



# wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 07:19 PM GMT

PDB ID : 4DR5  
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, crystallographically disordered cognate transfer RNA anticodon stem-loop and streptomycin bound  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-16  
Resolution : 3.45 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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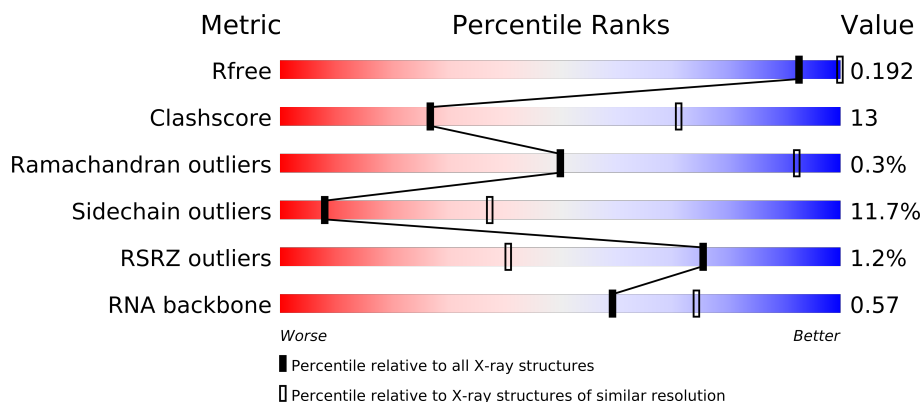
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.45 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.









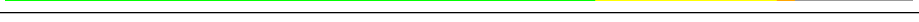




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)
RNA backbone	1838	1004 (4.10-2.76)

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	
22	V	3	
23	W	15	

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53065 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	6	0
			32641	14540	6039	10545	1517			

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	119	Total	C	N	O	S	0	0	0
			885	549	168	165	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
			492	312	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	100	Total	C	N	O	S	0	0	0
			834	534	156	142	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 a RNA chain called 5'-R(\*UP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	3	Total	C	N	O	P	0	0	0
			57	27	6	22	2			

- Molecule 23 is a RNA chain called 5'-R(\*GP\*GP\*GP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*AP\*UP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

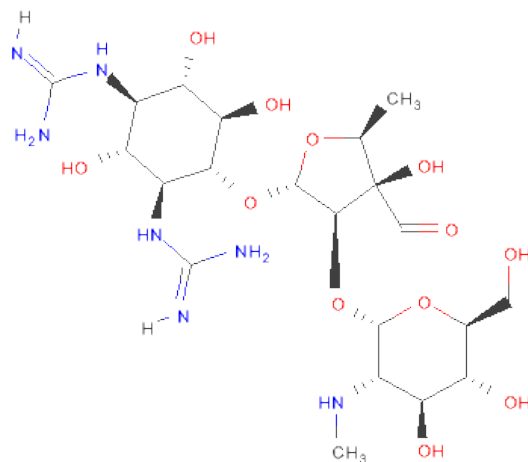
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	3	Total	Mg	0	0
			3	3		
24	G	1	Total	Mg	0	0
			1	1		
24	Q	1	Total	Mg	0	0
			1	1		
24	D	2	Total	Mg	0	0
			2	2		
24	E	1	Total	Mg	0	0
			1	1		
24	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	259	Total	Mg	0	0
			259	259		
24	N	1	Total	Mg	0	0
			1	1		
24	L	1	Total	Mg	0	0
			1	1		
24	S	1	Total	Mg	0	0
			1	1		
24	F	1	Total	Mg	0	0
			1	1		

- Molecule 25 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			40	21	7	12		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

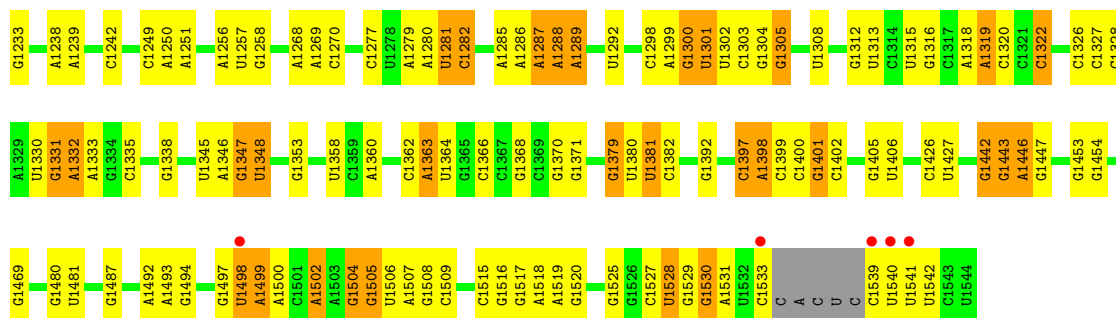
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total	Zn	0	0
			1	1		
26	N	1	Total	Zn	0	0
			1	1		

- Molecule 27 is water.



