



# wwPDB X-ray Structure Validation Summary Report

May 20, 2014 – 02:30 AM EDT

PDB ID : 4NXN  
Title : Crystal Structure of the 30S ribosomal subunit from a GidB (RsmG) mutant of *Thermus thermophilus* (HB8), bound with streptomycin  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2013-12-09  
Resolution : 3.54 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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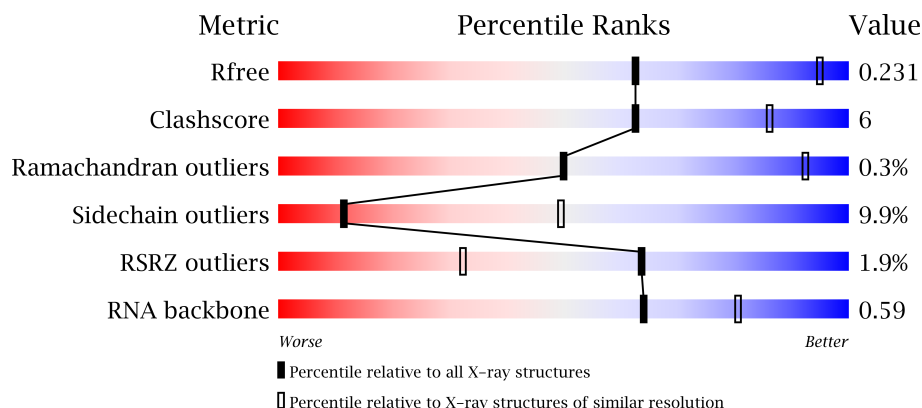
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
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) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 3.54 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.












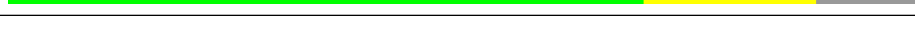
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1270 (3.78-3.30)
Clashscore	79885	1033 (3.70-3.38)
Ramachandran outliers	78287	1067 (3.72-3.36)
Sidechain outliers	78261	1067 (3.72-3.36)
RSRZ outliers	66119	1270 (3.78-3.30)
RNA backbone	1838	1011 (4.30-2.76)

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	

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Mol	Chain	Length	Quality of chain
12	L	135	
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 52137 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
			32506	14476	6011	10507	1512			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	SEE REMARK 999	GB M26923.1
A	1535	A	C	SEE REMARK 999	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 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 ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 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 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 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 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 ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called 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 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 ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

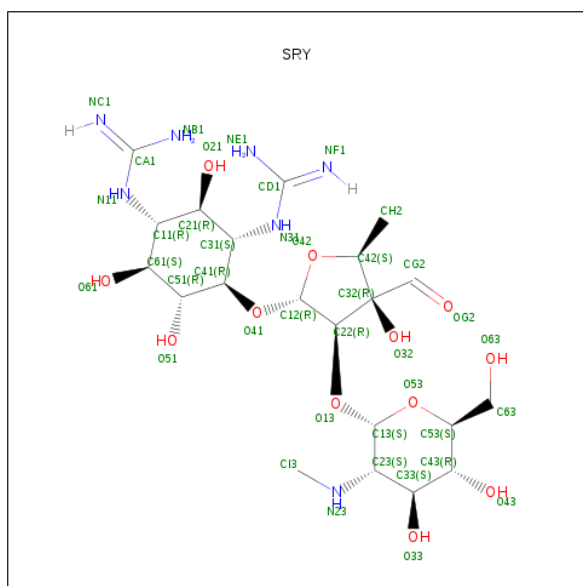
- Molecule 20 is a protein called ribosomal protein S20.

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 ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	3	Total 3	Mg 3	0	0
23	B	1	Total 1	Mg 1	0	0
23	A	227	Total 227	Mg 227	0	0
23	T	1	Total 1	Mg 1	0	0
23	N	1	Total 1	Mg 1	0	0
23	U	1	Total 1	Mg 1	0	0
23	M	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.

