F:202:ASP:O	2.33	0.46
4:I:120:PRO:HG3	4:I:164:ASN:HB2	1.98	0.46
2:J:168:ASN:OD1	2:J:171:GLY:N	2.47	0.46
7:N:19:SER:O	7:N:24:ARG:NH1	2.49	0.46
3:C:67:VAL:CG2	3:C:186:LEU:HB3	2.45	0.46
4:F:346:LEU:O	4:F:348:ALA:N	2.48	0.46
4:H:14:TYR:CD1	4:H:200:GLU:OE2	2.67	0.46
4:I:18:ASN:HD21	4:I:39:SER:H	1.63	0.46
4:I:187:GLN:HB2	4:I:236:ASN:HB2	1.98	0.46
7:N:33:SER:HB3	7:N:202:ASP:O	2.15	0.46
3:C:522:ARG:H	3:C:522:ARG:CD	2.25	0.46
4:D:28:VAL:HG21	4:D:37:ARG:HD3	1.96	0.46
4:F:62:THR:HG23	4:G:209:ASP:HB2	1.97	0.46
4:F:96:LYS:HG2	4:F:97:LYS:H	1.80	0.46
4:F:260:LEU:HD23	4:F:286:ILE:HD13	1.97	0.46
4:G:344:THR:HG22	4:G:346:LEU:H	1.81	0.46
1:A:113:ARG:NH2	5:K:58:G:O6	2.49	0.46
1:A:126:LEU:HB2	5:K:43:G:H1'	1.97	0.46
4:E:64:ARG:HD2	4:F:210:ILE:HD11	1.98	0.46
4:E:313:ARG:O	4:E:317:GLU:HG2	2.16	0.46
4:G:64:ARG:HH12	4:H:215:ASP:CG	2.24	0.46
4:H:61:ARG:HB2	4:H:118:TYR:CD1	2.51	0.46
4:H:289:ARG:HH12	4:H:294:ILE:CD1	2.17	0.46
4:I:291:ASP:N	4:I:291:ASP:OD1	2.48	0.46
4:I:331:ASP:OD1	4:I:331:ASP:N	2.49	0.46
4:D:278:MET:HG3	4:H:293:PRO:HG2	1.98	0.46
1:A:47:GLN:CD	5:K:60:G:H5'	2.41	0.45
1:A:160:LEU:HA	4:I:14:TYR:HD1	1.81	0.45
4:D:172:ARG:HD2	4:D:178:PRO:HA	1.98	0.45
4:G:17:ILE:O	4:G:270:GLY:HA3	2.16	0.45
4:H:194:VAL:HG13	4:H:300:PHE:CD1	2.51	0.45
4:I:289:ARG:HH12	4:I:335:ARG:NH2	2.14	0.45
2:J:158:GLU:OE2	2:J:162:HIS:NE2	2.48	0.45
1:A:2:THR:HG22	1:A:3:TRP:N	2.31	0.45
4:D:193:THR:HG23	4:D:231:PHE:HE1	1.81	0.45
4:E:253:ARG:NH2	4:E:368:PHE:HB3	2.31	0.45
2:J:77:VAL:CG1	2:J:78:GLU:N	2.68	0.45
1:A:126:LEU:HD12	5:K:43:G:O2'	2.16	0.45
2:B:28:ARG:HA	2:B:31:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:PRO:HB3	3:C:191:TYR:CD2	2.52	0.45
3:C:145:THR:HG22	3:C:295:TRP:CZ2	2.51	0.45
3:C:315:TYR:O	3:C:349:ASN:HB2	2.16	0.45
4:E:212:LYS:HZ1	4:I:109:GLU:CD	2.21	0.45
4:I:38:VAL:CG1	4:I:191:ALA:HB3	2.46	0.45
1:A:183:ILE:CB	5:K:46:C:C2	3.00	0.45
3:C:355:LEU:HD22	3:C:355:LEU:HA	1.67	0.45
3:C:472:ARG:HH21	4:D:29:VAL:HG21	1.82	0.45
4:E:64:ARG:CD	4:F:210:ILE:HD11	2.46	0.45
4:F:17:ILE:HD12	4:F:268:PRO:HG2	1.98	0.45
4:G:51:VAL:HG22	4:G:258:GLU:OE1	2.17	0.45
4:G:104:LYS:HD2	4:G:105:GLU:O	2.17	0.45
7:N:35:LEU:O	7:N:38:MET:HG2	2.17	0.45
2:B:44:MET:HB3	2:B:44:MET:HE2	1.75	0.45
3:C:227:THR:OG1	3:C:230:GLU:OE1	2.33	0.45
4:E:55:LEU:HD23	4:E:165:VAL:HG21	1.99	0.45
4:G:43:TRP:HB3	4:G:188:PHE:CE2	2.51	0.45
2:J:39:PRO:HD3	2:J:79:ARG:HD2	1.99	0.45
2:J:146:ALA:HB2	2:J:188:VAL:HG11	1.98	0.45
2:J:168:ASN:O	2:J:172:VAL:HG13	2.17	0.45
5:K:8:G:O6	7:N:79:GLY:HA3	2.17	0.45
2:B:146:ALA:HB2	2:B:188:VAL:HG11	1.98	0.45
3:C:155:ARG:HH22	3:C:174:HIS:CE1	2.34	0.45
3:C:441:TRP:CD1	3:C:441:TRP:C	2.95	0.45
4:G:205:THR:HG22	4:G:206:ALA:N	2.32	0.45
4:G:292:ARG:HH11	4:H:278:MET:HE3	1.81	0.45
2:B:202:TRP:CE3	2:B:206:PRO:HB3	2.51	0.45
4:E:30:TYR:CD2	4:E:35:ARG:NH2	2.85	0.45
4:E:200:GLU:OE2	4:E:226:PHE:HB2	2.16	0.45
4:F:123:ALA:HA	4:F:126:GLU:OE1	2.17	0.45
4:H:289:ARG:HD2	4:H:333:ALA:HB1	1.99	0.45
2:J:95:ALA:HB1	2:J:184:ARG:CG	2.47	0.45
7:N:148:LEU:CD1	7:N:246:VAL:HG21	2.47	0.45
7:N:162:LEU:HD12	7:N:163:VAL:N	2.32	0.45
2:B:174:ARG:NH2	4:E:29:VAL:HG21	2.32	0.45
2:B:179:LEU:HD12	2:B:180:VAL:HG13	1.99	0.45
3:C:139:ARG:HH12	3:C:283:HIS:CD2	2.35	0.45
3:C:343:HIS:C	3:C:345:GLY:N	2.72	0.45
4:D:19:ARG:NH2	5:K:10:C:O2'	2.50	0.45
3:C:326:ARG:NH2	3:C:349:ASN:HD22	2.14	0.45
4:E:195:HIS:CE1	4:E:230:THR:HG22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:324:ARG:HG2	4:F:340:VAL:O	2.17	0.45
4:H:187:GLN:HB2	4:H:236:ASN:HB2	1.98	0.45
4:H:356:TYR:HB2	4:H:357:PRO:HD3	1.99	0.45
4:I:264:LEU:HD12	4:I:360:ILE:HD11	1.99	0.45
2:J:28:ARG:HA	2:J:31:LEU:CD2	2.47	0.45
2:J:202:TRP:CE3	2:J:206:PRO:HB3	2.51	0.45
7:N:63:VAL:HG12	7:N:113:PHE:CD1	2.52	0.45
1:A:34:SER:OG	1:A:37:LEU:HD21	2.16	0.45
4:E:27:THR:HG22	4:E:36:THR:HG22	1.98	0.45
4:F:45:ARG:HA	4:F:48:ARG:HG2	1.99	0.45
4:G:312:LEU:O	4:G:316:GLN:HG3	2.17	0.45
4:I:49:HIS:HA	4:I:52:GLU:HG2	1.98	0.45
4:I:72:ARG:HH22	4:I:121:VAL:CG1	2.24	0.45
2:J:54:TYR:O	2:J:55:VAL:C	2.60	0.45
2:J:179:LEU:HD12	2:J:180:VAL:HG13	1.99	0.45
7:N:162:LEU:HD13	7:N:184:LEU:HD11	1.99	0.45
1:A:5:THR:O	1:A:66:VAL:HG22	2.16	0.44
2:B:10:ALA:O	2:B:14:VAL:HG13	2.17	0.44
2:B:16:ARG:HD2	2:B:54:TYR:OH	2.17	0.44
3:C:133:LEU:HD13	3:C:133:LEU:HA	1.85	0.44
3:C:208:ARG:NH2	6:M:47:DC:O2	2.50	0.44
3:C:504:PHE:CA	3:C:507:VAL:HG12	2.44	0.44
4:F:35:ARG:HD3	4:F:193:THR:O	2.17	0.44
4:F:35:ARG:NH2	4:F:303:ALA:HB2	2.32	0.44
4:H:90:VAL:HG22	4:H:131:ALA:HB2	1.99	0.44
7:N:45:VAL:HG21	7:N:54:TYR:HE2	1.82	0.44
1:A:43:ALA:HB1	5:K:50:A:O2'	2.17	0.44
2:B:167:GLN:HE21	2:B:171:GLY:HA3	1.82	0.44
3:C:161:GLN:HB3	7:N:101:ILE:HD11	1.98	0.44
3:C:317:THR:HG22	3:C:323:VAL:HG22	1.99	0.44
4:D:43:TRP:O	4:D:47:VAL:HG23	2.16	0.44
4:E:225:GLN:C	4:E:226:PHE:HD1	2.25	0.44
4:I:191:ALA:CB	4:I:233:ARG:HG2	2.46	0.44
2:J:192:TRP:O	2:J:196:ILE:HG13	2.17	0.44
2:B:24:GLU:OE1	2:B:27:ALA:N	2.31	0.44
3:C:171:LEU:O	3:C:172:ASP:OD1	2.34	0.44
3:C:228:LEU:H	3:C:228:LEU:HD23	1.83	0.44
4:D:19:ARG:HH12	4:D:271:LYS:HG2	1.82	0.44
4:F:212:LYS:HD3	4:F:215:ASP:H	1.82	0.44
4:H:21:ASP:N	4:H:21:ASP:OD1	2.50	0.44
1:A:32:ARG:HH12	1:A:75:ASP:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:VAL:O	2:B:18:SER:CB	2.65	0.44
3:C:33:ARG:O	3:C:33:ARG:HG2	2.17	0.44
4:D:4:VAL:HG12	4:D:288:VAL:HG22	2.00	0.44
4:D:187:GLN:NE2	7:N:144:VAL:HG12	2.32	0.44
4:F:186:VAL:HG22	4:F:237:VAL:HG22	2.00	0.44
4:F:187:GLN:HB2	4:F:236:ASN:HB2	1.98	0.44
4:H:96:LYS:HG3	4:H:97:LYS:N	2.32	0.44
4:H:151:LEU:H	4:H:151:LEU:HD22	1.83	0.44
5:K:2:U:O4	7:N:137:TYR:N	2.43	0.44
3:C:58:GLU:CD	3:C:375:ARG:HH12	2.21	0.44
3:C:139:ARG:NH1	3:C:295:TRP:HH2	2.16	0.44
4:E:323:GLU:HB3	4:E:348:ALA:HB2	1.99	0.44
4:F:10:GLN:NE2	4:F:279:THR:O	2.51	0.44
4:F:205:THR:HA	4:F:221:MET:CG	2.46	0.44
4:G:151:LEU:HD22	4:G:151:LEU:H	1.81	0.44
2:B:84:VAL:CG1	2:B:196:ILE:HG12	2.34	0.44
3:C:123:PHE:CZ	3:C:249:TRP:HZ3	2.36	0.44
3:C:197:CYS:SG	3:C:198:THR:N	2.84	0.44
3:C:219:VAL:HG13	3:C:221:TYR:CE2	2.53	0.44
4:D:6:ILE:HD11	4:D:260:LEU:HD21	1.99	0.44
4:G:33:LYS:HD3	4:G:196:GLY:HA3	1.98	0.44
4:G:291:ASP:OD1	4:G:291:ASP:N	2.50	0.44
4:H:24:SER:HB3	4:H:225:GLN:OE1	2.17	0.44
5:K:7:C:HO2'	7:N:76:ILE:HG22	1.82	0.44
5:K:8:G:H5''	7:N:75:THR:O	2.17	0.44
5:K:52:G:H2'	5:K:54:A:H2	1.82	0.44
4:E:14:TYR:HE1	4:E:200:GLU:CD	2.26	0.44
4:E:118:TYR:CE2	4:E:167:VAL:HG22	2.53	0.44
4:E:120:PRO:HG3	4:E:164:ASN:HB2	1.99	0.44
4:E:268:PRO:O	4:E:269:SER:OG	2.30	0.44
4:H:118:TYR:CD2	4:H:167:VAL:HG12	2.53	0.44
4:I:33:LYS:HE3	4:I:33:LYS:HB2	1.76	0.44
3:C:196:MET:HG2	8:O:10:DA:C2	2.53	0.44
4:G:306:GLY:C	4:G:308:ASP:H	2.25	0.44
4:H:152:PRO:HG3	4:H:155:ARG:HD3	2.00	0.44
4:I:323:GLU:HB3	4:I:348:ALA:CB	2.47	0.44
7:N:35:LEU:HD21	7:N:115:VAL:HG11	2.00	0.44
7:N:63:VAL:HG23	7:N:63:VAL:O	2.18	0.44
1:A:208:ASN:OD1	1:A:209:GLY:N	2.51	0.44
3:C:94:TRP:O	3:C:98:ARG:HB2	2.18	0.44
3:C:140:GLU:O	3:C:141:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:20:ASP:OD1	4:F:26:LYS:HG2	2.18	0.44
4:F:225:GLN:O	4:F:226:PHE:CD1	2.71	0.44
4:F:291:ASP:OD1	4:F:291:ASP:N	2.51	0.44
1:A:3:TRP:HH2	1:A:72:LEU:HB3	1.83	0.43
2:B:95:ALA:HB1	2:B:184:ARG:CG	2.47	0.43
