



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:51 PM GMT

PDB ID : 4G5V
Title : Crystal Structure of the 70S ribosome with tigecycline. This entry contains the 30S subunit of molecule B.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2012-07-18
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

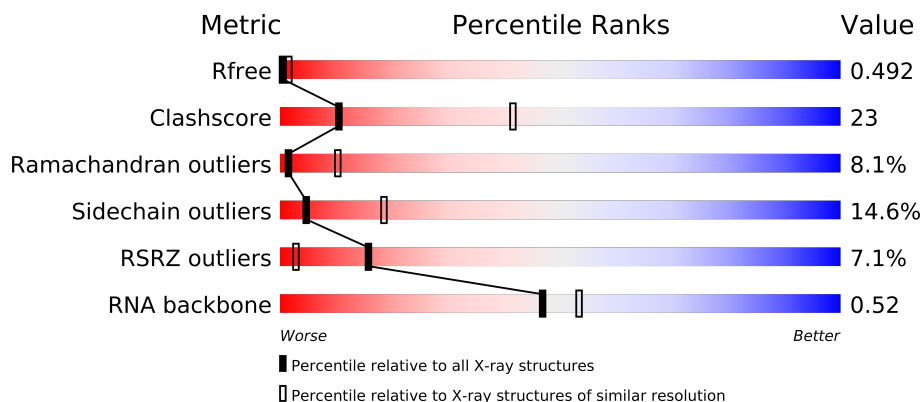
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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.



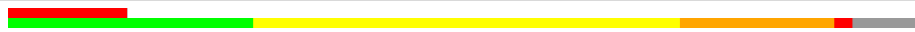
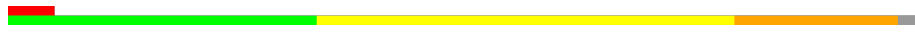




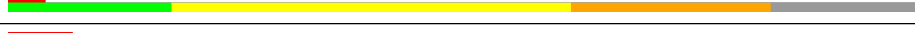


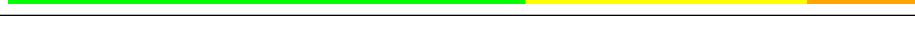

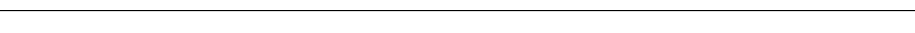
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	1506	
2	E	256	
3	F	239	
4	G	208	
5	H	162	
6	I	101	
7	J	156	
8	K	138	
9	L	128	
10	M	105	
11	N	129	
12	O	128	

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Mol	Chain	Length	Quality of chain
13	P	126	
14	Q	61	
15	R	89	
16	S	88	
17	T	105	
18	U	88	
19	V	93	
20	W	106	
21	X	27	
22	C	77	
22	D	77	
23	1	6	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 55763 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	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	G	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	H	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	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	J	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	K	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	L	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	M	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	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	O	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Q	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	R	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	S	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	T	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	U	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	V	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	W	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	X	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	D	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17A	C	U	CONFLICT	GB AP008226.1
C	50	U	C	CONFLICT	GB AP008226.1
C	51	C	G	CONFLICT	GB AP008226.1
C	63	G	C	CONFLICT	GB AP008226.1
D	17A	C	U	CONFLICT	GB AP008226.1
D	50	U	C	CONFLICT	GB AP008226.1
D	51	C	G	CONFLICT	GB AP008226.1
D	63	G	C	CONFLICT	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

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

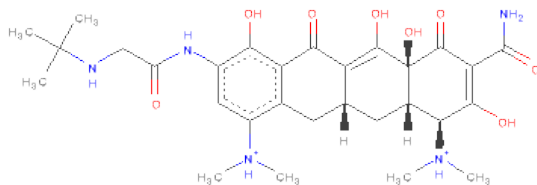
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	G	2	Total	Mg	0	0
			2	2		
24	D	24	Total	Mg	0	0
			24	24		
24	C	46	Total	Mg	0	0
			46	46		
24	A	686	Total	Mg	0	0
			686	686		
24	T	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	N	1	Total	Mg	0	0
			1	1		
24	X	1	Total	Mg	0	0
			1	1		
24	R	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		

- Molecule 25 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			42	29	5	8		

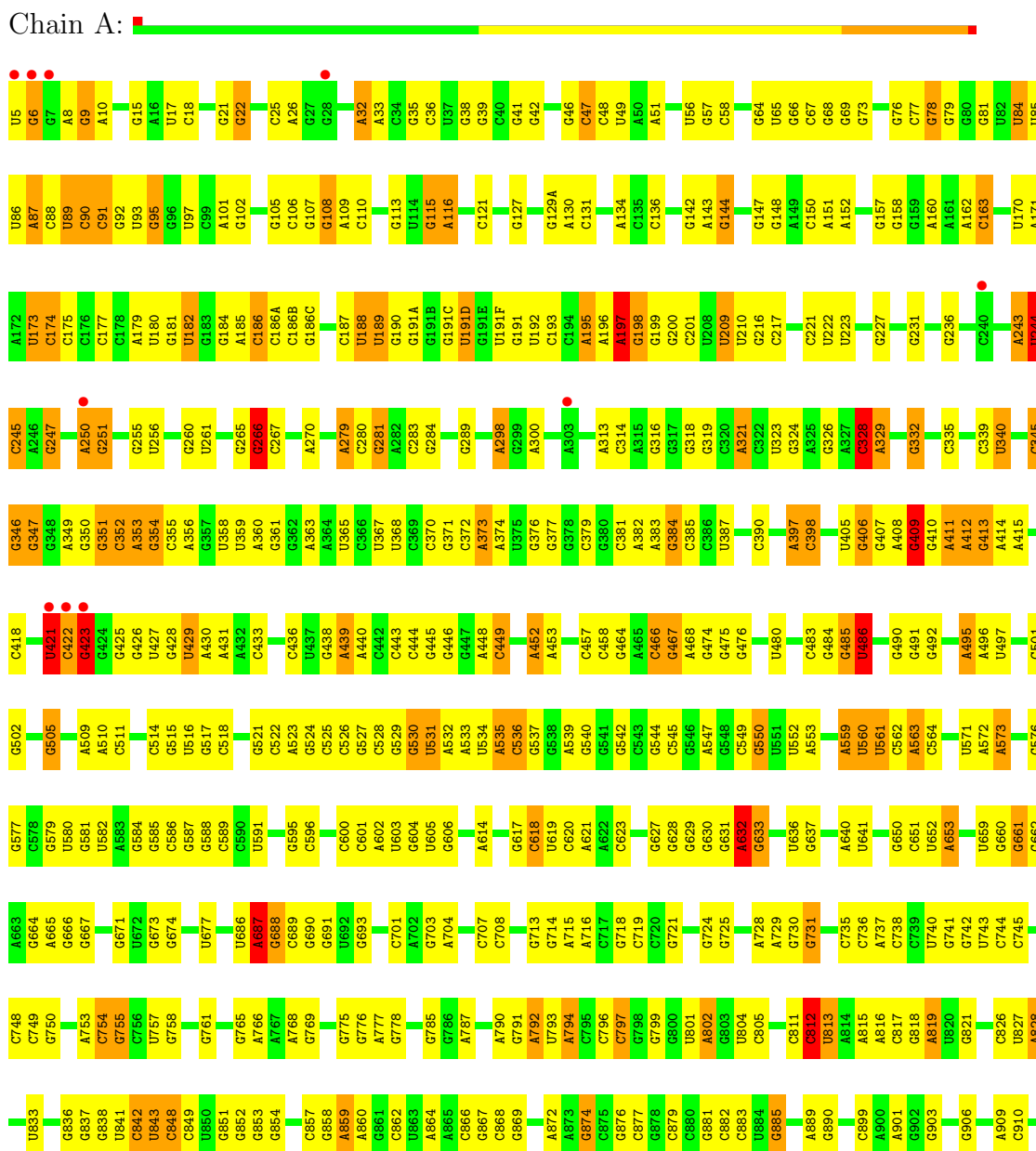
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

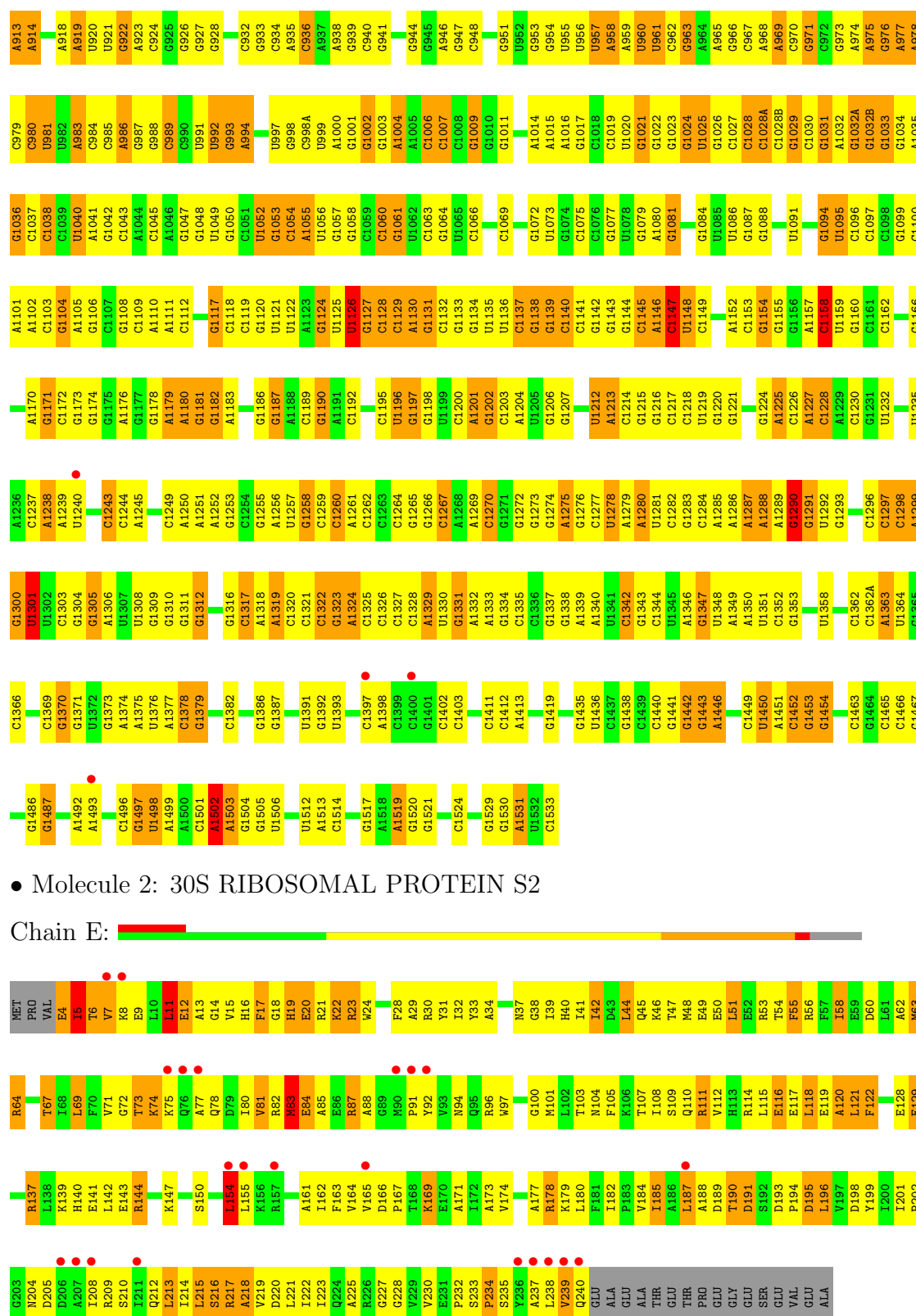
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	G	1	Total	Zn	0	0
			1	1		
26	Q	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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

