



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:25 AM UTC

PDB ID : 8WRC / pdb_00008wrc
Title : Time-Resolved Ambient Temperature Kineto-Crystallographic Structure of Initiation Factor in Complex with Ribosome
Authors : DeMirci, H.; Yapici, I.
Deposited on : 2023-10-13
Resolution : 3.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

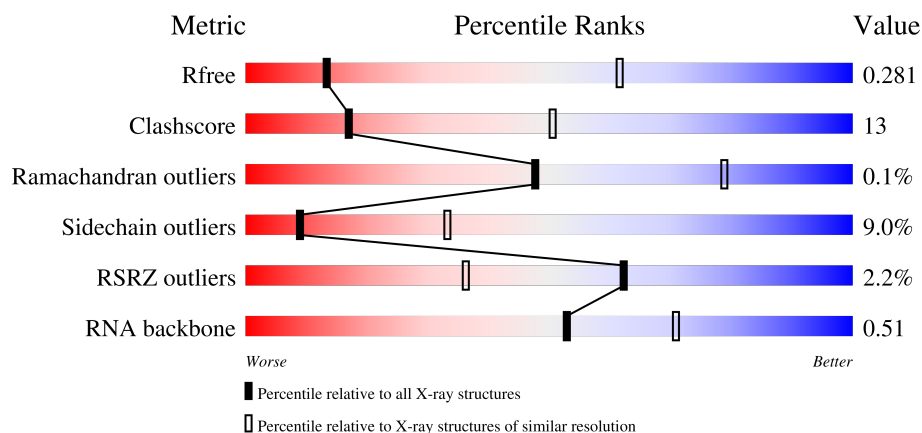
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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.



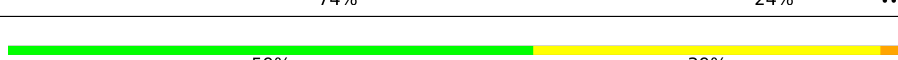
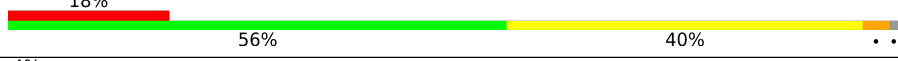
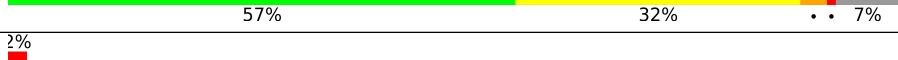
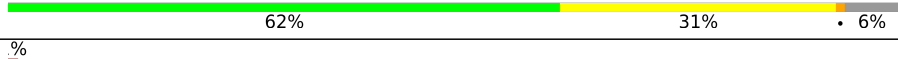
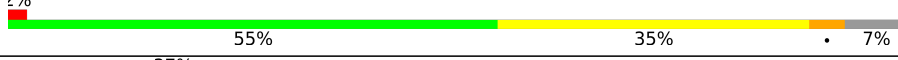
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
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	
22	W	71	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1511	Total	C	N	O	P	0	6	0
			32623	14530	6037	10539	1517			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	U	-	conflict	GB NR_037066
A	13	C	U	conflict	GB NR_037066
A	1027	C	-	insertion	GB NR_037066
A	1031	G	-	insertion	GB NR_037066
A	1244	C	-	insertion	GB NR_037066
A	1245	A	-	insertion	GB NR_037066
A	1534	C	A	conflict	GB NR_037066
A	1535	A	C	conflict	GB NR_037066
A	1540	PSU	-	insertion	GB NR_037066
A	1541	PSU	-	insertion	GB NR_037066
A	1543	C	U	conflict	GB NR_037066

- Molecule 2 is a protein called 30S 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 30S 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 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	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called 30S 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 Small ribosomal subunit protein uS12.

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 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 type Z.

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	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S 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 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 18 is a protein called 30S 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 30S 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 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	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	71	Total	C	N	O	S	0	0	0
			570	362	103	103	2			

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	233	Total	Mg	0	0
			233	233		
23	B	1	Total	Mg	0	0
			1	1		
23	C	3	Total	Mg	0	0
			3	3		
23	D	3	Total	Mg	0	0
			3	3		
23	E	2	Total	Mg	0	0
			2	2		
23	F	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	1	Total 1	Mg 1	0	0
23	I	3	Total 3	Mg 3	0	0
23	L	1	Total 1	Mg 1	0	0
23	N	1	Total 1	Mg 1	0	0
23	P	2	Total 2	Mg 2	0	0
23	Q	1	Total 1	Mg 1	0	0
23	S	1	Total 1	Mg 1	0	0
23	W	1	Total 1	Mg 1	0	0

- Molecule 24 is ZINC ION (CCD ID: 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	237	Total 237	O 237	0	0
25	C	1	Total 1	O 1	0	0
25	D	3	Total 3	O 3	0	0
25	E	1	Total 1	O 1	0	0
25	L	2	Total 2	O 2	0	0
25	N	3	Total 3	O 3	0	0
25	O	1	Total 1	O 1	0	0

Continued on next page...

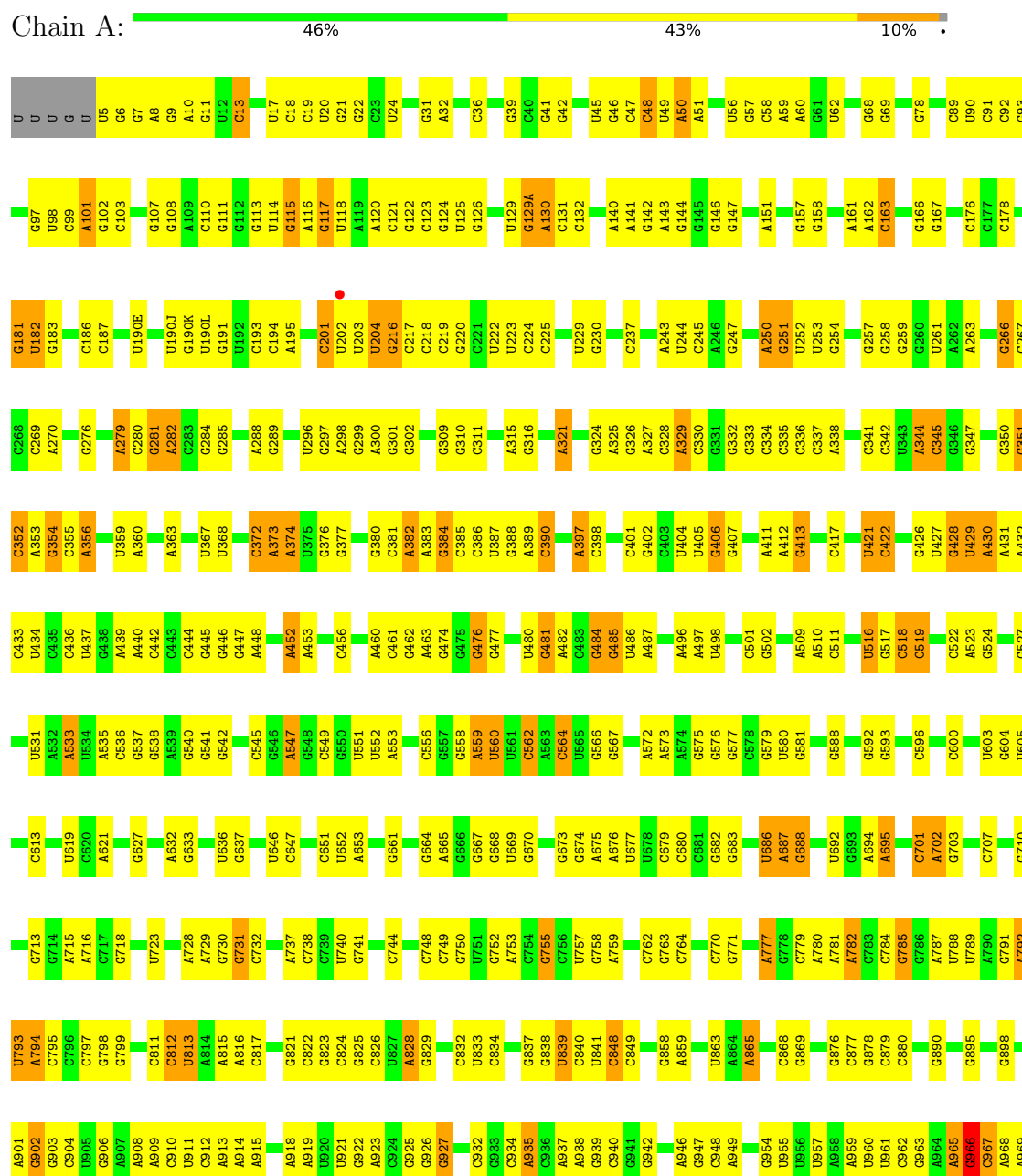
Continued from previous page...

