wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 02:59 PM EDT

PDB ID	:	6NY6 / pdb_00006ny6
Title	:	Structure of dimeric Escherichia coli toxin YoeB bound to the Thermus thermophilus 30S ribosome
Authors	:	Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-02-11
Resolution	:	3.74 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 (i) 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 (i)) were used in the production of this report:

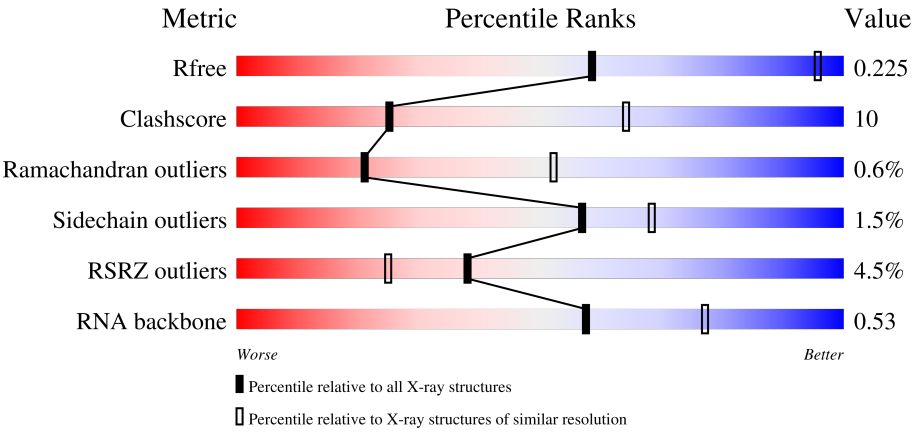
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 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.



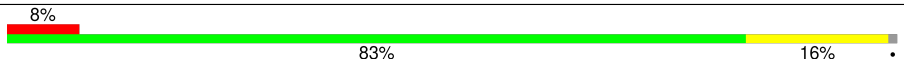
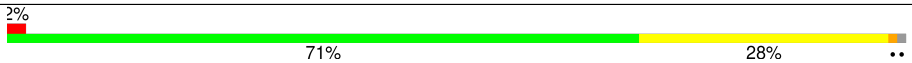
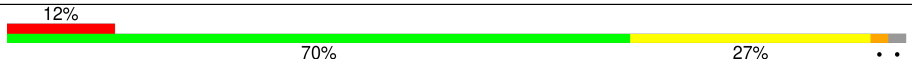
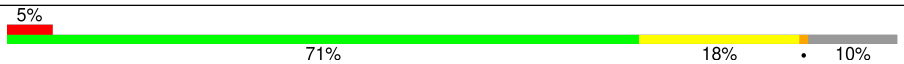
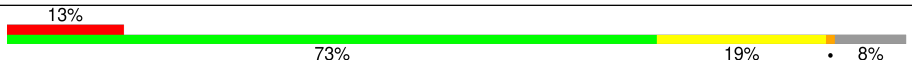
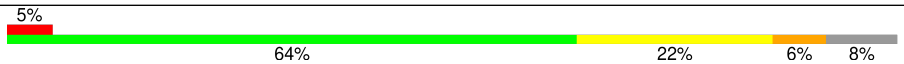
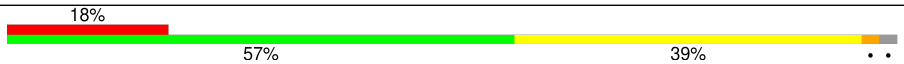
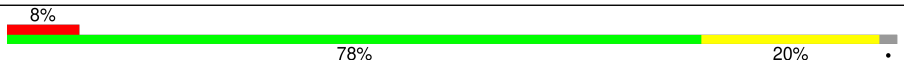
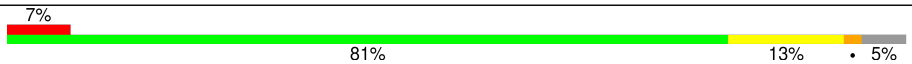
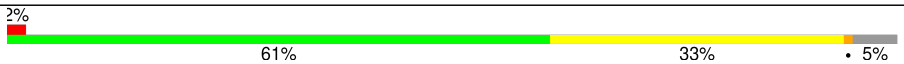
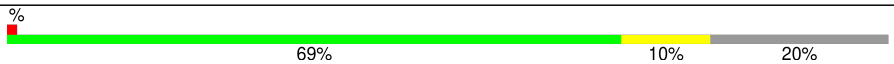
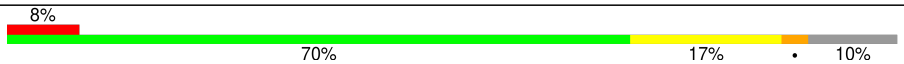
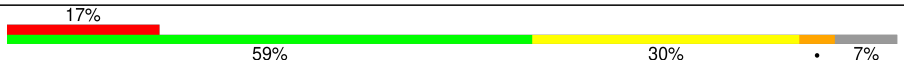
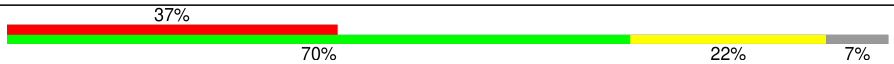
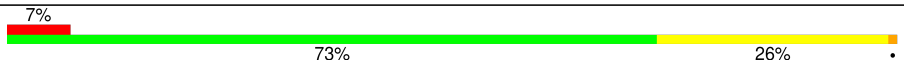
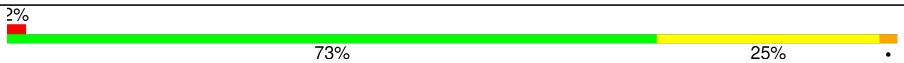
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1234 (3.88-3.60)
Clashscore	190562	1274 (3.88-3.60)
Ramachandran outliers	187476	1226 (3.88-3.60)
Sidechain outliers	187428	1221 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)
RNA backbone	3983	1012 (4.40-3.08)