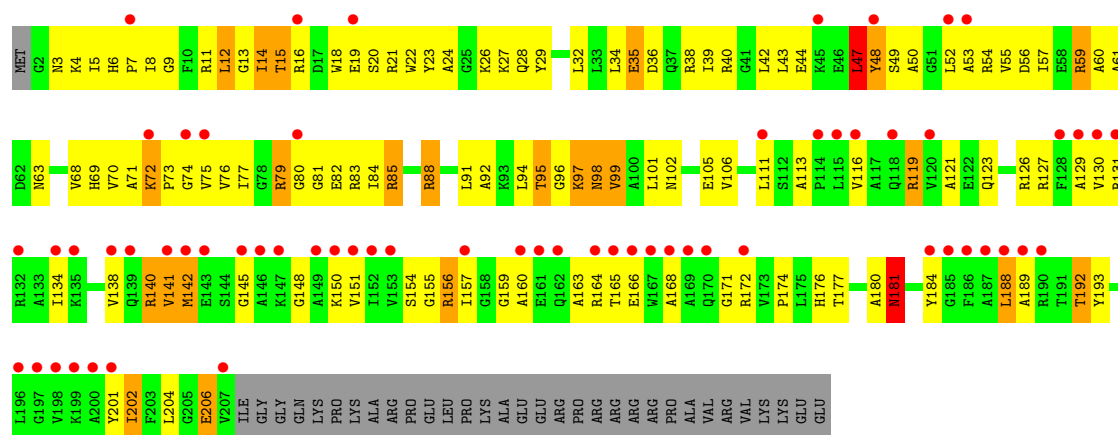
• Molecule 1: 16S ribosomal RNA





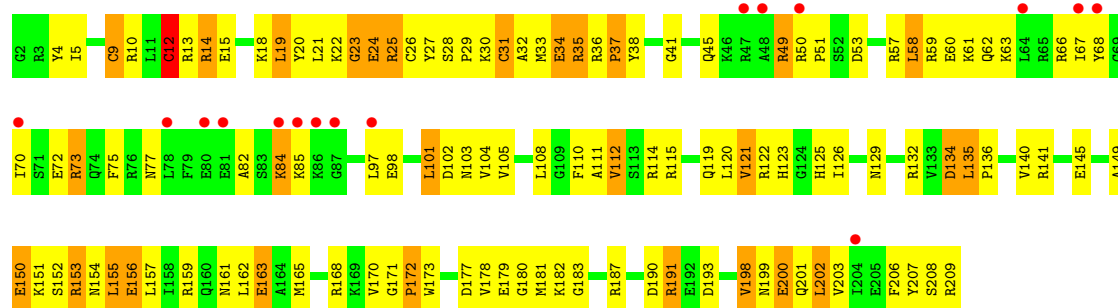
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain F:



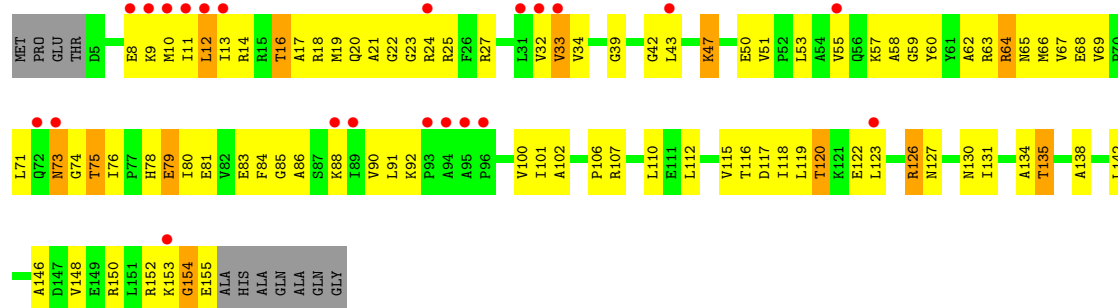
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain G:



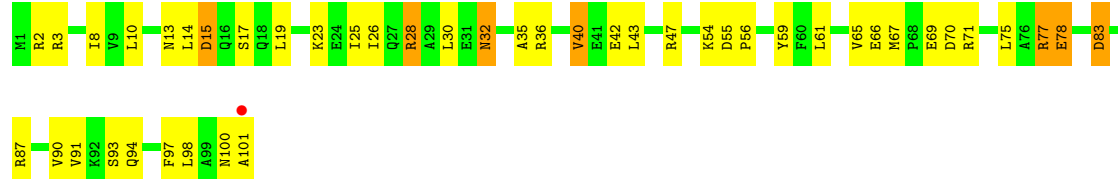
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain H:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain I:



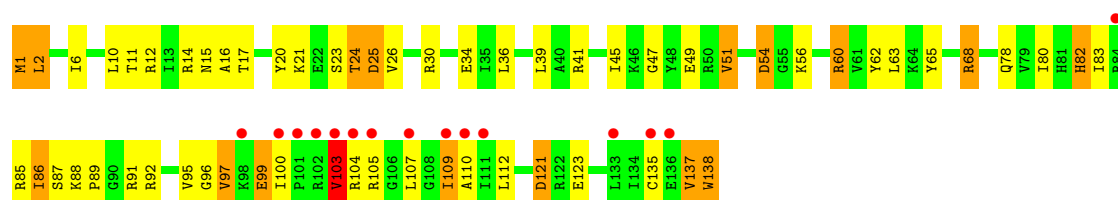
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain J: 



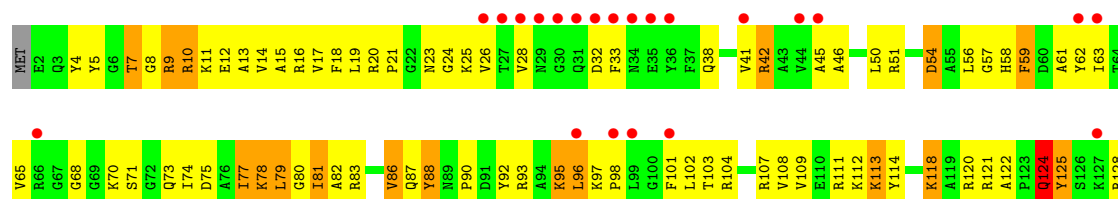
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain K: 



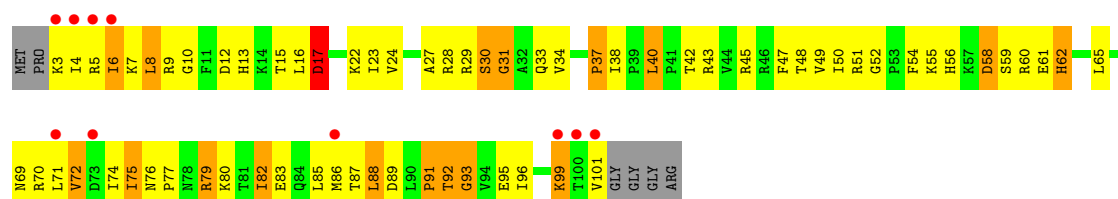
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain L: 



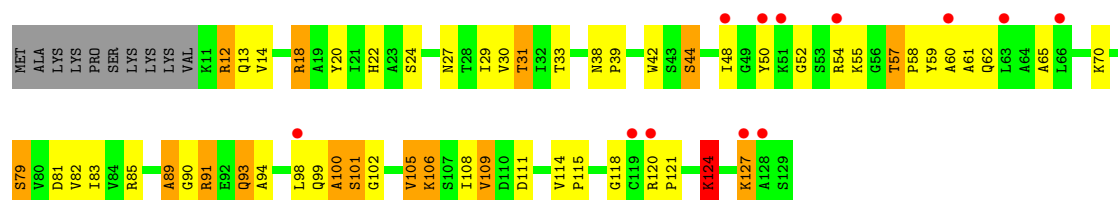
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain M: 



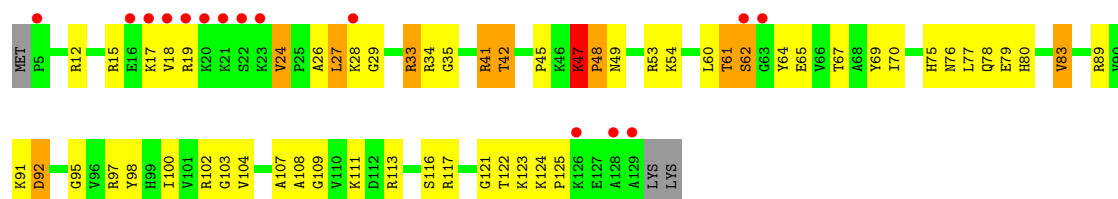
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain N: 



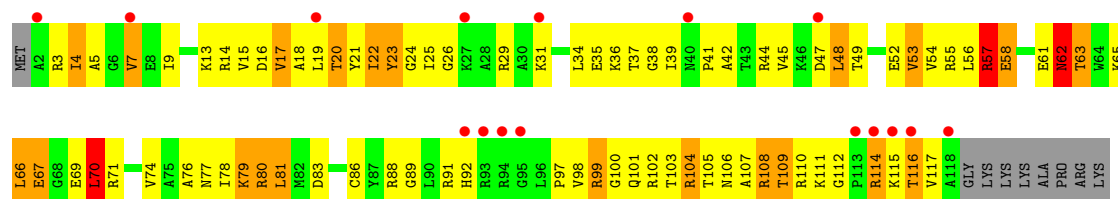
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain O:



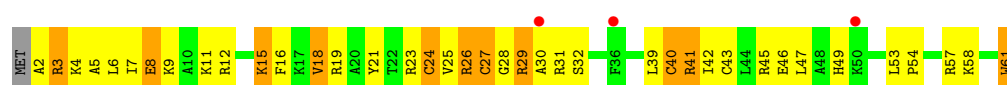
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain P:



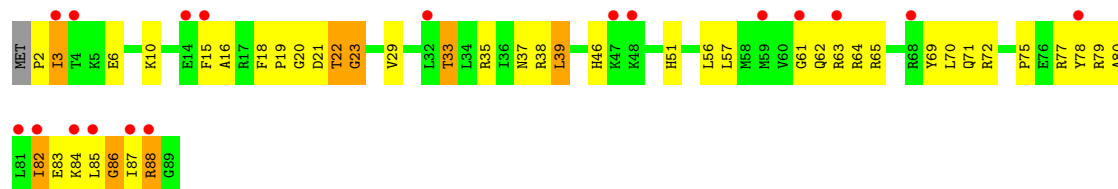
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain Q:



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain R:



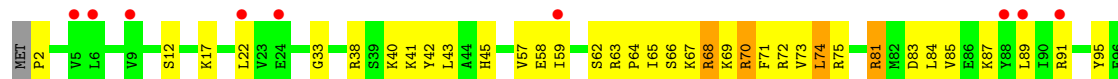
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

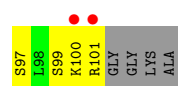
Chain S:



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

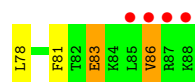
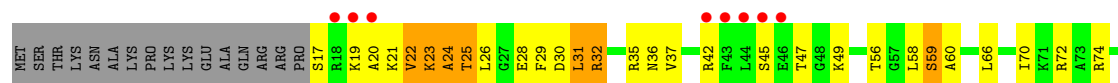
Chain T:





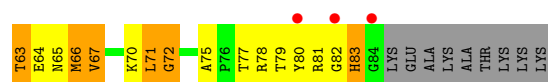
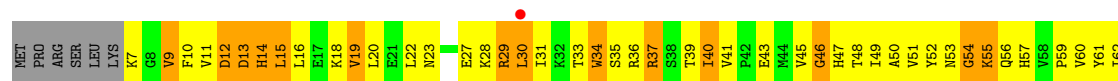
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain U:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain V:



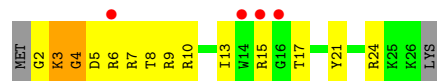
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain W:



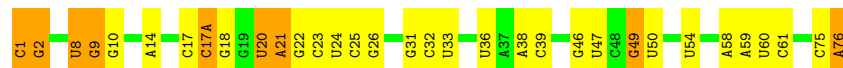
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain X:



• Molecule 22: TRNA-FMET

Chain C:



• Molecule 22: TRNA-FMET

Chain D:





- Molecule 23: MRNA

Chain 1: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 450.27Å 616.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.59 – 3.10 254.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (153.59-3.10) 93.4 (254.47-3.10)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_987)	Depositor
R, R_{free}	0.213 , 0.269 0.479 , 0.492	Depositor DCC
R_{free} test set	921 reflections (0.09%)	DCC
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 68.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1045188 reflections	Xtriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	55763	wwPDB-VP
Average B, all atoms (Å ²)	128.0	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T1C

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	0.50	5/36237 (0.0%)	0.95	67/56558 (0.1%)
2	E	0.38	0/1959	0.68	4/2642 (0.2%)
3	F	0.37	0/1636	0.56	0/2205
4	G	0.45	1/1733 (0.1%)	0.63	1/2318 (0.0%)
5	H	0.38	0/1171	0.57	0/1576
6	I	0.37	0/856	0.52	0/1154
7	J	0.39	0/1276	0.59	0/1709
8	K	0.35	0/1136	0.56	0/1527
9	L	0.41	0/1029	0.62	0/1379
10	M	0.38	0/814	0.58	0/1095
11	N	0.52	1/900 (0.1%)	0.66	1/1213 (0.1%)
12	O	0.42	0/991	0.65	1/1327 (0.1%)
13	P	0.35	0/943	0.63	1/1265 (0.1%)
14	Q	0.45	0/501	0.64	0/664
15	R	0.42	0/745	0.54	0/992
16	S	0.40	0/721	0.58	0/970
17	T	0.39	0/847	0.55	0/1131
18	U	0.41	0/596	0.60	0/790
19	V	0.47	0/638	0.78	0/860
20	W	0.37	0/765	0.58	0/1007
21	X	0.36	0/221	0.63	0/288
22	C	0.56	2/1832 (0.1%)	1.00	9/2855 (0.3%)
22	D	0.54	2/1832 (0.1%)	1.15	11/2855 (0.4%)
23	1	0.55	0/144	0.86	0/222
All	All	0.48	11/59523 (0.0%)	0.87	95/88602 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	17(A)	C	C4-N4	-11.41	1.23	1.33
22	D	17(A)	C	C4-N4	-11.38	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	124	LYS	CD-CE	8.56	1.72	1.51
22	D	17(A)	C	N3-C4	6.33	1.38	1.33
22	C	17(A)	C	N3-C4	5.78	1.38	1.33

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	17(A)	C	N3-C4-C5	-19.72	114.01	121.90
22	C	17(A)	C	N3-C4-C5	-18.15	114.64	121.90
22	D	17(A)	C	C2-N3-C4	15.12	127.46	119.90
22	C	17(A)	C	C2-N3-C4	13.98	126.89	119.90
1	A	1104	G	N3-C4-C5	11.78	134.49	128.60

There are no chirality outliers.

There are no planarity outliers.

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	32372	0	16336	878	0
2	E	1924	0	1975	144	0
3	F	1612	0	1677	118	0
4	G	1703	0	1764	215	0
5	H	1155	0	1212	56	0
6	I	843	0	857	27	0
7	J	1257	0	1296	67	0
8	K	1116	0	1177	43	0
9	L	1010	0	1037	94	0
10	M	801	0	849	56	0
11	N	885	0	904	39	0
12	O	975	0	1062	44	0
13	P	933	0	992	84	0
14	Q	492	0	531	43	0
15	R	734	0	771	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	S	705	0	725	29	0
17	T	834	0	904	28	0
18	U	591	0	662	25	0
19	V	624	0	636	78	0
20	W	763	0	861	48	0
21	X	217	0	234	20	0
22	C	1640	0	836	23	0
22	D	1640	0	836	89	0
23	I	129	0	65	0	0
24	A	686	0	0	0	0
24	C	46	0	0	0	0
24	D	24	0	0	0	0
24	G	2	0	0	0	0
24	L	1	0	0	0	0
24	N	1	0	0	0	0
24	R	1	0	0	0	0
24	S	1	0	0	0	0
24	T	1	0	0	0	0
24	X	1	0	0	0	0
25	A	42	0	38	5	0
26	G	1	0	0	0	0
26	Q	1	0	0	0	0
All	All	55763	0	38237	1977	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 23.

The worst 5 of 1977 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:412:A:N6	4:G:35:ARG:HG3	1.34	1.41
4:G:22:LYS:HG2	4:G:26:CYS:CB	1.50	1.39
4:G:9:CYS:SG	4:G:31:CYS:SG	1.40	1.39
4:G:22:LYS:HG3	4:G:26:CYS:N	1.47	1.28
4:G:9:CYS:SG	4:G:22:LYS:HE3	1.76	1.24

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	E	235/256 (92%)	165 (70%)	38 (16%)	32 (14%)	0	2
3	F	204/239 (85%)	135 (66%)	48 (24%)	21 (10%)	1	6
4	G	206/208 (99%)	150 (73%)	36 (18%)	20 (10%)	1	6
5	H	149/162 (92%)	130 (87%)	13 (9%)	6 (4%)	5	28
6	I	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	11	49
7	J	153/156 (98%)	120 (78%)	25 (16%)	8 (5%)	3	21
8	K	136/138 (99%)	120 (88%)	10 (7%)	6 (4%)	4	25
9	L	125/128 (98%)	90 (72%)	31 (25%)	4 (3%)	6	35
10	M	97/105 (92%)	65 (67%)	24 (25%)	8 (8%)	1	10
11	N	117/129 (91%)	96 (82%)	16 (14%)	5 (4%)	4	26
12	O	123/128 (96%)	103 (84%)	10 (8%)	10 (8%)	1	10
13	P	115/126 (91%)	75 (65%)	22 (19%)	18 (16%)	0	1
14	Q	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	1	6
15	R	86/89 (97%)	73 (85%)	6 (7%)	7 (8%)	1	10
16	S	82/88 (93%)	66 (80%)	15 (18%)	1 (1%)	19	62
17	T	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	11	49
18	U	70/88 (80%)	56 (80%)	7 (10%)	7 (10%)	1	6
19	V	76/93 (82%)	44 (58%)	17 (22%)	15 (20%)	0	0
20	W	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	1	7
21	X	23/27 (85%)	17 (74%)	3 (13%)	3 (13%)	0	3
All	All	2349/2533 (93%)	1787 (76%)	372 (16%)	190 (8%)	1	10

5 of 190 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	5	ILE
2	E	7	VAL
2	E	13	ALA

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Mol	Chain	Res	Type
2	E	64	ARG
2	E	74	LYS

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	E	205/220 (93%)	166 (81%)	39 (19%)	2	9
3	F	160/188 (85%)	138 (86%)	22 (14%)	5	21
4	G	180/180 (100%)	160 (89%)	20 (11%)	9	33
5	H	116/123 (94%)	102 (88%)	14 (12%)	7	27
6	I	90/90 (100%)	77 (86%)	13 (14%)	5	19
7	J	126/127 (99%)	107 (85%)	19 (15%)	4	16
8	K	119/119 (100%)	102 (86%)	17 (14%)	5	19
9	L	98/99 (99%)	80 (82%)	18 (18%)	2	9
10	M	89/92 (97%)	72 (81%)	17 (19%)	2	9
11	N	90/99 (91%)	73 (81%)	17 (19%)	2	9
12	O	104/107 (97%)	93 (89%)	11 (11%)	10	35
13	P	94/101 (93%)	75 (80%)	19 (20%)	2	8
14	Q	49/50 (98%)	40 (82%)	9 (18%)	2	9
15	R	79/80 (99%)	72 (91%)	7 (9%)	14	47
16	S	72/74 (97%)	61 (85%)	11 (15%)	4	15
17	T	95/97 (98%)	87 (92%)	8 (8%)	16	52
18	U	63/77 (82%)	55 (87%)	8 (13%)	6	24
19	V	67/80 (84%)	54 (81%)	13 (19%)	2	8
20	W	76/82 (93%)	68 (90%)	8 (10%)	10	35
21	X	20/22 (91%)	19 (95%)	1 (5%)	34	75
All	All	1992/2107 (94%)	1701 (85%)	291 (15%)	5	18

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	K	51	VAL
10	M	6	ILE
18	U	86	VAL
8	K	82	HIS
9	L	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
7	J	28	ASN
11	N	26	ASN
17	T	45	HIS
4	G	119	GLN
19	V	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1506 (99%)	312 (20%)	30 (1%)
22	C	77/77 (100%)	12 (15%)	1 (1%)
22	D	76/77 (98%)	45 (59%)	5 (6%)
23	1	5/6 (83%)	1 (20%)	0
All	All	1663/1666 (99%)	370 (22%)	36 (2%)

5 of 370 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	748	C
1	A	1126	U
22	D	12	G
1	A	913	A
1	A	1128	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 767 ligands modelled in this entry, 766 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	T1C	A	1984	24	45,45,45	1.54	6 (13%)	72,72,72	1.72	17 (23%)

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	T1C	A	1984	24	-	1/22/80/80	0/0/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1984	T1C	C7-N7	-7.03	1.41	1.48
25	A	1984	T1C	C4-N4	-3.41	1.47	1.51
25	A	1984	T1C	C9-N9	-2.62	1.36	1.41
25	A	1984	T1C	C1B-C12	-2.28	1.33	1.36
25	A	1984	T1C	C93-N92	-2.07	1.45	1.48

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1984	T1C	O12-C12-C1B	-6.49	117.73	123.90
25	A	1984	T1C	C1-C1C-C12	4.09	114.71	109.79
25	A	1984	T1C	O12-C12-C1C	3.51	119.25	113.57
25	A	1984	T1C	C51-C5-C41	-3.34	104.07	110.59
25	A	1984	T1C	O1C-C1C-C41	-3.24	105.98	110.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1984	T1C	C92-C91-N9-C9

