



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:27 PM UTC

PDB ID : 9QIW / pdb_00009qiw
EMDB ID : EMD-53196
Title : Human pre-60S - State 3
Authors : Thoms, M.; Denk, T.; Beckmann, R.
Deposited on : 2025-03-17
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

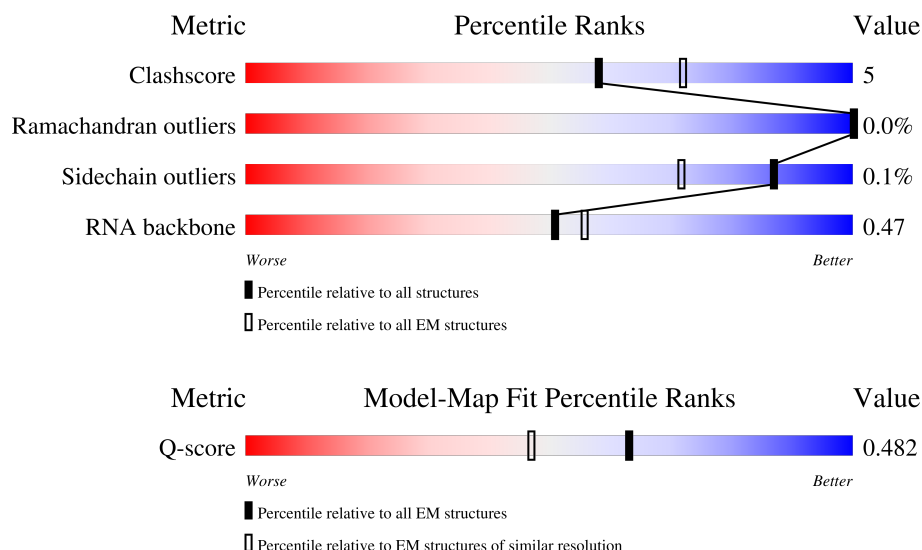
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.04 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.



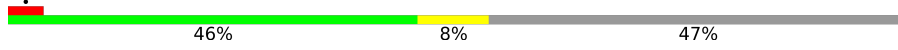
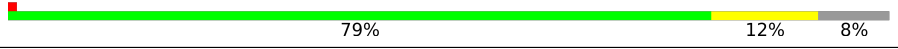
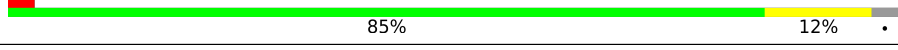
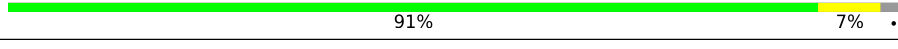
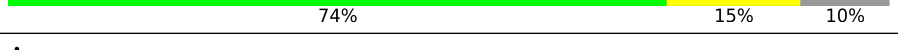
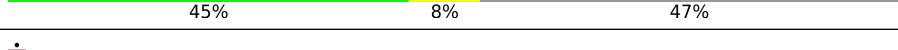
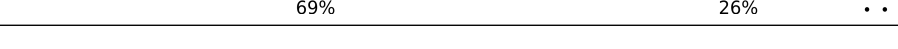
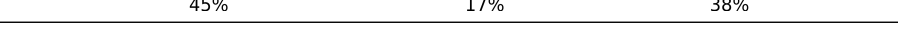
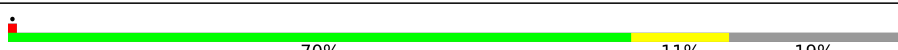
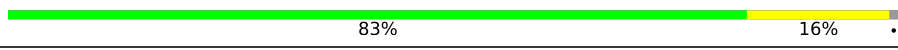
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13952 (2.54 - 3.54)

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	CA	245	
2	CB	731	
3	CC	549	

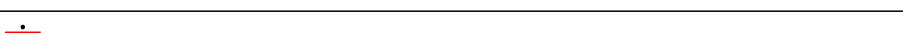
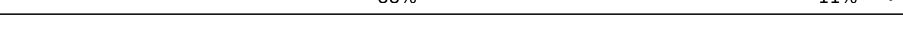
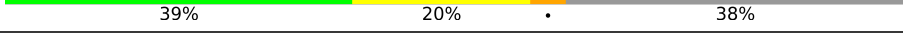
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Mol	Chain	Length	Quality of chain
4	CD	634	
5	CE	129	
6	CF	239	
7	CG	485	
8	CH	260	
9	CI	163	
10	CJ	306	
11	CK	365	
12	L7	121	
13	LA	257	
14	LB	403	
15	LC	427	
16	LD	297	
17	LE	288	
18	LF	248	
19	LG	266	
20	LH	192	
21	LJ	178	
22	LL	211	
23	LM	215	
24	LN	204	
25	LO	203	
26	LP	184	
27	LQ	188	
28	LR	196	

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Mol	Chain	Length	Quality of chain
29	LS	176	
30	LT	160	
31	LU	128	
32	LV	140	
33	LX	156	
34	LY	145	
35	LZ	136	
36	La	148	
37	Lc	115	
38	Ld	125	
39	Le	135	
40	Lf	110	
41	Lg	117	
42	Lh	123	
43	Li	105	
44	Lj	97	
45	Lk	70	
46	Ll	51	
47	Lp	92	
48	Lr	137	
49	Lt	165	
50	L5	5070	
51	L8	157	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 142067 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 Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CA	245	Total	C	N	O	S	0	0
			1860	1153	319	375	13		

- Molecule 2 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CB	441	Total	C	N	O	S	0	0
			3555	2259	634	650	12		

- Molecule 3 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	80	Total	C	N	O	S	0	0
			594	369	126	96	3		

- Molecule 4 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CD	577	Total	C	N	O	S	0	0
			4650	2930	840	855	25		

- Molecule 5 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CE	69	Total	C	N	O	S	0	0
			569	354	125	88	2		

- Molecule 6 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CF	219	Total	C	N	O	S	0	0
			1783	1136	313	322	12		

- Molecule 7 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CG	471	Total	C	N	O	S	0	0
			3449	2149	641	648	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CG	85	ALA	GLU	engineered mutation	UNP Q9NVX2

- Molecule 8 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CH	253	Total	C	N	O	S	0	0
			2036	1297	383	347	9		

- Molecule 9 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CI	140	Total	C	N	O	S	0	0
			1188	756	230	192	10		

- Molecule 10 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CJ	274	Total	C	N	O	S	0	0
			2203	1411	389	392	11		

- Molecule 11 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CK	195	Total	C	N	O	S	0	0
			1559	976	307	275	1		

- Molecule 12 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 13 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LA	159	Total	C	N	O	S	0	0
			1207	763	231	209	4		

- Molecule 14 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LB	383	Total	C	N	O	S	0	0
			3070	1953	571	533	13		

- Molecule 15 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LC	362	Total	C	N	O	S	0	0
			2870	1806	574	477	13		

- Molecule 16 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LD	231	Total	C	N	O	S	0	0
			1886	1197	339	337	13		

- Molecule 17 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LE	209	Total	C	N	O	S	0	0
			1680	1086	316	274	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LF	219	Total	C	N	O	S	0	0
			1790	1148	341	292	9		

- Molecule 19 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LG	216	Total	C	N	O	S	0	0
			1721	1096	332	289	4		

- Molecule 20 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LH	190	Total	C	N	O	S	0	0
			1510	950	282	272	6		

- Molecule 21 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LJ	170	Total	C	N	O	S	0	0
			1335	845	245	239	6		

- Molecule 22 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL	193	Total	C	N	O	S	0	0
			1564	983	326	252	3		

- Molecule 23 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LM	135	Total	C	N	O	S	0	0
			1105	707	213	178	7		

- Molecule 24 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LN	183	Total	C	N	O	S	0	0
			1542	972	324	242	4		

- Molecule 25 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LO	201	Total	C	N	O	S	0	0
			1642	1058	320	259	5		

- Molecule 26 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LP	155	Total	C	N	O	S	0	0
			1248	780	243	216	9		

- Molecule 27 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LQ	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 28 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LR	130	Total	C	N	O	S	0	0
			1095	688	227	172	8		

- Molecule 29 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LS	176	Total	C	N	O	S	0	0
			1457	927	283	236	11		

- Molecule 30 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LT	127	Total	C	N	O	S	0	0
			990	627	189	172	2		

- Molecule 31 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LU	102	Total	C	N	O	S	0	0
			833	533	146	152	2		

- Molecule 32 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LV	137	Total	C	N	O	S	0	0
			1019	639	196	179	5		

- Molecule 33 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LY	132	Total	C	N	O	S	0	0
			1098	689	222	184	3		

- Molecule 35 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 36 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	La	105	Total	C	N	O	S	0	0
			823	524	160	136	3		

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lc	95	Total	C	N	O	S	0	0
			715	457	126	126	6		

- Molecule 38 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ld	105	Total	C	N	O	S	0	0
			857	545	168	142	2		

- Molecule 39 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 40 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lf	109	Total	C	N	O	S	0	0
			872	552	173	144	3		

- Molecule 41 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lg	111	Total	C	N	O	S	0	0
			874	548	180	140	6		

- Molecule 42 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lh	121	Total	C	N	O	S	0	0
			1010	638	204	167	1		

- Molecule 43 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Li	104	Total	C	N	O	S	0	0
			839	524	178	132	5		

- Molecule 44 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lj	77	Total	C	N	O	S	0	0
			636	392	141	98	5		

- Molecule 45 is a protein called 60S ribosomal protein L38.

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

- Molecule 46 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lp	74	Total	C	N	O	S	0	0
			539	336	102	95	6		

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lr	123	Total	C	N	O	S	0	0
			984	611	205	164	4		

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lt	159	Total	C	N	O	S	0	0
			1186	736	223	223	4		

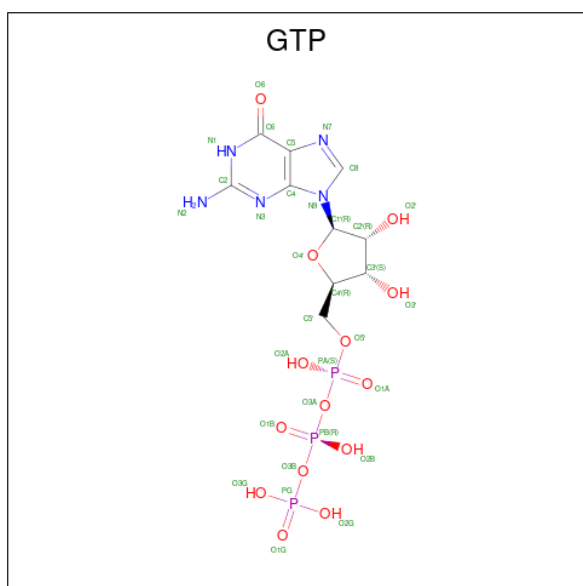
- Molecule 50 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L5	3145	Total	C	N	O	P	0	0
			67476	30040	12384	21908	3144		

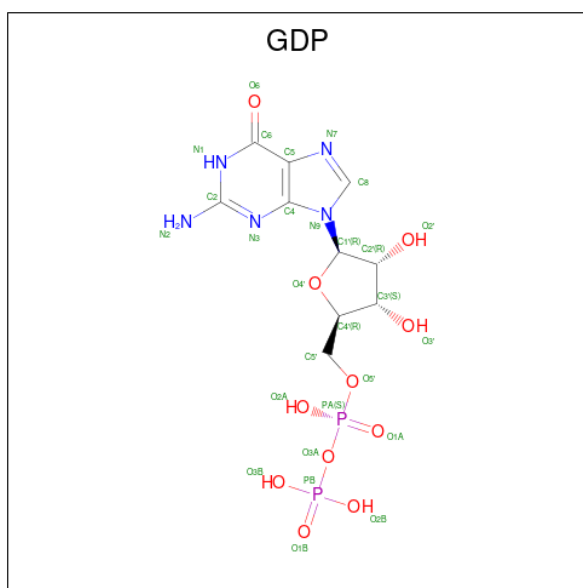
- Molecule 51 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	L8	148	Total	C	N	O	P	0	0
			3150	1406	560	1037	147		

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



- Molecule 53 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
53	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	CD	1	Total	Mg	0
			1	1	

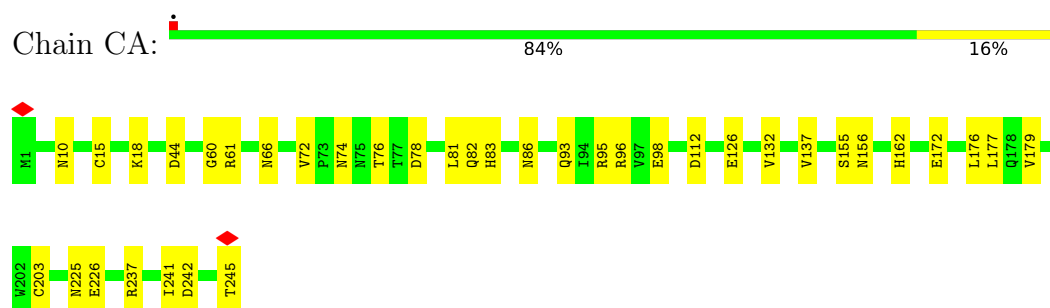
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	CI	1	Total	Zn	0
			1	1	
55	Lg	1	Total	Zn	0
			1	1	
55	Lj	1	Total	Zn	0
			1	1	
55	Lp	1	Total	Zn	0
			1	1	

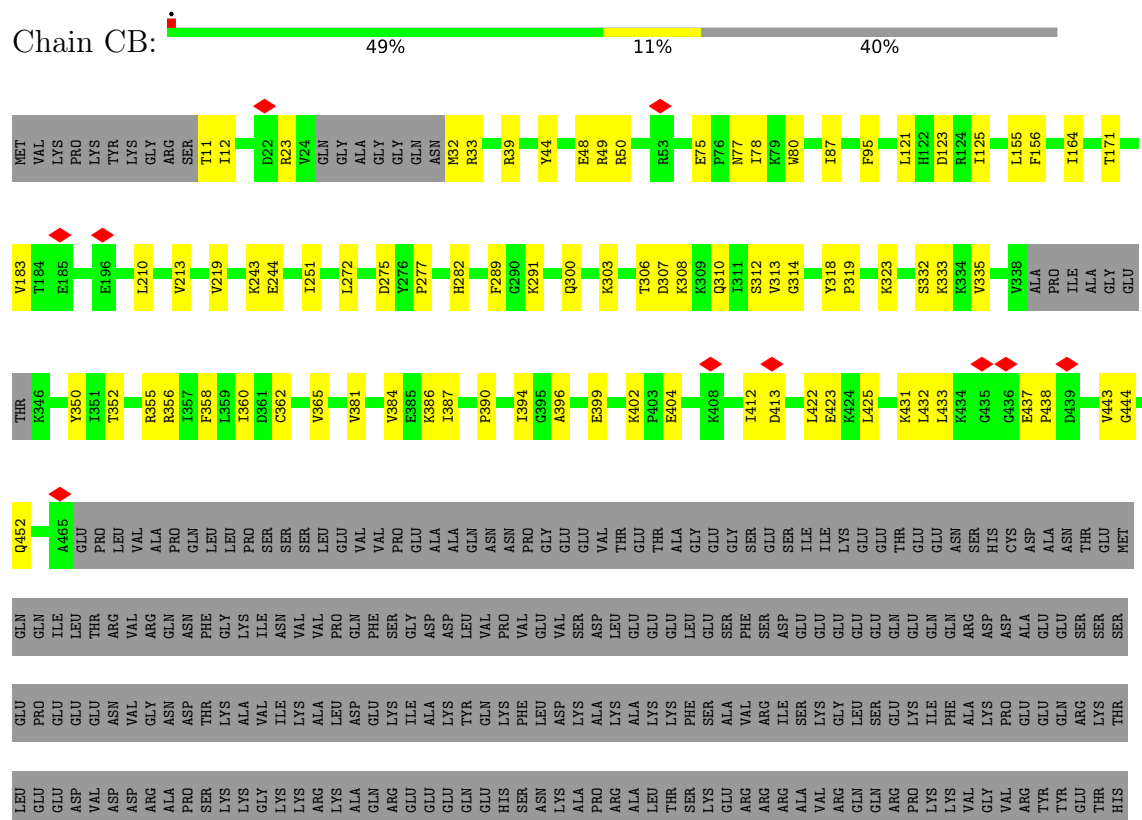
3 Residue-property plots

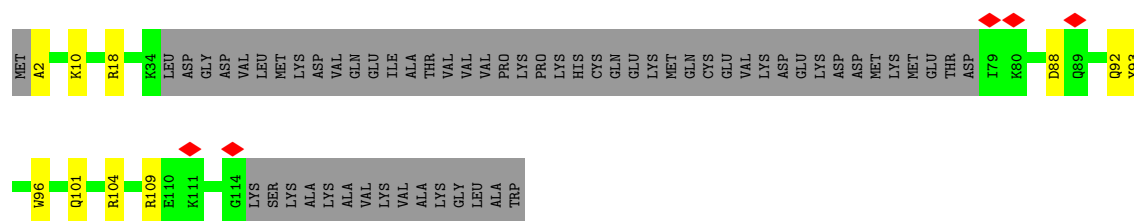
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Eukaryotic translation initiation factor 6

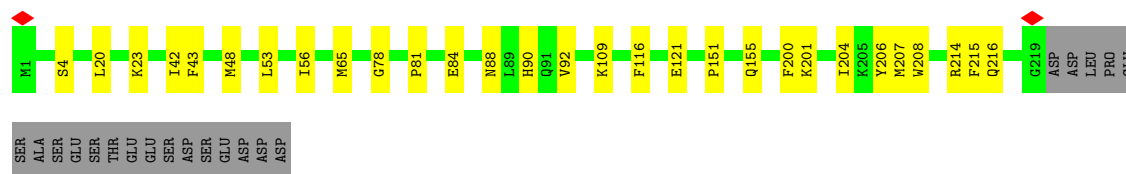
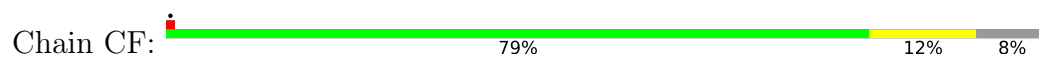


- Molecule 2: Nucleolar GTP-binding protein 2

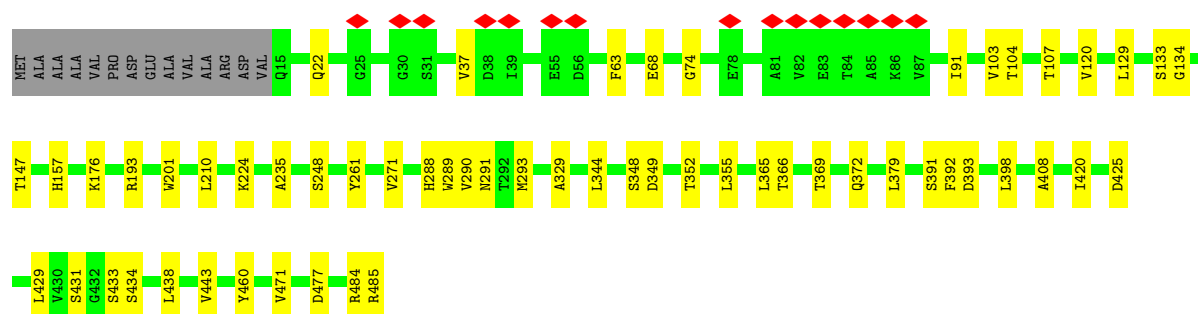
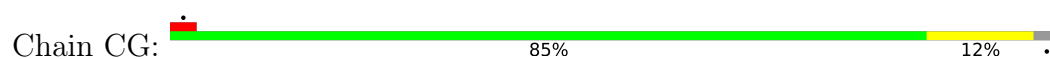




- Molecule 6: mRNA turnover protein 4 homolog



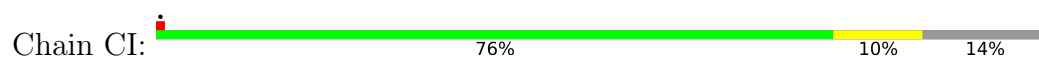
- Molecule 7: Notchless protein homolog 1



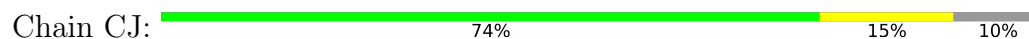
- Molecule 8: Ribosome biogenesis protein NSA2 homolog

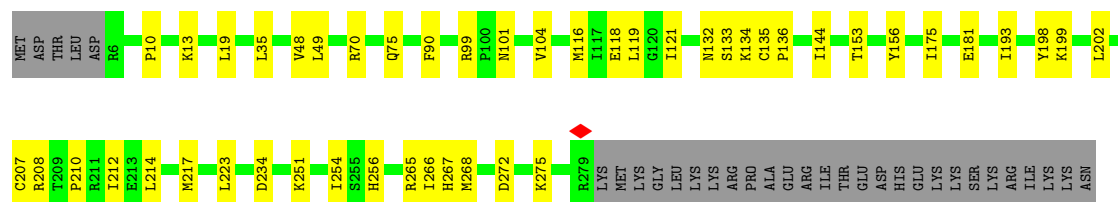


- Molecule 9: Probable ribosome biogenesis protein RLP24

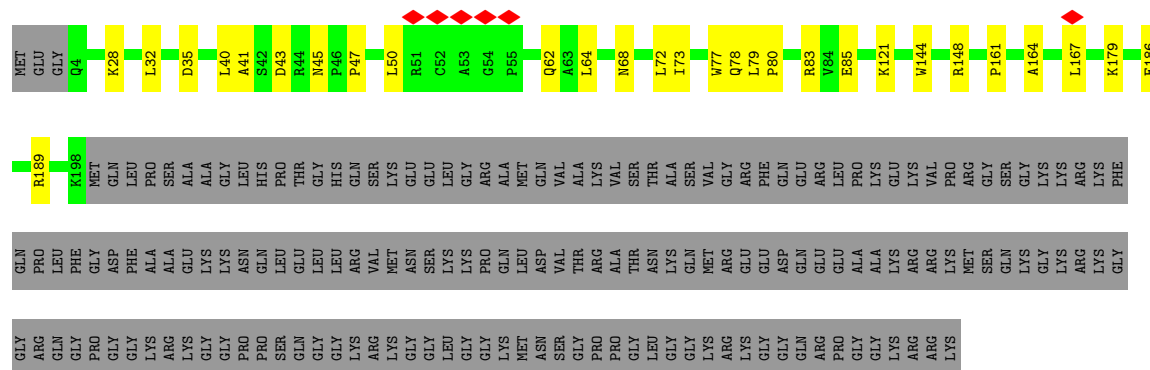


- Molecule 10: Ribosome production factor 2 homolog





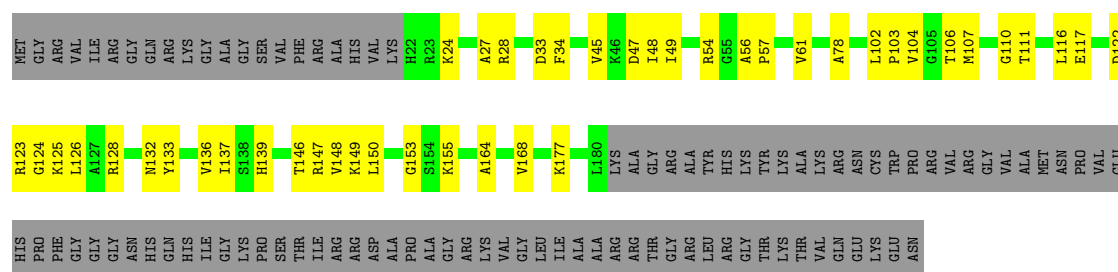
• Molecule 11: Ribosome biogenesis regulatory protein homolog



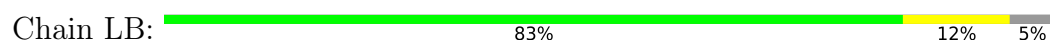
• Molecule 12: 5S rRNA



• Molecule 13: 60S ribosomal protein L8



• Molecule 14: 60S ribosomal protein L3







- Molecule 19: 60S ribosomal protein L7a



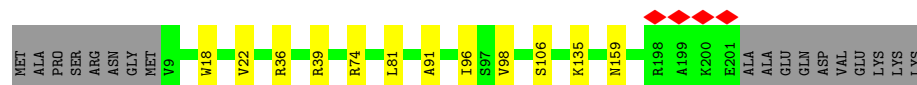
- Molecule 20: 60S ribosomal protein L9



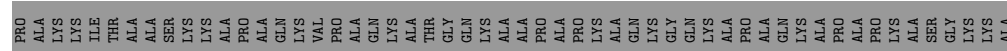
- Molecule 21: 60S ribosomal protein L11



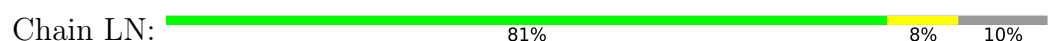
- Molecule 22: 60S ribosomal protein L13

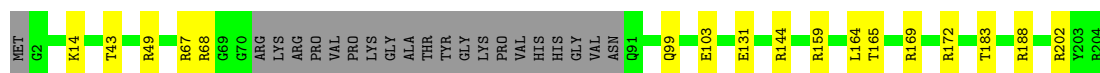


- Molecule 23: 60S ribosomal protein L14



- Molecule 24: 60S ribosomal protein L15





- Molecule 25: 60S ribosomal protein L13a

Chain LO: 83% 16%



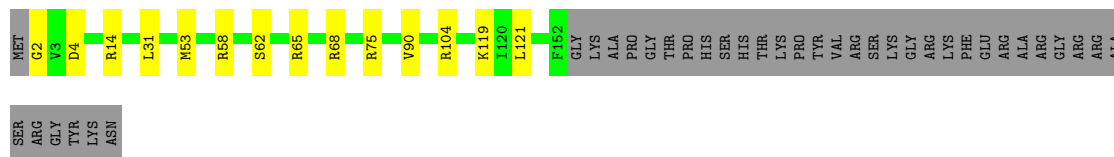
- Molecule 26: 60S ribosomal protein L17