3:C:57:VAL:HG13	3:C:228:LEU:HD13	2.00	0.43
3:C:444:SER:C	3:C:446:SER:H	2.25	0.43
4:D:260:LEU:HA	4:D:260:LEU:HD23	1.41	0.43
4:H:88:ARG:O	4:H:92:LEU:HB2	2.18	0.43
1:A:163:THR:O	4:I:19:ARG:HD3	2.18	0.43
2:B:168:ASN:O	2:B:172:VAL:HG13	2.17	0.43
2:B:192:TRP:O	2:B:196:ILE:HG13	2.17	0.43
3:C:123:PHE:HA	3:C:132:TRP:HE3	1.82	0.43
2:J:44:MET:HB3	2:J:44:MET:HE2	1.75	0.43
2:J:164:ILE:HD12	2:J:179:LEU:HD21	2.00	0.43
7:N:72:ASP:HB3	7:N:105:ARG:O	2.18	0.43
1:A:98:LYS:HB2	1:A:196:ILE:O	2.19	0.43
1:A:113:ARG:HD2	5:K:57:U:C5	2.53	0.43
3:C:140:GLU:O	3:C:141:GLU:CG	2.66	0.43
4:D:45:ARG:NH1	5:K:8:G:O4'	2.52	0.43
4:D:305:TYR:O	4:D:313:ARG:NH1	2.51	0.43
4:E:254:THR:O	4:E:258:GLU:OE1	2.35	0.43
4:F:253:ARG:CZ	4:F:368:PHE:O	2.65	0.43
8:O:6:DA:H2''	8:O:7:DC:C6	2.52	0.43
1:A:51:LEU:O	1:A:52:LEU:HD22	2.18	0.43
2:B:143:LEU:CD1	2:B:161:LEU:HD21	2.41	0.43
2:B:169:LEU:O	2:B:173:HIS:HD2	2.01	0.43
3:C:35:VAL:HG12	3:C:37:ALA:HB3	2.01	0.43
3:C:81:GLY:O	3:C:94:TRP:HH2	2.01	0.43
4:D:4:VAL:HG22	4:D:237:VAL:HG13	2.00	0.43
4:D:218:SER:OG	4:D:219:GLY:N	2.52	0.43
4:D:283:LEU:HD23	4:D:284:VAL:N	2.33	0.43
4:E:86:GLY:O	4:E:90:VAL:HG23	2.18	0.43
4:G:335:ARG:O	4:G:363:MET:HE1	2.18	0.43
4:H:35:ARG:NH1	4:H:300:PHE:O	2.44	0.43
4:I:304:LEU:HD23	4:I:304:LEU:HA	1.66	0.43
3:C:100:GLN:OE1	3:C:104:LYS:HB2	2.18	0.43
3:C:314:ILE:HD11	3:C:341:LEU:HD21	2.01	0.43
4:D:326:ARG:HH11	4:D:335:ARG:HH12	1.64	0.43
4:H:188:PHE:CE1	4:H:263:PHE:HE1	2.35	0.43
4:I:68:GLU:OE1	4:I:124:ILE:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:10:ALA:O	2:J:14:VAL:HG13	2.17	0.43
7:N:224:THR:HG22	7:N:225:GLU:N	2.33	0.43
1:A:124:LEU:HD23	1:A:126:LEU:N	2.33	0.43
3:C:82:LEU:O	3:C:84:GLN:N	2.50	0.43
3:C:273:LEU:HD23	3:C:273:LEU:HA	1.82	0.43
4:D:205:THR:HA	4:D:220:HIS:O	2.19	0.43
4:E:10:GLN:OE1	4:E:233:ARG:NH1	2.51	0.43
4:E:14:TYR:CE2	4:E:226:PHE:CD2	3.07	0.43
4:E:190:HIS:HD2	4:F:275:THR:HG22	1.84	0.43
4:H:205:THR:HA	4:H:221:MET:CB	2.49	0.43
4:I:337:TYR:CZ	4:I:352:ARG:HB2	2.54	0.43
7:N:148:LEU:HD13	7:N:148:LEU:HA	1.89	0.43
1:A:45:PRO:HB2	1:A:46:ARG:H	1.71	0.43
2:B:13:LEU:HD23	2:B:13:LEU:HA	1.84	0.43
3:C:132:TRP:CD1	3:C:133:LEU:HD23	2.54	0.43
4:D:21:ASP:HA	5:K:9:C:H5	1.84	0.43
4:D:340:VAL:O	4:H:324:ARG:NE	2.50	0.43
4:E:151:LEU:H	4:E:151:LEU:HD22	1.84	0.43
4:F:97:LYS:H	4:F:97:LYS:HD2	1.83	0.43
4:G:325:LEU:HD23	4:G:325:LEU:HA	1.71	0.43
4:H:137:ALA:HB1	4:H:150:ILE:HG21	2.00	0.43
1:A:52:LEU:HD11	1:A:214:LYS:HD3	1.99	0.43
1:A:170:ASP:N	2:B:23:ASN:HD21	2.12	0.43
3:C:163:TRP:CZ2	5:K:6:C:C2	3.06	0.43
3:C:280:VAL:HA	3:C:295:TRP:O	2.19	0.43
4:D:28:VAL:CG2	7:N:12:MET:HE2	2.49	0.43
4:E:130:ILE:HD12	4:E:131:ALA:N	2.34	0.43
4:E:213:GLU:HA	4:E:216:HIS:CE1	2.53	0.43
4:E:292:ARG:NH1	4:F:278:MET:HE3	2.33	0.43
4:F:62:THR:HG22	4:G:210:ILE:H	1.84	0.43
4:H:33:LYS:HD3	4:H:196:GLY:HA3	2.01	0.43
4:I:123:ALA:HA	4:I:126:GLU:OE1	2.18	0.43
4:D:3:PHE:CE2	4:D:293:PRO:HD3	2.51	0.43
4:E:19:ARG:HB3	4:E:23:GLY:HA2	2.01	0.43
4:E:253:ARG:CZ	4:E:368:PHE:HB3	2.48	0.43
4:F:169:LEU:HG	4:F:186:VAL:HG21	2.01	0.43
4:G:257:ALA:HB2	4:G:364:VAL:HG11	2.00	0.43
4:I:89:GLN:NE2	4:I:141:GLU:OE1	2.52	0.43
2:J:75:HIS:ND1	2:J:75:HIS:C	2.76	0.43
2:J:160:ARG:HG2	2:J:179:LEU:HD23	2.01	0.43
2:B:5:TYR:O	2:B:6:ILE:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ASP:O	2:B:15:LYS:HD3	2.19	0.43
2:B:33:ARG:NH1	2:B:43:ARG:O	2.52	0.43
4:D:168:ASN:HD21	4:D:245:ASN:HB3	1.83	0.43
4:E:148:LYS:HA	4:E:148:LYS:HE2	2.00	0.43
4:F:61:ARG:HA	4:F:117:PHE:O	2.18	0.43
4:F:65:ILE:HD12	4:F:66:ILE:N	2.34	0.43
4:G:35:ARG:NH1	4:G:300:PHE:O	2.37	0.43
4:G:88:ARG:O	4:G:92:LEU:HB2	2.19	0.43
4:G:188:PHE:HE1	4:G:263:PHE:CE1	2.36	0.43
4:H:207:VAL:HG12	5:K:20:U:OP1	2.19	0.43
2:J:157:THR:O	2:J:161:LEU:HD23	2.18	0.43
1:A:46:ARG:HA	5:K:59:G:H5"	2.01	0.42
2:B:160:ARG:HG2	2:B:179:LEU:HD23	2.01	0.42
3:C:61:LEU:HA	3:C:62:PRO:HD2	1.94	0.42
3:C:395:THR:O	3:C:396:PRO:O	2.37	0.42
3:C:423:ARG:HD2	3:C:427:GLU:OE1	2.19	0.42
3:C:428:ALA:HA	3:C:431:ARG:NH1	2.34	0.42
4:F:183:ASP:OD1	4:F:183:ASP:N	2.50	0.42
4:G:43:TRP:CZ2	4:G:233:ARG:CZ	3.02	0.42
4:H:61:ARG:HB2	4:H:118:TYR:HD1	1.84	0.42
4:I:18:ASN:HD21	4:I:39:SER:N	2.17	0.42
4:I:259:PHE:HD2	4:I:260:LEU:HD12	1.83	0.42
2:B:157:THR:O	2:B:161:LEU:HD23	2.18	0.42
2:B:160:ARG:CD	2:B:179:LEU:HB3	2.50	0.42
3:C:59:ILE:HD11	3:C:65:ALA:N	2.34	0.42
4:D:225:GLN:O	4:D:226:PHE:HD1	2.01	0.42
4:F:326:ARG:NH1	4:F:335:ARG:HH12	2.16	0.42
7:N:51:LEU:H	7:N:51:LEU:HD23	1.84	0.42
7:N:178:ALA:HA	7:N:228:ALA:HB2	2.01	0.42
1:A:203:ARG:HH12	1:A:207:LEU:HB2	1.81	0.42
4:F:16:ASN:ND2	4:F:225:GLN:O	2.52	0.42
4:F:50:GLU:OE1	4:F:266:THR:HG22	2.18	0.42
4:I:55:LEU:HD22	4:I:258:GLU:OE2	2.18	0.42
1:A:13:TYR:CG	1:A:14:ARG:N	2.87	0.42
4:E:94:VAL:O	4:E:99:GLY:HA2	2.19	0.42
4:F:101:LYS:H	4:F:101:LYS:HD3	1.84	0.42
4:F:174:LEU:HA	4:F:174:LEU:HD12	1.75	0.42
4:H:14:TYR:OH	4:H:202:ASP:HB2	2.19	0.42
2:J:33:ARG:NH1	2:J:43:ARG:O	2.52	0.42
2:J:160:ARG:CD	2:J:179:LEU:HB3	2.50	0.42
6:M:47:DC:H2"	6:M:48:DG:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:14:SER:OG	7:N:143:PHE:HE2	2.03	0.42
1:A:145:ALA:O	1:A:148:TRP:HB3	2.20	0.42
3:C:45:ARG:HH11	3:C:113:ASP:CG	2.28	0.42
3:C:139:ARG:NH1	3:C:283:HIS:HD2	2.18	0.42
3:C:207:GLU:C	3:C:209:ASN:H	2.27	0.42
3:C:252:PRO:HG2	3:C:253:GLU:OE2	2.18	0.42
3:C:260:LEU:HD13	3:C:261:PRO:C	2.45	0.42
4:D:212:LYS:HE3	4:H:64:ARG:NH2	2.35	0.42
4:F:319:ASN:HB2	4:F:346:LEU:CB	2.50	0.42
4:G:356:TYR:HB2	4:G:357:PRO:HD3	2.01	0.42
4:H:34:GLU:CB	2:J:207:ARG:HH22	2.27	0.42
7:N:43:GLN:HE21	7:N:125:ILE:HA	1.83	0.42
7:N:170:HIS:CG	7:N:234:PRO:HA	2.55	0.42
1:A:27:HIS:CD2	1:A:215:SER:HB2	2.52	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.77	0.42
2:B:28:ARG:O	2:B:31:LEU:HD23	2.19	0.42
3:C:158:GLY:O	7:N:89:ALA:HB3	2.18	0.42
4:E:121:VAL:N	4:E:122:PRO:HD2	2.35	0.42
4:E:212:LYS:HD3	4:I:64:ARG:NH2	2.35	0.42
4:F:85:ALA:O	4:F:89:GLN:HG2	2.19	0.42
4:G:324:ARG:NH1	4:G:327:GLU:HG2	2.35	0.42
4:I:121:VAL:N	4:I:122:PRO:HD2	2.35	0.42
4:I:176:GLU:OE1	4:I:176:GLU:N	2.45	0.42
7:N:4:PHE:CE1	7:N:125:ILE:HD11	2.54	0.42
7:N:13:GLN:O	7:N:108:LEU:N	2.52	0.42
1:A:51:LEU:HG	1:A:68:SER:HA	2.02	0.42
1:A:161:LEU:O	1:A:163:THR:HG23	2.20	0.42
4:F:39:SER:HA	4:F:190:HIS:ND1	2.35	0.42
4:I:27:THR:HG22	4:I:36:THR:HG22	2.02	0.42
4:I:103:GLU:OE1	4:I:114:SER:HA	2.19	0.42
2:J:5:TYR:O	2:J:6:ILE:C	2.62	0.42
8:O:9:DA:C8	8:O:10:DA:N7	2.87	0.42
3:C:329:GLU:O	3:C:332:ARG:HG3	2.19	0.42
3:C:527:LYS:CB	2:J:218:HIS:HE1	2.33	0.42
4:D:191:ALA:CB	4:D:233:ARG:HG2	2.49	0.42
4:F:141:GLU:HA	4:F:144:LYS:HE2	2.01	0.42
2:J:11:ASP:O	2:J:15:LYS:HD3	2.19	0.42
1:A:147:GLU:HG2	1:A:150:HIS:NE2	2.35	0.42
1:A:203:ARG:HH12	1:A:207:LEU:HD12	1.85	0.42
2:B:164:ILE:HD12	2:B:179:LEU:HD21	2.00	0.42
3:C:79:ILE:HG22	3:C:80:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:329:GLU:HB2	3:C:332:ARG:CG	2.50	0.42
3:C:384:GLN:HB3	6:M:44:DC:O2	2.20	0.42
4:F:189:ALA:HB2	4:G:276:ALA:HB3	2.02	0.42
4:H:91:VAL:HG22	4:H:100:ILE:HB	2.01	0.42
4:H:217:GLY:N	5:K:22:G:H22	2.18	0.42
5:K:50:A:C6	5:K:58:G:C6	3.08	0.42
3:C:137:ARG:NH1	3:C:257:PRO:HD3	2.33	0.42
3:C:137:ARG:HA	3:C:140:GLU:OE2	2.20	0.42
4:E:169:LEU:HD21	4:E:259:PHE:HB2	2.00	0.42