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, 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	1506/1506 (100%)	-0.50	14 (0%) 81 25	76, 117, 189, 249	0
2	E	237/256 (92%)	0.18	22 (9%) 9 2	126, 162, 192, 208	0
3	F	206/239 (86%)	1.45	63 (30%) 1 0	121, 145, 174, 184	0
4	G	208/208 (100%)	0.14	16 (7%) 13 2	93, 113, 133, 142	0
5	H	151/162 (93%)	0.74	22 (14%) 3 1	97, 117, 139, 165	0
6	I	101/101 (100%)	-0.32	1 (0%) 79 23	90, 107, 128, 148	0
7	J	155/156 (99%)	0.83	25 (16%) 2 1	116, 133, 162, 173	0
8	K	138/138 (100%)	0.37	15 (10%) 6 1	105, 122, 135, 143	0
9	L	127/128 (99%)	0.71	22 (17%) 2 0	114, 155, 170, 176	0
10	M	99/105 (94%)	0.35	10 (10%) 7 2	117, 159, 174, 180	0
11	N	119/129 (92%)	0.24	12 (10%) 7 2	91, 112, 138, 163	0
12	O	125/128 (97%)	0.65	15 (12%) 5 1	84, 104, 129, 170	0
13	P	117/126 (92%)	0.62	16 (13%) 4 1	121, 155, 170, 177	0
14	Q	60/61 (98%)	0.37	3 (5%) 28 4	130, 139, 155, 162	0
15	R	88/89 (98%)	1.11	18 (20%) 1 0	89, 113, 131, 136	0
16	S	84/88 (95%)	-0.24	0 100 100	91, 107, 126, 167	0
17	T	100/105 (95%)	0.63	11 (11%) 6 1	91, 111, 128, 149	0
18	U	72/88 (81%)	0.75	12 (16%) 2 0	96, 117, 152, 173	0
19	V	78/93 (83%)	-0.02	4 (5%) 27 4	135, 166, 181, 188	0
20	W	99/106 (93%)	0.07	7 (7%) 16 3	91, 116, 148, 165	0
21	X	25/27 (92%)	0.99	4 (16%) 3 1	117, 138, 154, 170	0
22	C	77/77 (100%)	-0.37	0 100 100	80, 118, 151, 171	0
22	D	77/77 (100%)	0.26	0 100 100	93, 220, 238, 248	0
23	1	6/6 (100%)	-0.14	1 (16%) 2 0	103, 111, 138, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4055/4199 (96%)	0.10	313 (7%) 16 2	76, 125, 183, 249	0

