



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 01:22 pm BST

PDB ID : 7Q4K / pdb_00007q4k
EMDB ID : EMD-13805
Title : Erythromycin-stalled Escherichia coli 70S ribosome with streptococcal MsrDL nascent chain
Authors : Fostier, C.R.; Ousalem, F.; Soufari, H.; Leroy, E.C.; Ngo, S.; Innis, A.; Hashem, Y.; Boel, G.
Deposited on : 2021-10-31
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

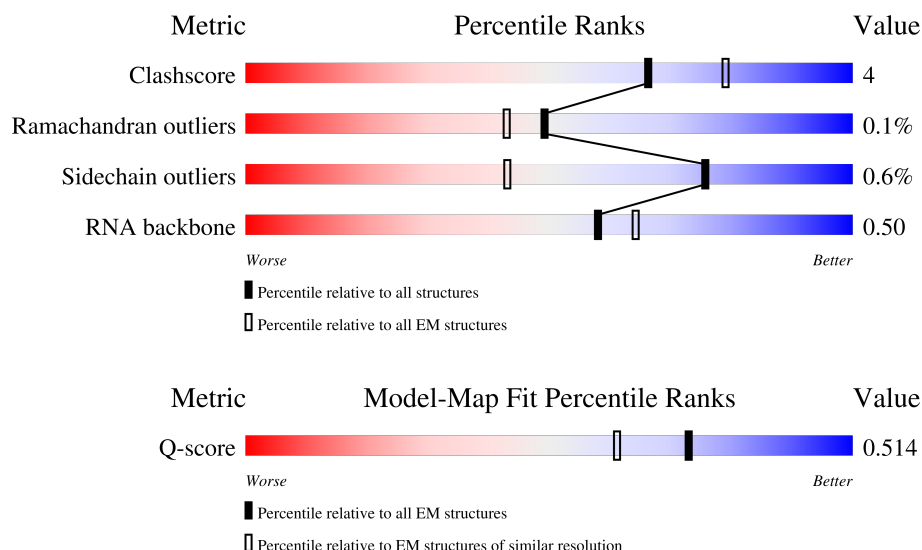
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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	14081 (2.50 - 3.50)

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	1534	
2	AB	241	
3	AC	233	

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Mol	Chain	Length	Quality of chain
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	BA	2903	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	

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Mol	Chain	Length	Quality of chain
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	
33	BL	144	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	
53	D1	6	

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Mol	Chain	Length	Quality of chain
54	D2	77	43%31%19%5%
55	D3	76	86%28%38%24%9%
56	D4	9	11%22%67%11%

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 146607 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- 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	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- 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	99	Total	C	N	O	S	0	0
			795	498	152	144	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
			957	591	196	165	5		

- 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	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP C3SR07

- 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
			714	439	144	130	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	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BI	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BK	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BY	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	51	Total	C	N	O		0	0
			414	266	76	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called MsrDL: FME-TYR-LEU-ILE-PHE-MET.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	D1	6	Total	C	N	O	S	0	0
			57	41	6	8	2		

- Molecule 54 is a RNA chain called Met-tRNA (P site).

Mol	Chain	Residues	Atoms						AltConf	Trace
54	D2	76	Total	C	N	O	P	S	0	0
			1634	733	290	534	76	1		

- Molecule 55 is a RNA chain called Phe-tRNA (E site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
55	D3	75	Total	C	N	O	P	S	0	0
			1604	715	288	525	75	1		

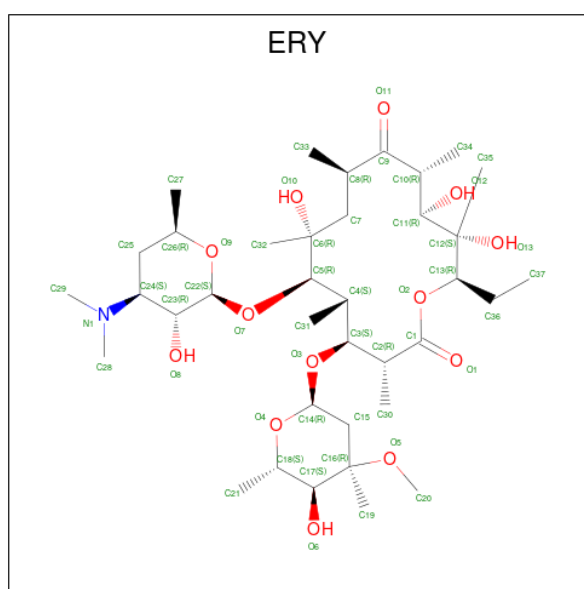
- Molecule 56 is a RNA chain called MsrDL mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	D4	9	Total	C	N	O	P	0	0
			189	85	31	64	9		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	AA	35	Total	Mg	0
			35	35	
57	BA	134	Total	Mg	0
			134	134	
57	BC	1	Total	Mg	0
			1	1	
57	BD	1	Total	Mg	0
			1	1	
57	D2	1	Total	Mg	0
			1	1	

- Molecule 58 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).



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

- Molecule 59 is water.

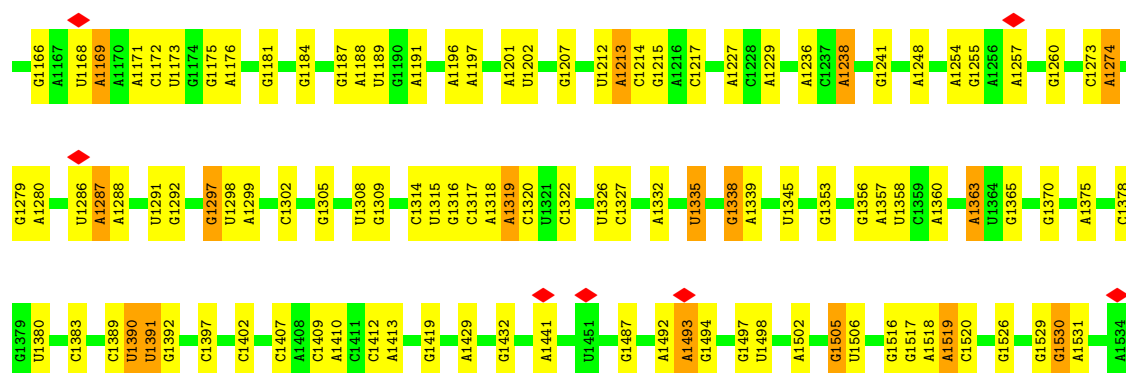
Mol	Chain	Residues	Atoms				AltConf
59	AA	166	Total	O			0
			166	166			
59	AK	2	Total	O			0
			2	2			
59	AM	1	Total	O			0
			1	1			
59	AN	2	Total	O			0
			2	2			
59	AQ	1	Total	O			0
			1	1			
59	BA	614	Total	O			0
			614	614			
59	BC	6	Total	O			0
			6	6			
59	BD	3	Total	O			0
			3	3			
59	BE	1	Total	O			0
			1	1			
59	BJ	1	Total	O			0
			1	1			
59	BL	1	Total	O			0
			1	1			
59	BN	2	Total	O			0
			2	2			

3 Residue-property plots

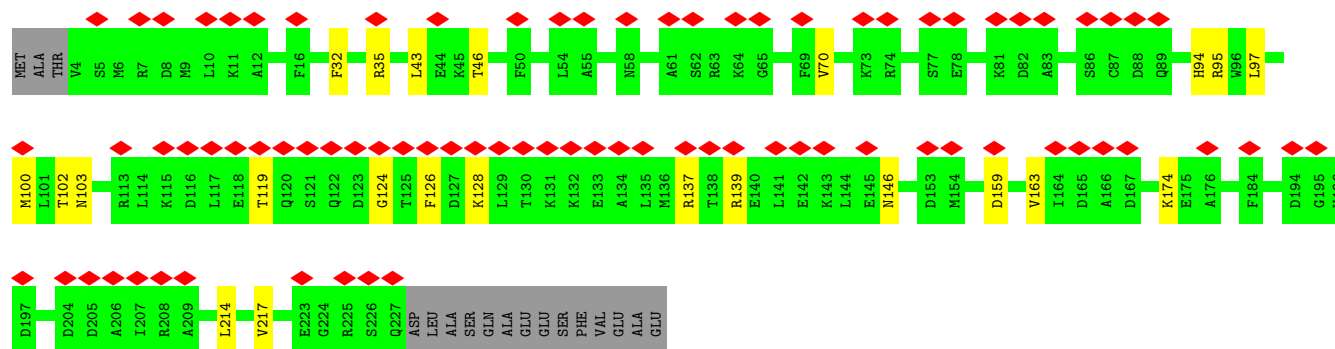
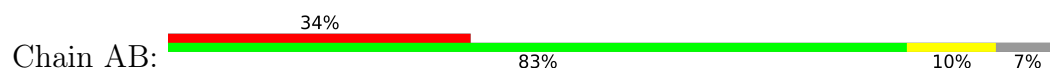
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

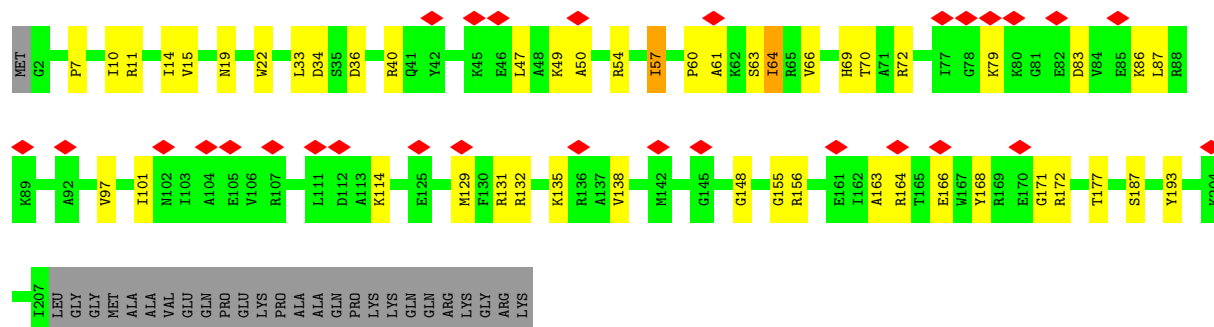




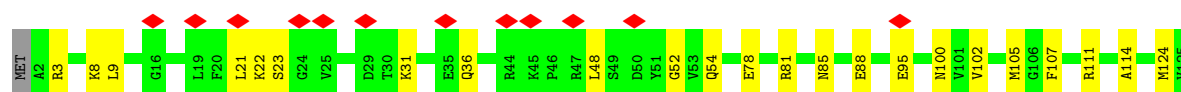
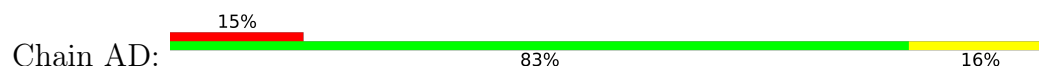
• Molecule 2: 30S ribosomal protein S2

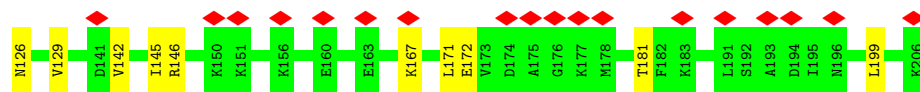


• Molecule 3: 30S ribosomal protein S3

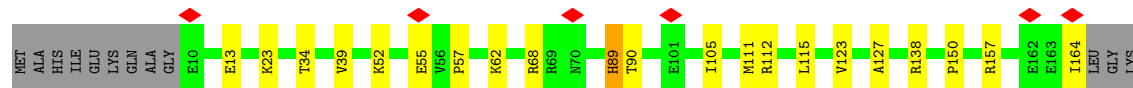
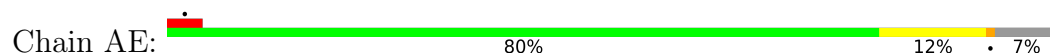


• Molecule 4: 30S ribosomal protein S4

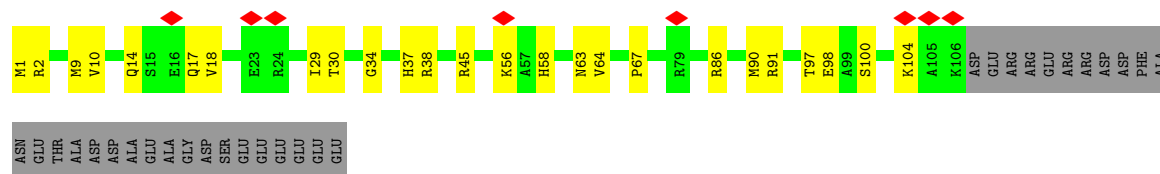




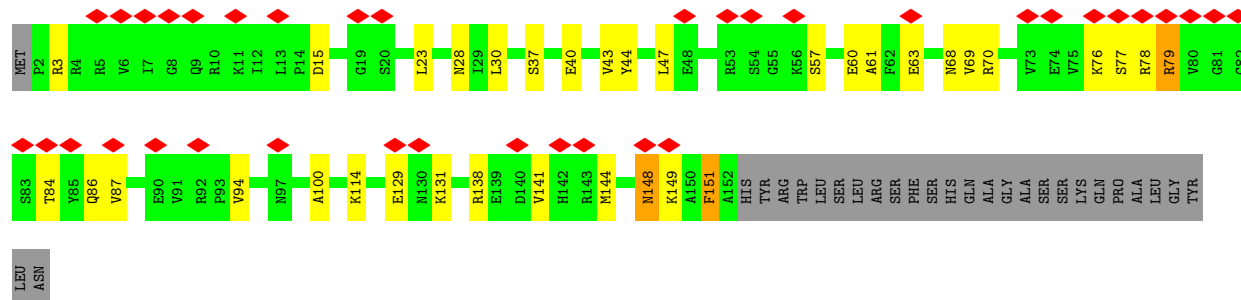
- Molecule 5: 30S ribosomal protein S5



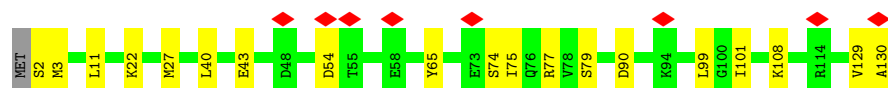
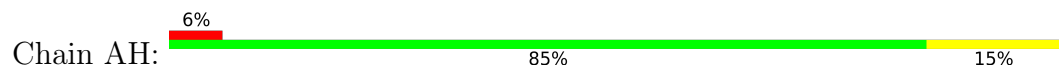
- Molecule 6: 30S ribosomal protein S6



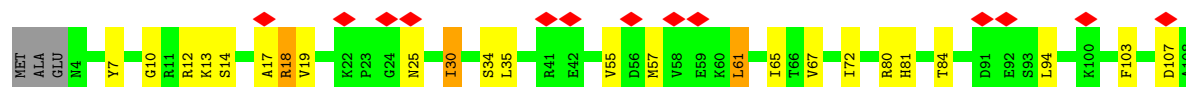
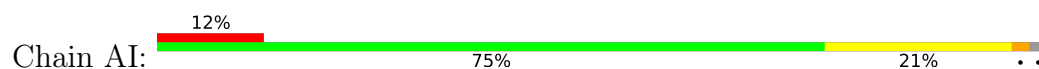
- Molecule 7: 30S ribosomal protein S7

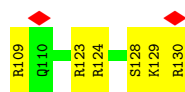


- Molecule 8: 30S ribosomal protein S8

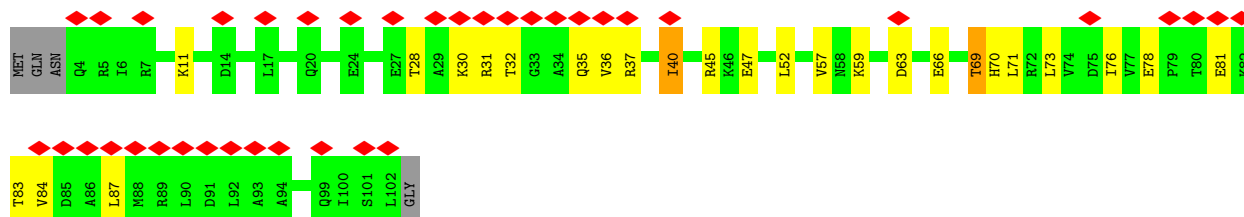
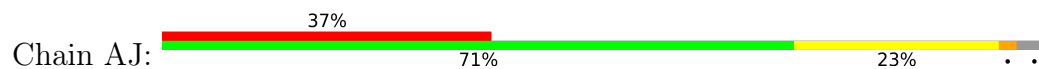


- Molecule 9: 30S ribosomal protein S9

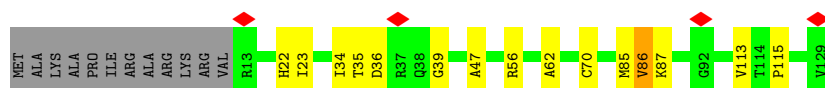
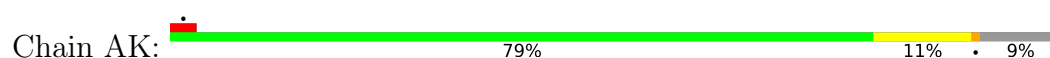




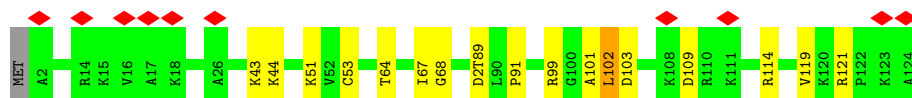
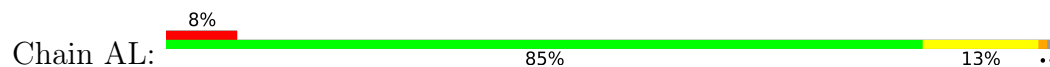
- Molecule 10: 30S ribosomal protein S10



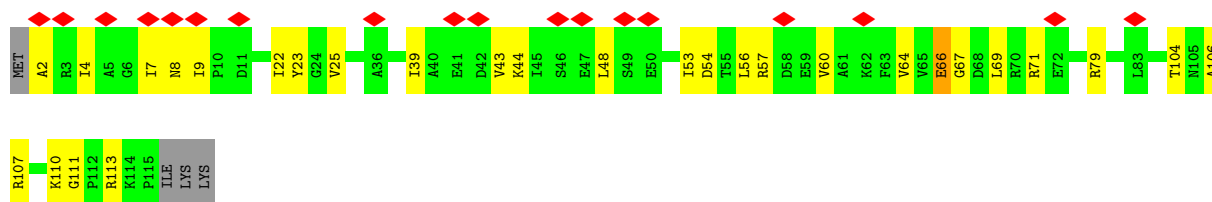
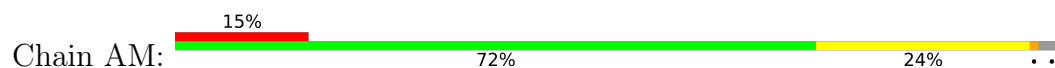
- Molecule 11: 30S ribosomal protein S11



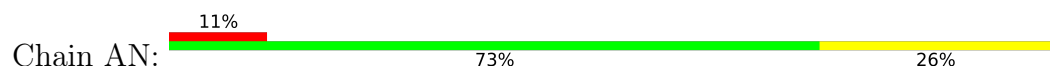
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

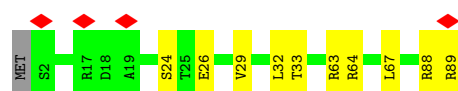


- Molecule 14: 30S ribosomal protein S14



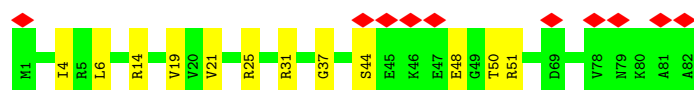
- Molecule 15: 30S ribosomal protein S15

Chain AO:  88% 11%



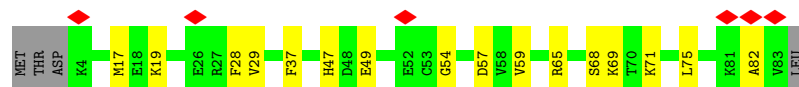
- Molecule 16: 30S ribosomal protein S16

Chain AP:  12% 85% 15%



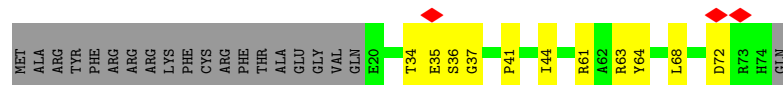
- Molecule 17: 30S ribosomal protein S17

Chain AQ:  7% 76% 19% 5%



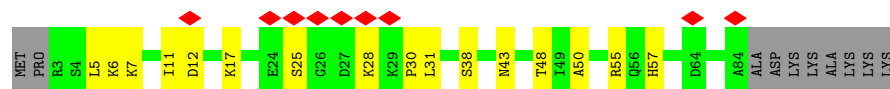
- Molecule 18: 30S ribosomal protein S18

Chain AR:  59% 15% 27%

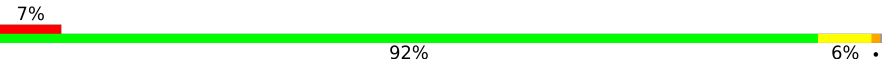


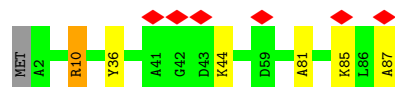
- Molecule 19: 30S ribosomal protein S19

Chain AS:  10% 72% 17% 11%



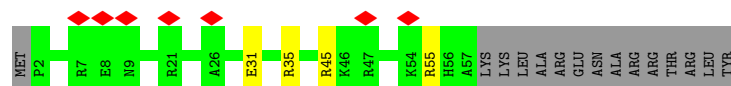
- Molecule 20: 30S ribosomal protein S20

Chain AT:  7% 92% 6% 2%



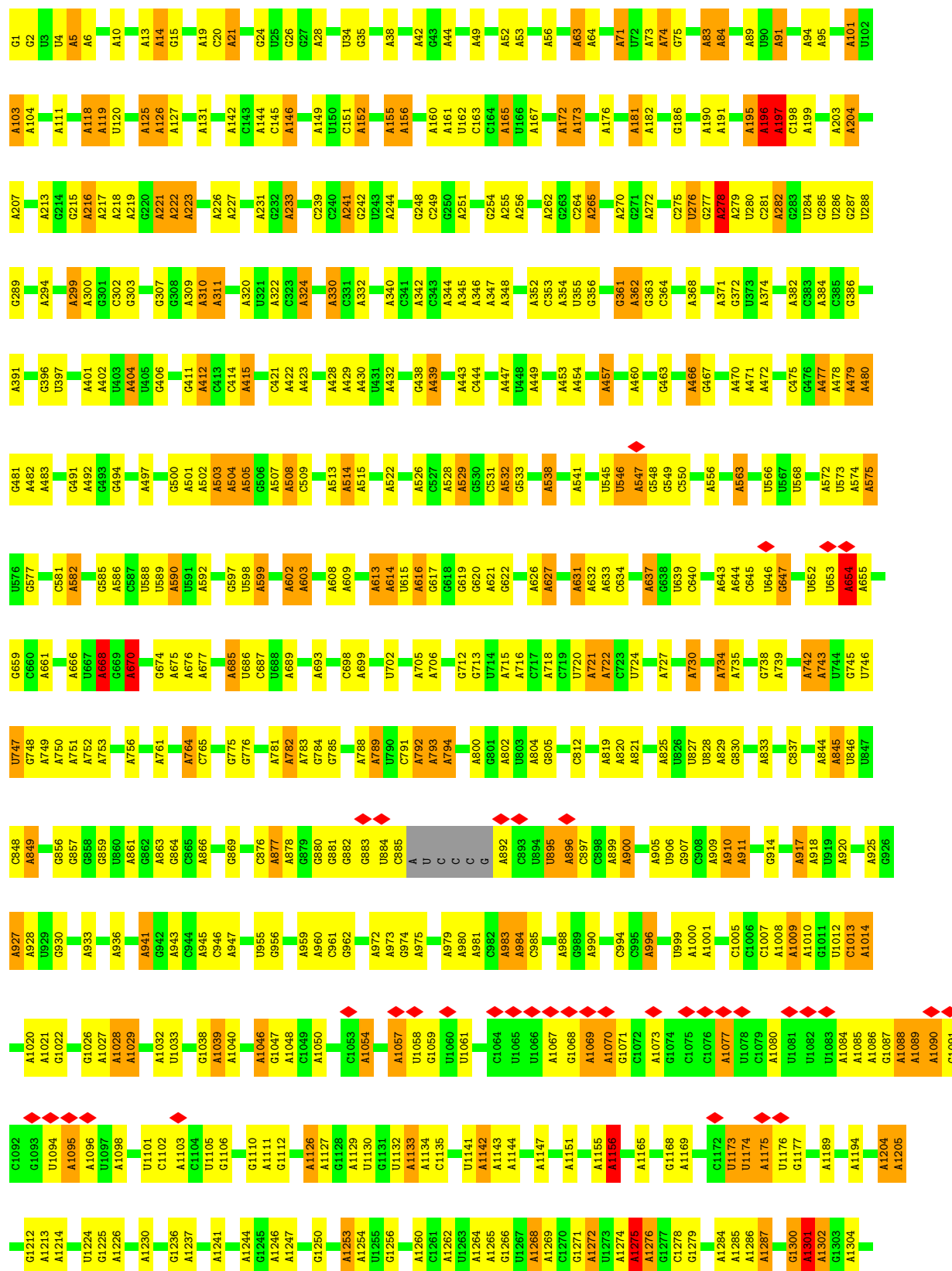
- Molecule 21: 30S ribosomal protein S21

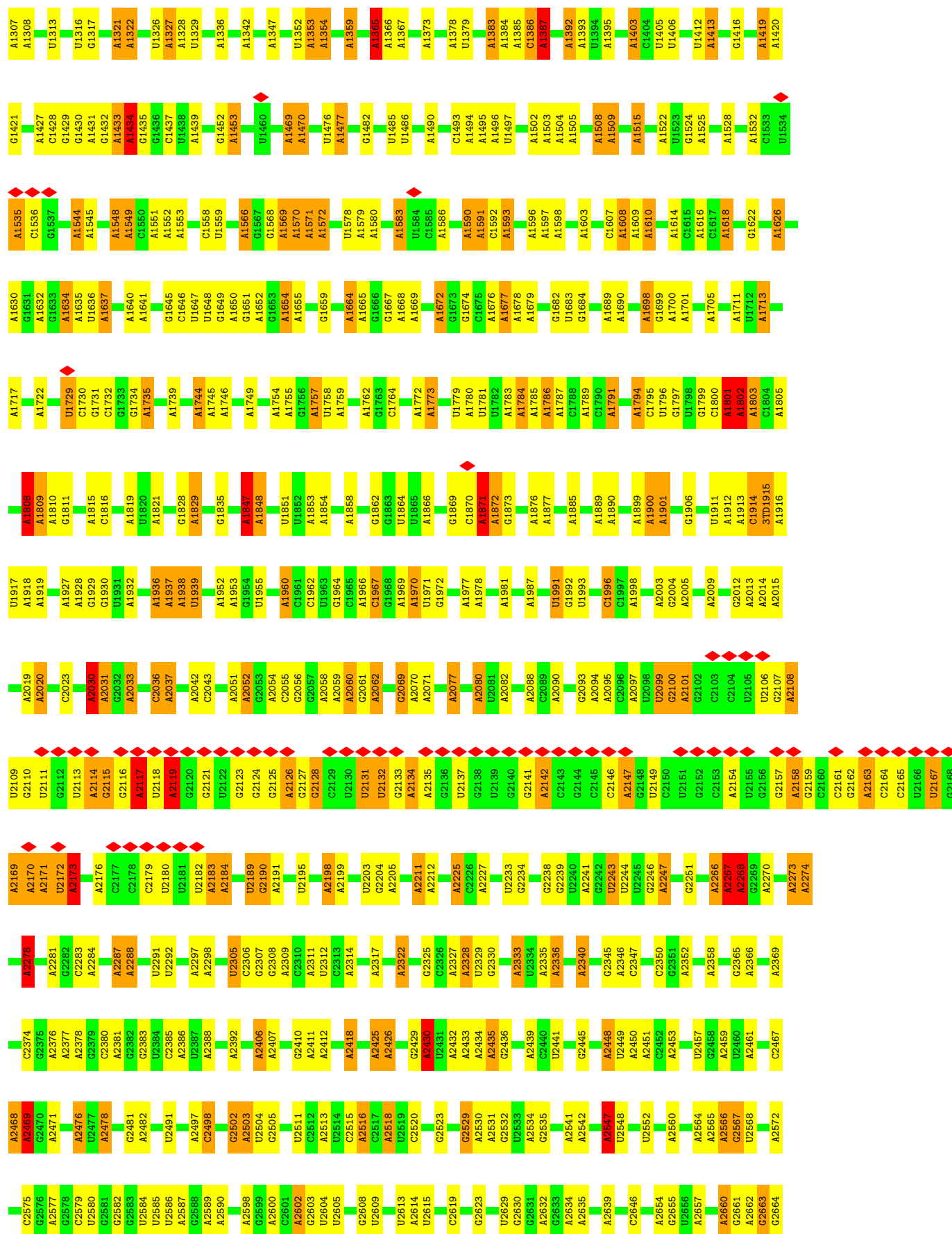
Chain AU:  10% 73% 6% 21%

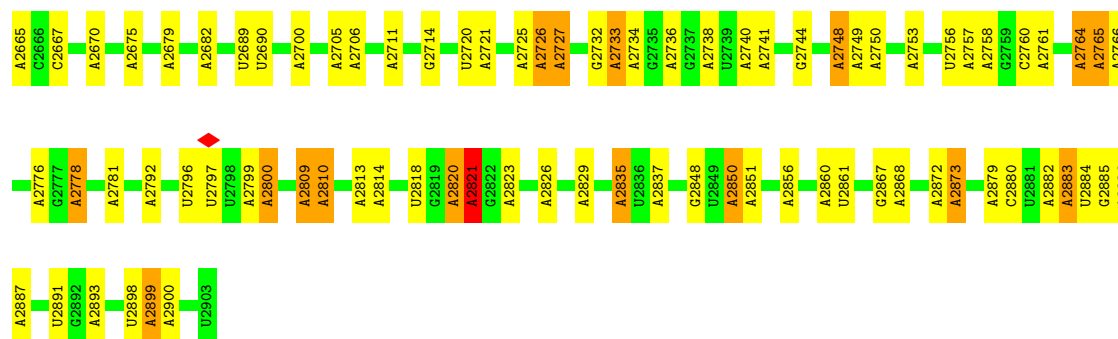


• Molecule 22: 23S rRNA

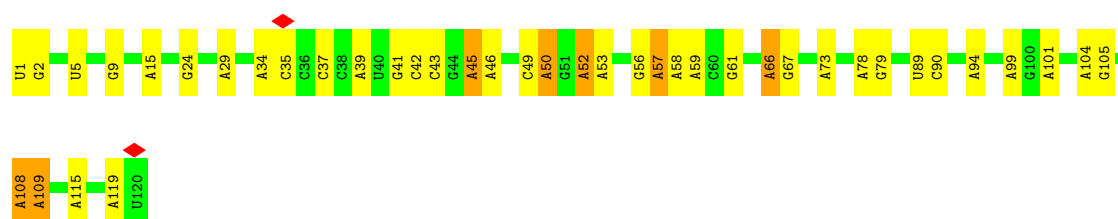
Chain BA:







• Molecule 23: 5S rRNA



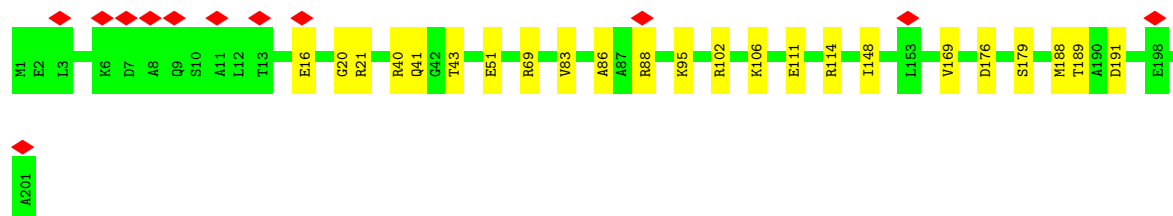
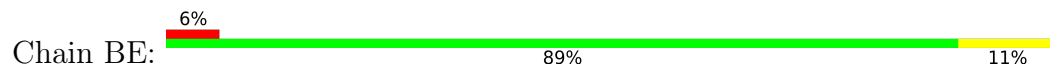
• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3



• Molecule 26: 50S ribosomal protein L4



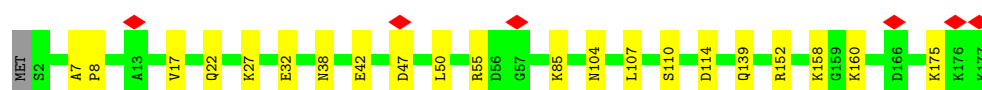
• Molecule 27: 50S ribosomal protein L5

Chain BF:  87% 12%



- Molecule 28: 50S ribosomal protein L6

Chain BG:  88% 12%



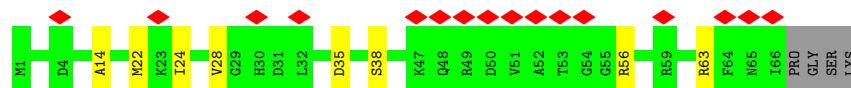
- Molecule 29: 50S ribosomal protein L9

Chain BH:  66% 87% 13%

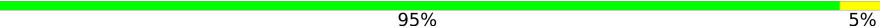


- Molecule 30: 50S ribosomal protein L31

Chain BI:  23% 83% 11% 6%



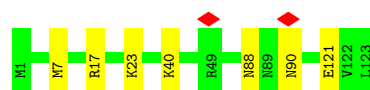
- Molecule 31: 50S ribosomal protein L13

Chain BJ:  95% 5%



- Molecule 32: 50S ribosomal protein L14

Chain BK:  94% 6%

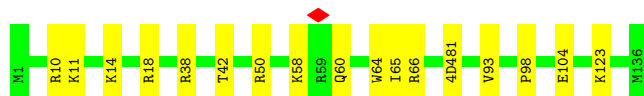
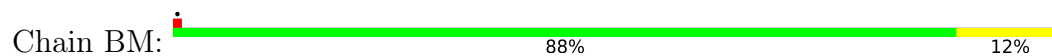


- Molecule 33: 50S ribosomal protein L15

Chain BL:  93% 7%



- Molecule 34: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L19



- Molecule 38: 50S ribosomal protein L20

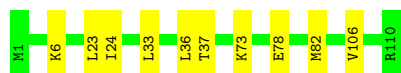


- Molecule 39: 50S ribosomal protein L21



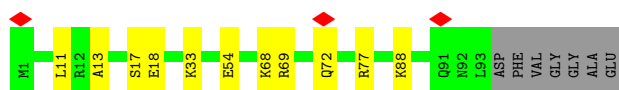
- Molecule 40: 50S ribosomal protein L22

Chain BS:  91% 9%

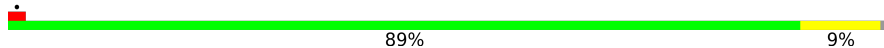


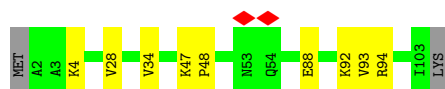
- Molecule 41: 50S ribosomal protein L23

Chain BT:  82% 11% 7%

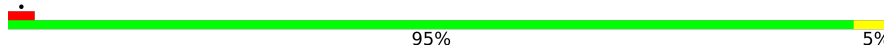


- Molecule 42: 50S ribosomal protein L24

Chain BU:  89% 9% .

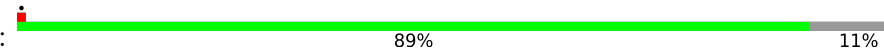


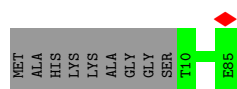
- Molecule 43: 50S ribosomal protein L25

Chain BV:  95% 5%

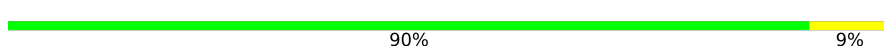


- Molecule 44: 50S ribosomal protein L27

Chain BW:  89% 11%



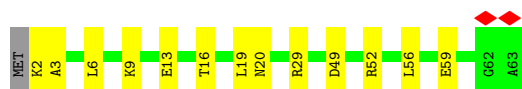
- Molecule 45: 50S ribosomal protein L28

Chain BX:  90% 9% .

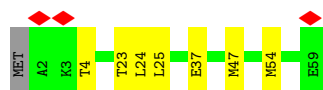
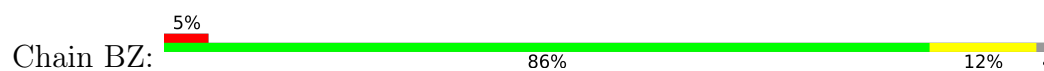


- Molecule 46: 50S ribosomal protein L29

Chain BY:  78% 21% .