4:G:94:VAL:HG23	4:G:100:ILE:HG12	2.02	0.42
4:H:78:TRP:HZ2	4:H:132:ASP:HA	1.85	0.42
4:I:68:GLU:OE2	4:I:72:ARG:NE	2.47	0.42
2:J:169:LEU:O	2:J:173:HIS:HD2	2.01	0.42
2:J:185:SER:O	2:J:186:ASP:HB2	2.20	0.42
4:D:17:ILE:O	4:D:270:GLY:HA3	2.20	0.41
4:E:44:LYS:HG3	4:E:170:PHE:CE1	2.55	0.41
4:E:333:ALA:O	4:E:335:ARG:HD2	2.20	0.41
4:F:40:SER:HB2	4:F:188:PHE:HD2	1.85	0.41
4:F:151:LEU:HD22	4:F:151:LEU:H	1.84	0.41
4:F:221:MET:HE3	4:F:222:ASN:OD1	2.20	0.41
4:G:63:ARG:CG	4:G:116:LEU:HG	2.48	0.41
1:A:74:VAL:HG23	1:A:79:PRO:HD2	2.01	0.41
2:B:95:ALA:HB1	2:B:184:ARG:HG2	2.02	0.41
4:D:54:ARG:HG2	4:D:258:GLU:OE2	2.20	0.41
4:D:215:ASP:OD2	4:D:216:HIS:ND1	2.53	0.41
4:E:59:ALA:HB2	4:E:164:ASN:HD22	1.85	0.41
4:E:271:LYS:HG2	4:E:274:ALA:HB3	2.01	0.41
4:F:97:LYS:HE2	4:F:99:GLY:O	2.20	0.41
4:F:167:VAL:HG11	4:F:172:ARG:HH11	1.84	0.41
4:F:195:HIS:CE1	4:F:230:THR:H	2.37	0.41
4:F:213:GLU:OE1	4:I:178:PRO:HG3	2.20	0.41
4:I:48:ARG:HH21	4:I:59:ALA:HB3	1.84	0.41
7:N:63:VAL:HG12	7:N:113:PHE:HD1	1.85	0.41
1:A:161:LEU:N	4:I:14:TYR:HE1	2.06	0.41
3:C:121:GLU:HG3	3:C:127:HIS:HE2	1.85	0.41
3:C:317:THR:HG21	3:C:350:TYR:CE2	2.52	0.41
3:C:379:PHE:O	3:C:381:GLN:OE1	2.37	0.41
4:D:43:TRP:CH2	4:D:263:PHE:CD1	3.08	0.41
4:D:169:LEU:HD12	4:D:170:PHE:CD2	2.55	0.41
4:F:18:ASN:HD21	4:F:39:SER:N	2.16	0.41
4:G:14:TYR:HD1	4:G:200:GLU:OE2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:21:ASP:OD2	2:J:178:ARG:NH1	2.54	0.41
7:N:78:GLY:HA2	7:N:100:THR:CG2	2.40	0.41
1:A:54:ARG:HE	1:A:220:LEU:HD23	1.85	0.41
4:F:188:PHE:CE1	4:F:263:PHE:HE1	2.37	0.41
4:G:188:PHE:HE1	4:G:263:PHE:HE1	1.67	0.41
4:H:43:TRP:CD1	4:H:43:TRP:C	2.96	0.41
4:I:304:LEU:HD21	4:I:317:GLU:OE2	2.21	0.41
2:J:21:ILE:C	2:J:23:ASN:N	2.77	0.41
2:J:87:ILE:HG21	2:J:87:ILE:HD13	1.77	0.41
2:J:209:VAL:HG23	2:J:212:GLU:OE2	2.21	0.41
7:N:92:GLU:OE1	7:N:92:GLU:N	2.54	0.41
1:A:160:LEU:O	1:A:192:GLY:HA3	2.21	0.41
3:C:64:GLY:O	3:C:68:LEU:HB2	2.20	0.41
3:C:261:PRO:HG3	3:C:300:TRP:CE3	2.54	0.41
3:C:271:LEU:CD2	3:C:273:LEU:HD12	2.50	0.41
4:H:10:GLN:NE2	4:H:279:THR:O	2.53	0.41
4:H:240:ASP:OD1	4:H:241:ARG:N	2.53	0.41
2:J:160:ARG:HD3	2:J:179:LEU:HB3	2.03	0.41
2:J:171:GLY:HA2	2:J:174:ARG:HG2	2.03	0.41
1:A:30:LEU:HD13	1:A:53:PHE:CD2	2.56	0.41
2:B:185:SER:O	2:B:186:ASP:HB2	2.20	0.41
3:C:285:SER:OG	3:C:286:PRO:HD2	2.21	0.41
3:C:519:TYR:C	3:C:521:GLU:H	2.28	0.41
4:D:305:TYR:CD2	4:D:306:GLY:N	2.89	0.41
4:D:326:ARG:NH1	4:D:335:ARG:HH12	2.18	0.41
4:G:19:ARG:HD2	4:G:23:GLY:HA2	2.03	0.41
2:J:13:LEU:HD23	2:J:13:LEU:HA	1.85	0.41
7:N:51:LEU:HD11	7:N:204:PRO:O	2.20	0.41
3:C:339:ASP:CG	3:C:419:ILE:HG22	2.45	0.41
3:C:429:LEU:O	3:C:432:ARG:HG2	2.20	0.41
4:D:4:VAL:HG13	4:D:239:LEU:HD13	2.03	0.41
4:D:7:HIS:ND1	4:D:7:HIS:N	2.68	0.41
4:D:207:VAL:HG12	5:K:14:G:OP1	2.20	0.41
4:D:225:GLN:O	4:D:226:PHE:CD1	2.74	0.41
4:E:14:TYR:CE1	4:E:200:GLU:OE2	2.74	0.41
4:E:164:ASN:O	4:E:168:ASN:ND2	2.54	0.41
4:F:8:ALA:HA	4:F:283:LEU:O	2.21	0.41
4:F:216:HIS:HD2	5:K:35:G:H21	1.68	0.41
4:G:35:ARG:HH22	4:G:301:GLU:C	2.27	0.41
4:G:152:PRO:HG3	4:G:155:ARG:HD3	2.02	0.41
4:H:65:ILE:HD11	4:H:124:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:5:A:N7	5:K:6:C:N4	2.68	0.41
2:B:87:ILE:HG21	2:B:87:ILE:HD13	1.77	0.41
2:B:206:PRO:O	2:B:209:VAL:HG12	2.21	0.41
3:C:196:MET:SD	6:M:46:DT:O2	2.79	0.41
4:D:214:ASN:OD1	4:D:214:ASN:C	2.63	0.41
4:E:9:ILE:O	4:E:282:ASP:N	2.54	0.41
4:H:43:TRP:CD1	4:H:43:TRP:O	2.74	0.41
2:J:11:ASP:O	2:J:14:VAL:HG22	2.21	0.41
7:N:35:LEU:HA	7:N:38:MET:HG2	2.03	0.41
7:N:88:THR:HB	7:N:91:GLY:H	1.85	0.41
7:N:232:ALA:HB1	7:N:237:ASP:OD2	2.20	0.41
2:B:171:GLY:HA2	2:B:174:ARG:HG2	2.03	0.41
3:C:33:ARG:NH1	3:C:227:THR:HG23	2.36	0.41
3:C:63:PRO:HB3	3:C:191:TYR:HD2	1.86	0.41
3:C:189:LEU:HG	3:C:276:PHE:CD2	2.55	0.41
3:C:202:VAL:HG21	3:C:257:PRO:HG3	2.01	0.41
3:C:226:ARG:N	3:C:230:GLU:OE2	2.53	0.41
4:D:41:GLN:HG2	4:D:42:SER:N	2.36	0.41
4:D:210:ILE:HB	4:H:64:ARG:HD2	2.03	0.41
4:F:55:LEU:HD13	4:F:258:GLU:OE1	2.20	0.41
4:G:118:TYR:CE2	4:G:167:VAL:HG22	2.56	0.41
4:G:336:GLY:HA3	4:G:363:MET:CE	2.50	0.41
4:H:39:SER:HA	4:H:190:HIS:ND1	2.36	0.41
4:I:137:ALA:HA	4:I:140:LYS:HZ3	1.86	0.41
5:K:5:A:H5"	7:N:141:ARG:CG	2.51	0.41
1:A:110:PRO:HA	1:A:148:TRP:CE2	2.56	0.41
2:B:207:ARG:H	2:B:207:ARG:HG2	1.40	0.41
2:B:209:VAL:HG23	2:B:212:GLU:OE2	2.21	0.41
3:C:211:THR:OG1	3:C:303:ARG:NH2	2.53	0.41
3:C:216:ARG:CZ	3:C:383:GLY:HA2	2.50	0.41
4:F:45:ARG:NE	4:G:207:VAL:HG11	2.36	0.41
4:F:249:ALA:O	4:F:253:ARG:HG2	2.21	0.41
4:F:305:TYR:N	4:F:305:TYR:CD1	2.89	0.41
4:G:20:ASP:OD1	4:G:26:LYS:HG2	2.20	0.41
4:G:40:SER:HB2	4:G:188:PHE:HD2	1.86	0.41
4:G:268:PRO:O	4:G:269:SER:OG	2.37	0.41
4:H:55:LEU:HD13	4:H:258:GLU:OE1	2.20	0.41
4:I:27:THR:HG22	4:I:36:THR:HA	2.02	0.41
4:I:151:LEU:H	4:I:151:LEU:HD22	1.86	0.41
2:J:28:ARG:O	2:J:31:LEU:HD23	2.19	0.41
5:K:33:G:H21	5:K:34:G:N2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:48:DG:H2''	6:M:49:DT:C6	2.56	0.41
3:C:30:ALA:HB2	3:C:57:VAL:HG12	2.04	0.40
3:C:70:ARG:HG2	3:C:312:TYR:HE2	1.86	0.40
3:C:214:PRO:HG2	3:C:215:LEU:HD22	2.03	0.40
3:C:380:ASP:OD1	3:C:389:GLN:HB3	2.21	0.40
4:D:30:TYR:CE1	4:D:301:GLU:HG3	2.56	0.40
4:E:30:TYR:HD2	4:E:35:ARG:NH2	2.13	0.40
4:F:14:TYR:CZ	4:F:226:PHE:HD2	2.38	0.40
4:F:61:ARG:HB2	4:F:118:TYR:CD1	2.56	0.40
4:H:216:HIS:CG	4:H:217:GLY:H	2.38	0.40
2:J:95:ALA:HB1	2:J:184:ARG:HG2	2.02	0.40
2:J:176:LEU:HD13	2:J:180:VAL:CG2	2.51	0.40
6:M:42:DG:O3'	7:N:98:LYS:NZ	2.54	0.40
1:A:77:LEU:HG	1:A:77:LEU:O	2.20	0.40
3:C:218:THR:HG21	3:C:325:PRO:HB2	2.03	0.40
3:C:468:HIS:CE1	3:C:472:ARG:NE	2.89	0.40
4:D:35:ARG:NH2	4:D:303:ALA:HB2	2.35	0.40
4:D:305:TYR:CE1	2:J:205:THR:HG22	2.55	0.40
4:I:14:TYR:CD2	4:I:14:TYR:O	2.74	0.40
7:N:217:ARG:HD2	7:N:218:GLN:O	2.21	0.40
2:B:41:ASP:HB3	2:B:43:ARG:HD3	2.03	0.40
3:C:417:ARG:HH12	3:C:498:ALA:HB1	1.87	0.40
3:C:472:ARG:HH11	3:C:514:GLU:HB3	1.86	0.40
4:E:164:ASN:HB3	4:E:167:VAL:HG23	2.03	0.40
4:H:17:ILE:HD12	4:H:268:PRO:HG2	2.04	0.40
2:J:207:ARG:H	2:J:207:ARG:HG2	1.40	0.40
1:A:170:ASP:OD1	1:A:171:VAL:N	2.54	0.40
2:B:11:ASP:O	2:B:14:VAL:HG22	2.21	0.40
3:C:245:ASP:HB2	3:C:266:GLY:HA3	2.03	0.40
4:E:123:ALA:HA	4:E:126:GLU:OE1	2.20	0.40
4:E:162:SER:O	4:E:172:ARG:NH1	2.54	0.40
4:F:33:LYS:HD3	4:F:196:GLY:HA3	2.04	0.40
2:B:179:LEU:HD12	2:B:180:VAL:N	2.36	0.40
4:D:305:TYR:OH	2:J:205:THR:HA	2.21	0.40
4:E:43:TRP:HB3	4:E:188:PHE:CE2	2.56	0.40
2:J:17:VAL:O	2:J:19:LYS:N	2.55	0.40
2:J:206:PRO:O	2:J:209:VAL:HG12	2.21	0.40
7:N:174:GLU:HB2	7:N:177:ALA:HB2	2.02	0.40
8:O:10:DA:C2'	8:O:11:DG:C8	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/232 (73%)	153 (90%)	9 (5%)	8 (5%)	2	18
2	B	153/244 (63%)	146 (95%)	6 (4%)	1 (1%)	18	51
2	J	164/244 (67%)	145 (88%)	12 (7%)	7 (4%)	2	19
3	C	485/549 (88%)	433 (89%)	40 (8%)	12 (2%)	4	28
4	D	256/373 (69%)	235 (92%)	19 (7%)	2 (1%)	16	48
4	E	365/373 (98%)	354 (97%)	11 (3%)	0	100	100
4	F	365/373 (98%)	353 (97%)	9 (2%)	3 (1%)	16	48
4	G	364/373 (98%)	353 (97%)	10 (3%)	1 (0%)	36	67
4	H	364/373 (98%)	349 (96%)	13 (4%)	2 (0%)	24	57
4	I	323/373 (87%)	313 (97%)	9 (3%)	1 (0%)	36	67
7	N	237/254 (93%)	218 (92%)	19 (8%)	0	100	100
All	All	3246/3761 (86%)	3052 (94%)	157 (5%)	37 (1%)	14	41