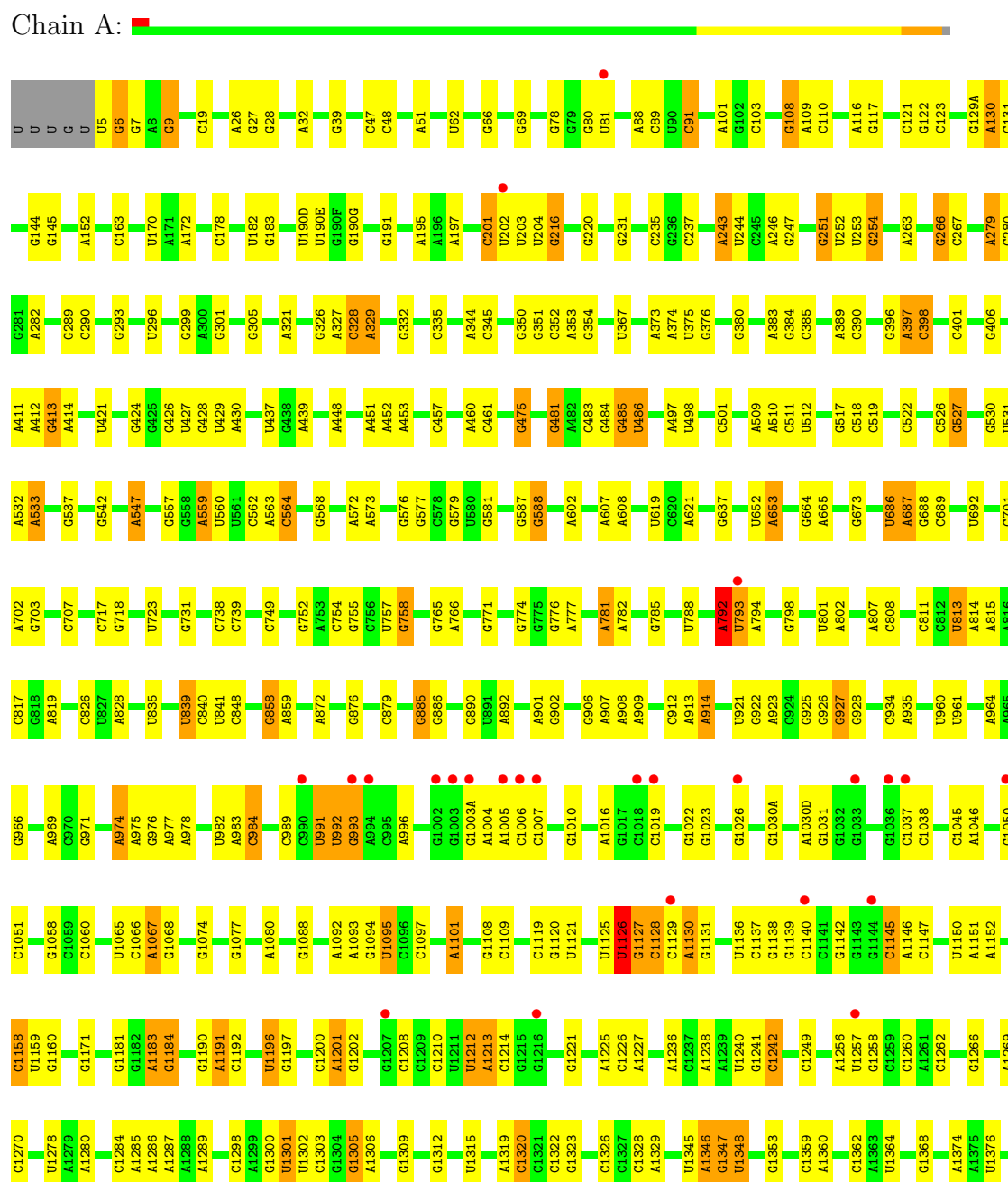
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	254	Total 254	O 254	0	0
25	D	1	Total 1	O 1	0	0
25	E	4	Total 4	O 4	0	0
25	L	1	Total 1	O 1	0	0

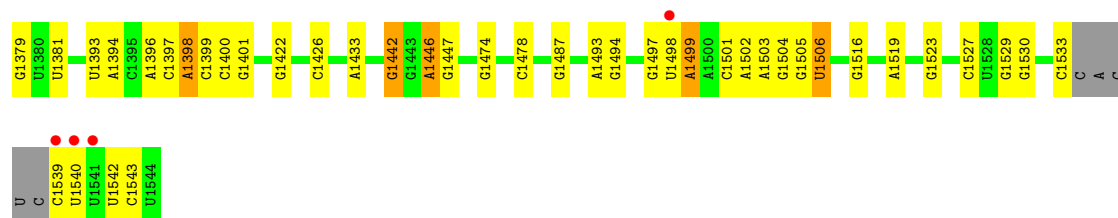


### 3 Residue-property plots

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

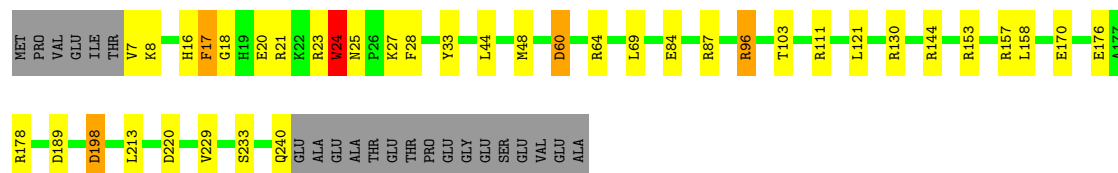
#### • Molecule 1: 16S rRNA





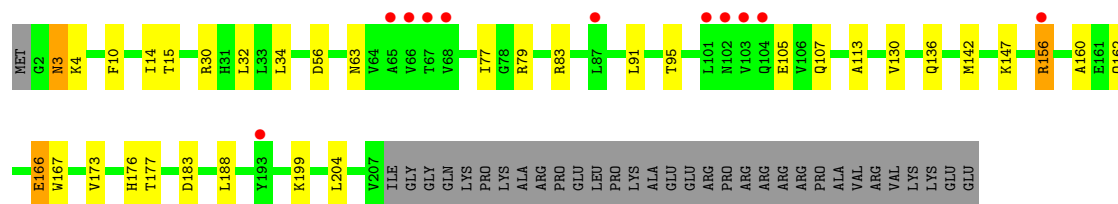
• Molecule 2: ribosomal protein S2

Chain B:



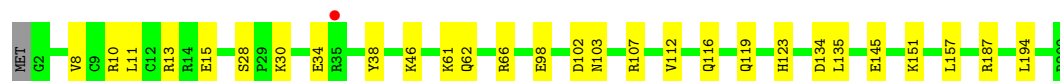
• Molecule 3: ribosomal protein S3

Chain C:



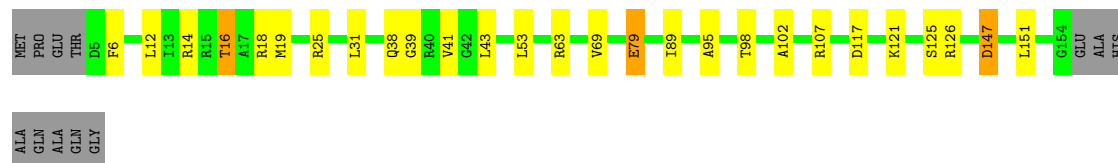
• Molecule 4: ribosomal protein S4

Chain D:



• Molecule 5: ribosomal protein S5

Chain E:



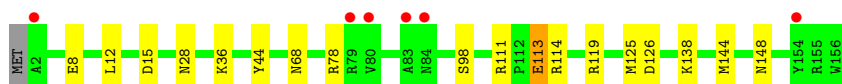
• Molecule 6: ribosomal protein S6

Chain F:



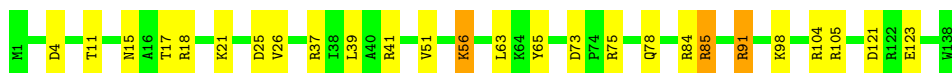
• Molecule 7: ribosomal protein S7

Chain G:



- Molecule 8: ribosomal protein S8

Chain H:



- Molecule 9: ribosomal protein S9

Chain I:



- Molecule 10: ribosomal protein S10

Chain J:



- Molecule 11: ribosomal protein S11

Chain K:



- Molecule 12: ribosomal protein S12

Chain L:



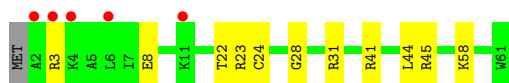
- Molecule 13: ribosomal protein S13

Chain M:



- Molecule 14: ribosomal protein S14

Chain N:



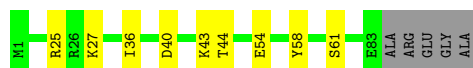
- Molecule 15: ribosomal protein S15

Chain O: 



- Molecule 16: ribosomal protein S16

Chain P: 



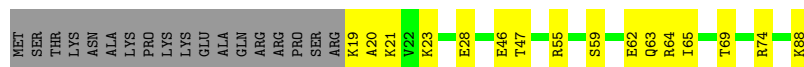
- Molecule 17: ribosomal protein S17

Chain Q: 



- Molecule 18: ribosomal protein S18

Chain R: 



- Molecule 19: ribosomal protein S19

Chain S: 



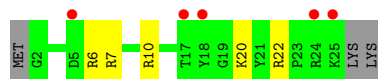
- Molecule 20: ribosomal protein S20

Chain T: 



- Molecule 21: 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, $\alpha$ , $\beta$ , $\gamma$	403.06Å 403.06Å 173.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.74 – 3.54 34.74 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.74-3.54) 98.9 (34.74-3.54)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1555)	Depositor
R, $R_{free}$	0.193 , 0.231 0.193 , 0.231	Depositor DCC
$R_{free}$ test set	8490 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	124.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 74.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 170323 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	52137	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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, 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	0.45	0/36066	0.79	26/56284 (0.0%)
2	B	0.33	0/1935	0.52	0/2609
3	C	0.25	0/1636	0.46	0/2205
4	D	0.31	0/1733	0.44	0/2318
5	E	0.38	0/1162	0.53	0/1564
6	F	0.26	0/856	0.42	0/1154
7	G	0.26	0/1276	0.43	0/1709
8	H	0.46	0/1136	0.52	0/1527
9	I	0.27	0/1029	0.47	0/1379
10	J	0.25	0/805	0.49	0/1082
11	K	0.32	0/879	0.46	0/1187
12	L	0.34	0/977	0.52	0/1306
13	M	0.26	0/947	0.47	0/1270
14	N	0.26	0/501	0.45	0/664
15	O	0.31	0/740	0.45	0/987
16	P	0.37	0/716	0.50	0/963
17	Q	0.40	0/836	0.55	0/1117
18	R	0.30	0/579	0.46	0/768
19	S	0.23	0/661	0.50	0/890
20	T	0.32	0/765	0.50	0/1007
21	U	0.26	0/212	0.38	0/277
All	All	0.41	0/55447	0.71	26/82267 (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
3	C	0	1
20	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	U	C2-N1-C1'	7.82	127.08	117.70
1	A	839	U	N1-C2-O2	7.53	128.07	122.80
1	A	1158	C	N1-C2-O2	7.36	123.32	118.90
1	A	1158	C	C2-N1-C1'	7.16	126.67	118.80
1	A	839	U	N3-C2-O2	-6.66	117.54	122.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
20	T	93	GLU	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	32506	0	32	182	0
2	B	1900	0	0	13	0
3	C	1612	0	0	8	0
4	D	1703	0	0	12	0
5	E	1146	0	0	13	0
6	F	843	0	0	5	0
7	G	1257	0	0	9	0
8	H	1116	0	0	12	0
9	I	1010	0	0	14	0
10	J	792	0	0	4	0
11	K	864	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	972	0	0	6	0
13	M	937	0	0	6	0
14	N	492	0	0	5	0
15	O	729	0	0	4	0
16	P	700	0	0	3	0
17	Q	823	0	0	5	0
18	R	574	0	0	8	0
19	S	647	0	0	7	0
20	T	763	0	0	6	0
21	U	208	0	0	4	0
22	A	40	0	36	4	0
23	A	227	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	3	0	0	0	0
23	M	1	0	0	0	0
23	N	1	0	0	0	0
23	P	2	0	0	0	0
23	Q	2	0	0	0	0
23	T	1	0	0	0	0
23	U	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	254	0	0	3	0
25	D	1	0	0	0	0
25	E	4	0	0	0	0
25	L	1	0	0	0	0
All	All	52137	0	68	265	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 6.

