



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 09:03 AM GMT

PDB ID : 4DR2
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with multiple copies of paromomycin molecules bound
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-16
Resolution : 3.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

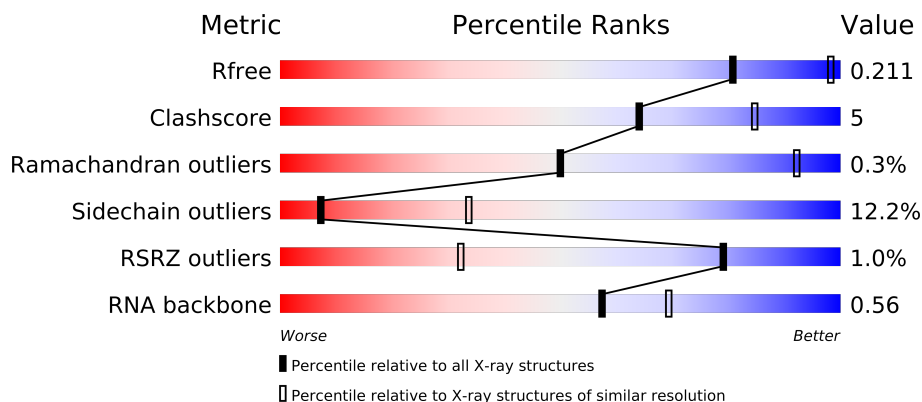
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.25 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1080 (3.30-3.18)
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RSRZ outliers	66119	1081 (3.30-3.18)
RNA backbone	1838	1006 (3.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	

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Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 53227 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32504	14477	6011	10505	1511			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			491	311	104	72	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	101	Total	C	N	O	S	0	0	0
			838	536	157	143	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O		0	0	0
			598	381	118	99				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

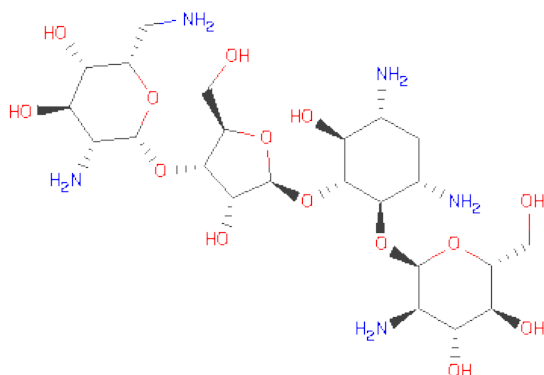
- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		
22	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	1	Total	Mg	0	0
			1	1		
23	Q	1	Total	Mg	0	0
			1	1		
23	D	2	Total	Mg	0	0
			2	2		
23	E	2	Total	Mg	0	0
			2	2		
23	H	2	Total	Mg	0	0
			2	2		
23	I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	305	Total 311	Mg 311	0	6
23	T	2	Total 2	Mg 2	0	0
23	N	1	Total 1	Mg 1	0	0
23	O	1	Total 1	Mg 1	0	0
23	L	1	Total 1	Mg 1	0	0
23	S	1	Total 1	Mg 1	0	0
23	F	1	Total 1	Mg 1	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total 1	Zn 1	0	0
24	N	1	Total 1	Zn 1	0	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	512	Total 512	O 512	0	0
25	C	1	Total 1	O 1	0	0
25	D	7	Total 7	O 7	0	0
25	E	6	Total 6	O 6	0	0
25	H	4	Total 4	O 4	0	0
25	L	2	Total 2	O 2	0	0
25	O	3	Total 3	O 3	0	0
25	T	1	Total 1	O 1	0	0

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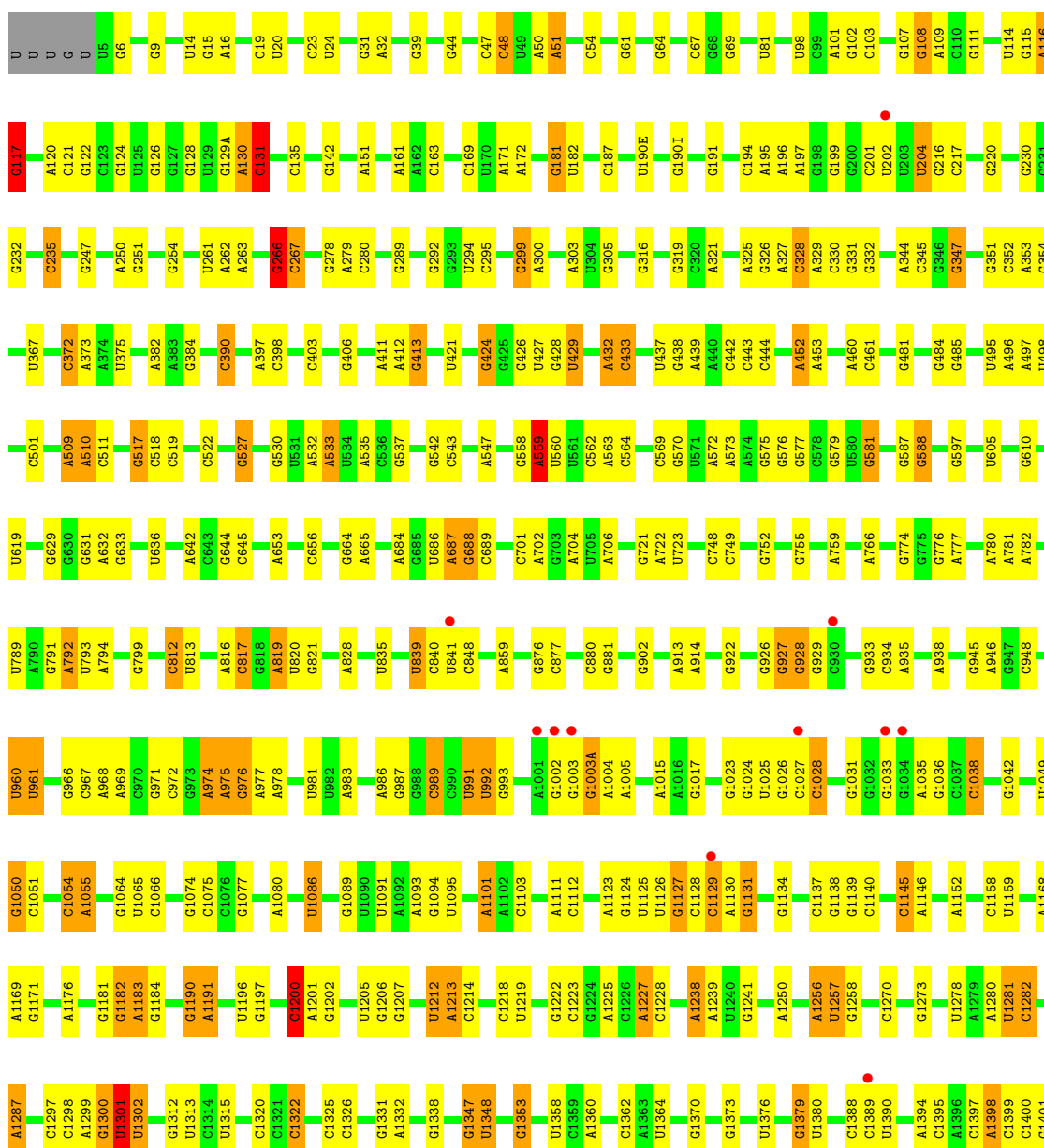
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	U	1	Total	O	0	0
			1	1		

3 Residue-property plots

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

- Molecule 1: 16S rRNA

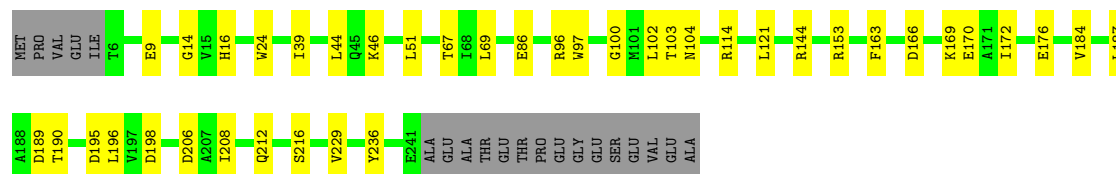
Chain A:





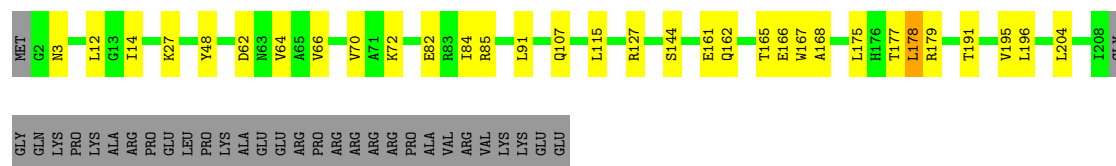
- Molecule 2: 30S ribosomal protein S2

Chain B:



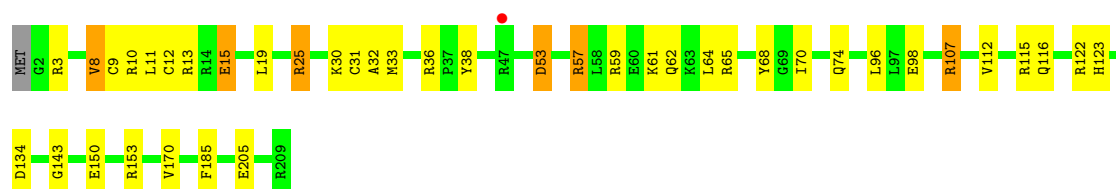
- Molecule 3: 30S ribosomal protein S3

Chain C:



- Molecule 4: 30S ribosomal protein S4

Chain D:



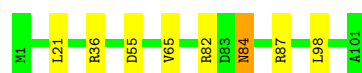
- Molecule 5: 30S ribosomal protein S5

Chain E:



- Molecule 6: 30S ribosomal protein S6

Chain F:



- Molecule 7: 30S ribosomal protein S7

Chain G:



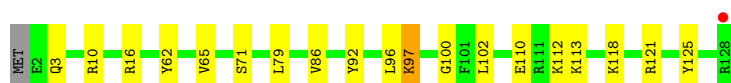
- Molecule 8: 30S ribosomal protein S8

Chain H:



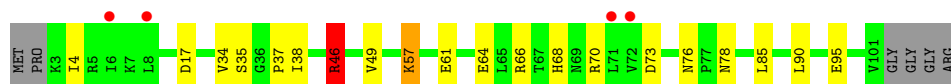
- Molecule 9: 30S ribosomal protein S9

Chain I:



- Molecule 10: 30S ribosomal protein S10

Chain J:



- Molecule 11: 30S ribosomal protein S11

Chain K:



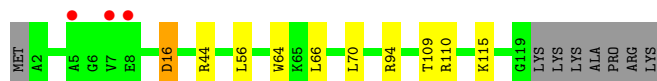
- Molecule 12: 30S ribosomal protein S12

Chain L:



- Molecule 13: 30S ribosomal protein S13

Chain M:



- Molecule 14: 30S ribosomal protein S14

Chain N:



- Molecule 15: 30S ribosomal protein S15

Chain O:



- Molecule 16: 30S ribosomal protein S16

Chain P:



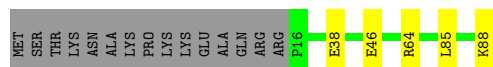
- Molecule 17: 30S ribosomal protein S17

Chain Q:



- Molecule 18: 30S ribosomal protein S18

Chain R:



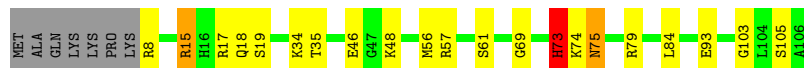
- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein THX

Chain U:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.60Å 402.60Å 177.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.39 – 3.25 44.39 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.39-3.25) 99.4 (44.39-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, R_{free}	0.171 , 0.211 0.171 , 0.211	Depositor DCC
R_{free} test set	11374 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 226283 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53227	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, MG, 0TD, PAR, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	3/36037 (0.0%)	1.03	121/56239 (0.2%)
2	B	0.41	0/1931	0.65	0/2607
3	C	0.42	0/1637	0.63	0/2207
4	D	0.49	3/1733 (0.2%)	0.63	1/2318 (0.0%)
5	E	0.51	0/1163	0.75	2/1566 (0.1%)
6	F	0.37	0/856	0.59	0/1154
7	G	0.37	0/1276	0.55	0/1709
8	H	0.50	0/1136	0.71	0/1527
9	I	0.39	0/1029	0.66	0/1379
10	J	0.38	0/806	0.68	1/1084 (0.1%)
11	K	0.43	0/888	0.69	0/1198
12	L	0.49	0/978	0.70	0/1308
13	M	0.38	0/947	0.59	0/1270
14	N	0.43	0/500	0.67	0/663
15	O	0.41	0/745	0.61	0/992
16	P	0.48	0/717	0.71	0/965
17	Q	0.52	0/851	0.74	0/1136
18	R	0.40	0/604	0.60	0/801
19	S	0.34	0/662	0.61	0/892
20	T	0.48	0/765	0.70	0/1007
21	U	0.44	0/213	0.69	0/279
All	All	0.57	6/55474 (0.0%)	0.93	125/82301 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	975	A	N9-C4	-6.19	1.34	1.37
4	D	31	CYS	CB-SG	6.06	1.92	1.82
1	A	1502	A	N9-C4	-5.34	1.34	1.37
1	A	1502	A	N7-C5	-5.24	1.36	1.39
4	D	9	CYS	CB-SG	5.06	1.90	1.82
4	D	12	CYS	CB-SG	5.04	1.90	1.82