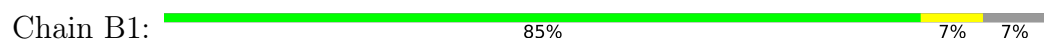
- Molecule 47: 50S ribosomal protein L30



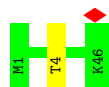
- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33



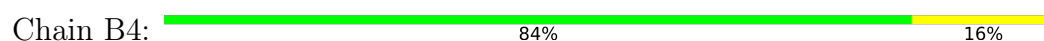
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36

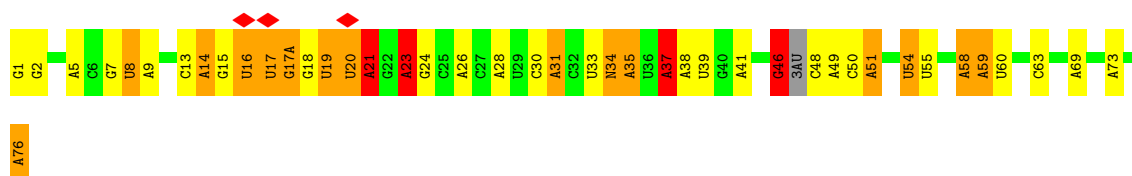


- Molecule 53: MsrDL: FME-TYR-LEU-ILE-PHE-MET

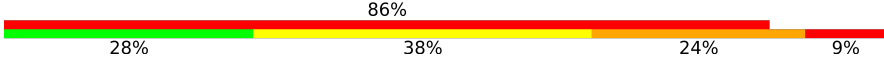


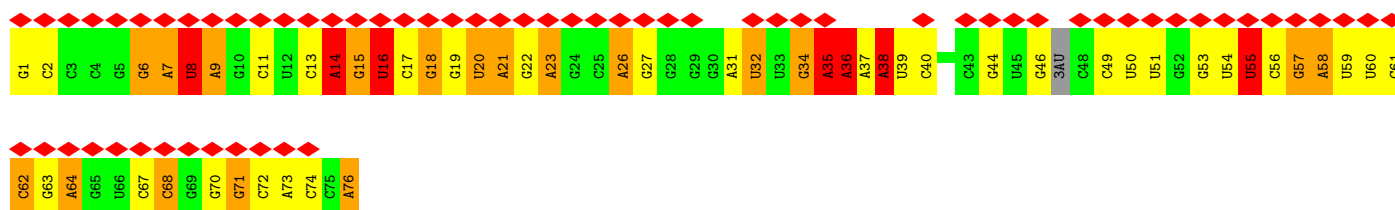
- Molecule 54: Met-tRNA (P site)

Chain D2: 



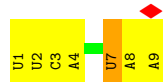
- Molecule 55: Phe-tRNA (E site)

Chain D3: 



- Molecule 56: MsrDL mRNA

Chain D4: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.089	Depositor
Minimum map value	-11.414	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.85	Depositor
Map size (Å)	414.0, 414.0, 414.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 4AC, MG, 4D4, H2U, OMG, 4OC, 1MG, 2MG, 6MZ, OMU, T6A, 2MA, MEQ, PSU, 3TD, G7M, D2T, OMC, ERY, 4SU, 5MC, 5MU, MA6, FME

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	0.66	0/36593	0.47	0/57081
2	AB	0.37	0/1784	0.62	0/2403
3	AC	0.67	0/1651	0.71	0/2225
4	AD	0.54	0/1665	0.63	0/2227
5	AE	0.53	0/1157	0.63	0/1557
6	AF	0.43	0/881	0.66	0/1189
7	AG	0.56	0/1195	0.71	0/1602
8	AH	0.52	0/989	0.59	0/1326
9	AI	0.75	0/1034	0.81	0/1375
10	AJ	0.69	0/805	0.74	0/1089
11	AK	0.50	0/893	0.56	0/1205
12	AL	0.56	0/960	0.91	7/1286 (0.5%)
13	AM	0.64	0/892	0.77	0/1193
14	AN	0.77	0/811	0.79	0/1081
15	AO	0.48	0/722	0.53	0/964
16	AP	0.54	0/659	0.84	1/884 (0.1%)
17	AQ	0.53	0/657	0.62	0/881
18	AR	0.53	0/462	0.58	0/621
19	AS	0.74	0/672	0.74	0/904
20	AT	0.44	0/676	0.53	0/895
21	AU	0.41	0/472	0.60	0/627
22	BA	0.92	758/69099 (1.1%)	0.74	0/107794
23	BB	0.78	23/2872 (0.8%)	0.63	0/4478
24	BC	0.35	0/2121	0.51	0/2852
25	BD	0.34	0/1576	0.48	0/2119
26	BE	0.29	0/1571	0.51	0/2113
27	BF	0.23	0/1434	0.52	0/1926
28	BG	0.25	0/1343	0.45	0/1816
29	BH	0.24	0/1121	0.66	0/1515
30	BI	0.24	0/531	0.55	0/709
31	BJ	0.31	0/1152	0.46	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	0.32	0/955	0.52	0/1279
33	BL	0.32	0/1062	0.51	0/1413
34	BM	0.33	0/1081	0.50	0/1443
35	BN	0.34	0/958	0.57	0/1281
36	BO	0.27	0/910	0.45	0/1219
37	BP	0.33	0/929	0.44	0/1242
38	BQ	0.36	0/960	0.46	0/1278
39	BR	0.31	0/829	0.47	0/1107
40	BS	0.32	0/864	0.49	0/1156
41	BT	0.29	0/744	0.49	0/994
42	BU	0.28	0/787	0.50	0/1051
43	BV	0.29	0/766	0.51	0/1025
44	BW	0.34	0/587	0.46	0/776
45	BX	0.34	0/635	0.50	0/848
46	BY	0.24	0/502	0.42	0/667
47	BZ	0.31	0/453	0.51	0/605
48	B0	0.34	0/450	0.51	0/599
49	B1	0.26	0/421	0.46	0/561
50	B2	0.36	0/380	0.59	0/498
51	B3	0.37	0/513	0.73	0/676
52	B4	0.33	0/303	0.46	0/397
53	D1	0.87	0/48	1.04	0/63
54	D2	0.93	18/1531 (1.2%)	0.74	0/2380
55	D3	0.83	15/1636 (0.9%)	0.77	0/2547
56	D4	0.43	0/210	0.57	0/324
All	All	0.74	814/156964 (0.5%)	0.64	8/234917 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AC	0	1
5	AE	0	1
29	BH	0	1
51	B3	0	1
All	All	0	4

All (814) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1872	A	C6-N6	6.89	1.47	1.33
55	D3	23	A	C6-N6	6.81	1.47	1.33
22	BA	1086	A	C6-N6	6.80	1.47	1.33
22	BA	2101	A	C6-N6	6.79	1.47	1.33
22	BA	1420	A	C6-N6	6.79	1.47	1.33
22	BA	1089	A	C6-N6	6.78	1.47	1.33
22	BA	2158	A	C6-N6	6.78	1.47	1.33
22	BA	2170	A	C6-N6	6.78	1.47	1.33
22	BA	2126	A	C6-N6	6.78	1.47	1.33
22	BA	1096	A	C6-N6	6.77	1.47	1.33
22	BA	1098	A	C6-N6	6.77	1.47	1.33
22	BA	1077	A	C6-N6	6.76	1.47	1.33
22	BA	1048	A	C6-N6	6.76	1.47	1.33
22	BA	896	A	C6-N6	6.76	1.47	1.33
22	BA	1175	A	C6-N6	6.75	1.47	1.33
22	BA	1084	A	C6-N6	6.75	1.47	1.33
22	BA	1871	A	C6-N6	6.75	1.47	1.33
22	BA	2163	A	C6-N6	6.75	1.47	1.33
22	BA	2602	A	C6-N6	6.74	1.47	1.33
22	BA	1095	A	C6-N6	6.74	1.47	1.33
55	D3	37	A	C6-N6	6.74	1.47	1.33
22	BA	1046	A	C6-N6	6.74	1.47	1.33
22	BA	877	A	C6-N6	6.73	1.47	1.33
22	BA	2134	A	C6-N6	6.73	1.47	1.33
22	BA	547	A	C6-N6	6.72	1.47	1.33
22	BA	2108	A	C6-N6	6.72	1.47	1.33
22	BA	1027	A	C6-N6	6.72	1.47	1.33
22	BA	1103	A	C6-N6	6.72	1.47	1.33
22	BA	2176	A	C6-N6	6.72	1.47	1.33
22	BA	362	A	C6-N6	6.71	1.47	1.33
22	BA	1528	A	C6-N6	6.71	1.47	1.33
22	BA	2082	A	C6-N6	6.71	1.47	1.33
22	BA	2171	A	C6-N6	6.71	1.47	1.33
22	BA	94	A	C6-N6	6.71	1.47	1.33
22	BA	614	A	C6-N6	6.71	1.47	1.33
22	BA	1069	A	C6-N6	6.71	1.47	1.33
55	D3	9	A	C6-N6	6.71	1.47	1.33
22	BA	1067	A	C6-N6	6.70	1.47	1.33
55	D3	58	A	C6-N6	6.70	1.47	1.33
22	BA	1057	A	C6-N6	6.70	1.47	1.33
22	BA	1085	A	C6-N6	6.70	1.47	1.33
22	BA	613	A	C6-N6	6.70	1.47	1.33
22	BA	1080	A	C6-N6	6.69	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	D3	73	A	C6-N6	6.69	1.47	1.33
22	BA	2117	A	C6-N6	6.69	1.47	1.33
22	BA	1070	A	C6-N6	6.69	1.47	1.33
22	BA	718	A	C6-N6	6.69	1.47	1.33
22	BA	2211	A	C6-N6	6.69	1.47	1.33
22	BA	1913	A	C6-N6	6.69	1.47	1.33
54	D2	73	A	C6-N6	6.68	1.47	1.33
22	BA	1490	A	C6-N6	6.68	1.47	1.33
22	BA	716	A	C6-N6	6.68	1.47	1.33
22	BA	1810	A	C6-N6	6.68	1.47	1.33
22	BA	1508	A	C6-N6	6.67	1.47	1.33
22	BA	1535	A	C6-N6	6.67	1.47	1.33
22	BA	2412	A	C6-N6	6.67	1.47	1.33
55	D3	38	A	C6-N6	6.67	1.47	1.33
22	BA	278	A	C6-N6	6.67	1.47	1.33
22	BA	1111	A	C6-N6	6.67	1.47	1.33
22	BA	2142	A	C6-N6	6.66	1.47	1.33
22	BA	1073	A	C6-N6	6.66	1.47	1.33
22	BA	1722	A	C6-N6	6.66	1.47	1.33
54	D2	51	A	C6-N6	6.65	1.47	1.33
22	BA	1866	A	C6-N6	6.65	1.47	1.33
54	D2	9	A	C6-N6	6.65	1.47	1.33
22	BA	95	A	C6-N6	6.65	1.47	1.33
22	BA	1937	A	C6-N6	6.65	1.47	1.33
22	BA	213	A	C6-N6	6.64	1.47	1.33
22	BA	1745	A	C6-N6	6.64	1.47	1.33
22	BA	1373	A	C6-N6	6.64	1.47	1.33
22	BA	1735	A	C6-N6	6.64	1.47	1.33
55	D3	35	A	C6-N6	6.64	1.47	1.33
22	BA	165	A	C6-N6	6.64	1.47	1.33
22	BA	878	A	C6-N6	6.64	1.47	1.33
22	BA	354	A	C6-N6	6.64	1.47	1.33
22	BA	892	A	C6-N6	6.64	1.47	1.33
22	BA	2042	A	C6-N6	6.64	1.47	1.33
22	BA	2814	A	C6-N6	6.64	1.47	1.33
22	BA	1580	A	C6-N6	6.63	1.47	1.33
55	D3	31	A	C6-N6	6.63	1.47	1.33
22	BA	1916	A	C6-N6	6.63	1.47	1.33
22	BA	251	A	C6-N6	6.63	1.47	1.33
22	BA	1509	A	C6-N6	6.63	1.47	1.33
22	BA	2820	A	C6-N6	6.63	1.47	1.33
22	BA	101	A	C6-N6	6.63	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2184	A	C6-N6	6.63	1.47	1.33
22	BA	2733	A	C6-N6	6.63	1.47	1.33
22	BA	2800	A	C6-N6	6.63	1.47	1.33
22	BA	2665	A	C6-N6	6.63	1.47	1.33
22	BA	633	A	C6-N6	6.62	1.47	1.33
22	BA	1395	A	C6-N6	6.62	1.47	1.33
22	BA	2309	A	C6-N6	6.62	1.47	1.33
22	BA	2662	A	C6-N6	6.62	1.47	1.33
54	D2	49	A	C6-N6	6.62	1.47	1.33
22	BA	1029	A	C6-N6	6.62	1.47	1.33
54	D2	14	A	C6-N6	6.62	1.47	1.33
22	BA	332	A	C6-N6	6.62	1.47	1.33
22	BA	1090	A	C6-N6	6.62	1.47	1.33
22	BA	1586	A	C6-N6	6.62	1.47	1.33
22	BA	2781	A	C6-N6	6.62	1.47	1.33
22	BA	2872	A	C6-N6	6.62	1.47	1.33
54	D2	69	A	C6-N6	6.62	1.47	1.33
22	BA	1532	A	C6-N6	6.62	1.47	1.33
54	D2	58	A	C6-N6	6.62	1.47	1.33
54	D2	59	A	C6-N6	6.62	1.47	1.33
22	BA	480	A	C6-N6	6.61	1.47	1.33
22	BA	2660	A	C6-N6	6.61	1.47	1.33
22	BA	2887	A	C6-N6	6.61	1.47	1.33
22	BA	508	A	C6-N6	6.61	1.47	1.33
22	BA	2154	A	C6-N6	6.61	1.47	1.33
22	BA	111	A	C6-N6	6.61	1.47	1.33
22	BA	749	A	C6-N6	6.61	1.47	1.33
22	BA	142	A	C6-N6	6.61	1.47	1.33
22	BA	279	A	C6-N6	6.61	1.47	1.33
22	BA	1583	A	C6-N6	6.61	1.47	1.33
22	BA	2748	A	C6-N6	6.61	1.47	1.33
22	BA	504	A	C6-N6	6.60	1.47	1.33
22	BA	1054	A	C6-N6	6.60	1.47	1.33
22	BA	265	A	C6-N6	6.60	1.47	1.33
22	BA	1050	A	C6-N6	6.60	1.47	1.33
22	BA	1156	A	C6-N6	6.60	1.47	1.33
22	BA	1434	A	C6-N6	6.60	1.47	1.33
22	BA	2879	A	C6-N6	6.60	1.47	1.33
23	BB	15	A	C6-N6	6.60	1.47	1.33
55	D3	36	A	C6-N6	6.60	1.47	1.33
23	BB	29	A	C6-N6	6.60	1.47	1.33
22	BA	2191	A	C6-N6	6.60	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2212	A	C6-N6	6.60	1.47	1.33
23	BB	52	A	C6-N6	6.60	1.47	1.33
54	D2	26	A	C6-N6	6.60	1.47	1.33
23	BB	108	A	C6-N6	6.59	1.47	1.33
22	BA	1367	A	C6-N6	6.59	1.47	1.33
54	D2	21	A	C6-N6	6.59	1.47	1.33
22	BA	849	A	C6-N6	6.59	1.47	1.33
22	BA	975	A	C6-N6	6.59	1.47	1.33
22	BA	2287	A	C6-N6	6.59	1.47	1.33
22	BA	345	A	C6-N6	6.59	1.47	1.33
22	BA	2135	A	C6-N6	6.59	1.47	1.33
22	BA	2173	A	C6-N6	6.59	1.47	1.33
54	D2	35	A	C6-N6	6.59	1.47	1.33
22	BA	739	A	C6-N6	6.58	1.47	1.33
22	BA	2297	A	C6-N6	6.58	1.47	1.33
22	BA	2468	A	C6-N6	6.58	1.47	1.33
22	BA	960	A	C6-N6	6.58	1.47	1.33
22	BA	71	A	C6-N6	6.58	1.47	1.33
22	BA	900	A	C6-N6	6.58	1.47	1.33
22	BA	1690	A	C6-N6	6.58	1.47	1.33
23	BB	34	A	C6-N6	6.58	1.47	1.33
23	BB	53	A	C6-N6	6.58	1.47	1.33
22	BA	91	A	C6-N6	6.58	1.47	1.33
22	BA	104	A	C6-N6	6.58	1.47	1.33
22	BA	1919	A	C6-N6	6.58	1.47	1.33
22	BA	2406	A	C6-N6	6.58	1.47	1.33
22	BA	2513	A	C6-N6	6.58	1.47	1.33
22	BA	2886	A	C6-N6	6.58	1.47	1.33
22	BA	1755	A	C6-N6	6.58	1.47	1.33
22	BA	2750	A	C6-N6	6.58	1.47	1.33
23	BB	39	A	C6-N6	6.57	1.47	1.33
22	BA	990	A	C6-N6	6.57	1.47	1.33
22	BA	347	A	C6-N6	6.57	1.47	1.33
22	BA	1039	A	C6-N6	6.57	1.47	1.33
22	BA	1284	A	C6-N6	6.57	1.47	1.33
22	BA	1328	A	C6-N6	6.57	1.47	1.33
22	BA	2119	A	C6-N6	6.57	1.47	1.33
22	BA	502	A	C6-N6	6.57	1.47	1.33
22	BA	655	A	C6-N6	6.57	1.47	1.33
22	BA	1593	A	C6-N6	6.57	1.47	1.33
22	BA	1876	A	C6-N6	6.57	1.47	1.33
23	BB	119	A	C6-N6	6.57	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	31	A	C6-N6	6.57	1.47	1.33
54	D2	38	A	C6-N6	6.57	1.47	1.33
22	BA	83	A	C6-N6	6.57	1.47	1.33
22	BA	155	A	C6-N6	6.57	1.47	1.33
22	BA	270	A	C6-N6	6.57	1.47	1.33
22	BA	344	A	C6-N6	6.57	1.47	1.33
22	BA	2335	A	C6-N6	6.57	1.47	1.33
22	BA	2377	A	C6-N6	6.57	1.47	1.33
22	BA	2547	A	C6-N6	6.57	1.47	1.33
22	BA	167	A	C6-N6	6.56	1.47	1.33
22	BA	282	A	C6-N6	6.56	1.47	1.33
22	BA	1453	A	C6-N6	6.56	1.47	1.33
22	BA	330	A	C6-N6	6.56	1.47	1.33
22	BA	1413	A	C6-N6	6.56	1.47	1.33
22	BA	1744	A	C6-N6	6.56	1.47	1.33
22	BA	2541	A	C6-N6	6.56	1.47	1.33
23	BB	66	A	C6-N6	6.56	1.47	1.33
22	BA	294	A	C6-N6	6.56	1.47	1.33
22	BA	626	A	C6-N6	6.56	1.47	1.33
22	BA	1544	A	C6-N6	6.56	1.47	1.33
22	BA	2378	A	C6-N6	6.56	1.47	1.33
22	BA	2169	A	C6-N6	6.56	1.47	1.33
22	BA	2657	A	C6-N6	6.56	1.47	1.33
22	BA	2721	A	C6-N6	6.56	1.47	1.33
22	BA	342	A	C6-N6	6.56	1.47	1.33
22	BA	352	A	C6-N6	6.56	1.47	1.33
22	BA	538	A	C6-N6	6.55	1.47	1.33
22	BA	1591	A	C6-N6	6.55	1.47	1.33
22	BA	1626	A	C6-N6	6.55	1.47	1.33
22	BA	1952	A	C6-N6	6.55	1.47	1.33
22	BA	2205	A	C6-N6	6.55	1.47	1.33
22	BA	2376	A	C6-N6	6.55	1.47	1.33
22	BA	2893	A	C6-N6	6.55	1.47	1.33
22	BA	933	A	C6-N6	6.55	1.47	1.33
22	BA	1502	A	C6-N6	6.55	1.47	1.33
22	BA	2033	A	C6-N6	6.55	1.47	1.33
23	BB	45	A	C6-N6	6.55	1.47	1.33
22	BA	782	A	C6-N6	6.55	1.47	1.33
22	BA	2298	A	C6-N6	6.55	1.47	1.33
22	BA	2478	A	C6-N6	6.55	1.47	1.33
22	BA	2598	A	C6-N6	6.55	1.47	1.33
22	BA	2850	A	C6-N6	6.55	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2821	A	C6-N6	6.55	1.47	1.33
23	BB	50	A	C6-N6	6.55	1.47	1.33
22	BA	1009	A	C6-N6	6.55	1.47	1.33
54	D2	76	A	C6-N6	6.55	1.47	1.33
22	BA	218	A	C6-N6	6.55	1.47	1.33
22	BA	996	A	C6-N6	6.55	1.47	1.33
22	BA	2439	A	C6-N6	6.55	1.47	1.33
22	BA	2753	A	C6-N6	6.55	1.47	1.33
55	D3	7	A	C6-N6	6.54	1.47	1.33
22	BA	1598	A	C6-N6	6.54	1.47	1.33
22	BA	2757	A	C6-N6	6.54	1.47	1.33
22	BA	482	A	C6-N6	6.54	1.47	1.33
22	BA	1495	A	C6-N6	6.54	1.47	1.33
22	BA	1503	A	C6-N6	6.54	1.47	1.33
22	BA	2311	A	C6-N6	6.54	1.47	1.33
22	BA	2654	A	C6-N6	6.54	1.47	1.33
22	BA	227	A	C6-N6	6.54	1.47	1.33
22	BA	401	A	C6-N6	6.54	1.47	1.33
22	BA	983	A	C6-N6	6.54	1.47	1.33
22	BA	1205	A	C6-N6	6.54	1.47	1.33
22	BA	1927	A	C6-N6	6.54	1.47	1.33
22	BA	64	A	C6-N6	6.54	1.47	1.33
22	BA	156	A	C6-N6	6.54	1.47	1.33
22	BA	391	A	C6-N6	6.54	1.47	1.33
22	BA	802	A	C6-N6	6.54	1.47	1.33
22	BA	1353	A	C6-N6	6.54	1.47	1.33
22	BA	1383	A	C6-N6	6.54	1.47	1.33
22	BA	1545	A	C6-N6	6.54	1.47	1.33
22	BA	1632	A	C6-N6	6.54	1.47	1.33
55	D3	64	A	C6-N6	6.54	1.47	1.33
22	BA	2482	A	C6-N6	6.53	1.47	1.33
22	BA	833	A	C6-N6	6.53	1.47	1.33
22	BA	2381	A	C6-N6	6.53	1.47	1.33
22	BA	125	A	C6-N6	6.53	1.47	1.33
22	BA	299	A	C6-N6	6.53	1.47	1.33
22	BA	2432	A	C6-N6	6.53	1.47	1.33
23	BB	59	A	C6-N6	6.53	1.47	1.33
22	BA	1272	A	C6-N6	6.53	1.47	1.33
22	BA	1640	A	C6-N6	6.53	1.47	1.33
22	BA	2632	A	C6-N6	6.53	1.47	1.33
22	BA	721	A	C6-N6	6.53	1.47	1.33
22	BA	1901	A	C6-N6	6.53	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2198	A	C6-N6	6.53	1.47	1.33
22	BA	2738	A	C6-N6	6.53	1.47	1.33
55	D3	21	A	C6-N6	6.53	1.47	1.33
22	BA	221	A	C6-N6	6.53	1.47	1.33
22	BA	608	A	C6-N6	6.53	1.47	1.33
22	BA	1739	A	C6-N6	6.53	1.47	1.33
22	BA	2080	A	C6-N6	6.53	1.47	1.33
22	BA	2873	A	C6-N6	6.53	1.47	1.33
22	BA	2741	A	C6-N6	6.52	1.47	1.33
22	BA	428	A	C6-N6	6.52	1.47	1.33
22	BA	899	A	C6-N6	6.52	1.47	1.33
22	BA	1322	A	C6-N6	6.52	1.47	1.33
22	BA	1590	A	C6-N6	6.52	1.47	1.33
22	BA	2453	A	C6-N6	6.52	1.47	1.33
22	BA	2705	A	C6-N6	6.52	1.47	1.33
54	D2	5	A	C6-N6	6.52	1.47	1.33
22	BA	1385	A	C6-N6	6.52	1.47	1.33
22	BA	311	A	C6-N6	6.52	1.47	1.33
22	BA	715	A	C6-N6	6.52	1.47	1.33
22	BA	2392	A	C6-N6	6.52	1.47	1.33
22	BA	637	A	C6-N6	6.52	1.47	1.33
22	BA	654	A	C6-N6	6.52	1.47	1.33
22	BA	2813	A	C6-N6	6.52	1.47	1.33
23	BB	57	A	C6-N6	6.52	1.47	1.33
54	D2	41	A	C6-N6	6.52	1.47	1.33
22	BA	63	A	C6-N6	6.52	1.47	1.33
22	BA	1393	A	C6-N6	6.52	1.47	1.33
22	BA	1504	A	C6-N6	6.51	1.47	1.33
22	BA	2856	A	C6-N6	6.51	1.47	1.33
22	BA	84	A	C6-N6	6.51	1.47	1.33
22	BA	752	A	C6-N6	6.51	1.47	1.33
55	D3	14	A	C6-N6	6.51	1.47	1.33
22	BA	503	A	C6-N6	6.51	1.47	1.33
22	BA	2900	A	C6-N6	6.51	1.47	1.33
22	BA	172	A	C6-N6	6.51	1.47	1.33
22	BA	309	A	C6-N6	6.51	1.47	1.33
22	BA	1928	A	C6-N6	6.51	1.47	1.33
22	BA	2114	A	C6-N6	6.51	1.47	1.33
22	BA	2199	A	C6-N6	6.51	1.47	1.33
22	BA	44	A	C6-N6	6.51	1.47	1.33
22	BA	644	A	C6-N6	6.51	1.47	1.33
22	BA	1877	A	C6-N6	6.51	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	322	A	C6-N6	6.51	1.47	1.33
22	BA	430	A	C6-N6	6.51	1.47	1.33
22	BA	905	A	C6-N6	6.51	1.47	1.33
22	BA	1147	A	C6-N6	6.51	1.47	1.33
22	BA	1307	A	C6-N6	6.51	1.47	1.33
22	BA	1609	A	C6-N6	6.51	1.47	1.33
22	BA	1900	A	C6-N6	6.51	1.47	1.33
22	BA	1912	A	C6-N6	6.51	1.47	1.33
22	BA	2097	A	C6-N6	6.51	1.47	1.33
22	BA	2476	A	C6-N6	6.51	1.47	1.33
22	BA	2761	A	C6-N6	6.51	1.47	1.33
22	BA	1134	A	C6-N6	6.50	1.47	1.33
22	BA	89	A	C6-N6	6.50	1.47	1.33
22	BA	340	A	C6-N6	6.50	1.47	1.33
22	BA	501	A	C6-N6	6.50	1.47	1.33
22	BA	541	A	C6-N6	6.50	1.47	1.33
22	BA	829	A	C6-N6	6.50	1.47	1.33
22	BA	1553	A	C6-N6	6.50	1.47	1.33
22	BA	1634	A	C6-N6	6.50	1.47	1.33
22	BA	1847	A	C6-N6	6.50	1.47	1.33
22	BA	1978	A	C6-N6	6.50	1.47	1.33
22	BA	2147	A	C6-N6	6.50	1.47	1.33
22	BA	2183	A	C6-N6	6.50	1.47	1.33
22	BA	2758	A	C6-N6	6.50	1.47	1.33
22	BA	477	A	C6-N6	6.50	1.47	1.33
22	BA	507	A	C6-N6	6.50	1.47	1.33
22	BA	1040	A	C6-N6	6.50	1.47	1.33
22	BA	1204	A	C6-N6	6.50	1.47	1.33
22	BA	1918	A	C6-N6	6.50	1.47	1.33
22	BA	2314	A	C6-N6	6.50	1.47	1.33
22	BA	2792	A	C6-N6	6.50	1.47	1.33
23	BB	109	A	C6-N6	6.50	1.47	1.33
22	BA	1885	A	C6-N6	6.50	1.47	1.33
22	BA	2288	A	C6-N6	6.50	1.47	1.33
54	D2	23	A	C6-N6	6.50	1.47	1.33
22	BA	1287	A	C6-N6	6.50	1.47	1.33
22	BA	1304	A	C6-N6	6.50	1.47	1.33
22	BA	1608	A	C6-N6	6.50	1.47	1.33
22	BA	2734	A	C6-N6	6.50	1.47	1.33
22	BA	2860	A	C6-N6	6.50	1.47	1.33
23	BB	73	A	C6-N6	6.50	1.47	1.33
22	BA	14	A	C6-N6	6.50	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	616	A	C6-N6	6.50	1.47	1.33
22	BA	73	A	C6-N6	6.49	1.47	1.33
22	BA	429	A	C6-N6	6.49	1.47	1.33
22	BA	1155	A	C6-N6	6.49	1.47	1.33
22	BA	1241	A	C6-N6	6.49	1.47	1.33
22	BA	1551	A	C6-N6	6.49	1.47	1.33
22	BA	1596	A	C6-N6	6.49	1.47	1.33
22	BA	1773	A	C6-N6	6.49	1.47	1.33
22	BA	2530	A	C6-N6	6.49	1.47	1.33
22	BA	2776	A	C6-N6	6.49	1.47	1.33
22	BA	1783	A	C6-N6	6.49	1.47	1.33
22	BA	320	A	C6-N6	6.49	1.47	1.33
22	BA	368	A	C6-N6	6.49	1.47	1.33
22	BA	734	A	C6-N6	6.49	1.47	1.33
22	BA	2322	A	C6-N6	6.49	1.47	1.33
22	BA	2572	A	C6-N6	6.49	1.47	1.33
22	BA	526	A	C6-N6	6.49	1.47	1.33
22	BA	602	A	C6-N6	6.49	1.47	1.33
22	BA	1327	A	C6-N6	6.49	1.47	1.33
22	BA	1678	A	C6-N6	6.49	1.47	1.33
22	BA	2366	A	C6-N6	6.49	1.47	1.33
23	BB	115	A	C6-N6	6.49	1.47	1.33
22	BA	988	A	C6-N6	6.49	1.47	1.33
22	BA	2531	A	C6-N6	6.49	1.47	1.33
22	BA	478	A	C6-N6	6.49	1.47	1.33
22	BA	603	A	C6-N6	6.49	1.47	1.33
22	BA	945	A	C6-N6	6.49	1.47	1.33
22	BA	1347	A	C6-N6	6.49	1.47	1.33
22	BA	1780	A	C6-N6	6.49	1.47	1.33
22	BA	404	A	C6-N6	6.48	1.47	1.33
22	BA	497	A	C6-N6	6.48	1.47	1.33
22	BA	1000	A	C6-N6	6.48	1.47	1.33
22	BA	1433	A	C6-N6	6.48	1.47	1.33
22	BA	1757	A	C6-N6	6.48	1.47	1.33
22	BA	2587	A	C6-N6	6.48	1.47	1.33
22	BA	196	A	C6-N6	6.48	1.47	1.33
22	BA	244	A	C6-N6	6.48	1.47	1.33
22	BA	384	A	C6-N6	6.48	1.47	1.33
22	BA	412	A	C6-N6	6.48	1.47	1.33
22	BA	866	A	C6-N6	6.48	1.47	1.33
22	BA	1470	A	C6-N6	6.48	1.47	1.33
22	BA	2095	A	C6-N6	6.48	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	182	A	C6-N6	6.48	1.47	1.33
22	BA	1133	A	C6-N6	6.48	1.47	1.33
22	BA	2799	A	C6-N6	6.48	1.47	1.33
22	BA	819	A	C6-N6	6.48	1.47	1.33
22	BA	2336	A	C6-N6	6.48	1.47	1.33
22	BA	146	A	C6-N6	6.48	1.47	1.33
22	BA	447	A	C6-N6	6.48	1.47	1.33
22	BA	643	A	C6-N6	6.48	1.47	1.33
22	BA	675	A	C6-N6	6.48	1.47	1.33
22	BA	1384	A	C6-N6	6.48	1.47	1.33
22	BA	1597	A	C6-N6	6.48	1.47	1.33
22	BA	219	A	C6-N6	6.47	1.46	1.33
22	BA	927	A	C6-N6	6.47	1.46	1.33
22	BA	980	A	C6-N6	6.47	1.47	1.33
22	BA	1165	A	C6-N6	6.47	1.46	1.33
22	BA	1672	A	C6-N6	6.47	1.46	1.33
22	BA	1759	A	C6-N6	6.47	1.47	1.33
22	BA	2430	A	C6-N6	6.47	1.47	1.33
23	BB	46	A	C6-N6	6.47	1.46	1.33
22	BA	1253	A	C6-N6	6.47	1.46	1.33
22	BA	1746	A	C6-N6	6.47	1.46	1.33
22	BA	2051	A	C6-N6	6.47	1.46	1.33
22	BA	2077	A	C6-N6	6.47	1.46	1.33
22	BA	1525	A	C6-N6	6.47	1.46	1.33
22	BA	460	A	C6-N6	6.47	1.46	1.33
22	BA	609	A	C6-N6	6.47	1.46	1.33
22	BA	789	A	C6-N6	6.47	1.46	1.33
22	BA	1969	A	C6-N6	6.47	1.46	1.33
22	BA	2518	A	C6-N6	6.47	1.46	1.33
22	BA	2835	A	C6-N6	6.47	1.46	1.33
22	BA	979	A	C6-N6	6.47	1.46	1.33
22	BA	2829	A	C6-N6	6.47	1.46	1.33
22	BA	936	A	C6-N6	6.47	1.46	1.33
22	BA	943	A	C6-N6	6.47	1.46	1.33
22	BA	1981	A	C6-N6	6.47	1.46	1.33
22	BA	2534	A	C6-N6	6.47	1.46	1.33
22	BA	917	A	C6-N6	6.46	1.46	1.33
22	BA	1321	A	C6-N6	6.46	1.46	1.33
22	BA	1635	A	C6-N6	6.46	1.46	1.33
22	BA	1641	A	C6-N6	6.46	1.46	1.33
22	BA	2450	A	C6-N6	6.46	1.46	1.33
22	BA	126	A	C6-N6	6.46	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1274	A	C6-N6	6.46	1.46	1.33
22	BA	1494	A	C6-N6	6.46	1.46	1.33
22	BA	2317	A	C6-N6	6.46	1.46	1.33
22	BA	2706	A	C6-N6	6.46	1.46	1.33
22	BA	2899	A	C6-N6	6.46	1.46	1.33
22	BA	127	A	C6-N6	6.46	1.46	1.33
22	BA	173	A	C6-N6	6.46	1.46	1.33
22	BA	1754	A	C6-N6	6.46	1.46	1.33
22	BA	2227	A	C6-N6	6.46	1.46	1.33
22	BA	2851	A	C6-N6	6.46	1.46	1.33
22	BA	984	A	C6-N6	6.46	1.46	1.33
22	BA	1469	A	C6-N6	6.46	1.46	1.33
22	BA	1664	A	C6-N6	6.46	1.46	1.33
22	BA	1717	A	C6-N6	6.46	1.46	1.33
22	BA	223	A	C6-N6	6.46	1.46	1.33
22	BA	751	A	C6-N6	6.46	1.46	1.33
22	BA	1654	A	C6-N6	6.46	1.46	1.33
22	BA	2425	A	C6-N6	6.46	1.46	1.33
22	BA	256	A	C6-N6	6.46	1.46	1.33
22	BA	471	A	C6-N6	6.46	1.46	1.33
22	BA	699	A	C6-N6	6.46	1.46	1.33
22	BA	928	A	C6-N6	6.46	1.46	1.33
22	BA	1010	A	C6-N6	6.46	1.46	1.33
22	BA	1268	A	C6-N6	6.46	1.46	1.33
22	BA	1713	A	C6-N6	6.46	1.46	1.33
22	BA	160	A	C6-N6	6.46	1.46	1.33
22	BA	781	A	C6-N6	6.46	1.46	1.33
22	BA	1571	A	C6-N6	6.46	1.46	1.33
22	BA	2727	A	C6-N6	6.46	1.46	1.33
22	BA	2764	A	C6-N6	6.46	1.46	1.33
22	BA	42	A	C6-N6	6.45	1.46	1.33
22	BA	272	A	C6-N6	6.45	1.46	1.33
22	BA	556	A	C6-N6	6.45	1.46	1.33
22	BA	2019	A	C6-N6	6.45	1.46	1.33
22	BA	2352	A	C6-N6	6.45	1.46	1.33
22	BA	1970	A	C6-N6	6.45	1.46	1.33
23	BB	104	A	C6-N6	6.45	1.46	1.33
22	BA	181	A	C6-N6	6.45	1.46	1.33
22	BA	454	A	C6-N6	6.45	1.46	1.33
22	BA	492	A	C6-N6	6.45	1.46	1.33
22	BA	1226	A	C6-N6	6.45	1.46	1.33
22	BA	1275	A	C6-N6	6.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	149	A	C6-N6	6.45	1.46	1.33
22	BA	1020	A	C6-N6	6.45	1.46	1.33
22	BA	1403	A	C6-N6	6.45	1.46	1.33
22	BA	1808	A	C6-N6	6.45	1.46	1.33
22	BA	666	A	C6-N6	6.45	1.46	1.33
22	BA	2003	A	C6-N6	6.45	1.46	1.33
22	BA	131	A	C6-N6	6.45	1.46	1.33
22	BA	483	A	C6-N6	6.45	1.46	1.33
22	BA	2418	A	C6-N6	6.45	1.46	1.33
22	BA	2434	A	C6-N6	6.45	1.46	1.33
22	BA	2566	A	C6-N6	6.45	1.46	1.33
22	BA	2823	A	C6-N6	6.45	1.46	1.33
22	BA	1794	A	C6-N6	6.44	1.46	1.33
22	BA	470	A	C6-N6	6.44	1.46	1.33
22	BA	1194	A	C6-N6	6.44	1.46	1.33
22	BA	1427	A	C6-N6	6.44	1.46	1.33
22	BA	2060	A	C6-N6	6.44	1.46	1.33
22	BA	627	A	C6-N6	6.44	1.46	1.33
22	BA	825	A	C6-N6	6.44	1.46	1.33
22	BA	1579	A	C6-N6	6.44	1.46	1.33
22	BA	1785	A	C6-N6	6.44	1.46	1.33
22	BA	1821	A	C6-N6	6.44	1.46	1.33
22	BA	2328	A	C6-N6	6.44	1.46	1.33
22	BA	2542	A	C6-N6	6.44	1.46	1.33
22	BA	49	A	C6-N6	6.44	1.46	1.33
22	BA	513	A	C6-N6	6.44	1.46	1.33
22	BA	1214	A	C6-N6	6.44	1.46	1.33
22	BA	1566	A	C6-N6	6.44	1.46	1.33
22	BA	2031	A	C6-N6	6.44	1.46	1.33
22	BA	2340	A	C6-N6	6.44	1.46	1.33
22	BA	300	A	C6-N6	6.44	1.46	1.33
22	BA	310	A	C6-N6	6.44	1.46	1.33
22	BA	443	A	C6-N6	6.44	1.46	1.33
22	BA	783	A	C6-N6	6.44	1.46	1.33
22	BA	1143	A	C6-N6	6.44	1.46	1.33
22	BA	1762	A	C6-N6	6.44	1.46	1.33
22	BA	1987	A	C6-N6	6.44	1.46	1.33
22	BA	1630	A	C6-N6	6.44	1.46	1.33
54	D2	28	A	C6-N6	6.44	1.46	1.33
22	BA	161	A	C6-N6	6.43	1.46	1.33
22	BA	217	A	C6-N6	6.43	1.46	1.33
22	BA	1285	A	C6-N6	6.43	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1786	A	C6-N6	6.43	1.46	1.33
22	BA	2058	A	C6-N6	6.43	1.46	1.33
22	BA	2411	A	C6-N6	6.43	1.46	1.33
22	BA	592	A	C6-N6	6.43	1.46	1.33
22	BA	735	A	C6-N6	6.43	1.46	1.33
22	BA	941	A	C6-N6	6.43	1.46	1.33
22	BA	1342	A	C6-N6	6.43	1.46	1.33
22	BA	1614	A	C6-N6	6.43	1.46	1.33
22	BA	1014	A	C6-N6	6.43	1.46	1.33
22	BA	1548	A	C6-N6	6.43	1.46	1.33
22	BA	1552	A	C6-N6	6.43	1.46	1.33
22	BA	2273	A	C6-N6	6.43	1.46	1.33
22	BA	574	A	C6-N6	6.43	1.46	1.33
22	BA	1260	A	C6-N6	6.43	1.46	1.33
22	BA	1366	A	C6-N6	6.43	1.46	1.33
22	BA	1749	A	C6-N6	6.43	1.46	1.33
22	BA	1854	A	C6-N6	6.43	1.46	1.33
22	BA	2274	A	C6-N6	6.43	1.46	1.33
22	BA	2448	A	C6-N6	6.43	1.46	1.33
22	BA	2560	A	C6-N6	6.43	1.46	1.33
22	BA	1809	A	C6-N6	6.43	1.46	1.33
22	BA	792	A	C6-N6	6.43	1.46	1.33
22	BA	1496	A	C6-N6	6.43	1.46	1.33
22	BA	1610	A	C6-N6	6.43	1.46	1.33
22	BA	1698	A	C6-N6	6.43	1.46	1.33
22	BA	2810	A	C6-N6	6.43	1.46	1.33
22	BA	103	A	C6-N6	6.42	1.46	1.33
22	BA	422	A	C6-N6	6.42	1.46	1.33
22	BA	1276	A	C6-N6	6.42	1.46	1.33
22	BA	1572	A	C6-N6	6.42	1.46	1.33
22	BA	1701	A	C6-N6	6.42	1.46	1.33
22	BA	2094	A	C6-N6	6.42	1.46	1.33
22	BA	1549	A	C6-N6	6.42	1.46	1.33
22	BA	255	A	C6-N6	6.42	1.46	1.33
22	BA	1144	A	C6-N6	6.42	1.46	1.33
22	BA	1890	A	C6-N6	6.42	1.46	1.33
22	BA	1772	A	C6-N6	6.42	1.46	1.33
22	BA	2670	A	C6-N6	6.42	1.46	1.33
22	BA	346	A	C6-N6	6.42	1.46	1.33
22	BA	529	A	C6-N6	6.42	1.46	1.33
22	BA	972	A	C6-N6	6.42	1.46	1.33
22	BA	1127	A	C6-N6	6.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1265	A	C6-N6	6.42	1.46	1.33
22	BA	1953	A	C6-N6	6.42	1.46	1.33
22	BA	2778	A	C6-N6	6.42	1.46	1.33
23	BB	58	A	C6-N6	6.42	1.46	1.33
22	BA	432	A	C6-N6	6.42	1.46	1.33
22	BA	706	A	C6-N6	6.42	1.46	1.33
22	BA	1603	A	C6-N6	6.42	1.46	1.33
22	BA	2015	A	C6-N6	6.42	1.46	1.33
22	BA	1189	A	C6-N6	6.41	1.46	1.33
22	BA	1439	A	C6-N6	6.41	1.46	1.33
22	BA	1677	A	C6-N6	6.41	1.46	1.33
22	BA	2564	A	C6-N6	6.41	1.46	1.33
22	BA	631	A	C6-N6	6.41	1.46	1.33
22	BA	1679	A	C6-N6	6.41	1.46	1.33
23	BB	99	A	C6-N6	6.41	1.46	1.33
22	BA	13	A	C6-N6	6.41	1.46	1.33
22	BA	1008	A	C6-N6	6.41	1.46	1.33
22	BA	1169	A	C6-N6	6.41	1.46	1.33
22	BA	191	A	C6-N6	6.41	1.46	1.33
22	BA	371	A	C6-N6	6.41	1.46	1.33
22	BA	505	A	C6-N6	6.41	1.46	1.33
22	BA	528	A	C6-N6	6.41	1.46	1.33
22	BA	532	A	C6-N6	6.41	1.46	1.33
22	BA	1711	A	C6-N6	6.41	1.46	1.33
22	BA	1998	A	C6-N6	6.41	1.46	1.33
22	BA	2635	A	C6-N6	6.41	1.46	1.33
55	D3	26	A	C6-N6	6.41	1.46	1.33
22	BA	1431	A	C6-N6	6.41	1.46	1.33
22	BA	1264	A	C6-N6	6.41	1.46	1.33
22	BA	1419	A	C6-N6	6.40	1.46	1.33
22	BA	586	A	C6-N6	6.40	1.46	1.33
22	BA	668	A	C6-N6	6.40	1.46	1.33
22	BA	820	A	C6-N6	6.40	1.46	1.33
22	BA	1286	A	C6-N6	6.40	1.46	1.33
22	BA	1477	A	C6-N6	6.40	1.46	1.33
22	BA	74	A	C6-N6	6.40	1.46	1.33
22	BA	226	A	C6-N6	6.40	1.46	1.33
22	BA	241	A	C6-N6	6.40	1.46	1.33
22	BA	1700	A	C6-N6	6.40	1.46	1.33
22	BA	1784	A	C6-N6	6.40	1.46	1.33
22	BA	1853	A	C6-N6	6.40	1.46	1.33
22	BA	2600	A	C6-N6	6.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2682	A	C6-N6	6.40	1.46	1.33
22	BA	2711	A	C6-N6	6.40	1.46	1.33
22	BA	1668	A	C6-N6	6.40	1.46	1.33
22	BA	1889	A	C6-N6	6.40	1.46	1.33
22	BA	2433	A	C6-N6	6.40	1.46	1.33
22	BA	910	A	C6-N6	6.40	1.46	1.33
22	BA	925	A	C6-N6	6.40	1.46	1.33
22	BA	1522	A	C6-N6	6.40	1.46	1.33
22	BA	2059	A	C6-N6	6.40	1.46	1.33
22	BA	1308	A	C6-N6	6.40	1.46	1.33
22	BA	415	A	C6-N6	6.39	1.46	1.33
22	BA	423	A	C6-N6	6.39	1.46	1.33
22	BA	1230	A	C6-N6	6.39	1.46	1.33
22	BA	1336	A	C6-N6	6.39	1.46	1.33
22	BA	1848	A	C6-N6	6.39	1.46	1.33
22	BA	144	A	C6-N6	6.39	1.46	1.33
22	BA	262	A	C6-N6	6.39	1.46	1.33
22	BA	1129	A	C6-N6	6.39	1.46	1.33
22	BA	1676	A	C6-N6	6.39	1.46	1.33
22	BA	1787	A	C6-N6	6.39	1.46	1.33
22	BA	1789	A	C6-N6	6.39	1.46	1.33
22	BA	1803	A	C6-N6	6.39	1.46	1.33
22	BA	1936	A	C6-N6	6.39	1.46	1.33
22	BA	2749	A	C6-N6	6.39	1.46	1.33
22	BA	981	A	C6-N6	6.39	1.46	1.33
22	BA	5	A	C6-N6	6.39	1.46	1.33
22	BA	233	A	C6-N6	6.39	1.46	1.33
22	BA	1669	A	C6-N6	6.39	1.46	1.33
22	BA	6	A	C6-N6	6.39	1.46	1.33
22	BA	753	A	C6-N6	6.39	1.46	1.33
22	BA	1247	A	C6-N6	6.38	1.46	1.33
22	BA	1354	A	C6-N6	6.38	1.46	1.33
22	BA	861	A	C6-N6	6.38	1.46	1.33
22	BA	1244	A	C6-N6	6.38	1.46	1.33
22	BA	1365	A	C6-N6	6.38	1.46	1.33
22	BA	2071	A	C6-N6	6.38	1.46	1.33
22	BA	10	A	C6-N6	6.38	1.46	1.33
22	BA	449	A	C6-N6	6.38	1.46	1.33
22	BA	1262	A	C6-N6	6.38	1.46	1.33
22	BA	1570	A	C6-N6	6.38	1.46	1.33
22	BA	2740	A	C6-N6	6.38	1.46	1.33
22	BA	2868	A	C6-N6	6.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	207	A	C6-N6	6.38	1.46	1.33
22	BA	2700	A	C6-N6	6.38	1.46	1.33
22	BA	661	A	C6-N6	6.38	1.46	1.33
22	BA	920	A	C6-N6	6.38	1.46	1.33
22	BA	1301	A	C6-N6	6.38	1.46	1.33
22	BA	1505	A	C6-N6	6.38	1.46	1.33
22	BA	2088	A	C6-N6	6.38	1.46	1.33
22	BA	2388	A	C6-N6	6.38	1.46	1.33
22	BA	2459	A	C6-N6	6.38	1.46	1.33
22	BA	2883	A	C6-N6	6.38	1.46	1.33
22	BA	670	A	C6-N6	6.38	1.46	1.33
22	BA	909	A	C6-N6	6.38	1.46	1.33
22	BA	844	A	C6-N6	6.38	1.46	1.33
22	BA	2009	A	C6-N6	6.38	1.46	1.33
22	BA	2589	A	C6-N6	6.38	1.46	1.33
22	BA	231	A	C6-N6	6.37	1.46	1.33
22	BA	466	A	C6-N6	6.37	1.46	1.33
22	BA	1032	A	C6-N6	6.37	1.46	1.33
22	BA	1515	A	C6-N6	6.37	1.46	1.33
22	BA	2426	A	C6-N6	6.37	1.46	1.33
22	BA	1088	A	C6-N6	6.37	1.46	1.33
22	BA	2725	A	C6-N6	6.37	1.46	1.33
22	BA	52	A	C6-N6	6.37	1.46	1.33
22	BA	761	A	C6-N6	6.37	1.46	1.33
22	BA	1966	A	C6-N6	6.37	1.46	1.33
22	BA	2270	A	C6-N6	6.37	1.46	1.33
22	BA	599	A	C6-N6	6.37	1.46	1.33
22	BA	911	A	C6-N6	6.37	1.46	1.33
22	BA	2451	A	C6-N6	6.37	1.46	1.33
22	BA	199	A	C6-N6	6.37	1.46	1.33
22	BA	563	A	C6-N6	6.37	1.46	1.33
22	BA	1213	A	C6-N6	6.37	1.46	1.33
22	BA	2386	A	C6-N6	6.37	1.46	1.33
22	BA	793	A	C6-N6	6.37	1.46	1.33
22	BA	804	A	C6-N6	6.37	1.46	1.33
22	BA	152	A	C6-N6	6.36	1.46	1.33
22	BA	197	A	C6-N6	6.36	1.46	1.33
22	BA	845	A	C6-N6	6.36	1.46	1.33
22	BA	2037	A	C6-N6	6.36	1.46	1.33
22	BA	2565	A	C6-N6	6.36	1.46	1.33
22	BA	2247	A	C6-N6	6.36	1.46	1.33
22	BA	402	A	C6-N6	6.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	216	A	C6-N6	6.36	1.46	1.33
22	BA	348	A	C6-N6	6.36	1.46	1.33
22	BA	590	A	C6-N6	6.36	1.46	1.33
22	BA	2241	A	C6-N6	6.36	1.46	1.33
22	BA	2278	A	C6-N6	6.36	1.46	1.33
22	BA	918	A	C6-N6	6.36	1.46	1.33
22	BA	53	A	C6-N6	6.35	1.46	1.33
22	BA	756	A	C6-N6	6.35	1.46	1.33
22	BA	21	A	C6-N6	6.35	1.46	1.33
22	BA	190	A	C6-N6	6.35	1.46	1.33
22	BA	1650	A	C6-N6	6.35	1.46	1.33
22	BA	2358	A	C6-N6	6.35	1.46	1.33
22	BA	472	A	C6-N6	6.35	1.46	1.33
22	BA	730	A	C6-N6	6.35	1.46	1.33
22	BA	19	A	C6-N6	6.35	1.46	1.33
22	BA	1269	A	C6-N6	6.35	1.46	1.33
22	BA	1801	A	C6-N6	6.35	1.46	1.33
22	BA	2435	A	C6-N6	6.35	1.46	1.33
23	BB	94	A	C6-N6	6.35	1.46	1.33
22	BA	1938	A	C6-N6	6.35	1.46	1.33
22	BA	2013	A	C6-N6	6.34	1.46	1.33
22	BA	2497	A	C6-N6	6.34	1.46	1.33
22	BA	947	A	C6-N6	6.34	1.46	1.33
22	BA	1359	A	C6-N6	6.34	1.46	1.33
22	BA	2281	A	C6-N6	6.34	1.46	1.33
22	BA	382	A	C6-N6	6.34	1.46	1.33
22	BA	453	A	C6-N6	6.34	1.46	1.33
22	BA	515	A	C6-N6	6.34	1.46	1.33
22	BA	689	A	C6-N6	6.34	1.46	1.33
22	BA	2346	A	C6-N6	6.34	1.46	1.33
22	BA	203	A	C6-N6	6.34	1.46	1.33
22	BA	1665	A	C6-N6	6.34	1.46	1.33
55	D3	76	A	C6-N6	6.34	1.46	1.33
22	BA	800	A	C6-N6	6.34	1.46	1.33
22	BA	1151	A	C6-N6	6.34	1.46	1.33
22	BA	1829	A	C6-N6	6.34	1.46	1.33
22	BA	195	A	C6-N6	6.33	1.46	1.33
22	BA	1126	A	C6-N6	6.33	1.46	1.33
22	BA	1805	A	C6-N6	6.33	1.46	1.33
22	BA	2634	A	C6-N6	6.33	1.46	1.33
22	BA	1960	A	C6-N6	6.33	1.46	1.33
22	BA	2327	A	C6-N6	6.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2516	A	C6-N6	6.33	1.46	1.33
23	BB	101	A	C6-N6	6.33	1.46	1.33
22	BA	788	A	C6-N6	6.33	1.46	1.33
22	BA	2266	A	C6-N6	6.33	1.46	1.33
22	BA	722	A	C6-N6	6.33	1.46	1.33
22	BA	56	A	C6-N6	6.33	1.46	1.33
22	BA	374	A	C6-N6	6.33	1.46	1.33
22	BA	1652	A	C6-N6	6.33	1.46	1.33
22	BA	2225	A	C6-N6	6.33	1.46	1.33
22	BA	2471	A	C6-N6	6.33	1.46	1.33
22	BA	2675	A	C6-N6	6.33	1.46	1.33
22	BA	632	A	C6-N6	6.32	1.46	1.33
22	BA	794	A	C6-N6	6.32	1.46	1.33
22	BA	2726	A	C6-N6	6.32	1.46	1.33
22	BA	2070	A	C6-N6	6.32	1.46	1.33
22	BA	2590	A	C6-N6	6.32	1.46	1.33
22	BA	1802	A	C6-N6	6.32	1.46	1.33
22	BA	2826	A	C6-N6	6.32	1.46	1.33
22	BA	176	A	C6-N6	6.32	1.46	1.33
22	BA	1932	A	C6-N6	6.32	1.46	1.33
22	BA	1977	A	C6-N6	6.32	1.46	1.33
22	BA	2882	A	C6-N6	6.32	1.46	1.33
22	BA	621	A	C6-N6	6.32	1.46	1.33
22	BA	2736	A	C6-N6	6.32	1.46	1.33
22	BA	2765	A	C6-N6	6.32	1.46	1.33
22	BA	572	A	C6-N6	6.31	1.46	1.33
22	BA	959	A	C6-N6	6.31	1.46	1.33
22	BA	118	A	C6-N6	6.31	1.46	1.33
22	BA	28	A	C6-N6	6.31	1.46	1.33
22	BA	119	A	C6-N6	6.31	1.46	1.33
22	BA	676	A	C6-N6	6.31	1.46	1.33
22	BA	2614	A	C6-N6	6.30	1.46	1.33
22	BA	2461	A	C6-N6	6.30	1.46	1.33
22	BA	1569	A	C6-N6	6.30	1.46	1.33
22	BA	38	A	C6-N6	6.30	1.46	1.33
22	BA	2090	A	C6-N6	6.30	1.46	1.33
22	BA	2268	A	C6-N6	6.30	1.46	1.33
22	BA	1392	A	C6-N6	6.29	1.46	1.33
22	BA	1689	A	C6-N6	6.29	1.46	1.33
22	BA	2369	A	C6-N6	6.29	1.46	1.33
22	BA	439	A	C6-N6	6.28	1.46	1.33
22	BA	1378	A	C6-N6	6.28	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1246	A	C6-N6	6.28	1.46	1.33
22	BA	2020	A	C6-N6	6.28	1.46	1.33
22	BA	2679	A	C6-N6	6.28	1.46	1.33
22	BA	1001	A	C6-N6	6.27	1.46	1.33
22	BA	2014	A	C6-N6	6.27	1.46	1.33
22	BA	677	A	C6-N6	6.27	1.46	1.33
22	BA	1387	A	C6-N6	6.27	1.46	1.33
22	BA	1899	A	C6-N6	6.27	1.46	1.33
22	BA	2333	A	C6-N6	6.27	1.46	1.33
22	BA	693	A	C6-N6	6.27	1.46	1.33
22	BA	1302	A	C6-N6	6.27	1.46	1.33
22	BA	1858	A	C6-N6	6.27	1.46	1.33
22	BA	1616	A	C6-N6	6.26	1.46	1.33
22	BA	685	A	C6-N6	6.26	1.46	1.33
22	BA	2809	A	C6-N6	6.26	1.46	1.33
22	BA	1705	A	C6-N6	6.26	1.46	1.33
22	BA	2639	A	C6-N6	6.26	1.46	1.33
22	BA	2062	A	C6-N6	6.25	1.46	1.33
22	BA	821	A	C6-N6	6.24	1.46	1.33
22	BA	2407	A	C6-N6	6.24	1.46	1.33
22	BA	1637	A	C6-N6	6.24	1.46	1.33
22	BA	1655	A	C6-N6	6.24	1.46	1.33
22	BA	2577	A	C6-N6	6.23	1.46	1.33
22	BA	863	A	C6-N6	6.22	1.46	1.33
22	BA	1815	A	C6-N6	6.22	1.46	1.33
22	BA	743	A	C6-N6	6.22	1.46	1.33
22	BA	1791	A	C6-N6	6.22	1.46	1.33
22	BA	727	A	C6-N6	6.21	1.46	1.33
22	BA	742	A	C6-N6	6.21	1.46	1.33
22	BA	2284	A	C6-N6	6.20	1.46	1.33
22	BA	2837	A	C6-N6	6.20	1.46	1.33
22	BA	204	A	C6-N6	6.20	1.46	1.33
22	BA	522	A	C6-N6	6.20	1.46	1.33
22	BA	705	A	C6-N6	6.20	1.46	1.33
22	BA	1254	A	C6-N6	6.19	1.46	1.33
22	BA	222	A	C6-N6	6.18	1.46	1.33
22	BA	457	A	C6-N6	6.18	1.46	1.33
22	BA	582	A	C6-N6	6.18	1.46	1.33
22	BA	973	A	C6-N6	6.18	1.46	1.33
22	BA	575	A	C6-N6	6.18	1.46	1.33
22	BA	764	A	C6-N6	6.17	1.46	1.33
23	BB	78	A	C6-N6	6.16	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	479	A	C6-N6	6.16	1.46	1.33
22	BA	2766	A	C6-N6	6.16	1.46	1.33
22	BA	1819	A	C6-N6	6.15	1.46	1.33
22	BA	2005	A	C6-N6	6.15	1.46	1.33
22	BA	2469	A	C6-N6	6.15	1.46	1.33
22	BA	1237	A	C6-N6	6.13	1.46	1.33
22	BA	324	A	C6-N6	6.12	1.46	1.33
22	BA	2054	A	C6-N6	6.08	1.46	1.33
22	BA	1142	A	C6-N6	6.08	1.46	1.33
22	BA	1021	A	C6-N6	6.06	1.46	1.33
22	BA	2267	A	C6-N6	6.05	1.46	1.33
22	BA	1028	A	C6-N6	6.04	1.46	1.33
22	BA	750	A	C6-N6	6.04	1.46	1.33
22	BA	2052	A	C6-N6	5.94	1.45	1.33
22	BA	514	A	C6-N6	5.93	1.45	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AL	101	ALA	N-CA-C	13.57	128.13	109.54
16	AP	48	GLU	CB-CA-C	-12.72	89.59	110.19
12	AL	103	ASP	N-CA-C	12.01	128.30	113.17
12	AL	103	ASP	N-CA-CB	-8.48	97.94	110.49
12	AL	102	LEU	CB-CA-C	6.70	123.75	110.42
12	AL	102	LEU	N-CA-C	-5.84	98.36	110.80
12	AL	101	ALA	CA-C-N	5.10	131.28	121.54
12	AL	101	ALA	C-N-CA	5.10	131.28	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AC	60	PRO	Peptide
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide
29	BH	41	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	185	0
2	AB	1753	0	1780	19	0
3	AC	1624	0	1696	38	0
4	AD	1643	0	1707	22	0
5	AE	1144	0	1184	14	0
6	AF	862	0	864	15	0
7	AG	1181	0	1238	26	0
8	AH	979	0	1031	13	0
9	AI	1022	0	1070	24	0
10	AJ	795	0	836	21	0
11	AK	877	0	887	12	0
12	AL	957	0	1017	8	0
13	AM	883	0	941	66	0
14	AN	799	0	841	18	0
15	AO	714	0	734	10	0
16	AP	649	0	666	11	0
17	AQ	648	0	691	11	0
18	AR	455	0	478	11	0
19	AS	656	0	680	22	0
20	AT	670	0	719	4	0
21	AU	465	0	491	4	0
22	BA	62209	0	31307	235	0
23	BB	2569	0	1301	7	0
24	BC	2082	0	2154	13	0
25	BD	1566	0	1618	11	0
26	BE	1552	0	1619	13	0
27	BF	1410	0	1444	36	0
28	BG	1323	0	1371	13	0
29	BH	1110	0	1148	9	0
30	BI	522	0	522	16	0
31	BJ	1129	0	1162	4	0
32	BK	946	0	1023	4	0
33	BL	1053	0	1129	8	0
34	BM	1075	0	1155	11	0
35	BN	945	0	989	5	0
36	BO	900	0	935	1	0
37	BP	917	0	962	6	0
38	BQ	947	0	1019	3	0
39	BR	816	0	839	6	0
40	BS	857	0	922	7	0
41	BT	738	0	807	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BU	779	0	831	5	0
43	BV	753	0	780	3	0
44	BW	580	0	594	0	0
45	BX	625	0	652	5	0
46	BY	501	0	531	8	0
47	BZ	449	0	488	4	0
48	B0	444	0	458	3	0
49	B1	414	0	442	2	0
50	B2	377	0	418	1	0
51	B3	504	0	572	8	0
52	B4	302	0	343	5	0
53	D1	57	0	59	7	0
54	D2	1634	0	842	19	0
55	D3	1604	0	817	29	0
56	D4	189	0	96	13	0
57	AA	35	0	0	1	0
57	BA	134	0	0	1	0
57	BC	1	0	0	0	0
57	BD	1	0	0	0	0
57	D2	1	0	0	0	0
58	BA	51	0	67	4	0
59	AA	166	0	0	4	0
59	AK	2	0	0	0	0
59	AM	1	0	0	0	0
59	AN	2	0	0	0	0
59	AQ	1	0	0	0	0
59	BA	614	0	0	4	0
59	BC	6	0	0	0	0
59	BD	3	0	0	0	0
59	BE	1	0	0	0	0
59	BJ	1	0	0	0	0
59	BL	1	0	0	0	0
59	BN	2	0	0	0	0
All	All	146607	0	97558	903	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 4.