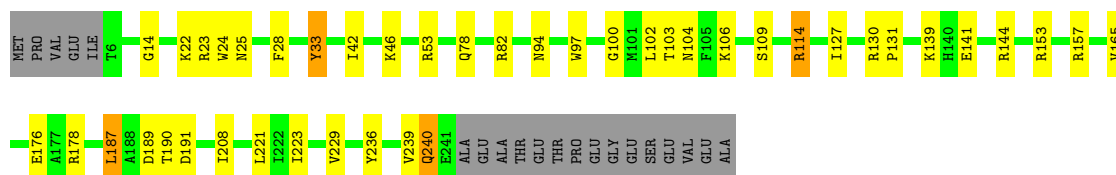
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	572	Total 572	O 572	0	0
27	D	2	Total 2	O 2	0	0
27	E	3	Total 3	O 3	0	0
27	L	1	Total 1	O 1	0	0
27	O	1	Total 1	O 1	0	0
27	P	1	Total 1	O 1	0	0
27	Q	1	Total 1	O 1	0	0
27	T	1	Total 1	O 1	0	0





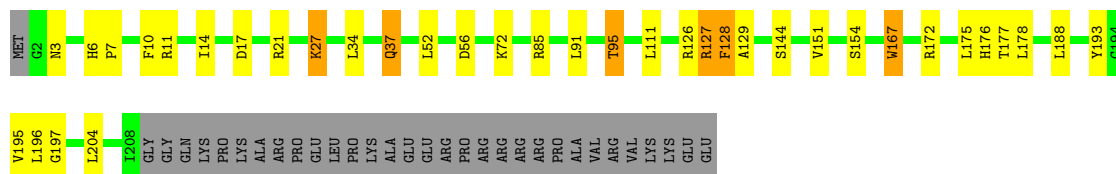
- Molecule 2: 30S ribosomal protein S2

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:



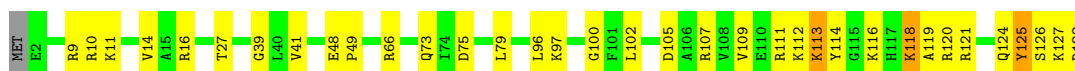
- Molecule 8: 30S ribosomal protein S8

Chain H:



- Molecule 9: 30S ribosomal protein S9

Chain I:



- Molecule 10: 30S ribosomal protein S10

Chain J:



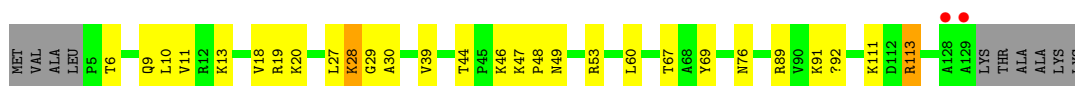
- Molecule 11: 30S ribosomal protein S11

Chain K:



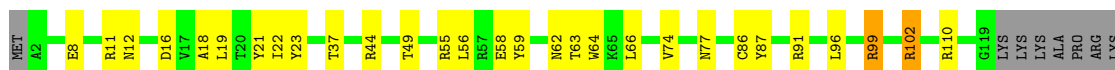
- Molecule 12: 30S ribosomal protein S12

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: 



- Molecule 22: 5'-R(\*UP\*UP\*U)-3'

Chain V: 



- Molecule 23: 5'-R(\*GP\*GP\*GP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*AP\*UP\*CP\*CP\*C)-3'

Chain W: 

G28	G29	G30	A31	U32	U33	G34	A35	A36	A37	A38	U39	C40	C41	C42

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.51 Å   400.51 Å   175.41 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.90 – 3.45 19.90 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.90-3.45) 100.0 (19.90-3.45)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.44 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, $R_{free}$	0.152 , 0.192 0.152 , 0.192	Depositor DCC
$R_{free}$ test set	9331 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	111.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 82.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 184810 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	53065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 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	0.49	0/36136	0.87	37/56392 (0.1%)
2	B	0.31	0/1931	0.53	0/2607
3	C	0.31	0/1637	0.50	0/2207
4	D	0.34	0/1733	0.53	0/2318
5	E	0.43	0/1163	0.64	0/1566
6	F	0.31	0/856	0.51	0/1154
7	G	0.33	0/1276	0.52	0/1709
8	H	0.41	0/1136	0.62	0/1527
9	I	0.30	0/1029	0.56	1/1379 (0.1%)
10	J	0.32	0/806	0.57	0/1084
11	K	0.38	0/900	0.65	0/1213
12	L	0.38	0/978	0.67	0/1308
13	M	0.31	0/947	0.52	0/1270
14	N	0.36	0/501	0.54	0/664
15	O	0.36	0/745	0.54	0/992
16	P	0.42	0/717	0.62	0/965
17	Q	0.45	0/847	0.66	0/1131
18	R	0.33	0/604	0.54	0/801
19	S	0.27	0/662	0.54	0/892
20	T	0.39	0/765	0.67	0/1007
21	U	0.34	0/213	0.57	0/279
22	V	0.23	0/62	0.67	0/94
23	W	0.18	0/357	0.47	0/555
All	All	0.45	0/56001	0.78	38/83114 (0.0%)

