Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Apr 11, 2018 – 12:45 PM EDT

PDB ID	:	6ERI
EMDB ID:	:	EMD-3941
Title	:	Structure of the chloroplast ribosome with chl-RRF and hibernation-promoting factor
Authors	:	Perez Borema, A.; Aibara, S.; Paul, B.; Tobiasson, V.; Kimanius, D.; Forsberg, B.O.; Wallden, K.; Lindahl, E.; Amunts, A.
Deposited on	:	2017-10-18
Resolution	:	3.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB 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 (i) symbol.

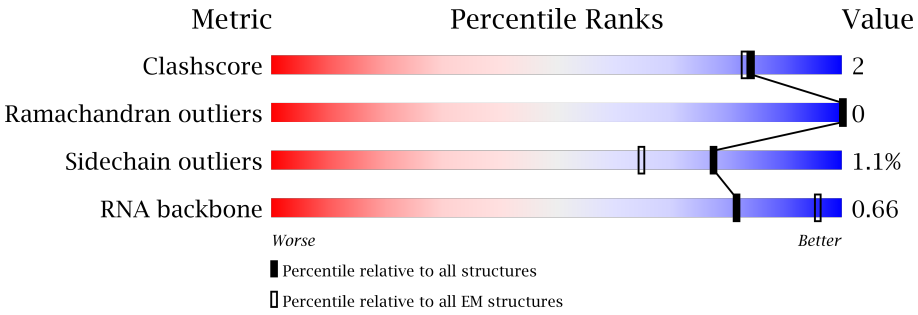
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	AA	2810	78% 17% • •
2	AB	106	83% 13% •
3	AC	246	92% 8%
4	AD	221	93% 7%
5	AE	212	93% 7%
6	AF	207	75% 7% 17%
7	AG	172	93% 7%
8	AH	46	96% •

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Mol	Chain	Length	Quality of chain
9	AJ	200	93% 7%
10	AK	121	91% 8%
11	AL	184	90% 10%
12	AM	134	88% 12%
13	AN	116	88% 12%
14	AO	121	95% 5%
15	AP	118	93% 6%
16	AQ	115	90% 10%
17	AR	165	88% 12%
18	AS	171	94% 6%
19	AT	92	97%
20	AU	127	89% 11%
21	AW	114	94% 6%
22	AX	76	93% 7%
23	AY	99	98%
24	AZ	66	89% 11%
25	Aa	48	100%
26	Ab	60	100%
27	Ac	61	100%
28	Ad	72	99%
29	Ae	37	100%
30	Af	47	98%
31	Aw	49	100%
32	Ax	118	93% 7%
33	Az	191	100%

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Mol	Chain	Length	Quality of chain
34	BA	1481	81% 18%
35	BB	215	87% 10%
36	BC	217	94% 6%
37	BD	200	88% 12%
38	BE	158	85% 15%
39	BF	113	96%
40	BG	151	96%
41	BH	134	82% 10% 7%
42	BI	141	90% 8%
43	BJ	98	93% 7%
44	BK	110	92% 8%
45	BL	122	92% 8%
46	BM	111	95% 5%
47	BN	99	88% 12%
48	BO	72	94% 6%
49	BP	81	91% 7%
50	BQ	84	89% 11%
51	BR	53	85% 15%
52	BS	81	86% 14%
53	BT	102	92% 8%
54	BU	59	92% 8%
55	BV	106	95% 5%
56	BW	37	89% 11%
57	BY	170	97%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 145026 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	2696	57902	25833	10727	18646	2696	0	0

- Molecule 2 is a RNA chain called 4.5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AB	106	2277	1017	423	731	106	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	246	1896	1175	388	327	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	221	1686	1066	308	301	11	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	212	1676	1061	312	300	3	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	77	SER	PRO	conflict	UNP O49937
AE	79	THR	LYS	conflict	UNP O49937
AE	130	ARG	GLY	conflict	UNP O49937

- Molecule 6 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	171	Total	C	N	O	S	0	0
			1328	843	231	246	8		

- Molecule 7 is a protein called 50S ribosomal protein L6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	172	Total	C	N	O	S	0	0
			1343	849	246	244	4		

- Molecule 8 is a protein called 50S ribosomal protein L9, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	46	Total	C	N	O	0	0
			367	241	66	60		

- Molecule 9 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	200	Total	C	N	O	S	0	0
			1619	1030	300	284	5		

- Molecule 10 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	120	Total	C	N	O	S	0	0
			934	582	178	169	5		

- Molecule 11 is a protein called 50S ribosomal protein L15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	184	Total	C	N	O	S	0	0
			1405	876	279	244	6		

- Molecule 12 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	134	Total	C	N	O	S	0	0
			1071	675	217	173	6		

- Molecule 13 is a protein called 50S ribosomal protein L17, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 14 is a protein called 50S ribosomal protein L18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	121	Total	C	N	O	S	0	0
			952	592	184	171	5		

- Molecule 15 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	118	Total	C	N	O	S	0	0
			953	610	186	156	1		

- Molecule 16 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	115	Total	C	N	O	S	0	0
			994	631	207	154	2		

- Molecule 17 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AR	165	Total	C	N	O	0	0
			1326	857	228	241		

- Molecule 18 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	171	Total	C	N	O	S	0	0
			1388	887	256	236	9		

- Molecule 19 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	92	Total	C	N	O	S	0	0
			743	480	129	132	2		

- Molecule 20 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	127	Total	C	N	O	S	0	0
			1015	639	189	184	3		

- Molecule 21 is a protein called 50S ribosomal protein L27, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AW	114	Total	C	N	O	0	0
			914	573	182	159		

- Molecule 22 is a protein called 50S ribosomal protein L28, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AX	76	Total	C	N	O	S	0	0
			625	397	127	100	1		

- Molecule 23 is a protein called 50S ribosomal protein L29, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AY	99	Total	C	N	O	S	0	0
			832	520	164	145	3		

- Molecule 24 is a protein called 50S ribosomal protein L31, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AZ	66	Total	C	N	O	S	0	0
			536	338	94	102	2		

- Molecule 25 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Aa	48	Total	C	N	O	0	0
			396	261	75	60		

- Molecule 26 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ab	60	Total	C	N	O	S	0	0
			489	304	98	83	4		

- Molecule 27 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ac	61	Total	C	N	O	S	0	0
			471	284	108	76	3		

- Molecule 28 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ad	72	Total	C	N	O	S	0	0
			588	370	124	93	1		

- Molecule 29 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ae	37	Total	C	N	O	S	0	0
			305	186	70	45	4		

- Molecule 30 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Af	47	Total	C	N	O	S	0	0
			375	240	72	62	1		

- Molecule 31 is a protein called 50S ribosomal protein 5 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Aw	49	Total	C	N	O	S	0	0
			423	269	92	58	4		

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ax	118	Total	C	N	O	P	0	0
			2522	1126	457	821	118		

- Molecule 33 is a protein called Ribosome-recycling factor, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Az	191	Total	C	N	O	S	0	0
			1512	939	260	308	5		

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	1481	Total	C	N	O	P	0	0
			31806	14180	5870	10275	1481		

- Molecule 35 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BB	209	Total	C	N	O	S	0	0
			1639	1032	303	293	11		

- Molecule 36 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BC	217	Total	C	N	O	S	0	0
			1745	1113	314	312	6		

- Molecule 37 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BD	199	Total	C	N	O	S	0	0
			1633	1032	319	278	4		

- Molecule 38 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BE	158	Total	C	N	O	S	0	0
			1189	742	230	211	6		

- Molecule 39 is a protein called 30S ribosomal protein S6 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BF	113	Total	C	N	O	S	0	0
			911	583	152	172	4		

- Molecule 40 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BG	151	Total	C	N	O	S	0	0
			1178	732	236	207	3		

- Molecule 41 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BH	124	Total	C	N	O	S	0	0
			1004	633	192	174	5		

- Molecule 42 is a protein called 30S ribosomal protein S9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BI	141	Total	C	N	O	S	0	0
			1091	696	205	189	1		

- Molecule 43 is a protein called 30S ribosomal protein S10 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BJ	98	Total	C	N	O	S	0	0
			796	512	142	137	5		

- Molecule 44 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BK	110	Total	C	N	O	S	0	0
			828	512	169	142	5		

- Molecule 45 is a protein called 30S ribosomal protein S12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BL	122	Total	C	N	O	S	0	0
			959	599	197	161	2		

- Molecule 46 is a protein called 30S ribosomal protein S13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BM	111	Total	C	N	O	S	0	0
			913	562	184	162	5		

- Molecule 47 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BN	99	Total	C	N	O	S	0	0
			824	510	174	137	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	73	TYR	ILE	conflict	UNP P06507

- Molecule 48 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BO	72	Total	C	N	O	S	0	0
			606	388	117	100	1		

- Molecule 49 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BP	81	Total	C	N	O	S	0	0
			675	431	127	115	2		

- Molecule 50 is a protein called 30S ribosomal protein S17, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BQ	84	Total	C	N	O	S	0	0
			677	423	133	117	4		

- Molecule 51 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BR	53	Total	C	N	O	S	0	0
			440	279	87	73	1		

- Molecule 52 is a protein called 30S ribosomal protein S19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BS	81	Total	C	N	O	S	0	0
			653	421	123	107	2		

- Molecule 53 is a protein called 30S ribosomal protein S20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BT	102	Total	C	N	O	S	0	0
			818	506	168	143	1		

- Molecule 54 is a protein called 30S ribosomal protein S21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BU	59	Total	C	N	O	S	0	0
			514	310	109	93	2		

- Molecule 55 is a protein called Ribosome-binding factor PSRP1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BV	106	Total	C	N	O	S	0	0
			836	514	164	157	1		

- Molecule 56 is a protein called 30S ribosomal protein S31, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	BW	37	Total	C	N	O	0	0
			289	179	65	45		

- Molecule 57 is a protein called bS1c.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	BY	170	Total	C	N	O	0	0
			850	510	170	170		

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	BA	82	Total	Mg	0
			82	82	
58	BN	1	Total	Mg	0
			1	1	
58	AB	9	Total	Mg	0
			9	9	
58	Aw	1	Total	Mg	0
			1	1	
58	AA	247	Total	Mg	0
			247	247	
58	Ax	2	Total	Mg	0
			2	2	
58	Af	1	Total	Mg	0
			1	1	

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

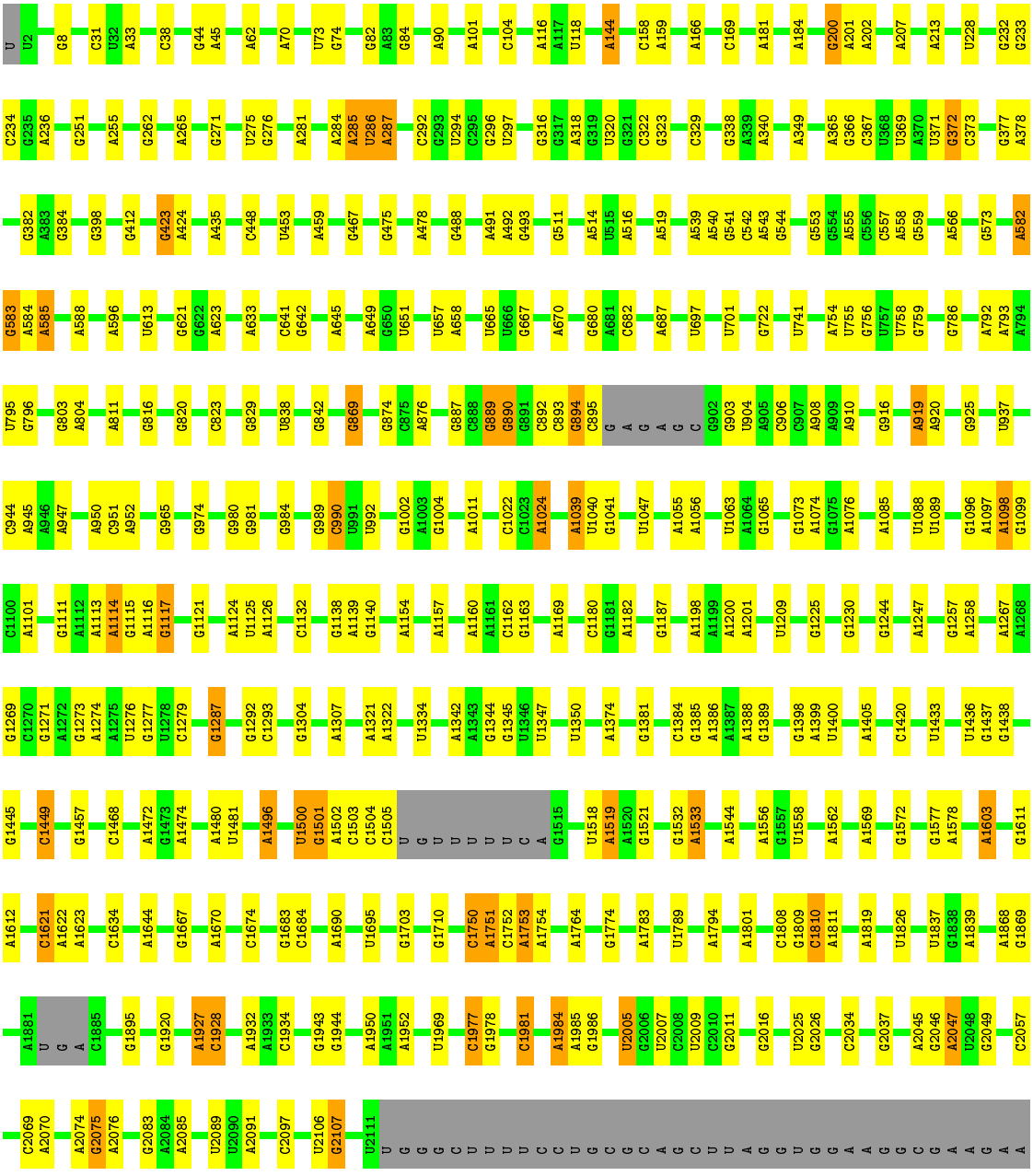
Mol	Chain	Residues	Atoms	AltConf
59	Ab	1	Total Zn 1 1	0
59	Ae	1	Total Zn 1 1	0

