

Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 21, 2017 – 07:31 PM EST

PDB ID : 5MMJ
EMDB ID: : EMD-3532
Title : Structure of the small subunit of the chloroplast ribosome
Authors : Bieri, P.; Leibundgut, M.; Saurer, M.; Boehringer, D.; Ban, N.
Deposited on : 2016-12-10
Resolution : 3.65 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

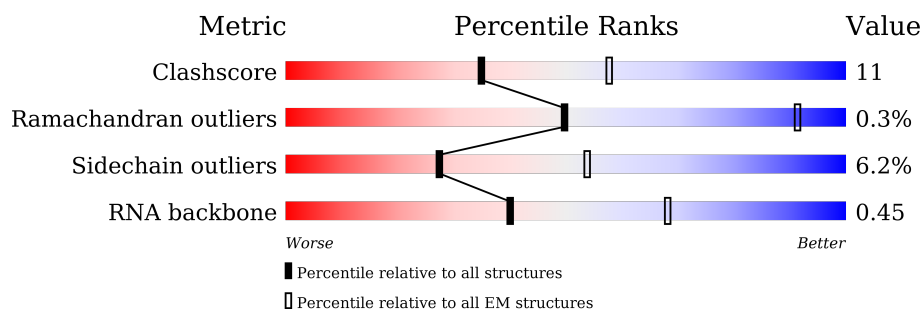
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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.



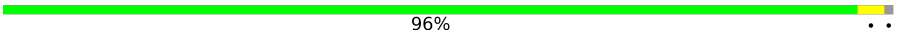




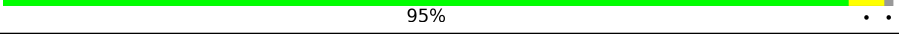


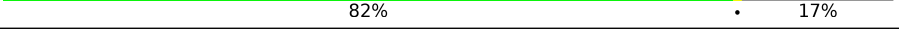

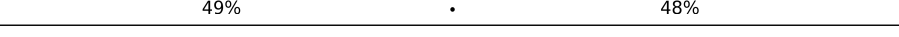
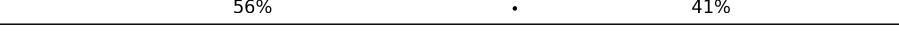

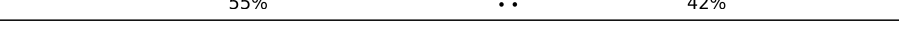


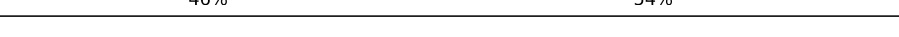

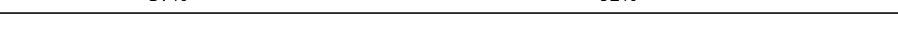
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	130	8% 92%
2	8	174	99% .
3	a	1491	71% 27% .
4	b	236	92% 7% .
5	c	218	92% 7% .
6	d	201	93% 6% .
7	e	308	58% . 39%
8	f	211	51% . 46%

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Mol	Chain	Length	Quality of chain
9	g	155	 96% . .
10	h	134	 92% 7% .
11	i	208	 62% 8% 31%
12	j	195	 47% . 49%
13	k	138	 79% 6% 15%
14	l	123	 95% . .
15	m	172	 59% 5% 36%
16	n	100	 88% 11% .
17	o	90	 82% . 17%
18	p	88	 85% 6% 9%
19	q	165	 49% . 48%
20	r	101	 56% . 41%
21	s	92	 82% . 15%
22	t	183	 55% . . 42%
23	u	180	 33% . 64%
24	v	260	 31% 69%
25	w	179	 46% 54%
26	x	101	 39% . 60%
27	y	302	 37% . 62%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 55315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	11	Total	C	N	O	0	0
			98	63	18	17		

- Molecule 2 is a protein called plastid ribosomal protein bS1c.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	8	174	Total	C	N	O	0	0
			870	522	174	174		

- Molecule 3 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	1484	Total	C	N	O	P	0	0
			31868	14208	5881	10295	1484		

- Molecule 4 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	233	Total	C	N	O	S	0	0
			1844	1163	339	329	13		

- Molecule 5 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	216	Total	C	N	O	S	0	0
			1736	1108	313	309	6		

- Molecule 6 is a protein called 30S ribosomal protein S4, chloroplastic.

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

- Molecule 7 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	187	Total	C	N	O	S	0	0
			1331	826	259	240	6		

- Molecule 8 is a protein called plastid ribosomal protein bS6c.

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

- Molecule 9 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	154	Total	C	N	O	S	0	0
			1210	753	244	210	3		

- Molecule 10 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	h	133	Total	C	N	O	S	0	0
			1079	679	210	185	5		

- Molecule 11 is a protein called plastid ribosomal protein uS9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	144	Total	C	N	O	S	0	0
			1119	712	211	195	1		

- Molecule 12 is a protein called plastid ribosomal protein uS10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	j	99	Total	C	N	O	S	0	0
			805	517	144	139	5		

- Molecule 13 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	k	117	Total	C	N	O	S	0	0
			882	546	181	150	5		

- Molecule 14 is a protein called 30S ribosomal protein S12, chloroplastic.