The worst 5 of 265 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1126:U:O4	1:A:1147:C:N4	2.14	0.81
1:A:1158:C:N3	1:A:1181:G:N2	2.29	0.80
1:A:279:A:OP2	17:Q:95:TYR:OH	2.04	0.76
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.20	0.74
1:A:1266:G:N2	1:A:1269:A:OP2	2.23	0.72

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	232/256 (91%)	209 (90%)	20 (9%)	3 (1%)	18	73
3	C	204/239 (85%)	178 (87%)	26 (13%)	0	100	100
4	D	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
5	E	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
9	I	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	27	82
10	J	96/105 (91%)	79 (82%)	15 (16%)	2 (2%)	11	63
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	L	121/135 (90%)	111 (92%)	10 (8%)	0	100	100
13	M	116/126 (92%)	106 (91%)	10 (9%)	0	100	100
14	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	Q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
18	R	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
19	S	78/93 (84%)	68 (87%)	8 (10%)	2 (3%)	8	58
20	T	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
21	U	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
All	All	2336/2541 (92%)	2146 (92%)	182 (8%)	8 (0%)	50	92

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
2	B	21	ARG
2	B	24	TRP

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Mol	Chain	Res	Type
9	I	119	ALA
19	S	14	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	202/220 (92%)	180 (89%)	22 (11%)	9	44
3	C	160/188 (85%)	136 (85%)	24 (15%)	4	26
4	D	180/181 (99%)	170 (94%)	10 (6%)	30	77
5	E	115/123 (94%)	100 (87%)	15 (13%)	6	33
6	F	90/90 (100%)	83 (92%)	7 (8%)	18	63
7	G	126/127 (99%)	120 (95%)	6 (5%)	35	82
8	H	119/119 (100%)	106 (89%)	13 (11%)	9	44
9	I	98/99 (99%)	87 (89%)	11 (11%)	9	41
10	J	87/92 (95%)	82 (94%)	5 (6%)	29	76
11	K	88/99 (89%)	82 (93%)	6 (7%)	22	70
12	L	103/110 (94%)	88 (85%)	15 (15%)	5	27
13	M	94/101 (93%)	79 (84%)	15 (16%)	3	22
14	N	49/50 (98%)	44 (90%)	5 (10%)	11	48
15	O	79/80 (99%)	72 (91%)	7 (9%)	14	57
16	P	72/74 (97%)	68 (94%)	4 (6%)	30	77
17	Q	94/97 (97%)	87 (93%)	7 (7%)	20	66
18	R	61/77 (79%)	55 (90%)	6 (10%)	12	50
19	S	71/80 (89%)	59 (83%)	12 (17%)	3	19
20	T	76/82 (93%)	71 (93%)	5 (7%)	24	71
21	U	19/22 (86%)	18 (95%)	1 (5%)	32	78
All	All	1983/2111 (94%)	1787 (90%)	196 (10%)	11	49

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	39	LEU
10	J	57	LYS
19	S	15	LEU
8	H	63	LEU
9	I	29	ASN

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%)	258 (17%)	0

5 of 258 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G

There are no RNA pucker outliers to report.

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

14 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	1.67	6 (25%)	33,38,41	9.76	5 (15%)
1	5MC	A	1400	1	20,22,23	1.74	1 (5%)	26,32,35	1.09	2 (7%)
1	4OC	A	1402	1	21,23,24	1.48	2 (9%)	26,32,35	0.89	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1404	1	20,22,23	1.49	1 (5%)	26,32,35	1.13	2 (7%)
1	5MC	A	1407	1	20,22,23	1.69	1 (5%)	26,32,35	1.06	2 (7%)
1	UR3	A	1498	1	20,22,23	1.59	1 (5%)	23,32,35	1.11	2 (8%)
1	MA6	A	1518	1	26,26,27	1.19	2 (7%)	37,38,41	0.99	2 (5%)
1	MA6	A	1519	1	26,26,27	1.25	2 (7%)	37,38,41	0.97	2 (5%)
1	PSU	A	1540	1,23	19,21,22	0.88	0	23,30,33	1.17	2 (8%)
1	PSU	A	1541	1	19,21,22	0.89	0	23,30,33	1.02	2 (8%)
1	PSU	A	516	1,23	19,21,22	0.91	0	23,30,33	0.96	2 (8%)
1	M2G	A	966	1	25,27,28	1.83	5 (20%)	35,40,43	8.59	5 (14%)
1	5MC	A	967	1	20,22,23	1.47	1 (5%)	26,32,35	1.12	2 (7%)
12	0TD	L	92	12	9,9,10	6.86	2 (22%)	9,11,13	1.82	2 (22%)

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	0/3/3/3
1	5MC	A	1400	1	-	0/6/25/26	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	0/3/3/3
1	MA6	A	1519	1	-	0/13/29/30	0/3/3/3
1	PSU	A	1540	1,23	-	1/8/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/8/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/8/25/26	0/2/2/2
1	M2G	A	966	1	-	0/12/29/30	0/3/3/3
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 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	O-C	20.29	1.25	1.11
1	A	1400	5MC	C2-N1	6.68	1.45	1.38
1	A	1407	5MC	C2-N1	6.33	1.45	1.38
1	A	1498	UR3	C5-C4	5.92	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C2-N1	5.74	1.44	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C6-C5-N7	-55.65	126.65	134.14
1	A	966	M2G	C6-C5-N7	-49.94	127.42	134.14
1	A	966	M2G	C6-N1-C2	7.20	123.33	120.18
12	L	92	0TD	CSB-SB-CB	-3.97	94.32	101.29
1	A	1540	PSU	C5-C1'-C2'	-3.83	108.63	115.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1540	PSU	OP2-P-O5'-C5'