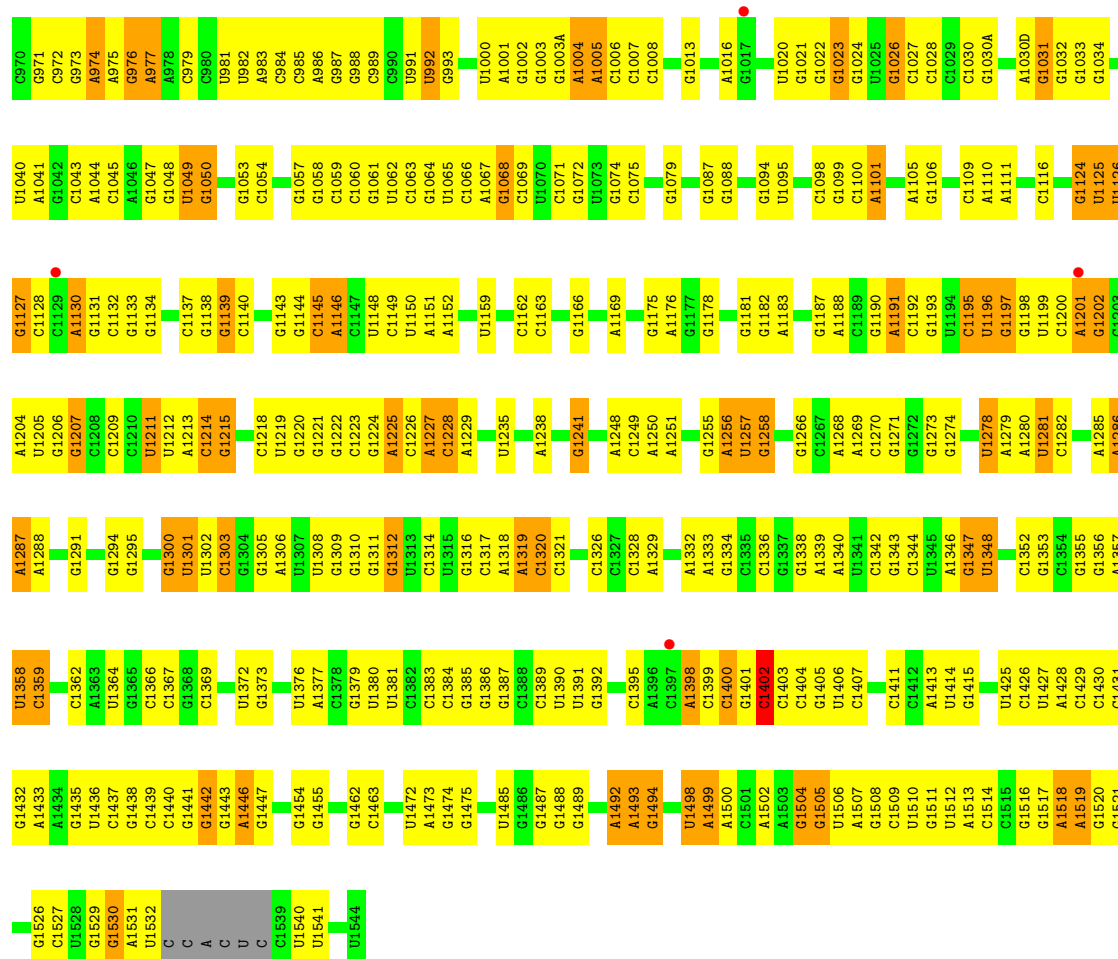
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	T	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