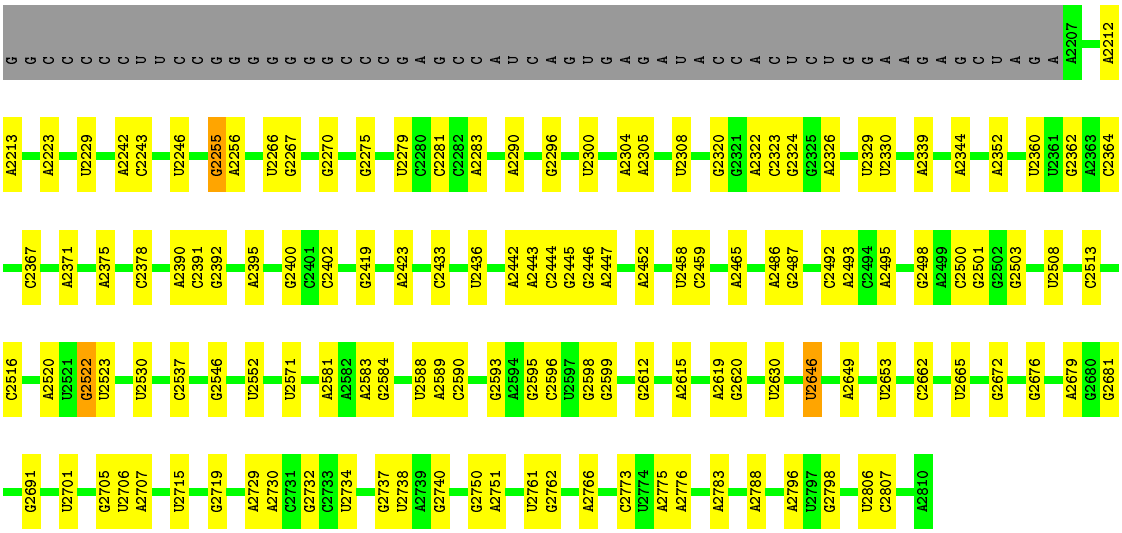
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: 23S ribosomal RNA

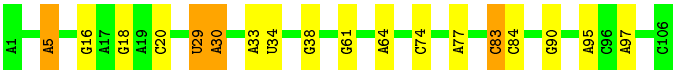
Chain AA: 78% 17%





- Molecule 2: 4.5S ribosomal RNA

Chain AB:

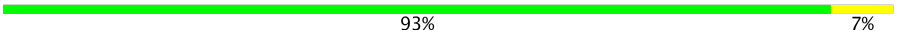


- Molecule 3: 50S ribosomal protein L2, chloroplastic

Chain AC:

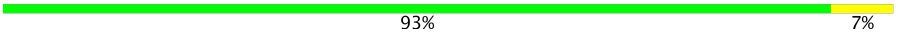
- Molecule 4: 50S ribosomal protein L3, chloroplastic

Chain AD:



- Molecule 5: 50S ribosomal protein L4, chloroplastic

Chain AE:

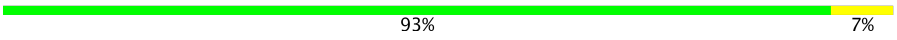


- Molecule 6: 50S ribosomal protein L5, chloroplastic

Chain AF:

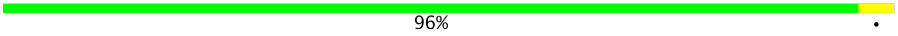
- Molecule 7: 50S ribosomal protein L6, chloroplastic

Chain AG:



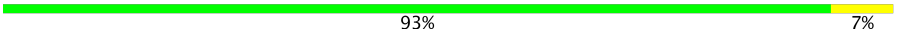
- Molecule 8: 50S ribosomal protein L9, chloroplastic

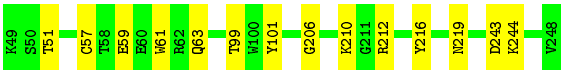
Chain AH:



- Molecule 9: 50S ribosomal protein L13, chloroplastic

Chain AJ:





- Molecule 10: 50S ribosomal protein L14, chloroplastic

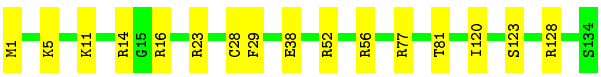
Chain AK:

- Molecule 11: 50S ribosomal protein L15, chloroplastic

Chain AL:

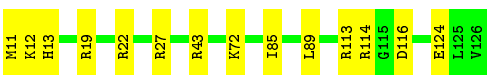
- Molecule 12: 50S ribosomal protein L16, chloroplastic

Chain AM:



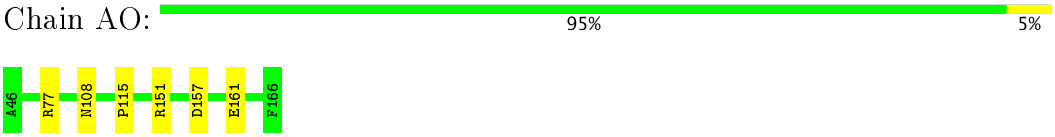
- Molecule 13: 50S ribosomal protein L17, chloroplastic

Chain AN:



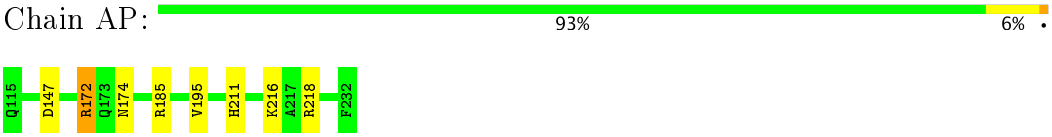
- Molecule 14: 50S ribosomal protein L18, chloroplastic

Chain AO:



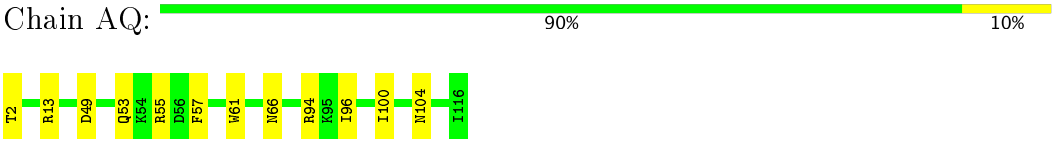
- Molecule 15: 50S ribosomal protein L19, chloroplastic

Chain AP:



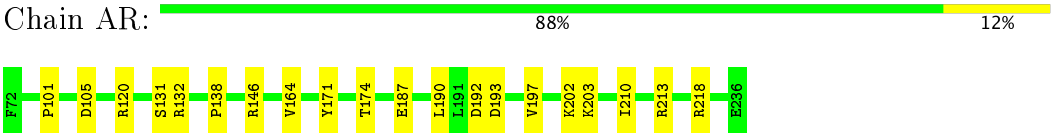
- Molecule 16: 50S ribosomal protein L20, chloroplastic

Chain AQ:



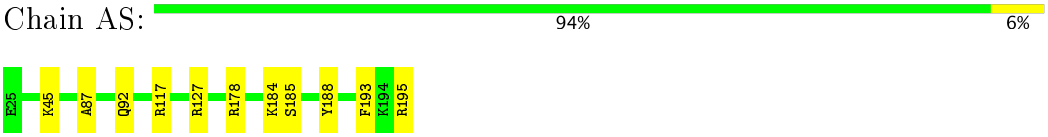
- Molecule 17: 50S ribosomal protein L21, chloroplastic

Chain AR:



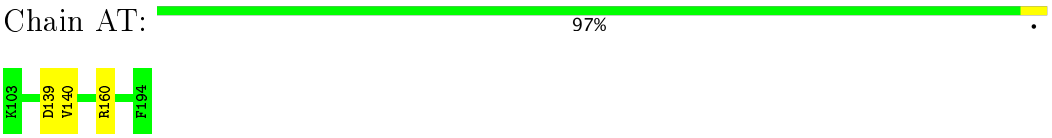
- Molecule 18: 50S ribosomal protein L22, chloroplastic

Chain AS:



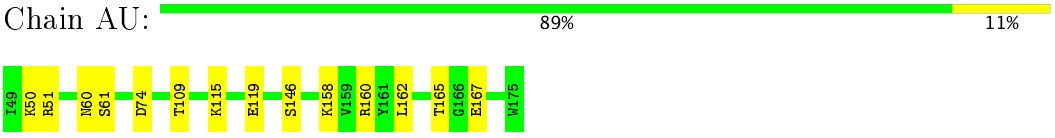
- Molecule 19: 50S ribosomal protein L23, chloroplastic

Chain AT:



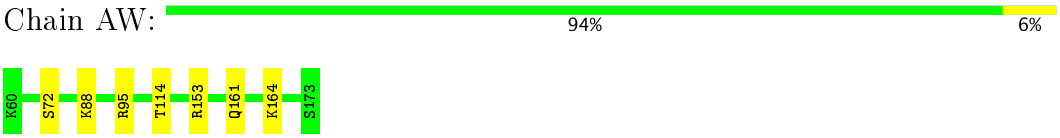
- Molecule 20: 50S ribosomal protein L24, chloroplastic

Chain AU:



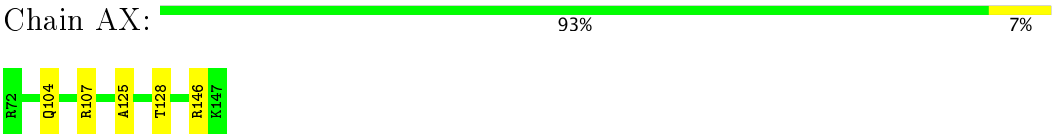
- Molecule 21: 50S ribosomal protein L27, chloroplastic

Chain AW:



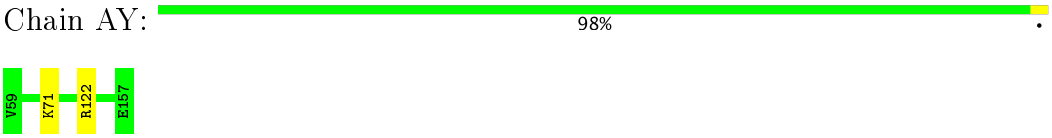
- Molecule 22: 50S ribosomal protein L28, chloroplastic

Chain AX:



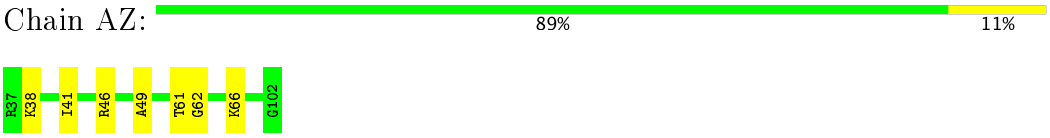
- Molecule 23: 50S ribosomal protein L29, chloroplastic

Chain AY:



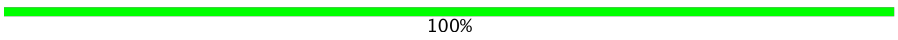
- Molecule 24: 50S ribosomal protein L31, chloroplastic

Chain AZ:



- Molecule 25: 50S ribosomal protein L32, chloroplastic

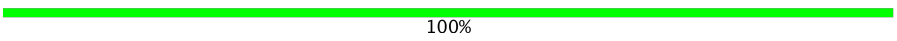
Chain Aa:



There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L33, chloroplastic

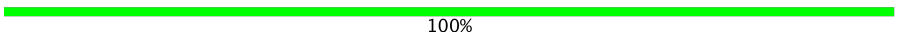
Chain Ab:



There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L34, chloroplastic

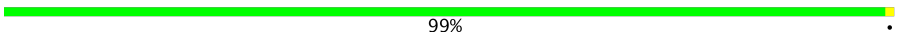
Chain Ac:



There are no outlier residues recorded for this chain.