All (903) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:7:ILE:HD12	27:BF:112:ARG:CD	1.04	1.50
13:AM:7:ILE:CD1	27:BF:112:ARG:HD2	1.36	1.48
13:AM:7:ILE:CD1	27:BF:112:ARG:CD	1.89	1.44
13:AM:7:ILE:HD12	27:BF:112:ARG:CG	1.51	1.40
13:AM:43:VAL:CG1	13:AM:48:LEU:HD11	1.54	1.37
13:AM:7:ILE:CD1	27:BF:112:ARG:CG	2.08	1.30
13:AM:7:ILE:HD11	27:BF:112:ARG:HD2	1.24	1.19
13:AM:43:VAL:HG13	13:AM:48:LEU:HD11	1.28	1.14
13:AM:7:ILE:HD12	27:BF:112:ARG:HD3	1.29	1.14
13:AM:43:VAL:HG11	13:AM:48:LEU:HD11	1.30	1.13
1:AA:1493:A:H1'	56:D4:7:U:H5	1.13	1.12
19:AS:5:LEU:HD12	19:AS:7:LYS:H	1.05	1.07
13:AM:7:ILE:CD1	27:BF:112:ARG:HG2	1.80	1.07
13:AM:71:ARG:NH1	27:BF:115:ARG:HH22	1.54	1.04
1:AA:1493:A:H1'	56:D4:7:U:C5	1.93	1.04
1:AA:1076:U:OP1	2:AB:174:LYS:NZ	1.93	1.01
13:AM:7:ILE:HD13	27:BF:112:ARG:CG	1.93	0.98
22:BA:2099:U:H3	22:BA:2190:G:H1	1.10	0.98
13:AM:43:VAL:CG1	13:AM:48:LEU:CD1	2.43	0.97
54:D2:15:G:H22	54:D2:48:C:H42	1.01	0.96
22:BA:881:G:H1	22:BA:895:U:H3	0.95	0.95
1:AA:458:U:O2	1:AA:474:G:N1	2.00	0.94
55:D3:35:A:N6	56:D4:2:U:O4	2.03	0.92
18:AR:34:THR:HG22	18:AR:35:GLU:H	1.35	0.90
16:AP:6:LEU:HD23	16:AP:19:VAL:HG12	1.50	0.90
19:AS:5:LEU:CD1	19:AS:7:LYS:H	1.84	0.90
13:AM:43:VAL:HG13	13:AM:48:LEU:CD1	2.00	0.90
1:AA:1009:U:H3	1:AA:1020:G:H1	1.18	0.87
1:AA:823:C:HO2'	8:AH:2:SER:N	1.70	0.87
19:AS:5:LEU:HD12	19:AS:7:LYS:N	1.89	0.86
15:AO:89:ARG:NH2	22:BA:712:G:O5'	2.08	0.86
54:D2:15:G:H22	54:D2:48:C:N4	1.74	0.86
54:D2:15:G:N2	54:D2:48:C:H42	1.74	0.85
13:AM:57:ARG:NH2	30:BI:35:ASP:OD1	2.10	0.83
13:AM:43:VAL:HG11	13:AM:48:LEU:CD1	2.07	0.83
1:AA:694:A:HO2'	55:D3:38:A:HO2'	1.06	0.82
58:BA:3001:ERY:O6	53:D1:3:LEU:O	1.97	0.81
13:AM:71:ARG:HH11	27:BF:115:ARG:HH22	1.27	0.80
19:AS:5:LEU:CD1	19:AS:7:LYS:HB2	2.12	0.79
22:BA:2099:U:O2	22:BA:2190:G:N2	2.14	0.79
13:AM:7:ILE:HD12	27:BF:112:ARG:HG2	1.50	0.77
1:AA:458:U:O2	1:AA:474:G:N2	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:7:ILE:HD13	27:BF:112:ARG:HG2	1.54	0.76
1:AA:458:U:O2	1:AA:474:G:C2	2.39	0.75
13:AM:79:ARG:NH1	30:BI:56:ARG:HH21	1.84	0.75
1:AA:1305:G:H21	1:AA:1332:A:H2	1.35	0.74
3:AC:57:ILE:HG22	3:AC:66:VAL:HG23	1.69	0.74
55:D3:36:A:N1	56:D4:1:U:O4	2.21	0.74
13:AM:43:VAL:HG11	13:AM:48:LEU:HD21	1.68	0.74
13:AM:7:ILE:HD13	27:BF:112:ARG:CB	2.17	0.73
13:AM:79:ARG:CZ	30:BI:56:ARG:NH2	2.52	0.73
13:AM:71:ARG:NH1	27:BF:115:ARG:NH2	2.36	0.73
18:AR:34:THR:HG22	18:AR:35:GLU:N	2.02	0.73
13:AM:79:ARG:NH1	30:BI:56:ARG:NH2	2.38	0.72
22:BA:475:C:O2	22:BA:479:A:N6	2.24	0.70
1:AA:1073:U:O2'	2:AB:103:ASN:OD1	2.03	0.70
25:BD:13:ARG:HH12	37:BP:56:HIS:HA	1.56	0.70
15:AO:33:THR:HG22	15:AO:63:ARG:HH11	1.57	0.70
55:D3:36:A:C2	56:D4:1:U:H5	2.09	0.70
16:AP:6:LEU:CD2	16:AP:19:VAL:HG12	2.21	0.70
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.56	0.69
19:AS:5:LEU:HD13	19:AS:7:LYS:HB2	1.74	0.69
1:AA:1076:U:P	2:AB:174:LYS:HZ1	2.13	0.69
1:AA:1078:U:H4'	5:AE:138:ARG:CZ	2.23	0.69
13:AM:43:VAL:HG21	13:AM:48:LEU:CD2	2.23	0.68
9:AI:130:ARG:NH2	54:D2:33:U:H5	1.91	0.68
1:AA:352:C:OP2	59:AA:1704:HOH:O	2.11	0.68
54:D2:37:T6A:H8	54:D2:37:T6A:H5''	1.58	0.68
55:D3:15:G:H3'	55:D3:16:H2U:H2'	1.76	0.68
1:AA:1055:A:O2'	3:AC:156:ARG:NH1	2.26	0.67
13:AM:8:ASN:HD22	13:AM:22:ILE:HA	1.60	0.67
4:AD:105:MET:HG2	4:AD:171:LEU:HD13	1.77	0.67
13:AM:57:ARG:NH2	30:BI:35:ASP:CG	2.53	0.67
9:AI:130:ARG:NH2	54:D2:33:U:C5	2.63	0.67
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.75	0.67
13:AM:7:ILE:CD1	27:BF:112:ARG:CB	2.73	0.66
55:D3:15:G:H5'	55:D3:16:H2U:H62	1.78	0.65
6:AF:29:ILE:HD13	6:AF:64:VAL:HG11	1.79	0.65
22:BA:2821:A:OP2	57:BA:3109:MG:MG	1.40	0.65
22:BA:2134:A:OP2	22:BA:2157:G:N2	2.30	0.65
6:AF:90:MET:SD	18:AR:61:ARG:NH1	2.71	0.64
1:AA:1009:U:O2	1:AA:1020:G:N2	2.27	0.64
1:AA:1229:A:OP2	13:AM:113:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BL:109:LYS:HG2	33:BL:126:ARG:HB2	1.79	0.64
7:AG:148:ASN:O	7:AG:148:ASN:ND2	2.30	0.64
1:AA:1086:U:H2'	1:AA:1087:G:H8	1.63	0.64
1:AA:212:G:H2'	1:AA:213:G:H8	1.63	0.63
5:AE:55:GLU:HG3	5:AE:57:PRO:HD2	1.80	0.63
22:BA:2114:A:H61	22:BA:2119:A:H62	1.46	0.63
55:D3:55:PSU:HN1	55:D3:57:G:H5''	1.62	0.63
1:AA:352:C:OP2	57:AA:1608:MG:MG	1.41	0.63
1:AA:429:U:H5'	4:AD:9:LEU:HD11	1.81	0.63
16:AP:6:LEU:HD23	16:AP:19:VAL:CG1	2.27	0.63
22:BA:2760:C:H1'	28:BG:139:GLN:HE22	1.61	0.63
9:AI:123:ARG:NH1	9:AI:124:ARG:O	2.32	0.63
29:BH:84:ALA:HB2	29:BH:90:LEU:HD23	1.81	0.62
1:AA:1086:U:H2'	1:AA:1087:G:C8	2.34	0.62
22:BA:585:G:N7	38:BQ:6:ARG:NH1	2.47	0.62
15:AO:89:ARG:NH2	22:BA:712:G:P	2.73	0.62
55:D3:34:G:O6	56:D4:3:C:N3	2.32	0.62
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.32	0.62
4:AD:129:VAL:HG21	4:AD:146:ARG:HH21	1.65	0.62
13:AM:9:ILE:HG21	27:BF:143:TYR:HE2	1.64	0.62
22:BA:652:U:OP1	22:BA:654:A:N6	2.31	0.62
1:AA:110:C:O2'	16:AP:25:ARG:O	2.18	0.62
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.33	0.62
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.33	0.62
55:D3:51:U:O4	55:D3:63:G:O6	2.18	0.62
1:AA:1012:A:OP2	19:AS:17:LYS:NZ	2.33	0.61
13:AM:79:ARG:NH2	30:BI:56:ARG:NH2	2.48	0.61
1:AA:208:U:N3	1:AA:211:G:N1	2.47	0.61
7:AG:151:PHE:CZ	11:AK:56:ARG:HG2	2.36	0.61
7:AG:79:ARG:CG	7:AG:79:ARG:HH21	2.13	0.61
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.29	0.61
17:AQ:68:SER:OG	17:AQ:69:LYS:N	2.32	0.61
19:AS:5:LEU:HD13	19:AS:7:LYS:HE2	1.82	0.61
1:AA:694:A:O2'	55:D3:38:A:O2'	1.92	0.61
3:AC:83:ASP:O	3:AC:87:LEU:N	2.33	0.61
4:AD:102:VAL:HG23	4:AD:114:ALA:HB1	1.83	0.61
13:AM:43:VAL:CG2	13:AM:48:LEU:HG	2.30	0.61
8:AH:43:GLU:HG3	8:AH:101:ILE:HD13	1.83	0.60
22:BA:2365:G:N7	51:B3:39:LYS:NZ	2.45	0.60
3:AC:129:MET:HE2	3:AC:131:ARG:HB2	1.81	0.60
41:BT:11:LEU:O	46:BY:29:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:97:LEU:H	2:AB:100:MET:HE3	1.65	0.60
13:AM:4:ILE:HG22	13:AM:60:VAL:HG11	1.83	0.60
22:BA:2107:G:H1	22:BA:2182:U:H3	1.48	0.60
24:BC:262:ARG:O	24:BC:265:LYS:NZ	2.33	0.60
22:BA:2469:A:N6	22:BA:2481:G:O2'	2.34	0.60
55:D3:62:C:H2'	55:D3:63:G:H8	1.67	0.60
1:AA:958:A:OP1	19:AS:55:ARG:NH2	2.32	0.60
34:BM:50:ARG:HG3	34:BM:65:ILE:HD11	1.83	0.60
1:AA:411:A:H4'	1:AA:412:A:H5'	1.83	0.60
1:AA:1144:G:H21	1:AA:1146:A:H62	1.49	0.60
6:AF:30:THR:HA	6:AF:34:GLY:H	1.67	0.60
9:AI:17:ALA:HB2	9:AI:67:VAL:HG12	1.82	0.60
22:BA:2523:G:HO2'	22:BA:2764:A:HO2'	1.50	0.60
5:AE:105:ILE:O	5:AE:112:ARG:NH2	2.34	0.59
10:AJ:28:THR:O	10:AJ:32:THR:OG1	2.16	0.59
13:AM:43:VAL:HG22	13:AM:48:LEU:HG	1.84	0.59
22:BA:1174:U:O2	22:BA:1177:G:N1	2.33	0.59
2:AB:43:LEU:HA	2:AB:46:THR:HG22	1.84	0.59
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.85	0.59
23:BB:43:C:O2	27:BF:92:ARG:NH2	2.36	0.59
1:AA:1073:U:O2	2:AB:103:ASN:ND2	2.35	0.59
13:AM:71:ARG:HH12	27:BF:115:ARG:HH22	1.45	0.59
7:AG:129:GLU:O	7:AG:131:LYS:NZ	2.36	0.59
13:AM:43:VAL:HG11	13:AM:48:LEU:CD2	2.33	0.59
22:BA:2848:G:O2'	22:BA:2867:G:N2	2.32	0.59
13:AM:43:VAL:HG21	13:AM:48:LEU:HD21	1.83	0.59
52:B4:2:LYS:NZ	52:B4:32:LYS:O	2.36	0.59
1:AA:1005:A:N7	1:AA:1024:G:O2'	2.36	0.59
9:AI:18:ARG:NH1	9:AI:18:ARG:HG3	2.16	0.59
9:AI:128:SER:OG	9:AI:130:ARG:O	2.20	0.58
22:BA:1779:U:OP2	22:BA:1784:A:N6	2.35	0.58
55:D3:6:G:N2	55:D3:68:C:O2	2.36	0.58
22:BA:877:A:O2'	22:BA:900:A:N6	2.36	0.58
25:BD:181:ASP:HB3	25:BD:186:LEU:HB2	1.85	0.58
28:BG:27:LYS:HG2	28:BG:32:GLU:HG3	1.84	0.58
6:AF:37:HIS:HB3	6:AF:97:THR:HG22	1.85	0.58
14:AN:19:TYR:O	14:AN:23:ARG:N	2.31	0.58
53:D1:4:ILE:O	53:D1:4:ILE:HG13	2.03	0.58
1:AA:1081:A:OP1	5:AE:23:LYS:HB2	2.03	0.58
22:BA:1007:C:OP1	31:BJ:37:ARG:NH2	2.36	0.58
22:BA:2511:U:O4	22:BA:2575:C:N3	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:202:G:O2'	1:AA:467:U:O4	2.21	0.58
3:AC:57:ILE:CG2	3:AC:66:VAL:HG23	2.32	0.58
10:AJ:83:THR:O	10:AJ:87:LEU:N	2.37	0.58
14:AN:47:LYS:O	14:AN:50:THR:OG1	2.19	0.58
1:AA:210:C:O2	1:AA:211:G:N1	2.36	0.57
1:AA:264:C:O3'	17:AQ:65:ARG:NH1	2.37	0.57
13:AM:67:GLY:HA3	27:BF:113:ASP:OD2	2.04	0.57
8:AH:74:SER:HB3	8:AH:130:ALA:HB3	1.86	0.57
22:BA:2467:C:O2	34:BM:123:LYS:NZ	2.36	0.57
28:BG:22:GLN:NE2	28:BG:38:ASN:O	2.37	0.57
1:AA:683:G:N2	11:AK:39:GLY:O	2.37	0.57
1:AA:445:G:H1	1:AA:489:C:H5	1.53	0.57
7:AG:68:ASN:O	7:AG:138:ARG:NH1	2.38	0.57
9:AI:18:ARG:HG3	9:AI:18:ARG:HH11	1.70	0.57
9:AI:130:ARG:HD3	54:D2:35:A:OP1	2.05	0.57
3:AC:7:PRO:O	3:AC:11:ARG:NH1	2.38	0.57
20:AT:81:ALA:O	20:AT:85:LYS:HG2	2.05	0.57
22:BA:2796:U:H2'	22:BA:2797:U:H2'	1.87	0.56
21:AU:31:GLU:HG3	21:AU:35:ARG:HE	1.70	0.56
22:BA:568:U:H1'	22:BA:2030:6MZ:H9C1	1.86	0.56
1:AA:718:A:O2'	21:AU:35:ARG:NH2	2.39	0.56
13:AM:9:ILE:HG12	27:BF:143:TYR:CE2	2.40	0.56
32:BK:88:ASN:ND2	32:BK:90:ASN:OD1	2.38	0.56
8:AH:77:ARG:NH1	8:AH:79:SER:O	2.39	0.56
10:AJ:45:ARG:NH2	10:AJ:47:GLU:OE1	2.38	0.56
22:BA:1392:A:N6	41:BT:18:GLU:OE1	2.38	0.56
26:BE:189:THR:HG22	26:BE:191:ASP:H	1.70	0.56
55:D3:51:U:H3	55:D3:63:G:H1	0.86	0.56
55:D3:16:H2U:HN3	55:D3:60:U:H1'	1.71	0.56
22:BA:882:G:N2	22:BA:883:G:N7	2.54	0.56
1:AA:500:G:H5''	12:AL:121:ARG:HH12	1.70	0.56
22:BA:2478:A:H5'	52:B4:32:LYS:HE2	1.88	0.56
22:BA:2131:U:H5'	22:BA:2132:U:H5''	1.88	0.56
22:BA:881:G:O6	22:BA:895:U:O4	2.24	0.56
22:BA:627:A:OP1	33:BL:78:ARG:NH1	2.39	0.55
1:AA:352:C:OP2	59:AA:1706:HOH:O	2.18	0.55
1:AA:929:G:C2	1:AA:1389:C:O2	2.60	0.55
5:AE:13:GLU:OE2	5:AE:68:ARG:NH2	2.39	0.55
22:BA:1607:C:N4	22:BA:1622:G:OP2	2.38	0.55
46:BY:49:ASP:OD1	46:BY:52:ARG:NH2	2.38	0.55
47:BZ:24:LEU:HD11	47:BZ:54:MET:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1308:U:H2'	1:AA:1309:G:H8	1.71	0.55
15:AO:64:ARG:HH12	15:AO:88:ARG:HD3	1.70	0.55
22:BA:2821:A:OP2	35:BN:3:HIS:NE2	2.40	0.55
3:AC:34:ASP:OD2	14:AN:65:ARG:NH1	2.39	0.55
22:BA:281:C:H2'	22:BA:282:A:H8	1.71	0.55
1:AA:1391:U:H2'	1:AA:1392:G:H8	1.71	0.55
19:AS:5:LEU:HD12	19:AS:5:LEU:C	2.32	0.55
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.24	0.55
1:AA:1291:U:H2'	1:AA:1292:G:H8	1.72	0.55
22:BA:404:A:N6	22:BA:421:C:O2'	2.40	0.55
22:BA:2109:U:OP1	22:BA:2149:U:O2'	2.24	0.55
25:BD:46:ARG:NH2	25:BD:88:GLU:O	2.39	0.55
13:AM:79:ARG:CZ	30:BI:56:ARG:HH21	2.16	0.55
27:BF:102:ARG:HG2	30:BI:24:ILE:HD12	1.88	0.55
54:D2:15:G:O6	54:D2:48:C:O2	2.25	0.55
55:D3:36:A:C2	56:D4:1:U:C5	2.94	0.55
22:BA:994:C:O2	39:BR:10:LYS:NZ	2.38	0.54
22:BA:2515:C:H2'	22:BA:2516:A:H8	1.72	0.54
9:AI:12:ARG:HG3	9:AI:13:LYS:H	1.72	0.54
14:AN:83:LYS:NZ	14:AN:86:GLU:OE1	2.39	0.54
28:BG:104:ASN:ND2	28:BG:114:ASP:OD1	2.41	0.54
40:BS:73:LYS:HB2	40:BS:106:VAL:HB	1.88	0.54
14:AN:26:LEU:HD23	14:AN:48:LEU:HD13	1.87	0.54
54:D2:51:A:H61	54:D2:63:C:H42	1.54	0.54
18:AR:34:THR:CG2	18:AR:35:GLU:H	2.14	0.54
19:AS:25:SER:HB2	19:AS:28:LYS:HZ1	1.73	0.54
22:BA:2278:A:OP1	34:BM:10:ARG:NH2	2.40	0.54
7:AG:151:PHE:CE1	11:AK:56:ARG:HG2	2.43	0.54
1:AA:464:U:N3	1:AA:466:A:OP2	2.41	0.54
7:AG:84:THR:HG21	55:D3:32:PSU:O2'	2.07	0.54
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.89	0.54
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.54
17:AQ:47:HIS:NE2	17:AQ:49:GLU:OE1	2.40	0.54
36:BO:31:THR:O	36:BO:102:ARG:NH1	2.33	0.54
3:AC:66:VAL:CG1	3:AC:101:ILE:HD13	2.38	0.54
5:AE:157:ARG:NH2	8:AH:99:LEU:O	2.41	0.54
7:AG:57:SER:O	7:AG:61:ALA:N	2.33	0.54
22:BA:880:G:H2'	22:BA:881:G:H8	1.72	0.54
1:AA:87:C:H2'	1:AA:88:U:H4'	1.90	0.54
22:BA:2267:A:H5''	22:BA:2268:A:H5'	1.89	0.54
1:AA:85:U:OP2	1:AA:86:G:N2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1027:C:N3	1:AA:1028:C:N4	2.56	0.53
19:AS:6:LYS:HZ1	30:BI:63:ARG:HD3	1.73	0.53
27:BF:105:THR:HA	30:BI:38:SER:HB2	1.90	0.53
10:AJ:63:ASP:OD2	14:AN:85:ARG:NH1	2.42	0.53
28:BG:107:LEU:O	28:BG:152:ARG:NH2	2.36	0.53
4:AD:54:GLN:HG2	4:AD:199:LEU:HD22	1.91	0.53
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	1.89	0.53
22:BA:2608:G:C6	53:D1:1:FME:HCN	2.43	0.53
1:AA:147:G:H2'	1:AA:148:G:C8	2.44	0.53
22:BA:275:C:H2'	22:BA:276:U:H4'	1.91	0.53
22:BA:2106:U:H2'	22:BA:2107:G:H8	1.74	0.53
22:BA:2756:U:OP2	52:B4:19:ARG:NE	2.39	0.53
55:D3:15:G:H5'	55:D3:16:H2U:H2'	1.90	0.53
3:AC:177:THR:O	3:AC:177:THR:OG1	2.26	0.53
16:AP:44:SER:O	16:AP:44:SER:OG	2.27	0.53
22:BA:1:G:H2'	22:BA:2:G:H8	1.74	0.53
1:AA:426:U:OP1	4:AD:36:GLN:NE2	2.42	0.52
10:AJ:35:GLN:N	10:AJ:78:GLU:OE1	2.41	0.52
19:AS:5:LEU:CD1	19:AS:7:LYS:N	2.61	0.52
1:AA:17:U:O4'	1:AA:1080:A:H1'	2.09	0.52
1:AA:673:A:H2'	1:AA:674:G:C8	2.45	0.52
1:AA:1074:G:H4'	2:AB:102:THR:O	2.09	0.52
4:AD:124:MET:HE3	4:AD:146:ARG:HG3	1.91	0.52
11:AK:23:ILE:HD11	11:AK:86:VAL:HG22	1.91	0.52
19:AS:12:ASP:OD1	19:AS:38:SER:OG	2.26	0.52
24:BC:260:ASN:ND2	24:BC:263:THR:OG1	2.37	0.52
25:BD:39:ASP:N	25:BD:39:ASP:OD1	2.41	0.52
1:AA:157:U:O2	1:AA:164:G:O6	2.28	0.52
22:BA:2608:G:O6	53:D1:1:FME:HCN	2.09	0.52
42:BU:4:LYS:O	42:BU:94:ARG:NH2	2.43	0.52
1:AA:486:U:H2'	1:AA:487:A:H8	1.75	0.52
27:BF:140:GLU:HA	30:BI:28:VAL:HG12	1.90	0.52
1:AA:108:G:H5'	1:AA:109:A:H5''	1.92	0.52
7:AG:63:GLU:OE2	7:AG:70:ARG:NH2	2.34	0.52
13:AM:9:ILE:HD13	27:BF:143:TYR:OH	2.10	0.52
23:BB:1:U:H2'	23:BB:2:G:H8	1.73	0.52
37:BP:88:ARG:NH2	37:BP:110:ILE:O	2.39	0.52
3:AC:114:LYS:NZ	3:AC:187:SER:OG	2.43	0.52
5:AE:111:MET:HE2	5:AE:127:ALA:HB2	1.90	0.52
22:BA:864:G:O2'	22:BA:914:G:O6	2.26	0.52
18:AR:34:THR:CG2	18:AR:35:GLU:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2532:G:N2	22:BA:2663:G:O2'	2.43	0.52
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.45	0.52
2:AB:214:LEU:HA	2:AB:217:VAL:HG12	1.92	0.52
28:BG:17:VAL:HG11	28:BG:50:LEU:HD21	1.92	0.52
1:AA:1297:G:O2'	7:AG:114:LYS:NZ	2.43	0.51
6:AF:14:GLN:HG3	6:AF:17:GLN:HG3	1.91	0.51
16:AP:50:THR:HG23	16:AP:50:THR:O	2.09	0.51
22:BA:619:G:OP2	22:BA:620:G:N2	2.43	0.51
22:BA:1365:A:OP1	45:BX:3:ARG:NH2	2.37	0.51
24:BC:162:VAL:HG11	24:BC:174:LEU:HD13	1.91	0.51
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.76	0.51
3:AC:148:GLY:HA3	3:AC:172:ARG:H	1.75	0.51
9:AI:18:ARG:HH11	9:AI:18:ARG:CG	2.24	0.51
1:AA:858:G:O6	59:AA:1705:HOH:O	2.18	0.51
22:BA:1801:A:OP2	24:BC:150:LYS:NZ	2.41	0.51
22:BA:1419:A:O2'	22:BA:1421:G:N7	2.41	0.51
22:BA:1469:A:H2'	22:BA:1470:A:C8	2.45	0.51
22:BA:444:C:OP1	26:BE:40:ARG:NH2	2.44	0.51
1:AA:108:G:C6	20:AT:10:ARG:HG2	2.45	0.51
22:BA:589:U:H2'	22:BA:590:A:H8	1.75	0.51
31:BJ:32:LEU:HD22	31:BJ:54:ILE:HG21	1.92	0.51
1:AA:494:G:H2'	1:AA:496:A:H8	1.76	0.51
1:AA:1390:U:H6	1:AA:1390:U:O5'	1.94	0.51
3:AC:70:THR:HG22	3:AC:72:ARG:H	1.75	0.51
9:AI:14:SER:O	9:AI:14:SER:OG	2.22	0.51
13:AM:106:ALA:HB3	13:AM:110:LYS:HD3	1.93	0.51
55:D3:36:A:N1	56:D4:1:U:C4	2.78	0.51
13:AM:7:ILE:HG21	27:BF:112:ARG:HG2	1.92	0.51
59:BA:3213:HOH:O	53:D1:1:FME:CE	2.58	0.51
1:AA:208:U:O4	1:AA:211:G:N2	2.44	0.51
14:AN:15:LEU:HD23	14:AN:54:ASP:HB2	1.94	0.50
22:BA:2667:C:N3	28:BG:110:SER:OG	2.40	0.50
27:BF:8:TYR:HA	27:BF:12:VAL:HB	1.93	0.50
46:BY:16:THR:O	46:BY:20:ASN:ND2	2.44	0.50
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.42	0.50
22:BA:24:G:O2'	40:BS:78:GLU:O	2.29	0.50
23:BB:1:U:H2'	23:BB:2:G:C8	2.46	0.50
26:BE:111:GLU:OE1	26:BE:114:ARG:NH1	2.44	0.50
54:D2:21:A:N6	54:D2:46:G7M:O2'	2.41	0.50
3:AC:156:ARG:H	3:AC:163:ALA:HA	1.76	0.50
19:AS:6:LYS:HZ1	30:BI:63:ARG:CD	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1078:U:O4'	5:AE:89:HIS:HE1	1.94	0.50
22:BA:196:A:OP2	33:BL:47:ARG:NH1	2.43	0.50
22:BA:617:G:OP1	26:BE:102:ARG:NH2	2.40	0.50
22:BA:1068:G:N2	22:BA:1095:A:O3'	2.40	0.50
14:AN:24:ALA:O	14:AN:28:ALA:N	2.45	0.50
26:BE:148:ILE:HB	26:BE:169:VAL:HG22	1.94	0.50
22:BA:1799:G:OP1	24:BC:258:ARG:NH1	2.35	0.50
42:BU:47:LYS:HD3	42:BU:48:PRO:HD2	1.94	0.50
54:D2:58:A:O2'	54:D2:60:U:OP2	2.26	0.50
12:AL:109:ASP:OD1	12:AL:109:ASP:N	2.40	0.50
22:BA:646:U:O2'	22:BA:647:G:O4'	2.28	0.50
26:BE:51:GLU:OE2	26:BE:88:ARG:NH1	2.45	0.50
45:BX:72:ARG:NH1	45:BX:78:TYR:OH	2.43	0.50
1:AA:626:G:O2'	16:AP:51:ARG:NH2	2.41	0.50
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.93	0.50
46:BY:3:ALA:HB2	46:BY:52:ARG:HD3	1.93	0.50
5:AE:13:GLU:HG2	5:AE:39:VAL:HG12	1.92	0.49
7:AG:76:LYS:HD2	7:AG:77:SER:H	1.77	0.49
11:AK:87:LYS:HE3	11:AK:113:VAL:HG13	1.95	0.49
22:BA:2720:U:OP1	37:BP:53:ARG:NH2	2.45	0.49
1:AA:255:G:O3'	17:AQ:19:LYS:NZ	2.42	0.49
1:AA:1144:G:N2	1:AA:1146:A:H62	2.10	0.49
3:AC:57:ILE:HG22	3:AC:66:VAL:CG2	2.40	0.49
55:D3:36:A:N1	56:D4:1:U:C5	2.80	0.49
1:AA:713:G:H2'	1:AA:714:G:C8	2.47	0.49
1:AA:1028:C:O2'	1:AA:1030:U:O4	2.29	0.49
1:AA:1135:U:O2'	1:AA:1138:G:O6	2.28	0.49
1:AA:1526:G:OP1	21:AU:45:ARG:NH2	2.45	0.49
9:AI:80:ARG:O	9:AI:84:THR:HG23	2.11	0.49
3:AC:83:ASP:HA	3:AC:86:LYS:HB3	1.94	0.49
22:BA:1432:G:H2'	22:BA:1433:A:C8	2.47	0.49
24:BC:66:ASP:OD2	24:BC:102:ARG:NH1	2.46	0.49
40:BS:33:LEU:O	40:BS:37:THR:OG1	2.29	0.49
1:AA:1037:C:H2'	1:AA:1038:C:H6	1.78	0.49
8:AH:54:ASP:OD1	8:AH:54:ASP:N	2.36	0.49
10:AJ:81:GLU:O	10:AJ:84:VAL:N	2.44	0.49
13:AM:43:VAL:CG1	13:AM:48:LEU:CG	2.90	0.49
41:BT:13:ALA:HB3	41:BT:33:LYS:HE3	1.95	0.49
4:AD:172:GLU:HB2	4:AD:181:THR:HB	1.95	0.49
10:AJ:45:ARG:HB3	10:AJ:69:THR:HG23	1.94	0.49
22:BA:1028:A:H2'	22:BA:1029:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1434:A:H2'	22:BA:1435:G:C8	2.47	0.49
22:BA:1568:G:H4'	24:BC:59:LYS:HB3	1.95	0.49
1:AA:618:C:H1'	16:AP:14:ARG:HH12	1.77	0.49
22:BA:281:C:H2'	22:BA:282:A:C8	2.48	0.49
58:BA:3001:ERY:O10	58:BA:3001:ERY:H11	2.13	0.49
34:BM:42:THR:HG22	34:BM:93:VAL:HG12	1.93	0.49
52:B4:16:ILE:HG12	52:B4:25:VAL:HG22	1.95	0.49
2:AB:32:PHE:HE2	2:AB:35:ARG:HH12	1.60	0.49
11:AK:23:ILE:HG13	11:AK:86:VAL:HA	1.95	0.49
14:AN:39:GLU:O	14:AN:43:ASN:HB2	2.12	0.49
22:BA:195:A:H61	22:BA:198:C:H3'	1.77	0.49
22:BA:631:A:OP2	51:B3:23:LYS:NZ	2.45	0.49
22:BA:2502:G:H5''	22:BA:2503:2MA:H5''	1.95	0.49
1:AA:208:U:C4	1:AA:211:G:N1	2.81	0.49
1:AA:532:A:C6	3:AC:193:TYR:HE1	2.30	0.49
13:AM:107:ARG:NH1	13:AM:111:GLY:O	2.46	0.49
22:BA:856:G:H2'	22:BA:857:G:C8	2.47	0.49
22:BA:2306:C:N4	27:BF:39:GLY:O	2.41	0.49
13:AM:43:VAL:HG11	13:AM:48:LEU:CG	2.43	0.49
19:AS:6:LYS:HD2	19:AS:6:LYS:HA	1.59	0.49
1:AA:1097:C:O3'	2:AB:139:ARG:NH2	2.45	0.48
12:AL:53:CYS:HB2	12:AL:67:ILE:HD11	1.94	0.48
22:BA:280:U:O4	22:BA:361:G:N2	2.46	0.48
22:BA:1636:U:H2'	22:BA:1637:A:C8	2.49	0.48
1:AA:1060:U:OP1	14:AN:85:ARG:NH2	2.46	0.48
16:AP:19:VAL:HG22	16:AP:37:GLY:C	2.39	0.48
22:BA:151:C:H2'	22:BA:152:A:H8	1.78	0.48
22:BA:1316:U:H2'	22:BA:1317:G:H8	1.78	0.48
22:BA:2134:A:O2'	22:BA:2159:G:N3	2.44	0.48
1:AA:208:U:N3	1:AA:211:G:C6	2.81	0.48
1:AA:208:U:C2	1:AA:211:G:O6	2.65	0.48
15:AO:89:ARG:NH1	22:BA:713:G:N7	2.61	0.48
20:AT:44:LYS:HB3	20:AT:87:ALA:HB3	1.94	0.48
19:AS:12:ASP:OD1	19:AS:12:ASP:N	2.44	0.48
22:BA:1173:U:O2'	22:BA:1174:U:O4'	2.30	0.48
1:AA:1175:G:H2'	1:AA:1176:A:H8	1.77	0.48
22:BA:2172:U:H4'	22:BA:2173:A:H5'	1.96	0.48
32:BK:23:LYS:HB3	32:BK:40:LYS:HB3	1.95	0.48
51:B3:31:HIS:C	51:B3:33:LEU:H	2.22	0.48
25:BD:25:THR:OG1	25:BD:191:GLY:O	2.30	0.48
1:AA:946:A:H2'	1:AA:947:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:14:ILE:HG22	3:AC:15:VAL:HG23	1.94	0.48
24:BC:155:ALA:HB2	24:BC:162:VAL:HG23	1.95	0.48
1:AA:490:C:H2'	1:AA:491:G:H8	1.79	0.48
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.79	0.48
25:BD:49:GLN:HE21	25:BD:79:LEU:HB3	1.77	0.48
1:AA:259:G:OP1	20:AT:36:TYR:OH	2.25	0.48
3:AC:132:ARG:HA	3:AC:135:LYS:HG2	1.95	0.48
22:BA:1322:A:H5''	40:BS:82:MET:HE1	1.95	0.48
22:BA:1386:C:H2'	22:BA:1387:A:C8	2.49	0.48
23:BB:79:G:N7	43:BV:14:LYS:NZ	2.58	0.48
28:BG:42:GLU:HA	28:BG:55:ARG:HH21	1.78	0.48
22:BA:172:A:H2'	22:BA:173:A:C8	2.49	0.48
22:BA:414:C:H2'	22:BA:415:A:C8	2.48	0.48
22:BA:463:G:N2	22:BA:466:A:OP2	2.39	0.48
22:BA:687:C:H1'	50:B2:4:THR:HG22	1.96	0.48
59:BA:3213:HOH:O	53:D1:1:FME:HE3	2.13	0.48
25:BD:184:ARG:HG3	25:BD:186:LEU:HG	1.94	0.48
27:BF:103:LEU:HA	27:BF:107:ALA:HB3	1.96	0.48
34:BM:64:TRP:HB2	34:BM:104:GLU:HB2	1.95	0.48
47:BZ:4:THR:HG21	47:BZ:37:GLU:HG3	1.95	0.48
7:AG:40:GLU:HA	7:AG:43:VAL:HG12	1.96	0.47
22:BA:2233:U:H2'	22:BA:2234:G:C8	2.49	0.47
29:BH:78:VAL:HG23	29:BH:144:VAL:HG23	1.95	0.47
22:BA:2305:U:H5''	27:BF:131:GLY:HA3	1.96	0.47
29:BH:116:ARG:HD3	29:BH:133:GLN:HG2	1.97	0.47
1:AA:664:G:H22	1:AA:741:G:H1	1.61	0.47
1:AA:486:U:H2'	1:AA:487:A:C8	2.49	0.47
14:AN:20:PHE:C	14:AN:22:LYS:H	2.21	0.47
18:AR:41:PRO:HG2	18:AR:44:ILE:HG12	1.96	0.47
22:BA:1791:A:N6	22:BA:1828:G:O2'	2.43	0.47
22:BA:2106:U:H2'	22:BA:2107:G:C8	2.49	0.47
22:BA:2183:A:H2'	22:BA:2184:A:C8	2.49	0.47
23:BB:5:U:OP1	23:BB:61:G:O2'	2.29	0.47
1:AA:1213:A:O2'	1:AA:1215:G:N7	2.39	0.47
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	1.96	0.47
13:AM:71:ARG:HH12	27:BF:115:ARG:NH2	2.07	0.47
22:BA:414:C:H2'	22:BA:415:A:H8	1.79	0.47
22:BA:2291:U:H2'	22:BA:2292:U:C6	2.49	0.47
46:BY:56:LEU:HA	46:BY:59:GLU:HG2	1.95	0.47
1:AA:216:U:H2'	1:AA:217:C:C6	2.49	0.47
1:AA:1005:A:H3'	1:AA:1006:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.49	0.47
1:AA:1493:A:H4'	56:D4:7:U:H6	1.79	0.47
22:BA:597:G:O2'	33:BL:11:GLY:O	2.26	0.47
1:AA:17:U:C1'	1:AA:1080:A:H1'	2.44	0.47
1:AA:79:G:H2'	1:AA:80:A:H8	1.79	0.47
1:AA:865:A:H5'	1:AA:1078:U:O4	2.14	0.47
5:AE:34:THR:HG22	5:AE:52:LYS:HG2	1.97	0.47
22:BA:1796:U:H2'	22:BA:1797:G:H8	1.79	0.47
22:BA:1864:U:OP1	22:BA:2410:G:O2'	2.28	0.47
22:BA:2547:A:H2'	22:BA:2548:U:C6	2.50	0.47
26:BE:16:GLU:O	26:BE:20:GLY:N	2.47	0.47
43:BV:40:ILE:HD12	43:BV:42:LEU:HD21	1.96	0.47
54:D2:15:G:N1	54:D2:48:C:N3	2.45	0.47
55:D3:8:4SU:HN3	55:D3:14:A:H62	1.62	0.47
3:AC:63:SER:OG	3:AC:64:ILE:N	2.48	0.47
9:AI:30:ILE:HG23	9:AI:65:ILE:HB	1.96	0.47
42:BU:88:GLU:HG2	42:BU:93:VAL:HG11	1.97	0.47
55:D3:16:H2U:H4'	55:D3:18:G:OP2	2.15	0.47
4:AD:95:GLU:HA	4:AD:100:ASN:ND2	2.30	0.47
22:BA:155:A:H2'	22:BA:156:A:C8	2.50	0.47
22:BA:249:C:O2	51:B3:12:LYS:NZ	2.47	0.47
22:BA:1592:C:H2'	22:BA:1593:A:C8	2.49	0.47
38:BQ:97:ASP:OD2	39:BR:13:ARG:NH2	2.40	0.47
41:BT:54:GLU:HB3	41:BT:88:LYS:HD2	1.97	0.47
49:B1:11:LEU:HB3	49:B1:49:TYR:HB3	1.96	0.47
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.50	0.47