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

- Molecule 15 is a protein called plastid ribosomal protein uS13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	110	Total	C	N	O	S	0	0
			904	556	182	161	5		

- Molecule 16 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	99	Total	C	N	O	S	0	0
			820	507	174	136	3		

- Molecule 17 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	75	Total	C	N	O	S	0	0
			635	404	123	107	1		

- Molecule 18 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	80	Total	C	N	O	S	0	0
			664	425	123	114	2		

- Molecule 19 is a protein called plastid ribosomal protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	86	Total	C	N	O	S	0	0
			693	434	136	119	4		

- Molecule 20 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	r	60	Total	C	N	O	S	0	0
			490	308	96	85	1		

- Molecule 21 is a protein called 30S ribosomal protein S19 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	78	Total	C	N	O	S	0	0
			631	406	119	104	2		

- Molecule 22 is a protein called plastid ribosomal protein bS20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	t	107	Total	C	N	O	S	0	0
			853	528	173	151	1		

- Molecule 23 is a protein called plastid ribosomal protein bS21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	u	65	Total	C	N	O	S	0	0
			568	339	127	100	2		

- Molecule 24 is a protein called 30S ribosomal protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	80	Total	C	N	O		0	0
			613	388	104	121			

- Molecule 25 is a protein called 30S ribosomal protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	w	82	Total	C	N	O	S	0	0
			686	454	113	116	3		

- Molecule 26 is a protein called 30S ribosomal protein S31, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	40	Total	C	N	O		0	0
			309	192	69	48			

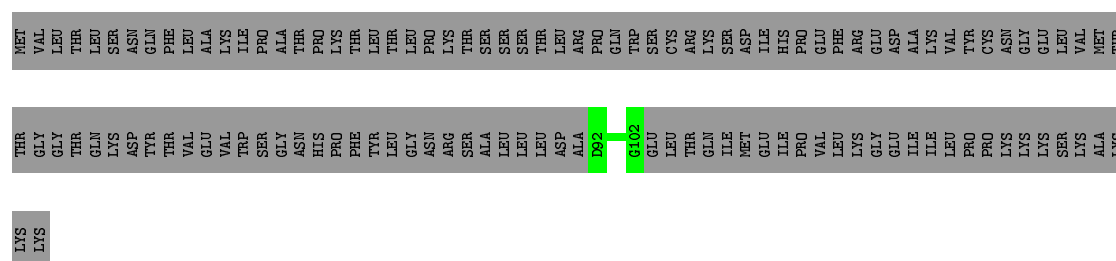
- Molecule 27 is a protein called Ribosome-binding factor PSRP1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	116	Total	C	N	O	S	0	0
			919	567	181	169	2		

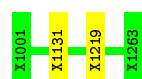
- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	x	1	Total 1	Mg 1	0
28	a	182	Total 182	Mg 182	0
28	l	1	Total 1	Mg 1	0
28	k	1	Total 1	Mg 1	0

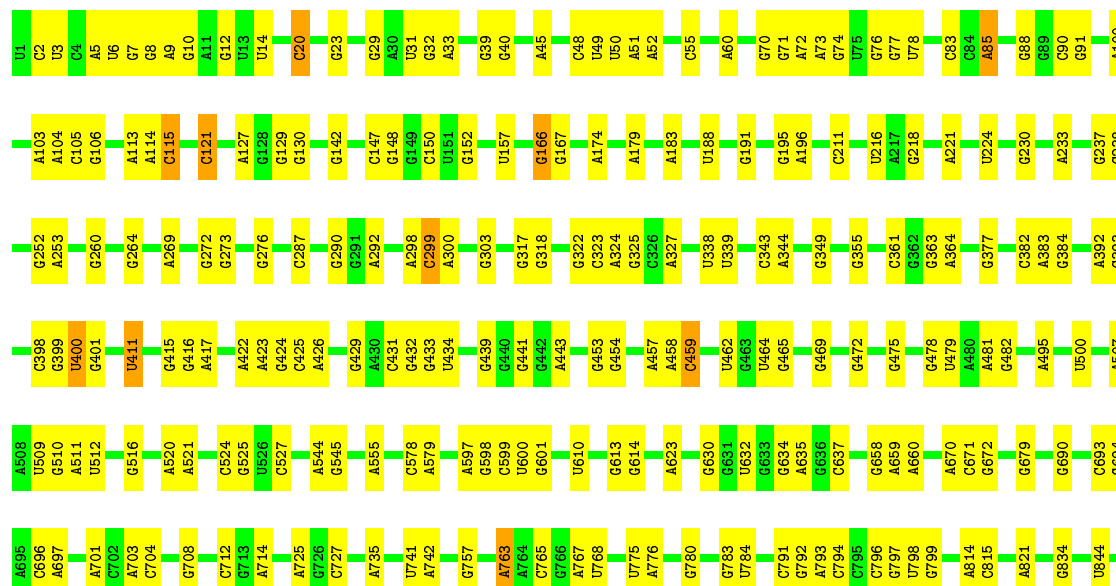
- Molecule 1: 50S ribosomal protein L31



- Chain 8:  99%



- Chain a: 71% 27%

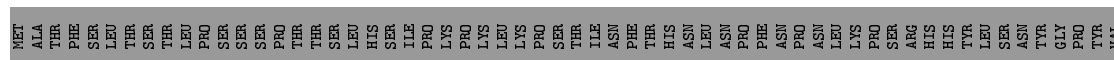






- Molecule 8: plastid ribosomal protein bS6c

Chain f: 51% 46%



- Molecule 9: 30S ribosomal protein S7, chloroplastic

Chain g: 96%



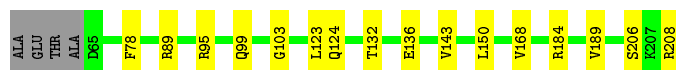
- Molecule 10: 30S ribosomal protein S8, chloroplastic

Chain h: 92% 7%



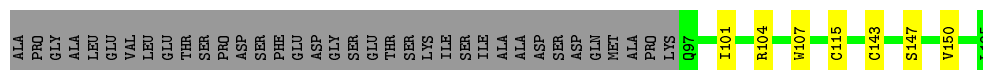
- Molecule 11: plastid ribosomal protein uS9c

Chain i: 62% 8% 31%



- Molecule 12: plastid ribosomal protein uS10c

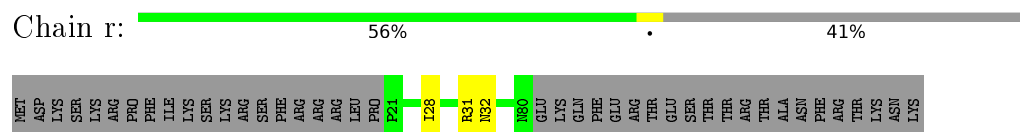
Chain j: 47% 49%



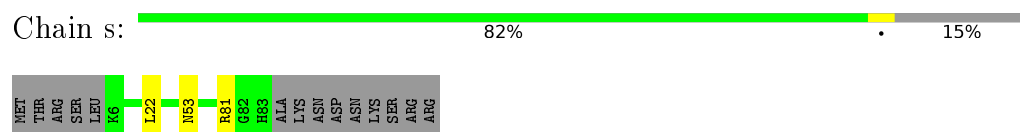
- Molecule 13: 30S ribosomal protein S11, chloroplastic