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	G	C4-C5-N7	10.01	114.81	110.80
1	A	108	G	C5-N7-C8	-9.95	99.32	104.30
1	A	1128	C	C6-N1-C2	-9.70	116.42	120.30
1	A	328	C	N1-C2-O2	9.68	124.71	118.90
1	A	1502	A	C5-N7-C8	-9.64	99.08	103.90
1	A	1054	C	N1-C2-O2	9.01	124.31	118.90
1	A	1502	A	C2-N3-C4	-8.94	106.13	110.60
1	A	1054	C	C2-N1-C1'	8.79	128.47	118.80
1	A	927	G	C4-N9-C1'	8.77	137.90	126.50
1	A	108	G	N7-C8-N9	8.49	117.34	113.10
1	A	1502	A	N7-C8-N9	8.30	117.95	113.80
1	A	1502	A	C6-C5-N7	-8.19	126.57	132.30
1	A	266	G	C8-N9-C4	-8.07	103.17	106.40
1	A	929	G	C8-N9-C4	7.98	109.59	106.40
1	A	1200	C	N1-C2-O2	7.92	123.65	118.90
1	A	975	A	C5-N7-C8	-7.86	99.97	103.90
1	A	1502	A	C4-C5-N7	7.72	114.56	110.70
1	A	1502	A	N1-C6-N6	7.67	123.20	118.60
1	A	204	U	C2-N1-C1'	7.65	126.89	117.70
1	A	1532	U	C5-C6-N1	7.53	126.47	122.70
1	A	204	U	N3-C2-O2	-7.41	117.01	122.20
1	A	328	C	N3-C2-O2	-7.32	116.77	121.90
1	A	204	U	N1-C2-O2	7.31	127.92	122.80
1	A	124	G	C5-C6-N1	7.30	115.15	111.50
1	A	1054	C	C6-N1-C1'	-7.23	112.12	120.80
1	A	839	U	C2-N1-C1'	7.23	126.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	927	G	C8-N9-C1'	-7.23	117.60	127.00
1	A	328	C	C2-N1-C1'	7.12	126.63	118.80
1	A	299	G	C4-C5-N7	6.96	113.58	110.80
1	A	108	G	C6-C5-N7	-6.84	126.30	130.40
1	A	1389	C	C6-N1-C2	-6.83	117.57	120.30
1	A	108	G	C4-N9-C1'	6.74	135.26	126.50
1	A	812	C	C2-N1-C1'	6.73	126.21	118.80
1	A	1502	A	N1-C2-N3	6.63	132.62	129.30
1	A	266	G	N7-C8-N9	6.61	116.40	113.10
1	A	299	G	N9-C4-C5	-6.58	102.77	105.40
1	A	1505	G	C8-N9-C4	-6.56	103.78	106.40
1	A	1128	C	C5-C6-N1	6.55	124.28	121.00
1	A	1388	C	C6-N1-C2	6.50	122.90	120.30
1	A	1388	C	C5-C6-N1	-6.50	117.75	121.00
1	A	372	C	N1-C2-O2	6.48	122.79	118.90
1	A	108	G	N1-C6-O6	6.47	123.78	119.90
1	A	722	A	N1-C6-N6	6.42	122.45	118.60
1	A	235	C	C6-N1-C2	6.34	122.84	120.30
1	A	975	A	C2-N3-C4	-6.32	107.44	110.60
1	A	927	G	N7-C8-N9	6.28	116.24	113.10
1	A	1064	G	N9-C4-C5	6.27	107.91	105.40
1	A	1505	G	C5-C6-O6	6.21	132.33	128.60
1	A	839	U	N1-C2-O2	6.19	127.13	122.80
1	A	117	G	N1-C6-O6	6.19	123.61	119.90
1	A	303	A	C8-N9-C4	6.17	108.27	105.80
1	A	1390	U	C5-C4-O4	-6.13	122.22	125.90
10	J	46	ARG	NE-CZ-NH1	6.12	123.36	120.30
5	E	12	LEU	CA-CB-CG	6.11	129.35	115.30
5	E	41	VAL	CB-CA-C	-6.11	99.80	111.40
1	A	328	C	N3-C4-N4	-6.08	113.74	118.00
1	A	839	U	N3-C2-O2	-6.04	117.97	122.20
1	A	135	C	N1-C2-O2	-5.98	115.31	118.90
1	A	1227	A	C5-N7-C8	-5.97	100.92	103.90
1	A	1416	G	N1-C6-O6	5.97	123.48	119.90
1	A	559	A	C8-N9-C4	-5.96	103.42	105.80
1	A	570	G	C8-N9-C4	-5.95	104.02	106.40
1	A	24	U	C5-C6-N1	-5.92	119.74	122.70
1	A	266	G	C5-N7-C8	-5.90	101.35	104.30
1	A	1054	C	C5-C6-N1	5.89	123.94	121.00
1	A	328	C	C6-N1-C1'	-5.88	113.74	120.80
1	A	1227	A	N7-C8-N9	5.86	116.73	113.80
1	A	1389	C	N3-C4-C5	-5.83	119.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	12	CYS	CA-CB-SG	5.78	124.41	114.00
1	A	232	G	N9-C4-C5	-5.78	103.09	105.40
1	A	975	A	N1-C6-N6	5.77	122.06	118.60
1	A	927	G	C8-N9-C4	-5.76	104.10	106.40
1	A	372	C	C6-N1-C2	5.75	122.60	120.30
1	A	299	G	C5-C6-O6	-5.71	125.17	128.60
1	A	929	G	N3-C4-C5	5.69	131.44	128.60
1	A	1227	A	C8-N9-C4	-5.68	103.53	105.80
1	A	1200	C	C2-N1-C1'	5.68	125.05	118.80
1	A	1503	A	C2-N3-C4	5.68	113.44	110.60
1	A	1299	A	C6-C5-N7	-5.67	128.33	132.30
1	A	981	U	N3-C4-O4	5.67	123.37	119.40
1	A	372	C	N1-C2-N3	-5.66	115.24	119.20
1	A	232	G	C8-N9-C4	5.66	108.66	106.40
1	A	108	G	C5-C6-O6	-5.64	125.21	128.60
1	A	181	G	C8-N9-C4	-5.64	104.14	106.40
1	A	812	C	N1-C2-O2	5.61	122.27	118.90
1	A	266	G	N3-C4-N9	-5.60	122.64	126.00
1	A	722	A	C2-N3-C4	-5.60	107.80	110.60
1	A	328	C	C5-C4-N4	5.58	124.11	120.20
1	A	128	G	C8-N9-C4	5.57	108.63	106.40
1	A	1301	U	P-O3'-C3'	5.56	126.37	119.70
1	A	15	G	C4-N9-C1'	5.52	133.68	126.50
1	A	752	G	C8-N9-C4	5.50	108.60	106.40
1	A	975	A	C4-C5-N7	5.48	113.44	110.70
1	A	1509	C	C6-N1-C2	5.47	122.49	120.30
1	A	929	G	C4-N9-C1'	-5.47	119.39	126.50
1	A	108	G	C8-N9-C1'	-5.47	119.89	127.00
1	A	817	C	C6-N1-C2	5.45	122.48	120.30
1	A	15	G	C8-N9-C1'	-5.45	119.92	127.00
1	A	1158	C	C2-N1-C1'	5.44	124.79	118.80
1	A	1299	A	N7-C8-N9	5.44	116.52	113.80
1	A	6	G	C4-N9-C1'	5.42	133.54	126.50
1	A	1222	G	C5-C6-N1	-5.41	108.79	111.50
1	A	1200	C	C6-N1-C1'	-5.41	114.31	120.80
1	A	960	U	C2-N1-C1'	5.38	124.16	117.70
1	A	325	A	N1-C6-N6	-5.34	115.40	118.60
1	A	948	C	N3-C2-O2	5.33	125.64	121.90
1	A	975	A	N7-C8-N9	5.33	116.46	113.80
1	A	706	A	N1-C6-N6	5.28	121.77	118.60
1	A	812	C	C6-N1-C1'	-5.26	114.48	120.80
1	A	1502	A	C8-N9-C4	-5.26	103.69	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	C	P-O3'-C3'	5.21	125.96	119.70
1	A	1086	U	C5-C6-N1	5.21	125.31	122.70
1	A	1322	C	C6-N1-C2	5.20	122.38	120.30
1	A	199	G	C8-N9-C4	5.18	108.47	106.40
1	A	295	C	C6-N1-C2	5.14	122.36	120.30
1	A	1373	G	C5-C6-O6	5.13	131.68	128.60
1	A	481	G	N1-C6-O6	5.11	122.96	119.90
1	A	131	C	N3-C2-O2	-5.09	118.33	121.90
1	A	1502	A	C5-C6-N1	-5.09	115.16	117.70
1	A	1299	A	C4-N9-C1'	5.06	135.40	126.30
1	A	108	G	C8-N9-C4	-5.04	104.38	106.40
1	A	686	U	C2-N1-C1'	-5.04	111.65	117.70
1	A	881	G	C8-N9-C4	5.03	108.41	106.40
1	A	819	A	N7-C8-N9	5.03	116.31	113.80
1	A	20	U	C5-C4-O4	-5.01	122.89	125.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	0	166	0
2	B	1896	0	0	8	0
3	C	1613	0	0	4	0
4	D	1703	0	0	17	0
5	E	1147	0	0	7	0
6	F	843	0	0	1	0
7	G	1257	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1116	0	0	8	0
9	I	1010	0	0	6	0
10	J	793	0	0	9	0
11	K	873	0	0	2	0
12	L	973	0	0	6	0
13	M	937	0	0	2	0
14	N	491	0	0	7	0
15	O	734	0	0	5	0
16	P	701	0	0	4	0
17	Q	838	0	0	7	0
18	R	598	0	0	3	0
19	S	648	0	0	4	0
20	T	763	0	0	9	0
21	U	209	0	0	2	0
22	A	714	0	765	34	0
23	A	311	0	0	0	0
23	D	2	0	0	0	0
23	E	2	0	0	0	0
23	F	1	0	0	0	0
23	H	2	0	0	0	0
23	I	1	0	0	0	0
23	L	1	0	0	0	0
23	N	1	0	0	0	0
23	O	1	0	0	0	0
23	P	1	0	0	0	0
23	Q	1	0	0	0	0
23	S	1	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	512	0	0	8	0
25	C	1	0	0	0	0
25	D	7	0	0	0	0
25	E	6	0	0	0	0
25	H	4	0	0	0	0
25	L	2	0	0	0	0
25	O	3	0	0	0	0
25	T	1	0	0	0	0
25	U	1	0	0	0	0
All	All	53227	0	765	248	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (248) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:427:U:OP1	4:D:13:ARG:NH2	2.12	0.83
1:A:972:C:OP1	10:J:57:LYS:NZ	2.13	0.81
1:A:279:A:OP2	17:Q:95:TYR:OH	1.99	0.79
1:A:835:U:OP1	18:R:64:ARG:NH2	2.16	0.79
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.16	0.79
1:A:230:G:O6	22:A:1611:PAR:N24	2.14	0.79
1:A:542:G:OP1	4:D:10:ARG:NH2	2.16	0.78
1:A:821:G:N7	22:A:1602:PAR:H641	1.99	0.77
1:A:774:G:OP2	22:A:1614:PAR:N64	2.18	0.76
20:T:75:ASN:N	20:T:75:ASN:OD1	2.18	0.76
1:A:1182:G:O2'	1:A:1183:A:OP2	2.03	0.75
1:A:235:C:N4	25:A:2155:HOH:O	2.20	0.73
1:A:1127:G:N2	1:A:1145:C:N3	2.37	0.72
4:D:98:GLU:OE2	4:D:107:ARG:NH1	2.23	0.71
7:G:15:ASP:OD1	7:G:18:TYR:N	2.24	0.70
10:J:17:ASP:OD1	10:J:70:ARG:NH1	2.24	0.70
1:A:1313:U:O4	19:S:4:SER:OG	2.08	0.70
1:A:390:C:O3'	16:P:28:ARG:NH2	2.26	0.69
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.25	0.69
1:A:1505:G:O2'	1:A:1506:U:OP2	2.10	0.69
1:A:619:U:N3	4:D:134:ASP:OD2	2.25	0.69
1:A:261:U:OP2	20:T:79:ARG:NH2	2.26	0.68
1:A:1028:C:N3	1:A:1033:G:N2	2.43	0.67
22:A:1610:PAR:H241	22:A:1610:PAR:H33	1.58	0.67
20:T:46:GLU:OE2	20:T:48:LYS:NZ	2.27	0.67
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.28	0.66
1:A:69:G:O6	22:A:1613:PAR:H221	1.96	0.66
19:S:36:ARG:NH2	19:S:75:ALA:O	2.28	0.66
1:A:1024:G:N1	25:A:2509:HOH:O	2.29	0.65
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.15	0.65
22:A:1614:PAR:O44	22:A:1614:PAR:N64	2.30	0.65
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.29	0.65
1:A:1134:G:N2	1:A:1140:C:N3	2.45	0.65
6:F:84:ASN:OD1	6:F:84:ASN:N	2.30	0.65
5:E:152:ARG:NH2	8:H:107:LEU:O	2.30	0.64
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.30	0.64
1:A:424:G:N7	22:A:1617:PAR:N21	2.40	0.64
1:A:411:A:OP2	4:D:25:ARG:NH2	2.31	0.64
1:A:933:G:O6	7:G:3:ARG:NH2	2.31	0.64
1:A:1131:G:OP1	9:I:3:GLN:NE2	2.31	0.64
1:A:1077:G:N2	1:A:1080:A:OP2	2.31	0.63
1:A:1281:U:O2'	1:A:1282:C:OP1	2.16	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1003(A):G:N2	1:A:1038:C:O2	2.32	0.63
1:A:413:G:N2	1:A:429:U:OP2	2.32	0.63
4:D:57:ARG:NH1	4:D:205:GLU:OE2	2.32	0.62
1:A:991:U:O2'	1:A:992:U:O5'	2.16	0.62
1:A:537:G:OP1	12:L:113:ARG:NH2	2.32	0.62
12:L:27:LEU:O	12:L:29:GLY:N	2.32	0.62
1:A:51:A:OP2	22:A:1604:PAR:H24	1.99	0.61
1:A:103:C:OP1	20:T:17:ARG:NH1	2.32	0.61
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.33	0.61
1:A:130:A:OP2	1:A:190(E):U:O2'	2.18	0.61
1:A:1023:G:O6	1:A:1024:G:N2	2.34	0.61
1:A:517:G:N1	1:A:533:A:OP2	2.33	0.61
4:D:32:ALA:O	4:D:36:ARG:N	2.33	0.61
22:A:1609:PAR:N21	22:A:1609:PAR:O43	2.34	0.61
19:S:10:PHE:O	19:S:39:THR:OG1	2.19	0.61
1:A:877:C:OP1	8:H:88:LYS:NZ	2.34	0.60
1:A:587:G:O2'	1:A:588:G:OP2	2.19	0.60
7:G:111:ARG:NH2	7:G:126:ASP:OD1	2.35	0.60