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



Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	H	0	1
12	L	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	G	C4-C5-N7	7.91	113.97	110.80
1	A	108	G	N7-C8-N9	7.26	116.73	113.10
1	A	108	G	C5-N7-C8	-7.26	100.67	104.30
1	A	108	G	C6-C5-N7	-7.07	126.16	130.40
1	A	108	G	C4-N9-C1'	7.03	135.64	126.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
8	H	90	GLY	Peptide
12	L	46	LYS	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	32641	0	0	383	1
2	B	1896	0	0	16	0
3	C	1613	0	0	13	0
4	D	1703	0	0	24	0
5	E	1147	0	0	8	0
6	F	843	0	0	4	0
7	G	1257	0	0	15	0
8	H	1116	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1010	0	0	18	0
10	J	793	0	0	12	0
11	K	885	0	0	7	0
12	L	973	0	0	15	0
13	M	937	0	0	13	0
14	N	492	0	0	9	0
15	O	734	0	0	13	0
16	P	701	0	0	9	0
17	Q	834	0	0	13	0
18	R	598	0	0	8	0
19	S	648	0	0	9	0
20	T	763	0	0	11	0
21	U	209	0	0	3	0
22	V	57	0	0	0	0
23	W	319	0	0	4	0
24	A	259	0	0	0	0
24	D	2	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	G	1	0	0	0	0
24	H	1	0	0	0	0
24	L	1	0	0	0	0
24	N	1	0	0	0	0
24	P	3	0	0	0	0
24	Q	1	0	0	0	0
24	S	1	0	0	0	0
25	A	40	0	37	7	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	572	0	0	20	0
27	D	2	0	0	0	0
27	E	3	0	0	0	0
27	L	1	0	0	0	0
27	O	1	0	0	0	0
27	P	1	0	0	0	0
27	Q	1	0	0	0	0
27	T	1	0	0	0	0
All	All	53065	0	37	555	1

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 13.

The worst 5 of 555 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1498:UR3:O2'	1:A:1499:A:OP2	1.75	1.04
1:A:1005:A:N3	1:A:1026:G:N2	2.11	0.98
1:A:1182:G:O2'	1:A:1183:A:OP2	1.82	0.97
1:A:451:A:O2'	27:A:2407:HOH:O	1.83	0.96
1:A:413:G:N2	1:A:429:U:OP2	1.99	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:702:A:N6	1:A:1447:G:OP1[4_554]	2.18	0.02

## 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%)	209 (89%)	24 (10%)	1 (0%)	43	90
3	C	205/239 (86%)	183 (89%)	22 (11%)	0	100	100
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
5	E	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
8	H	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	27	81
10	J	97/105 (92%)	80 (82%)	16 (16%)	1 (1%)	22	78
11	K	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	25	79
12	L	122/135 (90%)	109 (89%)	12 (10%)	1 (1%)	27	81
13	M	116/126 (92%)	105 (90%)	11 (10%)	0	100	100
14	N	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
15	O	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	P	82/88 (93%)	78 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	68 (96%)	3 (4%)	0	100	100
19	S	79/93 (85%)	69 (87%)	8 (10%)	2 (2%)	9	57
20	T	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2353/2541 (93%)	2152 (92%)	194 (8%)	7 (0%)	50	92

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
19	S	6	LYS
11	K	117	ASN
9	I	119	ALA

### 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%)	181 (90%)	20 (10%)	11	47
3	C	160/188 (85%)	136 (85%)	24 (15%)	4	25
4	D	180/181 (99%)	161 (89%)	19 (11%)	10	43
5	E	115/123 (94%)	101 (88%)	14 (12%)	7	35
6	F	90/90 (100%)	78 (87%)	12 (13%)	6	30
7	G	126/127 (99%)	114 (90%)	12 (10%)	12	50
8	H	119/119 (100%)	105 (88%)	14 (12%)	8	37
9	I	98/99 (99%)	83 (85%)	15 (15%)	4	24
10	J	87/92 (95%)	76 (87%)	11 (13%)	7	33
11	K	90/99 (91%)	81 (90%)	9 (10%)	11	47
12	L	103/110 (94%)	90 (87%)	13 (13%)	7	33
13	M	94/101 (93%)	83 (88%)	11 (12%)	8	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	49/50 (98%)	42 (86%)	7 (14%)	5	27
15	O	79/80 (99%)	72 (91%)	7 (9%)	14	54
16	P	72/74 (97%)	67 (93%)	5 (7%)	22	68
17	Q	95/97 (98%)	84 (88%)	11 (12%)	8	38
18	R	64/77 (83%)	58 (91%)	6 (9%)	13	50
19	S	71/80 (89%)	61 (86%)	10 (14%)	5	28
20	T	76/82 (93%)	65 (86%)	11 (14%)	5	26
21	U	19/22 (86%)	17 (90%)	2 (10%)	10	44
All	All	1988/2111 (94%)	1755 (88%)	233 (12%)	8	37

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	85	ARG
10	J	6	ILE
19	S	30	LEU
8	H	97	VAL
9	I	66	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	1503/1522 (98%)	248 (16%)	43 (2%)
22	V	2/3 (66%)	0	0
23	W	14/15 (93%)	3 (21%)	0
All	All	1519/1540 (98%)	251 (16%)	43 (2%)

5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	1026	G
1	A	1397	C
1	A	812	C
1	A	913	A