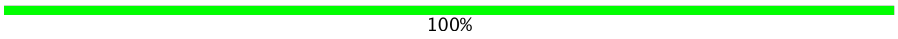
- Molecule 28: 50S ribosomal protein L35, chloroplastic

Chain Ad:



- Molecule 29: 50S ribosomal protein L36, chloroplastic

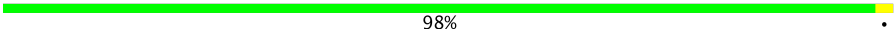
Chain Ae:



There are no outlier residues recorded for this chain.

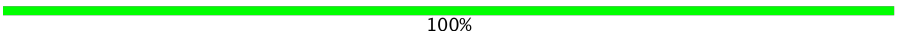
- Molecule 30: 50S ribosomal protein 6, chloroplastic

Chain Af:



- Molecule 31: 50S ribosomal protein 5 alpha, chloroplastic

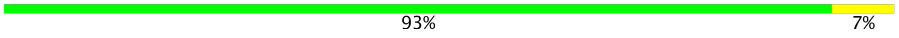
Chain Aw:

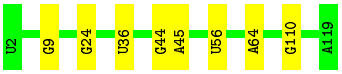


There are no outlier residues recorded for this chain.

- Molecule 32: 5S ribosomal RNA

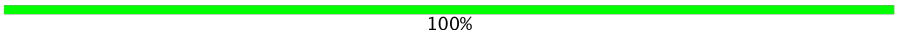
Chain Ax:





- Molecule 33: Ribosome-recycling factor, chloroplastic

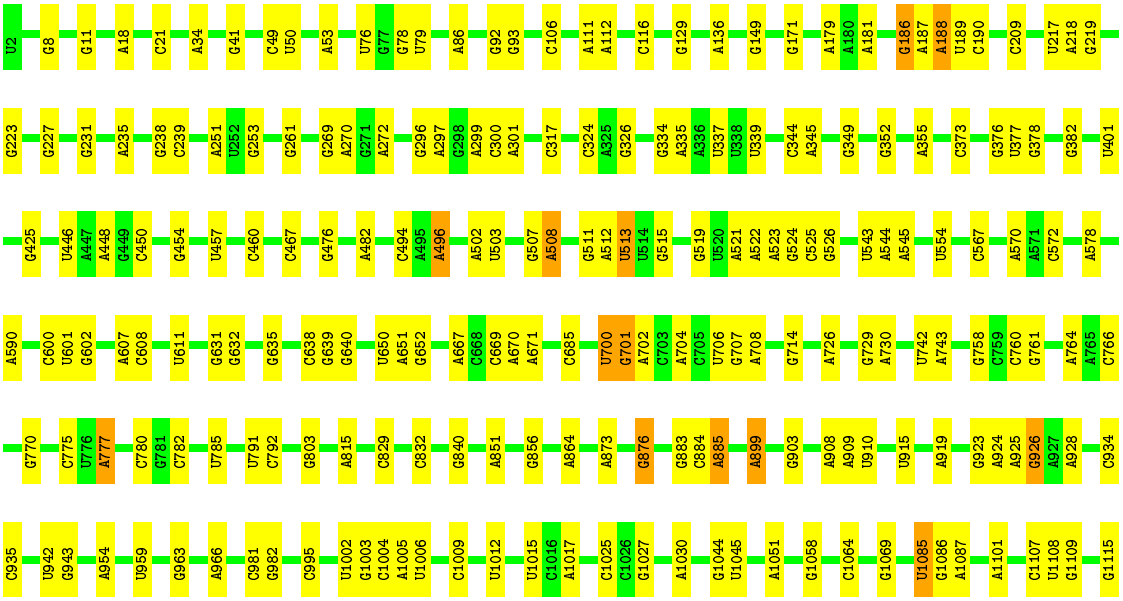
Chain Az:

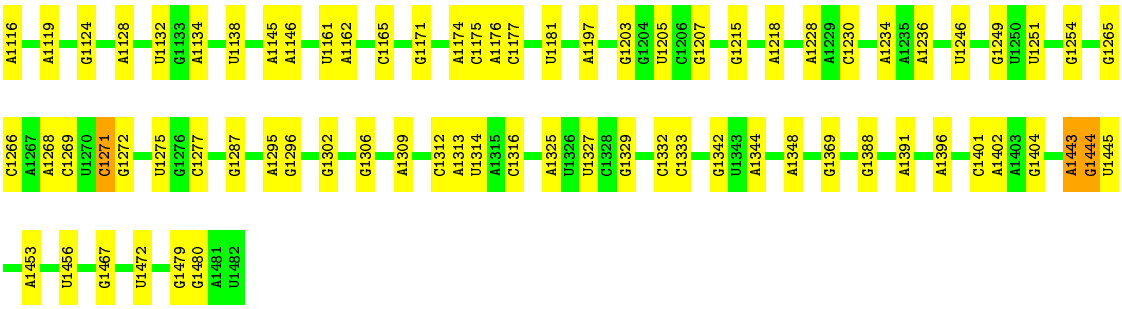


There are no outlier residues recorded for this chain.

- Molecule 34: 16S ribosomal RNA

Chain BA:



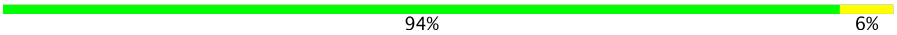


- Molecule 35: 30S ribosomal protein S2, chloroplastic

Chain BB:

- Molecule 36: 30S ribosomal protein S3, chloroplastic

Chain BC:



- Molecule 37: 30S ribosomal protein S4, chloroplastic

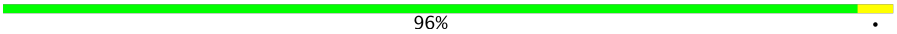
Chain BD:

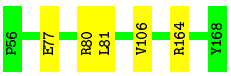
- Molecule 38: 30S ribosomal protein S5, chloroplastic

Chain BE:

- Molecule 39: 30S ribosomal protein S6 alpha, chloroplastic

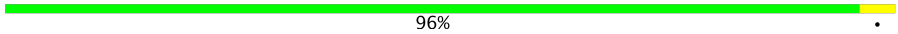
Chain BF:

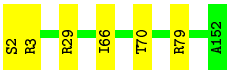




- Molecule 40: 30S ribosomal protein S7, chloroplastic

Chain BG:





- Molecule 41: 30S ribosomal protein S8, chloroplastic

Chain BH:

- Molecule 42: 30S ribosomal protein S9, chloroplastic

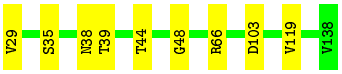
Chain BI:

- Molecule 43: 30S ribosomal protein S10 alpha, chloroplastic

Chain BJ:

- Molecule 44: 30S ribosomal protein S11, chloroplastic

Chain BK:

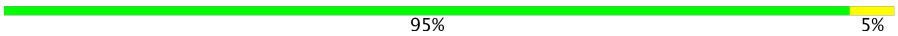


- Molecule 45: 30S ribosomal protein S12, chloroplastic

Chain BL:

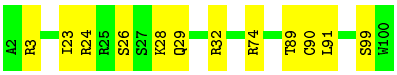
- Molecule 46: 30S ribosomal protein S13, chloroplastic

Chain BM:



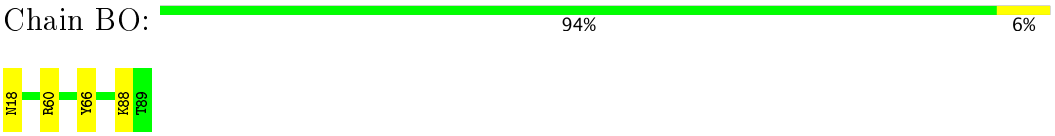
- Molecule 47: 30S ribosomal protein S14, chloroplastic

Chain BN:



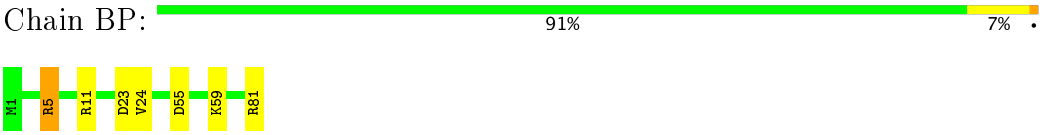
- Molecule 48: 30S ribosomal protein S15, chloroplastic

Chain BO:



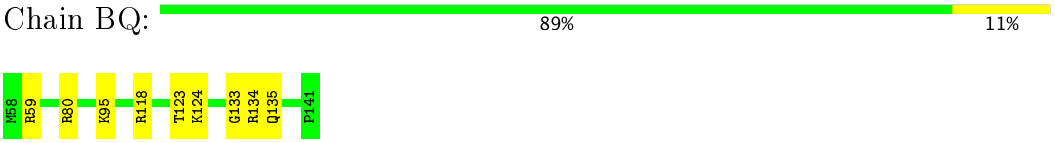
- Molecule 49: 30S ribosomal protein S16, chloroplastic

Chain BP:



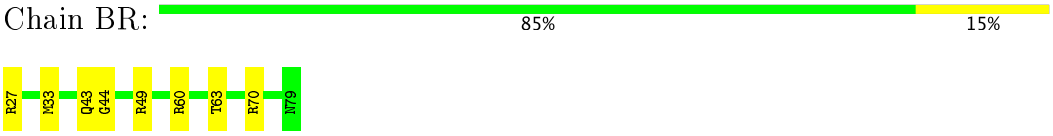
- Molecule 50: 30S ribosomal protein S17, chloroplastic

Chain BQ:



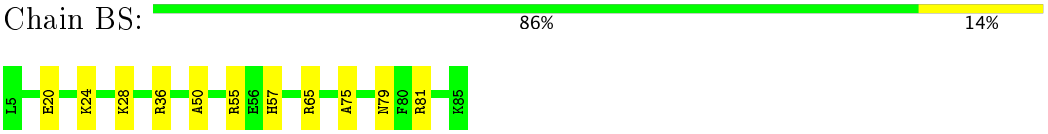
- Molecule 51: 30S ribosomal protein S18, chloroplastic

Chain BR:



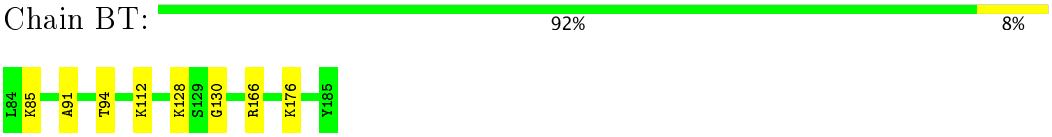
- Molecule 52: 30S ribosomal protein S19, chloroplastic

Chain BS:



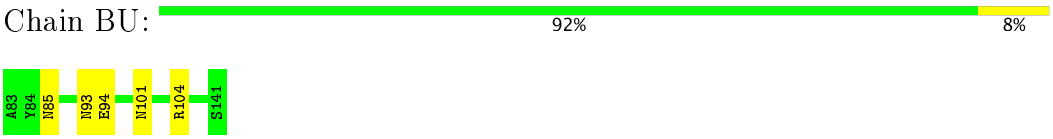
- Molecule 53: 30S ribosomal protein S20, chloroplastic

Chain BT:



- Molecule 54: 30S ribosomal protein S21, chloroplastic

Chain BU:

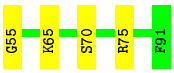


- Molecule 55: Ribosome-binding factor PSRP1, chloroplastic

Chain BV:

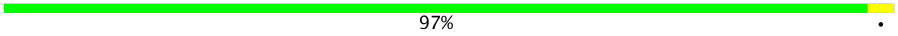
- Molecule 56: 30S ribosomal protein S31, chloroplastic

Chain BW:



- Molecule 57: bS1c

Chain BY:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130300	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 ($e^-/Å^2$)	4	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	AA	0.25	0/64858	0.70	2/101177 (0.0%)
10	AK	0.26	0/943	0.59	0/1271
11	AL	0.28	0/1425	0.58	0/1889
12	AM	0.28	0/1093	0.60	0/1466
13	AN	0.26	0/959	0.56	0/1280
14	AO	0.27	0/968	0.51	0/1300
15	AP	0.27	0/967	0.57	0/1300
16	AQ	0.27	0/1011	0.60	0/1350
17	AR	0.28	0/1359	0.55	0/1850
18	AS	0.27	0/1412	0.57	0/1889
19	AT	0.26	0/753	0.53	0/1011
2	AB	0.24	0/2551	0.72	0/3977
20	AU	0.25	0/1030	0.53	0/1375
21	AW	0.28	0/930	0.56	0/1235
22	AX	0.26	0/635	0.54	0/844
23	AY	0.26	0/840	0.53	0/1113
24	AZ	0.27	0/548	0.59	0/737
25	Aa	0.28	0/405	0.53	0/537
26	Ab	0.26	0/497	0.57	0/664
27	Ac	0.25	0/474	0.63	0/624
28	Ad	0.27	0/594	0.58	0/784
29	Ae	0.27	0/307	0.66	0/403
3	AC	0.27	0/1929	0.58	0/2588
30	Af	0.27	0/389	0.51	0/528
31	Aw	0.25	0/426	0.68	0/552
32	Ax	0.21	0/2821	0.70	0/4396
33	Az	0.25	0/1525	0.50	0/2048
34	BA	0.19	0/35618	0.69	1/55573 (0.0%)
35	BB	0.26	0/1666	0.55	0/2251
36	BC	0.26	0/1772	0.55	0/2382
37	BD	0.26	0/1661	0.57	0/2230
38	BE	0.26	0/1203	0.57	0/1620