Chain LP: 71% 13% 16%



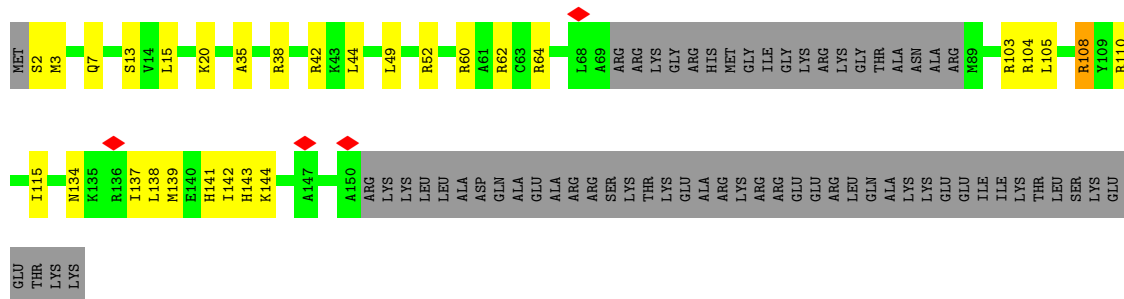
- Molecule 27: 60S ribosomal protein L18

Chain LQ: 73% 7% 20%



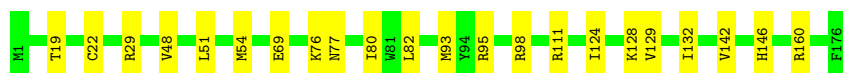
- Molecule 28: 60S ribosomal protein L19

Chain LR: 52% 14% 34%



- Molecule 29: 60S ribosomal protein L18a

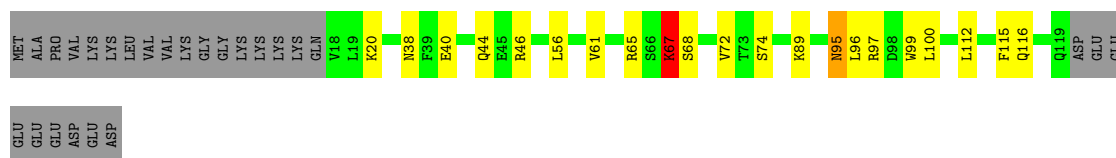
Chain LS: 88% 13%



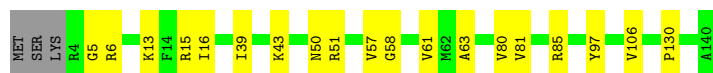
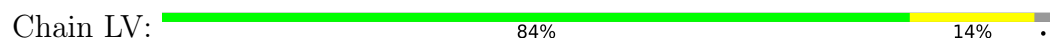
- Molecule 30: 60S ribosomal protein L21



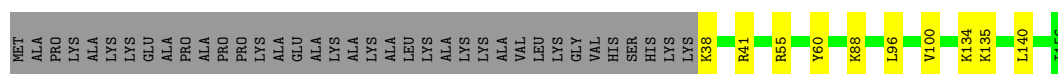
- Molecule 31: 60S ribosomal protein L22



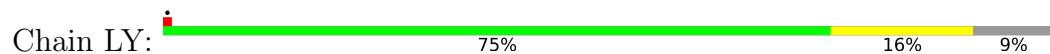
- Molecule 32: 60S ribosomal protein L23



- Molecule 33: 60S ribosomal protein L23a

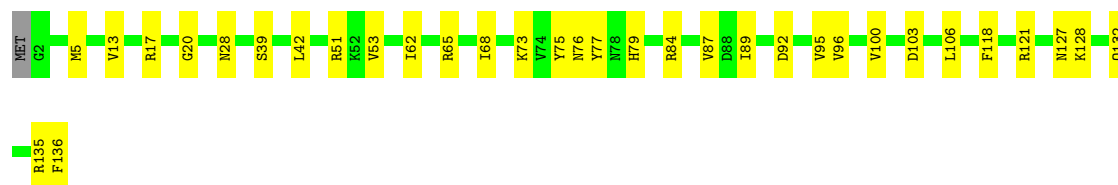


- Molecule 34: 60S ribosomal protein L26

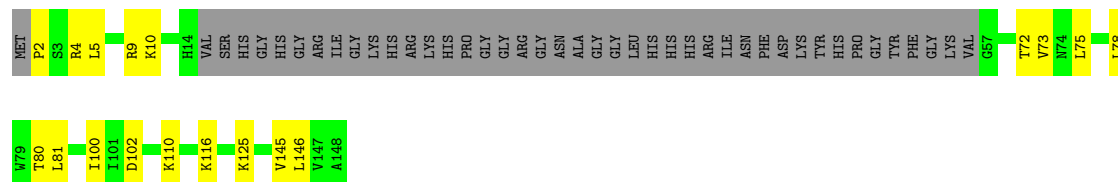


- Molecule 35: 60S ribosomal protein L27





- Molecule 36: 60S ribosomal protein L27a



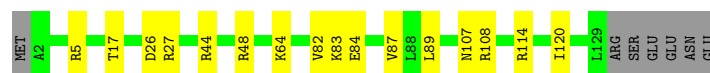
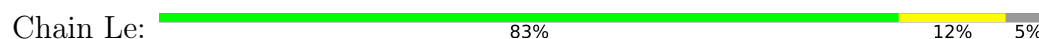
- Molecule 37: 60S ribosomal protein L30



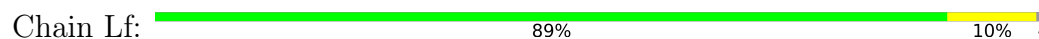
- Molecule 38: 60S ribosomal protein L31



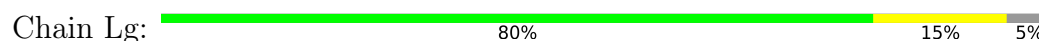
- Molecule 39: 60S ribosomal protein L32



- Molecule 40: 60S ribosomal protein L35a



- Molecule 41: 60S ribosomal protein L34





- Molecule 42: 60S ribosomal protein L35

Chain Lh: 89% 10% .



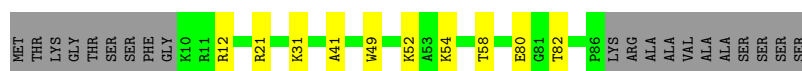
- Molecule 43: 60S ribosomal protein L36

Chain Li: 88% 11% .



- Molecule 44: Large ribosomal subunit protein eL37

Chain Lj: 69% 10% 21%



- Molecule 45: 60S ribosomal protein L38

Chain Lk: 71% 27% .



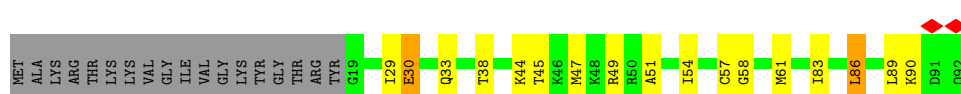
- Molecule 46: 60S ribosomal protein L39

Chain Ll: 69% 29% .



- Molecule 47: 60S ribosomal protein L37a

Chain Lp: 62% 16% 20%



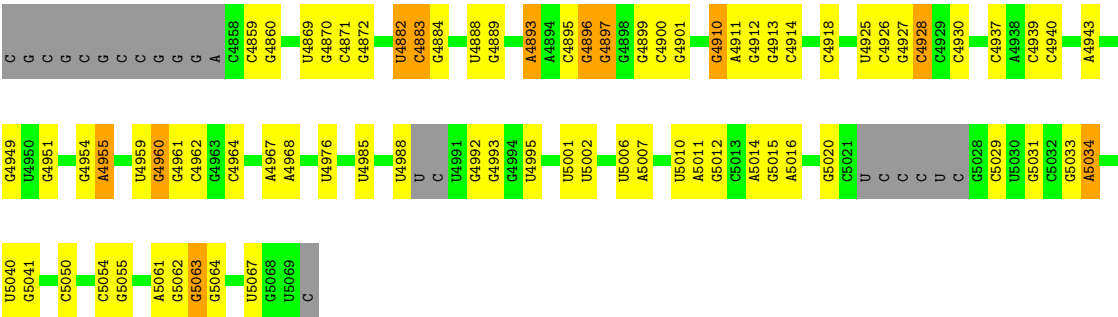
- Molecule 48: 60S ribosomal protein L28

Chain Lr: 75% 15% 10%

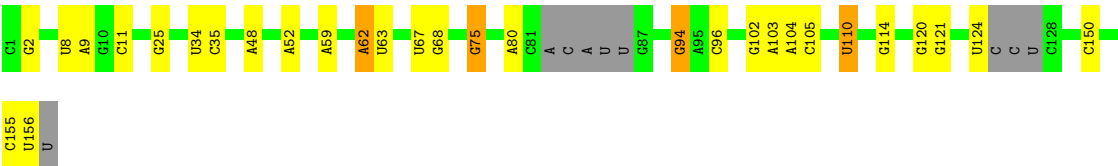








● Molecule 51: 5.8S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33891	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.588	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GTP, GDP, MG

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	CA	0.21	0/1885	0.49	1/2564 (0.0%)
2	CB	0.20	0/3629	0.45	3/4897 (0.1%)
3	CC	0.21	0/602	0.41	0/800
4	CD	0.23	0/4728	0.50	0/6366
5	CE	0.22	0/575	0.48	0/755
6	CF	0.20	0/1818	0.45	0/2436
7	CG	0.26	0/3526	0.45	0/4799
8	CH	0.26	0/2075	0.46	0/2775
9	CI	0.25	0/1211	0.46	0/1605
10	CJ	0.20	0/2245	0.45	0/3011
11	CK	0.20	0/1591	0.46	3/2159 (0.1%)
12	L7	0.21	0/2861	0.30	0/4459
13	LA	0.25	0/1229	0.56	0/1652
14	LB	0.27	0/3132	0.45	0/4189
15	LC	0.26	0/2924	0.45	0/3929
16	LD	0.26	0/1924	0.49	0/2577
17	LE	0.22	0/1712	0.44	0/2300
18	LF	0.27	0/1824	0.49	0/2437
19	LG	0.24	0/1752	0.47	0/2368
20	LH	0.26	0/1529	0.48	0/2058
21	LJ	0.20	0/1358	0.43	0/1820
22	LL	0.22	0/1594	0.46	0/2135
23	LM	0.25	0/1127	0.47	0/1508
24	LN	0.31	0/1580	0.46	0/2112
25	LO	0.28	0/1674	0.43	0/2241
26	LP	0.27	0/1274	0.44	0/1710
27	LQ	0.26	0/1239	0.43	0/1658
28	LR	0.25	0/1109	0.60	1/1472 (0.1%)
29	LS	0.26	0/1497	0.45	0/2009
30	LT	0.22	0/1011	0.53	0/1361
31	LU	0.25	0/847	0.63	1/1137 (0.1%)
32	LV	0.25	0/1033	0.54	0/1383

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
33	LX	0.24	0/993	0.41	0/1334
34	LY	0.25	0/1115	0.48	0/1484
35	LZ	0.22	0/1130	0.47	0/1507
36	La	0.24	0/837	0.50	0/1118
37	Lc	0.20	0/725	0.59	0/978
38	Ld	0.24	0/872	0.48	0/1175
39	Le	0.30	0/1071	0.52	0/1429
40	Lf	0.30	0/891	0.43	0/1194
41	Lg	0.27	0/884	0.60	0/1179
42	Lh	0.25	0/1018	0.51	0/1344
43	Li	0.25	0/850	0.56	0/1125
44	Lj	0.30	0/650	0.51	0/861
45	Lk	0.23	0/575	0.57	0/761
46	Ll	0.29	0/454	0.49	0/599
47	Lp	0.30	0/547	0.71	2/733 (0.3%)
48	Lr	0.24	0/999	0.48	0/1340
49	Lt	0.18	0/1202	0.41	0/1622
50	L5	0.24	0/75446	0.35	0/117599
51	L8	0.30	0/3517	0.33	0/5476
All	All	0.25	0/151891	0.41	11/221540 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
37	Lc	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Lp	86	LEU	CA-CB-CG	6.10	137.65	116.30
31	LU	67	LYS	CA-CB-CG	6.09	126.29	114.10
11	CK	77	TRP	CA-C-N	-6.07	111.39	122.38
11	CK	77	TRP	C-N-CA	-6.07	111.39	122.38
11	CK	78	GLN	N-CA-CB	5.29	118.53	110.44
1	CA	172	GLU	N-CA-CB	5.17	118.26	110.30
2	CB	452	GLN	N-CA-CB	5.12	118.19	110.30
2	CB	171	THR	CA-C-N	-5.07	112.27	121.14
2	CB	171	THR	C-N-CA	-5.07	112.27	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Lp	30	GLU	N-CA-CB	5.05	118.08	110.30
28	LR	108	ARG	CB-CG-CD	5.04	122.89	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	Lc	87	LYS	Peptide

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	CA	1860	0	1835	25	0
2	CB	3555	0	3608	59	0
3	CC	594	0	584	8	0
4	CD	4650	0	4677	63	0
5	CE	569	0	615	10	0
6	CF	1783	0	1824	17	0
7	CG	3449	0	3178	37	0
8	CH	2036	0	2155	15	0
9	CI	1188	0	1251	14	0
10	CJ	2203	0	2275	32	0
11	CK	1559	0	1558	21	0
12	L7	2561	0	1295	16	0
13	LA	1207	0	1268	26	0
14	LB	3070	0	3182	31	0
15	LC	2870	0	3027	24	0
16	LD	1886	0	1895	24	0
17	LE	1680	0	1812	19	0
18	LF	1790	0	1873	25	0
19	LG	1721	0	1800	22	0
20	LH	1510	0	1579	12	0
21	LJ	1335	0	1345	10	0
22	LL	1564	0	1673	9	0
23	LM	1105	0	1156	13	0
24	LN	1542	0	1579	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	LO	1642	0	1779	27	0
26	LP	1248	0	1269	15	0
27	LQ	1223	0	1330	12	0
28	LR	1095	0	1201	22	0
29	LS	1457	0	1491	15	0
30	LT	990	0	985	8	0
31	LU	833	0	856	14	0
32	LV	1019	0	1079	18	0
33	LX	976	0	1053	8	0
34	LY	1098	0	1178	15	0
35	LZ	1107	0	1182	24	0
36	La	823	0	879	14	0
37	Lc	715	0	728	9	0
38	Ld	857	0	906	9	0
39	Le	1053	0	1147	13	0
40	Lf	872	0	901	9	0
41	Lg	874	0	960	15	0
42	Lh	1010	0	1143	8	0
43	Li	839	0	910	10	0
44	Lj	636	0	661	8	0
45	Lk	569	0	637	13	0
46	Ll	444	0	483	12	0
47	Lp	539	0	525	13	0
48	Lr	984	0	1048	16	0
49	Lt	1186	0	1226	14	0
50	L5	67476	0	34130	498	0
51	L8	3150	0	1600	12	0
52	CB	32	0	12	0	0
53	CD	28	0	12	0	0
54	CD	1	0	0	0	0
55	CI	1	0	0	0	0
55	Lg	1	0	0	0	0
55	Lj	1	0	0	0	0
55	Lp	1	0	0	0	0
All	All	142067	0	108355	1134	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 5.