14:AN:63:ARG:NH1	14:AN:68:GLY:O	2.47	0.47
22:BA:1667:G:O2'	22:BA:1991:U:O4	2.26	0.47
22:BA:2127:G:H2'	22:BA:2128:G:C8	2.50	0.47
42:BU:28:VAL:HG22	42:BU:34:VAL:HG12	1.97	0.47
3:AC:22:TRP:NE1	3:AC:36:ASP:OD2	2.46	0.46
8:AH:40:LEU:HD21	8:AH:129:VAL:HG21	1.97	0.46
22:BA:674:G:H1'	26:BE:69:ARG:HD3	1.96	0.46
24:BC:5:LYS:HG3	24:BC:17:VAL:HG22	1.96	0.46
24:BC:133:ARG:HB3	24:BC:186:ALA:HB1	1.97	0.46
1:AA:382:A:H2'	1:AA:383:A:C8	2.50	0.46
1:AA:481:G:O2'	1:AA:483:C:N4	2.45	0.46
1:AA:1106:G:H2'	1:AA:1107:C:C6	2.50	0.46
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.96	0.46
22:BA:2246:G:H2'	22:BA:2247:A:C8	2.50	0.46
6:AF:1:MET:HE2	6:AF:67:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:68:ARG:HD3	29:BH:134:VAL:HG21	1.98	0.46
1:AA:1124:G:H5''	10:AJ:37:ARG:HD2	1.96	0.46
3:AC:138:VAL:HG21	3:AC:168:TYR:HD2	1.80	0.46
4:AD:8:LYS:HG2	4:AD:21:LEU:HD12	1.98	0.46
7:AG:78:ARG:NH1	7:AG:87:VAL:HG21	2.30	0.46
22:BA:917:A:H5''	22:BA:2268:A:H61	1.80	0.46
22:BA:1434:A:H2'	22:BA:1435:G:H8	1.80	0.46
52:B4:15:LYS:HB3	52:B4:15:LYS:HE2	1.70	0.46
1:AA:920:U:O4'	1:AA:1080:A:N1	2.49	0.46
8:AH:22:LYS:O	8:AH:65:TYR:OH	2.23	0.46
13:AM:66:GLU:O	13:AM:69:LEU:N	2.48	0.46
22:BA:589:U:H2'	22:BA:590:A:C8	2.50	0.46
22:BA:1476:U:H2'	22:BA:1477:A:H8	1.80	0.46
4:AD:167:LYS:HA	4:AD:167:LYS:HD3	1.67	0.46
8:AH:27:MET:HE2	8:AH:27:MET:HB3	1.81	0.46
22:BA:288:U:H2'	22:BA:289:G:H8	1.81	0.46
1:AA:204:G:H2'	1:AA:205:A:C4	2.51	0.46
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.48	0.46
7:AG:79:ARG:CG	7:AG:79:ARG:NH2	2.73	0.46
22:BA:2167:U:N3	22:BA:2170:A:OP2	2.43	0.46
1:AA:1078:U:C6	5:AE:90:THR:HG21	2.50	0.46
8:AH:90:ASP:OD1	8:AH:90:ASP:N	2.36	0.46
17:AQ:54:GLY:N	17:AQ:57:ASP:OD2	2.48	0.46
22:BA:1:G:H2'	22:BA:2:G:C8	2.49	0.46
22:BA:639:U:H2'	22:BA:640:C:C6	2.50	0.46
22:BA:659:G:O2'	26:BE:95:LYS:O	2.33	0.46
22:BA:1156:A:C8	38:BQ:51:ARG:HG2	2.51	0.46
27:BF:44:ILE:HG21	27:BF:79:ILE:HG22	1.98	0.46
28:BG:47:ASP:OD1	28:BG:47:ASP:N	2.49	0.46
1:AA:1098:C:P	2:AB:139:ARG:HH22	2.39	0.46
13:AM:79:ARG:NH2	30:BI:56:ARG:HH22	2.13	0.46
22:BA:2328:A:H2'	22:BA:2329:U:C6	2.51	0.46
35:BN:79:LEU:HD23	35:BN:83:LEU:HD12	1.98	0.46
1:AA:1238:A:OP1	1:AA:1335:U:O2'	2.25	0.46
10:AJ:30:LYS:HE3	10:AJ:36:VAL:HG22	1.99	0.46
11:AK:35:THR:OG1	11:AK:36:ASP:N	2.49	0.46
22:BA:1570:A:H2'	22:BA:1571:A:C8	2.50	0.46
1:AA:521:G:OP2	12:AL:51:LYS:NZ	2.49	0.45
22:BA:1590:A:H2'	22:BA:1591:A:C8	2.51	0.45
34:BM:18:ARG:HE	34:BM:18:ARG:HB3	1.61	0.45
13:AM:44:LYS:O	13:AM:48:LEU:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:11:ILE:HG13	19:AS:38:SER:HB3	1.97	0.45
22:BA:285:G:H1	22:BA:355:U:H3	1.64	0.45
58:BA:3001:ERY:O8	58:BA:3001:ERY:H293	2.16	0.45
48:B0:38:HIS:ND1	48:B0:39:LEU:O	2.50	0.45
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.98	0.45
1:AA:1021:A:H2'	1:AA:1022:A:C8	2.51	0.45
1:AA:1027:C:O2	1:AA:1034:G:N1	2.50	0.45
12:AL:43:LYS:HD3	12:AL:91:PRO:HG3	1.98	0.45
3:AC:164:ARG:NH1	3:AC:166:GLU:OE2	2.49	0.45
22:BA:1275:A:OP2	22:BA:1646:C:N4	2.45	0.45
13:AM:8:ASN:ND2	13:AM:23:TYR:H	2.14	0.45
15:AO:24:SER:OG	15:AO:26:GLU:OE1	2.35	0.45
22:BA:1571:A:H2'	22:BA:1572:A:C8	2.52	0.45
22:BA:2189:U:H2'	22:BA:2190:G:H8	1.81	0.45
1:AA:720:C:H5''	18:AR:41:PRO:HB3	1.99	0.45
22:BA:906:U:HO2'	34:BM:66:ARG:HH21	1.61	0.45
33:BL:64:PHE:HB3	51:B3:25:LYS:HD3	1.98	0.45
1:AA:1086:U:H3	1:AA:1099:G:H1	1.65	0.45
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.17	0.45
19:AS:5:LEU:HD11	19:AS:7:LYS:HB2	1.96	0.45
22:BA:2273:A:H2'	22:BA:2274:A:C8	2.51	0.45
26:BE:83:VAL:HB	26:BE:86:ALA:HB2	1.97	0.45
30:BI:14:ALA:O	30:BI:22:MET:N	2.50	0.45
49:B1:17:THR:HG22	49:B1:19:HIS:H	1.81	0.45
1:AA:407:U:H2'	1:AA:408:A:C8	2.51	0.45
1:AA:492:C:H2'	1:AA:493:A:C8	2.52	0.45
1:AA:1175:G:H2'	1:AA:1176:A:C8	2.52	0.45
22:BA:151:C:H2'	22:BA:152:A:C8	2.52	0.45
22:BA:286:U:H2'	22:BA:287:G:H8	1.81	0.45
22:BA:721:A:H2'	22:BA:722:A:C8	2.51	0.45
22:BA:1590:A:H2'	22:BA:1591:A:H8	1.81	0.45
22:BA:1964:G:O2'	22:BA:1967:C:OP2	2.30	0.45
22:BA:2619:C:H5''	25:BD:157:LYS:HG2	1.99	0.45
33:BL:20:GLY:HA2	33:BL:28:GLY:HA2	1.99	0.45
55:D3:62:C:H2'	55:D3:63:G:C8	2.48	0.45
1:AA:723:U:OP1	21:AU:55:ARG:NH1	2.34	0.45
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.52	0.45
9:AI:55:VAL:HG22	9:AI:94:LEU:HD22	1.99	0.45
19:AS:30:PRO:HA	19:AS:48:THR:O	2.17	0.45
22:BA:1013:C:H2'	22:BA:1014:A:H8	1.82	0.45
24:BC:157:SER:OG	24:BC:158:ALA:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:55:VAL:HG12	9:AI:57:MET:HG2	1.98	0.45
22:BA:277:G:H4'	22:BA:278:A:C5	2.52	0.45
22:BA:307:G:N1	22:BA:310:A:OP2	2.45	0.45
22:BA:2898:U:H2'	22:BA:2899:A:C8	2.53	0.45
31:BJ:8:PRO:HG3	31:BJ:48:VAL:HG13	1.98	0.45
41:BT:68:LYS:HG3	41:BT:77:ARG:HH21	1.82	0.45
54:D2:23:A:H2'	54:D2:24:G:C8	2.52	0.45
1:AA:1326:U:H2'	1:AA:1327:C:C6	2.53	0.44
10:AJ:11:LYS:HA	10:AJ:70:HIS:O	2.17	0.44
22:BA:545:U:O2'	22:BA:546:U:O4'	2.34	0.44
45:BX:43:GLU:OE1	45:BX:45:ARG:NH2	2.49	0.44
9:AI:34:SER:OG	9:AI:35:LEU:N	2.50	0.44
22:BA:239:C:HO2'	22:BA:622:G:HO2'	1.61	0.44
22:BA:668:A:H2'	22:BA:670:A:H62	1.82	0.44
27:BF:22:TYR:OH	27:BF:165:GLU:OE2	2.27	0.44
37:BP:87:LYS:HA	37:BP:87:LYS:HD3	1.83	0.44
7:AG:23:LEU:HD23	7:AG:23:LEU:HA	1.69	0.44
3:AC:57:ILE:H	3:AC:57:ILE:HG12	1.58	0.44
6:AF:97:THR:N	6:AF:98:GLU:OE1	2.48	0.44
9:AI:7:TYR:CE1	9:AI:18:ARG:HB2	2.44	0.44
22:BA:2579:C:O2'	25:BD:136:ASN:OD1	2.34	0.44
46:BY:9:LYS:HD3	46:BY:13:GLU:HG2	1.99	0.44
3:AC:66:VAL:O	3:AC:66:VAL:HG13	2.18	0.44
15:AO:89:ARG:HH22	22:BA:712:G:H3'	1.83	0.44
22:BA:397:U:OP2	45:BX:10:LYS:NZ	2.42	0.44
34:BM:58:LYS:O	34:BM:60:GLN:NE2	2.38	0.44
51:B3:31:HIS:O	51:B3:33:LEU:N	2.51	0.44
55:D3:60:U:H5''	55:D3:61:C:H5	1.83	0.44
1:AA:1037:C:H2'	1:AA:1038:C:C6	2.53	0.44
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.17	0.44
8:AH:3:MET:HE2	8:AH:3:MET:HB3	1.82	0.44
6:AF:10:VAL:HB	6:AF:58:HIS:HB3	2.00	0.44
10:AJ:37:ARG:HA	10:AJ:37:ARG:HD3	1.85	0.44
22:BA:581:C:H2'	22:BA:582:A:C8	2.52	0.44
22:BA:2141:G:H2'	22:BA:2142:A:C8	2.52	0.44
22:BA:2655:G:O2'	22:BA:2664:G:O6	2.33	0.44
55:D3:16:H2U:N3	55:D3:60:U:H1'	2.33	0.44
1:AA:1098:C:OP1	2:AB:139:ARG:NH2	2.50	0.44
1:AA:1308:U:H2'	1:AA:1309:G:C8	2.52	0.44
3:AC:64:ILE:HG22	3:AC:97:VAL:HG23	1.99	0.44
3:AC:148:GLY:HA2	3:AC:171:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:78:GLU:OE2	4:AD:81:ARG:NH2	2.39	0.44
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.99	0.44
10:AJ:35:GLN:H	10:AJ:78:GLU:CD	2.26	0.44
17:AQ:57:ASP:OD1	17:AQ:82:ALA:N	2.50	0.44
22:BA:1266:G:O2'	22:BA:2012:G:O6	2.30	0.44
22:BA:1412:U:H2'	22:BA:1413:A:C8	2.53	0.44
22:BA:1802:A:H2'	22:BA:1803:A:C8	2.53	0.44
1:AA:736:C:H2'	1:AA:737:C:C6	2.53	0.44
1:AA:999:C:H2'	1:AA:1000:A:C8	2.53	0.44
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.53	0.44
23:BB:66:A:OP2	23:BB:108:A:N6	2.50	0.44
1:AA:294:U:OP1	1:AA:610:U:O2'	2.26	0.43
1:AA:1072:G:OP1	5:AE:62:LYS:NZ	2.51	0.43
7:AG:79:ARG:NH2	7:AG:79:ARG:HG3	2.33	0.43
9:AI:129:LYS:HE3	9:AI:129:LYS:HB2	1.78	0.43
22:BA:1386:C:H2'	22:BA:1387:A:H8	1.84	0.43
22:BA:1729:U:O2	22:BA:1731:G:N2	2.44	0.43
29:BH:14:SER:N	29:BH:17:ASP:OD2	2.44	0.43
29:BH:69:ALA:O	29:BH:73:ASN:N	2.48	0.43
54:D2:1:G:H2'	54:D2:2:G:H8	1.83	0.43
1:AA:1375:A:P	7:AG:28:ASN:HD22	2.41	0.43
12:AL:44:LYS:HD2	12:AL:44:LYS:HA	1.85	0.43
13:AM:113:ARG:H	13:AM:113:ARG:HG2	1.62	0.43
22:BA:155:A:H2'	22:BA:156:A:H8	1.83	0.43
22:BA:500:G:N1	22:BA:503:A:OP2	2.48	0.43
22:BA:1101:U:H2'	22:BA:1102:C:C6	2.53	0.43
22:BA:1278:C:H2'	22:BA:1279:G:H8	1.83	0.43
22:BA:2107:G:O6	22:BA:2182:U:O4	2.35	0.43
23:BB:49:C:H2'	23:BB:50:A:C8	2.53	0.43
55:D3:36:A:H2	56:D4:1:U:H5	1.61	0.43
1:AA:928:G:C2	1:AA:1390:U:O2	2.70	0.43
6:AF:9:MET:HE2	6:AF:9:MET:HB3	1.79	0.43
6:AF:18:VAL:HG21	6:AF:58:HIS:CD2	2.53	0.43
10:AJ:47:GLU:OE2	14:AN:76:LYS:NZ	2.50	0.43
14:AN:33:VAL:HG13	14:AN:41:ARG:HH12	1.83	0.43
22:BA:743:A:O2'	22:BA:1659:G:OP1	2.32	0.43
22:BA:1651:G:H4'	35:BN:39:PRO:HG2	2.00	0.43
1:AA:458:U:H2'	1:AA:459:A:H8	1.83	0.43
11:AK:22:HIS:HD2	11:AK:85:MET:HB2	1.84	0.43
17:AQ:59:VAL:HG21	17:AQ:75:LEU:HD11	2.00	0.43
35:BN:117:ASP:OD1	35:BN:117:ASP:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:12:ARG:HD2	9:AI:12:ARG:HA	1.78	0.43
22:BA:848:C:H2'	22:BA:849:A:H8	1.83	0.43
55:D3:35:A:N6	56:D4:2:U:C4	2.70	0.43
1:AA:746:A:H2'	1:AA:747:A:C8	2.53	0.43
3:AC:54:ARG:HB3	3:AC:69:HIS:HB2	2.01	0.43
13:AM:79:ARG:HH22	30:BI:56:ARG:HH22	1.67	0.43
22:BA:288:U:H2'	22:BA:289:G:C8	2.54	0.43
22:BA:581:C:H2'	22:BA:582:A:H8	1.83	0.43
22:BA:720:U:H2'	22:BA:721:A:C8	2.54	0.43
22:BA:1734:G:H2'	22:BA:1735:A:H8	1.83	0.43
26:BE:41:GLN:NE2	26:BE:43:THR:OG1	2.37	0.43
28:BG:158:LYS:HB2	28:BG:160:LYS:HG3	2.01	0.43
1:AA:18:C:H5'	1:AA:1079:G:H1'	1.99	0.43
1:AA:1286:U:O2'	1:AA:1287:A:H5'	2.19	0.43
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.53	0.43
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.18	0.43
22:BA:172:A:H2'	22:BA:173:A:H8	1.83	0.43
22:BA:1796:U:H2'	22:BA:1797:G:C8	2.53	0.43
22:BA:2291:U:OP1	22:BA:2380:C:O2'	2.35	0.43
54:D2:1:G:H2'	54:D2:2:G:C8	2.54	0.43
54:D2:23:A:H2'	54:D2:24:G:H8	1.84	0.43
1:AA:356:A:N3	1:AA:368:U:O2'	2.39	0.43
1:AA:674:G:H2'	1:AA:675:A:C8	2.54	0.43
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.48	0.43
2:AB:94:HIS:CE1	2:AB:146:ASN:HB2	2.54	0.43
10:AJ:36:VAL:HG12	10:AJ:76:ILE:HG13	2.01	0.43
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.58	0.43
13:AM:2:ALA:HB1	13:AM:53:ILE:HG12	2.01	0.43
19:AS:5:LEU:CD1	19:AS:7:LYS:CB	2.93	0.43
29:BH:135:HIS:CG	29:BH:136:SER:H	2.37	0.43
2:AB:70:VAL:HB	2:AB:163:VAL:HG22	2.00	0.43
10:AJ:52:LEU:HD11	10:AJ:59:LYS:HD2	2.01	0.43
22:BA:1794:A:H2'	22:BA:1795:C:C6	2.54	0.43
2:AB:159:ASP:OD1	2:AB:159:ASP:N	2.51	0.43
3:AC:66:VAL:HG13	3:AC:101:ILE:HD13	1.99	0.43
11:AK:87:LYS:HG3	11:AK:115:PRO:HD3	2.00	0.43
22:BA:538:A:H4'	31:BJ:7:LYS:HG2	2.00	0.43
3:AC:114:LYS:HA	3:AC:114:LYS:HD2	1.84	0.42
7:AG:37:SER:HA	7:AG:40:GLU:HG2	2.00	0.42
22:BA:438:G:H2'	22:BA:439:A:C8	2.55	0.42
22:BA:2515:C:H2'	22:BA:2516:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BL:57:LEU:HD22	51:B3:54:ASP:HB3	2.01	0.42
1:AA:1027:C:H2'	1:AA:1028:C:C6	2.54	0.42
4:AD:107:PHE:CG	4:AD:145:ILE:HD11	2.54	0.42
7:AG:15:ASP:OD1	7:AG:44:TYR:OH	2.27	0.42
24:BC:21:ASN:HB3	24:BC:24:LEU:HD13	2.01	0.42
39:BR:1:MET:HE3	39:BR:101:ILE:HB	2.01	0.42
1:AA:447:G:N1	1:AA:486:U:OP2	2.38	0.42
3:AC:132:ARG:HA	3:AC:135:LYS:HE2	2.01	0.42
5:AE:150:PRO:HB2	5:AE:164:ILE:HG23	2.01	0.42
13:AM:22:ILE:HB	13:AM:25:VAL:HG22	2.01	0.42
22:BA:598:U:H2'	22:BA:599:A:H8	1.84	0.42
22:BA:837:C:N3	22:BA:941:A:N6	2.67	0.42
22:BA:930:G:H1'	47:BZ:25:LEU:HD21	2.01	0.42
22:BA:956:G:N7	34:BM:14:LYS:NZ	2.66	0.42
22:BA:1058:U:H2'	22:BA:1059:G:C8	2.54	0.42
22:BA:1869:G:N2	22:BA:1871:A:O2'	2.51	0.42
22:BA:2529:G:H4'	28:BG:175:LYS:HD2	2.01	0.42
29:BH:80:ILE:HB	29:BH:146:VAL:HG12	2.01	0.42
46:BY:2:LYS:HD2	46:BY:6:LEU:HD21	2.00	0.42
55:D3:35:A:N6	56:D4:2:U:H3	2.17	0.42
1:AA:458:U:H2'	1:AA:459:A:C8	2.55	0.42
1:AA:1032:G:C5	1:AA:1033:G:H1'	2.54	0.42
1:AA:1338:G:H2'	1:AA:1339:A:C4	2.55	0.42
10:AJ:66:GLU:HB3	14:AN:99:ALA:HB2	2.01	0.42
22:BA:598:U:H2'	22:BA:599:A:C8	2.54	0.42
22:BA:1672:A:C2	22:BA:2582:G:H5'	2.55	0.42
22:BA:2291:U:O2'	22:BA:2374:C:O2	2.38	0.42
26:BE:21:ARG:HD3	26:BE:106:LYS:HB3	2.02	0.42
37:BP:100:LEU:HD11	37:BP:110:ILE:HD11	2.00	0.42
39:BR:16:GLU:HG3	39:BR:101:ILE:HG12	2.01	0.42
1:AA:936:C:C2	1:AA:937:A:C8	3.07	0.42
4:AD:105:MET:HE3	4:AD:107:PHE:CE2	2.54	0.42
1:AA:299:G:H2'	1:AA:300:A:C8	2.54	0.42
1:AA:921:U:H5''	1:AA:1082:A:OP1	2.20	0.42
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.54	0.42
1:AA:1316:G:H22	1:AA:1319:A:H5''	1.84	0.42
2:AB:126:PHE:CZ	2:AB:137:ARG:HD2	2.54	0.42
3:AC:33:LEU:HD11	14:AN:93:ILE:HD13	2.01	0.42
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.02	0.42
22:BA:742:A:H2'	22:BA:743:A:C8	2.54	0.42
22:BA:1847:A:O2'	22:BA:1848:A:H8	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2052:A:O2'	25:BD:148:GLN:O	2.34	0.42
47:BZ:23:THR:HG23	47:BZ:47:MET:HG2	2.02	0.42
1:AA:925:G:C6	1:AA:1392:G:C6	3.07	0.42
22:BA:197:A:H62	22:BA:2430:A:H2'	1.84	0.42
22:BA:911:A:N6	34:BM:11:LYS:O	2.52	0.42
58:BA:3001:ERY:H353	58:BA:3001:ERY:H10	1.76	0.42
40:BS:24:ILE:HD13	40:BS:36:LEU:HD11	2.00	0.42
1:AA:56:U:H2'	1:AA:57:G:C8	2.54	0.42
9:AI:61:LEU:HD13	9:AI:61:LEU:HA	1.87	0.42
22:BA:242:G:O2'	22:BA:254:G:O6	2.35	0.42
22:BA:962:G:P	59:BA:3202:HOH:O	2.75	0.42
28:BG:85:LYS:HE2	28:BG:85:LYS:HB2	1.96	0.42
41:BT:17:SER:OG	41:BT:18:GLU:N	2.52	0.42
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.55	0.42
22:BA:372:G:OP2	45:BX:62:LYS:NZ	2.43	0.42
22:BA:1105:U:H2'	22:BA:1106:G:H8	1.84	0.42
22:BA:1326:U:H2'	22:BA:1327:A:H8	1.85	0.42
24:BC:133:ARG:NH2	24:BC:187:ASP:OD1	2.53	0.42
34:BM:38:ARG:HB3	34:BM:98:PRO:HD3	2.02	0.42
39:BR:60:LYS:O	39:BR:99:THR:OG1	2.36	0.42
1:AA:88:U:H1'	1:AA:89:U:H5	1.85	0.42
1:AA:950:U:H2'	1:AA:951:G:C8	2.55	0.42
1:AA:1130:A:H2'	1:AA:1131:G:H8	1.85	0.42
6:AF:2:ARG:HD3	6:AF:91:ARG:HE	1.84	0.42
9:AI:10:GLY:HA2	9:AI:81:HIS:ND1	2.35	0.42
11:AK:87:LYS:HB2	11:AK:113:VAL:HG13	2.00	0.42
17:AQ:68:SER:HB3	17:AQ:71:LYS:HB2	2.02	0.42
22:BA:1914:C:H2'	22:BA:1915:3TD:H6	2.01	0.42
22:BA:2100:G:H4'	22:BA:2100:G:OP1	2.19	0.42
55:D3:61:C:H2'	55:D3:62:C:C6	2.55	0.42
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.54	0.41
3:AC:49:LYS:HD3	3:AC:49:LYS:HA	1.91	0.41
6:AF:100:SER:O	6:AF:104:LYS:HG2	2.20	0.41
8:AH:108:LYS:HD3	8:AH:108:LYS:HA	1.86	0.41
13:AM:43:VAL:CG2	13:AM:48:LEU:CG	2.98	0.41
18:AR:37:GLY:O	18:AR:63:ARG:NH2	2.50	0.41
22:BA:1429:G:H2'	22:BA:1430:G:H8	1.85	0.41
22:BA:1808:A:H3'	22:BA:1809:A:C8	2.55	0.41
22:BA:1851:U:O2'	55:D3:71:G:O2'	2.34	0.41
22:BA:2418:A:OP1	51:B3:45:ARG:NH1	2.48	0.41
35:BN:106:ASP:OD1	35:BN:106:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:10:ILE:HD12	3:AC:10:ILE:HA	1.83	0.41
13:AM:107:ARG:NH2	13:AM:110:LYS:HE2	2.35	0.41
22:BA:494:G:H4'	40:BS:6:LYS:HB2	2.02	0.41
22:BA:1645:G:H5''	22:BA:1646:C:H5'	2.02	0.41
22:BA:2179:C:H2'	22:BA:2180:U:H6	1.84	0.41
29:BH:100:ALA:HA	29:BH:103:VAL:HG12	2.01	0.41
1:AA:79:G:H2'	1:AA:80:A:C8	2.55	0.41
1:AA:235:C:H2'	1:AA:236:A:C8	2.56	0.41
1:AA:254:G:OP1	17:AQ:68:SER:OG	2.36	0.41
1:AA:1166:G:H22	1:AA:1169:A:H5''	1.85	0.41
3:AC:19:ASN:O	3:AC:40:ARG:NH2	2.52	0.41
13:AM:79:ARG:HH12	30:BI:56:ARG:NH2	2.17	0.41
22:BA:4:U:H2'	22:BA:5:A:H8	1.85	0.41
22:BA:1316:U:H2'	22:BA:1317:G:C8	2.54	0.41
22:BA:1682:G:H2'	22:BA:1683:U:C6	2.55	0.41
22:BA:2567:G:H2'	22:BA:2568:U:C6	2.55	0.41
32:BK:17:ARG:HD3	32:BK:17:ARG:HA	1.88	0.41
32:BK:121:GLU:OE1	37:BP:65:SER:OG	2.29	0.41
1:AA:920:U:O4'	1:AA:1080:A:C2	2.74	0.41
1:AA:935:A:O2'	1:AA:1383:C:O2	2.38	0.41
13:AM:113:ARG:HH11	13:AM:113:ARG:HD3	1.75	0.41
15:AO:29:VAL:O	15:AO:33:THR:HG23	2.20	0.41
22:BA:566:U:H5''	33:BL:29:LYS:HE3	2.02	0.41
54:D2:37:T6A:N1	54:D2:37:T6A:N11	2.69	0.41
1:AA:253:A:O2'	17:AQ:17:MET:SD	2.77	0.41
1:AA:927:G:OP1	1:AA:1505:G:N2	2.42	0.41
2:AB:119:THR:O	2:AB:124:GLY:N	2.41	0.41
13:AM:7:ILE:CD1	27:BF:112:ARG:HB3	2.50	0.41
22:BA:26:G:H1'	22:BA:514:A:N6	2.36	0.41
22:BA:1476:U:H2'	22:BA:1477:A:C8	2.55	0.41
1:AA:588:G:P	59:AA:1711:HOH:O	2.78	0.41
1:AA:1380:U:O2'	7:AG:3:ARG:NH1	2.46	0.41
7:AG:86:GLN:NE2	7:AG:148:ASN:OD1	2.54	0.41
22:BA:145:C:H2'	22:BA:146:A:C8	2.56	0.41
22:BA:698:C:O2'	22:BA:734:A:N6	2.54	0.41
22:BA:1992:G:N2	22:BA:1996:C:O2'	2.53	0.41
22:BA:2898:U:H2'	22:BA:2899:A:H8	1.85	0.41
27:BF:147:ASP:OD1	27:BF:147:ASP:N	2.53	0.41
4:AD:9:LEU:HD23	4:AD:22:LYS:HD2	2.03	0.41
4:AD:22:LYS:HD3	4:AD:31:LYS:HE2	2.03	0.41
10:AJ:28:THR:HA	10:AJ:31:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:39:ILE:HD13	13:AM:56:LEU:HD21	2.03	0.41
22:BA:83:A:OP1	42:BU:92:LYS:NZ	2.41	0.41
22:BA:195:A:H8	59:BA:3391:HOH:O	1.99	0.41
22:BA:363:G:H2'	22:BA:364:C:C6	2.56	0.41
22:BA:1071:G:N2	22:BA:1091:G:OP2	2.54	0.41
22:BA:1300:G:H4'	22:BA:1301:A:H5''	2.02	0.41
28:BG:7:ALA:HA	28:BG:8:PRO:HD3	1.95	0.41
54:D2:50:C:H2'	54:D2:51:A:C8	2.56	0.41
1:AA:744:C:H2'	1:AA:745:G:C8	2.56	0.41
1:AA:1004:A:N6	1:AA:1025:U:OP1	2.52	0.41
1:AA:1026:G:H22	1:AA:1034:G:H1	1.69	0.41
7:AG:47:LEU:HD23	7:AG:47:LEU:HA	1.91	0.41
22:BA:1353:A:H2'	22:BA:1354:A:C8	2.56	0.41
22:BA:1548:A:H2'	22:BA:1549:A:C8	2.55	0.41
26:BE:176:ASP:OD1	26:BE:179:SER:OG	2.30	0.41
41:BT:69:ARG:NH1	41:BT:72:GLN:O	2.54	0.41
1:AA:1016:A:O2'	1:AA:1217:C:O2'	2.35	0.41
1:AA:1020:G:H8	1:AA:1020:G:OP2	2.03	0.41
1:AA:1119:C:H2'	1:AA:1120:C:H6	1.86	0.41
6:AF:38:ARG:HG2	6:AF:63:ASN:HB2	2.02	0.41
7:AG:60:GLU:OE1	7:AG:60:GLU:N	2.54	0.41
9:AI:107:ASP:OD2	9:AI:109:ARG:NH1	2.53	0.41
10:AJ:40:ILE:HG13	10:AJ:73:LEU:HB3	2.01	0.41
22:BA:1683:U:H2'	22:BA:1684:G:H8	1.85	0.41
22:BA:2243:U:H2'	22:BA:2244:U:C6	2.56	0.41
22:BA:2329:U:H2'	22:BA:2330:G:C8	2.56	0.41
27:BF:64:LYS:HA	27:BF:65:PRO:HD3	1.91	0.41
1:AA:500:G:H2'	1:AA:501:C:C6	2.56	0.41
1:AA:1011:C:H2'	1:AA:1012:A:H8	1.85	0.41
1:AA:1023:U:H2'	1:AA:1024:G:N3	2.36	0.41
1:AA:1048:G:OP1	14:AN:3:GLN:HB2	2.21	0.41
2:AB:128:LYS:HB2	2:AB:128:LYS:HE2	1.82	0.41
15:AO:32:LEU:HD23	15:AO:32:LEU:HA	1.88	0.41
15:AO:67:LEU:HD23	15:AO:67:LEU:HA	1.86	0.41
17:AQ:29:VAL:O	17:AQ:37:PHE:HA	2.21	0.41
22:BA:1734:G:H2'	22:BA:1735:A:C8	2.56	0.41
25:BD:109:VAL:HG22	25:BD:203:VAL:HG13	2.03	0.41
43:BV:4:ILE:HG12	43:BV:50:MET:HE1	2.02	0.41
46:BY:19:LEU:HD23	46:BY:19:LEU:HA	1.94	0.41
1:AA:384:G:H2'	1:AA:385:C:C6	2.56	0.40
1:AA:821:G:H2'	1:AA:822:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1016:A:HO2'	1:AA:1217:C:HO2'	1.62	0.40
1:AA:1188:A:H2'	1:AA:1189:U:O4'	2.21	0.40
22:BA:848:C:H2'	22:BA:849:A:C8	2.56	0.40
22:BA:1174:U:H1'	22:BA:1177:G:C2	2.56	0.40
48:B0:39:LEU:HD23	48:B0:39:LEU:HA	1.90	0.40
1:AA:96:U:H2'	1:AA:97:G:C8	2.57	0.40
3:AC:87:LEU:HD23	3:AC:87:LEU:HA	1.85	0.40
4:AD:126:ASN:ND2	4:AD:142:VAL:H	2.18	0.40
19:AS:43:ASN:OD1	19:AS:43:ASN:N	2.42	0.40
22:BA:20:C:H2'	22:BA:21:A:H8	1.86	0.40
22:BA:1224:U:H2'	22:BA:1225:G:C8	2.56	0.40
22:BA:1405:U:H2'	22:BA:1406:U:C6	2.56	0.40
22:BA:2036:C:H2'	22:BA:2037:A:C8	2.56	0.40
40:BS:23:LEU:HD22	48:B0:24:ALA:HB2	2.02	0.40
1:AA:715:A:H2'	1:AA:716:A:C8	2.57	0.40
4:AD:48:LEU:HD22	4:AD:52:GLY:HA3	2.02	0.40
11:AK:47:ALA:HB1	11:AK:62:ALA:HB1	2.02	0.40
18:AR:68:LEU:HD23	18:AR:68:LEU:HA	1.84	0.40
22:BA:1636:U:H2'	22:BA:1637:A:H8	1.84	0.40
22:BA:2115:G:H2'	22:BA:2117:A:N7	2.37	0.40
22:BA:2233:U:H2'	22:BA:2234:G:H8	1.86	0.40
22:BA:2809:A:H2'	22:BA:2810:A:C8	2.56	0.40
39:BR:38:VAL:HG23	39:BR:54:VAL:HB	2.02	0.40
3:AC:79:LYS:HA	3:AC:79:LYS:HD3	1.96	0.40
4:AD:85:ASN:HB3	4:AD:88:GLU:HG2	2.04	0.40
7:AG:57:SER:HB3	7:AG:60:GLU:HB2	2.02	0.40
22:BA:2586:U:OP2	53:D1:1:FME:N	2.55	0.40
54:D2:30:C:H2'	54:D2:31:A:H8	1.87	0.40
1:AA:408:A:O3'	4:AD:23:SER:OG	2.38	0.40
1:AA:1254:A:H2'	1:AA:1255:G:H8	1.86	0.40
1:AA:1409:C:H2'	1:AA:1410:A:C8	2.57	0.40
4:AD:3:ARG:HH11	4:AD:3:ARG:HD3	1.75	0.40
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	2.03	0.40
7:AG:141:VAL:HA	7:AG:144:MET:HE2	2.02	0.40
10:AJ:11:LYS:HE2	10:AJ:71:LEU:HD21	2.04	0.40
10:AJ:52:LEU:HD21	10:AJ:59:LYS:HA	2.03	0.40
22:BA:20:C:H2'	22:BA:21:A:C8	2.57	0.40
22:BA:284:U:H3	22:BA:356:G:H1	1.69	0.40
22:BA:876:C:H2'	22:BA:877:A:O4'	2.22	0.40
22:BA:1038:G:H2'	22:BA:1039:A:C8	2.57	0.40
22:BA:1485:U:H2'	22:BA:1486:U:C6	2.57	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	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
3	AC	204/233 (88%)	192 (94%)	11 (5%)	1 (0%)	24	60
4	AD	203/206 (98%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/167 (92%)	143 (94%)	10 (6%)	0	100	100
6	AF	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
7	AG	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
8	AH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	AI	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	16	50
10	AJ	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	12	45
11	AK	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
12	AL	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	16	50
13	AM	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	14	48
14	AN	99/102 (97%)	83 (84%)	16 (16%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	AP	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	AR	53/75 (71%)	50 (94%)	3 (6%)	0	100	100
19	AS	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
24	BC	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
25	BD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
27	BF	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
28	BG	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
32	BK	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	BL	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	BM	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	BN	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
36	BO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
37	BP	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
40	BS	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
41	BT	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
42	BU	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
43	BV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	BW	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	BX	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	BY	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
47	BZ	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
48	B0	54/57 (95%)	54 (100%)	0	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	44 (100%)	0	0	100	100
51	B3	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	3	18
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	D1	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	5579/5920 (94%)	5322 (95%)	249 (4%)	8 (0%)	49	80