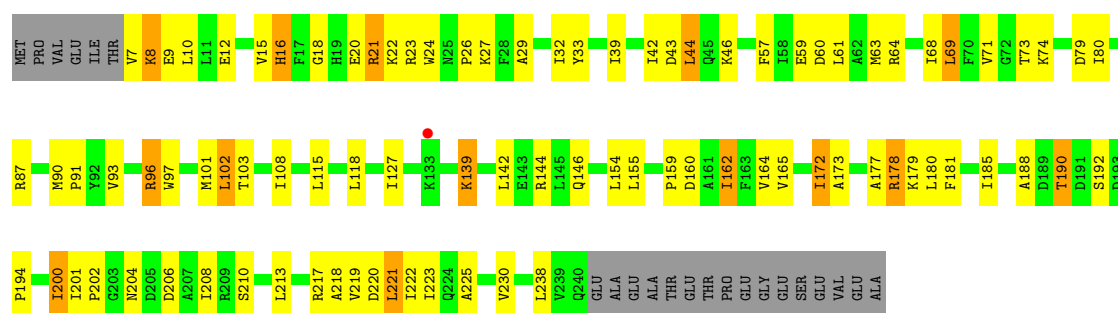
• Molecule 1: 16S rRNA





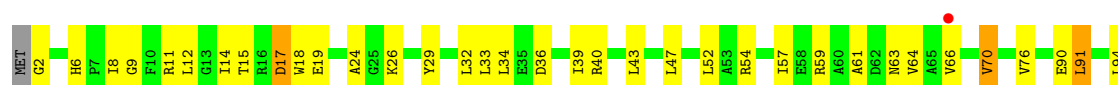
• Molecule 2: 30S ribosomal protein S2

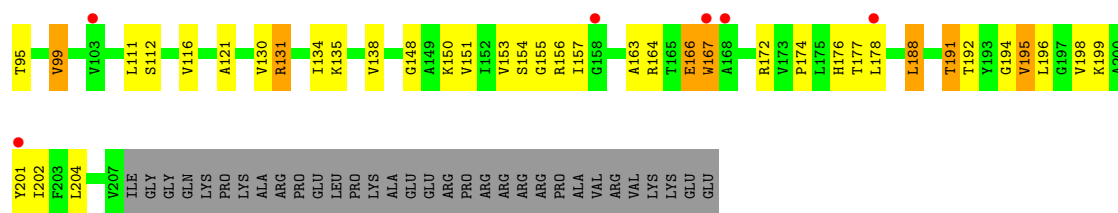
Chain B: 56% 30% 5% 9%



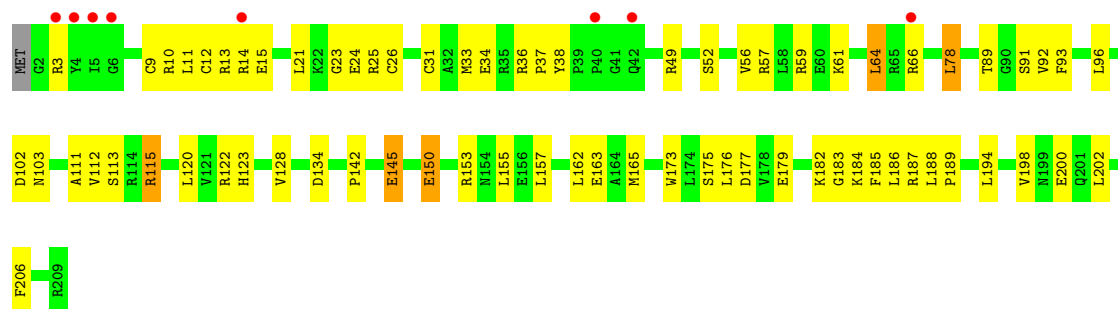
• Molecule 3: 30S ribosomal protein S3

Chain C: 3% 55% 27% 14%

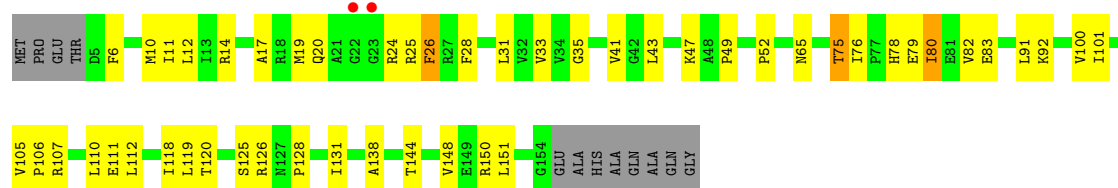




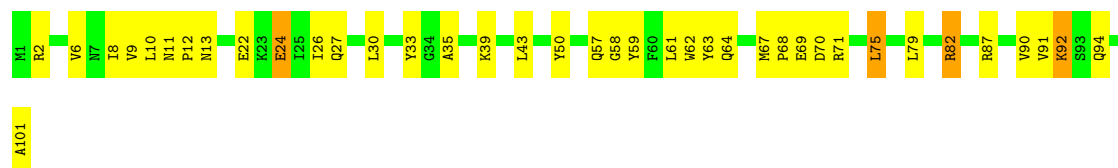
• Molecule 4: 30S ribosomal protein S4



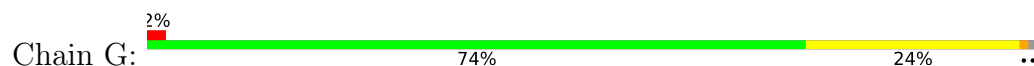
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



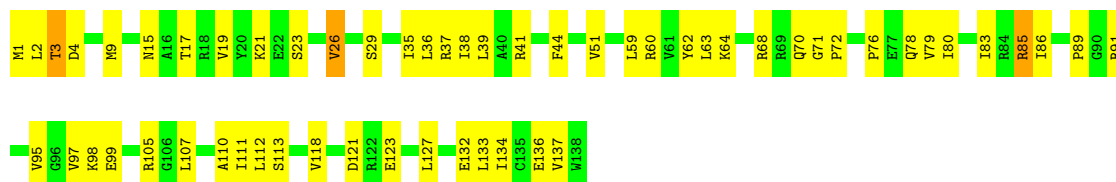
• Molecule 7: 30S ribosomal protein S7





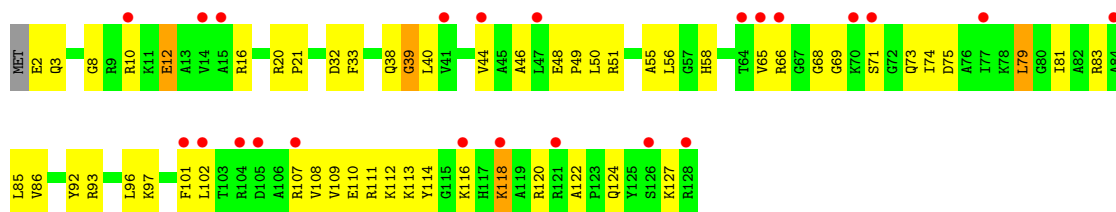
- Molecule 8: 30S ribosomal protein S8

Chain H: 59% 39%



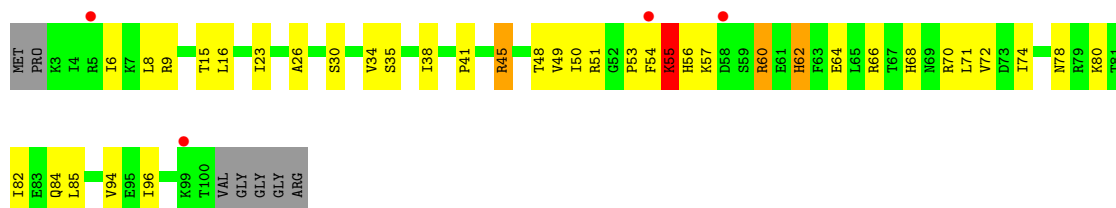
- Molecule 9: 30S ribosomal protein S9

Chain I: 18% 56% 40%



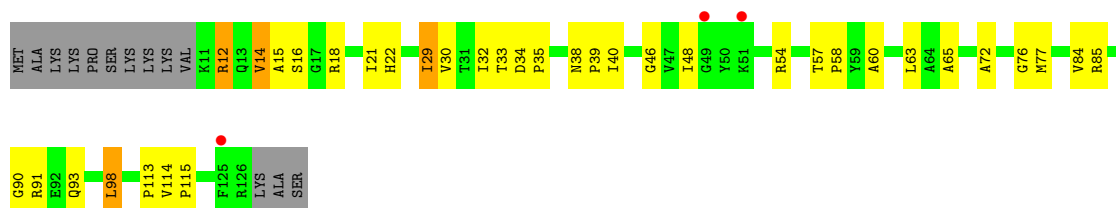
- Molecule 10: 30S ribosomal protein S10

Chain J: 4% 57% 32% 7%



- Molecule 11: 30S ribosomal protein S11

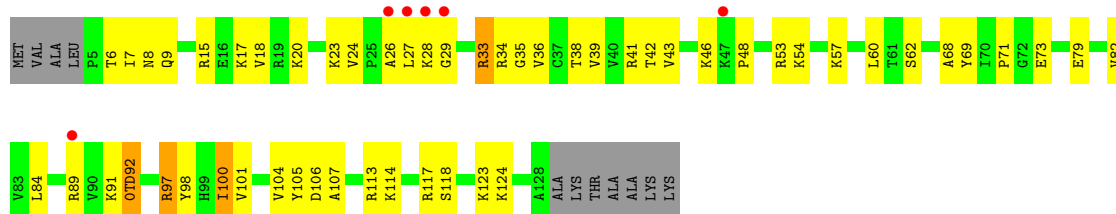
Chain K: 2% 62% 25% 10%



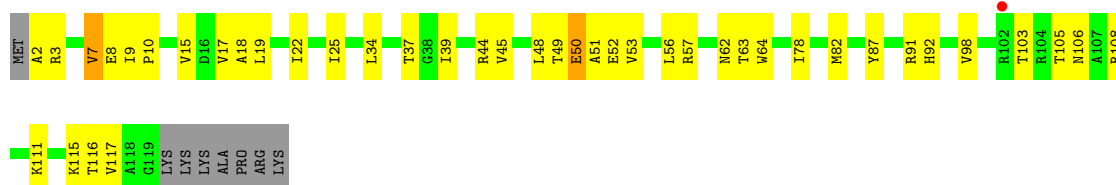
- Molecule 12: Small ribosomal subunit protein uS12

