



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 02:14 am BST

PDB ID : 7O1A / pdb_00007o1a
EMDB ID : EMD-12694
Title : Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome complex stalled in response to L-tryptophan
Authors : van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on : 2021-03-29
Resolution : 2.40 Å(reported)
Based on initial model : 6TBV

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:

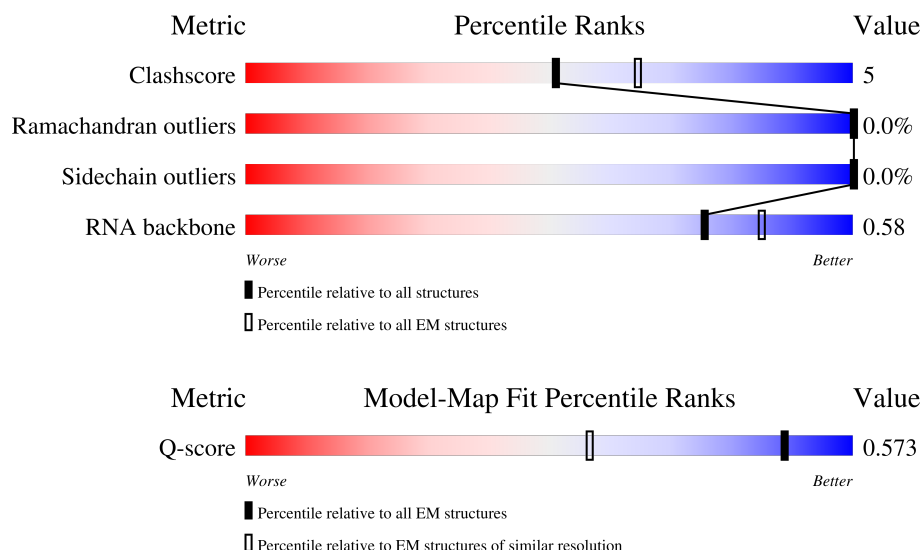
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.40 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.



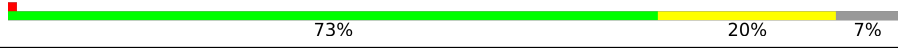
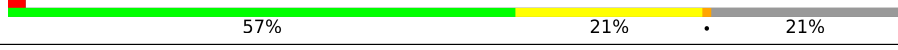
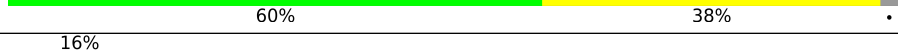
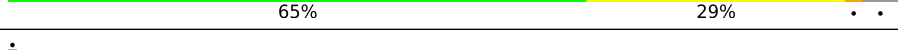
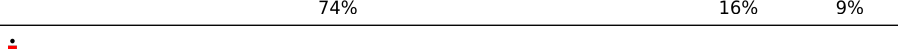
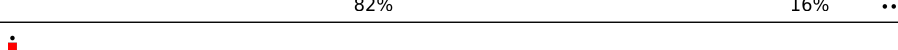
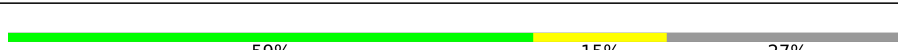
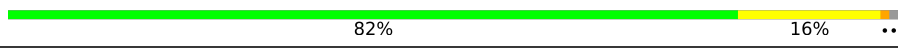
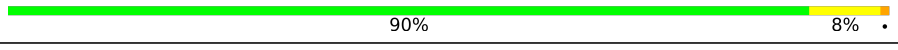
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	240	

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Mol	Chain	Length	Quality of chain
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	

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Mol	Chain	Length	Quality of chain
28	BG	177	
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	

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Mol	Chain	Length	Quality of chain
53	B5	17	76% 18% 6%
54	B7	9	56% 33% 11%
55	B8	77	49% 39% 8%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 146602 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 Ribosomal RNA 16S.

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 P0AG59

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			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 Ribosomal RNA 23S.

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 Ribosomal RNA 5S.

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 TnaC - Tryptophanase leader peptide - R23F.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	97	24	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	9	Total	C	N	O	P	0	0
			191	85	34	63	9		

- Molecule 55 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total	C	N	O	P	0	0
			1648	735	295	541	77		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	86	Total	Mg	0
			86	86	
56	BA	233	Total	Mg	0
			233	233	
56	BB	1	Total	Mg	0
			1	1	
56	BC	1	Total	Mg	0
			1	1	
56	BD	2	Total	Mg	0
			2	2	
56	BL	1	Total	Mg	0
			1	1	
56	B8	2	Total	Mg	0
			2	2	

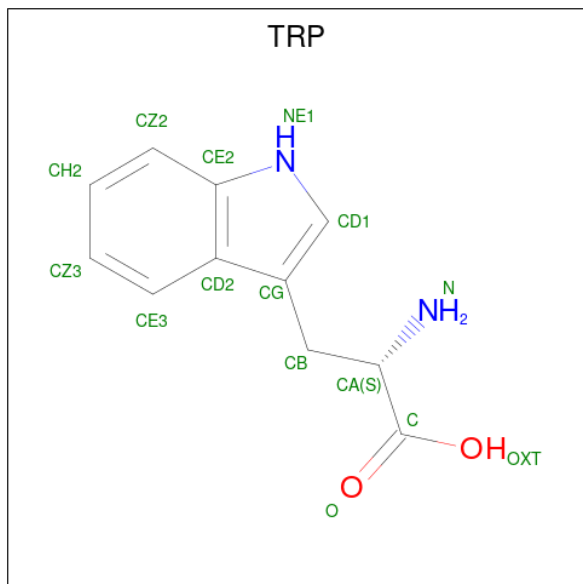
- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	AA	38	Total	K	0
			38	38	
57	AM	1	Total	K	0
			1	1	
57	BA	104	Total	K	0
			104	104	
57	BB	1	Total	K	0
			1	1	
57	BC	1	Total	K	0
			1	1	
57	BD	1	Total	K	0
			1	1	
57	BM	1	Total	K	0
			1	1	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	AB	1	Total	Zn	0
			1	1	
58	BI	1	Total	Zn	0
			1	1	
58	B4	1	Total	Zn	0
			1	1	

- Molecule 59 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
59	BA	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	AA	184	Total	O	0
			184	184	
60	AK	1	Total	O	0
			1	1	
60	AN	1	Total	O	0
			1	1	
60	BA	1672	Total	O	0
			1672	1672	
60	BB	2	Total	O	0
			2	2	
60	BC	38	Total	O	0
			38	38	

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Mol	Chain	Residues	Atoms		AltConf
60	BD	14	Total 14	O 14	0
60	BE	21	Total 21	O 21	0
60	BF	1	Total 1	O 1	0
60	BJ	2	Total 2	O 2	0
60	BK	3	Total 3	O 3	0
60	BL	14	Total 14	O 14	0
60	BM	2	Total 2	O 2	0
60	BN	9	Total 9	O 9	0
60	BO	1	Total 1	O 1	0
60	BP	2	Total 2	O 2	0
60	BQ	12	Total 12	O 12	0
60	BR	4	Total 4	O 4	0
60	BS	7	Total 7	O 7	0
60	BT	3	Total 3	O 3	0
60	BU	1	Total 1	O 1	0
60	BW	5	Total 5	O 5	0
60	BX	4	Total 4	O 4	0
60	B0	4	Total 4	O 4	0
60	B2	6	Total 6	O 6	0
60	B3	7	Total 7	O 7	0
60	B4	1	Total 1	O 1	0

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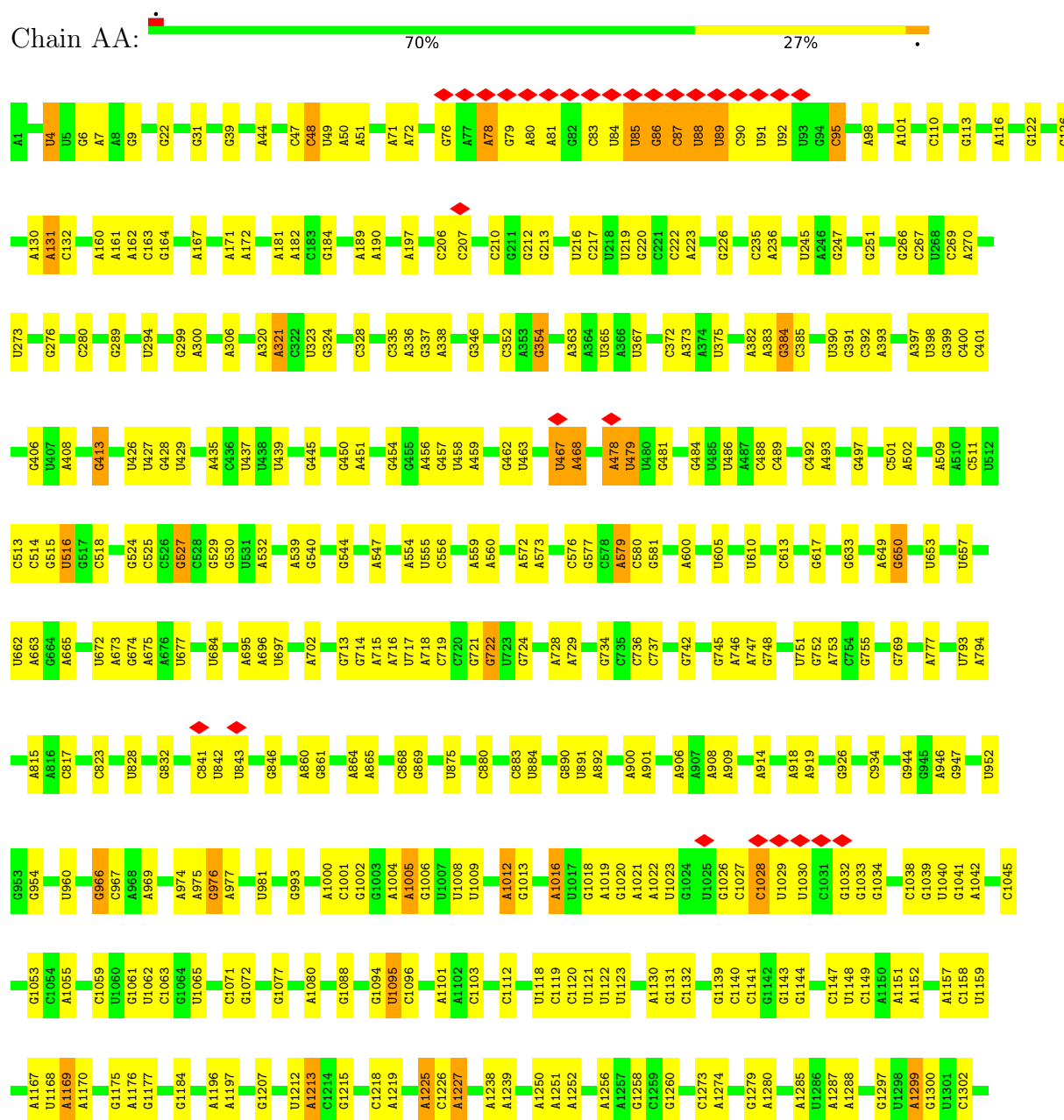
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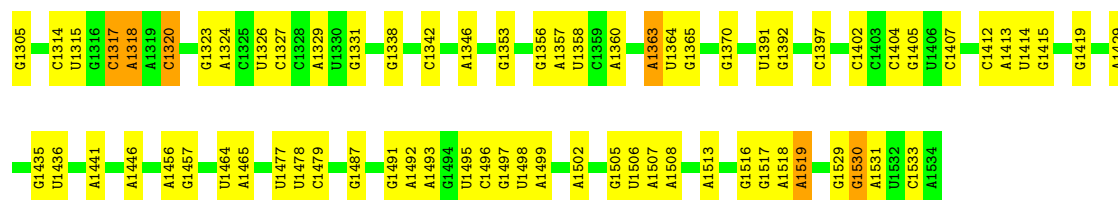
Mol	Chain	Residues	Atoms		AltConf
60	B5	2	Total	O	0
			2	2	
60	B8	3	Total	O	0
			3	3	

3 Residue-property plots

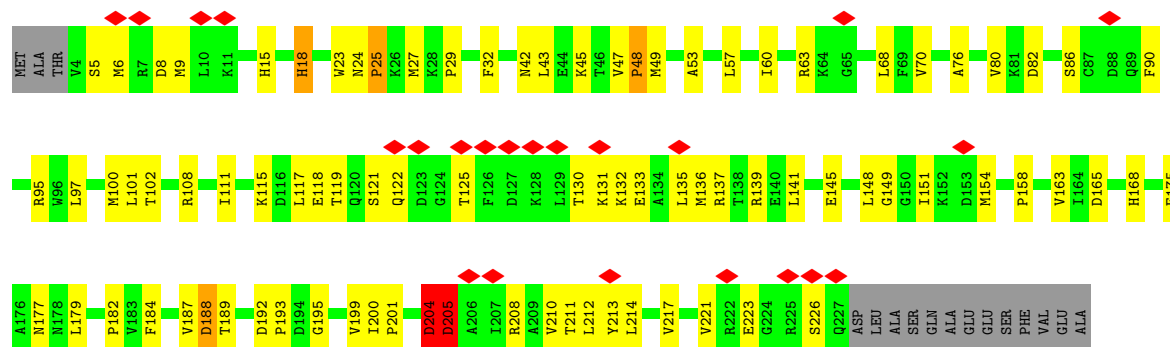
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ribosomal RNA 16S

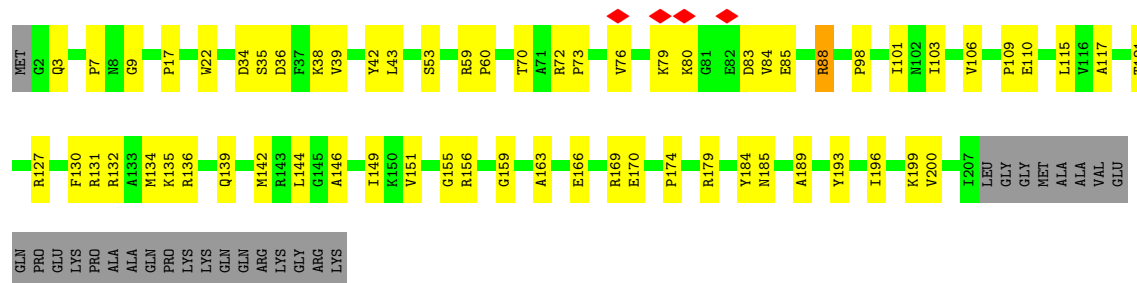




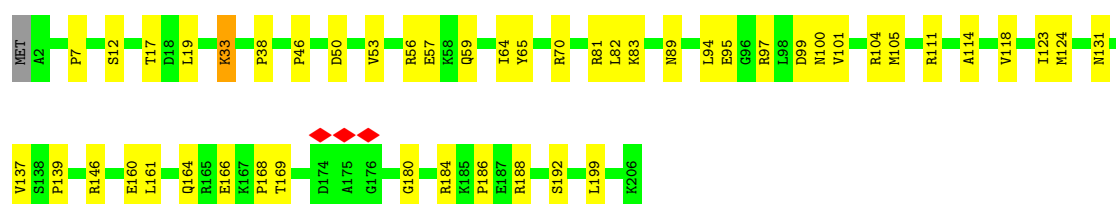
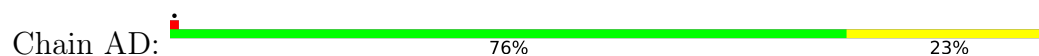
• Molecule 2: 30S ribosomal protein S2



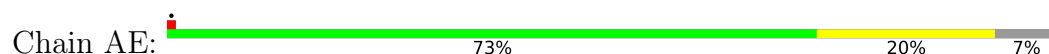
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

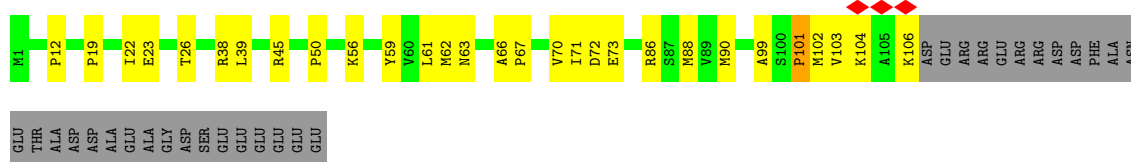


• Molecule 5: 30S ribosomal protein S5

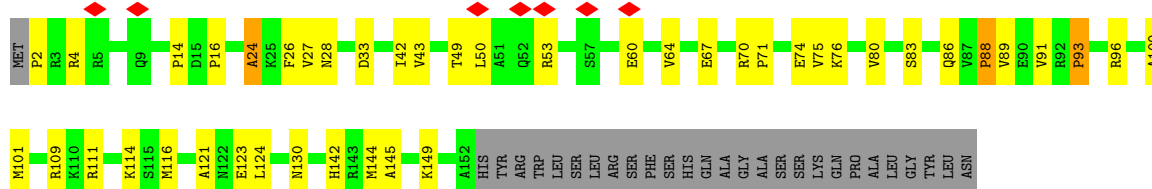




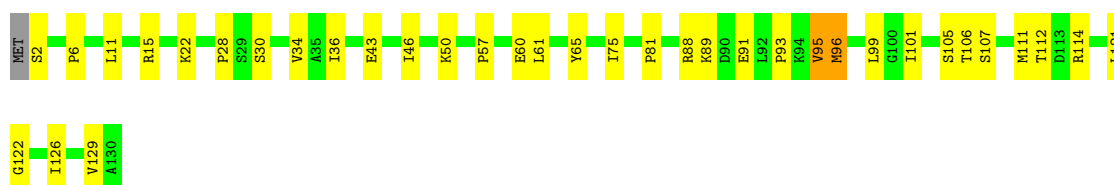
- Molecule 6: 30S ribosomal protein S6



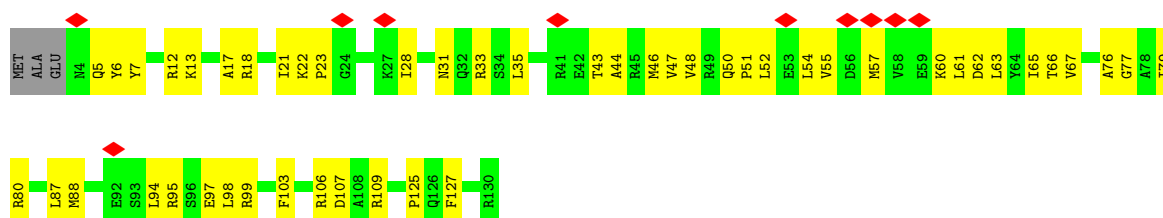
- Molecule 7: 30S ribosomal protein S7



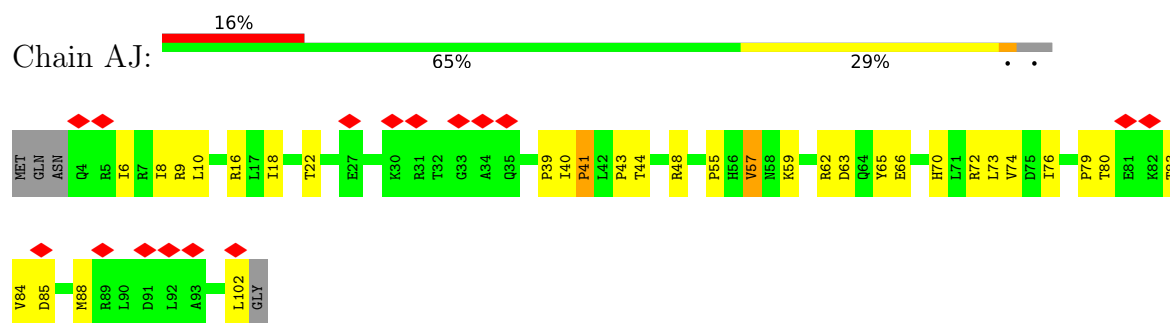
- Molecule 8: 30S ribosomal protein S8



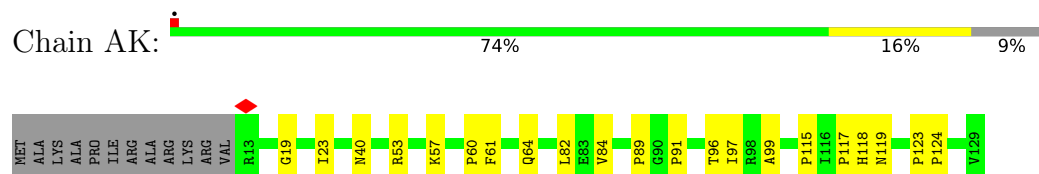
- Molecule 9: 30S ribosomal protein S9



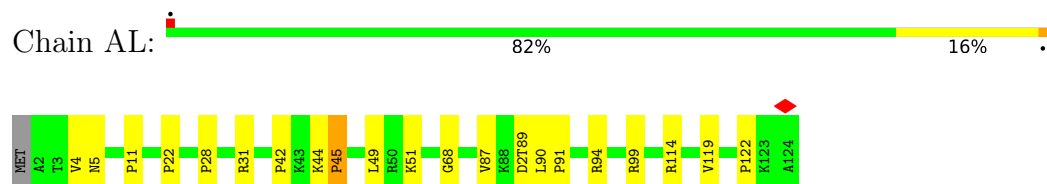
- Molecule 10: 30S ribosomal protein S10



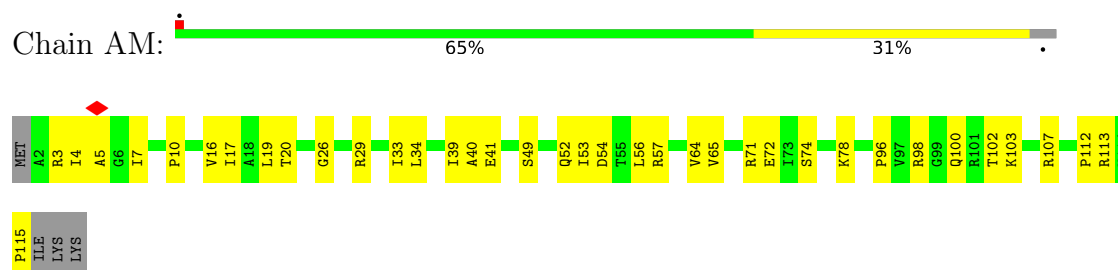
- Molecule 11: 30S ribosomal protein S11



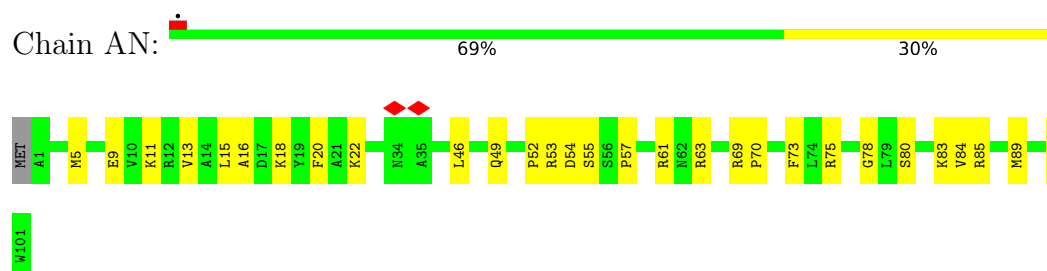
- Molecule 12: 30S ribosomal protein S12



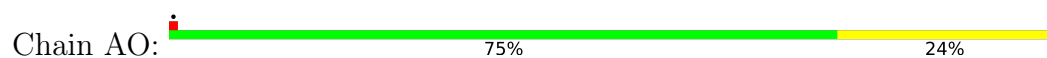
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

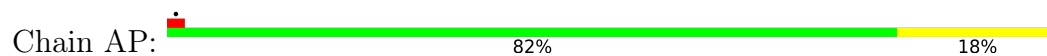


- Molecule 15: 30S ribosomal protein S15

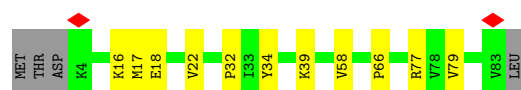
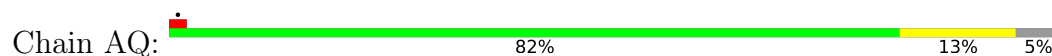




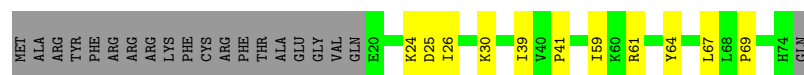
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



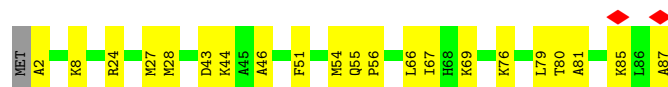
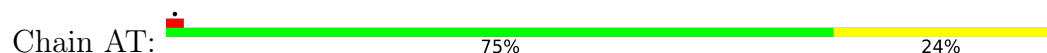
- Molecule 18: 30S ribosomal protein S18



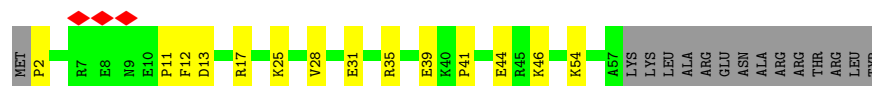
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

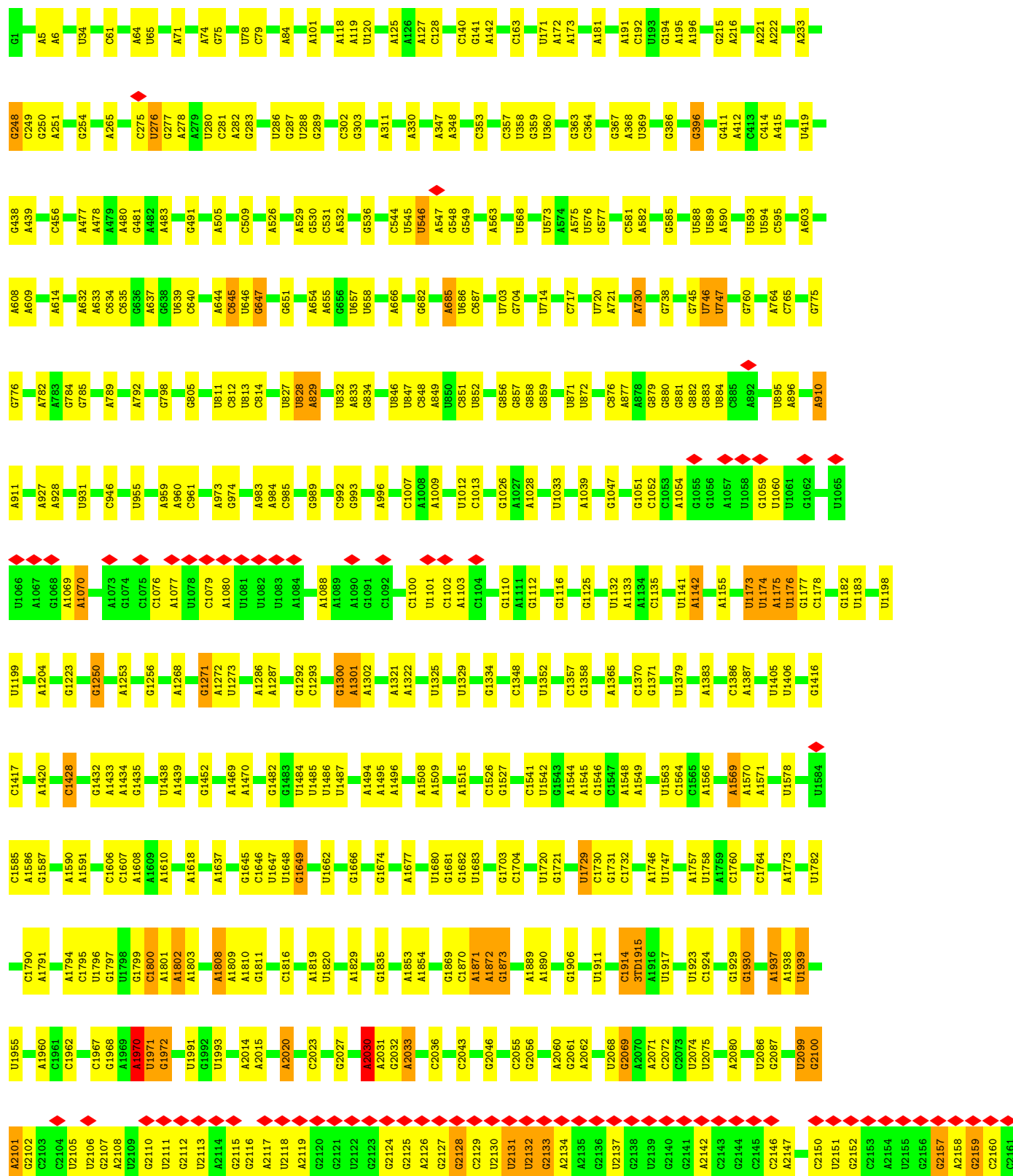


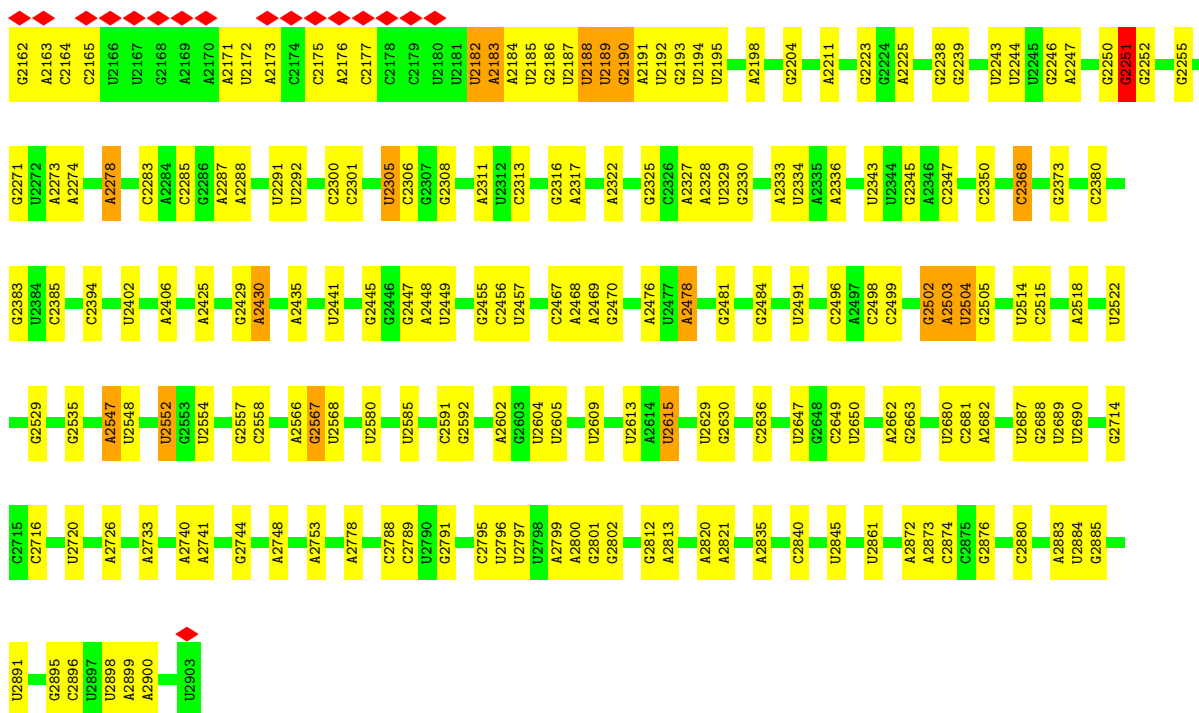
- Molecule 21: 30S ribosomal protein S21



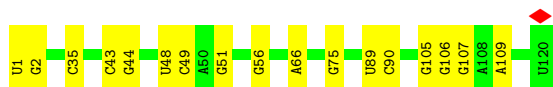
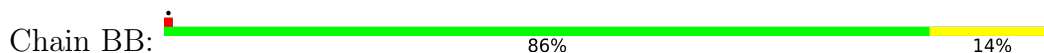
● Molecule 22: Ribosomal RNA 23S

Chain BA:

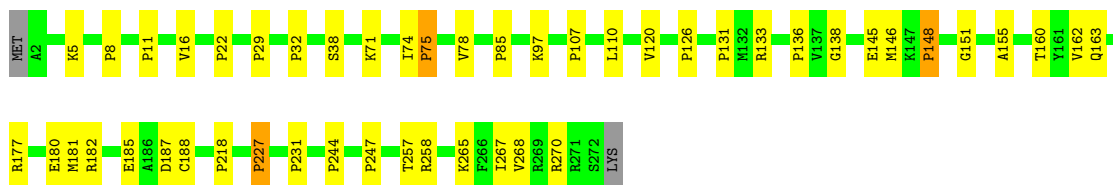
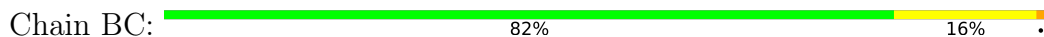