The worst 5 of 313 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	240	GLN	12.5
12	O	19	ARG	12.2
7	J	12	LEU	10.7
7	J	11	GLN	10.0
12	O	129	ALA	9.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	MG	A	2068	1/1	0.28	-	62,62,62,62	0
24	MG	A	2147	1/1	0.36	-	79,79,79,79	0
24	MG	A	1877	1/1	0.07	-	71,71,71,71	0
24	MG	A	1779	1/1	0.31	-	95,95,95,95	0
24	MG	A	1997	1/1	0.34	-	87,87,87,87	0
24	MG	D	120	1/1	0.14	-	81,81,81,81	0
24	MG	A	2012	1/1	0.18	-	63,63,63,63	0
24	MG	C	126	1/1	0.15	-	77,77,77,77	0
24	MG	A	2063	1/1	0.31	-	105,105,105,105	0
24	MG	C	131	1/1	0.44	-	77,77,77,77	0
24	MG	A	2258	1/1	0.32	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2077	1/1	0.56	-	68,68,68,68	0
24	MG	A	1911	1/1	0.18	-	88,88,88,88	0
24	MG	A	2194	1/1	0.36	-	85,85,85,85	0
24	MG	A	1892	1/1	0.12	-	77,77,77,77	0
24	MG	A	2007	1/1	0.38	-	54,54,54,54	0
24	MG	C	136	1/1	0.58	-	71,71,71,71	0
24	MG	A	2260	1/1	2.15	-	111,111,111,111	0
24	MG	A	1784	1/1	0.09	-	121,121,121,121	0
24	MG	A	1633	1/1	0.11	-	67,67,67,67	0
24	MG	C	101	1/1	0.20	-	110,110,110,110	0
24	MG	A	1634	1/1	0.11	-	108,108,108,108	0
24	MG	D	119	1/1	0.12	-	83,83,83,83	0
24	MG	C	111	1/1	0.17	-	51,51,51,51	0
24	MG	A	1950	1/1	0.30	-	93,93,93,93	0
24	MG	A	1696	1/1	1.50	-	119,119,119,119	0
24	MG	A	1800	1/1	0.20	-	90,90,90,90	0
24	MG	A	2182	1/1	0.48	-	73,73,73,73	0
24	MG	A	1988	1/1	0.35	-	58,58,58,58	0
24	MG	A	1617	1/1	0.13	-	97,97,97,97	0
24	MG	C	113	1/1	0.18	-	70,70,70,70	0
24	MG	A	1651	1/1	0.31	-	110,110,110,110	0
24	MG	A	1716	1/1	0.81	-	91,91,91,91	0
24	MG	A	1733	1/1	0.23	-	95,95,95,95	0
24	MG	A	1622	1/1	0.30	-	74,74,74,74	0
24	MG	A	1956	1/1	0.14	-	67,67,67,67	0
24	MG	A	1928	1/1	0.22	-	101,101,101,101	0
24	MG	C	118	1/1	0.07	-	63,63,63,63	0
24	MG	A	2211	1/1	0.56	-	107,107,107,107	0
24	MG	A	1666	1/1	0.25	-	91,91,91,91	0
24	MG	A	1865	1/1	0.60	-	102,102,102,102	0
24	MG	A	2249	1/1	0.59	-	95,95,95,95	0
24	MG	A	1708	1/1	0.05	-	88,88,88,88	0
24	MG	A	1905	1/1	0.30	-	100,100,100,100	0
24	MG	A	2084	1/1	0.07	-	90,90,90,90	0
24	MG	A	1967	1/1	0.42	-	105,105,105,105	0
24	MG	C	123	1/1	0.14	-	73,73,73,73	0
24	MG	A	2034	1/1	0.10	-	74,74,74,74	0
24	MG	A	1752	1/1	0.14	-	85,85,85,85	0
24	MG	A	2103	1/1	0.51	-	84,84,84,84	0
24	MG	A	1822	1/1	0.07	-	85,85,85,85	0
24	MG	A	2151	1/1	0.59	-	91,91,91,91	0
24	MG	A	2033	1/1	0.09	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2218	1/1	0.24	-	84,84,84,84	0
24	MG	A	1698	1/1	0.23	-	80,80,80,80	0
24	MG	A	1885	1/1	0.27	-	110,110,110,110	0
24	MG	A	2185	1/1	0.66	-	82,82,82,82	0
24	MG	A	1795	1/1	0.25	-	85,85,85,85	0
24	MG	L	201	1/1	0.17	-	104,104,104,104	0
24	MG	A	1859	1/1	0.13	-	70,70,70,70	0
24	MG	A	1812	1/1	0.76	-	119,119,119,119	0
24	MG	A	2142	1/1	0.18	-	82,82,82,82	0
24	MG	A	1819	1/1	0.21	-	104,104,104,104	0
24	MG	A	2132	1/1	0.08	-	76,76,76,76	0
24	MG	A	1944	1/1	0.08	-	74,74,74,74	0
24	MG	A	2046	1/1	0.23	-	75,75,75,75	0
24	MG	A	1902	1/1	0.24	-	86,86,86,86	0
24	MG	A	2160	1/1	0.22	-	96,96,96,96	0
24	MG	A	1685	1/1	0.22	-	82,82,82,82	0
24	MG	A	1936	1/1	0.49	-	86,86,86,86	0
24	MG	A	1722	1/1	0.38	-	70,70,70,70	0
24	MG	A	1926	1/1	0.28	-	97,97,97,97	0
24	MG	C	139	1/1	0.10	-	72,72,72,72	0
24	MG	A	2162	1/1	0.17	-	91,91,91,91	0
24	MG	A	2054	1/1	0.09	-	74,74,74,74	0
24	MG	A	1608	1/1	0.14	-	87,87,87,87	0
24	MG	A	2253	1/1	0.31	-	101,101,101,101	0
24	MG	A	2129	1/1	0.07	-	54,54,54,54	0
24	MG	A	2040	1/1	0.51	-	67,67,67,67	0
24	MG	A	1906	1/1	0.21	-	63,63,63,63	0
24	MG	A	1787	1/1	0.37	-	91,91,91,91	0
24	MG	A	1985	1/1	0.15	-	53,53,53,53	0
24	MG	A	2255	1/1	1.04	-	81,81,81,81	0
24	MG	A	2036	1/1	0.55	-	73,73,73,73	0
24	MG	A	2089	1/1	0.40	-	76,76,76,76	0
24	MG	A	1687	1/1	0.08	-	88,88,88,88	0
24	MG	A	1694	1/1	0.28	-	101,101,101,101	0
24	MG	A	2042	1/1	0.39	-	57,57,57,57	0
24	MG	A	2157	1/1	0.32	-	68,68,68,68	0
24	MG	A	2241	1/1	0.45	-	97,97,97,97	0
24	MG	A	1721	1/1	0.06	-	60,60,60,60	0
24	MG	A	2248	1/1	0.15	-	82,82,82,82	0
24	MG	A	1602	1/1	0.72	-	95,95,95,95	0
24	MG	A	2131	1/1	0.31	-	95,95,95,95	0
24	MG	A	2094	1/1	0.08	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1735	1/1	0.14	-	88,88,88,88	0
24	MG	A	2285	1/1	0.47	-	91,91,91,91	0
24	MG	A	1982	1/1	0.33	-	115,115,115,115	0
24	MG	A	1874	1/1	0.22	-	70,70,70,70	0
24	MG	A	2216	1/1	0.14	-	73,73,73,73	0
24	MG	A	1788	1/1	0.12	-	80,80,80,80	0
24	MG	A	1724	1/1	0.41	-	80,80,80,80	0
24	MG	A	2201	1/1	0.32	-	94,94,94,94	0
24	MG	G	302	1/1	0.64	-	114,114,114,114	0
24	MG	A	1834	1/1	0.22	-	112,112,112,112	0
24	MG	A	1830	1/1	0.14	-	88,88,88,88	0
24	MG	A	1675	1/1	0.12	-	85,85,85,85	0
24	MG	A	1755	1/1	0.26	-	75,75,75,75	0
24	MG	D	114	1/1	0.13	-	81,81,81,81	0
24	MG	A	2059	1/1	0.51	-	89,89,89,89	0
24	MG	A	1879	1/1	0.23	-	102,102,102,102	0
24	MG	A	2000	1/1	0.21	-	83,83,83,83	0
24	MG	A	1884	1/1	0.25	-	56,56,56,56	0
24	MG	A	2213	1/1	0.30	-	92,92,92,92	0
24	MG	A	2027	1/1	0.73	-	69,69,69,69	0
24	MG	A	1741	1/1	0.20	-	81,81,81,81	0
24	MG	A	2015	1/1	0.17	-	60,60,60,60	0
24	MG	C	115	1/1	0.06	-	66,66,66,66	0
24	MG	A	1661	1/1	0.09	-	93,93,93,93	0
24	MG	A	2172	1/1	0.13	-	84,84,84,84	0
24	MG	A	1642	1/1	0.17	-	113,113,113,113	0
24	MG	A	1908	1/1	0.83	-	80,80,80,80	0
24	MG	A	1743	1/1	0.44	-	77,77,77,77	0
24	MG	A	1957	1/1	0.16	-	83,83,83,83	0
24	MG	A	2133	1/1	0.58	-	67,67,67,67	0
24	MG	C	122	1/1	0.16	-	54,54,54,54	0
24	MG	A	1940	1/1	0.23	-	84,84,84,84	0
24	MG	A	2180	1/1	0.35	-	92,92,92,92	0
24	MG	A	1914	1/1	0.07	-	84,84,84,84	0
24	MG	A	1702	1/1	0.93	-	103,103,103,103	0
24	MG	A	1951	1/1	0.11	-	80,80,80,80	0
24	MG	A	1669	1/1	0.10	-	78,78,78,78	0
24	MG	A	2156	1/1	0.30	-	83,83,83,83	0
24	MG	A	1723	1/1	0.14	-	65,65,65,65	0
24	MG	A	2197	1/1	0.97	-	88,88,88,88	0
24	MG	A	2078	1/1	0.10	-	91,91,91,91	0
24	MG	A	1657	1/1	0.27	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2257	1/1	0.31	-	91,91,91,91	0
24	MG	A	2158	1/1	0.27	-	90,90,90,90	0
24	MG	A	1826	1/1	0.26	-	94,94,94,94	0
24	MG	A	1654	1/1	0.30	-	91,91,91,91	0
24	MG	A	1835	1/1	0.09	-	76,76,76,76	0
24	MG	A	1939	1/1	0.13	-	102,102,102,102	0
24	MG	A	1818	1/1	0.17	-	73,73,73,73	0
24	MG	C	121	1/1	0.64	-	55,55,55,55	0
24	MG	A	2038	1/1	0.23	-	57,57,57,57	0
24	MG	A	1842	1/1	0.58	-	70,70,70,70	0
24	MG	A	2009	1/1	0.07	-	72,72,72,72	0
24	MG	A	2137	1/1	0.36	-	78,78,78,78	0
24	MG	A	2011	1/1	0.18	-	57,57,57,57	0
24	MG	C	107	1/1	0.10	-	77,77,77,77	0
24	MG	A	1711	1/1	0.16	-	90,90,90,90	0
24	MG	A	1878	1/1	0.07	-	71,71,71,71	0
24	MG	A	2017	1/1	0.23	-	71,71,71,71	0
24	MG	A	1710	1/1	0.27	-	88,88,88,88	0
24	MG	A	2031	1/1	0.25	-	56,56,56,56	0
24	MG	A	1855	1/1	0.11	-	60,60,60,60	0
24	MG	A	2121	1/1	0.10	-	78,78,78,78	0
24	MG	A	1866	1/1	0.52	-	57,57,57,57	0
24	MG	C	137	1/1	0.68	-	96,96,96,96	0
24	MG	A	2262	1/1	0.36	-	101,101,101,101	0
24	MG	A	2221	1/1	0.92	-	93,93,93,93	0
24	MG	A	1907	1/1	0.24	-	94,94,94,94	0
24	MG	A	1718	1/1	0.45	-	92,92,92,92	0
24	MG	A	2163	1/1	0.30	-	93,93,93,93	0
24	MG	A	2214	1/1	0.34	-	75,75,75,75	0
24	MG	A	1904	1/1	0.09	-	90,90,90,90	0
24	MG	A	1965	1/1	0.15	-	82,82,82,82	0
24	MG	A	2086	1/1	0.17	-	65,65,65,65	0
24	MG	A	1780	1/1	0.24	-	89,89,89,89	0
24	MG	A	2159	1/1	0.11	-	72,72,72,72	0
24	MG	A	2016	1/1	0.38	-	73,73,73,73	0
24	MG	A	2179	1/1	1.22	-	79,79,79,79	0
24	MG	C	108	1/1	0.08	-	47,47,47,47	0
24	MG	A	2274	1/1	0.40	-	80,80,80,80	0
24	MG	A	1740	1/1	0.10	-	61,61,61,61	0
24	MG	A	2127	1/1	0.57	-	74,74,74,74	0
24	MG	A	1882	1/1	0.66	-	91,91,91,91	0
24	MG	A	2277	1/1	0.58	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1763	1/1	0.27	-	94,94,94,94	0
24	MG	A	1690	1/1	0.48	-	92,92,92,92	0
24	MG	A	2234	1/1	0.26	-	89,89,89,89	0
24	MG	A	2231	1/1	0.13	-	95,95,95,95	0
24	MG	A	2150	1/1	0.31	-	84,84,84,84	0
24	MG	A	2079	1/1	0.28	-	87,87,87,87	0
24	MG	A	1990	1/1	0.18	-	65,65,65,65	0
24	MG	A	2085	1/1	0.30	-	67,67,67,67	0
25	T1C	A	1984	42/42	0.36	-	101,116,124,127	0
24	MG	A	1699	1/1	0.07	-	93,93,93,93	0
