



# wwPDB X-ray Structure Validation Summary Report

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 wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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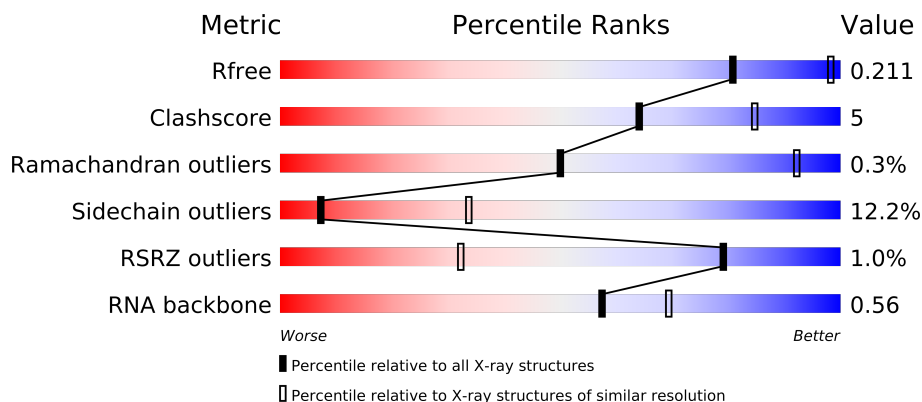
The following versions of software and data (see [references](#)) were used in the production of this report:

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.








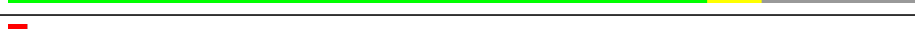
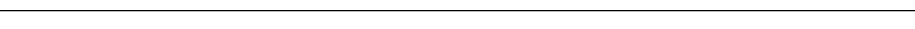


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1080 (3.30-3.18)
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RSRZ outliers	66119	1081 (3.30-3.18)
RNA backbone	1838	1006 (3.78-2.70)

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  $\geq 3$ , 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	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			

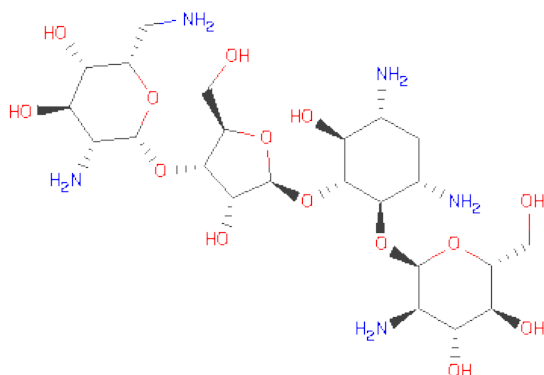
- Molecule 20 is a protein called 30S ribosomal protein S20.

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 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0
22	A	1	Total 42	C 23	N 5	O 14	0	0

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

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

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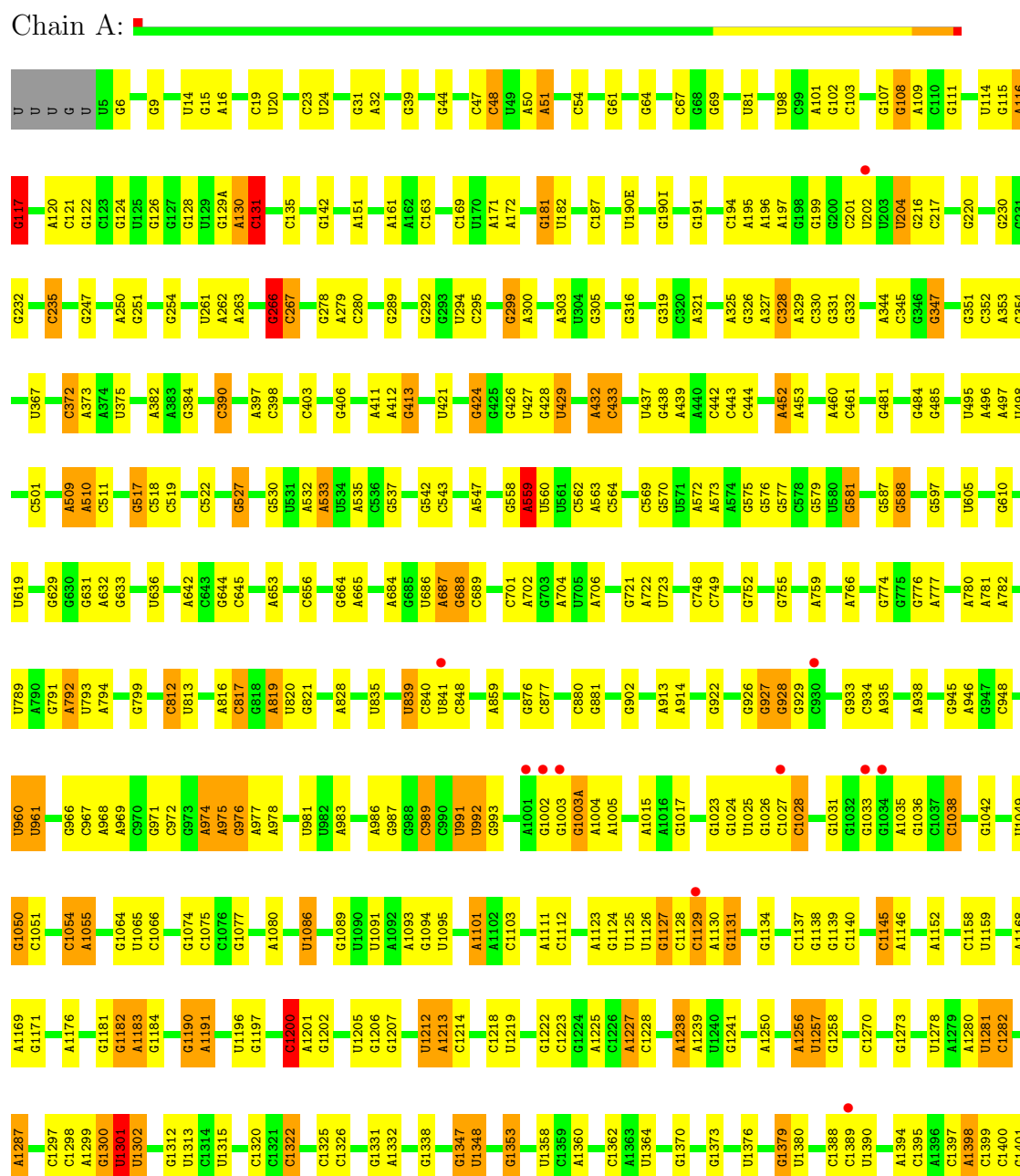
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	U	1	Total	O	0	0
			1	1		

