



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 11:33 am BST

PDB ID : 5JU8 / pdb_00005ju8
EMDB ID : EMD-8176
Title : Cryo-EM structure of an ErmBL-stalled ribosome in complex with P-, and E-tRNA
Authors : Arenz, S.; Bock, L.V.; Graf, M.; Innis, C.A.; Beckmann, R.; Grubmueller, H.; Vaiana, A.C.; Wilson, D.N.
Deposited on : 2016-05-10
Resolution : 3.60 Å (reported)
Based on initial model : 5AFI

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:

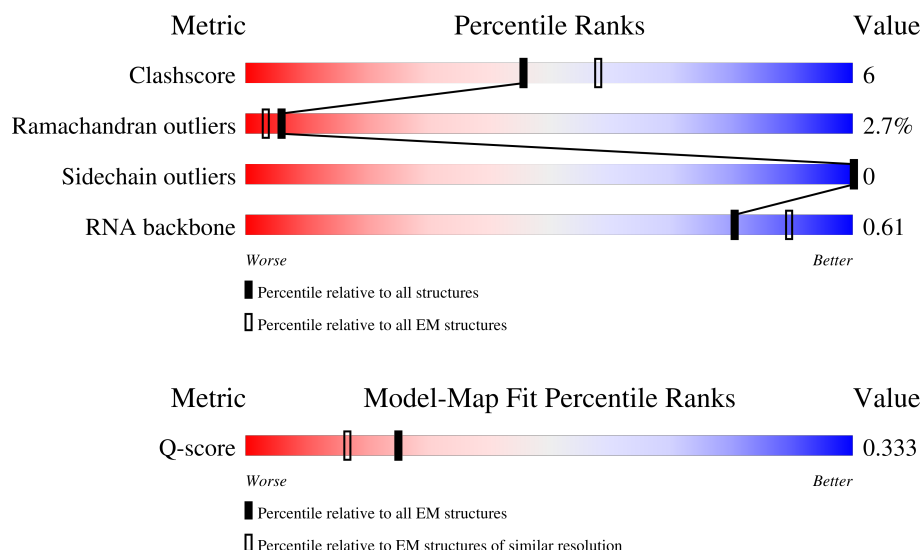
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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	12797 (3.10 - 4.10)

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	AA	1539	15% 54% 34% 10% •
2	AB	240	90% 66% 24% • 9%

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Mol	Chain	Length	Quality of chain
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	10	
23	AX	77	
24	AY	71	
25	BA	2903	
26	BB	120	
27	BC	273	

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Mol	Chain	Length	Quality of chain
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	
32	BH	149	
33	BI	142	
34	BJ	142	
35	BK	123	
36	BL	144	
37	BM	136	
38	BN	127	
39	BO	117	
40	BP	115	
41	BQ	118	
42	BR	103	
43	BS	110	
44	BT	100	
45	BU	104	
46	BV	94	
47	BW	85	
48	BX	78	
49	BY	63	
50	BZ	59	
51	B0	57	
52	B1	55	

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Mol	Chain	Length	Quality of chain
53	B2	46	17% 70% 30%
54	B3	65	32% 74% 25%
55	B4	38	24% 79% 21%
56	B5	9	67% 44% 56%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	36	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

- Molecule 23 is a RNA chain called P-site tRNA Aspartate.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AX	77	Total	C	N	O	P	S	0	0
			1656	741	290	547	77	1		

- Molecule 24 is a RNA chain called E-site tRNA Valine.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AY	71	Total	C	N	O	P	S	0	0
			1525	682	276	496	70	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	A	-	expression tag	GB 991970073

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BF	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BK	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	BO	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	BQ	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	BU	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

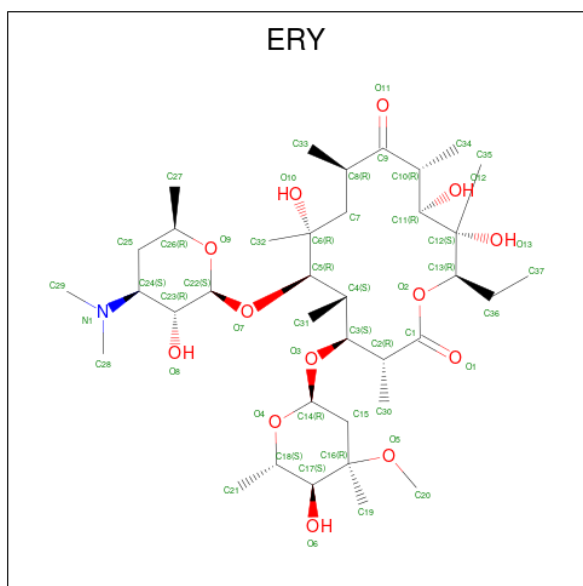
- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called ErmBL.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	9	Total	C	N	O	S	0	0
			74	46	14	13	1		

- Molecule 57 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$).

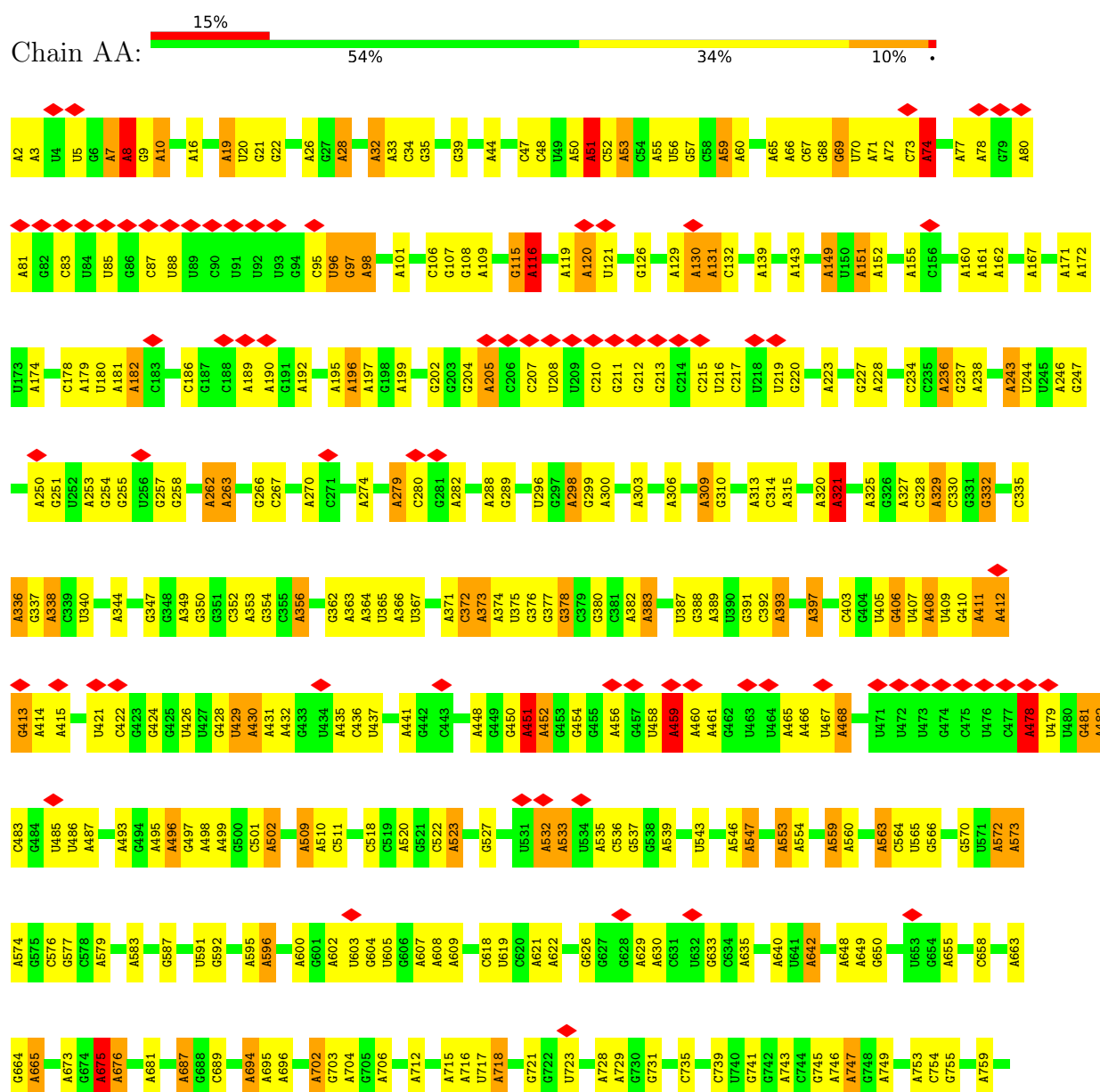


Mol	Chain	Residues	Atoms				AltConf
57	BA	1	Total	C	N	O	0
			51	37	1	13	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

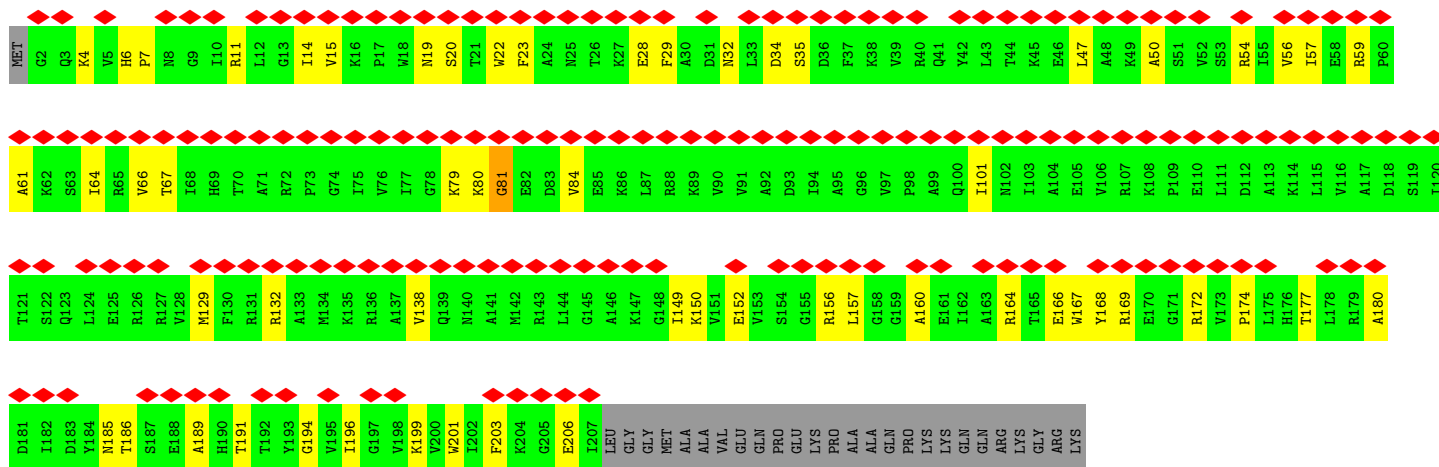
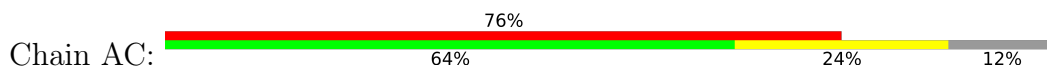
• Molecule 1: 16S ribosomal RNA



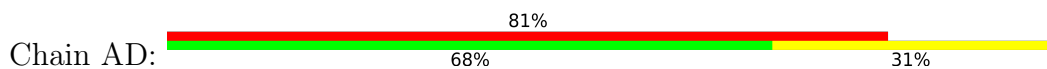




• Molecule 3: 30S ribosomal protein S3

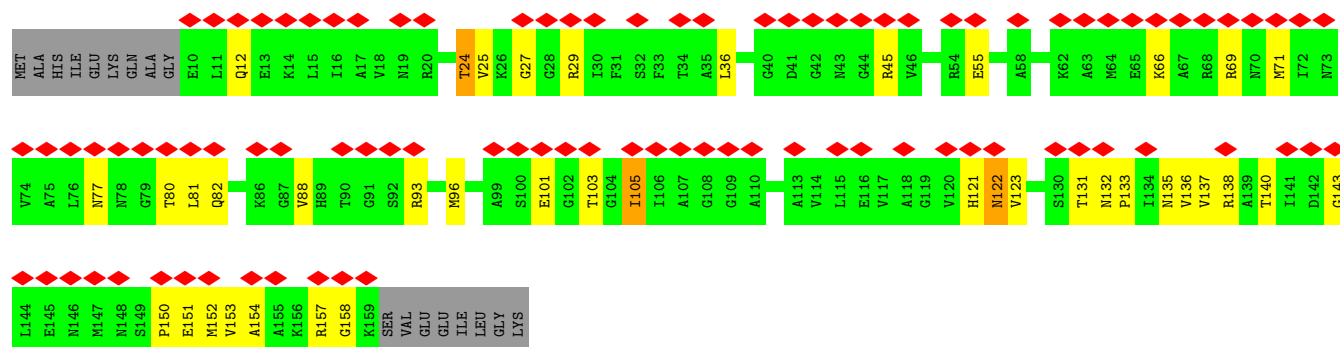


• Molecule 4: 30S ribosomal protein S4

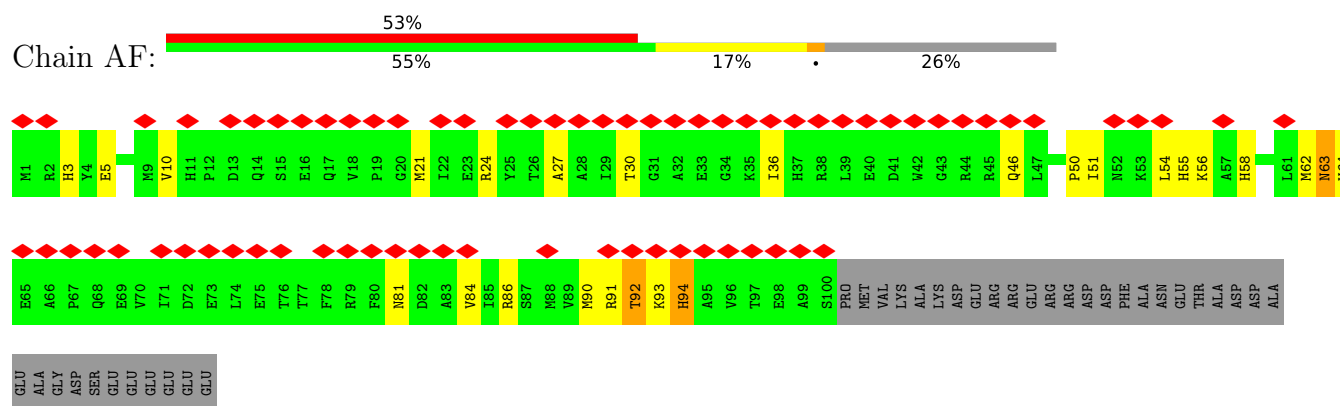


• Molecule 5: 30S ribosomal protein S5

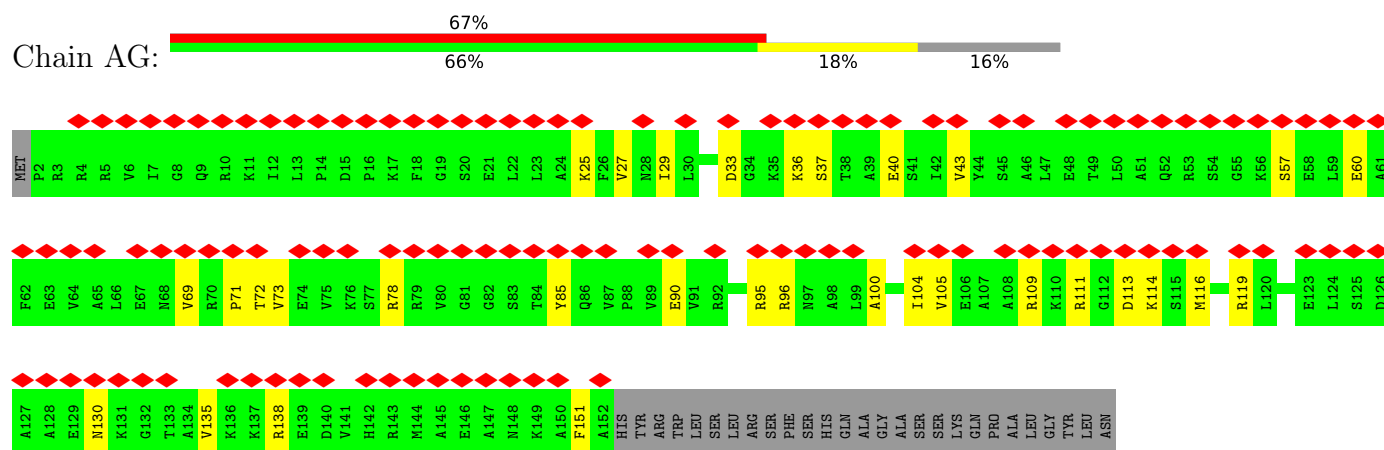




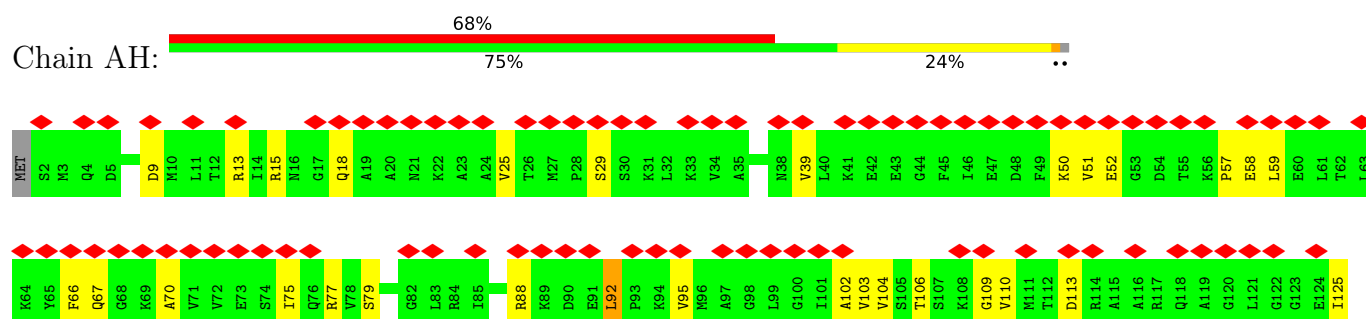
• Molecule 6: 30S ribosomal protein S6

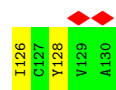


• Molecule 7: 30S ribosomal protein S7

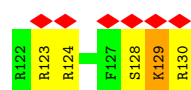
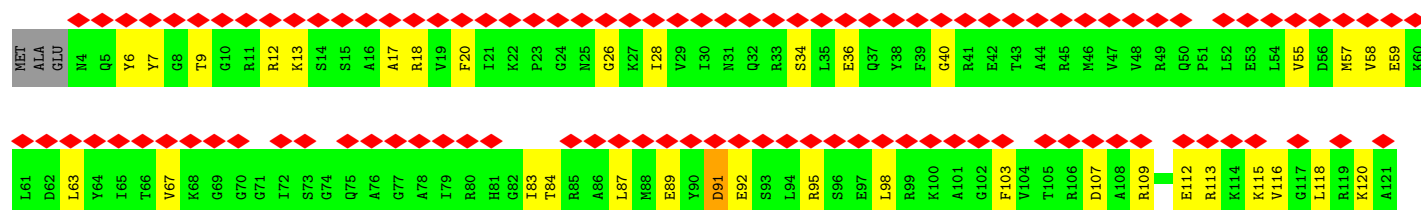
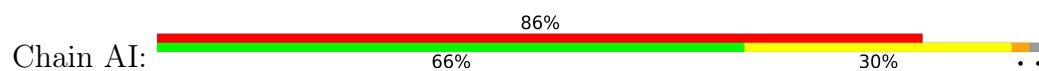


• Molecule 8: 30S ribosomal protein S8





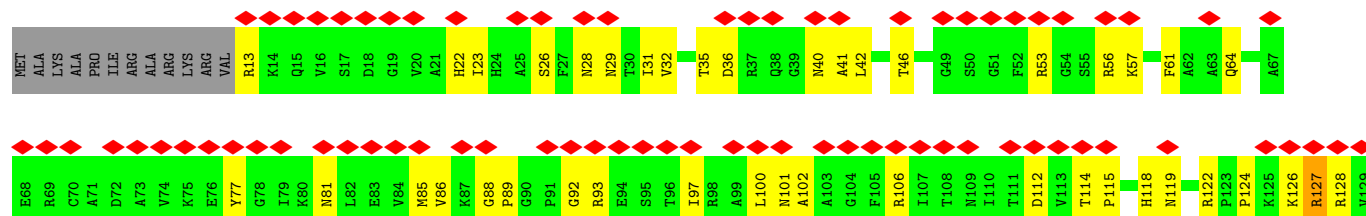
- Molecule 9: 30S ribosomal protein S9



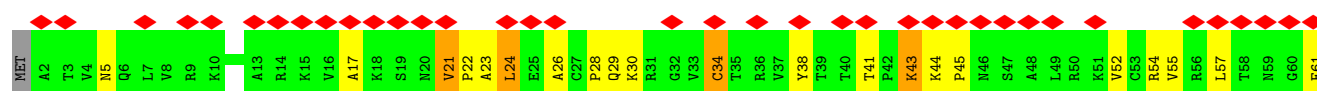
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

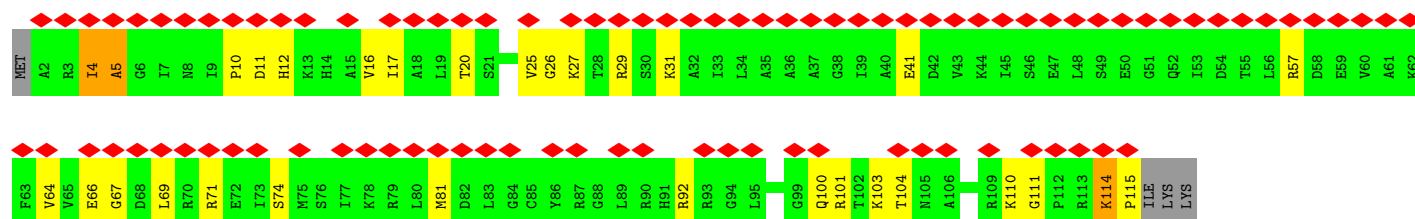
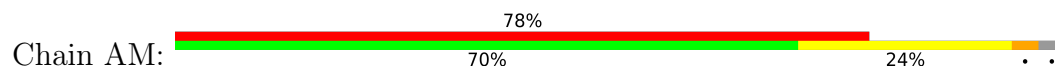


- Molecule 12: 30S ribosomal protein S12

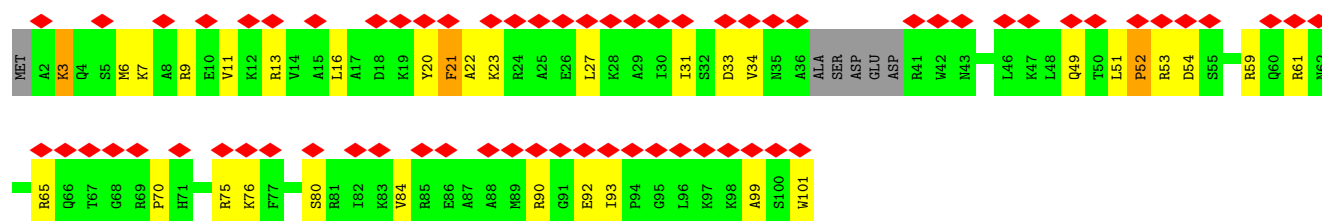




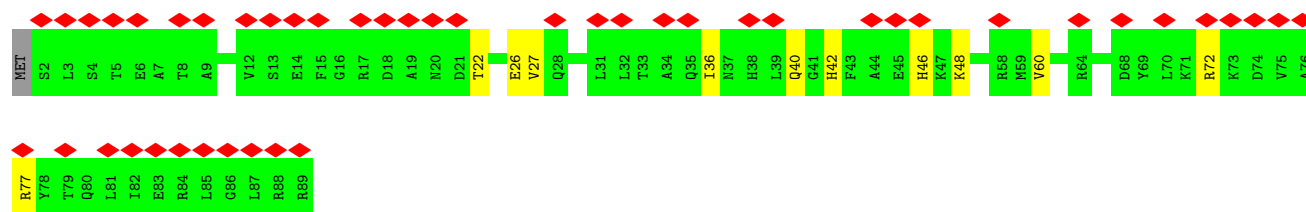
• Molecule 13: 30S ribosomal protein S13



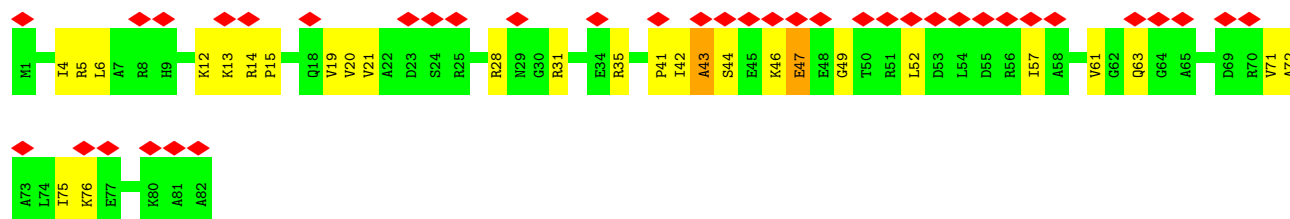
• Molecule 14: 30S ribosomal protein S14



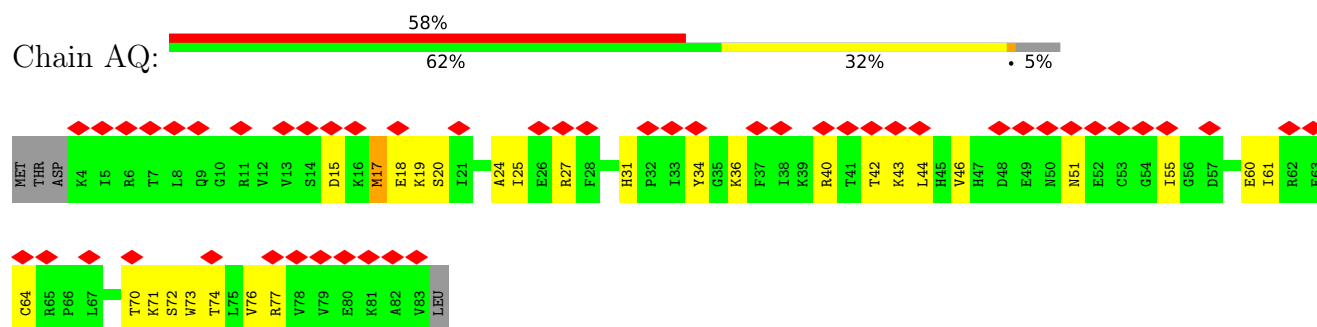
• Molecule 15: 30S ribosomal protein S15



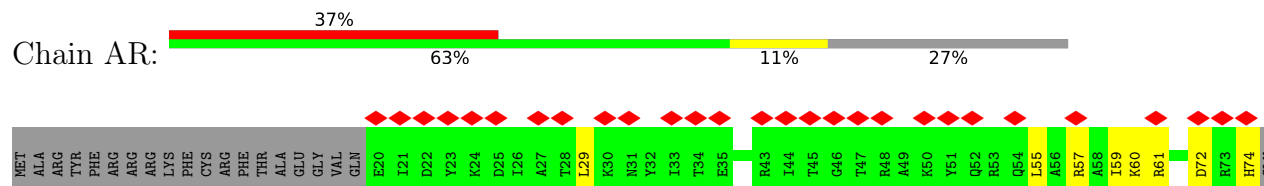
• Molecule 16: 30S ribosomal protein S16



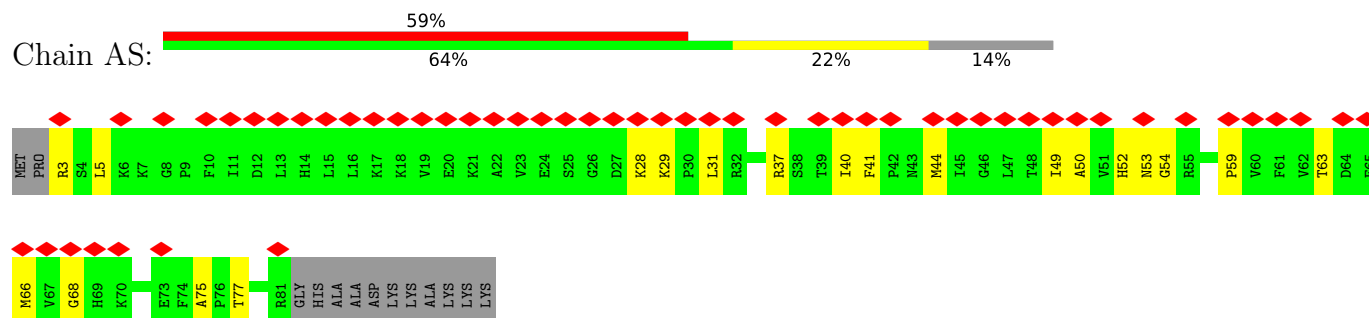
• Molecule 17: 30S ribosomal protein S17



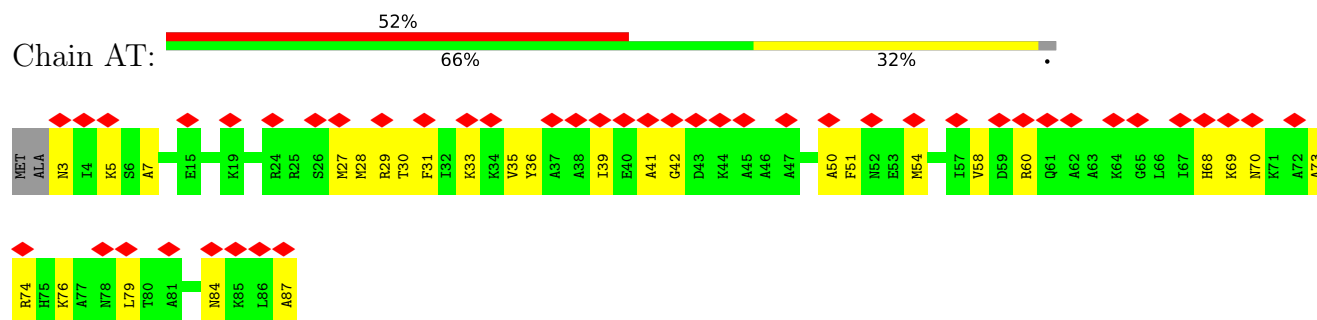
- Molecule 18: 30S ribosomal protein S18



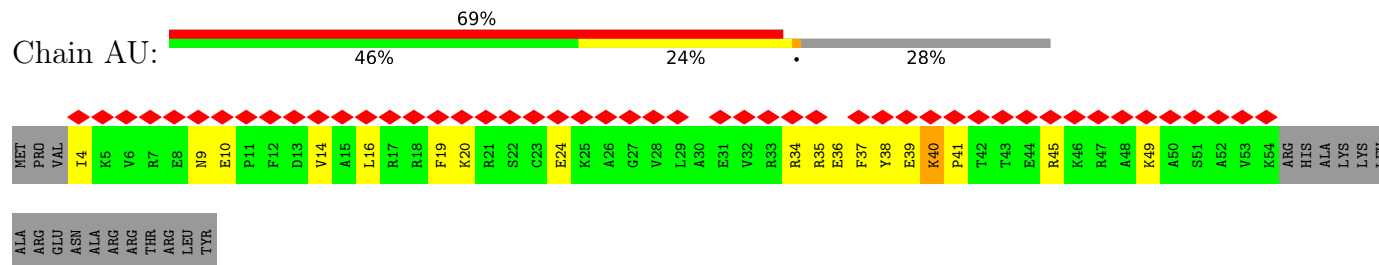
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



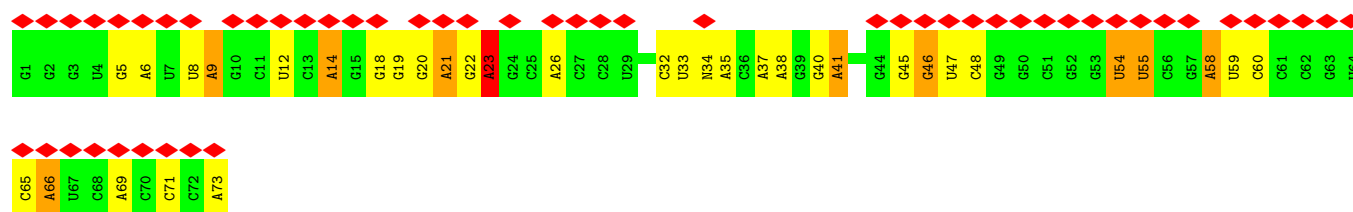
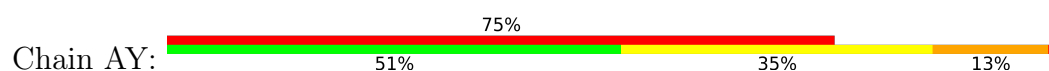
- Molecule 22: mRNA