24	MG	A	1913	1/1	0.15	-	103,103,103,103	0
24	MG	A	1935	1/1	0.20	-	113,113,113,113	0
24	MG	T	201	1/1	1.38	-	94,94,94,94	0
24	MG	D	103	1/1	0.11	-	67,67,67,67	0
24	MG	A	1828	1/1	0.26	-	115,115,115,115	0
24	MG	A	2140	1/1	0.29	-	90,90,90,90	0
24	MG	A	1603	1/1	0.07	-	87,87,87,87	0
24	MG	A	1774	1/1	0.27	-	86,86,86,86	0
24	MG	A	1636	1/1	0.36	-	75,75,75,75	0
24	MG	A	2098	1/1	0.23	-	76,76,76,76	0
24	MG	A	1794	1/1	0.21	-	84,84,84,84	0
24	MG	A	1632	1/1	0.26	-	109,109,109,109	0
24	MG	A	2111	1/1	0.14	-	104,104,104,104	0
24	MG	A	1872	1/1	0.42	-	90,90,90,90	0
24	MG	R	101	1/1	0.93	-	93,93,93,93	0
24	MG	A	2071	1/1	0.51	-	86,86,86,86	0
24	MG	A	2003	1/1	0.49	-	67,67,67,67	0
24	MG	A	2203	1/1	0.22	-	87,87,87,87	0
24	MG	A	1942	1/1	0.15	-	78,78,78,78	0
24	MG	D	124	1/1	0.12	-	90,90,90,90	0
24	MG	A	2204	1/1	0.18	-	81,81,81,81	0
24	MG	A	1610	1/1	0.19	-	105,105,105,105	0
24	MG	A	1888	1/1	0.10	-	97,97,97,97	0
24	MG	C	130	1/1	0.12	-	95,95,95,95	0
24	MG	A	1662	1/1	0.24	-	100,100,100,100	0
24	MG	A	1748	1/1	0.31	-	86,86,86,86	0
24	MG	A	1732	1/1	0.09	-	60,60,60,60	0
24	MG	A	1978	1/1	1.29	-	81,81,81,81	0
24	MG	A	1896	1/1	0.12	-	104,104,104,104	0
24	MG	A	1860	1/1	0.34	-	93,93,93,93	0
24	MG	A	1821	1/1	0.19	-	74,74,74,74	0
24	MG	C	132	1/1	0.09	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1660	1/1	0.20	-	87,87,87,87	0
24	MG	A	2181	1/1	1.35	-	102,102,102,102	0
24	MG	A	2227	1/1	0.09	-	113,113,113,113	0
24	MG	A	2261	1/1	0.93	-	92,92,92,92	0
24	MG	A	1786	1/1	0.65	-	96,96,96,96	0
24	MG	A	1758	1/1	0.13	-	109,109,109,109	0
24	MG	A	2212	1/1	1.08	-	82,82,82,82	0
24	MG	A	1766	1/1	0.54	-	93,93,93,93	0
24	MG	A	1994	1/1	0.08	-	78,78,78,78	0
24	MG	A	1992	1/1	0.13	-	73,73,73,73	0
24	MG	A	2008	1/1	0.34	-	82,82,82,82	0
24	MG	A	1820	1/1	0.18	-	86,86,86,86	0
24	MG	A	1704	1/1	0.10	-	78,78,78,78	0
24	MG	A	1809	1/1	0.15	-	99,99,99,99	0
24	MG	A	1631	1/1	0.07	-	64,64,64,64	0
24	MG	C	144	1/1	0.20	-	92,92,92,92	0
24	MG	A	1637	1/1	0.63	-	105,105,105,105	0
24	MG	A	1854	1/1	0.10	-	61,61,61,61	0
24	MG	A	1867	1/1	0.14	-	103,103,103,103	0
24	MG	A	1796	1/1	0.24	-	99,99,99,99	0
24	MG	A	1655	1/1	0.27	-	102,102,102,102	0
24	MG	A	1922	1/1	0.17	-	79,79,79,79	0
24	MG	A	1976	1/1	0.28	-	87,87,87,87	0
24	MG	A	1640	1/1	0.08	-	82,82,82,82	0
24	MG	C	117	1/1	0.16	-	67,67,67,67	0
24	MG	A	1971	1/1	0.66	-	105,105,105,105	0
24	MG	A	1618	1/1	0.44	-	77,77,77,77	0
24	MG	A	1973	1/1	0.13	-	69,69,69,69	0
24	MG	A	2134	1/1	0.50	-	88,88,88,88	0
24	MG	A	1898	1/1	0.16	-	96,96,96,96	0
24	MG	A	2069	1/1	0.21	-	60,60,60,60	0
24	MG	A	2135	1/1	0.86	-	97,97,97,97	0
24	MG	A	1613	1/1	0.47	-	99,99,99,99	0
24	MG	A	1810	1/1	0.22	-	81,81,81,81	0
24	MG	A	1912	1/1	0.25	-	83,83,83,83	0
24	MG	C	127	1/1	0.21	-	103,103,103,103	0
24	MG	A	1952	1/1	0.07	-	71,71,71,71	0
24	MG	A	1791	1/1	1.00	-	90,90,90,90	0
24	MG	A	1857	1/1	0.30	-	58,58,58,58	0
24	MG	C	143	1/1	0.64	-	71,71,71,71	0
24	MG	A	1615	1/1	0.16	-	121,121,121,121	0
24	MG	A	1707	1/1	0.36	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2279	1/1	0.13	-	95,95,95,95	0
24	MG	C	142	1/1	0.61	-	86,86,86,86	0
24	MG	A	2113	1/1	0.46	-	73,73,73,73	0
24	MG	A	2238	1/1	0.30	-	92,92,92,92	0
24	MG	A	2064	1/1	0.20	-	87,87,87,87	0
24	MG	A	2164	1/1	0.15	-	79,79,79,79	0
24	MG	A	1783	1/1	0.52	-	74,74,74,74	0
24	MG	A	2190	1/1	2.78	-	107,107,107,107	0
24	MG	A	2062	1/1	0.48	-	74,74,74,74	0
24	MG	C	104	1/1	0.09	-	50,50,50,50	0
24	MG	A	1804	1/1	0.25	-	98,98,98,98	0
24	MG	A	1648	1/1	0.22	-	63,63,63,63	0
24	MG	A	1843	1/1	0.16	-	66,66,66,66	0
24	MG	A	1897	1/1	0.54	-	76,76,76,76	0
24	MG	A	1823	1/1	0.14	-	104,104,104,104	0
24	MG	C	112	1/1	0.06	-	88,88,88,88	0
24	MG	A	1832	1/1	0.07	-	89,89,89,89	0
24	MG	A	1751	1/1	0.39	-	90,90,90,90	0
24	MG	A	2010	1/1	0.22	-	82,82,82,82	0
24	MG	A	2265	1/1	0.58	-	86,86,86,86	0
24	MG	S	101	1/1	0.18	-	95,95,95,95	0
24	MG	A	2019	1/1	0.19	-	73,73,73,73	0
24	MG	A	2232	1/1	0.05	-	67,67,67,67	0
24	MG	A	1672	1/1	0.19	-	93,93,93,93	0
24	MG	A	2195	1/1	0.28	-	70,70,70,70	0
24	MG	A	1813	1/1	0.19	-	161,161,161,161	0
24	MG	A	1709	1/1	0.08	-	110,110,110,110	0
24	MG	A	1747	1/1	0.11	-	74,74,74,74	0
24	MG	A	2050	1/1	0.05	-	52,52,52,52	0
24	MG	A	1753	1/1	0.19	-	73,73,73,73	0
24	MG	A	1972	1/1	0.17	-	82,82,82,82	0
24	MG	D	108	1/1	0.18	-	117,117,117,117	0
24	MG	A	1948	1/1	0.22	-	148,148,148,148	0
24	MG	A	2245	1/1	0.40	-	83,83,83,83	0
24	MG	A	2091	1/1	0.71	-	76,76,76,76	0
24	MG	A	1790	1/1	0.07	-	133,133,133,133	0
24	MG	A	2183	1/1	0.14	-	78,78,78,78	0
24	MG	A	1991	1/1	0.11	-	70,70,70,70	0
24	MG	A	1688	1/1	0.57	-	82,82,82,82	0
24	MG	A	1831	1/1	0.66	-	88,88,88,88	0
24	MG	A	1947	1/1	0.17	-	49,49,49,49	0
24	MG	A	1901	1/1	0.17	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1836	1/1	0.08	-	108,108,108,108	0
24	MG	A	1789	1/1	0.65	-	97,97,97,97	0
24	MG	A	2106	1/1	0.09	-	84,84,84,84	0
24	MG	A	1736	1/1	0.14	-	76,76,76,76	0
24	MG	A	1929	1/1	0.21	-	65,65,65,65	0
24	MG	A	2251	1/1	0.35	-	86,86,86,86	0
24	MG	A	2272	1/1	4.12	-	99,99,99,99	0
24	MG	A	1954	1/1	0.42	-	81,81,81,81	0
24	MG	A	1785	1/1	0.31	-	95,95,95,95	0
24	MG	A	2104	1/1	0.19	-	110,110,110,110	0
24	MG	A	1851	1/1	0.19	-	86,86,86,86	0
24	MG	D	116	1/1	0.59	-	101,101,101,101	0
24	MG	A	1811	1/1	0.27	-	109,109,109,109	0
24	MG	D	107	1/1	0.06	-	91,91,91,91	0
24	MG	A	1701	1/1	0.09	-	114,114,114,114	0
24	MG	A	2161	1/1	0.14	-	82,82,82,82	0
24	MG	A	1862	1/1	0.59	-	66,66,66,66	0
24	MG	A	1989	1/1	0.20	-	66,66,66,66	0
24	MG	A	1894	1/1	0.18	-	80,80,80,80	0
24	MG	A	1745	1/1	0.12	-	79,79,79,79	0
24	MG	A	1797	1/1	0.44	-	67,67,67,67	0
24	MG	A	1703	1/1	0.20	-	82,82,82,82	0
24	MG	A	2259	1/1	0.13	-	134,134,134,134	0
24	MG	A	1627	1/1	0.15	-	95,95,95,95	0
24	MG	A	1845	1/1	0.20	-	65,65,65,65	0
24	MG	A	1713	1/1	0.14	-	93,93,93,93	0
24	MG	A	1871	1/1	0.16	-	109,109,109,109	0
24	MG	A	2267	1/1	0.65	-	105,105,105,105	0
24	MG	A	2060	1/1	0.80	-	76,76,76,76	0
24	MG	A	1886	1/1	0.16	-	91,91,91,91	0
24	MG	A	2170	1/1	0.10	-	83,83,83,83	0
24	MG	A	2264	1/1	1.75	-	95,95,95,95	0
24	MG	A	1899	1/1	0.14	-	76,76,76,76	0
24	MG	A	1681	1/1	0.20	-	84,84,84,84	0
24	MG	A	1612	1/1	0.09	-	94,94,94,94	0
24	MG	D	104	1/1	0.10	-	76,76,76,76	0
24	MG	A	1953	1/1	0.25	-	95,95,95,95	0
24	MG	G	301	1/1	0.14	-	113,113,113,113	0
24	MG	A	2124	1/1	0.14	-	78,78,78,78	0
24	MG	A	2005	1/1	0.18	-	92,92,92,92	0
24	MG	A	1815	1/1	0.25	-	103,103,103,103	0
24	MG	A	2287	1/1	1.79	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	D	122	1/1	0.64	-	104,104,104,104	0
24	MG	A	1653	1/1	0.15	-	107,107,107,107	0
24	MG	A	1900	1/1	0.89	-	79,79,79,79	0
24	MG	A	1749	1/1	0.31	-	87,87,87,87	0
24	MG	A	1616	1/1	0.71	-	76,76,76,76	0
24	MG	A	1737	1/1	0.27	-	82,82,82,82	0
24	MG	A	1807	1/1	0.41	-	102,102,102,102	0
24	MG	A	2099	1/1	0.35	-	57,57,57,57	0
24	MG	A	1769	1/1	0.27	-	82,82,82,82	0
24	MG	A	2073	1/1	0.13	-	72,72,72,72	0
24	MG	A	2139	1/1	0.59	-	84,84,84,84	0
24	MG	A	2118	1/1	1.31	-	94,94,94,94	0
24	MG	A	1765	1/1	0.14	-	86,86,86,86	0
24	MG	A	1931	1/1	0.11	-	79,79,79,79	0
24	MG	A	1730	1/1	0.09	-	78,78,78,78	0
24	MG	A	1837	1/1	0.13	-	60,60,60,60	0
24	MG	A	1719	1/1	0.39	-	67,67,67,67	0
24	MG	A	2047	1/1	0.12	-	94,94,94,94	0
24	MG	A	2107	1/1	0.11	-	78,78,78,78	0
24	MG	A	1801	1/1	0.24	-	109,109,109,109	0
24	MG	A	1970	1/1	0.29	-	91,91,91,91	0
24	MG	A	1849	1/1	0.20	-	56,56,56,56	0
24	MG	A	1937	1/1	0.14	-	105,105,105,105	0
24	MG	D	113	1/1	0.06	-	63,63,63,63	0
24	MG	A	1693	1/1	0.11	-	106,106,106,106	0
24	MG	A	1646	1/1	0.08	-	81,81,81,81	0
24	MG	A	2087	1/1	0.19	-	54,54,54,54	0
24	MG	A	2082	1/1	0.41	-	87,87,87,87	0
24	MG	A	1739	1/1	0.15	-	80,80,80,80	0
24	MG	A	1808	1/1	0.14	-	100,100,100,100	0
24	MG	A	1725	1/1	0.11	-	51,51,51,51	0
24	MG	A	2116	1/1	0.37	-	140,140,140,140	0
24	MG	A	1714	1/1	0.55	-	78,78,78,78	0
24	MG	A	2256	1/1	0.86	-	102,102,102,102	0
24	MG	A	1673	1/1	0.10	-	86,86,86,86	0