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 <=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	1523	51% 40% 9%
2	B	256	3% 65% 26% 8%
3	C	239	3% 68% 17% 14%
4	D	209	3% 69% 28%

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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	132	
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	Y	84	
22	Z	84	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1604	-	-	-	X
23	MG	A	1612	-	-	-	X
23	MG	A	1615	-	-	-	X
23	MG	A	1622	-	-	-	X
23	MG	A	1625	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1627	-	-	-	X
23	MG	A	1692	-	-	-	X
23	MG	A	1693	-	-	-	X
23	MG	A	1707	-	-	-	X
23	MG	A	1708	-	-	-	X
23	MG	A	1710	-	-	-	X
23	MG	A	1712	-	-	-	X
23	MG	A	1741	-	-	-	X
23	MG	A	1752	-	-	-	X
23	MG	A	1778	-	-	-	X
24	SF4	D	301	-	-	X	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 53243 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
			Total	C	N	O	P			
1	A	1513	32514	14472	6016	10513	1513	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1915	1223	343	344	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	205	1605	1011	313	280	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1155	729	218	204	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	100	837	528	154	152	3	0	0	0

- 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	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	126	Total	C	N	O	0	0	0
			998	633	193	172			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	96	Total	C	N	O	S	0	0	0
			777	487	153	136	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 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total 705	C 446	N 140	O 118	S 1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	84	Total 674	C 430	N 126	O 116	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total 763	C 470	N 162	O 129	S 2	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total 217	C 134	N 52	O 31	0	0	0