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

17 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	1.45	5 (20%)	32,38,41	9.48	3 (9%)
1	5MC	A	1400	1	20,22,23	1.79	2 (10%)	26,32,35	1.19	3 (11%)
1	4OC	A	1402	1	21,23,24	1.24	2 (9%)	26,32,35	0.87	1 (3%)
1	5MC	A	1404	1	20,22,23	2.03	4 (20%)	26,32,35	1.68	3 (11%)
1	5MC	A	1407	1	20,22,23	1.82	2 (10%)	26,32,35	1.33	3 (11%)
1	UR3	A	1498	1	20,22,23	1.50	2 (10%)	23,32,35	0.97	1 (4%)
1	MA6	A	1518[A]	1	26,26,27	1.14	2 (7%)	37,38,41	0.91	2 (5%)
1	MA6	A	1518[B]	1	26,26,27	1.18	2 (7%)	37,38,41	0.97	2 (5%)
1	MA6	A	1519[A]	1	26,26,27	0.90	1 (3%)	37,38,41	0.99	2 (5%)
1	MA6	A	1519[B]	1	26,26,27	1.20	2 (7%)	37,38,41	0.90	3 (8%)
1	PSU	A	1540	1	19,21,22	1.16	1 (5%)	23,30,33	1.67	4 (17%)
1	PSU	A	1541	1	19,21,22	1.21	1 (5%)	23,30,33	2.07	3 (13%)
1	PSU	A	516	1,24	19,21,22	1.06	1 (5%)	23,30,33	0.93	2 (8%)
1	7MG	A	527	1	24,26,27	3.90	5 (20%)	34,39,42	1.46	7 (20%)
1	M2G	A	966	1	25,27,28	1.47	6 (24%)	34,40,43	7.91	4 (11%)
1	5MC	A	967	1	20,22,23	1.53	2 (10%)	26,32,35	1.40	3 (11%)
12	0TD	L	92	12	9,9,10	7.36	3 (33%)	9,11,13	2.81	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[A]	1	-	0/13/29/30	0/1/3/3
1	MA6	A	1518[B]	1	-	0/13/29/30	0/1/3/3
1	MA6	A	1519[A]	1	-	0/13/29/30	0/1/3/3
1	MA6	A	1519[B]	1	-	1/13/29/30	0/1/3/3
1	PSU	A	1540	1	-	0/8/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/8/25/26	0/2/2/2
1	PSU	A	516	1,24	-	0/8/25/26	0/2/2/2
1	7MG	A	527	1	-	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 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	O-C	21.26	1.26	1.11
1	A	527	7MG	C8-N9	-15.85	1.33	1.46
1	A	527	7MG	C2-N2	7.59	1.44	1.32
1	A	1400	5MC	C2-N1	6.81	1.45	1.38
1	A	1407	5MC	C2-N1	6.38	1.45	1.38

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-C5-N7	-53.34	126.96	134.14
1	A	966	M2G	C6-C5-N7	-45.49	128.01	134.14
1	A	1541	PSU	C5-C1'-C2'	-7.18	102.94	115.61
1	A	1404	5MC	C6-N1-C2	6.34	121.74	118.62
1	A	1540	PSU	C5-C1'-C2'	-6.26	104.57	115.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1400	5MC	OP2-P-O5'-C5'
1	A	1519[B]	MA6	OP1-P-O5'-C5'

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 275 ligands modelled in this entry, 274 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
25	SRY	A	1860	-	42,42,42	2.26	11 (26%)	63,63,63	2.04	13 (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
25	SRY	A	1860	-	-	0/22/87/87	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1860	SRY	CD1-N31	8.57	1.49	1.33
25	A	1860	SRY	CA1-N11	6.72	1.45	1.33
25	A	1860	SRY	C32-CG2	-4.23	1.47	1.52
25	A	1860	SRY	O53-C53	-3.39	1.35	1.44
25	A	1860	SRY	C23-N23	-3.00	1.42	1.47



The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1860	SRY	CI3-N23-C23	-7.88	107.43	113.65
25	A	1860	SRY	C13-O13-C22	-7.51	103.22	116.28
25	A	1860	SRY	C12-O42-C42	-4.51	101.02	108.25
25	A	1860	SRY	O42-C42-C32	4.17	107.31	103.39
25	A	1860	SRY	C43-C33-C23	-3.68	105.21	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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%)	-0.35	19 (1%) 74 39	63, 101, 190, 333	0
2	B	236/256 (92%)	-0.25	0 100 100	93, 136, 194, 231	0
3	C	207/239 (86%)	-0.27	0 100 100	106, 142, 183, 216	0
4	D	208/209 (99%)	-0.22	2 (0%) 79 46	77, 113, 175, 202	0
5	E	151/162 (93%)	-0.32	1 (0%) 84 54	68, 95, 131, 177	0
6	F	101/101 (100%)	-0.32	0 100 100	93, 133, 164, 185	0
7	G	155/156 (99%)	-0.25	0 100 100	90, 120, 183, 219	0
8	H	138/138 (100%)	-0.39	0 100 100	62, 85, 115, 146	0
9	I	127/128 (99%)	-0.23	0 100 100	95, 144, 180, 216	0
10	J	99/105 (94%)	-0.09	2 (2%) 62 29	105, 165, 237, 271	0
11	K	119/129 (92%)	-0.22	2 (1%) 67 32	72, 101, 148, 212	0
12	L	124/135 (91%)	-0.23	2 (1%) 68 33	64, 110, 146, 220	0
13	M	118/126 (93%)	-0.39	0 100 100	92, 124, 162, 204	0
14	N	60/61 (98%)	-0.23	0 100 100	107, 133, 172, 248	0
15	O	88/89 (98%)	-0.33	0 100 100	68, 102, 144, 210	0
16	P	84/88 (95%)	-0.33	0 100 100	75, 96, 122, 171	0
17	Q	100/105 (95%)	-0.26	0 100 100	63, 89, 126, 182	0
18	R	73/88 (82%)	-0.21	3 (4%) 35 15	86, 109, 197, 245	0
19	S	81/93 (87%)	-0.19	1 (1%) 75 41	120, 154, 199, 254	0
20	T	99/106 (93%)	-0.43	0 100 100	73, 96, 140, 176	0
21	U	25/27 (92%)	-0.26	0 100 100	101, 121, 153, 171	0
22	V	3/3 (100%)	2.47	2 (66%) 0 1	191, 191, 198, 226	3 (100%)
23	W	15/15 (100%)	2.91	11 (73%) 0 0	194, 222, 273, 301	8 (53%)
All	All	3922/4081 (96%)	-0.29	45 (1%) 75 42	62, 112, 188, 333	11 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	28	G	5.6
23	W	42	C	5.3
1	A	1498	UR3	4.4
1	A	1540	PSU	4.3
23	W	41	C	4.2