1:A:1347:G:O2'	1:A:1348:U:OP2	2.19	0.60
1:A:776:G:O6	22:A:1614:PAR:N24	2.35	0.60
1:A:98:U:O4	22:A:1613:PAR:N12	2.35	0.60
1:A:983:A:O2'	1:A:1050:G:OP2	2.20	0.59
8:H:85:ARG:NE	8:H:87:SER:O	2.35	0.59
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.36	0.59
1:A:1376:U:OP1	7:G:98:SER:OG	2.20	0.59
1:A:1200:C:O2'	1:A:1205:U:O4	2.20	0.58
10:J:64:GLU:OE2	10:J:66:ARG:NH2	2.37	0.58
1:A:527:7MG:O2'	1:A:535:A:N1	2.37	0.58
20:T:69:GLY:O	20:T:73:HIS:ND1	2.37	0.58
1:A:1129:C:OP1	9:I:62:TYR:OH	2.22	0.58
1:A:1301:U:O2'	1:A:1302:U:O5'	2.21	0.58
22:A:1612:PAR:N64	22:A:1612:PAR:O33	2.36	0.58
1:A:1513:A:N6	25:A:2425:HOH:O	2.35	0.57
1:A:1347:G:O2'	1:A:1348:U:P	2.62	0.57
1:A:976:G:OP1	14:N:32:SER:N	2.38	0.56
1:A:664:G:OP1	18:R:64:ARG:NH1	2.37	0.56
1:A:1300:G:O2'	1:A:1301:U:O5'	2.22	0.56
22:A:1607:PAR:O44	22:A:1607:PAR:N64	2.38	0.56
5:E:140:ARG:O	5:E:143:ARG:NH2	2.39	0.56
1:A:581:G:O3'	15:O:64:ARG:NH2	2.38	0.56
22:A:1617:PAR:O44	22:A:1617:PAR:N64	2.35	0.55
15:O:36:ILE:O	15:O:40:SER:OG	2.25	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:U:OP1	1:A:610:G:O2'	2.25	0.55
1:A:684:A:O3'	11:K:12:ARG:NH2	2.39	0.55
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.41	0.54
22:A:1610:PAR:H33	22:A:1610:PAR:N24	2.22	0.54
10:J:35:SER:OG	10:J:73:ASP:O	2.26	0.54
1:A:1112:C:N3	3:C:178:LEU:N	2.55	0.54
2:B:195:ASP:O	8:H:68:ARG:NH2	2.42	0.53
2:B:189:ASP:OD2	2:B:190:THR:N	2.41	0.53
22:A:1610:PAR:N21	22:A:1610:PAR:O53	2.42	0.53
5:E:97:GLY:N	5:E:117:ASP:OD1	2.43	0.52
1:A:403:C:N4	25:A:2090:HOH:O	2.43	0.52
1:A:1502:A:C2	1:A:1505:G:N1	2.78	0.52
1:A:610:G:OP1	22:A:1606:PAR:H641	2.10	0.52
1:A:1347:G:N7	9:I:10:ARG:NH2	2.57	0.52
1:A:974:A:OP2	14:N:41:ARG:NH1	2.43	0.52
4:D:8:VAL:O	4:D:11:LEU:N	2.43	0.51
1:A:642:A:N3	8:H:113:SER:OG	2.43	0.51
22:A:1612:PAR:O43	22:A:1612:PAR:N21	2.42	0.51
4:D:112:VAL:N	4:D:116:GLN:OE1	2.43	0.51
1:A:1498:UR3:OP2	1:A:1542:U:O2'	2.28	0.51
13:M:16:ASP:N	13:M:16:ASP:OD1	2.43	0.51
7:G:15:ASP:N	7:G:20:ASP:O	2.43	0.51
1:A:1300:G:O2'	1:A:1301:U:P	2.68	0.51
1:A:1219:U:OP1	14:N:19:ARG:NH1	2.44	0.51
15:O:4:THR:N	15:O:7:GLU:OE1	2.44	0.51
1:A:194:C:OP1	20:T:61:SER:OG	2.29	0.50
1:A:688:G:O2'	1:A:704:A:N1	2.44	0.50
4:D:15:GLU:OE2	4:D:59:ARG:NE	2.44	0.50
1:A:432:A:O2'	1:A:433:C:OP1	2.29	0.50
22:A:1604:PAR:H11	22:A:1604:PAR:O52	2.11	0.50
1:A:191:G:N2	20:T:103:GLY:O	2.44	0.50
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.30	0.50
7:G:20:ASP:OD1	7:G:63:LYS:NZ	2.45	0.50
1:A:254:G:OP1	17:Q:67:LYS:O	2.30	0.49
22:A:1616:PAR:H33	22:A:1616:PAR:HN61	1.77	0.49
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.45	0.49
14:N:26:ARG:NH2	14:N:46:GLU:OE1	2.45	0.49
1:A:1325:C:OP1	21:U:15:ARG:NH1	2.46	0.49
1:A:1256:A:O2'	1:A:1257:U:O5'	2.31	0.49
1:A:1190:G:O2'	1:A:1191:A:P	2.70	0.49
2:B:100:GLY:O	2:B:104:ASN:N	2.46	0.49
1:A:1074:G:O2'	1:A:1101:A:N1	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:113:GLU:OE1	7:G:113:GLU:N	2.46	0.48
1:A:1402:4OC:O2	1:A:1500:A:N1	2.46	0.48
1:A:107:G:N7	20:T:15:ARG:NH2	2.62	0.48
1:A:558:G:OP2	1:A:559:A:O2'	2.32	0.48
15:O:2:PRO:O	15:O:38:ARG:NH1	2.47	0.48
1:A:1239:A:C4	1:A:1298:C:N4	2.82	0.47
1:A:509:A:O2'	1:A:510:A:OP1	2.32	0.47
1:A:142:G:O2'	1:A:196:A:N1	2.48	0.47
17:Q:62:SER:OG	17:Q:72:ARG:NE	2.47	0.47
1:A:61:G:O2'	25:A:2002:HOH:O	2.20	0.47
1:A:316:G:OP2	1:A:351:G:O2'	2.33	0.47
8:H:103:VAL:O	8:H:106:GLY:N	2.48	0.47
14:N:34:TYR:N	14:N:39:LEU:O	2.48	0.47
10:J:76:ASN:O	10:J:78:ASN:N	2.48	0.47
1:A:789:U:O2'	1:A:791:G:N7	2.47	0.47
16:P:75:ARG:O	16:P:78:GLY:N	2.48	0.47
1:A:299:G:C6	1:A:300:A:C6	3.03	0.46
1:A:187:C:N3	20:T:105:SER:OG	2.48	0.46
1:A:114:U:OP1	22:A:1604:PAR:H32	2.15	0.46
1:A:928:G:O2'	1:A:1533:C:OP1	2.33	0.46
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.49	0.46
1:A:1212:U:O2'	1:A:1213:A:P	2.74	0.46
1:A:1055:A:O2'	3:C:161:GLU:O	2.34	0.46
1:A:991:U:O2'	1:A:992:U:P	2.74	0.45
1:A:437:U:O2'	4:D:123:HIS:ND1	2.49	0.45
2:B:103:THR:N	2:B:176:GLU:OE1	2.49	0.45
1:A:120:A:O2'	1:A:122:G:OP1	2.35	0.45
1:A:1228:C:OP1	13:M:115:LYS:NZ	2.49	0.45
1:A:375:U:OP1	16:P:69:THR:OG1	2.35	0.45
22:A:1616:PAR:H24	25:A:2497:HOH:O	2.16	0.45
1:A:501:C:OP1	12:L:117:ARG:NH2	2.50	0.45
1:A:689:C:OP1	11:K:44:SER:OG	2.35	0.45
1:A:986:A:O2'	19:S:55:LYS:O	2.35	0.44
1:A:262:A:C6	1:A:263:A:C6	3.05	0.44
1:A:64:G:N1	22:A:1613:PAR:N32	2.66	0.44
1:A:687:A:O2'	1:A:688:G:OP2	2.35	0.44
1:A:1347:G:C2'	1:A:1348:U:OP2	2.66	0.44
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.36	0.44
8:H:21:LYS:O	8:H:65:TYR:OH	2.35	0.44
1:A:880:C:OP1	12:L:8:ASN:ND2	2.51	0.44
1:A:978:A:O2'	1:A:1322:C:N3	2.51	0.44
22:A:1616:PAR:H21	22:A:1616:PAR:H42	1.44	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1168:A:C6	1:A:1169:A:C6	3.06	0.44
1:A:1123:A:O2'	10:J:37:PRO:O	2.36	0.44
1:A:633:G:OP2	22:A:1612:PAR:H11	2.18	0.44
1:A:109:A:C6	1:A:326:G:C6	3.06	0.44
22:A:1601:PAR:O52	22:A:1601:PAR:H11	2.17	0.44
4:D:53:ASP:OD1	4:D:53:ASP:N	2.50	0.44
1:A:945:G:C2	1:A:946:A:C8	3.06	0.43
1:A:161:A:N1	1:A:347:G:O2'	2.51	0.43
1:A:1190:G:O2'	1:A:1191:A:O5'	2.36	0.43
1:A:922:G:O2'	1:A:1398:A:N1	2.52	0.43
1:A:656:C:O2'	15:O:28:GLN:OE1	2.36	0.43
18:R:38:GLU:OE1	18:R:38:GLU:N	2.51	0.43
1:A:411:A:OP1	4:D:30:LYS:NZ	2.51	0.43
1:A:517:G:N2	1:A:530:G:OP1	2.51	0.43
1:A:1111:A:N1	3:C:177:THR:OG1	2.52	0.43
1:A:1212:U:O2'	1:A:1213:A:OP2	2.36	0.43
1:A:989:C:O2'	1:A:1017:G:O2'	2.36	0.43
17:Q:48:GLU:OE1	17:Q:50:LYS:NZ	2.52	0.43
1:A:1206:G:C6	1:A:1207:2MG:C5	3.07	0.43
1:A:117:G:P	25:A:2020:HOH:O	2.77	0.43
1:A:1315:U:O2'	1:A:1360:A:N3	2.52	0.43
1:A:509:A:N3	1:A:543:C:O2'	2.52	0.43
1:A:426:G:OP1	4:D:38:TYR:OH	2.37	0.42
4:D:143:GLY:N	4:D:185:PHE:O	2.53	0.42
22:A:1613:PAR:H52	22:A:1613:PAR:H11	1.82	0.42
1:A:64:G:C6	22:A:1613:PAR:N32	2.88	0.42
12:L:53:ARG:NH1	12:L:92:0TD:OD1	2.52	0.42
1:A:791:G:C6	1:A:792:A:N7	2.88	0.42
2:B:166:ASP:O	2:B:170:GLU:N	2.52	0.42
1:A:629:G:N7	22:A:1615:PAR:H221	2.35	0.42
1:A:14:U:O2'	1:A:16:A:N7	2.53	0.42
1:A:636:U:O4	22:A:1612:PAR:H54	2.19	0.42
1:A:109:A:C6	1:A:327:A:C6	3.07	0.42
1:A:644:G:C5	1:A:645:C:C5	3.07	0.42
1:A:102:G:O2'	1:A:151:A:N3	2.53	0.42
1:A:67:C:O2'	1:A:171:A:N3	2.53	0.42
9:I:97:LYS:O	9:I:100:GLY:N	2.53	0.42
1:A:31:G:N2	1:A:48:C:OP1	2.53	0.42
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.53	0.42
1:A:217:C:O2'	1:A:461:C:N4	2.53	0.42
2:B:212:GLN:O	2:B:216:SER:OG	2.38	0.42
22:A:1607:PAR:O51	22:A:1607:PAR:N32	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1399:C:C2	1:A:1401:G:C5	3.08	0.42
1:A:522:C:OP2	12:L:69:TYR:OH	2.38	0.41
1:A:1074:G:C6	1:A:1075:C:C4	3.08	0.41
1:A:266:G:O2'	1:A:267:C:OP2	2.38	0.41
1:A:1379:G:C6	1:A:1380:U:C4	3.08	0.41
1:A:438:G:O2'	1:A:495:U:O4	2.38	0.41
1:A:961:U:OP1	1:A:1223:C:O2'	2.37	0.41
1:A:19:C:OP1	5:E:125:SER:OG	2.39	0.41
1:A:976:G:OP2	1:A:1358:U:O2'	2.38	0.41
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.53	0.41
1:A:1002:G:C6	1:A:1003:G:C6	3.08	0.41
1:A:1238:A:N3	1:A:1241:G:O2'	2.53	0.41
1:A:1500:A:OP2	1:A:1505:G:OP1	2.38	0.41
1:A:581:G:N1	1:A:759:A:OP2	2.53	0.41
1:A:111:G:O6	1:A:330:C:N4	2.53	0.41
1:A:938:A:N3	1:A:1376:U:O2'	2.53	0.41
1:A:1091:U:O2	1:A:1093:A:C8	2.73	0.41
1:A:292:G:OP2	1:A:305:G:N2	2.53	0.41
10:J:46:ARG:NH1	10:J:64:GLU:OE1	2.53	0.41
2:B:184:VAL:N	2:B:198:ASP:OD2	2.54	0.41
1:A:1480:G:C6	1:A:1481:U:C4	3.09	0.41
5:E:39:GLY:O	5:E:69:VAL:N	2.54	0.41
1:A:1287:A:N3	1:A:1353:G:O2'	2.54	0.41
22:A:1613:PAR:H13	22:A:1613:PAR:H42	1.60	0.41
1:A:103:C:O2'	1:A:172:A:N1	2.54	0.41
5:E:117:ASP:N	5:E:117:ASP:OD2	2.54	0.41
9:I:92:TYR:O	9:I:96:LEU:N	2.54	0.41
1:A:1015:A:N3	1:A:1218:C:O2'	2.54	0.41
1:A:23:C:N4	25:A:2102:HOH:O	2.53	0.41
16:P:40:ASP:N	16:P:48:TRP:O	2.54	0.41
1:A:116:A:OP2	1:A:116:A:C8	2.75	0.40
22:A:1606:PAR:O52	22:A:1606:PAR:H11	2.21	0.40
1:A:1112:C:O2	3:C:179:ARG:N	2.54	0.40
1:A:452:A:O2'	1:A:453:A:C8	2.74	0.40
1:A:1297:C:O2'	7:G:114:ARG:NH2	2.54	0.40
22:A:1608:PAR:H13	22:A:1608:PAR:H42	1.74	0.40
1:A:126:G:OP1	1:A:605:U:O2'	2.39	0.40
1:A:131:C:O2'	1:A:262:A:N3	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	218 (93%)	15 (6%)	1 (0%)	43	89
3	C	205/239 (86%)	187 (91%)	16 (8%)	2 (1%)	22	75
4	D	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	38	86
5	E	149/162 (92%)	143 (96%)	6 (4%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
9	I	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
10	J	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	22	75
11	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	27	78
13	M	116/126 (92%)	108 (93%)	8 (7%)	0	100	100
14	N	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	Q	99/105 (94%)	94 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	64 (90%)	7 (10%)	0	100	100
19	S	79/93 (85%)	70 (89%)	8 (10%)	1 (1%)	18	70
20	T	97/106 (92%)	88 (91%)	8 (8%)	1 (1%)	22	75
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2352/2541 (93%)	2203 (94%)	141 (6%)	8 (0%)	50	92