Chain L: 4% 52% 37% 8%

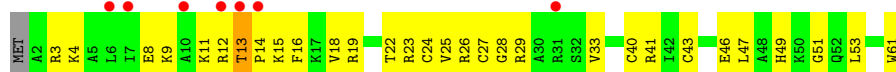




- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



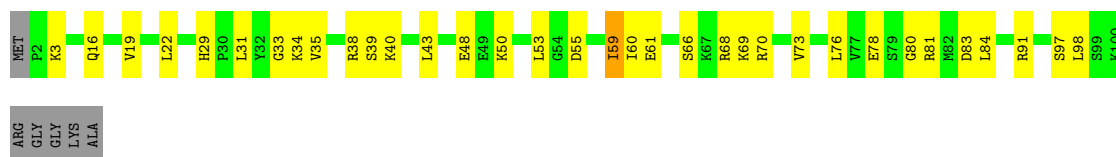
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



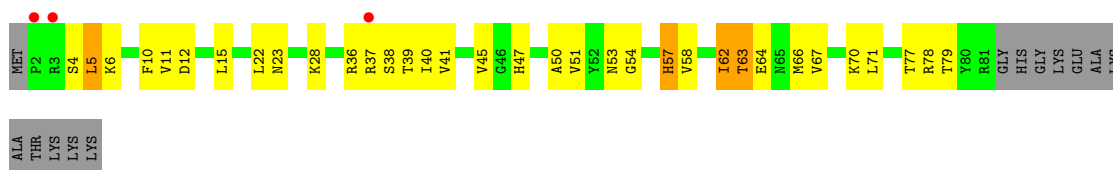
- Molecule 17: 30S ribosomal protein S17



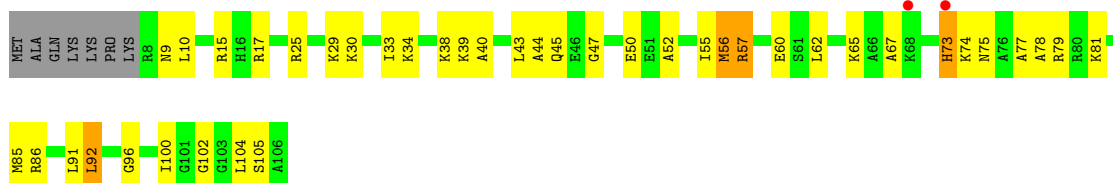
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: Translation initiation factor IF-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.60Å 402.60Å 175.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.91 – 3.59 51.91 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.2 (51.91-3.59) 98.1 (51.91-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.233 , 0.282 0.234 , 0.281	Depositor DCC
R_{free} test set	1999 reflections (0.32%)	wwPDB-VP
Wilson B-factor (Å ²)	138.5	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 210.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	52786	wwPDB-VP
Average B, all atoms (Å ²)	181.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 4OC, 0TD, ZN, MG, 5MC, PSU, M2G, 2MG, G7M, UR3

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	0.13	1/36114 (0.0%)	0.32	0/56355
2	B	0.13	0/1935	0.33	0/2609
3	C	0.13	0/1636	0.32	0/2205
4	D	0.11	0/1733	0.28	0/2318
5	E	0.14	0/1162	0.34	0/1564
6	F	0.11	0/856	0.28	0/1154
7	G	0.10	0/1276	0.26	0/1709
8	H	0.15	0/1136	0.35	0/1527
9	I	0.14	0/1029	0.42	1/1379 (0.1%)
10	J	0.16	0/805	0.35	0/1082
11	K	0.14	0/879	0.32	0/1187
12	L	0.14	0/977	0.39	0/1306
13	M	0.14	0/947	0.38	0/1270
14	N	0.13	0/501	0.35	0/664
15	O	0.11	0/740	0.26	0/987
16	P	0.12	0/716	0.34	0/963
17	Q	0.13	0/836	0.36	0/1117
18	R	0.12	0/579	0.33	0/768
19	S	0.11	0/661	0.37	0/890
20	T	0.12	0/765	0.29	0/1007
21	U	0.11	0/212	0.25	0/277
22	W	0.13	0/580	0.35	0/782
All	All	0.13	1/56075 (0.0%)	0.32	1/83120 (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

Continued on next page...

Continued from previous page...

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O3'-P	5.75	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	39	GLY	N-CA-C	-5.66	99.77	113.18

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
8	H	71	GLY	Peptide
13	M	111	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32623	0	16486	598	1
2	B	1900	0	1951	64	0
3	C	1612	0	1677	61	0
4	D	1703	0	1763	44	0
5	E	1146	0	1207	37	0
6	F	843	0	857	26	0
7	G	1257	0	1296	28	0
8	H	1116	0	1177	45	0
9	I	1010	0	1037	36	0
10	J	792	0	835	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	864	0	881	24	0
12	L	972	0	1058	49	0
13	M	937	0	995	27	0
14	N	492	0	529	35	0
15	O	729	0	768	16	0
16	P	700	0	720	17	0
17	Q	823	0	893	21	0
18	R	574	0	644	22	0
19	S	647	0	673	23	0
20	T	763	0	861	33	0
21	U	208	0	221	4	0
22	W	570	0	599	30	0
23	A	233	0	0	0	0
23	B	1	0	0	0	0
23	C	3	0	0	0	0
23	D	3	0	0	0	0
23	E	2	0	0	0	0
23	F	1	0	0	0	0
23	H	1	0	0	0	0
23	I	3	0	0	0	0
23	L	1	0	0	0	0
23	N	1	0	0	0	0
23	P	2	0	0	0	0
23	Q	1	0	0	0	0
23	S	1	0	0	0	0
23	W	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	237	0	0	0	0
25	C	1	0	0	0	0
25	D	3	0	0	0	0
25	E	1	0	0	0	0
25	L	2	0	0	0	0
25	N	3	0	0	0	0
25	O	1	0	0	0	0
25	T	1	0	0	0	0
All	All	52786	0	37128	1090	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1090 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:A:HO2'	7:G:2:ALA:N	1.62	0.96
1:A:481:G:HO2'	1:A:482:A:H8	1.01	0.94
1:A:664:G:H22	1:A:741:G:H1	1.09	0.93
1:A:955:U:H1'	1:A:1227:A:H61	1.32	0.92
1:A:463:A:OP1	16:P:75:ARG:NH1	2.13	0.82

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:G:OP1	1:A:1229:A:O2'[3_655]	2.14	0.06

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%)	211 (91%)	21 (9%)	0	100	100
3	C	204/239 (85%)	182 (89%)	22 (11%)	0	100	100
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
5	E	148/162 (91%)	139 (94%)	9 (6%)	0	100	100
6	F	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	G	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
8	H	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
9	I	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	12	45
11	K	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
12	L	121/135 (90%)	113 (93%)	8 (7%)	0	100	100
13	M	116/126 (92%)	101 (87%)	15 (13%)	0	100	100
14	N	58/61 (95%)	52 (90%)	6 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	Q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
18	R	68/88 (77%)	63 (93%)	5 (7%)	0	100	100
19	S	78/93 (84%)	70 (90%)	8 (10%)	0	100	100
20	T	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
22	W	69/71 (97%)	57 (83%)	11 (16%)	1 (1%)	9	38
All	All	2405/2612 (92%)	2219 (92%)	184 (8%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
22	W	45	ILE