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AL	102	LEU
25	BD	149	ASN
51	B3	32	ILE
10	AJ	57	VAL
51	B3	33	LEU
3	AC	61	ALA
9	AI	25	ASN
13	AM	66	GLU

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	186/199 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	168 (99%)	2 (1%)	63	82
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	118 (95%)	6 (5%)	23	57
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	100 (95%)	5 (5%)	23	57
10	AJ	87/90 (97%)	85 (98%)	2 (2%)	44	74
11	AK	90/99 (91%)	89 (99%)	1 (1%)	65	83
12	AL	102/103 (99%)	101 (99%)	1 (1%)	68	84
13	AM	92/96 (96%)	91 (99%)	1 (1%)	65	83
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	76/77 (99%)	76 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	73 (99%)	1 (1%)	59	80
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	70 (99%)	1 (1%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AT	65/66 (98%)	64 (98%)	1 (2%)	57	80
21	AU	48/61 (79%)	48 (100%)	0	100	100
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	162 (99%)	1 (1%)	78	88
26	BE	165/165 (100%)	164 (99%)	1 (1%)	78	88
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	113 (99%)	1 (1%)	70	85
30	BI	59/62 (95%)	59 (100%)	0	100	100
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	70	85
32	BK	104/104 (100%)	103 (99%)	1 (1%)	68	84
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	108 (100%)	0	100	100
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	87 (100%)	0	100	100
37	BP	99/100 (99%)	99 (100%)	0	100	100
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	83 (99%)	1 (1%)	63	82
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	47 (100%)	0	100	100
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52 (98%)	50 (98%)	1 (2%)	48	76
52	B4	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	D1	5/5 (100%)	4 (80%)	1 (20%)	1 7
All	All	4638/4832 (96%)	4609 (99%)	29 (1%)	76 88

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	57	ILE
3	AC	64	ILE
7	AG	30	LEU
7	AG	79	ARG
7	AG	94	VAL
7	AG	148	ASN
7	AG	149	LYS
7	AG	151	PHE
9	AI	18	ARG
9	AI	19	VAL
9	AI	30	ILE
9	AI	61	LEU
9	AI	72	ILE
10	AJ	40	ILE
10	AJ	69	THR
11	AK	86	VAL
12	AL	64	THR
13	AM	104	THR
17	AQ	28	PHE
19	AS	31	LEU
20	AT	10	ARG
25	BD	1	MET
26	BE	188	MET
29	BH	27	ARG
31	BJ	92	MET
32	BK	7	MET
39	BR	1	MET
51	B3	32	ILE
53	D1	6	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	170	HIS
4	AD	41	HIS

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Mol	Chain	Res	Type
4	AD	116	GLN
4	AD	126	ASN
4	AD	136	GLN
5	AE	89	HIS
7	AG	9	GLN
7	AG	86	GLN
9	AI	25	ASN
11	AK	15	GLN
11	AK	118	HIS
12	AL	5	ASN
12	AL	96	HIS
13	AM	8	ASN
14	AN	3	GLN
17	AQ	50	ASN
20	AT	3	ASN
20	AT	48	GLN
20	AT	52	ASN
20	AT	61	GLN
20	AT	70	ASN
21	AU	56	HIS
24	BC	25	HIS
24	BC	86	ASN
24	BC	90	ASN
24	BC	200	HIS
24	BC	260	ASN
27	BF	21	ASN
28	BG	22	GLN
28	BG	45	HIS
28	BG	104	ASN
28	BG	116	GLN
28	BG	128	GLN
28	BG	139	GLN
31	BJ	47	HIS
31	BJ	86	GLN
32	BK	9	ASN
32	BK	88	ASN
35	BN	73	ASN
36	BO	100	HIS
38	BQ	72	ASN
43	BV	24	ASN
46	BY	20	ASN
46	BY	58	ASN

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Mol	Chain	Res	Type
47	BZ	20	HIS
48	B0	42	HIS
49	B1	45	GLN
50	B2	26	ASN
52	B4	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	269 (17%)	4 (0%)
22	BA	2895/2903 (99%)	418 (14%)	16 (0%)
23	BB	119/120 (99%)	15 (12%)	0
54	D2	74/77 (96%)	18 (24%)	3 (4%)
55	D3	74/76 (97%)	43 (58%)	3 (4%)
56	D4	8/9 (88%)	4 (50%)	0
All	All	4703/4719 (99%)	767 (16%)	26 (0%)

All (767) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	22	G
1	AA	29	U
1	AA	32	A
1	AA	39	G
1	AA	44	A
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	70	U
1	AA	71	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U

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Mol	Chain	Res	Type
1	AA	85	U
1	AA	86	G
1	AA	87	C
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	98	A
1	AA	116	A
1	AA	121	U
1	AA	122	G
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	144	G
1	AA	159	G
1	AA	163	C
1	AA	164	G
1	AA	167	A
1	AA	181	A
1	AA	183	C
1	AA	197	A
1	AA	205	A
1	AA	210	C
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	280	C
1	AA	289	G
1	AA	316	C
1	AA	321	A
1	AA	327	A
1	AA	328	C
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A

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Mol	Chain	Res	Type
1	AA	384	G
1	AA	390	U
1	AA	392	C
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	428	G
1	AA	429	U
1	AA	436	C
1	AA	437	U
1	AA	439	U
1	AA	465	A
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	469	C
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	482	A
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	496	A
1	AA	499	A
1	AA	511	C
1	AA	515	G
1	AA	517	G
1	AA	518	C
1	AA	521	G
1	AA	527	G7M
1	AA	529	G
1	AA	532	A
1	AA	533	A
1	AA	542	G
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	572	A
1	AA	573	A

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Mol	Chain	Res	Type
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	607	A
1	AA	631	C
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	665	A
1	AA	687	A
1	AA	688	G
1	AA	694	A
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	722	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	758	C
1	AA	760	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	799	G
1	AA	810	C
1	AA	815	A
1	AA	817	C
1	AA	819	A
1	AA	820	U
1	AA	821	G
1	AA	828	U
1	AA	829	G
1	AA	832	G
1	AA	840	C
1	AA	841	C
1	AA	843	U
1	AA	845	A
1	AA	846	G
1	AA	871	U

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Mol	Chain	Res	Type
1	AA	889	A
1	AA	914	A
1	AA	929	G
1	AA	930	C
1	AA	934	C
1	AA	935	A
1	AA	942	G
1	AA	960	U
1	AA	966	2MG
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A
1	AA	989	U
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1009	U
1	AA	1018	G
1	AA	1019	A
1	AA	1020	G
1	AA	1021	A
1	AA	1022	A
1	AA	1023	U
1	AA	1024	G
1	AA	1025	U
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1036	A
1	AA	1043	G
1	AA	1044	A
1	AA	1045	C

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Mol	Chain	Res	Type
1	AA	1065	U
1	AA	1070	U
1	AA	1085	U
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1127	G
1	AA	1132	C
1	AA	1133	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1143	G
1	AA	1154	G
1	AA	1158	C
1	AA	1159	U
1	AA	1168	U
1	AA	1169	A
1	AA	1171	A
1	AA	1172	C
1	AA	1173	U
1	AA	1181	G
1	AA	1184	G
1	AA	1187	G
1	AA	1191	A
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	1214	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1241	G
1	AA	1248	A
1	AA	1257	A
1	AA	1260	G
1	AA	1274	A
1	AA	1279	G

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Mol	Chain	Res	Type
1	AA	1280	A
1	AA	1287	A
1	AA	1297	G
1	AA	1298	U
1	AA	1299	A
1	AA	1302	C
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C
1	AA	1322	C
1	AA	1335	U
1	AA	1338	G
1	AA	1345	U
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1378	C
1	AA	1390	U
1	AA	1391	U
1	AA	1397	C
1	AA	1419	G
1	AA	1429	A
1	AA	1432	G
1	AA	1441	A
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1502	A
1	AA	1505	G
1	AA	1506	U
1	AA	1517	G
1	AA	1519	MA6
1	AA	1520	C
1	AA	1529	G
1	AA	1530	G
22	BA	14	A
22	BA	15	G
22	BA	34	U
22	BA	35	G