- Molecule 23: Ribosomal RNA 5S



- Molecule 24: 50S ribosomal protein L2



- Molecule 25: 50S ribosomal protein L3



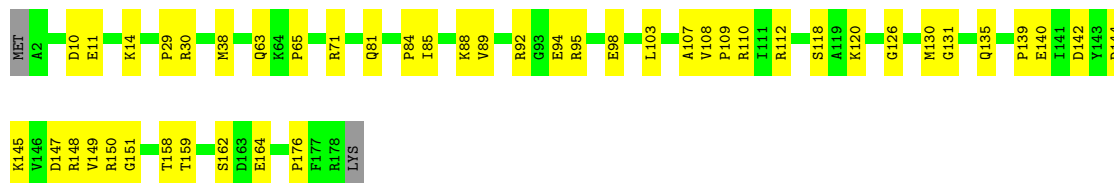
- Molecule 26: 50S ribosomal protein L4





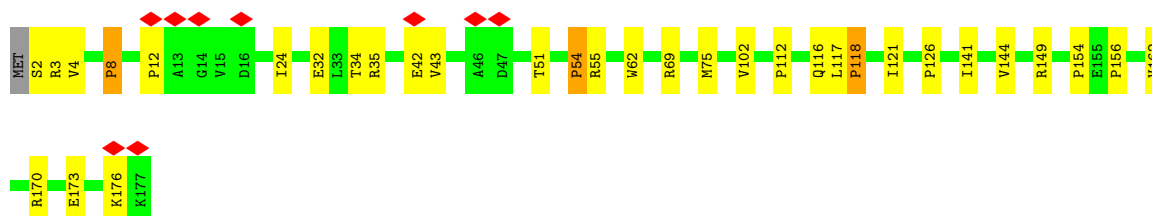
- Molecule 27: 50S ribosomal protein L5

Chain BF: 74% 25%



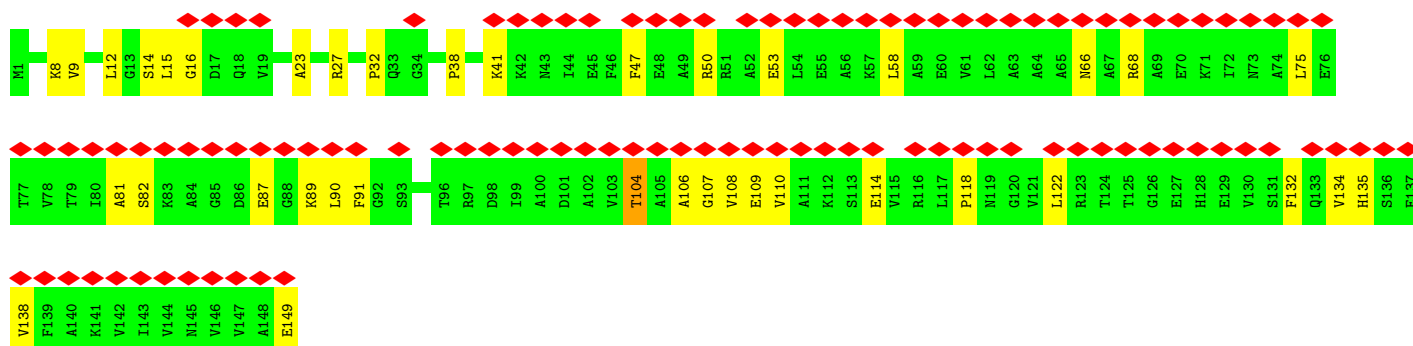
- Molecule 28: 50S ribosomal protein L6

Chain BG: 5% 81% 17%



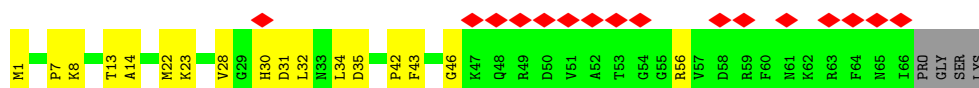
- Molecule 29: 50S ribosomal protein L9

Chain BH: 71% 74% 25%



- Molecule 30: 50S ribosomal protein L31

Chain BI: 23% 70% 24% 6%



- Molecule 31: 50S ribosomal protein L13

Chain BJ:  80% 20%



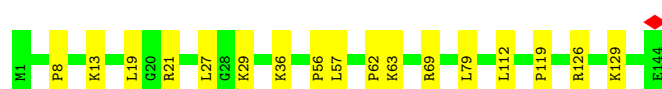
- Molecule 32: 50S ribosomal protein L14

Chain BK:  84% 16%



- Molecule 33: 50S ribosomal protein L15

Chain BL:  88% 12%



- Molecule 34: 50S ribosomal protein L16

Chain BM:  80% 19%



- Molecule 35: 50S ribosomal protein L17

Chain BN:  80% 13% 7%



- Molecule 36: 50S ribosomal protein L18

Chain BO:  91% 9%

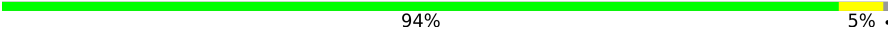


- Molecule 37: 50S ribosomal protein L19

Chain BP:  89% 10%



- Molecule 38: 50S ribosomal protein L20

Chain BQ:  94% 5%



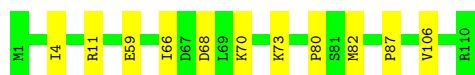
- Molecule 39: 50S ribosomal protein L21

Chain BR:  90% 10%



- Molecule 40: 50S ribosomal protein L22

Chain BS:  90% 10%



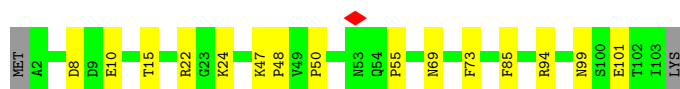
- Molecule 41: 50S ribosomal protein L23

Chain BT:  76% 16% 7%



- Molecule 42: 50S ribosomal protein L24

Chain BU:  84% 14%



- Molecule 43: 50S ribosomal protein L25

Chain BV:  77% 23%



- Molecule 44: 50S ribosomal protein L27

Chain BW:  75% 14% 11%



- Molecule 45: 50S ribosomal protein L28

Chain BX:  87% 12%



- Molecule 46: 50S ribosomal protein L29

Chain BY:  87% 11%



- Molecule 47: 50S ribosomal protein L30

Chain BZ:  88% 10%



- Molecule 48: 50S ribosomal protein L32

Chain B0:  82% 16%



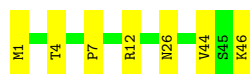
- Molecule 49: 50S ribosomal protein L33

Chain B1:  60% 33% 7%



- Molecule 50: 50S ribosomal protein L34

Chain B2:  85% 15%



- Molecule 51: 50S ribosomal protein L35

Chain B3:  88% 11%



- Molecule 52: 50S ribosomal protein L36

Chain B4:  84% 16%



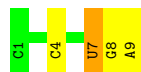
- Molecule 53: TnaC - Tryptophanase leader peptide - R23F

Chain B5:  76% 18% 6%



- Molecule 54: mRNA

Chain B7:  56% 33% 11%



- Molecule 55: P-site tRNA-Pro

Chain B8:  49% 39% 8% 4%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	191230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-1600	Depositor
Magnification	59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	271.375, 271.375, 271.375	wwPDB
Map dimensions	325, 325, 325	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.58	0/36593	0.70	1/57081 (0.0%)
2	AB	0.91	9/1784 (0.5%)	0.97	9/2403 (0.4%)
3	AC	0.84	7/1651 (0.4%)	0.67	2/2225 (0.1%)
4	AD	0.78	6/1665 (0.4%)	0.61	2/2227 (0.1%)
5	AE	0.85	5/1157 (0.4%)	0.58	0/1557
6	AF	0.92	5/881 (0.6%)	0.55	0/1189
7	AG	0.99	7/1195 (0.6%)	0.78	2/1602 (0.1%)
8	AH	0.96	6/989 (0.6%)	0.70	3/1326 (0.2%)
9	AI	0.71	3/1034 (0.3%)	0.69	0/1375
10	AJ	1.08	7/805 (0.9%)	0.75	0/1089
11	AK	1.11	7/893 (0.8%)	0.68	0/1205
12	AL	1.08	9/960 (0.9%)	0.58	1/1286 (0.1%)
13	AM	0.91	5/892 (0.6%)	0.73	2/1193 (0.2%)
14	AN	0.89	4/811 (0.5%)	0.63	0/1081
15	AO	0.25	0/722	0.53	0/964
16	AP	0.71	2/659 (0.3%)	0.58	0/884
17	AQ	0.70	2/657 (0.3%)	0.68	2/881 (0.2%)
18	AR	0.82	2/462 (0.4%)	0.49	0/621
19	AS	1.07	5/672 (0.7%)	0.66	1/904 (0.1%)
20	AT	0.53	1/676 (0.1%)	0.44	0/895
21	AU	1.14	5/472 (1.1%)	0.63	0/627
22	BA	0.65	2/69121 (0.0%)	0.75	3/107828 (0.0%)
23	BB	0.54	0/2872	0.62	0/4478
24	BC	1.12	17/2121 (0.8%)	0.58	0/2852
25	BD	0.84	8/1576 (0.5%)	0.51	0/2119
26	BE	0.73	5/1571 (0.3%)	0.52	0/2113
27	BF	0.82	6/1434 (0.4%)	0.59	1/1926 (0.1%)
28	BG	0.96	8/1343 (0.6%)	0.55	0/1816
29	BH	0.68	3/1121 (0.3%)	0.67	1/1515 (0.1%)
30	BI	0.77	2/531 (0.4%)	0.76	0/709
31	BJ	0.89	6/1152 (0.5%)	0.50	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	0.91	5/955 (0.5%)	0.53	0/1279
33	BL	0.81	4/1062 (0.4%)	0.49	0/1413
34	BM	1.00	7/1081 (0.6%)	0.55	0/1443
35	BN	0.84	4/958 (0.4%)	0.56	0/1281
36	BO	0.61	2/910 (0.2%)	0.42	0/1219
37	BP	0.77	3/929 (0.3%)	0.51	0/1242
38	BQ	0.33	0/960	0.48	0/1278
39	BR	0.61	3/829 (0.4%)	0.47	0/1107
40	BS	0.66	2/864 (0.2%)	0.50	0/1156
41	BT	0.66	1/744 (0.1%)	0.76	3/994 (0.3%)
42	BU	0.80	3/787 (0.4%)	0.51	0/1051
43	BV	0.91	4/766 (0.5%)	0.51	0/1025
44	BW	0.61	1/587 (0.2%)	0.48	0/776
45	BX	0.74	2/635 (0.3%)	0.52	0/848
46	BY	0.23	0/502	0.38	0/667
47	BZ	0.82	2/453 (0.4%)	0.48	0/605
48	B0	0.62	1/450 (0.2%)	0.51	0/599
49	B1	0.89	2/421 (0.5%)	0.55	0/561
50	B2	0.74	1/380 (0.3%)	0.51	0/498
51	B3	1.14	4/513 (0.8%)	0.57	0/676
52	B4	0.74	1/303 (0.3%)	0.49	0/397
53	B5	1.40	2/151 (1.3%)	1.10	1/205 (0.5%)
54	B7	0.94	1/212 (0.5%)	0.89	1/328 (0.3%)
55	B8	0.67	1/1765 (0.1%)	0.74	2/2750 (0.1%)
All	All	0.70	210/155689 (0.1%)	0.70	37/232920 (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
2	AB	0	2
7	AG	0	1
29	BH	0	2
43	BV	0	1
All	All	0	6

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AJ	41	PRO	N-CD	13.03	1.66	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AG	2	PRO	N-CD	12.99	1.66	1.47
21	AU	2	PRO	N-CD	12.59	1.65	1.47
51	B3	63	PRO	N-CD	12.24	1.64	1.47
24	BC	11	PRO	N-CD	12.16	1.64	1.47
12	AL	45	PRO	N-CD	12.15	1.64	1.47
29	BH	118	PRO	N-CD	12.11	1.64	1.47
10	AJ	39	PRO	N-CD	12.08	1.64	1.47
28	BG	156	PRO	N-CD	12.02	1.64	1.47
25	BD	152	PRO	N-CD	12.02	1.64	1.47
39	BR	52	PRO	N-CD	12.01	1.64	1.47
24	BC	8	PRO	N-CD	12.00	1.64	1.47
11	AK	117	PRO	N-CD	11.96	1.64	1.47
3	AC	174	PRO	N-CD	11.90	1.64	1.47
8	AH	93	PRO	N-CD	11.87	1.64	1.47
2	AB	29	PRO	N-CD	11.87	1.64	1.47
27	BF	84	PRO	N-CD	11.86	1.64	1.47
7	AG	14	PRO	N-CD	11.85	1.64	1.47
51	B3	2	PRO	N-CD	11.84	1.64	1.47
13	AM	115	PRO	N-CD	11.83	1.64	1.47
33	BL	8	PRO	N-CD	11.82	1.64	1.47
5	AE	150	PRO	N-CD	11.81	1.64	1.47
21	AU	11	PRO	N-CD	11.79	1.64	1.47
8	AH	6	PRO	N-CD	11.79	1.64	1.47
10	AJ	79	PRO	N-CD	11.79	1.64	1.47
50	B2	7	PRO	N-CD	11.74	1.64	1.47
40	BS	87	PRO	N-CD	11.68	1.64	1.47
25	BD	23	PRO	N-CD	11.67	1.64	1.47
35	BN	85	PRO	N-CD	11.67	1.64	1.47
5	AE	98	PRO	N-CD	11.66	1.64	1.47
36	BO	32	PRO	N-CD	11.63	1.64	1.47
20	AT	56	PRO	N-CD	11.63	1.64	1.47
3	AC	17	PRO	N-CD	11.63	1.64	1.47
2	AB	48	PRO	N-CD	11.62	1.64	1.47
7	AG	71	PRO	N-CD	11.62	1.64	1.47
4	AD	38	PRO	N-CD	11.60	1.64	1.47
43	BV	84	PRO	N-CD	11.58	1.64	1.47
24	BC	29	PRO	N-CD	11.57	1.64	1.47
53	B5	24	PRO	N-CD	11.56	1.64	1.47
14	AN	52	PRO	N-CD	11.56	1.64	1.47
34	BM	69	PRO	N-CD	11.56	1.64	1.47
42	BU	48	PRO	N-CD	11.56	1.64	1.47
28	BG	118	PRO	N-CD	11.52	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	193	PRO	N-CD	11.52	1.63	1.47
28	BG	154	PRO	N-CD	11.52	1.63	1.47
24	BC	247	PRO	N-CD	11.51	1.63	1.47
41	BT	14	PRO	N-CD	11.49	1.63	1.47
14	AN	57	PRO	N-CD	11.48	1.63	1.47
11	AK	89	PRO	N-CD	11.46	1.63	1.47
42	BU	55	PRO	N-CD	11.46	1.63	1.47
44	BW	74	PRO	N-CD	11.46	1.63	1.47
49	B1	31	PRO	N-CD	11.45	1.63	1.47
3	AC	109	PRO	N-CD	11.45	1.63	1.47
6	AF	67	PRO	N-CD	11.40	1.63	1.47
24	BC	85	PRO	N-CD	11.40	1.63	1.47
18	AR	69	PRO	N-CD	11.39	1.63	1.47
24	BC	126	PRO	N-CD	11.39	1.63	1.47
2	AB	158	PRO	N-CD	11.38	1.63	1.47
7	AG	88	PRO	N-CD	11.38	1.63	1.47
4	AD	7	PRO	N-CD	11.38	1.63	1.47
28	BG	54	PRO	N-CD	11.35	1.63	1.47
31	BJ	137	PRO	N-CD	11.35	1.63	1.47
26	BE	129	PRO	N-CD	11.33	1.63	1.47
37	BP	18	PRO	N-CD	11.32	1.63	1.47
4	AD	186	PRO	N-CD	11.31	1.63	1.47
19	AS	42	PRO	N-CD	11.30	1.63	1.47
27	BF	29	PRO	N-CD	11.30	1.63	1.47
45	BX	12	PRO	N-CD	11.28	1.63	1.47
32	BK	102	PRO	N-CD	11.27	1.63	1.47
4	AD	46	PRO	N-CD	11.27	1.63	1.47
37	BP	22	PRO	N-CD	11.26	1.63	1.47
11	AK	91	PRO	N-CD	11.26	1.63	1.47
3	AC	7	PRO	N-CD	11.23	1.63	1.47
12	AL	22	PRO	N-CD	11.23	1.63	1.47
8	AH	28	PRO	N-CD	11.22	1.63	1.47
13	AM	96	PRO	N-CD	11.22	1.63	1.47
9	AI	23	PRO	N-CD	11.21	1.63	1.47
31	BJ	97	PRO	N-CD	11.21	1.63	1.47
51	B3	46	PRO	N-CD	11.20	1.63	1.47
34	BM	72	PRO	N-CD	11.19	1.63	1.47
34	BM	125	PRO	N-CD	11.18	1.63	1.47
27	BF	176	PRO	N-CD	11.17	1.63	1.47
33	BL	62	PRO	N-CD	11.17	1.63	1.47
43	BV	37	PRO	N-CD	11.16	1.63	1.47
2	AB	201	PRO	N-CD	11.16	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AK	115	PRO	N-CD	11.15	1.63	1.47
11	AK	123	PRO	N-CD	11.14	1.63	1.47
24	BC	75	PRO	N-CD	11.14	1.63	1.47
43	BV	27	PRO	N-CD	11.13	1.63	1.47
10	AJ	43	PRO	N-CD	11.12	1.63	1.47
14	AN	70	PRO	N-CD	11.12	1.63	1.47
16	AP	41	PRO	N-CD	11.11	1.63	1.47
24	BC	32	PRO	N-CD	11.11	1.63	1.47
28	BG	126	PRO	N-CD	11.09	1.63	1.47
24	BC	107	PRO	N-CD	11.08	1.63	1.47
33	BL	119	PRO	N-CD	11.07	1.63	1.47
7	AG	93	PRO	N-CD	11.07	1.63	1.47
19	AS	59	PRO	N-CD	11.07	1.63	1.47
24	BC	22	PRO	N-CD	11.07	1.63	1.47
25	BD	194	PRO	N-CD	11.07	1.63	1.47
37	BP	79	PRO	N-CD	11.06	1.63	1.47
25	BD	63	PRO	N-CD	11.04	1.63	1.47
5	AE	57	PRO	N-CD	11.04	1.63	1.47
16	AP	15	PRO	N-CD	11.02	1.63	1.47
29	BH	32	PRO	N-CD	11.01	1.63	1.47
5	AE	84	PRO	N-CD	11.00	1.63	1.47
26	BE	89	PRO	N-CD	10.98	1.63	1.47
19	AS	30	PRO	N-CD	10.98	1.63	1.47
3	AC	60	PRO	N-CD	10.97	1.63	1.47
25	BD	205	PRO	N-CD	10.96	1.63	1.47
28	BG	112	PRO	N-CD	10.97	1.63	1.47
45	BX	31	PRO	N-CD	10.96	1.63	1.47
17	AQ	66	PRO	N-CD	10.96	1.63	1.47
42	BU	50	PRO	N-CD	10.96	1.63	1.47
12	AL	42	PRO	N-CD	10.96	1.63	1.47
13	AM	112	PRO	N-CD	10.95	1.63	1.47
8	AH	81	PRO	N-CD	10.95	1.63	1.47
12	AL	91	PRO	N-CD	10.95	1.63	1.47
2	AB	182	PRO	N-CD	10.95	1.63	1.47
30	BI	7	PRO	N-CD	10.92	1.63	1.47
26	BE	177	PRO	N-CD	10.91	1.63	1.47
12	AL	28	PRO	N-CD	10.91	1.63	1.47
33	BL	56	PRO	N-CD	10.90	1.63	1.47
36	BO	42	PRO	N-CD	10.89	1.63	1.47
26	BE	76	PRO	N-CD	10.88	1.62	1.47
34	BM	4	PRO	N-CD	10.87	1.62	1.47
49	B1	41	PRO	N-CD	10.88	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	BZ	42	PRO	N-CD	10.87	1.62	1.47
2	AB	25	PRO	N-CD	10.87	1.62	1.47
26	BE	59	PRO	N-CD	10.87	1.62	1.47
19	AS	9	PRO	N-CD	10.86	1.62	1.47
19	AS	76	PRO	N-CD	10.86	1.62	1.47
6	AF	101	PRO	N-CD	10.85	1.62	1.47
3	AC	98	PRO	N-CD	10.85	1.62	1.47
4	AD	168	PRO	N-CD	10.82	1.62	1.47
35	BN	39	PRO	N-CD	10.82	1.62	1.47
21	AU	41	PRO	N-CD	10.82	1.62	1.47
24	BC	131	PRO	N-CD	10.82	1.62	1.47
25	BD	143	PRO	N-CD	10.81	1.62	1.47
11	AK	124	PRO	N-CD	10.79	1.62	1.47
31	BJ	113	PRO	N-CD	10.79	1.62	1.47
12	AL	122	PRO	N-CD	10.77	1.62	1.47
30	BI	42	PRO	N-CD	10.77	1.62	1.47
43	BV	81	PRO	N-CD	10.77	1.62	1.47
34	BM	109	PRO	N-CD	10.75	1.62	1.47
32	BK	120	PRO	N-CD	10.74	1.62	1.47
27	BF	139	PRO	N-CD	10.73	1.62	1.47
35	BN	109	PRO	N-CD	10.73	1.62	1.47
52	B4	31	PRO	N-CD	10.73	1.62	1.47
6	AF	50	PRO	N-CD	10.72	1.62	1.47
11	AK	60	PRO	N-CD	10.71	1.62	1.47
28	BG	12	PRO	N-CD	10.69	1.62	1.47
24	BC	148	PRO	N-CD	10.69	1.62	1.47
34	BM	77	PRO	N-CD	10.68	1.62	1.47
29	BH	38	PRO	N-CD	10.68	1.62	1.47
4	AD	139	PRO	N-CD	10.67	1.62	1.47
6	AF	19	PRO	N-CD	10.64	1.62	1.47
6	AF	12	PRO	N-CD	10.63	1.62	1.47
9	AI	51	PRO	N-CD	10.63	1.62	1.47
24	BC	244	PRO	N-CD	10.61	1.62	1.47
8	AH	57	PRO	N-CD	10.61	1.62	1.47
32	BK	72	PRO	N-CD	10.59	1.62	1.47
35	BN	50	PRO	N-CD	10.58	1.62	1.47
31	BJ	110	PRO	N-CD	10.55	1.62	1.47
27	BF	109	PRO	N-CD	10.53	1.62	1.47
22	BA	2449	U	C5-C6	10.53	1.55	1.34
12	AL	11	PRO	N-CD	10.46	1.62	1.47
27	BF	65	PRO	N-CD	10.45	1.62	1.47
24	BC	218	PRO	N-CD	10.45	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	B0	8	PRO	N-CD	10.44	1.62	1.47
32	BK	94	PRO	N-CD	10.44	1.62	1.47
40	BS	80	PRO	N-CD	10.42	1.62	1.47
18	AR	41	PRO	N-CD	10.42	1.62	1.47
17	AQ	32	PRO	N-CD	10.41	1.62	1.47
34	BM	98	PRO	N-CD	10.41	1.62	1.47
24	BC	136	PRO	N-CD	10.36	1.62	1.47
28	BG	8	PRO	N-CD	10.35	1.62	1.47
9	AI	125	PRO	N-CD	10.34	1.62	1.47
10	AJ	55	PRO	N-CD	10.34	1.62	1.47
14	AN	94	PRO	N-CD	10.30	1.62	1.47
47	BZ	18	PRO	N-CD	10.27	1.62	1.47
13	AM	10	PRO	N-CD	10.26	1.62	1.47
3	AC	73	PRO	N-CD	10.21	1.62	1.47
7	AG	16	PRO	N-CD	10.21	1.62	1.47
32	BK	48	PRO	N-CD	10.20	1.62	1.47
31	BJ	46	PRO	N-CD	10.19	1.62	1.47
55	B8	20	U	C5-C6	10.12	1.54	1.34
24	BC	227	PRO	N-CD	10.06	1.61	1.47
5	AE	133	PRO	N-CD	10.02	1.61	1.47
31	BJ	8	PRO	N-CD	9.97	1.61	1.47
51	B3	2	PRO	N-CA	-9.82	1.32	1.47
7	AG	2	PRO	N-CA	-9.82	1.32	1.47
24	BC	231	PRO	N-CD	9.66	1.61	1.47
21	AU	2	PRO	N-CA	-9.35	1.33	1.47
13	AM	115	PRO	N-CA	-8.32	1.34	1.47
54	B7	7	U	O3'-P	-7.85	1.49	1.61
53	B5	24	PRO	N-CA	-7.62	1.35	1.47
2	AB	204	ASP	CB-CG	-7.39	1.33	1.52
25	BD	152	PRO	N-CA	-7.35	1.34	1.47
10	AJ	39	PRO	N-CA	-6.72	1.35	1.47
25	BD	152	PRO	CG-CD	-6.67	1.33	1.51
39	BR	52	PRO	N-CA	-6.54	1.36	1.47
8	AH	96	MET	CB-CG	-6.44	1.33	1.52
39	BR	52	PRO	CG-CD	-6.37	1.34	1.51
12	AL	45	PRO	N-CA	-6.36	1.36	1.47
10	AJ	39	PRO	CG-CD	-6.33	1.34	1.51
12	AL	45	PRO	CG-CD	-6.25	1.34	1.51
2	AB	204	ASP	C-N	-5.30	1.26	1.33
21	AU	2	PRO	CG-CD	-5.12	1.33	1.50
22	BA	2069	G7M	O3'-P	5.07	1.61	1.56