### 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 ( $\text{RSRZ} > 2$ ). 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.

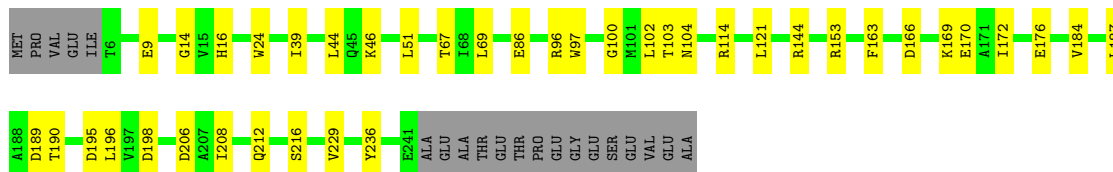
#### • Molecule 1: 16S rRNA





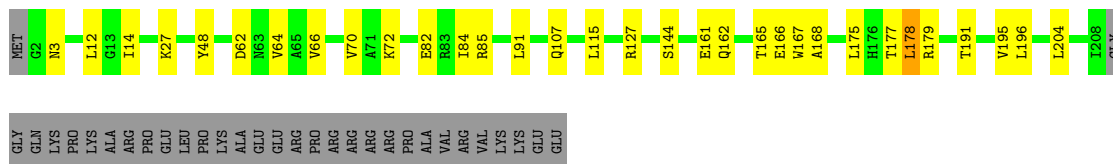
- Molecule 2: 30S ribosomal protein S2

Chain B:



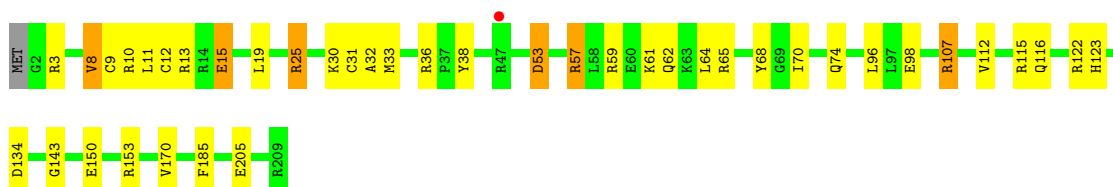
- Molecule 3: 30S ribosomal protein S3

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:



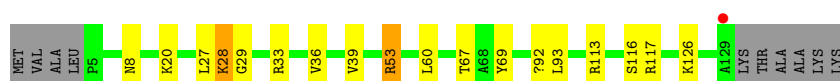
- Molecule 11: 30S ribosomal protein S11

Chain K:



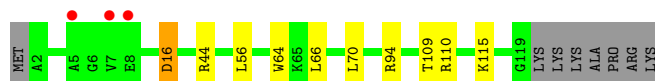
- Molecule 12: 30S ribosomal protein S12

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:



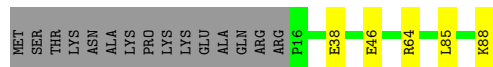
- Molecule 17: 30S ribosomal protein S17

Chain Q:



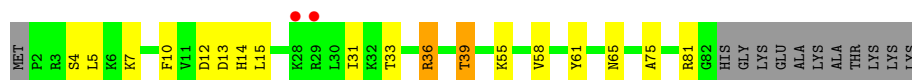
- Molecule 18: 30S ribosomal protein S18

Chain R:



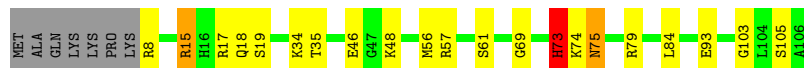
- Molecule 19: 30S ribosomal protein S19

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	88.7	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities 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

The worst 5 of 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

The worst 5 of 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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
3	C	168	ALA
4	D	3	ARG
20	T	73	HIS

### 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

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

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	18	ARG
9	I	125	TYR
19	S	58	VAL
8	H	26	VAL
8	H	102	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%)

5 of 256 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G

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Mol	Chain	Res	Type
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	812	C
1	A	1331	G
1	A	701	C
1	A	748	C

## 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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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 i

There are no carbohydrates in this entry.

## 5.6 Ligand geometry i

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%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
22	PAR	A	1616	-	-	1/18/94/94	2/4/4/4
22	PAR	A	1617	-	-	0/18/94/94	1/4/4/4

The worst 5 of 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

The worst 5 of 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

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

5 of 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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	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

The worst 5 of 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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MA6	A	1518	24/25	0.20	-	57,62,73,74	0
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, 95<sup>th</sup> 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 <sup>2</sup> )	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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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.