5.3.2 Protein sidechains [i](#)

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%)	182 (90%)	20 (10%)	7	31
3	C	160/188 (85%)	144 (90%)	16 (10%)	7	30
4	D	180/181 (99%)	165 (92%)	15 (8%)	10	35
5	E	115/123 (94%)	105 (91%)	10 (9%)	9	34
6	F	90/90 (100%)	84 (93%)	6 (7%)	15	42
7	G	126/127 (99%)	120 (95%)	6 (5%)	23	50
8	H	119/119 (100%)	110 (92%)	9 (8%)	12	39
9	I	98/99 (99%)	86 (88%)	12 (12%)	5	23
10	J	87/92 (95%)	79 (91%)	8 (9%)	8	33
11	K	88/99 (89%)	83 (94%)	5 (6%)	18	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	103/110 (94%)	96 (93%)	7 (7%)	14	42
13	M	94/101 (93%)	84 (89%)	10 (11%)	6	28
14	N	49/50 (98%)	46 (94%)	3 (6%)	17	45
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	14
16	P	72/74 (97%)	65 (90%)	7 (10%)	8	31
17	Q	94/97 (97%)	84 (89%)	10 (11%)	6	28
18	R	61/77 (79%)	58 (95%)	3 (5%)	22	49
19	S	71/80 (89%)	63 (89%)	8 (11%)	5	26
20	T	76/82 (93%)	68 (90%)	8 (10%)	6	29
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	29
22	W	62/62 (100%)	55 (89%)	7 (11%)	5	26
All	All	2045/2173 (94%)	1860 (91%)	185 (9%)	9	33

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	17	VAL
16	P	54	GLU
13	M	50	GLU
15	O	33	THR
17	Q	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	84	GLN
13	M	12	ASN
22	W	19	ASN
13	M	106	ASN
4	D	77	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	234 (15%)	48 (3%)

5 of 234 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	13	C
1	A	32	A
1	A	39	G

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1049	U
1	A	1201	A
1	A	1065	U
1	A	1145	C
1	A	1257	U

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

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	$\# Z > 2$
12	0TD	L	92	12	8,9,10	1.10	0	6,11,13	1.96	2 (33%)
1	MA6	A	1519[A]	1	23,26,27	1.19	3 (13%)	33,38,41	0.83	0
1	5MC	A	1404	1	19,22,23	1.14	3 (15%)	26,32,35	0.93	1 (3%)
1	5MC	A	1407	1	19,22,23	1.33	3 (15%)	26,32,35	1.11	1 (3%)
1	M2G	A	966	1	24,27,28	1.35	4 (16%)	33,40,43	0.87	1 (3%)
1	PSU	A	1540	1	18,21,22	1.11	1 (5%)	21,30,33	1.87	5 (23%)
1	5MC	A	967	1	19,22,23	1.15	2 (10%)	26,32,35	0.97	1 (3%)
1	G7M	A	527	1	23,26,27	1.36	3 (13%)	34,39,42	1.70	7 (20%)
1	4OC	A	1402	1	20,23,24	1.16	2 (10%)	25,32,35	0.77	0
1	MA6	A	1518[A]	1	23,26,27	1.18	2 (8%)	33,38,41	0.87	1 (3%)
1	MA6	A	1519[B]	1	23,26,27	1.25	3 (13%)	33,38,41	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1541	1	18,21,22	1.16	1 (5%)	21,30,33	1.74	5 (23%)
1	PSU	A	516	23,1	18,21,22	1.15	1 (5%)	21,30,33	1.92	6 (28%)
1	MA6	A	1518[B]	1	23,26,27	1.32	3 (13%)	33,38,41	0.91	1 (3%)
1	5MC	A	1400	1	19,22,23	1.12	3 (15%)	26,32,35	1.01	2 (7%)
1	UR3	A	1498	23,1	19,22,23	0.81	1 (5%)	26,32,35	0.91	1 (3%)
1	2MG	A	1207	1	23,26,27	1.43	5 (21%)	33,38,41	1.15	4 (12%)

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
12	0TD	L	92	12	-	3/7/12/14	-
1	MA6	A	1519[A]	1	-	5/11/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	7/11/29/30	0/3/3/3
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	G7M	A	527	1	-	2/7/25/26	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	A	1518[A]	1	-	0/11/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	3/11/29/30	0/3/3/3
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	PSU	A	516	23,1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	0/11/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	23,1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	G7M	C2-N2	4.19	1.44	1.34
1	A	1541	PSU	C6-C5	3.96	1.39	1.35
1	A	516	PSU	C6-C5	3.87	1.39	1.35
1	A	1540	PSU	C6-C5	3.74	1.39	1.35
1	A	966	M2G	C2-N2	3.64	1.41	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	4.88	120.31	115.17
1	A	1540	PSU	C4-N3-C2	-4.81	119.74	126.37
1	A	516	PSU	C4-N3-C2	-4.74	119.85	126.37
1	A	1541	PSU	C4-N3-C2	-4.57	120.08	126.37
1	A	1540	PSU	N1-C2-N3	4.53	119.94	115.17

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C4'-C5'-O5'-P
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	92	0TD	5	0
1	A	1519[A]	MA6	2	0
1	A	966	M2G	2	0
1	A	967	5MC	1	0
1	A	1402	4OC	2	0
1	A	1518[A]	MA6	3	0
1	A	1519[B]	MA6	3	0
1	A	516	PSU	1	0
1	A	1518[B]	MA6	3	0
1	A	1498	UR3	2	0
1	A	1207	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 256 ligands modelled in this entry, 256 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1497/1522 (98%)	-0.18	5 (0%) 90 75	67, 163, 304, 482	4 (0%)
2	B	234/256 (91%)	-0.22	1 (0%) 88 70	114, 177, 251, 306	0
3	C	206/239 (86%)	0.19	7 (3%) 48 27	202, 257, 322, 353	0
4	D	208/209 (99%)	0.14	8 (3%) 44 25	109, 166, 247, 301	0
5	E	150/162 (92%)	-0.14	2 (1%) 75 48	90, 133, 188, 216	0
6	F	101/101 (100%)	-0.25	0 100 100	133, 170, 203, 216	0
7	G	155/156 (99%)	-0.09	3 (1%) 66 39	137, 199, 268, 298	0
8	H	138/138 (100%)	-0.22	0 100 100	76, 117, 159, 238	0
9	I	127/128 (99%)	0.92	23 (18%) 3 4	164, 258, 332, 373	0
10	J	98/105 (93%)	0.29	4 (4%) 41 23	158, 253, 340, 363	0
11	K	116/129 (89%)	-0.28	3 (2%) 57 33	112, 151, 191, 218	0
12	L	123/135 (91%)	0.21	6 (4%) 35 20	100, 171, 206, 258	0
13	M	118/126 (93%)	0.01	1 (0%) 82 58	149, 188, 239, 319	0
14	N	60/61 (98%)	0.86	7 (11%) 9 8	179, 223, 289, 324	0
15	O	87/89 (97%)	-0.10	0 100 100	103, 143, 196, 219	0
16	P	83/88 (94%)	-0.14	0 100 100	115, 152, 190, 239	0
17	Q	99/105 (94%)	-0.03	0 100 100	99, 129, 164, 181	0
18	R	70/88 (79%)	-0.14	1 (1%) 73 46	102, 150, 218, 239	0
19	S	80/93 (86%)	0.19	3 (3%) 44 25	203, 239, 294, 312	0
20	T	99/106 (93%)	0.03	2 (2%) 65 38	127, 152, 214, 238	0
21	U	24/27 (88%)	1.88	10 (41%) 0 1	152, 213, 278, 302	0
22	W	71/71 (100%)	0.09	1 (1%) 73 46	91, 171, 228, 245	41 (57%)
All	All	3944/4134 (95%)	-0.03	87 (2%) 62 36	67, 172, 292, 482	45 (1%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	U	6	ARG	7.8
4	D	4	TYR	5.4
19	S	2	PRO	4.7
9	I	105	ASP	4.6
21	U	7	ARG	4.4