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	204	ASP	N-CA-CB	-16.02	84.67	111.27
2	AB	205	ASP	CB-CA-C	12.83	130.63	109.07
55	B8	19	G	OP1-P-O3'	-12.35	70.96	108.00
8	AH	96	MET	N-CA-CB	-10.50	96.34	112.30
41	BT	1	MET	CB-CG-SD	-9.56	84.01	112.70
2	AB	205	ASP	N-CA-CB	-9.05	98.09	110.67
41	BT	1	MET	CB-CA-C	-8.90	93.19	110.10
2	AB	188	ASP	CB-CG-OD1	8.36	137.62	118.40
2	AB	204	ASP	CA-CB-CG	8.31	120.91	112.60
17	AQ	16	LYS	CD-CE-NZ	7.76	136.75	111.90
7	AG	33	ASP	N-CA-CB	-7.39	100.95	112.41
41	BT	1	MET	N-CA-C	7.33	131.52	111.00
1	AA	1491	G	OP1-P-O3'	-6.81	87.58	108.00
3	AC	85	GLU	CA-CB-CG	6.75	127.59	114.10
27	BF	109	PRO	CA-N-CD	-6.34	103.12	112.00
53	B5	24	PRO	CA-N-CD	-6.12	103.43	112.00
3	AC	88	ARG	CG-CD-NE	5.96	125.11	112.00
29	BH	32	PRO	CA-N-CD	-5.69	104.03	112.00
2	AB	205	ASP	CB-CG-OD1	5.62	131.32	118.40
17	AQ	16	LYS	N-CA-CB	-5.57	100.64	110.39
55	B8	19	G	OP2-P-O3'	-5.50	91.50	108.00
22	BA	1970	A	O5'-P-OP1	-5.48	91.57	108.00
54	B7	7	U	O3'-P-O5'	5.47	112.21	104.00
13	AM	65	VAL	CA-C-N	5.44	131.93	121.54
13	AM	65	VAL	C-N-CA	5.44	131.93	121.54
19	AS	3	ARG	N-CA-C	-5.42	95.82	111.00
22	BA	2872	A	N1-C6-N6	-5.23	102.92	118.60
2	AB	188	ASP	N-CA-CB	-5.19	103.01	110.44
2	AB	188	ASP	OD1-CG-OD2	-5.17	110.49	122.90
8	AH	95	VAL	CA-C-N	-5.14	114.95	122.40
8	AH	95	VAL	C-N-CA	-5.14	114.95	122.40
2	AB	18	HIS	CB-CA-C	5.04	122.87	111.78
22	BA	2872	A	C5-C6-N6	5.04	138.81	123.70
4	AD	168	PRO	CA-N-CD	-5.03	104.95	112.00
7	AG	16	PRO	CA-N-CD	-5.03	104.96	112.00
12	AL	44	LYS	CB-CG-CD	-5.02	99.75	111.30
4	AD	33	LYS	CA-CB-CG	-5.02	104.07	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	204	ASP	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	205	ASP	Sidechain
7	AG	24	ALA	Mainchain
29	BH	104	THR	Peptide
29	BH	66	ASN	Peptide
43	BV	34	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	16580	238	0
2	AB	1753	0	1780	68	0
3	AC	1624	0	1696	43	0
4	AD	1643	0	1707	38	0
5	AE	1144	0	1185	28	0
6	AF	862	0	864	32	0
7	AG	1181	0	1238	34	0
8	AH	979	0	1031	32	0
9	AI	1022	0	1070	40	0
10	AJ	795	0	836	27	0
11	AK	877	0	887	16	0
12	AL	957	0	1017	11	0
13	AM	883	0	941	25	0
14	AN	799	0	841	25	0
15	AO	714	0	734	18	0
16	AP	649	0	666	10	0
17	AQ	648	0	691	14	0
18	AR	455	0	478	12	0
19	AS	656	0	680	25	0
20	AT	670	0	719	12	0
21	AU	465	0	491	9	0
22	BA	62209	0	31290	324	0
23	BB	2569	0	1301	8	0
24	BC	2082	0	2154	28	0
25	BD	1566	0	1617	12	0
26	BE	1552	0	1619	12	0
27	BF	1410	0	1444	30	0
28	BG	1323	0	1371	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BH	1110	0	1148	28	0
30	BI	522	0	520	14	0
31	BJ	1129	0	1162	17	0
32	BK	946	0	1023	13	0
33	BL	1053	0	1128	12	0
34	BM	1075	0	1155	15	0
35	BN	945	0	989	9	0
36	BO	900	0	935	8	0
37	BP	917	0	962	9	0
38	BQ	947	0	1019	7	0
39	BR	816	0	839	9	0
40	BS	857	0	922	8	0
41	BT	738	0	807	11	0
42	BU	779	0	831	11	0
43	BV	753	0	780	11	0
44	BW	580	0	594	20	0
45	BX	625	0	652	4	0
46	BY	501	0	531	5	0
47	BZ	449	0	488	3	0
48	B0	444	0	458	5	0
49	B1	414	0	442	12	0
50	B2	377	0	418	7	0
51	B3	504	0	572	4	0
52	B4	302	0	340	4	0
53	B5	146	0	139	3	0
54	B7	191	0	99	0	0
55	B8	1648	0	833	26	0
56	AA	86	0	0	0	0
56	B8	2	0	0	0	0
56	BA	233	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	2	0	0	0	0
56	BL	1	0	0	0	0
57	AA	38	0	0	0	0
57	AM	1	0	0	0	0
57	BA	104	0	0	1	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	1	0	0	0	0
57	BM	1	0	0	0	0
58	AB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B4	1	0	0	0	0
58	BI	1	0	0	0	0
59	BA	15	0	9	0	0
60	AA	184	0	0	1	0
60	AK	1	0	0	0	0
60	AN	1	0	0	0	0
60	B0	4	0	0	0	0
60	B2	6	0	0	0	0
60	B3	7	0	0	0	0
60	B4	1	0	0	0	0
60	B5	2	0	0	1	0
60	B8	3	0	0	1	0
60	BA	1672	0	0	25	0
60	BB	2	0	0	0	0
60	BC	38	0	0	1	0
60	BD	14	0	0	0	0
60	BE	21	0	0	2	0
60	BF	1	0	0	0	0
60	BJ	2	0	0	0	0
60	BK	3	0	0	0	0
60	BL	14	0	0	0	0
60	BM	2	0	0	0	0
60	BN	9	0	0	0	0
60	BO	1	0	0	0	0
60	BP	2	0	0	0	0
60	BQ	12	0	0	0	0
60	BR	4	0	0	0	0
60	BS	7	0	0	0	0
60	BT	3	0	0	0	0
60	BU	1	0	0	0	0
60	BW	5	0	0	3	0
60	BX	4	0	0	0	0
All	All	146602	0	96723	1305	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1305) 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)
6:AF:39:LEU:CD1	6:AF:62:MET:HE2	1.26	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:39:LEU:HD11	6:AF:62:MET:CE	1.55	1.34
6:AF:39:LEU:CD1	6:AF:62:MET:CE	2.07	1.28
42:BU:10:GLU:OE2	42:BU:73:PHE:HB3	1.34	1.23
6:AF:39:LEU:HD12	6:AF:62:MET:HG2	1.27	1.14
55:B8:22:G:N7	55:B8:46:G7M:N2	1.96	1.13
49:B1:35:GLU:OE1	49:B1:48:ILE:HG23	1.49	1.12
14:AN:49:GLN:NE2	19:AS:10:PHE:CE1	2.22	1.08
22:BA:2330:G:O2'	44:BW:44:LYS:NZ	1.87	1.06
44:BW:42:GLY:H	44:BW:44:LYS:HZ3	1.04	1.03
6:AF:39:LEU:HD13	6:AF:62:MET:HE2	1.39	1.01
42:BU:10:GLU:OE2	42:BU:73:PHE:CB	2.09	1.00
6:AF:39:LEU:HD12	6:AF:62:MET:CG	1.91	0.99
27:BF:94:GLU:OE2	27:BF:98:GLU:OE2	1.79	0.99
7:AG:74:GLU:HG2	7:AG:91:VAL:HG22	1.45	0.99
7:AG:74:GLU:HG2	7:AG:91:VAL:CG2	1.94	0.98
27:BF:38:MET:HE2	27:BF:151:GLY:O	1.68	0.93
5:AE:83:HIS:NE2	5:AE:147:MET:HG3	1.85	0.92
1:AA:49:U:C4	1:AA:365:U:O4	2.23	0.92
6:AF:39:LEU:CD1	6:AF:62:MET:HG2	2.00	0.92
14:AN:49:GLN:HE21	19:AS:10:PHE:HE1	1.18	0.91
6:AF:22:ILE:HG23	6:AF:62:MET:HE1	1.53	0.91
14:AN:49:GLN:NE2	19:AS:10:PHE:CZ	2.39	0.90
1:AA:49:U:O4	1:AA:365:U:O4	1.91	0.88
2:AB:151:ILE:HG13	2:AB:154:MET:HE3	1.56	0.88
1:AA:49:U:C5	1:AA:365:U:O4	2.28	0.87
17:AQ:77:ARG:HE	17:AQ:79:VAL:HG12	1.40	0.86
49:B1:35:GLU:OE1	49:B1:48:ILE:CG2	2.23	0.86
28:BG:24:ILE:HD11	28:BG:43:VAL:HG11	1.59	0.84
6:AF:101:PRO:HG2	18:AR:25:ASP:OD1	1.77	0.84
3:AC:9:GLY:HA3	14:AN:89:MET:HE3	1.62	0.82
44:BW:41:ARG:H	44:BW:44:LYS:HE2	1.43	0.82
25:BD:184:ARG:NH1	37:BP:7:GLN:OE1	2.14	0.81
3:AC:132:ARG:HG2	3:AC:136:ARG:NH1	1.95	0.81
44:BW:44:LYS:HD2	44:BW:44:LYS:H	1.45	0.81
2:AB:15:HIS:HB3	2:AB:43:LEU:HD21	1.61	0.81
5:AE:94:VAL:HG13	5:AE:111:MET:HE3	1.61	0.81
3:AC:135:LYS:O	3:AC:139:GLN:HG2	1.81	0.80
5:AE:112:ARG:HG3	5:AE:112:ARG:HH11	1.46	0.80
2:AB:165:ASP:HB2	2:AB:204:ASP:OD1	1.81	0.80
55:B8:18:G:O2'	55:B8:57:G:N2	2.15	0.80
6:AF:22:ILE:HG23	6:AF:62:MET:CE	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:81:ALA:HB1	29:BH:149:GLU:HG2	1.63	0.79
2:AB:6:MET:SD	2:AB:47:VAL:HG11	2.23	0.79
42:BU:8:ASP:OD1	42:BU:24:LYS:NZ	2.15	0.78
9:AI:28:ILE:HG12	9:AI:63:LEU:HD21	1.66	0.78
11:AK:53:ARG:HH12	11:AK:57:LYS:HD3	1.46	0.78
8:AH:95:VAL:O	8:AH:96:MET:HB3	1.84	0.78
7:AG:50:LEU:HD21	7:AG:124:LEU:HB3	1.64	0.78
3:AC:84:VAL:HG23	3:AC:88:ARG:NH1	1.99	0.77
3:AC:132:ARG:HG2	3:AC:136:ARG:HH12	1.48	0.77
6:AF:39:LEU:CD1	6:AF:62:MET:CG	2.59	0.77
1:AA:401:C:OP2	4:AD:70:ARG:NH1	2.16	0.76
22:BA:2189:U:H2'	22:BA:2190:G:C8	2.21	0.76
29:BH:82:SER:N	29:BH:149:GLU:HG3	2.01	0.76
22:BA:2840:C:H5''	35:BN:53:THR:HG21	1.67	0.75
6:AF:38:ARG:HH21	6:AF:61:LEU:HD21	1.51	0.75
22:BA:760:G:OP1	60:BA:3402:HOH:O	2.05	0.75
7:AG:74:GLU:CG	7:AG:91:VAL:HG22	2.16	0.75
6:AF:39:LEU:CD1	6:AF:62:MET:SD	2.74	0.75
22:BA:1800:C:OP2	24:BC:182:ARG:NH2	2.20	0.75
11:AK:23:ILE:HG12	11:AK:96:THR:HG21	1.66	0.74
11:AK:64:GLN:HG3	11:AK:99:ALA:HB2	1.68	0.74
10:AJ:22:THR:HG21	10:AJ:72:ARG:HG2	1.70	0.74
9:AI:18:ARG:HG2	9:AI:66:THR:HG22	1.69	0.74
55:B8:55:PSU:O2'	55:B8:57:G:N7	2.20	0.74
6:AF:39:LEU:HD13	6:AF:62:MET:SD	2.28	0.74
22:BA:1649:G:O2'	35:BN:106:ASP:OD2	2.06	0.74
1:AA:742:G:OP1	15:AO:58:ARG:NH2	2.21	0.73
4:AD:56:ARG:HE	4:AD:56:ARG:HA	1.53	0.73
60:BA:3713:HOH:O	38:BQ:41:LYS:HE3	1.88	0.73
1:AA:458:U:H2'	1:AA:459:A:C8	2.22	0.73
1:AA:458:U:H2'	1:AA:459:A:H8	1.52	0.73
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.23	0.73
24:BC:148:PRO:CD	24:BC:185:GLU:OE2	2.36	0.73
15:AO:89:ARG:NH2	22:BA:714:U:O4	2.22	0.73
13:AM:16:VAL:HB	13:AM:41:GLU:HB2	1.71	0.72
22:BA:2131:U:H5'	22:BA:2132:U:H5''	1.71	0.72
22:BA:2134:A:OP2	22:BA:2157:G:N2	2.22	0.72
18:AR:26:ILE:HD11	18:AR:67:LEU:HD22	1.71	0.72
7:AG:67:GLU:OE2	7:AG:70:ARG:NH2	2.22	0.72
57:BA:3260:K:K	60:BA:3487:HOH:O	2.00	0.72
22:BA:1047:G:HO2'	22:BA:1110:G:H1	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2898:U:O2'	31:BJ:136:GLN:NE2	2.23	0.71
2:AB:18:HIS:HE2	2:AB:188:ASP:CG	1.98	0.71
8:AH:43:GLU:HG2	8:AH:101:ILE:HG21	1.71	0.71
9:AI:106:ARG:NH1	9:AI:107:ASP:O	2.23	0.71
3:AC:84:VAL:O	3:AC:88:ARG:HG2	1.89	0.71
6:AF:39:LEU:HD11	6:AF:62:MET:HE2	0.72	0.71
26:BE:164:LEU:O	60:BE:301:HOH:O	2.07	0.71
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	1.71	0.71
22:BA:1155:A:OP2	60:BA:3403:HOH:O	2.09	0.71
22:BA:2470:G:OP1	34:BM:55:ARG:NH2	2.23	0.71
49:B1:5:ILE:HD12	49:B1:28:ARG:HH21	1.54	0.71
1:AA:1151:A:H5''	10:AJ:44:THR:HG23	1.71	0.71
1:AA:1061:G:OP2	3:AC:3:GLN:NE2	2.24	0.71
19:AS:67:VAL:O	30:BI:56:ARG:NH2	2.24	0.71
55:B8:12:G:OP2	60:B8:201:HOH:O	2.08	0.70
22:BA:1250:G:H5''	38:BQ:6:ARG:HD3	1.72	0.70
1:AA:544:G:OP1	4:AD:56:ARG:NH2	2.24	0.70
7:AG:50:LEU:HD11	7:AG:121:ALA:HA	1.73	0.70
44:BW:39:ARG:HD3	60:BW:104:HOH:O	1.90	0.70
44:BW:40:GLN:HB2	44:BW:44:LYS:HE2	1.73	0.70
2:AB:68:LEU:HD12	2:AB:154:MET:HE1	1.74	0.70
10:AJ:6:ILE:HG22	10:AJ:76:ILE:HB	1.73	0.70
40:BS:59:GLU:OE2	40:BS:66:ILE:HB	1.92	0.70
1:AA:1055:A:O2'	3:AC:156:ARG:NH1	2.25	0.69
22:BA:666:A:O2'	60:BA:3404:HOH:O	2.10	0.69
7:AG:75:VAL:HG21	7:AG:144:MET:HE3	1.74	0.69
1:AA:600:A:H5''	8:AH:89:LYS:HD2	1.75	0.69
2:AB:18:HIS:NE2	2:AB:205:ASP:OD2	2.26	0.69
30:BI:14:ALA:HB1	30:BI:34:LEU:HD21	1.75	0.69
2:AB:122:GLN:O	2:AB:125:THR:OG1	2.10	0.69
3:AC:151:VAL:HG22	3:AC:200:VAL:HG22	1.74	0.69
9:AI:12:ARG:NH1	9:AI:107:ASP:OD2	2.25	0.68
44:BW:42:GLY:H	44:BW:44:LYS:NZ	1.86	0.68
4:AD:12:SER:OG	4:AD:17:THR:O	2.11	0.68
25:BD:16:THR:HG22	25:BD:18:ASP:H	1.59	0.68
1:AA:600:A:H5''	8:AH:89:LYS:CD	2.24	0.68
3:AC:142:MET:HG3	3:AC:170:GLU:HG2	1.76	0.67
22:BA:1607:C:OP2	60:BA:3405:HOH:O	2.12	0.67
22:BA:2185:U:H2'	22:BA:2186:G:C8	2.29	0.67
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.28	0.67
22:BA:140:C:H5'	22:BA:141:G:N7	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	1.94	0.67
13:AM:17:ILE:O	13:AM:20:THR:OG1	2.11	0.67
22:BA:882:G:N2	22:BA:883:G:N7	2.42	0.67
10:AJ:40:ILE:HG22	10:AJ:73:LEU:HB3	1.77	0.66
29:BH:9:VAL:HG23	29:BH:12:LEU:HB2	1.76	0.66
14:AN:9:GLU:O	14:AN:13:VAL:HG23	1.96	0.66
6:AF:66:ALA:HB3	6:AF:71:ILE:HD11	1.76	0.66
1:AA:823:C:HO2'	8:AH:2:SER:N	1.92	0.66
1:AA:382:A:H2'	1:AA:383:A:C8	2.31	0.66
1:AA:1059:C:O3'	14:AN:85:ARG:NH2	2.29	0.66
1:AA:1147:C:O2	9:AI:18:ARG:NH1	2.29	0.66
22:BA:286:U:H2'	22:BA:287:G:H8	1.61	0.66
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.31	0.66
39:BR:1:MET:HE3	39:BR:101:ILE:HB	1.77	0.65
5:AE:112:ARG:HG3	5:AE:112:ARG:NH1	2.08	0.65
14:AN:16:ALA:HA	14:AN:55:SER:HA	1.77	0.65
22:BA:2033:A:OP1	60:BA:3406:HOH:O	2.15	0.65
48:B0:55:ILE:HD12	48:B0:57:LYS:HD2	1.79	0.65
1:AA:1225:A:H3'	13:AM:102:THR:HG21	1.79	0.65
4:AD:57:GLU:HG2	4:AD:199:LEU:HD12	1.79	0.65
1:AA:1505:G:OP2	60:AA:1802:HOH:O	0.65	0.65
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.29	0.65
32:BK:66:LYS:HE2	32:BK:81:GLY:HA2	1.77	0.65
1:AA:1320:C:H5''	19:AS:3:ARG:HH12	1.62	0.64
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.60	0.64
22:BA:248:G:N3	60:BA:3434:HOH:O	2.30	0.64
53:B5:17:ASN:ND2	60:B5:101:HOH:O	2.30	0.64
9:AI:47:VAL:CG2	9:AI:76:ALA:HB1	2.28	0.64
5:AE:80:THR:OG1	5:AE:122:ASN:O	2.14	0.64
7:AG:74:GLU:HG2	7:AG:91:VAL:HG21	1.77	0.64
21:AU:28:VAL:HA	21:AU:31:GLU:HB2	1.79	0.64
42:BU:10:GLU:OE1	42:BU:22:ARG:HD2	1.97	0.64
28:BG:42:GLU:HB3	28:BG:55:ARG:HH21	1.62	0.64
22:BA:568:U:H1'	22:BA:2030:6MZ:H9C1	1.79	0.64
1:AA:49:U:O4	1:AA:365:U:C4	2.51	0.64
49:B1:7:GLU:OE1	49:B1:9:ILE:HG23	1.98	0.64
1:AA:346:G:OP1	37:BP:39:ARG:NH1	2.28	0.63
6:AF:99:ALA:O	6:AF:104:LYS:NZ	2.31	0.63
22:BA:651:G:H5'	51:B3:19:LYS:HG3	1.81	0.63
41:BT:92:ASN:O	41:BT:93:LEU:HB2	1.97	0.63
3:AC:84:VAL:HG23	3:AC:88:ARG:HH12	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1434:A:H2'	22:BA:1435:G:C8	2.33	0.63
22:BA:1797:G:HO2'	24:BC:257:THR:HG1	1.45	0.63
22:BA:2327:A:H2'	22:BA:2328:A:C8	2.33	0.63
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.80	0.63
5:AE:83:HIS:CE1	5:AE:85:VAL:HG12	2.33	0.63
38:BQ:89:GLU:O	38:BQ:89:GLU:HG2	1.98	0.63
6:AF:39:LEU:HD13	6:AF:62:MET:CE	2.03	0.63
17:AQ:39:LYS:HZ3	17:AQ:39:LYS:C	2.07	0.63
2:AB:47:VAL:HG23	2:AB:48:PRO:HD3	1.81	0.63
3:AC:76:VAL:HG23	3:AC:103:ILE:HD13	1.79	0.63
46:BY:27:ASN:O	46:BY:31:GLN:HG3	1.99	0.63
4:AD:65:TYR:CE2	4:AD:94:LEU:HB3	2.34	0.62
10:AJ:8:ILE:HD12	10:AJ:74:VAL:HG13	1.80	0.62
22:BA:536:G:OP2	60:BA:3407:HOH:O	2.16	0.62
22:BA:1469:A:H2'	22:BA:1470:A:C8	2.33	0.62
27:BF:10:ASP:O	27:BF:14:LYS:NZ	2.29	0.62
10:AJ:18:ILE:O	10:AJ:22:THR:HG23	1.99	0.62
22:BA:2188:U:H2'	22:BA:2189:U:C6	2.34	0.62
31:BJ:13:ARG:NH2	31:BJ:49:ASP:O	2.32	0.62
33:BL:69:ARG:HG2	33:BL:69:ARG:HH11	1.64	0.62
2:AB:6:MET:HE1	2:AB:43:LEU:HB3	1.82	0.62
20:AT:44:LYS:HG3	20:AT:87:ALA:HB3	1.81	0.62
28:BG:32:GLU:OE2	28:BG:34:THR:OG1	2.17	0.62
17:AQ:17:MET:HE1	17:AQ:22:VAL:HG23	1.82	0.62
22:BA:1434:A:H2'	22:BA:1435:G:H8	1.64	0.62
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.32	0.62
2:AB:18:HIS:NE2	2:AB:188:ASP:CG	2.58	0.62
27:BF:103:LEU:O	27:BF:108:VAL:HG13	2.00	0.62
6:AF:45:ARG:O	6:AF:56:LYS:HA	1.98	0.61
9:AI:47:VAL:HG21	9:AI:76:ALA:HB1	1.82	0.61
15:AO:55:GLY:O	15:AO:59:MET:HG3	2.00	0.61
1:AA:673:A:H2'	1:AA:674:G:C8	2.35	0.61
17:AQ:77:ARG:HE	17:AQ:79:VAL:CG1	2.10	0.61
22:BA:2159:G:H2'	22:BA:2160:C:C6	2.36	0.61
11:AK:84:VAL:HG11	11:AK:97:ILE:HD11	1.81	0.61
12:AL:51:LYS:HD2	12:AL:51:LYS:N	2.16	0.61
14:AN:80:SER:O	14:AN:84:VAL:HG12	1.99	0.61
22:BA:992:C:OP1	39:BR:76:LYS:NZ	2.34	0.61
22:BA:2250:G:OP1	34:BM:84:LYS:NZ	2.32	0.61
3:AC:22:TRP:HB3	3:AC:59:ARG:HB2	1.81	0.61
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BG:170:ARG:NH1	52:B4:29:ALA:O	2.33	0.61
44:BW:44:LYS:H	44:BW:44:LYS:CD	2.14	0.61
10:AJ:10:LEU:HD12	10:AJ:22:THR:HG22	1.82	0.61
28:BG:117:LEU:HD13	28:BG:118:PRO:HD2	1.83	0.61
22:BA:2187:U:H2'	22:BA:2188:U:O4'	2.01	0.61
27:BF:118:SER:OG	27:BF:120:LYS:HG2	2.00	0.60
28:BG:4:VAL:O	28:BG:69:ARG:HD2	2.01	0.60
49:B1:33:LYS:HD3	49:B1:51:GLU:HB3	1.83	0.60
26:BE:80:SER:OG	60:BE:302:HOH:O	2.13	0.60
22:BA:2273:A:H2'	22:BA:2274:A:C8	2.37	0.60
22:BA:2032:G:C5	25:BD:150:MEQ:HE3	2.37	0.60
22:BA:2176:A:H2'	22:BA:2177:C:C6	2.37	0.60
3:AC:53:SER:HB3	3:AC:115:LEU:HD21	1.83	0.60
19:AS:65:GLU:O	30:BI:56:ARG:NH1	2.34	0.60
22:BA:275:C:H2'	22:BA:276:U:H4'	1.83	0.60
22:BA:2189:U:H2'	22:BA:2190:G:H8	1.61	0.60
31:BJ:125:TYR:HH	31:BJ:132:HIS:HE2	1.44	0.60
42:BU:10:GLU:OE2	42:BU:73:PHE:CD2	2.55	0.60
49:B1:37:LYS:NZ	49:B1:46:HIS:O	2.25	0.60
1:AA:337:G:H2'	1:AA:338:A:C8	2.36	0.60
2:AB:133:GLU:HB3	2:AB:137:ARG:HD2	1.84	0.60
6:AF:38:ARG:HG2	6:AF:63:ASN:HB3	1.84	0.60
8:AH:106:THR:HG22	8:AH:107:SER:N	2.15	0.60
2:AB:6:MET:SD	2:AB:47:VAL:CG1	2.89	0.60
1:AA:684:U:O4'	11:AK:40:ASN:ND2	2.35	0.59
7:AG:4:ARG:HG3	7:AG:4:ARG:HH11	1.67	0.59
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.35	0.59
1:AA:746:A:H2'	1:AA:747:A:C8	2.37	0.59
2:AB:204:ASP:C	2:AB:205:ASP:OD1	2.45	0.59
7:AG:149:LYS:HG2	11:AK:61:PHE:CE2	2.37	0.59
1:AA:613:C:OP1	4:AD:81:ARG:NH1	2.29	0.59
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.83	0.59
22:BA:1970:A:H5''	22:BA:1971:U:OP1	2.02	0.59
22:BA:2068:U:N3	22:BA:2430:A:C2	2.71	0.59
32:BK:105:ARG:HG2	32:BK:108:ARG:HD2	1.84	0.59
22:BA:2184:A:H2'	22:BA:2185:U:C6	2.37	0.59
43:BV:75:GLN:HB2	43:BV:92:VAL:HG23	1.83	0.59
44:BW:42:GLY:N	44:BW:44:LYS:HZ3	1.88	0.59
60:BA:4942:HOH:O	38:BQ:11:ARG:HD2	2.03	0.59
24:BC:148:PRO:CG	24:BC:185:GLU:OE2	2.51	0.59
35:BN:72:ASP:OD2	35:BN:75:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:105:MET:SD	4:AD:180:GLY:HA3	2.43	0.59
5:AE:157:ARG:NH2	8:AH:99:LEU:O	2.36	0.59
8:AH:30:SER:O	8:AH:34:VAL:HG23	2.01	0.59
8:AH:106:THR:HG21	8:AH:121:LEU:HB3	1.85	0.59
22:BA:2478:A:OP2	52:B4:2:LYS:NZ	2.26	0.59
6:AF:101:PRO:CG	18:AR:25:ASP:OD1	2.48	0.59
22:BA:281:C:H2'	22:BA:282:A:H8	1.68	0.59
22:BA:639:U:H2'	22:BA:640:C:C6	2.38	0.59
22:BA:1386:C:OP1	60:BA:3408:HOH:O	2.17	0.59
22:BA:2134:A:N6	22:BA:2157:G:O2'	2.36	0.59
24:BC:148:PRO:HD3	24:BC:185:GLU:OE2	2.02	0.59
41:BT:33:LYS:HG2	41:BT:80:TRP:CZ3	2.38	0.59
44:BW:44:LYS:HD2	44:BW:44:LYS:N	2.16	0.59
10:AJ:48:ARG:NH1	10:AJ:66:GLU:OE1	2.36	0.58
22:BA:832:U:H2'	22:BA:833:A:C8	2.38	0.58
22:BA:2107:G:H2'	22:BA:2108:A:C8	2.38	0.58
28:BG:117:LEU:HD12	28:BG:121:ILE:HB	1.84	0.58
30:BI:35:ASP:OD1	30:BI:35:ASP:N	2.34	0.58
3:AC:127:ARG:NH1	3:AC:127:ARG:HB2	2.18	0.58
22:BA:1007:C:OP1	31:BJ:37:ARG:NH1	2.37	0.58
25:BD:35:THR:HG22	25:BD:73:VAL:HG21	1.85	0.58
27:BF:140:GLU:HA	30:BI:28:VAL:HG12	1.85	0.58
29:BH:15:LEU:HD22	29:BH:15:LEU:H	1.67	0.58
11:AK:97:ILE:HG22	21:AU:12:PHE:CZ	2.38	0.58
1:AA:539:A:H2'	1:AA:540:G:C8	2.38	0.58
22:BA:250:G:H2'	22:BA:251:A:C8	2.38	0.58
22:BA:414:C:H2'	22:BA:415:A:C8	2.37	0.58
28:BG:2:SER:OG	28:BG:3:ARG:N	2.30	0.58
29:BH:108:VAL:HG13	29:BH:109:GLU:H	1.69	0.58
44:BW:41:ARG:N	44:BW:44:LYS:HE2	2.16	0.58
30:BI:43:PHE:HA	30:BI:46:GLY:HA3	1.84	0.58
22:BA:871:U:H2'	22:BA:872:U:C6	2.37	0.58
1:AA:445:G:H1	1:AA:489:C:H5	1.51	0.58
60:BA:4826:HOH:O	50:B2:46:LYS:HD3	2.02	0.58
4:AD:160:GLU:O	4:AD:164:GLN:HG2	2.03	0.57
22:BA:286:U:H2'	22:BA:287:G:C8	2.37	0.57
60:BA:3605:HOH:O	24:BC:227:PRO:HD2	2.04	0.57
42:BU:10:GLU:OE2	42:BU:73:PHE:CG	2.56	0.57
11:AK:53:ARG:NH1	11:AK:57:LYS:HD3	2.16	0.57
14:AN:15:LEU:O	14:AN:18:LYS:HB3	2.04	0.57
22:BA:2328:A:H2'	22:BA:2329:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:111:ILE:HG22	2:AB:148:LEU:HD13	1.86	0.57
22:BA:1869:G:N2	22:BA:1871:A:O2'	2.38	0.57
30:BI:30:HIS:CG	30:BI:31:ASP:H	2.21	0.57
7:AG:26:PHE:CD1	7:AG:101:MET:HG2	2.40	0.57
31:BJ:69:ARG:HG2	31:BJ:90:GLU:HG3	1.86	0.57
3:AC:127:ARG:HB2	3:AC:127:ARG:HH11	1.68	0.57
8:AH:106:THR:HG21	8:AH:121:LEU:CB	2.34	0.57
1:AA:1038:C:H2'	1:AA:1039:G:H8	1.67	0.57
42:BU:10:GLU:OE1	42:BU:22:ARG:HB3	2.04	0.57
1:AA:1320:C:OP2	19:AS:3:ARG:NH1	2.38	0.57
9:AI:88:MET:HE2	9:AI:95:ARG:CZ	2.35	0.57
10:AJ:84:VAL:HG13	10:AJ:85:ASP:H	1.69	0.57
10:AJ:84:VAL:O	10:AJ:88:MET:HG3	2.04	0.57
15:AO:58:ARG:CZ	15:AO:58:ARG:HB3	2.34	0.57
1:AA:375:U:H4'	16:AP:17:TYR:CE2	2.40	0.57
22:BA:254:G:N7	51:B3:5:LYS:NZ	2.53	0.57
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.40	0.57
7:AG:27:VAL:HG12	7:AG:43:VAL:HG21	1.87	0.57
9:AI:57:MET:HE1	9:AI:61:LEU:HG	1.87	0.57
55:B8:22:G:N7	55:B8:46:G7M:C2	2.67	0.57
1:AA:216:U:H2'	1:AA:217:C:C6	2.40	0.56
1:AA:492:C:H2'	1:AA:493:A:C8	2.40	0.56
13:AM:64:VAL:HG11	13:AM:72:GLU:OE2	2.04	0.56
15:AO:78:TYR:O	15:AO:82:ILE:HG23	2.05	0.56
22:BA:2636:C:O2'	25:BD:45:TYR:OH	2.19	0.56
20:AT:66:LEU:HD23	20:AT:67:ILE:HG23	1.87	0.56
22:BA:1177:G:H2'	22:BA:1178:C:H6	1.70	0.56
29:BH:104:THR:HA	29:BH:107:GLY:N	2.20	0.56
44:BW:40:GLN:HB2	44:BW:44:LYS:HD3	1.87	0.56
10:AJ:63:ASP:OD1	14:AN:98:LYS:NZ	2.39	0.56
22:BA:910:A:H2'	22:BA:911:A:C8	2.40	0.56
22:BA:2753:A:O2'	52:B4:15:LYS:HE3	2.04	0.56
29:BH:8:LYS:HD3	29:BH:14:SER:HB3	1.86	0.56
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.53	0.56
2:AB:97:LEU:HB2	2:AB:100:MET:SD	2.45	0.56
2:AB:70:VAL:HG12	2:AB:163:VAL:HA	1.86	0.56
12:AL:94:ARG:HG3	12:AL:94:ARG:HH11	1.71	0.56
3:AC:42:TYR:HD1	3:AC:43:LEU:HD12	1.69	0.56
1:AA:363:A:OP2	12:AL:31:ARG:NH2	2.35	0.56
22:BA:682:G:H5'	50:B2:26:ASN:OD1	2.06	0.56
29:BH:104:THR:HG21	29:BH:110:VAL:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BU:15:THR:HB	42:BU:69:ASN:ND2	2.21	0.56
1:AA:1040:U:H2'	1:AA:1041:G:H8	1.70	0.56
9:AI:43:THR:O	9:AI:47:VAL:HG13	2.06	0.56
24:BC:5:LYS:NZ	24:BC:16:VAL:O	2.39	0.56
27:BF:94:GLU:OE2	27:BF:98:GLU:CD	2.49	0.56
49:B1:27:LYS:HA	49:B1:27:LYS:HE2	1.87	0.56
22:BA:249:C:O2	51:B3:12:LYS:NZ	2.39	0.56
55:B8:2:G:O2'	55:B8:3:G:H2'	2.06	0.56
1:AA:299:G:H2'	1:AA:300:A:C8	2.41	0.55
1:AA:1320:C:O2	19:AS:36:ARG:NH2	2.39	0.55
2:AB:163:VAL:N	2:AB:184:PHE:O	2.30	0.55
1:AA:1250:A:H2'	1:AA:1251:A:C8	2.41	0.55
1:AA:944:G:N1	1:AA:1338:G:OP2	2.34	0.55
22:BA:2469:A:N6	22:BA:2481:G:O2'	2.40	0.55
24:BC:267:ILE:HD13	24:BC:270:ARG:HH21	1.70	0.55
7:AG:93:PRO:HA	7:AG:96:ARG:HG3	1.88	0.55
22:BA:526:A:H2'	60:BA:4631:HOH:O	2.06	0.55
22:BA:856:G:H2'	22:BA:857:G:C8	2.41	0.55
10:AJ:57:VAL:O	10:AJ:57:VAL:HG13	2.06	0.55
55:B8:3:G:H4'	55:B8:4:U:OP1	2.07	0.55
2:AB:90:PHE:HB3	2:AB:154:MET:HE2	1.89	0.55
3:AC:117:ALA:O	3:AC:121:THR:HG23	2.06	0.55
22:BA:2100:G:O6	22:BA:2189:U:O4	2.25	0.55
4:AD:50:ASP:HA	4:AD:53:VAL:HG22	1.89	0.55
4:AD:104:ARG:HG2	4:AD:104:ARG:HH11	1.71	0.55
6:AF:88:MET:HG2	6:AF:90:MET:HE2	1.89	0.55
23:BB:1:U:H2'	23:BB:2:G:H8	1.71	0.55
1:AA:1012:A:N6	1:AA:1018:G:O6	2.39	0.55
3:AC:142:MET:HE3	3:AC:149:ILE:HG22	1.89	0.55
49:B1:9:ILE:HG21	49:B1:51:GLU:OE1	2.07	0.55
55:B8:37:1MG:H2'	55:B8:38:A:C8	2.42	0.55
22:BA:2182:U:H2'	22:BA:2183:A:C8	2.42	0.55
4:AD:95:GLU:HA	4:AD:100:ASN:HD22	1.72	0.54
18:AR:26:ILE:HG22	18:AR:30:LYS:NZ	2.21	0.54
27:BF:135:GLN:HE21	27:BF:149:VAL:HA	1.71	0.54
1:AA:1008:U:H1'	1:AA:1009:U:C6	2.42	0.54
29:BH:104:THR:HA	29:BH:107:GLY:H	1.72	0.54
29:BH:114:GLU:OE1	29:BH:114:GLU:N	2.41	0.54
9:AI:47:VAL:HA	9:AI:50:GLN:HE21	1.71	0.54
22:BA:646:U:C5	22:BA:2368:C:H1'	2.42	0.54
48:B0:38:HIS:ND1	48:B0:39:LEU:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:390:U:H2'	1:AA:391:G:H8	1.73	0.54
21:AU:31:GLU:O	21:AU:35:ARG:HG3	2.07	0.54
22:BA:1223:G:OP1	39:BR:68:ARG:NH1	2.39	0.54
3:AC:184:TYR:O	3:AC:185:ASN:ND2	2.41	0.54
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.90	0.54
22:BA:358:U:C2	22:BA:359:G:C8	2.96	0.54
22:BA:832:U:H2'	22:BA:833:A:H8	1.72	0.54
18:AR:26:ILE:CG2	18:AR:30:LYS:NZ	2.71	0.54
22:BA:2128:G:H2'	22:BA:2129:C:H6	1.72	0.54
22:BA:2796:U:H2'	22:BA:2797:U:H2'	1.89	0.54
1:AA:1088:G:H21	1:AA:1167:A:H61	1.54	0.54
1:AA:1320:C:C5'	19:AS:3:ARG:HH12	2.20	0.54
22:BA:414:C:H2'	22:BA:415:A:H8	1.73	0.54
35:BN:114:GLU:OE1	35:BN:118:ARG:NH1	2.41	0.54
1:AA:280:C:H42	17:AQ:39:LYS:NZ	2.05	0.54
1:AA:714:G:H2'	1:AA:715:A:C8	2.43	0.54
5:AE:111:MET:CE	5:AE:125:ALA:HB1	2.38	0.54
22:BA:2394:C:H5''	33:BL:63:LYS:HE2	1.90	0.54
5:AE:111:MET:HE2	5:AE:125:ALA:HB1	1.89	0.54
7:AG:109:ARG:HA	7:AG:116:MET:HE1	1.90	0.54
17:AQ:39:LYS:O	17:AQ:39:LYS:HG3	2.08	0.54
22:BA:281:C:H2'	22:BA:282:A:C8	2.43	0.54
25:BD:156:PHE:CE1	31:BJ:81:ILE:HD13	2.42	0.54
41:BT:11:LEU:O	46:BY:29:ARG:NH1	2.41	0.54
55:B8:71:C:H2'	55:B8:72:G:C8	2.43	0.54
2:AB:204:ASP:C	2:AB:205:ASP:CG	2.77	0.53
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.90	0.53
9:AI:46:MET:O	9:AI:50:GLN:HG2	2.07	0.53
22:BA:2522:U:O2'	22:BA:2647:U:OP1	2.21	0.53