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	156	ASN
1	A	160	LEU
1	A	183	ILE
2	B	6	ILE
3	C	162	VAL
3	C	341	LEU
3	C	351	ARG
3	C	363	GLN
3	C	364	VAL
3	C	382	ASP
3	C	396	PRO
4	F	346	LEU

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Mol	Chain	Res	Type
4	H	217	GLY
2	J	6	ILE
2	J	77	VAL
4	D	218	SER
4	H	222	ASN
4	I	346	LEU
2	J	78	GLU
2	J	83	ALA
1	A	45	PRO
1	A	180	SER
3	C	83	ASP
4	F	219	GLY
4	F	347	ALA
4	G	97	LYS
2	J	16	ARG
2	J	25	PRO
3	C	308	GLU
3	C	328	ALA
3	C	345	GLY
4	D	211	PRO
1	A	186	PRO
2	J	17	VAL
3	C	352	PRO
1	A	9	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	145/193 (75%)	141 (97%)	4 (3%)	38	58
2	B	128/200 (64%)	116 (91%)	12 (9%)	8	30
2	J	126/200 (63%)	115 (91%)	11 (9%)	9	33
3	C	395/452 (87%)	380 (96%)	15 (4%)	29	53
4	D	209/299 (70%)	205 (98%)	4 (2%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	291/299 (97%)	289 (99%)	2 (1%)	76	77
4	F	292/299 (98%)	288 (99%)	4 (1%)	59	70
4	G	292/299 (98%)	290 (99%)	2 (1%)	76	77
4	H	293/299 (98%)	289 (99%)	4 (1%)	59	70
4	I	264/299 (88%)	262 (99%)	2 (1%)	73	76
7	N	201/211 (95%)	200 (100%)	1 (0%)	81	81
All	All	2636/3050 (86%)	2575 (98%)	61 (2%)	44	63