24	MG	A	1998	1/1	0.66	-	77,77,77,77	0
24	MG	A	1664	1/1	0.26	-	100,100,100,100	0
24	MG	C	106	1/1	0.23	-	72,72,72,72	0
24	MG	A	2233	1/1	0.27	-	88,88,88,88	0
24	MG	A	1656	1/1	0.12	-	78,78,78,78	0
24	MG	A	2193	1/1	0.06	-	62,62,62,62	0
24	MG	A	2206	1/1	0.11	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2202	1/1	0.40	-	94,94,94,94	0
24	MG	D	102	1/1	0.18	-	82,82,82,82	0
24	MG	A	1684	1/1	0.85	-	93,93,93,93	0
24	MG	A	2052	1/1	0.12	-	64,64,64,64	0
24	MG	A	2055	1/1	0.08	-	66,66,66,66	0
24	MG	A	2220	1/1	0.74	-	95,95,95,95	0
24	MG	A	2252	1/1	0.18	-	103,103,103,103	0
24	MG	A	1987	1/1	0.41	-	71,71,71,71	0
24	MG	A	1945	1/1	0.21	-	97,97,97,97	0
24	MG	A	1742	1/1	0.16	-	73,73,73,73	0
24	MG	A	2037	1/1	0.26	-	49,49,49,49	0
24	MG	A	1918	1/1	0.32	-	86,86,86,86	0
24	MG	A	2093	1/1	0.10	-	70,70,70,70	0
24	MG	D	115	1/1	0.14	-	92,92,92,92	0
24	MG	A	2250	1/1	0.19	-	74,74,74,74	0
24	MG	A	1863	1/1	0.28	-	120,120,120,120	0
24	MG	A	2070	1/1	0.20	-	56,56,56,56	0
24	MG	A	1706	1/1	0.09	-	92,92,92,92	0
24	MG	A	1958	1/1	0.19	-	69,69,69,69	0
24	MG	A	2061	1/1	0.47	-	93,93,93,93	0
24	MG	A	1881	1/1	0.20	-	97,97,97,97	0
24	MG	A	1920	1/1	0.30	-	122,122,122,122	0
24	MG	A	1620	1/1	0.12	-	71,71,71,71	0
24	MG	A	2022	1/1	0.20	-	61,61,61,61	0
24	MG	A	1825	1/1	1.18	-	88,88,88,88	0
24	MG	D	111	1/1	0.26	-	77,77,77,77	0
24	MG	A	1975	1/1	0.15	-	74,74,74,74	0
24	MG	A	1607	1/1	0.24	-	91,91,91,91	0
24	MG	C	134	1/1	0.11	-	77,77,77,77	0
24	MG	A	2136	1/1	0.09	-	105,105,105,105	0
24	MG	A	2092	1/1	0.31	-	91,91,91,91	0
24	MG	A	1782	1/1	0.36	-	119,119,119,119	0
24	MG	A	1883	1/1	0.09	-	96,96,96,96	0
24	MG	A	1695	1/1	0.34	-	124,124,124,124	0
24	MG	C	141	1/1	0.15	-	86,86,86,86	0
24	MG	A	1692	1/1	0.17	-	114,114,114,114	0
24	MG	A	2039	1/1	0.15	-	75,75,75,75	0
24	MG	A	1925	1/1	0.40	-	116,116,116,116	0
24	MG	A	2207	1/1	0.80	-	89,89,89,89	0
24	MG	A	1980	1/1	0.26	-	101,101,101,101	0
24	MG	A	1995	1/1	0.17	-	74,74,74,74	0
24	MG	A	2230	1/1	0.08	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2270	1/1	0.41	-	96,96,96,96	0
24	MG	A	1827	1/1	0.40	-	107,107,107,107	0
24	MG	A	1712	1/1	0.19	-	78,78,78,78	0
24	MG	A	2048	1/1	0.13	-	74,74,74,74	0
24	MG	A	2228	1/1	0.18	-	94,94,94,94	0
24	MG	A	1649	1/1	0.20	-	111,111,111,111	0
24	MG	A	1816	1/1	0.20	-	86,86,86,86	0
24	MG	C	103	1/1	0.12	-	89,89,89,89	0
24	MG	A	1817	1/1	0.04	-	100,100,100,100	0
24	MG	A	2223	1/1	0.38	-	62,62,62,62	0
24	MG	A	2109	1/1	0.20	-	77,77,77,77	0
24	MG	A	1792	1/1	0.26	-	90,90,90,90	0
24	MG	A	1968	1/1	0.12	-	95,95,95,95	0
24	MG	C	129	1/1	0.30	-	78,78,78,78	0
24	MG	A	1645	1/1	0.39	-	115,115,115,115	0
24	MG	C	116	1/1	0.18	-	66,66,66,66	0
24	MG	A	2006	1/1	0.08	-	76,76,76,76	0
24	MG	A	2225	1/1	0.30	-	153,153,153,153	0
24	MG	A	1764	1/1	0.19	-	102,102,102,102	0
24	MG	A	2269	1/1	0.51	-	133,133,133,133	0
24	MG	A	1847	1/1	0.17	-	66,66,66,66	0
24	MG	C	114	1/1	0.16	-	65,65,65,65	0
24	MG	A	1943	1/1	0.31	-	107,107,107,107	0
24	MG	A	2178	1/1	0.18	-	77,77,77,77	0
24	MG	A	1635	1/1	0.13	-	74,74,74,74	0
24	MG	A	1614	1/1	1.87	-	95,95,95,95	0
24	MG	A	2120	1/1	0.82	-	88,88,88,88	0
24	MG	A	1930	1/1	0.10	-	96,96,96,96	0
24	MG	A	1643	1/1	0.07	-	142,142,142,142	0
24	MG	A	2198	1/1	0.37	-	90,90,90,90	0
24	MG	A	2088	1/1	0.27	-	100,100,100,100	0
24	MG	A	1983	1/1	0.08	-	115,115,115,115	0
24	MG	A	1876	1/1	0.22	-	92,92,92,92	0
24	MG	A	1697	1/1	0.15	-	107,107,107,107	0
24	MG	D	121	1/1	0.28	-	99,99,99,99	0
24	MG	A	2004	1/1	0.42	-	62,62,62,62	0
24	MG	A	2278	1/1	0.14	-	81,81,81,81	0
24	MG	A	2035	1/1	0.50	-	82,82,82,82	0
24	MG	A	1641	1/1	0.10	-	79,79,79,79	0
24	MG	A	1966	1/1	0.17	-	64,64,64,64	0
24	MG	A	1959	1/1	0.51	-	136,136,136,136	0
24	MG	C	124	1/1	0.12	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1689	1/1	0.10	-	93,93,93,93	0
24	MG	A	1844	1/1	0.08	-	71,71,71,71	0
24	MG	A	2018	1/1	0.54	-	80,80,80,80	0
24	MG	A	1868	1/1	0.11	-	58,58,58,58	0
24	MG	A	2081	1/1	0.58	-	76,76,76,76	0
24	MG	A	2242	1/1	0.28	-	97,97,97,97	0
24	MG	A	1873	1/1	0.16	-	85,85,85,85	0
24	MG	A	1619	1/1	0.15	-	106,106,106,106	0
24	MG	A	1728	1/1	0.50	-	84,84,84,84	0
24	MG	A	1889	1/1	0.41	-	95,95,95,95	0
24	MG	A	2100	1/1	0.64	-	63,63,63,63	0
24	MG	A	2023	1/1	0.22	-	57,57,57,57	0
24	MG	A	1841	1/1	0.15	-	68,68,68,68	0
24	MG	A	1962	1/1	0.30	-	66,66,66,66	0
24	MG	A	1773	1/1	0.29	-	98,98,98,98	0
24	MG	A	1960	1/1	0.75	-	84,84,84,84	0
24	MG	A	1777	1/1	0.11	-	65,65,65,65	0
24	MG	A	2014	1/1	0.09	-	66,66,66,66	0
24	MG	A	2123	1/1	0.13	-	75,75,75,75	0
24	MG	A	2168	1/1	0.58	-	85,85,85,85	0
24	MG	A	1861	1/1	0.08	-	74,74,74,74	0
24	MG	A	1949	1/1	0.11	-	58,58,58,58	0
24	MG	A	1778	1/1	0.42	-	93,93,93,93	0
24	MG	A	1731	1/1	0.10	-	67,67,67,67	0
24	MG	A	1683	1/1	0.16	-	88,88,88,88	0
24	MG	A	1856	1/1	0.17	-	105,105,105,105	0
24	MG	A	2282	1/1	0.10	-	80,80,80,80	0
24	MG	A	2029	1/1	0.48	-	78,78,78,78	0
24	MG	A	1674	1/1	0.18	-	74,74,74,74	0
24	MG	A	2177	1/1	0.18	-	86,86,86,86	0
24	MG	A	1839	1/1	0.07	-	64,64,64,64	0
24	MG	A	2066	1/1	0.14	-	88,88,88,88	0
24	MG	A	2186	1/1	0.21	-	91,91,91,91	0
24	MG	A	2041	1/1	0.09	-	70,70,70,70	0
24	MG	A	2196	1/1	1.00	-	104,104,104,104	0
24	MG	A	1969	1/1	0.44	-	105,105,105,105	0
24	MG	A	1625	1/1	0.43	-	103,103,103,103	0
24	MG	A	2102	1/1	0.17	-	77,77,77,77	0
26	ZN	Q	101	1/1	0.06	-	123,123,123,123	0
24	MG	A	2122	1/1	0.26	-	88,88,88,88	0
24	MG	A	2155	1/1	0.09	-	76,76,76,76	0
24	MG	A	2141	1/1	0.17	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	N	201	1/1	0.07	-	95,95,95,95	0
24	MG	A	1999	1/1	0.11	-	84,84,84,84	0
24	MG	A	2217	1/1	0.59	-	52,52,52,52	0
24	MG	A	1909	1/1	0.09	-	100,100,100,100	0
24	MG	D	112	1/1	0.10	-	77,77,77,77	0
24	MG	A	1659	1/1	0.11	-	85,85,85,85	0
24	MG	A	2076	1/1	0.21	-	62,62,62,62	0
24	MG	A	2176	1/1	0.17	-	91,91,91,91	0
24	MG	A	2075	1/1	0.19	-	95,95,95,95	0
24	MG	A	1772	1/1	0.10	-	88,88,88,88	0
24	MG	A	1921	1/1	0.18	-	86,86,86,86	0
24	MG	A	2222	1/1	0.29	-	91,91,91,91	0
24	MG	A	2171	1/1	0.54	-	126,126,126,126	0
24	MG	A	1750	1/1	0.30	-	96,96,96,96	0
24	MG	A	1727	1/1	0.09	-	70,70,70,70	0
24	MG	A	1761	1/1	0.50	-	88,88,88,88	0
24	MG	D	109	1/1	0.11	-	65,65,65,65	0
24	MG	A	1802	1/1	0.10	-	88,88,88,88	0
24	MG	A	1629	1/1	0.09	-	67,67,67,67	0
24	MG	A	1670	1/1	0.47	-	76,76,76,76	0
24	MG	A	1715	1/1	0.20	-	169,169,169,169	0
24	MG	A	1891	1/1	0.86	-	94,94,94,94	0
24	MG	A	2263	1/1	0.11	-	82,82,82,82	0
24	MG	A	1676	1/1	1.08	-	96,96,96,96	0
24	MG	A	2025	1/1	0.48	-	48,48,48,48	0
24	MG	A	1759	1/1	0.28	-	104,104,104,104	0
24	MG	A	2226	1/1	0.25	-	97,97,97,97	0
24	MG	A	1893	1/1	1.08	-	105,105,105,105	0
24	MG	A	1609	1/1	0.12	-	83,83,83,83	0
24	MG	C	128	1/1	0.12	-	86,86,86,86	0
24	MG	A	2148	1/1	0.47	-	94,94,94,94	0
24	MG	A	2199	1/1	0.33	-	133,133,133,133	0
24	MG	A	2169	1/1	0.14	-	71,71,71,71	0
24	MG	A	1853	1/1	0.24	-	90,90,90,90	0
24	MG	A	1605	1/1	0.17	-	91,91,91,91	0
24	MG	A	2209	1/1	0.11	-	82,82,82,82	0
24	MG	A	1677	1/1	0.27	-	78,78,78,78	0
24	MG	C	119	1/1	0.23	-	68,68,68,68	0
24	MG	A	1762	1/1	0.12	-	76,76,76,76	0
24	MG	A	2028	1/1	0.21	-	68,68,68,68	0
24	MG	A	1979	1/1	0.13	-	64,64,64,64	0
24	MG	A	2049	1/1	0.11	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	D	117	1/1	0.10	-	76,76,76,76	0
24	MG	A	1917	1/1	0.15	-	79,79,79,79	0
24	MG	A	2095	1/1	0.69	-	92,92,92,92	0
24	MG	A	1746	1/1	0.27	-	72,72,72,72	0
24	MG	A	2173	1/1	0.33	-	84,84,84,84	0
24	MG	A	2284	1/1	0.19	-	84,84,84,84	0
24	MG	A	2276	1/1	2.02	-	88,88,88,88	0
24	MG	A	1691	1/1	0.07	-	114,114,114,114	0
24	MG	A	1658	1/1	0.26	-	110,110,110,110	0
24	MG	A	2125	1/1	0.35	-	64,64,64,64	0
24	MG	A	1974	1/1	0.09	-	112,112,112,112	0
24	MG	A	2200	1/1	0.12	-	93,93,93,93	0
24	MG	A	1964	1/1	0.08	-	84,84,84,84	0
24	MG	A	1915	1/1	0.10	-	83,83,83,83	0
24	MG	A	2146	1/1	0.18	-	95,95,95,95	0
24	MG	A	2165	1/1	0.09	-	90,90,90,90	0
24	MG	A	1606	1/1	0.19	-	115,115,115,115	0
24	MG	C	120	1/1	0.60	-	64,64,64,64	0