10:AJ:16:ARG:HG2	10:AJ:16:ARG:HH11	1.73	0.53
24:BC:133:ARG:NE	24:BC:187:ASP:OD1	2.39	0.53
1:AA:946:A:H2'	1:AA:947:G:C8	2.44	0.53
2:AB:223:GLU:HA	2:AB:226:SER:HB3	1.89	0.53
1:AA:1533:C:N3	21:AU:54:LYS:NZ	2.55	0.53
2:AB:45:LYS:O	2:AB:49:MET:HG2	2.09	0.53
2:AB:68:LEU:CD1	2:AB:154:MET:HE1	2.38	0.53
15:AO:76:ALA:O	15:AO:80:GLN:HG3	2.09	0.53
22:BA:685:A:OP2	60:BA:3411:HOH:O	2.19	0.53
55:B8:66:A:H2'	55:B8:67:U:C6	2.43	0.53
8:AH:88:ARG:HB2	8:AH:91:GLU:OE1	2.09	0.53
9:AI:87:LEU:HD11	9:AI:98:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BT:67:VAL:HG22	41:BT:76:ARG:HG3	1.91	0.53
9:AI:80:ARG:HH21	9:AI:103:PHE:HA	1.74	0.53
11:AK:53:ARG:NH1	11:AK:53:ARG:HA	2.24	0.53
22:BA:1417:C:O2'	22:BA:1587:G:O2'	2.18	0.53
22:BA:2291:U:H2'	22:BA:2292:U:C6	2.43	0.53
3:AC:36:ASP:OD1	3:AC:59:ARG:NH2	2.41	0.53
4:AD:97:ARG:O	4:AD:101:VAL:HG23	2.09	0.53
22:BA:78:U:H2'	22:BA:79:C:C6	2.44	0.53
22:BA:1009:A:OP1	31:BJ:39:LYS:NZ	2.41	0.53
22:BA:2185:U:H2'	22:BA:2186:G:H8	1.73	0.53
1:AA:212:G:H2'	1:AA:213:G:C8	2.43	0.53
4:AD:82:LEU:HB2	4:AD:89:ASN:HD22	1.73	0.53
4:AD:101:VAL:O	4:AD:105:MET:HG3	2.09	0.53
11:AK:97:ILE:HG22	21:AU:12:PHE:HZ	1.73	0.53
22:BA:140:C:H5'	22:BA:141:G:C8	2.44	0.53
22:BA:2191:A:H2'	22:BA:2192:U:C6	2.44	0.53
22:BA:2246:G:H2'	22:BA:2247:A:C8	2.44	0.53
22:BA:2250:G:O2'	22:BA:2496:C:OP1	2.26	0.53
44:BW:40:GLN:HB2	44:BW:44:LYS:CE	2.38	0.53
1:AA:717:U:H4'	11:AK:119:ASN:HD22	1.73	0.52
18:AR:39:ILE:HD12	18:AR:59:ILE:HD12	1.91	0.52
22:BA:1348:C:OP1	60:BA:3410:HOH:O	2.19	0.52
29:BH:104:THR:HG21	29:BH:110:VAL:H	1.74	0.52
1:AA:87:C:H2'	1:AA:88:U:H4'	1.91	0.52
1:AA:171:A:H2'	1:AA:172:A:C8	2.44	0.52
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.91	0.52
1:AA:1530:G:N7	21:AU:46:LYS:NZ	2.57	0.52
2:AB:208:ARG:HA	2:AB:211:THR:OG1	2.09	0.52
7:AG:26:PHE:HD1	7:AG:101:MET:HG2	1.73	0.52
2:AB:76:ALA:O	2:AB:80:VAL:HG23	2.09	0.52
3:AC:35:SER:O	3:AC:39:VAL:HG12	2.09	0.52
4:AD:65:TYR:CD2	4:AD:94:LEU:HB3	2.44	0.52
22:BA:1177:G:H2'	22:BA:1178:C:C6	2.44	0.52
26:BE:47:LYS:HA	26:BE:51:GLU:OE1	2.09	0.52
12:AL:94:ARG:HG3	12:AL:94:ARG:NH1	2.25	0.52
19:AS:5:LEU:HD12	19:AS:5:LEU:H	1.74	0.52
22:BA:585:G:N7	38:BQ:6:ARG:NH2	2.56	0.52
1:AA:384:G:H2'	1:AA:385:C:C6	2.44	0.52
1:AA:1279:G:OP1	10:AJ:9:ARG:NH2	2.42	0.52
13:AM:107:ARG:NH2	13:AM:113:ARG:HA	2.25	0.52
1:AA:529:G:H5'	1:AA:530:G:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:80:ARG:NH2	9:AI:103:PHE:HA	2.24	0.52
22:BA:456:C:O2'	41:BT:73:ARG:NH1	2.41	0.52
27:BF:94:GLU:O	27:BF:98:GLU:HG3	2.09	0.52
33:BL:69:ARG:HG2	33:BL:69:ARG:NH1	2.24	0.52
1:AA:745:G:H2'	1:AA:746:A:C8	2.44	0.52
9:AI:12:ARG:HG3	9:AI:77:GLY:HA3	1.92	0.52
11:AK:19:GLY:O	11:AK:82:LEU:HA	2.09	0.52
13:AM:4:ILE:HG22	13:AM:5:ALA:N	2.25	0.52
22:BA:880:G:H2'	22:BA:881:G:H8	1.73	0.52
3:AC:34:ASP:OD1	3:AC:38:LYS:NZ	2.40	0.52
43:BV:64:VAL:HG22	43:BV:69:GLU:HG2	1.91	0.52
37:BP:32:VAL:HG23	37:BP:39:ARG:HG3	1.90	0.52
4:AD:160:GLU:OE1	4:AD:160:GLU:N	2.39	0.52
7:AG:24:ALA:O	7:AG:28:ASN:OD1	2.27	0.52
13:AM:98:ARG:HB2	13:AM:100:GLN:HE22	1.74	0.52
22:BA:2255:G:O2'	55:B8:3:G:OP2	2.25	0.52
22:BA:2812:G:H2'	22:BA:2813:A:C8	2.45	0.52
1:AA:49:U:H5	1:AA:365:U:O4	1.89	0.51
1:AA:206:C:H2'	1:AA:207:C:C6	2.45	0.51
2:AB:6:MET:CE	2:AB:43:LEU:HB3	2.40	0.51
2:AB:130:THR:O	2:AB:131:LYS:HB2	2.10	0.51
10:AJ:66:GLU:HB3	14:AN:99:ALA:HB2	1.91	0.51
27:BF:142:ASP:HB3	27:BF:145:LYS:HE2	1.92	0.51
1:AA:728:A:H2'	1:AA:729:A:C8	2.45	0.51
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.38	0.51
3:AC:130:PHE:O	3:AC:134:MET:HG3	2.09	0.51
7:AG:70:ARG:HG2	7:AG:100:ALA:HB2	1.92	0.51
20:AT:2:ALA:HB3	20:AT:8:LYS:HG3	1.93	0.51
22:BA:1662:U:OP2	60:BA:3413:HOH:O	2.19	0.51
34:BM:75:GLU:HG3	34:BM:90:GLU:HG3	1.92	0.51
19:AS:12:ASP:OD2	19:AS:35:SER:OG	2.08	0.51
22:BA:1485:U:H2'	22:BA:1486:U:C6	2.46	0.51
28:BG:8:PRO:HB3	28:BG:51:THR:HG22	1.91	0.51
29:BH:8:LYS:CD	29:BH:14:SER:HB3	2.40	0.51
22:BA:1590:A:H2'	22:BA:1591:A:C8	2.45	0.51
31:BJ:95:ARG:HD2	31:BJ:96:ARG:NH1	2.25	0.51
1:AA:713:G:H2'	1:AA:714:G:C8	2.45	0.51
1:AA:1318:A:H1'	19:AS:37:ARG:CZ	2.40	0.51
13:AM:4:ILE:HG23	13:AM:57:ARG:HG2	1.93	0.51
1:AA:450:G:H5'	1:AA:451:A:H5''	1.92	0.51
1:AA:539:A:H2'	1:AA:540:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:52:LEU:HD21	16:AP:75:ILE:HG12	1.93	0.51
22:BA:2316:G:H2'	22:BA:2317:A:H8	1.76	0.51
45:BX:69:ALA:HA	45:BX:72:ARG:HE	1.76	0.51
7:AG:75:VAL:CG1	7:AG:86:GLN:HB3	2.41	0.51
1:AA:269:C:H2'	1:AA:270:A:C8	2.44	0.51
1:AA:390:U:H2'	1:AA:391:G:C8	2.46	0.51
1:AA:524:G:H2'	1:AA:525:C:C6	2.45	0.51
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.46	0.51
9:AI:60:LYS:HE3	9:AI:61:LEU:HD23	1.93	0.51
18:AR:61:ARG:HG3	18:AR:61:ARG:HH11	1.76	0.51
22:BA:2447:G:H1'	60:BA:4636:HOH:O	2.11	0.51
55:B8:62:C:H2'	55:B8:63:U:C6	2.46	0.51
6:AF:103:VAL:O	6:AF:106:LYS:HB2	2.11	0.51
22:BA:1796:U:H2'	22:BA:1797:G:H8	1.75	0.51
22:BA:2046:G:OP2	60:BA:3412:HOH:O	2.19	0.51
32:BK:38:ILE:HD11	32:BK:112:PHE:HZ	1.74	0.51
55:B8:69:A:H2'	55:B8:70:C:C6	2.46	0.51
1:AA:579:A:O2'	15:AO:54:ARG:NH1	2.43	0.51
1:AA:600:A:H5''	8:AH:89:LYS:HD3	1.93	0.51
1:AA:1033:G:H2'	1:AA:1034:G:C8	2.46	0.51
2:AB:187:VAL:HG11	2:AB:199:VAL:HG13	1.93	0.51
12:AL:4:VAL:HG13	17:AQ:34:TYR:HB3	1.93	0.51
22:BA:1079:C:H2'	22:BA:1080:A:H8	1.76	0.51
24:BC:78:VAL:HG21	24:BC:110:LEU:HD21	1.91	0.51
41:BT:6:ARG:HD2	41:BT:6:ARG:O	2.10	0.51
2:AB:8:ASP:OD1	2:AB:9:MET:N	2.43	0.50
5:AE:82:GLN:HB2	5:AE:83:HIS:HD2	1.76	0.50
8:AH:106:THR:CG2	8:AH:121:LEU:HB3	2.40	0.50
22:BA:1100:C:H2'	22:BA:1101:U:O4'	2.11	0.50
22:BA:1570:A:H2'	22:BA:1571:A:C8	2.46	0.50
30:BI:14:ALA:HB1	30:BI:34:LEU:CD2	2.40	0.50
53:B5:14:ASN:O	53:B5:20:VAL:HG21	2.11	0.50
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.76	0.50
22:BA:1300:G:H4'	22:BA:1301:A:H5''	1.93	0.50
1:AA:1317:C:C4	14:AN:53:ARG:HD2	2.46	0.50
2:AB:18:HIS:CE1	2:AB:205:ASP:OD2	2.64	0.50
2:AB:60:ILE:HA	2:AB:63:ARG:HH21	1.76	0.50
8:AH:106:THR:HG22	8:AH:107:SER:H	1.76	0.50
8:AH:106:THR:HG23	8:AH:122:GLY:O	2.12	0.50
20:AT:54:MET:HE2	20:AT:79:LEU:HD12	1.93	0.50
22:BA:959:A:H2'	22:BA:960:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BG:24:ILE:HD11	28:BG:43:VAL:CG1	2.36	0.50
34:BM:53:MET:HE1	34:BM:103:TYR:CG	2.46	0.50
4:AD:56:ARG:HA	4:AD:56:ARG:NE	2.23	0.50
7:AG:80:VAL:N	7:AG:83:SER:O	2.44	0.50
13:AM:54:ASP:HA	13:AM:57:ARG:HB2	1.93	0.50
1:AA:235:C:H2'	1:AA:236:A:C8	2.46	0.50
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.25	0.50
22:BA:608:A:H2'	22:BA:609:A:C8	2.47	0.50
27:BF:162:SER:HG	27:BF:164:GLU:CD	2.20	0.50
1:AA:219:U:H2'	1:AA:220:G:H8	1.77	0.50
1:AA:890:G:O2'	1:AA:906:A:N6	2.44	0.50
22:BA:798:G:OP1	60:BA:3414:HOH:O	2.20	0.50
46:BY:19:LEU:O	46:BY:23:ARG:HD3	2.11	0.50
1:AA:80:A:H2'	1:AA:81:A:O4'	2.12	0.50
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.47	0.50
21:AU:39:GLU:OE2	21:AU:44:GLU:HG3	2.11	0.50
26:BE:7:ASP:OD2	26:BE:122:GLU:HB2	2.11	0.50
31:BJ:1:MET:HE2	31:BJ:2:LYS:O	2.12	0.50
22:BA:848:C:H2'	22:BA:849:A:C8	2.47	0.50
22:BA:1870:C:O2'	22:BA:1871:A:O5'	2.30	0.50
25:BD:152:PRO:HG3	25:BD:156:PHE:CZ	2.47	0.50
6:AF:45:ARG:HD3	6:AF:59:TYR:CG	2.47	0.49
22:BA:191:A:H2'	22:BA:192:C:C6	2.47	0.49
30:BI:13:THR:HB	30:BI:23:LYS:HD3	1.92	0.49
32:BK:121:GLU:OE1	37:BP:65:SER:OG	2.29	0.49
1:AA:1314:C:H2'	1:AA:1315:U:H6	1.77	0.49
14:AN:46:LEU:HD11	19:AS:13:LEU:HB2	1.93	0.49
22:BA:172:A:H2'	22:BA:173:A:C8	2.47	0.49
2:AB:217:VAL:O	2:AB:221:VAL:HG13	2.11	0.49
7:AG:111:ARG:HH12	7:AG:123:GLU:N	2.10	0.49
19:AS:19:VAL:HG21	19:AS:44:MET:HB3	1.93	0.49
22:BA:276:U:H2'	22:BA:277:G:O4'	2.13	0.49
22:BA:879:G:H2'	22:BA:880:G:H8	1.76	0.49
22:BA:2193:G:H2'	22:BA:2194:U:C6	2.46	0.49
1:AA:674:G:H21	11:AK:118:HIS:HB2	1.78	0.49
22:BA:1173:U:O2'	22:BA:1174:U:O5'	2.30	0.49
1:AA:1130:A:H2'	1:AA:1131:G:C8	2.47	0.49
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.40	0.49
4:AD:124:MET:HG2	4:AD:146:ARG:HG3	1.95	0.49
9:AI:6:TYR:HB2	9:AI:21:ILE:CG1	2.43	0.49
19:AS:47:LEU:HD12	19:AS:48:THR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BB:51:G:OP1	36:BO:63:LYS:NZ	2.34	0.49
28:BG:102:VAL:HG22	28:BG:116:GLN:HG2	1.94	0.49
33:BL:57:LEU:HD22	51:B3:54:ASP:HB3	1.94	0.49
1:AA:426:U:P	4:AD:33:LYS:NZ	2.86	0.49
5:AE:13:GLU:OE2	5:AE:68:ARG:NH2	2.42	0.49
6:AF:70:VAL:HG23	6:AF:71:ILE:HD13	1.93	0.49
18:AR:61:ARG:HG3	18:AR:61:ARG:NH1	2.27	0.49
22:BA:833:A:H2'	22:BA:834:G:C8	2.47	0.49
22:BA:1386:C:H2'	22:BA:1387:A:C8	2.48	0.49
24:BC:180:GLU:OE2	24:BC:270:ARG:NH2	2.45	0.49
26:BE:23:PHE:CD1	26:BE:111:GLU:HG3	2.47	0.49
28:BG:117:LEU:HD11	28:BG:144:VAL:HG11	1.95	0.49
29:BH:16:GLY:HA2	29:BH:47:PHE:CE2	2.48	0.49
30:BI:30:HIS:CG	30:BI:31:ASP:N	2.80	0.49
4:AD:118:VAL:HG12	4:AD:123:ILE:HG13	1.94	0.49
22:BA:1590:A:H2'	22:BA:1591:A:H8	1.76	0.49
22:BA:2128:G:H2'	22:BA:2129:C:C6	2.47	0.49
1:AA:1112:C:O2'	3:AC:179:ARG:HD2	2.12	0.49
1:AA:1143:G:H2'	1:AA:1144:G:H8	1.78	0.49
2:AB:90:PHE:CB	2:AB:154:MET:HE2	2.42	0.49
13:AM:71:ARG:HG3	13:AM:71:ARG:HH11	1.77	0.49
22:BA:2334:U:HO2'	36:BO:13:ARG:NH1	2.11	0.49
22:BA:2334:U:H1'	36:BO:13:ARG:HD3	1.94	0.49
27:BF:63:GLN:HE21	27:BF:89:VAL:CG2	2.26	0.49
1:AA:891:U:H2'	1:AA:892:A:H8	1.76	0.49
1:AA:1414:U:H2'	1:AA:1415:G:H8	1.78	0.49
22:BA:1175:A:H8	22:BA:1176:U:C4	2.31	0.49
22:BA:2845:U:H5''	37:BP:52:ASN:O	2.13	0.49
42:BU:99:ASN:ND2	42:BU:101:GLU:OE2	2.45	0.49
55:B8:19:G:H4'	55:B8:20:U:OP2	2.11	0.49
1:AA:189:A:H2'	1:AA:190:A:C8	2.48	0.49
1:AA:880:C:OP1	12:AL:5:ASN:ND2	2.46	0.49
22:BA:2086:U:H2'	22:BA:2087:G:C8	2.48	0.49
22:BA:2305:U:H5''	27:BF:131:GLY:HA3	1.95	0.49
24:BC:145:GLU:HB2	24:BC:188:CYS:HB3	1.94	0.49
47:BZ:57:VAL:HG12	47:BZ:59:GLU:HG3	1.95	0.49
9:AI:22:LYS:HB2	9:AI:62:ASP:OD1	2.13	0.48
22:BA:989:G:OP2	47:BZ:12:SER:OG	2.27	0.48
22:BA:1322:A:H5'	40:BS:11:ARG:NH2	2.28	0.48
34:BM:50:ARG:HD3	34:BM:65:ILE:HD11	1.94	0.48
43:BV:2:PHE:HB2	43:BV:61:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:300:A:O5'	1:AA:300:A:H8	1.95	0.48
22:BA:1682:G:H2'	22:BA:1683:U:C6	2.47	0.48
22:BA:2313:C:H5''	27:BF:88:LYS:HD2	1.95	0.48
22:BA:2680:U:O2'	22:BA:2681:C:H5'	2.13	0.48
22:BA:2795:C:H2'	22:BA:2796:U:C6	2.48	0.48
11:AK:53:ARG:HH12	11:AK:57:LYS:CD	2.21	0.48
22:BA:396:G:OP2	45:BX:10:LYS:NZ	2.46	0.48
22:BA:594:U:H2'	22:BA:595:C:C6	2.49	0.48
22:BA:1485:U:H2'	22:BA:1486:U:H6	1.77	0.48
22:BA:1800:C:H3'	24:BC:146:MET:HE1	1.95	0.48
22:BA:2101:A:H2'	22:BA:2102:G:H8	1.78	0.48
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.49	0.48
2:AB:115:LYS:O	2:AB:119:THR:HG22	2.14	0.48
4:AD:188:ARG:NH1	4:AD:192:SER:O	2.44	0.48
7:AG:50:LEU:CD2	7:AG:124:LEU:HB3	2.39	0.48
9:AI:28:ILE:HG21	9:AI:35:LEU:HD12	1.94	0.48
20:AT:27:MET:HE3	20:AT:27:MET:HB3	1.78	0.48
22:BA:194:G:H2'	22:BA:195:A:O4'	2.13	0.48
24:BC:155:ALA:HB2	24:BC:162:VAL:HG23	1.95	0.48
22:BA:703:U:H2'	22:BA:704:G:O4'	2.13	0.48
22:BA:1494:A:H2'	22:BA:1495:A:C8	2.49	0.48
1:AA:1088:G:N2	1:AA:1167:A:H61	2.10	0.48
3:AC:184:TYR:OH	3:AC:199:LYS:HD3	2.13	0.48
4:AD:99:ASP:OD1	4:AD:100:ASN:N	2.45	0.48
22:BA:358:U:H2'	22:BA:359:G:H8	1.77	0.48
22:BA:545:U:O2'	22:BA:546:U:O4'	2.30	0.48
22:BA:2334:U:O2'	36:BO:13:ARG:NH1	2.46	0.48
23:BB:75:G:O2'	43:BV:88:HIS:NE2	2.46	0.48
1:AA:674:G:H2'	1:AA:675:A:C8	2.48	0.48
5:AE:105:ILE:HB	5:AE:112:ARG:NH1	2.29	0.48
8:AH:96:MET:CG	8:AH:99:LEU:HB2	2.43	0.48
16:AP:6:LEU:HB3	16:AP:17:TYR:HD2	1.78	0.48
22:BA:2291:U:OP1	22:BA:2380:C:O2'	2.32	0.48
22:BA:2649:C:H2'	22:BA:2650:U:H6	1.79	0.48
34:BM:66:ARG:NH1	34:BM:104:GLU:OE2	2.46	0.48
10:AJ:80:THR:HG22	10:AJ:83:THR:HG23	1.95	0.48
22:BA:5:A:H2'	22:BA:6:A:C8	2.48	0.48
22:BA:419:U:OP1	60:BA:3416:HOH:O	2.20	0.48
22:BA:1809:A:H2'	22:BA:1810:A:C8	2.48	0.48
35:BN:35:LYS:HE2	35:BN:100:CYS:SG	2.53	0.48
1:AA:1297:G:O2'	7:AG:114:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1173:U:O2'	22:BA:1174:U:O4'	2.32	0.48
22:BA:1495:A:H2'	22:BA:1496:A:C8	2.49	0.48
24:BC:38:SER:OG	60:BC:401:HOH:O	2.14	0.48
1:AA:280:C:N4	17:AQ:39:LYS:NZ	2.62	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.49	0.48
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.49	0.48
1:AA:1464:U:H2'	1:AA:1465:A:H8	1.79	0.48
4:AD:95:GLU:HA	4:AD:100:ASN:ND2	2.29	0.48
9:AI:17:ALA:HB2	9:AI:67:VAL:HG12	1.95	0.48
9:AI:63:LEU:HD12	9:AI:65:ILE:HD11	1.96	0.48
15:AO:70:LEU:HD11	15:AO:77:ARG:HB3	1.95	0.48
22:BA:2193:G:H2'	22:BA:2194:U:H6	1.78	0.48
32:BK:111:LYS:HG2	32:BK:112:PHE:CE1	2.49	0.48
1:AA:131:A:H2'	1:AA:132:C:C6	2.49	0.47
1:AA:868:C:H2'	1:AA:869:G:O4'	2.13	0.47
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.14	0.47
22:BA:645:C:H2'	22:BA:647:G:C8	2.49	0.47
22:BA:1102:C:H2'	22:BA:1103:A:H8	1.78	0.47
2:AB:165:ASP:OD2	2:AB:168:HIS:HB2	2.14	0.47
6:AF:23:GLU:HA	6:AF:26:THR:OG1	2.14	0.47
22:BA:347:A:H2'	22:BA:348:A:C8	2.49	0.47
22:BA:1729:U:O2	22:BA:1731:G:N2	2.38	0.47
1:AA:276:G:OP1	17:AQ:17:MET:HE2	2.13	0.47
1:AA:674:G:H2'	1:AA:675:A:H8	1.80	0.47
9:AI:5:GLN:HE22	9:AI:22:LYS:HD2	1.79	0.47
23:BB:75:G:HO2'	43:BV:88:HIS:HE2	1.60	0.47
34:BM:50:ARG:O	34:BM:54:THR:HG22	2.14	0.47
55:B8:23:C:H2'	55:B8:24:G:H8	1.79	0.47
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.43	0.47
3:AC:127:ARG:HH11	3:AC:127:ARG:CB	2.26	0.47
22:BA:589:U:H2'	22:BA:590:A:C8	2.49	0.47
22:BA:1937:A:H1'	22:BA:1939:5MU:H72	1.97	0.47
1:AA:337:G:H2'	1:AA:338:A:H8	1.80	0.47
8:AH:111:MET:HB3	8:AH:111:MET:HE2	1.77	0.47
22:BA:1322:A:H5'	40:BS:11:ARG:HH21	1.80	0.47
22:BA:2071:A:H2'	22:BA:2072:C:C6	2.50	0.47
22:BA:2311:A:N3	27:BF:85:ILE:HD11	2.30	0.47
22:BA:2788:C:H2'	22:BA:2789:C:C6	2.50	0.47
29:BH:68:ARG:HH21	29:BH:134:VAL:HB	1.79	0.47
34:BM:41:LEU:HG	34:BM:96:ILE:HG13	1.95	0.47
22:BA:1047:G:O2'	22:BA:1110:G:N1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1799:G:OP1	24:BC:258:ARG:NH1	2.40	0.47
22:BA:2100:G:C2	22:BA:2101:A:H1'	2.49	0.47
29:BH:122:LEU:HD12	29:BH:122:LEU:O	2.15	0.47
50:B2:1:MET:SD	50:B2:1:MET:N	2.82	0.47
1:AA:1218:C:H2'	1:AA:1219:A:H8	1.79	0.47
1:AA:1315:U:O2	1:AA:1360:A:H2	1.97	0.47
2:AB:53:ALA:O	2:AB:57:LEU:HD12	2.14	0.47
3:AC:110:GLU:HB2	3:AC:144:LEU:HD12	1.97	0.47
9:AI:7:TYR:CE1	9:AI:18:ARG:HB2	2.49	0.47
19:AS:29:LYS:H	19:AS:29:LYS:HD2	1.79	0.47
22:BA:1059:G:H2'	22:BA:1060:U:C5	2.49	0.47
22:BA:1720:U:H2'	22:BA:1721:G:O4'	2.14	0.47
22:BA:2455:G:H2'	22:BA:2456:C:C6	2.49	0.47
35:BN:35:LYS:HG3	35:BN:112:TYR:CE1	2.50	0.47
50:B2:12:ARG:NH2	50:B2:44:VAL:HG21	2.30	0.47
1:AA:696:A:H2'	1:AA:697:U:H6	1.80	0.47
1:AA:1279:G:P	10:AJ:9:ARG:HH22	2.38	0.47
2:AB:212:LEU:HD12	2:AB:213:TYR:N	2.30	0.47
4:AD:101:VAL:HG21	4:AD:137:VAL:HG21	1.96	0.47
13:AM:71:ARG:HG3	13:AM:71:ARG:NH1	2.29	0.47
15:AO:20:ASN:OD1	15:AO:21:ASP:N	2.48	0.47
22:BA:588:U:H2'	22:BA:589:U:C6	2.50	0.47
29:BH:50:ARG:HG3	29:BH:53:GLU:OE2	2.15	0.47
55:B8:23:C:H2'	55:B8:24:G:C8	2.50	0.47
6:AF:72:ASP:OD1	6:AF:73:GLU:N	2.47	0.47
7:AG:50:LEU:CD1	7:AG:121:ALA:HA	2.43	0.47
22:BA:646:U:H5	22:BA:2368:C:H1'	1.80	0.47
44:BW:40:GLN:HB2	44:BW:44:LYS:CD	2.44	0.47
1:AA:1225:A:OP1	13:AM:102:THR:HG22	2.15	0.47
22:BA:1334:G:OP1	41:BT:69:ARG:NH2	2.48	0.47
22:BA:2514:U:H2'	22:BA:2515:C:C6	2.50	0.47
25:BD:61:THR:HB	25:BD:63:PRO:HD2	1.97	0.47
3:AC:155:GLY:O	3:AC:196:ILE:HG12	2.14	0.46
16:AP:52:LEU:CD2	16:AP:75:ILE:HG12	2.46	0.46
22:BA:2278:A:OP1	34:BM:10:ARG:NH2	2.46	0.46
32:BK:63:VAL:HG12	32:BK:107:LEU:HD11	1.97	0.46
1:AA:695:A:H2'	1:AA:696:A:C8	2.51	0.46
2:AB:18:HIS:H	2:AB:189:THR:HG22	1.79	0.46
20:AT:81:ALA:O	20:AT:85:LYS:HD3	2.15	0.46
22:BA:64:A:H2'	22:BA:65:U:C6	2.51	0.46
22:BA:1796:U:H2'	22:BA:1797:G:C8	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BK:105:ARG:HG2	32:BK:108:ARG:CD	2.44	0.46
55:B8:51:A:H2'	55:B8:52:G:C8	2.50	0.46
3:AC:159:GLY:HA2	3:AC:193:TYR:CD2	2.50	0.46
22:BA:141:G:N2	22:BA:142:A:C8	2.83	0.46
22:BA:1370:C:H2'	22:BA:1371:G:O4'	2.15	0.46
22:BA:2567:G:H2'	22:BA:2568:U:C6	2.50	0.46
22:BA:2649:C:H2'	22:BA:2650:U:C6	2.51	0.46
24:BC:148:PRO:HG2	24:BC:185:GLU:OE2	2.15	0.46
28:BG:24:ILE:CD1	28:BG:43:VAL:HG11	2.36	0.46
29:BH:81:ALA:HB1	29:BH:149:GLU:CG	2.39	0.46
1:AA:1175:G:H2'	1:AA:1176:A:H8	1.80	0.46
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.50	0.46
2:AB:6:MET:HE1	2:AB:43:LEU:C	2.41	0.46
7:AG:60:GLU:O	7:AG:64:VAL:HG22	2.15	0.46
13:AM:49:SER:HB3	13:AM:52:GLN:HG3	1.98	0.46
22:BA:280:U:H2'	22:BA:281:C:C6	2.50	0.46
22:BA:2100:G:C6	22:BA:2101:A:C4	3.03	0.46
25:BD:105:LYS:HA	25:BD:105:LYS:HD3	1.60	0.46
1:AA:1239:A:H62	1:AA:1299:A:H62	1.64	0.46
5:AE:86:LYS:HD3	5:AE:95:PHE:HB2	1.97	0.46
10:AJ:40:ILE:O	10:AJ:72:ARG:HD3	2.15	0.46
10:AJ:40:ILE:CG2	10:AJ:73:LEU:HB3	2.43	0.46
22:BA:593:U:H2'	22:BA:594:U:C6	2.50	0.46
7:AG:74:GLU:O	7:AG:88:PRO:HA	2.15	0.46
22:BA:363:G:H2'	22:BA:364:C:C6	2.50	0.46
22:BA:2585:U:C2	53:B5:24:PRO:HG3	2.51	0.46
1:AA:751:U:H2'	1:AA:752:G:O4'	2.16	0.46
3:AC:121:THR:HB	3:AC:189:ALA:HB2	1.97	0.46
12:AL:87:VAL:HG11	12:AL:90:LEU:HD12	1.98	0.46
22:BA:2130:U:O2'	22:BA:2133:G:O2'	2.29	0.46
22:BA:2591:C:H2'	22:BA:2592:G:C8	2.50	0.46
22:BA:2740:A:H2'	22:BA:2741:A:C8	2.51	0.46
31:BJ:49:ASP:OD1	31:BJ:121:LYS:NZ	2.47	0.46
43:BV:6:ALA:HB2	43:BV:42:LEU:HD23	1.97	0.46
1:AA:89:U:H2'	1:AA:90:C:C6	2.50	0.46
1:AA:122:G:OP2	1:AA:122:G:H8	1.98	0.46
1:AA:126:G:OP1	1:AA:605:U:O2'	2.24	0.46
2:AB:108:ARG:HA	2:AB:111:ILE:HG12	1.97	0.46
3:AC:39:VAL:O	3:AC:43:LEU:HD13	2.15	0.46
14:AN:15:LEU:HD22	14:AN:54:ASP:HB2	1.97	0.46
15:AO:74:ASP:OD2	15:AO:77:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:357:C:H2'	22:BA:358:U:C6	2.50	0.46
22:BA:2099:U:H2'	22:BA:2100:G:O5'	2.16	0.46
29:BH:135:HIS:HB3	29:BH:138:VAL:HB	1.97	0.46
1:AA:883:C:O2'	1:AA:884:U:H5'	2.16	0.46
4:AD:169:THR:HG23	4:AD:184:ARG:HH22	1.81	0.46
6:AF:90:MET:HE3	6:AF:90:MET:HB2	1.81	0.46
7:AG:75:VAL:CG2	7:AG:144:MET:HE3	2.46	0.46
22:BA:828:U:H2'	22:BA:829:A:C8	2.51	0.46
22:BA:1802:A:H2'	22:BA:1803:A:C8	2.51	0.46
27:BF:10:ASP:OD1	27:BF:11:GLU:N	2.49	0.46
31:BJ:7:LYS:O	31:BJ:11:VAL:HG13	2.15	0.46
32:BK:40:LYS:HD3	32:BK:58:LEU:O	2.16	0.46
34:BM:135:VAL:HG13	43:BV:57:TYR:CD2	2.51	0.46
1:AA:478:A:OP2	1:AA:479:U:H5''	2.16	0.46
2:AB:18:HIS:CD2	2:AB:188:ASP:CG	2.94	0.46
5:AE:134:ILE:O	5:AE:138:ARG:HG2	2.16	0.46
21:AU:25:LYS:HE3	21:AU:25:LYS:HB3	1.68	0.46
27:BF:162:SER:OG	27:BF:164:GLU:CD	2.59	0.46
1:AA:719:C:O2	18:AR:39:ILE:HG22	2.16	0.45
1:AA:753:A:OP1	15:AO:69:TYR:OH	2.34	0.45
4:AD:19:LEU:HD22	4:AD:64:ILE:HG13	1.97	0.45
7:AG:75:VAL:HG11	7:AG:86:GLN:HB3	1.98	0.45
22:BA:1484:U:H2'	22:BA:1485:U:C6	2.51	0.45
39:BR:60:LYS:N	39:BR:60:LYS:HD3	2.30	0.45
1:AA:908:A:H2'	1:AA:909:A:C8	2.51	0.45
22:BA:2251:OMG:HM23	22:BA:2251:OMG:H1'	1.64	0.45
41:BT:53:VAL:CG1	41:BT:54:GLU:N	2.79	0.45
49:B1:6:ARG:HG3	49:B1:24:THR:HB	1.98	0.45
1:AA:501:C:H2'	1:AA:502:A:C8	2.51	0.45
1:AA:954:G:H21	1:AA:1227:A:H62	1.63	0.45
1:AA:1122:U:H2'	1:AA:1123:U:C6	2.51	0.45
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.51	0.45
23:BB:48:U:H2'	23:BB:49:C:C6	2.51	0.45
44:BW:65:GLY:HA2	44:BW:85:GLU:HG3	1.99	0.45
1:AA:918:A:H2'	1:AA:919:A:C8	2.52	0.45
4:AD:114:ALA:O	4:AD:118:VAL:HG13	2.15	0.45
1:AA:413:G:H1'	1:AA:428:G:N2	2.31	0.45
1:AA:426:U:OP1	4:AD:33:LYS:NZ	2.49	0.45
1:AA:672:U:H2'	1:AA:673:A:C8	2.51	0.45
6:AF:45:ARG:HD3	6:AF:59:TYR:HB2	1.98	0.45
15:AO:71:LYS:HE3	15:AO:71:LYS:HB3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BW:41:ARG:NH2	60:BW:101:HOH:O	2.42	0.45
46:BY:19:LEU:HD12	46:BY:19:LEU:HA	1.77	0.45
55:B8:25:C:H2'	55:B8:26:A:O4'	2.17	0.45
1:AA:426:U:H2'	1:AA:427:U:C6	2.52	0.45
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.49	0.45
4:AD:166:GLU:N	4:AD:166:GLU:OE1	2.49	0.45
8:AH:22:LYS:HB2	8:AH:22:LYS:HE2	1.63	0.45
10:AJ:59:LYS:NZ	10:AJ:62:ARG:HH22	2.14	0.45
22:BA:730:A:H5'	60:BA:3766:HOH:O	2.16	0.45
22:BA:1357:C:H2'	22:BA:1358:G:O4'	2.16	0.45
22:BA:1808:A:H3'	22:BA:1809:A:C8	2.52	0.45
22:BA:1923:U:H2'	22:BA:1924:C:C6	2.52	0.45
22:BA:2223:G:O3'	24:BC:265:LYS:HE3	2.16	0.45
25:BD:108:ASP:OD1	25:BD:173:GLN:HA	2.16	0.45
37:BP:6:LYS:HD3	37:BP:6:LYS:HA	1.66	0.45
55:B8:63:U:H2'	55:B8:64:C:C6	2.52	0.45
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.81	0.45
4:AD:118:VAL:O	4:AD:131:ASN:HA	2.17	0.45
22:BA:369:U:O2'	60:BA:3415:HOH:O	2.20	0.45
22:BA:927:A:H2'	22:BA:928:A:C8	2.51	0.45
22:BA:2100:G:O6	22:BA:2189:U:C4	2.70	0.45
2:AB:5:SER:O	2:AB:9:MET:HG3	2.17	0.45
2:AB:45:LYS:O	2:AB:48:PRO:HD2	2.17	0.45
7:AG:130:ASN:O	7:AG:130:ASN:ND2	2.48	0.45
19:AS:11:ILE:HG13	19:AS:38:SER:HB2	1.98	0.45
22:BA:359:G:C5	22:BA:360:U:C5	3.05	0.45
30:BI:14:ALA:HA	30:BI:32:LEU:O	2.17	0.45
44:BW:41:ARG:NE	60:BW:101:HOH:O	2.41	0.45
3:AC:142:MET:HE2	3:AC:146:ALA:HB3	1.99	0.45
5:AE:39:VAL:HG13	5:AE:71:MET:HE1	1.98	0.45
7:AG:49:THR:O	7:AG:53:ARG:HB2	2.16	0.45
22:BA:438:G:H2'	22:BA:439:A:C8	2.52	0.45
40:BS:73:LYS:HB2	40:BS:106:VAL:HB	1.98	0.45
1:AA:719:C:H2'	18:AR:39:ILE:HG23	1.98	0.45
8:AH:112:THR:HG22	8:AH:114:ARG:H	1.82	0.45
22:BA:1746:A:H2'	22:BA:1747:U:C6	2.52	0.45
22:BA:2662:A:O5'	22:BA:2662:A:H8	2.00	0.45
31:BJ:31:GLU:OE1	31:BJ:34:ARG:HD3	2.17	0.45
1:AA:715:A:H2'	1:AA:716:A:C8	2.53	0.44
1:AA:1358:U:OP1	14:AN:75:ARG:HB2	2.16	0.44
22:BA:191:A:H2'	22:BA:192:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1428:C:C5	22:BA:1569:A:H5''	2.52	0.44
22:BA:1794:A:H2'	22:BA:1795:C:C6	2.52	0.44
28:BG:35:ARG:HB2	28:BG:75:MET:HE1	2.00	0.44
35:BN:57:THR:HG23	35:BN:62:ASN:ND2	2.32	0.44
41:BT:7:LEU:HD22	41:BT:46:ALA:HB2	1.99	0.44
1:AA:900:A:H2'	1:AA:901:A:C8	2.52	0.44
5:AE:105:ILE:HB	5:AE:112:ARG:HH12	1.82	0.44
8:AH:106:THR:CG2	8:AH:107:SER:N	2.80	0.44
9:AI:52:LEU:HD22	9:AI:57:MET:HE3	1.98	0.44
21:AU:13:ASP:OD2	21:AU:17:ARG:NH2	2.51	0.44
22:BA:581:C:H2'	22:BA:582:A:C8	2.52	0.44
22:BA:1102:C:C2	22:BA:1103:A:C8	3.05	0.44
22:BA:1432:G:H2'	22:BA:1433:A:C8	2.52	0.44
22:BA:1819:A:H3'	24:BC:177:ARG:HG2	1.99	0.44
29:BH:41:LYS:HG3	29:BH:41:LYS:O	2.17	0.44
2:AB:23:TRP:CZ3	2:AB:25:PRO:HA	2.51	0.44
2:AB:32:PHE:HD2	2:AB:42:ASN:ND2	2.16	0.44
16:AP:76:LYS:O	16:AP:80:LYS:HD3	2.18	0.44
22:BA:363:G:H2'	22:BA:364:C:H6	1.83	0.44
22:BA:813:U:H2'	22:BA:814:C:C6	2.52	0.44
22:BA:1069:A:H4'	22:BA:1070:A:H5''	2.00	0.44
43:BV:55:GLU:O	43:BV:59:GLU:HG2	2.17	0.44
1:AA:31:G:O2'	1:AA:48:C:N4	2.49	0.44
1:AA:662:U:H2'	1:AA:663:A:C8	2.51	0.44
1:AA:1404:C:H2'	1:AA:1405:G:C8	2.52	0.44
9:AI:88:MET:HE2	9:AI:95:ARG:NH2	2.32	0.44
13:AM:29:ARG:O	13:AM:33:ILE:HG12	2.17	0.44
15:AO:73:LYS:HA	15:AO:73:LYS:HD2	1.80	0.44
19:AS:32:ARG:HG2	19:AS:57:HIS:CE1	2.51	0.44
22:BA:1548:A:H2'	22:BA:1549:A:C8	2.52	0.44