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	BF	0.28	0/929	0.58	0/1255
4	AD	0.27	0/1713	0.53	0/2291
40	BG	0.26	0/1192	0.55	0/1596
41	BH	0.26	0/1016	0.59	0/1363
42	BI	0.26	0/1110	0.54	0/1490
43	BJ	0.27	0/813	0.54	0/1099
44	BK	0.25	0/841	0.58	0/1135
45	BL	0.27	0/975	0.61	0/1312
46	BM	0.25	0/921	0.61	0/1230
47	BN	0.24	0/841	0.59	0/1123
48	BO	0.26	0/613	0.58	0/814
49	BP	0.27	0/685	0.58	0/916
5	AE	0.27	0/1707	0.56	0/2298
50	BQ	0.26	0/690	0.57	0/926
51	BR	0.26	0/443	0.57	0/591
52	BS	0.26	0/668	0.49	0/899
53	BT	0.25	0/826	0.54	0/1100
54	BU	0.27	0/518	0.58	0/685
55	BV	0.25	0/843	0.55	0/1126
56	BW	0.27	0/296	0.62	0/390
6	AF	0.27	0/1347	0.53	0/1813
7	AG	0.28	0/1364	0.58	0/1835
8	AH	0.25	0/370	0.60	0/490
9	AJ	0.27	0/1659	0.51	0/2242
All	All	0.24	0/155949	0.66	3/232263 (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
17	AR	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1334	U	C2-N1-C1'	6.57	125.58	117.70
34	BA	1107	C	C2-N1-C1'	6.41	125.85	118.80
1	AA	1621	C	C6-N1-C2	-5.10	118.26	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	AR	174	THR	Peptide

5.2 Too-close contacts (i)

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	57902	0	29161	195	0
2	AB	2277	0	1146	7	0
3	AC	1896	0	1977	14	0
4	AD	1686	0	1772	11	0
5	AE	1676	0	1737	11	0
6	AF	1328	0	1371	10	0
7	AG	1343	0	1405	6	0
8	AH	367	0	422	2	0
9	AJ	1619	0	1652	12	0
10	AK	934	0	985	6	0
11	AL	1405	0	1490	11	0
12	AM	1071	0	1131	11	0
13	AN	944	0	1004	9	0
14	AO	952	0	971	2	0
15	AP	953	0	1045	5	0
16	AQ	994	0	1056	9	0
17	AR	1326	0	1360	13	0
18	AS	1388	0	1474	8	0
19	AT	743	0	793	2	0
20	AU	1015	0	1074	9	0
21	AW	914	0	956	5	0
22	AX	625	0	678	3	0
23	AY	832	0	900	1	0
24	AZ	536	0	515	4	0
25	Aa	396	0	437	0	0
26	Ab	489	0	507	0	0
27	Ac	471	0	529	0	0
28	Ad	588	0	658	0	0
29	Ae	305	0	344	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Af	375	0	391	0	0
31	Aw	423	0	510	0	0
32	Ax	2522	0	1274	0	0
33	Az	1512	0	1572	0	0
34	BA	31806	0	16016	114	0
35	BB	1639	0	1694	13	0
36	BC	1745	0	1825	9	0
37	BD	1633	0	1730	13	0
38	BE	1189	0	1245	14	0
39	BF	911	0	923	2	0
40	BG	1178	0	1255	7	0
41	BH	1004	0	1056	10	0
42	BI	1091	0	1153	8	0
43	BJ	796	0	841	4	0
44	BK	828	0	863	9	0
45	BL	959	0	1035	8	0
46	BM	913	0	956	4	0
47	BN	824	0	856	9	0
48	BO	606	0	661	3	0
49	BP	675	0	716	5	0
50	BQ	677	0	709	7	0
51	BR	440	0	487	3	0
52	BS	653	0	690	6	0
53	BT	818	0	878	5	0
54	BU	514	0	516	3	0
55	BV	836	0	878	5	0
56	BW	289	0	301	3	0
57	BY	850	0	202	4	0
58	AA	247	0	0	0	0
58	AB	9	0	0	0	0
58	Af	1	0	0	0	0
58	Aw	1	0	0	0	0
58	Ax	2	0	0	0	0
58	BA	82	0	0	0	0
58	BN	1	0	0	0	0
59	Ab	1	0	0	0	0
59	Ae	1	0	0	0	0
All	All	145026	0	99783	473	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 2.