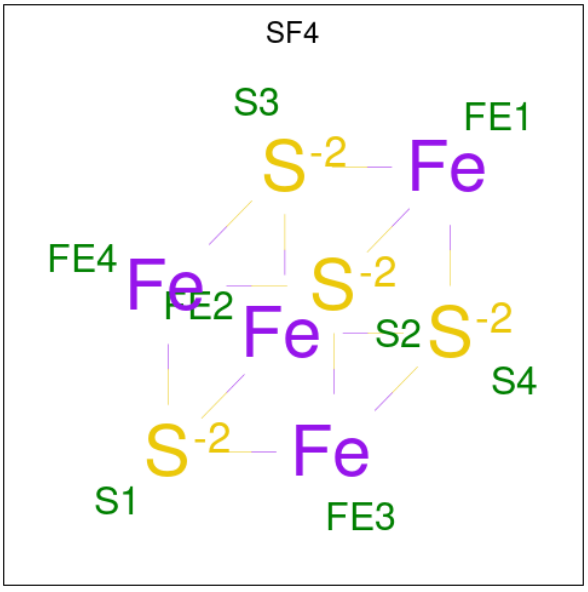
- Molecule 22 is a protein called Toxin YoeB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	84	Total 722	C 464	N 126	O 130	S 2	0	0	0
22	Z	84	Total 723	C 464	N 126	O 131	S 2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	182	Total 182	Mg 182	0	0
23	B	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	D	1	Total 8	Fe 4	S 4	0	0

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

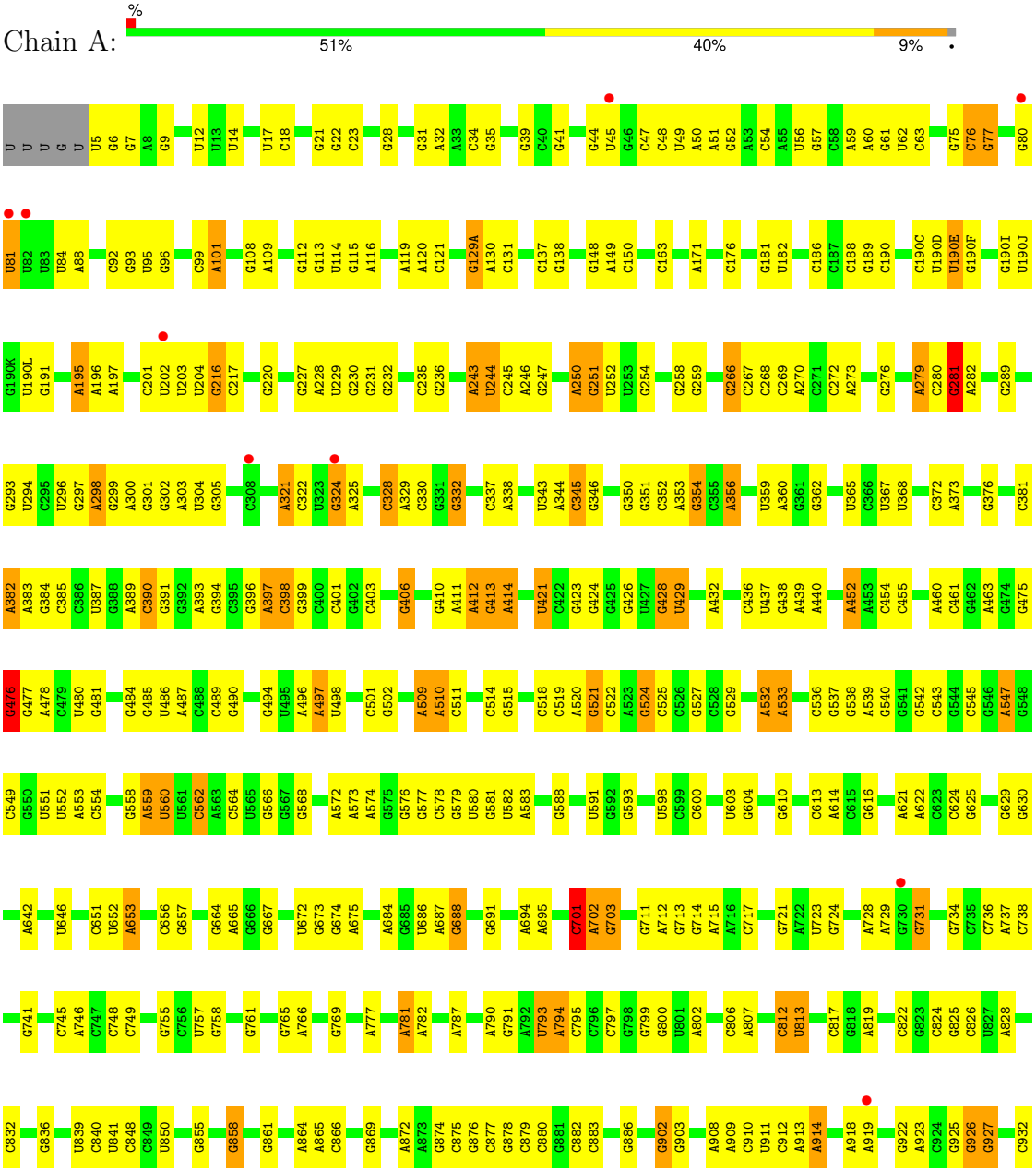
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	N	1	Total Zn 1 1	0	0