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 244 ligands modelled in this entry, 243 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
22	SRY	A	1601	-	42,42,42	2.24	13 (30%)	63,63,63	1.82	12 (19%)

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	SRY	A	1601	-	-	0/22/87/87	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	8.06	1.48	1.33
22	A	1601	SRY	CA1-N11	6.59	1.45	1.33
22	A	1601	SRY	O53-C53	-3.68	1.35	1.44
22	A	1601	SRY	C32-C42	-3.45	1.49	1.54
22	A	1601	SRY	C23-N23	-2.98	1.42	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	CI3-N23-C23	-5.47	109.34	113.65
22	A	1601	SRY	C13-O13-C22	-5.41	106.77	116.21
22	A	1601	SRY	C12-O42-C42	-4.75	100.68	108.36
22	A	1601	SRY	O41-C12-C22	4.24	115.47	107.32
22	A	1601	SRY	O41-C12-O42	-4.04	107.67	111.57

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%)	-0.23	29 (1%) 64 32	85, 130, 272, 382	0
2	B	234/256 (91%)	-0.13	0 100 100	98, 143, 227, 240	0
3	C	206/239 (86%)	0.31	11 (5%) 25 11	148, 207, 271, 304	0
4	D	208/209 (99%)	-0.12	1 (0%) 88 65	90, 127, 171, 259	0
5	E	150/162 (92%)	-0.19	0 100 100	77, 106, 136, 201	0
6	F	101/101 (100%)	-0.29	0 100 100	119, 143, 167, 214	0
7	G	155/156 (99%)	0.09	6 (3%) 37 17	135, 180, 230, 263	0
8	H	138/138 (100%)	-0.26	0 100 100	70, 93, 121, 166	0
9	I	127/128 (99%)	0.25	4 (3%) 47 22	136, 204, 249, 303	0
10	J	98/105 (93%)	0.70	7 (7%) 16 7	164, 247, 326, 391	0
11	K	116/129 (89%)	-0.13	0 100 100	96, 124, 170, 203	0
12	L	123/135 (91%)	0.01	1 (0%) 83 53	75, 128, 151, 199	0
13	M	118/126 (93%)	-0.05	1 (0%) 83 53	127, 156, 192, 327	0
14	N	60/61 (98%)	0.61	5 (8%) 11 7	165, 197, 252, 298	0
15	O	87/89 (97%)	-0.19	0 100 100	85, 113, 150, 163	0
16	P	83/88 (94%)	-0.14	0 100 100	104, 124, 153, 198	0
17	Q	99/105 (94%)	-0.22	0 100 100	85, 104, 135, 167	0
18	R	70/88 (79%)	-0.20	0 100 100	96, 124, 170, 215	0
19	S	80/93 (86%)	0.60	4 (5%) 28 12	159, 221, 278, 327	0
20	T	99/106 (93%)	-0.16	0 100 100	103, 119, 155, 199	0
21	U	24/27 (88%)	1.21	5 (20%) 1 2	141, 172, 202, 216	0
All	All	3887/4063 (95%)	-0.08	74 (1%) 64 32	70, 137, 253, 391	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1498	UR3	6.8
1	A	1018	C	6.2
3	C	103	VAL	6.2
1	A	1540	PSU	5.7
1	A	1541	PSU	5.4