Chain k: 79% 6% 15%

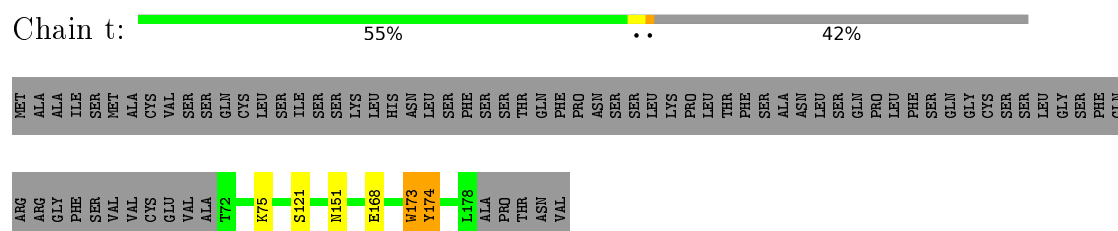
- Molecule 20: 30S ribosomal protein S18, chloroplatic



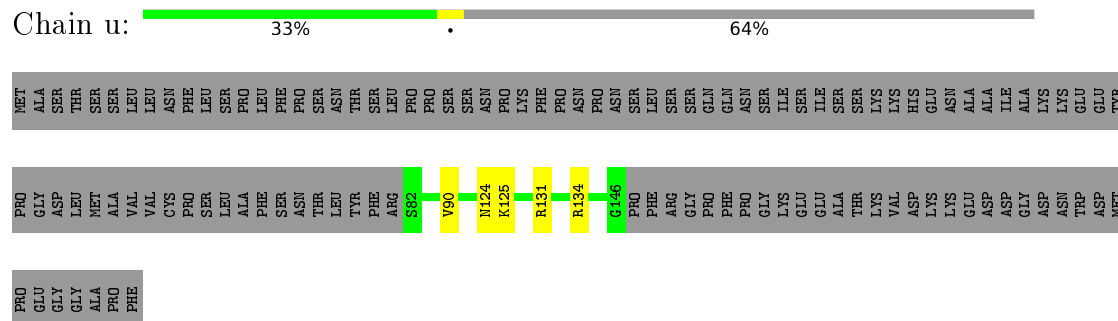
- Molecule 21: 30S ribosomal protein S19 alpha, chloroplatic



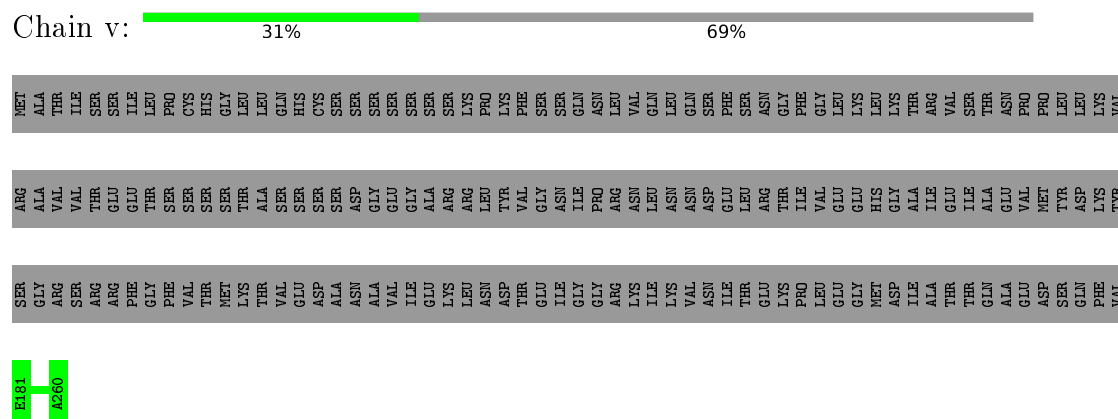
- Molecule 22: plastid ribosomal protein bS20c



- Molecule 23: plastid ribosomal protein bS21c



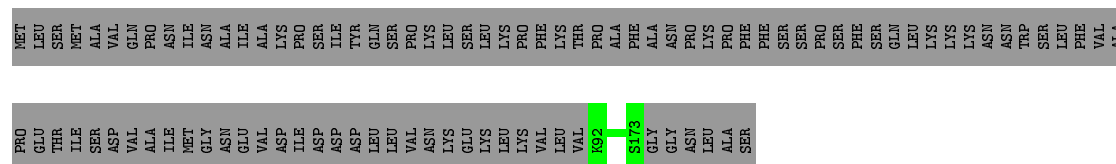
- Molecule 24: 30S ribosomal protein 2, chloroplatic



E1481
A260

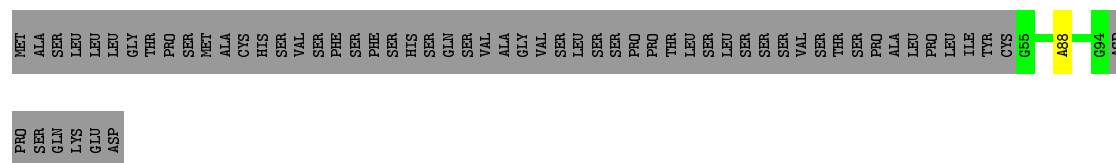
- Molecule 25: 30S ribosomal protein 3, chloroplastic