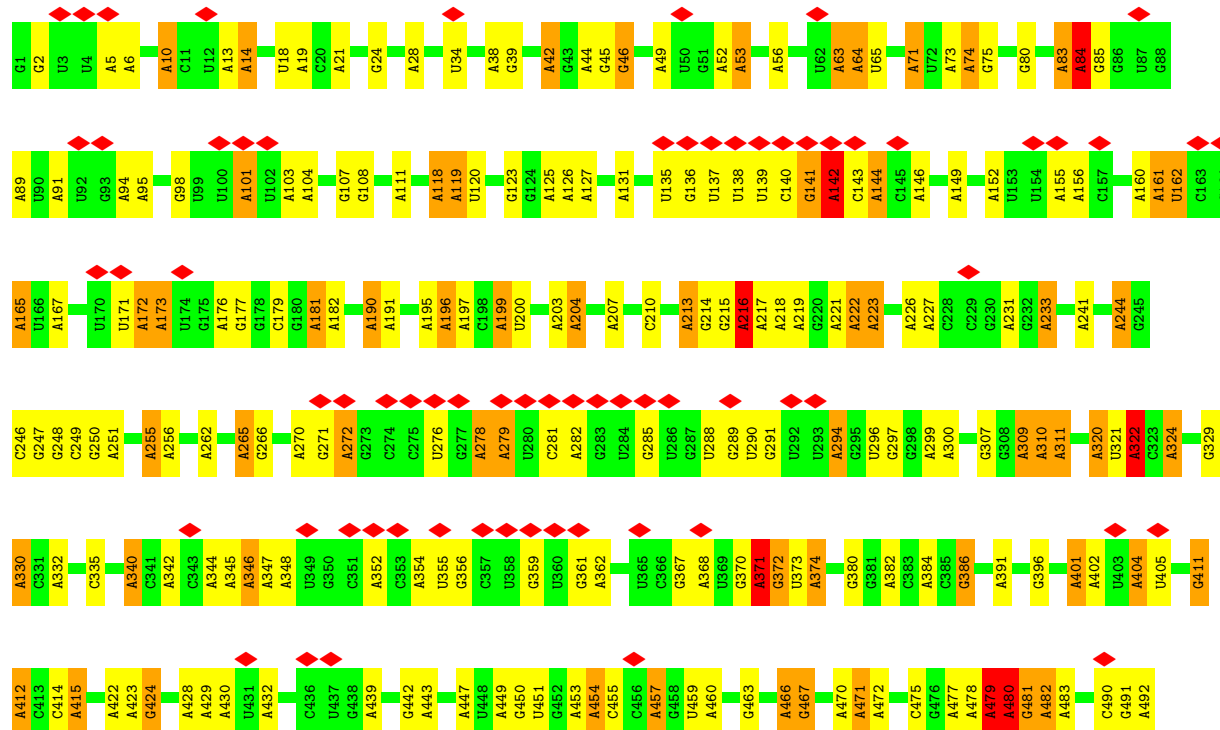
• Molecule 23: P-site tRNA Aspartate

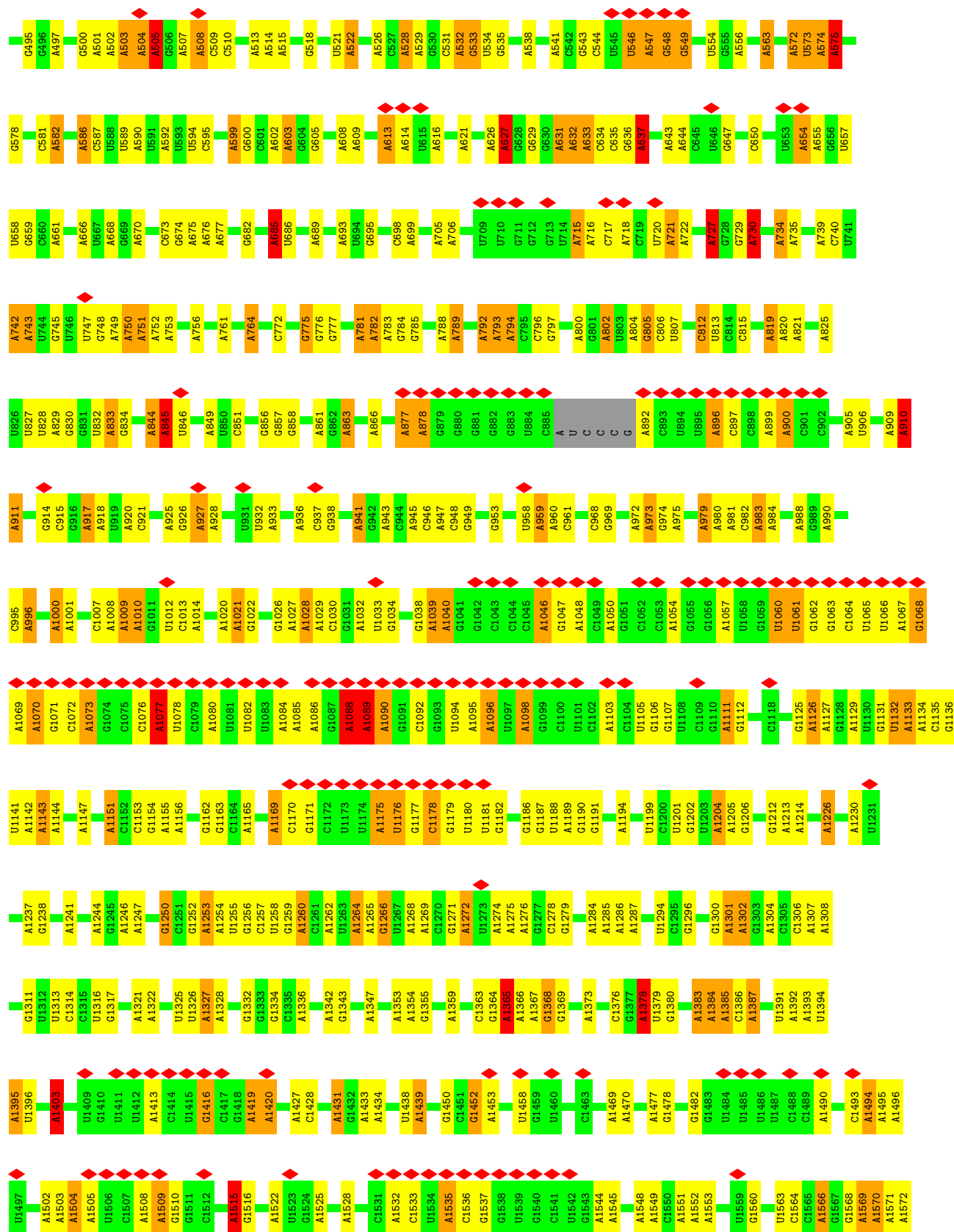


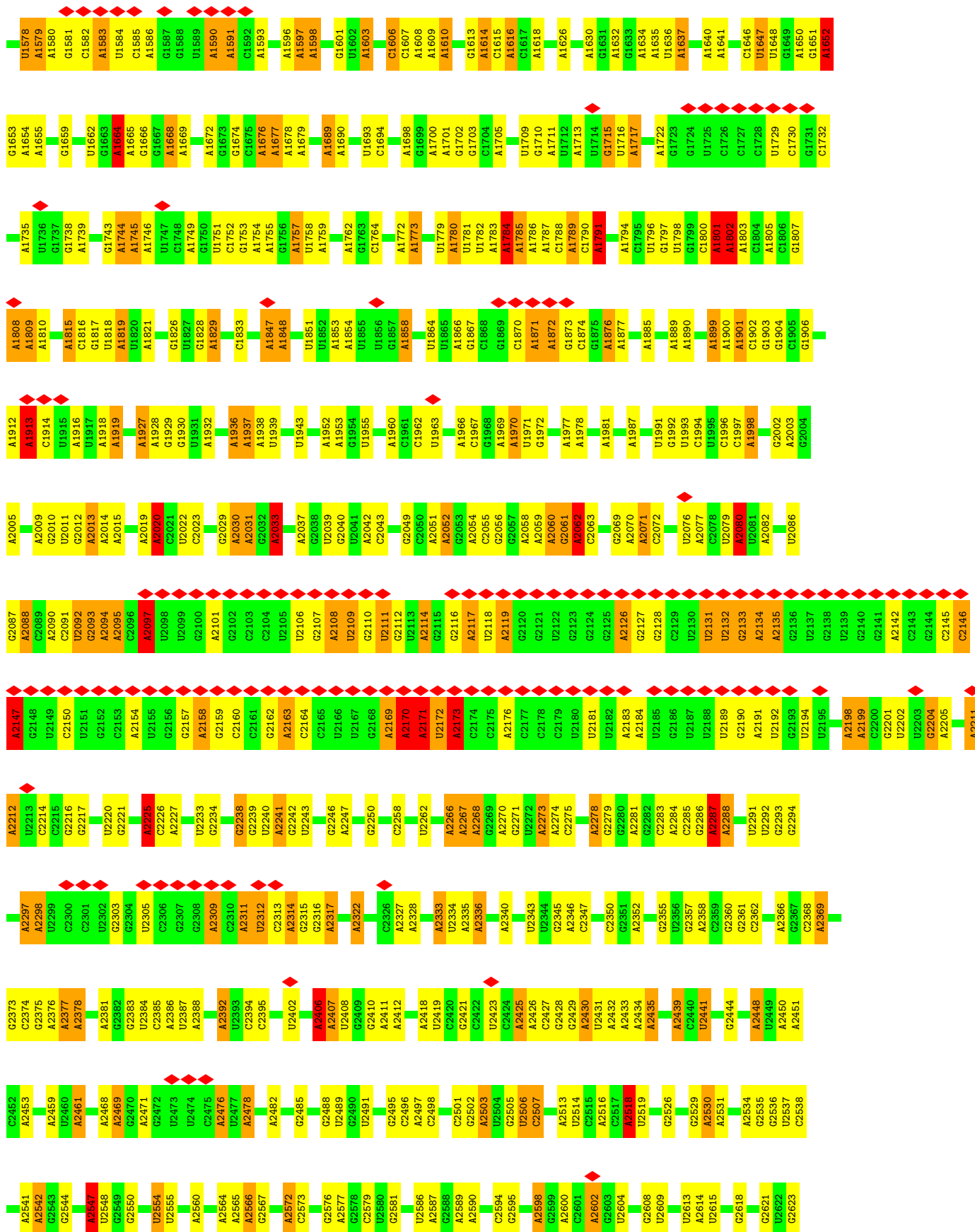
• Molecule 24: E-site tRNA Valine

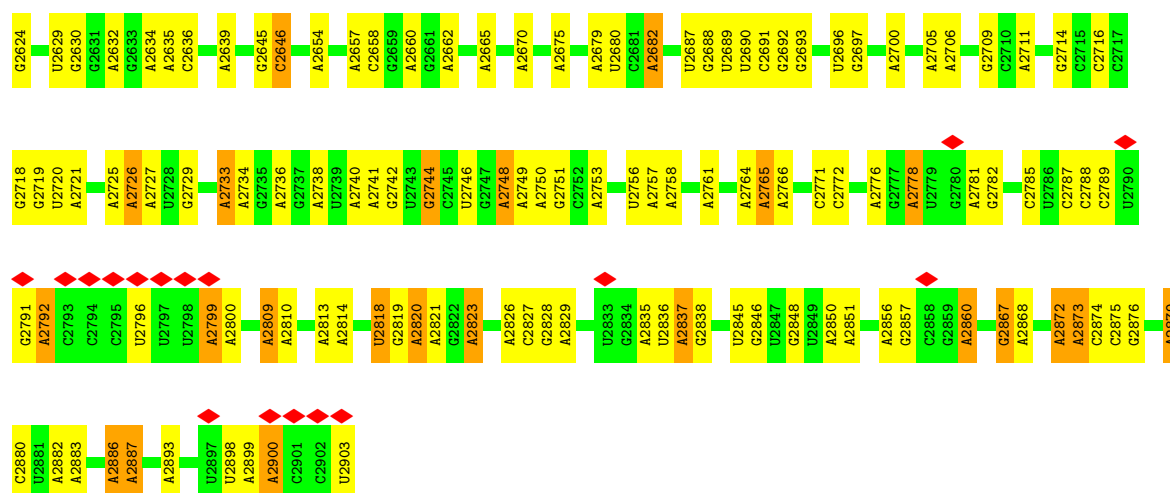


• Molecule 25: 23S ribosomal RNA

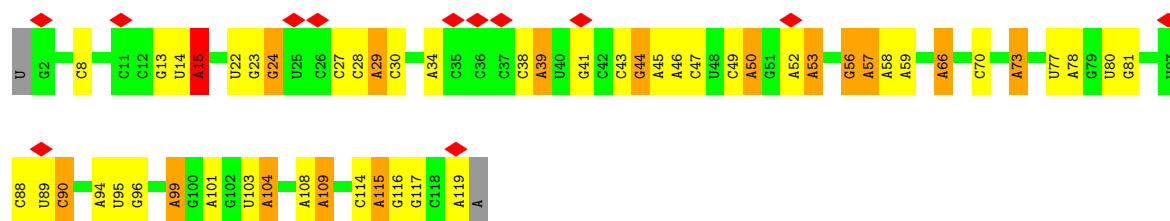




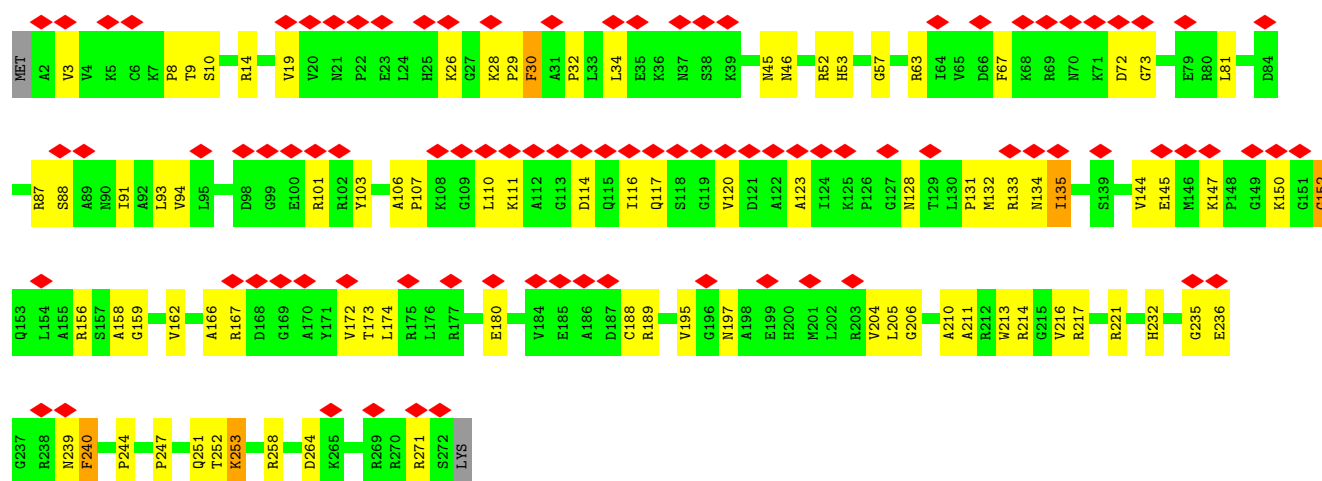




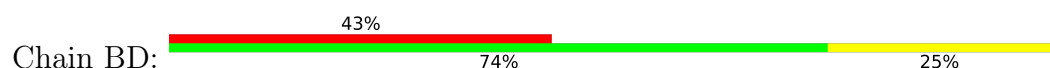
• Molecule 26: 5S ribosomal RNA

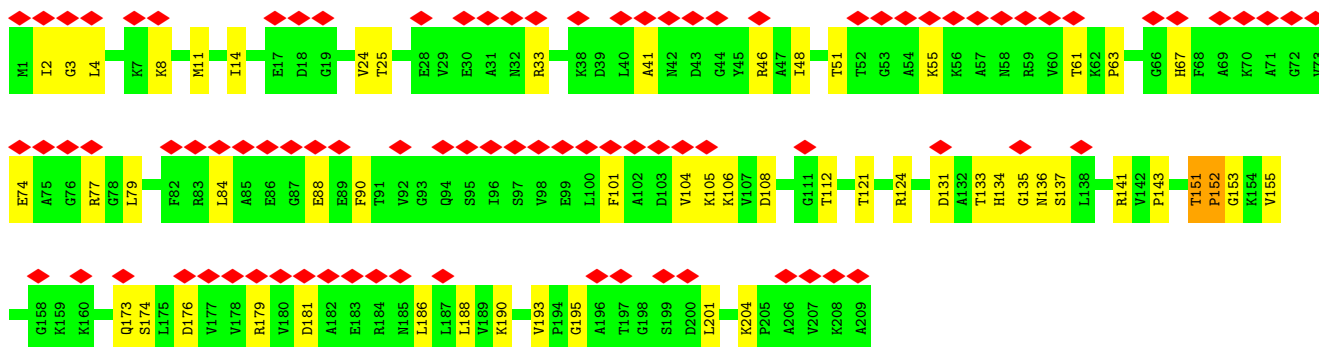


• Molecule 27: 50S ribosomal protein L2

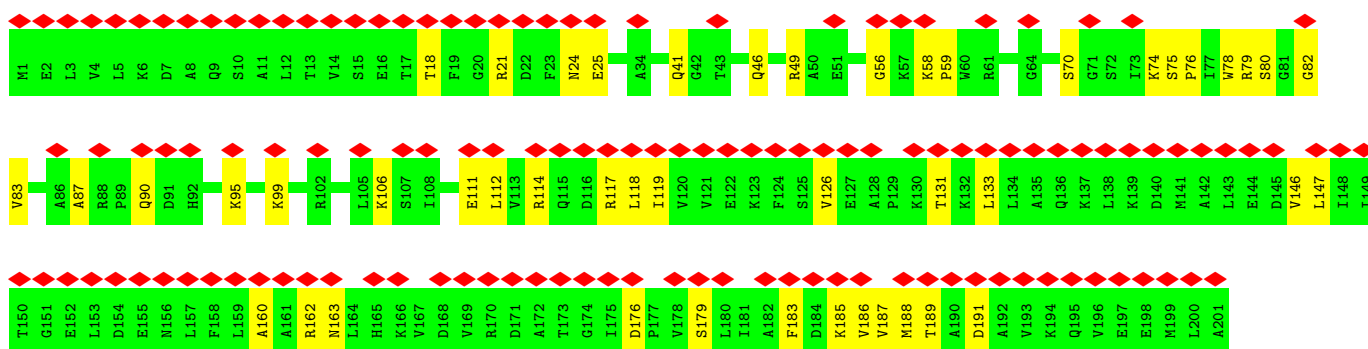
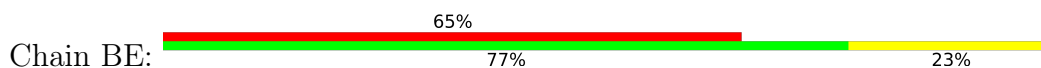


• Molecule 28: 50S ribosomal protein L3

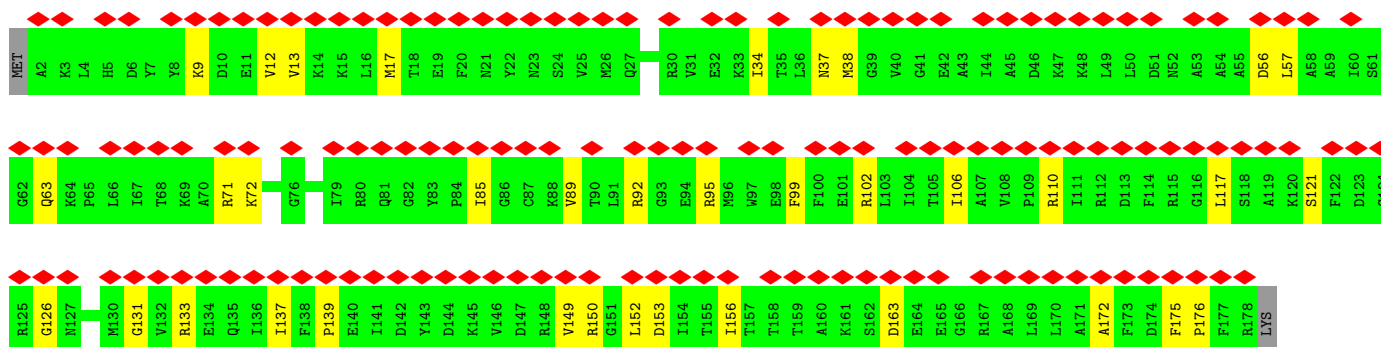
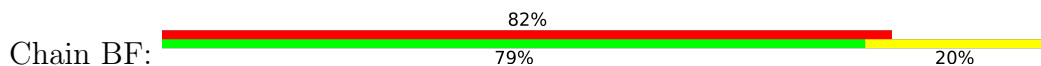




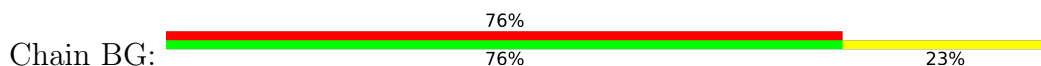
• Molecule 29: 50S ribosomal protein L4

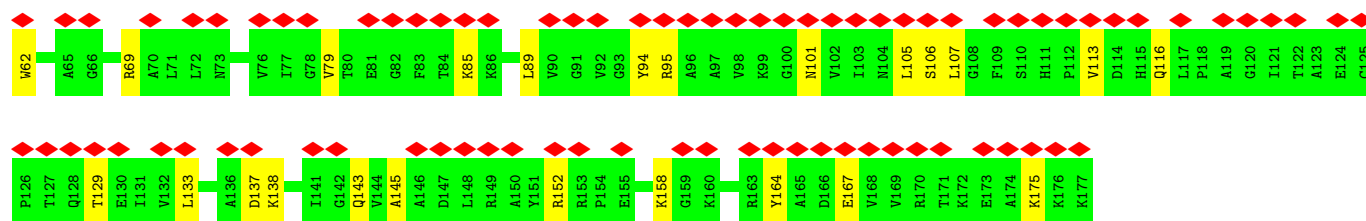


• Molecule 30: 50S ribosomal protein L5

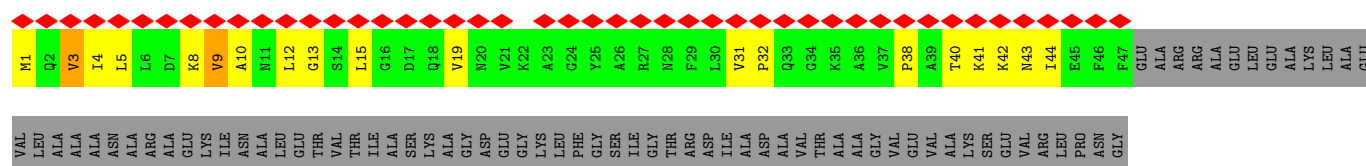


• Molecule 31: 50S ribosomal protein L6





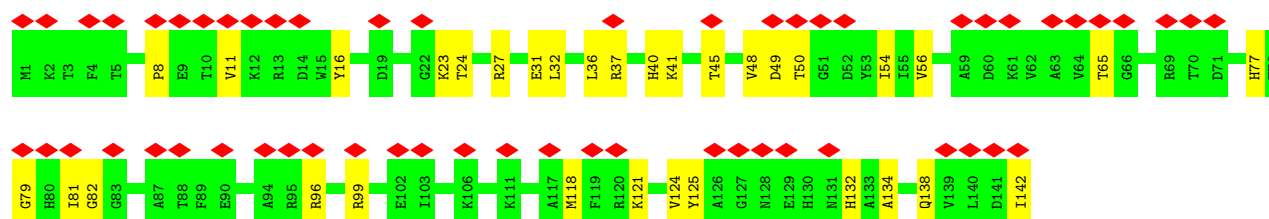
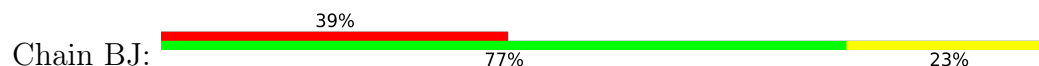
• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L11

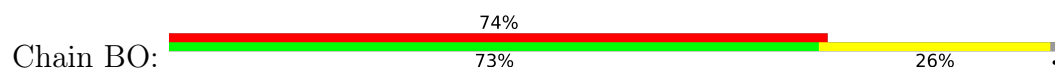


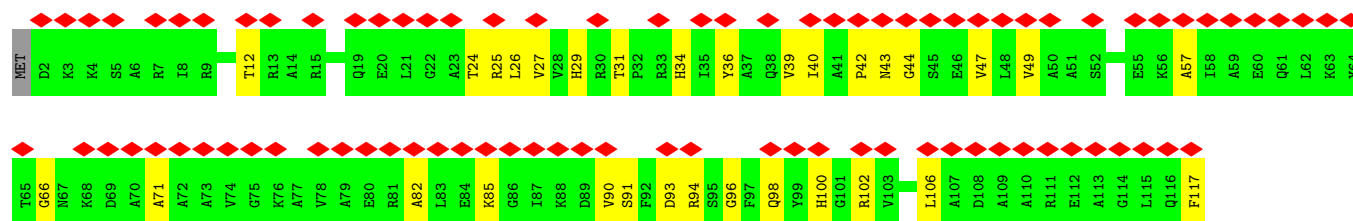
• Molecule 34: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L14

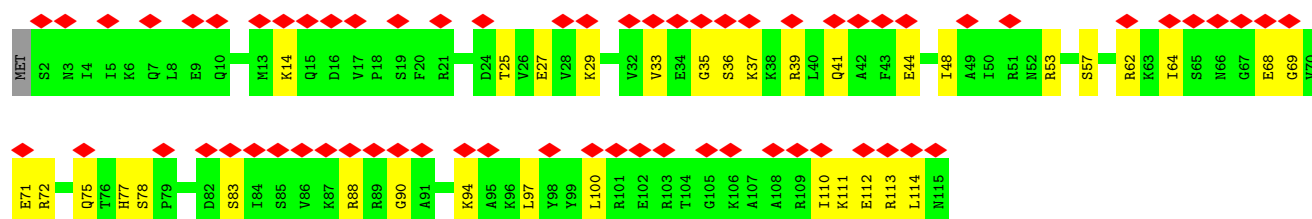






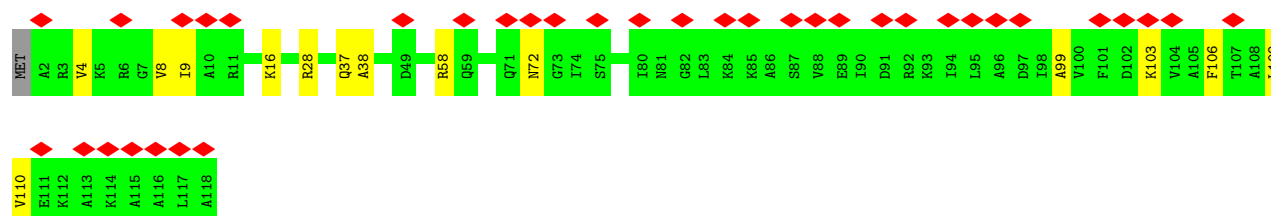
• Molecule 40: 50S ribosomal protein L19

Chain BP:



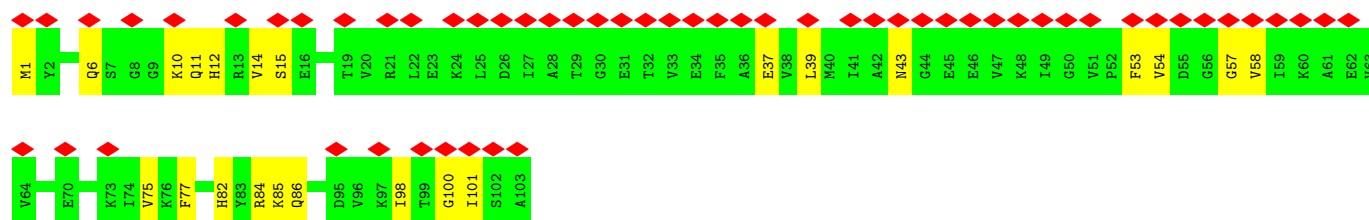
• Molecule 41: 50S ribosomal protein L20

Chain BQ:



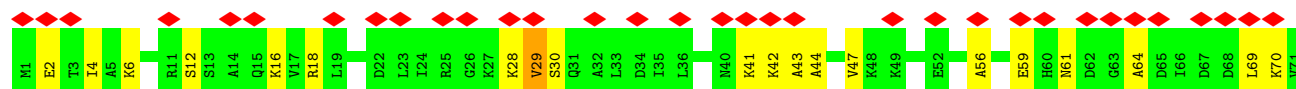
• Molecule 42: 50S ribosomal protein L21

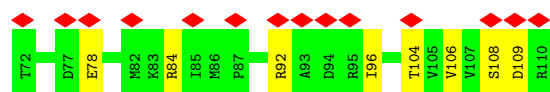
Chain BR:



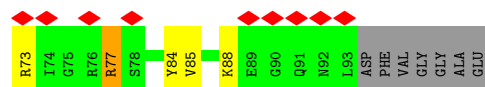
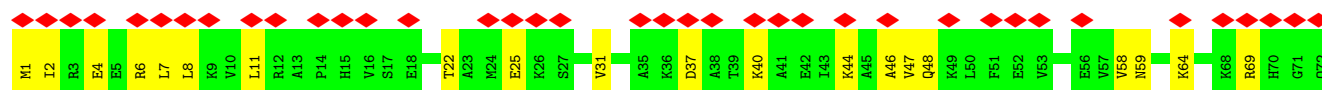
• Molecule 43: 50S ribosomal protein L22

Chain BS:

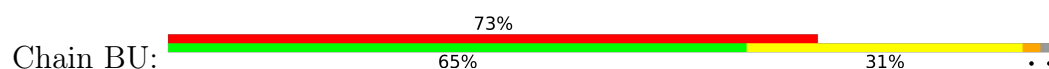




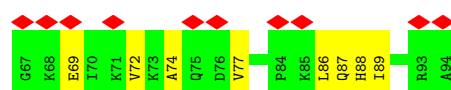
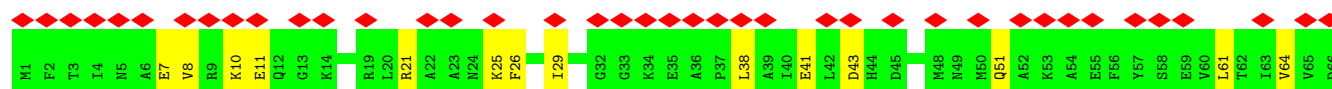
- Molecule 44: 50S ribosomal protein L23



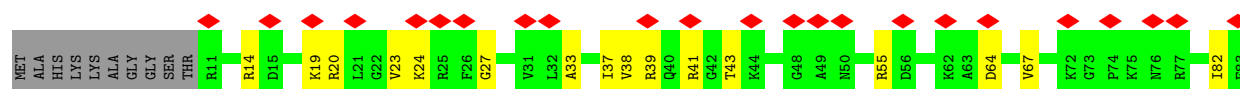
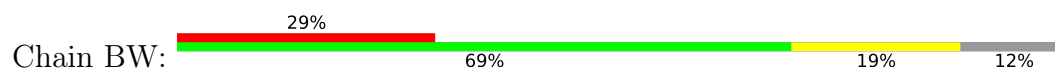
- Molecule 45: 50S ribosomal protein L24



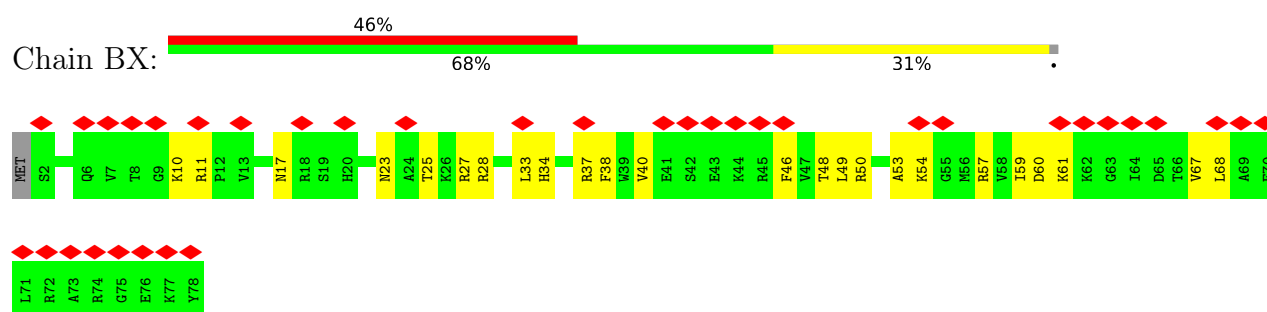
- Molecule 46: 50S ribosomal protein L25



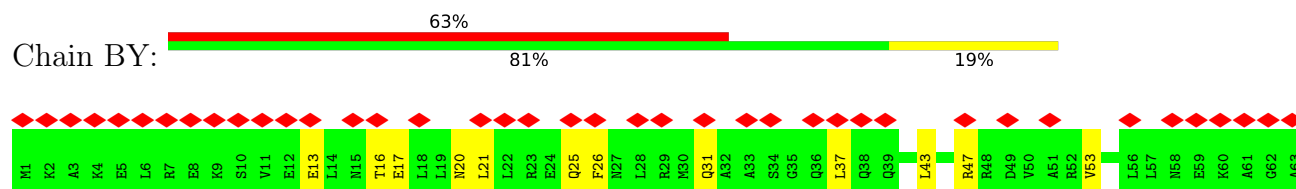
- Molecule 47: 50S ribosomal protein L27



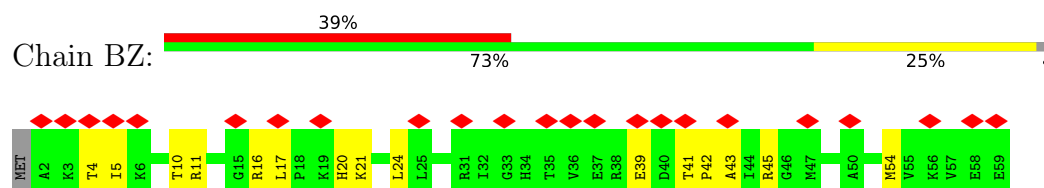
- Molecule 48: 50S ribosomal protein L28



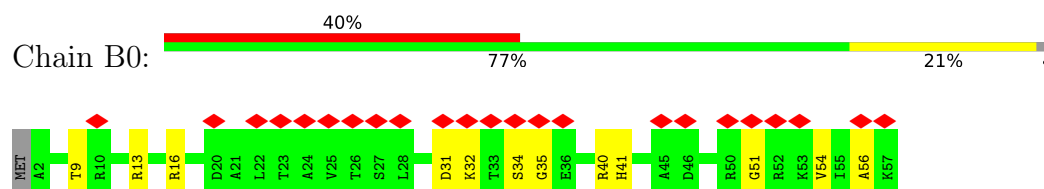
- Molecule 49: 50S ribosomal protein L29



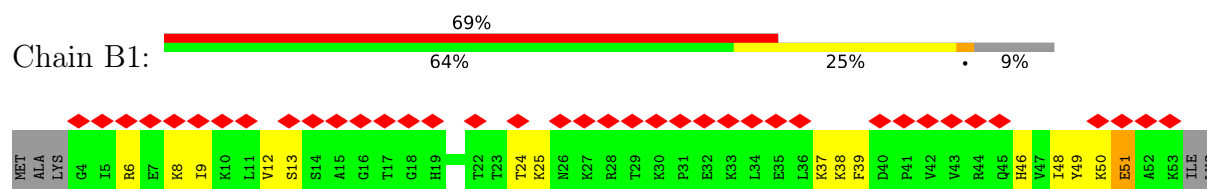
- Molecule 50: 50S ribosomal protein L30



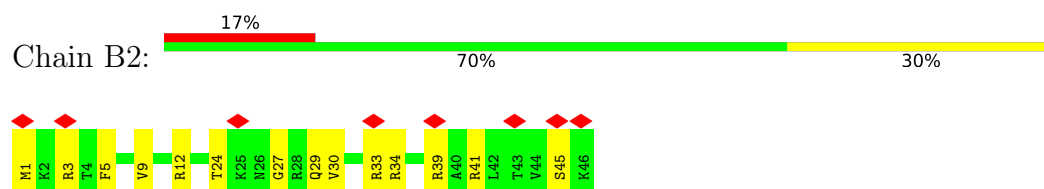
- Molecule 51: 50S ribosomal protein L32



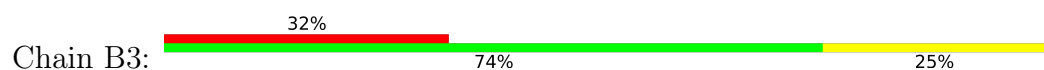
- Molecule 52: 50S ribosomal protein L33

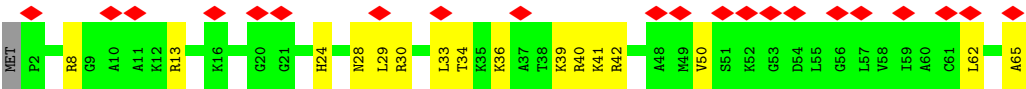


- Molecule 53: 50S ribosomal protein L34

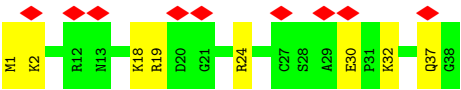
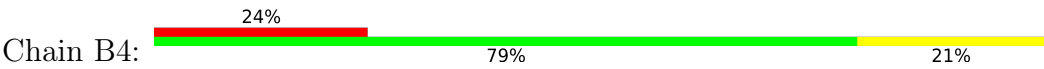


- Molecule 54: 50S ribosomal protein L35

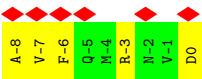




- Molecule 55: 50S ribosomal protein L36



- Molecule 56: ErmBL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.007	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00118	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, CM0, QUO, 7MG, H2U, 6MZ, 5MU, ERY, PSU, 2MA

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	AA	0.86	385/36965 (1.0%)	0.64	0/57662
2	AB	0.44	0/1735	0.74	1/2338 (0.0%)
3	AC	0.35	0/1651	0.72	0/2225
4	AD	0.37	0/1665	0.73	0/2227
5	AE	0.34	0/1118	0.79	0/1504
6	AF	0.36	0/835	0.73	0/1128
7	AG	0.33	0/1195	0.70	0/1602
8	AH	0.37	0/989	0.76	3/1326 (0.2%)
9	AI	0.41	1/1034 (0.1%)	0.75	0/1375
10	AJ	0.45	0/796	0.76	0/1077
11	AK	0.36	0/893	0.75	0/1205
12	AL	0.36	0/969	0.83	5/1300 (0.4%)
13	AM	0.38	0/892	0.76	2/1193 (0.2%)
14	AN	0.32	0/785	0.71	0/1043
15	AO	0.37	0/718	0.64	0/959
16	AP	0.36	0/659	0.71	0/884
17	AQ	0.42	0/657	0.80	0/881
18	AR	0.36	0/462	0.68	0/621
19	AS	0.38	0/652	0.74	0/877
20	AT	0.34	0/671	0.69	0/888
21	AU	0.35	0/430	0.77	2/570 (0.4%)
22	AV	1.32	6/245 (2.4%)	0.97	0/380
23	AX	0.68	10/1602 (0.6%)	0.50	0/2491
24	AY	0.78	13/1554 (0.8%)	0.58	0/2416
25	BA	0.88	761/69659 (1.1%)	0.65	0/108672
26	BB	0.76	23/2828 (0.8%)	0.56	0/4410
27	BC	0.37	0/2121	0.77	7/2852 (0.2%)
28	BD	0.39	0/1586	0.73	0/2134
29	BE	0.38	0/1571	0.69	0/2113
30	BF	0.41	0/1434	0.74	0/1926
31	BG	0.39	0/1343	0.74	0/1816
32	BH	0.42	0/364	0.75	0/490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BI	0.41	0/1046	0.80	4/1410 (0.3%)
34	BJ	0.37	0/1152	0.68	0/1551
35	BK	0.37	0/947	0.77	1/1268 (0.1%)
36	BL	0.35	0/1054	0.75	0/1403
37	BM	0.37	1/1093 (0.1%)	0.69	0/1460
38	BN	0.36	0/973	0.73	0/1301
39	BO	0.35	0/902	0.64	0/1209
40	BP	0.34	0/929	0.74	0/1242
41	BQ	0.31	0/960	0.65	0/1278
42	BR	0.32	0/829	0.68	0/1107
43	BS	0.41	0/864	0.74	1/1156 (0.1%)
44	BT	0.31	0/744	0.69	0/994
45	BU	0.38	0/787	0.75	0/1051
46	BV	0.36	0/766	0.73	2/1025 (0.2%)
47	BW	0.34	0/576	0.71	0/762
48	BX	0.30	0/635	0.72	0/848
49	BY	0.27	0/510	0.63	0/677
50	BZ	0.34	0/453	0.72	0/605
51	B0	0.37	0/450	0.71	0/599
52	B1	0.31	0/416	0.70	0/554
53	B2	0.26	0/380	0.63	0/498
54	B3	0.30	0/513	0.68	0/676
55	B4	0.35	0/303	0.74	0/397
56	B5	0.45	0/74	0.77	0/98
All	All	0.76	1200/157434 (0.8%)	0.67	28/235754 (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
28	BD	0	1