All (1134) 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)
50:L5:1550:G:H1	50:L5:1578:U:H3	0.93	0.92
50:L5:3759:A:H62	50:L5:3764:U:H3	1.11	0.90
50:L5:4745:G:H1	50:L5:4955:A:H61	1.19	0.90
50:L5:2845:A:H61	50:L5:3843:C:H42	1.13	0.89
19:LG:232:GLU:O	19:LG:236:HIS:HB2	1.77	0.83
50:L5:3759:A:N6	50:L5:3764:U:H3	1.77	0.81
50:L5:1079:C:C2	50:L5:1221:G:N2	2.49	0.81
50:L5:4077:A:H62	50:L5:4169:G:H21	1.28	0.81
50:L5:512:U:H3	50:L5:647:G:H1	1.30	0.79
50:L5:2483:G:H1	50:L5:2495:U:H3	1.30	0.77
14:LB:214:ASP:HA	14:LB:284:ILE:O	1.84	0.77
50:L5:2845:A:H61	50:L5:3843:C:N4	1.83	0.74
50:L5:2845:A:N6	50:L5:3843:C:H42	1.84	0.74
5:CE:2:ALA:N	50:L5:4468:U:HO2'	1.87	0.72
50:L5:1684:A:H62	50:L5:1853:G:H8	1.36	0.72
50:L5:3754:G:H1	50:L5:3770:U:H3	1.35	0.72
50:L5:4745:G:H1	50:L5:4955:A:N6	1.90	0.70
18:LF:93:ILE:HA	18:LF:119:ASN:O	1.92	0.69
25:LO:85:ARG:HG3	25:LO:99:LEU:HD11	1.75	0.69
34:LY:31:SER:HA	34:LY:48:PRO:HA	1.74	0.69
11:CK:167:LEU:HD13	30:LT:66:ASN:HD21	1.58	0.69
23:LM:24:LEU:HB2	23:LM:43:THR:HG21	1.75	0.69
50:L5:4077:A:H62	50:L5:4169:G:N2	1.90	0.69
2:CB:314:GLY:HA2	2:CB:360:ILE:HB	1.75	0.68
9:CI:109:MET:HE1	14:LB:399:LYS:HE2	1.74	0.68
33:LX:38:LYS:HE2	50:L5:1:C:H3'	1.75	0.68
24:LN:202:ARG:NH2	50:L5:1372:A:OP1	2.27	0.68
48:Lr:85:ASN:HD22	50:L5:690:C:H4'	1.58	0.68
14:LB:19:ARG:NH2	50:L5:4623:G:OP1	2.27	0.67
50:L5:3716:C:H2'	50:L5:3735:G:H22	1.59	0.67
41:Lg:61:PRO:HA	41:Lg:64:LEU:HD12	1.76	0.67
13:LA:116:LEU:HB3	13:LA:126:LEU:HB2	1.77	0.67
50:L5:3765:G:O2'	50:L5:3767:C:N4	2.27	0.67
50:L5:1079:C:O2	50:L5:1221:G:N2	2.27	0.67
50:L5:4134:C:H2'	50:L5:4135:G:H8	1.61	0.66
4:CD:482:GLN:OE1	4:CD:485:LYS:NZ	2.27	0.66
50:L5:268:G:H2'	50:L5:269:G:H8	1.61	0.66
45:Lk:54:GLU:HB3	45:Lk:58:GLN:HE22	1.61	0.66
50:L5:2552:G:H1'	50:L5:2766:A:H61	1.61	0.66
13:LA:147:ARG:HH12	13:LA:155:LYS:HD3	1.61	0.65
28:LR:60:ARG:NH1	50:L5:2808:G:O2'	2.29	0.65
15:LC:94:ASN:HD22	15:LC:102:PHE:HB2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:La:10:LYS:NZ	50:L5:2287:G:N7	2.43	0.65
9:CI:112:LEU:HB3	14:LB:396:ARG:HD3	1.77	0.65
6:CF:151:PRO:O	6:CF:155:GLN:NE2	2.30	0.65
50:L5:1584:G:H1	50:L5:1609:U:H3	1.45	0.65
50:L5:2049:G:HO2'	50:L5:3884:U:HO2'	1.45	0.65
27:LQ:53:MET:HE2	50:L5:1692:C:H5''	1.79	0.65
28:LR:60:ARG:HH12	50:L5:2809:G:H5'	1.61	0.64
10:CJ:272:ASP:HB3	10:CJ:275:LYS:HG2	1.79	0.64
44:Lj:12:ARG:NH1	50:L5:2801:U:O2	2.30	0.64
14:LB:224:LYS:HG3	14:LB:340:THR:HG22	1.80	0.64
25:LO:3:GLU:N	40:Lf:31:GLU:OE2	2.30	0.64
28:LR:104:ARG:HG3	28:LR:108:ARG:HH22	1.61	0.64
36:La:100:ILE:HD11	36:La:125:LYS:HD2	1.80	0.64
50:L5:1079:C:C2	50:L5:1221:G:C2	2.85	0.64
4:CD:105:LEU:HD21	50:L5:4436:U:H5'	1.79	0.64
45:Lk:47:ILE:HG22	45:Lk:49:ASP:H	1.62	0.64
14:LB:10:ARG:NH1	14:LB:11:HIS:O	2.30	0.64
37:Lc:17:ARG:HE	37:Lc:104:ILE:HG13	1.63	0.64
45:Lk:23:VAL:HG11	45:Lk:60:LEU:HD11	1.79	0.64
4:CD:273:GLN:HG2	4:CD:276:ARG:HH21	1.63	0.64
8:CH:17:ARG:NH1	20:LH:175:PHE:O	2.31	0.64
36:La:78:LEU:HA	36:La:81:LEU:HD12	1.79	0.64
45:Lk:54:GLU:O	45:Lk:58:GLN:NE2	2.32	0.64
50:L5:1079:C:N3	50:L5:1221:G:N1	2.45	0.64
15:LC:329:ASN:ND2	18:LF:188:GLU:OE2	2.30	0.63
40:Lf:29:LYS:HE2	40:Lf:83:MET:HE2	1.80	0.63
25:LO:176:ARG:HD3	50:L5:4769:G:H5''	1.81	0.63
31:LU:61:VAL:HG12	31:LU:74:SER:HB2	1.81	0.63
38:Ld:36:VAL:HG21	38:Ld:44:ARG:HG2	1.80	0.63
3:CC:52:ASN:HA	3:CC:57:LYS:HE2	1.81	0.63
14:LB:220:ILE:HG12	14:LB:278:THR:HG23	1.81	0.63
6:CF:42:ILE:HD11	6:CF:92:VAL:HG13	1.79	0.63
28:LR:62:ARG:NH1	50:L5:4648:A:OP1	2.32	0.63
36:La:73:VAL:HG21	36:La:81:LEU:HD11	1.80	0.63
2:CB:80:TRP:HB3	8:CH:259:LEU:HD13	1.79	0.63
14:LB:57:VAL:HG22	14:LB:73:VAL:HG22	1.79	0.63
35:LZ:51:ARG:HD2	35:LZ:65:ARG:HG2	1.81	0.63
3:CC:34:LYS:NZ	50:L5:1862:U:OP2	2.32	0.62
44:Lj:21:ARG:NH2	44:Lj:41:ALA:O	2.28	0.62
50:L5:2562:G:N2	50:L5:2565:A:OP2	2.32	0.62
39:Le:82:VAL:HG13	39:Le:114:ARG:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Lg:76:ARG:NH2	50:L5:2583:C:OP2	2.31	0.62
2:CB:33:ARG:NH2	50:L5:4541:G:O2'	2.32	0.62
28:LR:139:MET:O	28:LR:143:HIS:ND1	2.27	0.62
30:LT:56:CYS:SG	30:LT:57:TYR:N	2.72	0.62
26:LP:16:LYS:HG2	26:LP:149:ILE:HG12	1.80	0.62
32:LV:6:ARG:NH2	50:L5:4594:U:O2'	2.32	0.62
32:LV:15:ARG:HB2	50:L5:4618:G:H5''	1.82	0.62
27:LQ:90:VAL:HB	36:La:80:THR:HG21	1.82	0.62
50:L5:3715:U:H3	50:L5:3738:G:H1	1.45	0.62
50:L5:1525:A:H61	50:L5:1649:U:H3	1.48	0.61
19:LG:70:LEU:HA	19:LG:73:ARG:HG2	1.82	0.61
10:CJ:265:ARG:NH1	10:CJ:266:ILE:O	2.34	0.61
42:Lh:66:LYS:HD2	51:L8:96:C:H5''	1.82	0.61
50:L5:2020:U:H2'	50:L5:2021:G:H8	1.64	0.61
23:LM:11:ARG:NH1	23:LM:58:THR:O	2.34	0.61
2:CB:49:ARG:NH1	50:L5:3912:U:OP1	2.33	0.61
4:CD:296:ILE:HG13	4:CD:299:LEU:HD12	1.82	0.61
9:CI:22:VAL:HG22	9:CI:28:VAL:HG22	1.83	0.61
22:LL:39:ARG:NH2	50:L5:1362:G:OP1	2.26	0.60
2:CB:312:SER:HB3	2:CB:360:ILE:HD11	1.83	0.60
29:LS:19:THR:HG23	29:LS:22:CYS:H	1.64	0.60
50:L5:3897:G:N2	50:L5:3898:G:O6	2.34	0.60
50:L5:723:A:OP1	50:L5:934:C:N4	2.34	0.60
5:CE:109:ARG:NH2	50:L5:4739:C:OP1	2.32	0.60
11:CK:148:ARG:NH2	50:L5:4199:C:OP2	2.34	0.60
50:L5:4182:G:O2'	50:L5:4184:G:N7	2.35	0.60
4:CD:514:LYS:HG3	31:LU:116:GLN:HE22	1.66	0.60
2:CB:183:VAL:O	4:CD:1:MET:N	2.34	0.60
21:LJ:108:GLY:HA3	50:L5:4251:A:H5''	1.84	0.60
39:Le:5:ARG:NH2	50:L5:705:G:OP1	2.34	0.60
8:CH:36:SER:HG	50:L5:1946:G:HO2'	1.49	0.60
12:L7:3:C:OP1	12:L7:58:A:O2'	2.18	0.60
32:LV:58:GLY:N	32:LV:81:VAL:O	2.35	0.60
46:Ll:23:ILE:HB	46:Ll:27:ILE:HD11	1.83	0.60
50:L5:1576:G:O2'	50:L5:1577:G:N2	2.34	0.60
2:CB:210:LEU:HD22	2:CB:365:VAL:HG21	1.83	0.60
49:Lt:61:LYS:HB3	49:Lt:72:GLU:HG2	1.83	0.60
50:L5:3759:A:N7	50:L5:3764:U:O4	2.35	0.60
19:LG:150:LYS:NZ	19:LG:177:MET:O	2.35	0.59
26:LP:125:MET:HB2	26:LP:141:SER:HB3	1.83	0.59
36:La:75:LEU:HA	36:La:78:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:4101:C:H1'	50:L5:4110:C:H42	1.67	0.59
50:L5:2474:G:H22	50:L5:2503:G:H5''	1.67	0.59
4:CD:207:VAL:O	8:CH:3:GLN:NE2	2.34	0.59
38:Ld:61:ASP:OD2	38:Ld:63:ARG:NH1	2.35	0.59
47:Lp:49:ARG:NH2	50:L5:2739:C:OP2	2.33	0.59
16:LD:50:ARG:NH1	16:LD:147:ASP:OD2	2.35	0.59
50:L5:1079:C:O2	50:L5:1221:G:C2	2.56	0.59
50:L5:1553:A:H8	50:L5:1574:G:H21	1.48	0.59
29:LS:95:ARG:NH2	50:L5:1951:G:O2'	2.36	0.59
40:Lf:22:ARG:NH2	50:L5:2070:U:OP1	2.36	0.59
1:CA:10:ASN:HD21	32:LV:130:PRO:HG2	1.68	0.59
11:CK:32:LEU:HG	11:CK:43:ASP:HB3	1.85	0.59
22:LL:36:ARG:NH2	50:L5:1364:U:OP2	2.36	0.59
2:CB:352:THR:HG23	50:L5:4539:U:H5''	1.85	0.59
4:CD:399:ARG:NH2	50:L5:4597:U:O2'	2.36	0.59
32:LV:6:ARG:NH1	50:L5:4594:U:O3'	2.32	0.59
47:Lp:58:GLY:O	50:L5:2652:G:N1	2.33	0.59
49:Lt:20:GLY:HA2	49:Lt:51:GLY:HA2	1.83	0.59
5:CE:93:TYR:OH	5:CE:109:ARG:NH2	2.34	0.59
38:Ld:79:ASN:ND2	50:L5:4653:C:OP1	2.36	0.59
10:CJ:135:CYS:HB3	10:CJ:217:MET:HE1	1.84	0.58
14:LB:213:GLN:NE2	14:LB:285:TYR:O	2.35	0.58
41:Lg:97:ILE:HD11	50:L5:4122:G:N7	2.18	0.58
4:CD:81:ASP:OD2	4:CD:246:HIS:NE2	2.36	0.58
11:CK:83:ARG:NH1	16:LD:139:PRO:O	2.36	0.58
13:LA:117:GLU:HG3	13:LA:124:GLY:H	1.67	0.58
2:CB:394:ILE:HG13	2:CB:422:LEU:HD11	1.85	0.58
1:CA:237:ARG:HG3	4:CD:360:LEU:HD21	1.85	0.58
50:L5:1399:G:H2'	50:L5:1400:G:H8	1.69	0.58
6:CF:56:ILE:HD11	6:CF:116:PHE:HE1	1.69	0.58
8:CH:31:GLU:HA	8:CH:34:GLU:HB2	1.84	0.58
10:CJ:207:CYS:SG	10:CJ:208:ARG:N	2.77	0.58
2:CB:300:GLN:HE22	10:CJ:267:HIS:HB2	1.68	0.58
19:LG:108:GLN:O	19:LG:112:GLN:NE2	2.36	0.58
27:LQ:119:LYS:HE3	27:LQ:121:LEU:HD21	1.85	0.58
28:LR:13:SER:OG	28:LR:38:ARG:NH2	2.37	0.58
50:L5:679:C:H2'	50:L5:680:G:H8	1.69	0.58
4:CD:368:ARG:NH1	4:CD:369:ASP:OD2	2.37	0.57
50:L5:1743:A:N1	50:L5:1789:C:O2'	2.37	0.57
50:L5:2335:C:H2'	50:L5:2336:G:H8	1.69	0.57
10:CJ:99:ARG:NH1	12:L7:98:G:OP1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:67:C:OP2	50:L5:312:G:N2	2.35	0.57
32:LV:50:ASN:ND2	50:L5:4457:U:OP1	2.34	0.57
37:Lc:48:LEU:HD21	37:Lc:60:ILE:HG21	1.87	0.57
50:L5:1740:C:O2	50:L5:1786:A:N6	2.37	0.57
50:L5:255:C:N4	50:L5:256:G:O6	2.36	0.57
50:L5:4344:U:H3	50:L5:4368:G:H1	1.51	0.57
23:LM:100:ARG:NH1	25:LO:197:LYS:O	2.38	0.57
29:LS:51:LEU:HD12	30:LT:151:LEU:HD23	1.86	0.57
37:Lc:22:MET:HE2	37:Lc:85:CYS:HB3	1.86	0.57
39:Le:26:ASP:OD1	39:Le:27:ARG:N	2.37	0.57
10:CJ:214:LEU:O	11:CK:62:GLN:NE2	2.38	0.57
14:LB:10:ARG:NH2	14:LB:265:SER:O	2.37	0.57
17:LE:152:ILE:O	17:LE:159:GLY:N	2.37	0.57
31:LU:46:ARG:HH21	31:LU:89:LYS:HE2	1.70	0.57
32:LV:15:ARG:NH2	50:L5:4672:A:OP1	2.36	0.57
48:Lr:99:LYS:HD2	50:L5:677:G:H5'	1.86	0.57
50:L5:35:U:O2'	50:L5:1651:G:N3	2.38	0.57
12:L7:26:C:O2'	21:LJ:147:ARG:NH2	2.37	0.57
16:LD:111:ASN:C	16:LD:111:ASN:HD22	2.10	0.57
39:Le:108:ARG:NH2	50:L5:2326:G:OP1	2.37	0.57
1:CA:200:ASN:ND2	1:CA:203:CYS:SG	2.72	0.57
50:L5:184:U:H1'	50:L5:254:G:H22	1.69	0.57
25:LO:27:VAL:O	25:LO:101:ARG:NH1	2.38	0.56
39:Le:84:GLU:HA	39:Le:87:VAL:HG12	1.87	0.56
40:Lf:33:VAL:HG13	40:Lf:38:GLU:HG2	1.86	0.56
50:L5:498:C:H42	50:L5:656:C:H42	1.51	0.56
17:LE:141:ARG:NH2	17:LE:191:GLN:O	2.38	0.56
28:LR:20:LYS:NZ	50:L5:2822:G:N7	2.49	0.56
4:CD:102:ALA:HB2	4:CD:144:GLN:HG3	1.88	0.56
4:CD:581:ARG:HB3	4:CD:585:MET:HE2	1.87	0.56
11:CK:35:ASP:HB3	11:CK:40:LEU:HB3	1.87	0.56
31:LU:40:GLU:HG3	31:LU:65:ARG:HG3	1.87	0.56
50:L5:1406:G:H2'	50:L5:1409:C:H41	1.70	0.56
11:CK:47:PRO:HB2	11:CK:50:LEU:HB2	1.88	0.56
50:L5:1558:A:H2'	50:L5:1559:G:H8	1.71	0.56
6:CF:20:LEU:HD12	6:CF:23:LYS:HD2	1.88	0.56
43:Li:12:ASN:OD1	43:Li:16:LYS:NZ	2.38	0.56
43:Li:54:GLU:OE2	43:Li:86:LYS:NZ	2.39	0.56
45:Lk:8:ILE:HG23	45:Lk:56:LEU:HD11	1.87	0.56
6:CF:42:ILE:HB	6:CF:206:TYR:HB2	1.87	0.56
6:CF:48:MET:HE1	6:CF:201:LYS:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:66:ASP:OD1	9:CI:67:ASN:N	2.39	0.56
30:LT:54:HIS:O	30:LT:58:HIS:NE2	2.38	0.56
35:LZ:13:VAL:O	35:LZ:20:GLY:N	2.39	0.56
36:La:4:ARG:HG3	36:La:5:LEU:HD12	1.88	0.56
48:Lr:37:SER:OG	50:L5:2267:U:OP1	2.24	0.56
50:L5:515:C:H41	50:L5:647:G:H21	1.52	0.56
50:L5:4670:C:O2'	50:L5:4672:A:OP2	2.23	0.56
33:LX:135:LYS:NZ	50:L5:2436:U:OP2	2.39	0.56
41:Lg:99:GLU:HA	41:Lg:102:ILE:HG22	1.88	0.56
47:Lp:38:THR:HA	47:Lp:45:THR:HA	1.88	0.56
50:L5:4151:G:H2'	50:L5:4152:G:H8	1.69	0.56
26:LP:129:THR:HG22	26:LP:131:ARG:H	1.70	0.56
7:CG:147:THR:HG21	16:LD:196:ARG:HB2	1.88	0.56
3:CC:5:LYS:HB3	25:LO:52:LEU:HD13	1.88	0.55
4:CD:525:ARG:HH11	4:CD:531:MET:HB2	1.71	0.55
6:CF:214:ARG:NH1	6:CF:216:GLN:OE1	2.39	0.55
12:L7:23:A:N3	12:L7:118:C:O2'	2.36	0.55
2:CB:310:GLN:OE1	50:L5:4305:G:N1	2.39	0.55
2:CB:75:GLU:OE1	8:CH:201:LYS:NZ	2.38	0.55
17:LE:285:LYS:NZ	40:Lf:38:GLU:OE1	2.40	0.55
20:LH:165:THR:HG21	20:LH:179:ILE:HG13	1.88	0.55
26:LP:37:LYS:HG3	26:LP:117:ILE:HG22	1.87	0.55
47:Lp:83:ILE:HD13	47:Lp:86:LEU:HD23	1.88	0.55
50:L5:294:G:N2	50:L5:296:A:OP1	2.39	0.55
50:L5:2395:A:N6	50:L5:2820:C:O2	2.39	0.55
4:CD:480:ILE:HD12	9:CI:127:VAL:HG11	1.88	0.55
31:LU:67:LYS:HD2	31:LU:68:SER:H	1.71	0.55
40:Lf:68:ARG:NH1	50:L5:442:G:OP1	2.40	0.55
47:Lp:30:GLU:HA	47:Lp:33:GLN:HG2	1.88	0.55
50:L5:4174:U:H2'	50:L5:4175:G:H8	1.72	0.55
16:LD:62:CYS:HB3	16:LD:105:LEU:HD22	1.88	0.55
25:LO:188:LYS:NZ	50:L5:4893:A:OP1	2.40	0.55
10:CJ:175:ILE:HD12	16:LD:44:TYR:HB3	1.89	0.55
14:LB:39:LYS:HE2	14:LB:42:HIS:HE1	1.72	0.55
16:LD:50:ARG:NH2	16:LD:72:ASP:OD2	2.40	0.55
18:LF:148:LYS:HD3	18:LF:245:ARG:HH21	1.72	0.55
18:LF:151:ASN:HD21	50:L5:943:A:H62	1.55	0.55
2:CB:303:LYS:O	2:CB:306:THR:OG1	2.25	0.55
17:LE:141:ARG:NH1	40:Lf:110:ILE:O	2.40	0.55
50:L5:2740:U:O2	50:L5:2742:G:N2	2.39	0.55
50:L5:4733:C:H1'	50:L5:4734:A:H2'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LA:132:ASN:ND2	50:L5:3683:C:OP1	2.40	0.55
26:LP:3:ARG:O	26:LP:18:ARG:NH2	2.40	0.55
39:Le:48:ARG:NH2	50:L5:2279:A:O2'	2.39	0.55
22:LL:74:ARG:NH2	50:L5:109:G:OP2	2.39	0.55
50:L5:1750:G:N2	50:L5:1781:U:O2	2.40	0.55
35:LZ:92:ASP:HB3	35:LZ:95:VAL:HG12	1.89	0.55
50:L5:733:A:N6	50:L5:933:G:O6	2.39	0.55
50:L5:1558:A:H2'	50:L5:1559:G:C8	2.41	0.55
8:CH:103:SER:HB2	8:CH:109:LYS:HZ3	1.72	0.54
16:LD:53:VAL:HB	16:LD:159:VAL:HG13	1.89	0.54
35:LZ:17:ARG:NH2	50:L5:2578:G:N7	2.54	0.54
37:Lc:50:ASN:ND2	37:Lc:75:SER:O	2.40	0.54
50:L5:369:G:N2	50:L5:372:A:OP2	2.26	0.54
50:L5:4113:U:H2'	50:L5:4114:C:H4'	1.89	0.54
4:CD:188:VAL:HG13	4:CD:189:THR:HG23	1.89	0.54
4:CD:347:LYS:HZ1	4:CD:352:LYS:HE2	1.71	0.54
10:CJ:90:PHE:HZ	10:CJ:116:MET:HG2	1.71	0.54
11:CK:186:GLU:OE1	11:CK:189:ARG:NH1	2.40	0.54
18:LF:131:ASN:ND2	50:L5:1727:U:OP1	2.41	0.54
25:LO:106:ASP:O	50:L5:4910:G:N2	2.40	0.54
14:LB:385:LYS:NZ	50:L5:5002:U:OP2	2.40	0.54
7:CG:291:ASN:ND2	7:CG:349:ASP:OD1	2.41	0.54
19:LG:89:ARG:NH1	51:L8:155:C:OP2	2.41	0.54
50:L5:4145:C:O2'	50:L5:4146:G:N7	2.40	0.54
50:L5:4620:U:OP2	50:L5:4670:C:N4	2.39	0.54
50:L5:4992:G:H2'	50:L5:4993:G:C8	2.42	0.54
2:CB:425:LEU:HD11	2:CB:443:VAL:HB	1.90	0.54
39:Le:64:LYS:NZ	50:L5:2079:G:OP2	2.36	0.54
7:CG:485:ARG:NH2	16:LD:139:PRO:O	2.41	0.54
17:LE:266:GLN:NE2	50:L5:4930:C:OP1	2.39	0.54
24:LN:183:THR:HG22	24:LN:188:ARG:HG3	1.89	0.54
29:LS:69:GLU:OE2	29:LS:76:LYS:NZ	2.39	0.54
48:Lr:122:LYS:HD3	48:Lr:123:PRO:HD2	1.89	0.54
50:L5:184:U:O2	50:L5:254:G:N1	2.40	0.54
1:CA:66:ASN:HD22	1:CA:112:ASP:HA	1.72	0.54
10:CJ:202:LEU:HD11	10:CJ:210:PRO:HG2	1.89	0.54
18:LF:92:VAL:O	18:LF:120:GLY:HA2	2.08	0.54
48:Lr:87:ARG:NH1	50:L5:690:C:OP1	2.41	0.54
50:L5:468:U:H1'	50:L5:686:A:H61	1.72	0.54
7:CG:107:THR:HG21	7:CG:484:ARG:HD3	1.89	0.54
15:LC:144:ILE:HD12	15:LC:150:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LN:67:ARG:HD2	50:L5:2458:C:H5''	1.89	0.54
27:LQ:62:SER:OG	50:L5:1502:G:OP2	2.24	0.54
1:CA:78:ASP:OD1	1:CA:78:ASP:N	2.41	0.54
19:LG:232:GLU:O	19:LG:236:HIS:CB	2.55	0.54
16:LD:83:LEU:HB3	16:LD:88:VAL:HG23	1.89	0.53
21:LJ:159:LYS:HG2	21:LJ:163:MET:HE2	1.89	0.53
23:LM:4:ARG:NH2	50:L5:4765:G:O6	2.42	0.53
32:LV:85:ARG:NH2	50:L5:2847:G:OP1	2.37	0.53
44:Lj:31:LYS:NZ	50:L5:1532:G:OP2	2.39	0.53
18:LF:105:VAL:HG13	18:LF:136:VAL:HG12	1.90	0.53
18:LF:115:ARG:NH1	27:LQ:4:ASP:O	2.40	0.53
50:L5:989:U:O2	50:L5:1064:G:O6	2.26	0.53
50:L5:4541:G:N2	50:L5:4544:A:OP2	2.38	0.53
48:Lr:39:ARG:NH2	50:L5:2266:C:O2	2.41	0.53
10:CJ:144:ILE:HG12	11:CK:41:ALA:HB3	1.90	0.53
14:LB:80:GLU:OE1	14:LB:323:TYR:OH	2.26	0.53
48:Lr:32:LEU:O	48:Lr:113:ARG:NH1	2.37	0.53
49:Lt:59:THR:HB	49:Lt:74:VAL:HB	1.90	0.53
10:CJ:251:LYS:HB2	10:CJ:254:ILE:HB	1.89	0.53
1:CA:245:THR:HB	4:CD:347:LYS:HE3	1.91	0.53
2:CB:48:GLU:OE2	2:CB:50:ARG:NH1	2.42	0.53
8:CH:41:LYS:NZ	50:L5:1931:C:OP1	2.42	0.53
48:Lr:67:ARG:NH1	50:L5:480:C:OP1	2.42	0.53
50:L5:267:G:H2'	50:L5:268:G:C8	2.44	0.53
6:CF:4:SER:HB2	20:LH:64:ARG:HH12	1.74	0.53
7:CG:398:LEU:HD12	7:CG:408:ALA:HB3	1.91	0.53
15:LC:204:ARG:NH1	15:LC:205:ARG:O	2.42	0.53
50:L5:659:G:H3'	50:L5:660:A:H8	1.73	0.53
50:L5:4335:C:H3'	50:L5:4336:A:H8	1.73	0.53
28:LR:42:ARG:NH2	50:L5:2525:U:OP2	2.39	0.53
35:LZ:84:ARG:NH1	37:Lc:66:LEU:HG	2.24	0.53
50:L5:483:G:O6	50:L5:485:C:O2'	2.25	0.53
25:LO:94:ARG:NH2	50:L5:1915:C:OP2	2.42	0.52
13:LA:137:ILE:HD11	13:LA:149:LYS:HB2	1.91	0.52
26:LP:37:LYS:NZ	50:L5:425:U:OP1	2.41	0.52
39:Le:87:VAL:HG23	48:Lr:34:ALA:HB1	1.90	0.52
50:L5:1399:G:H2'	50:L5:1400:G:C8	2.44	0.52
50:L5:3700:C:H2'	50:L5:3746:A:H62	1.74	0.52
15:LC:6:PRO:HB3	50:L5:668:C:H4'	1.91	0.52
25:LO:72:HIS:O	25:LO:74:ARG:NH1	2.40	0.52
14:LB:128:LYS:NZ	50:L5:4728:U:OP1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LO:108:ILE:HD13	25:LO:117:ARG:HH12	1.74	0.52
42:Lh:109:ARG:NH2	50:L5:156:G:OP2	2.42	0.52
15:LC:289:LEU:HD11	27:LQ:31:LEU:HB2	1.92	0.52
24:LN:159:ARG:HB3	24:LN:164:LEU:HB2	1.90	0.52
38:Ld:64:ILE:HG23	38:Ld:68:LEU:HD23	1.92	0.52
39:Le:44:ARG:NH2	50:L5:1313:C:OP1	2.43	0.52
11:CK:121:LYS:NZ	50:L5:4195:G:O6	2.43	0.52
28:LR:44:LEU:HD22	28:LR:49:LEU:HD12	1.92	0.52
50:L5:1243:C:H2'	50:L5:1244:G:H8	1.74	0.52
50:L5:4305:G:O2'	50:L5:4307:A:OP2	2.25	0.52
12:L7:79:U:H3	12:L7:97:G:H1	1.57	0.52
17:LE:186:LEU:N	17:LE:250:GLN:OE1	2.41	0.52
50:L5:189:G:H2'	50:L5:190:G:C8	2.45	0.52
50:L5:3932:U:H2'	50:L5:3933:G:H8	1.74	0.52
50:L5:4496:A:H61	50:L5:4504:C:H42	1.57	0.52
13:LA:133:TYR:HB3	13:LA:168:VAL:HG23	1.92	0.52
22:LL:36:ARG:HH12	50:L5:1363:C:H3'	1.75	0.52
42:Lh:52:LYS:NZ	51:L8:62:A:OP1	2.41	0.52
46:Ll:8:ARG:NH2	51:L8:110:U:OP2	2.39	0.52
42:Lh:86:LYS:N	44:Lj:80:GLU:OE1	2.41	0.52
50:L5:1:C:H42	51:L8:156:U:H3	1.58	0.52
50:L5:3702:A:H5''	50:L5:3746:A:H61	1.75	0.52
2:CB:39:ARG:NH1	50:L5:4305:G:OP2	2.40	0.52
4:CD:275:ILE:HB	4:CD:278:LEU:HD12	1.90	0.52
16:LD:11:ALA:HA	16:LD:14:LYS:HG2	1.91	0.52
28:LR:105:LEU:HD11	28:LR:138:LEU:HD23	1.91	0.52
35:LZ:121:ARG:NH2	35:LZ:127:ASN:OD1	2.42	0.52
50:L5:1749:A:H2'	50:L5:1750:G:C8	2.44	0.52
50:L5:3711:A:H2'	50:L5:3712:A:H8	1.75	0.52
50:L5:4279:A:H5'	50:L5:4281:A:H1'	1.92	0.52
1:CA:18:LYS:HE2	1:CA:60:GLY:HA2	1.92	0.51
1:CA:93:GLN:NE2	9:CI:77:GLU:OE1	2.42	0.51
4:CD:597:GLN:NE2	50:L5:2416:G:O6	2.44	0.51
18:LF:135:ILE:HD11	50:L5:1726:U:H5'	1.92	0.51
28:LR:103:ARG:NH1	50:L5:2667:C:OP2	2.42	0.51
46:Ll:20:ASN:OD1	46:Ll:41:ARG:NH1	2.42	0.51
46:Ll:45:ARG:NH1	46:Ll:46:ARG:HH12	2.08	0.51
50:L5:3701:C:N4	50:L5:3745:U:C2	2.78	0.51
50:L5:5063:G:H2'	50:L5:5064:G:H8	1.75	0.51
1:CA:155:SER:OG	1:CA:156:ASN:N	2.43	0.51
4:CD:144:GLN:NE2	50:L5:4437:U:O4	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LR:62:ARG:HH22	50:L5:4645:C:H3'	1.75	0.51
35:LZ:42:LEU:HD21	35:LZ:96:VAL:HG12	1.92	0.51
50:L5:1550:G:O6	50:L5:1578:U:O4	2.28	0.51
50:L5:4736:C:H2'	50:L5:4737:G:H8	1.75	0.51
2:CB:431:LYS:NZ	50:L5:3628:G:O3'	2.44	0.51
4:CD:88:ASP:HB3	4:CD:91:HIS:HB2	1.91	0.51
12:L7:75:G:H4'	12:L7:76:U:H5'	1.92	0.51
13:LA:47:ASP:OD1	13:LA:48:ILE:N	2.43	0.51
22:LL:106:SER:OG	50:L5:73:A:OP1	2.27	0.51
26:LP:41:ILE:HG23	26:LP:42:ARG:HD2	1.91	0.51
50:L5:3932:U:H2'	50:L5:3933:G:C8	2.46	0.51
1:CA:74:ASN:HB3	1:CA:98:GLU:HA	1.93	0.51
9:CI:129:GLN:OE1	9:CI:130:ASN:ND2	2.43	0.51
36:La:116:LYS:HE2	50:L5:1398:A:H61	1.74	0.51
46:LI:41:ARG:NH2	50:L5:2431:A:OP1	2.43	0.51
17:LE:149:ILE:HD12	17:LE:271:LEU:HD21	1.91	0.51
18:LF:182:TYR:HB3	18:LF:200:ARG:HG3	1.92	0.51
6:CF:43:PHE:HB3	6:CF:204:ILE:HD13	1.92	0.51
13:LA:136:VAL:HA	13:LA:148:VAL:HG12	1.92	0.51
36:La:72:THR:HG22	36:La:110:LYS:HB3	1.93	0.51
50:L5:1943:A:N1	50:L5:4414:A:O2'	2.42	0.51
17:LE:206:VAL:HG21	17:LE:257:ILE:HG22	1.92	0.51
41:Lg:97:ILE:HG22	50:L5:4120:U:C4	2.45	0.51
50:L5:4102:C:N4	50:L5:4108:G:O6	2.44	0.51
21:LJ:23:ASN:ND2	50:L5:4258:C:O2	2.43	0.51
41:Lg:26:PRO:HD2	50:L5:2521:G:H4'	1.91	0.51
50:L5:512:U:O4	50:L5:647:G:O6	2.28	0.51
5:CE:93:TYR:HH	5:CE:109:ARG:HH21	1.58	0.51
7:CG:420:ILE:HB	7:CG:429:LEU:HD11	1.93	0.51
49:Lt:20:GLY:HA3	49:Lt:54:LYS:HD2	1.92	0.51
50:L5:85:G:O2'	50:L5:97:G:O6	2.24	0.51
50:L5:268:G:H2'	50:L5:269:G:C8	2.45	0.51
10:CJ:119:LEU:HD13	10:CJ:223:LEU:HD13	1.93	0.51
25:LO:85:ARG:NH2	50:L5:3886:G:OP1	2.42	0.51
38:Ld:28:ASN:HB3	38:Ld:31:LYS:HG2	1.93	0.51
43:Li:90:LEU:HA	43:Li:93:VAL:HG12	1.93	0.51
49:Lt:58:ILE:HD11	49:Lt:75:PRO:HA	1.92	0.51
50:L5:1786:A:H4'	50:L5:1787:A:H5'	1.93	0.51
2:CB:23:ARG:HH12	2:CB:32:MET:HE2	1.76	0.50
15:LC:184:TYR:OH	50:L5:226:G:N7	2.32	0.50
38:Ld:53:ALA:HA	38:Ld:88:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:3658:C:H2'	50:L5:3659:G:H8	1.77	0.50
50:L5:3861:A:H2'	50:L5:3862:A:C8	2.47	0.50
2:CB:350:TYR:CE1	2:CB:360:ILE:HG12	2.46	0.50
41:Lg:29:ARG:NH2	50:L5:2523:G:OP2	2.44	0.50
41:Lg:66:ARG:NH2	50:L5:2518:G:OP1	2.42	0.50
50:L5:1243:C:H2'	50:L5:1244:G:C8	2.47	0.50
17:LE:181:LEU:O	50:L5:4883:C:N4	2.36	0.50
43:Li:68:ARG:HH22	50:L5:3722:G:H5'	1.76	0.50
3:CC:30:ARG:NH1	50:L5:1860:U:OP2	2.45	0.50
4:CD:442:ILE:HD13	9:CI:89:THR:HG21	1.92	0.50
50:L5:1565:A:C5	50:L5:1566:C:H1'	2.47	0.50
21:LJ:120:ASP:HB3	21:LJ:123:ILE:HG12	1.94	0.50
29:LS:142:VAL:HG12	29:LS:146:HIS:CE1	2.47	0.50
34:LY:74:TYR:OH	51:L8:75:G:OP2	2.30	0.50
35:LZ:103:ASP:HB3	35:LZ:106:LEU:HB2	1.93	0.50
7:CG:391:SER:OG	7:CG:392:PHE:N	2.45	0.50
17:LE:66:LYS:HB3	17:LE:68:MET:HE3	1.94	0.50
33:LX:96:LEU:HD12	33:LX:140:LEU:HD21	1.92	0.50
50:L5:3661:G:N2	50:L5:3681:G:O2'	2.44	0.50
4:CD:210:MET:HE1	4:CD:332:LYS:HG3	1.94	0.50
33:LX:100:VAL:HG23	33:LX:134:LYS:HB3	1.94	0.50
2:CB:433:LEU:HB2	2:CB:437:GLU:HG2	1.93	0.50
12:L7:58:A:H2'	12:L7:59:G:H8	1.77	0.50
15:LC:218:ILE:O	15:LC:222:ARG:HB3	2.12	0.50
32:LV:6:ARG:HH12	50:L5:4595:G:H5'	1.76	0.50
32:LV:51:ARG:NH1	50:L5:4620:U:OP1	2.42	0.50
18:LF:59:LYS:O	18:LF:63:GLN:HG2	2.11	0.50
29:LS:80:ILE:HG12	29:LS:129:VAL:HG22	1.93	0.50
50:L5:188:G:N2	50:L5:191:G:O6	2.42	0.50
13:LA:57:PRO:HG2	13:LA:78:ALA:HB3	1.94	0.49
25:LO:43:ILE:HD11	25:LO:138:LEU:HD13	1.94	0.49
47:Lp:89:LEU:HD12	47:Lp:90:LYS:HD3	1.94	0.49
2:CB:95:PHE:HB3	2:CB:121:LEU:HD21	1.93	0.49
11:CK:64:LEU:O	11:CK:68:ASN:ND2	2.45	0.49
24:LN:68:ARG:NH2	50:L5:303:C:OP2	2.45	0.49
35:LZ:136:PHE:OXT	50:L5:4122:G:O2'	2.30	0.49
37:Lc:87:LYS:HD3	37:Lc:88:TYR:H	1.78	0.49
39:Le:107:ASN:ND2	50:L5:2303:C:OP1	2.43	0.49
48:Lr:47:LYS:O	48:Lr:103:ARG:NH1	2.42	0.49
50:L5:1390:G:N2	50:L5:1393:G:OP2	2.41	0.49
50:L5:4151:G:H2'	50:L5:4152:G:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:104:VAL:HG22	10:CJ:118:GLU:HG2	1.94	0.49
12:L7:65:G:O2'	16:LD:10:LYS:NZ	2.44	0.49
31:LU:40:GLU:OE2	31:LU:44:GLN:NE2	2.45	0.49
44:Lj:82:THR:HB	51:L8:94:G:H21	1.77	0.49
50:L5:658:C:H2'	50:L5:659:G:H8	1.77	0.49
50:L5:1583:A:N6	50:L5:1610:C:O2'	2.45	0.49
18:LF:223:LYS:HE3	50:L5:1907:A:H4'	1.94	0.49
23:LM:71:LYS:NZ	50:L5:737:C:OP2	2.45	0.49
34:LY:10:ASP:HB3	34:LY:13:LYS:HB2	1.95	0.49
50:L5:4407:G:H2'	50:L5:4408:G:C8	2.48	0.49
4:CD:447:MET:HE2	9:CI:88:LYS:HB3	1.94	0.49
4:CD:589:ALA:HB1	46:L1:25:GLN:HB3	1.94	0.49
10:CJ:234:ASP:OD2	10:CJ:234:ASP:N	2.45	0.49
19:LG:132:ARG:NH1	50:L5:119:G:N3	2.60	0.49
50:L5:1612:G:H2'	50:L5:1613:A:H3'	1.93	0.49
1:CA:95:ARG:HG3	1:CA:132:VAL:HG21	1.94	0.49
13:LA:117:GLU:OE2	13:LA:122:ASP:N	2.46	0.49
23:LM:4:ARG:NH1	50:L5:4869:U:O4	2.45	0.49
35:LZ:76:ASN:HB3	35:LZ:79:HIS:HD2	1.76	0.49
45:Lk:26:LYS:NZ	45:Lk:28:ASN:OD1	2.41	0.49
50:L5:300:A:H2'	50:L5:301:G:H8	1.76	0.49
10:CJ:70:ARG:HH21	12:L7:99:G:H4'	1.77	0.49
50:L5:4129:G:O6	50:L5:4156:G:N2	2.45	0.49
50:L5:4322:G:N2	50:L5:4325:A:OP2	2.45	0.49
1:CA:44:ASP:N	1:CA:44:ASP:OD1	2.45	0.49
2:CB:422:LEU:HD22	2:CB:443:VAL:HG23	1.95	0.49
14:LB:97:ARG:NH2	50:L5:4911:A:OP1	2.38	0.49
50:L5:2382:A:N1	50:L5:2829:U:O2'	2.36	0.49
50:L5:2495:U:H2'	50:L5:2496:G:C8	2.48	0.49
50:L5:3718:A:H2'	50:L5:3719:A:H8	1.77	0.49
50:L5:4537:C:H2'	50:L5:4538:G:H8	1.78	0.49
4:CD:90:ASP:O	4:CD:94:LEU:HB2	2.12	0.49
19:LG:94:GLN:HG3	19:LG:218:LEU:HD21	1.94	0.49
26:LP:62:ARG:NH1	50:L5:423:G:OP1	2.45	0.49
50:L5:2756:G:H2'	50:L5:2757:A:H8	1.77	0.49
7:CG:431:SER:O	7:CG:438:LEU:HA	2.13	0.49
14:LB:56:ILE:HD12	14:LB:365:LEU:HD22	1.93	0.49
23:LM:41:PRO:HG3	23:LM:73:VAL:HG12	1.94	0.49
25:LO:176:ARG:NH1	50:L5:4769:G:OP1	2.45	0.49
34:LY:89:LYS:NZ	50:L5:386:A:OP2	2.43	0.49
50:L5:1241:C:H2'	50:L5:1242:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:3718:A:H4'	50:L5:4178:A:H4'	1.94	0.48
6:CF:78:GLY:HA3	6:CF:84:GLU:HA	1.95	0.48
11:CK:179:LYS:NZ	50:L5:4226:G:OP1	2.44	0.48
41:Lg:28:ASN:ND2	50:L5:2637:U:OP1	2.46	0.48
10:CJ:268:MET:SD	10:CJ:268:MET:N	2.86	0.48
1:CA:177:LEU:HB3	1:CA:179:VAL:HG22	1.96	0.48
2:CB:384:VAL:HA	2:CB:387:ILE:HD12	1.95	0.48
10:CJ:35:LEU:HB3	10:CJ:49:LEU:HD22	1.95	0.48
13:LA:177:LYS:HB2	47:Lp:29:ILE:HD13	1.95	0.48
20:LH:120:GLU:OE1	20:LH:124:ARG:NH1	2.41	0.48
28:LR:2:SER:OG	28:LR:3:MET:N	2.43	0.48
30:LT:42:ILE:HD12	30:LT:91:VAL:HG21	1.96	0.48
36:La:125:LYS:HG2	36:La:145:VAL:HB	1.94	0.48
7:CG:433:SER:OG	7:CG:434:SER:N	2.47	0.48
13:LA:102:LEU:HB2	13:LA:107:MET:HE2	1.95	0.48
17:LE:191:GLN:HA	17:LE:194:VAL:HG22	1.96	0.48
35:LZ:5:MET:O	35:LZ:28:ASN:ND2	2.46	0.48
47:Lp:47:MET:HE2	47:Lp:57:CYS:HB2	1.95	0.48
50:L5:189:G:H2'	50:L5:190:G:H8	1.78	0.48
50:L5:1933:G:H2'	50:L5:1934:A:C8	2.49	0.48
11:CK:41:ALA:HB2	11:CK:72:LEU:HD22	1.94	0.48
50:L5:2478:C:N4	50:L5:2500:U:O2	2.47	0.48
4:CD:185:ILE:O	4:CD:189:THR:OG1	2.29	0.48
20:LH:94:SER:HB3	20:LH:142:ASP:HB3	1.95	0.48
50:L5:747:A:N7	50:L5:913:U:O2	2.46	0.48
15:LC:218:ILE:HA	15:LC:229:LEU:HD13	1.94	0.48
46:Ll:26:TRP:HA	46:Ll:29:MET:HG2	1.94	0.48
50:L5:2486:G:O6	50:L5:2493:G:O6	2.31	0.48
50:L5:5016:A:H2	50:L5:5033:G:H21	1.62	0.48
2:CB:402:LYS:HE2	2:CB:404:GLU:HB3	1.95	0.48
7:CG:460:TYR:O	8:CH:89:TYR:OH	2.32	0.48
13:LA:111:THR:HG23	47:Lp:86:LEU:HD21	1.95	0.48
17:LE:165:LEU:HD11	17:LE:176:THR:HB	1.95	0.48
29:LS:77:ASN:HB2	29:LS:132:ILE:HG13	1.95	0.48
43:Li:7:MET:HE3	43:Li:7:MET:HB3	1.78	0.48
1:CA:176:LEU:O	4:CD:368:ARG:NH2	2.47	0.48
15:LC:350:ARG:NH2	50:L5:931:C:OP1	2.46	0.48
19:LG:234:ARG:HD2	19:LG:235:ARG:HH11	1.77	0.48
28:LR:64:ARG:NH1	50:L5:2633:U:OP1	2.47	0.48
35:LZ:84:ARG:NH2	37:Lc:62:TYR:O	2.37	0.48
46:Ll:2:SER:O	46:Ll:5:LYS:NZ	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:62:A:N3	50:L5:77:U:O2'	2.36	0.48
50:L5:161:G:H2'	50:L5:162:A:H8	1.78	0.48
50:L5:3839:G:N2	50:L5:3843:C:O2'	2.47	0.48
50:L5:3848:U:H2'	50:L5:3849:A:H8	1.79	0.48
50:L5:4478:G:N2	50:L5:4608:G:O2'	2.47	0.48
50:L5:5010:U:H2'	50:L5:5011:A:H8	1.78	0.48
50:L5:2843:U:O2'	50:L5:4632:U:OP1	2.31	0.47
50:L5:5010:U:H2'	50:L5:5011:A:C8	2.49	0.47
5:CE:96:TRP:HB2	14:LB:136:LYS:HB2	1.97	0.47
7:CG:224:LYS:HG3	7:CG:248:SER:HB2	1.95	0.47
10:CJ:133:SER:OG	10:CJ:199:LYS:NZ	2.47	0.47
15:LC:284:MET:HE2	15:LC:287:THR:HA	1.95	0.47
26:LP:122:ALA:HB3	26:LP:143:PRO:HG2	1.96	0.47
27:LQ:65:ARG:HG3	27:LQ:68:ARG:HH21	1.80	0.47
32:LV:5:GLY:HA3	32:LV:43:LYS:HE2	1.96	0.47
32:LV:39:ILE:HD12	32:LV:61:VAL:HG21	1.96	0.47
45:Lk:35:LYS:NZ	50:L5:2695:A:OP1	2.39	0.47
50:L5:162:A:H2'	50:L5:163:A:H8	1.78	0.47
50:L5:486:C:H2'	50:L5:487:G:C8	2.49	0.47
2:CB:310:GLN:HG2	2:CB:358:PHE:HE1	1.80	0.47
13:LA:110:GLY:HA2	13:LA:136:VAL:O	2.14	0.47
14:LB:218:ASP:HB2	14:LB:348:ARG:HB3	1.97	0.47
34:LY:11:ARG:HG3	50:L5:229:G:H5''	1.95	0.47
38:Ld:32:ARG:NH2	50:L5:4995:U:O3'	2.48	0.47
2:CB:155:LEU:HD21	4:CD:238:MET:HE2	1.96	0.47
2:CB:412:ILE:HD11	2:CB:425:LEU:HB3	1.97	0.47
7:CG:348:SER:OG	7:CG:349:ASP:N	2.48	0.47
10:CJ:101:ASN:HB3	10:CJ:121:ILE:HB	1.96	0.47
20:LH:53:LYS:HA	20:LH:53:LYS:HD3	1.68	0.47
27:LQ:2:GLY:N	50:L5:2072:C:OP1	2.47	0.47
50:L5:4959:U:H2'	50:L5:4960:G:C8	2.48	0.47
1:CA:72:VAL:HG21	1:CA:81:LEU:HD13	1.96	0.47
7:CG:355:LEU:HB3	7:CG:366:THR:HG22	1.97	0.47
19:LG:88:ASP:OD1	19:LG:89:ARG:N	2.47	0.47
34:LY:87:ARG:NH2	50:L5:404:U:O3'	2.42	0.47
2:CB:386:LYS:HA	2:CB:386:LYS:HD3	1.75	0.47
7:CG:355:LEU:O	7:CG:365:LEU:N	2.47	0.47
14:LB:62:ARG:NH1	14:LB:361:GLU:OE1	2.47	0.47
15:LC:101:MET:SD	15:LC:104:PRO:HA	2.55	0.47
15:LC:242:PRO:HB2	50:L5:2297:G:H4'	1.97	0.47
15:LC:275:SER:N	50:L5:1376:C:OP1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LD:111:ASN:C	16:LD:111:ASN:ND2	2.70	0.47
23:LM:5:ARG:NH2	23:LM:59:ASP:OD2	2.48	0.47
50:L5:456:C:H2'	50:L5:457:G:C8	2.50	0.47
50:L5:1671:U:O4	50:L5:1685:G:N2	2.45	0.47
50:L5:1804:A:O2'	50:L5:1833:G:O6	2.31	0.47
50:L5:4150:G:H2'	50:L5:4151:G:C8	2.50	0.47
2:CB:282:HIS:HB3	2:CB:289:PHE:HB3	1.97	0.47
7:CG:104:THR:OG1	7:CG:485:ARG:O	2.32	0.47
16:LD:146:LEU:HD21	16:LD:159:VAL:HG12	1.97	0.47
21:LJ:18:ARG:HG3	21:LJ:135:GLY:HA3	1.96	0.47
31:LU:56:LEU:HD23	31:LU:61:VAL:HG23	1.97	0.47
45:Lk:7:GLU:OE2	45:Lk:9:LYS:NZ	2.48	0.47
50:L5:1989:G:H2'	50:L5:1990:A:H8	1.80	0.47
4:CD:521:GLU:HB3	4:CD:525:ARG:NH1	2.29	0.47
29:LS:111:ARG:NH2	50:L5:2062:C:O2'	2.48	0.47
50:L5:2745:A:H2'	50:L5:2746:A:C8	2.50	0.47
50:L5:4729:A:H61	50:L5:5067:U:H2'	1.80	0.47
2:CB:164:ILE:HD11	4:CD:278:LEU:HD23	1.96	0.46
25:LO:65:ASN:ND2	50:L5:4565:C:OP1	2.48	0.46
32:LV:16:ILE:HD11	32:LV:57:VAL:H	1.80	0.46