## 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	1519	24/25	0.17	-	118,122,123,128	0
1	4OC	A	1402	22/23	0.22	-	120,124,130,131	0
12	0TD	L	92	10/11	0.38	-	122,125,128,294	0
1	UR3	A	1498	21/22	0.24	-	120,124,127,129	0
1	M2G	A	966	25/26	0.21	-	123,127,159,162	0
1	5MC	A	967	21/22	0.16	-	119,121,126,126	0
1	5MC	A	1407	21/22	0.15	-	132,139,146,152	0
1	PSU	A	516	20/21	0.10	-	131,135,144,144	0
1	5MC	A	1404	21/22	0.24	-	119,121,132,135	0
1	MA6	A	1518	24/25	0.14	-	122,126,137,140	0
1	5MC	A	1400	21/22	0.18	-	116,122,125,126	0
1	PSU	A	1540	20/21	0.59	-	279,294,305,305	0
1	PSU	A	1541	20/21	0.57	-	288,305,333,335	0
1	2MG	A	1207	24/25	0.32	-	201,210,224,228	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( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1735	1/1	0.13	-	74,74,74,74	0
23	MG	A	1624	1/1	0.09	-	74,74,74,74	0
23	MG	A	1693	1/1	0.14	-	121,121,121,121	0
23	MG	A	1713	1/1	0.62	-	121,121,121,121	0
23	MG	A	1754	1/1	0.20	-	106,106,106,106	0
23	MG	A	1672	1/1	0.13	-	91,91,91,91	0
23	MG	A	1792	1/1	0.14	-	98,98,98,98	0
23	MG	A	1704	1/1	0.21	-	76,76,76,76	0
23	MG	A	1785	1/1	0.16	-	304,304,304,304	0
23	MG	A	1757	1/1	0.35	-	84,84,84,84	0
23	MG	A	1789	1/1	0.21	-	81,81,81,81	0
23	MG	A	1626	1/1	0.09	-	113,113,113,113	0
23	MG	Q	201	1/1	0.07	-	80,80,80,80	0
23	MG	A	1763	1/1	0.61	-	106,106,106,106	0
23	MG	A	1737	1/1	0.90	-	73,73,73,73	0
23	MG	A	1675	1/1	0.24	-	119,119,119,119	0
23	MG	A	1621	1/1	0.29	-	98,98,98,98	0
23	MG	A	1773	1/1	0.12	-	75,75,75,75	0
23	MG	A	1665	1/1	0.09	-	128,128,128,128	0
23	MG	A	1738	1/1	0.14	-	86,86,86,86	0
23	MG	A	1709	1/1	0.13	-	172,172,172,172	0
23	MG	A	1699	1/1	0.21	-	289,289,289,289	0
23	MG	A	1659	1/1	0.09	-	138,138,138,138	0
23	MG	A	1815	1/1	0.24	-	108,108,108,108	0
23	MG	A	1753	1/1	0.39	-	51,51,51,51	0
23	MG	A	1724	1/1	0.34	-	57,57,57,57	0
23	MG	A	1681	1/1	0.15	-	82,82,82,82	0
23	MG	A	1783	1/1	0.16	-	129,129,129,129	0
23	MG	A	1606	1/1	0.07	-	106,106,106,106	0
23	MG	A	1776	1/1	0.42	-	106,106,106,106	0
23	MG	A	1728	1/1	0.08	-	97,97,97,97	0
23	MG	A	1605	1/1	0.28	-	75,75,75,75	0
23	MG	A	1637	1/1	0.25	-	81,81,81,81	0
23	MG	A	1749	1/1	0.27	-	77,77,77,77	0
23	MG	A	1700	1/1	0.13	-	136,136,136,136	0
23	MG	A	1747	1/1	0.43	-	89,89,89,89	0
23	MG	A	1781	1/1	0.07	-	119,119,119,119	0
23	MG	A	1634	1/1	0.17	-	115,115,115,115	0
23	MG	A	1683	1/1	1.05	-	91,91,91,91	0
23	MG	A	1667	1/1	0.26	-	141,141,141,141	0
23	MG	A	1770	1/1	0.07	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1720	1/1	0.38	-	82,82,82,82	0
23	MG	A	1688	1/1	0.17	-	135,135,135,135	0
23	MG	A	1787	1/1	0.50	-	86,86,86,86	0
23	MG	A	1632	1/1	0.15	-	95,95,95,95	0
23	MG	A	1767	1/1	0.20	-	104,104,104,104	0
23	MG	A	1616	1/1	0.25	-	54,54,54,54	0
22	SRY	A	1601	40/40	0.22	-	86,104,124,135	0
23	MG	A	1643	1/1	0.09	-	81,81,81,81	0
23	MG	N	102	1/1	0.32	-	96,96,96,96	0
23	MG	A	1639	1/1	0.10	-	44,44,44,44	0
23	MG	A	1743	1/1	0.21	-	70,70,70,70	0
23	MG	A	1701	1/1	0.19	-	93,93,93,93	0
23	MG	A	1663	1/1	0.18	-	65,65,65,65	0
23	MG	D	302	1/1	0.12	-	92,92,92,92	0
23	MG	A	1614	1/1	0.16	-	66,66,66,66	0
23	MG	A	1730	1/1	0.14	-	148,148,148,148	0
23	MG	A	1692	1/1	0.09	-	143,143,143,143	0
23	MG	A	1646	1/1	0.19	-	111,111,111,111	0
23	MG	A	1612	1/1	0.08	-	101,101,101,101	0
23	MG	A	1800	1/1	0.41	-	131,131,131,131	0
23	MG	A	1679	1/1	0.21	-	121,121,121,121	0
23	MG	A	1630	1/1	0.18	-	79,79,79,79	0
23	MG	A	1677	1/1	0.16	-	126,126,126,126	0
23	MG	A	1654	1/1	0.12	-	115,115,115,115	0
23	MG	A	1641	1/1	0.10	-	101,101,101,101	0
23	MG	A	1826	1/1	0.15	-	119,119,119,119	0
23	MG	A	1694	1/1	0.15	-	144,144,144,144	0
23	MG	A	1674	1/1	0.26	-	68,68,68,68	0