24:BC:120:VAL:HG22	29:BH:91:PHE:HB3	1.99	0.44
24:BC:145:GLU:HG2	24:BC:151:GLY:C	2.43	0.44
1:AA:320:A:H2'	1:AA:321:A:O4'	2.18	0.44
1:AA:363:A:OP2	12:AL:31:ARG:NE	2.50	0.44
1:AA:1342:C:H4'	9:AI:127:PHE:O	2.17	0.44
13:AM:19:LEU:CD1	13:AM:34:LEU:HD11	2.48	0.44
14:AN:83:LYS:HD2	14:AN:83:LYS:HA	1.66	0.44
36:BO:40:ILE:HD13	36:BO:47:VAL:HG22	2.00	0.44
1:AA:1456:A:H2'	1:AA:1457:G:O4'	2.17	0.44
2:AB:118:GLU:O	2:AB:121:SER:OG	2.24	0.44
8:AH:50:LYS:HE3	8:AH:60:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:22:LYS:HE2	9:AI:62:ASP:OD1	2.18	0.44
10:AJ:6:ILE:HD12	10:AJ:102:LEU:HA	1.99	0.44
13:AM:49:SER:O	13:AM:53:ILE:HG13	2.17	0.44
22:BA:720:U:H2'	22:BA:721:A:C8	2.53	0.44
22:BA:1028:A:N6	22:BA:1125:G:H2'	2.32	0.44
22:BA:1292:G:H2'	22:BA:1293:C:C6	2.52	0.44
22:BA:1322:A:H5''	40:BS:82:MET:HE1	2.00	0.44
32:BK:70:ARG:HD3	32:BK:76:VAL:HG22	1.99	0.44
34:BM:74:THR:O	34:BM:75:GLU:HG2	2.18	0.44
40:BS:70:LYS:HB2	40:BS:70:LYS:NZ	2.33	0.44
2:AB:145:GLU:HG2	2:AB:149:GLY:HA3	1.98	0.44
3:AC:131:ARG:NH2	3:AC:166:GLU:OE2	2.50	0.44
9:AI:6:TYR:HB2	9:AI:21:ILE:HG13	1.99	0.44
22:BA:2074:U:H2'	22:BA:2075:U:C6	2.52	0.44
29:BH:75:LEU:HD23	29:BH:106:ALA:HB1	1.98	0.44
43:BV:1:MET:HE1	43:BV:60:VAL:O	2.17	0.44
1:AA:335:C:H2'	1:AA:336:A:C8	2.53	0.44
1:AA:384:G:H2'	1:AA:385:C:H6	1.82	0.44
2:AB:9:MET:HE2	2:AB:43:LEU:HD12	1.99	0.44
2:AB:177:ASN:HD21	2:AB:195:GLY:CA	2.30	0.44
2:AB:210:VAL:O	2:AB:214:LEU:HD12	2.18	0.44
22:BA:1141:U:H4'	22:BA:1142:A:O4'	2.17	0.44
32:BK:105:ARG:HG2	32:BK:108:ARG:NE	2.33	0.44
1:AA:91:U:H2'	1:AA:92:U:O4'	2.17	0.44
1:AA:456:A:H2'	1:AA:457:G:C8	2.53	0.44
11:AK:84:VAL:HG11	11:AK:97:ILE:CD1	2.48	0.44
20:AT:43:ASP:OD2	20:AT:46:ALA:HB3	2.17	0.44
22:BA:358:U:H2'	22:BA:359:G:C8	2.53	0.44
26:BE:22:ASP:OD1	26:BE:23:PHE:N	2.51	0.44
2:AB:82:ASP:O	2:AB:86:SER:HB3	2.18	0.43
3:AC:79:LYS:O	3:AC:80:LYS:HB3	2.18	0.43
5:AE:39:VAL:HG13	5:AE:71:MET:CE	2.48	0.43
10:AJ:84:VAL:HG13	10:AJ:85:ASP:N	2.32	0.43
16:AP:23:ASP:HB3	16:AP:26:ASN:OD1	2.17	0.43
20:AT:69:LYS:HB2	20:AT:69:LYS:HE2	1.73	0.43
22:BA:1703:G:H2'	22:BA:1704:C:C6	2.52	0.43
22:BA:2557:G:H2'	22:BA:2558:C:C6	2.53	0.43
22:BA:2801:G:H2'	22:BA:2802:G:H8	1.82	0.43
25:BD:7:LYS:HD3	25:BD:198:GLY:HA2	1.99	0.43
27:BF:95:ARG:NH1	30:BI:1:MET:HE1	2.33	0.43
39:BR:58:VAL:HG12	39:BR:60:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:78:A:C6	1:AA:79:G:C6	3.06	0.43
1:AA:85:U:H4'	1:AA:86:G:H4'	1.99	0.43
1:AA:335:C:H2'	1:AA:336:A:H8	1.83	0.43
1:AA:426:U:P	4:AD:33:LYS:HZ1	2.40	0.43
1:AA:684:U:C1'	11:AK:40:ASN:HD22	2.31	0.43
1:AA:981:U:O2'	14:AN:61:ARG:HD3	2.19	0.43
2:AB:102:THR:HG23	2:AB:175:GLU:CG	2.49	0.43
22:BA:1405:U:H2'	22:BA:1406:U:C6	2.53	0.43
22:BA:2899:A:H2'	22:BA:2900:A:C8	2.53	0.43
27:BF:30:ARG:H	27:BF:159:THR:HB	1.82	0.43
28:BG:42:GLU:CB	28:BG:55:ARG:HH21	2.29	0.43
45:BX:51:VAL:HG22	45:BX:52:SER:O	2.18	0.43
46:BY:49:ASP:OD1	46:BY:52:ARG:NH1	2.52	0.43
50:B2:12:ARG:CZ	50:B2:44:VAL:HG21	2.47	0.43
1:AA:4:U:O2'	1:AA:6:G:OP1	2.36	0.43
1:AA:555:U:H2'	1:AA:556:C:C6	2.53	0.43
7:AG:4:ARG:HH11	7:AG:4:ARG:CG	2.31	0.43
22:BA:880:G:H2'	22:BA:881:G:C8	2.52	0.43
22:BA:2467:C:H2'	22:BA:2468:A:O4'	2.18	0.43
1:AA:323:U:H2'	1:AA:324:G:O4'	2.18	0.43
22:BA:1889:A:H2'	22:BA:1890:A:C8	2.54	0.43
35:BN:53:THR:HA	35:BN:56:LYS:HD3	2.01	0.43
8:AH:75:ILE:HD12	8:AH:129:VAL:HG22	2.01	0.43
9:AI:31:ASN:O	9:AI:33:ARG:HD2	2.18	0.43
14:AN:11:LYS:HB3	14:AN:11:LYS:HE3	1.78	0.43
19:AS:17:LYS:O	19:AS:20:GLU:HG3	2.18	0.43
22:BA:127:A:H5''	22:BA:128:C:O4'	2.18	0.43
22:BA:632:A:H2'	22:BA:633:A:C8	2.54	0.43
22:BA:1271:G:N7	22:BA:1325:U:H5	2.16	0.43
22:BA:1486:U:H2'	22:BA:1487:U:C6	2.54	0.43
22:BA:2099:U:C2'	22:BA:2100:G:O5'	2.66	0.43
22:BA:2134:A:H8	22:BA:2157:G:H21	1.66	0.43
25:BD:16:THR:HG22	25:BD:18:ASP:N	2.29	0.43
27:BF:38:MET:SD	27:BF:150:ARG:HD3	2.58	0.43
27:BF:147:ASP:CG	27:BF:148:ARG:H	2.27	0.43
52:B4:25:VAL:HB	52:B4:35:GLN:HB2	2.01	0.43
7:AG:111:ARG:NH1	7:AG:123:GLU:N	2.66	0.43
22:BA:1484:U:H2'	22:BA:1485:U:H6	1.84	0.43
22:BA:1819:A:H5''	24:BC:160:THR:HG21	2.01	0.43
22:BA:2133:G:H2'	22:BA:2157:G:H22	1.83	0.43
22:BA:2316:G:H2'	22:BA:2317:A:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:15:LEU:H	29:BH:15:LEU:CD2	2.29	0.43
33:BL:19:LEU:HD22	33:BL:27:LEU:HD22	2.00	0.43
36:BO:88:LYS:HG2	36:BO:116:GLN:HG2	2.00	0.43
1:AA:974:A:OP1	14:AN:69:ARG:NH2	2.48	0.43
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.84	0.43
22:BA:1079:C:H2'	22:BA:1080:A:C8	2.53	0.43
22:BA:1526:C:H2'	22:BA:1527:G:O4'	2.18	0.43
22:BA:2030:6MZ:C2	22:BA:2499:C:H5''	2.49	0.43
22:BA:2285:C:P	49:B1:6:ARG:HH21	2.42	0.43
32:BK:105:ARG:HG2	32:BK:108:ARG:HE	1.84	0.43
33:BL:29:LYS:O	33:BL:29:LYS:HG2	2.19	0.43
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.37	0.43
1:AA:1148:U:H2'	1:AA:1149:C:O4'	2.19	0.43
1:AA:1226:C:H6	13:AM:102:THR:HG23	1.83	0.43
7:AG:76:LYS:HD3	7:AG:89:VAL:HG11	2.01	0.43
8:AH:96:MET:HG3	8:AH:99:LEU:HB2	2.01	0.43
9:AI:107:ASP:OD1	9:AI:109:ARG:HG3	2.19	0.43
22:BA:2455:G:H2'	22:BA:2456:C:H6	1.84	0.43
22:BA:2801:G:H2'	22:BA:2802:G:C8	2.54	0.43
44:BW:72:LYS:HE2	44:BW:72:LYS:HB2	1.88	0.43
1:AA:269:C:H2'	1:AA:270:A:H8	1.81	0.43
1:AA:383:A:O5'	1:AA:383:A:H8	2.02	0.43
1:AA:1213:A:O2'	1:AA:1215:G:N7	2.39	0.43
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	2.01	0.43
4:AD:83:LYS:HD3	4:AD:83:LYS:N	2.34	0.43
12:AL:49:LEU:HD23	12:AL:49:LEU:HA	1.88	0.43
19:AS:19:VAL:O	19:AS:23:VAL:HG13	2.19	0.43
19:AS:36:ARG:HD2	19:AS:52:HIS:O	2.18	0.43
22:BA:881:G:H2'	22:BA:882:G:H8	1.84	0.43
22:BA:2100:G:C6	22:BA:2190:G:C2	3.07	0.43
31:BJ:95:ARG:HD2	31:BJ:96:ARG:HH11	1.83	0.43
34:BM:74:THR:HG21	34:BM:86:LYS:HE3	2.01	0.43
1:AA:110:C:O2'	16:AP:25:ARG:O	2.36	0.43
1:AA:860:A:H2'	1:AA:861:G:O4'	2.19	0.43
16:AP:42:ILE:H	16:AP:42:ILE:HG13	1.70	0.43
22:BA:1301:A:O2'	22:BA:1302:A:H3'	2.19	0.43
22:BA:1666:G:OP1	32:BK:66:LYS:HE3	2.19	0.43
22:BA:2343:U:HO2'	22:BA:2373:G:HO2'	1.53	0.43
28:BG:54:PRO:HG3	28:BG:62:TRP:CE2	2.54	0.43
37:BP:34:GLU:OE2	37:BP:39:ARG:NH2	2.50	0.43
1:AA:78:A:H2'	1:AA:79:G:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:554:A:H2'	1:AA:555:U:C6	2.54	0.42
1:AA:657:U:H4'	15:AO:28:GLN:HG2	2.01	0.42
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.50	0.42
1:AA:1119:C:H2'	1:AA:1120:C:H6	1.83	0.42
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.53	0.42
2:AB:133:GLU:HB3	2:AB:137:ARG:CD	2.47	0.42
8:AH:111:MET:HG3	8:AH:112:THR:O	2.18	0.42
22:BA:993:G:OP2	38:BQ:51:ARG:NH2	2.53	0.42
27:BF:112:ARG:HB3	27:BF:112:ARG:NH1	2.34	0.42
1:AA:273:U:H1'	17:AQ:18:GLU:OE2	2.19	0.42
1:AA:559:A:H4'	1:AA:560:A:H3'	2.00	0.42
2:AB:101:LEU:HB3	2:AB:179:LEU:HD12	2.01	0.42
3:AC:156:ARG:HE	3:AC:193:TYR:HB3	1.84	0.42
5:AE:82:GLN:HB2	5:AE:83:HIS:CD2	2.52	0.42
9:AI:95:ARG:O	9:AI:99:ARG:HG2	2.19	0.42
20:AT:28:MET:HE1	20:AT:66:LEU:HD22	2.02	0.42
22:BA:2150:C:H2'	22:BA:2151:U:O4'	2.19	0.42
22:BA:2799:A:O2'	22:BA:2800:A:H5''	2.20	0.42
24:BC:71:LYS:HG2	24:BC:74:ILE:HD12	2.01	0.42
28:BG:173:GLU:OE2	28:BG:176:LYS:HE2	2.19	0.42
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.84	0.42
1:AA:1095:U:H2'	1:AA:1096:C:C6	2.54	0.42
2:AB:24:ASN:ND2	2:AB:192:ASP:HB3	2.33	0.42
2:AB:139:ARG:HD2	2:AB:139:ARG:HA	1.90	0.42
22:BA:477:A:H2'	22:BA:478:A:C8	2.53	0.42
22:BA:720:U:H2'	22:BA:721:A:H8	1.84	0.42
22:BA:1198:U:H2'	22:BA:1199:U:C6	2.55	0.42
22:BA:2175:C:H2'	22:BA:2176:A:C8	2.54	0.42
22:BA:2504:PSU:N1	60:BA:3459:HOH:O	2.37	0.42
29:BH:23:ALA:O	29:BH:27:ARG:HD2	2.19	0.42
44:BW:25:ARG:HH11	44:BW:31:VAL:HG12	1.85	0.42
55:B8:37:1MG:H2'	55:B8:38:A:H8	1.84	0.42
1:AA:1022:A:H2'	1:AA:1023:U:O4'	2.20	0.42
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.54	0.42
2:AB:101:LEU:N	2:AB:175:GLU:OE2	2.48	0.42
2:AB:135:LEU:HD22	2:AB:136:MET:SD	2.59	0.42
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	2.00	0.42
15:AO:8:THR:HG23	15:AO:31:LEU:HD21	2.01	0.42
22:BA:1637:A:H5'	22:BA:1760:C:O2'	2.19	0.42
55:B8:20:U:H6	55:B8:20:U:H2'	1.63	0.42
1:AA:89:U:H2'	1:AA:90:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:160:A:H2'	1:AA:161:A:O4'	2.19	0.42
1:AA:1038:C:H2'	1:AA:1039:G:C8	2.52	0.42
1:AA:1118:U:H2'	1:AA:1119:C:H6	1.84	0.42
2:AB:199:VAL:C	2:AB:200:ILE:HG13	2.43	0.42
5:AE:86:LYS:HD2	5:AE:94:VAL:O	2.19	0.42
15:AO:70:LEU:HD12	15:AO:70:LEU:O	2.19	0.42
22:BA:568:U:OP1	33:BL:36:LYS:HE2	2.19	0.42
1:AA:280:C:H42	17:AQ:39:LYS:HZ1	1.67	0.42
4:AD:161:LEU:HD23	4:AD:161:LEU:HA	1.88	0.42
5:AE:89:HIS:O	5:AE:90:THR:C	2.62	0.42
15:AO:36:ILE:HG13	15:AO:59:MET:CE	2.49	0.42
22:BA:483:A:OP1	42:BU:47:LYS:HE2	2.19	0.42
22:BA:687:C:H1'	50:B2:4:THR:HG22	2.01	0.42
22:BA:848:C:H2'	22:BA:849:A:H8	1.84	0.42
28:BG:149:ARG:HA	28:BG:162:VAL:HG13	2.00	0.42
31:BJ:98:GLU:H	31:BJ:98:GLU:CD	2.27	0.42
32:BK:106:GLU:OE1	32:BK:106:GLU:N	2.52	0.42
1:AA:294:U:OP1	1:AA:610:U:O2'	2.28	0.42
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.49	0.42
13:AM:39:ILE:HG22	13:AM:40:ALA:O	2.20	0.42
14:AN:20:PHE:C	14:AN:22:LYS:H	2.27	0.42
22:BA:682:G:H5'	50:B2:26:ASN:CG	2.45	0.42
22:BA:1545:A:H2'	22:BA:1546:G:O4'	2.20	0.42
29:BH:87:GLU:OE1	29:BH:89:LYS:HB3	2.20	0.42
39:BR:58:VAL:HG12	39:BR:60:LYS:CD	2.50	0.42
48:B0:43:ILE:HG22	48:B0:49:TYR:HB2	2.00	0.42
1:AA:736:C:H2'	1:AA:737:C:C6	2.54	0.42
2:AB:27:MET:HE3	2:AB:27:MET:HB2	1.42	0.42
2:AB:179:LEU:HD23	2:AB:179:LEU:HA	1.90	0.42
5:AE:105:ILE:O	5:AE:112:ARG:NH1	2.44	0.42
22:BA:1182:G:H2'	22:BA:1183:U:O4'	2.19	0.42
22:BA:1438:U:H2'	22:BA:1439:A:H8	1.85	0.42
27:BF:126:GLY:O	27:BF:158:THR:OG1	2.30	0.42
29:BH:15:LEU:HD21	29:BH:58:LEU:HD22	2.02	0.42
34:BM:75:GLU:HG3	34:BM:90:GLU:CG	2.50	0.42
2:AB:108:ARG:O	2:AB:111:ILE:HG12	2.20	0.42
2:AB:132:LYS:HB2	2:AB:133:GLU:HG2	2.01	0.42
4:AD:56:ARG:HH21	4:AD:59:GLN:HG3	1.83	0.42
9:AI:12:ARG:O	9:AI:13:LYS:C	2.62	0.42
13:AM:74:SER:O	13:AM:78:LYS:HG3	2.20	0.42
22:BA:367:G:H2'	22:BA:368:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1039:A:H2	22:BA:1116:G:H22	1.68	0.42
22:BA:1585:C:H2'	22:BA:1586:A:O4'	2.19	0.42
22:BA:2687:U:H2'	22:BA:2688:G:O4'	2.20	0.42
30:BI:8:LYS:HA	30:BI:8:LYS:HD2	1.83	0.42
1:AA:190:A:O5'	1:AA:190:A:H8	2.03	0.42
1:AA:1397:C:P	5:AE:29:ARG:HH22	2.43	0.42
1:AA:1477:U:H2'	1:AA:1478:U:C6	2.55	0.42
2:AB:117:LEU:CD1	2:AB:141:LEU:HG	2.50	0.42
9:AI:44:ALA:O	9:AI:48:VAL:HG23	2.19	0.42
19:AS:33:THR:HG23	19:AS:51:VAL:HA	2.01	0.42
22:BA:657:U:H2'	22:BA:658:U:C6	2.55	0.42
22:BA:1797:G:O2'	24:BC:257:THR:OG1	2.20	0.42
22:BA:2547:A:H2'	22:BA:2548:U:C6	2.54	0.42
26:BE:192:ALA:O	26:BE:196:VAL:HG13	2.20	0.42
1:AA:1027:C:H2'	1:AA:1028:C:C6	2.55	0.41
3:AC:70:THR:C	3:AC:106:VAL:HG12	2.45	0.41
5:AE:83:HIS:HE1	5:AE:85:VAL:HG12	1.82	0.41
9:AI:44:ALA:O	9:AI:47:VAL:HG22	2.19	0.41
22:BA:1680:U:H2'	22:BA:1681:G:O4'	2.20	0.41
22:BA:1872:A:H2'	22:BA:1873:G:O4'	2.20	0.41
24:BC:181:MET:HB2	24:BC:268:VAL:HB	2.02	0.41
29:BH:108:VAL:HG13	29:BH:109:GLU:N	2.33	0.41
31:BJ:35:ARG:HB2	31:BJ:54:ILE:HD11	2.02	0.41
35:BN:49:GLU:O	35:BN:53:THR:HG23	2.20	0.41
49:B1:11:LEU:HB3	49:B1:49:TYR:HB3	2.01	0.41
1:AA:462:G:H2'	1:AA:463:U:C6	2.55	0.41
1:AA:1279:G:P	10:AJ:9:ARG:NH2	2.93	0.41
1:AA:1507:A:H2'	1:AA:1508:A:C8	2.55	0.41
3:AC:72:ARG:HD3	3:AC:72:ARG:HA	1.91	0.41
4:AD:104:ARG:HG2	4:AD:104:ARG:NH1	2.35	0.41
5:AE:148:ASN:OD1	8:AH:96:MET:HE1	2.20	0.41
22:BA:746:PSU:H2'	60:BA:4751:HOH:O	2.19	0.41
22:BA:2243:U:H2'	22:BA:2244:U:C6	2.55	0.41
22:BA:2484:G:OP1	34:BM:44:ARG:NH1	2.46	0.41
26:BE:23:PHE:HA	26:BE:107:SER:OG	2.20	0.41
27:BF:110:ARG:HE	27:BF:110:ARG:HB3	1.65	0.41
28:BG:141:ILE:HD12	28:BG:141:ILE:HA	1.93	0.41
43:BV:63:ILE:HG22	43:BV:65:VAL:HG23	2.02	0.41
1:AA:467:U:H3'	1:AA:468:A:C5'	2.51	0.41
1:AA:1530:G:H2'	1:AA:1531:A:H8	1.85	0.41
9:AI:54:LEU:HD13	9:AI:97:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:15:LEU:HD23	14:AN:55:SER:HB3	2.02	0.41
22:BA:282:A:H2'	22:BA:283:G:C8	2.56	0.41
22:BA:1645:G:H5''	22:BA:1646:C:H5'	2.03	0.41
22:BA:1820:U:OP1	24:BC:177:ARG:NE	2.53	0.41
27:BF:103:LEU:HA	27:BF:107:ALA:HB3	2.02	0.41
27:BF:144:ASP:C	27:BF:145:LYS:HD3	2.46	0.41
36:BO:49:VAL:HG21	36:BO:81:ARG:HB2	2.02	0.41
40:BS:68:ASP:OD1	40:BS:68:ASP:N	2.52	0.41
1:AA:162:A:O5'	1:AA:162:A:H8	2.02	0.41
1:AA:514:C:C2	1:AA:515:G:C8	3.08	0.41
2:AB:8:ASP:OD1	2:AB:9:MET:HG3	2.20	0.41
5:AE:46:VAL:C	5:AE:71:MET:HG3	2.44	0.41
10:AJ:41:PRO:HA	10:AJ:72:ARG:HD3	2.03	0.41
23:BB:43:C:O2	27:BF:92:ARG:NH1	2.47	0.41
26:BE:153:LEU:HD21	26:BE:158:PHE:HB2	2.01	0.41
29:BH:132:PHE:CD1	29:BH:132:PHE:N	2.89	0.41
55:B8:71:C:H2'	55:B8:72:G:H8	1.83	0.41
1:AA:161:A:H2'	1:AA:162:A:C8	2.55	0.41
1:AA:722:G:N3	1:AA:722:G:H2'	2.35	0.41
1:AA:1326:U:H2'	1:AA:1327:C:H6	1.85	0.41
4:AD:95:GLU:CD	4:AD:100:ASN:HD21	2.29	0.41
9:AI:47:VAL:HA	9:AI:50:GLN:CG	2.50	0.41
22:BA:1970:A:H5'	22:BA:1972:G:H1'	2.03	0.41
22:BA:2552:OMU:HM23	22:BA:2554:U:C6	2.55	0.41
27:BF:94:GLU:OE2	27:BF:98:GLU:CG	2.69	0.41
28:BG:35:ARG:CB	28:BG:75:MET:HE1	2.50	0.41
31:BJ:31:GLU:OE1	31:BJ:31:GLU:HA	2.20	0.41
41:BT:1:MET:HE2	41:BT:1:MET:HB3	1.66	0.41
1:AA:1495:U:H2'	1:AA:1496:C:H6	1.85	0.41
1:AA:1495:U:H2'	1:AA:1496:C:C6	2.56	0.41
13:AM:56:LEU:HA	13:AM:56:LEU:HD12	1.77	0.41
14:AN:46:LEU:HD12	14:AN:46:LEU:O	2.19	0.41
17:AQ:77:ARG:HD2	17:AQ:77:ARG:C	2.46	0.41
22:BA:288:U:H2'	22:BA:289:G:H8	1.86	0.41
22:BA:871:U:H2'	22:BA:872:U:H6	1.86	0.41
22:BA:1076:C:H2'	22:BA:1077:A:C8	2.56	0.41
22:BA:1930:G:N2	22:BA:1968:G:H2'	2.36	0.41
23:BB:66:A:H61	23:BB:107:G:H2'	1.86	0.41
26:BE:172:ALA:O	26:BE:199:MET:HE1	2.21	0.41
39:BR:60:LYS:NZ	39:BR:102:SER:OG	2.53	0.41
40:BS:4:ILE:HG12	40:BS:106:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:454:G:N2	1:AA:479:U:O2	2.54	0.41
1:AA:864:A:H2'	1:AA:865:A:C8	2.55	0.41
1:AA:1005:A:C4	1:AA:1006:G:C8	3.08	0.41
10:AJ:65:TYR:OH	14:AN:85:ARG:HG3	2.21	0.41
22:BA:635:C:OP2	33:BL:126:ARG:NH2	2.50	0.41
22:BA:644:A:H2'	22:BA:645:C:O4'	2.21	0.41
22:BA:1563:U:H2'	22:BA:1564:C:C6	2.56	0.41
22:BA:2105:U:H2'	22:BA:2106:U:C6	2.55	0.41
26:BE:188:MET:HE2	26:BE:188:MET:HB3	1.93	0.41
33:BL:79:LEU:HD11	33:BL:112:LEU:HD12	2.03	0.41
38:BQ:86:ALA:O	39:BR:51:VAL:HG23	2.21	0.41
45:BX:6:GLN:HG3	45:BX:50:ARG:O	2.21	0.41
1:AA:1000:A:N6	1:AA:1041:G:O6	2.54	0.41
6:AF:56:LYS:HE3	6:AF:56:LYS:HB3	1.89	0.41
8:AH:22:LYS:O	8:AH:65:TYR:OH	2.34	0.41
22:BA:1810:A:O5'	22:BA:1810:A:H8	2.04	0.41
22:BA:1853:A:H2'	22:BA:1854:A:C8	2.56	0.41
22:BA:2720:U:OP1	37:BP:53:ARG:NH2	2.54	0.41
43:BV:73:LYS:NZ	43:BV:73:LYS:HB3	2.36	0.41
1:AA:113:G:H1'	1:AA:354:G:H5'	2.03	0.41
1:AA:649:A:H2'	1:AA:650:G:O4'	2.21	0.41
7:AG:142:HIS:O	7:AG:145:ALA:N	2.54	0.41
14:AN:73:PHE:CE1	14:AN:78:GLY:HA2	2.56	0.41
15:AO:36:ILE:HG13	15:AO:59:MET:HE2	2.01	0.41
19:AS:7:LYS:HZ3	19:AS:7:LYS:HG3	1.81	0.41
20:AT:76:LYS:O	20:AT:80:THR:HG23	2.21	0.41
22:BA:876:C:H2'	22:BA:877:A:O4'	2.21	0.41
22:BA:882:G:N2	22:BA:895:U:H1'	2.35	0.41
22:BA:2876:G:OP1	37:BP:2:SER:N	2.54	0.41
22:BA:2895:G:H2'	22:BA:2896:C:C6	2.56	0.41
24:BC:75:PRO:HB2	24:BC:97:LYS:HE2	2.02	0.41
27:BF:130:MET:HB2	27:BF:130:MET:HE3	1.76	0.41
33:BL:13:LYS:HD3	33:BL:13:LYS:HA	1.86	0.41
33:BL:129:LYS:HE3	33:BL:129:LYS:HB3	1.75	0.41
34:BM:77:PRO:HG2	34:BM:80:VAL:HG11	2.02	0.41
36:BO:39:VAL:HB	36:BO:49:VAL:HG13	2.03	0.41
55:B8:22:G:C5	55:B8:46:G7M:N2	2.68	0.41
55:B8:63:U:H2'	55:B8:64:C:H6	1.85	0.41
1:AA:1464:U:H2'	1:AA:1465:A:C8	2.56	0.41
3:AC:169:ARG:HD2	3:AC:170:GLU:N	2.36	0.41
8:AH:36:ILE:HD11	8:AH:126:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AQ:58:VAL:HG12	17:AQ:79:VAL:CG2	2.51	0.41
19:AS:32:ARG:HE	19:AS:57:HIS:CD2	2.38	0.41
20:AT:51:PHE:CE1	20:AT:55:GLN:HG3	2.56	0.41
22:BA:171:U:H2'	22:BA:172:A:H8	1.86	0.41
22:BA:288:U:H2'	22:BA:289:G:C8	2.56	0.41
22:BA:811:U:H2'	33:BL:21:ARG:HA	2.02	0.41
22:BA:1541:C:H2'	22:BA:1542:U:C6	2.56	0.41
22:BA:2014:A:H2'	22:BA:2015:A:C8	2.55	0.41
22:BA:2271:G:OP1	44:BW:18:ALA:HB1	2.21	0.41
22:BA:2300:C:H2'	22:BA:2301:C:H6	1.86	0.41
24:BC:138:GLY:O	24:BC:163:GLN:NE2	2.53	0.41
47:BZ:45:ARG:HH22	47:BZ:59:GLU:CD	2.29	0.41
1:AA:580:C:H2'	1:AA:581:G:O4'	2.21	0.40
1:AA:677:U:H3	1:AA:713:G:H22	1.69	0.40
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.56	0.40
20:AT:24:ARG:HA	20:AT:24:ARG:HD3	1.82	0.40
22:BA:2502:G:H5''	22:BA:2503:2MA:H5''	2.02	0.40
41:BT:1:MET:HB2	41:BT:2:ILE:H	1.50	0.40
42:BU:85:PHE:CE1	42:BU:94:ARG:HG2	2.56	0.40
3:AC:83:ASP:OD1	3:AC:84:VAL:N	2.54	0.40
8:AH:46:ILE:HD13	8:AH:61:LEU:HD23	2.04	0.40
9:AI:65:ILE:HD13	9:AI:79:ILE:HG23	2.03	0.40
13:AM:4:ILE:HA	13:AM:57:ARG:HG2	2.04	0.40
13:AM:78:LYS:HB2	13:AM:78:LYS:HE2	1.87	0.40
14:AN:5:MET:HE2	14:AN:63:ARG:CZ	2.51	0.40
22:BA:634:C:H2'	22:BA:635:C:C6	2.57	0.40
22:BA:851:C:H2'	22:BA:852:U:C6	2.55	0.40
22:BA:1544:A:H2'	22:BA:1545:A:C8	2.56	0.40
22:BA:1914:C:H2'	22:BA:1915:3TD:H6	2.03	0.40
22:BA:2246:G:H2'	22:BA:2247:A:H8	1.85	0.40
1:AA:79:G:H2'	1:AA:80:A:C8	2.56	0.40
1:AA:95:C:O2	1:AA:95:C:H2'	2.21	0.40
1:AA:216:U:H2'	1:AA:217:C:H6	1.83	0.40
1:AA:579:A:H2'	1:AA:580:C:C6	2.56	0.40
1:AA:1041:G:H2'	1:AA:1042:A:C8	2.55	0.40
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.85	0.40
3:AC:42:TYR:CD1	3:AC:43:LEU:HD12	2.54	0.40
5:AE:148:ASN:OD1	8:AH:96:MET:CE	2.70	0.40
22:BA:347:A:H2'	22:BA:348:A:H8	1.86	0.40
22:BA:1051:G:H2'	22:BA:1052:C:O4'	2.21	0.40
22:BA:1790:C:H2'	22:BA:1791:A:C5	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2020:A:H5'	48:B0:9:THR:CG2	2.50	0.40
22:BA:2615:U:C2	48:B0:4:GLN:HA	2.56	0.40
49:B1:13:SER:HB2	49:B1:49:TYR:CZ	2.56	0.40
55:B8:28:U:H2'	55:B8:29:U:H6	1.87	0.40
1:AA:182:A:C4	1:AA:184:G:C8	3.10	0.40
1:AA:672:U:H2'	1:AA:673:A:H8	1.86	0.40
1:AA:696:A:H2'	1:AA:697:U:C6	2.55	0.40
1:AA:952:U:O4	13:AM:103:LYS:HD3	2.21	0.40
3:AC:88:ARG:HB3	3:AC:101:ILE:HG13	2.03	0.40
5:AE:55:GLU:OE1	5:AE:55:GLU:HA	2.21	0.40
13:AM:3:ARG:HH22	13:AM:7:ILE:HG23	1.86	0.40
17:AQ:39:LYS:NZ	17:AQ:39:LYS:O	2.47	0.40
19:AS:19:VAL:CG2	19:AS:44:MET:HB3	2.51	0.40
22:BA:973:A:OP2	39:BR:81:LYS:NZ	2.43	0.40
22:BA:2305:U:H2'	22:BA:2306:C:C6	2.57	0.40
26:BE:69:ARG:H	26:BE:69:ARG:HG2	1.62	0.40
29:BH:82:SER:HB2	29:BH:90:LEU:HD13	2.04	0.40
1:AA:222:C:H2'	1:AA:223:A:H8	1.86	0.40
1:AA:235:C:H2'	1:AA:236:A:H8	1.84	0.40
1:AA:399:G:H2'	1:AA:400:C:C6	2.57	0.40
1:AA:1012:A:C6	1:AA:1018:G:C6	3.09	0.40
2:AB:102:THR:HG23	2:AB:175:GLU:HG3	2.02	0.40
7:AG:42:ILE:HD12	7:AG:116:MET:HB3	2.03	0.40
9:AI:55:VAL:HG22	9:AI:94:LEU:HD22	2.04	0.40
10:AJ:80:THR:O	10:AJ:83:THR:OG1	2.36	0.40
16:AP:71:VAL:O	16:AP:75:ILE:HG13	2.20	0.40
22:BA:576:U:H2'	22:BA:577:G:C8	2.56	0.40
22:BA:2151:U:H2'	22:BA:2152:G:H8	1.86	0.40
23:BB:106:G:H2'	23:BB:107:G:O4'	2.22	0.40
27:BF:71:ARG:O	27:BF:81:GLN:HG3	2.22	0.40
30:BI:14:ALA:N	30:BI:22:MET:O	2.55	0.40
31:BJ:92:MET:HE3	31:BJ:92:MET:HB3	1.89	0.40
55:B8:65:U:H2'	55:B8:66:A:C8	2.56	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	222/240 (92%)	211 (95%)	11 (5%)	0	100	100
3	AC	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
4	AD	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	AE	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	AF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	AG	149/179 (83%)	136 (91%)	13 (9%)	0	100	100
8	AH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	AI	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
10	AJ	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	12	20
11	AK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	AL	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	AM	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
14	AN	99/102 (97%)	91 (92%)	8 (8%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
17	AQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	74 (92%)	6 (8%)	0	100	100
20	AT	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
25	BD	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
28	BG	174/177 (98%)	173 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
35	BN	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
36	BO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
37	BP	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
40	BS	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	BT	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	BU	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
43	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
44	BW	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	BX	75/78 (96%)	75 (100%)	0	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	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%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
All	All	5590/5930 (94%)	5381 (96%)	208 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AJ	57	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/198 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	102/103 (99%)	101 (99%)	1 (1%)	68	84
13	AM	92/96 (96%)	92 (100%)	0	100	100
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%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	71 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
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%)	163 (100%)	0	100	100
26	BE	165/165 (100%)	165 (100%)	0	100	100
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%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BI	59/62 (95%)	59 (100%)	0	100	100
31	BJ	116/116 (100%)	116 (100%)	0	100	100
32	BK	104/104 (100%)	104 (100%)	0	100	100
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%)	84 (100%)	0	100	100
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%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	18	31
All	All	4650/4843 (96%)	4648 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	AL	45	PRO
53	B5	24	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	AC	123	GLN
3	AC	185	ASN
4	AD	36	GLN
4	AD	41	HIS
5	AE	132	ASN
6	AF	63	ASN
6	AF	81	ASN
7	AG	148	ASN
9	AI	50	GLN
11	AK	119	ASN
15	AO	35	GLN
20	AT	52	ASN
24	BC	15	HIS
24	BC	25	HIS
24	BC	128	ASN
24	BC	239	ASN
25	BD	173	GLN
26	BE	62	GLN
26	BE	115	GLN
27	BF	37	ASN
28	BG	22	GLN
28	BG	38	ASN
28	BG	73	ASN
29	BH	133	GLN
32	BK	88	ASN
38	BQ	20	GLN
40	BS	9	HIS
41	BT	70	HIS
44	BW	46	HIS
45	BX	36	HIS
47	BZ	9	GLN
50	B2	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	181 (11%)	1 (0%)
22	BA	2895/2897 (99%)	298 (10%)	15 (0%)
23	BB	119/120 (99%)	7 (5%)	0
54	B7	8/9 (88%)	4 (50%)	0
55	B8	76/77 (98%)	14 (18%)	4 (5%)
All	All	4631/4637 (99%)	504 (10%)	20 (0%)