35:LZ:53:VAL:HG13	35:LZ:62:ILE:HD12	1.97	0.46
4:CD:399:ARG:NH1	4:CD:402:GLU:OE1	2.46	0.46
10:CJ:153:THR:HG23	10:CJ:156:TYR:H	1.80	0.46
12:L7:33:U:H2'	12:L7:34:C:H6	1.79	0.46
14:LB:69:LYS:HA	14:LB:69:LYS:HD3	1.80	0.46
16:LD:23:ARG:NH1	16:LD:23:ARG:O	2.49	0.46
17:LE:272:ARG:NH2	50:L5:4884:G:O6	2.48	0.46
26:LP:115:GLU:OE2	26:LP:151:THR:OG1	2.30	0.46
50:L5:1332:C:H2'	50:L5:1333:A:H8	1.80	0.46
50:L5:2495:U:H2'	50:L5:2496:G:H8	1.79	0.46
2:CB:213:VAL:HG21	2:CB:362:CYS:HB2	1.98	0.46
4:CD:527:LEU:HD11	31:LU:95:ASN:HB3	1.97	0.46
7:CG:201:TRP:CZ2	7:CG:224:LYS:HD2	2.50	0.46
28:LR:141:HIS:HA	28:LR:144:LYS:HG2	1.97	0.46
45:Lk:5:ILE:HD11	45:Lk:11:PHE:HD1	1.80	0.46
50:L5:35:U:H4'	50:L5:1525:A:H2	1.79	0.46
50:L5:1389:U:OP1	50:L5:1496:G:O2'	2.32	0.46
50:L5:2521:G:H5'	50:L5:2640:G:H1'	1.96	0.46
4:CD:447:MET:HE3	9:CI:88:LYS:HZ1	1.81	0.46
15:LC:315:LYS:HD2	18:LF:168:ALA:HB1	1.97	0.46
18:LF:67:THR:O	18:LF:71:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LJ:92:TYR:HE1	21:LJ:170:TYR:HB3	1.81	0.46
25:LO:10:ASP:OD2	25:LO:37:ARG:NH2	2.47	0.46
51:L8:102:G:OP2	51:L8:104:A:O2'	2.26	0.46
4:CD:538:HIS:HA	4:CD:541:VAL:HG12	1.96	0.46
10:CJ:132:ASN:O	10:CJ:134:LYS:NZ	2.47	0.46
13:LA:27:ALA:O	13:LA:128:ARG:NH2	2.41	0.46
24:LN:49:ARG:NH1	50:L5:152:U:OP1	2.39	0.46
25:LO:49:ARG:NH2	50:L5:1932:A:OP2	2.48	0.46
31:LU:96:LEU:HB3	31:LU:100:LEU:HD13	1.96	0.46
50:L5:2745:A:H2'	50:L5:2746:A:H8	1.80	0.46
50:L5:4478:G:O2'	50:L5:4602:A:N1	2.46	0.46
10:CJ:10:PRO:HG3	10:CJ:19:LEU:HD12	1.97	0.46
29:LS:93:MET:HG2	50:L5:1952:G:H4'	1.97	0.46
50:L5:4140:C:N4	50:L5:4145:C:O2'	2.48	0.46
50:L5:5006:U:H4'	50:L5:5007:A:H5'	1.95	0.46
22:LL:91:ALA:HB1	22:LL:96:ILE:HB	1.96	0.46
30:LT:78:LYS:NZ	30:LT:79:GLN:O	2.41	0.46
15:LC:26:ALA:HB1	15:LC:267:TRP:CZ3	2.50	0.46
45:Lk:52:LYS:HA	45:Lk:55:LYS:HG2	1.98	0.46
50:L5:1503:A:H4'	50:L5:1504:G:H5'	1.98	0.46
50:L5:2757:A:H2'	50:L5:2758:G:C8	2.50	0.46
2:CB:432:LEU:HA	2:CB:438:PRO:HA	1.98	0.46
5:CE:18:ARG:NH2	50:L5:4678:G:OP1	2.40	0.46
6:CF:109:LYS:HD2	6:CF:207:MET:HE1	1.97	0.46
11:CK:144:TRP:HA	11:CK:148:ARG:HG3	1.98	0.46
14:LB:322:HIS:O	14:LB:342:LYS:NZ	2.44	0.46
15:LC:307:LYS:NZ	50:L5:2090:U:OP2	2.40	0.46
36:La:9:ARG:NH2	50:L5:2345:G:N7	2.64	0.46
50:L5:2757:A:H2'	50:L5:2758:G:H8	1.80	0.46
51:L8:67:U:H2'	51:L8:68:G:H8	1.80	0.46
4:CD:103:LYS:HB3	4:CD:103:LYS:HE2	1.75	0.46
4:CD:466:TYR:HA	9:CI:106:LYS:HE3	1.98	0.46
12:L7:58:A:H2'	12:L7:59:G:C8	2.51	0.46
14:LB:140:GLU:OE1	14:LB:144:LYS:NZ	2.49	0.46
19:LG:197:LYS:HB3	50:L5:6:C:H5''	1.98	0.46
23:LM:104:MET:HE2	25:LO:199:HIS:HB3	1.98	0.46
49:Lt:85:LEU:HD11	49:Lt:102:GLY:HA3	1.98	0.46
50:L5:517:C:H5	50:L5:645:G:H21	1.63	0.46
4:CD:20:ASP:OD1	50:L5:4405:G:N2	2.46	0.45
7:CG:157:HIS:CE1	7:CG:176:LYS:HD3	2.51	0.45
49:Lt:107:ASP:OD1	49:Lt:108:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:690:C:H2'	50:L5:691:C:C6	2.51	0.45
50:L5:1220:G:H2'	50:L5:1221:G:C8	2.50	0.45
50:L5:3944:G:H1	50:L5:4069:U:H3	1.63	0.45
25:LO:54:TYR:CE1	25:LO:145:VAL:HG11	2.50	0.45
50:L5:3946:G:H1	50:L5:4067:U:H3	1.63	0.45
50:L5:5063:G:H2'	50:L5:5064:G:C8	2.52	0.45
4:CD:167:ASN:O	4:CD:343:ARG:NH2	2.50	0.45
15:LC:287:THR:HG21	48:Lr:5:LEU:HD22	1.97	0.45
25:LO:68:ARG:NH2	50:L5:4564:A:OP1	2.50	0.45
26:LP:30:ARG:HD2	26:LP:63:TYR:HE2	1.80	0.45
34:LY:52:ASP:HB2	34:LY:110:LYS:HD2	1.97	0.45
41:Lg:69:LYS:HA	41:Lg:72:LYS:HE2	1.97	0.45
50:L5:300:A:H2'	50:L5:301:G:C8	2.51	0.45
50:L5:307:A:N3	50:L5:310:G:O2'	2.47	0.45
50:L5:1585:C:H2'	50:L5:1586:G:C8	2.50	0.45
50:L5:1792:U:H3'	50:L5:1793:A:H8	1.81	0.45
50:L5:4633:G:O2'	50:L5:4635:A:OP1	2.35	0.45
1:CA:126:GLU:HG3	1:CA:137:VAL:HG11	1.97	0.45
34:LY:124:LYS:HA	34:LY:127:GLN:HE21	1.81	0.45
35:LZ:39:SER:OG	37:Lc:36:LYS:NZ	2.50	0.45
47:Lp:86:LEU:HD12	47:Lp:90:LYS:NZ	2.31	0.45
1:CA:82:GLN:NE2	1:CA:86:ASN:OD1	2.47	0.45
2:CB:333:LYS:HG3	2:CB:335:VAL:HG13	1.98	0.45
19:LG:34:LYS:HG3	50:L5:4128:A:H2	1.82	0.45
50:L5:2447:U:H2'	50:L5:2448:G:H8	1.82	0.45
50:L5:2786:C:H5''	50:L5:2787:A:H5'	1.98	0.45
50:L5:4743:G:H2'	50:L5:4744:A:C8	2.52	0.45
4:CD:58:TYR:HE2	4:CD:137:MET:HB3	1.80	0.45
27:LQ:14:ARG:NH2	50:L5:1693:U:OP2	2.49	0.45
32:LV:6:ARG:NH1	50:L5:4595:G:H5'	2.32	0.45
50:L5:1083:U:H3	50:L5:1216:C:H41	1.63	0.45
50:L5:1559:G:H2'	50:L5:1560:A:C8	2.52	0.45
50:L5:1989:G:H2'	50:L5:1990:A:C8	2.52	0.45
7:CG:288:HIS:HD1	7:CG:289:TRP:H	1.65	0.45
7:CG:398:LEU:HD13	7:CG:443:VAL:HG13	1.99	0.45
20:LH:152:GLU:O	20:LH:156:ASN:HB2	2.16	0.45
50:L5:1348:U:H2'	50:L5:1349:G:H8	1.82	0.45
13:LA:24:LYS:HG3	13:LA:49:ILE:HD12	1.99	0.45
13:LA:104:VAL:HG12	13:LA:146:THR:HG21	1.97	0.45
14:LB:113:GLU:HB2	14:LB:178:ALA:HB2	1.99	0.45
28:LR:134:ASN:H	28:LR:137:ILE:HG22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LU:99:TRP:HA	31:LU:115:PHE:HD2	1.81	0.45
44:Lj:49:TRP:O	50:L5:1646:A:O2'	2.35	0.45
48:Lr:52:GLU:OE2	48:Lr:79:ARG:NH2	2.50	0.45
50:L5:315:G:OP2	50:L5:4354:U:O2'	2.31	0.45
50:L5:4140:C:H2'	50:L5:4143:G:H1	1.80	0.45
2:CB:291:LYS:NZ	2:CB:332:SER:OG	2.38	0.45
50:L5:2756:G:H2'	50:L5:2757:A:C8	2.52	0.45
5:CE:101:GLN:HA	5:CE:104:ARG:HB2	1.99	0.45
16:LD:80:ALA:HA	16:LD:83:LEU:HD23	1.98	0.45
19:LG:200:THR:OG1	50:L5:150:U:OP2	2.29	0.45
32:LV:39:ILE:HD13	32:LV:63:ALA:HB2	1.99	0.45
47:Lp:51:ALA:HB3	47:Lp:54:ILE:HD13	1.98	0.45
48:Lr:99:LYS:HB2	48:Lr:99:LYS:HE3	1.70	0.45
50:L5:484:U:N3	50:L5:487:G:O6	2.49	0.45
50:L5:662:C:H2'	50:L5:663:G:C8	2.52	0.45
50:L5:2662:G:H2'	50:L5:2663:G:C8	2.51	0.45
1:CA:225:ASN:OD1	1:CA:226:GLU:N	2.44	0.44
2:CB:272:LEU:HA	2:CB:275:ASP:HB2	1.98	0.44
11:CK:161:PRO:HD2	11:CK:164:ALA:HB2	1.99	0.44
48:Lr:58:LYS:HD2	48:Lr:58:LYS:HA	1.77	0.44
49:Lt:16:ARG:NH1	49:Lt:57:ARG:HD3	2.33	0.44
50:L5:1339:U:H2'	50:L5:1340:C:C6	2.52	0.44
50:L5:1742:A:H2'	50:L5:1743:A:H8	1.81	0.44
50:L5:4233:A:H2'	50:L5:4234:A:C8	2.51	0.44
7:CG:133:SER:OG	7:CG:134:GLY:N	2.51	0.44
7:CG:352:THR:HG22	7:CG:369:THR:HG22	1.99	0.44
12:L7:76:U:H2'	12:L7:77:A:H8	1.82	0.44
15:LC:140:LYS:NZ	15:LC:242:PRO:O	2.50	0.44
51:L8:8:U:H2'	51:L8:9:A:C8	2.52	0.44
51:L8:120:G:H2'	51:L8:121:G:H8	1.82	0.44
9:CI:37:HIS:NE2	32:LV:97:TYR:OH	2.41	0.44
10:CJ:193:ILE:HG23	10:CJ:223:LEU:HB2	1.99	0.44
18:LF:162:ILE:HD12	18:LF:167:ILE:HB	1.99	0.44
19:LG:132:ARG:HD2	50:L5:119:G:C4	2.52	0.44
50:L5:740:G:O6	50:L5:924:C:N4	2.50	0.44
50:L5:4967:A:H2'	50:L5:4968:A:C8	2.52	0.44
2:CB:307:ASP:OD1	2:CB:307:ASP:N	2.49	0.44
23:LM:117:LYS:NZ	50:L5:4882:U:OP1	2.49	0.44
32:LV:13:LYS:NZ	32:LV:57:VAL:O	2.50	0.44
50:L5:3717:A:H1'	50:L5:4179:G:H1'	1.99	0.44
1:CA:15:CYS:HA	1:CA:61:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:1:MET:HE3	50:L5:2041:A:H1'	1.97	0.44
4:CD:15:ALA:HB2	4:CD:145:LYS:HA	2.00	0.44
50:L5:1333:A:H2'	50:L5:1334:A:C8	2.53	0.44
2:CB:44:TYR:OH	8:CH:166:LYS:O	2.23	0.44
3:CC:37:LYS:NZ	50:L5:1861:U:OP1	2.38	0.44
4:CD:172:LEU:HD21	4:CD:247:LEU:HD12	2.00	0.44
6:CF:53:LEU:HA	6:CF:56:ILE:HG22	1.99	0.44
7:CG:22:GLN:O	7:CG:91:ILE:HA	2.17	0.44
19:LG:243:GLY:HA2	50:L5:4076:G:C6	2.53	0.44
36:La:102:ASP:OD1	36:La:102:ASP:N	2.50	0.44
47:Lp:44:LYS:NZ	50:L5:2672:C:OP1	2.39	0.44
50:L5:161:G:H2'	50:L5:162:A:C8	2.53	0.44
50:L5:516:C:N4	50:L5:645:G:H1	2.14	0.44
7:CG:293:MET:HE2	7:CG:344:LEU:HD11	2.00	0.44
10:CJ:256:HIS:HB2	50:L5:4298:A:C4	2.53	0.44
12:L7:83:A:O2'	12:L7:85:G:OP1	2.32	0.44
14:LB:90:VAL:HG22	14:LB:104:THR:HG23	1.99	0.44
18:LF:151:ASN:ND2	50:L5:943:A:N7	2.65	0.44
25:LO:107:GLY:HA3	50:L5:4910:G:H22	1.83	0.44
27:LQ:58:ARG:HE	27:LQ:58:ARG:HB2	1.56	0.44
35:LZ:51:ARG:HB2	35:LZ:65:ARG:HB3	2.00	0.44
49:Lt:52:ASP:N	49:Lt:52:ASP:OD1	2.49	0.44
50:L5:1346:C:H2'	50:L5:1347:G:H8	1.83	0.44
50:L5:4112:C:H3'	50:L5:4113:U:H5''	2.00	0.44
50:L5:4606:G:H2'	50:L5:4607:A:C8	2.53	0.44
6:CF:121:GLU:HB2	6:CF:200:PHE:HB3	2.00	0.44
16:LD:55:VAL:HG23	16:LD:60:ILE:HG12	1.98	0.44
16:LD:152:ARG:HG3	16:LD:154:THR:HG23	2.00	0.44
20:LH:91:LYS:HB2	20:LH:183:GLU:HB3	1.99	0.44
24:LN:14:LYS:HE2	50:L5:280:G:H5''	1.99	0.44
41:Lg:37:LYS:NZ	50:L5:2515:G:OP1	2.47	0.44
50:L5:3848:U:H2'	50:L5:3849:A:C8	2.53	0.44
2:CB:394:ILE:HD11	2:CB:444:GLY:HA2	1.99	0.44
17:LE:190:HIS:HB3	17:LE:193:PHE:HD2	1.83	0.44
28:LR:60:ARG:NH1	50:L5:2809:G:H5'	2.31	0.44
46:Ll:51:LEU:HD23	46:Ll:51:LEU:HA	1.82	0.44
2:CB:12:ILE:HD13	11:CK:121:LYS:HE3	1.99	0.43
10:CJ:48:VAL:HG21	10:CJ:121:ILE:HD13	2.00	0.43
24:LN:172:ARG:NH1	50:L5:62:A:OP1	2.51	0.43
50:L5:162:A:H2'	50:L5:163:A:C8	2.53	0.43
50:L5:2570:U:H2'	50:L5:2571:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:3752:C:H2'	50:L5:3753:G:H5''	2.00	0.43
1:CA:155:SER:OG	1:CA:201:ASP:OD1	2.36	0.43
14:LB:217:ILE:HD12	14:LB:347:LEU:HB3	2.00	0.43
17:LE:110:ARG:HD2	17:LE:110:ARG:HA	1.84	0.43
30:LT:42:ILE:HD11	30:LT:74:ILE:HG13	2.00	0.43
49:Lt:16:ARG:HH11	49:Lt:57:ARG:HD3	1.82	0.43
50:L5:493:G:H2'	50:L5:494:U:C6	2.52	0.43
50:L5:1332:C:H2'	50:L5:1333:A:C8	2.52	0.43
50:L5:1585:C:H2'	50:L5:1586:G:H8	1.83	0.43
50:L5:4460:U:H2'	50:L5:4461:C:H6	1.83	0.43
11:CK:28:LYS:HB3	11:CK:45:ASN:HD21	1.82	0.43
18:LF:213:LEU:O	50:L5:2072:C:O2'	2.35	0.43
42:Lh:104:THR:O	42:Lh:108:GLN:HG3	2.17	0.43
50:L5:66:A:O2'	50:L5:326:C:O2	2.34	0.43
50:L5:365:U:H2'	50:L5:366:A:H8	1.83	0.43
50:L5:2016:C:H2'	50:L5:2017:A:H8	1.83	0.43
50:L5:2395:A:O2'	50:L5:2807:A:OP2	2.36	0.43
50:L5:4318:C:H2'	50:L5:4319:C:H6	1.83	0.43
16:LD:68:ARG:HD2	16:LD:73:MET:HB2	2.00	0.43
27:LQ:75:ARG:NH2	50:L5:1457:G:O2'	2.46	0.43
29:LS:29:ARG:NE	30:LT:147:GLU:OE2	2.51	0.43
31:LU:100:LEU:HD23	31:LU:112:LEU:HD23	2.01	0.43
39:Le:83:LYS:HB3	39:Le:83:LYS:HE3	1.70	0.43
41:Lg:40:LYS:HB3	41:Lg:40:LYS:HE2	1.85	0.43
41:Lg:61:PRO:O	50:L5:2748:C:O2'	2.35	0.43
50:L5:679:C:H2'	50:L5:680:G:C8	2.51	0.43
50:L5:1725:U:H2'	50:L5:1726:U:C6	2.53	0.43
50:L5:1747:U:O2'	50:L5:1783:C:N3	2.37	0.43
15:LC:268:ARG:NH2	50:L5:655:C:OP1	2.52	0.43
20:LH:23:ARG:NH1	20:LH:39:ASN:OD1	2.52	0.43
26:LP:84:PRO:HB2	26:LP:87:SER:HB2	2.00	0.43
29:LS:160:ARG:NH2	50:L5:1921:C:O2'	2.41	0.43
46:Ll:45:ARG:NH1	50:L5:2796:G:N7	2.66	0.43
50:L5:10:A:H2'	50:L5:11:G:C8	2.54	0.43
50:L5:2280:G:N2	50:L5:2281:U:O4	2.51	0.43
13:LA:28:ARG:HH21	13:LA:123:ARG:HD3	1.84	0.43
16:LD:193:GLU:O	16:LD:197:LYS:HG2	2.19	0.43
42:Lh:10:ARG:NH2	42:Lh:63:GLN:OE1	2.41	0.43
46:Ll:28:ARG:NH1	46:Ll:36:ARG:O	2.51	0.43
50:L5:4309:G:H2'	50:L5:4310:A:H8	1.84	0.43
50:L5:4927:G:H5''	50:L5:4928:C:H5	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:18:PHE:HD2	4:CD:141:ILE:HG21	1.83	0.43
6:CF:81:PRO:HG3	6:CF:90:HIS:CD2	2.53	0.43
8:CH:2:PRO:HB2	8:CH:6:TYR:CD1	2.54	0.43
34:LY:126:ARG:NH2	50:L5:198:A:OP1	2.44	0.43
43:Li:76:ARG:O	50:L5:304:C:O2'	2.35	0.43
45:Lk:51:GLU:O	45:Lk:55:LYS:HE3	2.19	0.43
50:L5:174:C:H2'	50:L5:175:C:H6	1.83	0.43
50:L5:1557:C:H2'	50:L5:1558:A:C8	2.54	0.43
50:L5:1617:G:H1'	50:L5:2513:A:N6	2.34	0.43
50:L5:2669:C:H2'	50:L5:2670:C:O4'	2.19	0.43
50:L5:4699:U:H1'	50:L5:4700:A:H5''	1.99	0.43
2:CB:23:ARG:NH2	2:CB:33:ARG:O	2.52	0.43
2:CB:123:ASP:OD2	7:CG:393:ASP:HB2	2.19	0.43
2:CB:431:LYS:HA	2:CB:431:LYS:HD3	1.74	0.43
4:CD:172:LEU:HD23	4:CD:220:VAL:HB	2.01	0.43
28:LR:15:LEU:O	28:LR:52:ARG:NH1	2.51	0.43
35:LZ:73:LYS:HB3	35:LZ:75:TYR:CE2	2.54	0.43
50:L5:690:C:H2'	50:L5:691:C:H6	1.83	0.43
50:L5:1546:C:H3'	50:L5:1611:C:H41	1.84	0.43
50:L5:2467:U:H4'	50:L5:2468:U:H5'	2.01	0.43
50:L5:3897:G:O2'	50:L5:4559:A:N6	2.52	0.43
50:L5:4954:G:H2'	50:L5:4955:A:C8	2.54	0.43
7:CG:63:PHE:HA	7:CG:68:GLU:HA	2.01	0.43
10:CJ:199:LYS:HB3	10:CJ:199:LYS:HE2	1.86	0.43
16:LD:223:PHE:HB3	16:LD:226:TYR:HB2	2.01	0.43
17:LE:180:VAL:HG21	17:LE:258:LEU:HD11	2.01	0.43
18:LF:199:LYS:HD3	18:LF:199:LYS:HA	1.81	0.43
28:LR:115:ILE:HG21	28:LR:142:ILE:HD11	2.00	0.43
34:LY:59:ARG:HB2	34:LY:103:LYS:HD2	2.01	0.43
50:L5:10:A:H2'	50:L5:11:G:H8	1.83	0.43
50:L5:4393:G:H2'	50:L5:4394:A:C8	2.54	0.43
50:L5:4635:A:H5'	50:L5:4664:A:H61	1.84	0.43
12:L7:12:U:OP2	12:L7:67:C:O2'	2.36	0.43
15:LC:330:PRO:HB2	18:LF:51:TYR:HD2	1.84	0.43
19:LG:58:PRO:HD2	19:LG:61:ILE:HD12	2.01	0.43
23:LM:74:ARG:NH2	50:L5:736:C:OP1	2.52	0.43
29:LS:82:LEU:HD12	29:LS:124:ILE:HG23	2.00	0.43
33:LX:88:LYS:HA	33:LX:88:LYS:HD2	1.90	0.43
35:LZ:65:ARG:HH12	50:L5:2755:A:P	2.42	0.43
35:LZ:87:VAL:HG22	35:LZ:89:ILE:HG13	2.00	0.43
50:L5:1536:U:H2'	50:L5:1537:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:1559:G:H2'	50:L5:1560:A:H8	1.84	0.43
50:L5:2520:C:H2'	50:L5:2521:G:H8	1.83	0.43
2:CB:49:ARG:HD2	2:CB:49:ARG:HA	1.88	0.42
7:CG:379:LEU:HD23	7:CG:379:LEU:HA	1.89	0.42
13:LA:107:MET:O	13:LA:139:HIS:NE2	2.39	0.42
20:LH:75:SER:OG	50:L5:4691:A:OP1	2.31	0.42
48:Lr:90:LEU:HG	48:Lr:111:ILE:HG23	2.01	0.42
50:L5:2579:G:N2	50:L5:2582:A:OP2	2.34	0.42
1:CA:76:THR:O	1:CA:96:ARG:NH1	2.53	0.42
2:CB:11:THR:HB	50:L5:4335:C:H42	1.84	0.42
13:LA:125:LYS:HA	13:LA:128:ARG:HD2	2.01	0.42
14:LB:28:LYS:HD3	14:LB:30:LYS:HG2	2.00	0.42
18:LF:241:ASN:O	18:LF:245:ARG:HG2	2.20	0.42
50:L5:1400:G:H2'	50:L5:1401:C:H6	1.84	0.42
50:L5:1461:C:H2'	50:L5:1462:A:C8	2.54	0.42
50:L5:1565:A:N6	50:L5:1566:C:O2	2.53	0.42
50:L5:4185:G:H2'	50:L5:4186:A:H8	1.83	0.42
50:L5:4346:U:H2'	50:L5:4347:G:H8	1.84	0.42
1:CA:162:HIS:NE2	1:CA:191:GLU:OE2	2.50	0.42
4:CD:502:ASN:OD1	50:L5:4646:U:O2'	2.27	0.42
6:CF:208:TRP:HD1	6:CF:215:PHE:HB2	1.85	0.42
18:LF:222:LYS:N	18:LF:232:ASP:OD1	2.38	0.42
29:LS:48:VAL:HG11	29:LS:54:MET:HE3	2.01	0.42
29:LS:80:ILE:HA	29:LS:128:LYS:O	2.19	0.42
35:LZ:76:ASN:HB3	35:LZ:79:HIS:CD2	2.54	0.42
42:Lh:21:LEU:HB2	42:Lh:57:VAL:HG11	2.01	0.42
50:L5:174:C:H2'	50:L5:175:C:C6	2.54	0.42
50:L5:1398:A:H8	50:L5:1420:A:C5	2.38	0.42
6:CF:88:ASN:HB2	6:CF:208:TRP:HE1	1.84	0.42
7:CG:290:VAL:HA	7:CG:348:SER:HB2	2.02	0.42
10:CJ:212:ILE:HD13	11:CK:73:ILE:HG13	2.01	0.42
13:LA:150:LEU:O	13:LA:153:GLY:N	2.52	0.42
15:LC:28:PHE:CD1	15:LC:132:ALA:HB2	2.54	0.42
19:LG:105:GLU:OE2	19:LG:113:ARG:NH1	2.53	0.42
19:LG:157:ILE:HA	19:LG:201:THR:HG22	2.01	0.42
22:LL:81:LEU:HD11	22:LL:98:VAL:HG22	2.01	0.42
25:LO:108:ILE:HD13	25:LO:117:ARG:NH1	2.33	0.42
29:LS:98:ARG:HG3	29:LS:142:VAL:HG13	2.01	0.42
50:L5:2052:G:O2'	50:L5:2057:A:N1	2.50	0.42
50:L5:3939:G:H2'	50:L5:3940:U:C6	2.53	0.42
50:L5:4685:U:H2'	50:L5:4686:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:480:ILE:HG23	9:CI:127:VAL:HG11	2.01	0.42
4:CD:524:MET:HG3	4:CD:531:MET:HE2	2.02	0.42
19:LG:55:VAL:HG21	33:LX:41:ARG:HD2	2.00	0.42
35:LZ:68:ILE:HD13	35:LZ:118:PHE:HB3	2.01	0.42
35:LZ:135:ARG:HA	35:LZ:135:ARG:HD2	1.75	0.42
45:Lk:33:LYS:NZ	50:L5:2693:G:OP2	2.43	0.42
50:L5:506:C:H2'	50:L5:507:G:C8	2.54	0.42
2:CB:87:ILE:HG23	8:CH:236:VAL:HB	2.00	0.42
20:LH:92:MET:HB2	20:LH:144:LEU:HB2	2.01	0.42
22:LL:18:TRP:O	22:LL:22:VAL:HG23	2.19	0.42
41:Lg:62:LYS:HA	41:Lg:65:MET:HG2	2.00	0.42
45:Lk:49:ASP:HB3	45:Lk:52:LYS:HB2	2.02	0.42
50:L5:1265:G:H4'	50:L5:1266:G:N7	2.35	0.42
50:L5:1537:A:N1	50:L5:1623:A:H1'	2.35	0.42
50:L5:4146:G:H2'	50:L5:4147:G:C8	2.54	0.42
50:L5:4563:U:H2'	50:L5:4564:A:H8	1.84	0.42
7:CG:37:VAL:O	7:CG:74:GLY:N	2.53	0.42
13:LA:45:VAL:HG22	13:LA:61:VAL:HG22	2.01	0.42
28:LR:104:ARG:HG3	28:LR:108:ARG:NH2	2.30	0.42
36:La:2:PRO:HD2	50:L5:1509:C:H5''	2.02	0.42
1:CA:83:HIS:CE1	4:CD:413:LEU:HB3	2.55	0.42
2:CB:396:ALA:HA	2:CB:399:GLU:HG2	2.02	0.42
4:CD:88:ASP:OD2	4:CD:91:HIS:N	2.52	0.42
7:CG:120:VAL:HG13	7:CG:129:LEU:HD11	2.01	0.42
7:CG:210:LEU:HD23	7:CG:329:ALA:HB2	2.01	0.42
10:CJ:198:TYR:HB3	10:CJ:214:LEU:HB3	2.01	0.42
17:LE:109:LEU:HD12	17:LE:110:ARG:HG2	2.01	0.42
17:LE:178:PRO:HG3	17:LE:257:ILE:HD11	2.02	0.42
20:LH:171:ASP:HB3	20:LH:174:LYS:HB3	2.01	0.42
24:LN:43:THR:OG1	24:LN:131:GLU:OE2	2.32	0.42
33:LX:60:TYR:OH	50:L5:17:A:OP2	2.29	0.42
34:LY:15:ARG:NH1	50:L5:230:G:OP1	2.46	0.42
50:L5:190:G:H2'	50:L5:191:G:H8	1.85	0.42
50:L5:2492:C:H2'	50:L5:2493:G:O4'	2.18	0.42
50:L5:3871:A:H2'	50:L5:3872:A:C8	2.54	0.42
50:L5:4130:C:H2'	50:L5:4131:G:H8	1.85	0.42
50:L5:4389:C:H2'	50:L5:4390:A:C8	2.54	0.42
50:L5:4389:C:H2'	50:L5:4390:A:H8	1.85	0.42
1:CA:241:ILE:HG12	4:CD:356:VAL:HG11	2.02	0.42
2:CB:243:LYS:HE3	2:CB:244:GLU:HG2	2.02	0.42
2:CB:423:GLU:HG2	2:CB:438:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CG:425:ASP:OD1	7:CG:425:ASP:N	2.53	0.42
28:LR:7:GLN:NE2	28:LR:35:ALA:O	2.41	0.42
31:LU:20:LYS:HA	31:LU:72:VAL:O	2.20	0.42
35:LZ:128:LYS:O	35:LZ:132:GLN:HG2	2.20	0.42
36:La:146:LEU:HD23	36:La:146:LEU:HA	1.91	0.42
38:Ld:24:GLU:OE2	38:Ld:87:ARG:NH2	2.48	0.42
44:Lj:54:LYS:O	44:Lj:58:THR:HB	2.20	0.42
50:L5:1475:G:H2'	50:L5:1476:C:C6	2.55	0.42
50:L5:1552:G:O2'	50:L5:1574:G:N2	2.42	0.42
50:L5:4239:A:H2'	50:L5:4240:G:H8	1.84	0.42
50:L5:4460:U:H2'	50:L5:4461:C:C6	2.55	0.42
50:L5:4743:G:H2'	50:L5:4744:A:H8	1.83	0.42
2:CB:355:ARG:HH22	2:CB:356:ARG:HD2	1.84	0.42
14:LB:46:PHE:CZ	14:LB:84:MET:HG3	2.55	0.42
34:LY:30:MET:HE1	34:LY:75:ARG:HG2	2.02	0.42
50:L5:190:G:H2'	50:L5:191:G:C8	2.55	0.42
50:L5:1536:U:H2'	50:L5:1537:A:H8	1.85	0.42
50:L5:2844:A:N6	50:L5:3839:G:O2'	2.53	0.42
50:L5:3718:A:H2'	50:L5:3719:A:C8	2.55	0.42
50:L5:3948:C:H3'	50:L5:3949:A:H8	1.85	0.42
50:L5:4089:G:H2'	50:L5:4090:G:C8	2.55	0.42
50:L5:4685:U:H2'	50:L5:4686:G:C8	2.55	0.42
50:L5:5011:A:H2'	50:L5:5012:G:C8	2.55	0.42
4:CD:594:LYS:O	4:CD:598:LYS:HB2	2.20	0.41
12:L7:49:A:H3'	16:LD:225:GLN:HE21	1.85	0.41
21:LJ:31:ASP:OD1	21:LJ:32:ARG:N	2.52	0.41
23:LM:51:PRO:O	23:LM:55:MET:HG3	2.20	0.41
24:LN:165:THR:O	24:LN:169:ARG:HG3	2.20	0.41
28:LR:110:ARG:HE	28:LR:110:ARG:HB3	1.65	0.41
31:LU:97:ARG:HA	31:LU:97:ARG:HD2	1.91	0.41
35:LZ:76:ASN:OD1	35:LZ:77:TYR:N	2.54	0.41
50:L5:710:G:H2'	50:L5:711:A:H8	1.85	0.41
50:L5:909:A:H2'	50:L5:910:G:H8	1.85	0.41
50:L5:4077:A:N6	50:L5:4169:G:H21	2.06	0.41
50:L5:4414:A:H1'	50:L5:4428:A:H62	1.84	0.41
2:CB:308:LYS:O	2:CB:356:ARG:NH2	2.53	0.41
11:CK:85:GLU:OE1	16:LD:43:LYS:NZ	2.42	0.41
50:L5:1076:C:H2'	50:L5:1077:C:O4'	2.20	0.41
50:L5:2411:C:H2'	50:L5:2412:A:C8	2.55	0.41
50:L5:2479:G:H2'	50:L5:2480:G:H8	1.85	0.41
50:L5:4093:G:O6	50:L5:4158:C:N4	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:4522:G:H2'	50:L5:4523:A:H8	1.84	0.41
2:CB:319:PRO:HG2	2:CB:381:VAL:HG13	2.01	0.41
7:CG:103:VAL:HG11	7:CG:471:VAL:HG23	2.01	0.41
10:CJ:75:GLN:HE21	10:CJ:116:MET:HE1	1.85	0.41
14:LB:315:ASN:ND2	14:LB:326:VAL:H	2.18	0.41
32:LV:80:VAL:HG23	32:LV:106:VAL:HG21	2.01	0.41
50:L5:382:G:N1	50:L5:385:A:OP2	2.47	0.41
50:L5:669:C:N4	50:L5:670:G:O6	2.53	0.41
50:L5:4589:A:N1	50:L5:4621:C:O2'	2.43	0.41
2:CB:390:PRO:O	2:CB:394:ILE:HG12	2.20	0.41
4:CD:79:TYR:O	4:CD:83:MET:HG3	2.20	0.41
15:LC:298:ILE:HD12	15:LC:298:ILE:H	1.85	0.41
21:LJ:64:ARG:NH1	50:L5:4204:C:OP1	2.53	0.41
23:LM:94:LYS:NZ	50:L5:4872:G:OP2	2.50	0.41
39:Le:17:THR:HG22	50:L5:1302:U:H5'	2.02	0.41
43:Li:44:ILE:HD13	43:Li:44:ILE:HA	1.95	0.41
44:Lj:52:LYS:NZ	50:L5:375:G:OP2	2.36	0.41
49:Lt:38:SER:HA	49:Lt:39:PRO:HD3	1.96	0.41
50:L5:183:C:H1'	50:L5:184:U:H5	1.85	0.41
50:L5:2477:A:O2'	50:L5:2478:C:H5'	2.21	0.41
50:L5:2722:G:H2'	50:L5:2723:U:O4'	2.20	0.41
50:L5:3658:C:H2'	50:L5:3659:G:C8	2.55	0.41
2:CB:318:TYR:O	2:CB:323:LYS:NZ	2.51	0.41
2:CB:413:ASP:OD1	2:CB:413:ASP:N	2.53	0.41
4:CD:301:GLU:HB3	4:CD:305:LYS:NZ	2.36	0.41
18:LF:62:ARG:HE	18:LF:62:ARG:HB3	1.65	0.41
18:LF:216:PRO:HG3	18:LF:220:MET:HE3	2.02	0.41
25:LO:28:LEU:HA	25:LO:28:LEU:HD23	1.85	0.41
27:LQ:104:ARG:NH2	50:L5:1353:G:N7	2.53	0.41
48:Lr:66:ARG:NH1	50:L5:478:G:OP1	2.54	0.41
50:L5:197:A:N3	50:L5:222:C:O2'	2.46	0.41
50:L5:1738:A:H2'	50:L5:1739:G:C8	2.56	0.41
3:CC:13:MET:HE3	3:CC:18:ARG:HB2	2.02	0.41
4:CD:144:GLN:HE22	50:L5:4437:U:H3	1.68	0.41
8:CH:19:ASP:N	8:CH:19:ASP:OD2	2.52	0.41
10:CJ:13:LYS:HE3	10:CJ:13:LYS:HB3	1.84	0.41
18:LF:37:PHE:O	18:LF:41:MET:HG2	2.21	0.41
19:LG:106:THR:H	19:LG:109:GLU:CD	2.29	0.41
26:LP:96:LYS:HB3	26:LP:96:LYS:HE2	1.78	0.41
37:Lc:47:ILE:HD12	37:Lc:94:LEU:HD11	2.03	0.41
40:Lf:91:ASN:O	50:L5:440:U:O2'	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Lp:57:CYS:O	47:Lp:61:MET:HA	2.21	0.41
50:L5:1784:U:H2'	50:L5:1785:C:H6	1.86	0.41
50:L5:5015:G:H21	50:L5:5034:A:H62	1.67	0.41
2:CB:251:ILE:HG22	2:CB:277:PRO:HB2	2.02	0.41
4:CD:588:LYS:HA	4:CD:588:LYS:HD2	1.84	0.41
10:CJ:136:PRO:HD2	10:CJ:181:GLU:HG3	2.03	0.41
11:CK:79:LEU:HD12	11:CK:80:PRO:HD2	2.02	0.41
24:LN:144:ARG:NH2	50:L5:137:G:OP2	2.53	0.41
26:LP:153:LYS:HA	26:LP:153:LYS:HD3	1.80	0.41
46:Ll:45:ARG:HH11	46:Ll:46:ARG:HH12	1.68	0.41
50:L5:218:A:O2'	50:L5:219:G:O4'	2.26	0.41
50:L5:456:C:H2'	50:L5:457:G:H8	1.86	0.41
50:L5:1264:C:O2'	50:L5:1265:G:O5'	2.30	0.41
50:L5:4197:G:H2'	50:L5:4198:G:H8	1.85	0.41
13:LA:107:MET:HE1	13:LA:164:ALA:HB3	2.02	0.41
25:LO:55:LEU:HD23	25:LO:58:LEU:HD12	2.03	0.41
38:Ld:37:GLY:O	38:Ld:41:ARG:HG3	2.21	0.41
49:Lt:32:ILE:HD12	49:Lt:35:LEU:HD12	2.03	0.41
50:L5:1725:U:H2'	50:L5:1726:U:H6	1.84	0.41
50:L5:1980:U:O2'	50:L5:1982:G:N7	2.49	0.41
50:L5:3626:G:H2'	50:L5:3627:G:C8	2.55	0.41
5:CE:10:LYS:HA	5:CE:10:LYS:HD2	1.91	0.41
7:CG:365:LEU:HD23	7:CG:365:LEU:HA	1.90	0.41
13:LA:54:ARG:HG2	13:LA:56:ALA:H	1.86	0.41
17:LE:210:LYS:HA	17:LE:210:LYS:HE3	2.03	0.41
24:LN:99:GLN:O	24:LN:103:GLU:HG3	2.21	0.41
40:Lf:50:VAL:HG22	40:Lf:69:VAL:HG22	2.02	0.41
43:Li:76:ARG:HD3	43:Li:76:ARG:HA	1.74	0.41
43:Li:82:ARG:NH1	50:L5:282:C:O2	2.47	0.41
50:L5:2610:G:H2'	50:L5:2611:A:C8	2.56	0.41
50:L5:2640:G:H2'	50:L5:2641:A:C8	2.56	0.41
50:L5:3868:G:H1	50:L5:3900:G:H21	1.69	0.41
50:L5:3871:A:H2'	50:L5:3872:A:H8	1.85	0.41
50:L5:3931:C:N4	50:L5:4180:G:O6	2.54	0.41
50:L5:4098:A:H3'	50:L5:4099:G:H4'	2.02	0.41
50:L5:4133:C:N3	50:L5:4152:G:N1	2.68	0.41
2:CB:156:PHE:HZ	4:CD:89:LYS:HD3	1.86	0.41
3:CC:20:LYS:HE2	3:CC:20:LYS:HB3	1.87	0.41
4:CD:251:VAL:HG11	4:CD:279:PHE:CE2	2.56	0.41
4:CD:251:VAL:HG11	4:CD:279:PHE:HE2	1.86	0.41
7:CG:477:ASP:OD1	7:CG:477:ASP:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CH:44:GLY:HA2	50:L5:2040:A:H1'	2.01	0.41
22:LL:135:LYS:HA	22:LL:135:LYS:HD2	1.78	0.41
25:LO:108:ILE:HD12	25:LO:160:ARG:CZ	2.50	0.41
25:LO:190:ASP:OD1	25:LO:191:LYS:N	2.53	0.41
26:LP:5:SER:O	51:L8:11:C:O2'	2.33	0.41
42:Lh:88:THR:HB	42:Lh:91:MET:HG3	2.03	0.41
50:L5:461:G:H2'	50:L5:462:G:C8	2.57	0.41
1:CA:242:ASP:OD1	4:CD:343:ARG:NH1	2.54	0.40
4:CD:181:LYS:HE2	4:CD:181:LYS:HB2	1.82	0.40
4:CD:399:ARG:NH2	50:L5:4598:C:OP1	2.54	0.40
13:LA:103:PRO:HB2	13:LA:106:THR:HG22	2.03	0.40
33:LX:55:ARG:HD2	33:LX:55:ARG:HA	1.90	0.40
50:L5:4239:A:H2'	50:L5:4240:G:C8	2.55	0.40
50:L5:4318:C:H2'	50:L5:4319:C:C6	2.56	0.40
50:L5:4896:G:H2'	50:L5:4897:G:H8	1.86	0.40
2:CB:219:VAL:O	2:CB:313:VAL:HA	2.22	0.40
5:CE:18:ARG:HH21	14:LB:352:LEU:HD13	1.86	0.40
13:LA:33:ASP:OD2	13:LA:34:PHE:N	2.47	0.40
19:LG:173:LEU:HB2	43:Li:43:MET:HE1	2.03	0.40
21:LJ:92:TYR:HB3	21:LJ:172:GLY:HA2	2.04	0.40
25:LO:99:LEU:HD23	25:LO:99:LEU:HA	1.97	0.40
31:LU:97:ARG:NH1	31:LU:100:LEU:O	2.54	0.40
49:Lt:63:THR:HB	49:Lt:65:GLN:HE22	1.86	0.40
50:L5:460:C:H2'	50:L5:461:G:H8	1.86	0.40
50:L5:2045:G:O2'	50:L5:2046:G:H5''	2.22	0.40
50:L5:2411:C:H2'	50:L5:2412:A:H8	1.86	0.40
50:L5:2520:C:H2'	50:L5:2521:G:C8	2.56	0.40
2:CB:77:ASN:OD1	2:CB:78:ILE:N	2.54	0.40
7:CG:261:TYR:HD2	7:CG:271:VAL:HG22	1.87	0.40
12:L7:110:G:H2'	12:L7:111:C:C6	2.56	0.40
14:LB:315:ASN:HD21	14:LB:326:VAL:H	1.70	0.40
19:LG:232:GLU:H	19:LG:232:GLU:HG2	1.76	0.40
34:LY:101:PRO:HA	34:LY:104:VAL:HG22	2.04	0.40
50:L5:710:G:H2'	50:L5:711:A:C8	2.56	0.40
50:L5:1346:C:H2'	50:L5:1347:G:C8	2.57	0.40
50:L5:2491:C:H2'	50:L5:2492:C:C6	2.56	0.40
50:L5:3707:U:H2'	50:L5:3708:C:C6	2.56	0.40
50:L5:4309:G:H2'	50:L5:4310:A:C8	2.56	0.40
50:L5:4346:U:H2'	50:L5:4347:G:C8	2.56	0.40
50:L5:4643:G:H2'	50:L5:4644:G:C8	2.57	0.40
50:L5:4643:G:H2'	50:L5:4644:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:292:ASP:OD1	4:CD:292:ASP:N	2.51	0.40
6:CF:56:ILE:HG23	6:CF:65:MET:HE1	2.03	0.40
8:CH:41:LYS:HD2	8:CH:41:LYS:HA	1.77	0.40
11:CK:121:LYS:HD3	11:CK:121:LYS:HA	1.88	0.40
14:LB:372:SER:OG	50:L5:5001:U:O2'	2.38	0.40
15:LC:335:MET:HE2	15:LC:335:MET:HB3	1.83	0.40
16:LD:211:LEU:HD13	16:LD:219:TYR:HA	2.02	0.40
18:LF:56:HIS:NE2	18:LF:60:GLU:OE2	2.55	0.40
34:LY:112:ASP:H	34:LY:115:ARG:HB3	1.86	0.40
35:LZ:100:VAL:HG12	35:LZ:106:LEU:HB3	2.04	0.40
39:Le:89:LEU:HA	39:Le:120:ILE:HD11	2.02	0.40
50:L5:738:C:H5'	50:L5:739:G:H5''	2.03	0.40
50:L5:1928:C:H42	50:L5:2054:U:H1'	1.85	0.40
50:L5:1983:A:O2'	50:L5:2011:C:OP1	2.39	0.40
50:L5:2029:A:H2'	50:L5:2030:A:C8	2.56	0.40
2:CB:125:ILE:HG22	7:CG:372:GLN:HB3	2.04	0.40
5:CE:88:ASP:OD1	5:CE:92:GLN:N	2.38	0.40
7:CG:193:ARG:NH1	7:CG:235:ALA:O	2.53	0.40
9:CI:45:ASN:HD22	9:CI:48:LYS:HG3	1.86	0.40
34:LY:109:LEU:HD23	34:LY:115:ARG:HD2	2.03	0.40
41:Lg:33:LEU:HD23	41:Lg:33:LEU:HA	1.83	0.40
49:Lt:117:ARG:HA	49:Lt:117:ARG:HD2	1.90	0.40
50:L5:703:G:H2'	50:L5:704:C:H4'	2.04	0.40
50:L5:1560:A:H2'	50:L5:1561:G:C8	2.56	0.40
50:L5:1939:A:H2'	50:L5:1940:G:C8	2.56	0.40
50:L5:2489:C:O3'	50:L5:2491:C:N4	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CA	243/245 (99%)	228 (94%)	15 (6%)	0	100	100
2	CB	435/731 (60%)	428 (98%)	7 (2%)	0	100	100
3	CC	78/549 (14%)	76 (97%)	2 (3%)	0	100	100
4	CD	571/634 (90%)	564 (99%)	7 (1%)	0	100	100
5	CE	65/129 (50%)	63 (97%)	2 (3%)	0	100	100
6	CF	217/239 (91%)	208 (96%)	9 (4%)	0	100	100
7	CG	469/485 (97%)	451 (96%)	18 (4%)	0	100	100
8	CH	249/260 (96%)	242 (97%)	7 (3%)	0	100	100
9	CI	138/163 (85%)	136 (99%)	2 (1%)	0	100	100
10	CJ	272/306 (89%)	266 (98%)	6 (2%)	0	100	100
11	CK	193/365 (53%)	189 (98%)	4 (2%)	0	100	100
13	LA	157/257 (61%)	152 (97%)	5 (3%)	0	100	100
14	LB	379/403 (94%)	363 (96%)	15 (4%)	1 (0%)	36	67
15	LC	360/427 (84%)	347 (96%)	13 (4%)	0	100	100
16	LD	227/297 (76%)	219 (96%)	8 (4%)	0	100	100
17	LE	201/288 (70%)	191 (95%)	10 (5%)	0	100	100
18	LF	217/248 (88%)	210 (97%)	6 (3%)	1 (0%)	24	57
19	LG	212/266 (80%)	205 (97%)	7 (3%)	0	100	100
20	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
21	LJ	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
22	LL	191/211 (90%)	187 (98%)	4 (2%)	0	100	100
23	LM	133/215 (62%)	128 (96%)	5 (4%)	0	100	100
24	LN	179/204 (88%)	175 (98%)	4 (2%)	0	100	100
25	LO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
26	LP	153/184 (83%)	148 (97%)	5 (3%)	0	100	100
27	LQ	149/188 (79%)	144 (97%)	5 (3%)	0	100	100
28	LR	126/196 (64%)	122 (97%)	4 (3%)	0	100	100
29	LS	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
30	LT	125/160 (78%)	123 (98%)	2 (2%)	0	100	100
31	LU	100/128 (78%)	96 (96%)	3 (3%)	1 (1%)	12	41
32	LV	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
33	LX	117/156 (75%)	114 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	LY	130/145 (90%)	125 (96%)	5 (4%)	0	100	100
35	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
36	La	101/148 (68%)	96 (95%)	5 (5%)	0	100	100
37	Lc	93/115 (81%)	90 (97%)	3 (3%)	0	100	100
38	Ld	103/125 (82%)	103 (100%)	0	0	100	100
39	Le	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
40	Lf	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
41	Lg	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
42	Lh	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
43	Li	102/105 (97%)	99 (97%)	3 (3%)	0	100	100
44	Lj	75/97 (77%)	74 (99%)	1 (1%)	0	100	100
45	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
46	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
47	Lp	72/92 (78%)	71 (99%)	1 (1%)	0	100	100
48	Lr	121/137 (88%)	119 (98%)	2 (2%)	0	100	100
49	Lt	157/165 (95%)	155 (99%)	2 (1%)	0	100	100
All	All	8483/10694 (79%)	8244 (97%)	236 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	LU	67	LYS
14	LB	29	VAL
18	LF	197	VAL