## 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	M2G	A	966	25/26	0.15	-	88,105,117,123	0
1	PSU	A	1540	20/21	0.49	-	193,205,213,214	0
1	UR3	A	1498	21/22	0.20	-	87,96,109,112	0
1	4OC	A	1402	22/23	0.17	-	89,101,107,111	0
1	7MG	A	527	24/25	0.13	-	66,86,94,104	0
1	5MC	A	1407	21/22	0.21	-	107,119,130,134	0
1	5MC	A	967	21/22	0.12	-	90,98,107,115	0
1	PSU	A	1541	20/21	0.46	-	188,196,202,203	0
12	0TD	L	92	10/11	0.14	-	83,93,97,207	0
1	2MG	A	1207	24/25	0.15	-	120,123,131,135	0
1	5MC	A	1404	21/22	0.14	-	84,88,103,117	0
1	5MC	A	1400	21/22	0.22	-	71,102,119,121	0
1	MA6	A	1519[A]	24/25	0.16	-	77,81,91,95	24
1	MA6	A	1518[B]	24/25	0.18	-	79,88,110,112	24
1	MA6	A	1518[A]	24/25	0.18	-	81,85,92,101	24
1	MA6	A	1519[B]	24/25	0.16	-	76,83,90,91	24
1	PSU	A	516	20/21	0.15	-	120,125,133,136	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
24	MG	A	1842	1/1	0.72	-	334,334,334,334	0
24	MG	A	1852	1/1	0.32	-	84,84,84,84	0
24	MG	A	1722	1/1	0.44	-	118,118,118,118	0
24	MG	A	1706	1/1	0.28	-	174,174,174,174	0
24	MG	A	1708	1/1	0.10	-	211,211,211,211	0
24	MG	A	1604	1/1	0.09	-	153,153,153,153	0
24	MG	A	1691	1/1	0.20	-	139,139,139,139	0
24	MG	A	1762	1/1	0.22	-	83,83,83,83	0
24	MG	A	1644	1/1	0.46	-	95,95,95,95	0
24	MG	A	1826	1/1	0.26	-	354,354,354,354	0
24	MG	A	1716	1/1	0.08	-	70,70,70,70	0
24	MG	A	1794	1/1	0.45	-	120,120,120,120	0
24	MG	A	1757	1/1	0.33	-	83,83,83,83	0
24	MG	A	1603	1/1	0.18	-	97,97,97,97	0
24	MG	A	1807	1/1	0.40	-	397,397,397,397	0
24	MG	A	1720	1/1	0.20	-	64,64,64,64	0
24	MG	A	1677	1/1	0.10	-	113,113,113,113	0
24	MG	A	1684	1/1	0.25	-	90,90,90,90	0
24	MG	A	1711	1/1	0.54	-	109,109,109,109	0
24	MG	P	101	1/1	0.37	-	67,67,67,67	0
24	MG	A	1617	1/1	0.14	-	81,81,81,81	0
24	MG	A	1768	1/1	0.52	-	99,99,99,99	0
24	MG	A	1755	1/1	0.11	-	131,131,131,131	0
24	MG	A	1856	1/1	0.16	-	104,104,104,104	0
24	MG	A	1821	1/1	0.21	-	178,178,178,178	0
24	MG	A	1742	1/1	0.30	-	89,89,89,89	0
24	MG	A	1783	1/1	0.30	-	89,89,89,89	0
24	MG	A	1623	1/1	0.10	-	84,84,84,84	0
24	MG	A	1723	1/1	0.23	-	117,117,117,117	0
24	MG	A	1822	1/1	0.26	-	209,209,209,209	0
24	MG	A	1717	1/1	0.60	-	125,125,125,125	0
24	MG	A	1776	1/1	0.20	-	96,96,96,96	0
24	MG	A	1637	1/1	0.21	-	86,86,86,86	0
24	MG	A	1670	1/1	0.19	-	109,109,109,109	0
24	MG	A	1758	1/1	0.16	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1830	1/1	0.26	-	273,273,273,273	0
24	MG	A	1681	1/1	0.10	-	160,160,160,160	0
24	MG	A	1833	1/1	0.14	-	335,335,335,335	0
24	MG	A	1799	1/1	0.25	-	277,277,277,277	0
24	MG	A	1673	1/1	0.38	-	102,102,102,102	0
24	MG	A	1730	1/1	0.39	-	90,90,90,90	0
24	MG	A	1715	1/1	0.12	-	89,89,89,89	0
24	MG	A	1695	1/1	0.41	-	88,88,88,88	0
24	MG	A	1849	1/1	0.19	-	74,74,74,74	0
24	MG	A	1734	1/1	0.18	-	99,99,99,99	0
24	MG	A	1806	1/1	0.55	-	211,211,211,211	0
24	MG	A	1784	1/1	0.74	-	92,92,92,92	0
24	MG	A	1774	1/1	0.64	-	61,61,61,61	0
24	MG	A	1615	1/1	0.42	-	72,72,72,72	0
24	MG	A	1802	1/1	0.30	-	206,206,206,206	0
26	ZN	D	301	1/1	0.33	-	114,114,114,114	0
24	MG	D	302	1/1	0.13	-	86,86,86,86	0
24	MG	A	1687	1/1	0.28	-	116,116,116,116	0
24	MG	A	1689	1/1	0.14	-	132,132,132,132	0