All (504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	22	G
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	71	A
1	AA	72	A
1	AA	76	G
1	AA	78	A
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	87	C
1	AA	88	U
1	AA	89	U
1	AA	95	C
1	AA	98	A
1	AA	101	A
1	AA	116	A
1	AA	130	A
1	AA	131	A
1	AA	163	C
1	AA	164	G
1	AA	167	A
1	AA	181	A
1	AA	197	A
1	AA	210	C
1	AA	226	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	306	A
1	AA	321	A

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Mol	Chain	Res	Type
1	AA	328	C
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	G
1	AA	392	C
1	AA	393	A
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	408	A
1	AA	413	G
1	AA	429	U
1	AA	435	A
1	AA	437	U
1	AA	439	U
1	AA	467	U
1	AA	468	A
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	488	C
1	AA	497	G
1	AA	509	A
1	AA	511	C
1	AA	513	C
1	AA	516	PSU
1	AA	518	C
1	AA	527	G7M
1	AA	532	A
1	AA	547	A
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	617	G
1	AA	633	G

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Mol	Chain	Res	Type
1	AA	650	G
1	AA	653	U
1	AA	665	A
1	AA	702	A
1	AA	718	A
1	AA	721	G
1	AA	722	G
1	AA	724	G
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	832	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	846	G
1	AA	914	A
1	AA	926	G
1	AA	934	C
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	993	G
1	AA	1004	A
1	AA	1005	A
1	AA	1012	A
1	AA	1016	A
1	AA	1019	A
1	AA	1020	G
1	AA	1021	A
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U

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Mol	Chain	Res	Type
1	AA	1030	U
1	AA	1032	G
1	AA	1045	C
1	AA	1053	G
1	AA	1065	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1132	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1157	A
1	AA	1158	C
1	AA	1159	U
1	AA	1168	U
1	AA	1169	A
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1212	U
1	AA	1213	A
1	AA	1227	A
1	AA	1238	A
1	AA	1256	A
1	AA	1258	G
1	AA	1260	G
1	AA	1280	A
1	AA	1285	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1317	C
1	AA	1318	A
1	AA	1320	C
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1370	G
1	AA	1419	G
1	AA	1429	A

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Mol	Chain	Res	Type
1	AA	1441	A
1	AA	1446	A
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1497	G
1	AA	1499	A
1	AA	1502	A
1	AA	1506	U
1	AA	1517	G
1	AA	1519	MA6
1	AA	1529	G
1	AA	1530	G
22	BA	34	U
22	BA	61	C
22	BA	71	A
22	BA	74	A
22	BA	75	G
22	BA	84	A
22	BA	101	A
22	BA	118	A
22	BA	119	A
22	BA	120	U
22	BA	163	C
22	BA	181	A
22	BA	196	A
22	BA	215	G
22	BA	216	A
22	BA	221	A
22	BA	222	A
22	BA	233	A
22	BA	248	G
22	BA	265	A
22	BA	276	U
22	BA	278	A
22	BA	302	C
22	BA	303	G
22	BA	311	A
22	BA	330	A
22	BA	353	C
22	BA	386	G
22	BA	396	G

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Mol	Chain	Res	Type
22	BA	411	G
22	BA	412	A
22	BA	480	A
22	BA	481	G
22	BA	491	G
22	BA	505	A
22	BA	509	C
22	BA	529	A
22	BA	530	G
22	BA	531	C
22	BA	532	A
22	BA	544	C
22	BA	546	U
22	BA	547	A
22	BA	548	G
22	BA	549	G
22	BA	563	A
22	BA	573	U
22	BA	575	A
22	BA	603	A
22	BA	614	A
22	BA	637	A
22	BA	645	C
22	BA	647	G
22	BA	654	A
22	BA	655	A
22	BA	685	A
22	BA	686	U
22	BA	717	C
22	BA	730	A
22	BA	738	G
22	BA	747	5MU
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	792	A
22	BA	805	G

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Mol	Chain	Res	Type
22	BA	812	C
22	BA	827	U
22	BA	828	U
22	BA	829	A
22	BA	846	U
22	BA	847	U
22	BA	858	G
22	BA	859	G
22	BA	884	U
22	BA	896	A
22	BA	910	A
22	BA	931	U
22	BA	946	C
22	BA	961	C
22	BA	974	G
22	BA	983	A
22	BA	984	A
22	BA	985	C
22	BA	996	A
22	BA	1012	U
22	BA	1013	C
22	BA	1026	G
22	BA	1033	U
22	BA	1054	A
22	BA	1070	A
22	BA	1088	A
22	BA	1112	G
22	BA	1132	U
22	BA	1133	A
22	BA	1135	C
22	BA	1142	A
22	BA	1173	U
22	BA	1174	U
22	BA	1175	A
22	BA	1176	U
22	BA	1204	A
22	BA	1250	G
22	BA	1253	A
22	BA	1256	G
22	BA	1268	A
22	BA	1271	G
22	BA	1272	A

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Mol	Chain	Res	Type
22	BA	1273	U
22	BA	1287	A
22	BA	1300	G
22	BA	1301	A
22	BA	1321	A
22	BA	1329	U
22	BA	1352	U
22	BA	1365	A
22	BA	1379	U
22	BA	1383	A
22	BA	1416	G
22	BA	1420	A
22	BA	1428	C
22	BA	1452	G
22	BA	1482	G
22	BA	1508	A
22	BA	1509	A
22	BA	1515	A
22	BA	1566	A
22	BA	1569	A
22	BA	1578	U
22	BA	1606	C
22	BA	1608	A
22	BA	1610	A
22	BA	1647	U
22	BA	1648	U
22	BA	1649	G
22	BA	1674	G
22	BA	1677	A
22	BA	1729	U
22	BA	1730	C
22	BA	1732	C
22	BA	1757	A
22	BA	1758	U
22	BA	1764	C
22	BA	1773	A
22	BA	1782	U
22	BA	1800	C
22	BA	1801	A
22	BA	1802	A
22	BA	1808	A
22	BA	1811	G

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Mol	Chain	Res	Type
22	BA	1816	C
22	BA	1829	A
22	BA	1871	A
22	BA	1872	A
22	BA	1873	G
22	BA	1906	G
22	BA	1914	C
22	BA	1929	G
22	BA	1930	G
22	BA	1937	A
22	BA	1938	A
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	2020	A
22	BA	2023	C
22	BA	2027	G
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	2080	A
22	BA	2099	U
22	BA	2100	G
22	BA	2101	A
22	BA	2110	G
22	BA	2111	U
22	BA	2112	G
22	BA	2113	U
22	BA	2115	G

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Mol	Chain	Res	Type
22	BA	2116	G
22	BA	2117	A
22	BA	2118	U
22	BA	2119	A
22	BA	2124	G
22	BA	2125	G
22	BA	2126	A
22	BA	2127	G
22	BA	2128	G
22	BA	2131	U
22	BA	2132	U
22	BA	2133	G
22	BA	2137	U
22	BA	2142	A
22	BA	2147	A
22	BA	2157	G
22	BA	2158	A
22	BA	2159	G
22	BA	2163	A
22	BA	2164	C
22	BA	2165	C
22	BA	2171	A
22	BA	2172	U
22	BA	2173	A
22	BA	2182	U
22	BA	2183	A
22	BA	2188	U
22	BA	2189	U
22	BA	2190	G
22	BA	2195	U
22	BA	2198	A
22	BA	2204	G
22	BA	2211	A
22	BA	2225	A
22	BA	2238	G
22	BA	2239	G
22	BA	2252	G
22	BA	2278	A
22	BA	2283	C
22	BA	2287	A
22	BA	2288	A
22	BA	2305	U

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Mol	Chain	Res	Type
22	BA	2308	G
22	BA	2322	A
22	BA	2325	G
22	BA	2333	A
22	BA	2336	A
22	BA	2345	G
22	BA	2347	C
22	BA	2350	C
22	BA	2368	C
22	BA	2383	G
22	BA	2385	C
22	BA	2402	U
22	BA	2406	A
22	BA	2425	A
22	BA	2429	G
22	BA	2430	A
22	BA	2435	A
22	BA	2441	U
22	BA	2448	A
22	BA	2476	A
22	BA	2478	A
22	BA	2491	U
22	BA	2502	G
22	BA	2505	G
22	BA	2518	A
22	BA	2529	G
22	BA	2535	G
22	BA	2547	A
22	BA	2566	A
22	BA	2567	G
22	BA	2602	A
22	BA	2609	U
22	BA	2613	U
22	BA	2615	U
22	BA	2629	U
22	BA	2630	G
22	BA	2663	G
22	BA	2682	A
22	BA	2689	U
22	BA	2690	U
22	BA	2714	G
22	BA	2716	C

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Mol	Chain	Res	Type
22	BA	2726	A
22	BA	2733	A
22	BA	2744	G
22	BA	2748	A
22	BA	2778	A
22	BA	2791	G
22	BA	2820	A
22	BA	2821	A
22	BA	2835	A
22	BA	2861	U
22	BA	2873	A
22	BA	2874	C
22	BA	2880	C
22	BA	2883	A
22	BA	2884	U
22	BA	2885	G
22	BA	2891	U
23	BB	35	C
23	BB	44	G
23	BB	56	G
23	BB	89	U
23	BB	90	C
23	BB	105	G
23	BB	109	A
54	B7	4	C
54	B7	7	U
54	B7	8	G
54	B7	9	A
55	B8	3	G
55	B8	4	U
55	B8	5	G
55	B8	6	A
55	B8	14	A
55	B8	17	C
55	B8	19	G
55	B8	20	U
55	B8	21	A
55	B8	22	G
55	B8	36	G
55	B8	46	G7M
55	B8	47	U
55	B8	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1225	A
22	BA	125	A
22	BA	764	A
22	BA	784	G
22	BA	984	A
22	BA	1286	A
22	BA	1608	A
22	BA	1970	A
22	BA	2099	U
22	BA	2146	C
22	BA	2162	G
22	BA	2188	U
22	BA	2189	U
22	BA	2251	OMG
22	BA	2518	A
22	BA	2873	A
55	B8	2	G
55	B8	3	G
55	B8	19	G
55	B8	20	U

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

40 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	$\# Z > 2$
1	UR3	AA	1498	1	19,22,23	3.02	8 (42%)	26,32,35	1.42	2 (7%)
55	G7M	B8	46	55	23,26,27	2.56	8 (34%)	35,39,42	2.38	12 (34%)
1	5MC	AA	1407	1	18,22,23	3.53	7 (38%)	26,32,35	1.02	1 (3%)
22	2MG	BA	1835	22	23,26,27	2.68	8 (34%)	32,38,41	2.21	13 (40%)
22	5MU	BA	1939	57,22	19,22,23	0.75	0	28,32,35	1.19	4 (14%)
22	PSU	BA	1917	22	18,21,22	4.24	7 (38%)	22,30,33	1.71	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	AA	527	1	23,26,27	2.71	8 (34%)	35,39,42	2.36	11 (31%)
22	6MZ	BA	1618	22	22,25,26	3.97	6 (27%)	30,36,39	2.29	9 (30%)
22	OMC	BA	2498	22,56	19,22,23	2.91	8 (42%)	26,31,34	1.17	2 (7%)
22	5MC	BA	1962	57,22	18,22,23	3.39	7 (38%)	26,32,35	1.15	2 (7%)
22	6MZ	BA	2030	22	22,25,26	3.77	6 (27%)	30,36,39	2.53	11 (36%)
34	4D4	BM	81	34	9,11,12	2.52	3 (33%)	8,13,15	1.06	0
22	PSU	BA	2580	57,22	18,21,22	4.19	8 (44%)	22,30,33	2.02	6 (27%)
1	MA6	AA	1519	1	23,26,27	1.74	4 (17%)	34,38,41	3.38	12 (35%)
22	5MU	BA	747	22	19,22,23	0.78	0	28,32,35	1.10	2 (7%)
22	PSU	BA	2457	22	18,21,22	4.13	7 (38%)	22,30,33	1.70	5 (22%)
1	2MG	AA	966	1	23,26,27	2.78	9 (39%)	32,38,41	2.18	11 (34%)
22	PSU	BA	2604	22	18,21,22	4.11	6 (33%)	22,30,33	1.86	5 (22%)
55	PSU	B8	55	55	18,21,22	4.26	8 (44%)	22,30,33	1.94	5 (22%)
1	MA6	AA	1518	1	23,26,27	1.75	4 (17%)	34,38,41	3.32	11 (32%)
55	1MG	B8	37	55	22,26,27	2.55	7 (31%)	33,39,42	1.70	8 (24%)
1	PSU	AA	516	1,56	18,21,22	4.35	7 (38%)	22,30,33	1.66	4 (18%)
25	MEQ	BD	150	25	8,9,10	1.64	2 (25%)	5,10,12	1.76	2 (40%)
22	OMG	BA	2251	57,22,55	23,26,27	2.37	8 (34%)	33,38,41	2.14	15 (45%)
1	4OC	AA	1402	1,56	20,23,24	3.13	8 (40%)	26,32,35	1.02	2 (7%)
22	PSU	BA	1911	22	18,21,22	4.28	7 (38%)	22,30,33	1.86	5 (22%)
22	3TD	BA	1915	22	18,22,23	4.17	8 (44%)	22,32,35	1.65	3 (13%)
1	5MC	AA	967	1	18,22,23	3.50	7 (38%)	26,32,35	0.98	1 (3%)
22	PSU	BA	2504	57,22	18,21,22	4.25	7 (38%)	22,30,33	1.83	5 (22%)
22	2MG	BA	2445	22	23,26,27	2.68	9 (39%)	32,38,41	2.30	13 (40%)
22	PSU	BA	955	22	18,21,22	4.18	7 (38%)	22,30,33	1.50	4 (18%)
22	OMU	BA	2552	22,56	19,22,23	2.83	7 (36%)	26,31,34	1.72	5 (19%)
22	G7M	BA	2069	57,22	23,26,27	2.59	8 (34%)	35,39,42	2.22	11 (31%)
22	2MA	BA	2503	57,22,56	22,25,26	3.71	8 (36%)	33,37,40	2.21	11 (33%)
22	PSU	BA	2605	22	18,21,22	4.13	7 (38%)	22,30,33	1.71	3 (13%)
1	2MG	AA	1207	57,1	23,26,27	2.86	8 (34%)	32,38,41	2.30	12 (37%)
1	2MG	AA	1516	1	23,26,27	2.77	9 (39%)	32,38,41	2.16	13 (40%)
22	1MG	BA	745	22	22,26,27	2.53	6 (27%)	33,39,42	1.92	8 (24%)
12	D2T	AL	89	12	7,9,10	1.09	0	6,11,13	2.51	3 (50%)
22	PSU	BA	746	22,56	18,21,22	4.26	8 (44%)	22,30,33	1.81	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
55	G7M	B8	46	55	-	0/7/25/26	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/9/27/28	0/3/3/3
22	5MU	BA	1939	57,22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
22	6MZ	BA	1618	22	-	0/9/27/28	0/3/3/3
22	OMC	BA	2498	22,56	-	0/9/27/28	0/2/2/2
22	5MC	BA	1962	57,22	-	0/7/25/26	0/2/2/2
22	6MZ	BA	2030	22	-	2/9/27/28	0/3/3/3
34	4D4	BM	81	34	-	3/11/12/14	-
22	PSU	BA	2580	57,22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
22	5MU	BA	747	22	-	1/7/25/26	0/2/2/2
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
55	PSU	B8	55	55	-	2/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
55	1MG	B8	37	55	-	0/7/25/26	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
25	MEQ	BD	150	25	-	3/8/9/11	-
22	OMG	BA	2251	57,22,55	-	3/9/27/28	0/3/3/3
1	4OC	AA	1402	1,56	-	2/9/29/30	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	3TD	BA	1915	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	2504	57,22	-	2/7/25/26	0/2/2/2
22	2MG	BA	2445	22	-	1/9/27/28	0/3/3/3
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
22	OMU	BA	2552	22,56	-	1/9/27/28	0/2/2/2
22	G7M	BA	2069	57,22	-	2/7/25/26	0/3/3/3
22	2MA	BA	2503	57,22,56	-	2/7/25/26	0/3/3/3
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	57,1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
22	1MG	BA	745	22	-	0/7/25/26	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
22	PSU	BA	746	22,56	-	1/7/25/26	0/2/2/2

All (260) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1618	6MZ	C6-N6	17.34	1.53	1.34
22	BA	2030	6MZ	C6-N6	16.27	1.51	1.34
22	BA	1915	3TD	C6-C5	11.97	1.49	1.35
22	BA	746	PSU	C6-C5	11.78	1.49	1.35
22	BA	2504	PSU	C6-C5	11.65	1.48	1.35
1	AA	516	PSU	C6-C5	11.65	1.48	1.35
22	BA	2580	PSU	C6-C5	11.49	1.48	1.35
22	BA	1911	PSU	C6-C5	11.36	1.48	1.35
22	BA	2503	2MA	C4-N3	11.32	1.48	1.34
22	BA	2605	PSU	C6-C5	11.29	1.48	1.35
22	BA	955	PSU	C6-C5	11.24	1.48	1.35
22	BA	2457	PSU	C6-C5	11.21	1.48	1.35
22	BA	1917	PSU	C6-C5	11.21	1.48	1.35
22	BA	2604	PSU	C6-C5	11.15	1.48	1.35
55	B8	55	PSU	C6-C5	11.12	1.48	1.35
55	B8	55	PSU	C2-N1	9.84	1.50	1.36
22	BA	1911	PSU	C2-N1	9.77	1.50	1.36
1	AA	516	PSU	C2-N1	9.62	1.49	1.36
22	BA	746	PSU	C2-N1	9.54	1.49	1.36
22	BA	1917	PSU	C2-N1	9.45	1.49	1.36
22	BA	2605	PSU	C2-N1	9.39	1.49	1.36
22	BA	2504	PSU	C2-N1	9.36	1.49	1.36
1	AA	1407	5MC	C6-C5	9.26	1.49	1.34
22	BA	2604	PSU	C2-N1	9.14	1.49	1.36
1	AA	967	5MC	C6-C5	8.89	1.49	1.34
22	BA	1962	5MC	C6-C5	8.85	1.49	1.34
22	BA	955	PSU	C2-N1	8.82	1.48	1.36
22	BA	2580	PSU	C2-N1	8.80	1.48	1.36
22	BA	2457	PSU	C2-N1	8.77	1.48	1.36
22	BA	1915	3TD	C2-N1	8.71	1.48	1.37
1	AA	1498	UR3	C2-N1	8.25	1.50	1.38
1	AA	1207	2MG	C2-N3	7.48	1.46	1.31
1	AA	516	PSU	C2-N3	7.31	1.50	1.37
22	BA	2580	PSU	C2-N3	7.22	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	966	2MG	C2-N3	7.15	1.45	1.31
1	AA	1516	2MG	C2-N3	7.12	1.45	1.31
22	BA	1911	PSU	C2-N3	7.07	1.49	1.37
22	BA	2503	2MA	C2-N3	7.02	1.46	1.34
22	BA	1917	PSU	C2-N3	6.99	1.49	1.37
22	BA	955	PSU	C2-N3	6.92	1.49	1.37
55	B8	55	PSU	C2-N3	6.88	1.49	1.37
22	BA	2504	PSU	C2-N3	6.82	1.49	1.37
22	BA	2457	PSU	C2-N3	6.81	1.49	1.37
22	BA	2604	PSU	C2-N3	6.79	1.49	1.37
22	BA	1835	2MG	C2-N3	6.75	1.44	1.31
22	BA	2445	2MG	C2-N3	6.69	1.44	1.31
1	AA	527	G7M	C4-N3	6.66	1.50	1.34
1	AA	1402	4OC	C4-N3	6.64	1.44	1.32
22	BA	746	PSU	C2-N3	6.61	1.48	1.37
1	AA	967	5MC	C4-N3	6.48	1.45	1.34
1	AA	1402	4OC	C6-C5	6.45	1.50	1.35
1	AA	1207	2MG	C4-N3	6.45	1.49	1.34
22	BA	2069	G7M	C4-N3	6.43	1.49	1.34
55	B8	37	1MG	C4-N3	6.39	1.49	1.34
55	B8	37	1MG	C2-N3	6.37	1.46	1.34
22	BA	2552	OMU	C2-N3	6.33	1.49	1.38
22	BA	745	1MG	C4-N3	6.33	1.49	1.34
22	BA	745	1MG	C2-N3	6.20	1.45	1.34
1	AA	1407	5MC	C4-N3	6.20	1.44	1.34
1	AA	966	2MG	C4-N3	6.12	1.48	1.34
22	BA	2503	2MA	C2-N1	6.11	1.44	1.34
34	BM	81	4D4	CZ-NE	6.09	1.45	1.33
22	BA	2605	PSU	C2-N3	6.08	1.47	1.37
22	BA	1962	5MC	C4-N3	6.06	1.44	1.34
22	BA	2552	OMU	C2-N1	6.06	1.48	1.38
22	BA	2251	OMG	C4-N3	6.05	1.48	1.34
1	AA	967	5MC	C2-N3	6.05	1.48	1.36
1	AA	1516	2MG	C4-N3	6.04	1.48	1.34
1	AA	1402	4OC	C2-N3	5.98	1.48	1.36
22	BA	2498	OMC	C6-C5	5.94	1.48	1.35
1	AA	527	G7M	C2-N3	5.93	1.47	1.33
1	AA	1407	5MC	C2-N3	5.88	1.48	1.36
22	BA	2503	2MA	C6-N1	5.86	1.43	1.35
22	BA	1835	2MG	C4-N3	5.79	1.48	1.34
55	B8	46	G7M	C4-N3	5.76	1.48	1.34
22	BA	2445	2MG	C4-N3	5.76	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1962	5MC	C2-N3	5.73	1.48	1.36
22	BA	2498	OMC	C2-N3	5.69	1.47	1.36
1	AA	1498	UR3	C6-C5	5.57	1.48	1.35
1	AA	1519	MA6	C6-N6	5.56	1.53	1.36
1	AA	1207	2MG	C2-N2	5.48	1.45	1.33
1	AA	966	2MG	C2-N2	5.42	1.45	1.33
1	AA	1518	MA6	C6-N6	5.42	1.52	1.36
22	BA	1915	3TD	C6-N1	5.37	1.45	1.36
1	AA	1516	2MG	C2-N2	5.32	1.45	1.33
55	B8	46	G7M	C5-N7	-5.32	1.33	1.39
22	BA	2069	G7M	C2-N3	5.26	1.45	1.33
22	BA	2552	OMU	C6-C5	5.22	1.47	1.35
55	B8	46	G7M	C2-N3	5.19	1.45	1.33
22	BA	2069	G7M	C5-N7	-5.17	1.33	1.39
1	AA	527	G7M	C5-N7	-5.06	1.33	1.39
22	BA	1917	PSU	C6-N1	5.01	1.44	1.36
22	BA	2445	2MG	C2-N2	5.00	1.44	1.33
55	B8	55	PSU	C6-N1	4.95	1.44	1.36
22	BA	2251	OMG	C2-N3	4.94	1.45	1.33
22	BA	1911	PSU	C6-N1	4.89	1.44	1.36
1	AA	1207	2MG	C2-N1	4.89	1.44	1.36
22	BA	2498	OMC	C2-N1	4.88	1.50	1.40
1	AA	1498	UR3	C2-N3	4.87	1.48	1.39
22	BA	2605	PSU	C6-N1	4.83	1.44	1.36
22	BA	1835	2MG	C2-N2	4.83	1.44	1.33
1	AA	516	PSU	C6-N1	4.83	1.44	1.36
1	AA	966	2MG	C2-N1	4.81	1.44	1.36
1	AA	1516	2MG	C2-N1	4.77	1.44	1.36
22	BA	1915	3TD	C1'-C5	-4.74	1.39	1.50
22	BA	2504	PSU	C6-N1	4.69	1.44	1.36
55	B8	37	1MG	C2-N2	4.62	1.42	1.34
1	AA	1402	4OC	C4-N4	4.61	1.45	1.35
22	BA	1915	3TD	C2-N3	4.58	1.48	1.38
22	BA	2251	OMG	C2-N2	4.57	1.45	1.34
1	AA	1407	5MC	C6-N1	4.56	1.45	1.38
22	BA	955	PSU	C6-N1	4.56	1.43	1.36
22	BA	746	PSU	C6-N1	4.55	1.43	1.36
22	BA	2457	PSU	C6-N1	4.54	1.43	1.36
22	BA	1835	2MG	C2-N1	4.52	1.43	1.36
22	BA	745	1MG	C2-N2	4.52	1.42	1.34
22	BA	2503	2MA	C5-C6	4.43	1.53	1.41
22	BA	2498	OMC	C4-N4	4.42	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	967	5MC	C6-N1	4.38	1.45	1.38
22	BA	2604	PSU	C6-N1	4.35	1.43	1.36
22	BA	2445	2MG	C2-N1	4.34	1.43	1.36
22	BA	2580	PSU	C6-N1	4.31	1.43	1.36
1	AA	1498	UR3	O4-C4	-4.29	1.14	1.23
22	BA	2498	OMC	C4-N3	4.29	1.43	1.34
1	AA	1407	5MC	C4-N4	4.20	1.45	1.34
1	AA	967	5MC	C4-N4	4.19	1.45	1.34
1	AA	527	G7M	C5-C6	4.16	1.55	1.43
22	BA	1962	5MC	C6-N1	4.13	1.45	1.38
1	AA	516	PSU	C4-N3	4.08	1.46	1.38
1	AA	527	G7M	C2-N2	4.08	1.43	1.34
22	BA	2069	G7M	C5-C6	4.03	1.54	1.43
1	AA	967	5MC	C2-N1	4.01	1.48	1.40
22	BA	1917	PSU	C4-N3	4.01	1.46	1.38
1	AA	1407	5MC	C2-N1	3.98	1.48	1.40
22	BA	1962	5MC	C4-N4	3.97	1.44	1.34
22	BA	955	PSU	C4-N3	3.94	1.46	1.38
22	BA	2552	OMU	C4-N3	3.93	1.45	1.38
1	AA	1402	4OC	C2-N1	3.89	1.48	1.40
1	AA	1402	4OC	C5-C4	3.86	1.49	1.40
22	BA	1962	5MC	C2-N1	3.82	1.48	1.40
22	BA	2069	G7M	C2-N2	3.80	1.43	1.34
22	BA	1911	PSU	C4-N3	3.71	1.45	1.38
22	BA	2457	PSU	C4-N3	3.69	1.45	1.38
55	B8	46	G7M	C4-N9	-3.64	1.28	1.38
55	B8	55	PSU	C4-N3	3.64	1.45	1.38
22	BA	2030	6MZ	C5-N7	-3.59	1.32	1.39
22	BA	2580	PSU	C4-N3	3.59	1.45	1.38
22	BA	2503	2MA	C6-N6	-3.57	1.25	1.34
22	BA	1835	2MG	C5-N7	-3.56	1.32	1.39
55	B8	46	G7M	C5-C6	3.54	1.53	1.43
55	B8	46	G7M	C2-N2	3.53	1.42	1.34
22	BA	2552	OMU	O4-C4	-3.47	1.17	1.24
22	BA	745	1MG	C5-C6	3.47	1.54	1.45
22	BA	2504	PSU	C4-N3	3.46	1.45	1.38
22	BA	2498	OMC	O2-C2	-3.45	1.17	1.23
22	BA	2503	2MA	C8-N7	3.43	1.38	1.31
22	BA	2604	PSU	C4-N3	3.39	1.45	1.38
55	B8	37	1MG	C5-N7	-3.37	1.32	1.39
1	AA	527	G7M	C6-N1	3.35	1.45	1.38
22	BA	2498	OMC	C6-N1	3.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1402	4OC	C6-N1	3.26	1.45	1.38
22	BA	1618	6MZ	C5-N7	-3.23	1.32	1.39
22	BA	2605	PSU	C4-N3	3.18	1.44	1.38
1	AA	1402	4OC	O2-C2	-3.16	1.17	1.23
55	B8	46	G7M	C6-N1	3.16	1.44	1.38
1	AA	1516	2MG	C5-N7	-3.16	1.33	1.39
22	BA	1835	2MG	O6-C6	-3.14	1.17	1.23
22	BA	745	1MG	C5-N7	-3.13	1.33	1.39
22	BA	746	PSU	C4-N3	3.12	1.44	1.38
22	BA	2069	G7M	C6-N1	3.12	1.44	1.38
22	BA	2251	OMG	C5-N7	-3.11	1.33	1.39
55	B8	37	1MG	C5-C6	3.08	1.53	1.45
1	AA	966	2MG	C5-N7	-3.08	1.33	1.39
22	BA	2445	2MG	C5-N7	-3.07	1.33	1.39
22	BA	2445	2MG	O6-C6	-3.06	1.17	1.23
1	AA	1518	MA6	C5-C4	-3.05	1.33	1.39
34	BM	81	4D4	CZ-NH2	3.04	1.44	1.32
22	BA	2251	OMG	O6-C6	-3.04	1.17	1.23
25	BD	150	MEQ	OE1-CD	-3.03	1.17	1.23
22	BA	1962	5MC	O2-C2	-2.98	1.18	1.23
22	BA	745	1MG	O6-C6	-2.98	1.16	1.23
1	AA	1407	5MC	O2-C2	-2.94	1.18	1.23
1	AA	1498	UR3	C5-C4	2.93	1.51	1.43
1	AA	1207	2MG	C5-N7	-2.92	1.33	1.39
22	BA	2552	OMU	O2-C2	-2.92	1.17	1.23
22	BA	1618	6MZ	C8-N9	-2.91	1.32	1.37
1	AA	527	G7M	C2-N1	2.88	1.44	1.37
22	BA	2030	6MZ	C8-N9	-2.87	1.32	1.37
22	BA	2069	G7M	C4-N9	-2.84	1.30	1.38
22	BA	955	PSU	C1'-C5	2.83	1.56	1.50
1	AA	1519	MA6	C5-N7	-2.83	1.33	1.39
22	BA	2445	2MG	C5-C6	2.80	1.54	1.44
55	B8	46	G7M	C2-N1	2.80	1.44	1.37
22	BA	955	PSU	O4-C4	-2.77	1.18	1.23
1	AA	1498	UR3	O2-C2	-2.76	1.17	1.22
1	AA	967	5MC	O2-C2	-2.76	1.18	1.23
1	AA	1519	MA6	C5-C4	-2.75	1.33	1.39
22	BA	2457	PSU	C1'-C5	2.75	1.56	1.50
22	BA	2457	PSU	O4-C4	-2.75	1.18	1.23
22	BA	2604	PSU	O4-C4	-2.74	1.18	1.23
1	AA	1518	MA6	C5-N7	-2.71	1.33	1.39
22	BA	2552	OMU	C6-N1	2.69	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1516	2MG	O6-C6	-2.68	1.18	1.23
1	AA	1518	MA6	C8-N9	-2.68	1.32	1.37
1	AA	1207	2MG	C5-C6	2.65	1.54	1.44
22	BA	2030	6MZ	C5-C4	-2.64	1.34	1.39
22	BA	746	PSU	C1'-C5	2.64	1.56	1.50
1	AA	1516	2MG	C5-C6	2.63	1.54	1.44
1	AA	1207	2MG	C6-N1	2.60	1.43	1.38
22	BA	2251	OMG	C2-N1	2.60	1.44	1.37
1	AA	966	2MG	O6-C6	-2.60	1.18	1.23
55	B8	55	PSU	O4-C4	-2.53	1.18	1.23
22	BA	2580	PSU	O4-C4	-2.52	1.18	1.23
22	BA	2251	OMG	C4-N9	-2.51	1.31	1.38
22	BA	2605	PSU	C1'-C5	2.50	1.55	1.50
22	BA	1915	3TD	C4-N3	2.50	1.45	1.40
22	BA	1618	6MZ	C9-N6	2.49	1.49	1.45
1	AA	1207	2MG	O6-C6	-2.49	1.18	1.23
22	BA	2504	PSU	C1'-C5	2.48	1.55	1.50
22	BA	2069	G7M	C2-N1	2.48	1.43	1.37
1	AA	966	2MG	C6-N1	2.47	1.43	1.38
22	BA	1915	3TD	O2-C2	-2.46	1.18	1.23
22	BA	1618	6MZ	C5-C4	-2.45	1.34	1.39
1	AA	516	PSU	C1'-C5	2.45	1.55	1.50
22	BA	1835	2MG	C5-C6	2.45	1.53	1.44
22	BA	746	PSU	O4-C4	-2.43	1.19	1.23
22	BA	1917	PSU	C1'-C5	2.41	1.55	1.50
1	AA	1519	MA6	C8-N9	-2.41	1.33	1.37
22	BA	2605	PSU	O4-C4	-2.41	1.19	1.23
1	AA	1498	UR3	C6-N1	2.40	1.43	1.38
22	BA	2504	PSU	O4-C4	-2.38	1.19	1.23
22	BA	2503	2MA	C5-N7	-2.37	1.34	1.39
34	BM	81	4D4	CZ-NH1	-2.36	1.25	1.34
22	BA	2498	OMC	C5-C4	2.35	1.48	1.42
1	AA	966	2MG	C5-C6	2.35	1.53	1.44
55	B8	37	1MG	O6-C6	-2.35	1.18	1.23
22	BA	2445	2MG	C4-N9	-2.34	1.32	1.38
22	BA	1835	2MG	C4-N9	-2.34	1.32	1.38
1	AA	527	G7M	C4-N9	-2.29	1.32	1.38
22	BA	2251	OMG	C5-C6	2.28	1.52	1.44
22	BA	2445	2MG	C6-N1	2.28	1.43	1.38
22	BA	2030	6MZ	C8-N7	2.25	1.35	1.31
22	BA	1911	PSU	C1'-C5	2.25	1.55	1.50
22	BA	2580	PSU	C1'-C5	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	516	PSU	O4-C4	-2.22	1.19	1.23
55	B8	55	PSU	O4'-C1'	-2.20	1.40	1.43
1	AA	1516	2MG	C4-N9	-2.20	1.32	1.38
1	AA	966	2MG	C4-N9	-2.20	1.32	1.38
55	B8	37	1MG	C4-N9	-2.19	1.32	1.38
25	BD	150	MEQ	CD-NE2	2.19	1.44	1.34
1	AA	1516	2MG	C6-N1	2.19	1.42	1.38
22	BA	2030	6MZ	C9-N6	2.19	1.48	1.45
22	BA	1618	6MZ	C8-N7	2.17	1.35	1.31
55	B8	55	PSU	C1'-C5	2.17	1.55	1.50
22	BA	1911	PSU	O4-C4	-2.16	1.19	1.23
22	BA	2580	PSU	O4'-C1'	-2.15	1.40	1.43
22	BA	1917	PSU	O4-C4	-2.15	1.19	1.23
1	AA	1498	UR3	C3U-N3	-2.10	1.43	1.47
22	BA	1915	3TD	O4-C4	-2.02	1.18	1.23
22	BA	746	PSU	O4'-C1'	-2.00	1.41	1.43