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	CA	213/213 (100%)	213 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CB	394/654 (60%)	394 (100%)	0	100	100
3	CC	51/485 (10%)	51 (100%)	0	100	100
4	CD	500/574 (87%)	500 (100%)	0	100	100
5	CE	56/115 (49%)	56 (100%)	0	100	100
6	CF	195/214 (91%)	195 (100%)	0	100	100
7	CG	327/403 (81%)	327 (100%)	0	100	100
8	CH	217/228 (95%)	217 (100%)	0	100	100
9	CI	128/149 (86%)	128 (100%)	0	100	100
10	CJ	242/279 (87%)	242 (100%)	0	100	100
11	CK	156/300 (52%)	156 (100%)	0	100	100
13	LA	125/199 (63%)	125 (100%)	0	100	100
14	LB	329/349 (94%)	329 (100%)	0	100	100
15	LC	297/348 (85%)	297 (100%)	0	100	100
16	LD	194/250 (78%)	193 (100%)	1 (0%)	81	86
17	LE	184/252 (73%)	184 (100%)	0	100	100
18	LF	182/215 (85%)	182 (100%)	0	100	100
19	LG	179/223 (80%)	179 (100%)	0	100	100
20	LH	167/171 (98%)	167 (100%)	0	100	100
21	LJ	137/149 (92%)	137 (100%)	0	100	100
22	LL	161/177 (91%)	160 (99%)	1 (1%)	78	85
23	LM	113/161 (70%)	113 (100%)	0	100	100
24	LN	154/172 (90%)	154 (100%)	0	100	100
25	LO	171/174 (98%)	171 (100%)	0	100	100
26	LP	133/163 (82%)	133 (100%)	0	100	100
27	LQ	136/165 (82%)	136 (100%)	0	100	100
28	LR	120/175 (69%)	120 (100%)	0	100	100
29	LS	156/157 (99%)	156 (100%)	0	100	100
30	LT	100/140 (71%)	100 (100%)	0	100	100
31	LU	92/115 (80%)	90 (98%)	2 (2%)	45	71
32	LV	104/107 (97%)	104 (100%)	0	100	100
33	LX	107/133 (80%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	LY	122/135 (90%)	122 (100%)	0	100	100
35	LZ	117/118 (99%)	117 (100%)	0	100	100
36	La	87/121 (72%)	87 (100%)	0	100	100
37	Lc	72/97 (74%)	72 (100%)	0	100	100
38	Ld	92/110 (84%)	92 (100%)	0	100	100
39	Le	114/121 (94%)	114 (100%)	0	100	100
40	Lf	87/89 (98%)	87 (100%)	0	100	100
41	Lg	93/100 (93%)	93 (100%)	0	100	100
42	Lh	109/110 (99%)	109 (100%)	0	100	100
43	Li	85/89 (96%)	85 (100%)	0	100	100
44	Lj	65/80 (81%)	65 (100%)	0	100	100
45	Lk	64/65 (98%)	64 (100%)	0	100	100
46	Ll	47/48 (98%)	47 (100%)	0	100	100
47	Lp	51/75 (68%)	51 (100%)	0	100	100
48	Lr	106/121 (88%)	106 (100%)	0	100	100
49	Lt	127/137 (93%)	127 (100%)	0	100	100
All	All	7258/9225 (79%)	7254 (100%)	4 (0%)	87	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LD	111	ASN
22	LL	159	ASN
31	LU	38	ASN
31	LU	95	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	CA	68	HIS
2	CB	89	GLN
2	CB	93	GLN
2	CB	113	GLN
2	CB	129	ASN
2	CB	161	GLN