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Mol	Chain	Res	Type
22	BA	63	A
22	BA	71	A
22	BA	74	A
22	BA	75	G
22	BA	84	A
22	BA	91	A
22	BA	101	A
22	BA	103	A
22	BA	118	A
22	BA	119	A
22	BA	120	U
22	BA	125	A
22	BA	126	A
22	BA	162	U
22	BA	163	C
22	BA	165	A
22	BA	181	A
22	BA	186	G
22	BA	196	A
22	BA	197	A
22	BA	204	A
22	BA	215	G
22	BA	216	A
22	BA	221	A
22	BA	222	A
22	BA	223	A
22	BA	233	A
22	BA	241	A
22	BA	248	G
22	BA	264	C
22	BA	265	A
22	BA	276	U
22	BA	278	A
22	BA	299	A
22	BA	302	C
22	BA	303	G
22	BA	311	A
22	BA	324	A
22	BA	330	A
22	BA	353	C
22	BA	361	G
22	BA	362	A

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Mol	Chain	Res	Type
22	BA	386	G
22	BA	396	G
22	BA	406	G
22	BA	411	G
22	BA	412	A
22	BA	457	A
22	BA	467	G
22	BA	477	A
22	BA	480	A
22	BA	481	G
22	BA	491	G
22	BA	504	A
22	BA	505	A
22	BA	508	A
22	BA	509	C
22	BA	529	A
22	BA	531	C
22	BA	532	A
22	BA	533	G
22	BA	546	U
22	BA	547	A
22	BA	548	G
22	BA	549	G
22	BA	550	C
22	BA	563	A
22	BA	573	U
22	BA	575	A
22	BA	577	G
22	BA	588	U
22	BA	602	A
22	BA	603	A
22	BA	613	A
22	BA	614	A
22	BA	615	U
22	BA	616	A
22	BA	634	C
22	BA	637	A
22	BA	645	C
22	BA	647	G
22	BA	653	U
22	BA	654	A
22	BA	668	A

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Mol	Chain	Res	Type
22	BA	670	A
22	BA	685	A
22	BA	686	U
22	BA	702	U
22	BA	724	U
22	BA	730	A
22	BA	738	G
22	BA	747	5MU
22	BA	748	G
22	BA	764	A
22	BA	765	C
22	BA	775	G
22	BA	776	G
22	BA	782	A
22	BA	784	G
22	BA	785	G
22	BA	789	A
22	BA	791	C
22	BA	792	A
22	BA	793	A
22	BA	794	A
22	BA	805	G
22	BA	812	C
22	BA	827	U
22	BA	828	U
22	BA	830	G
22	BA	845	A
22	BA	846	U
22	BA	859	G
22	BA	869	G
22	BA	884	U
22	BA	885	C
22	BA	895	U
22	BA	896	A
22	BA	897	C
22	BA	907	G
22	BA	910	A
22	BA	927	A
22	BA	946	C
22	BA	961	C
22	BA	974	G
22	BA	983	A

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Mol	Chain	Res	Type
22	BA	984	A
22	BA	985	C
22	BA	996	A
22	BA	999	U
22	BA	1005	C
22	BA	1009	A
22	BA	1012	U
22	BA	1013	C
22	BA	1022	G
22	BA	1026	G
22	BA	1033	U
22	BA	1046	A
22	BA	1047	G
22	BA	1054	A
22	BA	1057	A
22	BA	1061	U
22	BA	1069	A
22	BA	1070	A
22	BA	1077	A
22	BA	1087	G
22	BA	1088	A
22	BA	1089	A
22	BA	1090	A
22	BA	1094	U
22	BA	1110	G
22	BA	1112	G
22	BA	1126	A
22	BA	1130	U
22	BA	1132	U
22	BA	1133	A
22	BA	1135	C
22	BA	1141	U
22	BA	1142	A
22	BA	1156	A
22	BA	1168	G
22	BA	1173	U
22	BA	1174	U
22	BA	1175	A
22	BA	1176	U
22	BA	1204	A
22	BA	1205	A
22	BA	1212	G

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Mol	Chain	Res	Type
22	BA	1236	G
22	BA	1250	G
22	BA	1253	A
22	BA	1256	G
22	BA	1268	A
22	BA	1271	G
22	BA	1272	A
22	BA	1275	A
22	BA	1276	A
22	BA	1287	A
22	BA	1300	G
22	BA	1301	A
22	BA	1302	A
22	BA	1313	U
22	BA	1321	A
22	BA	1329	U
22	BA	1352	U
22	BA	1359	A
22	BA	1365	A
22	BA	1379	U
22	BA	1383	A
22	BA	1386	C
22	BA	1387	A
22	BA	1403	A
22	BA	1416	G
22	BA	1428	C
22	BA	1434	A
22	BA	1437	C
22	BA	1452	G
22	BA	1453	A
22	BA	1482	G
22	BA	1493	C
22	BA	1497	U
22	BA	1508	A
22	BA	1509	A
22	BA	1515	A
22	BA	1524	G
22	BA	1535	A
22	BA	1536	C
22	BA	1544	A
22	BA	1558	C
22	BA	1559	U

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Mol	Chain	Res	Type
22	BA	1566	A
22	BA	1569	A
22	BA	1578	U
22	BA	1583	A
22	BA	1608	A
22	BA	1610	A
22	BA	1618	6MZ
22	BA	1626	A
22	BA	1634	A
22	BA	1647	U
22	BA	1648	U
22	BA	1649	G
22	BA	1654	A
22	BA	1664	A
22	BA	1674	G
22	BA	1677	A
22	BA	1698	A
22	BA	1699	G
22	BA	1713	A
22	BA	1729	U
22	BA	1730	C
22	BA	1732	C
22	BA	1744	A
22	BA	1757	A
22	BA	1758	U
22	BA	1764	C
22	BA	1773	A
22	BA	1781	U
22	BA	1786	A
22	BA	1800	C
22	BA	1801	A
22	BA	1802	A
22	BA	1808	A
22	BA	1811	G
22	BA	1816	C
22	BA	1829	A
22	BA	1847	A
22	BA	1862	G
22	BA	1870	C
22	BA	1871	A
22	BA	1872	A
22	BA	1873	G

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Mol	Chain	Res	Type
22	BA	1900	A
22	BA	1901	A
22	BA	1906	G
22	BA	1914	C
22	BA	1929	G
22	BA	1930	G
22	BA	1936	A
22	BA	1937	A
22	BA	1938	A
22	BA	1939	5MU
22	BA	1955	U
22	BA	1960	A
22	BA	1967	C
22	BA	1970	A
22	BA	1971	U
22	BA	1972	G
22	BA	1991	U
22	BA	1993	U
22	BA	1996	C
22	BA	2004	G
22	BA	2020	A
22	BA	2023	C
22	BA	2030	6MZ
22	BA	2031	A
22	BA	2033	A
22	BA	2036	C
22	BA	2043	C
22	BA	2055	C
22	BA	2056	G
22	BA	2060	A
22	BA	2061	G
22	BA	2062	A
22	BA	2069	G7M
22	BA	2077	A
22	BA	2080	A
22	BA	2093	G
22	BA	2099	U
22	BA	2100	G
22	BA	2101	A
22	BA	2108	A
22	BA	2110	G
22	BA	2111	U

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Mol	Chain	Res	Type
22	BA	2113	U
22	BA	2115	G
22	BA	2116	G
22	BA	2117	A
22	BA	2118	U
22	BA	2119	A
22	BA	2121	G
22	BA	2123	G
22	BA	2124	G
22	BA	2125	G
22	BA	2126	A
22	BA	2128	G
22	BA	2131	U
22	BA	2132	U
22	BA	2133	G
22	BA	2137	U
22	BA	2146	C
22	BA	2147	A
22	BA	2158	A
22	BA	2161	C
22	BA	2162	G
22	BA	2163	A
22	BA	2164	C
22	BA	2165	C
22	BA	2167	U
22	BA	2169	A
22	BA	2171	A
22	BA	2172	U
22	BA	2173	A
22	BA	2189	U
22	BA	2190	G
22	BA	2195	U
22	BA	2198	A
22	BA	2203	U
22	BA	2204	G
22	BA	2211	A
22	BA	2225	A
22	BA	2238	G
22	BA	2239	G
22	BA	2243	U
22	BA	2266	A
22	BA	2267	A

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Mol	Chain	Res	Type
22	BA	2268	A
22	BA	2278	A
22	BA	2283	C
22	BA	2287	A
22	BA	2288	A
22	BA	2305	U
22	BA	2307	G
22	BA	2308	G
22	BA	2312	U
22	BA	2322	A
22	BA	2325	G
22	BA	2333	A
22	BA	2336	A
22	BA	2340	A
22	BA	2345	G
22	BA	2347	C
22	BA	2350	C
22	BA	2383	G
22	BA	2385	C
22	BA	2406	A
22	BA	2425	A
22	BA	2426	A
22	BA	2429	G
22	BA	2430	A
22	BA	2435	A
22	BA	2436	G
22	BA	2441	U
22	BA	2448	A
22	BA	2469	A
22	BA	2476	A
22	BA	2491	U
22	BA	2498	OMC
22	BA	2502	G
22	BA	2505	G
22	BA	2518	A
22	BA	2520	C
22	BA	2529	G
22	BA	2535	G
22	BA	2547	A
22	BA	2566	A
22	BA	2567	G
22	BA	2584	U

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Mol	Chain	Res	Type
22	BA	2585	U
22	BA	2602	A
22	BA	2603	G
22	BA	2609	U
22	BA	2613	U
22	BA	2615	U
22	BA	2623	G
22	BA	2629	U
22	BA	2630	G
22	BA	2646	C
22	BA	2660	A
22	BA	2661	G
22	BA	2663	G
22	BA	2689	U
22	BA	2690	U
22	BA	2714	G
22	BA	2726	A
22	BA	2727	A
22	BA	2732	G
22	BA	2733	A
22	BA	2744	G
22	BA	2748	A
22	BA	2765	A
22	BA	2778	A
22	BA	2800	A
22	BA	2818	U
22	BA	2820	A
22	BA	2821	A
22	BA	2835	A
22	BA	2850	A
22	BA	2861	U
22	BA	2880	C
22	BA	2883	A
22	BA	2884	U
22	BA	2885	G
22	BA	2891	U
23	BB	9	G
23	BB	24	G
23	BB	35	C
23	BB	37	C
23	BB	41	G
23	BB	42	C

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Mol	Chain	Res	Type
23	BB	45	A
23	BB	52	A
23	BB	56	G
23	BB	57	A
23	BB	67	G
23	BB	89	U
23	BB	90	C
23	BB	105	G
23	BB	109	A
54	D2	7	G
54	D2	8	4SU
54	D2	13	C
54	D2	14	A
54	D2	16	H2U
54	D2	17	H2U
54	D2	17(A)	OMG
54	D2	18	G
54	D2	19	H2U
54	D2	20	H2U
54	D2	21	A
54	D2	23	A
54	D2	34	4AC
54	D2	37	T6A
54	D2	46	G7M
54	D2	54	5MU
54	D2	59	A
54	D2	76	A
55	D3	2	C
55	D3	6	G
55	D3	7	A
55	D3	8	4SU
55	D3	9	A
55	D3	11	C
55	D3	13	C
55	D3	14	A
55	D3	15	G
55	D3	16	H2U
55	D3	17	C
55	D3	18	G
55	D3	19	G
55	D3	20	H2U
55	D3	21	A

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Mol	Chain	Res	Type
55	D3	22	G
55	D3	23	A
55	D3	26	A
55	D3	27	G
55	D3	34	G
55	D3	35	A
55	D3	36	A
55	D3	38	A
55	D3	40	C
55	D3	44	G
55	D3	46	G
55	D3	49	C
55	D3	50	U
55	D3	53	G
55	D3	55	PSU
55	D3	56	C
55	D3	57	G
55	D3	58	A
55	D3	59	U
55	D3	62	C
55	D3	64	A
55	D3	67	C
55	D3	68	C
55	D3	70	G
55	D3	71	G
55	D3	72	C
55	D3	74	C
55	D3	76	A
56	D4	4	A
56	D4	7	U
56	D4	8	A
56	D4	9	A

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	81	A
1	AA	428	G
1	AA	722	G
1	AA	1493	A
22	BA	125	A
22	BA	196	A

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Mol	Chain	Res	Type
22	BA	221	A
22	BA	764	A
22	BA	984	A
22	BA	1046	A
22	BA	1089	A
22	BA	1142	A
22	BA	1275	A
22	BA	1634	A
22	BA	1900	A
22	BA	2116	G
22	BA	2189	U
22	BA	2468	A
22	BA	2602	A
22	BA	2873	A
54	D2	16	H2U
54	D2	17	H2U
54	D2	17(A)	OMG
55	D3	1	G
55	D3	8	4SU
55	D3	58	A

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

58 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$
22	5MC	BA	1962	22	18,22,23	3.31	7 (38%)	26,32,35	1.02	2 (7%)
22	2MG	BA	1835	22	23,26,27	2.81	7 (30%)	32,38,41	2.33	9 (28%)
1	2MG	AA	1516	1	23,26,27	2.66	7 (30%)	32,38,41	2.25	10 (31%)
22	5MU	BA	1939	22	19,22,23	4.66	7 (36%)	28,32,35	3.72	9 (32%)
22	5MU	BA	747	22	19,22,23	4.72	7 (36%)	28,32,35	3.70	9 (32%)
22	2MG	BA	2445	22	23,26,27	2.79	7 (30%)	32,38,41	2.24	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	G7M	BA	2069	22	23,26,27	2.47	9 (39%)	35,39,42	2.14	11 (31%)
54	H2U	D2	17	54	18,21,22	3.06	5 (27%)	21,30,33	2.03	5 (23%)
54	H2U	D2	19	54	18,21,22	3.27	4 (22%)	21,30,33	1.77	5 (23%)
54	PSU	D2	55	54	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
12	D2T	AL	89	12	7,9,10	1.37	1 (14%)	6,11,13	1.45	0
22	PSU	BA	1911	22	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)
34	4D4	BM	81	34	9,11,12	2.03	2 (22%)	8,13,15	1.97	3 (37%)
22	PSU	BA	2580	22	18,21,22	1.10	3 (16%)	22,30,33	1.90	5 (22%)
22	1MG	BA	745	22	22,26,27	2.58	7 (31%)	33,39,42	1.80	7 (21%)
22	PSU	BA	2457	22	18,21,22	1.00	1 (5%)	22,30,33	1.91	4 (18%)
55	4SU	D3	8	55	18,21,22	3.69	8 (44%)	26,30,33	2.24	5 (19%)
1	5MC	AA	1407	1	18,22,23	3.18	7 (38%)	26,32,35	1.05	1 (3%)
22	OMG	BA	2251	22,54	23,26,27	2.36	9 (39%)	33,38,41	2.46	10 (30%)
55	H2U	D3	16	55	18,21,22	3.19	5 (27%)	21,30,33	1.65	4 (19%)
1	MA6	AA	1519	1	23,26,27	1.47	3 (13%)	34,38,41	3.84	13 (38%)
1	MA6	AA	1518	1	23,26,27	1.37	3 (13%)	34,38,41	3.84	13 (38%)
22	2MA	BA	2503	22,57	22,25,26	3.49	6 (27%)	33,37,40	2.09	9 (27%)
22	PSU	BA	746	22,57	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
55	H2U	D3	20	55	18,21,22	3.15	5 (27%)	21,30,33	1.90	4 (19%)
22	6MZ	BA	1618	22	22,25,26	2.76	3 (13%)	30,36,39	2.39	11 (36%)
22	PSU	BA	955	22	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
1	2MG	AA	966	1	23,26,27	2.65	7 (30%)	32,38,41	2.10	8 (25%)
22	OMC	BA	2498	22,57	19,22,23	2.73	7 (36%)	26,31,34	0.98	1 (3%)
22	H2U	BA	2449	22	18,21,22	2.86	5 (27%)	21,30,33	2.01	5 (23%)
22	PSU	BA	2605	22	18,21,22	0.99	1 (5%)	22,30,33	1.77	3 (13%)
54	H2U	D2	20	54	18,21,22	3.02	5 (27%)	21,30,33	2.12	5 (23%)
54	T6A	D2	37	54	31,34,35	1.42	6 (19%)	44,49,52	2.24	13 (29%)
1	2MG	AA	1207	1	23,26,27	2.71	7 (30%)	32,38,41	2.21	9 (28%)
22	PSU	BA	2604	22	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
1	5MC	AA	967	1	18,22,23	3.25	7 (38%)	26,32,35	1.15	1 (3%)
22	PSU	BA	1917	22	18,21,22	1.00	1 (5%)	22,30,33	1.65	4 (18%)
22	OMU	BA	2552	22	19,22,23	2.99	8 (42%)	26,31,34	1.78	5 (19%)
25	MEQ	BD	150	25	8,9,10	0.93	0	5,10,12	0.75	0
1	4OC	AA	1402	1	20,23,24	2.89	8 (40%)	26,32,35	0.97	1 (3%)
1	G7M	AA	527	1	23,26,27	2.51	9 (39%)	35,39,42	2.26	10 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	3TD	BA	1915	22	18,22,23	4.18	6 (33%)	22,32,35	1.69	3 (13%)
22	PSU	BA	2504	22	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
54	4AC	D2	34	54	21,24,25	3.25	9 (42%)	29,34,37	2.03	9 (31%)
54	PSU	D2	39	54	18,21,22	0.93	1 (5%)	22,30,33	1.66	4 (18%)
55	PSU	D3	55	55	18,21,22	1.15	1 (5%)	22,30,33	1.63	4 (18%)
54	OMG	D2	17(A)	54	23,26,27	2.47	9 (39%)	33,38,41	2.75	11 (33%)
55	5MU	D3	54	55	19,22,23	4.88	7 (36%)	28,32,35	3.58	9 (32%)
55	PSU	D3	39	55	18,21,22	1.06	1 (5%)	22,30,33	1.74	5 (22%)
22	6MZ	BA	2030	22	22,25,26	2.68	4 (18%)	30,36,39	2.66	11 (36%)
54	4SU	D2	8	54	18,21,22	3.61	8 (44%)	26,30,33	2.14	5 (19%)
53	FME	D1	1	53	8,9,10	0.59	0	7,9,11	1.10	1 (14%)
54	5MU	D2	54	54	19,22,23	4.83	7 (36%)	28,32,35	3.68	9 (32%)
54	G7M	D2	46	54	23,26,27	2.49	8 (34%)	35,39,42	2.15	10 (28%)
55	PSU	D3	32	55	18,21,22	1.11	1 (5%)	22,30,33	1.72	5 (22%)
1	PSU	AA	516	57,1	18,21,22	1.03	3 (16%)	22,30,33	1.92	4 (18%)
54	H2U	D2	16	54	18,21,22	3.21	5 (27%)	21,30,33	1.77	5 (23%)
1	UR3	AA	1498	1	19,22,23	2.60	6 (31%)	26,32,35	1.28	2 (7%)

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
22	5MC	BA	1962	22	-	0/7/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/9/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
22	5MU	BA	1939	22	-	2/7/25/26	0/2/2/2
22	5MU	BA	747	22	-	0/7/25/26	0/2/2/2
22	2MG	BA	2445	22	-	2/9/27/28	0/3/3/3
22	G7M	BA	2069	22	-	3/7/25/26	0/3/3/3
54	H2U	D2	17	54	-	1/7/38/39	0/2/2/2
54	H2U	D2	19	54	-	6/7/38/39	0/2/2/2
54	PSU	D2	55	54	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
34	4D4	BM	81	34	-	3/11/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
22	1MG	BA	745	22	-	0/7/25/26	0/3/3/3
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
55	4SU	D3	8	55	-	7/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	OMG	BA	2251	22,54	-	0/9/27/28	0/3/3/3
55	H2U	D3	16	55	-	2/7/38/39	0/2/2/2
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
22	2MA	BA	2503	22,57	-	2/7/25/26	0/3/3/3
22	PSU	BA	746	22,57	-	1/7/25/26	0/2/2/2
55	H2U	D3	20	55	-	4/7/38/39	0/2/2/2
22	6MZ	BA	1618	22	-	2/9/27/28	0/3/3/3
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
22	OMC	BA	2498	22,57	-	1/9/27/28	0/2/2/2
22	H2U	BA	2449	22	-	0/7/38/39	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
54	H2U	D2	20	54	-	3/7/38/39	0/2/2/2
54	T6A	D2	37	54	-	7/23/41/42	0/3/3/3
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
22	OMU	BA	2552	22	-	0/9/27/28	0/2/2/2
25	MEQ	BD	150	25	-	3/8/9/11	-
1	4OC	AA	1402	1	-	2/9/29/30	0/2/2/2
1	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
22	3TD	BA	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2504	22	-	2/7/25/26	0/2/2/2
54	4AC	D2	34	54	-	5/11/29/30	0/2/2/2
54	PSU	D2	39	54	-	3/7/25/26	0/2/2/2
55	PSU	D3	55	55	-	4/7/25/26	0/2/2/2
54	OMG	D2	17(A)	54	-	0/9/27/28	0/3/3/3
55	5MU	D3	54	55	-	2/7/25/26	0/2/2/2
55	PSU	D3	39	55	-	0/7/25/26	0/2/2/2
22	6MZ	BA	2030	22	-	2/9/27/28	0/3/3/3
54	4SU	D2	8	54	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	FME	D1	1	53	-	3/7/9/11	-
54	5MU	D2	54	54	-	2/7/25/26	0/2/2/2
54	G7M	D2	46	54	-	2/7/25/26	0/3/3/3
55	PSU	D3	32	55	-	2/7/25/26	0/2/2/2
1	PSU	AA	516	57,1	-	0/7/25/26	0/2/2/2
54	H2U	D2	16	54	-	5/7/38/39	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2

All (276) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	12.07	1.49	1.35
22	BA	1618	6MZ	C6-N6	11.85	1.47	1.34
54	D2	54	5MU	C2-N1	11.23	1.56	1.38
55	D3	54	5MU	C2-N1	11.22	1.56	1.38
22	BA	2030	6MZ	C6-N6	11.20	1.46	1.34
22	BA	2503	2MA	C4-N3	11.04	1.48	1.34
55	D3	54	5MU	C6-N1	10.79	1.56	1.38
55	D3	16	H2U	C2-N1	10.54	1.50	1.35
54	D2	19	H2U	C2-N1	10.45	1.50	1.35
22	BA	747	5MU	C2-N1	10.40	1.55	1.38
54	D2	54	5MU	C6-N1	10.29	1.55	1.38
54	D2	16	H2U	C2-N1	10.22	1.50	1.35
22	BA	1939	5MU	C2-N1	10.19	1.54	1.38
22	BA	747	5MU	C6-N1	10.19	1.55	1.38
22	BA	1939	5MU	C6-N1	10.00	1.55	1.38
54	D2	54	5MU	C4-C5	9.90	1.61	1.44
55	D3	20	H2U	C2-N1	9.89	1.49	1.35
55	D3	54	5MU	C4-C5	9.86	1.61	1.44
22	BA	1939	5MU	C4-C5	9.55	1.60	1.44
22	BA	747	5MU	C4-C5	9.49	1.60	1.44
54	D2	17	H2U	C2-N1	9.31	1.48	1.35
54	D2	20	H2U	C2-N1	9.27	1.48	1.35
22	BA	1915	3TD	C2-N1	9.02	1.48	1.37
1	AA	967	5MC	C6-C5	8.69	1.48	1.34
22	BA	2449	H2U	C2-N1	8.50	1.47	1.35
22	BA	747	5MU	C4-N3	-8.32	1.23	1.38
22	BA	1962	5MC	C6-C5	8.29	1.48	1.34
22	BA	1939	5MU	C4-N3	-8.25	1.23	1.38
1	AA	1407	5MC	C6-C5	8.05	1.47	1.34
54	D2	54	5MU	C4-N3	-7.94	1.24	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	D3	54	5MU	C4-N3	-7.78	1.24	1.38
55	D3	8	4SU	C4-N3	7.42	1.45	1.37
55	D3	8	4SU	C2-N1	7.23	1.50	1.38
54	D2	8	4SU	C4-N3	7.19	1.45	1.37
54	D2	8	4SU	C2-N1	7.16	1.49	1.38
22	BA	1835	2MG	C2-N3	7.07	1.45	1.31
22	BA	2552	OMU	C2-N3	7.01	1.50	1.38
22	BA	2445	2MG	C2-N3	6.97	1.45	1.31
55	D3	8	4SU	C2-N3	6.89	1.50	1.38
54	D2	34	4AC	C4-N3	6.87	1.44	1.32
1	AA	1207	2MG	C2-N3	6.80	1.44	1.31
22	BA	2503	2MA	C2-N3	6.76	1.46	1.34
54	D2	8	4SU	C2-N3	6.61	1.49	1.38
54	D2	19	H2U	C2-N3	6.58	1.49	1.38
55	D3	20	H2U	C2-N3	6.56	1.49	1.38
54	D2	16	H2U	C2-N3	6.52	1.49	1.38
1	AA	966	2MG	C2-N3	6.48	1.44	1.31
54	D2	17(A)	OMG	C4-N3	6.47	1.49	1.34
54	D2	17	H2U	C2-N3	6.46	1.49	1.38
1	AA	1516	2MG	C2-N3	6.41	1.44	1.31
22	BA	1835	2MG	C4-N3	6.40	1.49	1.34
1	AA	1207	2MG	C2-N2	6.37	1.47	1.33
22	BA	2552	OMU	C2-N1	6.36	1.48	1.38
54	D2	20	H2U	C2-N3	6.34	1.49	1.38
1	AA	1498	UR3	C6-C5	6.33	1.49	1.35
22	BA	1835	2MG	C2-N2	6.30	1.47	1.33
22	BA	2445	2MG	C4-N3	6.28	1.49	1.34
1	AA	1498	UR3	C2-N1	6.25	1.47	1.38
22	BA	745	1MG	C2-N3	6.21	1.45	1.34
22	BA	1962	5MC	C4-N3	6.16	1.44	1.34
22	BA	2445	2MG	C2-N2	6.15	1.47	1.33
55	D3	16	H2U	C2-N3	6.11	1.48	1.38
55	D3	54	5MU	C6-C5	6.07	1.44	1.34
22	BA	745	1MG	C4-N3	6.07	1.48	1.34
22	BA	2251	OMG	C4-N3	6.04	1.48	1.34
54	D2	34	4AC	C6-C5	6.02	1.49	1.35
22	BA	2449	H2U	C2-N3	5.93	1.48	1.38
1	AA	966	2MG	C2-N2	5.92	1.46	1.33
22	BA	1962	5MC	C2-N3	5.87	1.48	1.36
1	AA	1516	2MG	C4-N3	5.86	1.48	1.34
54	D2	34	4AC	C2-N3	5.82	1.48	1.36
1	AA	1516	2MG	C2-N2	5.80	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	54	5MU	C6-C5	5.79	1.44	1.34
1	AA	527	G7M	C5-N7	-5.79	1.32	1.39
22	BA	745	1MG	C2-N2	5.78	1.44	1.34
1	AA	1207	2MG	C4-N3	5.77	1.48	1.34
22	BA	2552	OMU	C6-C5	5.77	1.48	1.35
22	BA	747	5MU	C6-C5	5.74	1.44	1.34
54	D2	46	G7M	C4-N3	5.69	1.47	1.34
55	D3	8	4SU	C6-C5	5.69	1.48	1.35
1	AA	1407	5MC	C4-N3	5.66	1.43	1.34
22	BA	2498	OMC	C2-N3	5.63	1.47	1.36
54	D2	8	4SU	C6-C5	5.63	1.48	1.35
22	BA	2503	2MA	C2-N1	5.61	1.44	1.34
54	D2	17(A)	OMG	C2-N3	5.59	1.46	1.33
1	AA	966	2MG	C4-N3	5.59	1.47	1.34
22	BA	2498	OMC	C6-C5	5.57	1.48	1.35
1	AA	1407	5MC	C2-N3	5.54	1.47	1.36
22	BA	1939	5MU	C6-C5	5.52	1.43	1.34
22	BA	2069	G7M	C4-N3	5.48	1.47	1.34
1	AA	967	5MC	C4-N3	5.46	1.43	1.34
22	BA	1915	3TD	C6-N1	5.45	1.45	1.36
1	AA	1402	4OC	C2-N3	5.43	1.47	1.36
1	AA	1402	4OC	C4-N3	5.42	1.42	1.32
22	BA	2503	2MA	C6-N1	5.41	1.42	1.35
1	AA	1402	4OC	C6-C5	5.35	1.47	1.35
1	AA	967	5MC	C2-N3	5.32	1.47	1.36
1	AA	527	G7M	C4-N3	5.27	1.46	1.34
22	BA	2069	G7M	C5-N7	-5.15	1.33	1.39
22	BA	1915	3TD	C2-N3	5.05	1.49	1.38
54	D2	19	H2U	C4-N3	5.00	1.46	1.37
54	D2	17	H2U	C4-N3	4.96	1.46	1.37
55	D3	20	H2U	C4-N3	4.93	1.46	1.37
1	AA	1402	4OC	C4-N4	4.91	1.46	1.35
22	BA	2251	OMG	C2-N3	4.90	1.45	1.33
54	D2	34	4AC	C7-N4	4.89	1.46	1.37
54	D2	46	G7M	C2-N2	4.87	1.45	1.34
54	D2	16	H2U	C4-N3	4.86	1.45	1.37
54	D2	20	H2U	C4-N3	4.86	1.45	1.37
54	D2	46	G7M	C5-N7	-4.84	1.33	1.39
22	BA	1835	2MG	C2-N1	4.84	1.44	1.36
54	D2	17(A)	OMG	C2-N2	4.83	1.45	1.34
55	D3	8	4SU	C5-C4	4.74	1.48	1.42
34	BM	81	4D4	CZ-NE	4.71	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	34	4AC	C4-N4	4.67	1.46	1.39
22	BA	2069	G7M	C2-N2	4.66	1.45	1.34
54	D2	8	4SU	C4-S4	-4.66	1.59	1.68
22	BA	2445	2MG	C2-N1	4.65	1.44	1.36
1	AA	527	G7M	C2-N2	4.60	1.45	1.34
1	AA	1498	UR3	C2-N3	4.59	1.47	1.39
55	D3	16	H2U	C4-N3	4.55	1.45	1.37
22	BA	2251	OMG	C2-N2	4.52	1.44	1.34
22	BA	2498	OMC	C4-N4	4.50	1.44	1.33
55	D3	8	4SU	C4-S4	-4.47	1.59	1.68
1	AA	1402	4OC	O2-C2	-4.42	1.15	1.23
1	AA	1519	MA6	C5-C4	-4.39	1.30	1.39
54	D2	8	4SU	C5-C4	4.31	1.48	1.42
22	BA	2498	OMC	C4-N3	4.31	1.43	1.34
54	D2	34	4AC	C2-N1	4.30	1.49	1.40
1	AA	1516	2MG	C2-N1	4.29	1.43	1.36
22	BA	2449	H2U	C4-N3	4.28	1.44	1.37
22	BA	2552	OMU	C4-N3	4.25	1.46	1.38
22	BA	2498	OMC	C2-N1	4.20	1.49	1.40
22	BA	1962	5MC	C4-N4	4.16	1.44	1.34
54	D2	46	G7M	C2-N3	4.15	1.43	1.33
1	AA	1207	2MG	C2-N1	4.13	1.43	1.36
1	AA	966	2MG	C2-N1	4.11	1.43	1.36
22	BA	2503	2MA	C5-C6	4.07	1.52	1.41
22	BA	1915	3TD	O2-C2	-4.03	1.15	1.23
1	AA	1518	MA6	C5-C4	-4.00	1.31	1.39
1	AA	967	5MC	C4-N4	3.98	1.44	1.34
22	BA	1962	5MC	C6-N1	3.96	1.44	1.38
1	AA	527	G7M	O6-C6	-3.95	1.16	1.23
1	AA	1407	5MC	C6-N1	3.94	1.44	1.38
54	D2	34	4AC	C5-C4	3.94	1.49	1.40
54	D2	37	T6A	C5-C4	3.93	1.46	1.39
55	D3	55	PSU	C6-C5	3.83	1.39	1.35
1	AA	1407	5MC	C4-N4	3.80	1.44	1.34
22	BA	2069	G7M	O6-C6	-3.77	1.16	1.23
1	AA	967	5MC	C6-N1	3.72	1.44	1.38
1	AA	527	G7M	C2-N3	3.69	1.42	1.33
22	BA	1962	5MC	C2-N1	3.67	1.48	1.40
22	BA	2069	G7M	C2-N3	3.62	1.41	1.33
55	D3	32	PSU	C6-C5	3.60	1.39	1.35
1	AA	967	5MC	O2-C2	-3.59	1.17	1.23
22	BA	745	1MG	C5-N7	-3.57	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	46	G7M	O6-C6	-3.53	1.16	1.23
1	AA	1402	4OC	C2-N1	3.42	1.47	1.40
1	AA	1407	5MC	C2-N1	3.42	1.47	1.40
54	D2	55	PSU	C6-C5	3.41	1.39	1.35
55	D3	39	PSU	C6-C5	3.37	1.39	1.35
1	AA	1516	2MG	C5-N7	-3.27	1.32	1.39
22	BA	2251	OMG	C5-N7	-3.26	1.32	1.39
1	AA	966	2MG	C5-N7	-3.20	1.32	1.39
1	AA	1407	5MC	O2-C2	-3.13	1.17	1.23
1	AA	967	5MC	C2-N1	3.13	1.46	1.40
54	D2	46	G7M	C5-C6	3.11	1.52	1.43
22	BA	955	PSU	C6-C5	3.10	1.38	1.35
1	AA	1402	4OC	C5-C4	3.10	1.47	1.40
22	BA	1911	PSU	C6-C5	3.09	1.38	1.35
1	AA	1402	4OC	CM4-N4	3.06	1.51	1.45
1	AA	527	G7M	C4-N9	-3.04	1.30	1.38
54	D2	34	4AC	C6-N1	3.04	1.45	1.38
22	BA	2503	2MA	C5-N7	-3.01	1.33	1.39
34	BM	81	4D4	CZ-NH2	2.98	1.44	1.32
22	BA	747	5MU	O2-C2	-2.96	1.17	1.23
22	BA	2498	OMC	O2-C2	-2.95	1.18	1.23
22	BA	746	PSU	C6-C5	2.94	1.38	1.35
22	BA	747	5MU	O4-C4	-2.94	1.18	1.23
22	BA	2069	G7M	C4-N9	-2.93	1.30	1.38
22	BA	2504	PSU	C6-C5	2.91	1.38	1.35
1	AA	1207	2MG	C5-N7	-2.91	1.33	1.39
22	BA	1962	5MC	O2-C2	-2.91	1.18	1.23
22	BA	2251	OMG	O6-C6	-2.91	1.18	1.23
22	BA	1939	5MU	O4-C4	-2.91	1.18	1.23
54	D2	46	G7M	C2-N1	2.90	1.44	1.37
55	D3	8	4SU	C6-N1	2.89	1.45	1.38
22	BA	1835	2MG	C5-N7	-2.89	1.33	1.39
22	BA	1917	PSU	C6-C5	2.88	1.38	1.35
22	BA	2552	OMU	C6-N1	2.85	1.44	1.38
54	D2	37	T6A	C5-N7	-2.85	1.33	1.39
22	BA	2604	PSU	C6-C5	2.84	1.38	1.35
22	BA	2030	6MZ	C5-C4	-2.84	1.33	1.39
54	D2	34	4AC	O2-C2	-2.82	1.18	1.23
54	D2	17(A)	OMG	C2-N1	2.82	1.44	1.37
22	BA	2445	2MG	C5-N7	-2.81	1.33	1.39
54	D2	8	4SU	C6-N1	2.78	1.44	1.38
22	BA	1939	5MU	O2-C2	-2.76	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2069	G7M	C5-C6	2.76	1.51	1.43
54	D2	54	5MU	O4-C4	-2.75	1.18	1.23
22	BA	2449	H2U	O2-C2	-2.74	1.18	1.23
22	BA	2580	PSU	C6-C5	2.74	1.38	1.35
22	BA	2069	G7M	C2-N1	2.73	1.44	1.37
54	D2	39	PSU	C6-C5	2.73	1.38	1.35
22	BA	2552	OMU	O2-C2	-2.71	1.18	1.23
1	AA	966	2MG	C4-N9	-2.68	1.31	1.38
54	D2	17(A)	OMG	C5-N7	-2.67	1.33	1.39
22	BA	2498	OMC	C6-N1	2.67	1.44	1.38
22	BA	745	1MG	C5-C6	2.65	1.52	1.45
1	AA	1498	UR3	O4-C4	-2.63	1.17	1.23
54	D2	8	4SU	O2-C2	-2.59	1.18	1.23
1	AA	1498	UR3	C6-N1	2.58	1.44	1.38
1	AA	527	G7M	C5-C6	2.57	1.50	1.43
54	D2	19	H2U	O2-C2	-2.57	1.18	1.23
1	AA	1516	2MG	C4-N9	-2.56	1.31	1.38
22	BA	2030	6MZ	C5-N7	-2.56	1.34	1.39
1	AA	1518	MA6	C6-N6	2.56	1.44	1.36
54	D2	17(A)	OMG	C5-C6	2.55	1.53	1.44
54	D2	17(A)	OMG	C6-N1	2.55	1.43	1.38
55	D3	54	5MU	O4-C4	-2.54	1.18	1.23
54	D2	37	T6A	C6-N6	-2.54	1.34	1.39
54	D2	16	H2U	O2-C2	-2.54	1.18	1.23
22	BA	1618	6MZ	C5-N7	-2.53	1.34	1.39
22	BA	2449	H2U	O4-C4	-2.52	1.18	1.23
1	AA	1519	MA6	C8-N9	-2.51	1.33	1.37
54	D2	17(A)	OMG	O6-C6	-2.51	1.18	1.23
54	D2	46	G7M	C4-N9	-2.48	1.31	1.38
22	BA	745	1MG	O6-C6	-2.48	1.17	1.23
54	D2	20	H2U	O2-C2	-2.48	1.18	1.23
1	AA	527	G7M	C2-N1	2.47	1.43	1.37
22	BA	2605	PSU	C6-C5	2.46	1.38	1.35
55	D3	54	5MU	O2-C2	-2.46	1.18	1.23
54	D2	17	H2U	O2-C2	-2.46	1.18	1.23
22	BA	2251	OMG	C4-N9	-2.44	1.31	1.38
55	D3	16	H2U	O2-C2	-2.43	1.18	1.23
22	BA	1915	3TD	O4-C4	-2.40	1.18	1.23
22	BA	2445	2MG	C5-C6	2.40	1.53	1.44
22	BA	2251	OMG	C2-N1	2.38	1.43	1.37
22	BA	1835	2MG	C5-C6	2.37	1.53	1.44
1	AA	1519	MA6	C6-N6	2.36	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	D3	20	H2U	O2-C2	-2.35	1.18	1.23
55	D3	8	4SU	O2-C2	-2.35	1.18	1.23
54	D2	37	T6A	C10-N6	-2.34	1.32	1.37
1	AA	1518	MA6	C8-N9	-2.33	1.33	1.37
1	AA	1207	2MG	C4-N9	-2.33	1.32	1.38
22	BA	2552	OMU	C5-C4	2.31	1.48	1.43
22	BA	2580	PSU	O4'-C1'	-2.29	1.40	1.43
22	BA	1618	6MZ	C5-C4	-2.27	1.34	1.39
54	D2	54	5MU	O2-C2	-2.24	1.18	1.23
1	AA	527	G7M	CN7-N7	-2.22	1.43	1.46
22	BA	2030	6MZ	C4-N9	-2.20	1.32	1.37
22	BA	2552	OMU	O4-C4	-2.19	1.20	1.24
22	BA	2457	PSU	C6-C5	2.18	1.37	1.35
54	D2	20	H2U	O4-C4	-2.17	1.18	1.23
22	BA	2251	OMG	C6-N1	2.16	1.42	1.38
1	AA	516	PSU	C6-C5	2.16	1.37	1.35
22	BA	2069	G7M	CN7-N7	-2.15	1.43	1.46
22	BA	745	1MG	C4-N9	-2.14	1.32	1.38
12	AL	89	D2T	CB1-SB	-2.14	1.75	1.79
54	D2	17	H2U	O4-C4	-2.14	1.18	1.23
22	BA	2251	OMG	C5-C6	2.13	1.52	1.44
54	D2	16	H2U	O4-C4	-2.13	1.18	1.23
54	D2	37	T6A	C8-N9	-2.13	1.33	1.37
55	D3	20	H2U	O4-C4	-2.12	1.19	1.23
1	AA	1516	2MG	C5-C6	2.11	1.52	1.44
55	D3	16	H2U	O4-C4	-2.10	1.19	1.23
1	AA	516	PSU	C4-C5	-2.08	1.38	1.44
1	AA	1207	2MG	O6-C6	-2.08	1.19	1.23
1	AA	516	PSU	O4'-C1'	-2.06	1.41	1.43
54	D2	37	T6A	C5-C6	2.06	1.47	1.41
1	AA	1498	UR3	O2-C2	-2.05	1.18	1.22
22	BA	2445	2MG	C4-N9	-2.05	1.32	1.38
54	D2	17(A)	OMG	C4-N9	-2.05	1.32	1.38
1	AA	966	2MG	O6-C6	-2.03	1.19	1.23
22	BA	2580	PSU	C4-C5	-2.02	1.38	1.44
22	BA	1835	2MG	C6-N1	2.01	1.42	1.38