All (473) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:540:A:OP2	9:AJ:212:ARG:NH2	2.02	0.92
1:AA:1789:U:OP2	1:AA:1794:A:N6	2.09	0.85
34:BA:1228:A:O2'	34:BA:1230:C:OP2	1.96	0.84
34:BA:1388:G:OP2	53:BT:112:LYS:NZ	2.10	0.83
1:AA:1927:A:O2'	1:AA:1928:C:OP2	1.97	0.83
34:BA:607:A:HO2'	48:BO:18:ASN:N	1.77	0.83
1:AA:1225:G:OP2	5:AE:204:LYS:NZ	2.13	0.82
34:BA:334:G:N2	34:BA:337:U:OP2	2.15	0.79
2:AB:61:G:N2	2:AB:64:A:OP2	2.15	0.79
46:BM:127:GLU:OE2	52:BS:65:ARG:NH1	2.17	0.77
34:BA:714:G:H1	34:BA:761:G:HO2'	1.33	0.76
9:AJ:59:GLU:OE2	9:AJ:63:GLN:NE2	2.19	0.76
34:BA:572:C:O2	49:BP:11:ARG:NH2	2.19	0.75
34:BA:450:C:OP1	45:BL:114:ARG:NH2	2.20	0.75
34:BA:296:G:N1	34:BA:299:A:OP2	2.20	0.75
1:AA:2016:G:OP2	13:AN:19:ARG:NH2	2.20	0.74
1:AA:1180:C:OP1	16:AQ:94:ARG:NH2	2.20	0.74
1:AA:2593:G:O2'	1:AA:2596:C:OP2	2.05	0.74
1:AA:2662:C:HO2'	1:AA:2750:G:HO2'	1.30	0.74
34:BA:926:G:N2	34:BA:1312:C:OP2	2.19	0.74
1:AA:2500:C:O2'	12:AM:52:ARG:NH2	2.21	0.73
34:BA:1115:G:N2	34:BA:1119:A:OP2	2.21	0.73
37:BD:58:TYR:OH	37:BD:88:GLU:OE2	2.07	0.73
1:AA:1098:A:N6	1:AA:1126:A:OP2	2.20	0.73
1:AA:1837:U:OP2	3:AC:217:ARG:NH1	2.22	0.72
37:BD:14:ARG:NH1	37:BD:49:GLU:OE2	2.22	0.72
34:BA:513:U:OP2	45:BL:12:ARG:NH1	2.22	0.72
1:AA:366:G:O2'	1:AA:367:C:O4'	2.07	0.72
1:AA:2701:U:O2'	10:AK:68:GLU:OE1	2.08	0.71
34:BA:1215:G:N2	34:BA:1218:A:OP2	2.23	0.71
34:BA:1165:C:OP1	47:BN:3:ARG:NH1	2.23	0.71
1:AA:2598:G:N2	1:AA:2598:G:OP2	2.20	0.71
34:BA:780:C:OP1	35:BB:25:ARG:NH2	2.22	0.71
1:AA:488:G:O6	20:AU:50:LYS:NZ	2.24	0.71
1:AA:492:A:O2'	20:AU:109:THR:O	2.09	0.70
1:AA:8:G:O2'	1:AA:2646:U:O4	2.06	0.70
1:AA:2283:A:N6	1:AA:2290:A:OP2	2.23	0.70
1:AA:2737:G:OP1	15:AP:218:ARG:NH1	2.24	0.70
5:AE:116:TYR:OH	5:AE:124:ALA:O	2.10	0.70
1:AA:1344:G:OP2	18:AS:127:ARG:NH1	2.25	0.69
12:AM:77:ARG:NH1	12:AM:81:THR:O	2.25	0.69
34:BA:1275:U:OP1	56:BW:65:LYS:NZ	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BE:298:ASP:O	41:BH:64:ARG:NH1	2.24	0.69
1:AA:756:G:O2'	1:AA:759:G:O2'	2.11	0.69
34:BA:840:G:O2'	34:BA:856:G:O6	2.11	0.69
45:BL:10:ASN:O	45:BL:13:GLN:NE2	2.26	0.69
1:AA:1703:G:O2'	1:AA:2005:U:O4	2.10	0.69
1:AA:1279:C:OP1	5:AE:134:ARG:NH1	2.25	0.69
1:AA:2308:U:O2'	1:AA:2391:C:O2	2.11	0.68
34:BA:1306:G:N2	34:BA:1316:C:O2	2.27	0.68
2:AB:29:U:O2'	2:AB:83:C:N3	2.27	0.68
34:BA:503:U:OP1	45:BL:19:THR:OG1	2.10	0.68
24:AZ:49:ALA:N	24:AZ:61:THR:O	2.27	0.68
34:BA:1266:C:OP1	47:BN:24:ARG:NH1	2.26	0.68
1:AA:566:A:N1	9:AJ:101:TYR:OH	2.26	0.67
34:BA:171:G:O3'	53:BT:176:LYS:NZ	2.25	0.67
34:BA:377:U:O4	37:BD:2:SER:N	2.27	0.67
1:AA:2275:G:O2'	1:AA:2444:C:OP2	2.10	0.67
47:BN:29:GLN:OE1	47:BN:32:ARG:NH1	2.27	0.67
34:BA:760:C:O2'	34:BA:851:A:N1	2.28	0.67
1:AA:1533:A:N3	1:AA:1611:G:O2'	2.28	0.67
35:BB:92:ARG:NH1	57:BY:1254:UNK:O	2.27	0.67
1:AA:2323:C:OP2	1:AA:2324:G:O2'	2.02	0.67
35:BB:122:ARG:NH2	35:BB:149:GLN:OE1	2.28	0.67
34:BA:601:U:O4	34:BA:701:G:O2'	2.09	0.67
1:AA:804:A:OP2	1:AA:2085:A:O2'	2.13	0.67
1:AA:1022:C:O2'	17:AR:132:ARG:NH1	2.27	0.67
3:AC:34:ARG:NH2	3:AC:35:CYS:O	2.28	0.67
11:AL:163:ARG:NH2	11:AL:203:GLU:OE1	2.28	0.66
34:BA:376:G:OP2	37:BD:108:ARG:NH2	2.28	0.66
1:AA:1518:U:O2	1:AA:1519:A:N6	2.26	0.66
1:AA:1562:A:N6	1:AA:1577:G:O2'	2.29	0.66
34:BA:1128:A:OP2	42:BI:162:ARG:NH2	2.28	0.66
1:AA:893:C:N4	1:AA:904:U:O2	2.28	0.66
1:AA:511:G:N1	1:AA:514:A:OP2	2.28	0.66
41:BH:97:PRO:O	41:BH:121:ARG:NH2	2.29	0.66
1:AA:755:U:OP2	4:AD:227:LYS:NZ	2.27	0.66
34:BA:928:A:OP2	34:BA:1312:C:N4	2.29	0.66
34:BA:1329:G:O6	40:BG:2:SER:N	2.29	0.66
34:BA:1332:C:O2'	40:BG:79:ARG:NH2	2.28	0.66
1:AA:641:C:O2	1:AA:651:U:O2'	2.13	0.65
34:BA:1445:U:OP1	55:BV:97:LYS:NZ	2.28	0.65
1:AA:754:A:O2'	1:AA:1695:U:OP1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1801:A:O2'	3:AC:201:LEU:O	2.08	0.65
6:AF:117:ARG:NH2	24:AZ:62:GLY:O	2.30	0.65
34:BA:885:A:O2'	34:BA:1333:C:N3	2.27	0.65
1:AA:2520:A:O2'	1:AA:2522:G:OP2	2.14	0.65
1:AA:2588:U:O2'	4:AD:240:THR:OG1	2.15	0.65
1:AA:1927:A:N7	34:BA:1444:G:O2'	2.28	0.65
1:AA:555:A:O5'	18:AS:195:ARG:NH2	2.29	0.65
42:BI:78:ARG:NH1	42:BI:144:GLN:OE1	2.30	0.65
1:AA:475:G:N2	1:AA:478:A:OP2	2.28	0.65
34:BA:502:A:O2'	45:BL:26:GLY:O	2.15	0.65
1:AA:1445:G:OP1	3:AC:27:ASN:ND2	2.30	0.65
7:AG:94:LYS:NZ	7:AG:102:ASN:OD1	2.29	0.65
1:AA:1287:G:O2'	1:AA:2026:G:O6	2.10	0.65
34:BA:1266:C:OP2	47:BN:28:LYS:NZ	2.30	0.65
37:BD:155:SER:O	37:BD:157:ARG:NH1	2.30	0.65
1:AA:1269:G:OP1	16:AQ:2:THR:N	2.30	0.64
44:BK:35:SER:OG	44:BK:38:ASN:O	2.11	0.64
1:AA:329:C:O2	5:AE:222:ASN:ND2	2.30	0.64
34:BA:1309:A:OP2	47:BN:74:ARG:NH2	2.30	0.64
1:AA:889:G:O2'	1:AA:890:G:OP2	2.14	0.64
34:BA:632:G:N2	44:BK:48:GLY:O	2.30	0.64
1:AA:2807:C:O2'	2:AB:95:A:O2'	2.09	0.64
1:AA:285:A:O2'	1:AA:372:G:O6	2.13	0.64
1:AA:792:A:OP1	3:AC:213:ARG:NH2	2.31	0.64
34:BA:1254:G:OP2	56:BW:55:GLY:N	2.30	0.64
7:AG:160:GLU:OE1	7:AG:176:ARG:NH2	2.31	0.64
34:BA:1265:G:N1	34:BA:1268:A:OP2	2.30	0.64
1:AA:1273:G:OP2	16:AQ:13:ARG:NH1	2.30	0.64
1:AA:2360:U:O2'	1:AA:2390:A:O2'	2.13	0.64
34:BA:1086:G:OP2	34:BA:1086:G:N2	2.25	0.64
34:BA:607:A:O2'	48:BO:18:ASN:N	2.32	0.63
15:AP:172:ARG:NE	15:AP:174:ASN:OD1	2.31	0.63
20:AU:74:ASP:OD2	20:AU:160:ARG:NH1	2.32	0.63
34:BA:1132:U:O2'	34:BA:1134:A:OP2	2.17	0.63
43:BJ:136:PRO:O	43:BJ:164:GLN:NE2	2.31	0.63
1:AA:2320:G:O2'	6:AF:136:SER:O	2.15	0.63
1:AA:2107:G:OP2	8:AH:70:ARG:NH2	2.32	0.63
36:BC:61:ALA:O	36:BC:125:ASN:ND2	2.32	0.62
1:AA:2075:G:OP1	5:AE:119:LYS:NZ	2.29	0.62
1:AA:869:G:O2'	1:AA:925:G:O6	2.13	0.62
34:BA:269:G:N2	34:BA:272:A:OP2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AN:113:ARG:NH2	13:AN:116:ASP:OD2	2.32	0.62
34:BA:915:U:O2'	55:BV:115:ARG:NH1	2.32	0.62
1:AA:232:G:OP2	1:AA:234:C:N4	2.28	0.62
1:AA:2371:A:OP1	21:AW:88:LYS:NZ	2.30	0.62
5:AE:55:LEU:N	5:AE:68:THR:O	2.33	0.62
10:AK:58:ILE:HD13	10:AK:86:ILE:HG22	1.82	0.62
34:BA:873:A:N6	34:BA:1342:G:O6	2.33	0.62
1:AA:992:U:O2'	1:AA:2290:A:N3	2.31	0.61
1:AA:2740:G:O2'	13:AN:13:HIS:O	2.10	0.61
34:BA:909:A:HO2'	34:BA:934:C:HO2'	1.48	0.61
1:AA:553:G:OP1	18:AS:185:SER:OG	2.17	0.61
34:BA:111:A:OP1	34:BA:554:U:O2'	2.11	0.61
51:BR:44:GLY:O	51:BR:70:ARG:NH2	2.33	0.61
1:AA:1927:A:HO2'	1:AA:1928:C:P	2.22	0.61
1:AA:2047:A:O2'	1:AA:2049:G:OP2	2.12	0.61
4:AD:115:ILE:HD12	4:AD:278:ILE:HD13	1.82	0.60
1:AA:1751:A:O2'	1:AA:1753:A:OP2	2.19	0.60
1:AA:2267:G:O2'	1:AA:2513:C:OP1	2.12	0.60
38:BE:294:ASP:OD1	38:BE:297:ARG:NH2	2.34	0.60
1:AA:1111:G:N2	1:AA:1114:A:OP2	2.34	0.60
4:AD:142:GLU:OE2	4:AD:166:ARG:NH1	2.35	0.60
12:AM:120:ILE:O	12:AM:123:SER:OG	2.15	0.60
1:AA:104:C:OP1	20:AU:60:ASN:ND2	2.35	0.60
1:AA:1024:A:OP2	17:AR:132:ARG:NH2	2.35	0.60
34:BA:227:G:OP1	50:BQ:124:LYS:NZ	2.32	0.60
6:AF:177:THR:OG1	6:AF:180:GLU:OE1	2.20	0.60
1:AA:2691:G:O2'	10:AK:28:SER:O	2.20	0.59
38:BE:247:VAL:O	38:BE:254:ARG:NH1	2.36	0.59
56:BW:70:SER:O	56:BW:75:ARG:NH2	2.34	0.59
47:BN:89:THR:HG23	47:BN:91:LEU:HD23	1.84	0.59
34:BA:544:A:N6	34:BA:590:A:O2'	2.36	0.59
34:BA:611:U:O2'	34:BA:785:U:OP1	2.19	0.59
34:BA:1004:C:O2'	55:BV:119:ARG:NH2	2.35	0.59
37:BD:73:ARG:NH2	37:BD:197:TYR:O	2.36	0.59
42:BI:173:ARG:NH1	42:BI:174:ASP:O	2.35	0.59
1:AA:1113:A:O2'	1:AA:1132:C:O2	2.16	0.59
15:AP:147:ASP:OD1	15:AP:211:HIS:ND1	2.36	0.58
16:AQ:49:ASP:O	16:AQ:53:GLN:N	2.36	0.58
37:BD:131:LYS:N	37:BD:134:ASP:OD2	2.36	0.58
51:BR:43:GLN:NE2	54:BU:85:ASN:O	2.35	0.58
38:BE:299:ARG:NH1	41:BH:42:GLU:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2798:G:OP2	9:AJ:219:ASN:ND2	2.35	0.58
1:AA:1809:G:OP1	3:AC:256:ARG:NH2	2.36	0.58
34:BA:511:G:N2	45:BL:11:THR:O	2.36	0.58
38:BE:279:ALA:O	38:BE:282:THR:OG1	2.19	0.58
1:AA:1978:G:O2'	1:AA:1981:C:OP2	2.16	0.58
34:BA:494:C:OP1	37:BD:51:LYS:NZ	2.36	0.58
34:BA:512:A:O2'	34:BA:515:G:O3'	2.22	0.58
34:BA:448:A:O4'	34:BA:496:A:N6	2.37	0.58
34:BA:876:G:N7	55:BV:170:LYS:NZ	2.52	0.57
1:AA:82:G:OP1	20:AU:158:LYS:NZ	2.32	0.57
11:AL:134:MET:O	11:AL:139:ARG:NH2	2.35	0.57
35:BB:38:LYS:N	57:BY:1206:UNK:O	2.36	0.57
1:AA:213:A:OP1	11:AL:238:ARG:NH2	2.38	0.57
34:BA:1027:G:N2	34:BA:1030:A:OP2	2.33	0.57
36:BC:83:LEU:O	36:BC:87:ASN:ND2	2.38	0.57
34:BA:1327:U:HO2'	40:BG:2:SER:N	2.02	0.57
1:AA:1932:A:O2'	1:AA:1934:C:N4	2.38	0.57
1:AA:2581:A:OP1	1:AA:2665:U:O2'	2.20	0.57
11:AL:187:ILE:HG22	11:AL:189:PRO:HD3	1.87	0.57
34:BA:883:G:N7	40:BG:3:ARG:NH1	2.53	0.56
17:AR:192:ASP:O	17:AR:213:ARG:NE	2.35	0.56
34:BA:567:C:O2	49:BP:11:ARG:NH1	2.37	0.56
34:BA:209:C:OP2	50:BQ:95:LYS:NZ	2.38	0.56
11:AL:205:GLU:OE2	11:AL:207:SER:OG	2.23	0.56
34:BA:1069:G:OP2	42:BI:77:ARG:NH2	2.39	0.56
17:AR:146:ARG:NH1	17:AR:190:LEU:O	2.39	0.56
1:AA:2612:G:N2	1:AA:2615:A:OP2	2.38	0.56
49:BP:55:ASP:OD1	49:BP:59:LYS:NZ	2.38	0.56
1:AA:588:A:OP1	1:AA:1276:U:O2'	2.23	0.56
34:BA:352:G:N2	34:BA:355:A:OP2	2.38	0.56
1:AA:642:G:N2	1:AA:645:A:OP2	2.35	0.55
24:AZ:38:LYS:HD2	24:AZ:41:ILE:HD11	1.88	0.55
41:BH:112:ARG:NH2	41:BH:123:GLU:OE2	2.39	0.55
52:BS:79:ASN:OD1	52:BS:81:ARG:NH1	2.40	0.55
52:BS:20:GLU:O	52:BS:24:LYS:NZ	2.36	0.55
34:BA:112:A:O2'	50:BQ:59:ARG:NH2	2.40	0.55
1:AA:1667:G:N2	1:AA:1670:A:OP2	2.36	0.55
1:AA:2761:U:OP2	1:AA:2773:C:N4	2.40	0.55
1:AA:2025:U:OP2	18:AS:45:LYS:NZ	2.37	0.54
1:AA:1438:G:O2'	1:AA:1623:A:O2'	2.25	0.54
38:BE:305:GLU:OE2	41:BH:118:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1039:A:OP2	16:AQ:66:ASN:ND2	2.40	0.54
1:AA:169:C:O2'	1:AA:202:A:N3	2.39	0.54
17:AR:120:ARG:NH1	17:AR:138:PRO:O	2.40	0.54
34:BA:218:A:O2'	34:BA:251:A:N6	2.40	0.54
34:BA:775:C:O2	41:BH:15:ASN:ND2	2.40	0.54
50:BQ:133:GLY:O	50:BQ:134:ARG:NE	2.37	0.54
43:BJ:159:GLU:OE1	43:BJ:159:GLU:N	2.40	0.54
2:AB:74:C:OP1	13:AN:72:LYS:NZ	2.27	0.53
41:BH:4:ASP:OD2	41:BH:7:ALA:N	2.38	0.53
17:AR:187:GLU:OE1	17:AR:218:ARG:NE	2.42	0.53
1:AA:1808:C:OP2	3:AC:270:ARG:NH2	2.42	0.53
1:AA:2329:U:OP2	6:AF:86:LYS:NZ	2.37	0.53
38:BE:274:ASN:ND2	38:BE:277:ASN:OD1	2.39	0.53
52:BS:50:ALA:HB1	52:BS:57:HIS:HB3	1.91	0.53
1:AA:1690:A:OP2	13:AN:11:MET:N	2.42	0.53
1:AA:232:G:N2	1:AA:236:A:OP2	2.36	0.53
34:BA:1171:G:OP2	34:BA:1271:C:N4	2.37	0.53
1:AA:1457:G:O2'	1:AA:1496:A:N1	2.41	0.52
1:AA:984:G:OP2	12:AM:14:ARG:NH1	2.37	0.52
1:AA:255:A:OP2	1:AA:271:G:N1	2.36	0.52
34:BA:519:G:O6	34:BA:815:A:N6	2.43	0.52
1:AA:2676:G:O2'	7:AG:215:LYS:NZ	2.39	0.51
1:AA:670:A:N3	5:AE:86:ARG:NH2	2.58	0.51
1:AA:2662:C:O2'	1:AA:2750:G:O2'	2.07	0.51
1:AA:687:A:HO2'	1:AA:2459:C:HO2'	1.56	0.51
1:AA:919:A:N3	1:AA:2281:C:O2'	2.41	0.51
21:AW:161:GLN:OE1	21:AW:164:LYS:NZ	2.43	0.51
34:BA:523:A:HO2'	34:BA:832:C:HO2'	1.55	0.51
34:BA:76:U:N3	34:BA:79:U:OP1	2.41	0.51
1:AA:583:G:OP2	17:AR:203:LYS:NZ	2.40	0.51
18:AS:188:TYR:HH	18:AS:193:PHE:HE2	1.59	0.50
1:AA:1056:A:OP2	1:AA:1154:A:N6	2.40	0.50
1:AA:488:G:N1	1:AA:491:A:OP2	2.41	0.50
34:BA:1025:C:OP1	38:BE:210:ARG:NH2	2.45	0.50
1:AA:286:U:O2'	1:AA:287:A:O4'	2.29	0.50
1:AA:1182:A:O3'	16:AQ:55:ARG:NH2	2.44	0.50
44:BK:103:ASP:OD2	54:BU:104:ARG:NH1	2.43	0.50
35:BB:97:ASN:OD1	35:BB:98:LYS:N	2.45	0.50
42:BI:104:TYR:OH	42:BI:142:GLN:OE1	2.24	0.50
1:AA:384:G:O2'	1:AA:412:G:O6	2.24	0.50
1:AA:842:G:O2'	11:AL:117:GLN:OE1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BE:215:VAL:HG12	38:BE:286:VAL:HG11	1.94	0.50
34:BA:915:U:O3'	55:BV:115:ARG:NH1	2.45	0.50
1:AA:1121:G:H21	1:AA:1126:A:H62	1.60	0.50
1:AA:1500:U:O2'	1:AA:1501:G:OP1	2.28	0.50
35:BB:124:GLU:OE1	35:BB:129:ARG:NH1	2.43	0.50
1:AA:423:G:OP2	1:AA:2423:A:O2'	2.22	0.49
1:AA:2486:A:N6	1:AA:2498:G:O2'	2.43	0.49
34:BA:706:U:O2'	34:BA:829:C:O2	2.29	0.49
1:AA:1950:A:N6	1:AA:1977:C:N3	2.58	0.49
1:AA:1420:C:OP1	19:AT:160:ARG:NH2	2.45	0.49
1:AA:1304:G:N2	1:AA:1307:A:OP2	2.44	0.49
1:AA:2091:A:OP1	1:AA:2255:G:N2	2.39	0.49
1:AA:382:G:OP1	1:AA:435:A:N6	2.46	0.49
34:BA:1085:U:O2'	34:BA:1087:A:N6	2.41	0.49
1:AA:1468:C:O2'	1:AA:1578:A:N3	2.42	0.49
53:BT:128:LYS:NZ	53:BT:130:GLY:O	2.46	0.49
1:AA:2106:U:N3	1:AA:2243:C:OP2	2.37	0.48
1:AA:1096:G:N2	1:AA:1124:A:O4'	2.46	0.48
1:AA:8:G:OP1	9:AJ:216:TYR:OH	2.15	0.48
34:BA:373:C:O2'	34:BA:570:A:N3	2.36	0.48
34:BA:730:A:O2'	34:BA:1472:U:O2	2.30	0.48
35:BB:30:ARG:NH1	35:BB:198:ASP:OD2	2.45	0.48
1:AA:1230:G:O2'	1:AA:1258:A:N1	2.35	0.48
1:AA:2097:C:O2	3:AC:248:TYR:OH	2.18	0.48
34:BA:543:U:O4'	50:BQ:135:GLN:NE2	2.47	0.48
6:AF:73:ALA:O	6:AF:77:GLY:N	2.42	0.48
1:AA:1271:G:OP2	11:AL:100:ARG:NE	2.46	0.48
13:AN:85:ILE:O	13:AN:89:LEU:N	2.46	0.48
34:BA:1002:U:O2'	34:BA:1005:A:OP2	2.14	0.48
53:BT:91:ALA:O	53:BT:94:THR:OG1	2.20	0.48
1:AA:2523:U:OP2	1:AA:2593:G:N1	2.38	0.48
1:AA:892:C:N4	1:AA:903:G:O6	2.46	0.48
42:BI:105:LEU:HD12	42:BI:111:TRP:HB3	1.94	0.48
52:BS:36:ARG:NH2	52:BS:75:ALA:O	2.46	0.48
1:AA:1449:C:O2'	1:AA:1603:A:OP2	2.20	0.48
1:AA:2009:U:O2	10:AK:32:TYR:OH	2.28	0.48
1:AA:585:A:OP2	1:AA:2516:C:O2'	2.31	0.48
1:AA:682:C:OP1	11:AL:122:GLY:N	2.47	0.48
1:AA:2330:U:O4'	6:AF:52:ASN:ND2	2.47	0.48
17:AR:101:PRO:O	17:AR:105:ASP:N	2.46	0.48
3:AC:138:HIS:ND1	3:AC:189:GLY:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AX:125:ALA:O	22:AX:128:THR:OG1	2.22	0.48
34:BA:1064:C:O2	47:BN:99:SER:OG	2.31	0.48
34:BA:669:C:OP2	34:BA:670:A:O2'	2.26	0.48
1:AA:1750:C:O2'	1:AA:1751:A:O3'	2.29	0.47
1:AA:759:G:OP1	18:AS:117:ARG:NH1	2.46	0.47
36:BC:190:ARG:NH2	36:BC:217:GLU:OE2	2.47	0.47
18:AS:87:ALA:O	18:AS:92:GLN:N	2.46	0.47
34:BA:335:A:N6	45:BL:27:CYS:SG	2.87	0.47
3:AC:113:VAL:N	3:AC:124:ASN:OD1	2.45	0.47