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

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.83	0.23	362,405,482,541	0
1	PSU	A	1540	20/21	0.88	0.19	274,296,321,345	0
1	2MG	A	1207	24/25	0.89	0.11	262,276,288,300	0
1	PSU	A	516	20/21	0.92	0.07	183,200,205,207	0
1	5MC	A	1407	21/22	0.94	0.08	169,180,191,196	0
1	5MC	A	1404	21/22	0.95	0.11	114,141,154,158	0
1	5MC	A	967	21/22	0.95	0.12	165,179,199,201	0
1	UR3	A	1498	21/22	0.96	0.12	134,148,155,162	0
1	MA6	A	1518[A]	24/25	0.96	0.13	121,125,132,133	24
1	MA6	A	1518[B]	24/25	0.96	0.13	125,131,138,139	24
1	G7M	A	527	24/25	0.96	0.09	137,149,162,167	0
1	5MC	A	1400	21/22	0.96	0.11	150,172,187,191	0
1	4OC	A	1402	22/23	0.97	0.09	113,158,174,180	0
1	M2G	A	966	25/26	0.97	0.10	147,187,194,201	0
1	MA6	A	1519[A]	24/25	0.98	0.10	116,125,141,143	24
1	MA6	A	1519[B]	24/25	0.98	0.10	118,135,139,150	24
12	0TD	L	92	10/11	0.99	0.07	154,164,189,189	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1622	1/1	0.53	0.18	191,191,191,191	0
23	MG	A	1795	1/1	0.58	0.24	200,200,200,200	0
23	MG	A	1602	1/1	0.65	0.18	164,164,164,164	0
23	MG	A	1683	1/1	0.66	0.14	143,143,143,143	0
23	MG	A	1770	1/1	0.68	0.22	153,153,153,153	0
23	MG	A	1776	1/1	0.71	0.13	147,147,147,147	0
23	MG	A	1730	1/1	0.72	0.06	135,135,135,135	0
23	MG	A	1812	1/1	0.72	0.13	71,71,71,71	0
23	MG	A	1700	1/1	0.74	0.18	111,111,111,111	0
23	MG	A	1780	1/1	0.75	0.11	146,146,146,146	0
23	MG	C	302	1/1	0.75	0.13	180,180,180,180	0
23	MG	L	201	1/1	0.75	0.15	128,128,128,128	0
23	MG	A	1686	1/1	0.76	0.09	182,182,182,182	0
23	MG	A	1669	1/1	0.76	0.16	119,119,119,119	0
23	MG	A	1827	1/1	0.77	0.13	109,109,109,109	0
23	MG	A	1688	1/1	0.77	0.16	131,131,131,131	0
23	MG	D	303	1/1	0.77	0.10	87,87,87,87	0
23	MG	A	1817	1/1	0.77	0.23	120,120,120,120	0
23	MG	A	1668	1/1	0.78	0.09	134,134,134,134	0
23	MG	A	1739	1/1	0.78	0.17	123,123,123,123	0
23	MG	A	1757	1/1	0.79	0.17	156,156,156,156	0
23	MG	A	1675	1/1	0.80	0.15	139,139,139,139	0
23	MG	A	1704	1/1	0.80	0.14	86,86,86,86	0
23	MG	C	301	1/1	0.80	0.09	137,137,137,137	0
23	MG	A	1777	1/1	0.81	0.13	150,150,150,150	0
23	MG	A	1822	1/1	0.81	0.14	97,97,97,97	0
23	MG	A	1749	1/1	0.81	0.34	128,128,128,128	0
23	MG	A	1831	1/1	0.81	0.13	133,133,133,133	0
23	MG	A	1653	1/1	0.82	0.32	83,83,83,83	0
23	MG	A	1717	1/1	0.82	0.10	88,88,88,88	0
23	MG	A	1719	1/1	0.82	0.11	132,132,132,132	0
23	MG	S	101	1/1	0.82	0.10	114,114,114,114	0
23	MG	A	1665	1/1	0.83	0.30	164,164,164,164	0
23	MG	A	1703	1/1	0.83	0.15	96,96,96,96	0
23	MG	A	1752	1/1	0.83	0.12	109,109,109,109	0
23	MG	F	201	1/1	0.83	0.14	148,148,148,148	0
23	MG	A	1672	1/1	0.83	0.11	140,140,140,140	0
23	MG	A	1762	1/1	0.83	0.10	94,94,94,94	0
23	MG	A	1684	1/1	0.84	0.14	136,136,136,136	0
23	MG	A	1734	1/1	0.84	0.14	170,170,170,170	0
23	MG	A	1758	1/1	0.84	0.07	127,127,127,127	0
23	MG	A	1825	1/1	0.84	0.15	96,96,96,96	0
23	MG	A	1716	1/1	0.85	0.23	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1604	1/1	0.85	0.18	145,145,145,145	0
23	MG	A	1677	1/1	0.85	0.12	143,143,143,143	0
23	MG	A	1682	1/1	0.85	0.21	135,135,135,135	0
23	MG	A	1805	1/1	0.85	0.23	202,202,202,202	0
23	MG	A	1808	1/1	0.85	0.27	172,172,172,172	0
23	MG	A	1761	1/1	0.85	0.36	110,110,110,110	0
23	MG	I	202	1/1	0.85	0.07	151,151,151,151	0
23	MG	A	1657	1/1	0.85	0.08	123,123,123,123	0
23	MG	A	1633	1/1	0.85	0.13	117,117,117,117	0
23	MG	A	1634	1/1	0.86	0.10	65,65,65,65	0
23	MG	A	1708	1/1	0.86	0.14	142,142,142,142	0
23	MG	A	1742	1/1	0.86	0.18	70,70,70,70	0
23	MG	A	1748	1/1	0.86	0.23	92,92,92,92	0
23	MG	A	1689	1/1	0.86	0.09	155,155,155,155	0
23	MG	A	1796	1/1	0.86	0.13	169,169,169,169	0
23	MG	A	1800	1/1	0.86	0.14	145,145,145,145	0
23	MG	A	1828	1/1	0.86	0.08	172,172,172,172	0
23	MG	A	1632	1/1	0.87	0.15	103,103,103,103	0
23	MG	A	1711	1/1	0.87	0.08	189,189,189,189	0
23	MG	A	1656	1/1	0.87	0.10	136,136,136,136	0
23	MG	B	301	1/1	0.87	0.08	145,145,145,145	0
23	MG	A	1609	1/1	0.87	0.16	109,109,109,109	0
23	MG	A	1662	1/1	0.87	0.19	102,102,102,102	0
23	MG	A	1721	1/1	0.87	0.14	101,101,101,101	0
23	MG	A	1680	1/1	0.87	0.15	87,87,87,87	0
23	MG	A	1631	1/1	0.87	0.11	150,150,150,150	0
23	MG	A	1644	1/1	0.87	0.19	129,129,129,129	0
23	MG	A	1706	1/1	0.87	0.11	116,116,116,116	0