24	MG	A	1838	1/1	0.18	-	181,181,181,181	0
24	MG	A	1848	1/1	0.36	-	87,87,87,87	0
24	MG	A	1813	1/1	0.28	-	181,181,181,181	0
24	MG	A	1664	1/1	0.33	-	131,131,131,131	0
24	MG	A	1805	1/1	0.36	-	280,280,280,280	0
24	MG	A	1727	1/1	0.28	-	79,79,79,79	0
24	MG	A	1835	1/1	0.14	-	299,299,299,299	0
24	MG	A	1654	1/1	0.18	-	97,97,97,97	0
24	MG	A	1790	1/1	0.60	-	88,88,88,88	0
24	MG	A	1713	1/1	0.07	-	112,112,112,112	0
24	MG	A	1694	1/1	0.13	-	116,116,116,116	0
24	MG	A	1611	1/1	0.12	-	120,120,120,120	0
24	MG	A	1641	1/1	0.39	-	92,92,92,92	0
24	MG	A	1666	1/1	0.18	-	103,103,103,103	0
24	MG	A	1620	1/1	0.18	-	141,141,141,141	0
24	MG	A	1707	1/1	0.24	-	163,163,163,163	0
24	MG	A	1740	1/1	0.26	-	89,89,89,89	0
24	MG	A	1759	1/1	0.27	-	75,75,75,75	0
24	MG	A	1660	1/1	0.07	-	104,104,104,104	0
24	MG	A	1678	1/1	0.16	-	133,133,133,133	0
24	MG	A	1801	1/1	0.21	-	248,248,248,248	0
24	MG	A	1601	1/1	0.13	-	86,86,86,86	0
24	MG	A	1797	1/1	0.15	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1701	1/1	0.50	-	73,73,73,73	0
24	MG	A	1750	1/1	0.55	-	92,92,92,92	0
24	MG	A	1602	1/1	0.09	-	108,108,108,108	0
24	MG	A	1751	1/1	0.24	-	83,83,83,83	0
24	MG	A	1770	1/1	0.75	-	98,98,98,98	0
24	MG	A	1847	1/1	0.31	-	334,334,334,334	0
24	MG	A	1831	1/1	0.33	-	160,160,160,160	0
24	MG	A	1841	1/1	0.17	-	266,266,266,266	0
24	MG	A	1662	1/1	0.16	-	145,145,145,145	0
24	MG	A	1629	1/1	0.06	-	151,151,151,151	0
24	MG	A	1858	1/1	0.28	-	98,98,98,98	0
24	MG	A	1824	1/1	0.15	-	202,202,202,202	0
24	MG	A	1823	1/1	0.16	-	281,281,281,281	0
24	MG	A	1754	1/1	0.28	-	105,105,105,105	0
24	MG	A	1834	1/1	0.37	-	231,231,231,231	0
24	MG	A	1749	1/1	0.52	-	98,98,98,98	0
24	MG	A	1777	1/1	0.40	-	100,100,100,100	0
24	MG	A	1639	1/1	0.29	-	73,73,73,73	0
24	MG	A	1780	1/1	0.60	-	80,80,80,80	0
24	MG	A	1605	1/1	0.08	-	72,72,72,72	0
24	MG	A	1789	1/1	0.33	-	92,92,92,92	0
24	MG	N	102	1/1	0.65	-	99,99,99,99	0
24	MG	A	1645	1/1	0.09	-	108,108,108,108	0
24	MG	A	1683	1/1	0.52	-	110,110,110,110	0
24	MG	A	1606	1/1	0.23	-	87,87,87,87	0
24	MG	A	1771	1/1	0.39	-	82,82,82,82	0
24	MG	A	1653	1/1	0.53	-	89,89,89,89	0
24	MG	A	1846	1/1	0.12	-	225,225,225,225	0
24	MG	A	1817	1/1	0.25	-	180,180,180,180	0
24	MG	A	1825	1/1	0.41	-	401,401,401,401	0
24	MG	A	1714	1/1	0.48	-	99,99,99,99	0
24	MG	A	1753	1/1	0.80	-	110,110,110,110	0
24	MG	A	1786	1/1	0.31	-	96,96,96,96	0
24	MG	A	1699	1/1	0.42	-	100,100,100,100	0
24	MG	A	1773	1/1	0.62	-	88,88,88,88	0
24	MG	A	1837	1/1	0.19	-	244,244,244,244	0
24	MG	A	1855	1/1	0.41	-	115,115,115,115	0
24	MG	A	1832	1/1	0.23	-	112,112,112,112	0
24	MG	A	1668	1/1	0.18	-	138,138,138,138	0
24	MG	A	1815	1/1	0.32	-	309,309,309,309	0
24	MG	A	1732	1/1	0.63	-	97,97,97,97	0
24	MG	A	1626	1/1	0.17	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1787	1/1	0.14	-	78,78,78,78	0
24	MG	A	1854	1/1	0.57	-	89,89,89,89	0
24	MG	A	1744	1/1	0.21	-	109,109,109,109	0
24	MG	A	1657	1/1	0.32	-	189,189,189,189	0
24	MG	A	1614	1/1	0.18	-	79,79,79,79	0
24	MG	A	1610	1/1	0.14	-	71,71,71,71	0
24	MG	A	1761	1/1	0.22	-	107,107,107,107	0
24	MG	A	1621	1/1	0.43	-	131,131,131,131	0
24	MG	A	1850	1/1	0.56	-	117,117,117,117	0