All (1200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	454	A	C6-N6	6.88	1.47	1.33
1	AA	860	A	C6-N6	6.86	1.47	1.33
1	AA	1227	A	C6-N6	6.85	1.47	1.33
1	AA	1155	A	C6-N6	6.83	1.47	1.33
25	BA	633	A	C6-N6	6.83	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1570	A	C6-N6	6.83	1.47	1.33
25	BA	1937	A	C6-N6	6.83	1.47	1.33
1	AA	149	A	C6-N6	6.82	1.47	1.33
1	AA	1418	A	C6-N6	6.82	1.47	1.33
25	BA	52	A	C6-N6	6.82	1.47	1.33
25	BA	1590	A	C6-N6	6.81	1.47	1.33
1	AA	253	A	C6-N6	6.81	1.47	1.33
1	AA	74	A	C6-N6	6.80	1.47	1.33
25	BA	104	A	C6-N6	6.80	1.47	1.33
25	BA	190	A	C6-N6	6.80	1.47	1.33
1	AA	313	A	C6-N6	6.80	1.47	1.33
25	BA	165	A	C6-N6	6.80	1.47	1.33
25	BA	344	A	C6-N6	6.80	1.47	1.33
25	BA	1722	A	C6-N6	6.80	1.47	1.33
26	BB	34	A	C6-N6	6.80	1.47	1.33
1	AA	1005	A	C6-N6	6.80	1.47	1.33
1	AA	1410	A	C6-N6	6.80	1.47	1.33
25	BA	453	A	C6-N6	6.80	1.47	1.33
25	BA	19	A	C6-N6	6.79	1.47	1.33
25	BA	819	A	C6-N6	6.79	1.47	1.33
25	BA	1385	A	C6-N6	6.79	1.47	1.33
1	AA	139	A	C6-N6	6.79	1.47	1.33
1	AA	179	A	C6-N6	6.79	1.47	1.33
1	AA	431	A	C6-N6	6.79	1.47	1.33
25	BA	975	A	C6-N6	6.79	1.47	1.33
25	BA	1027	A	C6-N6	6.79	1.47	1.33
25	BA	2381	A	C6-N6	6.79	1.47	1.33
25	BA	2453	A	C6-N6	6.79	1.47	1.33
1	AA	162	A	C6-N6	6.79	1.47	1.33
25	BA	825	A	C6-N6	6.79	1.47	1.33
25	BA	1111	A	C6-N6	6.79	1.47	1.33
25	BA	1810	A	C6-N6	6.79	1.47	1.33
25	BA	2748	A	C6-N6	6.79	1.47	1.33
25	BA	1014	A	C6-N6	6.79	1.47	1.33
25	BA	1952	A	C6-N6	6.79	1.47	1.33
25	BA	2268	A	C6-N6	6.79	1.47	1.33
1	AA	908	A	C6-N6	6.79	1.47	1.33
25	BA	1046	A	C6-N6	6.79	1.47	1.33
25	BA	1308	A	C6-N6	6.79	1.47	1.33
1	AA	109	A	C6-N6	6.79	1.47	1.33
25	BA	504	A	C6-N6	6.79	1.47	1.33
25	BA	1579	A	C6-N6	6.79	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1630	A	C6-N6	6.79	1.47	1.33
1	AA	344	A	C6-N6	6.79	1.47	1.33
1	AA	560	A	C6-N6	6.79	1.47	1.33
1	AA	749	A	C6-N6	6.79	1.47	1.33
25	BA	1080	A	C6-N6	6.79	1.47	1.33
25	BA	1749	A	C6-N6	6.79	1.47	1.33
25	BA	1889	A	C6-N6	6.79	1.47	1.33
25	BA	2019	A	C6-N6	6.79	1.47	1.33
25	BA	2392	A	C6-N6	6.79	1.47	1.33
25	BA	2873	A	C6-N6	6.79	1.47	1.33
1	AA	80	A	C6-N6	6.78	1.47	1.33
1	AA	250	A	C6-N6	6.78	1.47	1.33
1	AA	1004	A	C6-N6	6.78	1.47	1.33
1	AA	1110	A	C6-N6	6.78	1.47	1.33
1	AA	1213	A	C6-N6	6.78	1.47	1.33
1	AA	1375	A	C6-N6	6.78	1.47	1.33
25	BA	176	A	C6-N6	6.78	1.47	1.33
25	BA	637	A	C6-N6	6.78	1.47	1.33
25	BA	981	A	C6-N6	6.78	1.47	1.33
25	BA	1395	A	C6-N6	6.78	1.47	1.33
25	BA	1872	A	C6-N6	6.78	1.47	1.33
25	BA	2163	A	C6-N6	6.78	1.47	1.33
25	BA	2530	A	C6-N6	6.78	1.47	1.33
25	BA	2662	A	C6-N6	6.78	1.47	1.33
1	AA	554	A	C6-N6	6.78	1.47	1.33
25	BA	219	A	C6-N6	6.78	1.47	1.33
25	BA	721	A	C6-N6	6.78	1.47	1.33
25	BA	866	A	C6-N6	6.78	1.47	1.33
25	BA	1287	A	C6-N6	6.78	1.47	1.33
25	BA	1970	A	C6-N6	6.78	1.47	1.33
25	BA	2682	A	C6-N6	6.78	1.47	1.33
1	AA	160	A	C6-N6	6.78	1.47	1.33
1	AA	1360	A	C6-N6	6.78	1.47	1.33
1	AA	1374	A	C6-N6	6.78	1.47	1.33
1	AA	1408	A	C6-N6	6.78	1.47	1.33
25	BA	556	A	C6-N6	6.78	1.47	1.33
25	BA	905	A	C6-N6	6.78	1.47	1.33
25	BA	945	A	C6-N6	6.78	1.47	1.33
25	BA	960	A	C6-N6	6.78	1.47	1.33
25	BA	1032	A	C6-N6	6.78	1.47	1.33
25	BA	1089	A	C6-N6	6.78	1.47	1.33
25	BA	2051	A	C6-N6	6.78	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2108	A	C6-N6	6.78	1.47	1.33
25	BA	2266	A	C6-N6	6.78	1.47	1.33
25	BA	2589	A	C6-N6	6.78	1.47	1.33
25	BA	2657	A	C6-N6	6.78	1.47	1.33
22	AV	19	A	C6-N6	6.78	1.47	1.33
25	BA	472	A	C6-N6	6.78	1.47	1.33
25	BA	1069	A	C6-N6	6.78	1.47	1.33
25	BA	1127	A	C6-N6	6.78	1.47	1.33
25	BA	1593	A	C6-N6	6.78	1.47	1.33
25	BA	2435	A	C6-N6	6.78	1.47	1.33
1	AA	181	A	C6-N6	6.78	1.47	1.33
1	AA	648	A	C6-N6	6.78	1.47	1.33
1	AA	676	A	C6-N6	6.78	1.47	1.33
1	AA	1250	A	C6-N6	6.78	1.47	1.33
1	AA	1257	A	C6-N6	6.78	1.47	1.33
1	AA	1413	A	C6-N6	6.78	1.47	1.33
1	AA	1428	A	C6-N6	6.78	1.47	1.33
1	AA	1518	A	C6-N6	6.78	1.47	1.33
25	BA	299	A	C6-N6	6.78	1.47	1.33
25	BA	1705	A	C6-N6	6.78	1.47	1.33
25	BA	2082	A	C6-N6	6.78	1.47	1.33
25	BA	2176	A	C6-N6	6.78	1.47	1.33
25	BA	2270	A	C6-N6	6.78	1.47	1.33
25	BA	2322	A	C6-N6	6.78	1.47	1.33
25	BA	2513	A	C6-N6	6.78	1.47	1.33
25	BA	2899	A	C6-N6	6.78	1.47	1.33
1	AA	602	A	C6-N6	6.78	1.47	1.33
1	AA	1339	A	C6-N6	6.78	1.47	1.33
1	AA	1433	A	C6-N6	6.78	1.47	1.33
23	AX	14	A	C6-N6	6.78	1.47	1.33
25	BA	155	A	C6-N6	6.78	1.47	1.33
25	BA	294	A	C6-N6	6.78	1.47	1.33
25	BA	522	A	C6-N6	6.78	1.47	1.33
25	BA	1165	A	C6-N6	6.78	1.47	1.33
25	BA	1532	A	C6-N6	6.78	1.47	1.33
25	BA	1580	A	C6-N6	6.78	1.47	1.33
25	BA	1616	A	C6-N6	6.78	1.47	1.33
25	BA	1759	A	C6-N6	6.78	1.47	1.33
25	BA	1786	A	C6-N6	6.78	1.47	1.33
25	BA	2173	A	C6-N6	6.78	1.47	1.33
25	BA	2241	A	C6-N6	6.78	1.47	1.33
25	BA	2433	A	C6-N6	6.78	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2590	A	C6-N6	6.78	1.47	1.33
25	BA	2600	A	C6-N6	6.78	1.47	1.33
25	BA	2632	A	C6-N6	6.78	1.47	1.33
25	BA	2634	A	C6-N6	6.78	1.47	1.33
1	AA	10	A	C6-N6	6.77	1.47	1.33
1	AA	120	A	C6-N6	6.77	1.47	1.33
1	AA	393	A	C6-N6	6.77	1.47	1.33
1	AA	681	A	C6-N6	6.77	1.47	1.33
25	BA	1084	A	C6-N6	6.77	1.47	1.33
25	BA	1490	A	C6-N6	6.77	1.47	1.33
25	BA	1609	A	C6-N6	6.77	1.47	1.33
25	BA	2886	A	C6-N6	6.77	1.47	1.33
1	AA	51	A	C6-N6	6.77	1.47	1.33
1	AA	190	A	C6-N6	6.77	1.47	1.33
1	AA	825	A	C6-N6	6.77	1.47	1.33
1	AA	1319	A	C6-N6	6.77	1.47	1.33
25	BA	374	A	C6-N6	6.77	1.47	1.33
25	BA	479	A	C6-N6	6.77	1.47	1.33
25	BA	749	A	C6-N6	6.77	1.47	1.33
25	BA	1057	A	C6-N6	6.77	1.47	1.33
25	BA	1134	A	C6-N6	6.77	1.47	1.33
25	BA	1156	A	C6-N6	6.77	1.47	1.33
25	BA	2071	A	C6-N6	6.77	1.47	1.33
25	BA	2288	A	C6-N6	6.77	1.47	1.33
25	BA	2430	A	C6-N6	6.77	1.47	1.33
25	BA	2476	A	C6-N6	6.77	1.47	1.33
25	BA	2635	A	C6-N6	6.77	1.47	1.33
1	AA	197	A	C6-N6	6.77	1.47	1.33
1	AA	456	A	C6-N6	6.77	1.47	1.33
1	AA	807	A	C6-N6	6.77	1.47	1.33
1	AA	901	A	C6-N6	6.77	1.47	1.33
1	AA	1280	A	C6-N6	6.77	1.47	1.33
1	AA	1288	A	C6-N6	6.77	1.47	1.33
1	AA	1483	A	C6-N6	6.77	1.47	1.33
24	AY	35	A	C6-N6	6.77	1.47	1.33
25	BA	482	A	C6-N6	6.77	1.47	1.33
1	AA	119	A	C6-N6	6.77	1.47	1.33
1	AA	298	A	C6-N6	6.77	1.47	1.33
1	AA	790	A	C6-N6	6.77	1.47	1.33
1	AA	949	A	C6-N6	6.77	1.47	1.33
25	BA	191	A	C6-N6	6.77	1.47	1.33
25	BA	348	A	C6-N6	6.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	432	A	C6-N6	6.77	1.47	1.33
25	BA	1085	A	C6-N6	6.77	1.47	1.33
25	BA	1821	A	C6-N6	6.77	1.47	1.33
25	BA	1877	A	C6-N6	6.77	1.47	1.33
25	BA	2126	A	C6-N6	6.77	1.47	1.33
25	BA	2352	A	C6-N6	6.77	1.47	1.33
25	BA	2665	A	C6-N6	6.77	1.47	1.33
1	AA	152	A	C6-N6	6.77	1.47	1.33
1	AA	243	A	C6-N6	6.77	1.47	1.33
1	AA	777	A	C6-N6	6.77	1.47	1.33
1	AA	1500	A	C6-N6	6.77	1.47	1.33
25	BA	492	A	C6-N6	6.77	1.47	1.33
25	BA	1021	A	C6-N6	6.77	1.47	1.33
25	BA	1103	A	C6-N6	6.77	1.47	1.33
25	BA	1853	A	C6-N6	6.77	1.47	1.33
25	BA	2670	A	C6-N6	6.77	1.47	1.33
1	AA	364	A	C6-N6	6.77	1.47	1.33
1	AA	448	A	C6-N6	6.77	1.47	1.33
1	AA	533	A	C6-N6	6.77	1.47	1.33
1	AA	563	A	C6-N6	6.77	1.47	1.33
1	AA	702	A	C6-N6	6.77	1.47	1.33
24	AY	6	A	C6-N6	6.77	1.47	1.33
25	BA	256	A	C6-N6	6.77	1.47	1.33
25	BA	1618	A	C6-N6	6.77	1.47	1.33
25	BA	1773	A	C6-N6	6.77	1.47	1.33
25	BA	1928	A	C6-N6	6.77	1.47	1.33
25	BA	2733	A	C6-N6	6.77	1.47	1.33
25	BA	2753	A	C6-N6	6.77	1.47	1.33
26	BB	29	A	C6-N6	6.77	1.47	1.33
1	AA	143	A	C6-N6	6.76	1.47	1.33
1	AA	262	A	C6-N6	6.76	1.47	1.33
1	AA	349	A	C6-N6	6.76	1.47	1.33
1	AA	459	A	C6-N6	6.76	1.47	1.33
1	AA	496	A	C6-N6	6.76	1.47	1.33
1	AA	767	A	C6-N6	6.76	1.47	1.33
1	AA	873	A	C6-N6	6.76	1.47	1.33
1	AA	1067	A	C6-N6	6.76	1.47	1.33
1	AA	1236	A	C6-N6	6.76	1.47	1.33
23	AX	9	A	C6-N6	6.76	1.47	1.33
23	AX	41	A	C6-N6	6.76	1.47	1.33
25	BA	21	A	C6-N6	6.76	1.47	1.33
25	BA	101	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	127	A	C6-N6	6.76	1.47	1.33
25	BA	340	A	C6-N6	6.76	1.47	1.33
25	BA	742	A	C6-N6	6.76	1.47	1.33
25	BA	988	A	C6-N6	6.76	1.47	1.33
25	BA	1040	A	C6-N6	6.76	1.47	1.33
25	BA	1569	A	C6-N6	6.76	1.47	1.33
25	BA	1650	A	C6-N6	6.76	1.47	1.33
25	BA	1689	A	C6-N6	6.76	1.47	1.33
25	BA	1794	A	C6-N6	6.76	1.47	1.33
25	BA	1848	A	C6-N6	6.76	1.47	1.33
25	BA	1871	A	C6-N6	6.76	1.47	1.33
25	BA	1913	A	C6-N6	6.76	1.47	1.33
25	BA	1977	A	C6-N6	6.76	1.47	1.33
25	BA	1998	A	C6-N6	6.76	1.47	1.33
25	BA	2314	A	C6-N6	6.76	1.47	1.33
25	BA	2317	A	C6-N6	6.76	1.47	1.33
25	BA	2761	A	C6-N6	6.76	1.47	1.33
25	BA	2778	A	C6-N6	6.76	1.47	1.33
25	BA	2813	A	C6-N6	6.76	1.47	1.33
25	BA	2882	A	C6-N6	6.76	1.47	1.33
26	BB	99	A	C6-N6	6.76	1.47	1.33
26	BB	101	A	C6-N6	6.76	1.47	1.33
1	AA	1000	A	C6-N6	6.76	1.47	1.33
25	BA	278	A	C6-N6	6.76	1.47	1.33
25	BA	354	A	C6-N6	6.76	1.47	1.33
25	BA	575	A	C6-N6	6.76	1.47	1.33
25	BA	829	A	C6-N6	6.76	1.47	1.33
25	BA	1029	A	C6-N6	6.76	1.47	1.33
25	BA	1096	A	C6-N6	6.76	1.47	1.33
25	BA	2823	A	C6-N6	6.76	1.47	1.33
1	AA	71	A	C6-N6	6.76	1.47	1.33
1	AA	182	A	C6-N6	6.76	1.47	1.33
1	AA	196	A	C6-N6	6.76	1.47	1.33
1	AA	787	A	C6-N6	6.76	1.47	1.33
1	AA	845	A	C6-N6	6.76	1.47	1.33
1	AA	959	A	C6-N6	6.76	1.47	1.33
1	AA	1019	A	C6-N6	6.76	1.47	1.33
1	AA	1150	A	C6-N6	6.76	1.47	1.33
1	AA	1180	A	C6-N6	6.76	1.47	1.33
25	BA	126	A	C6-N6	6.76	1.47	1.33
25	BA	320	A	C6-N6	6.76	1.47	1.33
25	BA	346	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	603	A	C6-N6	6.76	1.47	1.33
25	BA	613	A	C6-N6	6.76	1.47	1.33
25	BA	1126	A	C6-N6	6.76	1.47	1.33
25	BA	1304	A	C6-N6	6.76	1.47	1.33
25	BA	1383	A	C6-N6	6.76	1.47	1.33
25	BA	1469	A	C6-N6	6.76	1.47	1.33
25	BA	1549	A	C6-N6	6.76	1.47	1.33
25	BA	1596	A	C6-N6	6.76	1.47	1.33
25	BA	1632	A	C6-N6	6.76	1.47	1.33
25	BA	1866	A	C6-N6	6.76	1.47	1.33
25	BA	2020	A	C6-N6	6.76	1.47	1.33
25	BA	2042	A	C6-N6	6.76	1.47	1.33
25	BA	2736	A	C6-N6	6.76	1.47	1.33
25	BA	2740	A	C6-N6	6.76	1.47	1.33
25	BA	2860	A	C6-N6	6.76	1.47	1.33
1	AA	77	A	C6-N6	6.76	1.47	1.33
1	AA	306	A	C6-N6	6.76	1.47	1.33
1	AA	315	A	C6-N6	6.76	1.47	1.33
1	AA	461	A	C6-N6	6.76	1.47	1.33
1	AA	510	A	C6-N6	6.76	1.47	1.33
1	AA	559	A	C6-N6	6.76	1.47	1.33
1	AA	609	A	C6-N6	6.76	1.47	1.33
1	AA	780	A	C6-N6	6.76	1.47	1.33
1	AA	1082	A	C6-N6	6.76	1.47	1.33
1	AA	1225	A	C6-N6	6.76	1.47	1.33
1	AA	1318	A	C6-N6	6.76	1.47	1.33
1	AA	1329	A	C6-N6	6.76	1.47	1.33
1	AA	1513	A	C6-N6	6.76	1.47	1.33
24	AY	73	A	C6-N6	6.76	1.47	1.33
25	BA	63	A	C6-N6	6.76	1.47	1.33
25	BA	221	A	C6-N6	6.76	1.47	1.33
25	BA	447	A	C6-N6	6.76	1.47	1.33
25	BA	513	A	C6-N6	6.76	1.47	1.33
25	BA	735	A	C6-N6	6.76	1.47	1.33
25	BA	849	A	C6-N6	6.76	1.47	1.33
25	BA	1095	A	C6-N6	6.76	1.47	1.33
25	BA	1213	A	C6-N6	6.76	1.47	1.33
25	BA	1286	A	C6-N6	6.76	1.47	1.33
25	BA	1392	A	C6-N6	6.76	1.47	1.33
25	BA	1502	A	C6-N6	6.76	1.47	1.33
25	BA	1809	A	C6-N6	6.76	1.47	1.33
25	BA	1978	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2336	A	C6-N6	6.76	1.47	1.33
25	BA	2879	A	C6-N6	6.76	1.47	1.33
1	AA	65	A	C6-N6	6.76	1.47	1.33
1	AA	1311	A	C6-N6	6.76	1.47	1.33
25	BA	255	A	C6-N6	6.76	1.47	1.33
25	BA	342	A	C6-N6	6.76	1.47	1.33
25	BA	401	A	C6-N6	6.76	1.47	1.33
25	BA	507	A	C6-N6	6.76	1.47	1.33
25	BA	627	A	C6-N6	6.76	1.47	1.33
25	BA	1247	A	C6-N6	6.76	1.47	1.33
25	BA	1322	A	C6-N6	6.76	1.47	1.33
25	BA	1640	A	C6-N6	6.76	1.47	1.33
25	BA	2377	A	C6-N6	6.76	1.47	1.33
1	AA	383	A	C6-N6	6.76	1.47	1.33
1	AA	579	A	C6-N6	6.76	1.47	1.33
1	AA	878	A	C6-N6	6.76	1.47	1.33
1	AA	913	A	C6-N6	6.76	1.47	1.33
1	AA	1021	A	C6-N6	6.76	1.47	1.33
1	AA	1080	A	C6-N6	6.76	1.47	1.33
1	AA	1201	A	C6-N6	6.76	1.47	1.33
1	AA	1252	A	C6-N6	6.76	1.47	1.33
1	AA	1456	A	C6-N6	6.76	1.47	1.33
23	AX	58	A	C6-N6	6.76	1.47	1.33
25	BA	38	A	C6-N6	6.76	1.47	1.33
25	BA	146	A	C6-N6	6.76	1.47	1.33
25	BA	149	A	C6-N6	6.76	1.47	1.33
25	BA	404	A	C6-N6	6.76	1.47	1.33
25	BA	439	A	C6-N6	6.76	1.47	1.33
25	BA	654	A	C6-N6	6.76	1.47	1.33
25	BA	734	A	C6-N6	6.76	1.47	1.33
25	BA	789	A	C6-N6	6.76	1.47	1.33
25	BA	947	A	C6-N6	6.76	1.47	1.33
25	BA	990	A	C6-N6	6.76	1.47	1.33
25	BA	1039	A	C6-N6	6.76	1.47	1.33
25	BA	1302	A	C6-N6	6.76	1.47	1.33
25	BA	1321	A	C6-N6	6.76	1.47	1.33
25	BA	1354	A	C6-N6	6.76	1.47	1.33
25	BA	1365	A	C6-N6	6.76	1.47	1.33
25	BA	1420	A	C6-N6	6.76	1.47	1.33
25	BA	1515	A	C6-N6	6.76	1.47	1.33
25	BA	1668	A	C6-N6	6.76	1.47	1.33
25	BA	1900	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2097	A	C6-N6	6.76	1.47	1.33
25	BA	2468	A	C6-N6	6.76	1.47	1.33
25	BA	2534	A	C6-N6	6.76	1.47	1.33
25	BA	2750	A	C6-N6	6.76	1.47	1.33
26	BB	58	A	C6-N6	6.76	1.47	1.33
1	AA	174	A	C6-N6	6.75	1.47	1.33
1	AA	300	A	C6-N6	6.75	1.47	1.33
1	AA	325	A	C6-N6	6.75	1.47	1.33
1	AA	329	A	C6-N6	6.75	1.47	1.33
1	AA	441	A	C6-N6	6.75	1.47	1.33
1	AA	1016	A	C6-N6	6.75	1.47	1.33
1	AA	1437	A	C6-N6	6.75	1.47	1.33
1	AA	1468	A	C6-N6	6.75	1.47	1.33
25	BA	103	A	C6-N6	6.75	1.47	1.33
25	BA	223	A	C6-N6	6.75	1.47	1.33
25	BA	761	A	C6-N6	6.75	1.47	1.33
25	BA	804	A	C6-N6	6.75	1.47	1.33
25	BA	1508	A	C6-N6	6.75	1.47	1.33
25	BA	1553	A	C6-N6	6.75	1.47	1.33
25	BA	1919	A	C6-N6	6.75	1.47	1.33
25	BA	2278	A	C6-N6	6.75	1.47	1.33
25	BA	2311	A	C6-N6	6.75	1.47	1.33
1	AA	2	A	C6-N6	6.75	1.47	1.33
1	AA	53	A	C6-N6	6.75	1.47	1.33
1	AA	172	A	C6-N6	6.75	1.47	1.33
1	AA	189	A	C6-N6	6.75	1.47	1.33
1	AA	373	A	C6-N6	6.75	1.47	1.33
1	AA	415	A	C6-N6	6.75	1.47	1.33
1	AA	466	A	C6-N6	6.75	1.47	1.33
1	AA	696	A	C6-N6	6.75	1.47	1.33
1	AA	831	A	C6-N6	6.75	1.47	1.33
1	AA	937	A	C6-N6	6.75	1.47	1.33
1	AA	969	A	C6-N6	6.75	1.47	1.33
1	AA	1191	A	C6-N6	6.75	1.47	1.33
1	AA	1246	A	C6-N6	6.75	1.47	1.33
1	AA	1499	A	C6-N6	6.75	1.47	1.33
24	AY	26	A	C6-N6	6.75	1.47	1.33
24	AY	66	A	C6-N6	6.75	1.47	1.33
25	BA	172	A	C6-N6	6.75	1.47	1.33
25	BA	282	A	C6-N6	6.75	1.47	1.33
25	BA	466	A	C6-N6	6.75	1.47	1.33
25	BA	471	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	478	A	C6-N6	6.75	1.47	1.33
25	BA	483	A	C6-N6	6.75	1.47	1.33
25	BA	502	A	C6-N6	6.75	1.47	1.33
25	BA	508	A	C6-N6	6.75	1.47	1.33
25	BA	515	A	C6-N6	6.75	1.47	1.33
25	BA	655	A	C6-N6	6.75	1.47	1.33
25	BA	668	A	C6-N6	6.75	1.47	1.33
25	BA	833	A	C6-N6	6.75	1.47	1.33
25	BA	896	A	C6-N6	6.75	1.47	1.33
25	BA	1050	A	C6-N6	6.75	1.47	1.33
25	BA	1285	A	C6-N6	6.75	1.47	1.33
25	BA	1535	A	C6-N6	6.75	1.47	1.33
25	BA	1572	A	C6-N6	6.75	1.47	1.33
25	BA	1780	A	C6-N6	6.75	1.47	1.33
25	BA	1936	A	C6-N6	6.75	1.47	1.33
25	BA	2031	A	C6-N6	6.75	1.47	1.33
25	BA	2094	A	C6-N6	6.75	1.47	1.33
1	AA	7	A	C6-N6	6.75	1.47	1.33
1	AA	55	A	C6-N6	6.75	1.47	1.33
1	AA	583	A	C6-N6	6.75	1.47	1.33
1	AA	792	A	C6-N6	6.75	1.47	1.33
1	AA	794	A	C6-N6	6.75	1.47	1.33
1	AA	892	A	C6-N6	6.75	1.47	1.33
1	AA	1197	A	C6-N6	6.75	1.47	1.33
1	AA	1306	A	C6-N6	6.75	1.47	1.33
25	BA	28	A	C6-N6	6.75	1.47	1.33
25	BA	89	A	C6-N6	6.75	1.47	1.33
25	BA	125	A	C6-N6	6.75	1.47	1.33
25	BA	196	A	C6-N6	6.75	1.47	1.33
25	BA	213	A	C6-N6	6.75	1.47	1.33
25	BA	216	A	C6-N6	6.75	1.47	1.33
25	BA	382	A	C6-N6	6.75	1.47	1.33
25	BA	631	A	C6-N6	6.75	1.47	1.33
25	BA	699	A	C6-N6	6.75	1.47	1.33
25	BA	716	A	C6-N6	6.75	1.47	1.33
25	BA	844	A	C6-N6	6.75	1.47	1.33
25	BA	925	A	C6-N6	6.75	1.47	1.33
25	BA	1129	A	C6-N6	6.75	1.47	1.33
25	BA	1147	A	C6-N6	6.75	1.47	1.33
25	BA	1241	A	C6-N6	6.75	1.47	1.33
25	BA	1269	A	C6-N6	6.75	1.47	1.33
25	BA	1384	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1494	A	C6-N6	6.75	1.47	1.33
25	BA	1571	A	C6-N6	6.75	1.47	1.33
25	BA	1610	A	C6-N6	6.75	1.47	1.33
25	BA	1679	A	C6-N6	6.75	1.47	1.33
25	BA	1772	A	C6-N6	6.75	1.47	1.33
25	BA	1953	A	C6-N6	6.75	1.47	1.33
25	BA	2013	A	C6-N6	6.75	1.47	1.33
25	BA	2033	A	C6-N6	6.75	1.47	1.33
25	BA	2776	A	C6-N6	6.75	1.47	1.33
1	AA	59	A	C6-N6	6.75	1.47	1.33
1	AA	600	A	C6-N6	6.75	1.47	1.33
1	AA	649	A	C6-N6	6.75	1.47	1.33
1	AA	1169	A	C6-N6	6.75	1.47	1.33
1	AA	1394	A	C6-N6	6.75	1.47	1.33
25	BA	788	A	C6-N6	6.75	1.47	1.33
25	BA	1009	A	C6-N6	6.75	1.47	1.33
25	BA	1268	A	C6-N6	6.75	1.47	1.33
25	BA	2378	A	C6-N6	6.75	1.47	1.33
1	AA	28	A	C6-N6	6.75	1.47	1.33
1	AA	32	A	C6-N6	6.75	1.47	1.33
1	AA	81	A	C6-N6	6.75	1.47	1.33
1	AA	192	A	C6-N6	6.75	1.47	1.33
1	AA	228	A	C6-N6	6.75	1.47	1.33
1	AA	374	A	C6-N6	6.75	1.47	1.33
1	AA	435	A	C6-N6	6.75	1.47	1.33
1	AA	495	A	C6-N6	6.75	1.47	1.33
1	AA	630	A	C6-N6	6.75	1.47	1.33
1	AA	640	A	C6-N6	6.75	1.47	1.33
1	AA	655	A	C6-N6	6.75	1.47	1.33
1	AA	781	A	C6-N6	6.75	1.47	1.33
1	AA	819	A	C6-N6	6.75	1.47	1.33
1	AA	906	A	C6-N6	6.75	1.47	1.33
1	AA	914	A	C6-N6	6.75	1.47	1.33
1	AA	964	A	C6-N6	6.75	1.47	1.33
1	AA	1117	A	C6-N6	6.75	1.47	1.33
1	AA	1163	A	C6-N6	6.75	1.47	1.33
1	AA	1271	A	C6-N6	6.75	1.47	1.33
1	AA	1368	A	C6-N6	6.75	1.47	1.33
1	AA	1476	A	C6-N6	6.75	1.47	1.33
23	AX	21	A	C6-N6	6.75	1.47	1.33
25	BA	352	A	C6-N6	6.75	1.47	1.33
25	BA	501	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	505	A	C6-N6	6.75	1.47	1.33
25	BA	599	A	C6-N6	6.75	1.47	1.33
25	BA	626	A	C6-N6	6.75	1.47	1.33
25	BA	861	A	C6-N6	6.75	1.47	1.33
25	BA	878	A	C6-N6	6.75	1.47	1.33
25	BA	1010	A	C6-N6	6.75	1.47	1.33
25	BA	1205	A	C6-N6	6.75	1.47	1.33
25	BA	1262	A	C6-N6	6.75	1.47	1.33
25	BA	1275	A	C6-N6	6.75	1.47	1.33
25	BA	1413	A	C6-N6	6.75	1.47	1.33
25	BA	1528	A	C6-N6	6.75	1.47	1.33
25	BA	1552	A	C6-N6	6.75	1.47	1.33
25	BA	1805	A	C6-N6	6.75	1.47	1.33
25	BA	1927	A	C6-N6	6.75	1.47	1.33
25	BA	2014	A	C6-N6	6.75	1.47	1.33
25	BA	2015	A	C6-N6	6.75	1.47	1.33
25	BA	2114	A	C6-N6	6.75	1.47	1.33
25	BA	2309	A	C6-N6	6.75	1.47	1.33
25	BA	2411	A	C6-N6	6.75	1.47	1.33
25	BA	2497	A	C6-N6	6.75	1.47	1.33
25	BA	2814	A	C6-N6	6.75	1.47	1.33
25	BA	2850	A	C6-N6	6.75	1.47	1.33
1	AA	3	A	C6-N6	6.75	1.47	1.33
1	AA	309	A	C6-N6	6.75	1.47	1.33
1	AA	363	A	C6-N6	6.75	1.47	1.33
1	AA	704	A	C6-N6	6.75	1.47	1.33
1	AA	802	A	C6-N6	6.75	1.47	1.33
1	AA	872	A	C6-N6	6.75	1.47	1.33
1	AA	996	A	C6-N6	6.75	1.47	1.33
1	AA	1042	A	C6-N6	6.75	1.47	1.33
1	AA	1229	A	C6-N6	6.75	1.47	1.33
1	AA	1287	A	C6-N6	6.75	1.47	1.33
1	AA	1289	A	C6-N6	6.75	1.47	1.33
1	AA	1362	A	C6-N6	6.75	1.47	1.33
1	AA	1446	A	C6-N6	6.75	1.47	1.33
24	AY	41	A	C6-N6	6.75	1.47	1.33
24	AY	58	A	C6-N6	6.75	1.47	1.33
25	BA	428	A	C6-N6	6.75	1.47	1.33
25	BA	529	A	C6-N6	6.75	1.47	1.33
25	BA	670	A	C6-N6	6.75	1.47	1.33
25	BA	793	A	C6-N6	6.75	1.47	1.33
25	BA	899	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	917	A	C6-N6	6.75	1.47	1.33
25	BA	1272	A	C6-N6	6.75	1.47	1.33
25	BA	1284	A	C6-N6	6.75	1.47	1.33
25	BA	1336	A	C6-N6	6.75	1.47	1.33
25	BA	1525	A	C6-N6	6.75	1.47	1.33
25	BA	1548	A	C6-N6	6.75	1.47	1.33
25	BA	1603	A	C6-N6	6.75	1.47	1.33
25	BA	1641	A	C6-N6	6.75	1.47	1.33
25	BA	1678	A	C6-N6	6.75	1.47	1.33
25	BA	1746	A	C6-N6	6.75	1.47	1.33
25	BA	1987	A	C6-N6	6.75	1.47	1.33
25	BA	2009	A	C6-N6	6.75	1.47	1.33
25	BA	2366	A	C6-N6	6.75	1.47	1.33
25	BA	2425	A	C6-N6	6.75	1.47	1.33
25	BA	2700	A	C6-N6	6.75	1.47	1.33
25	BA	2711	A	C6-N6	6.75	1.47	1.33
25	BA	2749	A	C6-N6	6.75	1.47	1.33
25	BA	2829	A	C6-N6	6.75	1.47	1.33
26	BB	57	A	C6-N6	6.75	1.47	1.33
26	BB	115	A	C6-N6	6.75	1.47	1.33
1	AA	16	A	C6-N6	6.75	1.47	1.33
1	AA	44	A	C6-N6	6.75	1.47	1.33
1	AA	130	A	C6-N6	6.75	1.47	1.33
1	AA	535	A	C6-N6	6.75	1.47	1.33
1	AA	746	A	C6-N6	6.75	1.47	1.33
1	AA	753	A	C6-N6	6.75	1.47	1.33
1	AA	1036	A	C6-N6	6.75	1.47	1.33
25	BA	197	A	C6-N6	6.75	1.47	1.33
25	BA	203	A	C6-N6	6.75	1.47	1.33
25	BA	739	A	C6-N6	6.75	1.47	1.33
25	BA	1054	A	C6-N6	6.75	1.47	1.33
25	BA	2284	A	C6-N6	6.75	1.47	1.33
25	BA	2327	A	C6-N6	6.75	1.47	1.33
25	BA	2346	A	C6-N6	6.75	1.47	1.33
25	BA	2792	A	C6-N6	6.75	1.47	1.33
25	BA	2868	A	C6-N6	6.75	1.47	1.33
25	BA	2872	A	C6-N6	6.75	1.47	1.33
1	AA	101	A	C6-N6	6.74	1.47	1.33
1	AA	116	A	C6-N6	6.74	1.47	1.33
1	AA	282	A	C6-N6	6.74	1.47	1.33
1	AA	288	A	C6-N6	6.74	1.47	1.33
1	AA	408	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	595	A	C6-N6	6.74	1.47	1.33
1	AA	784	A	C6-N6	6.74	1.47	1.33
1	AA	816	A	C6-N6	6.74	1.47	1.33
1	AA	900	A	C6-N6	6.74	1.47	1.33
1	AA	1171	A	C6-N6	6.74	1.47	1.33
1	AA	1216	A	C6-N6	6.74	1.47	1.33
1	AA	1285	A	C6-N6	6.74	1.47	1.33
1	AA	1398	A	C6-N6	6.74	1.47	1.33
1	AA	1447	A	C6-N6	6.74	1.47	1.33
25	BA	94	A	C6-N6	6.74	1.47	1.33
25	BA	480	A	C6-N6	6.74	1.47	1.33
25	BA	632	A	C6-N6	6.74	1.47	1.33
25	BA	689	A	C6-N6	6.74	1.47	1.33
25	BA	730	A	C6-N6	6.74	1.47	1.33
25	BA	743	A	C6-N6	6.74	1.47	1.33
25	BA	752	A	C6-N6	6.74	1.47	1.33
25	BA	845	A	C6-N6	6.74	1.47	1.33
25	BA	1088	A	C6-N6	6.74	1.47	1.33
25	BA	1230	A	C6-N6	6.74	1.47	1.33
25	BA	1453	A	C6-N6	6.74	1.47	1.33
25	BA	1509	A	C6-N6	6.74	1.47	1.33
25	BA	1744	A	C6-N6	6.74	1.47	1.33
25	BA	1762	A	C6-N6	6.74	1.47	1.33
25	BA	1847	A	C6-N6	6.74	1.47	1.33
25	BA	1969	A	C6-N6	6.74	1.47	1.33
25	BA	2142	A	C6-N6	6.74	1.47	1.33
25	BA	2406	A	C6-N6	6.74	1.47	1.33
25	BA	2448	A	C6-N6	6.74	1.47	1.33
25	BA	2679	A	C6-N6	6.74	1.47	1.33
25	BA	2856	A	C6-N6	6.74	1.47	1.33
25	BA	2893	A	C6-N6	6.74	1.47	1.33
26	BB	39	A	C6-N6	6.74	1.47	1.33
1	AA	19	A	C6-N6	6.74	1.47	1.33
1	AA	78	A	C6-N6	6.74	1.47	1.33
1	AA	382	A	C6-N6	6.74	1.47	1.33
1	AA	460	A	C6-N6	6.74	1.47	1.33
1	AA	1046	A	C6-N6	6.74	1.47	1.33
1	AA	1431	A	C6-N6	6.74	1.47	1.33
25	BA	10	A	C6-N6	6.74	1.47	1.33
25	BA	422	A	C6-N6	6.74	1.47	1.33
25	BA	643	A	C6-N6	6.74	1.47	1.33
25	BA	936	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1001	A	C6-N6	6.74	1.47	1.33
25	BA	1073	A	C6-N6	6.74	1.47	1.33
25	BA	1194	A	C6-N6	6.74	1.47	1.33
25	BA	1477	A	C6-N6	6.74	1.47	1.33
25	BA	1598	A	C6-N6	6.74	1.47	1.33
25	BA	1802	A	C6-N6	6.74	1.47	1.33
25	BA	1981	A	C6-N6	6.74	1.47	1.33
25	BA	2183	A	C6-N6	6.74	1.47	1.33
25	BA	2211	A	C6-N6	6.74	1.47	1.33
25	BA	2450	A	C6-N6	6.74	1.47	1.33
25	BA	2564	A	C6-N6	6.74	1.47	1.33
25	BA	2726	A	C6-N6	6.74	1.47	1.33
26	BB	15	A	C6-N6	6.74	1.47	1.33
26	BB	94	A	C6-N6	6.74	1.47	1.33
1	AA	72	A	C6-N6	6.74	1.47	1.33
1	AA	274	A	C6-N6	6.74	1.47	1.33
1	AA	487	A	C6-N6	6.74	1.47	1.33
1	AA	635	A	C6-N6	6.74	1.47	1.33
1	AA	768	A	C6-N6	6.74	1.47	1.33
1	AA	983	A	C6-N6	6.74	1.47	1.33
1	AA	1055	A	C6-N6	6.74	1.47	1.33
1	AA	1256	A	C6-N6	6.74	1.47	1.33
1	AA	1349	A	C6-N6	6.74	1.47	1.33
22	AV	20	A	C6-N6	6.74	1.47	1.33
25	BA	13	A	C6-N6	6.74	1.47	1.33
25	BA	73	A	C6-N6	6.74	1.47	1.33
25	BA	270	A	C6-N6	6.74	1.47	1.33
25	BA	528	A	C6-N6	6.74	1.47	1.33
25	BA	614	A	C6-N6	6.74	1.47	1.33
25	BA	675	A	C6-N6	6.74	1.47	1.33
25	BA	677	A	C6-N6	6.74	1.47	1.33
25	BA	727	A	C6-N6	6.74	1.47	1.33
25	BA	751	A	C6-N6	6.74	1.47	1.33
25	BA	980	A	C6-N6	6.74	1.47	1.33
25	BA	1133	A	C6-N6	6.74	1.47	1.33
25	BA	1367	A	C6-N6	6.74	1.47	1.33
25	BA	1403	A	C6-N6	6.74	1.47	1.33
25	BA	1431	A	C6-N6	6.74	1.47	1.33
25	BA	1634	A	C6-N6	6.74	1.47	1.33
25	BA	1739	A	C6-N6	6.74	1.47	1.33
25	BA	1854	A	C6-N6	6.74	1.47	1.33
25	BA	1885	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1938	A	C6-N6	6.74	1.47	1.33
25	BA	2134	A	C6-N6	6.74	1.47	1.33
25	BA	2297	A	C6-N6	6.74	1.47	1.33
25	BA	2434	A	C6-N6	6.74	1.47	1.33
25	BA	2809	A	C6-N6	6.74	1.47	1.33
1	AA	155	A	C6-N6	6.74	1.47	1.33
1	AA	199	A	C6-N6	6.74	1.47	1.33
1	AA	320	A	C6-N6	6.74	1.47	1.33
1	AA	321	A	C6-N6	6.74	1.47	1.33
1	AA	573	A	C6-N6	6.74	1.47	1.33
1	AA	687	A	C6-N6	6.74	1.47	1.33
1	AA	718	A	C6-N6	6.74	1.47	1.33
1	AA	815	A	C6-N6	6.74	1.47	1.33
1	AA	978	A	C6-N6	6.74	1.47	1.33
1	AA	1092	A	C6-N6	6.74	1.47	1.33
1	AA	1176	A	C6-N6	6.74	1.47	1.33
1	AA	1179	A	C6-N6	6.74	1.47	1.33
1	AA	1204	A	C6-N6	6.74	1.47	1.33
1	AA	1299	A	C6-N6	6.74	1.47	1.33
1	AA	1346	A	C6-N6	6.74	1.47	1.33
1	AA	1441	A	C6-N6	6.74	1.47	1.33
23	AX	23	A	C6-N6	6.74	1.47	1.33
24	AY	23	A	C6-N6	6.74	1.47	1.33
25	BA	42	A	C6-N6	6.74	1.47	1.33
25	BA	590	A	C6-N6	6.74	1.47	1.33
25	BA	608	A	C6-N6	6.74	1.47	1.33
25	BA	782	A	C6-N6	6.74	1.47	1.33
25	BA	1155	A	C6-N6	6.74	1.47	1.33
25	BA	1274	A	C6-N6	6.74	1.47	1.33
25	BA	1393	A	C6-N6	6.74	1.47	1.33
25	BA	1637	A	C6-N6	6.74	1.47	1.33
25	BA	1654	A	C6-N6	6.74	1.47	1.33
25	BA	1665	A	C6-N6	6.74	1.47	1.33
25	BA	1754	A	C6-N6	6.74	1.47	1.33
25	BA	1858	A	C6-N6	6.74	1.47	1.33
25	BA	1890	A	C6-N6	6.74	1.47	1.33
25	BA	1916	A	C6-N6	6.74	1.47	1.33
25	BA	1918	A	C6-N6	6.74	1.47	1.33
25	BA	2090	A	C6-N6	6.74	1.47	1.33
25	BA	2170	A	C6-N6	6.74	1.47	1.33
25	BA	2541	A	C6-N6	6.74	1.47	1.33
25	BA	2660	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2900	A	C6-N6	6.74	1.47	1.33
26	BB	108	A	C6-N6	6.74	1.47	1.33
1	AA	66	A	C6-N6	6.74	1.47	1.33
1	AA	129	A	C6-N6	6.74	1.47	1.33
1	AA	414	A	C6-N6	6.74	1.47	1.33
1	AA	547	A	C6-N6	6.74	1.47	1.33
1	AA	782	A	C6-N6	6.74	1.47	1.33
1	AA	1340	A	C6-N6	6.74	1.47	1.33
1	AA	1465	A	C6-N6	6.74	1.47	1.33
1	AA	1502	A	C6-N6	6.74	1.47	1.33
1	AA	1507	A	C6-N6	6.74	1.47	1.33
25	BA	310	A	C6-N6	6.74	1.47	1.33
25	BA	423	A	C6-N6	6.74	1.47	1.33
25	BA	547	A	C6-N6	6.74	1.47	1.33
25	BA	918	A	C6-N6	6.74	1.47	1.33
25	BA	1503	A	C6-N6	6.74	1.47	1.33
25	BA	1690	A	C6-N6	6.74	1.47	1.33
25	BA	1785	A	C6-N6	6.74	1.47	1.33
25	BA	2135	A	C6-N6	6.74	1.47	1.33
25	BA	2154	A	C6-N6	6.74	1.47	1.33
25	BA	2482	A	C6-N6	6.74	1.47	1.33
25	BA	2727	A	C6-N6	6.74	1.47	1.33
1	AA	238	A	C6-N6	6.74	1.47	1.33
1	AA	279	A	C6-N6	6.74	1.47	1.33
1	AA	498	A	C6-N6	6.74	1.47	1.33
1	AA	607	A	C6-N6	6.74	1.47	1.33
1	AA	673	A	C6-N6	6.74	1.47	1.33
1	AA	1035	A	C6-N6	6.74	1.47	1.33
1	AA	1151	A	C6-N6	6.74	1.47	1.33
1	AA	1519	A	C6-N6	6.74	1.47	1.33
1	AA	1534	A	C6-N6	6.74	1.47	1.33
25	BA	111	A	C6-N6	6.74	1.47	1.33
25	BA	156	A	C6-N6	6.74	1.47	1.33
25	BA	233	A	C6-N6	6.74	1.47	1.33
25	BA	300	A	C6-N6	6.74	1.47	1.33
25	BA	538	A	C6-N6	6.74	1.47	1.33
25	BA	718	A	C6-N6	6.74	1.47	1.33
25	BA	722	A	C6-N6	6.74	1.47	1.33
25	BA	792	A	C6-N6	6.74	1.47	1.33
25	BA	820	A	C6-N6	6.74	1.47	1.33
25	BA	877	A	C6-N6	6.74	1.47	1.33
25	BA	941	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	996	A	C6-N6	6.74	1.47	1.33
25	BA	1264	A	C6-N6	6.74	1.47	1.33
25	BA	1505	A	C6-N6	6.74	1.47	1.33
25	BA	1566	A	C6-N6	6.74	1.47	1.33
25	BA	1597	A	C6-N6	6.74	1.47	1.33
25	BA	1672	A	C6-N6	6.74	1.47	1.33
25	BA	2117	A	C6-N6	6.74	1.47	1.33
25	BA	2598	A	C6-N6	6.74	1.47	1.33
26	BB	53	A	C6-N6	6.74	1.47	1.33
26	BB	66	A	C6-N6	6.74	1.47	1.33
26	BB	73	A	C6-N6	6.74	1.47	1.33
1	AA	468	A	C6-N6	6.73	1.47	1.33
1	AA	1014	A	C6-N6	6.73	1.47	1.33
24	AY	38	A	C6-N6	6.73	1.47	1.33
25	BA	181	A	C6-N6	6.73	1.47	1.33
25	BA	322	A	C6-N6	6.73	1.47	1.33
25	BA	460	A	C6-N6	6.73	1.47	1.33
25	BA	497	A	C6-N6	6.73	1.47	1.33
25	BA	526	A	C6-N6	6.73	1.47	1.33
25	BA	1070	A	C6-N6	6.73	1.47	1.33
25	BA	1204	A	C6-N6	6.73	1.47	1.33
25	BA	1755	A	C6-N6	6.73	1.47	1.33
25	BA	1808	A	C6-N6	6.73	1.47	1.33
25	BA	2198	A	C6-N6	6.73	1.47	1.33
25	BA	2333	A	C6-N6	6.73	1.47	1.33
25	BA	2418	A	C6-N6	6.73	1.47	1.33
25	BA	2587	A	C6-N6	6.73	1.47	1.33
25	BA	2781	A	C6-N6	6.73	1.47	1.33
1	AA	223	A	C6-N6	6.73	1.47	1.33
1	AA	246	A	C6-N6	6.73	1.47	1.33
1	AA	263	A	C6-N6	6.73	1.47	1.33
1	AA	629	A	C6-N6	6.73	1.47	1.33
1	AA	663	A	C6-N6	6.73	1.47	1.33
1	AA	747	A	C6-N6	6.73	1.47	1.33
1	AA	918	A	C6-N6	6.73	1.47	1.33
1	AA	977	A	C6-N6	6.73	1.47	1.33
1	AA	994	A	C6-N6	6.73	1.47	1.33
1	AA	1430	A	C6-N6	6.73	1.47	1.33
22	AV	22	A	C6-N6	6.73	1.47	1.33
24	AY	14	A	C6-N6	6.73	1.47	1.33
25	BA	74	A	C6-N6	6.73	1.47	1.33
25	BA	84	A	C6-N6	6.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	160	A	C6-N6	6.73	1.47	1.33
25	BA	182	A	C6-N6	6.73	1.47	1.33
25	BA	195	A	C6-N6	6.73	1.47	1.33
25	BA	217	A	C6-N6	6.73	1.47	1.33
25	BA	311	A	C6-N6	6.73	1.47	1.33
25	BA	368	A	C6-N6	6.73	1.47	1.33
25	BA	477	A	C6-N6	6.73	1.47	1.33
25	BA	586	A	C6-N6	6.73	1.47	1.33
25	BA	602	A	C6-N6	6.73	1.47	1.33
25	BA	616	A	C6-N6	6.73	1.47	1.33
25	BA	800	A	C6-N6	6.73	1.47	1.33
25	BA	927	A	C6-N6	6.73	1.47	1.33
25	BA	928	A	C6-N6	6.73	1.47	1.33
25	BA	1189	A	C6-N6	6.73	1.47	1.33
25	BA	1495	A	C6-N6	6.73	1.47	1.33
25	BA	1626	A	C6-N6	6.73	1.47	1.33
25	BA	1677	A	C6-N6	6.73	1.47	1.33
25	BA	1735	A	C6-N6	6.73	1.47	1.33
25	BA	1960	A	C6-N6	6.73	1.47	1.33
25	BA	2062	A	C6-N6	6.73	1.47	1.33
25	BA	2101	A	C6-N6	6.73	1.47	1.33
25	BA	2358	A	C6-N6	6.73	1.47	1.33
25	BA	2432	A	C6-N6	6.73	1.47	1.33
25	BA	2439	A	C6-N6	6.73	1.47	1.33
25	BA	2471	A	C6-N6	6.73	1.47	1.33
25	BA	2705	A	C6-N6	6.73	1.47	1.33
1	AA	131	A	C6-N6	6.73	1.47	1.33
1	AA	327	A	C6-N6	6.73	1.47	1.33
1	AA	665	A	C6-N6	6.73	1.47	1.33
1	AA	919	A	C6-N6	6.73	1.47	1.33
1	AA	946	A	C6-N6	6.73	1.47	1.33
1	AA	968	A	C6-N6	6.73	1.47	1.33
1	AA	975	A	C6-N6	6.73	1.47	1.33
1	AA	1093	A	C6-N6	6.73	1.47	1.33
1	AA	1152	A	C6-N6	6.73	1.47	1.33
1	AA	1196	A	C6-N6	6.73	1.47	1.33
1	AA	1377	A	C6-N6	6.73	1.47	1.33
24	AY	21	A	C6-N6	6.73	1.47	1.33
25	BA	49	A	C6-N6	6.73	1.47	1.33
25	BA	64	A	C6-N6	6.73	1.47	1.33
25	BA	144	A	C6-N6	6.73	1.47	1.33
25	BA	345	A	C6-N6	6.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	705	A	C6-N6	6.73	1.47	1.33
25	BA	920	A	C6-N6	6.73	1.47	1.33
25	BA	1175	A	C6-N6	6.73	1.47	1.33
25	BA	1237	A	C6-N6	6.73	1.47	1.33
25	BA	1544	A	C6-N6	6.73	1.47	1.33
25	BA	1745	A	C6-N6	6.73	1.47	1.33
25	BA	1757	A	C6-N6	6.73	1.47	1.33
25	BA	2060	A	C6-N6	6.73	1.47	1.33
25	BA	2158	A	C6-N6	6.73	1.47	1.33
25	BA	2205	A	C6-N6	6.73	1.47	1.33
25	BA	2227	A	C6-N6	6.73	1.47	1.33
25	BA	2247	A	C6-N6	6.73	1.47	1.33
25	BA	2281	A	C6-N6	6.73	1.47	1.33
25	BA	2426	A	C6-N6	6.73	1.47	1.33
25	BA	2503	A	C6-N6	6.73	1.47	1.33
25	BA	2572	A	C6-N6	6.73	1.47	1.33
25	BA	2577	A	C6-N6	6.73	1.47	1.33
25	BA	2738	A	C6-N6	6.73	1.47	1.33
25	BA	2757	A	C6-N6	6.73	1.47	1.33
25	BA	2758	A	C6-N6	6.73	1.47	1.33
25	BA	2821	A	C6-N6	6.73	1.47	1.33
25	BA	2883	A	C6-N6	6.73	1.47	1.33
25	BA	2887	A	C6-N6	6.73	1.47	1.33
1	AA	236	A	C6-N6	6.73	1.47	1.33
1	AA	303	A	C6-N6	6.73	1.47	1.33
25	BA	262	A	C6-N6	6.73	1.47	1.33
25	BA	412	A	C6-N6	6.73	1.47	1.33
25	BA	693	A	C6-N6	6.73	1.47	1.33
25	BA	706	A	C6-N6	6.73	1.47	1.33
25	BA	715	A	C6-N6	6.73	1.47	1.33
25	BA	2070	A	C6-N6	6.73	1.47	1.33
25	BA	2560	A	C6-N6	6.73	1.47	1.33
25	BA	2602	A	C6-N6	6.73	1.47	1.33
25	BA	2614	A	C6-N6	6.73	1.47	1.33
25	BA	2826	A	C6-N6	6.73	1.47	1.33
25	BA	2837	A	C6-N6	6.73	1.47	1.33
1	AA	50	A	C6-N6	6.73	1.47	1.33
1	AA	338	A	C6-N6	6.73	1.47	1.33
1	AA	478	A	C6-N6	6.73	1.47	1.33
1	AA	502	A	C6-N6	6.73	1.47	1.33
1	AA	706	A	C6-N6	6.73	1.47	1.33
1	AA	712	A	C6-N6	6.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1111	A	C6-N6	6.73	1.47	1.33
1	AA	1238	A	C6-N6	6.73	1.47	1.33
1	AA	1324	A	C6-N6	6.73	1.47	1.33
1	AA	1396	A	C6-N6	6.73	1.47	1.33
25	BA	14	A	C6-N6	6.73	1.47	1.33
25	BA	44	A	C6-N6	6.73	1.47	1.33
25	BA	222	A	C6-N6	6.73	1.47	1.33
25	BA	371	A	C6-N6	6.73	1.47	1.33
25	BA	541	A	C6-N6	6.73	1.47	1.33
25	BA	563	A	C6-N6	6.73	1.47	1.33
25	BA	802	A	C6-N6	6.73	1.47	1.33
25	BA	1265	A	C6-N6	6.73	1.47	1.33
25	BA	1347	A	C6-N6	6.73	1.47	1.33
25	BA	1652	A	C6-N6	6.73	1.47	1.33
25	BA	1783	A	C6-N6	6.73	1.47	1.33
25	BA	1815	A	C6-N6	6.73	1.47	1.33
25	BA	2037	A	C6-N6	6.73	1.47	1.33
25	BA	2212	A	C6-N6	6.73	1.47	1.33
25	BA	2376	A	C6-N6	6.73	1.47	1.33
25	BA	2412	A	C6-N6	6.73	1.47	1.33
25	BA	2639	A	C6-N6	6.73	1.47	1.33
25	BA	2721	A	C6-N6	6.73	1.47	1.33
1	AA	205	A	C6-N6	6.73	1.47	1.33
1	AA	465	A	C6-N6	6.73	1.47	1.33
1	AA	675	A	C6-N6	6.73	1.47	1.33
1	AA	1012	A	C6-N6	6.73	1.47	1.33
1	AA	1251	A	C6-N6	6.73	1.47	1.33
24	AY	69	A	C6-N6	6.73	1.47	1.33
25	BA	429	A	C6-N6	6.73	1.47	1.33
25	BA	979	A	C6-N6	6.73	1.47	1.33
25	BA	1090	A	C6-N6	6.73	1.47	1.33
25	BA	1169	A	C6-N6	6.73	1.47	1.33
25	BA	1342	A	C6-N6	6.73	1.47	1.33
25	BA	1608	A	C6-N6	6.73	1.47	1.33
25	BA	1717	A	C6-N6	6.73	1.47	1.33
25	BA	2764	A	C6-N6	6.73	1.47	1.33
1	AA	60	A	C6-N6	6.72	1.47	1.33
1	AA	336	A	C6-N6	6.72	1.47	1.33
1	AA	430	A	C6-N6	6.72	1.47	1.33
1	AA	432	A	C6-N6	6.72	1.47	1.33
1	AA	539	A	C6-N6	6.72	1.47	1.33
1	AA	1105	A	C6-N6	6.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1167	A	C6-N6	6.72	1.47	1.33
1	AA	1248	A	C6-N6	6.72	1.47	1.33
1	AA	1269	A	C6-N6	6.72	1.47	1.33
1	AA	1274	A	C6-N6	6.72	1.47	1.33
1	AA	1275	A	C6-N6	6.72	1.47	1.33
1	AA	1434	A	C6-N6	6.72	1.47	1.33
25	BA	83	A	C6-N6	6.72	1.47	1.33
25	BA	272	A	C6-N6	6.72	1.47	1.33
25	BA	309	A	C6-N6	6.72	1.47	1.33
25	BA	470	A	C6-N6	6.72	1.47	1.33
25	BA	532	A	C6-N6	6.72	1.47	1.33
25	BA	781	A	C6-N6	6.72	1.47	1.33
25	BA	959	A	C6-N6	6.72	1.47	1.33
25	BA	1020	A	C6-N6	6.72	1.47	1.33
25	BA	1246	A	C6-N6	6.72	1.47	1.33
25	BA	1353	A	C6-N6	6.72	1.47	1.33
25	BA	1698	A	C6-N6	6.72	1.47	1.33
25	BA	2199	A	C6-N6	6.72	1.47	1.33
25	BA	2274	A	C6-N6	6.72	1.47	1.33
25	BA	2328	A	C6-N6	6.72	1.47	1.33
25	BA	2835	A	C6-N6	6.72	1.47	1.33
26	BB	109	A	C6-N6	6.72	1.47	1.33
1	AA	8	A	C6-N6	6.72	1.47	1.33
1	AA	366	A	C6-N6	6.72	1.47	1.33
1	AA	493	A	C6-N6	6.72	1.47	1.33
1	AA	574	A	C6-N6	6.72	1.47	1.33
1	AA	621	A	C6-N6	6.72	1.47	1.33
1	AA	715	A	C6-N6	6.72	1.47	1.33
1	AA	907	A	C6-N6	6.72	1.47	1.33
1	AA	915	A	C6-N6	6.72	1.47	1.33
1	AA	1188	A	C6-N6	6.72	1.47	1.33
1	AA	1254	A	C6-N6	6.72	1.47	1.33
1	AA	1508	A	C6-N6	6.72	1.47	1.33
23	AX	24	A	C6-N6	6.72	1.47	1.33
25	BA	5	A	C6-N6	6.72	1.47	1.33
25	BA	6	A	C6-N6	6.72	1.47	1.33
25	BA	347	A	C6-N6	6.72	1.47	1.33
25	BA	362	A	C6-N6	6.72	1.47	1.33
25	BA	666	A	C6-N6	6.72	1.47	1.33
25	BA	1008	A	C6-N6	6.72	1.47	1.33
25	BA	1048	A	C6-N6	6.72	1.47	1.33
25	BA	1307	A	C6-N6	6.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1387	A	C6-N6	6.72	1.47	1.33
25	BA	1591	A	C6-N6	6.72	1.47	1.33
25	BA	1635	A	C6-N6	6.72	1.47	1.33
25	BA	1669	A	C6-N6	6.72	1.47	1.33
25	BA	1932	A	C6-N6	6.72	1.47	1.33
25	BA	2058	A	C6-N6	6.72	1.47	1.33
25	BA	2147	A	C6-N6	6.72	1.47	1.33
25	BA	2287	A	C6-N6	6.72	1.47	1.33
25	BA	2335	A	C6-N6	6.72	1.47	1.33
25	BA	2547	A	C6-N6	6.72	1.47	1.33
25	BA	2820	A	C6-N6	6.72	1.47	1.33
26	BB	119	A	C6-N6	6.72	1.47	1.33
1	AA	572	A	C6-N6	6.72	1.47	1.33
22	AV	15	A	C6-N6	6.72	1.47	1.33
25	BA	199	A	C6-N6	6.72	1.47	1.33
25	BA	226	A	C6-N6	6.72	1.47	1.33
25	BA	241	A	C6-N6	6.72	1.47	1.33
25	BA	750	A	C6-N6	6.72	1.47	1.33
25	BA	984	A	C6-N6	6.72	1.47	1.33
25	BA	1067	A	C6-N6	6.72	1.47	1.33
25	BA	1789	A	C6-N6	6.72	1.47	1.33
25	BA	1801	A	C6-N6	6.72	1.47	1.33
25	BA	1819	A	C6-N6	6.72	1.47	1.33
25	BA	2810	A	C6-N6	6.72	1.47	1.33
1	AA	161	A	C6-N6	6.72	1.47	1.33
1	AA	642	A	C6-N6	6.72	1.47	1.33
1	AA	729	A	C6-N6	6.72	1.47	1.33
25	BA	71	A	C6-N6	6.72	1.47	1.33
25	BA	95	A	C6-N6	6.72	1.47	1.33
25	BA	152	A	C6-N6	6.72	1.47	1.33
25	BA	279	A	C6-N6	6.72	1.47	1.33
25	BA	332	A	C6-N6	6.72	1.47	1.33
25	BA	753	A	C6-N6	6.72	1.47	1.33
25	BA	943	A	C6-N6	6.72	1.47	1.33
25	BA	1433	A	C6-N6	6.72	1.47	1.33
25	BA	1787	A	C6-N6	6.72	1.47	1.33
25	BA	2005	A	C6-N6	6.72	1.47	1.33
25	BA	2080	A	C6-N6	6.72	1.47	1.33
25	BA	2340	A	C6-N6	6.72	1.47	1.33
25	BA	2386	A	C6-N6	6.72	1.47	1.33
26	BB	52	A	C6-N6	6.72	1.47	1.33
1	AA	1081	A	C6-N6	6.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	21	A	C6-N6	6.72	1.47	1.33
25	BA	415	A	C6-N6	6.72	1.47	1.33
25	BA	1098	A	C6-N6	6.72	1.47	1.33
25	BA	1504	A	C6-N6	6.72	1.47	1.33
25	BA	1676	A	C6-N6	6.72	1.47	1.33
25	BA	1876	A	C6-N6	6.72	1.47	1.33
25	BA	2169	A	C6-N6	6.72	1.47	1.33
25	BA	2369	A	C6-N6	6.72	1.47	1.33
1	AA	411	A	C6-N6	6.72	1.47	1.33
1	AA	523	A	C6-N6	6.72	1.47	1.33
1	AA	694	A	C6-N6	6.72	1.47	1.33
1	AA	695	A	C6-N6	6.72	1.47	1.33
1	AA	909	A	C6-N6	6.72	1.47	1.33
1	AA	1261	A	C6-N6	6.72	1.47	1.33
1	AA	1332	A	C6-N6	6.72	1.47	1.33
1	AA	1363	A	C6-N6	6.72	1.47	1.33
23	AX	3	A	C6-N6	6.72	1.47	1.33
25	BA	173	A	C6-N6	6.72	1.47	1.33
25	BA	384	A	C6-N6	6.72	1.47	1.33
25	BA	582	A	C6-N6	6.72	1.47	1.33
25	BA	621	A	C6-N6	6.72	1.47	1.33
25	BA	1028	A	C6-N6	6.72	1.47	1.33
25	BA	1439	A	C6-N6	6.72	1.47	1.33
25	BA	1470	A	C6-N6	6.72	1.47	1.33
25	BA	1496	A	C6-N6	6.72	1.47	1.33
25	BA	1700	A	C6-N6	6.72	1.47	1.33
25	BA	1912	A	C6-N6	6.72	1.47	1.33
25	BA	2030	A	C6-N6	6.72	1.47	1.33
25	BA	2225	A	C6-N6	6.72	1.47	1.33
25	BA	2273	A	C6-N6	6.72	1.47	1.33
25	BA	2531	A	C6-N6	6.72	1.47	1.33
1	AA	759	A	C6-N6	6.71	1.47	1.33
1	AA	938	A	C6-N6	6.71	1.47	1.33
1	AA	1531	A	C6-N6	6.71	1.47	1.33
23	AX	76	A	C6-N6	6.71	1.47	1.33
25	BA	131	A	C6-N6	6.71	1.47	1.33
25	BA	391	A	C6-N6	6.71	1.47	1.33
25	BA	764	A	C6-N6	6.71	1.47	1.33
25	BA	892	A	C6-N6	6.71	1.47	1.33
25	BA	900	A	C6-N6	6.71	1.47	1.33
25	BA	1328	A	C6-N6	6.71	1.47	1.33
25	BA	2003	A	C6-N6	6.71	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2077	A	C6-N6	6.71	1.47	1.33
25	BA	2654	A	C6-N6	6.71	1.47	1.33
25	BA	2765	A	C6-N6	6.71	1.47	1.33
26	BB	46	A	C6-N6	6.71	1.47	1.33
26	BB	104	A	C6-N6	6.71	1.47	1.33
1	AA	728	A	C6-N6	6.71	1.47	1.33
25	BA	1253	A	C6-N6	6.71	1.47	1.33
25	BA	1583	A	C6-N6	6.71	1.47	1.33
25	BA	2059	A	C6-N6	6.71	1.47	1.33
25	BA	2407	A	C6-N6	6.71	1.47	1.33
25	BA	2461	A	C6-N6	6.71	1.47	1.33
25	BA	2518	A	C6-N6	6.71	1.47	1.33
1	AA	33	A	C6-N6	6.71	1.47	1.33
1	AA	397	A	C6-N6	6.71	1.47	1.33
1	AA	499	A	C6-N6	6.71	1.47	1.33
1	AA	532	A	C6-N6	6.71	1.47	1.33
1	AA	1146	A	C6-N6	6.71	1.47	1.33
1	AA	1157	A	C6-N6	6.71	1.47	1.33
1	AA	1480	A	C6-N6	6.71	1.47	1.33
22	AV	17	A	C6-N6	6.71	1.47	1.33
25	BA	244	A	C6-N6	6.71	1.47	1.33
25	BA	756	A	C6-N6	6.71	1.47	1.33
25	BA	1151	A	C6-N6	6.71	1.47	1.33
25	BA	1244	A	C6-N6	6.71	1.47	1.33
25	BA	1327	A	C6-N6	6.71	1.47	1.33
25	BA	1366	A	C6-N6	6.71	1.47	1.33
25	BA	1373	A	C6-N6	6.71	1.47	1.33
25	BA	1434	A	C6-N6	6.71	1.47	1.33
25	BA	2119	A	C6-N6	6.71	1.47	1.33
25	BA	2706	A	C6-N6	6.71	1.47	1.33
1	AA	167	A	C6-N6	6.71	1.47	1.33
1	AA	889	A	C6-N6	6.71	1.47	1.33
25	BA	910	A	C6-N6	6.71	1.47	1.33
25	BA	2088	A	C6-N6	6.71	1.47	1.33
26	BB	45	A	C6-N6	6.71	1.47	1.33
1	AA	353	A	C6-N6	6.71	1.47	1.33
1	AA	553	A	C6-N6	6.71	1.47	1.33
1	AA	974	A	C6-N6	6.71	1.47	1.33
1	AA	1022	A	C6-N6	6.71	1.47	1.33
1	AA	1219	A	C6-N6	6.71	1.47	1.33
1	AA	1333	A	C6-N6	6.71	1.47	1.33
25	BA	91	A	C6-N6	6.71	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	592	A	C6-N6	6.71	1.47	1.33
25	BA	863	A	C6-N6	6.71	1.47	1.33
25	BA	972	A	C6-N6	6.71	1.47	1.33
25	BA	983	A	C6-N6	6.71	1.47	1.33
25	BA	1077	A	C6-N6	6.71	1.47	1.33
25	BA	1226	A	C6-N6	6.71	1.47	1.33
25	BA	1301	A	C6-N6	6.71	1.47	1.33
25	BA	2734	A	C6-N6	6.71	1.47	1.33
25	BA	2799	A	C6-N6	6.71	1.47	1.33
1	AA	171	A	C6-N6	6.71	1.47	1.33
1	AA	509	A	C6-N6	6.71	1.47	1.33
1	AA	520	A	C6-N6	6.71	1.47	1.33
1	AA	716	A	C6-N6	6.71	1.47	1.33
1	AA	743	A	C6-N6	6.71	1.47	1.33
1	AA	935	A	C6-N6	6.71	1.47	1.33
1	AA	1503	A	C6-N6	6.71	1.47	1.33
25	BA	118	A	C6-N6	6.71	1.47	1.33
25	BA	430	A	C6-N6	6.71	1.47	1.33
25	BA	1142	A	C6-N6	6.71	1.47	1.33
25	BA	1144	A	C6-N6	6.71	1.47	1.33
25	BA	2095	A	C6-N6	6.71	1.47	1.33
25	BA	2191	A	C6-N6	6.71	1.47	1.33
25	BA	2451	A	C6-N6	6.71	1.47	1.33
25	BA	2566	A	C6-N6	6.71	1.47	1.33
25	BA	2675	A	C6-N6	6.71	1.47	1.33
1	AA	864	A	C6-N6	6.71	1.47	1.33
25	BA	911	A	C6-N6	6.71	1.47	1.33
25	BA	1614	A	C6-N6	6.71	1.47	1.33
1	AA	1350	A	C6-N6	6.70	1.47	1.33
23	AX	26	A	C6-N6	6.70	1.47	1.33
25	BA	161	A	C6-N6	6.70	1.47	1.33
25	BA	231	A	C6-N6	6.70	1.47	1.33
25	BA	973	A	C6-N6	6.70	1.47	1.33
25	BA	1143	A	C6-N6	6.70	1.47	1.33
25	BA	1378	A	C6-N6	6.70	1.47	1.33
25	BA	1966	A	C6-N6	6.70	1.47	1.33
25	BA	2184	A	C6-N6	6.70	1.47	1.33
1	AA	151	A	C6-N6	6.70	1.47	1.33
25	BA	251	A	C6-N6	6.70	1.47	1.33
25	BA	2171	A	C6-N6	6.70	1.47	1.33
1	AA	371	A	C6-N6	6.70	1.47	1.33
1	AA	1130	A	C6-N6	6.70	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1170	A	C6-N6	6.70	1.47	1.33
1	AA	1239	A	C6-N6	6.70	1.47	1.33
25	BA	167	A	C6-N6	6.70	1.47	1.33
25	BA	1254	A	C6-N6	6.70	1.47	1.33
25	BA	1551	A	C6-N6	6.70	1.47	1.33
25	BA	2052	A	C6-N6	6.70	1.47	1.33
25	BA	2298	A	C6-N6	6.70	1.47	1.33
1	AA	482	A	C6-N6	6.70	1.47	1.33
24	AY	9	A	C6-N6	6.70	1.47	1.33
25	BA	402	A	C6-N6	6.70	1.47	1.33
25	BA	609	A	C6-N6	6.70	1.47	1.33
25	BA	661	A	C6-N6	6.70	1.47	1.33
25	BA	1829	A	C6-N6	6.70	1.47	1.33
25	BA	2388	A	C6-N6	6.70	1.47	1.33
1	AA	546	A	C6-N6	6.70	1.47	1.33
25	BA	265	A	C6-N6	6.70	1.47	1.33
25	BA	1086	A	C6-N6	6.70	1.47	1.33
1	AA	452	A	C6-N6	6.70	1.47	1.33
1	AA	622	A	C6-N6	6.70	1.47	1.33
1	AA	1101	A	C6-N6	6.70	1.47	1.33
25	BA	821	A	C6-N6	6.70	1.47	1.33
25	BA	1701	A	C6-N6	6.70	1.47	1.33
25	BA	1713	A	C6-N6	6.70	1.47	1.33
25	BA	2516	A	C6-N6	6.70	1.47	1.33
25	BA	2542	A	C6-N6	6.70	1.47	1.33
1	AA	195	A	C6-N6	6.69	1.47	1.33
1	AA	412	A	C6-N6	6.69	1.47	1.33
25	BA	574	A	C6-N6	6.69	1.47	1.33
25	BA	1427	A	C6-N6	6.69	1.47	1.33
25	BA	1586	A	C6-N6	6.69	1.47	1.33
25	BA	1803	A	C6-N6	6.69	1.47	1.33
1	AA	865	A	C6-N6	6.69	1.47	1.33
25	BA	1359	A	C6-N6	6.69	1.47	1.33
25	BA	2851	A	C6-N6	6.69	1.47	1.33
26	BB	50	A	C6-N6	6.69	1.47	1.33
26	BB	78	A	C6-N6	6.69	1.47	1.33
1	AA	958	A	C6-N6	6.69	1.47	1.33
25	BA	207	A	C6-N6	6.69	1.47	1.33
25	BA	449	A	C6-N6	6.69	1.47	1.33
25	BA	676	A	C6-N6	6.69	1.47	1.33
25	BA	909	A	C6-N6	6.69	1.47	1.33
25	BA	1711	A	C6-N6	6.69	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1791	A	C6-N6	6.69	1.47	1.33
25	BA	2741	A	C6-N6	6.69	1.47	1.33
25	BA	227	A	C6-N6	6.69	1.47	1.33
25	BA	2478	A	C6-N6	6.69	1.47	1.33
1	AA	389	A	C6-N6	6.69	1.47	1.33
25	BA	572	A	C6-N6	6.69	1.47	1.33
25	BA	2565	A	C6-N6	6.69	1.47	1.33
1	AA	26	A	C6-N6	6.69	1.47	1.33
1	AA	1102	A	C6-N6	6.68	1.47	1.33
1	AA	1429	A	C6-N6	6.68	1.47	1.33
25	BA	119	A	C6-N6	6.68	1.47	1.33
25	BA	794	A	C6-N6	6.68	1.47	1.33
25	BA	330	A	C6-N6	6.68	1.47	1.33
25	BA	933	A	C6-N6	6.68	1.47	1.33
25	BA	1260	A	C6-N6	6.68	1.47	1.33
1	AA	356	A	C6-N6	6.68	1.47	1.33
1	AA	1357	A	C6-N6	6.68	1.47	1.33
25	BA	1664	A	C6-N6	6.68	1.47	1.33
1	AA	814	A	C6-N6	6.68	1.47	1.33
25	BA	685	A	C6-N6	6.68	1.47	1.33
25	BA	2267	A	C6-N6	6.68	1.47	1.33
1	AA	596	A	C6-N6	6.68	1.47	1.33
25	BA	457	A	C6-N6	6.68	1.47	1.33
25	BA	218	A	C6-N6	6.68	1.47	1.33
25	BA	503	A	C6-N6	6.68	1.47	1.33
1	AA	1044	A	C6-N6	6.67	1.47	1.33
25	BA	443	A	C6-N6	6.67	1.47	1.33
25	BA	644	A	C6-N6	6.67	1.47	1.33
25	BA	2766	A	C6-N6	6.67	1.47	1.33
1	AA	270	A	C6-N6	6.67	1.47	1.33
25	BA	1522	A	C6-N6	6.67	1.47	1.33
25	BA	1419	A	C6-N6	6.67	1.47	1.33
1	AA	451	A	C6-N6	6.67	1.47	1.33
25	BA	324	A	C6-N6	6.67	1.47	1.33
25	BA	1000	A	C6-N6	6.67	1.47	1.33
25	BA	1655	A	C6-N6	6.67	1.47	1.33
25	BA	1901	A	C6-N6	6.67	1.47	1.33
1	AA	923	A	C6-N6	6.67	1.47	1.33
25	BA	1276	A	C6-N6	6.67	1.47	1.33
25	BA	2459	A	C6-N6	6.67	1.47	1.33
25	BA	53	A	C6-N6	6.67	1.47	1.33
25	BA	204	A	C6-N6	6.66	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	783	A	C6-N6	6.66	1.47	1.33
25	BA	1214	A	C6-N6	6.66	1.47	1.33
26	BB	59	A	C6-N6	6.66	1.47	1.33
1	AA	98	A	C6-N6	6.66	1.47	1.33
25	BA	1784	A	C6-N6	6.66	1.47	1.33
25	BA	1545	A	C6-N6	6.66	1.47	1.33
25	BA	2725	A	C6-N6	6.66	1.47	1.33
1	AA	1145	A	C6-N6	6.65	1.47	1.33
25	BA	1899	A	C6-N6	6.65	1.47	1.33
25	BA	2054	A	C6-N6	6.65	1.47	1.33
1	AA	608	A	C6-N6	6.64	1.47	1.33
1	AA	766	A	C6-N6	6.64	1.47	1.33
25	BA	2469	A	C6-N6	6.64	1.47	1.33
25	BA	56	A	C6-N6	6.64	1.47	1.33
25	BA	142	A	C6-N6	6.63	1.47	1.33
25	BA	2800	A	C6-N6	6.62	1.47	1.33
25	BA	514	A	C6-N6	6.57	1.47	1.33
9	AI	91	ASP	N-CA	5.42	1.53	1.46
37	BM	70	ASP	N-CA	5.28	1.53	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AL	21	VAL	CA-C-N	6.27	126.18	119.28
12	AL	21	VAL	C-N-CA	6.27	126.18	119.28
33	BI	73	THR	CA-C-N	6.10	124.11	119.66
33	BI	73	THR	C-N-CA	6.10	124.11	119.66
27	BC	135	ILE	CA-C-N	5.88	125.83	119.78
27	BC	135	ILE	C-N-CA	5.88	125.83	119.78
27	BC	135	ILE	N-CA-C	5.83	113.65	108.63
33	BI	25	GLY	CA-C-N	5.81	125.67	119.28
33	BI	25	GLY	C-N-CA	5.81	125.67	119.28
12	AL	102	LEU	CB-CA-C	-5.77	109.91	116.54
12	AL	41	THR	CA-C-N	5.72	125.67	119.78
12	AL	41	THR	C-N-CA	5.72	125.67	119.78
27	BC	106	ALA	CA-C-N	5.68	125.58	119.85
27	BC	106	ALA	C-N-CA	5.68	125.58	119.85
2	AB	129	LEU	CB-CA-C	-5.53	109.21	115.79
27	BC	28	LYS	CA-C-N	5.40	125.30	119.85
27	BC	28	LYS	C-N-CA	5.40	125.30	119.85
21	AU	10	GLU	CA-C-N	-5.40	113.09	119.84
21	AU	10	GLU	C-N-CA	-5.40	113.09	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BK	92	GLU	CB-CA-C	-5.32	109.46	115.79
8	AH	51	VAL	N-CA-C	5.30	111.88	106.21
46	BV	26	PHE	CA-C-N	5.28	125.22	119.78
46	BV	26	PHE	C-N-CA	5.28	125.22	119.78
8	AH	92	LEU	CA-C-N	5.12	125.02	119.85
8	AH	92	LEU	C-N-CA	5.12	125.02	119.85
43	BS	64	ALA	CB-CA-C	-5.12	110.27	117.23
13	AM	111	GLY	CA-C-N	5.11	125.05	119.78
13	AM	111	GLY	C-N-CA	5.11	125.05	119.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BD	151	THR	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	AA	33015	0	16618	250	0
2	AB	1704	0	1732	32	0
3	AC	1624	0	1696	36	0
4	AD	1643	0	1707	46	0
5	AE	1105	0	1148	25	0
6	AF	817	0	808	14	0
7	AG	1181	0	1238	22	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	23	0
10	AJ	786	0	828	32	0
11	AK	877	0	887	30	0
12	AL	955	0	1016	27	0
13	AM	883	0	941	20	0
14	AN	774	0	824	26	0
15	AO	710	0	728	9	0
16	AP	649	0	666	21	0
17	AQ	648	0	691	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	AR	455	0	478	7	0
19	AS	637	0	665	12	0
20	AT	665	0	714	22	0
21	AU	425	0	449	9	0
22	AV	218	0	109	2	0
23	AX	1656	0	855	5	0
24	AY	1525	0	780	7	0
25	BA	62195	0	31280	423	0
26	BB	2529	0	1281	24	0
27	BC	2082	0	2154	56	0
28	BD	1565	0	1616	41	0
29	BE	1552	0	1619	31	0
30	BF	1410	0	1444	21	0
31	BG	1323	0	1371	24	0
32	BH	359	0	381	12	0
33	BI	1032	0	1085	24	0
34	BJ	1129	0	1162	20	0
35	BK	938	0	1012	25	0
36	BL	1045	0	1117	30	0
37	BM	1074	0	1157	26	0
38	BN	960	0	1000	26	0
39	BO	892	0	923	19	0
40	BP	917	0	962	23	0
41	BQ	947	0	1019	11	0
42	BR	816	0	839	13	0
43	BS	857	0	922	18	0
44	BT	738	0	807	18	0
45	BU	779	0	831	24	0
46	BV	753	0	780	14	0
47	BW	569	0	581	14	0
48	BX	625	0	652	19	0
49	BY	509	0	543	8	0
50	BZ	449	0	488	9	0
51	B0	444	0	458	9	0
52	B1	409	0	440	11	0
53	B2	377	0	418	12	0
54	B3	504	0	572	14	0
55	B4	302	0	343	9	0
56	B5	74	0	74	8	0
57	BA	51	0	67	4	0
All	All	145158	0	97077	1457	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 6.