23	MG	A	1687	1/1	0.24	-	76,76,76,76	0
23	MG	H	201	1/1	0.23	-	56,56,56,56	0
23	MG	A	1813	1/1	0.10	-	81,81,81,81	0
23	MG	A	1802	1/1	0.72	-	101,101,101,101	0
23	MG	A	1725	1/1	0.18	-	74,74,74,74	0
23	MG	A	1610	1/1	0.18	-	102,102,102,102	0
23	MG	A	1653	1/1	0.17	-	87,87,87,87	0
23	MG	A	1805	1/1	0.50	-	108,108,108,108	0
23	MG	A	1752	1/1	0.12	-	110,110,110,110	0
23	MG	A	1708	1/1	0.12	-	111,111,111,111	0
23	MG	A	1715	1/1	0.47	-	110,110,110,110	0
23	MG	A	1680	1/1	0.18	-	139,139,139,139	0
23	MG	A	1807	1/1	0.21	-	222,222,222,222	0
23	MG	A	1727	1/1	0.23	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1673	1/1	0.11	-	88,88,88,88	0
23	MG	A	1734	1/1	0.14	-	77,77,77,77	0
23	MG	A	1774	1/1	0.21	-	79,79,79,79	0
23	MG	A	1670	1/1	0.21	-	170,170,170,170	0
23	MG	A	1686	1/1	0.20	-	102,102,102,102	0
23	MG	A	1629	1/1	0.16	-	180,180,180,180	0
23	MG	A	1748	1/1	0.25	-	63,63,63,63	0
23	MG	A	1822	1/1	1.23	-	104,104,104,104	0
23	MG	E	201	1/1	0.07	-	83,83,83,83	0
23	MG	A	1710	1/1	0.07	-	168,168,168,168	0
23	MG	A	1821	1/1	0.09	-	106,106,106,106	0
23	MG	A	1619	1/1	0.09	-	49,49,49,49	0
23	MG	A	1828	1/1	0.26	-	91,91,91,91	0
23	MG	A	1684	1/1	0.13	-	168,168,168,168	0
23	MG	A	1645	1/1	0.11	-	164,164,164,164	0
23	MG	A	1761	1/1	0.14	-	89,89,89,89	0
23	MG	A	1742	1/1	0.15	-	97,97,97,97	0
23	MG	A	1810	1/1	0.10	-	433,433,433,433	0
23	MG	Q	202	1/1	0.28	-	55,55,55,55	0
23	MG	A	1750	1/1	0.31	-	77,77,77,77	0
23	MG	P	102	1/1	0.27	-	80,80,80,80	0
23	MG	A	1782	1/1	0.12	-	93,93,93,93	0
23	MG	A	1716	1/1	0.22	-	68,68,68,68	0
23	MG	A	1718	1/1	0.28	-	90,90,90,90	0
23	MG	A	1666	1/1	0.21	-	104,104,104,104	0
23	MG	A	1816	1/1	0.14	-	132,132,132,132	0
23	MG	A	1662	1/1	0.25	-	89,89,89,89	0
23	MG	A	1625	1/1	0.33	-	137,137,137,137	0
23	MG	A	1759	1/1	0.81	-	70,70,70,70	0
23	MG	A	1784	1/1	0.15	-	170,170,170,170	0
23	MG	A	1755	1/1	0.29	-	73,73,73,73	0
23	MG	A	1617	1/1	0.20	-	87,87,87,87	0
23	MG	A	1765	1/1	0.33	-	53,53,53,53	0
23	MG	A	1604	1/1	0.17	-	90,90,90,90	0
23	MG	A	1682	1/1	0.46	-	107,107,107,107	0
23	MG	A	1644	1/1	0.16	-	78,78,78,78	0
23	MG	A	1691	1/1	0.15	-	186,186,186,186	0
23	MG	A	1790	1/1	0.37	-	78,78,78,78	0
23	MG	A	1678	1/1	0.17	-	91,91,91,91	0
23	MG	A	1736	1/1	0.11	-	114,114,114,114	0
23	MG	A	1799	1/1	0.30	-	79,79,79,79	0
23	MG	A	1793	1/1	0.17	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1620	1/1	0.15	-	85,85,85,85	0
23	MG	A	1779	1/1	0.28	-	139,139,139,139	0
23	MG	A	1707	1/1	0.10	-	120,120,120,120	0
23	MG	A	1814	1/1	0.88	-	98,98,98,98	0
23	MG	A	1651	1/1	0.08	-	96,96,96,96	0
23	MG	A	1627	1/1	0.17	-	76,76,76,76	0
23	MG	A	1818	1/1	0.24	-	79,79,79,79	0
23	MG	A	1652	1/1	0.19	-	129,129,129,129	0
23	MG	A	1819	1/1	0.22	-	68,68,68,68	0
23	MG	A	1669	1/1	0.23	-	104,104,104,104	0
23	MG	A	1729	1/1	0.40	-	124,124,124,124	0
23	MG	A	1705	1/1	0.16	-	185,185,185,185	0
23	MG	A	1628	1/1	0.13	-	99,99,99,99	0
23	MG	A	1798	1/1	0.78	-	85,85,85,85	0
23	MG	A	1794	1/1	0.64	-	56,56,56,56	0
23	MG	A	1702	1/1	0.12	-	153,153,153,153	0
23	MG	A	1671	1/1	0.41	-	73,73,73,73	0
23	MG	A	1726	1/1	1.05	-	106,106,106,106	0
23	MG	H	203	1/1	0.39	-	76,76,76,76	0
23	MG	A	1636	1/1	0.32	-	76,76,76,76	0
23	MG	A	1746	1/1	0.17	-	100,100,100,100	0
23	MG	A	1739	1/1	0.23	-	55,55,55,55	0
23	MG	A	1655	1/1	0.24	-	116,116,116,116	0
23	MG	A	1613	1/1	0.06	-	102,102,102,102	0
23	MG	A	1695	1/1	0.23	-	273,273,273,273	0
23	MG	A	1712	1/1	0.15	-	83,83,83,83	0
23	MG	A	1656	1/1	0.15	-	76,76,76,76	0
23	MG	A	1668	1/1	0.09	-	105,105,105,105	0
23	MG	A	1603	1/1	0.23	-	90,90,90,90	0
23	MG	A	1731	1/1	0.07	-	90,90,90,90	0
23	MG	A	1795	1/1	0.57	-	108,108,108,108	0
23	MG	A	1685	1/1	0.43	-	72,72,72,72	0