24	MG	A	1709	1/1	0.31	-	250,250,250,250	0
24	MG	A	1731	1/1	0.53	-	114,114,114,114	0
24	MG	A	1665	1/1	0.14	-	99,99,99,99	0
24	MG	A	1779	1/1	1.17	-	94,94,94,94	0
24	MG	A	1672	1/1	0.82	-	92,92,92,92	0
24	MG	A	1775	1/1	0.09	-	114,114,114,114	0
24	MG	A	1736	1/1	0.13	-	119,119,119,119	0
24	MG	A	1704	1/1	0.22	-	116,116,116,116	0
24	MG	A	1688	1/1	0.14	-	120,120,120,120	0
24	MG	A	1836	1/1	0.30	-	300,300,300,300	0
24	MG	A	1646	1/1	0.34	-	79,79,79,79	0
24	MG	A	1800	1/1	0.34	-	203,203,203,203	0
24	MG	A	1795	1/1	0.38	-	85,85,85,85	0
24	MG	D	303	1/1	0.79	-	97,97,97,97	0
24	MG	Q	201	1/1	0.24	-	84,84,84,84	0
24	MG	A	1765	1/1	0.12	-	93,93,93,93	0
24	MG	A	1692	1/1	0.17	-	119,119,119,119	0
24	MG	A	1625	1/1	0.23	-	194,194,194,194	0
24	MG	A	1648	1/1	0.09	-	96,96,96,96	0
24	MG	A	1818	1/1	0.26	-	249,249,249,249	0
24	MG	A	1608	1/1	0.44	-	84,84,84,84	0
24	MG	A	1628	1/1	0.40	-	104,104,104,104	0
25	SRY	A	1860	40/40	0.15	-	60,79,97,101	0
24	MG	A	1811	1/1	0.06	-	121,121,121,121	0
24	MG	A	1845	1/1	0.10	-	293,293,293,293	0
24	MG	A	1690	1/1	0.34	-	193,193,193,193	0
24	MG	L	201	1/1	0.17	-	81,81,81,81	0
24	MG	A	1652	1/1	0.31	-	96,96,96,96	0
24	MG	A	1767	1/1	0.54	-	64,64,64,64	0
24	MG	A	1724	1/1	0.25	-	99,99,99,99	0
24	MG	A	1697	1/1	1.00	-	102,102,102,102	0
24	MG	A	1607	1/1	0.13	-	102,102,102,102	0
24	MG	A	1728	1/1	0.20	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	S	101	1/1	0.22	-	80,80,80,80	0
24	MG	A	1816	1/1	0.33	-	318,318,318,318	0
24	MG	A	1851	1/1	0.69	-	92,92,92,92	0
24	MG	A	1769	1/1	0.27	-	92,92,92,92	0
24	MG	A	1808	1/1	0.49	-	377,377,377,377	0
24	MG	A	1650	1/1	0.07	-	107,107,107,107	0
24	MG	A	1843	1/1	0.11	-	115,115,115,115	0
24	MG	H	201	1/1	0.24	-	63,63,63,63	0
24	MG	A	1661	1/1	0.22	-	121,121,121,121	0
24	MG	A	1700	1/1	0.17	-	272,272,272,272	0
24	MG	F	201	1/1	0.50	-	79,79,79,79	0
24	MG	A	1782	1/1	0.22	-	65,65,65,65	0
26	ZN	N	101	1/1	0.11	-	129,129,129,129	0
24	MG	A	1810	1/1	0.37	-	295,295,295,295	0
24	MG	A	1675	1/1	0.14	-	223,223,223,223	0
24	MG	A	1633	1/1	0.13	-	85,85,85,85	0
24	MG	A	1772	1/1	0.33	-	78,78,78,78	0
24	MG	A	1844	1/1	0.39	-	310,310,310,310	0
24	MG	A	1685	1/1	0.20	-	134,134,134,134	0
24	MG	A	1618	1/1	0.63	-	85,85,85,85	0
24	MG	A	1659	1/1	0.51	-	121,121,121,121	0
24	MG	A	1616	1/1	0.04	-	93,93,93,93	0
24	MG	A	1778	1/1	0.30	-	78,78,78,78	0
24	MG	A	1686	1/1	0.12	-	194,194,194,194	0
24	MG	A	1631	1/1	0.12	-	101,101,101,101	0
24	MG	A	1718	1/1	0.21	-	220,220,220,220	0
24	MG	A	1788	1/1	0.24	-	84,84,84,84	0
24	MG	A	1640	1/1	0.07	-	98,98,98,98	0
24	MG	A	1819	1/1	0.95	-	371,371,371,371	0
24	MG	A	1840	1/1	0.20	-	289,289,289,289	0
24	MG	A	1671	1/1	0.30	-	99,99,99,99	0
24	MG	A	1733	1/1	0.34	-	68,68,68,68	0
24	MG	P	102	1/1	0.67	-	96,96,96,96	0
24	MG	A	1680	1/1	0.24	-	250,250,250,250	0
24	MG	A	1737	1/1	0.33	-	81,81,81,81	0
24	MG	A	1747	1/1	0.48	-	111,111,111,111	0
24	MG	A	1679	1/1	0.24	-	168,168,168,168	0
24	MG	A	1647	1/1	0.10	-	127,127,127,127	0
24	MG	E	201	1/1	0.49	-	87,87,87,87	0
24	MG	A	1760	1/1	0.11	-	101,101,101,101	0
24	MG	A	1612	1/1	0.16	-	97,97,97,97	0