All (1457) 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)
1:AA:1493:A:H3'	25:BA:1913:A:N1	1.74	1.02
1:AA:1493:A:C3'	25:BA:1913:A:N1	2.26	0.98
1:AA:1409:C:O2	1:AA:1492:A:N6	2.00	0.95
1:AA:1493:A:O3'	25:BA:1913:A:N1	2.02	0.92
1:AA:1493:A:O2'	1:AA:1494:G:OP1	1.91	0.88
1:AA:1492:A:O2'	1:AA:1493:A:N7	2.08	0.86
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.47	0.80
1:AA:1127:G:H1	1:AA:1145:A:H61	1.32	0.79
53:B2:39:ARG:HG3	53:B2:41:ARG:H	1.50	0.77
39:BO:40:ILE:HG12	39:BO:47:VAL:HG12	1.68	0.76
1:AA:1493:A:H3'	25:BA:1913:A:C2	2.21	0.76
37:BM:64:TRP:HB2	37:BM:104:GLU:HB2	1.67	0.75
1:AA:664:G:H22	1:AA:741:G:H1	1.35	0.74
10:AJ:49:PHE:HB2	10:AJ:65:TYR:HB2	1.70	0.74
5:AE:81:LEU:HD13	5:AE:123:VAL:HG11	1.68	0.73
1:AA:1522:U:H5''	11:AK:128:ARG:HH22	1.54	0.72
10:AJ:45:ARG:HB3	10:AJ:69:THR:HB	1.69	0.72
29:BE:146:VAL:HG12	29:BE:185:LYS:HB2	1.71	0.72
4:AD:11:LEU:HB3	4:AD:63:ARG:HD3	1.71	0.72
20:AT:5:LYS:HG3	20:AT:7:ALA:H	1.54	0.72
28:BD:151:THR:HG22	28:BD:152:PRO:HD2	1.70	0.71
27:BC:107:PRO:HG2	27:BC:110:LEU:HB2	1.74	0.70
7:AG:113:ASP:HB2	7:AG:119:ARG:HG2	1.73	0.70
25:BA:136:G:H1	25:BA:143:C:H42	1.39	0.70
30:BF:63:GLN:HE21	30:BF:95:ARG:HH11	1.38	0.70
25:BA:1779:U:OP2	25:BA:1784:A:N6	2.25	0.70
3:AC:14:ILE:HG22	3:AC:15:VAL:HG13	1.74	0.70
35:BK:21:CYS:HA	35:BK:41:ILE:HG22	1.74	0.70
36:BL:93:ASN:O	36:BL:95:LEU:N	2.23	0.70
1:AA:1124:G:O2'	1:AA:1145:A:N6	2.23	0.69
12:AL:5:ASN:HD21	17:AQ:36:LYS:HE2	1.56	0.69
34:BJ:56:VAL:HB	34:BJ:124:VAL:HA	1.74	0.69
2:AB:219:ALA:O	2:AB:222:ARG:NH1	2.26	0.69
33:BI:49:ILE:HG13	33:BI:50:GLU:H	1.58	0.69
34:BJ:118:MET:HA	34:BJ:121:LYS:HE2	1.75	0.69
4:AD:58:LYS:NZ	4:AD:59:GLN:OE1	2.26	0.69
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.58	0.69
1:AA:69:G:O6	1:AA:98:A:N6	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1359:C:O2'	1:AA:1361:G:N7	2.26	0.68
29:BE:58:LYS:NZ	29:BE:70:SER:O	2.26	0.68
10:AJ:25:ILE:HD11	10:AJ:87:LEU:HG	1.75	0.68
47:BW:37:ILE:HG22	47:BW:38:VAL:HG23	1.74	0.68
4:AD:85:ASN:OD1	5:AE:103:THR:OG1	2.11	0.68
1:AA:1397:C:H42	22:AV:22:A:H3'	1.58	0.68
6:AF:90:MET:SD	18:AR:61:ARG:NH1	2.67	0.68
54:B3:24:HIS:HD2	54:B3:50:VAL:HG22	1.59	0.68
25:BA:1062:G:H21	33:BI:135:SER:HB3	1.58	0.67
30:BF:117:LEU:HD13	30:BF:176:PRO:HG2	1.76	0.67
29:BE:126:VAL:HG13	29:BE:133:LEU:HD22	1.76	0.67
1:AA:237:G:H4'	17:AQ:27:ARG:HH12	1.60	0.67
6:AF:91:ARG:HH21	6:AF:93:LYS:HD3	1.59	0.67
31:BG:164:TYR:HB2	31:BG:167:GLU:HG2	1.76	0.67
12:AL:34:CYS:HA	12:AL:55:VAL:HA	1.77	0.67
27:BC:67:PHE:HZ	27:BC:87:ARG:HH22	1.40	0.67
55:B4:19:ARG:HD2	55:B4:24:ARG:HD2	1.75	0.67
50:BZ:10:THR:HG23	50:BZ:11:ARG:HG3	1.77	0.67
1:AA:1221:G:H4'	19:AS:77:THR:HG21	1.76	0.66
25:BA:807:U:OP2	36:BL:41:ARG:NH1	2.29	0.66
40:BP:27:GLU:HA	40:BP:44:GLU:HA	1.75	0.66
39:BO:31:THR:O	39:BO:102:ARG:NH1	2.28	0.66
45:BU:10:GLU:HA	45:BU:24:LYS:HA	1.76	0.66
38:BN:28:LEU:HD23	38:BN:48:VAL:HG21	1.77	0.66
13:AM:101:ARG:NH1	13:AM:104:THR:OG1	2.28	0.66
25:BA:45:G:H5''	25:BA:46:G:H5'	1.78	0.66
28:BD:46:ARG:HB3	28:BD:84:LEU:HD12	1.78	0.66
34:BJ:36:LEU:O	34:BJ:121:LYS:NZ	2.26	0.66
4:AD:95:GLU:HA	4:AD:100:ASN:HD22	1.61	0.65
33:BI:34:ASN:HB3	33:BI:37:GLU:HG2	1.78	0.65
20:AT:69:LYS:HG3	20:AT:70:ASN:H	1.61	0.65
3:AC:34:ASP:OD2	14:AN:65:ARG:NH1	2.30	0.65
1:AA:1373:G:H5''	7:AG:36:LYS:HE2	1.79	0.65
20:AT:73:ALA:HA	20:AT:76:LYS:HG2	1.79	0.65
17:AQ:70:THR:HG22	17:AQ:71:LYS:H	1.60	0.65
25:BA:1614:A:N6	43:BS:92:ARG:O	2.29	0.65
14:AN:3:LYS:HD2	14:AN:6:MET:HG2	1.78	0.65
14:AN:13:ARG:HE	14:AN:59:ARG:HE	1.45	0.65
3:AC:11:ARG:NH1	3:AC:180:ALA:O	2.30	0.64
40:BP:33:VAL:HG12	40:BP:35:GLY:H	1.60	0.64
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:482:A:H4'	45:BU:45:HIS:HE1	1.62	0.64
32:BH:9:VAL:HB	32:BH:13:GLY:HA3	1.78	0.64
1:AA:19:A:OP1	5:AE:135:ASN:ND2	2.31	0.64
25:BA:2312:U:H2'	30:BF:37:ASN:HD21	1.61	0.64
37:BM:11:LYS:HD3	37:BM:86:LYS:HD3	1.80	0.64
25:BA:1082:U:H5'	33:BI:119:GLY:HA2	1.79	0.64
25:BA:1601:G:OP1	44:BT:64:LYS:NZ	2.31	0.64
5:AE:133:PRO:HA	5:AE:136:VAL:HG12	1.79	0.64
25:BA:682:G:O6	25:BA:794:A:N6	2.31	0.64
33:BI:8:TYR:HB2	33:BI:59:ILE:H	1.62	0.64
1:AA:10:A:OP2	5:AE:131:THR:OG1	2.15	0.64
1:AA:570:G:O6	1:AA:865:A:N6	2.32	0.64
2:AB:130:THR:HG22	2:AB:132:LYS:H	1.63	0.64
1:AA:1072:G:O6	1:AA:1102:A:N6	2.31	0.63
27:BC:159:GLY:H	27:BC:195:VAL:HG13	1.64	0.63
13:AM:25:VAL:HG23	13:AM:29:ARG:HB3	1.80	0.63
1:AA:1493:A:C3'	25:BA:1913:A:C2	2.79	0.63
25:BA:2271:G:H5'	47:BW:20:ARG:HG2	1.80	0.63
29:BE:18:THR:HA	29:BE:106:LYS:HD2	1.80	0.63
39:BO:90:VAL:HG23	39:BO:117:PHE:HB3	1.78	0.63
41:BQ:28:ARG:HH21	41:BQ:38:ALA:HB1	1.64	0.63
3:AC:129:MET:SD	3:AC:132:ARG:NH1	2.72	0.63
2:AB:166:ALA:HB3	2:AB:191:SER:HB3	1.81	0.63
25:BA:1226:A:OP1	41:BQ:16:LYS:NZ	2.31	0.63
56:B5:-8:ALA:O	56:B5:-6:PHE:N	2.25	0.63
6:AF:27:ALA:O	6:AF:30:THR:OG1	2.15	0.63
25:BA:1068:G:O6	25:BA:1073:A:N6	2.32	0.63
27:BC:210:ALA:O	27:BC:214:ARG:NH1	2.32	0.63
50:BZ:5:ILE:HD13	50:BZ:45:ARG:HH22	1.64	0.63
52:B1:50:LYS:HG2	52:B1:51:GLU:H	1.64	0.63
6:AF:21:MET:HG2	6:AF:24:ARG:HH21	1.63	0.62
25:BA:1154:G:OP2	41:BQ:58:ARG:NH1	2.32	0.62
25:BA:2495:G:OP1	37:BM:81:ARG:NH1	2.31	0.62
1:AA:1492:A:O2'	1:AA:1493:A:C8	2.51	0.62
25:BA:2469:A:O2'	37:BM:55:ARG:NH2	2.30	0.62
25:BA:1789:A:OP2	27:BC:221:ARG:NH1	2.32	0.62
34:BJ:11:VAL:HG11	34:BJ:50:THR:HA	1.80	0.62
2:AB:70:VAL:HB	2:AB:163:VAL:HA	1.82	0.62
11:AK:124:PRO:HB2	11:AK:126:LYS:HG2	1.82	0.62
25:BA:1394:U:H4'	25:BA:1603:A:H4'	1.81	0.62
31:BG:8:PRO:HB2	31:BG:49:THR:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BN:43:GLU:OE1	38:BN:46:ARG:NH1	2.32	0.62
25:BA:1788:C:OP1	27:BC:221:ARG:NH2	2.33	0.62
25:BA:210:C:OP1	53:B2:29:GLN:NE2	2.30	0.62
27:BC:73:GLY:O	27:BC:117:GLN:NE2	2.33	0.62
27:BC:94:VAL:HG11	27:BC:116:ILE:HD11	1.82	0.62
30:BF:34:ILE:HG12	30:BF:156:ILE:HG12	1.80	0.62
5:AE:77:ASN:HB2	5:AE:82:GLN:HG2	1.82	0.62
25:BA:24:G:O2'	43:BS:78:GLU:O	2.17	0.62
26:BB:8:C:O2'	39:BO:25:ARG:NH1	2.33	0.62
1:AA:1097:C:OP1	2:AB:139:ARG:NH2	2.29	0.61
2:AB:146:ASN:OD1	2:AB:147:SER:N	2.33	0.61
10:AJ:47:GLU:OE1	14:AN:76:LYS:NZ	2.32	0.61
25:BA:1992:G:N2	25:BA:1996:C:O2'	2.33	0.61
49:BY:16:THR:O	49:BY:20:ASN:ND2	2.33	0.61
25:BA:335:C:O2	45:BU:68:SER:OG	2.17	0.61
25:BA:2771:C:O2'	28:BD:173:GLN:NE2	2.30	0.61
42:BR:6:GLN:HB3	42:BR:37:GLU:HB3	1.82	0.61
3:AC:28:GLU:O	3:AC:32:ASN:ND2	2.32	0.61
38:BN:114:GLU:OE1	38:BN:118:ARG:NH2	2.33	0.61
52:B1:37:LYS:HG2	52:B1:48:ILE:HG13	1.82	0.61
53:B2:34:ARG:HH21	53:B2:39:ARG:HG2	1.66	0.61
1:AA:243:A:H4'	1:AA:244:U:H3'	1.83	0.61
1:AA:978:A:OP2	1:AA:1362:A:N6	2.34	0.61
25:BA:1264:A:H5''	51:B0:16:ARG:HH22	1.66	0.61
1:AA:970:C:OP1	10:AJ:59:LYS:NZ	2.32	0.61
3:AC:180:ALA:HB1	3:AC:203:PHE:HE1	1.65	0.61
9:AI:123:ARG:NH1	9:AI:124:ARG:O	2.33	0.61
25:BA:793:A:OP2	25:BA:2071:A:O2'	2.17	0.61
25:BA:2688:G:N1	25:BA:2720:U:OP2	2.32	0.61
25:BA:877:A:O2'	25:BA:900:A:N6	2.33	0.61
25:BA:2441:U:OP2	56:B5:-3:ARG:NH2	2.33	0.61
36:BL:79:LEU:HD12	36:BL:113:ALA:H	1.65	0.61
3:AC:185:ASN:OD1	3:AC:186:THR:N	2.34	0.61
6:AF:81:ASN:HB3	6:AF:84:VAL:HG12	1.82	0.61
1:AA:848:C:OP1	2:AB:37:LYS:NZ	2.33	0.61
1:AA:1491:G:C8	1:AA:1491:G:H5''	2.36	0.61
26:BB:30:C:H1'	26:BB:57:A:H61	1.65	0.61
7:AG:71:PRO:O	7:AG:96:ARG:NH1	2.34	0.60
25:BA:863:A:OP1	37:BM:22:GLN:NE2	2.34	0.60
11:AK:97:ILE:HA	11:AK:100:LEU:HD13	1.83	0.60
28:BD:33:ARG:NH1	28:BD:74:GLU:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:40:ILE:HD12	10:AJ:73:LEU:HD22	1.83	0.60
25:BA:2581:G:OP2	25:BA:2581:G:N2	2.33	0.60
40:BP:37:LYS:HE3	40:BP:39:ARG:HB2	1.83	0.60
27:BC:145:GLU:HB2	27:BC:188:CYS:HB3	1.83	0.60
47:BW:23:VAL:HG13	47:BW:38:VAL:HG22	1.84	0.60
25:BA:320:A:O2'	25:BA:322:A:OP2	2.15	0.60
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.82	0.60
28:BD:131:ASP:O	28:BD:136:ASN:ND2	2.34	0.60
25:BA:1716:U:H2'	25:BA:1717:A:H8	1.66	0.60
1:AA:926:G:N2	22:AV:16:G:OP1	2.35	0.60
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.35	0.60
49:BY:25:GLN:HE22	49:BY:47:ARG:HG2	1.66	0.60
3:AC:56:VAL:HB	3:AC:67:THR:HB	1.83	0.60
25:BA:1450:G:N2	25:BA:1452:G:O6	2.34	0.60
25:BA:2595:G:N2	25:BA:2598:A:OP2	2.35	0.60
29:BE:46:GLN:HB2	29:BE:87:ALA:H	1.66	0.60
30:BF:106:ILE:HD12	30:BF:139:PRO:HG2	1.83	0.60
27:BC:235:GLY:O	27:BC:239:ASN:ND2	2.34	0.60
1:AA:350:G:OP1	20:AT:3:ASN:N	2.35	0.59
2:AB:163:VAL:HG21	2:AB:173:ILE:HD11	1.83	0.59
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.83	0.59
21:AU:4:ILE:HD13	21:AU:19:PHE:HE2	1.67	0.59
25:BA:2091:C:H3'	25:BA:2092:U:H5''	1.82	0.59
1:AA:68:G:H1'	1:AA:151:A:H61	1.66	0.59
1:AA:1020:G:H2'	1:AA:1021:A:H8	1.67	0.59
2:AB:68:LEU:HD12	2:AB:154:MET:HE1	1.84	0.59
25:BA:2303:G:O2'	30:BF:121:SER:O	2.20	0.59
25:BA:1998:A:OP2	28:BD:141:ARG:NH1	2.35	0.59
35:BK:40:LYS:HA	35:BK:59:LYS:HA	1.83	0.59
51:B0:32:LYS:HE2	51:B0:51:GLY:HA3	1.83	0.59
2:AB:72:THR:HG23	2:AB:95:ARG:HA	1.84	0.59
3:AC:59:ARG:HE	3:AC:64:ILE:HD12	1.66	0.59
27:BC:133:ARG:O	27:BC:167:ARG:NH1	2.33	0.59
1:AA:1491:G:C8	1:AA:1491:G:C5'	2.85	0.59
25:BA:1693:U:O2'	27:BC:14:ARG:NH1	2.35	0.59
36:BL:74:THR:HG22	36:BL:107:PHE:HB2	1.85	0.59
27:BC:244:PRO:O	27:BC:251:GLN:NE2	2.35	0.59
35:BK:43:ILE:HD12	35:BK:56:ASP:HB2	1.85	0.59
25:BA:1936:A:H2	25:BA:1943:U:H3	1.49	0.59
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.34	0.59
25:BA:2298:A:OP1	30:BF:71:ARG:NH2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B2:30:VAL:HG22	53:B2:33:ARG:HH11	1.66	0.59
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.36	0.59
1:AA:1492:A:C8	1:AA:1492:A:H3'	2.37	0.59
12:AL:110:ARG:HH21	12:AL:113:ALA:HB3	1.67	0.59
25:BA:2485:G:H5''	37:BM:45:GLN:HE21	1.68	0.59
1:AA:362:G:N2	1:AA:365:U:OP2	2.31	0.59
27:BC:53:HIS:HA	27:BC:217:ARG:HB2	1.85	0.59
27:BC:252:THR:HG22	27:BC:253:LYS:HG3	1.85	0.59
39:BO:29:HIS:HB3	39:BO:36:TYR:HB2	1.85	0.59
4:AD:54:GLN:NE2	4:AD:202:GLU:OE1	2.27	0.58
7:AG:57:SER:HB3	7:AG:60:GLU:HG2	1.85	0.58
7:AG:135:VAL:HA	7:AG:138:ARG:HG2	1.85	0.58
16:AP:20:VAL:HG12	16:AP:35:ARG:HA	1.83	0.58
45:BU:74:ASN:ND2	45:BU:77:THR:OG1	2.36	0.58
1:AA:255:G:H4'	17:AQ:19:LYS:HE3	1.85	0.58
1:AA:618:C:O2'	16:AP:14:ARG:NH2	2.36	0.58
3:AC:22:TRP:HB3	3:AC:59:ARG:H	1.68	0.58
25:BA:1343:G:O6	25:BA:1403:A:N6	2.36	0.58
25:BA:2092:U:O2	25:BA:2225:A:O2'	2.21	0.58
44:BT:59:ASN:HB2	44:BT:84:TYR:HB2	1.86	0.58
1:AA:1359:C:H3'	14:AN:75:ARG:HH22	1.68	0.58
9:AI:112:GLU:OE2	9:AI:115:LYS:NZ	2.36	0.58
25:BA:1334:G:OP1	44:BT:69:ARG:NH2	2.35	0.58
42:BR:11:GLN:HE22	42:BR:39:LEU:HD22	1.68	0.58
1:AA:1492:A:H2'	1:AA:1493:A:O5'	2.03	0.58
25:BA:463:G:N2	25:BA:466:A:OP2	2.30	0.58
25:BA:1326:U:H2'	25:BA:1327:A:H8	1.67	0.58
35:BK:105:ARG:NH2	40:BP:41:GLN:OE1	2.37	0.58
45:BU:29:LEU:HD12	45:BU:33:LYS:HB2	1.85	0.58
48:BX:34:HIS:HD2	48:BX:53:ALA:HB2	1.67	0.58
4:AD:14:ARG:HG3	4:AD:56:ARG:HH12	1.68	0.58
9:AI:92:GLU:OE1	9:AI:95:ARG:NH1	2.37	0.58
25:BA:1226:A:H5'	42:BR:86:GLN:HE22	1.68	0.58
25:BA:2489:U:O2'	25:BA:2518:A:N6	2.36	0.58
35:BK:80:ASP:HB2	40:BP:68:GLU:HB2	1.86	0.58
36:BL:63:LYS:HA	54:B3:13:ARG:HG2	1.85	0.58
1:AA:8:A:N6	4:AD:202:GLU:O	2.36	0.58
1:AA:132:C:H5''	20:AT:69:LYS:HE3	1.86	0.58
1:AA:717:U:H4'	11:AK:119:ASN:HD22	1.68	0.58
1:AA:1492:A:H3'	1:AA:1492:A:H8	1.69	0.58
4:AD:201:VAL:HG21	5:AE:103:THR:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:27:VAL:HG12	7:AG:43:VAL:HG21	1.85	0.58
10:AJ:5:ARG:HG3	10:AJ:6:ILE:HG13	1.85	0.58
25:BA:1007:C:OP1	34:BJ:37:ARG:NH2	2.36	0.58
25:BA:135:U:H3	25:BA:144:A:H61	1.50	0.57
38:BN:103:ARG:HG2	38:BN:105:GLY:H	1.68	0.57
1:AA:1064:G:O2'	1:AA:1190:G:N2	2.37	0.57
25:BA:2898:U:O2'	34:BJ:134:ALA:O	2.21	0.57
27:BC:57:GLY:HA2	27:BC:213:TRP:HA	1.86	0.57
28:BD:3:GLY:HA3	28:BD:204:LYS:HG2	1.86	0.57
30:BF:99:PHE:HA	30:BF:102:ARG:HE	1.69	0.57
38:BN:12:ARG:O	38:BN:17:ARG:NH2	2.37	0.57
25:BA:750:A:OP1	25:BA:1615:C:N4	2.35	0.57
21:AU:14:VAL:HG12	21:AU:16:LEU:H	1.68	0.57
24:AY:18:G:H1	24:AY:55:PSU:H1'	1.69	0.57
25:BA:2857:G:N2	25:BA:2860:A:OP2	2.34	0.57
31:BG:3:ARG:HA	31:BG:6:LYS:HE2	1.86	0.57
36:BL:81:ASP:O	36:BL:83:ALA:N	2.32	0.57
45:BU:33:LYS:HB3	45:BU:64:ALA:HB1	1.85	0.57
52:B1:39:PHE:HA	52:B1:46:HIS:HA	1.86	0.57
1:AA:972:C:H4'	10:AJ:59:LYS:HD3	1.86	0.57
1:AA:976:G:N2	1:AA:1362:A:O2'	2.38	0.57
8:AH:106:THR:OG1	8:AH:109:GLY:O	2.19	0.57
1:AA:553:A:H5''	12:AL:21:VAL:HG21	1.86	0.57
30:BF:56:ASP:OD2	30:BF:150:ARG:NH2	2.38	0.57
30:BF:57:LEU:HD13	30:BF:89:VAL:HG23	1.85	0.57
1:AA:375:U:O2	16:AP:28:ARG:NH2	2.38	0.57
1:AA:1396:A:O2'	5:AE:29:ARG:NH2	2.38	0.57
25:BA:1864:U:OP1	25:BA:2410:G:O2'	2.23	0.57
29:BE:147:LEU:HB2	29:BE:183:PHE:HD2	1.70	0.57
1:AA:59:A:H5''	1:AA:387:U:H5''	1.86	0.57
5:AE:154:ALA:HA	5:AE:157:ARG:HB3	1.86	0.57
12:AL:57:LEU:HD12	12:AL:61:PHE:HB2	1.86	0.57
25:BA:815:C:OP2	42:BR:85:LYS:NZ	2.38	0.57
25:BA:2199:A:OP1	48:BX:37:ARG:NH1	2.37	0.57
27:BC:8:PRO:HB3	27:BC:14:ARG:HG3	1.87	0.57
39:BO:26:LEU:N	39:BO:91:SER:O	2.37	0.57
48:BX:17:ASN:HB2	48:BX:25:THR:HB	1.86	0.57
1:AA:537:G:H5''	12:AL:110:ARG:HH12	1.68	0.56
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.68	0.56
32:BH:4:ILE:HD11	32:BH:44:ILE:HG22	1.86	0.56
3:AC:150:LYS:HG3	3:AC:169:ARG:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:105:ILE:HD13	5:AE:121:HIS:HA	1.88	0.56
6:AF:46:GLN:HA	6:AF:56:LYS:HG2	1.87	0.56
11:AK:28:ASN:O	11:AK:57:LYS:NZ	2.37	0.56
12:AL:38:TYR:HB2	12:AL:52:VAL:HG13	1.87	0.56
25:BA:1365:A:OP1	48:BX:28:ARG:NH2	2.34	0.56
29:BE:76:PRO:HA	29:BE:82:GLY:HA2	1.86	0.56
52:B1:8:LYS:HG2	52:B1:24:THR:HG22	1.85	0.56
55:B4:2:LYS:NZ	55:B4:32:LYS:O	2.31	0.56
1:AA:1317:C:O2'	14:AN:49:GLN:NE2	2.27	0.56
8:AH:18:GLN:HE21	8:AH:70:ALA:HB1	1.71	0.56
14:AN:16:LEU:HD22	14:AN:20:TYR:CE2	2.40	0.56
1:AA:406:G:H21	4:AD:116:GLN:HE22	1.52	0.56
3:AC:157:LEU:O	3:AC:164:ARG:NH2	2.34	0.56
25:BA:600:G:OP1	29:BE:24:ASN:ND2	2.39	0.56
25:BA:2384:U:OP2	47:BW:55:ARG:NH2	2.38	0.56
19:AS:3:ARG:NH2	19:AS:68:GLY:O	2.38	0.56
20:AT:27:MET:O	20:AT:30:THR:OG1	2.20	0.56
27:BC:72:ASP:OD2	27:BC:189:ARG:NH1	2.39	0.56
28:BD:151:THR:O	28:BD:153:GLY:N	2.38	0.56
12:AL:114:ARG:HG3	12:AL:119:VAL:HB	1.86	0.56
25:BA:2279:G:N7	47:BW:14:ARG:NH2	2.54	0.56
44:BT:7:LEU:HD21	44:BT:46:ALA:HA	1.87	0.56
4:AD:147:GLU:HA	4:AD:150:LYS:HE2	1.87	0.56
9:AI:57:MET:O	9:AI:59:GLU:N	2.39	0.56
25:BA:1030:C:OP2	37:BM:127:LYS:NZ	2.38	0.56
25:BA:1125:G:H5''	55:B4:37:GLN:HE21	1.71	0.56
16:AP:12:LYS:HG2	16:AP:13:LYS:HG2	1.88	0.56
25:BA:589:U:O3'	29:BE:90:GLN:NE2	2.39	0.56
28:BD:46:ARG:NH2	28:BD:88:GLU:O	2.36	0.56
31:BG:28:GLY:HA3	31:BG:79:VAL:HB	1.88	0.56
1:AA:890:G:O2'	1:AA:906:A:N6	2.39	0.55
1:AA:1351:U:O4	9:AI:120:LYS:NZ	2.39	0.55
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.71	0.55
25:BA:851:C:O2'	50:BZ:43:ALA:O	2.24	0.55
26:BB:13:G:O2'	26:BB:15:A:OP2	2.24	0.55
28:BD:121:THR:HG21	28:BD:143:PRO:HB3	1.89	0.55
1:AA:1462:C:O2'	40:BP:111:LYS:NZ	2.39	0.55
29:BE:25:GLU:OE2	36:BL:7:SER:N	2.38	0.55
35:BK:30:ARG:NH2	35:BK:37:ASP:OD2	2.39	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
25:BA:1028:A:OP2	25:BA:1126:A:N6	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BM:36:VAL:HG23	37:BM:129:THR:H	1.71	0.55
48:BX:33:LEU:HD23	48:BX:50:ARG:HE	1.70	0.55
2:AB:73:LYS:O	2:AB:77:SER:OG	2.23	0.55
4:AD:95:GLU:OE1	4:AD:100:ASN:ND2	2.39	0.55
19:AS:53:ASN:HB3	19:AS:75:ALA:HB1	1.89	0.55
25:BA:1078:U:O2'	25:BA:1088:A:OP1	2.24	0.55
25:BA:2478:A:O2'	25:BA:2536:G:N2	2.39	0.55
45:BU:18:ASP:HB3	45:BU:21:LYS:HD2	1.87	0.55
16:AP:15:PRO:HG2	16:AP:41:PRO:HG3	1.89	0.55
44:BT:40:LYS:NZ	44:BT:58:VAL:O	2.32	0.55
46:BV:51:GLN:HE22	46:BV:86:LEU:HD21	1.72	0.55
7:AG:111:ARG:O	7:AG:119:ARG:NH2	2.39	0.55
25:BA:1613:G:O2'	53:B2:3:ARG:NH1	2.40	0.55
25:BA:2355:G:O2'	47:BW:24:LYS:NZ	2.39	0.55
26:BB:14:U:OP2	26:BB:70:C:O2'	2.23	0.55
27:BC:211:ALA:HB1	27:BC:216:VAL:HB	1.89	0.55
1:AA:180:U:O2	1:AA:196:A:N6	2.39	0.55
54:B3:28:ASN:HB3	54:B3:36:LYS:HE2	1.89	0.55
25:BA:2293:G:H5''	39:BO:94:ARG:HH22	1.71	0.55
46:BV:77:VAL:HG23	46:BV:89:ILE:HG12	1.89	0.55
1:AA:1439:G:OP2	20:AT:33:LYS:NZ	2.36	0.55
25:BA:627:A:O4'	25:BA:637:A:N6	2.40	0.55
26:BB:90:C:O3'	37:BM:38:ARG:NH2	2.40	0.55
49:BY:43:LEU:O	49:BY:47:ARG:NH2	2.40	0.55
1:AA:1239:A:H61	1:AA:1296:C:H2'	1.71	0.54
1:AA:1458:G:H5'	20:AT:27:MET:HB3	1.87	0.54
17:AQ:25:ILE:HB	17:AQ:42:THR:HB	1.89	0.54
25:BA:2377:A:O2'	39:BO:117:PHE:O	2.24	0.54
25:BA:2645:G:OP2	25:BA:2645:G:N2	2.31	0.54
39:BO:24:THR:HG22	39:BO:42:PRO:HD3	1.89	0.54
25:BA:2258:C:O2'	25:BA:2427:C:OP2	2.23	0.54
34:BJ:45:THR:HB	34:BJ:48:VAL:HB	1.87	0.54
44:BT:47:VAL:HG21	44:BT:85:VAL:HG11	1.88	0.54
25:BA:411:G:OP2	25:BA:2406:A:O2'	2.24	0.54
25:BA:1653:G:O6	38:BN:11:ASN:N	2.36	0.54
53:B2:3:ARG:HG3	53:B2:5:PHE:H	1.71	0.54
2:AB:66:LYS:NZ	2:AB:154:MET:O	2.35	0.54
25:BA:372:G:O6	48:BX:57:ARG:NH1	2.41	0.54
25:BA:845:A:H61	25:BA:932:U:H3	1.54	0.54
25:BA:2063:C:N4	25:BA:2501:C:O2	2.40	0.54
33:BI:19:ASN:HB2	33:BI:39:CYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BK:2:ILE:HD12	35:BK:8:LEU:HD11	1.89	0.54
1:AA:451:A:H61	1:AA:481:G:H5'	1.72	0.54
3:AC:156:ARG:NH1	3:AC:160:ALA:O	2.40	0.54
10:AJ:78:GLU:OE2	10:AJ:80:THR:OG1	2.25	0.54
54:B3:39:LYS:HG3	54:B3:42:ARG:HH12	1.73	0.54
1:AA:115:G:H4'	1:AA:116:A:O5'	2.08	0.54
1:AA:766:A:OP2	1:AA:812:G:N2	2.40	0.54
2:AB:120:GLN:HG3	2:AB:124:GLY:HA3	1.90	0.54
25:BA:415:A:H61	25:BA:2408:U:H3	1.54	0.54
1:AA:982:U:H4'	1:AA:983:A:H5'	1.89	0.54
1:AA:1359:C:OP2	14:AN:75:ARG:NH1	2.41	0.54
25:BA:1801:A:OP2	27:BC:150:LYS:NZ	2.38	0.54
25:BA:2294:G:OP1	39:BO:98:GLN:NE2	2.38	0.54
26:BB:27:C:OP1	39:BO:34:HIS:NE2	2.40	0.54
4:AD:124:MET:HA	4:AD:129:VAL:HA	1.88	0.54
25:BA:370:G:O2'	25:BA:424:G:OP1	2.25	0.54
25:BA:479:A:H1'	25:BA:481:G:H5'	1.88	0.54
25:BA:1653:G:OP2	38:BN:8:ARG:NH2	2.40	0.54
36:BL:124:GLY:HA2	36:BL:144:GLU:HA	1.89	0.54
48:BX:59:ILE:HG12	48:BX:67:VAL:HG21	1.89	0.54
49:BY:31:GLN:HG2	49:BY:37:LEU:HB2	1.89	0.54
1:AA:1347:G:N7	9:AI:12:ARG:NH2	2.48	0.54
4:AD:91:LEU:HD13	4:AD:191:LEU:HD11	1.89	0.54
8:AH:13:ARG:HB3	8:AH:25:VAL:HG11	1.89	0.54
43:BS:29:VAL:HG21	43:BS:69:LEU:HG	1.90	0.54
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.35	0.54
25:BA:1798:U:OP2	27:BC:271:ARG:NH2	2.34	0.54
27:BC:145:GLU:HA	27:BC:152:GLY:HA2	1.90	0.54
36:BL:54:GLN:HE21	36:BL:60:ARG:HH12	1.57	0.54
38:BN:28:LEU:HD13	38:BN:34:ILE:HG12	1.90	0.54
4:AD:101:VAL:HG21	4:AD:137:VAL:HG21	1.90	0.53
25:BA:958:U:OP2	37:BM:14:LYS:NZ	2.29	0.53
1:AA:765:G:N1	1:AA:812:G:O2'	2.38	0.53
25:BA:2108:A:H4'	25:BA:2150:C:H4'	1.89	0.53
8:AH:50:LYS:HG2	8:AH:52:GLU:HG2	1.89	0.53
9:AI:95:ARG:HA	9:AI:98:LEU:HB3	1.91	0.53
28:BD:108:ASP:OD1	28:BD:174:SER:N	2.32	0.53
31:BG:89:LEU:HD23	31:BG:94:TYR:HB3	1.89	0.53
16:AP:42:ILE:O	16:AP:44:SER:N	2.39	0.53
25:BA:137:U:H3	25:BA:142:A:H61	1.55	0.53
27:BC:111:LYS:N	27:BC:114:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BP:64:ILE:HA	40:BP:69:GLY:HA2	1.89	0.53
4:AD:132:ILE:HG22	4:AD:134:SER:H	1.74	0.53
25:BA:2586:U:H1'	56:B5:-3:ARG:HD3	1.90	0.53
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.40	0.53
1:AA:1307:U:OP1	13:AM:100:GLN:NE2	2.40	0.53
17:AQ:31:HIS:HD2	17:AQ:34:TYR:H	1.57	0.53
25:BA:1801:A:N6	25:BA:2201:G:O2'	2.35	0.53
25:BA:2343:U:O2'	25:BA:2373:G:O2'	2.26	0.53
12:AL:54:ARG:HA	12:AL:64:THR:HA	1.88	0.53
20:AT:84:ASN:HA	20:AT:87:ALA:HB3	1.89	0.53
25:BA:505:A:O2'	25:BA:509:C:O2'	2.22	0.53
25:BA:1651:G:N7	38:BN:11:ASN:ND2	2.57	0.53
25:BA:1796:U:H2'	25:BA:1797:G:H8	1.74	0.53
1:AA:922:G:H4'	5:AE:25:VAL:HA	1.91	0.53
1:AA:1125:U:H4'	10:AJ:7:ARG:HH12	1.74	0.53
33:BI:12:GLN:HE21	33:BI:55:ILE:H	1.56	0.53
38:BN:24:MET:HE3	38:BN:44:LEU:HD13	1.90	0.53
1:AA:429:U:H5'	4:AD:9:LEU:HD23	1.90	0.53
3:AC:79:LYS:O	3:AC:81:GLY:N	2.42	0.53
25:BA:250:G:O5'	36:BL:59:ARG:NH1	2.42	0.53
48:BX:37:ARG:HA	48:BX:48:THR:HA	1.90	0.53
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.37	0.53
5:AE:24:THR:HA	5:AE:29:ARG:HA	1.91	0.53
25:BA:1826:G:O2'	25:BA:1971:U:OP2	2.21	0.53
25:BA:2079:U:O2'	48:BX:23:ASN:OD1	2.26	0.53
36:BL:61:LEU:O	54:B3:13:ARG:NE	2.42	0.53
46:BV:64:VAL:HG22	46:BV:69:GLU:HG2	1.91	0.53
14:AN:27:LEU:HA	14:AN:31:ILE:HD13	1.91	0.52
27:BC:158:ALA:HB1	27:BC:197:ASN:HB3	1.90	0.52
31:BG:85:LYS:HB2	31:BG:133:LEU:HD11	1.91	0.52
50:BZ:16:ARG:O	50:BZ:21:LYS:NZ	2.42	0.52
1:AA:1475:G:H4'	25:BA:1689:A:H4'	1.90	0.52
8:AH:77:ARG:NH2	8:AH:79:SER:O	2.41	0.52
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.92	0.52
1:AA:426:U:H4'	4:AD:40:GLN:HA	1.90	0.52
1:AA:1492:A:C8	1:AA:1492:A:C3'	2.92	0.52
9:AI:34:SER:OG	9:AI:36:GLU:OE1	2.27	0.52
25:BA:85:G:OP1	45:BU:7:ARG:N	2.40	0.52
25:BA:1363:C:H2'	25:BA:1364:G:H8	1.75	0.52
27:BC:52:ARG:HH12	27:BC:247:PRO:HG2	1.74	0.52
27:BC:180:GLU:HB2	27:BC:271:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BE:119:ILE:HB	29:BE:187:VAL:HG22	1.91	0.52
45:BU:11:VAL:HG12	45:BU:72:ILE:HA	1.92	0.52
1:AA:405:U:O4	4:AD:2:ALA:N	2.42	0.52
1:AA:754:C:OP1	15:AO:72:ARG:NH2	2.42	0.52
3:AC:138:VAL:HA	3:AC:149:ILE:HD13	1.90	0.52
3:AC:150:LYS:HB3	3:AC:201:TRP:HB2	1.92	0.52
16:AP:4:ILE:HG13	16:AP:21:VAL:HG22	1.92	0.52
17:AQ:17:MET:HG3	17:AQ:20:SER:HB3	1.91	0.52
24:AY:12:U:H3	24:AY:23:A:H61	1.58	0.52
25:BA:805:G:H5''	36:BL:38:GLN:HG3	1.90	0.52
25:BA:2131:U:H5'	25:BA:2132:U:H5''	1.92	0.52
25:BA:2266:A:N6	25:BA:2273:A:OP2	2.42	0.52
25:BA:2680:U:O2'	28:BD:11:MET:SD	2.68	0.52
1:AA:1228:C:OP2	13:AM:110:LYS:NZ	2.30	0.52
25:BA:632:A:H2'	25:BA:633:A:H8	1.75	0.52
25:BA:2419:U:OP1	54:B3:41:LYS:NZ	2.42	0.52
24:AY:71:C:O2'	25:BA:1851:U:O2'	2.26	0.52
25:BA:2172:U:H4'	25:BA:2173:A:H5'	1.90	0.52
26:BB:28:C:H2'	26:BB:29:A:C8	2.45	0.52
1:AA:126:G:OP1	1:AA:605:U:O2'	2.28	0.52
1:AA:458:U:H2'	1:AA:459:A:H8	1.75	0.52
7:AG:78:ARG:HB2	7:AG:85:TYR:HB2	1.91	0.52
25:BA:1169:A:H61	25:BA:1178:C:H41	1.56	0.52
25:BA:1306:C:H41	25:BA:1606:C:H2'	1.75	0.52
25:BA:1564:C:OP2	27:BC:26:LYS:NZ	2.43	0.52
25:BA:2250:G:O2'	25:BA:2496:C:OP1	2.27	0.52
25:BA:2796:U:H3	25:BA:2799:A:H61	1.57	0.52
29:BE:117:ARG:NH2	29:BE:183:PHE:O	2.43	0.52
36:BL:14:LYS:HG3	36:BL:16:GLY:H	1.74	0.52
1:AA:1409:C:C2	1:AA:1492:A:N6	2.72	0.52
1:AA:1503:A:H5'	1:AA:1531:A:H1'	1.92	0.52
14:AN:51:LEU:O	14:AN:53:ARG:N	2.42	0.52
25:BA:2334:U:H5'	39:BO:12:THR:HB	1.92	0.52
46:BV:25:LYS:HG2	46:BV:43:ASP:HA	1.92	0.52
1:AA:780:A:N6	1:AA:801:U:OP2	2.39	0.52
14:AN:52:PRO:O	14:AN:54:ASP:N	2.36	0.52
25:BA:373:U:H2'	25:BA:374:A:H8	1.75	0.52
25:BA:636:G:N2	36:BL:76:GLU:OE2	2.40	0.52
25:BA:2133:G:H2'	25:BA:2157:G:H22	1.75	0.52
1:AA:809:G:OP2	15:AO:48:LYS:NZ	2.42	0.51
13:AM:17:ILE:O	13:AM:20:THR:OG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BR:1:MET:HE2	42:BR:101:ILE:HB	1.92	0.51
1:AA:262:A:H5''	20:AT:74:ARG:HH22	1.75	0.51
1:AA:859:G:OP2	1:AA:869:G:N1	2.32	0.51
1:AA:1020:G:H2'	1:AA:1021:A:C8	2.45	0.51
2:AB:128:LYS:HG3	2:AB:129:LEU:HG	1.93	0.51
4:AD:83:LYS:O	4:AD:89:ASN:ND2	2.39	0.51
25:BA:685:A:O2'	25:BA:772:C:N4	2.43	0.51
25:BA:1902:C:H5''	27:BC:240:PHE:HE2	1.75	0.51
25:BA:2461:A:N6	25:BA:2488:G:O6	2.43	0.51
25:BA:2526:G:N3	55:B4:1:MET:N	2.57	0.51
28:BD:51:THR:HB	28:BD:79:LEU:HD23	1.92	0.51
42:BR:10:LYS:HG3	42:BR:12:HIS:CE1	2.45	0.51
4:AD:95:GLU:HG2	4:AD:186:PRO:HG3	1.91	0.51
8:AH:103:VAL:HG12	8:AH:126:ILE:HD13	1.92	0.51
25:BA:1141:U:OP2	34:BJ:65:THR:OG1	2.29	0.51
7:AG:72:THR:HA	7:AG:96:ARG:HH12	1.75	0.51
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.46	0.51
11:AK:35:THR:HA	11:AK:42:LEU:H	1.75	0.51
25:BA:578:G:OP1	25:BA:1255:U:O2'	2.29	0.51
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.92	0.51
3:AC:19:ASN:ND2	14:AN:90:ARG:O	2.43	0.51
8:AH:52:GLU:O	8:AH:58:GLU:N	2.44	0.51
25:BA:2262:U:OP1	47:BW:41:ARG:NH2	2.43	0.51
38:BN:2:ARG:HA	38:BN:5:LYS:HD2	1.92	0.51
40:BP:90:GLY:O	40:BP:113:ARG:NH1	2.44	0.51
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.46	0.51
20:AT:36:TYR:HA	20:AT:39:ILE:HD12	1.92	0.51
40:BP:25:THR:HB	40:BP:88:ARG:HB3	1.92	0.51
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.46	0.51
25:BA:2062:A:H8	56:B5:-3:ARG:HA	1.75	0.51
32:BH:40:THR:O	32:BH:42:LYS:N	2.42	0.51
43:BS:84:ARG:HB2	43:BS:96:ILE:HG13	1.92	0.51
49:BY:17:GLU:HB2	49:BY:53:VAL:HG11	1.93	0.51
25:BA:1416:G:H1	25:BA:1582:C:H42	1.57	0.51
30:BF:131:GLY:HA2	30:BF:153:ASP:HA	1.93	0.51
9:AI:26:GLY:H	9:AI:59:GLU:HG3	1.76	0.51
20:AT:51:PHE:HA	20:AT:54:MET:HG2	1.93	0.51
27:BC:120:VAL:HG13	27:BC:134:ASN:HD21	1.75	0.51
34:BJ:96:ARG:HH21	34:BJ:99:ARG:HG2	1.74	0.51
37:BM:17:ASN:O	37:BM:38:ARG:NH1	2.44	0.51
1:AA:51:A:H61	1:AA:314:C:H1'	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1405:G:HO2'	1:AA:1518:A:HO2'	1.56	0.51
4:AD:50:ASP:O	4:AD:54:GLN:HG2	2.10	0.51
5:AE:36:LEU:HD11	5:AE:137:VAL:HG11	1.93	0.51
25:BA:1817:G:H5''	27:BC:87:ARG:HE	1.76	0.51
38:BN:69:ARG:O	38:BN:71:ARG:N	2.34	0.51
12:AL:74:LEU:HD21	12:AL:80:ILE:HG21	1.91	0.50
25:BA:1380:G:H21	25:BA:1570:A:H2	1.59	0.50
25:BA:2134:A:H8	25:BA:2157:G:H21	1.59	0.50
36:BL:57:LEU:HA	36:BL:60:ARG:HG2	1.93	0.50
1:AA:1429:A:O2'	25:BA:1703:G:O2'	2.29	0.50
9:AI:129:LYS:HG3	9:AI:130:ARG:H	1.75	0.50
57:BA:9000:ERY:H352	57:BA:9000:ERY:H4	1.93	0.50
40:BP:48:ILE:HA	40:BP:97:LEU:HD12	1.93	0.50
9:AI:17:ALA:HB2	9:AI:67:VAL:HG23	1.94	0.50
15:AO:22:THR:HA	15:AO:27:VAL:HG11	1.92	0.50
25:BA:1365:A:O2'	48:BX:11:ARG:NH1	2.43	0.50
25:BA:1939:U:OP1	25:BA:2604:U:O2'	2.28	0.50
44:BT:1:MET:HB3	44:BT:2:ILE:HD12	1.92	0.50
1:AA:202:G:H1	1:AA:215:C:H42	1.59	0.50
1:AA:335:C:H2'	1:AA:336:A:C8	2.46	0.50
25:BA:471:A:OP1	29:BE:79:ARG:NH1	2.32	0.50
25:BA:1652:A:N6	38:BN:11:ASN:OD1	2.38	0.50
27:BC:131:PRO:HA	27:BC:189:ARG:HA	1.93	0.50
29:BE:111:GLU:OE2	29:BE:114:ARG:NH2	2.45	0.50
30:BF:110:ARG:NH2	30:BF:137:ILE:O	2.44	0.50
43:BS:28:LYS:O	43:BS:30:SER:N	2.45	0.50
1:AA:236:A:H5''	17:AQ:44:LEU:HD21	1.94	0.50
1:AA:1414:U:H2'	1:AA:1415:G:H8	1.75	0.50
25:BA:290:U:H2'	25:BA:291:G:H8	1.76	0.50
25:BA:500:G:N1	25:BA:503:A:OP2	2.44	0.50
29:BE:56:GLY:HA2	29:BE:74:LYS:HZ1	1.76	0.50
44:BT:6:ARG:NH2	44:BT:37:ASP:OD2	2.44	0.50
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.94	0.50
25:BA:2316:G:H2'	25:BA:2317:A:H8	1.77	0.50
1:AA:1494:G:O5'	1:AA:1494:G:H8	1.94	0.50
4:AD:62:ARG:O	4:AD:66:GLY:N	2.42	0.50
7:AG:73:VAL:HG12	7:AG:90:GLU:HA	1.93	0.50
17:AQ:24:ALA:HA	17:AQ:43:LYS:HA	1.93	0.50
25:BA:246:C:H41	54:B3:8:ARG:HG2	1.77	0.50
27:BC:29:PRO:HG2	27:BC:34:LEU:HD11	1.93	0.50
36:BL:110:VAL:HG11	36:BL:135:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BN:38:LEU:HD22	38:BN:99:LYS:HD3	1.94	0.50
36:BL:79:LEU:HD12	36:BL:114:GLY:H	1.77	0.50
45:BU:72:ILE:HD13	45:BU:83:VAL:HG22	1.93	0.50
48:BX:10:LYS:HE3	48:BX:54:LYS:HD3	1.94	0.50
12:AL:22:PRO:O	12:AL:24:LEU:N	2.39	0.50
25:BA:414:C:H2'	25:BA:415:A:C8	2.47	0.50
25:BA:1568:G:OP2	27:BC:63:ARG:NH1	2.45	0.50
25:BA:2011:U:OP2	43:BS:16:LYS:NZ	2.41	0.50
30:BF:38:MET:HG2	30:BF:152:LEU:HB3	1.93	0.50
1:AA:1105:A:H2'	1:AA:1106:G:H8	1.76	0.49
26:BB:49:C:H2'	26:BB:50:A:H8	1.77	0.49
36:BL:33:ARG:NH2	36:BL:40:SER:O	2.36	0.49
36:BL:78:ARG:NH2	36:BL:80:SER:OG	2.45	0.49
1:AA:1491:G:H8	1:AA:1491:G:O5'	1.95	0.49
9:AI:113:ARG:NH1	14:AN:101:TRP:OXT	2.45	0.49
13:AM:4:ILE:HD11	13:AM:10:PRO:HD2	1.94	0.49
40:BP:62:ARG:HA	40:BP:71:GLU:HA	1.93	0.49
5:AE:25:VAL:HG23	5:AE:27:GLY:H	1.77	0.49
5:AE:88:VAL:HG12	5:AE:93:ARG:HG2	1.94	0.49
20:AT:29:ARG:O	20:AT:33:LYS:HG2	2.12	0.49
25:BA:107:G:H2'	25:BA:108:G:H8	1.77	0.49
25:BA:1296:G:OP1	25:BA:2709:G:O2'	2.21	0.49
25:BA:2374:C:N4	25:BA:2375:G:O6	2.45	0.49
27:BC:147:LYS:HB2	27:BC:150:LYS:HB2	1.93	0.49
29:BE:21:ARG:HH21	29:BE:106:LYS:HE3	1.78	0.49
31:BG:24:ILE:HD11	31:BG:43:VAL:HG11	1.95	0.49
34:BJ:40:HIS:CE1	34:BJ:41:LYS:HG3	2.48	0.49
1:AA:522:C:OP2	12:AL:66:TYR:OH	2.25	0.49
9:AI:36:GLU:HA	9:AI:40:GLY:HA3	1.94	0.49
10:AJ:27:GLU:HA	10:AJ:30:LYS:HE3	1.93	0.49
12:AL:5:ASN:ND2	17:AQ:36:LYS:HE2	2.27	0.49
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.41	0.49
25:BA:1313:U:H4'	25:BA:1332:G:H4'	1.92	0.49
25:BA:2387:U:O2'	47:BW:19:LYS:NZ	2.44	0.49
25:BA:2751:G:OP2	31:BG:3:ARG:NH1	2.45	0.49
28:BD:2:ILE:HD13	28:BD:90:PHE:HE2	1.77	0.49
32:BH:3:VAL:HG12	32:BH:38:PRO:HA	1.94	0.49
33:BI:109:ILE:O	33:BI:112:THR:OG1	2.27	0.49
1:AA:340:U:OP2	35:BK:98:ARG:NH2	2.46	0.49
9:AI:18:ARG:HH21	9:AI:20:PHE:HZ	1.59	0.49
25:BA:2202:U:O2'	25:BA:2204:G:OP1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BG:105:LEU:HB2	31:BG:113:VAL:HB	1.93	0.49
46:BV:61:LEU:HB2	46:BV:72:VAL:HG23	1.95	0.49
1:AA:816:A:OP1	1:AA:1526:G:O2'	2.26	0.49
13:AM:71:ARG:HA	13:AM:74:SER:HB3	1.94	0.49
25:BA:309:A:H5'	45:BU:17:LYS:HD2	1.94	0.49
25:BA:1807:G:O2'	25:BA:1809:A:N6	2.45	0.49
25:BA:2029:G:N1	25:BA:2033:A:OP2	2.32	0.49
25:BA:2241:A:H2'	25:BA:2242:G:H8	1.76	0.49
25:BA:2336:A:H61	47:BW:43:THR:HG21	1.78	0.49
33:BI:53:LEU:HD21	33:BI:82:LYS:HE2	1.93	0.49
1:AA:1317:C:N3	14:AN:53:ARG:NH1	2.60	0.49
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.46	0.49
7:AG:37:SER:HA	7:AG:40:GLU:HG2	1.94	0.49
25:BA:1089:A:H2	25:BA:1090:A:H62	1.61	0.49
26:BB:77:U:OP1	46:BV:21:ARG:NH1	2.46	0.49
38:BN:24:MET:HE1	38:BN:40:LYS:HG2	1.93	0.49
43:BS:44:ALA:HA	43:BS:47:VAL:HG12	1.95	0.49
14:AN:61:ARG:HE	14:AN:70:PRO:HB2	1.78	0.49
16:AP:71:VAL:O	16:AP:75:ILE:HD12	2.12	0.49
17:AQ:64:CYS:SG	17:AQ:74:THR:OG1	2.63	0.49
25:BA:123:G:H4'	25:BA:1376:C:H5'	1.94	0.49
25:BA:832:U:H2'	25:BA:833:A:C8	2.48	0.49
25:BA:1515:A:H3'	25:BA:1516:G:H8	1.78	0.49
25:BA:1781:U:H5	53:B2:1:MET:HE1	1.77	0.49
50:BZ:17:LEU:HB2	50:BZ:20:HIS:HD2	1.77	0.49
51:B0:31:ASP:HB3	51:B0:35:GLY:H	1.77	0.49
51:B0:40:ARG:HG2	51:B0:41:HIS:ND1	2.28	0.49
1:AA:1279:G:OP1	10:AJ:9:ARG:NH2	2.46	0.49
9:AI:107:ASP:OD1	9:AI:109:ARG:NE	2.41	0.49
25:BA:1796:U:H2'	25:BA:1797:G:C8	2.48	0.49
25:BA:2080:A:H61	25:BA:2240:U:H3	1.60	0.49
43:BS:41:LYS:HG3	43:BS:43:ALA:H	1.78	0.49
1:AA:34:C:N4	1:AA:35:G:O6	2.46	0.48
1:AA:380:G:N2	1:AA:383:A:OP2	2.37	0.48
25:BA:1385:A:O2'	25:BA:1396:U:O2	2.27	0.48
31:BG:95:ARG:HB2	31:BG:106:SER:HB2	1.94	0.48
11:AK:23:ILE:HD11	11:AK:86:VAL:HG22	1.95	0.48
11:AK:35:THR:OG1	11:AK:41:ALA:N	2.46	0.48
15:AO:26:GLU:OE2	15:AO:77:ARG:NH2	2.46	0.48
25:BA:2756:U:OP2	55:B4:19:ARG:NE	2.38	0.48
30:BF:13:VAL:O	30:BF:17:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BU:86:ARG:HH12	45:BU:100:SER:HA	1.78	0.48
1:AA:458:U:H2'	1:AA:459:A:C8	2.48	0.48
25:BA:142:A:H1'	44:BT:1:MET:HE3	1.95	0.48
25:BA:475:C:H4'	25:BA:510:C:H5'	1.94	0.48
25:BA:500:G:OP1	45:BU:43:LYS:NZ	2.39	0.48
25:BA:1181:U:H2'	25:BA:1182:G:C8	2.47	0.48
37:BM:33:LEU:HD13	37:BM:117:PHE:HB3	1.94	0.48
40:BP:88:ARG:NH2	40:BP:110:ILE:O	2.43	0.48
52:B1:38:LYS:HB2	52:B1:49:TYR:CE2	2.47	0.48
1:AA:1121:U:H3	1:AA:1152:A:H61	1.62	0.48
7:AG:116:MET:HA	7:AG:119:ARG:HD3	1.94	0.48
23:AX:16:H2U:H5'	23:AX:59:G:H1	1.79	0.48
24:AY:9:A:N6	24:AY:22:G:N7	2.61	0.48
25:BA:450:G:N1	25:BA:454:A:OP2	2.45	0.48
25:BA:1176:U:H2'	25:BA:1177:G:C8	2.48	0.48
27:BC:204:VAL:O	27:BC:206:GLY:N	2.46	0.48
28:BD:8:LYS:HB2	28:BD:201:LEU:HD11	1.94	0.48
30:BF:37:ASN:OD1	30:BF:38:MET:N	2.47	0.48
52:B1:8:LYS:HD2	54:B3:34:THR:HG21	1.96	0.48
4:AD:29:ASP:O	4:AD:31:LYS:N	2.47	0.48
25:BA:1038:G:H2'	25:BA:1039:A:H8	1.77	0.48
26:BB:22:U:H2'	26:BB:23:G:C8	2.48	0.48
35:BK:77:ILE:HG12	40:BP:72:ARG:HG2	1.94	0.48
1:AA:450:G:H4'	16:AP:41:PRO:HB2	1.94	0.48
1:AA:954:G:H21	1:AA:1227:A:N6	2.12	0.48
20:AT:35:VAL:HG21	20:AT:54:MET:SD	2.54	0.48
25:BA:2576:G:O2'	25:BA:2579:C:OP2	2.30	0.48
28:BD:55:LYS:HB2	28:BD:77:ARG:HA	1.95	0.48
1:AA:1492:A:C2'	1:AA:1493:A:O5'	2.62	0.48
25:BA:1034:G:O4'	55:B4:18:LYS:NZ	2.46	0.48
39:BO:71:ALA:HB1	39:BO:106:LEU:HB2	1.94	0.48
43:BS:4:ILE:HG12	43:BS:106:VAL:HG22	1.95	0.48
1:AA:407:U:H2'	1:AA:408:A:C8	2.49	0.48
1:AA:1366:C:O2'	10:AJ:62:ARG:NH1	2.30	0.48
18:AR:55:LEU:O	18:AR:59:ILE:HG12	2.14	0.48
25:BA:1817:G:P	27:BC:87:ARG:HH21	2.37	0.48
25:BA:2233:U:H2'	25:BA:2234:G:C8	2.49	0.48
1:AA:970:C:N4	9:AI:128:SER:OG	2.47	0.48
9:AI:118:LEU:HG	9:AI:124:ARG:HA	1.96	0.48
13:AM:101:ARG:NH2	13:AM:103:LYS:HD2	2.29	0.48
25:BA:1064:C:H5'	33:BI:90:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BC:132:MET:HA	27:BC:135:ILE:HD12	1.95	0.48
1:AA:1058:G:OP1	3:AC:199:LYS:NZ	2.44	0.48
1:AA:1201:A:H4'	1:AA:1202:U:O5'	2.14	0.48
12:AL:114:ARG:HH22	12:AL:121:ARG:HH11	1.62	0.48
25:BA:727:A:OP1	25:BA:1431:A:O2'	2.28	0.48
25:BA:2586:U:O2'	56:B5:-3:ARG:NH2	2.46	0.48
54:B3:62:LEU:HB3	54:B3:65:ALA:HB2	1.96	0.48
25:BA:1257:C:H4'	29:BE:78:TRP:CD1	2.49	0.47
25:BA:674:G:H1	25:BA:806:C:H42	1.62	0.47
25:BA:1250:G:OP2	36:BL:21:ARG:NH2	2.47	0.47
26:BB:43:C:O2	30:BF:92:ARG:NH2	2.38	0.47
45:BU:45:HIS:HB3	45:BU:58:ILE:HA	1.96	0.47
1:AA:67:C:H2'	1:AA:68:G:C8	2.50	0.47
8:AH:9:ASP:O	8:AH:13:ARG:HG2	2.14	0.47
11:AK:22:HIS:NE2	11:AK:85:MET:SD	2.88	0.47
11:AK:26:SER:OG	11:AK:29:ASN:O	2.22	0.47
14:AN:21:PHE:O	14:AN:23:LYS:N	2.48	0.47
25:BA:2514:U:H5''	34:BJ:81:ILE:HD11	1.96	0.47
48:BX:38:PHE:HD2	48:BX:49:LEU:HD12	1.79	0.47
50:BZ:17:LEU:HB2	50:BZ:20:HIS:CD2	2.49	0.47
1:AA:299:G:N2	1:AA:565:U:O2	2.47	0.47
25:BA:518:G:O5'	43:BS:18:ARG:NH1	2.47	0.47
10:AJ:27:GLU:HA	10:AJ:30:LYS:HG2	1.96	0.47
25:BA:1038:G:H2'	25:BA:1039:A:C8	2.49	0.47
25:BA:2313:C:O4'	30:BF:37:ASN:ND2	2.40	0.47
26:BB:116:G:H2'	26:BB:117:G:H8	1.78	0.47
33:BI:33:VAL:HG13	33:BI:67:PHE:HE2	1.78	0.47
45:BU:41:LEU:HB3	45:BU:60:GLU:HG2	1.96	0.47
1:AA:234:C:O2'	17:AQ:72:SER:OG	2.29	0.47
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.78	0.47
3:AC:172:ARG:HG2	3:AC:174:PRO:HD3	1.97	0.47
17:AQ:27:ARG:HH21	17:AQ:40:ARG:HG2	1.80	0.47
25:BA:740:C:H5'	25:BA:1784:A:H2'	1.95	0.47
25:BA:1899:A:H4'	25:BA:1901:A:H5''	1.95	0.47
25:BA:2286:G:H4'	25:BA:2287:A:C4	2.49	0.47
35:BK:99:ILE:HD12	35:BK:118:LEU:HD12	1.97	0.47
1:AA:675:A:H1'	11:AK:118:HIS:CE1	2.50	0.47
2:AB:20:THR:OG1	2:AB:37:LYS:O	2.25	0.47
3:AC:152:GLU:HG2	3:AC:167:TRP:HB3	1.97	0.47
7:AG:25:LYS:O	7:AG:29:ILE:HG12	2.15	0.47
25:BA:1105:U:H2'	25:BA:1106:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1791:A:N6	25:BA:1828:G:O2'	2.45	0.47
25:BA:2097:A:H61	25:BA:2192:U:H3	1.62	0.47
25:BA:2109:U:O2	25:BA:2181:U:N3	2.46	0.47
25:BA:2623:G:H2'	25:BA:2624:G:H8	1.80	0.47
33:BI:79:LEU:HD21	33:BI:109:ILE:HD13	1.96	0.47
39:BO:94:ARG:HG3	39:BO:96:GLY:H	1.80	0.47
40:BP:75:GLN:HB2	40:BP:78:SER:HB2	1.95	0.47
25:BA:1068:G:N2	25:BA:1096:A:OP1	2.47	0.47
29:BE:189:THR:HG22	29:BE:191:ASP:H	1.80	0.47
31:BG:101:ASN:ND2	31:BG:116:GLN:HE22	2.13	0.47
1:AA:954:G:H1	1:AA:1226:C:H42	1.63	0.47
5:AE:96:MET:HE1	5:AE:140:THR:HG23	1.97	0.47
7:AG:151:PHE:CE2	11:AK:56:ARG:HG2	2.49	0.47
19:AS:40:ILE:HD13	19:AS:66:MET:HB3	1.97	0.47
25:BA:581:C:H2'	25:BA:582:A:C8	2.50	0.47
25:BA:927:A:O2'	50:BZ:39:GLU:OE2	2.30	0.47
33:BI:12:GLN:NE2	33:BI:55:ILE:O	2.48	0.47
42:BR:14:VAL:HG22	42:BR:15:SER:O	2.15	0.47
43:BS:69:LEU:HA	43:BS:109:ASP:HA	1.96	0.47
45:BU:10:GLU:OE2	45:BU:22:ARG:NE	2.45	0.47
53:B2:24:THR:HG23	53:B2:27:GLY:H	1.79	0.47
2:AB:205:ASP:OD1	2:AB:206:ALA:N	2.48	0.47