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Mol	Chain	Res	Type
4	CD	144	GLN
4	CD	146	GLN
4	CD	178	ASN
4	CD	274	ASN
4	CD	358	ASN
4	CD	437	ASN
4	CD	597	GLN
6	CF	70	ASN
6	CF	106	ASN
6	CF	155	GLN
7	CG	323	GLN
7	CG	376	ASN
8	CH	10	HIS
9	CI	76	ASN
9	CI	129	GLN
9	CI	130	ASN
10	CJ	75	GLN
11	CK	38	ASN
14	LB	208	ASN
15	LC	50	GLN
16	LD	225	GLN
18	LF	126	ASN
19	LG	112	GLN
19	LG	208	ASN
20	LH	98	HIS
20	LH	156	ASN
21	LJ	112	HIS
22	LL	19	GLN
22	LL	149	GLN
23	LM	20	HIS
23	LM	48	GLN
26	LP	21	ASN
26	LP	34	GLN
26	LP	116	HIS
26	LP	118	GLN
26	LP	133	HIS
28	LR	40	GLN
29	LS	77	ASN
29	LS	122	HIS
30	LT	98	HIS
31	LU	38	ASN
33	LX	57	GLN

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Mol	Chain	Res	Type
33	LX	73	HIS
33	LX	93	ASN
34	LY	127	GLN
37	Lc	51	ASN
38	Ld	28	ASN
40	Lf	21	GLN
42	Lh	107	GLN
44	Lj	76	HIS
45	Lk	58	GLN
46	Ll	17	GLN
48	Lr	36	ASN
49	Lt	97	ASN
49	Lt	118	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	L7	119/121 (98%)	17 (14%)	1 (0%)
50	L5	3090/5070 (60%)	736 (23%)	21 (0%)
51	L8	145/157 (92%)	18 (12%)	0
All	All	3354/5348 (62%)	771 (22%)	22 (0%)

All (771) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	L7	7	G
12	L7	22	A
12	L7	24	C
12	L7	38	U
12	L7	53	U
12	L7	54	A
12	L7	63	C
12	L7	64	G
12	L7	74	A
12	L7	75	G
12	L7	76	U
12	L7	84	U
12	L7	97	G
12	L7	100	A
12	L7	106	G
12	L7	110	G

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Mol	Chain	Res	Type
12	L7	120	U
50	L5	4	G
50	L5	17	A
50	L5	25	A
50	L5	30	C
50	L5	33	A
50	L5	48	G
50	L5	55	G
50	L5	56	A
50	L5	59	A
50	L5	64	A
50	L5	65	A
50	L5	66	A
50	L5	69	A
50	L5	72	C
50	L5	73	A
50	L5	74	G
50	L5	86	U
50	L5	92	C
50	L5	93	G
50	L5	95	G
50	L5	104	G
50	L5	108	A
50	L5	109	G
50	L5	110	C
50	L5	119	G
50	L5	120	A
50	L5	122	U
50	L5	128	C
50	L5	132	G
50	L5	135	G
50	L5	136	C
50	L5	144	G
50	L5	152	U
50	L5	157	U
50	L5	159	C
50	L5	165	A
50	L5	166	C
50	L5	183	C
50	L5	184	U
50	L5	185	C
50	L5	186	G

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Mol	Chain	Res	Type
50	L5	187	U
50	L5	188	G
50	L5	189	G
50	L5	200	U
50	L5	209	U
50	L5	217	C
50	L5	218	A
50	L5	219	G
50	L5	220	C
50	L5	233	U
50	L5	234	G
50	L5	235	A
50	L5	237	G
50	L5	255	C
50	L5	256	G
50	L5	258	G
50	L5	265	C
50	L5	266	C
50	L5	267	G
50	L5	280	G
50	L5	296	A
50	L5	297	U
50	L5	306	A
50	L5	315	G
50	L5	316	U
50	L5	322	C
50	L5	340	C
50	L5	349	A
50	L5	362	A
50	L5	363	A
50	L5	373	G
50	L5	387	G
50	L5	407	A
50	L5	409	G
50	L5	410	A
50	L5	412	G
50	L5	413	G
50	L5	432	U
50	L5	440	U
50	L5	449	C
50	L5	450	G
50	L5	452	A

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Mol	Chain	Res	Type
50	L5	453	G
50	L5	454	U
50	L5	465	G
50	L5	468	U
50	L5	479	G
50	L5	483	G
50	L5	484	U
50	L5	485	C
50	L5	486	C
50	L5	489	C
50	L5	494	U
50	L5	496	G
50	L5	497	G
50	L5	498	C
50	L5	509	A
50	L5	510	U
50	L5	511	C
50	L5	512	U
50	L5	513	U
50	L5	514	U
50	L5	515	C
50	L5	516	C
50	L5	518	G
50	L5	519	C
50	L5	643	C
50	L5	644	G
50	L5	646	G
50	L5	659	G
50	L5	660	A
50	L5	665	C
50	L5	666	G
50	L5	667	A
50	L5	668	C
50	L5	669	C
50	L5	670	G
50	L5	673	C
50	L5	674	G
50	L5	686	A
50	L5	688	U
50	L5	694	C
50	L5	696	C
50	L5	697	G

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Mol	Chain	Res	Type
50	L5	702	U
50	L5	703	G
50	L5	704	C
50	L5	731	G
50	L5	738	C
50	L5	739	G
50	L5	742	G
50	L5	744	G
50	L5	754	U
50	L5	758	G
50	L5	759	G
50	L5	912	G
50	L5	913	U
50	L5	914	U
50	L5	915	A
50	L5	917	A
50	L5	925	C
50	L5	926	G
50	L5	932	A
50	L5	933	G
50	L5	935	A
50	L5	943	A
50	L5	944	A
50	L5	945	U
50	L5	946	C
50	L5	956	A
50	L5	959	G
50	L5	960	A
50	L5	961	G
50	L5	983	C
50	L5	984	C
50	L5	985	C
50	L5	989	U
50	L5	990	C
50	L5	992	C
50	L5	993	G
50	L5	995	C
50	L5	1048	G
50	L5	1049	C
50	L5	1050	C
50	L5	1051	G
50	L5	1070	G

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Mol	Chain	Res	Type
50	L5	1072	C
50	L5	1075	G
50	L5	1083	U
50	L5	1217	G
50	L5	1235	G
50	L5	1240	G
50	L5	1241	C
50	L5	1242	G
50	L5	1246	G
50	L5	1265	G
50	L5	1266	G
50	L5	1267	C
50	L5	1269	G
50	L5	1274	A
50	L5	1275	G
50	L5	1277	G
50	L5	1280	C
50	L5	1284	G
50	L5	1287	G
50	L5	1293	G
50	L5	1295	C
50	L5	1301	C
50	L5	1304	C
50	L5	1313	C
50	L5	1314	C
50	L5	1315	C
50	L5	1354	A
50	L5	1359	G
50	L5	1377	G
50	L5	1378	C
50	L5	1379	C
50	L5	1381	U
50	L5	1387	A
50	L5	1394	G
50	L5	1397	A
50	L5	1398	A
50	L5	1399	G
50	L5	1400	G
50	L5	1403	G
50	L5	1405	C
50	L5	1408	G
50	L5	1410	U