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	46	ARG
1	A	179	ARG
1	A	180	SER
2	B	15	LYS
2	B	21	ILE
2	B	33	ARG
2	B	43	ARG
2	B	45	LEU
2	B	176	LEU
2	B	179	LEU
2	B	181	LEU
2	B	183	LEU
2	B	190	ILE
2	B	207	ARG
2	B	211	ARG
3	C	68	LEU
3	C	202	VAL
3	C	234	LEU
3	C	277	ARG
3	C	282	LEU
3	C	309	LEU
3	C	318	SER
3	C	341	LEU
3	C	342	LEU
3	C	347	ASP
3	C	355	LEU
3	C	358	CYS
3	C	364	VAL

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Mol	Chain	Res	Type
3	C	415	ILE
3	C	416	VAL
4	D	29	VAL
4	D	45	ARG
4	D	165	VAL
4	D	193	THR
4	E	92	LEU
4	E	286	ILE
4	F	52	GLU
4	F	183	ASP
4	F	218	SER
4	F	344	THR
4	G	97	LYS
4	G	183	ASP
4	H	50	GLU
4	H	115	VAL
4	H	177	LEU
4	H	183	ASP
4	I	174	LEU
4	I	183	ASP
2	J	15	LYS
2	J	33	ARG
2	J	43	ARG
2	J	45	LEU
2	J	176	LEU
2	J	179	LEU
2	J	181	LEU
2	J	183	LEU
2	J	190	ILE
2	J	207	ARG
2	J	211	ARG
7	N	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	44	ASN
2	B	9	HIS
2	B	23	ASN
2	B	48	HIS
2	B	91	GLN

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Mol	Chain	Res	Type
2	B	167	GLN
2	B	173	HIS
2	B	175	HIS
3	C	100	GLN
3	C	161	GLN
3	C	168	HIS
3	C	169	HIS
3	C	174	HIS
3	C	222	HIS
3	C	251	GLN
3	C	283	HIS
3	C	349	ASN
3	C	468	HIS
3	C	505	ASN
4	D	7	HIS
4	D	18	ASN
4	D	49	HIS
4	D	216	HIS
4	D	273	ASN
4	E	89	GLN
4	E	168	ASN
4	E	195	HIS
4	E	285	HIS
4	F	18	ASN
4	F	49	HIS
4	F	134	HIS
4	F	220	HIS
4	G	18	ASN
4	G	134	HIS
4	H	18	ASN
4	H	49	HIS
4	H	89	GLN
4	H	272	GLN
4	H	273	ASN
4	I	16	ASN
4	I	18	ASN
2	J	91	GLN
2	J	173	HIS
2	J	175	HIS
2	J	215	GLN
2	J	218	HIS
7	N	218	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	K	57/61 (93%)	25 (43%)	0

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	K	4	G
5	K	7	C
5	K	8	G
5	K	9	C
5	K	10	C
5	K	11	A
5	K	15	A
5	K	17	A
5	K	21	G
5	K	22	G
5	K	27	C
5	K	31	G
5	K	32	U
5	K	33	G
5	K	34	G
5	K	35	G
5	K	36	C
5	K	37	U
5	K	39	U
5	K	40	C
5	K	45	G
5	K	52	G
5	K	54	A
5	K	55	C
5	K	56	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

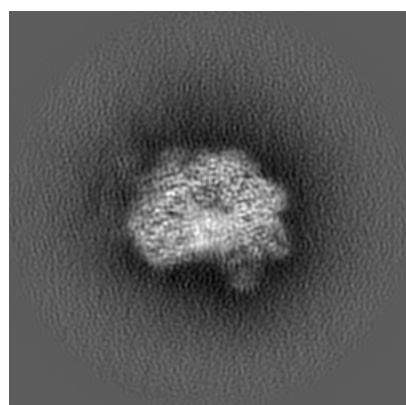
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8477. These allow visual inspection of the internal detail of the map and identification of artifacts.