Chain w:  46% 54%



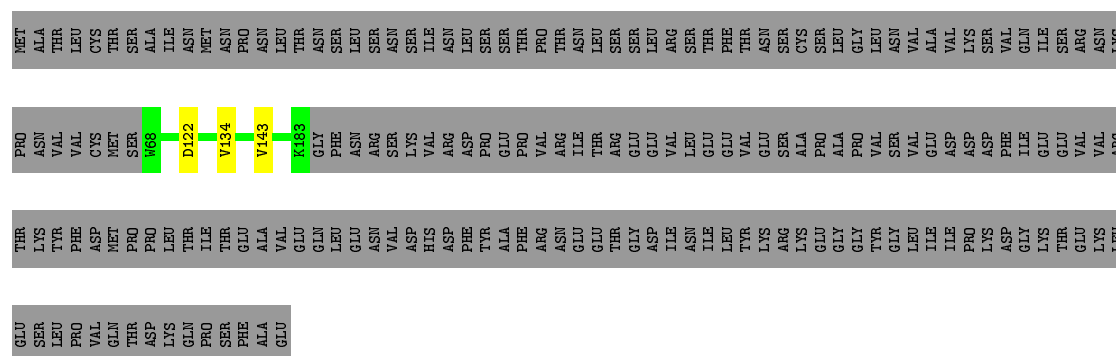
- Molecule 26: 30S ribosomal protein S31, chloroplastic

Chain x:  39% . 60%



- Molecule 27: Ribosome-binding factor PSRP1, chloroplastic

Chain y:  37% . 62%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	127031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0	0.34	0/99	0.47	0/128
10	h	0.48	0/1094	0.68	0/1467
11	i	0.52	0/1138	0.76	2/1526 (0.1%)
12	j	0.55	0/822	0.66	0/1111
13	k	0.43	0/896	0.64	0/1206
14	l	0.52	0/975	0.68	0/1312
15	m	0.46	0/912	0.67	0/1219
16	n	0.50	0/836	0.66	0/1116
17	o	0.40	0/642	0.53	0/852
18	p	0.46	0/674	0.70	0/902
19	q	0.44	0/707	0.62	0/949
20	r	0.45	0/494	0.67	0/660
21	s	0.51	0/646	0.77	0/870
22	t	0.49	0/862	0.68	0/1151
23	u	0.39	0/572	0.53	0/754
24	v	0.58	0/621	0.49	0/833
25	w	0.58	0/707	0.55	0/962
26	x	0.67	1/317 (0.3%)	0.80	0/418
27	y	0.45	0/930	0.65	0/1243
3	a	0.74	15/35687 (0.0%)	1.16	92/55680 (0.2%)
4	b	0.44	0/1878	0.60	0/2538
5	c	0.52	0/1763	0.70	1/2370 (0.0%)
6	d	0.46	0/1661	0.66	1/2230 (0.0%)
7	e	0.57	0/1345	0.70	0/1817
8	f	0.43	0/929	0.61	0/1255
9	g	0.39	0/1226	0.59	0/1641
All	All	0.66	16/58433 (0.0%)	1.01	96/86210 (0.1%)

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
22	t	0	2
4	b	0	1
5	c	0	1
7	e	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1152	A	C6-N6	-8.63	1.27	1.33
3	a	1006	G	N3-C4	-7.76	1.30	1.35
3	a	400	U	C4-C5	7.69	1.50	1.43
3	a	1152	A	N7-C5	-7.68	1.34	1.39
3	a	714	A	N9-C4	-7.31	1.33	1.37
3	a	400	U	N1-C2	7.15	1.45	1.38
3	a	868	A	N9-C4	-7.00	1.33	1.37
3	a	1152	A	N9-C4	-6.99	1.33	1.37
3	a	9	A	N9-C4	-6.11	1.34	1.37
26	x	88	ALA	CA-CB	5.85	1.64	1.52
3	a	1149	A	N9-C4	-5.63	1.34	1.37
3	a	1152	A	C5-C4	-5.57	1.34	1.38
3	a	815	C	N1-C6	-5.47	1.33	1.37
3	a	868	A	N3-C4	-5.17	1.31	1.34
3	a	1473	C	N1-C6	-5.10	1.34	1.37
3	a	1298	A	N9-C4	-5.00	1.34	1.37