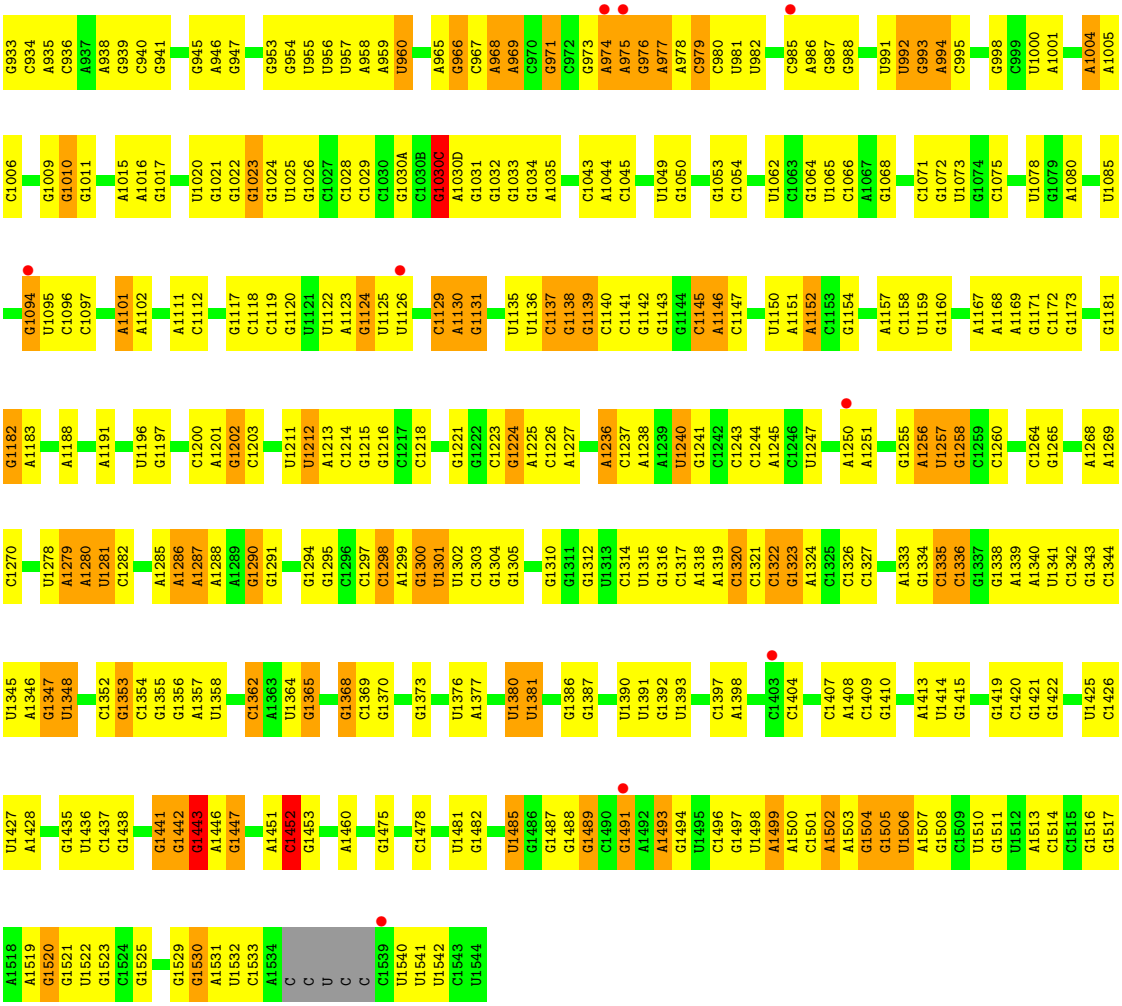
3 Residue-property plots (i)