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Mol	Chain	Res	Type
50	L5	1411	C
50	L5	1414	C
50	L5	1420	A
50	L5	1421	G
50	L5	1435	G
50	L5	1437	C
50	L5	1447	C
50	L5	1457	G
50	L5	1472	C
50	L5	1490	G
50	L5	1495	G
50	L5	1497	A
50	L5	1498	G
50	L5	1502	G
50	L5	1517	G
50	L5	1524	A
50	L5	1525	A
50	L5	1534	A
50	L5	1535	C
50	L5	1546	C
50	L5	1547	A
50	L5	1549	G
50	L5	1550	G
50	L5	1553	A
50	L5	1563	A
50	L5	1566	C
50	L5	1571	G
50	L5	1577	G
50	L5	1578	U
50	L5	1579	C
50	L5	1586	G
50	L5	1587	G
50	L5	1588	U
50	L5	1609	U
50	L5	1611	C
50	L5	1623	A
50	L5	1654	G
50	L5	1661	C
50	L5	1670	G
50	L5	1671	U
50	L5	1672	U
50	L5	1684	A

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Mol	Chain	Res	Type
50	L5	1694	C
50	L5	1726	U
50	L5	1730	U
50	L5	1733	G
50	L5	1734	G
50	L5	1735	U
50	L5	1741	G
50	L5	1742	A
50	L5	1782	U
50	L5	1783	C
50	L5	1786	A
50	L5	1787	A
50	L5	1788	A
50	L5	1789	C
50	L5	1794	A
50	L5	1795	A
50	L5	1796	U
50	L5	1797	G
50	L5	1798	G
50	L5	1799	G
50	L5	1803	G
50	L5	1804	A
50	L5	1806	G
50	L5	1810	G
50	L5	1829	G
50	L5	1832	C
50	L5	1836	G
50	L5	1837	A
50	L5	1842	G
50	L5	1843	A
50	L5	1865	G
50	L5	1869	G
50	L5	1870	C
50	L5	1872	G
50	L5	1874	A
50	L5	1881	C
50	L5	1882	U
50	L5	1891	A
50	L5	1897	A
50	L5	1917	A
50	L5	1918	U
50	L5	1919	G

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Mol	Chain	Res	Type
50	L5	1920	C
50	L5	1921	C
50	L5	1922	G
50	L5	1925	G
50	L5	1931	C
50	L5	1939	A
50	L5	1940	G
50	L5	1941	A
50	L5	1943	A
50	L5	1944	A
50	L5	1949	U
50	L5	1961	G
50	L5	1971	C
50	L5	1974	U
50	L5	1975	G
50	L5	1978	C
50	L5	1981	G
50	L5	1982	G
50	L5	1983	A
50	L5	1984	A
50	L5	1989	G
50	L5	1997	U
50	L5	2001	G
50	L5	2002	A
50	L5	2004	U
50	L5	2005	G
50	L5	2011	C
50	L5	2026	A
50	L5	2039	G
50	L5	2040	A
50	L5	2041	A
50	L5	2042	A
50	L5	2044	U
50	L5	2046	G
50	L5	2048	U
50	L5	2055	G
50	L5	2056	G
50	L5	2069	A
50	L5	2071	A
50	L5	2084	C
50	L5	2085	G
50	L5	2089	G

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Mol	Chain	Res	Type
50	L5	2090	U
50	L5	2091	C
50	L5	2268	A
50	L5	2289	C
50	L5	2300	A
50	L5	2301	G
50	L5	2306	G
50	L5	2313	A
50	L5	2314	G
50	L5	2316	G
50	L5	2332	A
50	L5	2333	G
50	L5	2344	U
50	L5	2345	G
50	L5	2348	G
50	L5	2351	C
50	L5	2395	A
50	L5	2396	A
50	L5	2397	G
50	L5	2412	A
50	L5	2416	G
50	L5	2421	G
50	L5	2425	U
50	L5	2428	A
50	L5	2437	C
50	L5	2438	A
50	L5	2448	G
50	L5	2469	C
50	L5	2470	C
50	L5	2471	G
50	L5	2474	G
50	L5	2475	G
50	L5	2478	C
50	L5	2483	G
50	L5	2484	A
50	L5	2485	U
50	L5	2486	G
50	L5	2487	G
50	L5	2490	U
50	L5	2511	A
50	L5	2513	A
50	L5	2517	A

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Mol	Chain	Res	Type
50	L5	2518	G
50	L5	2519	U
50	L5	2520	C
50	L5	2529	A
50	L5	2537	A
50	L5	2550	G
50	L5	2555	G
50	L5	2556	G
50	L5	2559	G
50	L5	2560	C
50	L5	2563	C
50	L5	2573	A
50	L5	2583	C
50	L5	2587	A
50	L5	2588	C
50	L5	2589	C
50	L5	2601	A
50	L5	2602	G
50	L5	2603	C
50	L5	2607	C
50	L5	2608	G
50	L5	2618	G
50	L5	2627	C
50	L5	2645	G
50	L5	2646	C
50	L5	2647	A
50	L5	2648	G
50	L5	2653	C
50	L5	2658	G
50	L5	2659	A
50	L5	2661	U
50	L5	2662	G
50	L5	2673	G
50	L5	2675	G
50	L5	2676	A
50	L5	2687	U
50	L5	2694	G
50	L5	2695	A
50	L5	2696	A
50	L5	2703	G
50	L5	2711	G
50	L5	2719	C

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Mol	Chain	Res	Type
50	L5	2721	G
50	L5	2724	G
50	L5	2726	G
50	L5	2730	U
50	L5	2731	C
50	L5	2734	U
50	L5	2735	G
50	L5	2738	C
50	L5	2739	C
50	L5	2742	G
50	L5	2743	A
50	L5	2744	A
50	L5	2746	A
50	L5	2748	C
50	L5	2749	C
50	L5	2755	A
50	L5	2758	G
50	L5	2769	U
50	L5	2770	C
50	L5	2787	A
50	L5	2788	U
50	L5	2790	U
50	L5	2794	C
50	L5	2801	U
50	L5	2806	A
50	L5	2814	C
50	L5	2815	A
50	L5	2825	A
50	L5	2835	A
50	L5	2840	A
50	L5	2848	G
50	L5	2855	G
50	L5	3630	A
50	L5	3662	A
50	L5	3664	G
50	L5	3667	C
50	L5	3678	G
50	L5	3691	G
50	L5	3701	C
50	L5	3702	A
50	L5	3706	C
50	L5	3710	G

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Mol	Chain	Res	Type
50	L5	3714	G
50	L5	3727	A
50	L5	3735	G
50	L5	3743	G
50	L5	3746	A
50	L5	3748	A
50	L5	3751	G
50	L5	3752	C
50	L5	3753	G
50	L5	3754	G
50	L5	3756	A
50	L5	3757	G
50	L5	3758	U
50	L5	3759	A
50	L5	3765	G
50	L5	3771	C
50	L5	3838	U
50	L5	3839	G
50	L5	3840	U
50	L5	3843	C
50	L5	3865	A
50	L5	3867	A
50	L5	3873	G
50	L5	3875	G
50	L5	3877	A
50	L5	3878	C
50	L5	3879	G
50	L5	3880	G
50	L5	3887	C
50	L5	3892	U
50	L5	3916	G
50	L5	3917	A
50	L5	3918	G
50	L5	3922	G
50	L5	3923	A
50	L5	3931	C
50	L5	3936	A
50	L5	3937	C
50	L5	3938	G
50	L5	3939	G
50	L5	3941	G
50	L5	3942	A

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Mol	Chain	Res	Type
50	L5	3943	A
50	L5	3944	G
50	L5	3946	G
50	L5	3947	A
50	L5	3952	A
50	L5	4062	A
50	L5	4066	U
50	L5	4073	A
50	L5	4074	C
50	L5	4077	A
50	L5	4078	C
50	L5	4080	C
50	L5	4081	G
50	L5	4084	G
50	L5	4088	C
50	L5	4092	G
50	L5	4093	G
50	L5	4096	C
50	L5	4097	G
50	L5	4099	G
50	L5	4101	C
50	L5	4102	C
50	L5	4104	G
50	L5	4108	G
50	L5	4109	G
50	L5	4111	U
50	L5	4112	C
50	L5	4113	U
50	L5	4114	C
50	L5	4115	G
50	L5	4116	C
50	L5	4117	U
50	L5	4119	C
50	L5	4120	U
50	L5	4121	G
50	L5	4122	G
50	L5	4127	A
50	L5	4138	C
50	L5	4139	G
50	L5	4141	G
50	L5	4142	C
50	L5	4143	G

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Mol	Chain	Res	Type
50	L5	4144	C
50	L5	4149	C
50	L5	4150	G
50	L5	4158	C
50	L5	4167	G
50	L5	4168	G
50	L5	4169	G
50	L5	4170	A
50	L5	4179	G
50	L5	4183	G
50	L5	4184	G
50	L5	4200	G
50	L5	4203	A
50	L5	4228	G
50	L5	4229	U
50	L5	4231	C
50	L5	4232	U
50	L5	4233	A
50	L5	4238	G
50	L5	4243	C
50	L5	4251	A
50	L5	4252	C
50	L5	4253	A
50	L5	4254	G
50	L5	4256	A
50	L5	4265	U
50	L5	4268	A
50	L5	4272	G
50	L5	4273	A
50	L5	4274	A
50	L5	4275	G
50	L5	4278	C
50	L5	4279	A
50	L5	4282	A
50	L5	4290	U
50	L5	4291	G
50	L5	4293	U
50	L5	4294	C
50	L5	4298	A
50	L5	4304	A
50	L5	4305	G
50	L5	4306	U

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Mol	Chain	Res	Type
50	L5	4309	G
50	L5	4313	A
50	L5	4316	G
50	L5	4317	A
50	L5	4325	A
50	L5	4326	G
50	L5	4331	G
50	L5	4335	C
50	L5	4348	A
50	L5	4349	C
50	L5	4354	U
50	L5	4360	U
50	L5	4368	G
50	L5	4384	U
50	L5	4386	C
50	L5	4387	C
50	L5	4388	A
50	L5	4391	G
50	L5	4401	G
50	L5	4404	U
50	L5	4428	A
50	L5	4431	U
50	L5	4432	C
50	L5	4437	U
50	L5	4439	U
50	L5	4440	G
50	L5	4443	C
50	L5	4446	U
50	L5	4447	C
50	L5	4454	G
50	L5	4455	G
50	L5	4464	A
50	L5	4465	U
50	L5	4466	C
50	L5	4471	U
50	L5	4475	G
50	L5	4476	C
50	L5	4488	A
50	L5	4498	U
50	L5	4500	U
50	L5	4501	U
50	L5	4502	C

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Mol	Chain	Res	Type
50	L5	4503	A
50	L5	4512	U
50	L5	4513	A
50	L5	4524	G
50	L5	4528	G
50	L5	4538	G
50	L5	4545	G
50	L5	4547	C
50	L5	4548	A
50	L5	4560	C
50	L5	4561	C
50	L5	4567	G
50	L5	4569	U
50	L5	4589	A
50	L5	4590	A
50	L5	4598	C
50	L5	4599	A
50	L5	4600	G
50	L5	4608	G
50	L5	4617	G
50	L5	4634	U
50	L5	4635	A
50	L5	4636	U
50	L5	4652	G
50	L5	4657	U
50	L5	4658	G
50	L5	4670	C
50	L5	4672	A
50	L5	4678	G
50	L5	4684	A
50	L5	4687	A
50	L5	4692	A
50	L5	4693	C
50	L5	4694	G
50	L5	4695	C
50	L5	4699	U
50	L5	4703	U
50	L5	4708	A
50	L5	4709	U
50	L5	4719	G
50	L5	4730	C
50	L5	4731	G

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Mol	Chain	Res	Type
50	L5	4733	C
50	L5	4734	A
50	L5	4740	G
50	L5	4741	C
50	L5	4742	G
50	L5	4745	G
50	L5	4751	G
50	L5	4754	G
50	L5	4757	C
50	L5	4759	C
50	L5	4761	G
50	L5	4764	A
50	L5	4765	G
50	L5	4771	C
50	L5	4773	C
50	L5	4775	C
50	L5	4859	C
50	L5	4860	G
50	L5	4870	G
50	L5	4871	C
50	L5	4882	U
50	L5	4883	C
50	L5	4888	U
50	L5	4889	G
50	L5	4893	A
50	L5	4895	C
50	L5	4896	G
50	L5	4897	G
50	L5	4899	G
50	L5	4900	C
50	L5	4901	G
50	L5	4910	G
50	L5	4912	G
50	L5	4914	C
50	L5	4918	C
50	L5	4925	U
50	L5	4926	C
50	L5	4928	C
50	L5	4937	C
50	L5	4939	C
50	L5	4940	C
50	L5	4943	A

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Mol	Chain	Res	Type
50	L5	4949	G
50	L5	4951	G
50	L5	4955	A
50	L5	4960	G
50	L5	4961	G
50	L5	4962	C
50	L5	4964	C
50	L5	4976	U
50	L5	4985	U
50	L5	4988	U
50	L5	5014	A
50	L5	5020	G
50	L5	5029	C
50	L5	5031	G
50	L5	5034	A
50	L5	5040	U
50	L5	5041	G
50	L5	5050	C
50	L5	5054	C
50	L5	5055	G
50	L5	5061	A
50	L5	5062	G
50	L5	5063	G
51	L8	2	G
51	L8	25	G
51	L8	34	U
51	L8	35	C
51	L8	48	A
51	L8	52	A
51	L8	59	A
51	L8	62	A
51	L8	63	U
51	L8	75	G
51	L8	80	A
51	L8	94	G
51	L8	103	A
51	L8	105	C
51	L8	110	U
51	L8	114	G
51	L8	124	U
51	L8	150	C

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	L7	74	A
50	L5	406	C
50	L5	493	G
50	L5	514	U
50	L5	673	C
50	L5	914	U
50	L5	1082	C
50	L5	1399	G
50	L5	1534	A
50	L5	1585	C
50	L5	2313	A
50	L5	2554	U
50	L5	2675	G
50	L5	2738	C
50	L5	3946	G
50	L5	4065	G
50	L5	4087	G
50	L5	4143	G
50	L5	4183	G
50	L5	4334	U
50	L5	4597	U
50	L5	4913	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	GDP	CD	801	54	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
52	GTP	CB	1001	-	33,34,34	0.93	1 (3%)	50,54,54	1.55	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	GDP	CD	801	54	-	4/16/32/32	0/3/3/3
52	GTP	CB	1001	-	-	7/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CD	801	GDP	C5-C4	3.01	1.47	1.38
53	CD	801	GDP	C6-N1	-2.53	1.34	1.38
52	CB	1001	GTP	C2-N3	2.15	1.38	1.33
53	CD	801	GDP	C5-N7	-2.12	1.34	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	CD	801	GDP	C5-C4-N3	-5.94	118.93	128.39
52	CB	1001	GTP	C5-C4-N3	-4.93	120.54	128.39
53	CD	801	GDP	C2-N3-C4	4.93	120.80	112.30
52	CB	1001	GTP	C2-N3-C4	4.49	120.04	112.30
53	CD	801	GDP	N9-C4-N3	4.36	134.68	125.95
53	CD	801	GDP	C6-C5-N7	3.35	136.39	130.29
52	CB	1001	GTP	N9-C4-N3	3.17	132.29	125.95
52	CB	1001	GTP	C2-N1-C6	-2.94	119.78	125.11
52	CB	1001	GTP	N9-C8-N7	-2.61	108.56	113.40
53	CD	801	GDP	C4-C5-N7	-2.54	106.64	110.67
52	CB	1001	GTP	C5-C6-N1	2.49	119.60	113.25
52	CB	1001	GTP	C8-N7-C5	2.45	108.63	104.26
52	CB	1001	GTP	O6-C6-C5	-2.40	120.19	126.53
53	CD	801	GDP	O6-C6-C5	-2.09	121.01	126.53
52	CB	1001	GTP	C3'-C2'-C1'	2.09	105.42	101.46

There are no chirality outliers.

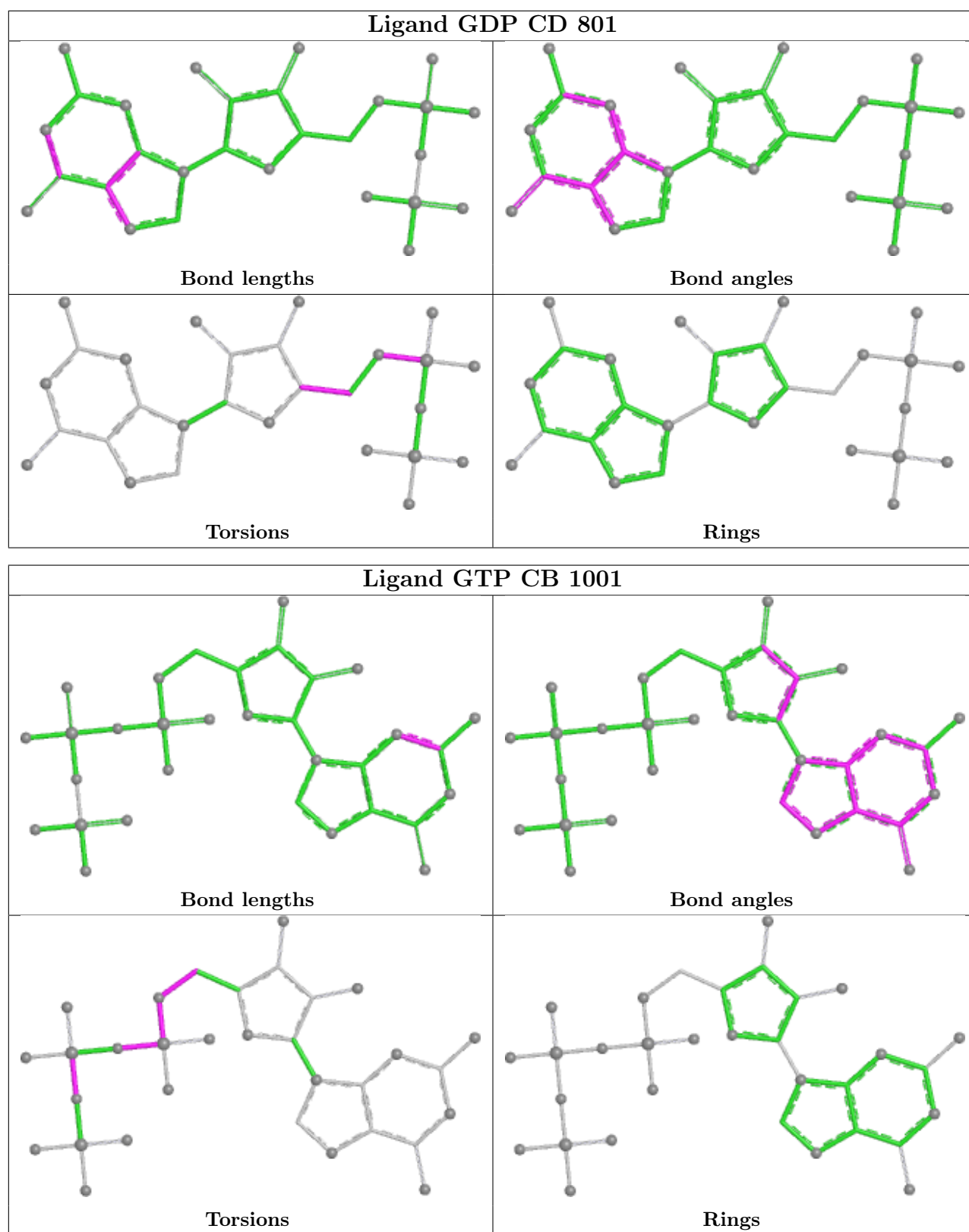
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	CB	1001	GTP	PB-O3A-PA-O5'
52	CB	1001	GTP	C5'-O5'-PA-O3A
52	CB	1001	GTP	C5'-O5'-PA-O1A
52	CB	1001	GTP	C5'-O5'-PA-O2A
53	CD	801	GDP	C5'-O5'-PA-O3A
53	CD	801	GDP	C5'-O5'-PA-O2A
53	CD	801	GDP	O4'-C4'-C5'-O5'
53	CD	801	GDP	C3'-C4'-C5'-O5'
52	CB	1001	GTP	PG-O3B-PB-O1B
52	CB	1001	GTP	C4'-C5'-O5'-PA
52	CB	1001	GTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

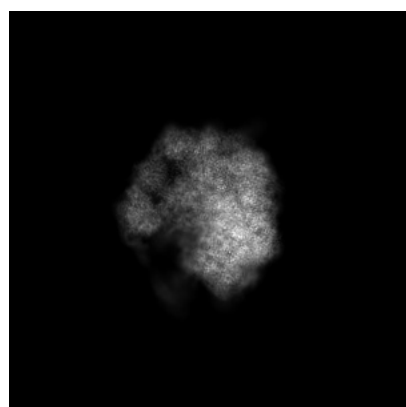
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53196. These allow visual inspection of the internal detail of the map and identification of artifacts.

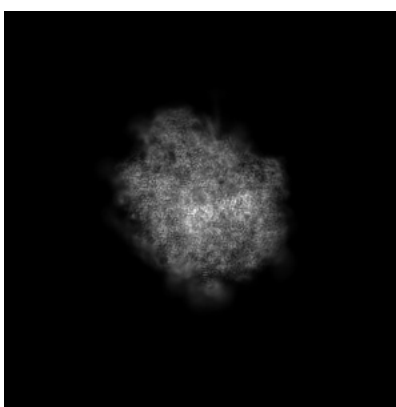
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

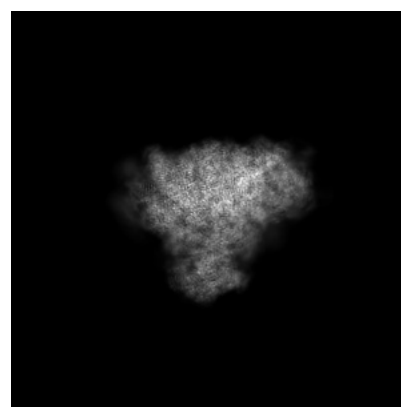
6.1.1 Primary map



X



Y

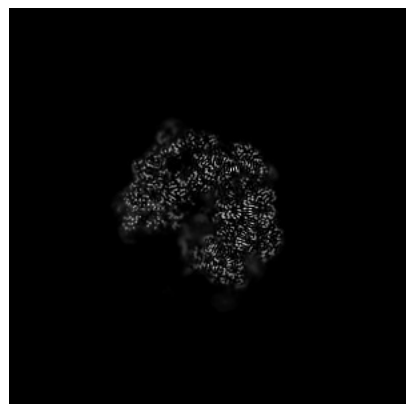


Z

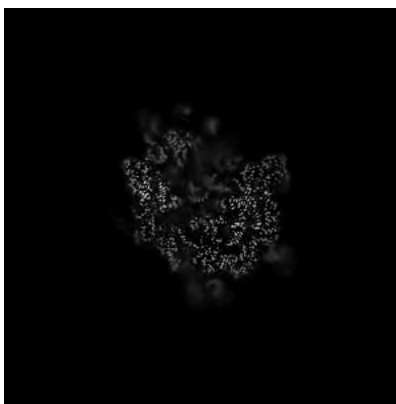
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

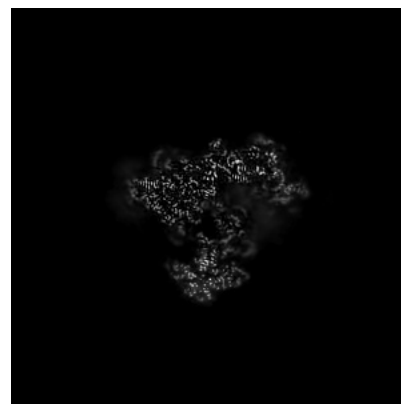
6.2.1 Primary map



X Index: 250



Y Index: 250

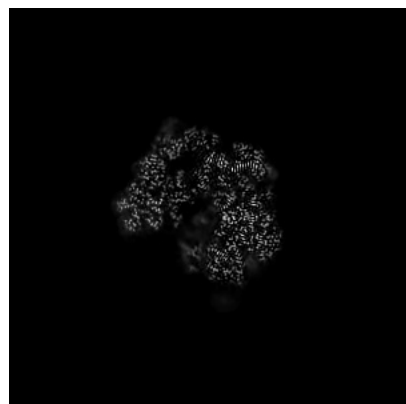


Z Index: 250

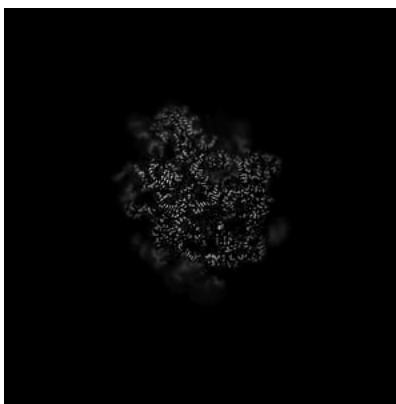
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

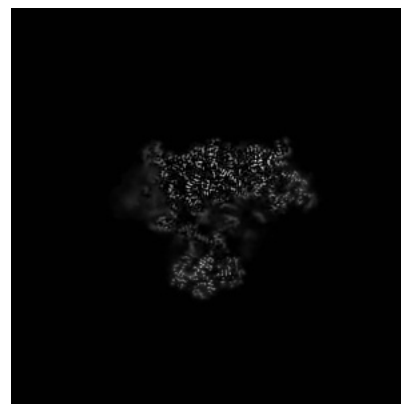
6.3.1 Primary map



X Index: 246



Y Index: 290

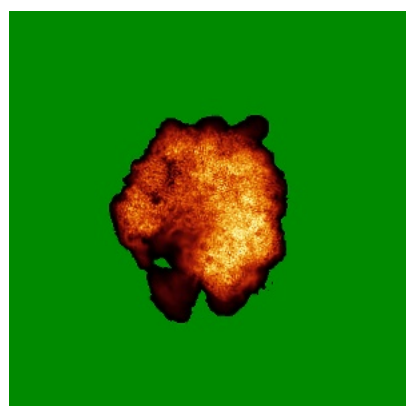


Z Index: 231

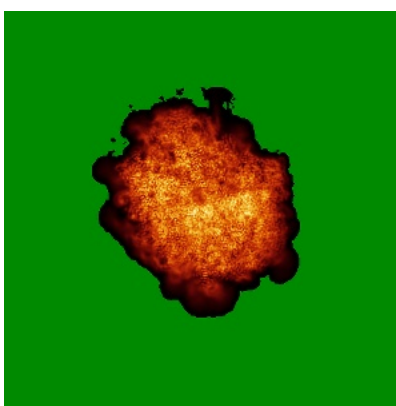
The images above show the largest variance slices of the map in three orthogonal directions.