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1152	A	C5-C6-N1	21.25	128.32	117.70
3	a	1152	A	C6-N1-C2	-20.10	106.54	118.60
3	a	1006	G	C5-C6-N1	-16.13	103.43	111.50
3	a	1152	A	N1-C2-N3	15.45	137.03	129.30
3	a	1006	G	N7-C8-N9	-15.28	105.46	113.10
3	a	1152	A	N1-C6-N6	-12.78	110.93	118.60
3	a	1006	G	N1-C6-O6	11.80	126.98	119.90
3	a	1148	C	C6-N1-C2	11.59	124.94	120.30
3	a	1152	A	C4-C5-C6	-10.96	111.52	117.00
3	a	1006	G	C5-N7-C8	10.18	109.39	104.30
3	a	1006	G	C8-N9-C4	9.86	110.34	106.40
3	a	1006	G	C6-N1-C2	9.60	130.86	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1152	A	C2-N3-C4	-9.60	105.80	110.60
3	a	1152	A	C5-N7-C8	-8.15	99.83	103.90
3	a	1006	G	C4-C5-C6	7.88	123.53	118.80
3	a	1152	A	C8-N9-C4	-7.59	102.76	105.80
3	a	1078	C	C5-C6-N1	7.18	124.59	121.00
3	a	1005	U	C6-N1-C2	6.92	125.15	121.00
3	a	704	C	C5-C6-N1	-6.92	117.54	121.00
3	a	1152	A	N7-C8-N9	6.85	117.22	113.80
3	a	1149	A	C8-N9-C4	6.71	108.49	105.80
3	a	290	G	C8-N9-C4	6.61	109.04	106.40
3	a	1006	G	C6-C5-N7	-6.56	126.47	130.40
3	a	871	G	C8-N9-C4	-6.56	103.78	106.40
3	a	1106	C	C6-N1-C2	-6.38	117.75	120.30
3	a	29	G	C8-N9-C4	-6.32	103.87	106.40
3	a	400	U	C5-C6-N1	-6.29	119.56	122.70
3	a	1106	C	N3-C2-O2	-6.23	117.54	121.90
3	a	12	G	C8-N9-C4	-6.17	103.93	106.40
3	a	299	C	C2-N1-C1'	6.13	125.55	118.80
3	a	1148	C	N3-C4-C5	6.11	124.34	121.90
3	a	1078	C	C6-N1-C2	-6.08	117.87	120.30
3	a	727	C	C6-N1-C2	-5.96	117.92	120.30
3	a	1106	C	C2-N1-C1'	5.94	125.34	118.80
3	a	1239	C	C6-N1-C2	5.91	122.67	120.30
3	a	856	A	C8-N9-C4	-5.88	103.45	105.80
3	a	1152	A	N3-C4-N9	-5.86	122.71	127.40
3	a	704	C	C6-N1-C2	5.81	122.62	120.30
3	a	1014	U	C5-C6-N1	-5.75	119.83	122.70
3	a	166	G	N3-C4-C5	-5.74	125.73	128.60
3	a	1454	G	N3-C4-C5	5.74	131.47	128.60
3	a	763	A	C8-N9-C4	5.74	108.09	105.80
3	a	516	G	N3-C4-C5	-5.71	125.74	128.60
3	a	115	C	C2-N1-C1'	5.70	125.07	118.80
3	a	1151	C	C6-N1-C2	-5.70	118.02	120.30
3	a	299	C	N1-C2-O2	5.70	122.32	118.90
3	a	1152	A	C4-C5-N7	5.67	113.53	110.70
3	a	1342	U	C6-N1-C2	5.65	124.39	121.00
3	a	1052	C	N3-C4-C5	5.64	124.16	121.90
5	c	27	LYS	CB-CG-CD	-5.63	96.96	111.60
3	a	1152	A	C8-N9-C1'	5.60	137.78	127.70
3	a	411	U	N1-C2-O2	5.59	126.72	122.80
3	a	85	A	N7-C8-N9	5.58	116.59	113.80
3	a	1469	G	N3-C4-C5	-5.58	125.81	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	91	G	C8-N9-C4	5.57	108.63	106.40
11	i	103	GLY	N-CA-C	-5.57	99.18	113.10
3	a	1152	A	N3-C4-C5	5.55	130.69	126.80
6	d	168	PRO	N-CA-C	5.52	126.46	112.10
3	a	276	G	N3-C4-C5	-5.50	125.85	128.60
3	a	509	U	C6-N1-C2	5.50	124.30	121.00
3	a	298	A	N1-C6-N6	-5.42	115.35	118.60
3	a	253	A	C8-N9-C4	-5.38	103.65	105.80
3	a	431	C	C6-N1-C2	5.37	122.45	120.30
3	a	632	U	C6-N1-C2	-5.36	117.78	121.00
3	a	871	G	N7-C8-N9	5.36	115.78	113.10
3	a	924	A	C8-N9-C4	5.35	107.94	105.80
3	a	1323	A	C8-N9-C4	-5.33	103.67	105.80
3	a	121	C	N1-C2-O2	5.33	122.10	118.90
3	a	166	G	C4-N9-C1'	5.31	133.40	126.50
3	a	1003	C	N3-C2-O2	-5.30	118.19	121.90
3	a	704	C	C2-N3-C4	-5.30	117.25	119.90
3	a	1043	G	O4'-C1'-N9	5.30	112.44	108.20
3	a	20	C	N1-C2-O2	-5.28	115.73	118.90
3	a	871	G	C4-N9-C1'	5.28	133.37	126.50
3	a	1325	U	C6-N1-C2	-5.25	117.85	121.00
3	a	299	C	N3-C2-O2	-5.24	118.23	121.90
3	a	578	C	C6-N1-C2	-5.24	118.20	120.30
3	a	459	C	C6-N1-C2	5.23	122.39	120.30
3	a	1291	G	C8-N9-C4	-5.22	104.31	106.40
3	a	929	C	C6-N1-C2	5.22	122.39	120.30
3	a	1279	G	O4'-C1'-N9	5.21	112.37	108.20
3	a	272	G	N1-C6-O6	-5.21	116.77	119.90
3	a	1479	G	C4-N9-C1'	-5.19	119.75	126.50
11	i	123	LEU	CB-CG-CD1	-5.19	102.17	111.00
3	a	999	G	C5'-C4'-O4'	5.19	115.33	109.10
3	a	1152	A	O5'-P-OP1	-5.18	101.04	105.70
3	a	1078	C	C2-N1-C1'	5.17	124.49	118.80
3	a	482	G	N3-C4-C5	5.13	131.16	128.60
3	a	1479	G	N3-C4-C5	5.12	131.16	128.60
3	a	966	G	C5-C6-O6	-5.10	125.54	128.60
3	a	298	A	N9-C4-C5	5.10	107.84	105.80
3	a	1311	C	C5-C6-N1	-5.09	118.45	121.00
3	a	880	C	C5-C6-N1	-5.08	118.46	121.00
3	a	1469	G	C8-N9-C4	-5.07	104.37	106.40
3	a	1297	A	C5-N7-C8	-5.07	101.37	103.90
3	a	712	C	C6-N1-C2	-5.05	118.28	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	b	74	VAL	Peptide
5	c	103	LEU	Peptide
7	e	144	LYS	Peptide
22	t	173	TRP	Peptide
22	t	75	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	0	98	0	99	0	0
2	8	870	0	184	1	0
3	a	31868	0	16048	0	0
4	b	1844	0	1887	0	0
5	c	1736	0	1819	0	0
6	d	1633	0	1730	0	0
7	e	1331	0	1312	0	0
8	f	911	0	923	0	0
9	g	1210	0	1284	0	0
10	h	1079	0	1137	0	0
11	i	1119	0	1181	0	0
12	j	805	0	849	0	0
13	k	882	0	928	0	0
14	l	959	0	1035	0	0
15	m	904	0	943	0	0
16	n	820	0	858	0	0
17	o	635	0	686	0	0
18	p	664	0	703	0	0
19	q	693	0	729	0	0
20	r	490	0	532	0	0
21	s	631	0	661	0	0
22	t	853	0	915	0	0
23	u	568	0	576	0	0
24	v	613	0	621	0	0
25	w	686	0	706	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	x	309	0	323	0	0
27	y	919	0	958	0	0
28	a	182	0	0	0	0
28	k	1	0	0	0	0
28	l	1	0	0	0	0
28	x	1	0	0	0	0
All	All	55315	0	39627	1	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 11.