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	54	5MU	C5-C4-N3	12.41	125.90	115.31
22	BA	1939	5MU	C5-C4-N3	12.30	125.81	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	747	5MU	C5-C4-N3	12.19	125.72	115.31
55	D3	54	5MU	C5-C4-N3	12.13	125.66	115.31
1	AA	1519	MA6	N1-C6-N6	-11.65	104.34	117.08
1	AA	1518	MA6	N1-C6-N6	-11.18	104.86	117.08
22	BA	1939	5MU	C5-C6-N1	-10.47	112.57	123.34
1	AA	1518	MA6	C1'-N9-C8	-10.45	103.54	127.14
22	BA	747	5MU	C5-C6-N1	-10.31	112.74	123.34
55	D3	54	5MU	C5-C6-N1	-9.93	113.12	123.34
54	D2	54	5MU	C5-C6-N1	-9.92	113.13	123.34
1	AA	1519	MA6	C1'-N9-C8	-9.84	104.91	127.14
1	AA	1518	MA6	C4-N9-C1'	9.41	149.02	126.59
54	D2	17(A)	OMG	C1'-N9-C8	-8.90	101.35	126.70
1	AA	1519	MA6	C4-N9-C1'	8.88	147.75	126.59
22	BA	2030	6MZ	C9-N6-C6	-8.59	115.47	122.87
55	D3	8	4SU	C4-N3-C2	-7.64	119.92	127.34
22	BA	2251	OMG	C1'-N9-C8	-7.49	105.38	126.70
54	D2	20	H2U	C4-N3-C2	-7.43	119.62	125.79
54	D2	17(A)	OMG	C1'-N9-C4	7.30	148.20	126.50
22	BA	1835	2MG	C2-N3-C4	7.08	120.82	112.04
54	D2	17	H2U	C4-N3-C2	-7.05	119.95	125.79
22	BA	2449	H2U	C4-N3-C2	-7.03	119.96	125.79
22	BA	2503	2MA	C5-C4-N3	-7.00	119.32	127.19
54	D2	8	4SU	C4-N3-C2	-6.94	120.60	127.34
54	D2	37	T6A	C5-C4-N3	-6.86	117.81	126.75
1	AA	1207	2MG	C2-N3-C4	6.78	120.45	112.04
54	D2	34	4AC	CM7-C7-N4	6.75	126.97	115.29
22	BA	2445	2MG	C2-N3-C4	6.55	120.16	112.04
55	D3	20	H2U	C4-N3-C2	-6.51	120.39	125.79
1	AA	1519	MA6	C5-C6-N6	6.39	136.43	125.30
22	BA	2251	OMG	C1'-N9-C4	6.24	145.03	126.50
1	AA	1516	2MG	C2-N3-C4	6.23	119.77	112.04
1	AA	1518	MA6	C5-C6-N6	6.08	135.90	125.30
22	BA	1835	2MG	C5-C4-N3	-6.02	118.69	128.46
22	BA	2030	6MZ	N1-C2-N3	-5.87	119.42	128.60
54	D2	37	T6A	N6-C10-N11	5.79	121.85	113.76
1	AA	1519	MA6	N1-C2-N3	-5.78	119.56	128.60
54	D2	16	H2U	C4-N3-C2	-5.77	121.01	125.79
1	AA	966	2MG	C2-N3-C4	5.62	119.01	112.04
22	BA	2552	OMU	C4-N3-C2	-5.59	119.21	126.58
22	BA	745	1MG	C5-C4-N3	-5.58	119.41	128.46
1	AA	1518	MA6	N1-C2-N3	-5.51	119.97	128.60
54	D2	19	H2U	C4-N3-C2	-5.49	121.23	125.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1915	3TD	N1-C2-N3	5.35	120.36	116.14
1	AA	527	G7M	CN7-N7-C5	5.35	133.41	126.77
54	D2	37	T6A	N3-C4-N9	5.33	135.86	127.08
22	BA	1618	6MZ	C9-N6-C6	-5.31	118.30	122.87
22	BA	2445	2MG	C5-C4-N3	-5.29	119.88	128.46
22	BA	1618	6MZ	C5-C4-N3	-5.26	119.88	126.75
22	BA	1618	6MZ	N1-C2-N3	-5.24	120.41	128.60
22	BA	1835	2MG	C2-N1-C6	-5.23	118.46	124.48
22	BA	2069	G7M	CN7-N7-C5	5.23	133.27	126.77
22	BA	1939	5MU	C4-N3-C2	-5.19	120.63	127.35
55	D3	54	5MU	O4-C4-C5	-5.17	118.91	124.90
22	BA	747	5MU	C4-N3-C2	-5.15	120.69	127.35
54	D2	54	5MU	O4-C4-C5	-5.12	118.97	124.90
1	AA	1207	2MG	C2-N1-C6	-5.12	118.59	124.48
22	BA	747	5MU	O4-C4-C5	-5.11	118.98	124.90
22	BA	1939	5MU	O4-C4-C5	-5.11	118.98	124.90
1	AA	1207	2MG	C5-C4-N3	-5.10	120.19	128.46
54	D2	8	4SU	C5-C4-N3	5.10	119.42	114.69
1	AA	966	2MG	C2-N1-C6	-5.07	118.64	124.48
55	D3	8	4SU	C5-C4-N3	5.05	119.38	114.69
1	AA	1516	2MG	C5-C4-N3	-5.05	120.27	128.46
22	BA	2457	PSU	N1-C2-N3	5.04	120.84	115.13
1	AA	1516	2MG	C2-N1-C6	-5.04	118.68	124.48
22	BA	747	5MU	N3-C2-N1	4.96	121.47	114.89
22	BA	2580	PSU	N1-C2-N3	4.91	120.69	115.13
54	D2	54	5MU	C4-N3-C2	-4.89	121.02	127.35
22	BA	2457	PSU	C4-N3-C2	-4.88	119.31	126.34
22	BA	1911	PSU	C4-N3-C2	-4.87	119.32	126.34
22	BA	2030	6MZ	N9-C8-N7	-4.87	107.25	113.91
22	BA	2605	PSU	C4-N3-C2	-4.87	119.33	126.34
22	BA	2445	2MG	C2-N1-C6	-4.86	118.89	124.48
1	AA	516	PSU	N1-C2-N3	4.85	120.63	115.13
22	BA	1911	PSU	N1-C2-N3	4.83	120.60	115.13
55	D3	54	5MU	C4-N3-C2	-4.82	121.12	127.35
54	D2	17(A)	OMG	C5-C4-N3	-4.79	120.70	128.46
1	AA	516	PSU	C4-N3-C2	-4.78	119.45	126.34
1	AA	966	2MG	C5-C4-N3	-4.78	120.71	128.46
54	D2	46	G7M	CN7-N7-C5	4.78	132.70	126.77
22	BA	1939	5MU	N3-C2-N1	4.72	121.16	114.89
22	BA	955	PSU	C4-N3-C2	-4.66	119.63	126.34
22	BA	746	PSU	C4-N3-C2	-4.64	119.65	126.34
55	D3	54	5MU	N3-C2-N1	4.62	121.02	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2504	PSU	N1-C2-N3	4.60	120.34	115.13
22	BA	2251	OMG	C5-C4-N3	-4.58	121.04	128.46
54	D2	55	PSU	C4-N3-C2	-4.55	119.78	126.34
22	BA	955	PSU	N1-C2-N3	4.55	120.28	115.13
1	AA	1518	MA6	C5-C4-N3	-4.55	120.82	126.75
54	D2	55	PSU	N1-C2-N3	4.52	120.25	115.13
1	AA	1498	UR3	C4-N3-C2	-4.52	120.31	124.56
54	D2	39	PSU	C4-N3-C2	-4.52	119.83	126.34
22	BA	2604	PSU	N1-C2-N3	4.50	120.23	115.13
55	D3	39	PSU	C4-N3-C2	-4.49	119.87	126.34
1	AA	1519	MA6	C5-C4-N3	-4.48	120.90	126.75
22	BA	2605	PSU	N1-C2-N3	4.46	120.18	115.13
1	AA	527	G7M	C2-N3-C4	4.46	120.24	112.30
1	AA	967	5MC	C5-C6-N1	-4.44	118.77	123.34
55	D3	32	PSU	C4-N3-C2	-4.44	119.94	126.34
55	D3	39	PSU	N1-C2-N3	4.44	120.16	115.13
22	BA	2580	PSU	C4-N3-C2	-4.41	119.98	126.34
22	BA	746	PSU	N1-C2-N3	4.36	120.08	115.13
22	BA	2030	6MZ	C5-C4-N3	-4.34	121.09	126.75
55	D3	16	H2U	C4-N3-C2	-4.33	122.20	125.79
54	D2	46	G7M	C2-N3-C4	4.33	120.01	112.30
22	BA	2069	G7M	C2-N3-C4	4.30	119.97	112.30
22	BA	2604	PSU	C4-N3-C2	-4.29	120.16	126.34
22	BA	2503	2MA	N9-C8-N7	-4.29	108.05	113.91
54	D2	54	5MU	N3-C2-N1	4.28	120.58	114.89
54	D2	17(A)	OMG	C2-N3-C4	4.28	119.93	112.30
1	AA	527	G7M	CN7-N7-C8	-4.27	118.24	124.84
55	D3	32	PSU	N1-C2-N3	4.27	119.97	115.13
22	BA	2504	PSU	C4-N3-C2	-4.26	120.19	126.34
22	BA	1917	PSU	N1-C2-N3	4.26	119.95	115.13
22	BA	1618	6MZ	N9-C8-N7	-4.21	108.16	113.91
54	D2	46	G7M	C1'-N9-C4	4.21	139.00	126.50
1	AA	527	G7M	C5-C6-N1	4.20	120.56	111.79
1	AA	527	G7M	C1'-N9-C8	-4.18	112.61	126.74
54	D2	54	5MU	C5M-C5-C4	4.18	123.37	118.77
22	BA	2069	G7M	CN7-N7-C8	-4.18	118.39	124.84
54	D2	46	G7M	C1'-N9-C8	-4.18	112.63	126.74
1	AA	527	G7M	C1'-N9-C4	4.16	138.86	126.50
54	D2	54	5MU	C5M-C5-C6	-4.16	117.29	122.85
22	BA	2503	2MA	N3-C4-N9	4.15	132.75	126.99
55	D3	55	PSU	N1-C2-N3	4.09	119.77	115.13
55	D3	8	4SU	N3-C2-N1	4.09	120.32	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2552	OMU	N3-C2-N1	4.07	120.29	114.89
1	AA	1519	MA6	N9-C8-N7	-4.06	108.36	113.91
22	BA	2251	OMG	C2-N3-C4	4.05	119.52	112.30
22	BA	1917	PSU	C4-N3-C2	-4.05	120.50	126.34
54	D2	39	PSU	N1-C2-N3	4.05	119.72	115.13
1	AA	1518	MA6	N9-C8-N7	-4.01	108.43	113.91
22	BA	1915	3TD	C4-N3-C2	-4.01	120.26	124.61
55	D3	55	PSU	C4-N3-C2	-3.95	120.65	126.34
54	D2	46	G7M	C5-C6-N1	3.91	119.96	111.79
22	BA	2069	G7M	C5-C6-N1	3.89	119.91	111.79
54	D2	46	G7M	CN7-N7-C8	-3.88	118.85	124.84
54	D2	37	T6A	C2-N3-C4	3.86	120.88	111.75
1	AA	1519	MA6	C2-N1-C6	3.86	120.87	111.75
54	D2	17(A)	OMG	N9-C8-N7	-3.86	106.13	113.39
22	BA	1939	5MU	C5M-C5-C6	-3.84	117.72	122.85
22	BA	1835	2MG	N9-C4-N3	3.83	133.62	125.94
22	BA	745	1MG	C2-N3-C4	3.82	120.56	111.98
54	D2	46	G7M	C5-C4-N3	-3.79	120.88	128.15
22	BA	1618	6MZ	C4-C5-C6	3.77	119.73	116.81
1	AA	966	2MG	CM2-N2-C2	-3.75	115.58	123.86
1	AA	1518	MA6	C2-N1-C6	3.73	120.57	111.75
22	BA	745	1MG	N9-C4-N3	3.73	133.42	125.94
22	BA	747	5MU	C5M-C5-C6	-3.71	117.90	122.85
1	AA	527	G7M	C5-C4-N3	-3.68	121.09	128.15
54	D2	8	4SU	N3-C2-N1	3.64	119.72	114.89
1	AA	1516	2MG	CM2-N2-C2	-3.57	115.97	123.86
22	BA	1618	6MZ	C2-N3-C4	3.57	120.18	111.75
22	BA	1939	5MU	C5M-C5-C4	3.55	122.68	118.77
22	BA	2069	G7M	C1'-N9-C8	-3.54	114.78	126.74
22	BA	2030	6MZ	C2-N3-C4	3.51	120.05	111.75
1	AA	1519	MA6	C2-N3-C4	3.48	119.97	111.75
54	D2	34	4AC	O7-C7-N4	-3.45	116.22	121.82
1	AA	527	G7M	O6-C6-C5	-3.45	120.28	128.06
1	AA	516	PSU	O2-C2-N1	-3.44	119.00	122.79
22	BA	2251	OMG	N9-C8-N7	-3.43	106.93	113.39
55	D3	8	4SU	C5-C4-S4	-3.43	120.05	124.47
22	BA	2069	G7M	C1'-N9-C4	3.42	136.66	126.50
22	BA	2552	OMU	C5-C4-N3	3.42	119.95	114.84
34	BM	81	4D4	NE-CZ-NH2	-3.41	114.69	120.70
1	AA	1518	MA6	C4-C5-C6	3.41	119.70	115.88
22	BA	2069	G7M	O6-C6-C5	-3.37	120.45	128.06
1	AA	1518	MA6	C2-N3-C4	3.36	119.69	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D3	54	5MU	C5M-C5-C6	-3.35	118.37	122.85
54	D2	8	4SU	C5-C4-S4	-3.33	120.18	124.47
54	D2	17(A)	OMG	N9-C4-N3	3.33	132.62	125.94
54	D2	19	H2U	C5-C6-N1	3.32	122.55	111.61
22	BA	747	5MU	C5M-C5-C4	3.31	122.41	118.77
54	D2	20	H2U	N3-C2-N1	3.29	120.13	116.65
22	BA	2069	G7M	C5-C4-N3	-3.27	121.88	128.15
55	D3	16	H2U	C5-C6-N1	3.26	122.35	111.61
1	AA	1207	2MG	C5-C6-N1	3.25	121.44	113.19
1	AA	1519	MA6	C4-C5-C6	3.25	119.51	115.88
22	BA	2449	H2U	N3-C2-N1	3.23	120.06	116.65
54	D2	37	T6A	C4-C5-N7	-3.22	106.69	110.62
22	BA	2503	2MA	C5-N7-C8	3.22	108.08	103.51
54	D2	17	H2U	N3-C2-N1	3.22	120.06	116.65
1	AA	1519	MA6	C5-C4-N9	3.21	109.52	105.78
22	BA	2503	2MA	N3-C2-N1	-3.21	119.83	125.72
22	BA	2580	PSU	C6-N1-C2	-3.19	119.42	122.68
55	D3	16	H2U	O2-C2-N3	-3.19	115.56	121.50
1	AA	527	G7M	C2-N1-C6	-3.18	119.30	125.10
22	BA	2030	6MZ	C5-N7-C8	3.15	107.99	103.51
22	BA	1618	6MZ	C5-N7-C8	3.08	107.88	103.51
55	D3	20	H2U	N3-C2-N1	3.07	119.90	116.65
34	BM	81	4D4	NH1-CZ-NE	3.07	126.27	119.19
54	D2	46	G7M	O6-C6-C5	-3.06	121.15	128.06
55	D3	54	5MU	C5M-C5-C4	3.05	122.12	118.77
22	BA	2445	2MG	CM2-N2-C2	-3.04	117.14	123.86
54	D2	37	T6A	O10-C10-N6	-3.04	118.47	123.62
54	D2	16	H2U	C5-C6-N1	3.04	121.61	111.61
22	BA	745	1MG	N9-C8-N7	-3.03	107.68	113.39
54	D2	8	4SU	C1'-N1-C2	3.01	123.03	117.57
22	BA	2445	2MG	N9-C4-N3	3.01	131.99	125.94
54	D2	16	H2U	N3-C2-N1	3.00	119.83	116.65
54	D2	46	G7M	C2-N1-C6	-3.00	119.64	125.10
54	D2	34	4AC	C5-C4-N3	-2.99	117.77	122.59
22	BA	1618	6MZ	N3-C4-N9	2.99	132.01	127.08
54	D2	19	H2U	N3-C2-N1	2.99	119.81	116.65
54	D2	20	H2U	C5-C4-N3	2.98	120.00	116.65
22	BA	2445	2MG	N9-C8-N7	-2.97	107.79	113.39
22	BA	2251	OMG	N9-C4-N3	2.95	131.87	125.94
22	BA	2251	OMG	C2-N1-C6	-2.93	119.75	125.10
22	BA	1835	2MG	C5-C6-N1	2.93	120.63	113.19
54	D2	34	4AC	C1'-N1-C2	2.91	124.91	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	747	5MU	O2-C2-N1	-2.91	118.92	122.79
22	BA	2457	PSU	O2-C2-N1	-2.89	119.61	122.79
1	AA	1519	MA6	C5-N7-C8	2.89	107.62	103.51
1	AA	1518	MA6	C5-N7-C8	2.89	107.61	103.51
1	AA	966	2MG	C5-C6-N1	2.86	120.46	113.19
22	BA	745	1MG	C5-C6-N1	2.85	120.42	114.91
54	D2	55	PSU	O2-C2-N1	-2.84	119.66	122.79
22	BA	2445	2MG	C5-C6-N1	2.84	120.40	113.19
1	AA	1516	2MG	O6-C6-C5	-2.84	119.07	126.60
54	D2	17(A)	OMG	C2-N1-C6	-2.84	119.93	125.10
22	BA	1962	5MC	C5-C6-N1	-2.83	120.42	123.34
54	D2	34	4AC	O7-C7-CM7	-2.83	116.81	122.06
22	BA	2030	6MZ	C4-N9-C8	2.83	108.79	105.73
54	D2	34	4AC	C6-C5-C4	2.82	120.41	116.96
1	AA	966	2MG	N9-C8-N7	-2.82	108.08	113.39
54	D2	17	H2U	C5-C4-N3	2.82	119.81	116.65
55	D3	20	H2U	C5-C6-N1	2.81	120.89	111.61
1	AA	1518	MA6	C5-C4-N9	2.80	109.04	105.78
22	BA	1939	5MU	O2-C2-N1	-2.80	119.07	122.79
22	BA	2552	OMU	O4-C4-C5	-2.79	120.25	125.16
1	AA	1207	2MG	N9-C4-N3	2.78	131.52	125.94
1	AA	1516	2MG	C5-C6-N1	2.77	120.23	113.19
54	D2	34	4AC	O2-C2-N3	-2.76	117.84	122.33
1	AA	1207	2MG	O6-C6-C5	-2.76	119.28	126.60
22	BA	2504	PSU	O2-C2-N1	-2.75	119.77	122.79
54	D2	37	T6A	N3-C2-N1	-2.74	124.32	128.60
22	BA	2504	PSU	C6-N1-C2	-2.73	119.90	122.68
22	BA	1917	PSU	C6-N1-C2	-2.72	119.90	122.68
22	BA	2580	PSU	O2-C2-N1	-2.72	119.80	122.79
53	D1	1	FME	O-C-CA	-2.71	117.68	124.78
1	AA	1407	5MC	C5-C6-N1	-2.71	120.56	123.34
1	AA	1519	MA6	C4-C5-N7	-2.70	107.32	110.62
54	D2	37	T6A	C5-N7-C8	2.70	107.35	103.51
22	BA	1835	2MG	CM2-N2-C2	-2.69	117.92	123.86
54	D2	37	T6A	N6-C6-N1	2.68	124.34	117.45
1	AA	966	2MG	N9-C4-N3	2.67	131.31	125.94
54	D2	17(A)	OMG	C5-C6-N1	2.67	119.97	113.19
22	BA	2069	G7M	C2-N1-C6	-2.65	120.26	125.10
22	BA	2449	H2U	C5-C4-N3	2.65	119.63	116.65
1	AA	1516	2MG	N9-C8-N7	-2.63	108.44	113.39
22	BA	2251	OMG	C5-C6-N1	2.62	119.84	113.19
22	BA	1917	PSU	O2-C2-N1	-2.62	119.91	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2457	PSU	C6-N1-C2	-2.62	120.00	122.68
54	D2	17	H2U	C5-C6-N1	2.62	120.24	111.61
22	BA	1835	2MG	O6-C6-C5	-2.61	119.67	126.60
1	AA	1516	2MG	N9-C4-N3	2.61	131.17	125.94
1	AA	966	2MG	O6-C6-C5	-2.60	119.70	126.60
1	AA	516	PSU	C6-N1-C2	-2.60	120.02	122.68
54	D2	54	5MU	O4-C4-N3	-2.60	115.13	120.12
22	BA	2498	OMC	O2-C2-N3	-2.59	118.12	122.33
22	BA	955	PSU	O2-C2-N1	-2.59	119.94	122.79
54	D2	17	H2U	O2-C2-N1	-2.58	119.87	123.11
1	AA	1518	MA6	C4-C5-N7	-2.57	107.49	110.62
54	D2	20	H2U	O2-C2-N1	-2.57	119.88	123.11
55	D3	20	H2U	C5-C4-N3	2.57	119.53	116.65
22	BA	1939	5MU	O4-C4-N3	-2.56	115.20	120.12
22	BA	2449	H2U	C5-C6-N1	2.56	120.05	111.61
22	BA	1911	PSU	O2-C2-N1	-2.54	119.99	122.79
55	D3	55	PSU	C6-N1-C2	-2.54	120.09	122.68
55	D3	55	PSU	O2-C2-N1	-2.52	120.02	122.79
22	BA	747	5MU	O4-C4-N3	-2.51	115.30	120.12
22	BA	746	PSU	O2-C2-N1	-2.51	120.03	122.79
1	AA	1207	2MG	N1-C2-N3	-2.51	120.08	123.95
22	BA	2604	PSU	O2-C2-N1	-2.49	120.05	122.79
54	D2	19	H2U	O2-C2-N3	-2.49	116.87	121.50
22	BA	2445	2MG	O6-C6-C5	-2.48	120.02	126.60
54	D2	17(A)	OMG	C8-N7-C5	2.48	108.73	104.24
22	BA	2251	OMG	O6-C6-C5	-2.47	120.05	126.60
22	BA	2580	PSU	O4'-C1'-C2'	2.47	108.63	105.14
54	D2	20	H2U	C5-C6-N1	2.46	119.73	111.61
22	BA	2069	G7M	N2-C2-N1	2.46	121.96	116.71
22	BA	1835	2MG	N9-C8-N7	-2.46	108.76	113.39
55	D3	39	PSU	O2-C2-N1	-2.46	120.08	122.79
22	BA	2552	OMU	O2-C2-N1	-2.46	119.52	122.79
55	D3	54	5MU	O4-C4-N3	-2.45	115.42	120.12
1	AA	1207	2MG	N9-C8-N7	-2.44	108.80	113.39
1	AA	1516	2MG	C1'-N9-C4	-2.43	119.27	126.50
22	BA	2030	6MZ	N3-C4-N9	2.43	131.09	127.08
55	D3	16	H2U	N3-C2-N1	2.43	119.22	116.65
54	D2	17(A)	OMG	O6-C6-C5	-2.42	120.19	126.60
1	AA	1402	4OC	C6-C5-C4	2.38	119.87	116.96
22	BA	2604	PSU	C6-N1-C2	-2.35	120.28	122.68
54	D2	55	PSU	C6-N1-C2	-2.34	120.29	122.68
22	BA	2030	6MZ	C4-C5-C6	2.33	118.62	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D3	54	5MU	O2-C2-N1	-2.33	119.69	122.79
22	BA	955	PSU	C6-N1-C2	-2.31	120.32	122.68
54	D2	37	T6A	C6-C5-N7	2.31	134.89	132.39
22	BA	2449	H2U	O2-C2-N1	-2.30	120.22	123.11
54	D2	46	G7M	N9-C4-N3	2.29	130.54	125.94
54	D2	34	4AC	C5-C4-N4	2.29	126.90	122.92
54	D2	17(A)	OMG	C8-N9-C4	2.29	110.40	106.05
22	BA	2503	2MA	CM2-C2-N1	2.28	120.70	117.15
1	AA	1516	2MG	C1'-N9-C8	2.28	133.18	126.70
1	AA	527	G7M	N9-C4-N3	2.27	130.49	125.94
22	BA	2503	2MA	C6-C5-C4	2.25	120.21	117.18
22	BA	1618	6MZ	C4-C5-N7	-2.24	107.89	110.62
55	D3	32	PSU	C6-N1-C2	-2.24	120.39	122.68
22	BA	1911	PSU	C6-N1-C2	-2.23	120.40	122.68
55	D3	32	PSU	O2-C2-N1	-2.22	120.35	122.79
34	BM	81	4D4	O-C-CA	-2.20	119.02	124.78
22	BA	2445	2MG	N1-C2-N3	-2.20	120.55	123.95
54	D2	16	H2U	C5-C4-N3	2.18	119.10	116.65
55	D3	8	4SU	C1'-N1-C2	2.18	121.52	117.57
22	BA	746	PSU	C6-N1-C2	-2.18	120.45	122.68
54	D2	16	H2U	O2-C2-N3	-2.18	117.45	121.50
22	BA	1915	3TD	C6-C5-C4	2.17	119.72	118.22
1	AA	1498	UR3	C6-N1-C2	-2.17	119.85	121.79
22	BA	2445	2MG	C8-N7-C5	2.16	108.14	104.24
22	BA	2251	OMG	C8-N7-C5	2.14	108.12	104.24
22	BA	1835	2MG	N1-C2-N3	-2.14	120.64	123.95
54	D2	19	H2U	C5-C4-N3	2.13	119.04	116.65
22	BA	2030	6MZ	C5-C6-N1	2.13	120.47	118.20
54	D2	37	T6A	C4-N9-C8	2.12	108.02	105.73
55	D3	39	PSU	O4'-C1'-C2'	2.11	108.12	105.14
22	BA	1962	5MC	CM5-C5-C6	-2.11	120.03	122.85
22	BA	2503	2MA	N6-C6-N1	2.10	120.00	117.03
54	D2	34	4AC	C1'-N1-C6	-2.09	116.29	120.84
22	BA	745	1MG	C1'-N9-C8	-2.08	120.77	126.70
54	D2	37	T6A	C4-C5-C6	2.08	118.42	116.81
55	D3	39	PSU	C6-N1-C2	-2.08	120.56	122.68
22	BA	745	1MG	C8-N7-C5	2.07	107.99	104.24
22	BA	2069	G7M	N1-C2-N3	-2.07	119.46	123.32
54	D2	39	PSU	O4-C4-N3	-2.07	116.16	120.12
54	D2	39	PSU	O2-C2-N1	-2.06	120.52	122.79
22	BA	2605	PSU	O2-C2-N1	-2.06	120.52	122.79
22	BA	1618	6MZ	C4-N9-C8	2.05	107.95	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1207	2MG	C1'-N9-C4	-2.05	120.42	126.50
54	D2	54	5MU	O2-C2-N1	-2.04	120.07	122.79
55	D3	32	PSU	O4'-C1'-C2'	2.04	108.02	105.14
22	BA	2030	6MZ	C4-C5-N7	-2.03	108.14	110.62
54	D2	37	T6A	C13-C12-N11	2.03	114.71	110.28
22	BA	2503	2MA	C4-C5-N7	-2.01	108.17	110.62
22	BA	1618	6MZ	C5-C6-N1	2.01	120.34	118.20

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
22	BA	1618	6MZ	O4'-C4'-C5'-O5'
22	BA	1618	6MZ	C3'-C4'-C5'-O5'
22	BA	2030	6MZ	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	C3'-C4'-C5'-O5'
34	BM	81	4D4	NE-CD-CG-CB
53	D1	1	FME	O1-CN-N-CA
53	D1	1	FME	CA-CB-CG-SD
54	D2	16	H2U	O4'-C1'-N1-C2
54	D2	16	H2U	O4'-C1'-N1-C6
54	D2	34	4AC	O4'-C4'-C5'-O5'
54	D2	37	T6A	C3'-C4'-C5'-O5'
54	D2	39	PSU	C2'-C1'-C5-C4
54	D2	39	PSU	O4'-C1'-C5-C4
54	D2	39	PSU	O4'-C1'-C5-C6
54	D2	54	5MU	C3'-C4'-C5'-O5'
54	D2	54	5MU	O4'-C4'-C5'-O5'
55	D3	8	4SU	C2'-C1'-N1-C2
55	D3	8	4SU	C2'-C1'-N1-C6
55	D3	16	H2U	O4'-C1'-N1-C2
55	D3	16	H2U	O4'-C1'-N1-C6
55	D3	20	H2U	O4'-C4'-C5'-O5'
55	D3	32	PSU	C2'-C1'-C5-C4
54	D2	19	H2U	C2'-C1'-N1-C2
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1402	4OC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	D2	19	H2U	O4'-C4'-C5'-O5'
54	D2	34	4AC	C3'-C4'-C5'-O5'
55	D3	20	H2U	C3'-C4'-C5'-O5'
55	D3	54	5MU	C3'-C4'-C5'-O5'
54	D2	8	4SU	O4'-C4'-C5'-O5'
54	D2	16	H2U	O4'-C4'-C5'-O5'
54	D2	16	H2U	C3'-C4'-C5'-O5'
54	D2	19	H2U	C3'-C4'-C5'-O5'
54	D2	20	H2U	O4'-C4'-C5'-O5'
55	D3	54	5MU	O4'-C4'-C5'-O5'
54	D2	19	H2U	C2'-C1'-N1-C6
54	D2	20	H2U	C3'-C4'-C5'-O5'
54	D2	37	T6A	C14-C12-C13-ODA
1	AA	1402	4OC	C3'-C4'-C5'-O5'
22	BA	2445	2MG	C3'-C4'-C5'-O5'
54	D2	8	4SU	C3'-C4'-C5'-O5'
54	D2	37	T6A	N11-C12-C13-ODA
22	BA	2069	G7M	O4'-C4'-C5'-O5'
22	BA	2069	G7M	C3'-C4'-C5'-O5'
22	BA	2504	PSU	O4'-C4'-C5'-O5'
54	D2	37	T6A	O4'-C4'-C5'-O5'
55	D3	8	4SU	O4'-C4'-C5'-O5'
22	BA	2580	PSU	O4'-C4'-C5'-O5'
55	D3	8	4SU	O4'-C1'-N1-C6
34	BM	81	4D4	OB-CB-CG-CD
55	D3	8	4SU	O4'-C1'-N1-C2
53	D1	1	FME	CB-CG-SD-CE
54	D2	37	T6A	C14-C12-C13-ODB
25	BD	150	MEQ	OE1-CD-CG-CB
54	D2	34	4AC	O7-C7-N4-C4
54	D2	34	4AC	CM7-C7-N4-C4
25	BD	150	MEQ	NE2-CD-CG-CB
22	BA	1939	5MU	O4'-C4'-C5'-O5'
22	BA	2503	2MA	O4'-C4'-C5'-O5'
54	D2	37	T6A	N11-C12-C13-ODB
54	D2	16	H2U	C4'-C5'-O5'-P
54	D2	17	H2U	C4'-C5'-O5'-P
55	D3	8	4SU	C3'-C4'-C5'-O5'
54	D2	46	G7M	C4'-C5'-O5'-P
55	D3	8	4SU	C4'-C5'-O5'-P
55	D3	55	PSU	C4'-C5'-O5'-P
25	BD	150	MEQ	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
55	D3	55	PSU	C3'-C4'-C5'-O5'
55	D3	55	PSU	O4'-C4'-C5'-O5'
22	BA	2069	G7M	C4'-C5'-O5'-P
54	D2	19	H2U	C4'-C5'-O5'-P
22	BA	2445	2MG	O4'-C4'-C5'-O5'
22	BA	1939	5MU	C3'-C4'-C5'-O5'
34	BM	81	4D4	CA-CB-CG-CD
54	D2	20	H2U	C2'-C1'-N1-C6
54	D2	37	T6A	N11-C12-C14-O14
22	BA	2498	OMC	O4'-C4'-C5'-O5'
22	BA	2503	2MA	C3'-C4'-C5'-O5'
22	BA	2504	PSU	C3'-C4'-C5'-O5'
22	BA	2580	PSU	C3'-C4'-C5'-O5'
54	D2	34	4AC	C2'-C1'-N1-C2
54	D2	46	G7M	C3'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
22	BA	746	PSU	O4'-C1'-C5-C6
55	D3	32	PSU	O4'-C1'-C5-C6
55	D3	55	PSU	O4'-C1'-C5-C6
54	D2	19	H2U	O4'-C1'-N1-C2
55	D3	20	H2U	C2'-C1'-N1-C2
55	D3	20	H2U	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	D3	8	4SU	1	0
55	D3	16	H2U	6	0
22	BA	2503	2MA	1	0
54	D2	37	T6A	2	0
22	BA	1915	3TD	1	0
55	D3	55	PSU	1	0
22	BA	2030	6MZ	1	0
53	D1	1	FME	5	0
54	D2	46	G7M	1	0
55	D3	32	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 173 ligands modelled in this entry, 172 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	ERY	BA	3001	-	53,53,53	0.43	0	82,82,82	0.95	5 (6%)