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE

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Mol	Chain	Res	Type
3	C	168	ALA
4	D	3	ARG
20	T	73	HIS
2	B	229	VAL
3	C	66	VAL
10	J	34	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 X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	201/220 (91%)	177 (88%)	24 (12%)	8	35
3	C	160/188 (85%)	134 (84%)	26 (16%)	3	17
4	D	180/181 (99%)	162 (90%)	18 (10%)	11	43
5	E	115/123 (94%)	96 (84%)	19 (16%)	3	17
6	F	90/90 (100%)	82 (91%)	8 (9%)	14	51
7	G	126/127 (99%)	112 (89%)	14 (11%)	9	38
8	H	119/119 (100%)	103 (87%)	16 (13%)	6	28
9	I	98/99 (99%)	87 (89%)	11 (11%)	9	38
10	J	87/92 (95%)	79 (91%)	8 (9%)	13	49
11	K	89/99 (90%)	79 (89%)	10 (11%)	9	38
12	L	103/110 (94%)	92 (89%)	11 (11%)	10	40
13	M	94/101 (93%)	85 (90%)	9 (10%)	12	46
14	N	48/50 (96%)	43 (90%)	5 (10%)	10	41
15	O	79/80 (99%)	66 (84%)	13 (16%)	3	17
16	P	72/74 (97%)	64 (89%)	8 (11%)	9	38
17	Q	95/97 (98%)	84 (88%)	11 (12%)	8	36
18	R	64/77 (83%)	61 (95%)	3 (5%)	36	80
19	S	71/80 (89%)	58 (82%)	13 (18%)	2	13
20	T	76/82 (93%)	63 (83%)	13 (17%)	3	16
21	U	19/22 (86%)	17 (90%)	2 (10%)	10	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1986/2111 (94%)	1744 (88%)	242 (12%)	7 34