All (1) 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)
2:8:1131:UNK:CB	2:8:1219:UNK:HA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	9/130 (7%)	8 (89%)	1 (11%)	0	100	100
4	b	231/236 (98%)	220 (95%)	11 (5%)	0	100	100
5	c	214/218 (98%)	200 (94%)	14 (6%)	0	100	100
6	d	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
7	e	185/308 (60%)	181 (98%)	4 (2%)	0	100	100
8	f	111/211 (53%)	106 (96%)	4 (4%)	1 (1%)	21	68
9	g	152/155 (98%)	146 (96%)	6 (4%)	0	100	100
10	h	131/134 (98%)	125 (95%)	4 (3%)	2 (2%)	13	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	i	142/208 (68%)	136 (96%)	6 (4%)	0	100	100
12	j	97/195 (50%)	92 (95%)	4 (4%)	1 (1%)	19	66
13	k	115/138 (83%)	107 (93%)	8 (7%)	0	100	100
14	l	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
15	m	108/172 (63%)	97 (90%)	10 (9%)	1 (1%)	21	68
16	n	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
17	o	73/90 (81%)	73 (100%)	0	0	100	100
18	p	78/88 (89%)	72 (92%)	6 (8%)	0	100	100
19	q	84/165 (51%)	78 (93%)	6 (7%)	0	100	100
20	r	58/101 (57%)	55 (95%)	3 (5%)	0	100	100
21	s	76/92 (83%)	74 (97%)	2 (3%)	0	100	100
22	t	105/183 (57%)	100 (95%)	4 (4%)	1 (1%)	19	66
23	u	63/180 (35%)	61 (97%)	2 (3%)	0	100	100
24	v	78/260 (30%)	76 (97%)	2 (3%)	0	100	100
25	w	80/179 (45%)	78 (98%)	2 (2%)	0	100	100
26	x	38/101 (38%)	37 (97%)	1 (3%)	0	100	100
27	y	114/302 (38%)	105 (92%)	8 (7%)	1 (1%)	21	68
All	All	2756/4270 (64%)	2614 (95%)	135 (5%)	7 (0%)	50	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	h	68	ASN
12	j	150	VAL
15	m	53	VAL
22	t	174	TYR
10	h	69	LYS
27	y	143	VAL
8	f	149	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	10/117 (8%)	10 (100%)	0	100	100
4	b	198/201 (98%)	182 (92%)	16 (8%)	15	54
5	c	186/188 (99%)	171 (92%)	15 (8%)	15	54
6	d	178/180 (99%)	167 (94%)	11 (6%)	23	65
7	e	121/255 (48%)	113 (93%)	8 (7%)	21	63
8	f	100/186 (54%)	96 (96%)	4 (4%)	38	76
9	g	125/126 (99%)	120 (96%)	5 (4%)	38	76
10	h	116/117 (99%)	108 (93%)	8 (7%)	19	61
11	i	114/169 (68%)	100 (88%)	14 (12%)	6	34
12	j	91/173 (53%)	85 (93%)	6 (7%)	21	63
13	k	91/109 (84%)	83 (91%)	8 (9%)	12	51
14	l	105/106 (99%)	100 (95%)	5 (5%)	31	72
15	m	99/151 (66%)	92 (93%)	7 (7%)	18	60
16	n	89/90 (99%)	78 (88%)	11 (12%)	6	34
17	o	70/85 (82%)	69 (99%)	1 (1%)	74	90
18	p	71/79 (90%)	66 (93%)	5 (7%)	19	61
19	q	77/149 (52%)	72 (94%)	5 (6%)	21	64
20	r	56/96 (58%)	53 (95%)	3 (5%)	27	69
21	s	68/81 (84%)	65 (96%)	3 (4%)	35	74
22	t	89/156 (57%)	84 (94%)	5 (6%)	26	68
23	u	59/160 (37%)	54 (92%)	5 (8%)	13	53
24	v	67/225 (30%)	67 (100%)	0	100	100
25	w	76/162 (47%)	76 (100%)	0	100	100
26	x	30/85 (35%)	30 (100%)	0	100	100
27	y	104/275 (38%)	102 (98%)	2 (2%)	65	87
All	All	2390/3721 (64%)	2243 (94%)	147 (6%)	27	65

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	b	7	ASN

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Mol	Chain	Res	Type
4	b	8	ILE
4	b	30	ARG
4	b	54	LEU
4	b	77	LYS
4	b	79	LYS
4	b	83	SER
4	b	114	ARG
4	b	119	ARG
4	b	121	LEU
4	b	163	ASP
4	b	175	THR
4	b	194	ASN
4	b	211	ILE
4	b	218	LEU
4	b	232	TYR
5	c	4	LYS
5	c	5	ILE
5	c	12	LEU
5	c	24	SER
5	c	50	ASN
5	c	58	GLU
5	c	72	ILE
5	c	83	LEU
5	c	103	LEU
5	c	105	CYS
5	c	107	ASN
5	c	116	ARG
5	c	196	CYS
5	c	202	THR
5	c	206	VAL
6	d	8	ARG
6	d	9	PHE
6	d	12	ILE
6	d	23	ASN
6	d	104	ILE
6	d	109	GLN
6	d	134	ASP
6	d	152	LEU
6	d	179	ILE
6	d	189	ASN
6	d	197	TYR
7	e	161	ARG