10:AJ:8:ILE:HD11	10:AJ:87:LEU:HD11	1.96	0.47
13:AM:16:VAL:HG23	13:AM:17:ILE:HG13	1.97	0.47
19:AS:28:LYS:HG3	19:AS:29:LYS:H	1.80	0.47
25:BA:1936:A:OP2	25:BA:1962:C:N4	2.39	0.47
25:BA:2519:U:O4'	25:BA:2542:A:N6	2.48	0.47
34:BJ:77:HIS:HD1	34:BJ:79:GLY:H	1.63	0.47
48:BX:34:HIS:CD2	48:BX:53:ALA:HB2	2.49	0.47
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.50	0.46
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.96	0.46
25:BA:475:C:O2	25:BA:479:A:N6	2.47	0.46
25:BA:1187:G:N2	25:BA:1188:U:O4	2.48	0.46
25:BA:1715:G:O2'	25:BA:1743:G:O6	2.25	0.46
25:BA:1790:C:H2'	25:BA:1791:A:C5	2.50	0.46
25:BA:2285:C:H5	52:B1:6:ARG:HH12	1.63	0.46
1:AA:403:C:H5'	4:AD:132:ILE:HG23	1.97	0.46
3:AC:191:THR:OG1	3:AC:194:GLY:O	2.32	0.46
4:AD:145:ILE:HD13	4:AD:178:MET:HB3	1.97	0.46
25:BA:2439:A:O4'	56:B5:-3:ARG:NH2	2.41	0.46
25:BA:2530:A:OP2	25:BA:2535:G:N2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:543:U:OP1	4:AD:14:ARG:NE	2.48	0.46
4:AD:54:GLN:HB3	4:AD:203:LEU:HD13	1.96	0.46
5:AE:45:ARG:HB3	5:AE:71:MET:SD	2.56	0.46
25:BA:813:U:OP1	42:BR:84:ARG:NH1	2.48	0.46
25:BA:1264:A:OP1	51:B0:16:ARG:NH1	2.47	0.46
25:BA:1363:C:H2'	25:BA:1364:G:C8	2.51	0.46
25:BA:1438:U:H2'	25:BA:1439:A:H8	1.80	0.46
25:BA:1666:G:H1	25:BA:1994:C:H42	1.62	0.46
25:BA:1818:U:H2'	27:BC:156:ARG:HB2	1.97	0.46
25:BA:2291:U:H2'	25:BA:2292:U:C6	2.51	0.46
25:BA:2788:C:H2'	25:BA:2789:C:C6	2.50	0.46
57:BA:9000:ERY:H312	57:BA:9000:ERY:H2	1.67	0.46
28:BD:48:ILE:HG23	28:BD:84:LEU:HD21	1.96	0.46
36:BL:82:LEU:HD13	36:BL:120:VAL:HG21	1.96	0.46
42:BR:98:ILE:HG22	42:BR:100:GLY:H	1.81	0.46
45:BU:84:GLY:O	45:BU:94:ARG:HA	2.14	0.46
1:AA:1060:U:H5''	10:AJ:53:ILE:HG12	1.96	0.46
1:AA:1437:A:H2'	1:AA:1438:G:H8	1.80	0.46
10:AJ:19:ASP:HA	10:AJ:22:THR:HG22	1.98	0.46
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.15	0.46
25:BA:659:G:OP1	29:BE:95:LYS:NZ	2.38	0.46
28:BD:61:THR:HB	28:BD:63:PRO:HD2	1.97	0.46
29:BE:112:LEU:HB3	29:BE:118:LEU:HB2	1.97	0.46
31:BG:38:ASN:OD1	31:BG:39:ASP:N	2.48	0.46
1:AA:954:G:H21	1:AA:1227:A:H61	1.62	0.46
3:AC:20:SER:HB3	3:AC:22:TRP:CD1	2.50	0.46
3:AC:20:SER:HB3	3:AC:22:TRP:NE1	2.30	0.46
3:AC:189:ALA:HB3	3:AC:196:ILE:HB	1.98	0.46
15:AO:60:VAL:HG11	25:BA:715:A:C8	2.51	0.46
25:BA:1326:U:H2'	25:BA:1327:A:C8	2.50	0.46
25:BA:2062:A:C8	56:B5:-3:ARG:HA	2.50	0.46
37:BM:75:GLU:HB2	37:BM:90:GLU:HG3	1.96	0.46
38:BN:69:ARG:C	38:BN:71:ARG:H	2.22	0.46
1:AA:372:C:N4	1:AA:388:G:OP2	2.45	0.46
1:AA:430:A:H4'	4:AD:7:PRO:HG3	1.98	0.46
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.36	0.46
3:AC:29:PHE:HZ	14:AN:93:ILE:HG23	1.81	0.46
9:AI:7:TYR:HD1	9:AI:20:PHE:HE1	1.63	0.46
11:AK:31:ILE:HG13	11:AK:46:THR:HG22	1.98	0.46
25:BA:482:A:H4'	45:BU:45:HIS:CE1	2.47	0.46
25:BA:1662:U:O2'	25:BA:2687:U:OP1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1782:U:O2	25:BA:2608:G:O2'	2.33	0.46
37:BM:41:LEU:HG	37:BM:96:ILE:HG13	1.96	0.46
51:B0:31:ASP:OD2	51:B0:34:SER:N	2.48	0.46
1:AA:106:C:H2'	1:AA:107:G:C8	2.51	0.46
1:AA:1031:C:H4'	1:AA:1032:G:C2	2.51	0.46
2:AB:166:ALA:HB2	2:AB:187:VAL:HG12	1.96	0.46
2:AB:203:ASN:OD1	2:AB:204:ASP:N	2.49	0.46
5:AE:150:PRO:HA	5:AE:153:VAL:HG22	1.97	0.46
25:BA:973:A:H5'	25:BA:1188:U:H1'	1.98	0.46
25:BA:2316:G:H2'	25:BA:2317:A:C8	2.51	0.46
27:BC:81:LEU:HD21	27:BC:110:LEU:HD22	1.98	0.46
28:BD:133:THR:OG1	28:BD:134:HIS:N	2.45	0.46
36:BL:79:LEU:H	36:BL:113:ALA:HB3	1.80	0.46
46:BV:8:VAL:HG22	46:BV:38:LEU:HD11	1.98	0.46
7:AG:130:ASN:C	7:AG:135:VAL:HG21	2.41	0.46
25:BA:657:U:H2'	25:BA:658:U:C6	2.50	0.46
25:BA:910:A:H2'	25:BA:911:A:C8	2.51	0.46
31:BG:12:PRO:HG2	31:BG:15:VAL:HG21	1.96	0.46
31:BG:89:LEU:N	31:BG:129:THR:O	2.45	0.46
33:BI:90:SER:HB3	33:BI:93:PRO:HG3	1.98	0.46
45:BU:45:HIS:O	45:BU:45:HIS:ND1	2.48	0.46
49:BY:21:LEU:HD23	49:BY:25:GLN:HG3	1.97	0.46
1:AA:939:G:OP1	7:AG:95:ARG:NH2	2.49	0.46
1:AA:1428:A:O2'	25:BA:1702:G:N2	2.46	0.46
7:AG:69:VAL:HA	7:AG:138:ARG:HD3	1.98	0.46
8:AH:75:ILE:HD12	8:AH:128:TYR:O	2.15	0.46
12:AL:83:ARG:HB2	12:AL:98:VAL:HG23	1.97	0.46
18:AR:57:ARG:HE	18:AR:61:ARG:HH21	1.61	0.46
25:BA:1190:G:H2'	25:BA:1191:G:H8	1.81	0.46
25:BA:1802:A:OP2	25:BA:1815:A:N6	2.46	0.46
25:BA:2061:G:N2	56:B5:0:ASP:OD2	2.49	0.46
33:BI:62:TYR:HD2	33:BI:67:PHE:HA	1.81	0.46
55:B4:30:GLU:HG3	55:B4:32:LYS:H	1.81	0.46
25:BA:2039:U:H2'	25:BA:2040:G:C8	2.50	0.46
28:BD:4:LEU:HB2	28:BD:101:PHE:HZ	1.80	0.46
32:BH:8:LYS:HD3	32:BH:15:LEU:HG	1.98	0.46
49:BY:13:GLU:HA	49:BY:16:THR:HG22	1.97	0.46
1:AA:28:A:O2'	1:AA:296:U:OP1	2.28	0.45
1:AA:321:A:H61	1:AA:332:G:H1	1.64	0.45
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.51	0.45
5:AE:137:VAL:O	5:AE:138:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:105:VAL:O	7:AG:109:ARG:HG2	2.16	0.45
15:AO:36:ILE:O	15:AO:40:GLN:HG2	2.17	0.45
23:AX:18:G:O2'	23:AX:57:G:N2	2.44	0.45
25:BA:18:U:O2'	25:BA:554:U:OP1	2.32	0.45
25:BA:2020:A:H5'	51:B0:9:THR:HG23	1.98	0.45
29:BE:75:SER:HB3	29:BE:78:TRP:CE3	2.51	0.45
40:BP:90:GLY:HA2	40:BP:112:GLU:HA	1.98	0.45
43:BS:2:GLU:HA	43:BS:108:SER:HB3	1.97	0.45
1:AA:950:U:H2'	1:AA:951:G:C8	2.50	0.45
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.49	0.45
1:AA:1493:A:HO2'	1:AA:1494:G:P	2.28	0.45
6:AF:36:ILE:HG13	6:AF:64:VAL:HG22	1.97	0.45
25:BA:442:G:O4'	29:BE:41:GLN:NE2	2.50	0.45
25:BA:466:A:OP1	53:B2:34:ARG:NH1	2.49	0.45
27:BC:166:ALA:HB3	27:BC:173:THR:HB	1.97	0.45
1:AA:830:G:H2'	1:AA:831:A:H8	1.82	0.45
1:AA:1222:G:OP2	1:AA:1322:C:N4	2.49	0.45
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.80	0.45
1:AA:1313:U:H3	1:AA:1324:A:H61	1.65	0.45
25:BA:2744:G:H21	31:BG:143:GLN:HE22	1.63	0.45
25:BA:2845:U:O3'	40:BP:53:ARG:NH1	2.50	0.45
30:BF:12:VAL:HG22	30:BF:172:ALA:HB1	1.98	0.45
35:BK:15:GLY:HA3	35:BK:50:GLY:HA3	1.98	0.45
41:BQ:72:ASN:HB3	41:BQ:110:VAL:HG11	1.98	0.45
45:BU:89:ASP:CG	45:BU:90:GLY:H	2.24	0.45
25:BA:371:A:H61	25:BA:401:A:H3'	1.82	0.45
25:BA:467:G:OP2	53:B2:34:ARG:HD3	2.17	0.45
25:BA:2744:G:N2	31:BG:143:GLN:HE22	2.14	0.45
28:BD:181:ASP:HB3	28:BD:186:LEU:HB2	1.99	0.45
39:BO:49:VAL:HG21	39:BO:82:ALA:HA	1.97	0.45
42:BR:77:PHE:HD1	42:BR:84:ARG:HB3	1.81	0.45
1:AA:56:U:H2'	1:AA:57:G:C8	2.52	0.45
1:AA:1191:A:H5''	3:AC:4:LYS:HE3	1.99	0.45
1:AA:1342:C:H2'	1:AA:1343:G:C8	2.52	0.45
24:AY:32:C:N4	24:AY:33:U:O4	2.50	0.45
25:BA:1201:U:H2'	25:BA:1202:G:H8	1.81	0.45
25:BA:2377:A:H2'	25:BA:2378:A:C8	2.51	0.45
25:BA:2658:C:OP1	31:BG:158:LYS:NZ	2.49	0.45
33:BI:61:VAL:HA	33:BI:67:PHE:HB3	1.98	0.45
37:BM:109:PRO:HB2	37:BM:112:LEU:HD13	1.97	0.45
46:BV:86:LEU:HD13	46:BV:89:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:979:C:H1'	1:AA:1317:C:H41	1.82	0.45
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.52	0.45
1:AA:1397:C:P	5:AE:29:ARG:HH22	2.40	0.45
4:AD:53:VAL:HA	4:AD:56:ARG:HB3	1.99	0.45
11:AK:112:ASP:OD1	11:AK:114:THR:HG23	2.16	0.45
25:BA:1313:U:H2'	25:BA:1313:U:O2	2.15	0.45
25:BA:2170:A:H1'	25:BA:2171:A:C8	2.51	0.45
37:BM:13:HIS:O	37:BM:71:LYS:NZ	2.49	0.45
37:BM:77:PRO:HB2	37:BM:80:VAL:HG21	1.98	0.45
37:BM:114:ARG:O	37:BM:118:LYS:HG2	2.17	0.45
39:BO:43:ASN:OD1	39:BO:44:GLY:N	2.50	0.45
1:AA:337:G:H2'	1:AA:338:A:C8	2.52	0.45
1:AA:501:C:H2'	1:AA:502:A:C8	2.51	0.45
1:AA:563:A:O2'	1:AA:566:G:O3'	2.35	0.45
8:AH:29:SER:HB2	8:AH:59:LEU:HB2	1.98	0.45
11:AK:61:PHE:HA	11:AK:64:GLN:HG2	1.97	0.45
25:BA:926:G:H2'	25:BA:927:A:C8	2.51	0.45
25:BA:1170:C:H2'	25:BA:1171:G:H8	1.82	0.45
25:BA:2618:G:H21	28:BD:155:VAL:HG21	1.82	0.45
27:BC:167:ARG:HA	27:BC:172:VAL:HG12	1.98	0.45
31:BG:7:ALA:O	31:BG:69:ARG:NE	2.31	0.45
43:BS:6:LYS:HE2	43:BS:104:THR:HG23	1.98	0.45
1:AA:960:U:H2'	1:AA:1225:A:H62	1.82	0.45
13:AM:5:ALA:H	13:AM:57:ARG:NH1	2.15	0.45
16:AP:52:LEU:HD21	16:AP:57:ILE:HD12	1.99	0.45
25:BA:372:G:H5''	48:BX:61:LYS:HD3	1.98	0.45
25:BA:533:G:H4'	41:BQ:28:ARG:HH22	1.82	0.45
25:BA:729:G:H5''	25:BA:730:A:H5''	1.98	0.45
25:BA:1063:G:N2	25:BA:1076:C:O2	2.50	0.45
25:BA:2013:A:H4'	43:BS:96:ILE:HG22	1.99	0.45
27:BC:9:THR:O	27:BC:10:SER:OG	2.28	0.45
28:BD:4:LEU:HB2	28:BD:101:PHE:CZ	2.52	0.45
28:BD:101:PHE:HA	28:BD:104:VAL:HG13	1.98	0.45
29:BE:58:LYS:HA	29:BE:59:PRO:HD3	1.84	0.45
33:BI:34:ASN:OD1	33:BI:35:ILE:N	2.50	0.45
40:BP:112:GLU:HG2	40:BP:114:LEU:H	1.81	0.45
4:AD:60:LYS:O	4:AD:64:ILE:HG13	2.16	0.45
11:AK:36:ASP:OD1	11:AK:40:ASN:N	2.50	0.45
11:AK:126:LYS:O	11:AK:127:ARG:HB2	2.17	0.45
17:AQ:61:ILE:HD11	17:AQ:73:TRP:HB3	1.98	0.45
25:BA:65:U:O3'	44:BT:73:ARG:NH1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:720:U:H2'	25:BA:721:A:C8	2.52	0.45
25:BA:742:A:H2'	25:BA:743:A:C8	2.52	0.45
25:BA:1000:A:OP2	25:BA:1154:G:N1	2.37	0.45
25:BA:2002:G:H5''	38:BN:9:GLN:HE21	1.82	0.45
25:BA:2818:U:H2'	25:BA:2819:G:C8	2.52	0.45
25:BA:2837:A:H2'	25:BA:2838:G:C8	2.52	0.45
26:BB:24:G:O2'	26:BB:56:G:N7	2.35	0.45
26:BB:95:U:H2'	26:BB:96:G:C8	2.52	0.45
32:BH:8:LYS:HA	32:BH:15:LEU:H	1.81	0.45
32:BH:41:LYS:O	32:BH:44:ILE:HG12	2.17	0.45
38:BN:53:THR:HA	38:BN:56:LYS:HG2	1.98	0.45
1:AA:1073:U:H3	1:AA:1102:A:H61	1.65	0.45
19:AS:31:LEU:H	19:AS:49:ILE:HA	1.81	0.45
25:BA:480:A:H5''	45:BU:44:LYS:HD2	1.99	0.45
25:BA:1077:A:N6	25:BA:1089:A:OP1	2.43	0.45
25:BA:1598:A:H5''	44:BT:40:LYS:HD3	1.97	0.45
25:BA:2355:G:H1'	47:BW:39:ARG:HH21	1.82	0.45
1:AA:1217:C:P	14:AN:9:ARG:HH21	2.40	0.44
4:AD:38:PRO:HD2	4:AD:42:GLY:HA3	2.00	0.44
4:AD:170:TRP:CD1	4:AD:171:LEU:HG	2.52	0.44
25:BA:2392:A:C2	36:BL:55:MET:HE3	2.51	0.44
28:BD:176:ASP:HB2	28:BD:190:LYS:HE2	1.99	0.44
1:AA:186:C:H5'	20:AT:73:ALA:HB1	1.98	0.44
1:AA:219:U:H2'	1:AA:220:G:C8	2.52	0.44
1:AA:689:C:OP2	11:AK:53:ARG:NH2	2.29	0.44
1:AA:1151:A:O2'	1:AA:1152:A:H5''	2.17	0.44
1:AA:1265:C:N4	1:AA:1266:G:O6	2.50	0.44
2:AB:106:THR:O	2:AB:109:GLN:NE2	2.49	0.44
25:BA:215:G:H4'	25:BA:216:A:H4'	1.99	0.44
25:BA:573:U:O2'	25:BA:575:A:OP1	2.29	0.44
25:BA:1867:G:H1	25:BA:1874:C:H42	1.65	0.44
28:BD:151:THR:HG22	28:BD:152:PRO:CD	2.42	0.44
41:BQ:106:PHE:HA	41:BQ:109:LEU:HD12	2.00	0.44
1:AA:219:U:H2'	1:AA:220:G:H8	1.82	0.44
11:AK:13:ARG:NH2	11:AK:77:TYR:OH	2.51	0.44
25:BA:247:G:O2'	25:BA:250:G:O6	2.35	0.44
27:BC:240:PHE:HZ	27:BC:244:PRO:HG3	1.81	0.44
29:BE:176:ASP:OD1	29:BE:179:SER:OG	2.31	0.44
35:BK:64:ARG:NE	40:BP:68:GLU:OE2	2.48	0.44
45:BU:6:ARG:HG2	45:BU:94:ARG:NH2	2.32	0.44
46:BV:10:LYS:HG3	46:BV:11:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BX:17:ASN:ND2	48:BX:27:ARG:HD2	2.33	0.44
1:AA:96:U:H2'	1:AA:97:G:C8	2.52	0.44
1:AA:413:G:H21	1:AA:428:G:H1'	1.82	0.44
1:AA:739:C:O2'	15:AO:42:HIS:ND1	2.50	0.44
1:AA:1414:U:H2'	1:AA:1415:G:C8	2.52	0.44
10:AJ:12:ALA:HB3	10:AJ:18:ILE:HB	2.00	0.44
13:AM:31:LYS:NZ	13:AM:41:GLU:OE1	2.50	0.44
25:BA:141:G:OP2	25:BA:142:A:N6	2.50	0.44
25:BA:1252:G:H1	41:BQ:37:GLN:HE21	1.66	0.44
25:BA:1378:A:O2'	25:BA:1380:G:OP2	2.26	0.44
25:BA:2093:G:H2'	25:BA:2094:A:H8	1.82	0.44
27:BC:144:VAL:HG11	27:BC:174:LEU:HD21	1.99	0.44
29:BE:118:LEU:HD11	29:BE:188:MET:HG3	1.98	0.44
40:BP:97:LEU:HB3	40:BP:100:LEU:HD12	1.99	0.44
1:AA:587:G:N2	1:AA:754:C:OP2	2.42	0.44
1:AA:675:A:OP1	18:AR:74:HIS:NE2	2.51	0.44
1:AA:676:A:H4'	11:AK:115:PRO:HB3	1.99	0.44
1:AA:1105:A:H2'	1:AA:1106:G:C8	2.52	0.44
14:AN:13:ARG:HE	14:AN:59:ARG:NE	2.12	0.44
20:AT:28:MET:HA	20:AT:31:PHE:HD2	1.82	0.44
25:BA:1131:G:N2	25:BA:1132:U:O4	2.37	0.44
25:BA:1653:G:C6	38:BN:9:GLN:HB3	2.53	0.44
27:BC:123:ALA:O	27:BC:128:ASN:ND2	2.51	0.44
33:BI:11:LEU:HD12	33:BI:11:LEU:O	2.17	0.44
34:BJ:49:ASP:OD1	34:BJ:121:LYS:NZ	2.46	0.44
44:BT:11:LEU:HB2	49:BY:26:PHE:HE1	1.83	0.44
1:AA:437:U:O2'	4:AD:120:HIS:ND1	2.51	0.44
3:AC:168:TYR:OH	5:AE:55:GLU:OE2	2.23	0.44
8:AH:95:VAL:HG23	8:AH:102:ALA:HB2	2.00	0.44
13:AM:114:LYS:H	13:AM:115:PRO:HD2	1.83	0.44
17:AQ:46:VAL:HG13	17:AQ:74:THR:HA	1.99	0.44
21:AU:40:LYS:HB3	21:AU:41:PRO:HD3	1.98	0.44
25:BA:548:G:O2'	25:BA:549:G:N7	2.50	0.44
25:BA:1170:C:H2'	25:BA:1171:G:C8	2.53	0.44
25:BA:1903:G:H2'	25:BA:1904:G:H8	1.81	0.44
25:BA:2076:U:OP2	25:BA:2238:G:N2	2.51	0.44
25:BA:2621:G:OP1	28:BD:124:ARG:NH2	2.45	0.44
52:B1:13:SER:HA	52:B1:49:TYR:CD1	2.52	0.44
12:AL:43:LYS:HD2	12:AL:91:PRO:HG3	2.00	0.44
17:AQ:60:GLU:OE2	17:AQ:77:ARG:NH2	2.51	0.44
25:BA:2506:U:O2'	25:BA:2507:C:OP1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BD:14:ILE:HG12	28:BD:24:VAL:HG21	2.00	0.44
25:BA:917:A:H5''	25:BA:2268:A:H61	1.82	0.44
25:BA:968:C:H2'	25:BA:969:G:C8	2.53	0.44
25:BA:1258:U:H2'	25:BA:1259:G:C8	2.52	0.44
25:BA:1278:C:H2'	25:BA:1279:G:H8	1.82	0.44
25:BA:1578:U:H2'	25:BA:1579:A:H8	1.82	0.44
40:BP:29:LYS:HD2	40:BP:83:SER:HB2	2.00	0.44
42:BR:82:HIS:O	42:BR:82:HIS:ND1	2.51	0.44
48:BX:40:VAL:HG11	48:BX:68:LEU:HD11	1.99	0.44
54:B3:33:LEU:HB3	54:B3:41:LYS:HD3	2.00	0.44
1:AA:409:U:OP2	4:AD:22:LYS:NZ	2.41	0.44
9:AI:28:ILE:HG23	9:AI:63:LEU:HD11	1.99	0.44
11:AK:93:ARG:HH21	21:AU:20:LYS:HG3	1.83	0.44
12:AL:38:TYR:OH	12:AL:54:ARG:NH1	2.50	0.44
25:BA:281:C:H42	25:BA:359:G:H1	1.66	0.44
25:BA:806:C:O2	25:BA:2444:G:O2'	2.36	0.44
25:BA:2106:U:H2'	25:BA:2107:G:C8	2.53	0.44
25:BA:2241:A:H2'	25:BA:2242:G:C8	2.53	0.44
25:BA:2368:C:H2'	25:BA:2369:A:C8	2.53	0.44
25:BA:2785:C:O2'	28:BD:67:HIS:ND1	2.44	0.44
28:BD:101:PHE:O	28:BD:104:VAL:HG22	2.18	0.44
30:BF:37:ASN:HB3	30:BF:153:ASP:OD1	2.18	0.44
34:BJ:23:LYS:NZ	34:BJ:142:ILE:OXT	2.51	0.44
34:BJ:31:GLU:HG2	34:BJ:142:ILE:HG12	2.00	0.44
1:AA:376:G:H5''	16:AP:5:ARG:HB2	2.00	0.43
1:AA:995:C:N3	1:AA:1046:A:O2'	2.46	0.43
14:AN:9:ARG:HG2	14:AN:13:ARG:HH12	1.82	0.43
25:BA:599:A:H2'	25:BA:600:G:C8	2.52	0.43
25:BA:812:C:H5	36:BL:21:ARG:HB3	1.82	0.43
25:BA:1311:G:H21	25:BA:1603:A:H62	1.65	0.43
25:BA:2298:A:H5''	30:BF:72:LYS:NZ	2.33	0.43
32:BH:5:LEU:HD13	32:BH:9:VAL:HG21	2.00	0.43
47:BW:33:ALA:N	47:BW:64:ASP:OD1	2.51	0.43
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.53	0.43
25:BA:2:G:O6	25:BA:2900:A:N6	2.51	0.43
25:BA:2691:C:H2'	25:BA:2692:G:C8	2.53	0.43
26:BB:116:G:H2'	26:BB:117:G:C8	2.53	0.43
34:BJ:125:TYR:OH	34:BJ:132:HIS:NE2	2.46	0.43
35:BK:10:VAL:HG12	35:BK:12:ASP:H	1.82	0.43
40:BP:53:ARG:N	40:BP:57:SER:OG	2.43	0.43
1:AA:808:C:H2'	1:AA:809:G:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:50:PRO:HG3	6:AF:55:HIS:CE1	2.53	0.43
10:AJ:11:LYS:HB2	10:AJ:97:ASP:HB3	1.99	0.43
16:AP:72:ALA:O	16:AP:76:LYS:HG2	2.18	0.43
17:AQ:31:HIS:CD2	17:AQ:34:TYR:H	2.34	0.43
25:BA:1190:G:H2'	25:BA:1191:G:C8	2.54	0.43
25:BA:2097:A:OP2	25:BA:2097:A:H8	2.00	0.43
25:BA:2623:G:H2'	25:BA:2624:G:C8	2.52	0.43
26:BB:24:G:N2	26:BB:28:C:O2	2.51	0.43
26:BB:95:U:H2'	26:BB:96:G:H8	1.83	0.43
33:BI:33:VAL:HG13	33:BI:67:PHE:CE2	2.53	0.43
37:BM:7:THR:HG21	37:BM:92:TRP:CH2	2.53	0.43
51:B0:13:ARG:HG3	51:B0:16:ARG:HH11	1.83	0.43
52:B1:50:LYS:HG2	52:B1:51:GLU:N	2.33	0.43
10:AJ:10:LEU:HD22	10:AJ:22:THR:HB	2.01	0.43
23:AX:63:C:H2'	23:AX:64:G:C8	2.52	0.43
25:BA:906:U:HO2'	37:BM:66:ARG:HH21	1.62	0.43
25:BA:1199:U:H1'	41:BQ:4:VAL:HG22	1.99	0.43
25:BA:1597:A:H5''	25:BA:1598:A:H5'	2.00	0.43
25:BA:1664:A:H61	25:BA:1996:C:H42	1.64	0.43
26:BB:44:G:H1'	26:BB:47:C:H42	1.82	0.43
32:BH:12:LEU:HD13	32:BH:19:VAL:HG21	1.99	0.43
38:BN:2:ARG:HG3	38:BN:5:LYS:HB2	1.98	0.43
2:AB:138:THR:HA	2:AB:141:LEU:HD13	2.00	0.43
2:AB:217:VAL:O	2:AB:221:VAL:HG23	2.18	0.43
8:AH:39:VAL:HG21	8:AH:110:VAL:HG12	1.99	0.43
11:AK:86:VAL:HB	11:AK:112:ASP:HA	2.00	0.43
15:AO:46:HIS:C	15:AO:48:LYS:H	2.26	0.43
25:BA:1636:U:H2'	25:BA:1637:A:C8	2.54	0.43
33:BI:21:SER:HB3	33:BI:22:PRO:HD3	1.99	0.43
35:BK:35:VAL:HG22	35:BK:69:VAL:HG12	2.01	0.43
1:AA:1217:C:OP2	14:AN:9:ARG:NH2	2.50	0.43
1:AA:1492:A:C2'	1:AA:1493:A:C8	3.01	0.43
4:AD:88:GLU:HG2	4:AD:188:ARG:HD3	2.01	0.43
6:AF:3:HIS:CD2	6:AF:94:HIS:HA	2.54	0.43
11:AK:127:ARG:HB2	21:AU:34:ARG:HE	1.83	0.43
13:AM:11:ASP:OD1	13:AM:12:HIS:N	2.51	0.43
25:BA:84:A:OP2	45:BU:6:ARG:NH1	2.51	0.43
25:BA:1010:A:H1'	25:BA:1153:C:H1'	2.01	0.43
28:BD:179:ARG:HB2	28:BD:188:LEU:HD12	2.00	0.43
29:BE:147:LEU:HB3	29:BE:186:VAL:HG22	2.00	0.43
43:BS:56:ALA:HA	43:BS:59:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BT:44:LYS:O	44:BT:48:GLN:HG2	2.19	0.43
1:AA:436:C:H2'	1:AA:437:U:C6	2.53	0.43
1:AA:891:U:H2'	1:AA:892:A:H8	1.83	0.43
1:AA:1106:G:O2'	3:AC:169:ARG:NH1	2.52	0.43
18:AR:29:LEU:HD23	18:AR:59:ILE:HD13	2.00	0.43
21:AU:37:PHE:O	21:AU:39:GLU:N	2.51	0.43
24:AY:65:C:H2'	24:AY:66:A:C8	2.54	0.43
25:BA:534:U:H2'	25:BA:535:G:C8	2.53	0.43
25:BA:673:C:OP1	29:BE:49:ARG:NH2	2.52	0.43
25:BA:958:U:H5'	37:BM:14:LYS:HE2	2.00	0.43
25:BA:979:A:H2'	25:BA:982:C:H42	1.84	0.43
25:BA:2087:G:H2'	25:BA:2088:A:H8	1.83	0.43
57:BA:9000:ERY:H151	57:BA:9000:ERY:H202	1.84	0.43
27:BC:162:VAL:HG11	27:BC:174:LEU:HD23	2.00	0.43
33:BI:94:ASN:ND2	33:BI:137:GLY:HA2	2.34	0.43
36:BL:29:LYS:C	36:BL:30:THR:HG1	2.25	0.43
1:AA:263:A:OP1	20:AT:74:ARG:NH1	2.52	0.43
1:AA:523:A:H61	12:AL:89:ASP:HB3	1.83	0.43
4:AD:124:MET:HG3	4:AD:146:ARG:HG2	2.00	0.43
4:AD:151:LYS:HB3	4:AD:178:MET:HE1	2.00	0.43
5:AE:151:GLU:HG3	5:AE:152:MET:HG2	2.01	0.43
13:AM:27:LYS:O	13:AM:31:LYS:HG2	2.18	0.43
20:AT:35:VAL:HG22	20:AT:50:ALA:HB1	1.99	0.43
25:BA:64:A:H5''	44:BT:77:ARG:HA	2.01	0.43
25:BA:296:U:H2'	25:BA:297:G:C8	2.54	0.43
25:BA:1105:U:H2'	25:BA:1106:G:H8	1.84	0.43
25:BA:2220:U:H2'	25:BA:2221:G:H8	1.84	0.43
25:BA:2874:C:H5''	38:BN:4:ARG:HH21	1.84	0.43
39:BO:39:VAL:N	39:BO:49:VAL:O	2.52	0.43
1:AA:407:U:H2'	1:AA:408:A:H8	1.84	0.43
1:AA:830:G:H2'	1:AA:831:A:C8	2.54	0.43
16:AP:6:LEU:HA	16:AP:19:VAL:HA	2.01	0.43
20:AT:35:VAL:HG11	20:AT:79:LEU:HD13	2.01	0.43
25:BA:459:U:OP2	53:B2:39:ARG:NH1	2.51	0.43
25:BA:1744:A:H3'	25:BA:1745:A:H8	1.84	0.43
25:BA:2146:C:O2'	25:BA:2147:A:O5'	2.23	0.43
25:BA:2838:G:H1'	38:BN:45:ARG:HH12	1.84	0.43
35:BK:9:ASN:OD1	35:BK:18:ARG:NH1	2.52	0.43
1:AA:309:A:H2'	1:AA:310:G:H8	1.84	0.43
1:AA:553:A:O2'	12:AL:26:ALA:O	2.28	0.43
1:AA:603:U:H2'	1:AA:604:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.54	0.43
8:AH:104:VAL:HA	8:AH:125:ILE:HA	2.01	0.43
10:AJ:19:ASP:OD1	10:AJ:20:GLN:N	2.50	0.43
25:BA:244:A:OP2	54:B3:8:ARG:NH1	2.50	0.43
25:BA:1779:U:H5''	25:BA:1780:A:H5''	2.00	0.43
1:AA:553:A:H1'	12:AL:28:PRO:HG3	2.01	0.42
2:AB:69:PHE:HB2	2:AB:91:PHE:HB3	2.01	0.42
16:AP:46:LYS:HG3	16:AP:47:GLU:HG2	2.02	0.42
25:BA:200:U:O2	25:BA:386:G:N2	2.52	0.42
25:BA:290:U:H2'	25:BA:291:G:C8	2.54	0.42
25:BA:634:C:H2'	25:BA:635:C:C6	2.55	0.42
25:BA:1266:G:O2'	25:BA:2012:G:O6	2.33	0.42
25:BA:2279:G:O6	47:BW:14:ARG:NE	2.50	0.42
25:BA:2428:G:N2	36:BL:60:ARG:HH22	2.17	0.42
25:BA:2537:U:H2'	25:BA:2538:C:C6	2.54	0.42
31:BG:54:PRO:HG3	31:BG:62:TRP:CD2	2.54	0.42
32:BH:1:MET:HE1	48:BX:60:ASP:HB3	2.00	0.42
51:B0:54:VAL:O	51:B0:56:ALA:N	2.49	0.42
1:AA:373:A:H61	1:AA:391:G:H1'	1.83	0.42
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.84	0.42
4:AD:188:ARG:NH2	4:AD:197:GLU:OE1	2.52	0.42
23:AX:23:A:H2'	23:AX:24:A:C8	2.54	0.42
25:BA:53:A:H2	25:BA:179:C:H4'	1.84	0.42
25:BA:322:A:P	29:BE:163:ASN:HD21	2.41	0.42
25:BA:2544:G:H1'	25:BA:2646:C:H5'	2.02	0.42
25:BA:2594:C:N4	25:BA:2595:G:O6	2.53	0.42
35:BK:109:SER:O	35:BK:111:LYS:N	2.52	0.42
1:AA:1268:G:N3	1:AA:1326:U:O2'	2.46	0.42
1:AA:1316:G:N2	1:AA:1319:A:OP2	2.52	0.42
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.31	0.42
21:AU:45:ARG:O	21:AU:49:LYS:HG2	2.18	0.42
25:BA:632:A:H2'	25:BA:633:A:C8	2.54	0.42
25:BA:2692:G:H2'	25:BA:2693:G:C8	2.55	0.42
33:BI:15:ALA:HB3	33:BI:52:GLY:H	1.83	0.42
39:BO:27:VAL:HA	39:BO:93:ASP:HB3	2.01	0.42
46:BV:29:ILE:HG22	46:BV:88:HIS:CE1	2.54	0.42
53:B2:9:VAL:HG13	53:B2:12:ARG:HH11	1.83	0.42
1:AA:68:G:C5	1:AA:69:G:H1'	2.53	0.42
1:AA:1350:A:O2'	7:AG:33:ASP:OD1	2.31	0.42
2:AB:47:VAL:HB	2:AB:48:PRO:HD3	2.01	0.42
3:AC:19:ASN:OD1	3:AC:54:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:62:MET:HG2	6:AF:64:VAL:HG23	2.02	0.42
17:AQ:15:ASP:HB2	17:AQ:55:ILE:HB	2.01	0.42
25:BA:775:G:OP1	25:BA:777:G:O2'	2.36	0.42
25:BA:948:C:H2'	25:BA:949:G:C8	2.55	0.42
25:BA:1076:C:H2'	25:BA:1077:A:O4'	2.19	0.42
25:BA:1259:G:H2'	25:BA:1260:A:C8	2.54	0.42
25:BA:1325:U:OP1	25:BA:1647:U:O2'	2.31	0.42
25:BA:1902:C:H5''	27:BC:240:PHE:CE2	2.53	0.42
33:BI:54:PRO:HG2	33:BI:78:VAL:HG21	2.02	0.42
54:B3:29:LEU:HA	54:B3:33:LEU:HD21	2.01	0.42
1:AA:745:G:OP1	1:AA:851:G:O2'	2.38	0.42
3:AC:84:VAL:HG13	3:AC:101:ILE:HD13	2.02	0.42
10:AJ:81:GLU:HA	10:AJ:84:VAL:HG12	2.02	0.42
25:BA:161:A:H3'	25:BA:162:U:H5''	2.00	0.42
25:BA:2719:G:H4'	25:BA:2846:G:H4'	2.01	0.42
28:BD:25:THR:HG21	28:BD:193:VAL:HG22	2.00	0.42
32:BH:31:VAL:HB	32:BH:32:PRO:HD3	2.02	0.42
41:BQ:99:ALA:O	41:BQ:103:LYS:NZ	2.44	0.42
42:BR:75:VAL:HG12	42:BR:77:PHE:H	1.84	0.42
1:AA:19:A:H2'	1:AA:20:U:C6	2.55	0.42
1:AA:52:C:H2'	1:AA:53:A:C8	2.55	0.42
2:AB:67:ILE:HD12	2:AB:160:ALA:HB3	2.01	0.42
6:AF:3:HIS:H	6:AF:92:THR:HG23	1.84	0.42
16:AP:43:ALA:HB1	16:AP:49:GLY:HA2	2.02	0.42
25:BA:45:G:H2'	25:BA:215:G:C5	2.54	0.42
25:BA:546:U:O2	25:BA:546:U:H2'	2.18	0.42
25:BA:743:A:O2'	25:BA:1659:G:OP1	2.33	0.42
25:BA:1106:G:H2'	25:BA:1107:G:H8	1.84	0.42
25:BA:2848:G:O2'	25:BA:2867:G:N2	2.42	0.42
26:BB:49:C:H2'	26:BB:50:A:C8	2.54	0.42
34:BJ:16:TYR:HE1	34:BJ:138:GLN:HE21	1.68	0.42
44:BT:22:THR:HA	44:BT:25:GLU:HG2	2.01	0.42
46:BV:21:ARG:NE	46:BV:87:GLN:OE1	2.51	0.42
47:BW:27:GLY:HA2	47:BW:67:VAL:HB	2.01	0.42
1:AA:73:C:O2'	1:AA:74:A:H8	2.02	0.42
2:AB:199:VAL:HG22	2:AB:201:PRO:HD3	2.02	0.42
25:BA:1060:U:H4'	25:BA:1061:U:H5'	2.01	0.42
25:BA:2394:C:OP1	54:B3:30:ARG:NH1	2.52	0.42
34:BJ:24:THR:HB	34:BJ:27:ARG:HB2	2.01	0.42
34:BJ:32:LEU:HD22	34:BJ:54:ILE:HG21	2.02	0.42
38:BN:78:LYS:HG2	38:BN:83:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1510:C:H42	1:AA:1525:G:H1	1.67	0.42
3:AC:6:HIS:HA	3:AC:7:PRO:HD3	1.87	0.42
3:AC:35:SER:OG	3:AC:59:ARG:NH2	2.46	0.42
4:AD:54:GLN:O	4:AD:203:LEU:HD22	2.20	0.42
5:AE:80:THR:HB	5:AE:122:ASN:HD21	1.85	0.42
25:BA:587:C:N4	36:BL:30:THR:O	2.53	0.42
25:BA:698:C:O2'	25:BA:734:A:N6	2.53	0.42
25:BA:906:U:O2'	37:BM:66:ARG:NH2	2.40	0.42
25:BA:1294:U:O2'	38:BN:23:ASN:OD1	2.31	0.42
25:BA:1368:G:H2'	25:BA:1369:G:H8	1.85	0.42
25:BA:2547:A:H4'	35:BK:29:HIS:CE1	2.55	0.42
35:BK:25:LEU:O	35:BK:30:ARG:NH1	2.53	0.42
35:BK:34:GLY:O	35:BK:36:GLY:N	2.53	0.42
40:BP:90:GLY:HA2	40:BP:113:ARG:H	1.85	0.42
1:AA:376:G:H4'	16:AP:5:ARG:HD2	2.01	0.42
1:AA:619:U:H3	4:AD:131:ASN:HB3	1.85	0.42
1:AA:1494:G:O5'	1:AA:1494:G:C8	2.72	0.42
19:AS:41:PHE:HB2	19:AS:44:MET:HG3	2.01	0.42
19:AS:52:HIS:CE1	19:AS:54:GLY:H	2.38	0.42
25:BA:288:U:H2'	25:BA:289:G:C8	2.55	0.42
25:BA:2742:G:OP2	55:B4:24:ARG:NH1	2.52	0.42
26:BB:114:C:H2'	26:BB:115:A:C8	2.54	0.42
31:BG:33:LEU:HD11	31:BG:137:ASP:HB2	2.02	0.42
37:BM:110:GLU:O	37:BM:114:ARG:HG2	2.19	0.42
44:BT:31:VAL:HG22	44:BT:84:TYR:CD1	2.55	0.42
46:BV:29:ILE:HG22	46:BV:88:HIS:HE1	1.85	0.42
1:AA:21:G:H2'	1:AA:22:G:C8	2.55	0.42
1:AA:626:G:OP1	16:AP:35:ARG:NH2	2.41	0.42
1:AA:718:A:C8	11:AK:118:HIS:HD2	2.38	0.42
1:AA:837:U:H2'	1:AA:838:G:H8	1.85	0.42
2:AB:210:VAL:O	2:AB:214:LEU:HB2	2.20	0.42
9:AI:83:ILE:O	9:AI:87:LEU:HG	2.20	0.42
13:AM:81:MET:HB3	13:AM:92:ARG:NH2	2.35	0.42
16:AP:57:ILE:O	16:AP:61:VAL:HG23	2.20	0.42
25:BA:213:A:H2'	25:BA:214:G:C8	2.55	0.42
25:BA:629:G:H5''	25:BA:650:C:O2'	2.20	0.42
25:BA:1278:C:H2'	25:BA:1279:G:C8	2.55	0.42
27:BC:45:ASN:OD1	27:BC:46:ASN:N	2.53	0.42
1:AA:257:G:H2'	1:AA:258:G:H8	1.84	0.41
10:AJ:6:ILE:HG22	10:AJ:8:ILE:HG13	2.02	0.41
10:AJ:9:ARG:NH2	10:AJ:99:GLN:OE1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:44:LYS:N	12:AL:45:PRO:HD2	2.35	0.41
14:AN:99:ALA:HB1	14:AN:101:TRP:HZ3	1.83	0.41
18:AR:72:ASP:OD2	21:AU:4:ILE:N	2.53	0.41
19:AS:63:THR:HB	19:AS:66:MET:HG2	2.02	0.41
25:BA:605:G:OP1	29:BE:99:LYS:NZ	2.53	0.41
25:BA:2086:U:H2'	25:BA:2087:G:C8	2.55	0.41
27:BC:91:ILE:HD12	27:BC:103:TYR:CD1	2.55	0.41
33:BI:122:ILE:HA	33:BI:125:MET:HE3	2.02	0.41
1:AA:536:C:N4	1:AA:537:G:O6	2.53	0.41
1:AA:948:C:H2'	1:AA:949:A:H8	1.85	0.41
10:AJ:78:GLU:HG3	10:AJ:80:THR:H	1.85	0.41
17:AQ:61:ILE:HG12	17:AQ:73:TRP:CE3	2.55	0.41
25:BA:177:G:OP2	25:BA:177:G:N2	2.30	0.41
25:BA:1709:U:H2'	25:BA:1710:G:C8	2.54	0.41
25:BA:2362:C:H5''	54:B3:40:ARG:HH11	1.84	0.41
46:BV:7:GLU:O	46:BV:41:GLU:HG2	2.20	0.41
47:BW:37:ILE:HD11	47:BW:82:ILE:HD11	2.02	0.41
50:BZ:24:LEU:HD11	50:BZ:54:MET:HE1	2.02	0.41
1:AA:205:A:N6	1:AA:213:G:O6	2.52	0.41
1:AA:410:G:N7	1:AA:429:U:O2'	2.52	0.41
1:AA:920:U:H2'	1:AA:921:U:C6	2.55	0.41
1:AA:1118:U:H2'	1:AA:1119:C:C6	2.55	0.41
9:AI:6:TYR:CE1	9:AI:89:GLU:HG2	2.56	0.41
25:BA:171:U:H2'	25:BA:172:A:C8	2.56	0.41
25:BA:307:G:N1	25:BA:310:A:OP2	2.49	0.41
25:BA:355:U:H2'	25:BA:356:G:C8	2.55	0.41
25:BA:1178:C:H2'	25:BA:1179:G:H8	1.85	0.41
25:BA:2787:C:H1'	28:BD:63:PRO:HG3	2.02	0.41
28:BD:11:MET:HA	28:BD:25:THR:HA	2.01	0.41
31:BG:107:LEU:HD13	31:BG:152:ARG:HB2	2.02	0.41
1:AA:254:G:O2'	17:AQ:18:GLU:O	2.38	0.41
1:AA:1163:A:H2'	1:AA:1164:G:C8	2.55	0.41
1:AA:1256:A:O2'	1:AA:1278:G:O6	2.35	0.41
12:AL:29:GLN:HB3	12:AL:81:LEU:HD11	2.02	0.41
14:AN:80:SER:O	14:AN:84:VAL:HG23	2.20	0.41
19:AS:50:ALA:HA	19:AS:59:PRO:HA	2.03	0.41
25:BA:340:A:O2'	29:BE:162:ARG:NH1	2.51	0.41
25:BA:594:U:H2'	25:BA:595:C:C6	2.55	0.41
27:BC:93:LEU:HD11	27:BC:101:ARG:HB3	2.02	0.41
37:BM:136:MET:HE1	46:BV:74:ALA:HB1	2.02	0.41
45:BU:28:VAL:HA	45:BU:34:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:B1:12:VAL:HG22	52:B1:51:GLU:HB3	2.03	0.41
4:AD:168:PRO:HB3	4:AD:170:TRP:CH2	2.55	0.41
14:AN:7:LYS:O	14:AN:11:VAL:HG23	2.20	0.41
25:BA:355:U:H2'	25:BA:356:G:H8	1.85	0.41
25:BA:745:G:O2'	25:BA:748:G:H1'	2.21	0.41
25:BA:1028:A:N6	25:BA:1125:G:H2'	2.36	0.41
25:BA:2696:U:H2'	25:BA:2697:G:C8	2.55	0.41
27:BC:258:ARG:NH2	27:BC:264:ASP:OD1	2.48	0.41
28:BD:112:THR:O	28:BD:195:GLY:HA2	2.20	0.41
35:BK:30:ARG:HH22	35:BK:37:ASP:CG	2.29	0.41
35:BK:92:GLU:HB3	35:BK:93:GLN:H	1.71	0.41
2:AB:193:PRO:O	2:AB:195:GLY:N	2.49	0.41
25:BA:2061:G:H2'	25:BA:2501:C:O2'	2.21	0.41
27:BC:34:LEU:HD23	27:BC:63:ARG:HG2	2.02	0.41
35:BK:103:VAL:HB	35:BK:107:LEU:HD22	2.01	0.41
43:BS:69:LEU:C	43:BS:70:LYS:HD2	2.45	0.41
1:AA:178:C:OP2	20:AT:60:ARG:NH2	2.53	0.41
1:AA:502:A:H61	1:AA:543:U:H3	1.68	0.41
1:AA:1320:C:N4	19:AS:37:ARG:HG2	2.36	0.41
1:AA:1395:C:O2'	1:AA:1401:G:O2'	2.31	0.41
4:AD:103:TYR:O	4:AD:165:ARG:NH1	2.52	0.41
8:AH:92:LEU:HD21	8:AH:113:ASP:HB2	2.03	0.41
25:BA:2395:C:H42	25:BA:2421:G:H1	1.68	0.41
34:BJ:8:PRO:HB3	34:BJ:48:VAL:HG13	2.03	0.41
50:BZ:41:THR:OG1	50:BZ:42:PRO:HD2	2.21	0.41
1:AA:377:G:H2'	1:AA:378:G:C8	2.55	0.41
1:AA:718:A:H5'	11:AK:119:ASN:ND2	2.36	0.41
1:AA:1130:A:H2'	1:AA:1131:G:C8	2.56	0.41
1:AA:1513:A:H2'	1:AA:1514:G:C8	2.55	0.41
11:AK:23:ILE:HG22	11:AK:32:VAL:HG22	2.02	0.41
12:AL:102:LEU:HB3	12:AL:103:ASP:H	1.57	0.41
14:AN:33:ASP:OD1	14:AN:34:VAL:N	2.49	0.41
16:AP:12:LYS:C	16:AP:14:ARG:H	2.28	0.41
25:BA:1752:C:H2'	25:BA:1753:G:C8	2.56	0.41
26:BB:115:A:H2'	26:BB:116:G:C8	2.56	0.41
27:BC:88:SER:O	27:BC:197:ASN:ND2	2.54	0.41
29:BE:131:THR:HG22	29:BE:160:ALA:HA	2.03	0.41
30:BF:126:GLY:HA2	30:BF:163:ASP:HA	2.01	0.41
36:BL:29:LYS:O	36:BL:31:GLY:N	2.54	0.41
41:BQ:8:VAL:HG13	41:BQ:9:ILE:HG23	2.03	0.41
44:BT:31:VAL:HG22	44:BT:84:TYR:HD1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:216:U:H2'	1:AA:217:C:C6	2.56	0.41
1:AA:658:C:H1'	15:AO:22:THR:HG21	2.03	0.41
1:AA:875:U:O3'	8:AH:15:ARG:NH1	2.54	0.41
1:AA:950:U:H2'	1:AA:951:G:H8	1.86	0.41
1:AA:1227:A:H5'	13:AM:110:LYS:NZ	2.35	0.41
2:AB:151:ILE:HA	2:AB:154:MET:HB2	2.01	0.41
2:AB:167:ASP:HB3	2:AB:191:SER:HA	2.03	0.41
4:AD:167:LYS:HD2	4:AD:173:VAL:HG11	2.03	0.41
5:AE:66:LYS:HA	5:AE:69:ARG:HH11	1.85	0.41
5:AE:132:ASN:HA	5:AE:133:PRO:HD2	1.95	0.41
6:AF:5:GLU:HG3	6:AF:63:ASN:ND2	2.36	0.41
7:AG:73:VAL:HG12	7:AG:90:GLU:HG3	2.03	0.41
10:AJ:9:ARG:NH1	10:AJ:11:LYS:HD2	2.36	0.41
11:AK:122:ARG:HG3	21:AU:36:GLU:HB2	2.02	0.41
12:AL:24:LEU:C	12:AL:26:ALA:H	2.29	0.41
20:AT:31:PHE:O	20:AT:35:VAL:HG23	2.21	0.41
25:BA:495:G:O2'	43:BS:61:ASN:ND2	2.54	0.41
25:BA:856:G:H1	25:BA:921:C:H42	1.67	0.41
25:BA:1751:U:H2'	25:BA:1752:C:C6	2.56	0.41
25:BA:2087:G:H2'	25:BA:2088:A:C8	2.55	0.41
25:BA:2275:C:H1'	37:BM:84:LYS:HA	2.01	0.41
25:BA:2548:U:O2'	35:BK:4:GLU:OE1	2.38	0.41
27:BC:30:PHE:CE2	27:BC:32:PRO:HG2	2.55	0.41
28:BD:105:LYS:HG2	28:BD:106:LYS:HG3	2.03	0.41
44:BT:4:GLU:O	44:BT:8:LEU:HG	2.21	0.41
52:B1:9:ILE:HG21	52:B1:25:LYS:HE2	2.03	0.41
1:AA:392:C:H2'	1:AA:393:A:C8	2.55	0.41
1:AA:944:G:N1	1:AA:1338:G:OP2	2.35	0.41
1:AA:1491:G:C5'	1:AA:1491:G:H8	2.32	0.41
24:AY:40:G:H2'	24:AY:41:A:C8	2.56	0.41
25:BA:743:A:OP1	28:BD:135:GLY:HA2	2.21	0.41
25:BA:856:G:H2'	25:BA:857:G:C8	2.56	0.41
25:BA:1563:U:H2'	25:BA:1564:C:C6	2.56	0.41
25:BA:1590:A:H2'	25:BA:1591:A:C8	2.55	0.41
25:BA:2010:G:H5''	43:BS:42:LYS:HB2	2.03	0.41
25:BA:2314:A:H2'	25:BA:2315:G:C8	2.55	0.41
25:BA:2772:C:H5'	28:BD:173:GLN:HE21	1.84	0.41
26:BB:38:C:H2'	26:BB:39:A:C8	2.56	0.41
31:BG:145:ALA:HB1	31:BG:164:TYR:HE1	1.84	0.41
38:BN:42:LYS:HA	38:BN:45:ARG:HE	1.85	0.41
1:AA:1318:A:O2'	19:AS:37:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:181:ILE:HA	2:AB:182:PRO:HD3	1.97	0.40
23:AX:50:C:H2'	23:AX:51:G:C8	2.56	0.40
25:BA:172:A:H2'	25:BA:173:A:C8	2.56	0.40
31:BG:38:ASN:HB3	31:BG:41:VAL:HG23	2.03	0.40
48:BX:38:PHE:CD2	48:BX:49:LEU:HD12	2.56	0.40
1:AA:591:U:H2'	1:AA:592:G:C8	2.56	0.40
1:AA:808:C:H2'	1:AA:809:G:C8	2.56	0.40
1:AA:1227:A:H5'	13:AM:110:LYS:HZ2	1.86	0.40
2:AB:176:ALA:O	2:AB:181:ILE:N	2.53	0.40
3:AC:20:SER:HA	3:AC:57:ILE:O	2.21	0.40
4:AD:198:HIS:O	4:AD:202:GLU:HG3	2.21	0.40
11:AK:101:ASN:OD1	11:AK:102:ALA:N	2.54	0.40
25:BA:2111:U:C5	25:BA:2145:C:H2'	2.57	0.40
25:BA:2159:G:H2'	25:BA:2160:C:C6	2.56	0.40
25:BA:2478:A:OP2	55:B4:2:LYS:HD3	2.21	0.40
25:BA:2554:U:H2'	25:BA:2555:U:C6	2.56	0.40
25:BA:2875:C:H2'	25:BA:2876:G:C8	2.56	0.40
32:BH:38:PRO:O	32:BH:43:ASN:ND2	2.47	0.40
35:BK:26:GLY:O	35:BK:30:ARG:HD2	2.20	0.40
36:BL:29:LYS:O	36:BL:30:THR:OG1	2.33	0.40
1:AA:227:G:O2'	16:AP:63:GLN:NE2	2.52	0.40
1:AA:392:C:HO2'	1:AA:483:C:HO2'	1.61	0.40
1:AA:454:G:H1	1:AA:478:A:H61	1.69	0.40
3:AC:23:PHE:CZ	10:AJ:11:LYS:HE2	2.56	0.40
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.02	0.40
11:AK:81:ASN:OD1	11:AK:106:ARG:HB3	2.21	0.40
25:BA:937:C:H2'	25:BA:938:G:C8	2.57	0.40
25:BA:1162:G:H2'	25:BA:1163:G:H8	1.87	0.40
25:BA:2106:U:H2'	25:BA:2107:G:H8	1.87	0.40
25:BA:2220:U:H2'	25:BA:2221:G:C8	2.56	0.40
25:BA:2746:U:H5''	31:BG:138:LYS:HE2	2.01	0.40
26:BB:103:U:H2'	26:BB:104:A:H8	1.85	0.40
27:BC:3:VAL:HG12	27:BC:19:VAL:HG22	2.03	0.40
35:BK:105:ARG:NH1	35:BK:122:VAL:O	2.55	0.40
38:BN:76:VAL:HA	38:BN:79:LEU:HD12	2.03	0.40
39:BO:49:VAL:HG22	39:BO:85:LYS:HD3	2.03	0.40
40:BP:14:LYS:HE3	40:BP:77:HIS:HA	2.03	0.40
6:AF:51:ILE:O	6:AF:51:ILE:HG13	2.22	0.40
12:AL:30:LYS:O	12:AL:82:ILE:HG22	2.21	0.40
25:BA:833:A:H2'	25:BA:834:G:C8	2.56	0.40
25:BA:1316:U:H2'	25:BA:1317:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1668:A:N6	25:BA:1676:A:H61	2.20	0.40
25:BA:2216:G:H2'	25:BA:2217:G:H8	1.86	0.40
25:BA:2357:G:N2	25:BA:2360:G:OP2	2.48	0.40
25:BA:2837:A:H2'	25:BA:2838:G:H8	1.86	0.40
57:BA:9000:ERY:H5	57:BA:9000:ERY:H18	2.03	0.40
27:BC:232:HIS:CE1	27:BC:244:PRO:HA	2.56	0.40
37:BM:76:LYS:HA	37:BM:77:PRO:HD3	1.97	0.40
48:BX:37:ARG:HD2	48:BX:46:PHE:HB3	2.03	0.40
2:AB:114:LEU:HD13	2:AB:144:LEU:HB2	2.03	0.40
4:AD:203:LEU:O	4:AD:206:LYS:HG2	2.21	0.40
6:AF:10:VAL:HB	6:AF:58:HIS:HB3	2.04	0.40
20:AT:28:MET:HE3	20:AT:58:VAL:HG13	2.04	0.40
25:BA:190:A:H5''	25:BA:204:A:H61	1.86	0.40
25:BA:521:U:H2'	25:BA:522:A:C8	2.57	0.40
25:BA:796:C:H2'	25:BA:797:G:C8	2.57	0.40
25:BA:1252:G:H1	41:BQ:37:GLN:NE2	2.19	0.40
25:BA:1903:G:H2'	25:BA:1904:G:C8	2.57	0.40
25:BA:2039:U:H2'	25:BA:2040:G:H8	1.86	0.40
25:BA:2827:C:H2'	25:BA:2828:G:H8	1.86	0.40
26:BB:80:U:H2'	26:BB:81:G:H8	1.86	0.40
28:BD:11:MET:HG2	28:BD:25:THR:OG1	2.22	0.40
28:BD:104:VAL:O	28:BD:106:LYS:N	2.53	0.40
28:BD:136:ASN:OD1	28:BD:137:SER:N	2.55	0.40
36:BL:96:LYS:HD3	36:BL:103:ILE:HA	2.04	0.40
42:BR:54:VAL:HG12	42:BR:57:GLY:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	216/240 (90%)	190 (88%)	19 (9%)	7 (3%)	3 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/233 (88%)	180 (88%)	18 (9%)	6 (3%)	3	26
4	AD	203/206 (98%)	187 (92%)	10 (5%)	6 (3%)	3	25
5	AE	148/167 (89%)	125 (84%)	16 (11%)	7 (5%)	2	17
6	AF	98/135 (73%)	85 (87%)	8 (8%)	5 (5%)	1	15
7	AG	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	18	51
8	AH	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	16	49
9	AI	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	2	16
10	AJ	96/103 (93%)	82 (85%)	8 (8%)	6 (6%)	1	12
11	AK	115/129 (89%)	98 (85%)	14 (12%)	3 (3%)	4	27
12	AL	121/124 (98%)	107 (88%)	7 (6%)	7 (6%)	1	13
13	AM	112/118 (95%)	104 (93%)	5 (4%)	3 (3%)	4	27
14	AN	92/102 (90%)	78 (85%)	9 (10%)	5 (5%)	1	14
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	AP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	4	28
17	AQ	78/84 (93%)	65 (83%)	10 (13%)	3 (4%)	2	21
18	AR	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	AS	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	9	39
20	AT	83/87 (95%)	77 (93%)	3 (4%)	3 (4%)	2	22
21	AU	49/71 (69%)	37 (76%)	7 (14%)	5 (10%)	0	5
27	BC	269/273 (98%)	246 (91%)	17 (6%)	6 (2%)	5	30
28	BD	207/209 (99%)	190 (92%)	15 (7%)	2 (1%)	12	45
29	BE	199/201 (99%)	187 (94%)	10 (5%)	2 (1%)	12	45
30	BF	175/179 (98%)	156 (89%)	14 (8%)	5 (3%)	3	26
31	BG	174/177 (98%)	161 (92%)	10 (6%)	3 (2%)	7	35
32	BH	45/149 (30%)	34 (76%)	8 (18%)	3 (7%)	1	11
33	BI	139/142 (98%)	117 (84%)	14 (10%)	8 (6%)	1	13
34	BJ	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	18	51
35	BK	120/123 (98%)	105 (88%)	10 (8%)	5 (4%)	2	19
36	BL	141/144 (98%)	117 (83%)	17 (12%)	7 (5%)	1	16
37	BM	134/136 (98%)	125 (93%)	6 (4%)	3 (2%)	5	30
38	BN	118/127 (93%)	105 (89%)	8 (7%)	5 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BO	114/117 (97%)	104 (91%)	7 (6%)	3 (3%)	4	27
40	BP	112/115 (97%)	104 (93%)	6 (5%)	2 (2%)	6	34
41	BQ	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
42	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	3	25
43	BS	108/110 (98%)	98 (91%)	8 (7%)	2 (2%)	6	33
44	BT	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	30
45	BU	100/104 (96%)	83 (83%)	12 (12%)	5 (5%)	1	16
46	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
47	BW	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
48	BX	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
49	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
50	BZ	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	6	34
51	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
52	B1	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	5	31
53	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	30
54	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	B4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
56	B5	7/9 (78%)	2 (29%)	4 (57%)	1 (14%)	0	3
All	All	5522/5994 (92%)	4969 (90%)	405 (7%)	148 (3%)	6	27