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
58	ERY	BA	3001	-	-	7/72/107/107	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	ERY	C12-C11-C10	-4.27	111.08	116.43
58	BA	3001	ERY	O5-C16-C15	-2.64	108.73	112.96
58	BA	3001	ERY	O7-C5-C6	2.33	109.26	106.39
58	BA	3001	ERY	C16-C15-C14	-2.30	111.08	115.07
58	BA	3001	ERY	C6-C5-C4	-2.12	111.04	114.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	ERY	C23-C24-N1-C29
58	BA	3001	ERY	C25-C24-N1-C28
58	BA	3001	ERY	C23-C24-N1-C28
58	BA	3001	ERY	C25-C24-N1-C29
58	BA	3001	ERY	O2-C13-C36-C37

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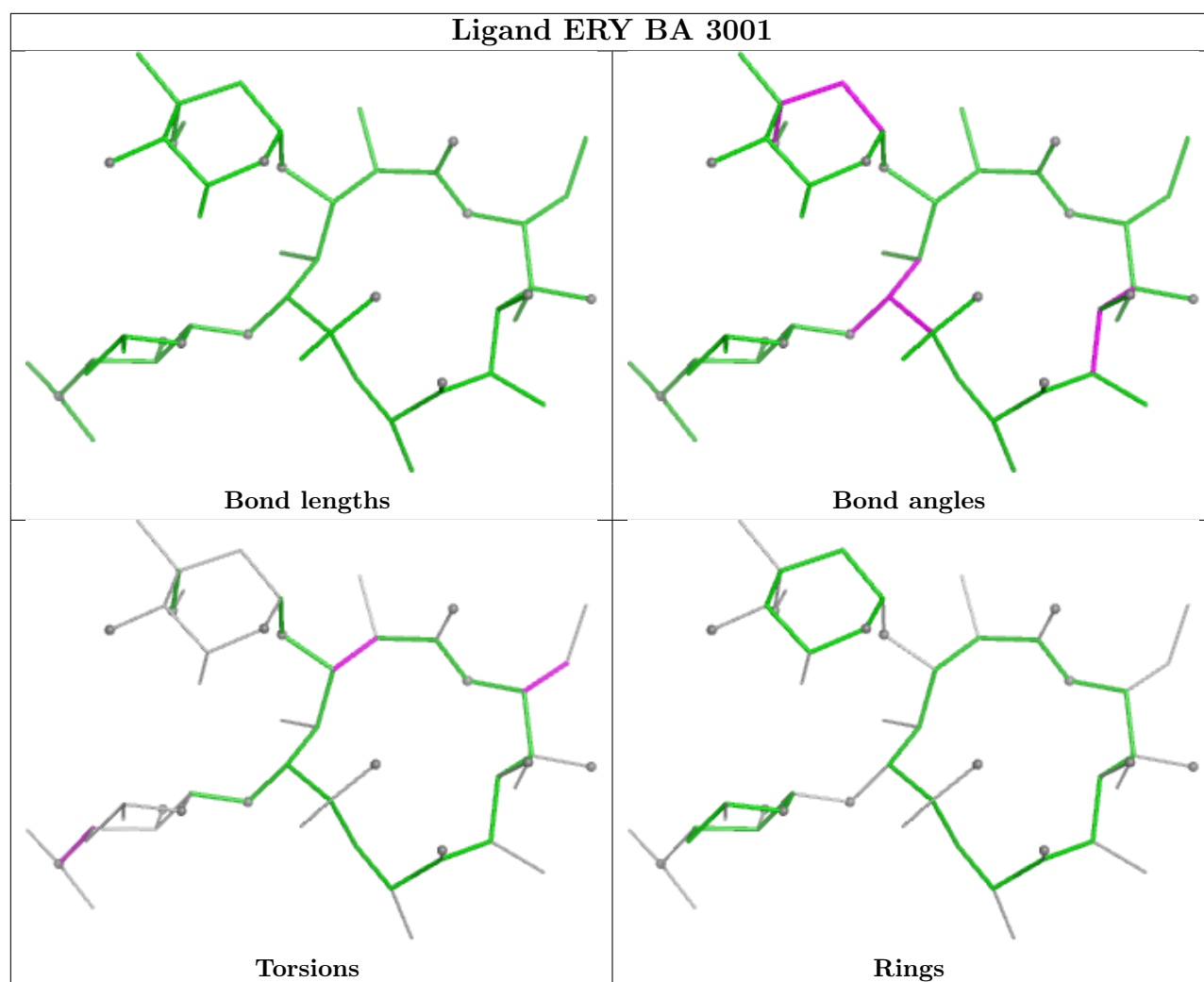
Mol	Chain	Res	Type	Atoms
58	BA	3001	ERY	C12-C13-C36-C37
58	BA	3001	ERY	C30-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	BA	3001	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](#)

There are no chain breaks in this entry.

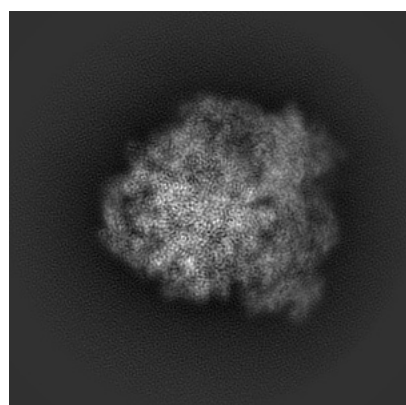
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13805. These allow visual inspection of the internal detail of the map and identification of artifacts.

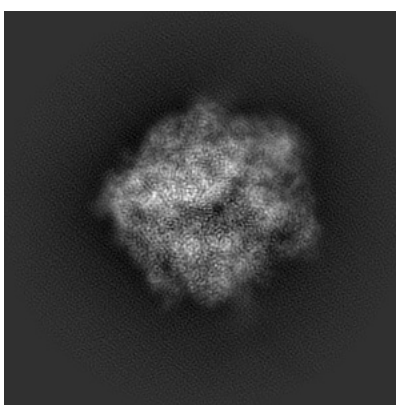
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

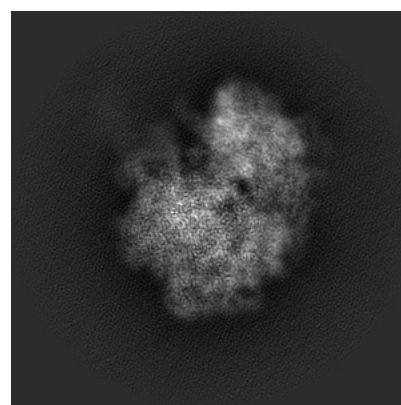
6.1.1 Primary map



X



Y

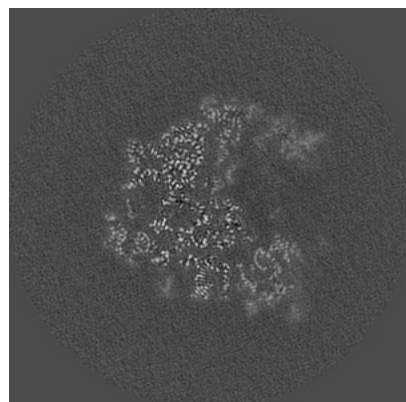


Z

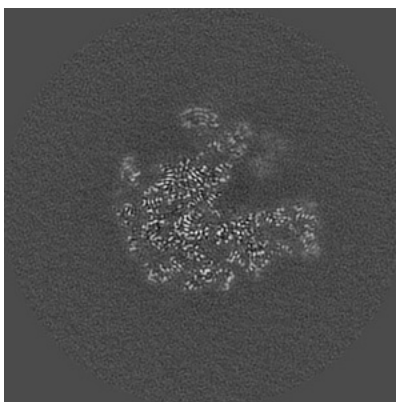
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

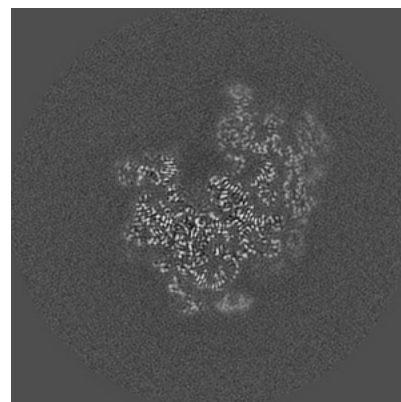
6.2.1 Primary map



X Index: 180



Y Index: 180

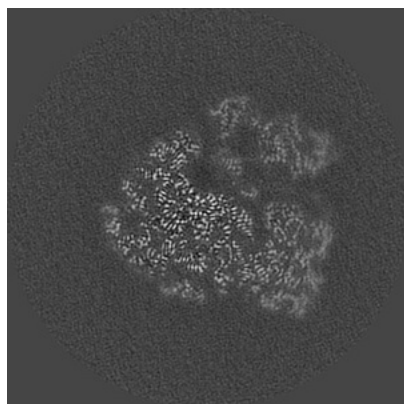


Z Index: 180

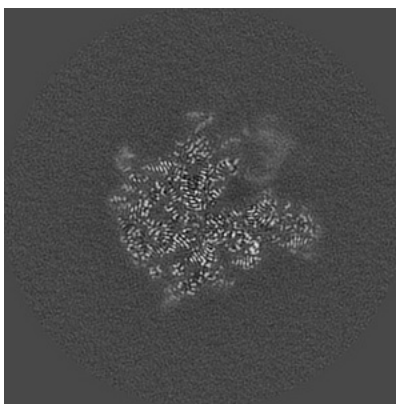
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

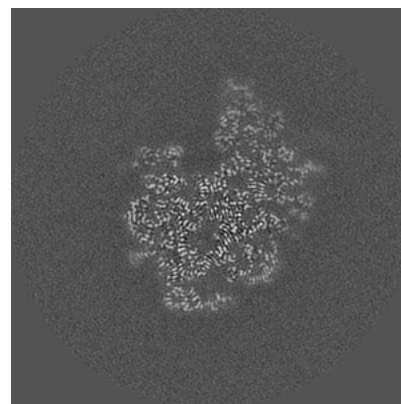
6.3.1 Primary map



X Index: 190



Y Index: 172

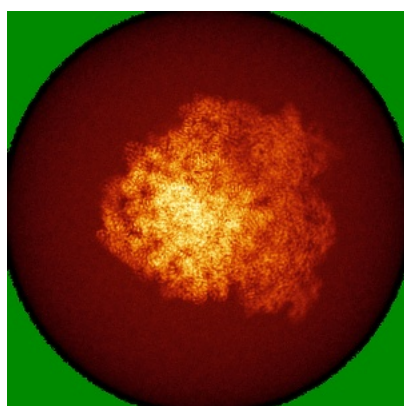


Z Index: 169

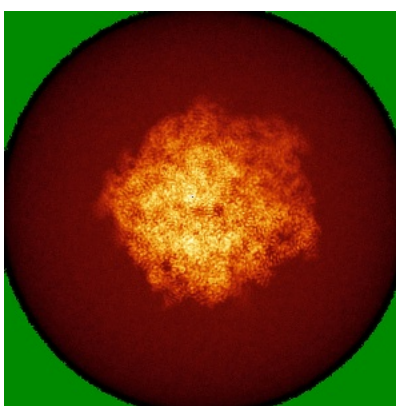
The images above show the largest variance slices of the map in three orthogonal directions.

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

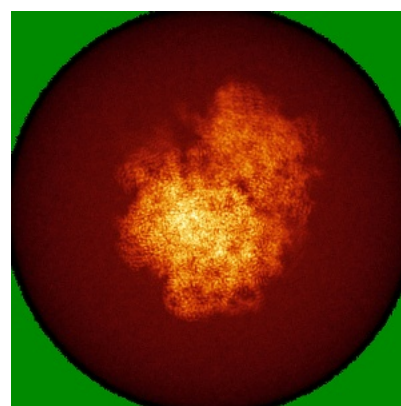
6.4.1 Primary map



X



Y

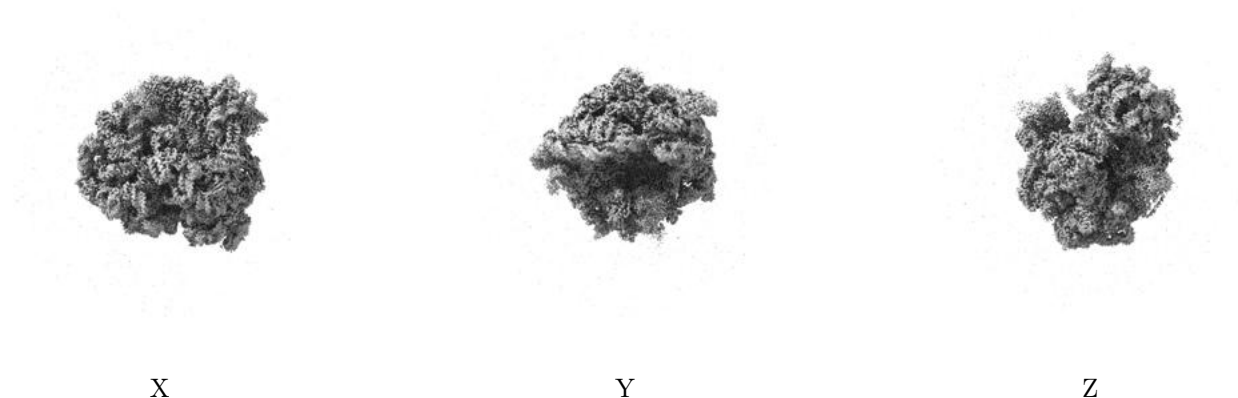


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

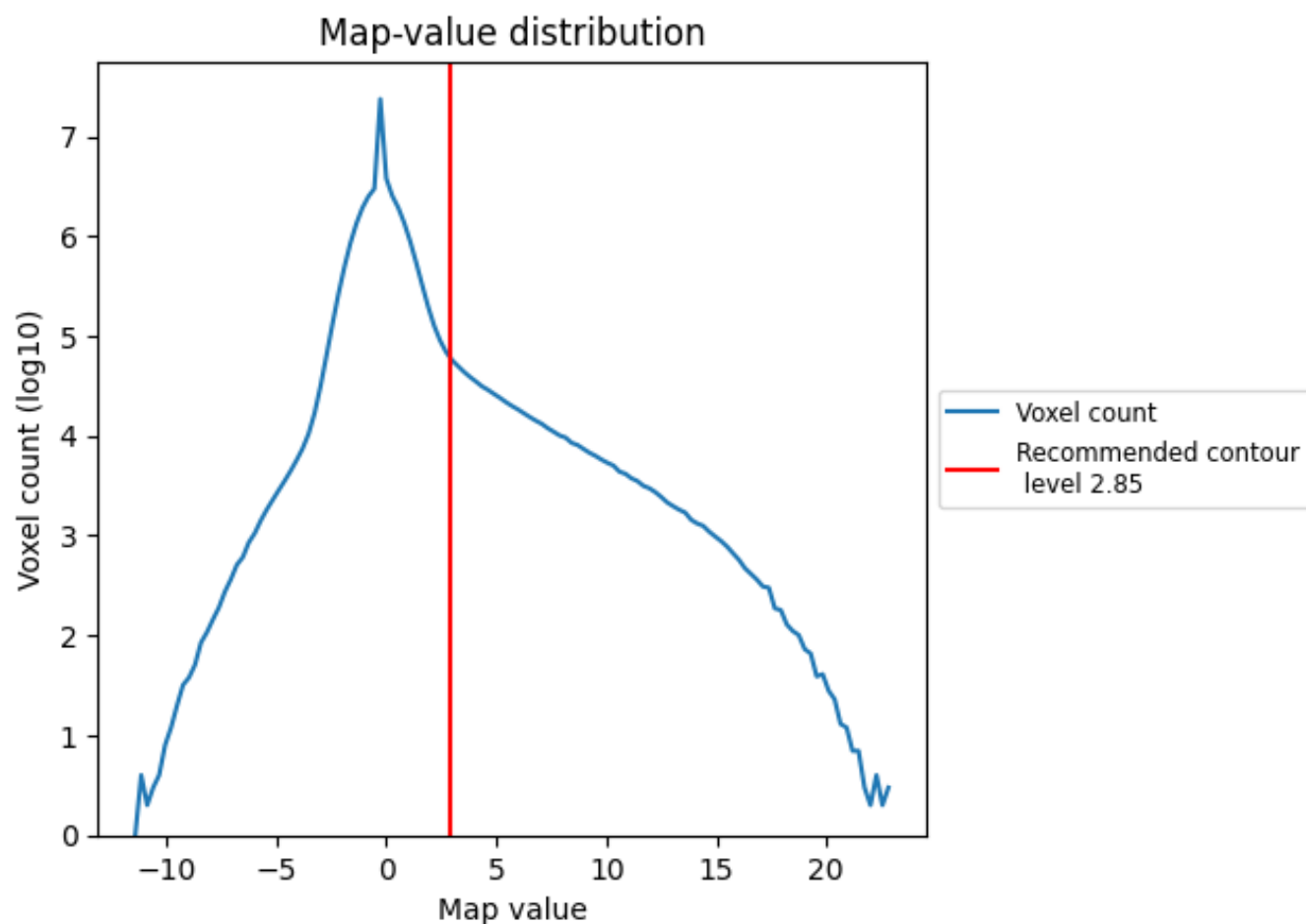
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

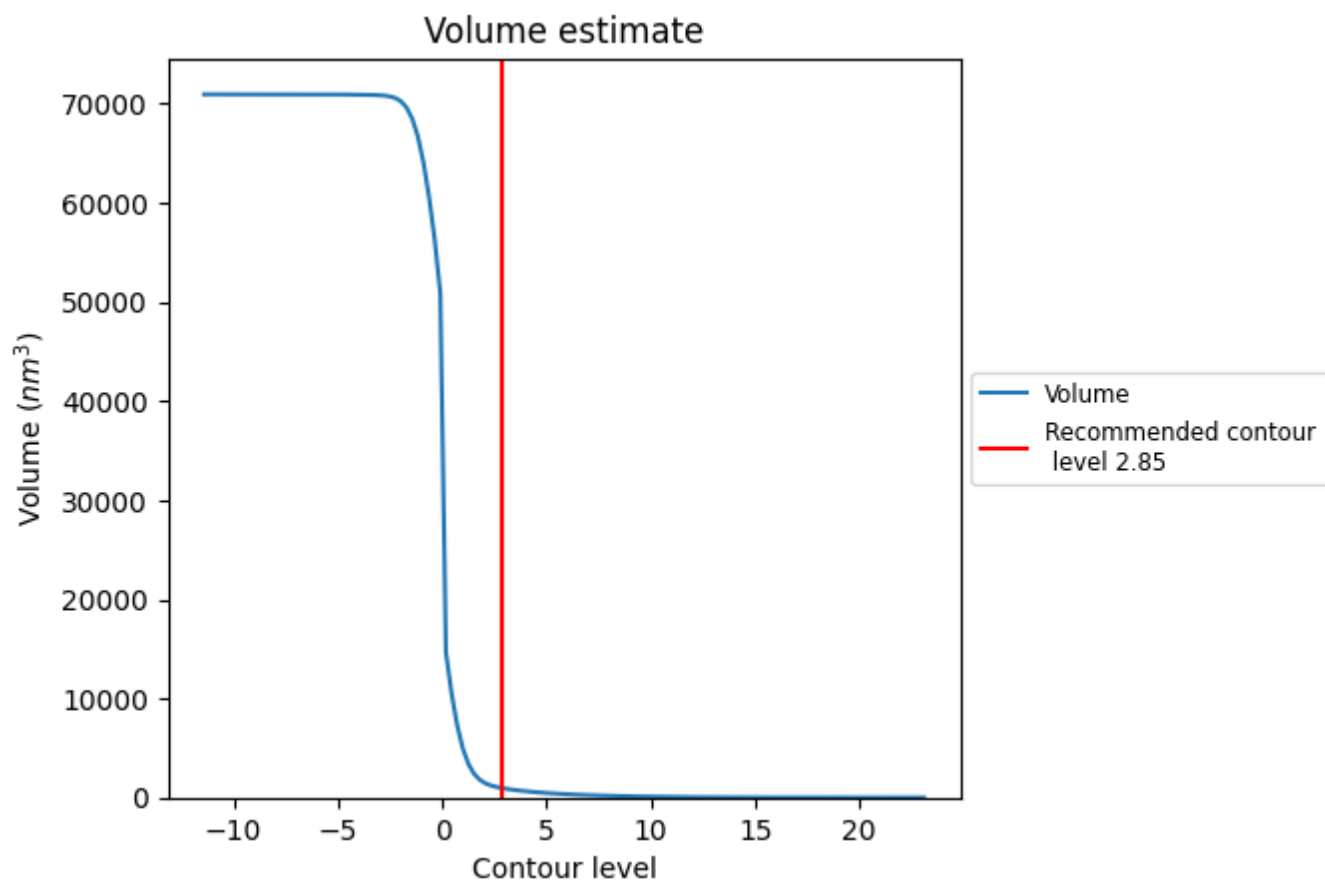
This section contains the results of statistical analysis of the map.

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.

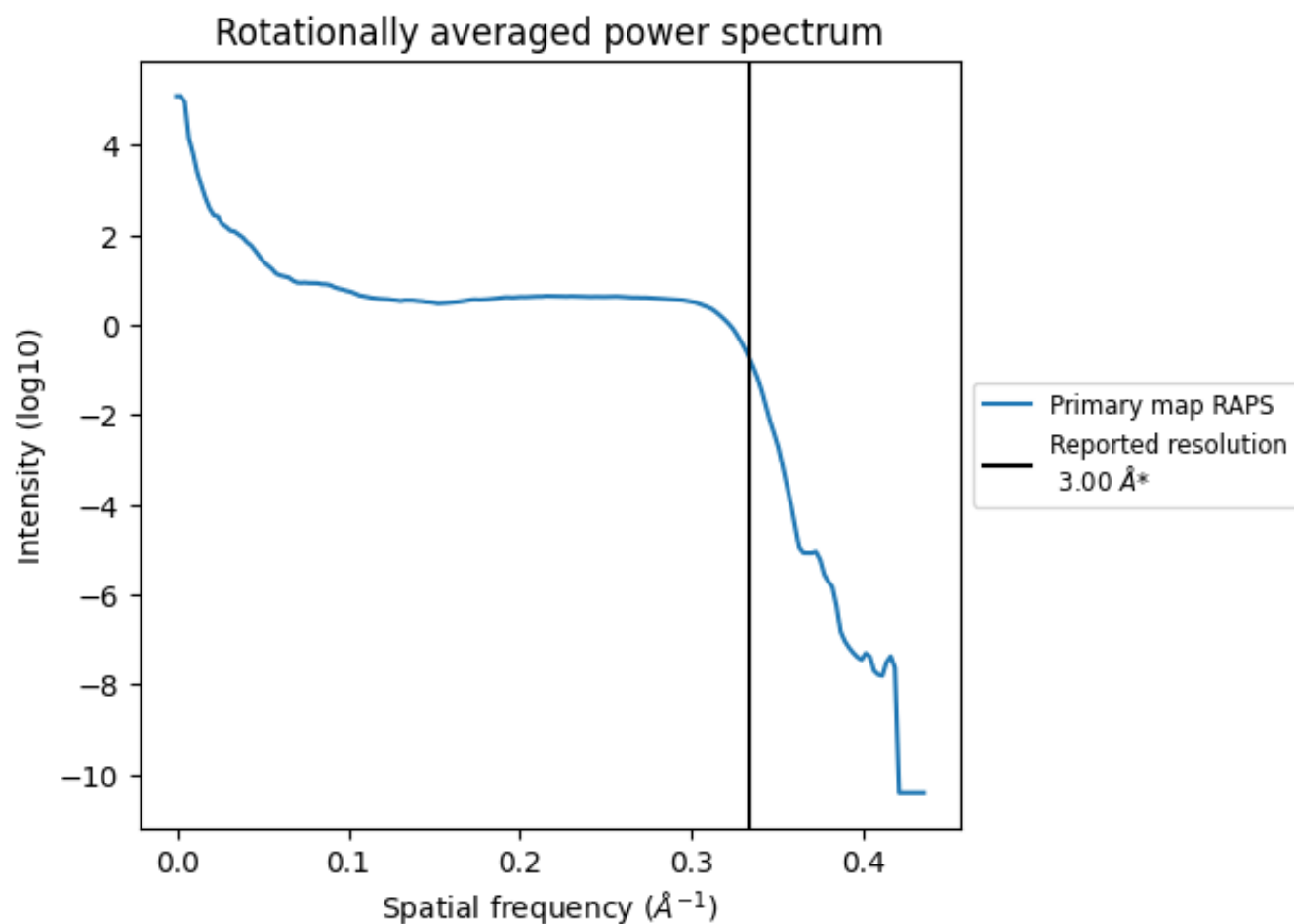
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 959 nm³; this corresponds to an approximate mass of 866 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 0.333 Å⁻¹

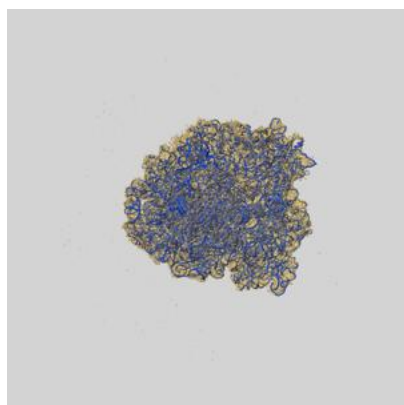
8 Fourier-Shell correlation

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

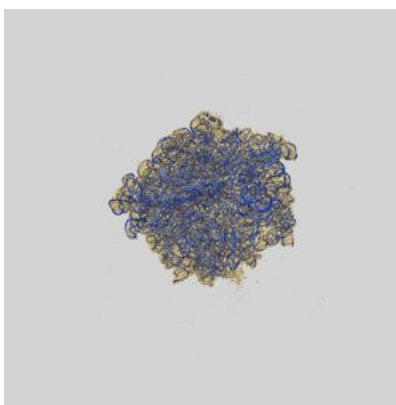
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13805 and PDB model 7Q4K. Per-residue inclusion information can be found in section 3 on page 16.

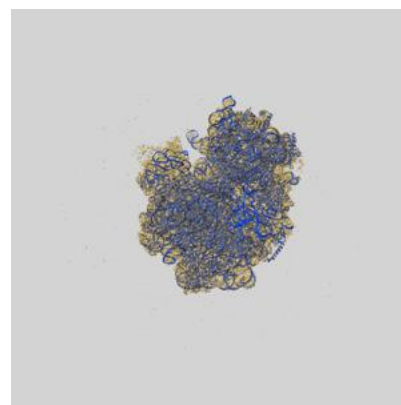
9.1 Map-model overlay [i](#)



X



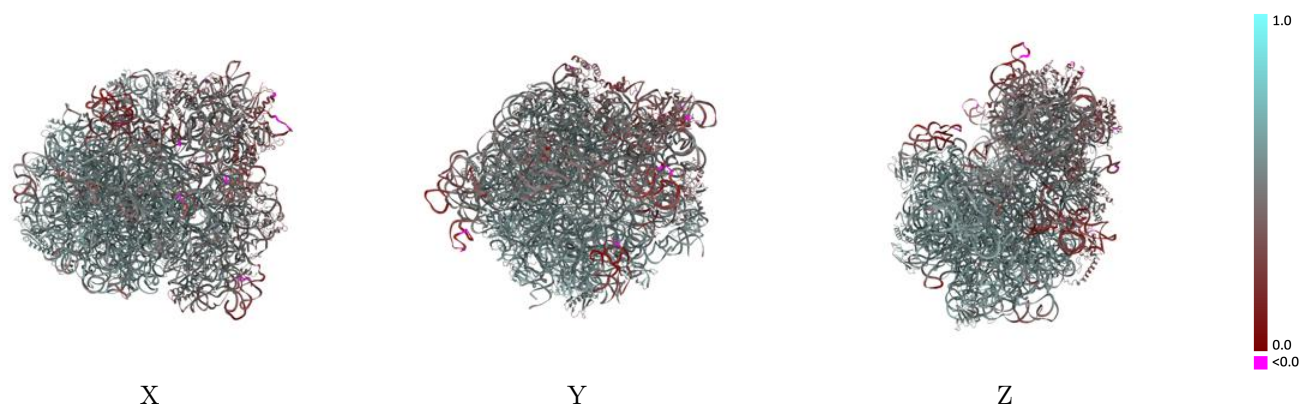
Y



Z

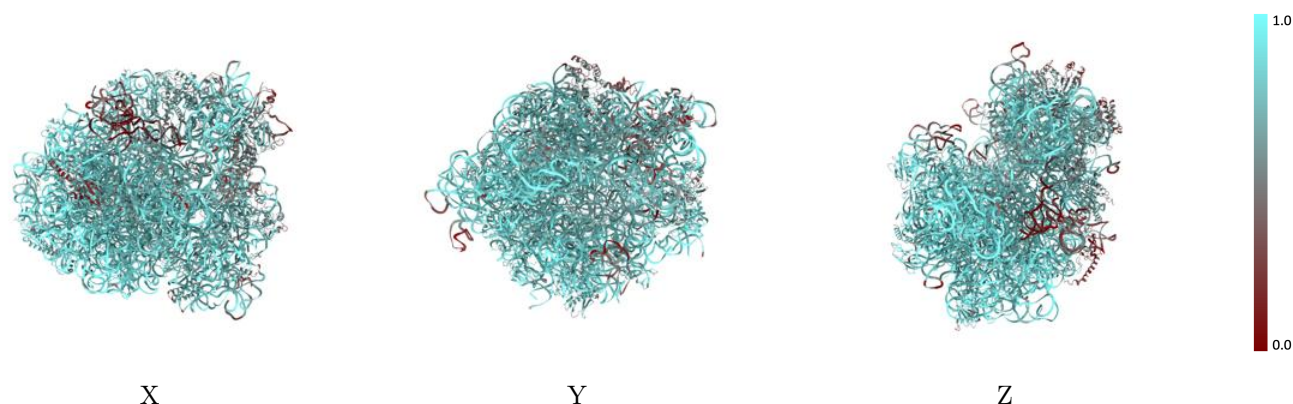
The images above show the 3D surface view of the map at the recommended contour level 2.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



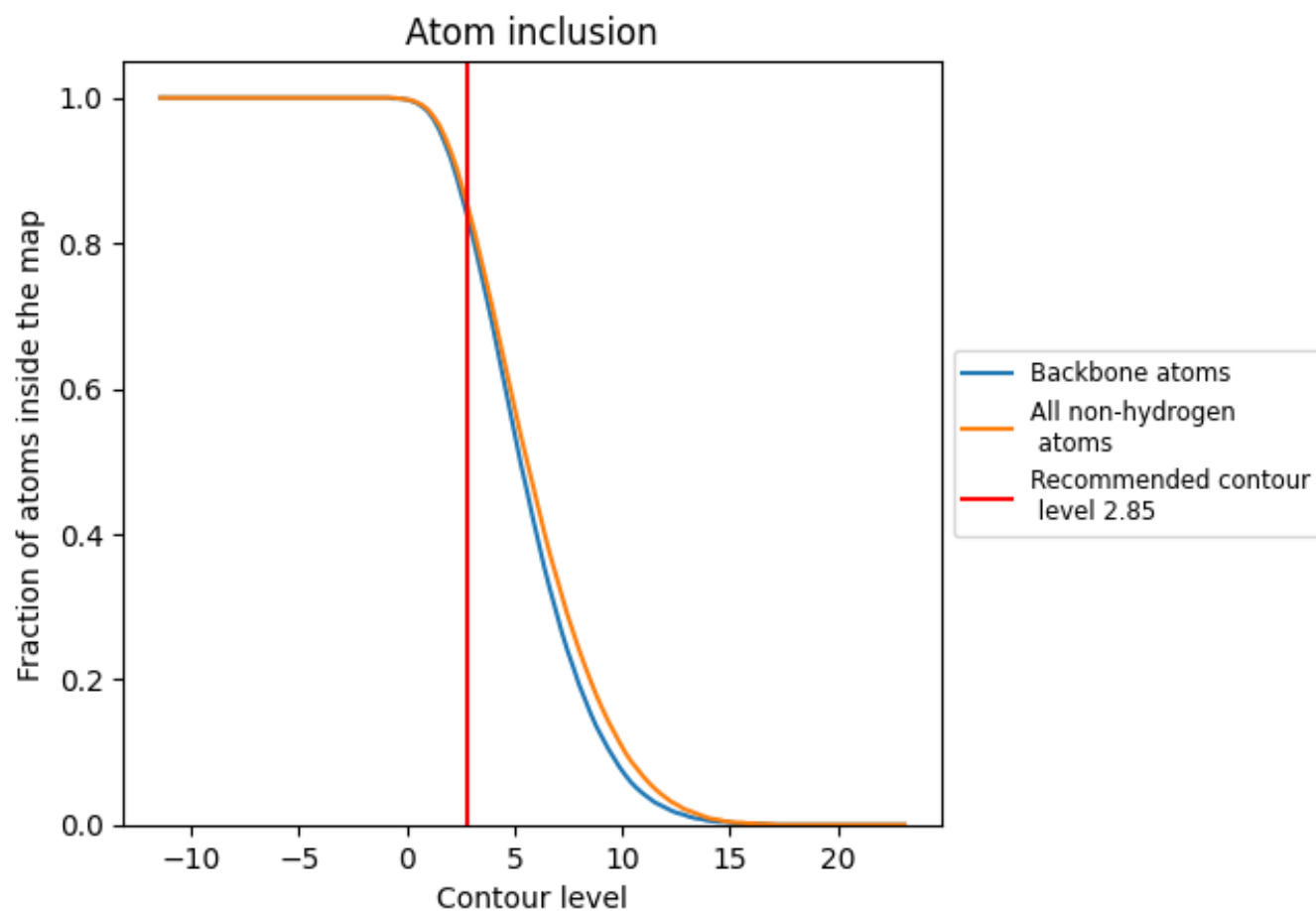
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.85).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (2.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.5140
AA	 0.8790	 0.4770
AB	 0.4950	 0.3570
AC	 0.6150	 0.4030
AD	 0.6160	 0.4130
AE	 0.7280	 0.4880
AF	 0.6710	 0.4290
AG	 0.5470	 0.3450
AH	 0.7160	 0.4960
AI	 0.6330	 0.3880
AJ	 0.5050	 0.3260
AK	 0.7350	 0.4870
AL	 0.7280	 0.5090
AM	 0.6490	 0.3910
AN	 0.6760	 0.4110
AO	 0.7590	 0.4920
AP	 0.7030	 0.4730
AQ	 0.6710	 0.4810
AR	 0.7390	 0.4760
AS	 0.6550	 0.4090
AT	 0.7360	 0.4740
AU	 0.6080	 0.4160
B0	 0.8600	 0.5770
B1	 0.8080	 0.5600
B2	 0.8840	 0.5990
B3	 0.9180	 0.5890
B4	 0.8870	 0.5830
BA	 0.9240	 0.5500
BB	 0.9420	 0.5430
BC	 0.8800	 0.5770
BD	 0.8780	 0.5810
BE	 0.8180	 0.5560
BF	 0.7400	 0.4930
BG	 0.7810	 0.5250
BH	 0.3300	 0.4060



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Chain	Atom inclusion	Q-score
BI	 0.5700	 0.3970
BJ	 0.8900	 0.5850
BK	 0.8360	 0.5700
BL	 0.8560	 0.5630
BM	 0.8630	 0.5740
BN	 0.9320	 0.5940
BO	 0.8520	 0.5480
BP	 0.8420	 0.5740
BQ	 0.9000	 0.5860
BR	 0.8630	 0.5730
BS	 0.8730	 0.5780
BT	 0.8120	 0.5570
BU	 0.8270	 0.5500
BV	 0.8360	 0.5560
BW	 0.8920	 0.5760
BX	 0.8650	 0.5680
BY	 0.8240	 0.5540
BZ	 0.8440	 0.5680
D1	 0.7680	 0.5620
D2	 0.7750	 0.4750
D3	 0.1840	 0.3060
D4	 0.7090	 0.4500