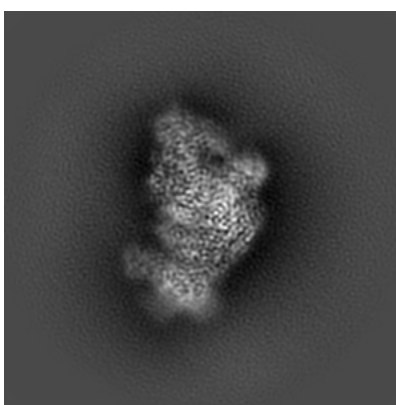
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

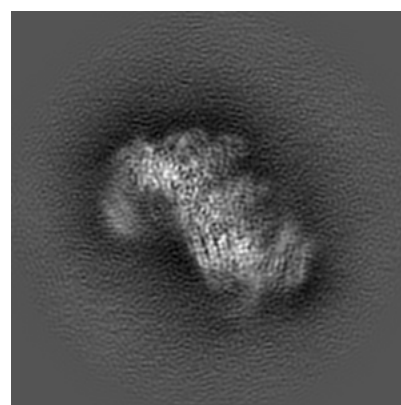
6.1.1 Primary map



X



Y

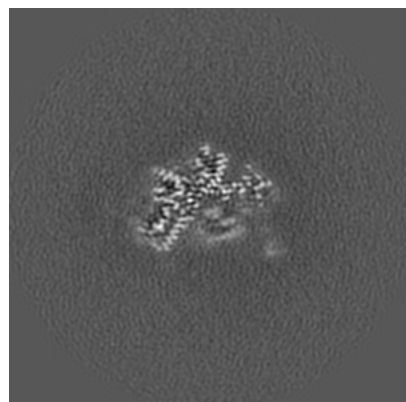


Z

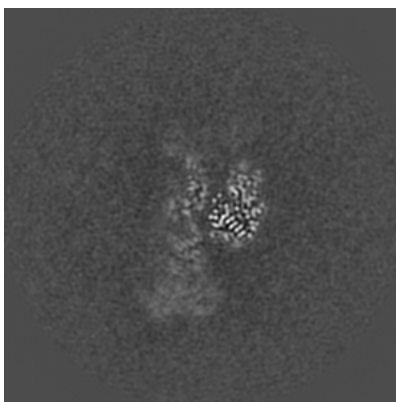
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

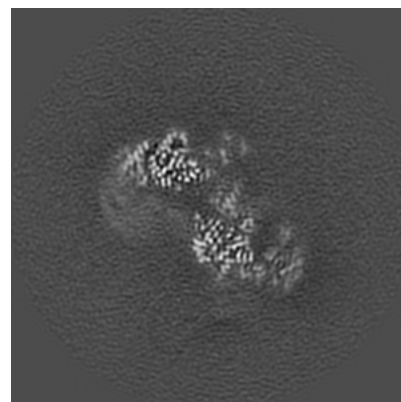
6.2.1 Primary map



X Index: 128



Y Index: 128

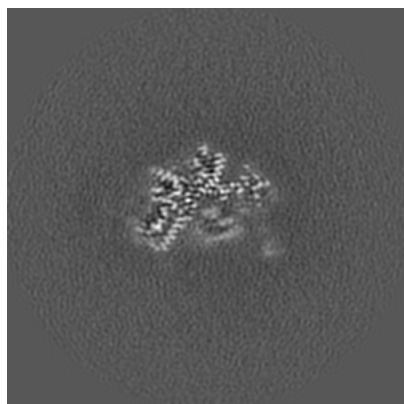


Z Index: 128

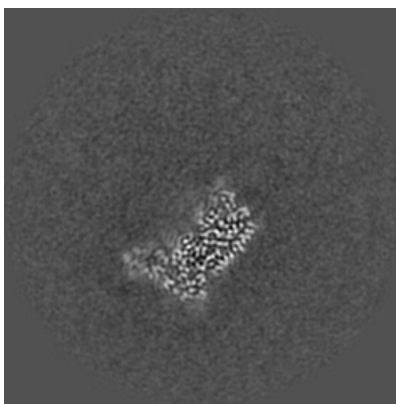
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

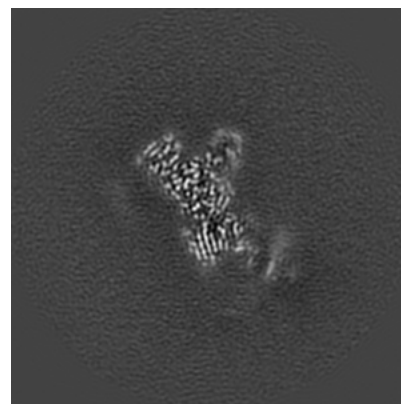
6.3.1 Primary map



X Index: 128



Y Index: 154

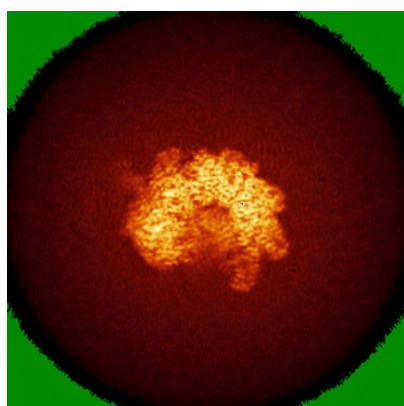


Z Index: 138

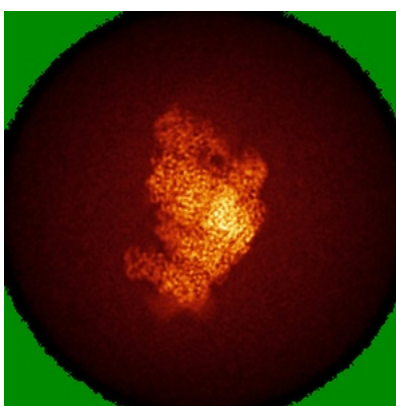
The images above show the largest variance slices of the map in three orthogonal directions.

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

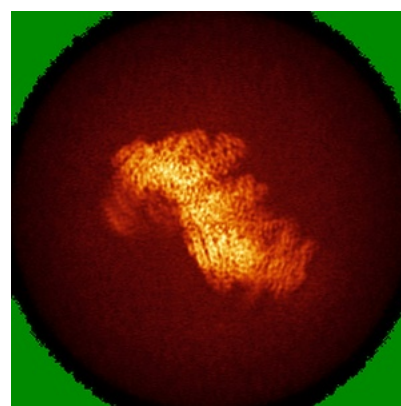
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

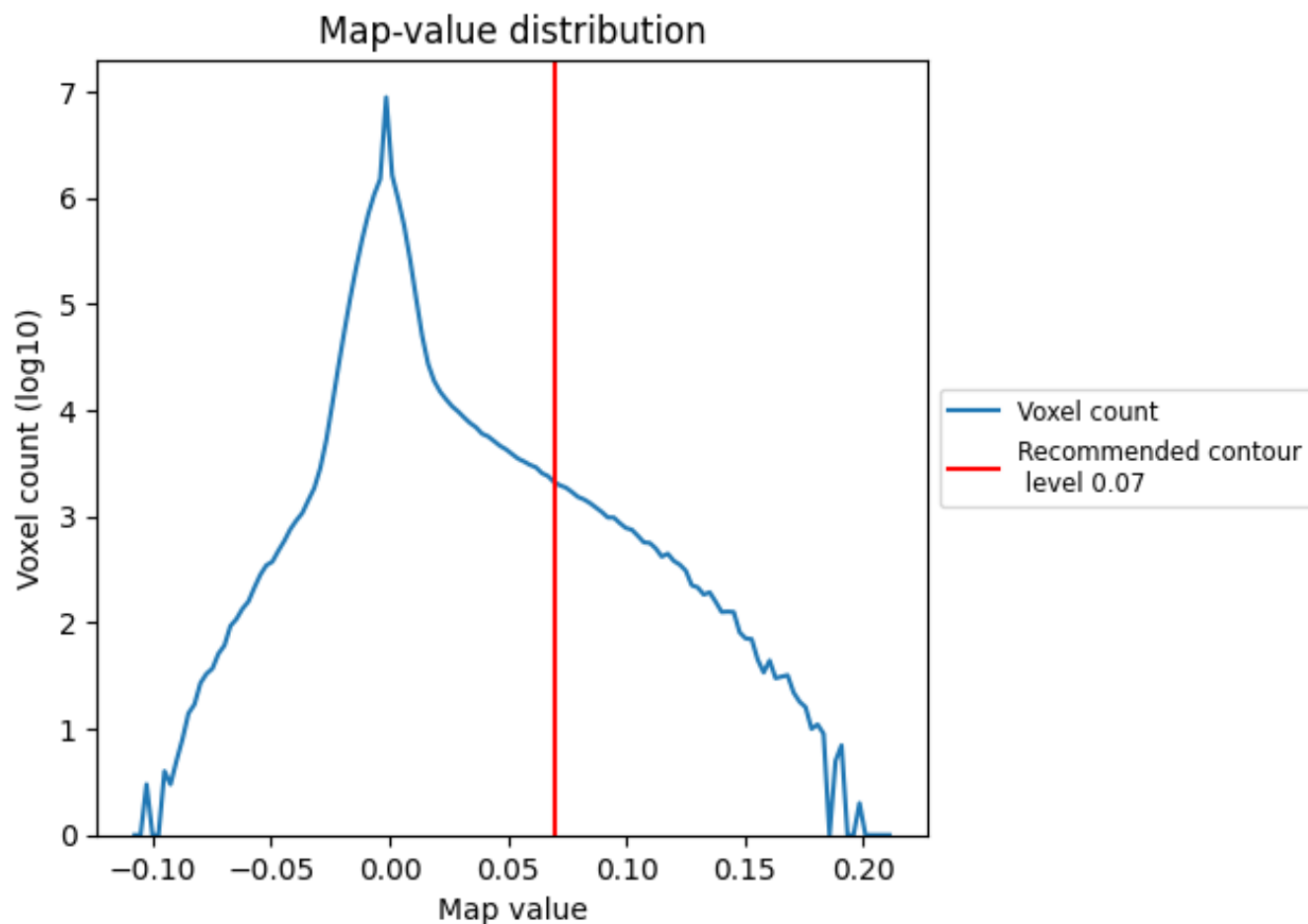
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