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	16	HIS
2	B	24	TRP
2	B	39	ILE
2	B	44	LEU
2	B	46	LYS
2	B	51	LEU
2	B	67	THR
2	B	69	LEU
2	B	86	GLU
2	B	97	TRP
2	B	102	LEU
2	B	114	ARG
2	B	121	LEU
2	B	144	ARG
2	B	153	ARG
2	B	163	PHE
2	B	169	LYS
2	B	172	ILE
2	B	187	LEU
2	B	196	LEU
2	B	206	ASP
2	B	208	ILE
2	B	236	TYR
3	C	3	ASN
3	C	12	LEU
3	C	14	ILE
3	C	27	LYS
3	C	48	TYR
3	C	62	ASP
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
3	C	82	GLU
3	C	84	ILE
3	C	85	ARG
3	C	91	LEU

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Mol	Chain	Res	Type
3	C	107	GLN
3	C	115	LEU
3	C	127	ARG
3	C	144	SER
3	C	162	GLN
3	C	165	THR
3	C	167	TRP
3	C	175	LEU
3	C	178	LEU
3	C	191	THR
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
4	D	8	VAL
4	D	15	GLU
4	D	19	LEU
4	D	25	ARG
4	D	33	MET
4	D	53	ASP
4	D	57	ARG
4	D	61	LYS
4	D	64	LEU
4	D	70	ILE
4	D	74	GLN
4	D	96	LEU
4	D	107	ARG
4	D	115	ARG
4	D	122	ARG
4	D	150	GLU
4	D	153	ARG
4	D	170	VAL
5	E	6	PHE
5	E	12	LEU
5	E	18	ARG
5	E	24	ARG
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	50	GLU
5	E	53	LEU
5	E	64	ARG
5	E	65	ASN

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Mol	Chain	Res	Type
5	E	79	GLU
5	E	80	ILE
5	E	92	LYS
5	E	116	THR
5	E	117	ASP
5	E	145	LYS
5	E	150	ARG
5	E	151	LEU
6	F	21	LEU
6	F	36	ARG
6	F	55	ASP
6	F	65	VAL
6	F	82	ARG
6	F	84	ASN
6	F	87	ARG
6	F	98	LEU
7	G	5	ARG
7	G	10	ARG
7	G	12	LEU
7	G	36	LYS
7	G	41	ARG
7	G	48	LYS
7	G	51	GLN
7	G	57	GLU
7	G	75	VAL
7	G	98	SER
7	G	114	ARG
7	G	124	LEU
7	G	149	ARG
7	G	156	TRP
8	H	18	ARG
8	H	21	LYS
8	H	23	SER
8	H	26	VAL
8	H	30	ARG
8	H	31	PHE
8	H	39	LEU
8	H	50	ARG
8	H	56	LYS
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG

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Mol	Chain	Res	Type
8	H	92	ARG
8	H	102	ARG
8	H	113	SER
8	H	133	LEU
9	I	16	ARG
9	I	65	VAL
9	I	71	SER
9	I	79	LEU
9	I	86	VAL
9	I	97	LYS
9	I	102	LEU
9	I	112	LYS
9	I	118	LYS
9	I	121	ARG
9	I	125	TYR
10	J	4	ILE
10	J	38	ILE
10	J	46	ARG
10	J	49	VAL
10	J	57	LYS
10	J	85	LEU
10	J	90	LEU
10	J	95	GLU
11	K	11	LYS
11	K	18	ARG
11	K	24	SER
11	K	48	ILE
11	K	51	LYS
11	K	77	MET
11	K	84	VAL
11	K	91	ARG
11	K	119	CYS
11	K	122	LYS
12	L	20	LYS
12	L	28	LYS
12	L	33	ARG
12	L	36	VAL
12	L	39	VAL
12	L	53	ARG
12	L	60	LEU
12	L	67	THR
12	L	93	LEU

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Mol	Chain	Res	Type
12	L	116	SER
12	L	126	LYS
13	M	16	ASP
13	M	44	ARG
13	M	56	LEU
13	M	64	TRP
13	M	66	LEU
13	M	70	LEU
13	M	94	ARG
13	M	109	THR
13	M	110	ARG
14	N	8	GLU
14	N	9	LYS
14	N	23	ARG
14	N	29	ARG
14	N	31	ARG
15	O	5	LYS
15	O	14	GLU
15	O	31	LEU
15	O	34	LEU
15	O	39	LEU
15	O	40	SER
15	O	43	LEU
15	O	44	LYS
15	O	48	LYS
15	O	57	LEU
15	O	70	LEU
15	O	81	LEU
15	O	88	ARG
16	P	2	VAL
16	P	8	ARG
16	P	27	LYS
16	P	31	LYS
16	P	42	ARG
16	P	54	GLU
16	P	55	ARG
16	P	62	VAL
17	Q	36	ILE
17	Q	38	ARG
17	Q	59	ILE
17	Q	68	ARG
17	Q	72	ARG

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Mol	Chain	Res	Type
17	Q	86	GLU
17	Q	96	GLN
17	Q	97	SER
17	Q	98	LEU
17	Q	99	SER
17	Q	101	ARG
18	R	46	GLU
18	R	85	LEU
18	R	88	LYS
19	S	5	LEU
19	S	7	LYS
19	S	12	ASP
19	S	13	ASP
19	S	14	HIS
19	S	15	LEU
19	S	33	THR
19	S	36	ARG
19	S	39	THR
19	S	58	VAL
19	S	61	TYR
19	S	65	ASN
19	S	81	ARG
20	T	8	ARG
20	T	15	ARG
20	T	18	GLN
20	T	19	SER
20	T	34	LYS
20	T	35	THR
20	T	56	MET
20	T	57	ARG
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	93	GLU
21	U	8	THR
21	U	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	256 (16%)	35 (2%)

All (256) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	81	U
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	169	C
1	A	182	U
1	A	190(I)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	319	G
1	A	321	A

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Mol	Chain	Res	Type
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G
1	A	429	U
1	A	432	A
1	A	433	C
1	A	439	A
1	A	442	C
1	A	443	C
1	A	444	C
1	A	452	A
1	A	460	A
1	A	485	G
1	A	496	A
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C

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Mol	Chain	Res	Type
1	A	527	7MG
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	569	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	588	G
1	A	597	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	721	G
1	A	723	U
1	A	749	C
1	A	755	G
1	A	766	A
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	813	U
1	A	816	A
1	A	817	C

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Mol	Chain	Res	Type
1	A	819	A
1	A	820	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	876	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	928	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	987	G
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1031	G
1	A	1035	A
1	A	1036	G

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Mol	Chain	Res	Type
1	A	1038	C
1	A	1042	G
1	A	1050	G
1	A	1051	C
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1086	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1146	A
1	A	1159	U
1	A	1171	G
1	A	1176	A
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A

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Mol	Chain	Res	Type
1	A	1227	A
1	A	1238	A
1	A	1250	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1273	G
1	A	1278	U
1	A	1280	A
1	A	1282	C
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1312	G
1	A	1320	C
1	A	1331	G
1	A	1332	A
1	A	1338	G
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1394	A
1	A	1395	C
1	A	1397	C
1	A	1398	A
1	A	1400	5MC
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1504	G

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	108	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	266	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	432	A
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	991	U
1	A	1049	U
1	A	1065	U
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1281	U

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Mol	Chain	Res	Type
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	1207	1	24,26,27	1.33	4 (16%)	32,38,41	10.15	3 (9%)
1	5MC	A	1400	1	20,22,23	1.91	4 (20%)	26,32,35	1.24	3 (11%)
1	4OC	A	1402	1	21,23,24	1.38	3 (14%)	26,32,35	0.70	0
1	5MC	A	1404	1	20,22,23	1.52	3 (15%)	26,32,35	1.26	4 (15%)
1	5MC	A	1407	1	20,22,23	1.29	1 (5%)	26,32,35	1.38	4 (15%)
1	UR3	A	1498	1	20,22,23	1.27	2 (10%)	23,32,35	1.09	2 (8%)
1	MA6	A	1518	1	26,26,27	1.04	1 (3%)	37,38,41	0.98	2 (5%)
1	MA6	A	1519	1	26,26,27	0.95	1 (3%)	37,38,41	1.17	4 (10%)
1	PSU	A	1540	1	19,21,22	1.11	1 (5%)	23,30,33	0.93	1 (4%)
1	PSU	A	1541	1,23	19,21,22	1.12	1 (5%)	23,30,33	0.92	2 (8%)
1	PSU	A	516	1,23	19,21,22	1.03	1 (5%)	23,30,33	1.03	3 (13%)
1	7MG	A	527	1,23	24,26,27	3.86	5 (20%)	34,39,42	1.36	5 (14%)
1	M2G	A	966	1	25,27,28	1.30	3 (12%)	34,40,43	6.98	4 (11%)
1	5MC	A	967	1	20,22,23	1.27	1 (5%)	26,32,35	1.31	3 (11%)
12	0TD	L	92	12	9,9,10	6.84	2 (22%)	9,11,13	3.44	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	0/10/27/28	0/1/3/3
1	5MC	A	1400	1	-	1/6/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/10/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/6/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/6/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/6/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/13/29/30	0/1/3/3
1	MA6	A	1519	1	-	0/13/29/30	0/1/3/3
1	PSU	A	1540	1	-	0/8/25/26	0/2/2/2
1	PSU	A	1541	1,23	-	0/8/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/8/25/26	0/2/2/2
1	7MG	A	527	1,23	-	0/8/37/38	0/1/3/3
1	M2G	A	966	1	-	0/12/29/30	0/1/3/3
1	5MC	A	967	1	-	0/6/25/26	0/2/2/2
12	0TD	L	92	12	-	0/10/12/14	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	O-C	19.86	1.25	1.11
1	A	527	7MG	C8-N9	-15.02	1.34	1.46
1	A	527	7MG	C2-N2	7.21	1.43	1.32
1	A	1400	5MC	C2-N1	6.87	1.45	1.38
1	A	527	7MG	C4-N3	6.74	1.43	1.34
1	A	1404	5MC	C2-N1	4.45	1.43	1.38
1	A	1402	4OC	C2-N1	4.40	1.43	1.38
1	A	967	5MC	C2-N1	4.22	1.42	1.38
12	L	92	0TD	CA-C	4.20	1.56	1.48
1	A	1407	5MC	C2-N1	4.02	1.42	1.38
1	A	966	M2G	C2-N2	3.98	1.39	1.34
1	A	527	7MG	C8-N7	-3.80	1.34	1.45
1	A	1541	PSU	C6-N1	3.74	1.35	1.32
1	A	1540	PSU	C6-N1	3.61	1.35	1.32
1	A	1519	MA6	C8-N9	3.59	1.42	1.36
1	A	1207	2MG	C8-N9	3.52	1.41	1.36
1	A	516	PSU	C6-N1	3.50	1.35	1.32
1	A	1498	UR3	C2-N1	3.43	1.42	1.38
1	A	1207	2MG	C6-N1	3.21	1.42	1.37
1	A	1404	5MC	C2-N3	3.14	1.43	1.35
1	A	966	M2G	C8-N9	3.12	1.41	1.36
1	A	1498	UR3	C2-N3	3.04	1.41	1.38
1	A	1518	MA6	C8-N9	2.98	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	CM7-N7	-2.91	1.41	1.46
1	A	1207	2MG	C2-N2	2.86	1.40	1.32
1	A	966	M2G	C6-N1	2.83	1.42	1.37
1	A	1400	5MC	C5-C4	2.50	1.45	1.41
1	A	1400	5MC	C2-N3	2.39	1.42	1.35
1	A	1207	2MG	C2-N1	2.38	1.42	1.36
1	A	1400	5MC	C4-N3	2.21	1.36	1.32
1	A	1402	4OC	C2-N3	2.06	1.41	1.35
1	A	1402	4OC	C4-N4	2.02	1.40	1.36
1	A	1404	5MC	C4-N4	2.00	1.39	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-C5-N7	-57.20	126.44	134.14
1	A	966	M2G	C6-C5-N7	-40.22	128.72	134.14
12	L	92	0TD	CSB-SB-CB	-7.10	89.17	101.48
12	L	92	0TD	CA-CB-CG	4.65	116.48	110.95
1	A	1407	5MC	C6-N1-C2	4.52	120.85	118.62
12	L	92	0TD	CG-CB-SB	-4.33	102.90	108.74
1	A	967	5MC	C6-N1-C2	3.88	120.53	118.62
12	L	92	0TD	C-CA-N	-3.83	105.71	111.94
1	A	1404	5MC	C6-N1-C2	3.60	120.39	118.62
1	A	1400	5MC	C6-N1-C2	3.59	120.39	118.62
1	A	966	M2G	C6-N1-C2	3.57	122.80	120.28
1	A	527	7MG	N7-C8-N9	3.43	107.61	103.08
1	A	527	7MG	N3-C4-N9	3.42	132.48	127.06
1	A	1407	5MC	C2-N3-C4	3.25	118.35	115.41
1	A	967	5MC	C2-N3-C4	3.18	118.29	115.41
1	A	527	7MG	C5-C4-N3	-3.12	120.99	126.61
1	A	1518	MA6	C2-N1-C6	2.81	117.62	111.53
1	A	1404	5MC	CM5-C5-C4	-2.78	118.62	121.43
1	A	1400	5MC	C2-N3-C4	2.74	117.89	115.41
1	A	1519	MA6	C2-N1-C6	2.71	117.41	111.53
1	A	1540	PSU	C4-N3-C2	-2.66	119.96	125.36
1	A	1541	PSU	C4-N3-C2	-2.61	120.06	125.36
1	A	516	PSU	C4-N3-C2	-2.59	120.10	125.36
1	A	1207	2MG	N3-C4-N9	2.51	130.59	126.91
1	A	967	5MC	N4-C4-N3	-2.51	114.41	118.73
1	A	1207	2MG	C4-C5-N7	2.45	111.62	109.52
1	A	1519	MA6	N1-C6-N6	-2.44	114.47	117.04
1	A	1404	5MC	C2-N3-C4	2.41	117.59	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	N3-C2-N1	2.38	130.70	128.71
1	A	527	7MG	CM7-N7-C8	2.34	125.02	119.23
1	A	1498	UR3	C3'-C2'-C1'	2.32	104.53	100.91
1	A	1518	MA6	C1'-N9-C4	-2.21	122.82	126.64
1	A	1519	MA6	C8-N9-C1'	2.20	130.71	126.38
1	A	1407	5MC	CM5-C5-C6	2.16	123.19	118.59
1	A	966	M2G	C8-N9-C1'	2.14	130.60	126.38
1	A	1407	5MC	N4-C4-N3	-2.14	115.05	118.73
1	A	516	PSU	C5-C1'-C2'	-2.14	111.84	115.61
1	A	1404	5MC	CM5-C5-C6	2.12	123.10	118.59
1	A	516	PSU	O4'-C1'-C2'	2.10	107.99	104.37
1	A	527	7MG	C8-N9-C1'	2.07	127.81	121.94
1	A	1400	5MC	N4-C4-N3	-2.07	115.17	118.73
1	A	1541	PSU	O4'-C1'-C2'	2.05	107.91	104.37
1	A	1498	UR3	C4'-O4'-C1'	2.03	111.95	109.75
1	A	966	M2G	N1-C2-N2	-2.01	115.88	118.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1400	5MC	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 346 ligands modelled in this entry, 329 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PAR	A	1601	-	45,45,45	1.03	4 (8%)	67,67,67	1.50	14 (20%)
22	PAR	A	1602	-	45,45,45	1.05	4 (8%)	67,67,67	1.68	14 (20%)
22	PAR	A	1603	-	45,45,45	1.29	3 (6%)	67,67,67	1.56	12 (17%)
22	PAR	A	1604	-	45,45,45	1.27	4 (8%)	67,67,67	1.59	13 (19%)
22	PAR	A	1605	-	45,45,45	1.20	3 (6%)	67,67,67	1.63	13 (19%)
22	PAR	A	1606	-	45,45,45	1.26	6 (13%)	67,67,67	1.59	15 (22%)
22	PAR	A	1607	-	45,45,45	1.26	4 (8%)	67,67,67	1.59	14 (20%)
22	PAR	A	1608	-	45,45,45	1.19	4 (8%)	67,67,67	1.63	13 (19%)
22	PAR	A	1609	-	45,45,45	1.15	5 (11%)	67,67,67	1.57	14 (20%)
22	PAR	A	1610	-	45,45,45	1.58	8 (17%)	67,67,67	1.64	13 (19%)
22	PAR	A	1611	-	45,45,45	2.00	13 (28%)	67,67,67	1.58	10 (14%)
22	PAR	A	1612	-	45,45,45	1.56	6 (13%)	67,67,67	1.66	14 (20%)
22	PAR	A	1613	-	45,45,45	1.63	10 (22%)	67,67,67	1.63	13 (19%)
22	PAR	A	1614	-	45,45,45	1.48	8 (17%)	67,67,67	1.63	12 (17%)
22	PAR	A	1615	-	45,45,45	1.51	8 (17%)	67,67,67	1.60	15 (22%)
22	PAR	A	1616	-	45,45,45	1.41	6 (13%)	67,67,67	1.60	13 (19%)
22	PAR	A	1617	-	45,45,45	1.35	5 (11%)	67,67,67	1.59	14 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PAR	A	1601	-	-	0/18/94/94	0/4/4/4
22	PAR	A	1602	-	-	0/18/94/94	1/4/4/4
22	PAR	A	1603	-	-	0/18/94/94	0/4/4/4
22	PAR	A	1604	-	-	0/18/94/94	0/4/4/4
22	PAR	A	1605	-	-	0/18/94/94	1/4/4/4
22	PAR	A	1606	-	-	0/18/94/94	0/4/4/4
22	PAR	A	1607	-	-	0/18/94/94	0/4/4/4
22	PAR	A	1608	-	-	0/18/94/94	0/4/4/4
22	PAR	A	1609	-	-	0/18/94/94	0/4/4/4
22	PAR	A	1610	-	-	1/18/94/94	0/4/4/4
22	PAR	A	1611	-	-	0/18/94/94	1/4/4/4
22	PAR	A	1612	-	-	1/18/94/94	1/4/4/4
22	PAR	A	1613	-	-	0/18/94/94	1/4/4/4
22	PAR	A	1614	-	-	0/18/94/94	1/4/4/4
22	PAR	A	1615	-	-	0/18/94/94	1/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PAR	A	1616	-	-	1/18/94/94	2/4/4/4
22	PAR	A	1617	-	-	0/18/94/94	1/4/4/4