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Mol	Chain	Res	Type
7	e	167	LYS
7	e	187	VAL
7	e	197	VAL
7	e	210	ARG
7	e	266	LEU
7	e	270	LEU
7	e	288	THR
8	f	107	GLN
8	f	118	MET
8	f	124	LEU
8	f	183	GLU
9	g	6	THR
9	g	10	LYS
9	g	15	ASP
9	g	25	MET
9	g	72	ASP
10	h	31	ILE
10	h	45	ILE
10	h	46	GLU
10	h	60	VAL
10	h	76	THR
10	h	103	MET
10	h	105	ILE
10	h	125	ILE
11	i	78	PHE
11	i	89	ARG
11	i	95	ARG
11	i	99	GLN
11	i	124	GLN
11	i	132	THR
11	i	136	GLU
11	i	143	VAL
11	i	150	LEU
11	i	168	VAL
11	i	184	ARG
11	i	189	VAL
11	i	206	SER
11	i	208	ARG
12	j	101	ILE
12	j	104	ARG
12	j	107	TRP
12	j	115	CYS

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Mol	Chain	Res	Type
12	j	143	CYS
12	j	147	SER
13	k	42	THR
13	k	45	ASP
13	k	49	ARG
13	k	51	VAL
13	k	55	SER
13	k	102	ARG
13	k	114	ILE
13	k	122	VAL
14	l	11	THR
14	l	24	LEU
14	l	31	ARG
14	l	78	SER
14	l	101	THR
15	m	69	HIS
15	m	110	ILE
15	m	113	ASP
15	m	118	ASN
15	m	142	CYS
15	m	151	CYS
15	m	152	ARG
16	n	3	ARG
16	n	5	SER
16	n	24	ARG
16	n	35	THR
16	n	37	LEU
16	n	49	SER
16	n	54	SER
16	n	63	CYS
16	n	68	ARG
16	n	90	CYS
16	n	92	LEU
17	o	35	ARG
18	p	22	ILE
18	p	26	SER
18	p	28	ARG
18	p	33	LEU
18	p	66	THR
19	q	70	ASN
19	q	89	ARG
19	q	112	VAL

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Mol	Chain	Res	Type
19	q	120	ILE
19	q	142	LYS
20	r	28	ILE
20	r	31	ARG
20	r	32	ASN
21	s	22	LEU
21	s	53	ASN
21	s	81	ARG
22	t	121	SER
22	t	151	ASN
22	t	168	GLU
22	t	173	TRP
22	t	174	TYR
23	u	90	VAL
23	u	124	ASN
23	u	125	LYS
23	u	131	ARG
23	u	134	ARG
27	y	122	ASP
27	y	134	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
4	b	94	HIS
4	b	170	GLN
4	b	194	ASN
5	c	50	ASN
5	c	104	ASN
6	d	57	HIS
6	d	149	GLN
7	e	211	ASN
7	e	225	HIS
7	e	277	ASN
8	f	160	ASN
9	g	20	ASN
10	h	19	ASN
11	i	138	ASN
12	j	117	GLN
12	j	149	HIS
12	j	151	HIS
13	k	31	HIS

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Mol	Chain	Res	Type
13	k	127	HIS
14	l	111	GLN
15	m	52	ASN
15	m	58	ASN
15	m	87	ASN
16	n	48	GLN
16	n	60	HIS
16	n	81	HIS
19	q	84	HIS
19	q	98	GLN
20	r	23	GLN
20	r	79	ASN
21	s	8	ASN
21	s	47	HIS
21	s	69	HIS
22	t	163	ASN
22	t	170	HIS
24	v	258	ASN
25	w	162	GLN
25	w	168	ASN
27	y	89	ASN
27	y	93	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	a	1483/1491 (99%)	389 (26%)	0

All (389) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	a	2	C
3	a	3	U
3	a	5	A
3	a	6	U
3	a	7	G
3	a	8	G
3	a	10	G
3	a	14	U
3	a	20	C
3	a	23	G

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Mol	Chain	Res	Type
3	a	31	U
3	a	32	G
3	a	33	A
3	a	39	G
3	a	40	G
3	a	45	A
3	a	48	C
3	a	49	U
3	a	50	U
3	a	51	A
3	a	52	A
3	a	55	C
3	a	60	A
3	a	70	G
3	a	71	G
3	a	72	A
3	a	73	A
3	a	74	G
3	a	76	G
3	a	77	G
3	a	78	U
3	a	83	C
3	a	85	A
3	a	88	G
3	a	90	C
3	a	100	A
3	a	103	A
3	a	104	A
3	a	105	C
3	a	106	G
3	a	113	A
3	a	114	A
3	a	115	C
3	a	121	C
3	a	127	A
3	a	129	G
3	a	130	G
3	a	142	G
3	a	147	C
3	a	148	G
3	a	150	C
3	a	152	G

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Mol	Chain	Res	Type
3	a	157	U
3	a	166	G
3	a	167	G
3	a	174	A
3	a	179	A
3	a	183	A
3	a	188	U
3	a	191	G
3	a	195	G
3	a	196	A
3	a	211	C
3	a	216	U
3	a	218	G
3	a	221	A
3	a	224	U
3	a	230	G
3	a	233	A
3	a	237	G
3	a	238	C
3	a	252	G
3	a	260	G
3	a	264	G
3	a	269	A
3	a	273	G
3	a	287	C
3	a	292	A
3	a	299	C
3	a	300	A
3	a	303	G
3	a	317	G
3	a	318	G
3	a	322	G
3	a	323	C
3	a	324	A
3	a	325	G
3	a	327	A
3	a	338	U
3	a	339	U
3	a	343	C
3	a	344	A
3	a	349	G
3	a	355	G

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Mol	Chain	Res	Type
3	a	361	C
3	a	363	G
3	a	364	A
3	a	377	G
3	a	382	C
3	a	383	A
3	a	384	G
3	a	392	A
3	a	393	C
3	a	398	C
3	a	399	G
3	a	400	U
3	a	401	G
3	a	411	U
3	a	415	G
3	a	416	G
3	a	417	A
3	a	422	A
3	a	423	A
3	a	424	G
3	a	425	C
3	a	426	A
3	a	429	G
3	a	432	G
3	a	433	G
3	a	434	U
3	a	439	G
3	a	441	G
3	a	443	A
3	a	453	G
3	a	454	G
3	a	457	A
3	a	458	A
3	a	459	C
3	a	462	U
3	a	464	U
3	a	465	G
3	a	469	G
3	a	472	G
3	a	475	G
3	a	478	G
3	a	479	U