34:BA:376:G:O5'	37:BD:112:ASN:ND2	2.47	0.47
1:AA:2705:G:N1	1:AA:2738:U:OP2	2.36	0.47
1:AA:349:A:O2'	5:AE:221:ARG:NH1	2.47	0.47
39:BF:77:GLU:O	39:BF:81:LEU:HD23	2.14	0.47
49:BP:23:ASP:OD1	49:BP:24:VAL:N	2.47	0.47
1:AA:1764:A:N1	1:AA:2734:U:O2'	2.40	0.47
1:AA:2106:U:OP2	8:AH:75:ARG:NH2	2.38	0.47
1:AA:2213:A:OP1	22:AX:107:ARG:NH1	2.48	0.47
1:AA:990:C:HO2'	1:AA:2513:C:HO2'	1.62	0.47
41:BH:117:ASP:OD1	41:BH:118:ARG:N	2.48	0.47
1:AA:1385:G:N2	1:AA:1388:A:OP2	2.42	0.47
1:AA:889:G:HO2'	1:AA:890:G:P	2.38	0.47
1:AA:2487:G:OP1	12:AM:56:ARG:NH1	2.48	0.47
1:AA:893:C:O2'	1:AA:894:G:O4'	2.31	0.47
9:AJ:243:ASP:OD1	9:AJ:244:LYS:N	2.48	0.47
34:BA:18:A:O4'	38:BE:163:THR:OG1	2.31	0.47
42:BI:100:ASP:OD1	42:BI:101:ALA:N	2.48	0.47
6:AF:150:GLN:N	6:AF:150:GLN:OE1	2.48	0.47
7:AG:83:GLU:OE1	7:AG:83:GLU:N	2.48	0.47
34:BA:635:G:H1	34:BA:652:G:HO2'	1.62	0.47
42:BI:116:LYS:O	42:BI:120:ALA:N	2.45	0.47
1:AA:2266:U:N3	1:AA:2270:G:OP2	2.43	0.46
1:AA:1089:U:O2'	1:AA:1098:A:O5'	2.32	0.46
9:AJ:206:GLY:O	9:AJ:210:LYS:NZ	2.48	0.46
18:AS:178:ARG:NH1	18:AS:184:LYS:O	2.48	0.46
34:BA:1017:A:N1	34:BA:1058:G:O2'	2.40	0.46
1:AA:1674:C:O2	1:AA:2715:U:O2'	2.33	0.46
1:AA:1384:C:O2'	1:AA:1819:A:N3	2.39	0.46
34:BA:349:G:OP1	49:BP:5:ARG:NH1	2.48	0.46
1:AA:44:G:N7	1:AA:200:G:O2'	2.34	0.46
1:AA:1056:A:N3	1:AA:2503:G:O2'	2.40	0.46
1:AA:2589:A:N7	4:AD:239:THR:OG1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:228:U:OP2	4:AD:96:LYS:NZ	117.13	0.46
2:AB:18:G:O2'	2:AB:20:C:OP2	2.19	0.46
34:BA:1006:U:OP1	36:BC:174:ALA:N	2.48	0.46
34:BA:92:G:OP1	34:BA:297:A:N6	2.49	0.46
1:AA:1521:G:OP2	1:AA:1521:G:N2	2.40	0.46
1:AA:2751:A:N6	1:AA:2788:A:N1	2.64	0.46
34:BA:1012:U:O4	36:BC:2:GLY:N	2.49	0.46
36:BC:57:VAL:HG12	36:BC:57:VAL:O	2.15	0.46
34:BA:235:A:OP1	53:BT:166:ARG:NE	2.49	0.45
51:BR:60:ARG:O	51:BR:63:THR:OG1	2.34	0.45
1:AA:1244:G:N2	1:AA:1247:A:OP2	2.44	0.45
14:AO:157:ASP:O	14:AO:161:GLU:N	2.50	0.45
1:AA:1097:A:H61	1:AA:1101:A:H62	1.65	0.45
1:AA:31:C:N4	1:AA:459:A:OP2	2.49	0.45
1:AA:874:G:OP1	12:AM:23:ARG:NH1	2.43	0.45
34:BA:639:G:OP2	44:BK:38:ASN:ND2	2.43	0.45
19:AT:139:ASP:OD1	19:AT:140:VAL:N	2.50	0.45
1:AA:2672:G:O2'	1:AA:2681:G:O6	2.20	0.45
1:AA:596:A:N1	1:AA:820:G:O2'	2.43	0.45
34:BA:8:G:O2'	34:BA:270:A:O4'	2.34	0.45
44:BK:38:ASN:OD1	44:BK:39:THR:N	2.49	0.45
5:AE:252:ILE:O	5:AE:256:ASN:ND2	2.50	0.45
9:AJ:57:CYS:HG	9:AJ:61:TRP:HE1	1.58	0.45
1:AA:937:U:OP2	21:AW:153:ARG:NH1	2.50	0.45
40:BG:66:ILE:O	40:BG:70:THR:OG1	2.19	0.45
41:BH:47:ASN:OD1	41:BH:48:ALA:N	2.49	0.45
1:AA:1374:A:OP2	1:AA:1398:G:N1	2.41	0.45
1:AA:1810:C:OP2	3:AC:178:ARG:NH1	2.50	0.45
12:AM:28:CYS:SG	12:AM:29:PHE:N	2.90	0.45
34:BA:1009:C:OP2	36:BC:210:LYS:NZ	2.41	0.45
36:BC:52:LYS:O	36:BC:53:THR:OG1	2.30	0.45
47:BN:23:ILE:O	47:BN:26:SER:OG	2.26	0.45
34:BA:700:U:O2'	34:BA:701:G:OP1	2.25	0.45
4:AD:176:VAL:O	4:AD:176:VAL:HG12	2.16	0.44
6:AF:122:ALA:HB1	6:AF:152:VAL:HG23	1.98	0.44
11:AL:79:ARG:O	11:AL:84:ASN:ND2	2.48	0.44
38:BE:227:ASN:ND2	38:BE:288:THR:OG1	2.51	0.44
47:BN:90:CYS:O	47:BN:91:LEU:HD22	2.17	0.44
34:BA:1316:C:O2'	43:BJ:155:ARG:NH2	2.50	0.44
9:AJ:99:THR:HG22	16:AQ:61:TRP:HE1	1.83	0.44
34:BA:1138:U:O2'	36:BC:187:GLN:OE1	2.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2089:U:OP1	3:AC:239:ARG:NH2	2.51	0.44
10:AK:88:ASP:OD1	10:AK:92:ASN:N	2.49	0.44
34:BA:640:G:O6	44:BK:66:ARG:NH2	2.50	0.44
37:BD:169:PHE:HB2	37:BD:170:PRO:HD3	2.00	0.44
1:AA:1004:G:O2'	1:AA:1182:A:O2'	2.24	0.44
1:AA:829:G:N1	1:AA:1209:U:OP2	2.40	0.44
34:BA:963:G:N2	34:BA:966:A:OP2	2.43	0.44
34:BA:507:G:OP2	34:BA:508:A:O2'	2.25	0.44
9:AJ:57:CYS:SG	9:AJ:61:TRP:NE1	2.89	0.44
1:AA:2392:G:N2	1:AA:2395:A:OP2	2.42	0.43
35:BB:201:ASP:OD1	35:BB:202:ILE:N	2.50	0.43
1:AA:583:G:N2	1:AA:2045:A:OP1	2.50	0.43
20:AU:146:SER:OG	20:AU:162:LEU:HD12	2.18	0.43
44:BK:29:VAL:N	44:BK:44:THR:O	2.52	0.43
24:AZ:46:ARG:NH1	24:AZ:66:LYS:O	2.52	0.43
34:BA:186:G:N1	34:BA:188:A:OP1	2.51	0.43
1:AA:1481:U:O2'	1:AA:2719:G:O2'	2.19	0.43
23:AY:71:LYS:O	23:AY:122:ARG:NH2	2.49	0.43
1:AA:1047:U:OP1	1:AA:1063:U:O2'	2.23	0.43
1:AA:981:G:OP2	12:AM:16:ARG:NE	2.51	0.43
35:BB:56:GLU:OE2	57:BY:1124:UNK:N	2.51	0.43
1:AA:2588:U:O3'	4:AD:240:THR:OG1	2.37	0.43
13:AN:22:ARG:O	13:AN:27:ARG:NH2	2.52	0.43
6:AF:39:ASN:OD1	6:AF:40:ILE:N	2.52	0.43
35:BB:189:CYS:SG	35:BB:190:LEU:N	2.86	0.43
35:BB:191:ILE:O	35:BB:191:ILE:HG22	2.19	0.43
44:BK:119:VAL:HG12	44:BK:119:VAL:O	2.18	0.43
1:AA:1808:C:OP2	3:AC:269:ARG:NH1	2.52	0.43
40:BG:2:SER:OG	40:BG:3:ARG:N	2.51	0.43
1:AA:1837:U:O2'	1:AA:1984:A:N3	2.42	0.43
9:AJ:99:THR:HG21	16:AQ:57:PHE:CD1	2.53	0.43
17:AR:192:ASP:OD1	17:AR:193:ASP:N	2.51	0.43
45:BL:18:VAL:HG12	45:BL:18:VAL:O	2.19	0.43
57:BY:1101:UNK:O	57:BY:1105:UNK:N	2.52	0.43
1:AA:322:C:N4	1:AA:323:G:O6	2.52	0.43
1:AA:945:A:H61	1:AA:950:A:H61	1.66	0.42
10:AK:76:ILE:HB	15:AP:195:VAL:HG12	2.01	0.42
34:BA:1443:A:O2'	34:BA:1444:G:O5'	2.36	0.42
1:AA:1503:C:O2'	1:AA:1519:A:N6	2.46	0.42
1:AA:262:G:N2	1:AA:265:A:OP2	2.44	0.42
1:AA:889:G:O2'	1:AA:890:G:O4'	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:923:G:OP2	34:BA:924:A:O2'	2.30	0.42
13:AN:43:ARG:NH1	13:AN:124:GLU:OE1	2.50	0.42
34:BA:908:A:N3	34:BA:935:C:O2'	2.48	0.42
34:BA:373:C:O3'	37:BD:67:LYS:NZ	2.51	0.42
35:BB:229:ARG:O	35:BB:230:SER:OG	2.34	0.42
6:AF:52:ASN:OD1	6:AF:53:CYS:N	2.52	0.42
38:BE:160:ARG:O	38:BE:175:ARG:N	2.49	0.42
34:BA:524:G:O2'	34:BA:770:G:OP2	2.08	0.42
35:BB:108:TRP:NE1	35:BB:112:GLU:OE2	2.52	0.42
1:AA:144:A:N3	1:AA:2223:A:O2'	2.48	0.42
12:AM:38:GLU:OE2	12:AM:128:ARG:NH2	2.53	0.42
14:AO:115:PRO:O	14:AO:151:ARG:NH1	2.50	0.42
2:AB:30:A:OP2	2:AB:38:G:O2'	2.26	0.42
3:AC:102:HIS:O	3:AC:192:GLY:N	2.50	0.42
17:AR:164:VAL:O	17:AR:171:TYR:N	2.52	0.42
34:BA:638:C:OP1	44:BK:38:ASN:ND2	2.49	0.42
54:BU:93:ASN:OD1	54:BU:94:GLU:N	2.52	0.42
1:AA:2806:U:O2'	2:AB:5:A:N3	2.40	0.41
7:AG:111:LEU:O	7:AG:115:MET:N	2.51	0.41
21:AW:95:ARG:NH1	21:AW:114:THR:OG1	2.53	0.41
34:BA:899:A:H62	34:BA:1181:U:H3	1.66	0.41
1:AA:2246:U:O2	22:AX:104:GLN:NE2	2.50	0.41
46:BM:132:ARG:O	46:BM:136:HIS:ND1	2.53	0.41
1:AA:1115:G:O2'	1:AA:1117:G:OP2	2.38	0.41
1:AA:1764:A:OP1	15:AP:216:LYS:NZ	2.50	0.41
4:AD:92:VAL:HG23	4:AD:292:LEU:HD21	2.02	0.41
37:BD:180:ASP:OD1	37:BD:181:SER:N	2.53	0.41
1:AA:1345:G:O2'	1:AA:1347:U:OP2	2.33	0.41
1:AA:2707:A:OP1	13:AN:27:ARG:NH1	2.53	0.41
1:AA:2766:A:O2'	7:AG:103:GLN:O	2.22	0.41
1:AA:1267:A:OP1	11:AL:92:ARG:NH2	2.53	0.41
34:BA:650:U:OP1	34:BA:651:A:O2'	2.19	0.41
39:BF:106:VAL:O	39:BF:106:VAL:HG12	2.19	0.41
34:BA:777:A:OP1	41:BH:19:ASN:ND2	2.53	0.41
1:AA:920:A:N6	12:AM:11:LYS:O	2.53	0.41
34:BA:702:A:OP1	48:BO:66:TYR:OH	2.39	0.41
1:AA:38:C:O2	5:AE:97:ARG:NH2	2.47	0.41
1:AA:1187:G:H21	17:AR:131:SER:HB2	1.85	0.41
34:BA:1325:A:O3'	40:BG:29:ARG:NH2	2.54	0.41
17:AR:197:VAL:N	17:AR:210:ILE:O	2.51	0.41
34:BA:903:G:O6	46:BM:148:LYS:NZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:908:A:OP1	52:BS:55:ARG:NH2	2.51	0.41
4:AD:288:ASN:OD1	4:AD:289:LEU:N	2.54	0.41
20:AU:60:ASN:O	20:AU:61:SER:OG	2.30	0.41
34:BA:1177:C:OP2	46:BM:155:LYS:NZ	2.54	0.41
34:BA:382:G:OP2	37:BD:24:LYS:NZ	2.42	0.41
38:BE:248:ILE:HD11	38:BE:266:LEU:HB2	2.03	0.41
50:BQ:123:THR:HG22	50:BQ:123:THR:O	2.21	0.41
34:BA:209:C:P	50:BQ:95:LYS:HZ2	2.44	0.41
1:AA:2433:C:O3'	11:AL:144:ARG:NH1	2.53	0.41
20:AU:165:THR:OG1	20:AU:167:GLU:OE1	2.29	0.41
1:AA:318:A:N3	1:AA:338:G:O2'	2.51	0.40
1:AA:453:U:O2	5:AE:97:ARG:NH1	2.54	0.40
16:AQ:96:ILE:HG22	16:AQ:100:ILE:HD12	2.04	0.40
20:AU:119:GLU:N	20:AU:119:GLU:OE1	2.54	0.40
38:BE:274:ASN:O	38:BE:278:ASN:ND2	2.53	0.40
43:BJ:112:GLU:OE2	43:BJ:165:ARG:NH2	2.53	0.40
1:AA:2653:U:O2'	4:AD:134:TYR:OH	2.38	0.40
1:AA:980:G:OP1	12:AM:16:ARG:NH2	2.54	0.40
1:AA:2279:U:OP2	21:AW:72:SER:OG	2.31	0.40
1:AA:582:A:OP2	17:AR:202:LYS:NZ	2.51	0.40
9:AJ:51:THR:O	9:AJ:51:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	244/246 (99%)	232 (95%)	12 (5%)	0	100	100
4	AD	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
5	AE	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
6	AF	167/207 (81%)	162 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
8	AH	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
9	AJ	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
10	AK	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
11	AL	182/184 (99%)	174 (96%)	8 (4%)	0	100	100
12	AM	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
13	AN	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
14	AO	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
15	AP	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
16	AQ	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	AR	163/165 (99%)	150 (92%)	13 (8%)	0	100	100
18	AS	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
19	AT	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
20	AU	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
21	AW	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
22	AX	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
23	AY	97/99 (98%)	97 (100%)	0	0	100	100
24	AZ	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
25	Aa	46/48 (96%)	46 (100%)	0	0	100	100
26	Ab	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
27	Ac	59/61 (97%)	59 (100%)	0	0	100	100
28	Ad	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
29	Ae	35/37 (95%)	35 (100%)	0	0	100	100
30	Af	45/47 (96%)	40 (89%)	5 (11%)	0	100	100
31	Aw	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
33	Az	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
35	BB	207/215 (96%)	187 (90%)	20 (10%)	0	100	100
36	BC	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
37	BD	197/200 (98%)	185 (94%)	12 (6%)	0	100	100
38	BE	156/158 (99%)	152 (97%)	4 (3%)	0	100	100
39	BF	111/113 (98%)	109 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BG	149/151 (99%)	143 (96%)	6 (4%)	0	100	100
41	BH	120/134 (90%)	117 (98%)	3 (2%)	0	100	100
42	BI	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
43	BJ	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
44	BK	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
45	BL	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
46	BM	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
47	BN	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
48	BO	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
49	BP	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
50	BQ	82/84 (98%)	73 (89%)	9 (11%)	0	100	100
51	BR	51/53 (96%)	51 (100%)	0	0	100	100
52	BS	79/81 (98%)	69 (87%)	10 (13%)	0	100	100
53	BT	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
54	BU	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
55	BV	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
56	BW	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	6070/6232 (97%)	5809 (96%)	261 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	
3	AC	194/194 (100%)	192 (99%)	2 (1%)	78	93
4	AD	182/182 (100%)	180 (99%)	2 (1%)	76	92
5	AE	179/179 (100%)	177 (99%)	2 (1%)	76	92
6	AF	146/176 (83%)	145 (99%)	1 (1%)	85	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	AG	146/146 (100%)	143 (98%)	3 (2%)	56 85
8	AH	40/40 (100%)	40 (100%)	0	100 100
9	AJ	173/173 (100%)	173 (100%)	0	100 100
10	AK	100/101 (99%)	98 (98%)	2 (2%)	58 86
11	AL	141/141 (100%)	139 (99%)	2 (1%)	69 90
12	AM	108/108 (100%)	106 (98%)	2 (2%)	60 87
13	AN	96/96 (100%)	94 (98%)	2 (2%)	56 85
14	AO	99/99 (100%)	97 (98%)	2 (2%)	58 86
15	AP	104/104 (100%)	102 (98%)	2 (2%)	60 87
16	AQ	102/102 (100%)	101 (99%)	1 (1%)	78 93
17	AR	147/147 (100%)	147 (100%)	0	100 100
18	AS	151/151 (100%)	151 (100%)	0	100 100
19	AT	81/81 (100%)	81 (100%)	0	100 100
20	AU	114/114 (100%)	112 (98%)	2 (2%)	62 87
21	AW	94/94 (100%)	94 (100%)	0	100 100
22	AX	66/66 (100%)	65 (98%)	1 (2%)	67 89
23	AY	92/92 (100%)	92 (100%)	0	100 100
24	AZ	57/57 (100%)	57 (100%)	0	100 100
25	Aa	41/41 (100%)	41 (100%)	0	100 100
26	Ab	56/56 (100%)	56 (100%)	0	100 100
27	Ac	50/50 (100%)	50 (100%)	0	100 100
28	Ad	62/62 (100%)	61 (98%)	1 (2%)	65 89
29	Ae	34/34 (100%)	34 (100%)	0	100 100
30	Af	41/41 (100%)	40 (98%)	1 (2%)	52 83
31	Aw	46/46 (100%)	46 (100%)	0	100 100
33	Az	175/175 (100%)	175 (100%)	0	100 100
35	BB	177/183 (97%)	176 (99%)	1 (1%)	87 96
36	BC	187/187 (100%)	185 (99%)	2 (1%)	76 92
37	BD	178/179 (99%)	175 (98%)	3 (2%)	63 88
38	BE	121/121 (100%)	120 (99%)	1 (1%)	83 94
39	BF	100/100 (100%)	98 (98%)	2 (2%)	58 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	BG	122/122 (100%)	122 (100%)	0	100 100
41	BH	109/117 (93%)	109 (100%)	0	100 100
42	BI	111/111 (100%)	108 (97%)	3 (3%)	48 81
43	BJ	90/90 (100%)	89 (99%)	1 (1%)	76 92
44	BK	86/86 (100%)	86 (100%)	0	100 100
45	BL	105/105 (100%)	104 (99%)	1 (1%)	78 93
46	BM	100/100 (100%)	99 (99%)	1 (1%)	78 93
47	BN	89/89 (100%)	89 (100%)	0	100 100
48	BO	67/67 (100%)	65 (97%)	2 (3%)	44 79
49	BP	72/72 (100%)	70 (97%)	2 (3%)	47 80
50	BQ	75/75 (100%)	73 (97%)	2 (3%)	48 81
51	BR	50/50 (100%)	47 (94%)	3 (6%)	21 57
52	BS	70/70 (100%)	69 (99%)	1 (1%)	69 90
53	BT	84/84 (100%)	83 (99%)	1 (1%)	74 92
54	BU	54/54 (100%)	53 (98%)	1 (2%)	60 87
55	BV	96/96 (100%)	95 (99%)	1 (1%)	78 93
56	BW	28/28 (100%)	28 (100%)	0	100 100
All	All	5288/5334 (99%)	5232 (99%)	56 (1%)	77 92