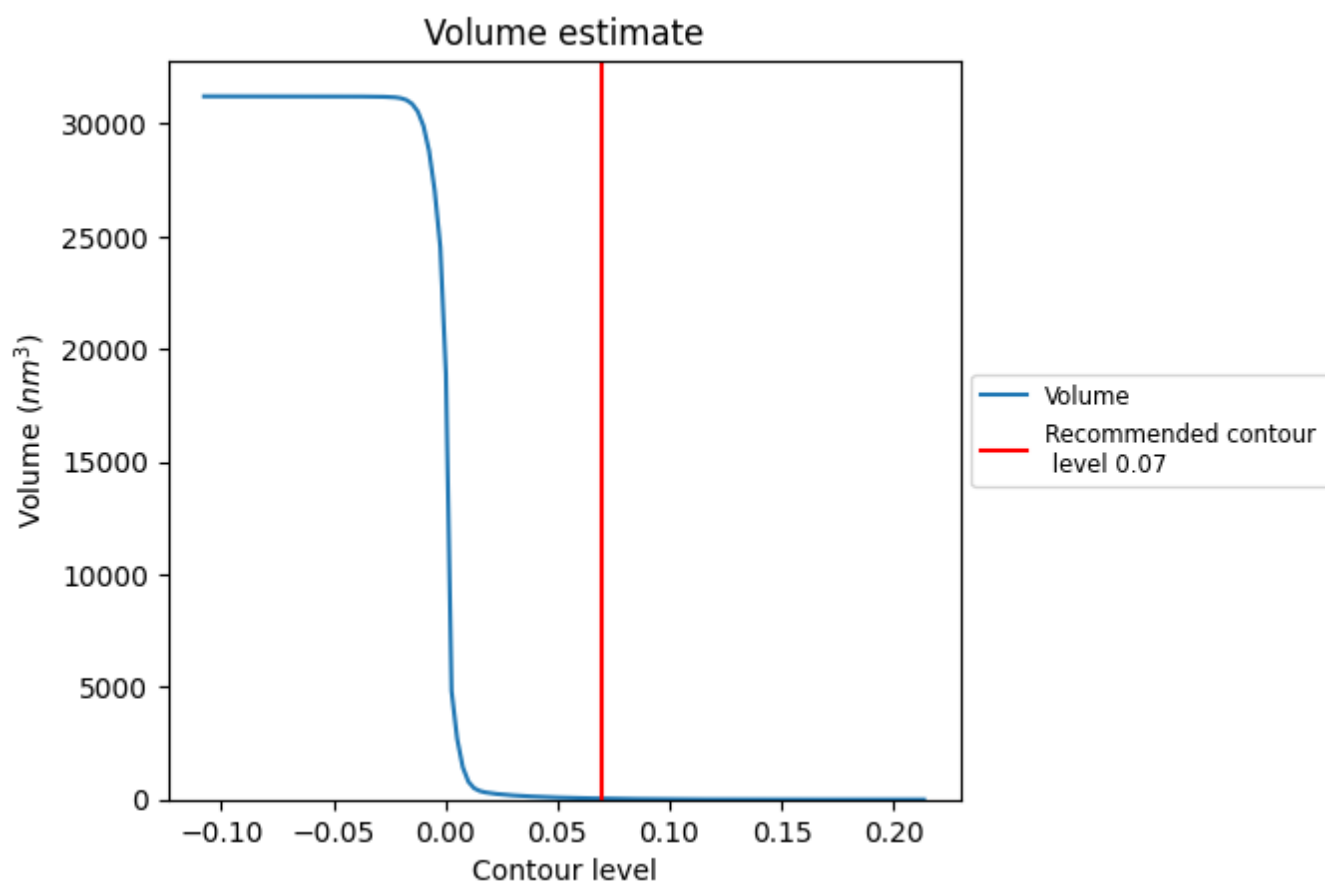
This section contains the results of statistical analysis of the map.

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.

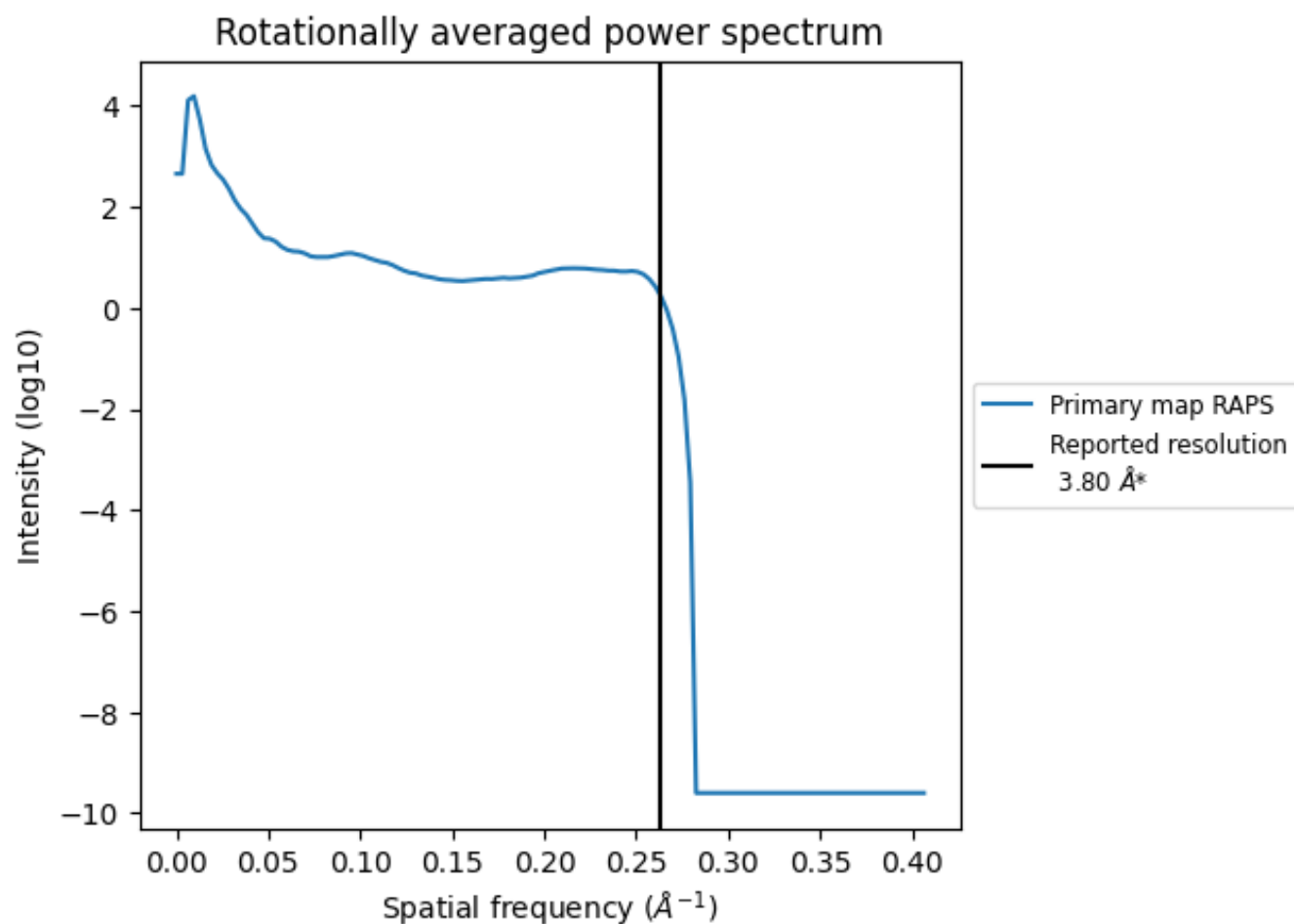
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 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 0.263 $\text{\AA}^{-1}$

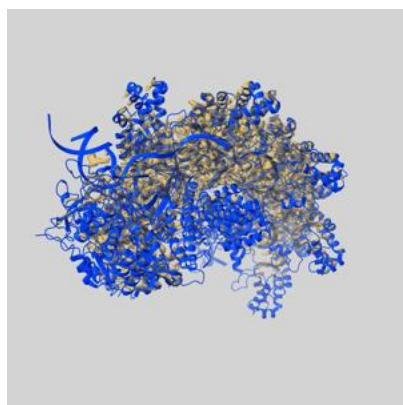
8 Fourier-Shell correlation

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

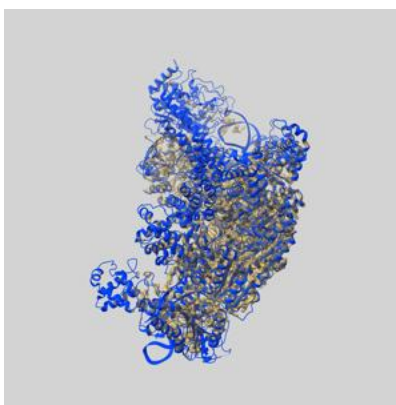
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8477 and PDB model 5U07. Per-residue inclusion information can be found in section [3](#) on page [6](#).