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Mol	Chain	Res	Type
3	a	481	A
3	a	495	A
3	a	500	U
3	a	507	A
3	a	510	G
3	a	511	A
3	a	512	U
3	a	520	A
3	a	521	A
3	a	524	C
3	a	525	G
3	a	527	C
3	a	544	A
3	a	545	G
3	a	555	A
3	a	579	A
3	a	597	A
3	a	598	G
3	a	599	C
3	a	600	U
3	a	601	G
3	a	610	U
3	a	613	G
3	a	614	G
3	a	623	A
3	a	630	G
3	a	634	G
3	a	635	A
3	a	637	C
3	a	658	G
3	a	659	A
3	a	660	A
3	a	670	A
3	a	671	C
3	a	672	G
3	a	679	G
3	a	690	G
3	a	693	C
3	a	694	G
3	a	696	C
3	a	697	A
3	a	701	A

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Mol	Chain	Res	Type
3	a	703	A
3	a	708	G
3	a	725	A
3	a	735	A
3	a	741	U
3	a	742	A
3	a	757	G
3	a	763	A
3	a	765	C
3	a	767	A
3	a	768	U
3	a	775	U
3	a	776	A
3	a	780	G
3	a	783	G
3	a	784	U
3	a	791	C
3	a	792	G
3	a	793	A
3	a	794	C
3	a	796	C
3	a	797	G
3	a	798	U
3	a	799	G
3	a	814	A
3	a	821	A
3	a	834	G
3	a	844	U
3	a	849	A
3	a	851	G
3	a	863	A
3	a	875	G
3	a	876	G
3	a	883	C
3	a	885	C
3	a	886	A
3	a	891	G
3	a	909	U
3	a	915	G
3	a	918	A
3	a	921	C
3	a	923	A

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Mol	Chain	Res	Type
3	a	924	A
3	a	925	G
3	a	926	A
3	a	941	U
3	a	942	G
3	a	943	A
3	a	944	C
3	a	945	A
3	a	948	C
3	a	953	A
3	a	957	C
3	a	958	U
3	a	961	U
3	a	963	A
3	a	966	G
3	a	968	G
3	a	969	A
3	a	972	G
3	a	973	G
3	a	975	G
3	a	976	C
3	a	978	U
3	a	979	U
3	a	980	C
3	a	981	G
3	a	982	G
3	a	984	A
3	a	985	A
3	a	986	C
3	a	992	C
3	a	999	G
3	a	1001	U
3	a	1002	G
3	a	1003	C
3	a	1004	A
3	a	1006	G
3	a	1014	U
3	a	1015	C
3	a	1019	U
3	a	1033	G
3	a	1034	U
3	a	1041	A

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Mol	Chain	Res	Type
3	a	1043	G
3	a	1044	U
3	a	1050	A
3	a	1067	U
3	a	1073	G
3	a	1075	U
3	a	1077	C
3	a	1078	C
3	a	1079	A
3	a	1080	A
3	a	1082	G
3	a	1083	U
3	a	1084	U
3	a	1085	G
3	a	1086	A
3	a	1088	U
3	a	1089	U
3	a	1091	G
3	a	1092	G
3	a	1095	C
3	a	1099	G
3	a	1100	A
3	a	1107	U
3	a	1114	G
3	a	1115	A
3	a	1116	U
3	a	1119	G
3	a	1131	U
3	a	1132	G
3	a	1134	G
3	a	1137	U
3	a	1144	A
3	a	1145	A
3	a	1149	A
3	a	1150	U
3	a	1151	C
3	a	1160	U
3	a	1161	A
3	a	1163	G
3	a	1169	G
3	a	1174	C
3	a	1175	A

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Mol	Chain	Res	Type
3	a	1184	A
3	a	1186	A
3	a	1187	A
3	a	1188	U
3	a	1189	G
3	a	1195	G
3	a	1198	A
3	a	1204	U
3	a	1205	C
3	a	1206	G
3	a	1208	G
3	a	1209	A
3	a	1217	A
3	a	1218	G
3	a	1222	G
3	a	1223	A
3	a	1227	A
3	a	1228	A
3	a	1229	C
3	a	1233	A
3	a	1234	A
3	a	1235	A
3	a	1242	U
3	a	1244	C
3	a	1245	U
3	a	1246	C
3	a	1247	A
3	a	1248	G
3	a	1249	U
3	a	1250	U
3	a	1253	G
3	a	1260	G
3	a	1265	C
3	a	1266	A
3	a	1270	C
3	a	1271	G
3	a	1280	A
3	a	1288	A
3	a	1294	A
3	a	1295	G
3	a	1301	G
3	a	1311	C

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Mol	Chain	Res	Type
3	a	1312	A
3	a	1313	U
3	a	1317	G
3	a	1319	G
3	a	1322	G
3	a	1328	G
3	a	1330	U
3	a	1346	C
3	a	1347	A
3	a	1363	U
3	a	1368	G
3	a	1371	G
3	a	1378	C
3	a	1379	C
3	a	1390	A
3	a	1395	A
3	a	1397	C
3	a	1399	G
3	a	1400	C
3	a	1401	A
3	a	1402	A
3	a	1403	G
3	a	1404	G
3	a	1405	A
3	a	1406	G
3	a	1407	G
3	a	1416	G
3	a	1418	A
3	a	1419	G
3	a	1436	G
3	a	1441	A
3	a	1446	G
3	a	1448	A
3	a	1452	A
3	a	1454	G
3	a	1455	U
3	a	1456	A
3	a	1464	U
3	a	1466	G
3	a	1474	G
3	a	1478	G
3	a	1479	G

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Mol	Chain	Res	Type
3	a	1482	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 185 ligands modelled in this entry, 185 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
2	8	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	1068:UNK	C	1101:UNK	N	66.30
1	8	1143:UNK	C	1201:UNK	N	11.98