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	33	ARG
3	AC	84	ASN
4	AD	121	ASN
4	AD	304	LYS
5	AE	81	ARG
5	AE	232	ARG
6	AF	193	ARG
7	AG	45	LYS
7	AG	164	LYS
7	AG	189	ARG
10	AK	31	ARG
10	AK	78	ARG
11	AL	115	ARG
11	AL	195	ARG

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Mol	Chain	Res	Type
12	AM	1	MET
12	AM	5	LYS
13	AN	12	LYS
13	AN	114	ARG
14	AO	77	ARG
14	AO	108	ASN
15	AP	172	ARG
15	AP	185	ARG
16	AQ	104	ASN
20	AU	51	ARG
20	AU	115	LYS
22	AX	146	ARG
28	Ad	112	ARG
30	Af	54	LYS
35	BB	123	MET
36	BC	52	LYS
36	BC	109	LYS
37	BD	8	ARG
37	BD	40	LYS
37	BD	93	ASN
38	BE	290	ARG
39	BF	80	ARG
39	BF	164	ARG
42	BI	77	ARG
42	BI	78	ARG
42	BI	173	ARG
43	BJ	98	LYS
45	BL	123	LYS
46	BM	158	LYS
48	BO	60	ARG
48	BO	88	LYS
49	BP	5	ARG
49	BP	81	ARG
50	BQ	80	ARG
50	BQ	118	ARG
51	BR	27	ARG
51	BR	33	MET
51	BR	49	ARG
52	BS	28	LYS
53	BT	85	LYS
54	BU	101	ASN
55	BV	110	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
16	AQ	104	ASN
50	BQ	135	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2691/2810 (95%)	284 (10%)	5 (0%)
2	AB	105/106 (99%)	11 (10%)	0
32	Ax	117/118 (99%)	8 (6%)	0
34	BA	1480/1481 (99%)	146 (9%)	3 (0%)
All	All	4393/4515 (97%)	449 (10%)	8 (0%)