24	MG	A	1698	1/1	0.16	-	218,218,218,218	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1814	1/1	0.06	-	113,113,113,113	0
24	MG	A	1658	1/1	0.18	-	102,102,102,102	0
24	MG	A	1857	1/1	0.27	-	89,89,89,89	0
24	MG	A	1803	1/1	0.71	-	324,324,324,324	0
24	MG	A	1745	1/1	0.71	-	82,82,82,82	0
24	MG	A	1703	1/1	0.23	-	106,106,106,106	0
24	MG	A	1624	1/1	0.23	-	97,97,97,97	0
24	MG	A	1663	1/1	0.35	-	94,94,94,94	0
24	MG	A	1743	1/1	0.07	-	76,76,76,76	0
24	MG	A	1781	1/1	0.37	-	75,75,75,75	0
24	MG	A	1643	1/1	0.26	-	99,99,99,99	0
24	MG	A	1682	1/1	0.29	-	228,228,228,228	0
24	MG	A	1726	1/1	0.25	-	86,86,86,86	0
24	MG	A	1820	1/1	0.28	-	152,152,152,152	0
24	MG	A	1622	1/1	0.64	-	75,75,75,75	0
24	MG	A	1725	1/1	0.52	-	109,109,109,109	0
24	MG	A	1635	1/1	0.13	-	75,75,75,75	0
24	MG	G	201	1/1	0.49	-	116,116,116,116	0
24	MG	A	1674	1/1	0.10	-	125,125,125,125	0
24	MG	A	1741	1/1	0.21	-	101,101,101,101	0
24	MG	A	1827	1/1	0.28	-	244,244,244,244	0
24	MG	A	1739	1/1	0.52	-	103,103,103,103	0
24	MG	A	1853	1/1	0.23	-	96,96,96,96	0
24	MG	A	1651	1/1	0.18	-	143,143,143,143	0
24	MG	A	1812	1/1	0.24	-	290,290,290,290	0
24	MG	A	1632	1/1	0.12	-	76,76,76,76	0
24	MG	A	1829	1/1	0.16	-	267,267,267,267	0
24	MG	A	1785	1/1	0.36	-	92,92,92,92	0
24	MG	A	1676	1/1	0.19	-	138,138,138,138	0
24	MG	A	1649	1/1	0.28	-	51,51,51,51	0
24	MG	A	1764	1/1	0.20	-	104,104,104,104	0
24	MG	A	1609	1/1	0.15	-	74,74,74,74	0
24	MG	A	1721	1/1	0.21	-	95,95,95,95	0
24	MG	A	1634	1/1	0.24	-	243,243,243,243	0
24	MG	A	1756	1/1	0.17	-	101,101,101,101	0
24	MG	A	1710	1/1	0.30	-	177,177,177,177	0
24	MG	P	103	1/1	0.17	-	93,93,93,93	0
24	MG	A	1763	1/1	0.18	-	72,72,72,72	0
24	MG	A	1619	1/1	0.13	-	72,72,72,72	0
24	MG	A	1656	1/1	0.27	-	177,177,177,177	0
24	MG	A	1655	1/1	0.29	-	210,210,210,210	0
24	MG	A	1748	1/1	0.22	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	A	1792	1/1	0.24	-	91,91,91,91	0
24	MG	A	1636	1/1	0.19	-	94,94,94,94	0
24	MG	A	1638	1/1	0.31	-	87,87,87,87	0
24	MG	A	1613	1/1	0.12	-	88,88,88,88	0
24	MG	A	1738	1/1	0.23	-	58,58,58,58	0
24	MG	A	1712	1/1	0.16	-	107,107,107,107	0
24	MG	A	1839	1/1	0.22	-	205,205,205,205	1
24	MG	A	1705	1/1	0.41	-	69,69,69,69	0
24	MG	A	1669	1/1	0.44	-	134,134,134,134	0
24	MG	A	1798	1/1	0.18	-	115,115,115,115	0
24	MG	A	1667	1/1	0.67	-	168,168,168,168	0
24	MG	A	1752	1/1	0.24	-	90,90,90,90	0
24	MG	A	1719	1/1	0.24	-	88,88,88,88	0
24	MG	A	1729	1/1	0.65	-	111,111,111,111	0
24	MG	A	1693	1/1	0.12	-	192,192,192,192	0
24	MG	A	1702	1/1	0.12	-	163,163,163,163	0
24	MG	A	1828	1/1	0.15	-	284,284,284,284	0
24	MG	A	1793	1/1	0.52	-	80,80,80,80	0
24	MG	A	1796	1/1	0.23	-	98,98,98,98	0
24	MG	A	1746	1/1	0.45	-	99,99,99,99	0
24	MG	A	1735	1/1	0.32	-	96,96,96,96	0
24	MG	A	1630	1/1	0.05	-	82,82,82,82	0
24	MG	A	1627	1/1	0.22	-	102,102,102,102	0
24	MG	A	1809	1/1	0.22	-	355,355,355,355	0
24	MG	A	1804	1/1	0.23	-	304,304,304,304	0
24	MG	A	1791	1/1	0.17	-	109,109,109,109	0
24	MG	A	1642	1/1	0.06	-	112,112,112,112	0
24	MG	A	1766	1/1	0.26	-	95,95,95,95	0
24	MG	A	1859	1/1	0.48	-	94,94,94,94	0
24	MG	A	1696	1/1	0.36	-	99,99,99,99	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.