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

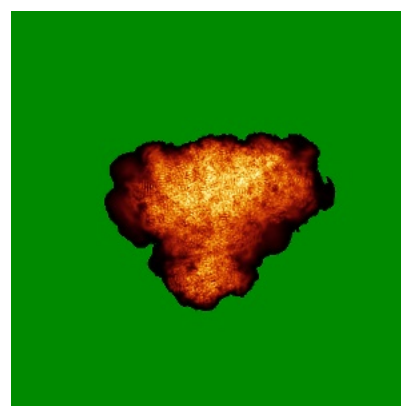
6.4.1 Primary map



X



Y

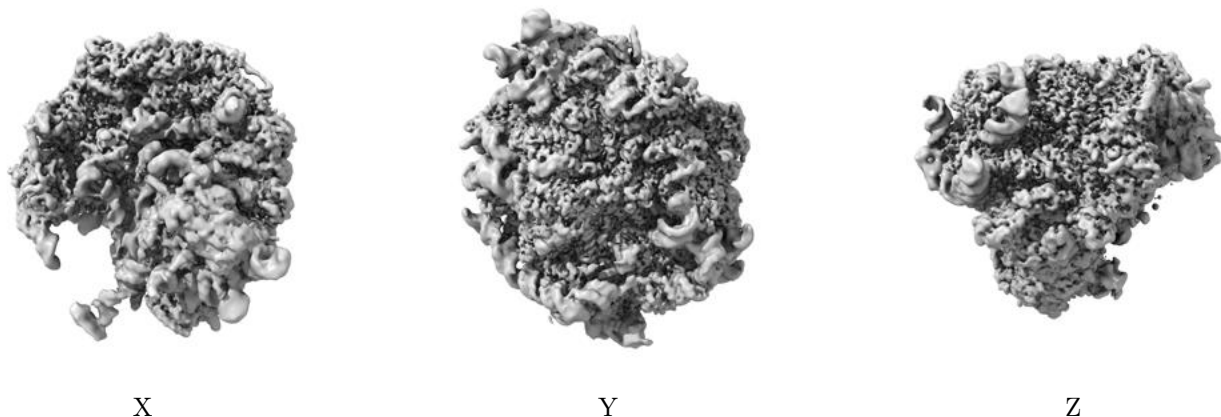


Z

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

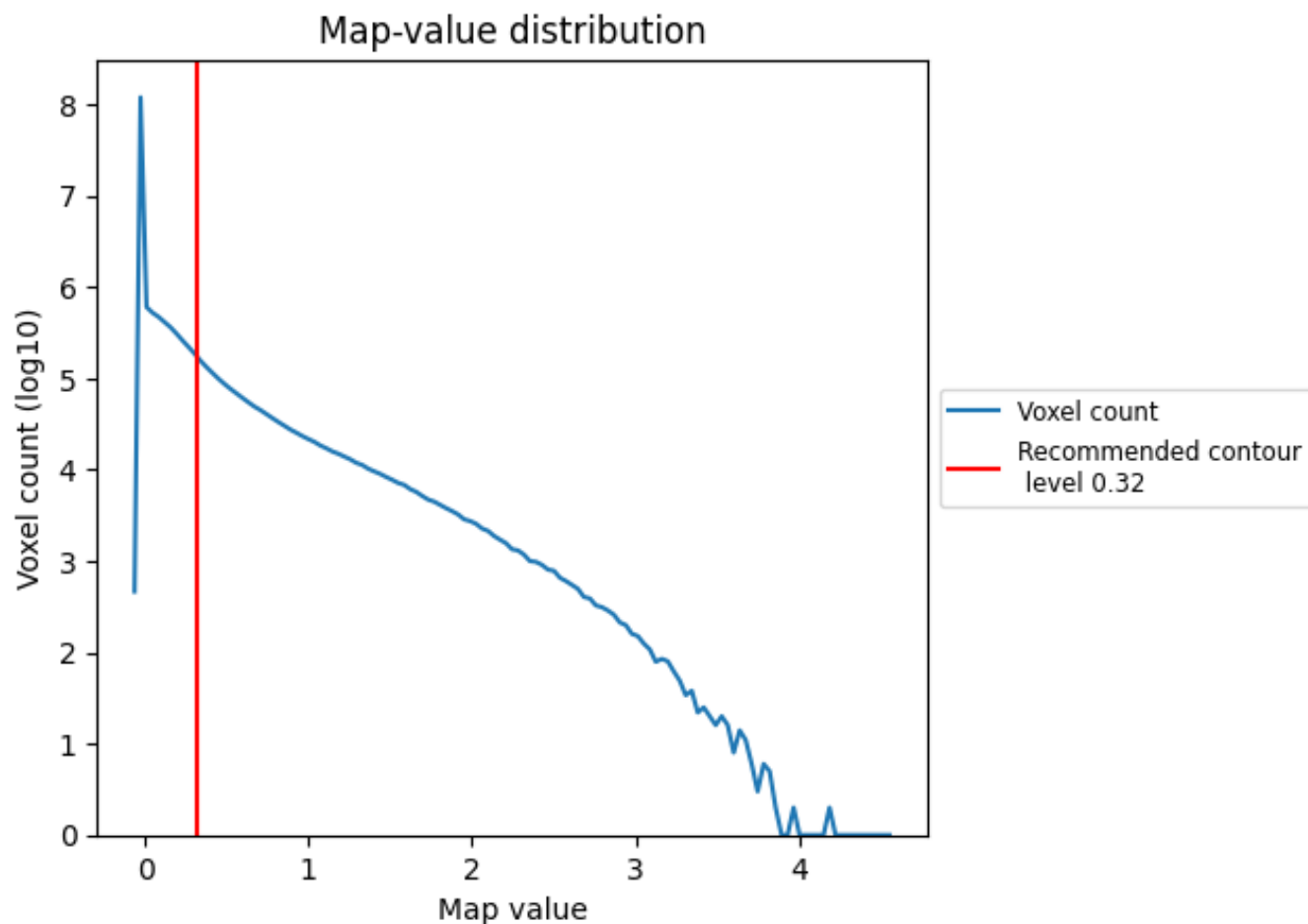
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

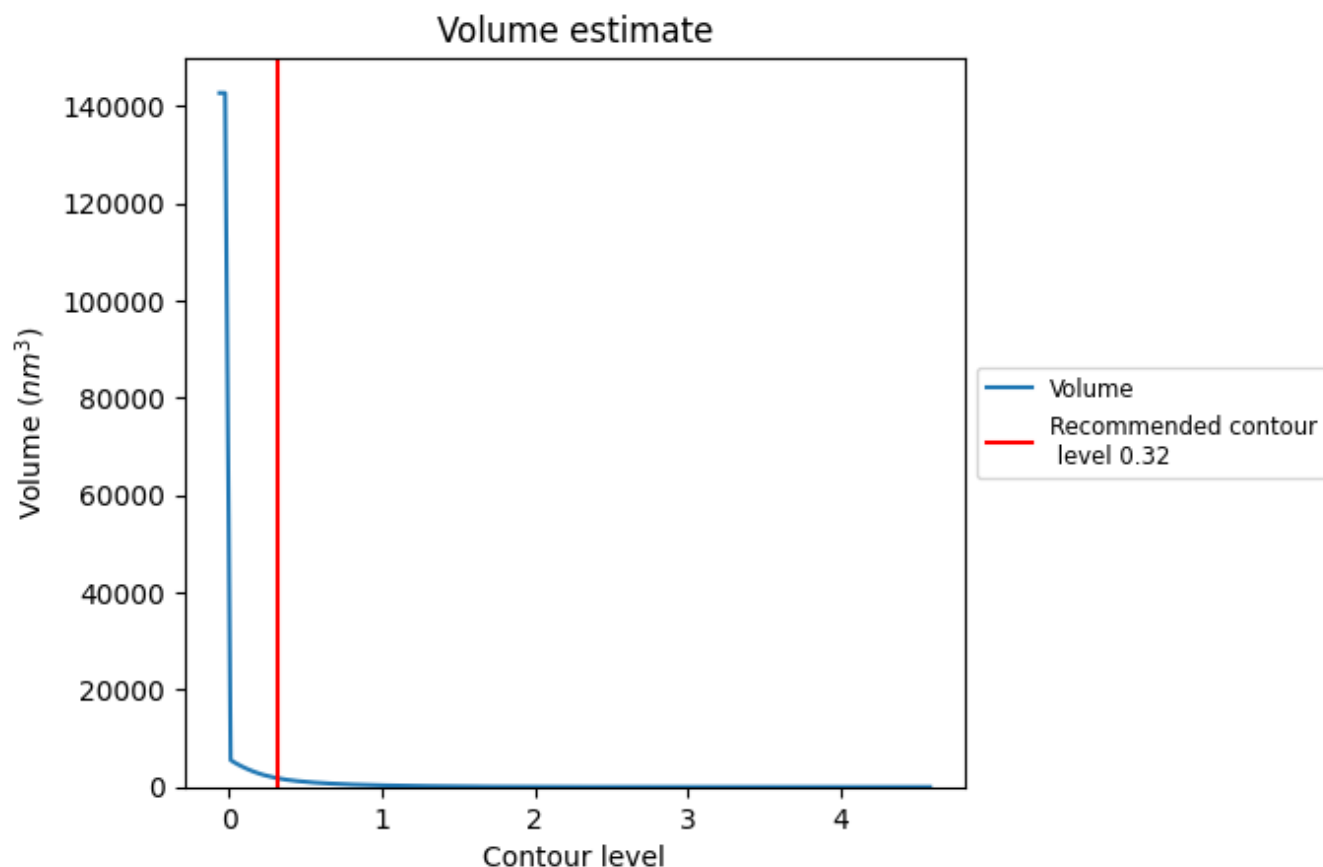
This section contains the results of statistical analysis of the map.

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.

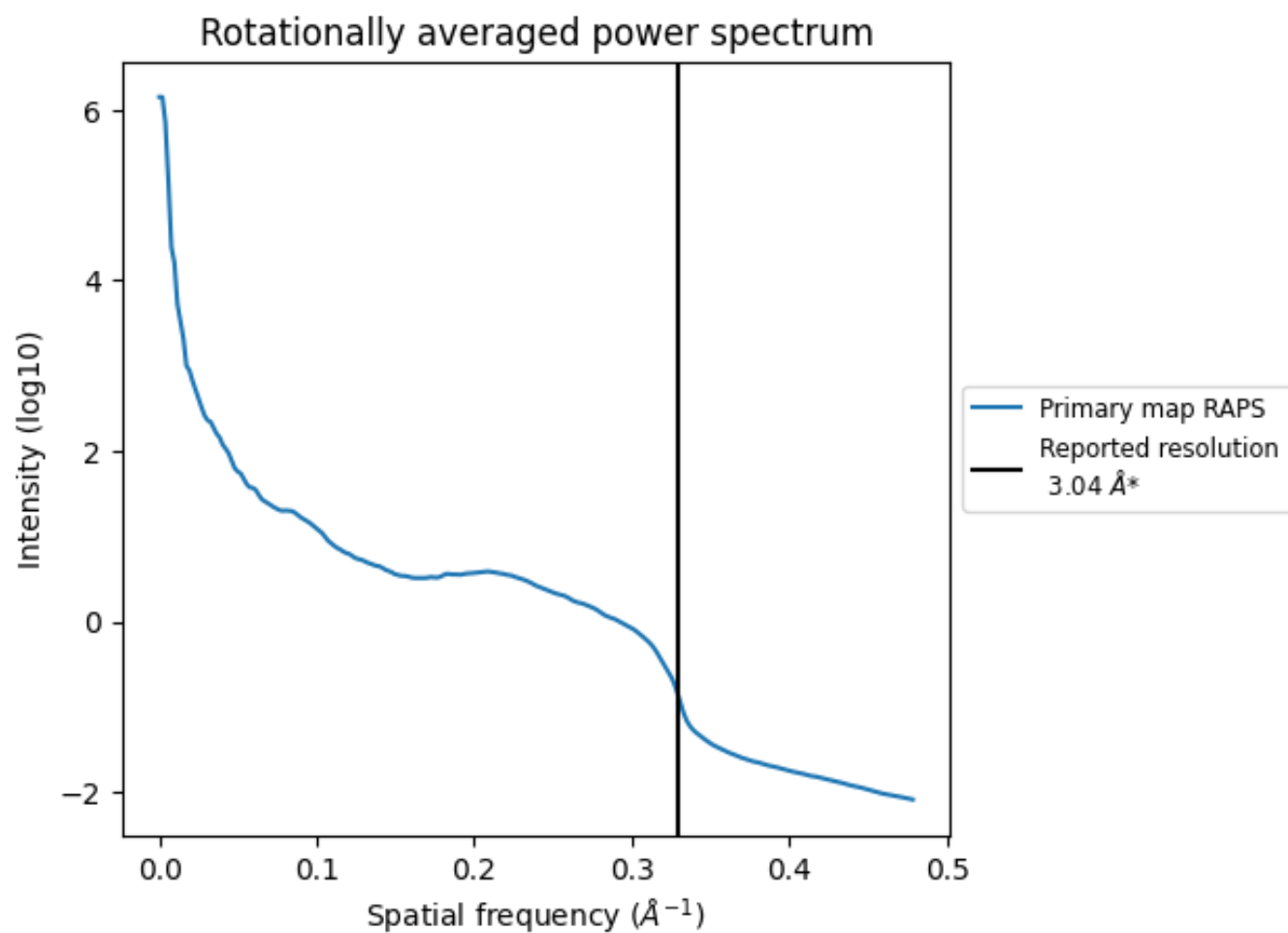
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1775 nm^3 ; this corresponds to an approximate mass of 1604 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 0.329 Å⁻¹

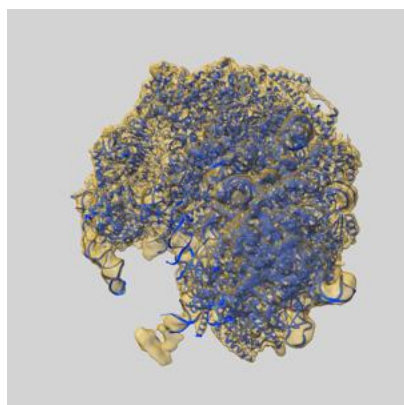
8 Fourier-Shell correlation

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

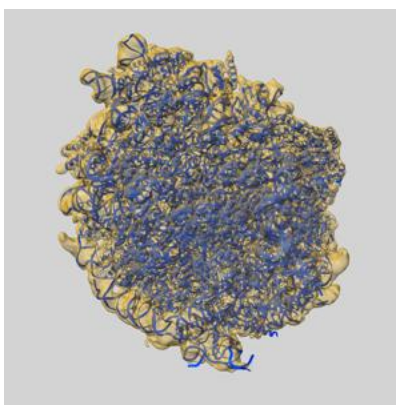
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53196 and PDB model 9QIW. Per-residue inclusion information can be found in section 3 on page 14.

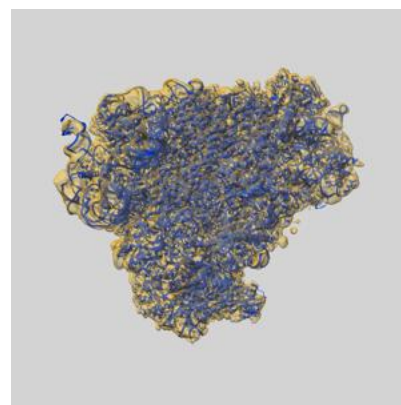
9.1 Map-model overlay [i](#)



X



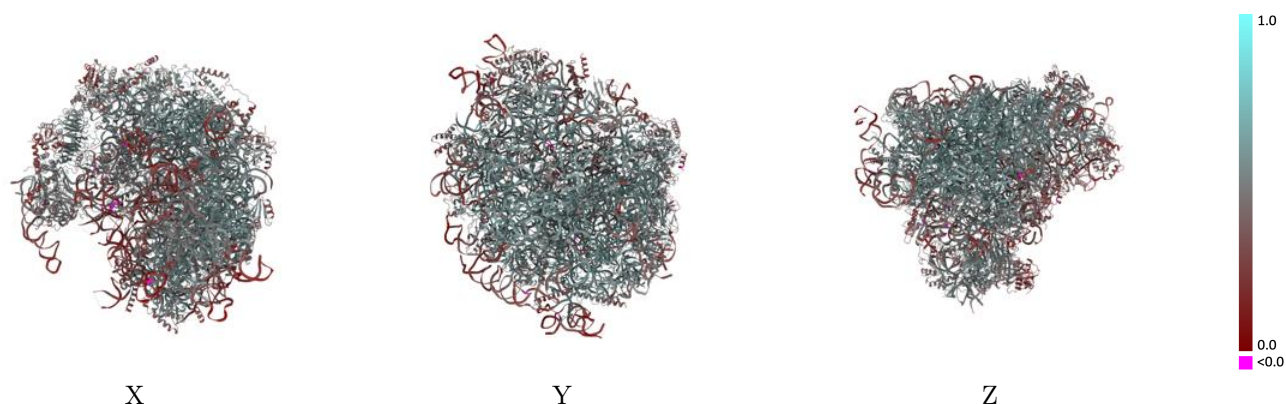
Y



Z

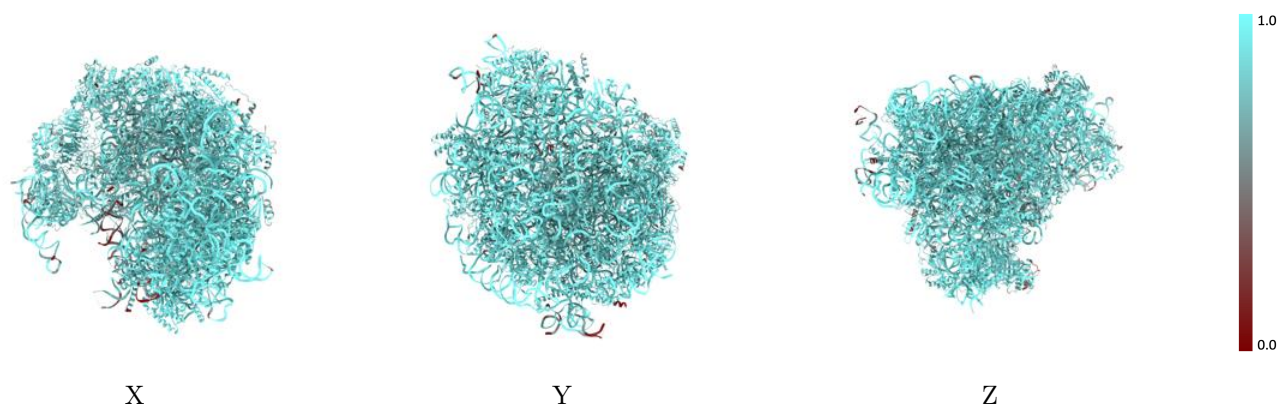
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



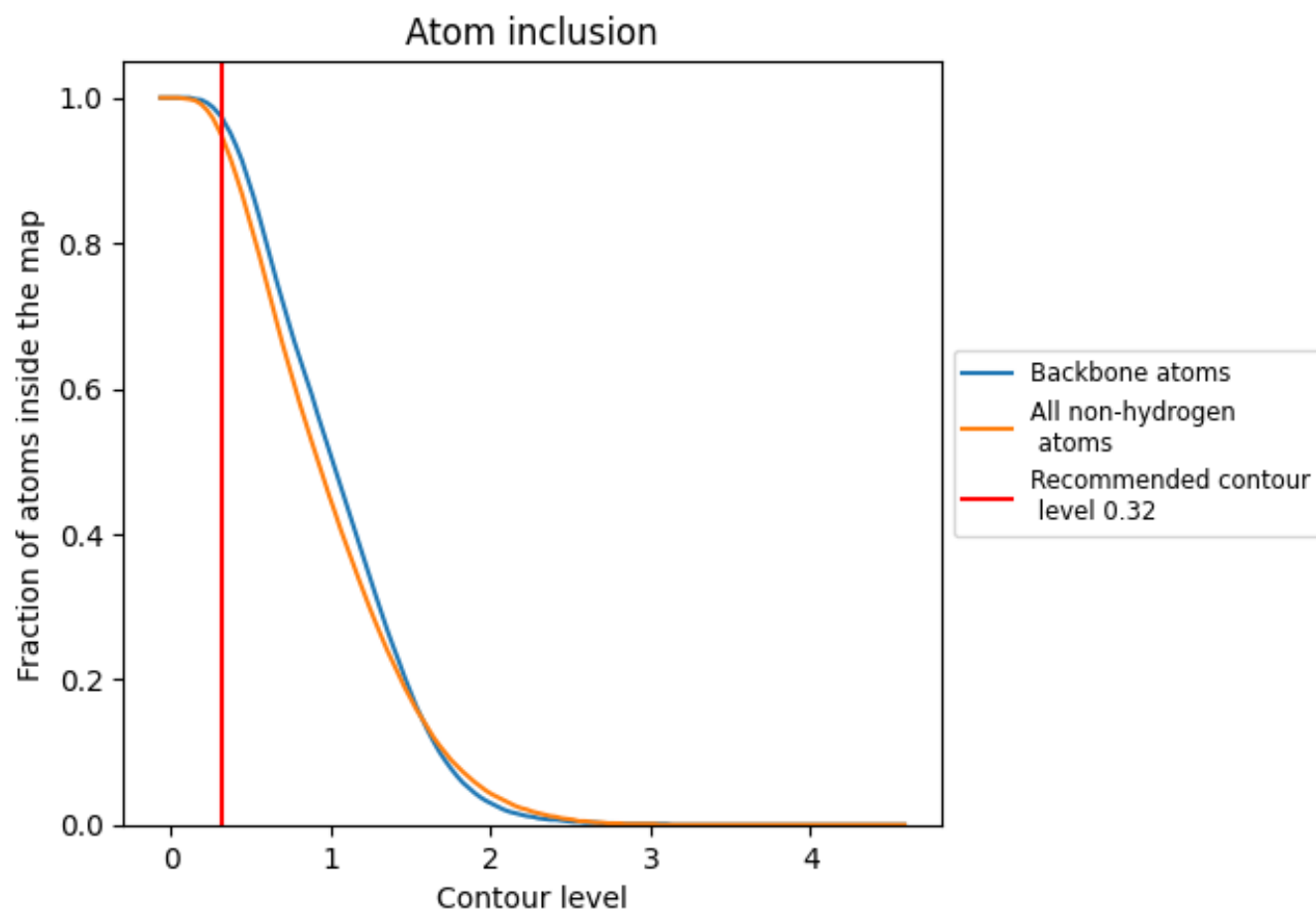
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.4820
CA	 0.9280	 0.4810
CB	 0.8420	 0.4000
CC	 0.7400	 0.4440
CD	 0.8970	 0.4710
CE	 0.8660	 0.4560
CF	 0.9070	 0.4400
CG	 0.9490	 0.4890
CH	 0.9460	 0.5440
CI	 0.9450	 0.4930
CJ	 0.9100	 0.4360
CK	 0.8100	 0.3580
L5	 0.9590	 0.4640
L7	 0.9500	 0.3950
L8	 0.9980	 0.5790
LA	 0.9370	 0.4770
LB	 0.9590	 0.5650
LC	 0.9600	 0.5640
LD	 0.9490	 0.4940
LE	 0.9530	 0.5180
LF	 0.9690	 0.5590
LG	 0.9540	 0.4860
LH	 0.9580	 0.5460
LJ	 0.9160	 0.4120
LL	 0.9340	 0.5010
LM	 0.9670	 0.5540
LN	 0.9970	 0.5960
LO	 0.9670	 0.5790
LP	 0.9520	 0.5770
LQ	 0.9620	 0.5510
LR	 0.9020	 0.4100
LS	 0.9650	 0.5660
LT	 0.8480	 0.3990
LU	 0.9360	 0.4510
LV	 0.9400	 0.5260



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Chain	Atom inclusion	Q-score
LX	 0.9660	 0.5460
LY	 0.9480	 0.5410
LZ	 0.9690	 0.4340
La	 0.9660	 0.5100
Lc	 0.9390	 0.3870
Ld	 0.9610	 0.5420
Le	 0.9690	 0.5760
Lf	 0.9890	 0.6180
Lg	 0.9680	 0.5280
Lh	 0.9560	 0.5220
Li	 0.9150	 0.4650
Lj	 0.9950	 0.5800
Lk	 0.8490	 0.4370
Ll	 0.9840	 0.5850
Lp	 0.8980	 0.3940
Lr	 0.9710	 0.5500
Lt	 0.8820	 0.3510