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	105	ILE
9	AI	55	VAL
11	AK	127	ARG
17	AQ	17	MET
17	AQ	51	ASN
21	AU	40	LYS
28	BD	152	PRO
32	BH	3	VAL
32	BH	9	VAL
32	BH	10	ALA
33	BI	93	PRO
36	BL	94	THR
56	B5	-7	VAL

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Mol	Chain	Res	Type
2	AB	193	PRO
4	AD	28	ILE
4	AD	30	THR
5	AE	12	GLN
5	AE	158	GLY
8	AH	88	ARG
9	AI	13	LYS
9	AI	58	VAL
9	AI	91	ASP
10	AJ	57	VAL
11	AK	89	PRO
12	AL	23	ALA
12	AL	24	LEU
12	AL	34	CYS
12	AL	43	LYS
14	AN	22	ALA
14	AN	52	PRO
14	AN	92	GLU
21	AU	9	ASN
21	AU	24	GLU
31	BG	175	LYS
33	BI	65	ARG
35	BK	108	ARG
36	BL	29	LYS
36	BL	111	ILE
38	BN	70	THR
38	BN	106	ASP
39	BO	57	ALA
44	BT	77	ARG
45	BU	7	ARG
45	BU	17	LYS
45	BU	76	ALA
2	AB	34	ALA
2	AB	68	LEU
2	AB	82	ASP
3	AC	80	LYS
3	AC	166	GLU
3	AC	206	GLU
4	AD	165	ARG
4	AD	175	ALA
5	AE	24	THR
5	AE	122	ASN