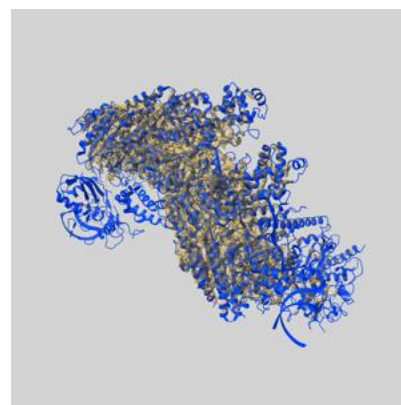
9.1 Map-model overlay [i](#)



X



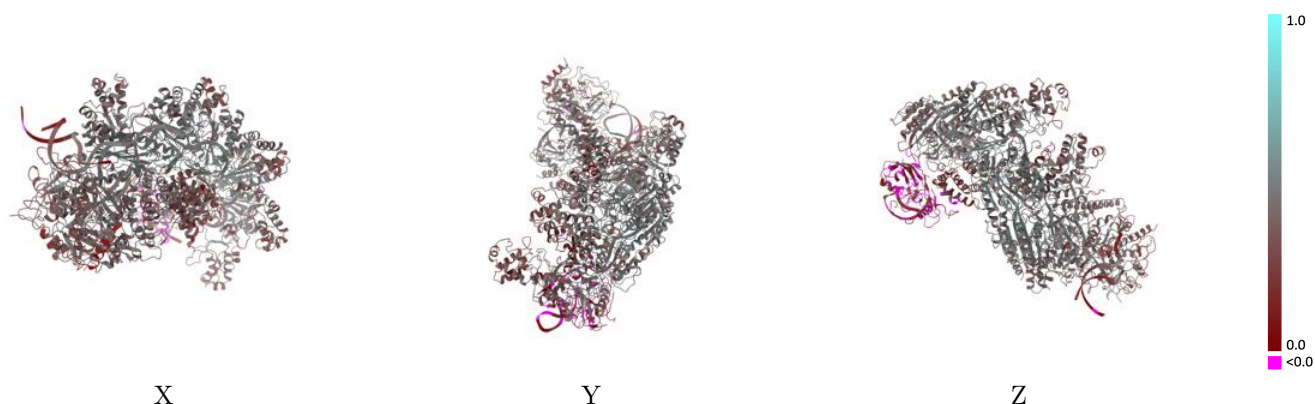
Y



Z

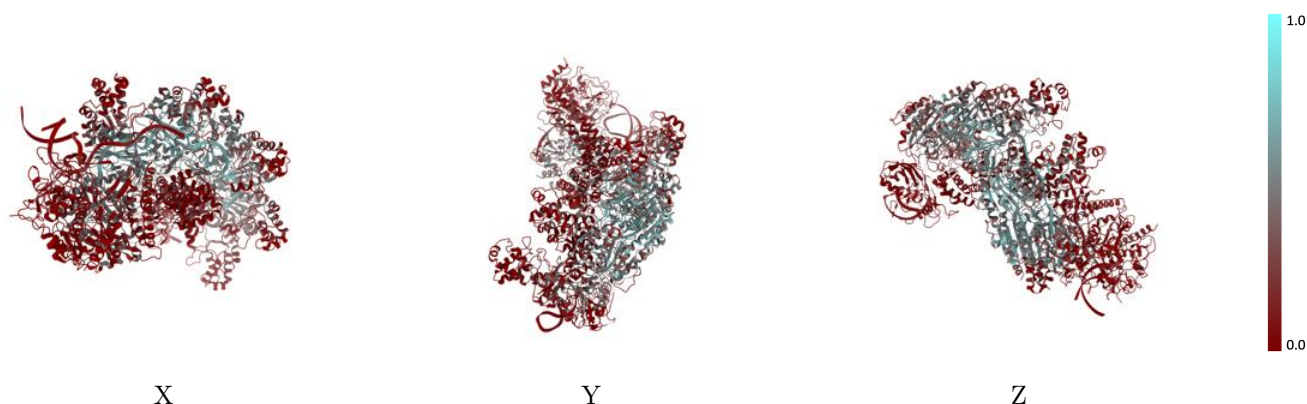
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



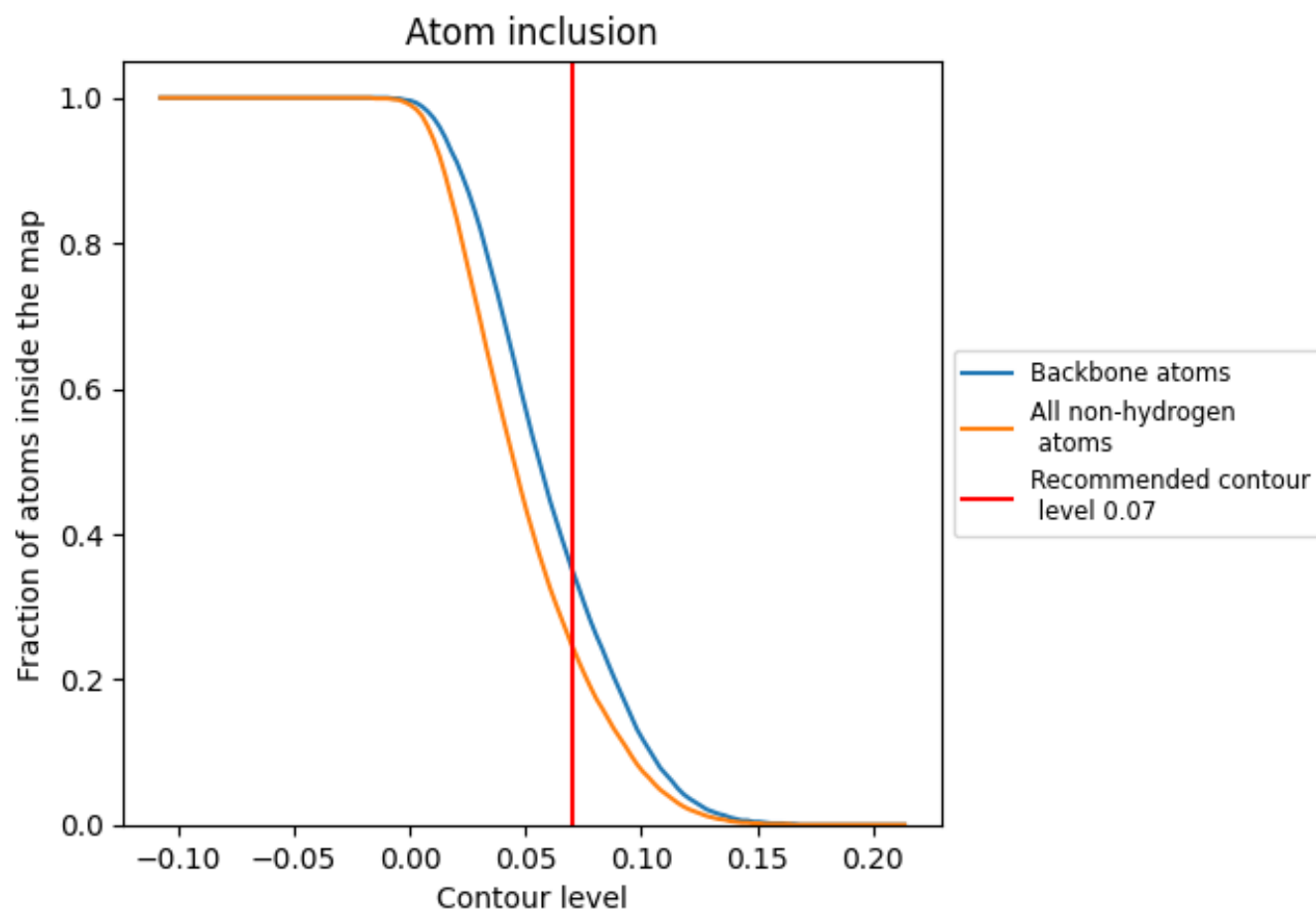
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 35% of all backbone atoms, 25% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2460	0.3850
A	0.0000	0.0560
B	0.0050	0.2560
C	0.0420	0.3710
D	0.3660	0.4470
E	0.3330	0.4240
F	0.3950	0.4460
G	0.4130	0.4590
H	0.3540	0.4470
I	0.2030	0.3750
J	0.0420	0.3400
K	0.4110	0.3450
M	0.0640	0.3590
N	0.2810	0.4370
O	0.0300	0.2130

1.0

0.0

<0.0