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1611	PAR	C13-C23	5.23	1.59	1.52
22	A	1611	PAR	C52-C42	5.04	1.62	1.52
22	A	1603	PAR	C31-C21	4.44	1.59	1.53
22	A	1612	PAR	C14-C24	4.38	1.60	1.52
22	A	1604	PAR	C52-C42	4.33	1.60	1.52
22	A	1614	PAR	C13-C23	4.31	1.58	1.52
22	A	1612	PAR	O43-C13	4.30	1.49	1.41
22	A	1611	PAR	C22-C12	-4.30	1.48	1.52
22	A	1615	PAR	C34-C24	4.23	1.59	1.53
22	A	1613	PAR	C13-C23	4.18	1.58	1.52
22	A	1617	PAR	O43-C13	4.14	1.49	1.41
22	A	1610	PAR	C34-C24	3.86	1.58	1.53
22	A	1613	PAR	C52-C42	3.74	1.59	1.52
22	A	1610	PAR	C52-C42	3.65	1.59	1.52
22	A	1607	PAR	O43-C13	3.62	1.48	1.41
22	A	1610	PAR	C13-C23	3.57	1.57	1.52
22	A	1613	PAR	C31-C21	3.48	1.58	1.53
22	A	1615	PAR	C52-C42	3.46	1.59	1.52
22	A	1604	PAR	C22-C32	-3.44	1.49	1.52
22	A	1611	PAR	C14-C24	3.43	1.59	1.52
22	A	1607	PAR	C13-C23	3.40	1.57	1.52
22	A	1603	PAR	C52-C42	3.38	1.59	1.52
22	A	1612	PAR	C52-C42	3.34	1.58	1.52
22	A	1616	PAR	O43-C13	3.34	1.47	1.41
22	A	1610	PAR	C14-C24	3.31	1.58	1.52
22	A	1617	PAR	C52-C42	3.31	1.58	1.52
22	A	1614	PAR	C52-C42	3.29	1.58	1.52
22	A	1611	PAR	C31-C21	3.28	1.58	1.53
22	A	1612	PAR	C34-C24	3.26	1.57	1.53
22	A	1606	PAR	C52-C42	3.22	1.58	1.52
22	A	1610	PAR	O43-C13	3.21	1.47	1.41
22	A	1614	PAR	C14-C24	3.19	1.58	1.52
22	A	1612	PAR	C13-C23	3.18	1.56	1.52
22	A	1616	PAR	C52-C42	3.15	1.58	1.52
22	A	1613	PAR	C34-C24	3.14	1.57	1.53
22	A	1611	PAR	O33-C14	3.12	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1615	PAR	C13-C23	3.01	1.56	1.52
22	A	1605	PAR	C13-C23	2.98	1.56	1.52
22	A	1615	PAR	C14-C24	2.92	1.58	1.52
22	A	1617	PAR	C34-C24	2.87	1.57	1.53
22	A	1611	PAR	C34-C24	2.84	1.57	1.53
22	A	1611	PAR	C62-C52	2.83	1.60	1.52
22	A	1608	PAR	O43-C13	2.83	1.46	1.41
22	A	1613	PAR	C14-C24	2.83	1.57	1.52
22	A	1616	PAR	C31-C21	2.81	1.57	1.53
22	A	1611	PAR	O52-C52	2.80	1.50	1.43
22	A	1601	PAR	C22-C12	-2.79	1.50	1.52
22	A	1609	PAR	C52-C42	2.78	1.57	1.52
22	A	1610	PAR	O33-C14	2.77	1.49	1.41
22	A	1613	PAR	C62-C52	2.76	1.60	1.52
22	A	1606	PAR	O43-C13	2.71	1.46	1.41
22	A	1605	PAR	C52-C42	2.68	1.57	1.52
22	A	1617	PAR	C13-C23	2.68	1.56	1.52
22	A	1606	PAR	C31-C21	2.66	1.57	1.53
22	A	1606	PAR	C13-C23	2.63	1.56	1.52
22	A	1608	PAR	C34-C24	2.60	1.57	1.53
22	A	1601	PAR	C52-C42	2.60	1.57	1.52
22	A	1604	PAR	C22-C12	-2.58	1.50	1.52
22	A	1616	PAR	C13-C23	2.57	1.56	1.52
22	A	1611	PAR	C42-C32	2.54	1.56	1.52
22	A	1608	PAR	C22-C12	2.54	1.54	1.52
22	A	1601	PAR	C31-C21	2.53	1.56	1.53
22	A	1607	PAR	C34-C24	2.53	1.56	1.53
22	A	1607	PAR	C52-C42	2.51	1.57	1.52
22	A	1612	PAR	O33-C14	2.49	1.48	1.41
22	A	1606	PAR	C42-C32	2.46	1.56	1.52
22	A	1616	PAR	O33-C14	2.44	1.48	1.41
22	A	1602	PAR	C11-C21	2.42	1.57	1.52
22	A	1613	PAR	O43-C13	2.41	1.45	1.41
22	A	1611	PAR	C22-C32	-2.39	1.50	1.52
22	A	1602	PAR	C42-C32	2.33	1.56	1.52
22	A	1602	PAR	O43-C13	2.31	1.45	1.41
22	A	1609	PAR	C33-C43	2.31	1.59	1.52
22	A	1614	PAR	C33-C43	2.29	1.59	1.52
22	A	1611	PAR	O33-C33	2.28	1.49	1.43
22	A	1609	PAR	C31-C21	2.27	1.56	1.53
22	A	1616	PAR	C22-C32	2.26	1.54	1.52
22	A	1615	PAR	O52-C52	2.23	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1614	PAR	O52-C52	2.22	1.49	1.43
22	A	1608	PAR	C13-C23	2.20	1.55	1.52
22	A	1606	PAR	C33-C43	2.18	1.59	1.52
22	A	1610	PAR	C42-C32	2.17	1.56	1.52
22	A	1615	PAR	C33-C43	2.16	1.59	1.52
22	A	1613	PAR	O11-C42	2.16	1.49	1.43
22	A	1604	PAR	C33-C43	2.15	1.59	1.52
22	A	1603	PAR	O43-C13	2.14	1.45	1.41
22	A	1614	PAR	C31-C21	2.13	1.56	1.53
22	A	1605	PAR	O43-C13	2.13	1.45	1.41
22	A	1609	PAR	C13-C23	2.12	1.55	1.52
22	A	1610	PAR	C44-C54	2.10	1.57	1.53
22	A	1614	PAR	C62-C52	2.09	1.58	1.52
22	A	1601	PAR	C33-C43	2.08	1.58	1.52
22	A	1615	PAR	C42-C32	2.08	1.55	1.52
22	A	1602	PAR	C33-C43	2.07	1.58	1.52
22	A	1613	PAR	O52-C52	2.07	1.49	1.43
22	A	1617	PAR	C31-C21	2.06	1.56	1.53
22	A	1609	PAR	C34-C24	2.06	1.56	1.53
22	A	1615	PAR	O43-C13	2.05	1.45	1.41
22	A	1613	PAR	C11-C21	2.04	1.56	1.52
22	A	1611	PAR	O43-C13	2.02	1.45	1.41
22	A	1614	PAR	O43-C13	2.01	1.45	1.41