23	MG	W	101	1/1	0.87	0.14	176,176,176,176	1
23	MG	A	1674	1/1	0.88	0.12	85,85,85,85	0
23	MG	A	1648	1/1	0.88	0.07	61,61,61,61	0
23	MG	A	1649	1/1	0.88	0.13	89,89,89,89	0
23	MG	A	1818	1/1	0.88	0.10	149,149,149,149	0
23	MG	A	1616	1/1	0.88	0.07	118,118,118,118	0
23	MG	A	1664	1/1	0.88	0.06	190,190,190,190	0
23	MG	A	1760	1/1	0.88	0.11	85,85,85,85	0
23	MG	A	1696	1/1	0.88	0.15	126,126,126,126	0
23	MG	A	1699	1/1	0.88	0.10	153,153,153,153	0
23	MG	A	1826	1/1	0.89	0.17	54,54,54,54	0
23	MG	D	302	1/1	0.89	0.16	152,152,152,152	0
23	MG	A	1619	1/1	0.89	0.07	72,72,72,72	0
23	MG	A	1701	1/1	0.89	0.11	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1830	1/1	0.89	0.11	82,82,82,82	0
23	MG	A	1802	1/1	0.89	0.08	205,205,205,205	0
23	MG	A	1660	1/1	0.89	0.11	103,103,103,103	0
23	MG	A	1673	1/1	0.89	0.09	127,127,127,127	0
23	MG	A	1618	1/1	0.90	0.13	109,109,109,109	0
23	MG	A	1756	1/1	0.90	0.16	100,100,100,100	0
23	MG	A	1685	1/1	0.90	0.12	90,90,90,90	0
23	MG	A	1725	1/1	0.90	0.14	84,84,84,84	0
23	MG	A	1666	1/1	0.90	0.09	154,154,154,154	0
23	MG	A	1623	1/1	0.90	0.12	101,101,101,101	0
23	MG	A	1809	1/1	0.90	0.08	121,121,121,121	0
23	MG	A	1810	1/1	0.90	0.21	102,102,102,102	0
23	MG	A	1679	1/1	0.90	0.11	136,136,136,136	0
23	MG	A	1765	1/1	0.90	0.09	160,160,160,160	0
23	MG	A	1601	1/1	0.90	0.12	100,100,100,100	0
23	MG	A	1746	1/1	0.90	0.09	142,142,142,142	0
23	MG	A	1640	1/1	0.90	0.12	142,142,142,142	0
23	MG	A	1655	1/1	0.90	0.15	91,91,91,91	0
23	MG	A	1736	1/1	0.91	0.06	58,58,58,58	0
23	MG	A	1813	1/1	0.91	0.06	115,115,115,115	0
23	MG	A	1798	1/1	0.91	0.14	104,104,104,104	0
23	MG	A	1728	1/1	0.91	0.12	125,125,125,125	0
23	MG	A	1821	1/1	0.91	0.14	105,105,105,105	0
23	MG	A	1714	1/1	0.91	0.05	61,61,61,61	0
23	MG	A	1804	1/1	0.91	0.30	162,162,162,162	0
23	MG	A	1779	1/1	0.91	0.10	138,138,138,138	0
23	MG	A	1743	1/1	0.91	0.08	113,113,113,113	0
23	MG	A	1788	1/1	0.91	0.10	58,58,58,58	0
23	MG	A	1678	1/1	0.91	0.13	157,157,157,157	0
23	MG	A	1816	1/1	0.92	0.26	83,83,83,83	0
23	MG	A	1784	1/1	0.92	0.09	90,90,90,90	0
23	MG	A	1654	1/1	0.92	0.06	107,107,107,107	0
23	MG	A	1790	1/1	0.92	0.17	131,131,131,131	0
23	MG	A	1792	1/1	0.92	0.06	116,116,116,116	0
23	MG	A	1793	1/1	0.92	0.10	86,86,86,86	0
23	MG	A	1747	1/1	0.92	0.50	140,140,140,140	0
23	MG	A	1612	1/1	0.92	0.07	142,142,142,142	0
23	MG	A	1764	1/1	0.92	0.07	134,134,134,134	0
23	MG	A	1799	1/1	0.92	0.21	110,110,110,110	0
23	MG	A	1629	1/1	0.92	0.11	85,85,85,85	0
23	MG	A	1750	1/1	0.92	0.15	104,104,104,104	0
23	MG	A	1803	1/1	0.92	0.08	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1670	1/1	0.92	0.09	116,116,116,116	0
23	MG	A	1692	1/1	0.92	0.11	146,146,146,146	0
23	MG	A	1806	1/1	0.92	0.08	149,149,149,149	0
23	MG	A	1695	1/1	0.92	0.09	135,135,135,135	0
23	MG	A	1630	1/1	0.92	0.10	62,62,62,62	0
23	MG	A	1781	1/1	0.92	0.07	110,110,110,110	0
23	MG	N	102	1/1	0.92	0.08	176,176,176,176	0
23	MG	P	101	1/1	0.92	0.26	89,89,89,89	0
23	MG	A	1782	1/1	0.92	0.06	92,92,92,92	0
23	MG	A	1783	1/1	0.92	0.05	109,109,109,109	0
23	MG	A	1646	1/1	0.93	0.09	119,119,119,119	0
23	MG	A	1731	1/1	0.93	0.29	144,144,144,144	0
23	MG	A	1815	1/1	0.93	0.10	88,88,88,88	0
23	MG	A	1636	1/1	0.93	0.25	113,113,113,113	0
23	MG	A	1801	1/1	0.93	0.11	120,120,120,120	0
23	MG	A	1620	1/1	0.93	0.14	92,92,92,92	0
23	MG	E	202	1/1	0.93	0.06	81,81,81,81	0
23	MG	A	1643	1/1	0.93	0.09	154,154,154,154	0
23	MG	H	201	1/1	0.93	0.10	104,104,104,104	0
23	MG	A	1767	1/1	0.93	0.06	125,125,125,125	0
23	MG	A	1753	1/1	0.93	0.15	83,83,83,83	0
23	MG	A	1772	1/1	0.93	0.13	88,88,88,88	0
23	MG	A	1707	1/1	0.93	0.07	102,102,102,102	0
23	MG	Q	201	1/1	0.93	0.08	113,113,113,113	0
23	MG	A	1687	1/1	0.93	0.08	138,138,138,138	0
23	MG	A	1627	1/1	0.93	0.11	170,170,170,170	0
23	MG	A	1769	1/1	0.94	0.19	106,106,106,106	0
23	MG	A	1744	1/1	0.94	0.09	108,108,108,108	0
23	MG	A	1645	1/1	0.94	0.06	139,139,139,139	0
23	MG	A	1775	1/1	0.94	0.07	118,118,118,118	0
23	MG	A	1652	1/1	0.94	0.08	122,122,122,122	0
23	MG	A	1709	1/1	0.94	0.08	126,126,126,126	0
23	MG	A	1778	1/1	0.94	0.05	100,100,100,100	0
23	MG	A	1638	1/1	0.94	0.08	121,121,121,121	0
23	MG	A	1611	1/1	0.94	0.08	132,132,132,132	0
23	MG	A	1763	1/1	0.94	0.07	109,109,109,109	0
23	MG	A	1715	1/1	0.94	0.10	91,91,91,91	0