23	MG	A	1721	1/1	0.15	-	100,100,100,100	0
23	MG	A	1780	1/1	0.16	-	84,84,84,84	0
23	MG	A	1633	1/1	0.28	-	130,130,130,130	0
23	MG	A	1649	1/1	0.22	-	67,67,67,67	0
23	MG	A	1772	1/1	0.35	-	107,107,107,107	0
23	MG	A	1623	1/1	0.12	-	58,58,58,58	0
23	MG	A	1664	1/1	0.07	-	135,135,135,135	0
23	MG	A	1764	1/1	0.28	-	146,146,146,146	0
23	MG	P	101	1/1	0.34	-	52,52,52,52	0
23	MG	A	1771	1/1	0.12	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	ZN	N	101	1/1	0.14	-	170,170,170,170	0
23	MG	A	1744	1/1	0.19	-	96,96,96,96	0
23	MG	T	201	1/1	0.33	-	87,87,87,87	0
23	MG	A	1786	1/1	0.19	-	180,180,180,180	0
23	MG	A	1635	1/1	0.13	-	61,61,61,61	0
23	MG	M	201	1/1	0.31	-	91,91,91,91	0
23	MG	A	1732	1/1	0.16	-	73,73,73,73	0
23	MG	A	1607	1/1	0.35	-	91,91,91,91	0
23	MG	A	1777	1/1	0.17	-	83,83,83,83	0
23	MG	A	1801	1/1	0.19	-	70,70,70,70	0
23	MG	A	1808	1/1	0.28	-	205,205,205,205	0
23	MG	A	1676	1/1	0.05	-	157,157,157,157	0
23	MG	A	1788	1/1	0.41	-	99,99,99,99	0
23	MG	A	1660	1/1	0.09	-	123,123,123,123	0
23	MG	A	1820	1/1	0.24	-	83,83,83,83	0
23	MG	A	1622	1/1	0.35	-	110,110,110,110	0
23	MG	A	1740	1/1	0.35	-	99,99,99,99	0
23	MG	A	1719	1/1	0.38	-	95,95,95,95	0
23	MG	A	1696	1/1	0.12	-	105,105,105,105	0
23	MG	A	1762	1/1	0.58	-	110,110,110,110	0
23	MG	A	1611	1/1	0.18	-	104,104,104,104	0
23	MG	A	1804	1/1	0.11	-	78,78,78,78	0
23	MG	A	1642	1/1	0.23	-	47,47,47,47	0
23	MG	A	1775	1/1	0.25	-	116,116,116,116	0
23	MG	A	1698	1/1	0.20	-	85,85,85,85	0
23	MG	A	1803	1/1	0.23	-	92,92,92,92	0
23	MG	A	1658	1/1	0.18	-	190,190,190,190	0
23	MG	A	1722	1/1	0.20	-	82,82,82,82	0
23	MG	A	1723	1/1	0.51	-	72,72,72,72	0
23	MG	A	1791	1/1	0.09	-	105,105,105,105	0
23	MG	A	1640	1/1	0.24	-	102,102,102,102	0
23	MG	A	1602	1/1	0.19	-	112,112,112,112	0
23	MG	B	301	1/1	0.59	-	120,120,120,120	0
23	MG	A	1756	1/1	0.08	-	94,94,94,94	0
23	MG	A	1769	1/1	0.38	-	102,102,102,102	0
23	MG	A	1647	1/1	0.14	-	89,89,89,89	0
23	MG	A	1657	1/1	0.24	-	96,96,96,96	0
23	MG	A	1751	1/1	0.96	-	94,94,94,94	0
23	MG	A	1618	1/1	0.33	-	73,73,73,73	0
23	MG	A	1809	1/1	0.22	-	187,187,187,187	0
23	MG	A	1797	1/1	0.19	-	75,75,75,75	0
23	MG	A	1760	1/1	0.34	-	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1806	1/1	0.21	-	334,334,334,334	0
23	MG	A	1778	1/1	0.26	-	149,149,149,149	0
23	MG	A	1631	1/1	0.14	-	80,80,80,80	0
23	MG	A	1758	1/1	0.10	-	81,81,81,81	0
23	MG	A	1827	1/1	0.12	-	74,74,74,74	0
23	MG	A	1825	1/1	0.15	-	96,96,96,96	0
23	MG	H	202	1/1	0.16	-	57,57,57,57	0
23	MG	A	1817	1/1	0.26	-	63,63,63,63	0
23	MG	A	1812	1/1	0.40	-	68,68,68,68	0
23	MG	A	1714	1/1	0.10	-	110,110,110,110	0
23	MG	A	1609	1/1	0.17	-	72,72,72,72	0
23	MG	A	1661	1/1	0.82	-	91,91,91,91	0
23	MG	A	1768	1/1	0.19	-	79,79,79,79	0
23	MG	A	1717	1/1	0.15	-	109,109,109,109	0
23	MG	A	1796	1/1	0.30	-	131,131,131,131	0
23	MG	A	1689	1/1	0.10	-	105,105,105,105	0
23	MG	A	1690	1/1	1.01	-	95,95,95,95	0
23	MG	A	1811	1/1	0.27	-	122,122,122,122	0
23	MG	A	1615	1/1	0.13	-	47,47,47,47	0
23	MG	A	1823	1/1	0.08	-	127,127,127,127	0
23	MG	A	1745	1/1	0.12	-	53,53,53,53	0
24	ZN	D	301	1/1	0.33	-	71,71,71,71	0
23	MG	A	1711	1/1	0.30	-	90,90,90,90	0
23	MG	A	1741	1/1	0.41	-	96,96,96,96	0
23	MG	A	1638	1/1	0.16	-	156,156,156,156	0
23	MG	A	1706	1/1	0.23	-	114,114,114,114	0
23	MG	A	1697	1/1	0.17	-	171,171,171,171	0
23	MG	A	1650	1/1	0.29	-	77,77,77,77	0
23	MG	A	1648	1/1	0.10	-	100,100,100,100	0
23	MG	A	1824	1/1	0.29	-	104,104,104,104	0
23	MG	A	1608	1/1	0.08	-	97,97,97,97	0
23	MG	A	1766	1/1	0.08	-	105,105,105,105	0
23	MG	A	1733	1/1	0.29	-	82,82,82,82	0
23	MG	U	101	1/1	0.25	-	129,129,129,129	0
23	MG	A	1703	1/1	0.15	-	79,79,79,79	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.