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-13.43	102.40	117.08
1	AA	1518	MA6	N1-C6-N6	-13.12	102.74	117.08
22	BA	2445	2MG	C2-N3-C4	7.55	121.40	112.04
55	B8	46	G7M	C1'-N9-C8	-7.18	102.50	126.74
1	AA	1519	MA6	C5-C6-N6	7.14	137.74	125.30
22	BA	2030	6MZ	C9-N6-C6	-7.09	116.76	122.87
1	AA	1518	MA6	C5-C6-N6	6.98	137.46	125.30
1	AA	1207	2MG	C2-N3-C4	6.95	120.65	112.04
1	AA	527	G7M	C1'-N9-C4	6.79	146.68	126.50
1	AA	527	G7M	C1'-N9-C8	-6.74	103.99	126.74
1	AA	1516	2MG	C2-N3-C4	6.37	119.94	112.04
55	B8	46	G7M	C1'-N9-C4	6.33	145.31	126.50
1	AA	966	2MG	C2-N3-C4	6.33	119.89	112.04
22	BA	2503	2MA	C5-C4-N3	-6.29	120.12	127.19
22	BA	1835	2MG	C2-N3-C4	6.27	119.81	112.04
22	BA	2069	G7M	C1'-N9-C8	-5.80	107.14	126.74
22	BA	745	1MG	C5-C4-N3	-5.58	119.41	128.46
1	AA	1518	MA6	N1-C2-N3	-5.51	119.99	128.60
22	BA	1618	6MZ	N1-C2-N3	-5.50	120.00	128.60
22	BA	2030	6MZ	N1-C2-N3	-5.50	120.00	128.60
22	BA	2069	G7M	C1'-N9-C4	5.49	142.80	126.50
1	AA	1519	MA6	C5-C4-N3	-5.42	119.68	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2552	OMU	C4-N3-C2	-5.40	119.45	126.58
1	AA	1519	MA6	N1-C2-N3	-5.40	120.16	128.60
1	AA	1498	UR3	C4-N3-C2	-5.34	119.53	124.56
1	AA	1518	MA6	C5-C4-N3	-5.29	119.85	126.75
22	BA	1915	3TD	N1-C2-N3	5.25	120.28	116.14
22	BA	2503	2MA	N9-C8-N7	-5.24	106.75	113.91
55	B8	55	PSU	C4-N3-C2	-5.23	118.81	126.34
1	AA	1207	2MG	C5-C4-N3	-5.20	120.02	128.46
22	BA	1618	6MZ	C5-C4-N3	-5.17	120.01	126.75
22	BA	2445	2MG	C5-C4-N3	-5.03	120.31	128.46
55	B8	37	1MG	C5-C4-N3	-4.87	120.56	128.46
22	BA	2030	6MZ	N9-C8-N7	-4.86	107.27	113.91
22	BA	1835	2MG	C5-C4-N3	-4.84	120.60	128.46
22	BA	1911	PSU	C4-N3-C2	-4.75	119.49	126.34
22	BA	2604	PSU	C4-N3-C2	-4.75	119.50	126.34
1	AA	1516	2MG	C5-C4-N3	-4.72	120.81	128.46
22	BA	2457	PSU	C4-N3-C2	-4.66	119.62	126.34
22	BA	746	PSU	C4-N3-C2	-4.63	119.67	126.34
22	BA	746	PSU	N1-C2-N3	4.62	120.36	115.13
1	AA	966	2MG	C5-C4-N3	-4.62	120.97	128.46
22	BA	1835	2MG	C2-N1-C6	-4.62	119.17	124.48
22	BA	2069	G7M	C2-N3-C4	4.60	120.49	112.30
22	BA	1618	6MZ	N9-C8-N7	-4.55	107.70	113.91
22	BA	2504	PSU	C4-N3-C2	-4.51	119.84	126.34
22	BA	2504	PSU	N1-C2-N3	4.49	120.21	115.13
22	BA	2604	PSU	N1-C2-N3	4.48	120.20	115.13
22	BA	2580	PSU	C4-N3-C2	-4.46	119.92	126.34
22	BA	1917	PSU	C4-N3-C2	-4.43	119.95	126.34
12	AL	89	D2T	CB1-SB-CB	4.41	110.43	102.44
22	BA	745	1MG	C2-N3-C4	4.40	121.87	111.98
22	BA	2503	2MA	N3-C4-N9	4.39	133.09	126.99
22	BA	1911	PSU	N1-C2-N3	4.38	120.09	115.13
22	BA	2030	6MZ	C5-C4-N3	-4.38	121.04	126.75
55	B8	55	PSU	N1-C2-N3	4.37	120.08	115.13
22	BA	2251	OMG	C5-C4-N3	-4.36	121.38	128.46
22	BA	2580	PSU	N1-C2-N3	4.36	120.07	115.13
1	AA	1518	MA6	N9-C8-N7	-4.34	107.98	113.91
22	BA	2605	PSU	C4-N3-C2	-4.29	120.15	126.34
1	AA	527	G7M	C2-N3-C4	4.27	119.91	112.30
1	AA	1516	2MG	C2-N1-C6	-4.19	119.66	124.48
22	BA	955	PSU	C4-N3-C2	-4.18	120.32	126.34
1	AA	1207	2MG	C2-N1-C6	-4.17	119.68	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N9-C8-N7	-4.17	108.21	113.91
1	AA	966	2MG	C2-N1-C6	-4.16	119.70	124.48
22	BA	2445	2MG	C2-N1-C6	-4.13	119.73	124.48
22	BA	2605	PSU	N1-C2-N3	4.12	119.80	115.13
1	AA	516	PSU	C4-N3-C2	-4.08	120.45	126.34
22	BA	1915	3TD	C4-N3-C2	-4.05	120.22	124.61
22	BA	2251	OMG	C2-N3-C4	4.01	119.45	112.30
22	BA	2069	G7M	C5-C6-N1	3.97	120.09	111.79
22	BA	1917	PSU	N1-C2-N3	3.93	119.59	115.13
22	BA	2251	OMG	N9-C8-N7	-3.91	106.03	113.39
1	AA	1518	MA6	C4-C5-C6	3.87	120.22	115.88
22	BA	2457	PSU	N1-C2-N3	3.85	119.50	115.13
1	AA	527	G7M	C5-C4-N3	-3.84	120.78	128.15
1	AA	1519	MA6	C4-C5-C6	3.84	120.18	115.88
1	AA	527	G7M	C5-C6-N1	3.82	119.76	111.79
22	BA	1618	6MZ	C4-C5-C6	3.77	119.73	116.81
55	B8	46	G7M	C5-C6-N1	3.77	119.66	111.79
22	BA	745	1MG	N9-C4-N3	3.77	133.50	125.94
1	AA	516	PSU	N1-C2-N3	3.76	119.39	115.13
55	B8	37	1MG	N9-C4-N3	3.74	133.44	125.94
22	BA	2552	OMU	N3-C2-N1	3.69	119.79	114.89
55	B8	46	G7M	O6-C6-C5	-3.68	119.76	128.06
22	BA	2580	PSU	O2-C2-N1	-3.64	118.78	122.79
1	AA	1519	MA6	C2-N3-C4	3.63	120.32	111.75
22	BA	2503	2MA	C5-N7-C8	3.58	108.60	103.51
22	BA	2552	OMU	C5-C4-N3	3.57	120.19	114.84
1	AA	1518	MA6	C2-N3-C4	3.57	120.17	111.75
55	B8	37	1MG	N9-C8-N7	-3.55	106.70	113.39
22	BA	1618	6MZ	C2-N3-C4	3.53	120.10	111.75
1	AA	966	2MG	C1'-N9-C8	-3.49	116.76	126.70
1	AA	1518	MA6	C2-N1-C6	3.49	119.99	111.75
22	BA	2498	OMC	O2-C2-N3	-3.43	116.75	122.33
22	BA	2030	6MZ	C5-N7-C8	3.43	108.38	103.51
22	BA	1618	6MZ	N3-C4-N9	3.43	132.73	127.08
55	B8	37	1MG	C2-N3-C4	3.41	119.64	111.98
22	BA	2580	PSU	C6-C5-C4	3.41	120.58	118.20
1	AA	1519	MA6	C2-N1-C6	3.40	119.79	111.75
22	BA	2069	G7M	C5-C4-N3	-3.40	121.63	128.15
22	BA	2503	2MA	C4-N9-C8	3.37	109.38	105.73
22	BA	1962	5MC	CM5-C5-C6	-3.35	118.37	122.85
22	BA	2251	OMG	O3'-C3'-C2'	3.32	120.59	111.17
22	BA	1962	5MC	C5-C6-N1	-3.32	119.93	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	745	1MG	N9-C8-N7	-3.31	107.16	113.39
22	BA	2030	6MZ	C2-N3-C4	3.31	119.56	111.75
1	AA	1518	MA6	N3-C4-N9	3.30	132.52	127.08
1	AA	1519	MA6	C5-N7-C8	3.30	108.19	103.51
55	B8	46	G7M	C2-N3-C4	3.29	118.16	112.30
22	BA	1618	6MZ	C5-N7-C8	3.26	108.15	103.51
12	AL	89	D2T	OD2-CG-CB	3.22	120.11	113.15
22	BA	2503	2MA	N3-C2-N1	-3.21	119.81	125.72
22	BA	955	PSU	N1-C2-N3	3.20	118.76	115.13
1	AA	1207	2MG	C1'-N9-C8	-3.20	117.59	126.70
1	AA	516	PSU	C6-N1-C2	-3.18	119.43	122.68
55	B8	46	G7M	N9-C8-N7	-3.17	104.36	112.21
22	BA	2069	G7M	O6-C6-C5	-3.16	120.94	128.06
22	BA	746	PSU	C6-N1-C2	-3.15	119.46	122.68
1	AA	1518	MA6	C5-N7-C8	3.14	107.96	103.51
1	AA	527	G7M	O6-C6-C5	-3.11	121.04	128.06
22	BA	745	1MG	C5-C6-N1	3.10	120.90	114.91
55	B8	46	G7M	C2-N1-C6	-3.08	119.47	125.10
1	AA	1519	MA6	N3-C4-N9	3.07	132.13	127.08
22	BA	2030	6MZ	C4-C5-C6	3.06	119.18	116.81
1	AA	966	2MG	N9-C8-N7	-3.06	107.63	113.39
1	AA	967	5MC	C5-C6-N1	-3.05	120.20	123.34
22	BA	1835	2MG	C1'-N9-C8	-3.02	118.11	126.70
22	BA	2503	2MA	N6-C6-N1	3.01	121.29	117.03
25	BD	150	MEQ	CG-CD-NE2	2.98	120.42	116.29
55	B8	46	G7M	N2-C2-N1	2.96	123.02	116.71
22	BA	1911	PSU	C6-N1-C2	-2.96	119.66	122.68
22	BA	2504	PSU	C6-N1-C2	-2.93	119.69	122.68
22	BA	1835	2MG	N9-C8-N7	-2.92	107.89	113.39
22	BA	2580	PSU	C6-N1-C2	-2.92	119.70	122.68
22	BA	2251	OMG	C1'-N9-C8	-2.90	118.43	126.70
22	BA	2445	2MG	N1-C2-N3	-2.90	119.47	123.95
22	BA	2251	OMG	N9-C4-N3	2.90	131.76	125.94
22	BA	2552	OMU	O4-C4-C5	-2.89	120.08	125.16
1	AA	1407	5MC	C5-C6-N1	-2.89	120.37	123.34
1	AA	527	G7M	C2-N1-C6	-2.88	119.84	125.10
1	AA	1516	2MG	N9-C8-N7	-2.85	108.02	113.39
1	AA	1207	2MG	N9-C8-N7	-2.85	108.03	113.39
55	B8	55	PSU	C6-C5-C4	2.84	120.19	118.20
22	BA	2504	PSU	O2-C2-N1	-2.84	119.67	122.79
1	AA	966	2MG	C1'-N9-C4	2.80	134.81	126.50
1	AA	1207	2MG	C1'-N9-C4	2.79	134.79	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2251	OMG	C2'-C1'-N9	-2.77	108.84	114.22
22	BA	2604	PSU	C6-C5-C4	2.77	120.13	118.20
22	BA	1917	PSU	C6-N1-C2	-2.77	119.85	122.68
22	BA	2251	OMG	C2-N1-C6	-2.75	120.08	125.10
1	AA	527	G7M	N9-C4-N3	2.75	131.46	125.94
22	BA	1939	5MU	C4-N3-C2	-2.73	123.81	127.35
1	AA	1207	2MG	N1-C2-N3	-2.71	119.75	123.95
22	BA	2445	2MG	C5-C6-N1	2.71	120.08	113.19
1	AA	1207	2MG	C5-C6-N1	2.71	120.06	113.19
1	AA	1402	4OC	C6-C5-C4	2.70	120.27	116.96
22	BA	2605	PSU	C6-N1-C2	-2.69	119.94	122.68
22	BA	1835	2MG	C1'-N9-C4	2.68	134.47	126.50
22	BA	2251	OMG	C8-N7-C5	2.66	109.05	104.24
1	AA	966	2MG	C5-C6-N1	2.66	119.93	113.19
22	BA	2030	6MZ	C4-N9-C8	2.65	108.60	105.73
22	BA	1911	PSU	C6-C5-C4	2.65	120.05	118.20
1	AA	1207	2MG	N9-C4-N3	2.64	131.24	125.94
1	AA	1516	2MG	C5-C6-N1	2.62	119.86	113.19
22	BA	1618	6MZ	C4-N9-C8	2.62	108.57	105.73
22	BA	1835	2MG	C5-C6-N1	2.62	119.85	113.19
22	BA	2445	2MG	N9-C8-N7	-2.62	108.46	113.39
22	BA	2251	OMG	C5-C6-N1	2.60	119.80	113.19
22	BA	2580	PSU	O4'-C1'-C2'	2.60	108.81	105.14
22	BA	745	1MG	C2-N1-C6	-2.60	118.84	120.95
1	AA	966	2MG	N1-C2-N3	-2.59	119.95	123.95
22	BA	2030	6MZ	N3-C4-N9	2.58	131.33	127.08
1	AA	966	2MG	O6-C6-C5	-2.57	119.78	126.60
22	BA	2445	2MG	C4-C5-N7	-2.57	106.65	110.72
22	BA	1835	2MG	CM2-N2-C2	-2.56	118.21	123.86
22	BA	2251	OMG	O6-C6-C5	-2.56	119.81	126.60
1	AA	966	2MG	N9-C4-N3	2.56	131.08	125.94
22	BA	747	5MU	C6-C5-C4	2.55	120.17	118.03
22	BA	2604	PSU	C6-N1-C2	-2.55	120.08	122.68
55	B8	37	1MG	C5-C6-N1	2.54	119.82	114.91
22	BA	2069	G7M	N9-C8-N7	-2.53	105.96	112.21
22	BA	1939	5MU	C6-C5-C4	2.52	120.14	118.03
22	BA	2445	2MG	C1'-N9-C8	-2.52	119.53	126.70
55	B8	46	G7M	C5-C4-N3	-2.50	123.36	128.15
1	AA	1516	2MG	C1'-N9-C8	-2.49	119.62	126.70
22	BA	2069	G7M	C2-N1-C6	-2.48	120.57	125.10
55	B8	55	PSU	C6-N1-C2	-2.45	120.18	122.68
22	BA	2069	G7M	N9-C4-N3	2.44	130.85	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	747	5MU	C4-N3-C2	-2.43	124.20	127.35
22	BA	2445	2MG	C1'-N9-C4	2.43	133.71	126.50
1	AA	1516	2MG	N1-C2-N3	-2.40	120.25	123.95
22	BA	1835	2MG	C8-N7-C5	2.38	108.55	104.24
22	BA	955	PSU	O2-C2-N1	-2.38	120.17	122.79
55	B8	37	1MG	C1'-N9-C4	-2.38	119.44	126.50
22	BA	745	1MG	C8-N7-C5	2.37	108.53	104.24
22	BA	2069	G7M	N2-C2-N1	2.37	121.75	116.71
1	AA	1207	2MG	O6-C6-C5	-2.37	120.33	126.60
55	B8	46	G7M	CN7-N7-C5	2.36	129.70	126.77
22	BA	746	PSU	C6-C5-C4	2.35	119.84	118.20
22	BA	2030	6MZ	C4-N9-C1'	-2.35	121.00	126.59
1	AA	527	G7M	N9-C8-N7	-2.34	106.41	112.21
22	BA	2457	PSU	O2-C2-N1	-2.34	120.21	122.79
1	AA	1516	2MG	C4-C5-N7	-2.34	107.02	110.72
22	BA	2552	OMU	O2-C2-N1	-2.34	119.68	122.79
25	BD	150	MEQ	OE1-CD-CG	-2.31	117.79	122.02
55	B8	46	G7M	CN7-N7-C8	-2.31	121.28	124.84
1	AA	1402	4OC	C5-C4-N3	-2.30	118.89	122.59
22	BA	1835	2MG	C4-C5-N7	-2.30	107.08	110.72
22	BA	2445	2MG	C8-N7-C5	2.29	108.39	104.24
1	AA	1518	MA6	C4-N9-C8	2.29	108.21	105.73
1	AA	1516	2MG	C8-N7-C5	2.29	108.38	104.24
1	AA	527	G7M	CN7-N7-C8	-2.28	121.32	124.84
22	BA	2251	OMG	C8-N9-C4	2.28	110.38	106.05
1	AA	1519	MA6	C4-C5-N7	-2.27	107.86	110.62
22	BA	745	1MG	C1'-N9-C4	-2.26	119.78	126.50
22	BA	2445	2MG	C5-C4-N9	2.26	109.73	105.63
22	BA	2069	G7M	N1-C2-N3	-2.26	119.10	123.32
22	BA	2251	OMG	C3'-C2'-C1'	-2.26	98.65	102.89
1	AA	527	G7M	CN7-N7-C5	2.26	129.57	126.77
22	BA	2251	OMG	O3'-C3'-C4'	2.25	117.55	111.05
55	B8	37	1MG	C8-N9-C4	2.24	110.31	106.05
1	AA	1516	2MG	CM2-N2-C2	-2.23	118.94	123.86
22	BA	2457	PSU	C6-N1-C2	-2.22	120.41	122.68
22	BA	2498	OMC	C6-C5-C4	2.22	121.08	117.50
1	AA	1207	2MG	C8-N7-C5	2.22	108.25	104.24
1	AA	1516	2MG	C1'-N9-C4	2.22	133.09	126.50
22	BA	2251	OMG	N2-C2-N1	2.21	121.42	116.71
22	BA	1911	PSU	O2-C2-N1	-2.20	120.36	122.79
22	BA	2445	2MG	C6-C5-N7	2.20	134.34	130.25
22	BA	1835	2MG	N9-C4-N3	2.18	130.31	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1835	2MG	O6-C6-C5	-2.17	120.84	126.60
22	BA	2503	2MA	C6-C5-C4	2.17	120.10	117.18
22	BA	2503	2MA	CM2-C2-N1	2.15	120.51	117.15
22	BA	2503	2MA	C5-C6-N6	-2.15	118.75	123.43
22	BA	2604	PSU	O2-C2-N1	-2.14	120.44	122.79
55	B8	37	1MG	C8-N7-C5	2.13	108.09	104.24
22	BA	1618	6MZ	C9-N6-C6	-2.13	121.04	122.87
22	BA	1917	PSU	O2-C2-N1	-2.12	120.45	122.79
1	AA	1207	2MG	C4-C5-N7	-2.12	107.37	110.72
22	BA	1835	2MG	N1-C2-N3	-2.10	120.70	123.95
1	AA	1516	2MG	O6-C6-C5	-2.09	121.06	126.60
22	BA	955	PSU	C6-N1-C2	-2.08	120.55	122.68
22	BA	1939	5MU	C5-C6-N1	-2.08	121.20	123.34
1	AA	516	PSU	O4'-C1'-C2'	2.07	108.06	105.14
22	BA	2504	PSU	C6-C5-C4	2.07	119.64	118.20
1	AA	966	2MG	C8-N7-C5	2.07	107.98	104.24
55	B8	55	PSU	O4'-C1'-C2'	2.06	108.06	105.14
22	BA	2457	PSU	O4'-C1'-C2'	2.06	108.05	105.14
1	AA	1498	UR3	C3U-N3-C4	2.06	120.83	117.89
1	AA	1519	MA6	C5-C4-N9	2.06	108.18	105.78
55	B8	46	G7M	N9-C4-N3	2.04	130.04	125.94
22	BA	2030	6MZ	C4-C5-N7	-2.04	108.14	110.62
22	BA	1939	5MU	O4-C4-N3	-2.03	116.22	120.12
22	BA	1917	PSU	O4'-C1'-C2'	2.03	108.01	105.14
12	AL	89	D2T	OD2-CG-OD1	-2.03	119.47	124.09
1	AA	1516	2MG	C5-C4-N9	2.02	109.30	105.63
22	BA	1915	3TD	O4'-C1'-C2'	2.01	107.98	105.14
22	BA	2503	2MA	C1'-N9-C8	-2.01	122.60	127.14
22	BA	2445	2MG	N9-C4-N3	2.00	129.96	125.94

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
25	BD	150	MEQ	N-CA-CB-CG
25	BD	150	MEQ	C-CA-CB-CG
25	BD	150	MEQ	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
55	B8	55	PSU	O4'-C1'-C5-C4
55	B8	55	PSU	O4'-C1'-C5-C6
22	BA	2030	6MZ	O4'-C4'-C5'-O5'
22	BA	2251	OMG	C1'-C2'-O2'-CM2
1	AA	527	G7M	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	C3'-C4'-C5'-O5'
22	BA	2504	PSU	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
22	BA	2504	PSU	C3'-C4'-C5'-O5'
1	AA	1402	4OC	O4'-C4'-C5'-O5'
22	BA	2251	OMG	O4'-C4'-C5'-O5'
34	BM	81	4D4	OB-CB-CG-CD
22	BA	2251	OMG	C3'-C4'-C5'-O5'
1	AA	1402	4OC	C3'-C4'-C5'-O5'
22	BA	2445	2MG	C3'-C4'-C5'-O5'
22	BA	747	5MU	C3'-C4'-C5'-O5'
22	BA	2069	G7M	C4'-C5'-O5'-P
22	BA	2552	OMU	C3'-C2'-O2'-CM2
22	BA	2069	G7M	O4'-C4'-C5'-O5'
34	BM	81	4D4	CG-CD-NE-CZ
34	BM	81	4D4	CA-CB-CG-CD
22	BA	2503	2MA	O4'-C4'-C5'-O5'
22	BA	746	PSU	O4'-C1'-C5-C6
22	BA	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	B8	46	G7M	3	0
22	BA	1939	5MU	1	0
22	BA	2030	6MZ	2	0
55	B8	55	PSU	1	0
55	B8	37	1MG	2	0
25	BD	150	MEQ	1	0
22	BA	2251	OMG	1	0
22	BA	1915	3TD	1	0
22	BA	2504	PSU	1	0
22	BA	2552	OMU	1	0
22	BA	2503	2MA	1	0
22	BA	746	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 477 ligands modelled in this entry, 476 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	$\# Z > 2$
59	TRP	BA	3001	-	14,16,16	0.92	0	20,22,22	1.37	2 (10%)

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
59	TRP	BA	3001	-	-	0/8/8/8	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	3001	TRP	CD2-CE2-NE1	-3.77	104.16	107.51
59	BA	3001	TRP	CE2-NE1-CD1	2.78	111.69	109.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.28

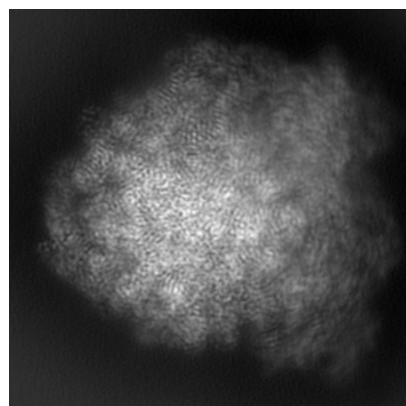
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12694. These allow visual inspection of the internal detail of the map and identification of artifacts.

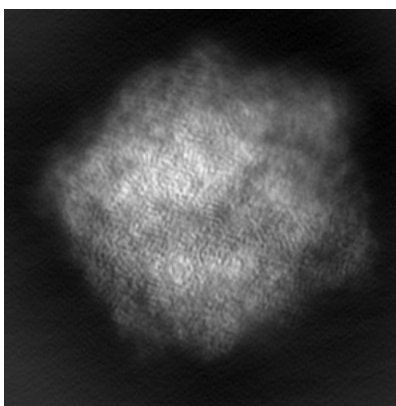
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

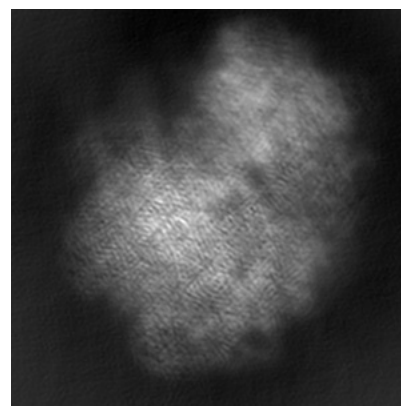
6.1.1 Primary map



X

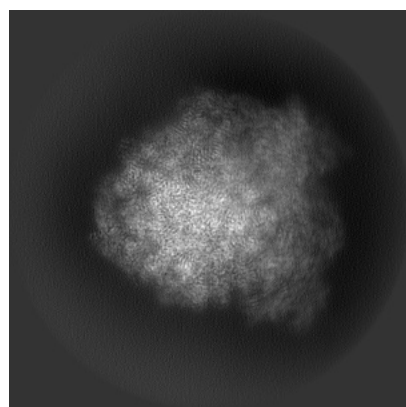


Y

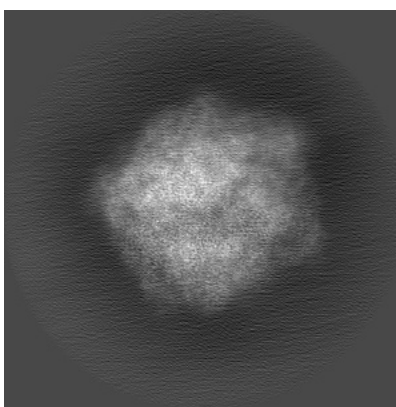


Z

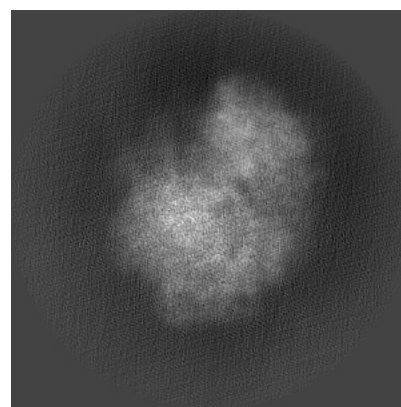
6.1.2 Raw map



X



Y

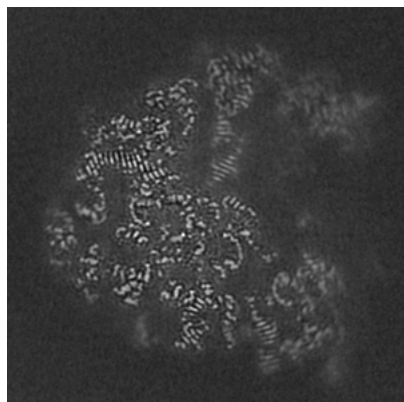


Z

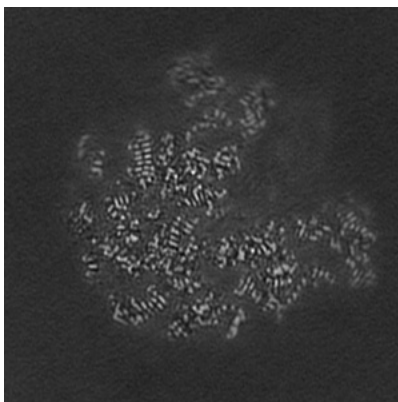
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

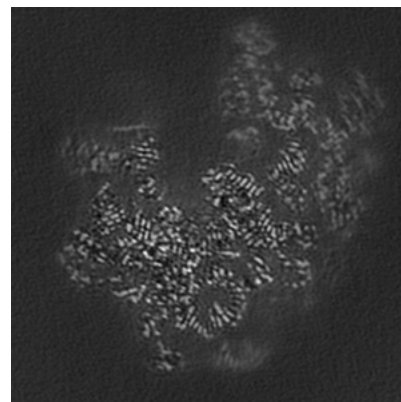
6.2.1 Primary map



X Index: 162

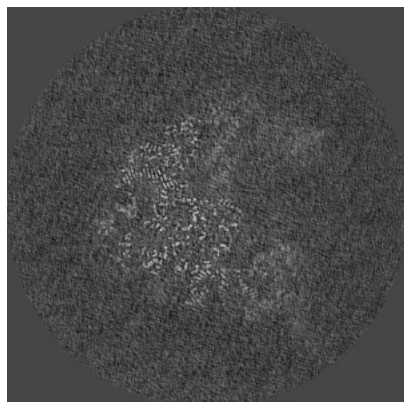


Y Index: 162

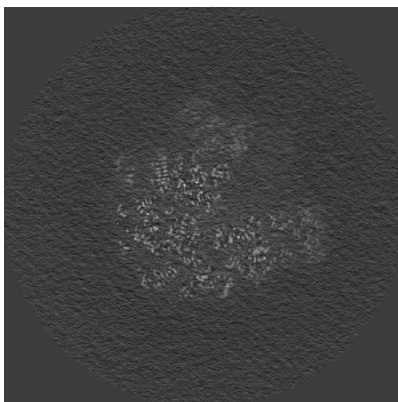


Z Index: 162

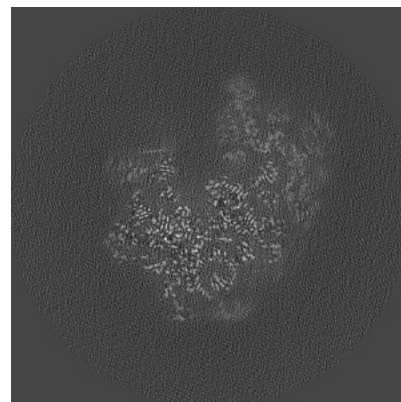
6.2.2 Raw map



X Index: 232



Y Index: 232

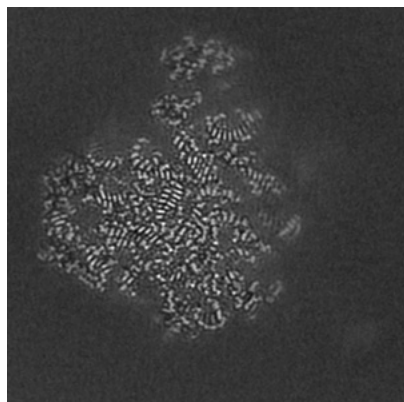


Z Index: 232

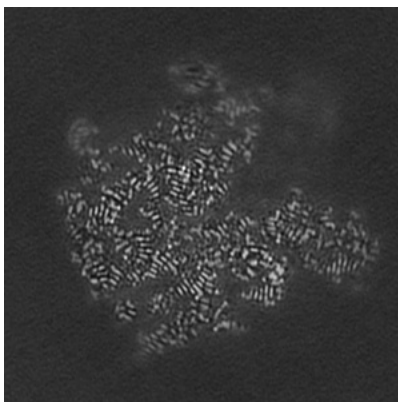
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

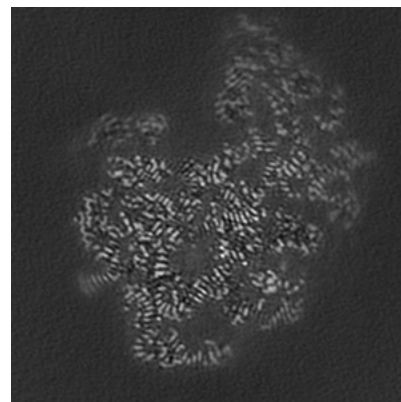
6.3.1 Primary map



X Index: 121

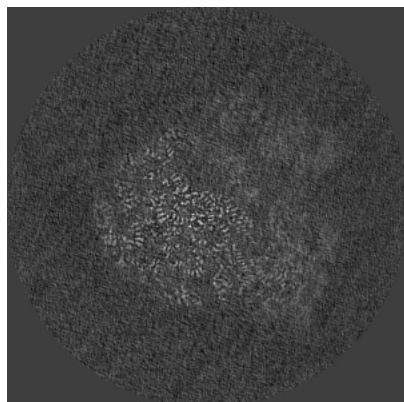


Y Index: 150

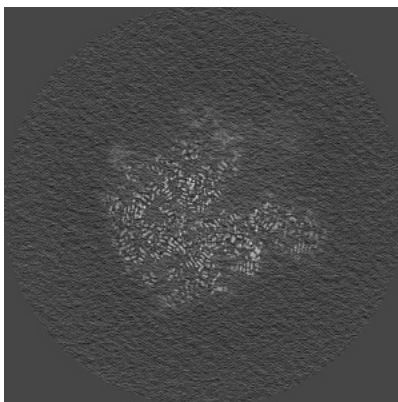


Z Index: 143

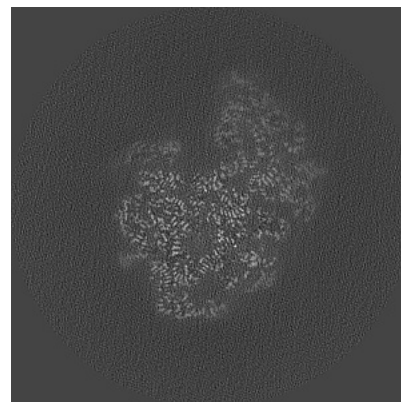
6.3.2 Raw map



X Index: 244



Y Index: 220

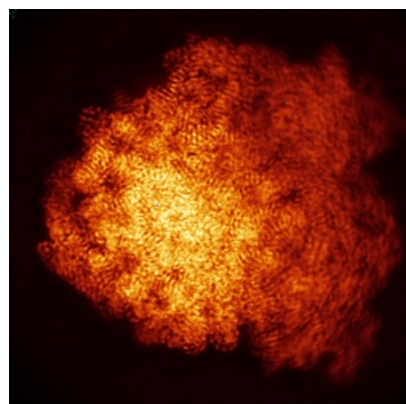


Z Index: 213

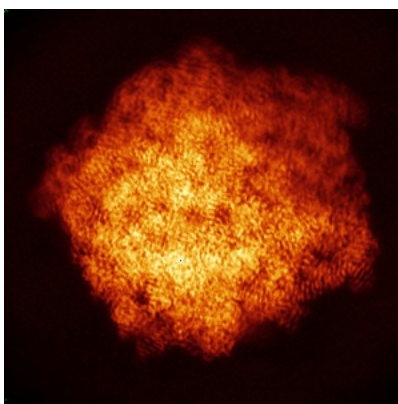
The images above show the largest variance slices of the map in three orthogonal directions.