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Mol	Chain	Res	Type
6	AF	54	LEU
6	AF	86	ARG
6	AF	94	HIS
7	AG	114	LYS
9	AI	129	LYS
12	AL	76	GLU
12	AL	78	SER
13	AM	114	LYS
14	AN	3	LYS
14	AN	21	PHE
16	AP	43	ALA
19	AS	5	LEU
21	AU	35	ARG
21	AU	38	TYR
27	BC	240	PHE
28	BD	41	ALA
30	BF	9	LYS
30	BF	133	ARG
31	BG	45	HIS
31	BG	46	ALA
33	BI	13	VAL
33	BI	88	SER
34	BJ	82	GLY
36	BL	30	THR
36	BL	82	LEU
38	BN	3	HIS
40	BP	36	SER
43	BS	12	SER
50	BZ	4	THR
53	B2	45	SER
2	AB	19	GLN
2	AB	75	ALA
4	AD	192	SER
5	AE	101	GLU
6	AF	63	ASN
9	AI	9	THR
10	AJ	95	GLY
10	AJ	101	SER
13	AM	5	ALA
16	AP	47	GLU
17	AQ	76	VAL
20	AT	41	ALA

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Mol	Chain	Res	Type
20	AT	42	GLY
20	AT	68	HIS
27	BC	30	PHE
27	BC	152	GLY
27	BC	253	LYS
33	BI	31	GLN
35	BK	93	GLN
35	BK	110	GLU
36	BL	70	LYS
37	BM	70	ASP
39	BO	100	HIS
40	BP	94	LYS
42	BR	43	ASN
42	BR	53	PHE
45	BU	55	PRO
45	BU	99	ASN
52	B1	51	GLU
6	AF	92	THR
10	AJ	36	VAL
12	AL	17	ALA
27	BC	205	LEU
27	BC	236	GLU
29	BE	83	VAL
30	BF	85	ILE
33	BI	21	SER
35	BK	119	ALA
37	BM	69	PRO
38	BN	118	ARG
39	BO	66	GLY
44	BT	88	LYS
2	AB	86	SER
3	AC	61	ALA
4	AD	167	LYS
10	AJ	42	LEU
29	BE	80	SER
30	BF	175	PHE
36	BL	100	ILE
37	BM	24	THR
38	BN	2	ARG
35	BK	35	VAL
43	BS	29	VAL
3	AC	66	VAL

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Mol	Chain	Res	Type
10	AJ	41	PRO
11	AK	92	GLY
3	AC	81	GLY
5	AE	143	GLY
13	AM	4	ILE
30	BF	149	VAL
33	BI	85	GLY
42	BR	58	VAL
33	BI	89	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/198 (91%)	180 (100%)	0	100	100
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	113/126 (90%)	113 (100%)	0	100	100
6	AF	87/116 (75%)	87 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	86/90 (96%)	86 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	103/104 (99%)	103 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	75/77 (97%)	75 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AS	70/79 (89%)	70 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	44/61 (72%)	44 (100%)	0	100	100
27	BC	216/218 (99%)	216 (100%)	0	100	100
28	BD	164/164 (100%)	164 (100%)	0	100	100
29	BE	165/165 (100%)	165 (100%)	0	100	100
30	BF	148/150 (99%)	148 (100%)	0	100	100
31	BG	137/138 (99%)	137 (100%)	0	100	100
32	BH	38/114 (33%)	38 (100%)	0	100	100
33	BI	109/110 (99%)	109 (100%)	0	100	100
34	BJ	116/116 (100%)	116 (100%)	0	100	100
35	BK	103/104 (99%)	103 (100%)	0	100	100
36	BL	102/103 (99%)	102 (100%)	0	100	100
37	BM	109/109 (100%)	109 (100%)	0	100	100
38	BN	100/103 (97%)	100 (100%)	0	100	100
39	BO	86/87 (99%)	86 (100%)	0	100	100
40	BP	99/100 (99%)	99 (100%)	0	100	100
41	BQ	89/90 (99%)	89 (100%)	0	100	100
42	BR	84/84 (100%)	84 (100%)	0	100	100
43	BS	93/93 (100%)	93 (100%)	0	100	100
44	BT	80/84 (95%)	80 (100%)	0	100	100
45	BU	83/85 (98%)	83 (100%)	0	100	100
46	BV	78/78 (100%)	78 (100%)	0	100	100
47	BW	56/63 (89%)	56 (100%)	0	100	100
48	BX	67/68 (98%)	67 (100%)	0	100	100
49	BY	55/55 (100%)	55 (100%)	0	100	100
50	BZ	48/49 (98%)	48 (100%)	0	100	100
51	B0	47/48 (98%)	47 (100%)	0	100	100
52	B1	45/49 (92%)	45 (100%)	0	100	100
53	B2	38/38 (100%)	38 (100%)	0	100	100
54	B3	51/52 (98%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	8/8 (100%)	8 (100%)	0	100	100
All	All	4594/4885 (94%)	4594 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	15	HIS
3	AC	8	ASN
3	AC	102	ASN
4	AD	74	ASN
4	AD	116	GLN
4	AD	140	ASN
4	AD	152	GLN
4	AD	196	ASN
5	AE	89	HIS
6	AF	3	HIS
6	AF	37	HIS
6	AF	55	HIS
6	AF	63	ASN
6	AF	94	HIS
7	AG	28	ASN
7	AG	86	GLN
7	AG	148	ASN
8	AH	4	GLN
8	AH	16	ASN
8	AH	76	GLN
10	AJ	56	HIS
11	AK	118	HIS
11	AK	119	ASN
12	AL	5	ASN
12	AL	77	HIS
13	AM	100	GLN
14	AN	49	GLN
15	AO	50	HIS
16	AP	63	GLN
17	AQ	31	HIS
19	AS	57	HIS
20	AT	48	GLN

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Mol	Chain	Res	Type
20	AT	75	HIS
27	BC	46	ASN
27	BC	86	ASN
27	BC	90	ASN
27	BC	134	ASN
28	BD	150	GLN
29	BE	41	GLN
29	BE	92	HIS
29	BE	163	ASN
30	BF	63	GLN
31	BG	22	GLN
31	BG	116	GLN
31	BG	143	GLN
32	BH	43	ASN
33	BI	12	GLN
33	BI	43	ASN
35	BK	29	HIS
35	BK	93	GLN
36	BL	35	HIS
36	BL	54	GLN
37	BM	22	GLN
38	BN	9	GLN
38	BN	31	HIS
41	BQ	20	GLN
41	BQ	37	GLN
41	BQ	52	GLN
42	BR	11	GLN
42	BR	86	GLN
43	BS	9	HIS
43	BS	40	ASN
43	BS	61	ASN
45	BU	66	GLN
45	BU	74	ASN
46	BV	51	GLN
47	BW	76	ASN
48	BX	16	ASN
48	BX	17	ASN
49	BY	25	GLN
49	BY	27	ASN
51	B0	38	HIS
52	B1	19	HIS
53	B2	13	ASN

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Mol	Chain	Res	Type
54	B3	24	HIS
55	B4	13	ASN
55	B4	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1539 (99%)	220 (14%)	6 (0%)
22	AV	9/10 (90%)	0	0
23	AX	76/77 (98%)	7 (9%)	0
24	AY	69/71 (97%)	13 (18%)	1 (1%)
25	BA	2895/2903 (99%)	428 (14%)	8 (0%)
26	BB	117/120 (97%)	13 (11%)	0
All	All	4704/4720 (99%)	681 (14%)	15 (0%)

All (681) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	69	G
1	AA	70	U
1	AA	74	A
1	AA	83	C
1	AA	85	U
1	AA	87	C
1	AA	88	U
1	AA	95	C
1	AA	97	G
1	AA	108	G
1	AA	116	A
1	AA	120	A
1	AA	121	U
1	AA	130	A

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Mol	Chain	Res	Type
1	AA	131	A
1	AA	149	A
1	AA	182	A
1	AA	204	G
1	AA	207	C
1	AA	208	U
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	280	C
1	AA	289	G
1	AA	298	A
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	347	G
1	AA	352	C
1	AA	354	G
1	AA	356	A
1	AA	367	U
1	AA	372	C
1	AA	378	G
1	AA	397	A
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	451	A
1	AA	452	A
1	AA	459	A
1	AA	467	U

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Mol	Chain	Res	Type
1	AA	468	A
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	482	A
1	AA	485	U
1	AA	486	U
1	AA	496	A
1	AA	497	G
1	AA	509	A
1	AA	511	C
1	AA	518	C
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	633	G
1	AA	642	A
1	AA	650	G
1	AA	665	A
1	AA	675	A
1	AA	687	A
1	AA	694	A
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	731	G
1	AA	747	A
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A

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Mol	Chain	Res	Type
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	829	G
1	AA	832	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	873	A
1	AA	885	G
1	AA	914	A
1	AA	926	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1026	G
1	AA	1027	C
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1034	G
1	AA	1036	A
1	AA	1043	G
1	AA	1044	A
1	AA	1050	G
1	AA	1054	C
1	AA	1065	U
1	AA	1073	U
1	AA	1094	G
1	AA	1095	U

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Mol	Chain	Res	Type
1	AA	1101	A
1	AA	1125	U
1	AA	1133	G
1	AA	1134	G
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1145	A
1	AA	1152	A
1	AA	1157	A
1	AA	1159	U
1	AA	1160	G
1	AA	1161	C
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1240	U
1	AA	1241	G
1	AA	1253	G
1	AA	1256	A
1	AA	1257	A
1	AA	1261	A
1	AA	1275	A
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1322	C

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Mol	Chain	Res	Type
1	AA	1337	G
1	AA	1346	A
1	AA	1347	G
1	AA	1363	A
1	AA	1364	U
1	AA	1377	A
1	AA	1379	G
1	AA	1394	A
1	AA	1398	A
1	AA	1413	A
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1452	C
1	AA	1491	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1505	G
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1535	C
1	AA	1536	C
23	AX	3	A
23	AX	19	H2U
23	AX	21	A
23	AX	47	U
23	AX	67	C
23	AX	68	G
23	AX	76	A
24	AY	5	G
24	AY	14	A
24	AY	19	G
24	AY	20	G
24	AY	21	A
24	AY	23	A

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Mol	Chain	Res	Type
24	AY	45	G
24	AY	46	7MG
24	AY	47	U
24	AY	48	C
24	AY	54	5MU
24	AY	59	U
24	AY	60	C
25	BA	10	A
25	BA	14	A
25	BA	34	U
25	BA	39	G
25	BA	42	A
25	BA	46	G
25	BA	63	A
25	BA	71	A
25	BA	74	A
25	BA	75	G
25	BA	80	G
25	BA	83	A
25	BA	84	A
25	BA	98	G
25	BA	101	A
25	BA	118	A
25	BA	119	A
25	BA	120	U
25	BA	138	U
25	BA	139	U
25	BA	140	C
25	BA	141	G
25	BA	142	A
25	BA	162	U
25	BA	165	A
25	BA	181	A
25	BA	196	A
25	BA	199	A
25	BA	216	A
25	BA	222	A
25	BA	223	A
25	BA	233	A
25	BA	248	G
25	BA	249	C
25	BA	255	A

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Mol	Chain	Res	Type
25	BA	265	A
25	BA	266	G
25	BA	271	G
25	BA	272	A
25	BA	276	U
25	BA	278	A
25	BA	279	A
25	BA	285	G
25	BA	294	A
25	BA	311	A
25	BA	321	U
25	BA	322	A
25	BA	324	A
25	BA	329	G
25	BA	330	A
25	BA	346	A
25	BA	361	G
25	BA	367	G
25	BA	371	A
25	BA	372	G
25	BA	380	G
25	BA	386	G
25	BA	396	G
25	BA	404	A
25	BA	405	U
25	BA	411	G
25	BA	412	A
25	BA	424	G
25	BA	451	U
25	BA	455	C
25	BA	457	A
25	BA	467	G
25	BA	479	A
25	BA	480	A
25	BA	481	G
25	BA	490	C
25	BA	491	G
25	BA	504	A
25	BA	505	A
25	BA	508	A
25	BA	528	A
25	BA	531	C

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Mol	Chain	Res	Type
25	BA	532	A
25	BA	533	G
25	BA	543	G
25	BA	544	C
25	BA	546	U
25	BA	547	A
25	BA	548	G
25	BA	549	G
25	BA	563	A
25	BA	572	A
25	BA	573	U
25	BA	574	A
25	BA	575	A
25	BA	586	A
25	BA	603	A
25	BA	613	A
25	BA	627	A
25	BA	631	A
25	BA	637	A
25	BA	647	G
25	BA	654	A
25	BA	685	A
25	BA	686	U
25	BA	695	G
25	BA	717	C
25	BA	727	A
25	BA	730	A
25	BA	747	U
25	BA	751	A
25	BA	764	A
25	BA	775	G
25	BA	776	G
25	BA	781	A
25	BA	782	A
25	BA	784	G
25	BA	785	G
25	BA	789	A
25	BA	792	A
25	BA	802	A
25	BA	805	G
25	BA	812	C
25	BA	819	A

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Mol	Chain	Res	Type
25	BA	827	U
25	BA	828	U
25	BA	830	G
25	BA	844	A
25	BA	845	A
25	BA	846	U
25	BA	858	G
25	BA	878	A
25	BA	896	A
25	BA	897	C
25	BA	910	A
25	BA	914	G
25	BA	915	C
25	BA	941	A
25	BA	946	C
25	BA	953	G
25	BA	959	A
25	BA	961	C
25	BA	974	G
25	BA	983	A
25	BA	995	C
25	BA	996	A
25	BA	1009	A
25	BA	1012	U
25	BA	1013	C
25	BA	1021	A
25	BA	1022	G
25	BA	1026	G
25	BA	1033	U
25	BA	1040	A
25	BA	1046	A
25	BA	1047	G
25	BA	1060	U
25	BA	1061	U
25	BA	1065	U
25	BA	1066	U
25	BA	1068	G
25	BA	1070	A
25	BA	1071	G
25	BA	1072	C
25	BA	1077	A
25	BA	1088	A

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Mol	Chain	Res	Type
25	BA	1089	A
25	BA	1092	C
25	BA	1094	U
25	BA	1098	A
25	BA	1111	A
25	BA	1112	G
25	BA	1132	U
25	BA	1133	A
25	BA	1135	C
25	BA	1136	G
25	BA	1143	A
25	BA	1151	A
25	BA	1175	A
25	BA	1176	U
25	BA	1178	C
25	BA	1180	U
25	BA	1186	G
25	BA	1204	A
25	BA	1206	G
25	BA	1212	G
25	BA	1238	G
25	BA	1250	G
25	BA	1253	A
25	BA	1256	G
25	BA	1266	G
25	BA	1271	G
25	BA	1272	A
25	BA	1300	G
25	BA	1301	A
25	BA	1302	A
25	BA	1314	C
25	BA	1355	G
25	BA	1365	A
25	BA	1368	G
25	BA	1378	A
25	BA	1379	U
25	BA	1383	A
25	BA	1384	A
25	BA	1386	C
25	BA	1387	A
25	BA	1391	U
25	BA	1395	A

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Mol	Chain	Res	Type
25	BA	1403	A
25	BA	1416	G
25	BA	1419	A
25	BA	1420	A
25	BA	1428	C
25	BA	1452	G
25	BA	1458	U
25	BA	1478	G
25	BA	1482	G
25	BA	1493	C
25	BA	1494	A
25	BA	1504	A
25	BA	1509	A
25	BA	1510	G
25	BA	1515	A
25	BA	1533	C
25	BA	1535	A
25	BA	1536	C
25	BA	1537	G
25	BA	1560	G
25	BA	1566	A
25	BA	1569	A
25	BA	1578	U
25	BA	1581	G
25	BA	1583	A
25	BA	1584	U
25	BA	1585	C
25	BA	1607	C
25	BA	1610	A
25	BA	1616	A
25	BA	1646	C
25	BA	1647	U
25	BA	1648	U
25	BA	1652	A
25	BA	1664	A
25	BA	1674	G
25	BA	1677	A
25	BA	1694	C
25	BA	1715	G
25	BA	1729	U
25	BA	1730	C
25	BA	1732	C

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Mol	Chain	Res	Type
25	BA	1738	G
25	BA	1757	A
25	BA	1758	U
25	BA	1764	C
25	BA	1773	A
25	BA	1784	A
25	BA	1785	A
25	BA	1791	A
25	BA	1800	C
25	BA	1801	A
25	BA	1802	A
25	BA	1808	A
25	BA	1816	C
25	BA	1819	A
25	BA	1829	A
25	BA	1833	C
25	BA	1847	A
25	BA	1848	A
25	BA	1858	A
25	BA	1870	C
25	BA	1871	A
25	BA	1872	A
25	BA	1873	G
25	BA	1876	A
25	BA	1906	G
25	BA	1913	A
25	BA	1914	C
25	BA	1919	A
25	BA	1927	A
25	BA	1929	G
25	BA	1930	G
25	BA	1937	A
25	BA	1955	U
25	BA	1963	U
25	BA	1967	C
25	BA	1970	A
25	BA	1972	G
25	BA	1991	U
25	BA	1993	U
25	BA	1997	C
25	BA	2020	A
25	BA	2022	U

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Mol	Chain	Res	Type
25	BA	2023	C
25	BA	2030	A
25	BA	2031	A
25	BA	2033	A
25	BA	2043	C
25	BA	2049	G
25	BA	2052	A
25	BA	2055	C
25	BA	2056	G
25	BA	2060	A
25	BA	2061	G
25	BA	2062	A
25	BA	2069	G
25	BA	2072	C
25	BA	2080	A
25	BA	2092	U
25	BA	2093	G
25	BA	2095	A
25	BA	2097	A
25	BA	2110	G
25	BA	2111	U
25	BA	2112	G
25	BA	2114	A
25	BA	2116	G
25	BA	2117	A
25	BA	2118	U
25	BA	2119	A
25	BA	2126	A
25	BA	2127	G
25	BA	2128	G
25	BA	2131	U
25	BA	2132	U
25	BA	2133	G
25	BA	2135	A
25	BA	2147	A
25	BA	2158	A
25	BA	2162	G
25	BA	2163	A
25	BA	2164	C
25	BA	2169	A
25	BA	2170	A
25	BA	2171	A

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Mol	Chain	Res	Type
25	BA	2172	U
25	BA	2173	A
25	BA	2189	U
25	BA	2190	G
25	BA	2194	U
25	BA	2198	A
25	BA	2204	G
25	BA	2211	A
25	BA	2212	A
25	BA	2214	C
25	BA	2225	A
25	BA	2226	C
25	BA	2238	G
25	BA	2239	G
25	BA	2243	U
25	BA	2246	G
25	BA	2267	A
25	BA	2278	A
25	BA	2283	C
25	BA	2287	A
25	BA	2288	A
25	BA	2297	A
25	BA	2305	U
25	BA	2309	A
25	BA	2311	A
25	BA	2312	U
25	BA	2322	A
25	BA	2333	A
25	BA	2345	G
25	BA	2347	C
25	BA	2350	C
25	BA	2361	G
25	BA	2383	G
25	BA	2385	C
25	BA	2402	U
25	BA	2406	A
25	BA	2407	A
25	BA	2423	U
25	BA	2425	A
25	BA	2429	G
25	BA	2430	A
25	BA	2431	U

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Mol	Chain	Res	Type
25	BA	2435	A
25	BA	2441	U
25	BA	2448	A
25	BA	2476	A
25	BA	2491	U
25	BA	2498	C
25	BA	2502	G
25	BA	2503	A
25	BA	2505	G
25	BA	2506	U
25	BA	2507	C
25	BA	2518	A
25	BA	2529	G
25	BA	2547	A
25	BA	2550	G
25	BA	2554	U
25	BA	2566	A
25	BA	2567	G
25	BA	2572	A
25	BA	2573	C
25	BA	2602	A
25	BA	2609	U
25	BA	2613	U
25	BA	2615	U
25	BA	2629	U
25	BA	2630	G
25	BA	2636	C
25	BA	2646	C
25	BA	2682	A
25	BA	2689	U
25	BA	2690	U
25	BA	2714	G
25	BA	2716	C
25	BA	2718	G
25	BA	2726	A
25	BA	2729	G
25	BA	2733	A
25	BA	2744	G
25	BA	2748	A
25	BA	2765	A
25	BA	2778	A
25	BA	2782	G

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Mol	Chain	Res	Type
25	BA	2791	G
25	BA	2792	A
25	BA	2809	A
25	BA	2818	U
25	BA	2820	A
25	BA	2823	A
25	BA	2836	U
25	BA	2867	G
25	BA	2872	A
25	BA	2873	A
25	BA	2879	A
25	BA	2880	C
25	BA	2886	A
25	BA	2887	A
25	BA	2903	U
26	BB	15	A
26	BB	24	G
26	BB	41	G
26	BB	44	G
26	BB	53	A
26	BB	56	G
26	BB	66	A
26	BB	73	A
26	BB	88	C
26	BB	89	U
26	BB	90	C
26	BB	99	A
26	BB	109	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	96	U
1	AA	115	G
1	AA	1201	A
1	AA	1362	A
1	AA	1491	G
1	AA	1493	A
24	AY	58	A
25	BA	271	G
25	BA	404	A
25	BA	479	A

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Mol	Chain	Res	Type
25	BA	1606	C
25	BA	2109	U
25	BA	2146	C
25	BA	2225	A
25	BA	2506	U

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

16 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CM0	AY	34	24	22,26,27	0.98	1 (4%)	28,37,40	1.24	3 (10%)
23	QUO	AX	34	23,22	31,35,36	1.13	3 (9%)	39,52,55	1.46	6 (15%)
23	H2U	AX	19	23	18,21,22	1.00	2 (11%)	21,30,33	1.00	2 (9%)
23	5MU	AX	54	23	19,22,23	0.92	2 (10%)	28,32,35	1.14	2 (7%)
24	5MU	AY	54	24	19,22,23	0.95	2 (10%)	28,32,35	1.14	2 (7%)
24	4SU	AY	8	24	18,21,22	1.08	2 (11%)	26,30,33	0.83	2 (7%)
23	7MG	AX	46	23	22,26,27	2.03	3 (13%)	29,39,42	1.21	4 (13%)
23	H2U	AX	20	23	18,21,22	1.04	2 (11%)	21,30,33	0.99	2 (9%)
23	H2U	AX	16	23	18,21,22	1.02	2 (11%)	21,30,33	1.00	2 (9%)
23	4SU	AX	8	23	18,21,22	1.08	2 (11%)	26,30,33	0.83	2 (7%)
24	6MZ	AY	37	24	22,25,26	1.68	5 (22%)	30,36,39	1.24	3 (10%)
23	PSU	AX	65	23	18,21,22	1.26	3 (16%)	22,30,33	1.53	5 (22%)
24	7MG	AY	46	24	22,26,27	2.04	3 (13%)	29,39,42	1.23	4 (13%)
24	PSU	AY	55	24	18,21,22	1.29	3 (16%)	22,30,33	1.60	3 (13%)
23	2MA	AX	37	23	22,25,26	2.13	4 (18%)	33,37,40	1.59	4 (12%)
23	PSU	AX	55	23	18,21,22	1.30	3 (16%)	22,30,33	1.63	4 (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
24	CM0	AY	34	24	-	3/12/30/31	0/2/2/2
23	QUO	AX	34	23,22	-	3/12/43/44	0/4/4/4
23	H2U	AX	19	23	-	6/7/38/39	0/2/2/2
23	5MU	AX	54	23	-	0/7/25/26	0/2/2/2
24	5MU	AY	54	24	-	2/7/25/26	0/2/2/2
24	4SU	AY	8	24	-	0/7/25/26	0/2/2/2
23	7MG	AX	46	23	-	0/7/37/38	0/3/3/3
23	H2U	AX	20	23	-	0/7/38/39	0/2/2/2
23	H2U	AX	16	23	-	3/7/38/39	0/2/2/2
23	4SU	AX	8	23	-	0/7/25/26	0/2/2/2
24	6MZ	AY	37	24	-	1/9/27/28	0/3/3/3
23	PSU	AX	65	23	-	4/7/25/26	0/2/2/2
24	7MG	AY	46	24	-	3/7/37/38	0/3/3/3
24	PSU	AY	55	24	-	0/7/25/26	0/2/2/2
23	2MA	AX	37	23	-	0/7/25/26	0/3/3/3
23	PSU	AX	55	23	-	0/7/25/26	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AX	37	2MA	C6-N1	6.85	1.44	1.35
24	AY	46	7MG	C8-N9	6.22	1.49	1.46
23	AX	46	7MG	C8-N9	6.20	1.49	1.46
24	AY	46	7MG	C5-N7	5.72	1.42	1.35
23	AX	46	7MG	C5-N7	5.69	1.42	1.35
24	AY	37	6MZ	C6-N6	4.45	1.39	1.34
23	AX	37	2MA	C4-N3	4.31	1.39	1.34
23	AX	37	2MA	C2-N1	3.83	1.40	1.34
24	AY	37	6MZ	C5-C4	3.52	1.45	1.39
23	AX	55	PSU	C2-N1	3.50	1.41	1.36
24	AY	55	PSU	C2-N1	3.40	1.41	1.36
23	AX	8	4SU	C4-S4	-3.21	1.62	1.68
24	AY	8	4SU	C4-S4	-3.17	1.62	1.68
23	AX	65	PSU	C2-N1	3.14	1.41	1.36
23	AX	16	H2U	C2-N1	2.74	1.39	1.35
23	AX	16	H2U	C2-N3	2.74	1.42	1.38
23	AX	20	H2U	C2-N3	2.72	1.42	1.38
23	AX	19	H2U	C2-N3	2.72	1.42	1.38
23	AX	20	H2U	C2-N1	2.70	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AX	34	QUO	C6-N1	2.68	1.43	1.38
23	AX	19	H2U	C2-N1	2.68	1.39	1.35
24	AY	54	5MU	C2-N1	2.63	1.42	1.38
23	AX	65	PSU	C4-N3	2.62	1.43	1.38
24	AY	55	PSU	C4-N3	2.55	1.43	1.38
23	AX	55	PSU	C4-N3	2.52	1.43	1.38
24	AY	46	7MG	C6-N1	2.51	1.43	1.38
23	AX	46	7MG	C6-N1	2.50	1.43	1.38
23	AX	54	5MU	C2-N1	2.45	1.42	1.38
23	AX	34	QUO	C4-N3	2.41	1.40	1.34
24	AY	37	6MZ	C8-N7	2.40	1.36	1.31
23	AX	37	2MA	C8-N7	2.38	1.36	1.31
24	AY	34	CM0	C4-N3	2.37	1.43	1.38
24	AY	37	6MZ	C2-N1	2.32	1.38	1.33
24	AY	8	4SU	C2-N3	2.31	1.42	1.38
23	AX	8	4SU	C2-N3	2.28	1.42	1.38
24	AY	55	PSU	C6-N1	2.28	1.40	1.36
23	AX	55	PSU	C6-N1	2.27	1.40	1.36
23	AX	54	5MU	C2-N3	2.25	1.42	1.38
24	AY	54	5MU	C2-N3	2.24	1.42	1.38
23	AX	34	QUO	C2-N2	2.21	1.39	1.34
24	AY	37	6MZ	C5-N7	2.18	1.43	1.39
23	AX	65	PSU	C6-N1	2.08	1.39	1.36