24	MG	A	2090	1/1	0.41	-	91,91,91,91	0
24	MG	A	2189	1/1	0.13	-	84,84,84,84	0
24	MG	A	2191	1/1	0.14	-	87,87,87,87	0
24	MG	A	1946	1/1	0.12	-	74,74,74,74	0
24	MG	C	105	1/1	0.16	-	123,123,123,123	0
24	MG	A	1793	1/1	1.54	-	89,89,89,89	0
24	MG	A	2243	1/1	0.44	-	84,84,84,84	0
24	MG	A	2097	1/1	0.13	-	69,69,69,69	0
26	ZN	G	303	1/1	0.21	-	139,139,139,139	0
24	MG	A	2254	1/1	0.34	-	110,110,110,110	0
24	MG	D	123	1/1	0.09	-	81,81,81,81	0
24	MG	A	1705	1/1	0.40	-	104,104,104,104	0
24	MG	D	118	1/1	0.08	-	80,80,80,80	0
24	MG	A	1668	1/1	0.69	-	96,96,96,96	0
24	MG	A	2080	1/1	0.20	-	78,78,78,78	0
24	MG	A	1833	1/1	0.10	-	128,128,128,128	0
24	MG	A	2266	1/1	0.16	-	111,111,111,111	0
24	MG	A	1875	1/1	0.23	-	84,84,84,84	0
24	MG	A	2057	1/1	0.33	-	89,89,89,89	0
24	MG	A	1869	1/1	0.33	-	114,114,114,114	0
24	MG	A	2053	1/1	0.94	-	86,86,86,86	0
24	MG	A	2117	1/1	0.42	-	64,64,64,64	0
24	MG	A	1993	1/1	0.08	-	68,68,68,68	0
24	MG	A	1955	1/1	0.75	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1650	1/1	0.10	-	61,61,61,61	0
24	MG	A	1680	1/1	0.51	-	72,72,72,72	0
24	MG	A	2152	1/1	0.17	-	90,90,90,90	0
24	MG	A	1734	1/1	0.10	-	82,82,82,82	0
24	MG	A	2187	1/1	0.10	-	87,87,87,87	0
24	MG	A	1938	1/1	0.15	-	88,88,88,88	0
24	MG	A	2138	1/1	0.24	-	104,104,104,104	0
24	MG	A	1700	1/1	0.05	-	127,127,127,127	0
24	MG	C	102	1/1	0.12	-	75,75,75,75	0
24	MG	A	2144	1/1	0.15	-	98,98,98,98	0
24	MG	A	2065	1/1	0.20	-	67,67,67,67	0
24	MG	A	2110	1/1	0.17	-	128,128,128,128	0
24	MG	A	1895	1/1	0.12	-	108,108,108,108	0
24	MG	A	2020	1/1	0.09	-	72,72,72,72	0
24	MG	A	2105	1/1	0.21	-	75,75,75,75	0
24	MG	A	1682	1/1	0.36	-	79,79,79,79	0
24	MG	A	2126	1/1	0.36	-	85,85,85,85	0
24	MG	A	2067	1/1	0.20	-	79,79,79,79	0
24	MG	A	2030	1/1	0.45	-	89,89,89,89	0
24	MG	A	1963	1/1	0.15	-	91,91,91,91	0
24	MG	A	1621	1/1	0.30	-	94,94,94,94	0
24	MG	A	1986	1/1	0.22	-	52,52,52,52	0
24	MG	A	1679	1/1	0.19	-	92,92,92,92	0
24	MG	A	1760	1/1	0.17	-	66,66,66,66	0
24	MG	A	2119	1/1	0.65	-	63,63,63,63	0
24	MG	A	2210	1/1	0.69	-	76,76,76,76	0
24	MG	A	1916	1/1	0.17	-	80,80,80,80	0
24	MG	C	138	1/1	0.55	-	90,90,90,90	0
24	MG	A	1829	1/1	0.48	-	82,82,82,82	0
24	MG	A	2237	1/1	0.22	-	92,92,92,92	0
24	MG	A	1814	1/1	0.17	-	102,102,102,102	0
24	MG	A	1744	1/1	0.16	-	93,93,93,93	0
24	MG	A	1628	1/1	0.34	-	113,113,113,113	0
24	MG	A	2056	1/1	0.13	-	71,71,71,71	0
24	MG	A	1798	1/1	0.19	-	135,135,135,135	0
24	MG	A	1996	1/1	0.07	-	70,70,70,70	0
24	MG	A	2280	1/1	0.24	-	92,92,92,92	0
24	MG	A	2074	1/1	0.27	-	97,97,97,97	0
24	MG	A	2083	1/1	0.10	-	97,97,97,97	0
24	MG	A	2166	1/1	0.14	-	78,78,78,78	0
24	MG	A	2043	1/1	0.14	-	64,64,64,64	0
24	MG	C	145	1/1	0.37	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	MG	A	2114	1/1	0.15	-	99,99,99,99	0
24	MG	A	2130	1/1	0.17	-	91,91,91,91	0
24	MG	A	1887	1/1	0.40	-	79,79,79,79	0
24	MG	A	1756	1/1	0.13	-	107,107,107,107	0
24	MG	A	1933	1/1	1.26	-	106,106,106,106	0
24	MG	C	110	1/1	0.15	-	54,54,54,54	0
24	MG	A	2112	1/1	0.25	-	84,84,84,84	0
24	MG	A	2174	1/1	0.12	-	123,123,123,123	0
24	MG	A	1850	1/1	0.11	-	78,78,78,78	0
24	MG	A	2026	1/1	0.14	-	64,64,64,64	0
24	MG	A	2188	1/1	0.17	-	98,98,98,98	0
24	MG	A	2275	1/1	0.07	-	89,89,89,89	0
24	MG	D	106	1/1	0.14	-	73,73,73,73	0
24	MG	A	1757	1/1	0.27	-	97,97,97,97	0
24	MG	C	133	1/1	0.10	-	79,79,79,79	0
24	MG	C	146	1/1	0.36	-	111,111,111,111	0
24	MG	A	2154	1/1	0.28	-	105,105,105,105	0
24	MG	A	1639	1/1	0.18	-	90,90,90,90	0
24	MG	D	110	1/1	0.15	-	64,64,64,64	0
24	MG	A	2205	1/1	0.18	-	63,63,63,63	0
24	MG	A	2153	1/1	0.49	-	80,80,80,80	0
24	MG	A	2224	1/1	0.18	-	86,86,86,86	0
24	MG	A	1806	1/1	0.33	-	110,110,110,110	0
24	MG	A	1663	1/1	0.14	-	97,97,97,97	0
24	MG	A	2273	1/1	0.10	-	120,120,120,120	0
24	MG	A	1805	1/1	0.30	-	97,97,97,97	0
24	MG	A	1665	1/1	0.88	-	95,95,95,95	0
24	MG	A	1846	1/1	0.42	-	108,108,108,108	0
24	MG	A	1726	1/1	1.14	-	97,97,97,97	0
24	MG	A	1880	1/1	0.14	-	67,67,67,67	0
24	MG	A	2271	1/1	0.16	-	101,101,101,101	0
24	MG	X	101	1/1	0.20	-	101,101,101,101	0
24	MG	A	1775	1/1	0.20	-	110,110,110,110	0
24	MG	A	1927	1/1	0.17	-	86,86,86,86	0
24	MG	C	109	1/1	0.26	-	50,50,50,50	0
24	MG	D	101	1/1	0.19	-	98,98,98,98	0
24	MG	A	1671	1/1	0.14	-	116,116,116,116	0
24	MG	A	1799	1/1	0.38	-	89,89,89,89	0
24	MG	A	1910	1/1	0.30	-	109,109,109,109	0
24	MG	A	1678	1/1	0.65	-	64,64,64,64	0
24	MG	A	1768	1/1	0.15	-	93,93,93,93	0
24	MG	A	2013	1/1	0.53	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2024	1/1	0.07	-	52,52,52,52	0
24	MG	A	2229	1/1	1.58	-	76,76,76,76	0
24	MG	A	1981	1/1	0.34	-	66,66,66,66	0
24	MG	A	2192	1/1	1.10	-	96,96,96,96	0
24	MG	A	1824	1/1	0.12	-	82,82,82,82	0
24	MG	A	2286	1/1	0.42	-	87,87,87,87	0
24	MG	A	1626	1/1	0.54	-	87,87,87,87	0
24	MG	A	1738	1/1	0.19	-	70,70,70,70	0
24	MG	A	2096	1/1	0.20	-	88,88,88,88	0
24	MG	A	1903	1/1	2.30	-	121,121,121,121	0
24	MG	A	2045	1/1	0.10	-	54,54,54,54	0
24	MG	A	2044	1/1	0.10	-	74,74,74,74	0
24	MG	A	1919	1/1	0.46	-	89,89,89,89	0
24	MG	A	1776	1/1	0.24	-	89,89,89,89	0
24	MG	A	2208	1/1	0.23	-	78,78,78,78	0
24	MG	C	140	1/1	0.17	-	125,125,125,125	0
24	MG	A	2281	1/1	0.31	-	90,90,90,90	0
24	MG	A	1771	1/1	0.21	-	84,84,84,84	0
24	MG	A	1623	1/1	0.10	-	86,86,86,86	0
24	MG	A	1934	1/1	0.17	-	128,128,128,128	0
24	MG	A	1890	1/1	0.44	-	52,52,52,52	0
24	MG	A	2108	1/1	0.30	-	72,72,72,72	0
24	MG	A	2244	1/1	0.15	-	86,86,86,86	0
24	MG	A	2143	1/1	0.42	-	75,75,75,75	0
24	MG	A	1941	1/1	0.09	-	98,98,98,98	0
24	MG	A	1864	1/1	0.53	-	60,60,60,60	0
24	MG	A	2128	1/1	0.58	-	81,81,81,81	0
24	MG	A	1870	1/1	0.50	-	60,60,60,60	0
24	MG	A	1754	1/1	0.46	-	68,68,68,68	0
24	MG	A	2175	1/1	0.29	-	113,113,113,113	0
24	MG	A	1838	1/1	0.10	-	117,117,117,117	0
24	MG	A	2215	1/1	0.13	-	103,103,103,103	0
24	MG	A	1638	1/1	0.09	-	75,75,75,75	0
24	MG	C	125	1/1	0.56	-	69,69,69,69	0
24	MG	A	2167	1/1	0.40	-	85,85,85,85	0
24	MG	A	1781	1/1	0.12	-	91,91,91,91	0
24	MG	A	1720	1/1	0.11	-	78,78,78,78	0
24	MG	A	1858	1/1	0.13	-	83,83,83,83	0
24	MG	A	1977	1/1	0.08	-	58,58,58,58	0
24	MG	A	2149	1/1	0.15	-	90,90,90,90	0
24	MG	A	1667	1/1	0.25	-	99,99,99,99	0
24	MG	A	2002	1/1	0.20	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1729	1/1	0.12	-	87,87,87,87	0
24	MG	A	1686	1/1	0.44	-	85,85,85,85	0
24	MG	A	2219	1/1	0.41	-	103,103,103,103	0
24	MG	A	2240	1/1	0.32	-	81,81,81,81	0
24	MG	A	1923	1/1	0.28	-	74,74,74,74	0
24	MG	A	2072	1/1	0.10	-	78,78,78,78	0
24	MG	A	1924	1/1	0.20	-	80,80,80,80	0
24	MG	A	2283	1/1	0.22	-	105,105,105,105	0
24	MG	A	2021	1/1	0.17	-	57,57,57,57	0
24	MG	A	1630	1/1	0.31	-	102,102,102,102	0
24	MG	A	2246	1/1	0.65	-	83,83,83,83	0
24	MG	A	2145	1/1	0.15	-	88,88,88,88	0
24	MG	A	1717	1/1	0.06	-	61,61,61,61	0
24	MG	A	2239	1/1	0.14	-	86,86,86,86	0
24	MG	A	2184	1/1	0.15	-	89,89,89,89	0
24	MG	A	2001	1/1	0.51	-	82,82,82,82	0
24	MG	A	1767	1/1	0.73	-	91,91,91,91	0
24	MG	A	1652	1/1	0.31	-	76,76,76,76	0
24	MG	A	1611	1/1	0.15	-	81,81,81,81	0
24	MG	A	1624	1/1	0.65	-	100,100,100,100	0
24	MG	A	1932	1/1	0.17	-	91,91,91,91	0
24	MG	A	2235	1/1	0.49	-	90,90,90,90	0
24	MG	A	2058	1/1	0.12	-	76,76,76,76	0
24	MG	C	135	1/1	0.27	-	105,105,105,105	0
24	MG	A	2247	1/1	0.27	-	114,114,114,114	0
24	MG	A	1770	1/1	0.75	-	96,96,96,96	0
24	MG	A	1852	1/1	0.14	-	65,65,65,65	0
24	MG	A	1644	1/1	0.16	-	92,92,92,92	0
24	MG	A	1647	1/1	0.23	-	115,115,115,115	0
24	MG	A	2032	1/1	0.56	-	70,70,70,70	0
24	MG	A	2101	1/1	1.23	-	102,102,102,102	0
24	MG	A	1848	1/1	0.11	-	79,79,79,79	0
24	MG	A	1604	1/1	0.33	-	77,77,77,77	0
24	MG	A	1601	1/1	0.60	-	77,77,77,77	0
24	MG	A	2268	1/1	0.23	-	85,85,85,85	0
24	MG	A	1961	1/1	0.27	-	81,81,81,81	0
24	MG	A	1803	1/1	0.21	-	79,79,79,79	0
24	MG	A	2051	1/1	0.16	-	65,65,65,65	0
24	MG	A	2115	1/1	0.76	-	83,83,83,83	0
24	MG	A	2236	1/1	0.38	-	84,84,84,84	0
24	MG	D	105	1/1	0.22	-	79,79,79,79	0
24	MG	A	1840	1/1	0.10	-	100,100,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.