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

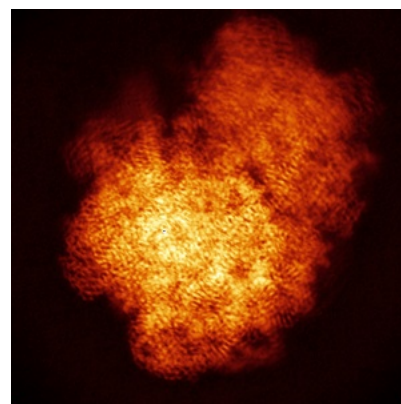
6.4.1 Primary map



X

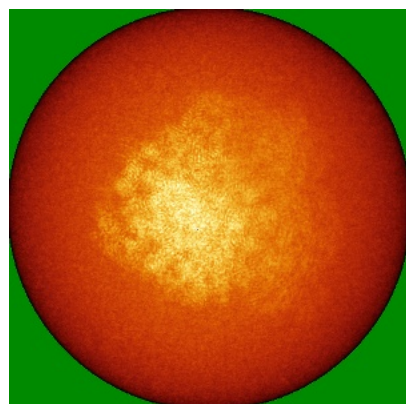


Y

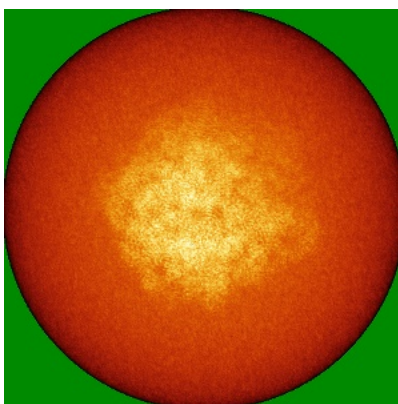


Z

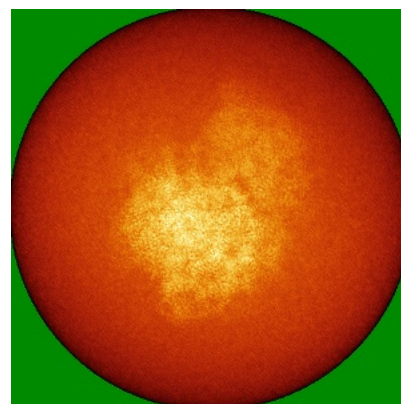
6.4.2 Raw map



X



Y

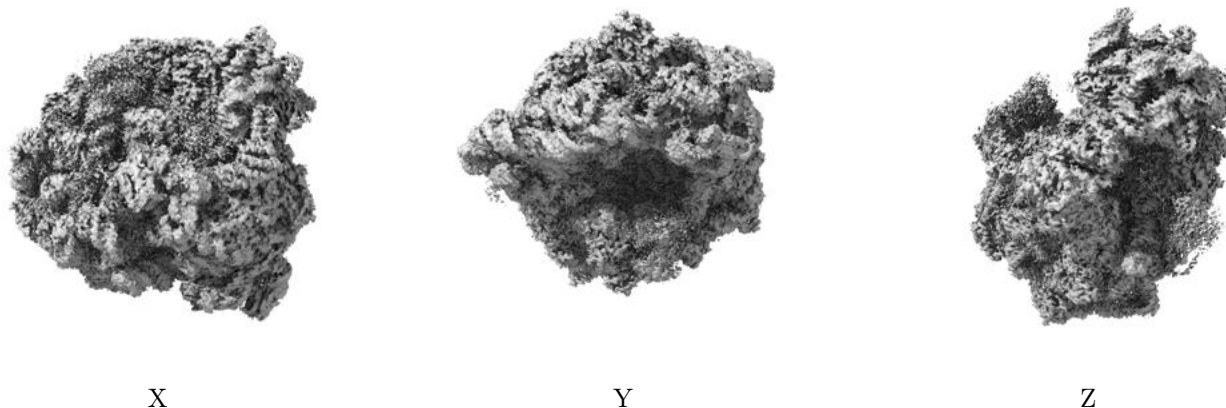


Z

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

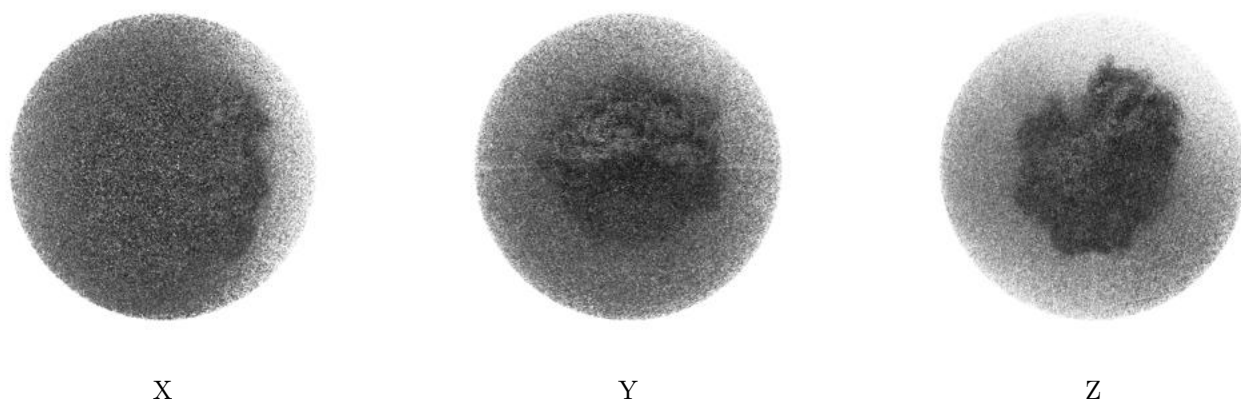
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

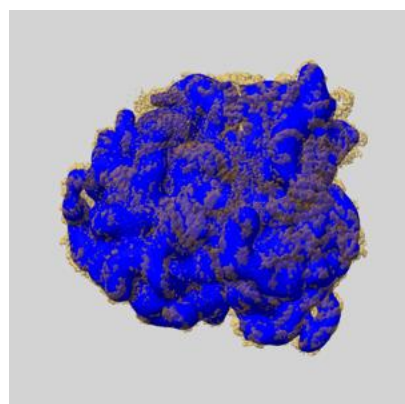
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

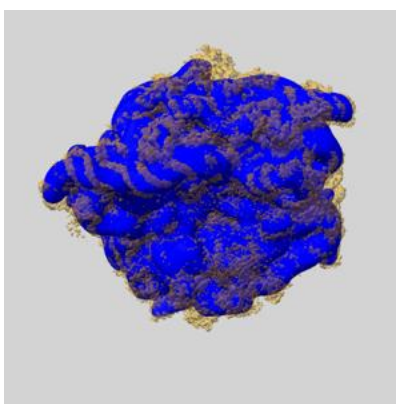
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

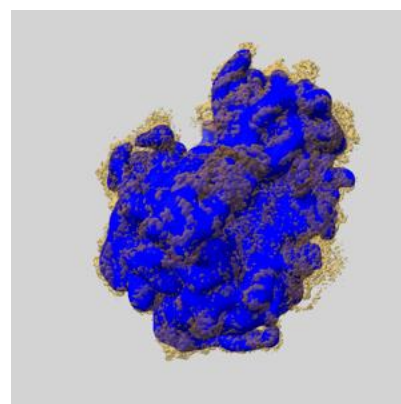
6.6.1 emd_12694_msk_1.map [i](#)



X



Y

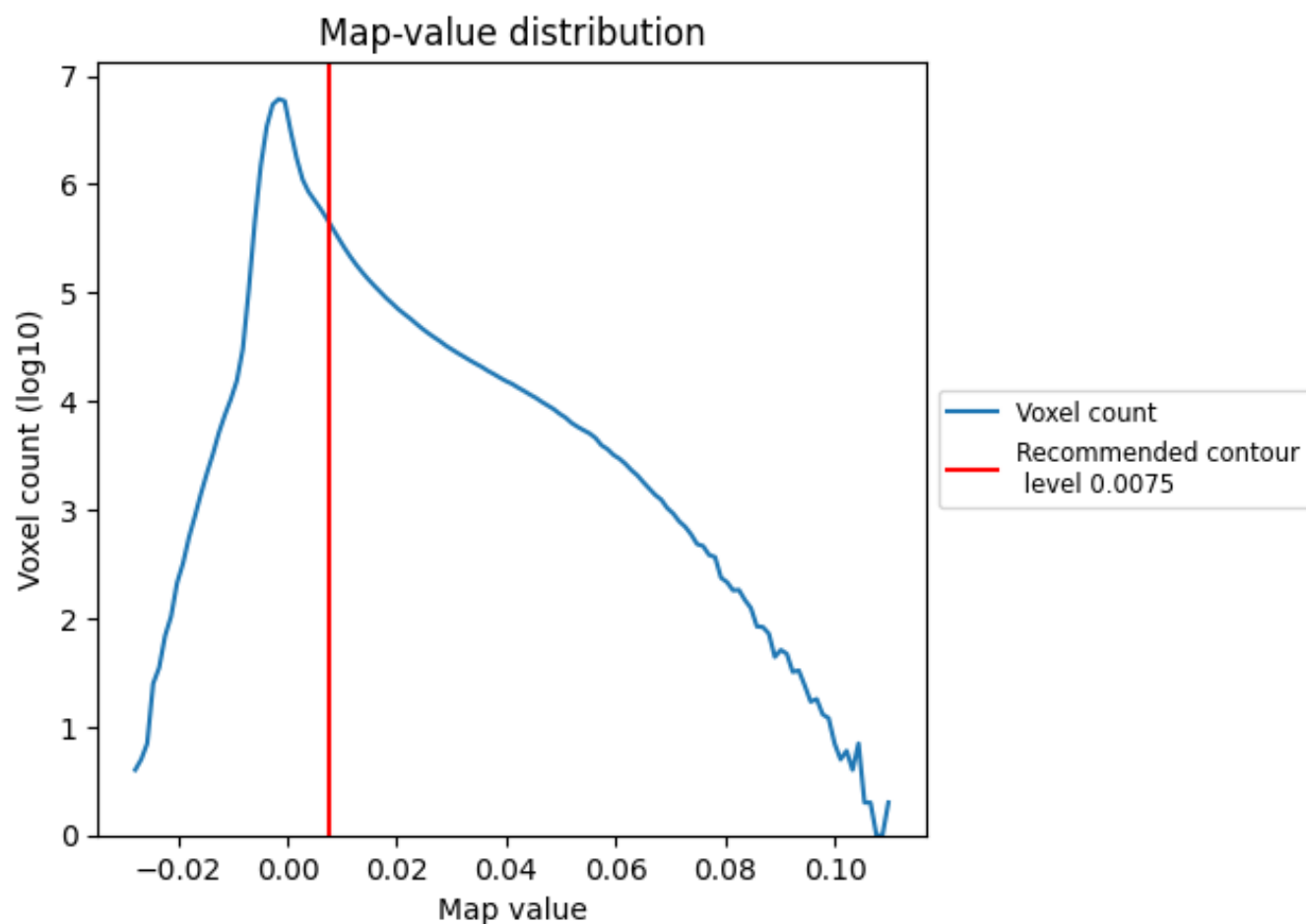


Z

7 Map analysis [i](#)

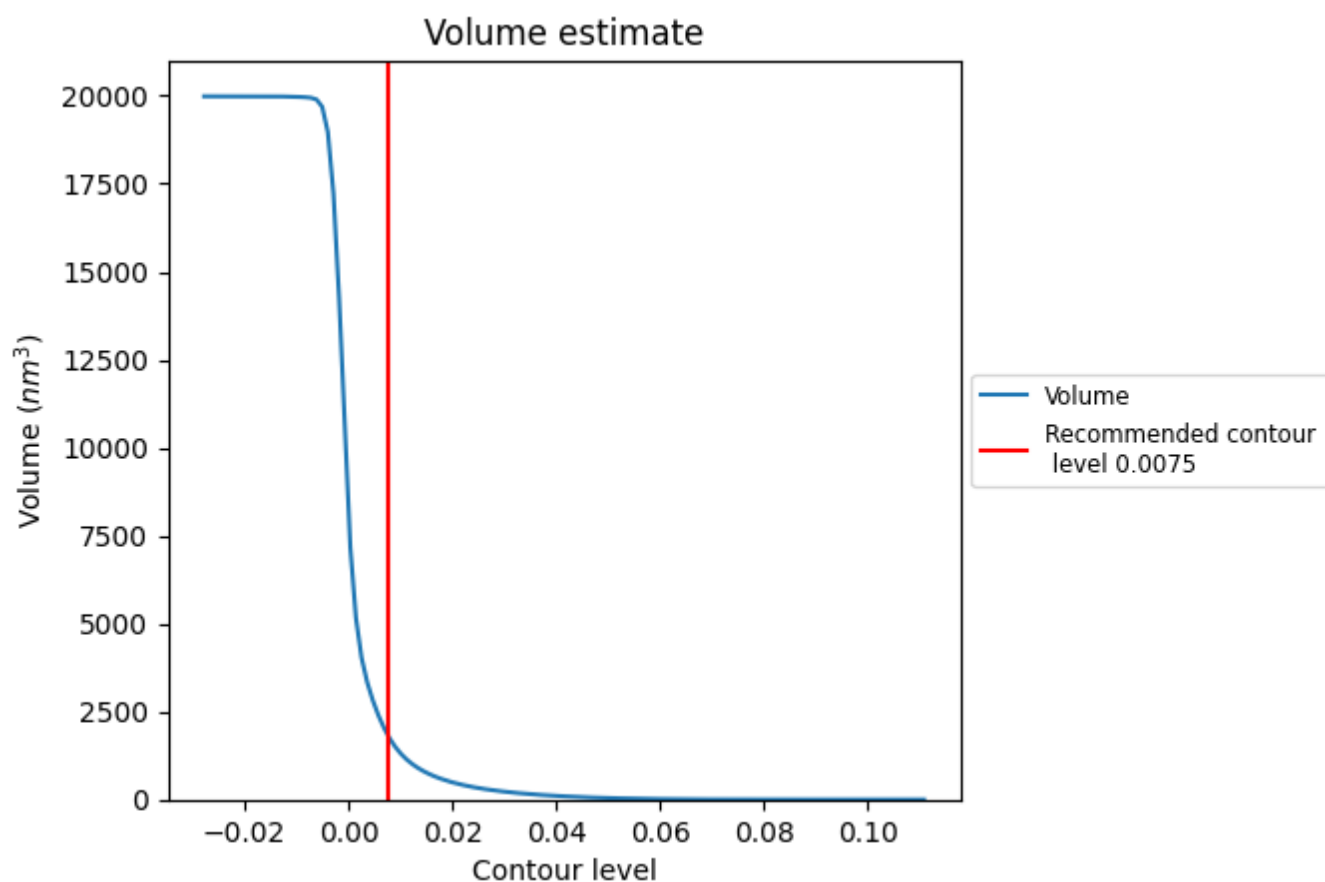
This section contains the results of statistical analysis of the map.

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.

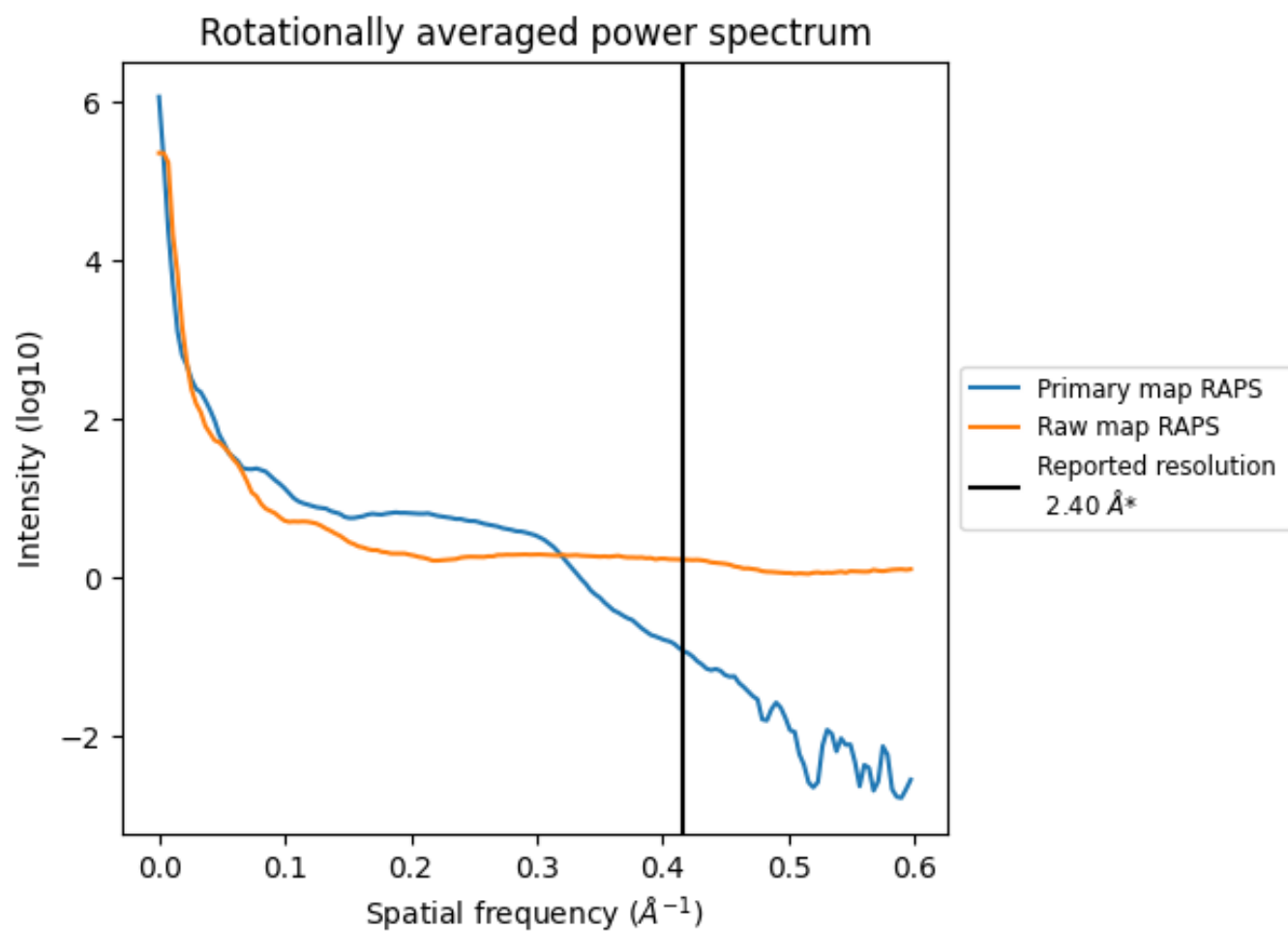
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1859 nm³; this corresponds to an approximate mass of 1680 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 ⓘ

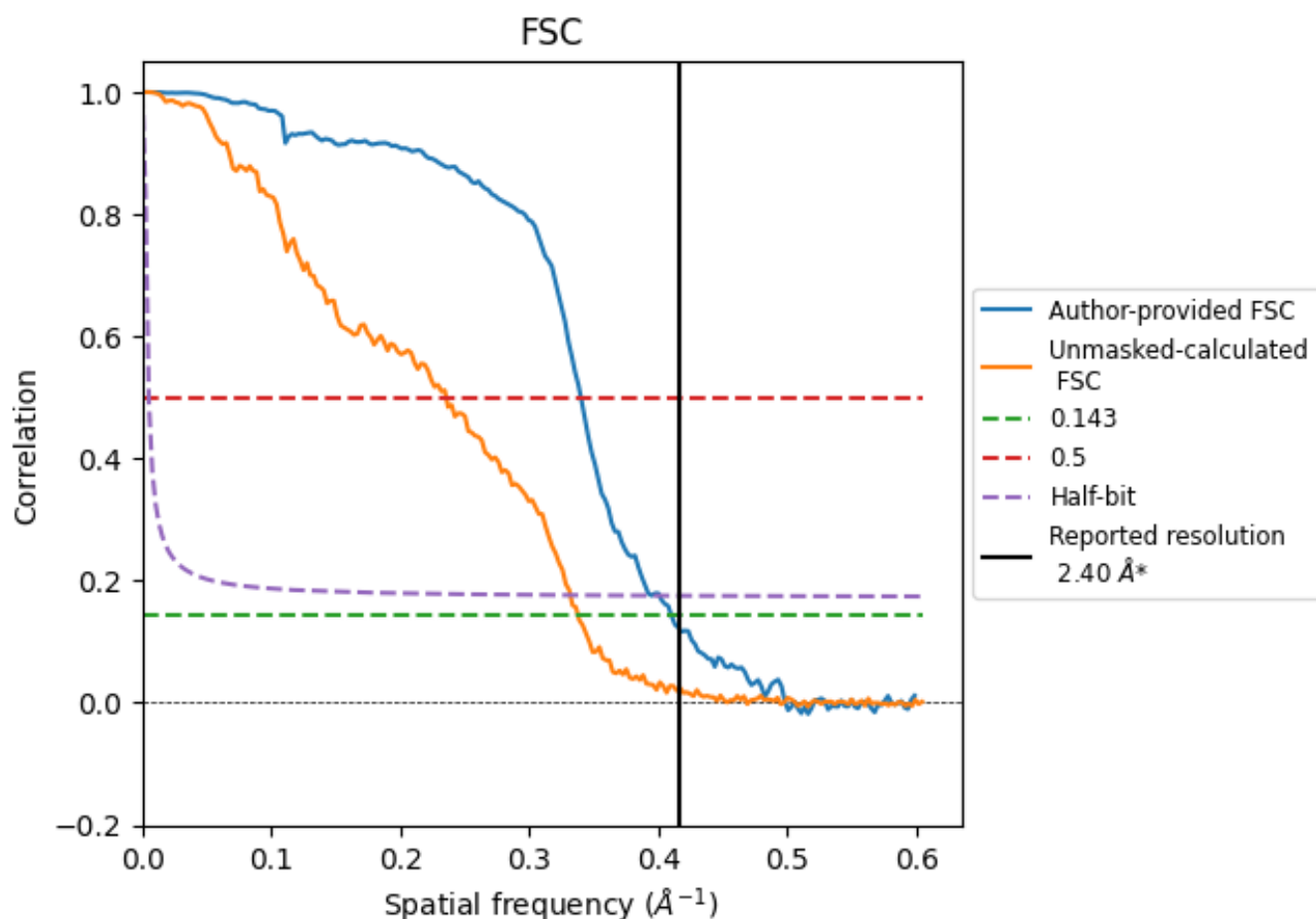


*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

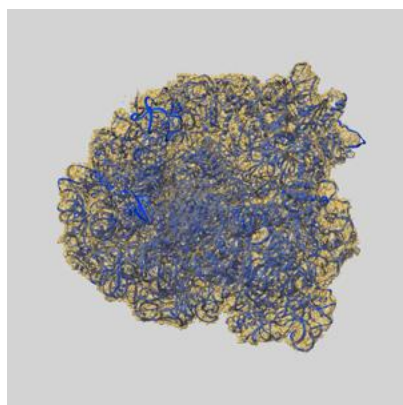
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.94	2.49
Unmasked-calculated*	2.96	4.24	3.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.96 differs from the reported value 2.4 by more than 10 %

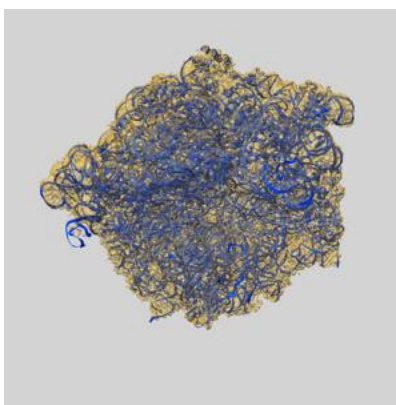
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12694 and PDB model 7O1A. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

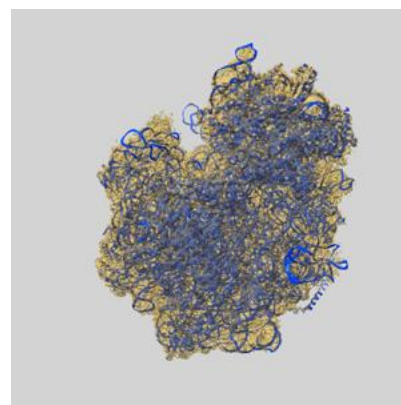
9.1 Map-model overlay [i](#)



X



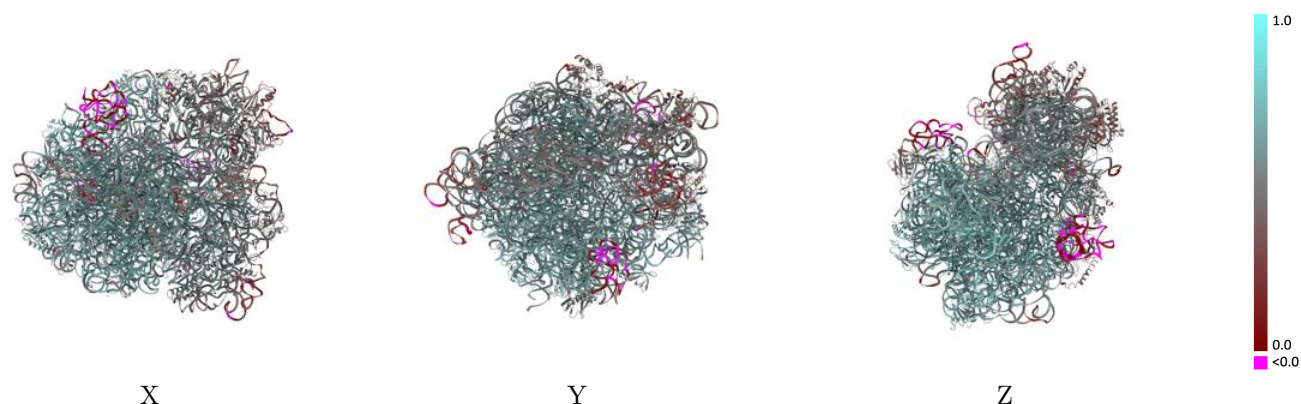
Y



Z

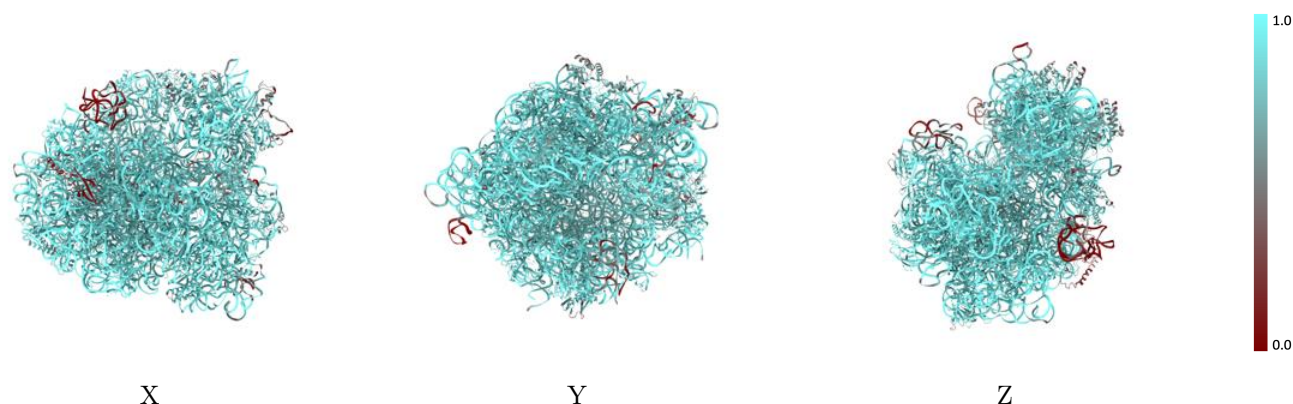
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



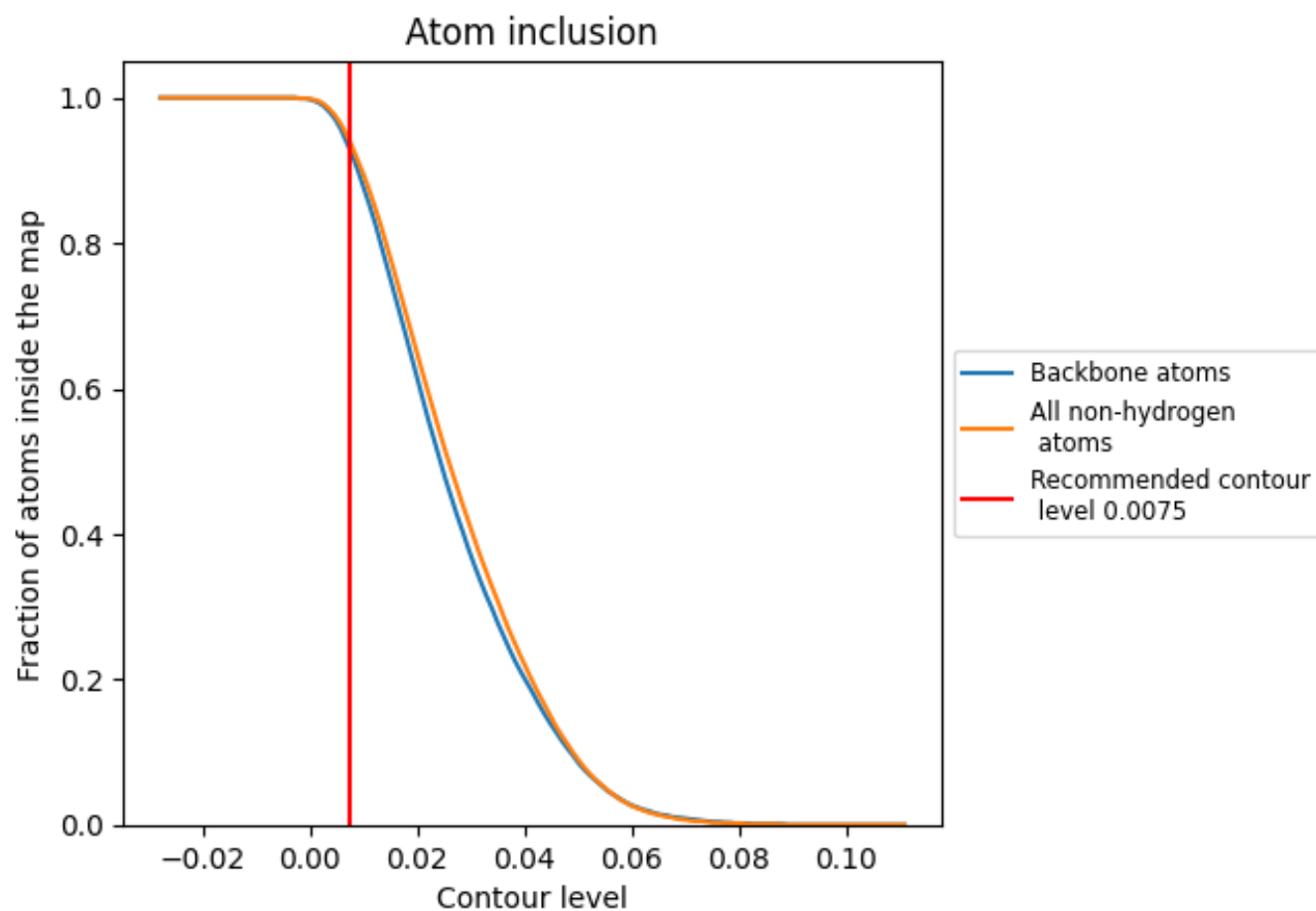
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.5730
AA	 0.9620	 0.5200
AB	 0.6970	 0.4140
AC	 0.8590	 0.4680
AD	 0.8550	 0.4620
AE	 0.9490	 0.5510
AF	 0.8450	 0.4420
AG	 0.7770	 0.4160
AH	 0.9200	 0.5320
AI	 0.7830	 0.4190
AJ	 0.7400	 0.4080
AK	 0.9300	 0.5220
AL	 0.9460	 0.5280
AM	 0.8570	 0.4650
AN	 0.8670	 0.4280
AO	 0.9100	 0.5140
AP	 0.8990	 0.4890
AQ	 0.9110	 0.4900
AR	 0.9520	 0.5250
AS	 0.7860	 0.4180
AT	 0.9020	 0.5080
AU	 0.7990	 0.4520
B0	 0.9560	 0.6460
B1	 0.9610	 0.6120
B2	 0.9830	 0.6660
B3	 1.0000	 0.6940
B4	 0.9800	 0.6310
B5	 1.0000	 0.6680
B7	 0.9950	 0.5260
B8	 0.9980	 0.5800
BA	 0.9590	 0.6150
BB	 0.9900	 0.6210
BC	 0.9940	 0.6630
BD	 0.9720	 0.6580
BE	 0.9160	 0.6240



Continued on next page...

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Chain	Atom inclusion	Q-score
BF	 0.9210	 0.5380
BG	 0.8300	 0.4980
BH	 0.3010	 0.3160
BI	 0.6390	 0.3620
BJ	 0.9800	 0.6500
BK	 0.9920	 0.6520
BL	 0.9690	 0.6470
BM	 0.9900	 0.6550
BN	 0.9930	 0.6780
BO	 0.9580	 0.6150
BP	 0.9750	 0.6430
BQ	 0.9930	 0.6810
BR	 0.9510	 0.6410
BS	 0.9800	 0.6590
BT	 0.9390	 0.6160
BU	 0.9430	 0.6080
BV	 0.9190	 0.5810
BW	 0.9820	 0.6580
BX	 0.9900	 0.6360
BY	 0.8960	 0.5870
BZ	 0.9410	 0.6470