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AX	37	2MA	N6-C6-N1	5.47	124.77	117.03
23	AX	34	QUO	C7-C5-C4	-5.13	106.73	112.66
23	AX	55	PSU	C6-C5-C4	5.07	121.74	118.20
24	AY	55	PSU	C6-C5-C4	4.92	121.64	118.20
23	AX	37	2MA	C5-C6-N1	-4.49	111.26	119.01
23	AX	65	PSU	C6-C5-C4	3.99	120.98	118.20
24	AY	37	6MZ	C4-N9-C8	3.90	109.95	105.73
24	AY	34	CM0	C7-O5-C5	-3.88	112.49	117.58
24	AY	54	5MU	C4-N3-C2	-3.15	123.27	127.35
23	AX	54	5MU	C4-N3-C2	-3.14	123.29	127.35
23	AX	54	5MU	C6-C5-C4	3.01	120.55	118.03
24	AY	54	5MU	C6-C5-C4	3.00	120.54	118.03
23	AX	37	2MA	C6-C5-C4	2.97	121.18	117.18
23	AX	34	QUO	C7-C8-N9	-2.87	108.25	111.06
23	AX	46	7MG	C5-C4-N9	2.85	110.05	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AX	34	QUO	C10-N11-C12	-2.78	109.14	114.89
24	AY	46	7MG	C5-C4-N9	2.77	109.94	106.35
23	AX	65	PSU	O2-C2-N1	-2.77	119.74	122.79
24	AY	8	4SU	C4-N3-C2	-2.74	124.68	127.34
23	AX	8	4SU	C4-N3-C2	-2.73	124.69	127.34
24	AY	55	PSU	O2-C2-N1	-2.70	119.82	122.79
24	AY	34	CM0	C4-N3-C2	-2.70	123.86	127.35
24	AY	37	6MZ	C6-C5-N7	2.69	135.30	132.39
23	AX	55	PSU	O2-C2-N1	-2.65	119.87	122.79
23	AX	37	2MA	C2-N1-C6	2.60	122.14	118.08
24	AY	37	6MZ	N9-C8-N7	-2.52	110.46	113.91
23	AX	34	QUO	O13-C13-C12	-2.42	106.45	112.92
23	AX	20	H2U	O2-C2-N3	-2.39	117.05	121.50
23	AX	65	PSU	O4-C4-N3	-2.39	115.54	120.12
23	AX	16	H2U	O2-C2-N3	-2.38	117.06	121.50
23	AX	19	H2U	O2-C2-N3	-2.37	117.09	121.50
24	AY	46	7MG	C4-C5-N7	2.32	108.75	105.53
23	AX	46	7MG	C2-N1-C6	-2.30	120.90	125.10
24	AY	46	7MG	C2-N1-C6	-2.30	120.91	125.10
24	AY	46	7MG	O6-C6-N1	-2.26	115.78	120.12
23	AX	46	7MG	C4-C5-N7	2.26	108.67	105.53
23	AX	46	7MG	O6-C6-N1	-2.24	115.82	120.12
23	AX	20	H2U	C5-C4-N3	2.23	119.15	116.65
23	AX	19	H2U	C5-C4-N3	2.19	119.11	116.65
23	AX	34	QUO	C16-C12-C13	2.18	106.42	103.18
23	AX	16	H2U	C5-C4-N3	2.17	119.08	116.65
23	AX	65	PSU	O4-C4-C5	2.13	129.63	124.05
23	AX	34	QUO	C2-N1-C6	-2.11	121.26	125.10
24	AY	8	4SU	C6-C5-C4	2.10	121.77	119.95
23	AX	8	4SU	C6-C5-C4	2.08	121.75	119.95
24	AY	34	CM0	O4-C4-N3	-2.07	116.14	120.12
23	AX	55	PSU	O4-C4-N3	-2.04	116.21	120.12
24	AY	55	PSU	N1-C2-N3	2.02	117.42	115.13
23	AX	55	PSU	N1-C2-N3	2.01	117.41	115.13
23	AX	65	PSU	N1-C2-N3	2.00	117.40	115.13

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AX	19	H2U	O4'-C4'-C5'-O5'
23	AX	19	H2U	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
23	AX	19	H2U	C2'-C1'-N1-C6
23	AX	34	QUO	C16-C12-N11-C10
23	AX	65	PSU	C2'-C1'-C5-C4
23	AX	65	PSU	O4'-C1'-C5-C4
23	AX	65	PSU	O4'-C1'-C5-C6
24	AY	46	7MG	C4'-C5'-O5'-P
24	AY	46	7MG	C2'-C1'-N9-C8
24	AY	54	5MU	C3'-C4'-C5'-O5'
24	AY	54	5MU	O4'-C4'-C5'-O5'
24	AY	34	CM0	O5-C7-C8-O8
23	AX	19	H2U	C2'-C1'-N1-C2
23	AX	19	H2U	C3'-C4'-C5'-O5'
23	AX	65	PSU	C4'-C5'-O5'-P
24	AY	34	CM0	O5-C7-C8-O9
23	AX	16	H2U	C2'-C1'-N1-C6
23	AX	19	H2U	O4'-C1'-N1-C2
23	AX	34	QUO	C13-C12-N11-C10
23	AX	16	H2U	C2'-C1'-N1-C2
23	AX	16	H2U	O4'-C1'-N1-C2
23	AX	34	QUO	N11-C10-C7-C8
24	AY	37	6MZ	C3'-C4'-C5'-O5'
24	AY	46	7MG	C2'-C1'-N9-C4
24	AY	34	CM0	C6-C5-O5-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AX	16	H2U	1	0
24	AY	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	ERY	BA	9000	-	53,53,53	1.14	4 (7%)	82,82,82	1.67	22 (26%)

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
57	ERY	BA	9000	-	-	15/72/107/107	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	9000	ERY	O13-C12	-2.82	1.39	1.44
57	BA	9000	ERY	O10-C6	-2.64	1.40	1.44
57	BA	9000	ERY	O9-C26	-2.52	1.39	1.44
57	BA	9000	ERY	O2-C13	-2.52	1.42	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	9000	ERY	C36-C13-C12	-3.88	107.85	115.20
57	BA	9000	ERY	C34-C10-C11	-3.87	109.56	114.38
57	BA	9000	ERY	C12-C11-C10	-3.41	112.15	116.43
57	BA	9000	ERY	O13-C12-C13	3.32	112.62	107.28
57	BA	9000	ERY	O2-C1-C2	3.28	118.76	111.56
57	BA	9000	ERY	C16-C15-C14	-3.11	109.68	115.07
57	BA	9000	ERY	C20-O5-C16	-2.99	111.31	117.55
57	BA	9000	ERY	O2-C1-O1	-2.87	118.58	123.94
57	BA	9000	ERY	C22-O9-C26	-2.57	108.84	112.91
57	BA	9000	ERY	O5-C16-C17	2.56	107.61	103.81
57	BA	9000	ERY	C35-C12-C13	-2.56	107.70	111.31
57	BA	9000	ERY	O6-C17-C16	-2.50	106.46	111.12
57	BA	9000	ERY	O3-C3-C2	2.45	115.40	111.14
57	BA	9000	ERY	C27-C26-C25	-2.43	109.58	113.40
57	BA	9000	ERY	C6-C5-C4	-2.38	110.68	114.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	9000	ERY	O8-C23-C24	-2.36	105.55	109.77
57	BA	9000	ERY	C7-C6-C5	-2.31	105.97	110.48
57	BA	9000	ERY	C22-O7-C5	-2.16	112.51	116.25
57	BA	9000	ERY	O5-C16-C15	-2.15	109.51	112.96
57	BA	9000	ERY	C15-C16-C17	2.11	111.45	107.67
57	BA	9000	ERY	O7-C22-O9	-2.08	104.86	110.67
57	BA	9000	ERY	O4-C18-C21	2.06	111.15	106.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	BA	9000	ERY	C9-C10-C11-C12
57	BA	9000	ERY	C34-C10-C11-C12
57	BA	9000	ERY	C34-C10-C11-O12
57	BA	9000	ERY	C35-C12-C13-O2
57	BA	9000	ERY	O13-C12-C13-O2
57	BA	9000	ERY	O13-C12-C13-C36
57	BA	9000	ERY	C35-C12-C13-C36
57	BA	9000	ERY	C11-C12-C13-O2
57	BA	9000	ERY	C11-C12-C13-C36
57	BA	9000	ERY	C25-C24-N1-C29
57	BA	9000	ERY	C25-C24-N1-C28
57	BA	9000	ERY	C23-C24-N1-C28
57	BA	9000	ERY	C9-C10-C11-O12
57	BA	9000	ERY	O2-C13-C36-C37
57	BA	9000	ERY	C12-C13-C36-C37

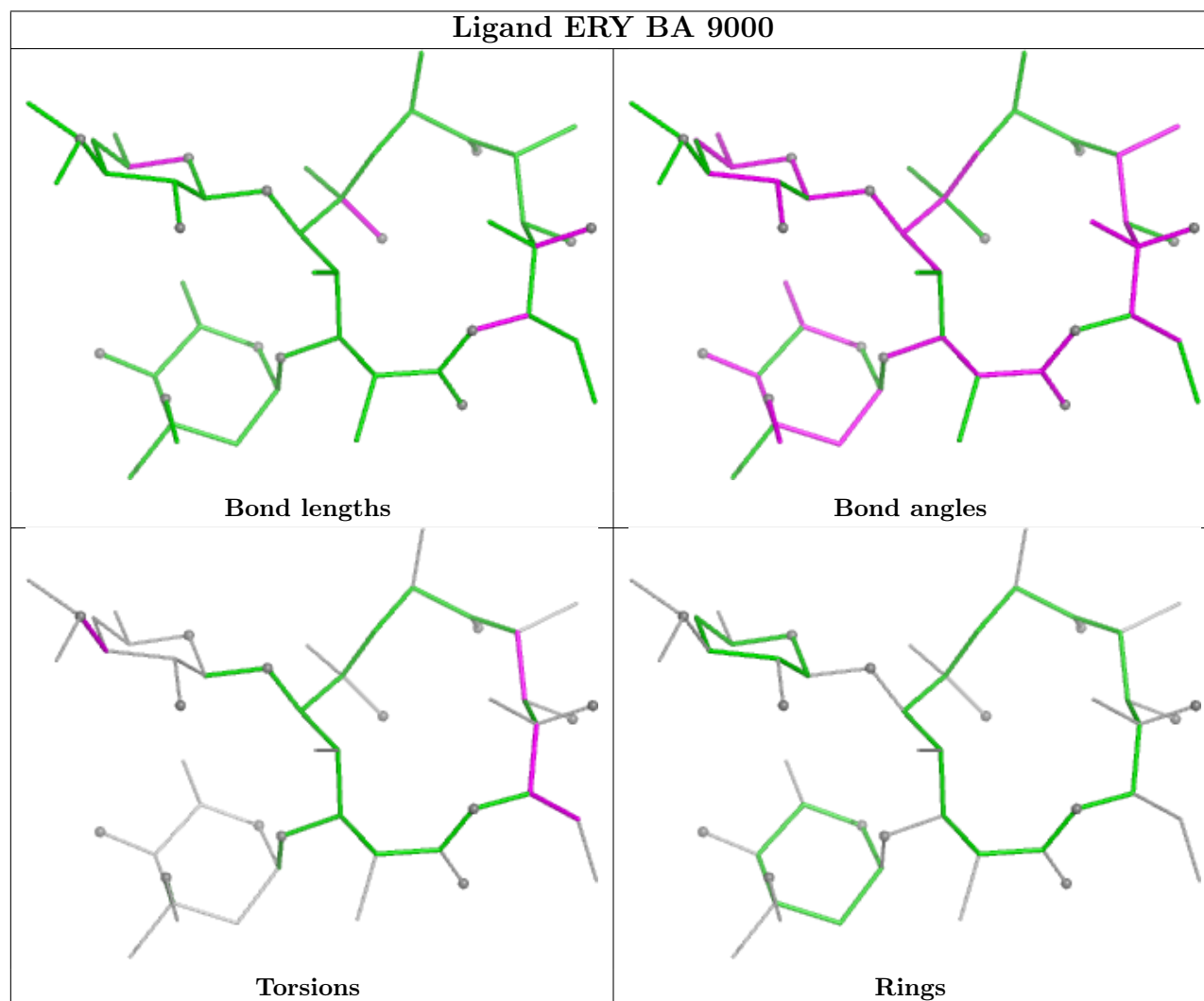
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	9000	ERY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	AY	1
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AY	15:G	O3'	18:G	P	6.79
1	AA	99:C	O3'	100:G	P	3.18

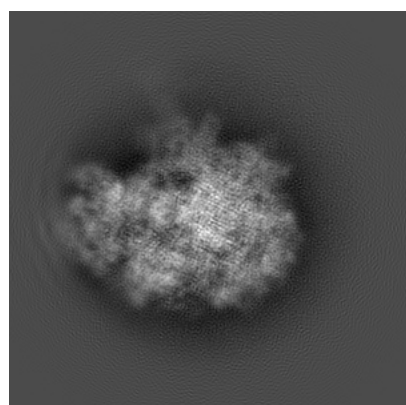
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8176. These allow visual inspection of the internal detail of the map and identification of artifacts.

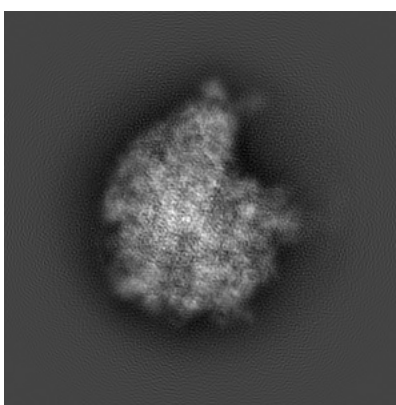
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

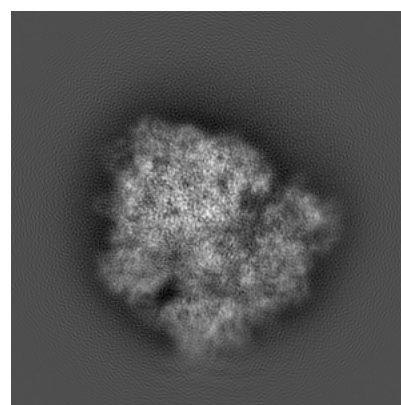
6.1.1 Primary map



X



Y

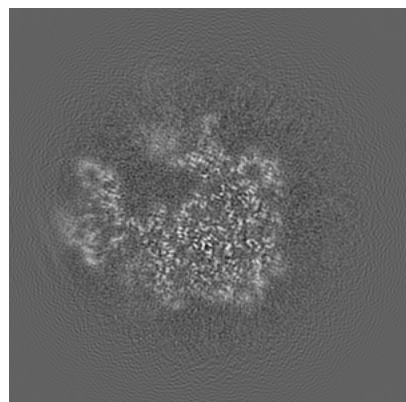


Z

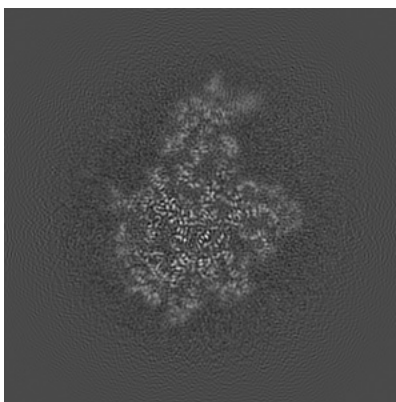
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

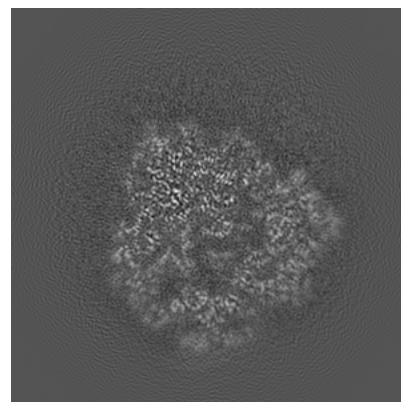
6.2.1 Primary map



X Index: 184



Y Index: 184

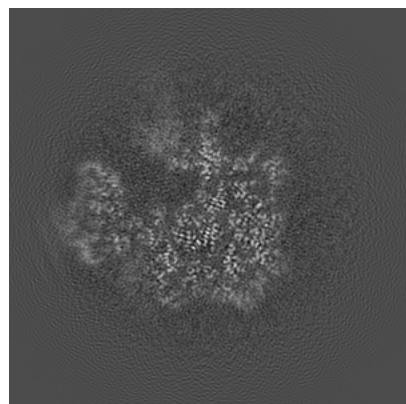


Z Index: 184

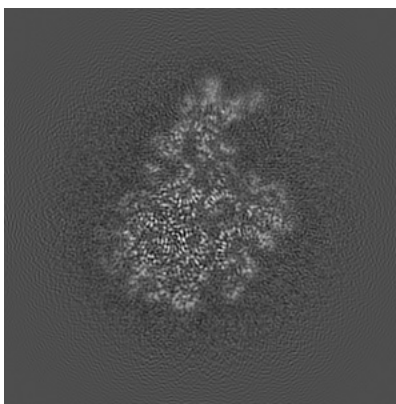
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

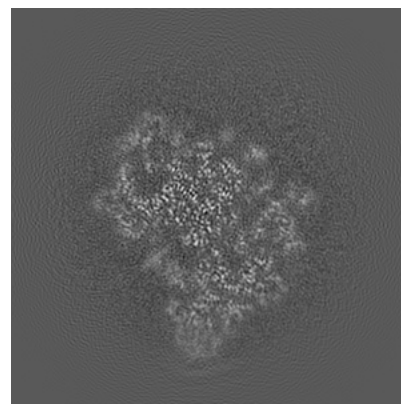
6.3.1 Primary map



X Index: 181



Y Index: 176

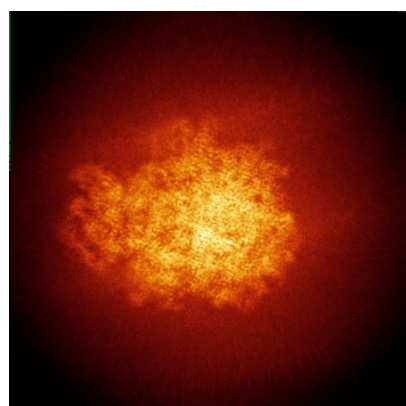


Z Index: 156

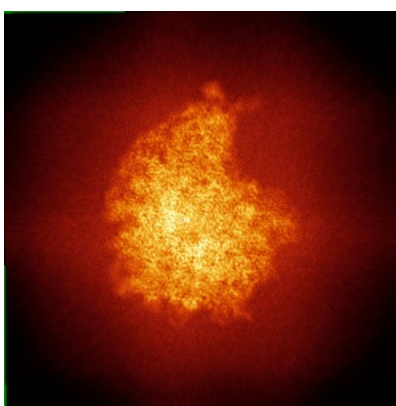
The images above show the largest variance slices of the map in three orthogonal directions.

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

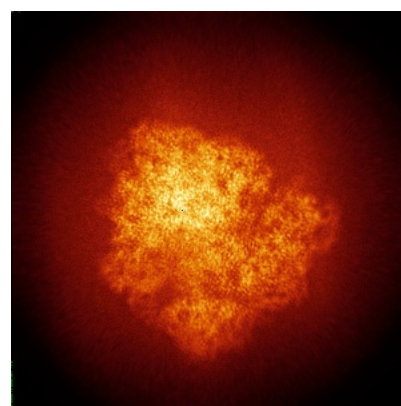
6.4.1 Primary map



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](#)

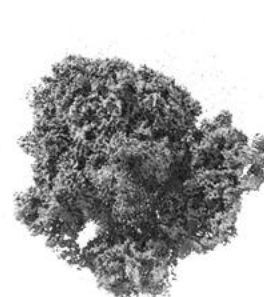
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

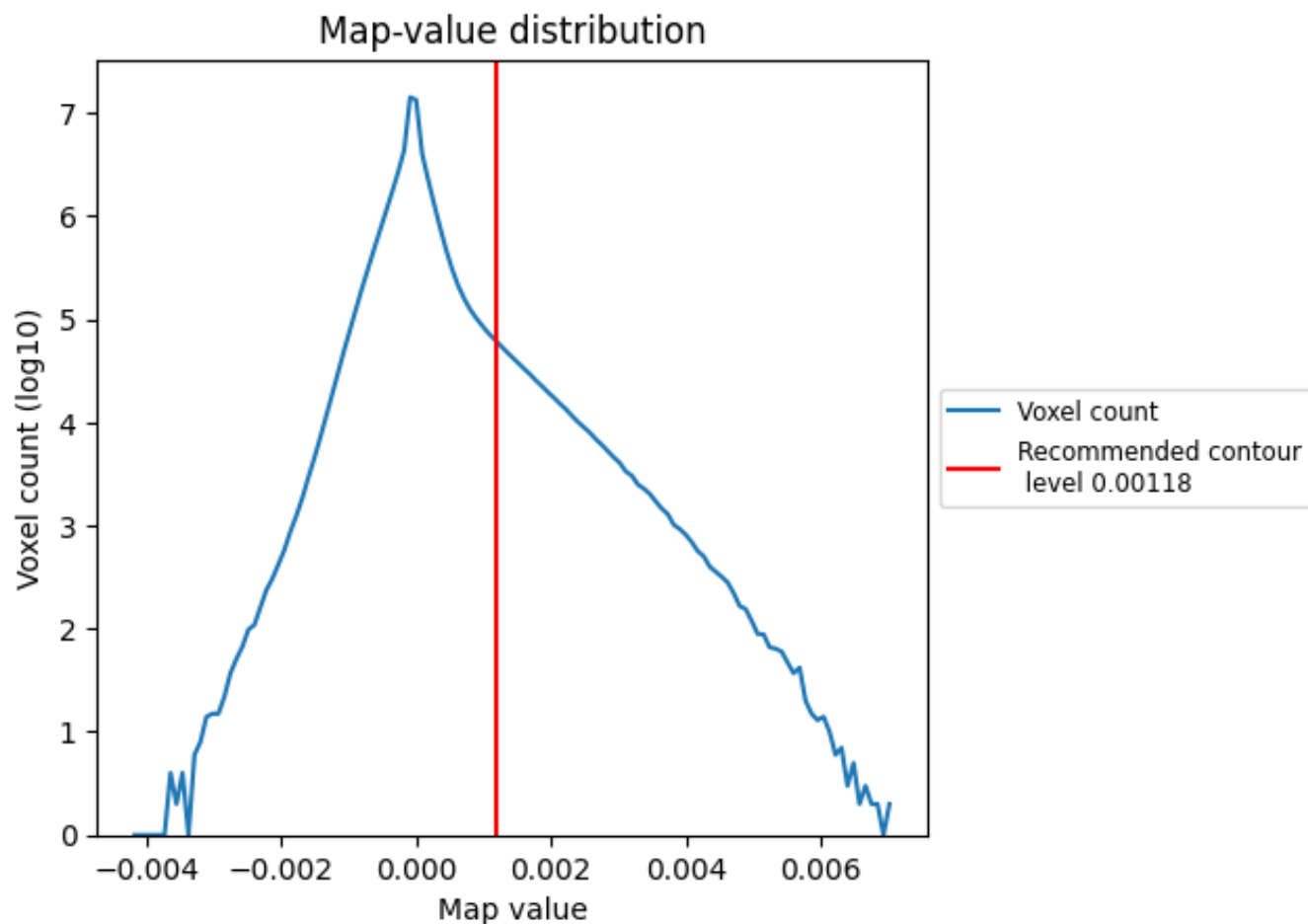
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

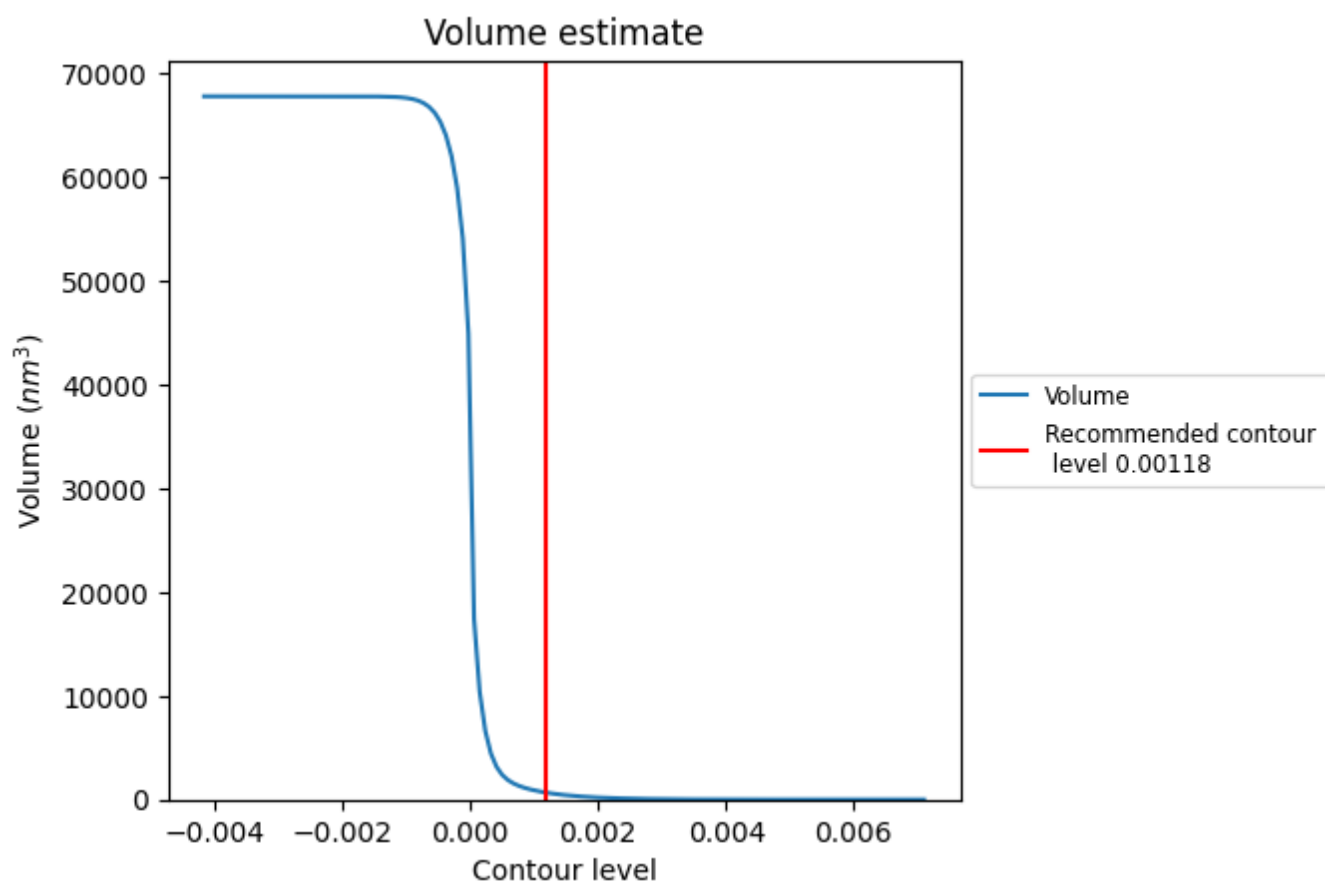
This section contains the results of statistical analysis of the map.

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.

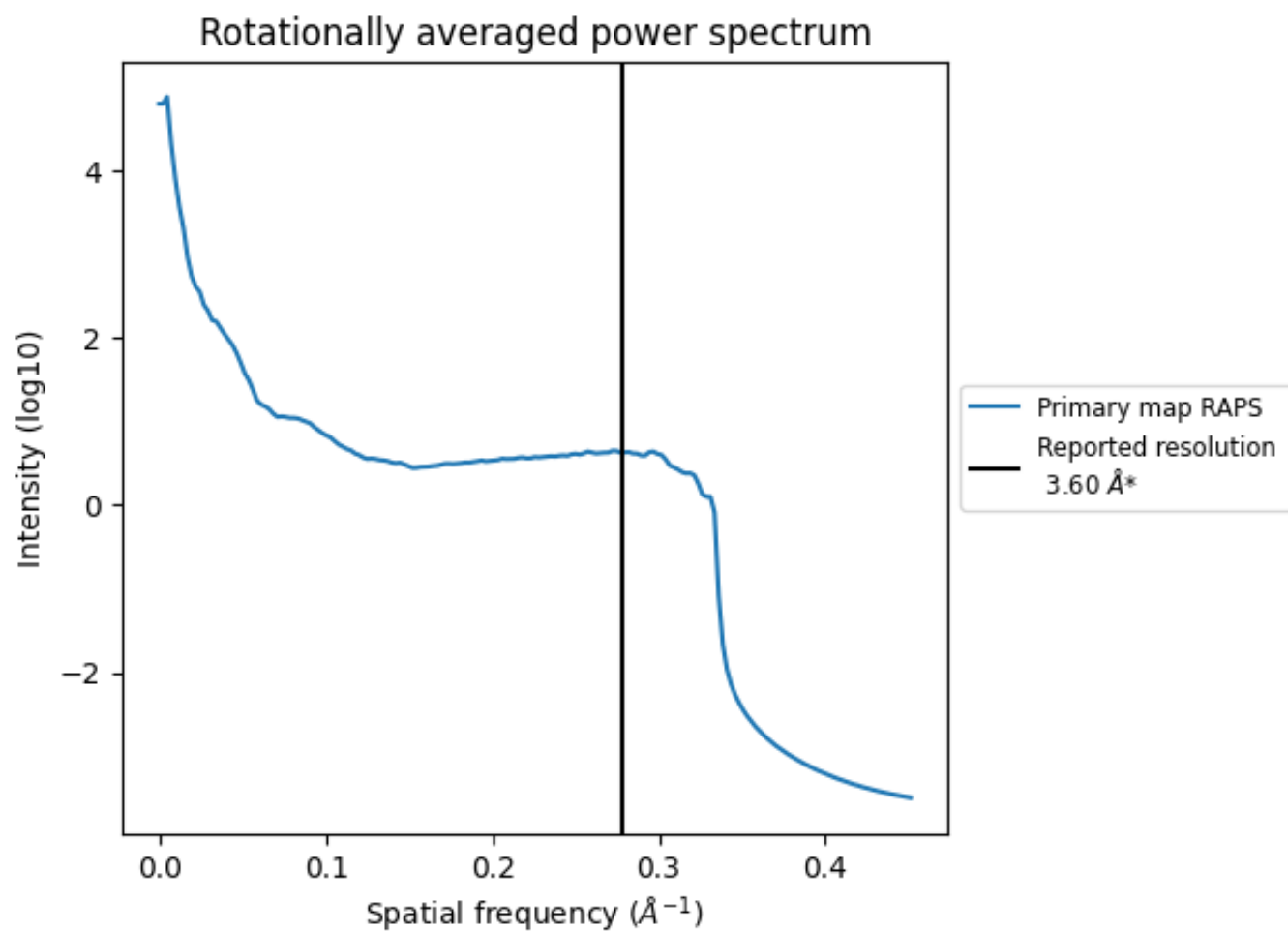
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 675 nm³; this corresponds to an approximate mass of 610 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 0.278 Å⁻¹

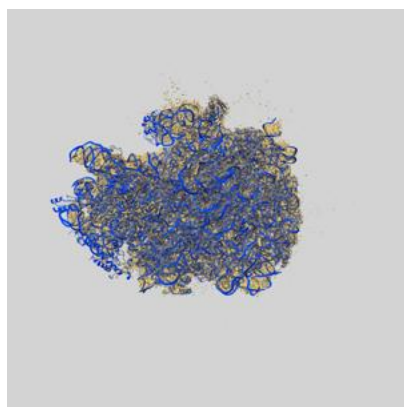
8 Fourier-Shell correlation

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

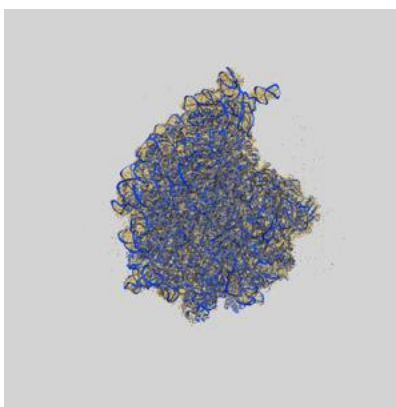
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8176 and PDB model 5JU8. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

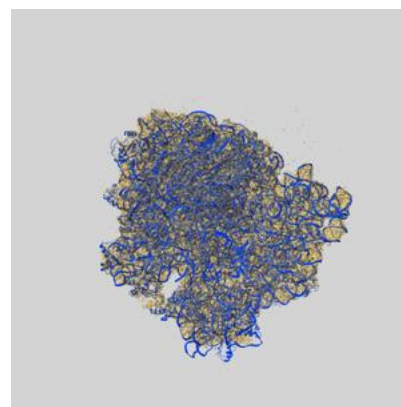
9.1 Map-model overlay [i](#)



X



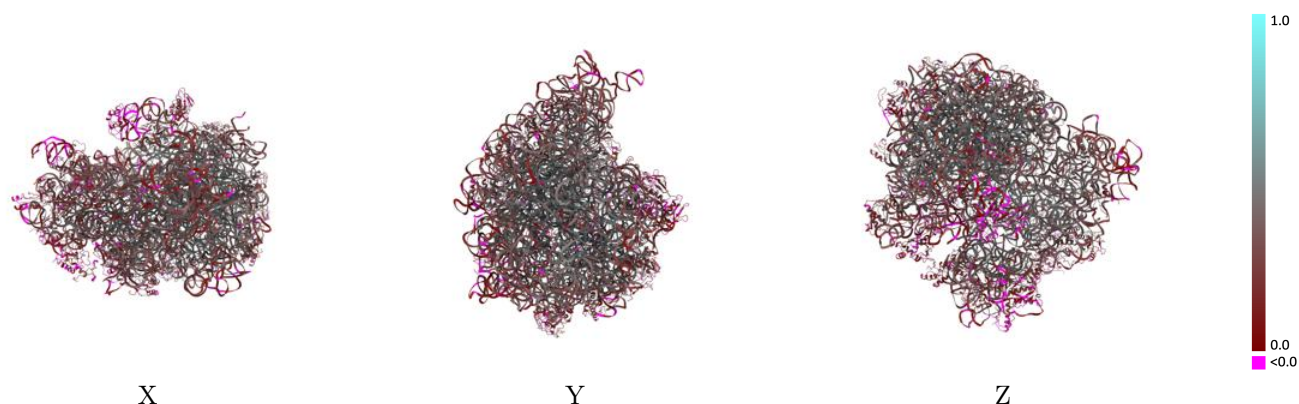
Y



Z

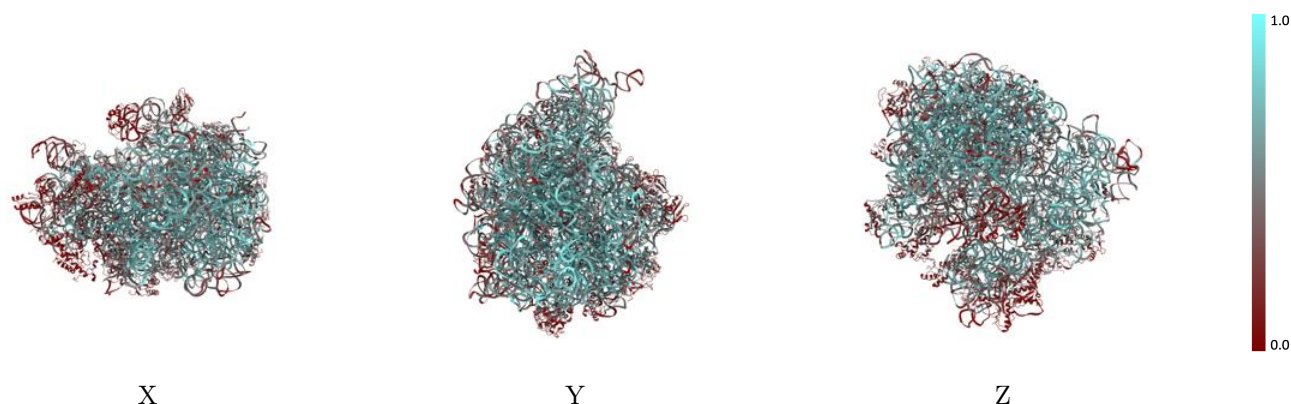
The images above show the 3D surface view of the map at the recommended contour level 0.00118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



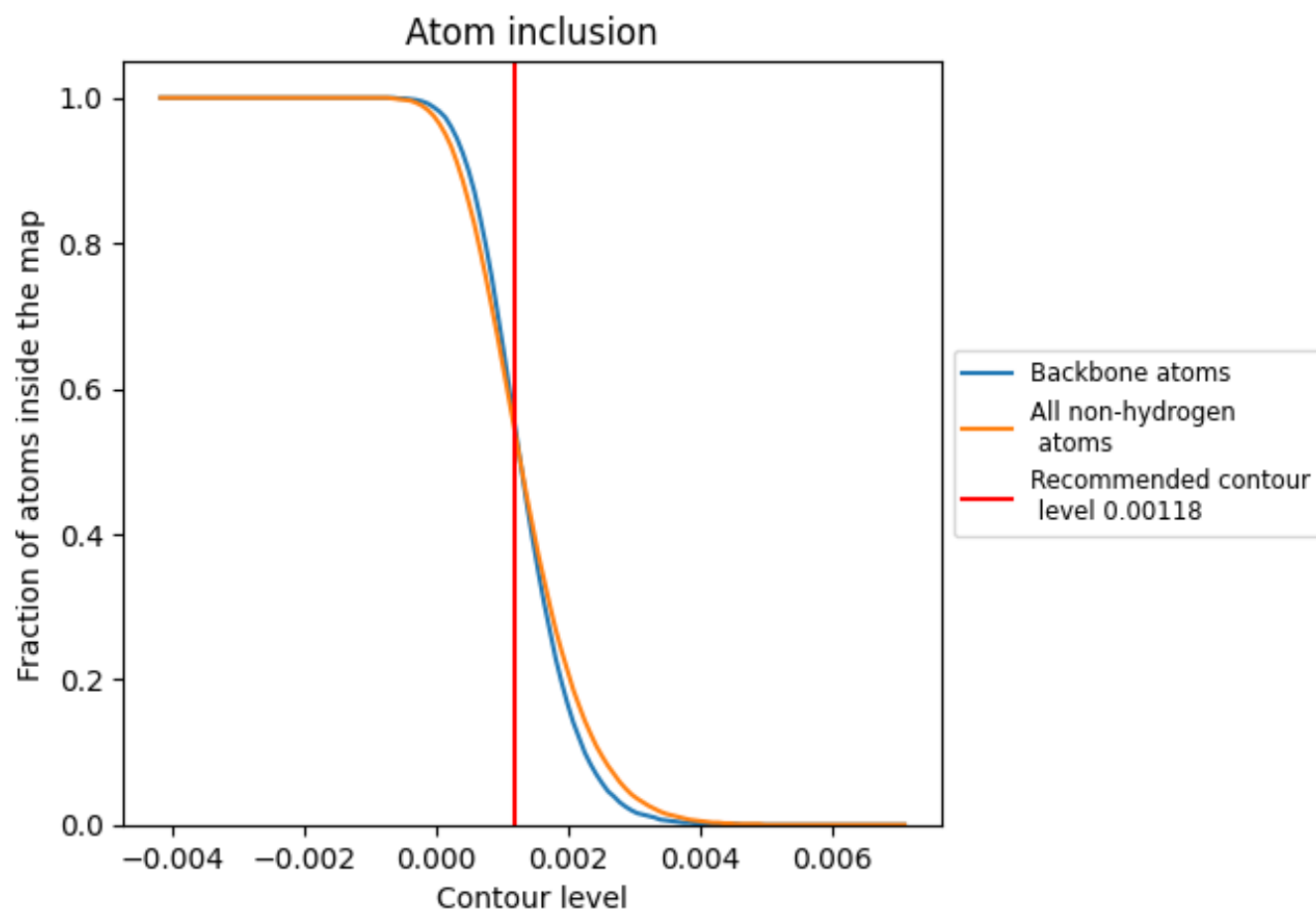
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00118).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 55% 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 (0.00118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5500	 0.3330
AA	 0.6140	 0.3450
AB	 0.0390	 0.1250
AC	 0.2100	 0.2590
AD	 0.2280	 0.2240
AE	 0.3350	 0.2930
AF	 0.2860	 0.2120
AG	 0.2390	 0.2060
AH	 0.3320	 0.2940
AI	 0.1730	 0.2140
AJ	 0.1280	 0.1560
AK	 0.3540	 0.2410
AL	 0.3530	 0.3030
AM	 0.2490	 0.2090
AN	 0.2870	 0.2540
AO	 0.4180	 0.2800
AP	 0.4040	 0.2630
AQ	 0.3320	 0.2440
AR	 0.3920	 0.2730
AS	 0.3290	 0.2330
AT	 0.3990	 0.2580
AU	 0.1060	 0.1150
AV	 0.6100	 0.4270
AX	 0.4840	 0.3130
AY	 0.3270	 0.1900
B0	 0.4670	 0.3370
B1	 0.2520	 0.2500
B2	 0.5630	 0.3770
B3	 0.4970	 0.3730
B4	 0.5340	 0.3630
B5	 0.2920	 0.2820
BA	 0.6710	 0.3830
BB	 0.6110	 0.3090
BC	 0.5130	 0.3560
BD	 0.4430	 0.3510



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Chain	Atom inclusion	Q-score
BE	 0.3200	 0.2700
BF	 0.2190	 0.1680
BG	 0.2710	 0.1930
BH	 0.0670	 0.1200
BI	 0.0080	 0.0070
BJ	 0.4720	 0.3350
BK	 0.3880	 0.3420
BL	 0.3900	 0.2860
BM	 0.4590	 0.3170
BN	 0.5030	 0.3620
BO	 0.2750	 0.2450
BP	 0.3890	 0.3140
BQ	 0.5400	 0.3480
BR	 0.3880	 0.2820
BS	 0.4580	 0.3300
BT	 0.3890	 0.2690
BU	 0.2840	 0.1930
BV	 0.4000	 0.2710
BW	 0.4880	 0.3560
BX	 0.4340	 0.2830
BY	 0.3440	 0.2020
BZ	 0.4260	 0.3180