All (449) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	33	A
1	AA	45	A
1	AA	62	A
1	AA	70	A
1	AA	73	U
1	AA	74	G
1	AA	84	G
1	AA	90	A
1	AA	101	A
1	AA	116	A
1	AA	118	U
1	AA	144	A
1	AA	158	C
1	AA	159	A
1	AA	166	A
1	AA	181	A
1	AA	184	A
1	AA	200	G
1	AA	201	A
1	AA	207	A
1	AA	233	G
1	AA	251	G
1	AA	275	U
1	AA	276	G
1	AA	281	A

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Mol	Chain	Res	Type
1	AA	284	A
1	AA	285	A
1	AA	286	U
1	AA	287	A
1	AA	292	C
1	AA	294	U
1	AA	296	G
1	AA	297	U
1	AA	316	G
1	AA	320	U
1	AA	340	A
1	AA	365	A
1	AA	369	U
1	AA	371	U
1	AA	372	G
1	AA	373	C
1	AA	377	G
1	AA	378	A
1	AA	398	G
1	AA	423	G
1	AA	424	A
1	AA	448	C
1	AA	467	G
1	AA	493	G
1	AA	516	A
1	AA	519	A
1	AA	539	A
1	AA	541	G
1	AA	542	C
1	AA	543	A
1	AA	544	G
1	AA	557	C
1	AA	558	A
1	AA	559	G
1	AA	573	G
1	AA	582	A
1	AA	583	G
1	AA	584	A
1	AA	585	A
1	AA	613	U
1	AA	621	G
1	AA	623	A

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Mol	Chain	Res	Type
1	AA	633	A
1	AA	649	A
1	AA	657	U
1	AA	658	A
1	AA	665	U
1	AA	667	G
1	AA	680	G
1	AA	697	U
1	AA	701	U
1	AA	722	G
1	AA	741	U
1	AA	758	U
1	AA	786	G
1	AA	793	A
1	AA	795	U
1	AA	796	G
1	AA	803	G
1	AA	811	A
1	AA	816	G
1	AA	823	C
1	AA	838	U
1	AA	869	G
1	AA	876	A
1	AA	887	G
1	AA	889	G
1	AA	890	G
1	AA	894	G
1	AA	895	C
1	AA	906	C
1	AA	908	A
1	AA	910	A
1	AA	916	G
1	AA	919	A
1	AA	944	C
1	AA	947	A
1	AA	951	C
1	AA	952	A
1	AA	965	G
1	AA	974	G
1	AA	989	G
1	AA	990	C
1	AA	1002	G

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Mol	Chain	Res	Type
1	AA	1011	A
1	AA	1024	A
1	AA	1039	A
1	AA	1040	U
1	AA	1041	G
1	AA	1055	A
1	AA	1065	G
1	AA	1073	G
1	AA	1074	A
1	AA	1076	A
1	AA	1085	A
1	AA	1088	U
1	AA	1098	A
1	AA	1099	G
1	AA	1114	A
1	AA	1116	A
1	AA	1117	G
1	AA	1125	U
1	AA	1138	G
1	AA	1139	A
1	AA	1140	G
1	AA	1157	A
1	AA	1160	A
1	AA	1162	C
1	AA	1163	G
1	AA	1169	A
1	AA	1198	A
1	AA	1201	A
1	AA	1257	G
1	AA	1274	A
1	AA	1277	G
1	AA	1287	G
1	AA	1292	G
1	AA	1293	C
1	AA	1321	A
1	AA	1322	A
1	AA	1342	A
1	AA	1350	U
1	AA	1381	G
1	AA	1386	A
1	AA	1389	G
1	AA	1399	A

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Mol	Chain	Res	Type
1	AA	1400	U
1	AA	1405	A
1	AA	1433	U
1	AA	1436	U
1	AA	1437	G
1	AA	1449	C
1	AA	1472	A
1	AA	1474	A
1	AA	1480	A
1	AA	1496	A
1	AA	1501	G
1	AA	1502	A
1	AA	1504	C
1	AA	1505	C
1	AA	1519	A
1	AA	1532	G
1	AA	1533	A
1	AA	1544	A
1	AA	1556	A
1	AA	1558	U
1	AA	1569	A
1	AA	1572	G
1	AA	1603	A
1	AA	1612	A
1	AA	1621	C
1	AA	1622	A
1	AA	1634	C
1	AA	1644	A
1	AA	1683	G
1	AA	1684	C
1	AA	1710	G
1	AA	1750	C
1	AA	1751	A
1	AA	1752	C
1	AA	1753	A
1	AA	1754	A
1	AA	1774	G
1	AA	1783	A
1	AA	1810	C
1	AA	1811	A
1	AA	1826	U
1	AA	1839	A

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Mol	Chain	Res	Type
1	AA	1868	A
1	AA	1869	G
1	AA	1895	G
1	AA	1920	G
1	AA	1928	C
1	AA	1943	G
1	AA	1944	G
1	AA	1952	A
1	AA	1969	U
1	AA	1977	C
1	AA	1981	C
1	AA	1984	A
1	AA	1985	A
1	AA	1986	G
1	AA	2005	U
1	AA	2007	U
1	AA	2011	G
1	AA	2034	C
1	AA	2037	G
1	AA	2046	G
1	AA	2047	A
1	AA	2057	C
1	AA	2069	C
1	AA	2070	A
1	AA	2074	A
1	AA	2075	G
1	AA	2076	A
1	AA	2083	G
1	AA	2107	G
1	AA	2212	A
1	AA	2229	U
1	AA	2242	A
1	AA	2255	G
1	AA	2256	A
1	AA	2296	G
1	AA	2300	U
1	AA	2304	A
1	AA	2305	A
1	AA	2322	A
1	AA	2326	A
1	AA	2339	A
1	AA	2344	A

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Mol	Chain	Res	Type
1	AA	2352	A
1	AA	2362	G
1	AA	2364	C
1	AA	2367	C
1	AA	2375	A
1	AA	2378	C
1	AA	2400	G
1	AA	2402	C
1	AA	2419	G
1	AA	2436	U
1	AA	2442	A
1	AA	2443	A
1	AA	2445	G
1	AA	2446	G
1	AA	2447	A
1	AA	2452	A
1	AA	2458	U
1	AA	2465	A
1	AA	2492	C
1	AA	2493	A
1	AA	2495	A
1	AA	2501	G
1	AA	2508	U
1	AA	2522	G
1	AA	2530	U
1	AA	2537	C
1	AA	2546	G
1	AA	2552	U
1	AA	2571	U
1	AA	2583	A
1	AA	2584	G
1	AA	2590	C
1	AA	2595	G
1	AA	2599	G
1	AA	2619	A
1	AA	2620	G
1	AA	2630	U
1	AA	2646	U
1	AA	2649	A
1	AA	2679	A
1	AA	2706	U
1	AA	2729	A

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Mol	Chain	Res	Type
1	AA	2730	A
1	AA	2732	G
1	AA	2762	G
1	AA	2775	A
1	AA	2776	A
1	AA	2783	A
1	AA	2796	A
2	AB	5	A
2	AB	16	G
2	AB	29	U
2	AB	30	A
2	AB	33	A
2	AB	34	U
2	AB	77	A
2	AB	83	C
2	AB	84	C
2	AB	90	G
2	AB	97	A
32	Ax	9	G
32	Ax	24	G
32	Ax	36	U
32	Ax	44	G
32	Ax	45	A
32	Ax	56	U
32	Ax	64	A
32	Ax	110	G
34	BA	11	G
34	BA	21	C
34	BA	34	A
34	BA	41	G
34	BA	49	C
34	BA	50	U
34	BA	53	A
34	BA	78	G
34	BA	86	A
34	BA	93	G
34	BA	106	C
34	BA	116	C
34	BA	129	G
34	BA	136	A
34	BA	149	G
34	BA	179	A

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Mol	Chain	Res	Type
34	BA	181	A
34	BA	186	G
34	BA	187	A
34	BA	188	A
34	BA	189	U
34	BA	190	C
34	BA	217	U
34	BA	219	G
34	BA	223	G
34	BA	231	G
34	BA	238	G
34	BA	239	C
34	BA	253	G
34	BA	261	G
34	BA	300	C
34	BA	301	A
34	BA	317	C
34	BA	324	C
34	BA	326	G
34	BA	339	U
34	BA	344	C
34	BA	345	A
34	BA	378	G
34	BA	401	U
34	BA	425	G
34	BA	446	U
34	BA	454	G
34	BA	457	U
34	BA	460	C
34	BA	467	C
34	BA	476	G
34	BA	482	A
34	BA	496	A
34	BA	508	A
34	BA	513	U
34	BA	521	A
34	BA	522	A
34	BA	525	C
34	BA	526	G
34	BA	545	A
34	BA	578	A
34	BA	600	C

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Mol	Chain	Res	Type
34	BA	602	G
34	BA	608	C
34	BA	631	G
34	BA	667	A
34	BA	671	A
34	BA	685	C
34	BA	701	G
34	BA	704	A
34	BA	708	A
34	BA	726	A
34	BA	729	G
34	BA	742	U
34	BA	743	A
34	BA	758	G
34	BA	764	A
34	BA	766	C
34	BA	777	A
34	BA	782	C
34	BA	791	U
34	BA	792	C
34	BA	803	G
34	BA	864	A
34	BA	876	G
34	BA	884	C
34	BA	885	A
34	BA	899	A
34	BA	910	U
34	BA	919	A
34	BA	925	A
34	BA	926	G
34	BA	942	U
34	BA	943	G
34	BA	954	A
34	BA	959	U
34	BA	981	C
34	BA	982	G
34	BA	995	C
34	BA	1003	G
34	BA	1015	U
34	BA	1044	G
34	BA	1045	U
34	BA	1051	A

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Mol	Chain	Res	Type
34	BA	1085	U
34	BA	1101	A
34	BA	1108	U
34	BA	1109	G
34	BA	1116	A
34	BA	1124	G
34	BA	1145	A
34	BA	1146	A
34	BA	1161	U
34	BA	1162	A
34	BA	1175	C
34	BA	1176	A
34	BA	1197	A
34	BA	1203	G
34	BA	1205	U
34	BA	1207	G
34	BA	1234	A
34	BA	1236	A
34	BA	1246	U
34	BA	1249	G
34	BA	1251	U
34	BA	1269	C
34	BA	1271	C
34	BA	1272	G
34	BA	1277	C
34	BA	1287	G
34	BA	1295	A
34	BA	1296	G
34	BA	1302	G
34	BA	1313	A
34	BA	1314	U
34	BA	1344	A
34	BA	1348	A
34	BA	1369	G
34	BA	1391	A
34	BA	1396	A
34	BA	1401	C
34	BA	1402	A
34	BA	1404	G
34	BA	1443	A
34	BA	1444	G
34	BA	1453	A

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Mol	Chain	Res	Type
34	BA	1456	U
34	BA	1467	G
34	BA	1479	G
34	BA	1480	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	795	U
1	AA	1200	A
1	AA	1399	A
1	AA	1500	U
1	AA	1927	A
34	BA	700	U
34	BA	707	G
34	BA	1174	A

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 345 ligands modelled in this entry, 345 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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
57	BY	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BY	1068:UNK	C	1101:UNK	N	65.42
1	BY	1143:UNK	C	1201:UNK	N	12.57