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1612	PAR	O33-C14-C24	6.49	120.94	108.09
22	A	1610	PAR	O33-C14-C24	6.22	120.40	108.09
22	A	1602	PAR	O33-C14-C24	6.00	119.96	108.09
22	A	1611	PAR	O33-C14-C24	5.75	119.46	108.09
22	A	1605	PAR	O33-C14-C24	5.72	119.40	108.09
22	A	1616	PAR	O33-C14-C24	5.70	119.38	108.09
22	A	1617	PAR	O33-C14-C24	5.66	119.29	108.09
22	A	1608	PAR	O33-C14-C24	5.65	119.28	108.09
22	A	1613	PAR	O33-C14-C24	5.44	118.86	108.09
22	A	1614	PAR	O33-C14-C24	5.38	118.73	108.09
22	A	1607	PAR	O33-C14-C24	5.33	118.64	108.09
22	A	1615	PAR	O33-C14-C24	5.25	118.47	108.09
22	A	1604	PAR	O33-C14-C24	4.95	117.89	108.09
22	A	1606	PAR	O52-C13-C23	4.74	115.95	107.50
22	A	1606	PAR	O33-C14-C24	4.74	117.46	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	PAR	O33-C14-C24	4.63	117.25	108.09
22	A	1609	PAR	O52-C13-C23	4.62	115.74	107.50
22	A	1603	PAR	O33-C14-C24	4.56	117.11	108.09
22	A	1609	PAR	O33-C14-C24	4.45	116.90	108.09
22	A	1614	PAR	O52-C13-C23	4.42	115.39	107.50
22	A	1602	PAR	O52-C13-O43	-4.41	107.29	111.51
22	A	1603	PAR	O52-C13-C23	4.39	115.34	107.50
22	A	1615	PAR	O52-C13-C23	4.39	115.33	107.50
22	A	1611	PAR	O52-C13-C23	4.28	115.15	107.50
22	A	1601	PAR	O52-C13-C23	4.07	114.76	107.50
22	A	1608	PAR	O52-C13-C23	3.99	114.62	107.50
22	A	1610	PAR	O52-C13-C23	3.90	114.47	107.50
22	A	1604	PAR	O52-C13-C23	3.85	114.37	107.50
22	A	1616	PAR	O52-C13-C23	3.85	114.37	107.50
22	A	1605	PAR	O52-C13-C23	3.82	114.32	107.50
22	A	1602	PAR	O43-C13-C23	-3.64	99.94	104.92
22	A	1607	PAR	O52-C13-C23	3.64	114.00	107.50
22	A	1613	PAR	O52-C13-C23	3.58	113.88	107.50
22	A	1612	PAR	O52-C13-C23	3.56	113.85	107.50
22	A	1613	PAR	O52-C13-O43	-3.53	108.13	111.51
22	A	1602	PAR	O34-C34-C44	-3.52	102.46	110.35
22	A	1613	PAR	C13-C23-C33	3.46	106.69	102.05
22	A	1617	PAR	O52-C13-C23	3.40	113.57	107.50
22	A	1612	PAR	O52-C13-O43	-3.37	108.28	111.51
22	A	1610	PAR	O52-C13-O43	-3.34	108.31	111.51
22	A	1614	PAR	O11-C11-O51	3.33	119.01	110.69
22	A	1612	PAR	O34-C34-C44	-3.31	102.93	110.35
22	A	1608	PAR	O52-C13-O43	-3.29	108.36	111.51
22	A	1614	PAR	C34-C24-N24	-3.29	104.41	110.91
22	A	1606	PAR	O11-C11-O51	3.28	118.88	110.69
22	A	1605	PAR	C34-C24-N24	-3.28	104.42	110.91
22	A	1605	PAR	C13-C23-C33	3.28	106.45	102.05
22	A	1606	PAR	C34-C24-N24	-3.27	104.43	110.91
22	A	1614	PAR	C13-C23-C33	3.27	106.43	102.05
22	A	1617	PAR	C14-O33-C33	-3.25	109.69	117.99
22	A	1609	PAR	C34-C24-N24	-3.25	104.49	110.91
22	A	1611	PAR	C13-C23-C33	3.23	106.39	102.05
22	A	1610	PAR	C34-C24-N24	-3.23	104.52	110.91
22	A	1615	PAR	O11-C11-O51	3.23	118.75	110.69
22	A	1609	PAR	O34-C34-C44	-3.20	103.18	110.35
22	A	1605	PAR	C14-O33-C33	-3.18	109.87	117.99
22	A	1611	PAR	O11-C11-O51	3.18	118.61	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1603	PAR	O34-C34-C44	-3.17	103.25	110.35
22	A	1611	PAR	C34-C24-N24	-3.17	104.65	110.91
22	A	1616	PAR	O11-C11-O51	3.16	118.58	110.69
22	A	1601	PAR	O34-C34-C44	-3.16	103.27	110.35
22	A	1613	PAR	O11-C11-O51	3.12	118.47	110.69
22	A	1607	PAR	O34-C34-C44	-3.10	103.41	110.35
22	A	1608	PAR	O34-C34-C44	-3.05	103.50	110.35
22	A	1603	PAR	C34-C24-N24	-3.05	104.87	110.91
22	A	1608	PAR	C34-C24-N24	-3.05	104.88	110.91
22	A	1601	PAR	C34-C24-N24	-3.05	104.89	110.91
22	A	1604	PAR	C34-C24-N24	-3.03	104.91	110.91
22	A	1617	PAR	O34-C34-C44	-3.03	103.56	110.35
22	A	1604	PAR	O11-C11-O51	3.03	118.24	110.69
22	A	1605	PAR	O34-C34-C44	-3.03	103.57	110.35
22	A	1617	PAR	O11-C11-O51	3.02	118.22	110.69
22	A	1612	PAR	O11-C11-O51	3.02	118.22	110.69
22	A	1607	PAR	C34-C24-N24	-3.01	104.95	110.91
22	A	1603	PAR	O11-C11-O51	3.01	118.20	110.69
22	A	1613	PAR	C34-C24-N24	-3.01	104.96	110.91
22	A	1612	PAR	C34-C24-N24	-3.00	104.97	110.91
22	A	1616	PAR	O52-C13-O43	-2.99	108.65	111.51
22	A	1609	PAR	O11-C11-O51	2.99	118.15	110.69
22	A	1607	PAR	O52-C13-O43	-2.99	108.65	111.51
22	A	1617	PAR	C34-C24-N24	-2.99	105.00	110.91
22	A	1604	PAR	O34-C34-C44	-2.95	103.74	110.35
22	A	1616	PAR	C14-O33-C33	-2.94	110.49	117.99
22	A	1616	PAR	C34-C24-N24	-2.94	105.09	110.91
22	A	1604	PAR	O52-C13-O43	-2.93	108.70	111.51
22	A	1610	PAR	O11-C11-O51	2.93	118.00	110.69
22	A	1613	PAR	C14-O33-C33	-2.92	110.54	117.99
22	A	1607	PAR	O11-C11-O51	2.91	117.96	110.69
22	A	1611	PAR	O34-C34-C44	-2.90	103.84	110.35
22	A	1607	PAR	C14-O33-C33	-2.90	110.59	117.99
22	A	1616	PAR	O34-C34-C44	-2.89	103.88	110.35
22	A	1601	PAR	O11-C11-O51	2.88	117.87	110.69
22	A	1613	PAR	O34-C34-C44	-2.88	103.90	110.35
22	A	1605	PAR	O11-C11-O51	2.86	117.82	110.69
22	A	1603	PAR	O52-C13-O43	-2.86	108.77	111.51
22	A	1602	PAR	O52-C13-C23	2.85	112.58	107.50
22	A	1614	PAR	O34-C34-C44	-2.84	103.98	110.35
22	A	1615	PAR	C34-C24-N24	-2.83	105.30	110.91
22	A	1605	PAR	O52-C13-O43	-2.82	108.81	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1605	PAR	O54-C54-C44	2.81	114.96	109.76
22	A	1607	PAR	O51-C51-C61	2.80	113.21	106.34
22	A	1615	PAR	O34-C34-C44	-2.79	104.09	110.35
22	A	1603	PAR	C13-O52-C52	-2.77	110.93	117.99
22	A	1606	PAR	C22-C32-C42	2.75	114.72	109.83
22	A	1612	PAR	O54-C54-C44	2.75	114.85	109.76
22	A	1602	PAR	O11-C11-O51	2.75	117.55	110.69
22	A	1608	PAR	O11-C11-O51	2.75	117.55	110.69
22	A	1602	PAR	C14-O33-C33	-2.73	111.02	117.99
22	A	1610	PAR	O34-C34-C44	-2.70	104.30	110.35
22	A	1606	PAR	O34-C34-C44	-2.69	104.31	110.35
22	A	1602	PAR	C34-C24-N24	-2.68	105.61	110.91
22	A	1609	PAR	C13-O52-C52	-2.67	111.17	117.99
22	A	1613	PAR	O11-C42-C52	2.66	114.25	107.41
22	A	1617	PAR	O52-C13-O43	-2.66	108.96	111.51
22	A	1610	PAR	O51-C51-C61	2.62	112.78	106.34
22	A	1608	PAR	C22-C12-C62	2.61	114.04	110.06
22	A	1616	PAR	O54-C54-C44	2.61	114.58	109.76
22	A	1616	PAR	O51-C51-C61	2.59	112.70	106.34
22	A	1612	PAR	C14-O33-C33	-2.57	111.42	117.99
22	A	1608	PAR	C14-O33-C33	-2.57	111.45	117.99
22	A	1615	PAR	C14-O33-C33	-2.54	111.52	117.99
22	A	1611	PAR	C14-O33-C33	-2.53	111.54	117.99
22	A	1615	PAR	C13-C23-C33	2.52	105.44	102.05
22	A	1604	PAR	O54-C54-C44	2.51	114.42	109.76
22	A	1606	PAR	C31-C41-C51	2.51	114.69	110.20
22	A	1614	PAR	C11-O51-C51	2.51	118.60	113.73
22	A	1604	PAR	C13-O52-C52	-2.50	111.62	117.99
22	A	1602	PAR	O34-C34-C24	-2.48	105.84	110.06
22	A	1606	PAR	C13-O52-C52	-2.48	111.67	117.99
22	A	1610	PAR	C11-O51-C51	2.47	118.54	113.73
22	A	1604	PAR	C13-C23-C33	2.46	105.36	102.05
22	A	1608	PAR	O51-C51-C61	2.46	112.40	106.34
22	A	1607	PAR	C22-C12-C62	2.46	113.81	110.06
22	A	1614	PAR	C14-O33-C33	-2.46	111.72	117.99
22	A	1614	PAR	C22-C12-C62	2.46	113.80	110.06
22	A	1615	PAR	C13-O52-C52	-2.45	111.74	117.99
22	A	1606	PAR	O52-C13-O43	-2.44	109.17	111.51
22	A	1614	PAR	O52-C13-O43	-2.44	109.17	111.51
22	A	1605	PAR	O51-C51-C61	2.44	112.33	106.34
22	A	1613	PAR	O52-C52-C42	2.43	113.65	107.41
22	A	1602	PAR	C22-C32-C42	2.43	114.14	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1610	PAR	C14-O33-C33	-2.43	111.80	117.99
22	A	1615	PAR	O52-C13-O43	-2.42	109.19	111.51
22	A	1613	PAR	O51-C51-C61	2.42	112.28	106.34
22	A	1615	PAR	O51-C51-C61	2.40	112.23	106.34
22	A	1611	PAR	C11-O51-C51	2.40	118.39	113.73
22	A	1605	PAR	C13-O52-C52	-2.40	111.88	117.99
22	A	1601	PAR	C13-O52-C52	-2.39	111.89	117.99
22	A	1613	PAR	C22-C12-C62	2.38	113.69	110.06
22	A	1610	PAR	O54-C54-C44	2.38	114.16	109.76
22	A	1601	PAR	O33-C14-O54	-2.38	104.76	110.69
22	A	1601	PAR	C22-C32-C42	2.37	114.03	109.83
22	A	1611	PAR	O51-C51-C61	2.36	112.14	106.34
22	A	1609	PAR	C14-O33-C33	-2.36	111.98	117.99
22	A	1609	PAR	O33-C14-O54	-2.36	104.82	110.69
22	A	1601	PAR	O34-C34-C24	-2.35	106.06	110.06
22	A	1606	PAR	O43-C13-C23	-2.34	101.72	104.92
22	A	1603	PAR	O34-C34-C24	-2.34	106.08	110.06
22	A	1609	PAR	O52-C13-O43	-2.33	109.28	111.51
22	A	1617	PAR	O51-C51-C61	2.32	112.05	106.34
22	A	1601	PAR	O51-C51-C61	2.32	112.05	106.34
22	A	1608	PAR	C13-C23-C33	2.32	105.17	102.05
22	A	1614	PAR	O51-C51-C61	2.31	112.02	106.34
22	A	1608	PAR	C13-O52-C52	-2.31	112.09	117.99
22	A	1616	PAR	C13-O52-C52	-2.31	112.11	117.99
22	A	1617	PAR	C22-C12-C62	2.31	113.57	110.06
22	A	1614	PAR	C13-O52-C52	-2.31	112.11	117.99
22	A	1603	PAR	O51-C51-C61	2.30	112.00	106.34
22	A	1604	PAR	C14-O33-C33	-2.30	112.12	117.99
22	A	1610	PAR	C13-O52-C52	-2.30	112.13	117.99
22	A	1611	PAR	C22-C32-C42	2.29	113.90	109.83
22	A	1604	PAR	O51-C51-C61	2.28	111.95	106.34
22	A	1616	PAR	C22-C32-C42	2.28	113.88	109.83
22	A	1612	PAR	C11-O51-C51	2.27	118.14	113.73
22	A	1609	PAR	O43-C13-C23	-2.26	101.83	104.92
22	A	1601	PAR	O52-C13-O43	-2.24	109.36	111.51
22	A	1609	PAR	C22-C12-C62	2.23	113.45	110.06
22	A	1617	PAR	C11-O51-C51	2.23	118.06	113.73
22	A	1617	PAR	C13-O52-C52	-2.23	112.31	117.99
22	A	1609	PAR	O51-C51-C61	2.22	111.80	106.34
22	A	1612	PAR	O51-C51-C61	2.20	111.76	106.34
22	A	1602	PAR	O51-C51-C61	2.20	111.76	106.34
22	A	1615	PAR	C22-C32-C42	2.19	113.72	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1617	PAR	O33-C14-O54	-2.18	105.26	110.69
22	A	1606	PAR	O51-C51-C61	2.18	111.69	106.34
22	A	1617	PAR	C22-C32-C42	2.17	113.69	109.83
22	A	1617	PAR	O54-C54-C44	2.17	113.79	109.76
22	A	1607	PAR	C13-C23-C33	2.17	104.96	102.05
22	A	1612	PAR	C23-C33-C43	-2.16	98.96	103.16
22	A	1602	PAR	C11-O51-C51	2.16	117.92	113.73
22	A	1604	PAR	O11-C11-C21	-2.15	103.83	108.09
22	A	1601	PAR	O43-C13-C23	-2.15	101.99	104.92
22	A	1601	PAR	C14-O33-C33	-2.14	112.53	117.99
22	A	1610	PAR	C22-C32-C42	2.14	113.62	109.83
22	A	1603	PAR	C14-O33-C33	-2.13	112.56	117.99
22	A	1609	PAR	O43-C43-C53	2.13	113.69	109.15
22	A	1606	PAR	O51-C51-C41	2.13	113.69	109.76
22	A	1612	PAR	C22-C32-C42	2.12	113.59	109.83
22	A	1616	PAR	C22-C12-C62	2.12	113.28	110.06
22	A	1615	PAR	C22-C12-C62	2.12	113.28	110.06
22	A	1607	PAR	O54-C54-C44	2.12	113.68	109.76
22	A	1608	PAR	O54-C54-C44	2.11	113.67	109.76
22	A	1605	PAR	O33-C14-O54	-2.11	105.43	110.69
22	A	1613	PAR	O33-C14-O54	-2.11	105.43	110.69
22	A	1606	PAR	O54-C54-C44	2.11	113.66	109.76
22	A	1607	PAR	C13-O52-C52	-2.11	112.62	117.99
22	A	1607	PAR	C11-O51-C51	2.10	117.82	113.73
22	A	1601	PAR	C23-C33-C43	-2.10	99.07	103.16
22	A	1603	PAR	C22-C32-C42	2.09	113.54	109.83
22	A	1603	PAR	O33-C14-O54	-2.09	105.48	110.69
22	A	1606	PAR	C11-O51-C51	2.09	117.78	113.73
22	A	1608	PAR	C11-O51-C51	2.07	117.76	113.73
22	A	1609	PAR	C11-O51-C51	2.07	117.76	113.73
22	A	1610	PAR	C13-C23-C33	2.06	104.82	102.05
22	A	1606	PAR	C23-C33-C43	-2.05	99.17	103.16
22	A	1604	PAR	C11-O51-C51	2.05	117.70	113.73
22	A	1612	PAR	C13-O52-C52	-2.04	112.79	117.99
22	A	1607	PAR	O33-C14-O54	-2.04	105.61	110.69
22	A	1612	PAR	O33-C14-O54	-2.03	105.63	110.69
22	A	1615	PAR	O54-C54-C44	2.03	113.51	109.76
22	A	1615	PAR	O52-C52-C42	2.02	112.61	107.41
22	A	1605	PAR	C22-C12-C62	2.02	113.14	110.06
22	A	1616	PAR	O33-C14-O54	-2.02	105.66	110.69
22	A	1602	PAR	O54-C54-C44	2.01	113.48	109.76
22	A	1615	PAR	O33-C14-O54	-2.00	105.70	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1602	PAR	C23-C33-C43	-2.00	99.27	103.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1616	PAR	C42-O11-C11-C21
22	A	1612	PAR	C33-O33-C14-C24
22	A	1610	PAR	C33-O33-C14-C24