23	MG	A	1729	1/1	0.94	0.09	144,144,144,144	0
23	MG	A	1755	1/1	0.94	0.08	134,134,134,134	0
23	MG	A	1768	1/1	0.94	0.14	74,74,74,74	0
23	MG	A	1829	1/1	0.94	0.12	89,89,89,89	0
23	MG	A	1789	1/1	0.94	0.18	182,182,182,182	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1726	1/1	0.95	0.10	124,124,124,124	0
23	MG	A	1727	1/1	0.95	0.07	110,110,110,110	0
23	MG	A	1713	1/1	0.95	0.17	117,117,117,117	0
23	MG	A	1671	1/1	0.95	0.06	95,95,95,95	0
23	MG	A	1650	1/1	0.95	0.30	118,118,118,118	0
23	MG	A	1751	1/1	0.95	0.04	111,111,111,111	0
23	MG	A	1603	1/1	0.95	0.06	119,119,119,119	0
23	MG	A	1791	1/1	0.95	0.07	61,61,61,61	0
23	MG	A	1647	1/1	0.95	0.13	69,69,69,69	0
23	MG	A	1754	1/1	0.95	0.08	74,74,74,74	0
23	MG	A	1773	1/1	0.95	0.12	168,168,168,168	0
23	MG	A	1718	1/1	0.95	0.08	72,72,72,72	0
23	MG	A	1797	1/1	0.95	0.09	151,151,151,151	0
23	MG	A	1819	1/1	0.95	0.12	64,64,64,64	0
23	MG	A	1639	1/1	0.95	0.09	100,100,100,100	0
23	MG	A	1710	1/1	0.95	0.04	108,108,108,108	0
23	MG	A	1724	1/1	0.95	0.15	139,139,139,139	0
23	MG	A	1610	1/1	0.95	0.08	141,141,141,141	0
23	MG	A	1745	1/1	0.95	0.10	83,83,83,83	0
24	ZN	N	101	1/1	0.95	0.10	276,276,276,276	0
23	MG	A	1823	1/1	0.96	0.18	167,167,167,167	0
23	MG	A	1607	1/1	0.96	0.04	138,138,138,138	0
23	MG	A	1774	1/1	0.96	0.10	101,101,101,101	0
23	MG	A	1624	1/1	0.96	0.11	85,85,85,85	0
23	MG	A	1712	1/1	0.96	0.12	90,90,90,90	0
23	MG	A	1625	1/1	0.96	0.14	98,98,98,98	0
23	MG	A	1697	1/1	0.96	0.06	154,154,154,154	0
23	MG	A	1735	1/1	0.96	0.11	61,61,61,61	0
23	MG	A	1681	1/1	0.96	0.08	131,131,131,131	0
23	MG	A	1759	1/1	0.96	0.08	127,127,127,127	0
23	MG	A	1608	1/1	0.96	0.07	80,80,80,80	0
23	MG	A	1606	1/1	0.96	0.09	108,108,108,108	0
23	MG	A	1659	1/1	0.96	0.13	153,153,153,153	0
23	MG	D	304	1/1	0.96	0.05	118,118,118,118	0
23	MG	A	1811	1/1	0.96	0.16	107,107,107,107	0
23	MG	A	1613	1/1	0.96	0.05	114,114,114,114	0
23	MG	A	1720	1/1	0.96	0.25	114,114,114,114	0
23	MG	A	1705	1/1	0.96	0.15	127,127,127,127	0
23	MG	A	1722	1/1	0.96	0.18	145,145,145,145	0
23	MG	A	1614	1/1	0.96	0.11	109,109,109,109	0
23	MG	A	1641	1/1	0.96	0.07	109,109,109,109	0
23	MG	A	1676	1/1	0.96	0.13	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1820	1/1	0.96	0.33	89,89,89,89	0
23	MG	A	1771	1/1	0.96	0.06	104,104,104,104	0
23	MG	A	1642	1/1	0.96	0.09	114,114,114,114	0
23	MG	A	1615	1/1	0.97	0.16	113,113,113,113	0
23	MG	A	1794	1/1	0.97	0.04	124,124,124,124	0
23	MG	A	1807	1/1	0.97	0.12	158,158,158,158	0
23	MG	A	1626	1/1	0.97	0.08	104,104,104,104	0
23	MG	A	1733	1/1	0.97	0.05	102,102,102,102	0
23	MG	A	1663	1/1	0.97	0.07	119,119,119,119	0
23	MG	A	1658	1/1	0.97	0.10	174,174,174,174	0
23	MG	I	201	1/1	0.97	0.06	106,106,106,106	0
23	MG	A	1786	1/1	0.97	0.04	75,75,75,75	0
23	MG	I	203	1/1	0.97	0.08	95,95,95,95	0
23	MG	A	1605	1/1	0.97	0.06	115,115,115,115	0
23	MG	A	1814	1/1	0.97	0.21	159,159,159,159	0
23	MG	A	1766	1/1	0.97	0.08	89,89,89,89	0
23	MG	A	1738	1/1	0.97	0.06	115,115,115,115	0
23	MG	A	1832	1/1	0.97	0.05	80,80,80,80	0
23	MG	A	1723	1/1	0.97	0.07	73,73,73,73	0
23	MG	A	1741	1/1	0.97	0.08	138,138,138,138	0
23	MG	A	1690	1/1	0.98	0.07	123,123,123,123	0
23	MG	A	1691	1/1	0.98	0.06	192,192,192,192	0
23	MG	A	1824	1/1	0.98	0.07	44,44,44,44	0
23	MG	E	201	1/1	0.98	0.04	70,70,70,70	0
23	MG	A	1651	1/1	0.98	0.04	55,55,55,55	0
23	MG	A	1693	1/1	0.98	0.03	176,176,176,176	0
23	MG	A	1694	1/1	0.98	0.09	122,122,122,122	0
23	MG	A	1635	1/1	0.98	0.06	133,133,133,133	0
23	MG	A	1621	1/1	0.98	0.07	86,86,86,86	0
23	MG	A	1637	1/1	0.98	0.05	124,124,124,124	0
23	MG	A	1698	1/1	0.98	0.12	139,139,139,139	0
23	MG	A	1737	1/1	0.98	0.04	104,104,104,104	0
23	MG	A	1833	1/1	0.98	0.06	82,82,82,82	0
23	MG	A	1628	1/1	0.98	0.06	90,90,90,90	0
23	MG	A	1667	1/1	0.98	0.10	101,101,101,101	0
23	MG	A	1661	1/1	0.98	0.05	100,100,100,100	0
23	MG	C	303	1/1	0.98	0.04	93,93,93,93	0
23	MG	A	1702	1/1	0.99	0.06	106,106,106,106	0
23	MG	A	1740	1/1	0.99	0.06	46,46,46,46	0
23	MG	P	102	1/1	0.99	0.05	75,75,75,75	0
23	MG	A	1785	1/1	0.99	0.04	92,92,92,92	0
23	MG	A	1617	1/1	0.99	0.04	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1787	1/1	0.99	0.04	94,94,94,94	0
24	ZN	D	301	1/1	0.99	0.12	168,168,168,168	0
23	MG	A	1732	1/1	0.99	0.04	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.