All (10) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1615	PAR	C12-C22-C32-C42-C52-C62
22	A	1617	PAR	C12-C22-C32-C42-C52-C62
22	A	1616	PAR	C12-C22-C32-C42-C52-C62
22	A	1616	PAR	C14-C24-C34-C44-C54-O54
22	A	1614	PAR	C14-C24-C34-C44-C54-O54
22	A	1611	PAR	C14-C24-C34-C44-C54-O54
22	A	1605	PAR	C14-C24-C34-C44-C54-O54
22	A	1612	PAR	C14-C24-C34-C44-C54-O54
22	A	1613	PAR	C14-C24-C34-C44-C54-O54
22	A	1602	PAR	C14-C24-C34-C44-C54-O54

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1511/1522 (99%)	-0.33	17 (1%) 77 30	48, 80, 189, 551	0
2	B	236/256 (92%)	-0.17	0 100 100	60, 104, 154, 168	0
3	C	207/239 (86%)	-0.18	0 100 100	69, 106, 153, 184	0
4	D	208/209 (99%)	-0.18	1 (0%) 88 48	53, 86, 123, 147	0
5	E	151/162 (93%)	-0.31	0 100 100	50, 70, 105, 144	0
6	F	101/101 (100%)	-0.13	0 100 100	73, 111, 136, 155	0
7	G	155/156 (99%)	-0.22	0 100 100	66, 100, 155, 187	0
8	H	138/138 (100%)	-0.32	0 100 100	45, 68, 95, 127	0
9	I	127/128 (99%)	0.01	1 (0%) 83 37	67, 110, 140, 169	0
10	J	99/105 (94%)	0.29	4 (4%) 36 8	69, 133, 194, 209	0
11	K	117/129 (90%)	-0.12	0 100 100	57, 85, 120, 137	0
12	L	124/135 (91%)	-0.09	1 (0%) 83 37	47, 87, 123, 166	0
13	M	118/126 (93%)	0.05	3 (2%) 54 13	72, 106, 131, 151	0
14	N	60/61 (98%)	-0.09	1 (1%) 67 21	76, 97, 143, 194	0
15	O	88/89 (98%)	-0.14	0 100 100	67, 87, 119, 163	0
16	P	84/88 (95%)	-0.20	0 100 100	61, 77, 109, 166	0
17	Q	101/105 (96%)	-0.18	0 100 100	54, 74, 108, 154	0
18	R	73/88 (82%)	-0.00	0 100 100	65, 87, 190, 221	0
19	S	81/93 (87%)	0.05	2 (2%) 54 13	93, 124, 165, 187	0
20	T	99/106 (93%)	-0.08	0 100 100	61, 85, 130, 156	0
21	U	25/27 (92%)	0.64	1 (4%) 36 8	77, 95, 129, 151	0
All	All	3903/4063 (96%)	-0.20	31 (0%) 79 37	45, 89, 157, 551	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1002	G	5.9
1	A	1129	C	5.7
1	A	1540	PSU	5.0
1	A	1003	G	4.7
14	N	12	ARG	4.3
9	I	128	ARG	4.0
1	A	841	U	3.9
21	U	26	LYS	3.9
1	A	930	C	3.6
19	S	29	ARG	3.6
1	A	1533	C	3.5
1	A	1532	U	3.4
1	A	1498	UR3	3.3
1	A	1539	C	2.8
10	J	71	LEU	2.7
13	M	8	GLU	2.7
13	M	5	ALA	2.6
12	L	129	ALA	2.6
4	D	47	ARG	2.6
1	A	1033	G	2.6
1	A	1389	C	2.6
1	A	1027	C	2.4
10	J	6	ILE	2.3
1	A	202	U	2.3
1	A	1001	A	2.3
1	A	1531	A	2.2
1	A	1034	G	2.2
13	M	7	VAL	2.1
19	S	28	LYS	2.1
10	J	8	LEU	2.1
10	J	72	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	MA6	A	1518	24/25	0.20	-	57,62,73,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	0TD	L	92	10/11	0.26	-	47,89,101,397	0
1	UR3	A	1498	21/22	0.19	-	57,68,78,81	0
1	7MG	A	527	24/25	0.17	-	60,65,76,80	0
1	5MC	A	967	21/22	0.13	-	53,66,76,80	0
1	MA6	A	1519	24/25	0.23	-	50,57,68,73	0
1	5MC	A	1407	21/22	0.17	-	58,69,78,82	0
1	5MC	A	1404	21/22	0.17	-	52,62,70,73	0
1	5MC	A	1400	21/22	0.18	-	56,78,91,92	0
1	PSU	A	516	20/21	0.13	-	91,99,107,112	0
1	PSU	A	1541	20/21	0.28	-	205,208,212,214	0
1	2MG	A	1207	24/25	0.14	-	84,91,99,100	0
1	PSU	A	1540	20/21	0.54	-	197,257,265,266	0
1	4OC	A	1402	22/23	0.17	-	56,67,76,80	0
1	M2G	A	966	25/26	0.14	-	65,74,83,93	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1628	1/1	0.19	-	44,44,44,44	0
23	MG	A	1736	1/1	0.24	-	138,138,138,138	0
23	MG	A	1694	1/1	0.30	-	97,97,97,97	0
23	MG	A	1779	1/1	0.17	-	70,70,70,70	0
23	MG	A	1831	1/1	0.43	-	85,85,85,85	0
23	MG	A	1713	1/1	0.19	-	95,95,95,95	0
23	MG	A	1770	1/1	0.24	-	101,101,101,101	0
23	MG	A	1842	1/1	0.32	-	70,70,70,70	0
23	MG	A	1621	1/1	0.08	-	131,131,131,131	0
23	MG	A	1899[B]	1/1	0.57	-	45,45,45,45	1
23	MG	A	1899[A]	1/1	0.57	-	45,45,45,45	1
23	MG	A	1892	1/1	0.18	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1673	1/1	0.13	-	70,70,70,70	0
23	MG	A	1667	1/1	0.17	-	78,78,78,78	0
23	MG	A	1620	1/1	0.16	-	91,91,91,91	0
23	MG	A	1783	1/1	0.35	-	132,132,132,132	0
22	PAR	A	1606	42/42	0.17	-	64,64,64,64	42
23	MG	A	1657	1/1	0.10	-	54,54,54,54	0
23	MG	H	202	1/1	0.17	-	72,72,72,72	0
23	MG	A	1858[A]	1/1	0.39	-	32,32,32,32	1
23	MG	A	1650	1/1	0.16	-	106,106,106,106	0
23	MG	A	1705	1/1	0.07	-	76,76,76,76	0
23	MG	A	1897	1/1	0.28	-	47,47,47,47	0
23	MG	A	1764	1/1	0.20	-	107,107,107,107	0
23	MG	A	1688	1/1	0.15	-	115,115,115,115	0
23	MG	A	1854	1/1	0.43	-	76,76,76,76	0
23	MG	A	1678	1/1	0.19	-	101,101,101,101	0
23	MG	A	1855	1/1	0.34	-	74,74,74,74	0
23	MG	A	1710	1/1	0.34	-	92,92,92,92	0
23	MG	A	1618	1/1	0.21	-	79,79,79,79	0
23	MG	A	1739	1/1	0.39	-	84,84,84,84	0
23	MG	A	1809	1/1	0.35	-	58,58,58,58	0
23	MG	A	1910	1/1	0.10	-	80,80,80,80	0
23	MG	A	1767	1/1	0.15	-	113,113,113,113	0
23	MG	A	1716	1/1	0.22	-	74,74,74,74	0
23	MG	A	1884	1/1	0.65	-	85,85,85,85	0
23	MG	A	1872	1/1	0.20	-	59,59,59,59	0
22	PAR	A	1603	42/42	0.19	-	83,83,83,83	3
23	MG	A	1861	1/1	1.09	-	75,75,75,75	0
23	MG	A	1754	1/1	0.08	-	111,111,111,111	0
23	MG	A	1655	1/1	0.10	-	87,87,87,87	0
23	MG	A	1623	1/1	0.10	-	62,62,62,62	0
23	MG	A	1793	1/1	1.28	-	84,84,84,84	0
23	MG	A	1921[A]	1/1	0.14	-	28,28,28,28	1
23	MG	A	1865	1/1	0.10	-	66,66,66,66	0
23	MG	A	1879	1/1	0.26	-	79,79,79,79	0
22	PAR	A	1604	42/42	0.20	-	70,70,70,70	0
23	MG	D	302	1/1	0.10	-	112,112,112,112	0
23	MG	A	1666	1/1	0.09	-	54,54,54,54	0
23	MG	A	1904	1/1	0.11	-	80,80,80,80	0
23	MG	A	1722	1/1	0.12	-	100,100,100,100	0
23	MG	A	1761	1/1	0.14	-	103,103,103,103	0
23	MG	A	1674	1/1	0.20	-	96,96,96,96	0
23	MG	A	1814	1/1	0.26	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1774	1/1	0.16	-	95,95,95,95	0
23	MG	A	1698	1/1	0.15	-	91,91,91,91	0
23	MG	A	1788	1/1	0.54	-	75,75,75,75	0
23	MG	A	1634	1/1	0.20	-	44,44,44,44	0
23	MG	A	1738	1/1	0.72	-	116,116,116,116	0
23	MG	A	1723	1/1	0.21	-	103,103,103,103	0
23	MG	A	1744	1/1	0.12	-	99,99,99,99	0
23	MG	A	1827	1/1	0.39	-	91,91,91,91	0
22	PAR	A	1615	42/42	0.28	-	169,169,169,169	0
23	MG	A	1752	1/1	0.25	-	105,105,105,105	0
23	MG	A	1893	1/1	0.25	-	71,71,71,71	0
23	MG	A	1711	1/1	0.09	-	102,102,102,102	0
23	MG	A	1911	1/1	0.11	-	62,62,62,62	0
23	MG	A	1798	1/1	0.63	-	75,75,75,75	0
23	MG	A	1800	1/1	0.19	-	83,83,83,83	0
23	MG	A	1725	1/1	0.09	-	94,94,94,94	0
23	MG	A	1818	1/1	0.18	-	79,79,79,79	0
23	MG	A	1660	1/1	0.05	-	66,66,66,66	0
23	MG	A	1819	1/1	1.05	-	96,96,96,96	0
23	MG	A	1652	1/1	0.46	-	86,86,86,86	0
23	MG	A	1715	1/1	0.20	-	107,107,107,107	0
23	MG	A	1775	1/1	0.14	-	83,83,83,83	0
23	MG	A	1895[A]	1/1	0.59	-	30,30,30,30	1
23	MG	A	1760	1/1	0.26	-	77,77,77,77	0
23	MG	A	1811	1/1	0.83	-	87,87,87,87	0
23	MG	A	1709	1/1	0.36	-	87,87,87,87	0
23	MG	A	1772	1/1	0.12	-	67,67,67,67	0
23	MG	Q	201	1/1	0.12	-	86,86,86,86	0
23	MG	P	101	1/1	0.43	-	63,63,63,63	0
23	MG	A	1762	1/1	0.07	-	127,127,127,127	0
23	MG	A	1646	1/1	0.11	-	85,85,85,85	0
23	MG	A	1728	1/1	0.17	-	144,144,144,144	0
23	MG	A	1753	1/1	0.10	-	109,109,109,109	0
23	MG	A	1700	1/1	0.10	-	90,90,90,90	0
23	MG	A	1687	1/1	0.24	-	92,92,92,92	0
23	MG	A	1797	1/1	0.50	-	85,85,85,85	0
23	MG	A	1676	1/1	0.20	-	82,82,82,82	0
23	MG	A	1921[B]	1/1	0.14	-	28,28,28,28	1
23	MG	A	1887	1/1	0.26	-	93,93,93,93	0
23	MG	A	1875	1/1	0.07	-	55,55,55,55	0
23	MG	A	1692	1/1	0.09	-	98,98,98,98	0
23	MG	A	1636	1/1	0.20	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1766	1/1	0.25	-	118,118,118,118	0
23	MG	A	1838	1/1	0.42	-	80,80,80,80	0
24	ZN	D	301	1/1	0.54	-	194,194,194,194	0
23	MG	A	1741	1/1	0.09	-	76,76,76,76	0
23	MG	A	1665	1/1	0.19	-	90,90,90,90	0
23	MG	A	1906	1/1	0.55	-	75,75,75,75	0
23	MG	A	1836	1/1	0.30	-	86,86,86,86	0
23	MG	A	1820	1/1	0.16	-	88,88,88,88	0
23	MG	A	1625	1/1	0.10	-	90,90,90,90	0
23	MG	A	1916[B]	1/1	0.30	-	50,50,50,50	1
23	MG	A	1856	1/1	0.20	-	90,90,90,90	0
23	MG	A	1907	1/1	0.45	-	81,81,81,81	0
23	MG	F	201	1/1	0.63	-	80,80,80,80	0
23	MG	A	1638	1/1	0.32	-	93,93,93,93	0
23	MG	A	1684	1/1	0.15	-	81,81,81,81	0
23	MG	A	1627	1/1	0.15	-	70,70,70,70	0
23	MG	A	1812	1/1	1.03	-	77,77,77,77	0
23	MG	A	1663	1/1	0.30	-	92,92,92,92	0
23	MG	A	1719	1/1	0.10	-	71,71,71,71	0
23	MG	A	1868	1/1	0.18	-	73,73,73,73	0
23	MG	A	1895[B]	1/1	0.59	-	30,30,30,30	1
23	MG	A	1784	1/1	0.14	-	127,127,127,127	0
23	MG	A	1909	1/1	0.12	-	91,91,91,91	0
23	MG	A	1717	1/1	0.23	-	110,110,110,110	0
23	MG	A	1721	1/1	0.09	-	93,93,93,93	0
23	MG	A	1649	1/1	0.17	-	90,90,90,90	0
23	MG	A	1888	1/1	0.51	-	71,71,71,71	0
23	MG	A	1846	1/1	0.74	-	81,81,81,81	0
23	MG	A	1801	1/1	0.68	-	87,87,87,87	0
22	PAR	A	1616	42/42	0.44	-	126,126,126,126	42
23	MG	A	1640	1/1	0.28	-	78,78,78,78	0
23	MG	A	1661	1/1	0.24	-	112,112,112,112	0
23	MG	A	1830	1/1	0.57	-	92,92,92,92	0
23	MG	A	1731	1/1	0.24	-	140,140,140,140	0
23	MG	A	1735	1/1	0.22	-	92,92,92,92	0
23	MG	O	101	1/1	0.25	-	104,104,104,104	0
23	MG	A	1633	1/1	0.14	-	64,64,64,64	0
23	MG	A	1773	1/1	0.31	-	91,91,91,91	0
23	MG	A	1922	1/1	0.28	-	77,77,77,77	0
23	MG	A	1746	1/1	0.12	-	88,88,88,88	0
23	MG	A	1898	1/1	0.19	-	55,55,55,55	0
23	MG	A	1729	1/1	0.10	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	PAR	A	1609	42/42	0.22	-	77,77,77,77	42
23	MG	A	1718	1/1	0.54	-	89,89,89,89	0
23	MG	A	1699	1/1	0.19	-	112,112,112,112	0
23	MG	A	1825	1/1	0.33	-	88,88,88,88	0
23	MG	A	1668	1/1	0.11	-	92,92,92,92	0
23	MG	A	1792	1/1	0.30	-	100,100,100,100	0
23	MG	A	1685	1/1	0.18	-	90,90,90,90	0
23	MG	A	1689	1/1	0.14	-	87,87,87,87	0
23	MG	A	1763	1/1	0.33	-	102,102,102,102	0
23	MG	A	1918	1/1	0.54	-	90,90,90,90	0
23	MG	A	1807	1/1	0.90	-	96,96,96,96	0
23	MG	A	1643	1/1	0.39	-	74,74,74,74	0
23	MG	A	1730	1/1	0.15	-	98,98,98,98	0
23	MG	A	1869	1/1	0.26	-	71,71,71,71	0
23	MG	E	202	1/1	0.49	-	74,74,74,74	0
22	PAR	A	1607	42/42	0.23	-	92,92,92,92	42
23	MG	A	1829	1/1	0.28	-	90,90,90,90	0
23	MG	A	1891	1/1	0.47	-	70,70,70,70	0
23	MG	A	1896	1/1	0.62	-	89,89,89,89	0
23	MG	A	1664	1/1	0.09	-	94,94,94,94	0
23	MG	A	1740	1/1	0.13	-	96,96,96,96	0
23	MG	A	1845	1/1	0.21	-	63,63,63,63	0
23	MG	A	1874	1/1	0.43	-	90,90,90,90	0
23	MG	A	1690	1/1	0.10	-	108,108,108,108	0
23	MG	A	1849	1/1	0.38	-	63,63,63,63	0
23	MG	A	1883	1/1	0.29	-	68,68,68,68	0
23	MG	A	1782	1/1	0.13	-	62,62,62,62	0
23	MG	A	1810	1/1	0.12	-	63,63,63,63	0
23	MG	A	1808	1/1	0.49	-	93,93,93,93	0
23	MG	A	1843	1/1	0.15	-	62,62,62,62	0
23	MG	A	1789	1/1	0.16	-	100,100,100,100	0
23	MG	A	1885	1/1	0.34	-	96,96,96,96	0
23	MG	A	1900	1/1	0.43	-	77,77,77,77	0
23	MG	A	1724	1/1	0.05	-	97,97,97,97	0
23	MG	A	1759	1/1	0.29	-	79,79,79,79	0
23	MG	A	1671	1/1	0.34	-	68,68,68,68	0
23	MG	A	1683	1/1	0.17	-	73,73,73,73	0
23	MG	A	1905	1/1	0.40	-	100,100,100,100	0
23	MG	A	1742	1/1	0.20	-	146,146,146,146	0
23	MG	A	1902	1/1	0.36	-	93,93,93,93	0
23	MG	A	1791	1/1	0.41	-	84,84,84,84	0
23	MG	A	1749	1/1	0.17	-	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1786	1/1	0.16	-	154,154,154,154	0
23	MG	A	1641	1/1	0.27	-	92,92,92,92	0
23	MG	A	1630	1/1	0.15	-	87,87,87,87	0
23	MG	A	1920	1/1	0.16	-	72,72,72,72	0
23	MG	A	1917	1/1	0.57	-	68,68,68,68	0
23	MG	A	1781	1/1	0.27	-	104,104,104,104	0
23	MG	A	1776	1/1	0.08	-	86,86,86,86	0
23	MG	L	201	1/1	0.14	-	81,81,81,81	0
23	MG	A	1631	1/1	0.05	-	78,78,78,78	0
23	MG	A	1837	1/1	0.57	-	84,84,84,84	0
23	MG	A	1654	1/1	0.19	-	104,104,104,104	0
23	MG	A	1727	1/1	0.08	-	117,117,117,117	0
23	MG	A	1769	1/1	0.14	-	108,108,108,108	0
23	MG	A	1693	1/1	0.27	-	129,129,129,129	0
23	MG	A	1862	1/1	0.88	-	70,70,70,70	0
23	MG	A	1821	1/1	0.27	-	82,82,82,82	0
23	MG	A	1670	1/1	0.11	-	84,84,84,84	0
23	MG	A	1629	1/1	0.20	-	96,96,96,96	0
23	MG	A	1794	1/1	0.49	-	80,80,80,80	0
23	MG	A	1659	1/1	0.14	-	84,84,84,84	0
23	MG	A	1828	1/1	0.24	-	100,100,100,100	0
23	MG	A	1642	1/1	0.15	-	77,77,77,77	0
23	MG	A	1859[B]	1/1	0.36	-	59,59,59,59	1
23	MG	A	1859[A]	1/1	0.36	-	59,59,59,59	1
23	MG	A	1850	1/1	0.17	-	60,60,60,60	0
23	MG	A	1747	1/1	0.43	-	166,166,166,166	0
23	MG	I	201	1/1	0.25	-	92,92,92,92	0
23	MG	A	1682	1/1	0.16	-	33,33,33,33	0
23	MG	A	1871	1/1	0.69	-	85,85,85,85	0
23	MG	A	1805	1/1	1.52	-	83,83,83,83	0
23	MG	A	1894	1/1	0.32	-	64,64,64,64	0
23	MG	A	1680	1/1	0.07	-	85,85,85,85	0
23	MG	A	1637	1/1	0.28	-	90,90,90,90	0
23	MG	A	1679	1/1	0.24	-	73,73,73,73	0
23	MG	A	1882	1/1	0.87	-	94,94,94,94	0
23	MG	A	1656	1/1	0.22	-	124,124,124,124	0
23	MG	A	1737	1/1	0.22	-	105,105,105,105	0
23	MG	A	1863	1/1	0.33	-	90,90,90,90	0
23	MG	A	1806	1/1	0.23	-	81,81,81,81	0
23	MG	A	1639	1/1	0.23	-	72,72,72,72	0
23	MG	A	1624	1/1	0.13	-	95,95,95,95	0
23	MG	A	1826	1/1	0.30	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1803	1/1	0.27	-	62,62,62,62	0
23	MG	A	1903	1/1	0.27	-	46,46,46,46	0
23	MG	A	1734	1/1	0.20	-	96,96,96,96	0
23	MG	A	1733	1/1	0.10	-	142,142,142,142	0
23	MG	A	1823	1/1	0.49	-	82,82,82,82	0
23	MG	A	1662	1/1	0.21	-	59,59,59,59	0
23	MG	A	1833	1/1	0.18	-	58,58,58,58	0
23	MG	A	1702	1/1	0.16	-	68,68,68,68	0
23	MG	A	1619	1/1	0.11	-	79,79,79,79	0
23	MG	A	1795	1/1	0.11	-	101,101,101,101	0
23	MG	A	1677	1/1	0.09	-	70,70,70,70	0
23	MG	A	1703	1/1	0.11	-	85,85,85,85	0
23	MG	A	1860	1/1	1.13	-	102,102,102,102	0
23	MG	A	1858[B]	1/1	0.39	-	32,32,32,32	1
23	MG	A	1695	1/1	0.12	-	62,62,62,62	0
22	PAR	A	1612	42/42	0.28	-	69,69,69,69	42
23	MG	A	1755	1/1	0.28	-	96,96,96,96	0
23	MG	A	1696	1/1	0.09	-	84,84,84,84	0
23	MG	A	1796	1/1	0.59	-	94,94,94,94	0
23	MG	A	1840	1/1	0.27	-	79,79,79,79	0
23	MG	A	1691	1/1	0.55	-	118,118,118,118	0
23	MG	A	1817	1/1	0.32	-	99,99,99,99	0
23	MG	A	1864	1/1	1.79	-	96,96,96,96	0
23	MG	A	1832	1/1	0.26	-	68,68,68,68	0
22	PAR	A	1611	42/42	0.35	-	130,130,130,130	0
23	MG	A	1780	1/1	0.09	-	66,66,66,66	0
23	MG	A	1712	1/1	0.10	-	112,112,112,112	0
23	MG	A	1681	1/1	0.14	-	89,89,89,89	0
23	MG	A	1672	1/1	0.14	-	58,58,58,58	0
23	MG	A	1824	1/1	0.30	-	92,92,92,92	0
23	MG	A	1835	1/1	0.52	-	72,72,72,72	0
23	MG	A	1732	1/1	0.41	-	86,86,86,86	0
23	MG	A	1675	1/1	0.35	-	101,101,101,101	0
23	MG	A	1908	1/1	0.09	-	69,69,69,69	0
23	MG	A	1878	1/1	0.14	-	49,49,49,49	0
23	MG	A	1750	1/1	0.12	-	100,100,100,100	0
23	MG	A	1848	1/1	0.32	-	71,71,71,71	0
23	MG	A	1866	1/1	0.49	-	83,83,83,83	0
23	MG	A	1632	1/1	0.11	-	68,68,68,68	0
23	MG	A	1707	1/1	0.17	-	112,112,112,112	0
22	PAR	A	1614	42/42	0.33	-	147,147,147,147	0
23	MG	A	1745	1/1	0.17	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1778	1/1	0.20	-	107,107,107,107	0
23	MG	A	1877	1/1	0.19	-	105,105,105,105	0
23	MG	A	1787	1/1	0.18	-	165,165,165,165	0
23	MG	A	1912	1/1	0.17	-	70,70,70,70	0
23	MG	A	1785	1/1	0.25	-	142,142,142,142	0
23	MG	A	1714	1/1	0.09	-	115,115,115,115	0
23	MG	A	1653	1/1	0.18	-	96,96,96,96	0
23	MG	A	1771	1/1	0.08	-	67,67,67,67	0
23	MG	A	1822	1/1	0.46	-	69,69,69,69	0
23	MG	A	1914	1/1	0.19	-	81,81,81,81	0
23	MG	A	1799	1/1	0.41	-	74,74,74,74	0
23	MG	D	303	1/1	0.11	-	63,63,63,63	0
23	MG	A	1645	1/1	0.29	-	64,64,64,64	0
23	MG	A	1669	1/1	0.14	-	76,76,76,76	0
23	MG	A	1622	1/1	0.20	-	111,111,111,111	0
23	MG	A	1816	1/1	0.31	-	75,75,75,75	0
23	MG	A	1697	1/1	0.62	-	66,66,66,66	0
23	MG	A	1890	1/1	0.13	-	86,86,86,86	0
23	MG	N	102	1/1	0.55	-	76,76,76,76	0
23	MG	A	1876	1/1	0.12	-	60,60,60,60	0
23	MG	A	1881	1/1	0.57	-	102,102,102,102	0
23	MG	A	1743	1/1	0.21	-	145,145,145,145	0
23	MG	A	1757	1/1	0.25	-	61,61,61,61	0
23	MG	A	1852	1/1	0.22	-	65,65,65,65	0
23	MG	A	1790	1/1	0.25	-	89,89,89,89	0
23	MG	A	1815	1/1	0.24	-	71,71,71,71	0
23	MG	A	1839	1/1	0.31	-	84,84,84,84	0
22	PAR	A	1610	42/42	0.31	-	111,111,111,111	0
23	MG	A	1844	1/1	0.29	-	71,71,71,71	0
23	MG	A	1847	1/1	0.68	-	70,70,70,70	0
23	MG	A	1686	1/1	0.14	-	73,73,73,73	0
23	MG	A	1919	1/1	0.26	-	85,85,85,85	0
23	MG	A	1748	1/1	0.11	-	115,115,115,115	0
23	MG	A	1648	1/1	0.10	-	86,86,86,86	0
23	MG	A	1804	1/1	1.24	-	103,103,103,103	0
23	MG	A	1851	1/1	0.51	-	89,89,89,89	0
23	MG	A	1901	1/1	0.27	-	81,81,81,81	0
23	MG	A	1777	1/1	0.30	-	84,84,84,84	0
23	MG	E	201	1/1	0.11	-	110,110,110,110	0
23	MG	A	1658	1/1	0.17	-	103,103,103,103	0
23	MG	A	1867	1/1	0.42	-	75,75,75,75	0
23	MG	A	1765	1/1	0.14	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	MG	A	1834	1/1	0.19	-	77,77,77,77	0
22	PAR	A	1602	42/42	0.19	-	58,58,58,58	0
23	MG	A	1886	1/1	0.23	-	86,86,86,86	0
23	MG	H	201	1/1	0.27	-	85,85,85,85	0
22	PAR	A	1605	42/42	0.25	-	93,93,93,93	0
23	MG	A	1635	1/1	0.18	-	65,65,65,65	0
22	PAR	A	1613	42/42	0.46	-	152,152,152,152	0
23	MG	A	1915	1/1	0.37	-	101,101,101,101	0
23	MG	A	1813	1/1	0.23	-	55,55,55,55	0
23	MG	A	1853	1/1	0.24	-	55,55,55,55	0
23	MG	A	1756	1/1	0.25	-	158,158,158,158	0
23	MG	A	1768	1/1	0.55	-	122,122,122,122	0
23	MG	A	1708	1/1	0.10	-	77,77,77,77	0
23	MG	A	1913	1/1	0.31	-	69,69,69,69	0
23	MG	A	1916[A]	1/1	0.30	-	50,50,50,50	1
23	MG	A	1706	1/1	0.30	-	123,123,123,123	0
24	ZN	N	101	1/1	0.24	-	141,141,141,141	0
23	MG	A	1873	1/1	0.55	-	59,59,59,59	0
23	MG	A	1701	1/1	0.28	-	83,83,83,83	0
23	MG	A	1626	1/1	0.14	-	53,53,53,53	0
23	MG	T	202	1/1	0.24	-	56,56,56,56	0
23	MG	A	1751	1/1	0.20	-	81,81,81,81	0
23	MG	A	1704	1/1	0.15	-	87,87,87,87	0
23	MG	A	1857	1/1	0.33	-	59,59,59,59	0
23	MG	A	1889	1/1	0.95	-	92,92,92,92	0
22	PAR	A	1608	42/42	0.22	-	97,97,97,97	0
23	MG	A	1758	1/1	0.30	-	149,149,149,149	0
22	PAR	A	1617	42/42	0.31	-	137,137,137,137	0
23	MG	A	1720	1/1	0.09	-	94,94,94,94	0
23	MG	S	101	1/1	0.11	-	83,83,83,83	0
23	MG	T	201	1/1	0.15	-	100,100,100,100	0
22	PAR	A	1601	42/42	0.20	-	70,70,70,70	0
23	MG	A	1880	1/1	0.29	-	96,96,96,96	0
23	MG	A	1647	1/1	0.14	-	101,101,101,101	0
23	MG	A	1726	1/1	0.04	-	91,91,91,91	0
23	MG	A	1870	1/1	0.53	-	75,75,75,75	0
23	MG	A	1651	1/1	0.52	-	61,61,61,61	0
23	MG	A	1841	1/1	0.23	-	74,74,74,74	0
23	MG	A	1644	1/1	0.09	-	50,50,50,50	0
23	MG	A	1802	1/1	0.30	-	71,71,71,71	0

6.5 Other polymers ⓘ

There are no such residues in this entry.