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

Chain A:

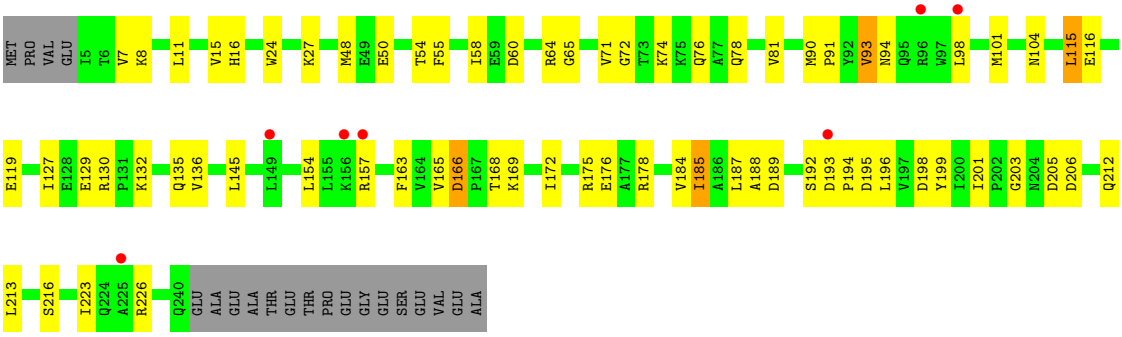




• Molecule 2: 30S ribosomal protein S2

Chain B:

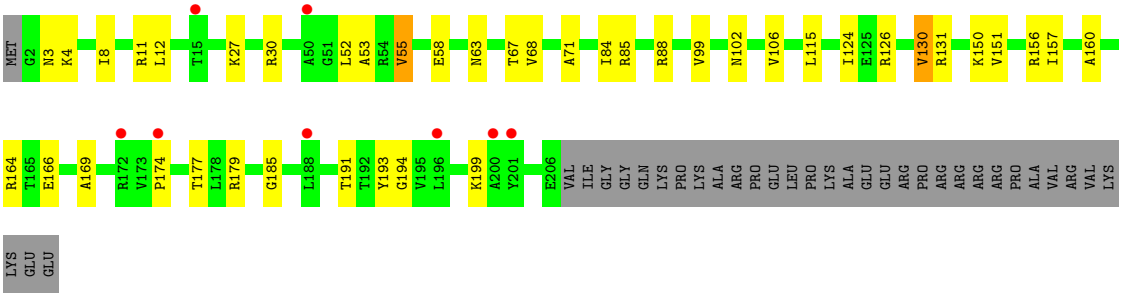




• Molecule 3: 30S ribosomal protein S3

Chain C:

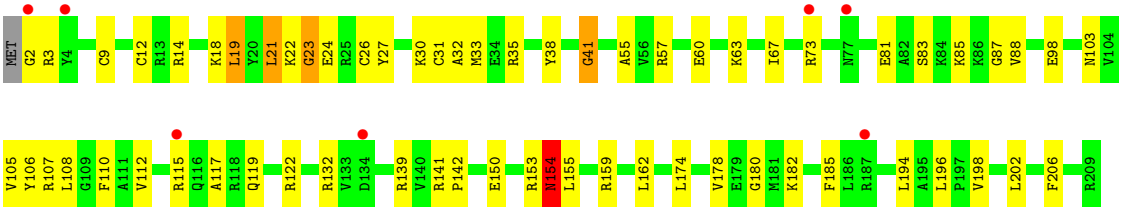




• Molecule 4: 30S ribosomal protein S4

Chain D:

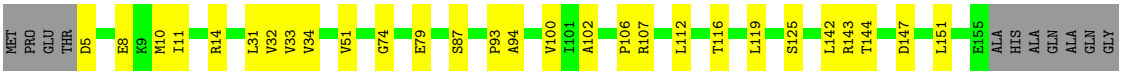




• Molecule 5: 30S ribosomal protein S5

Chain E:

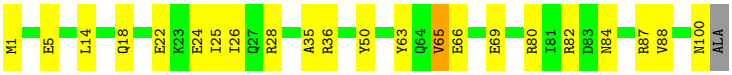




• Molecule 6: 30S ribosomal protein S6

Chain F:

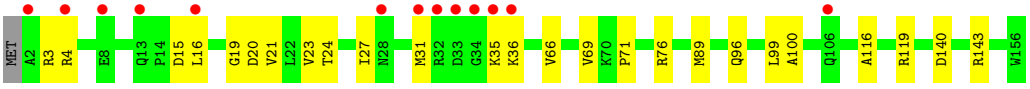




• Molecule 7: 30S ribosomal protein S7

Chain G:

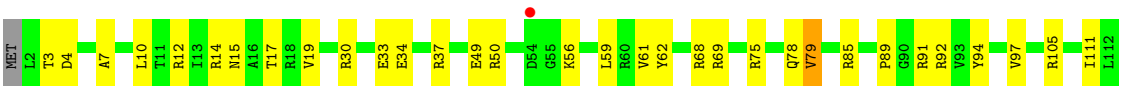


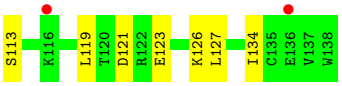


• Molecule 8: 30S ribosomal protein S8

Chain H:

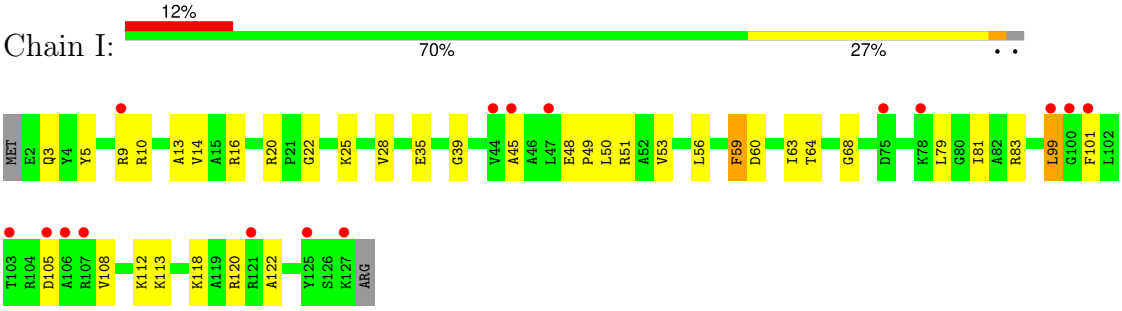






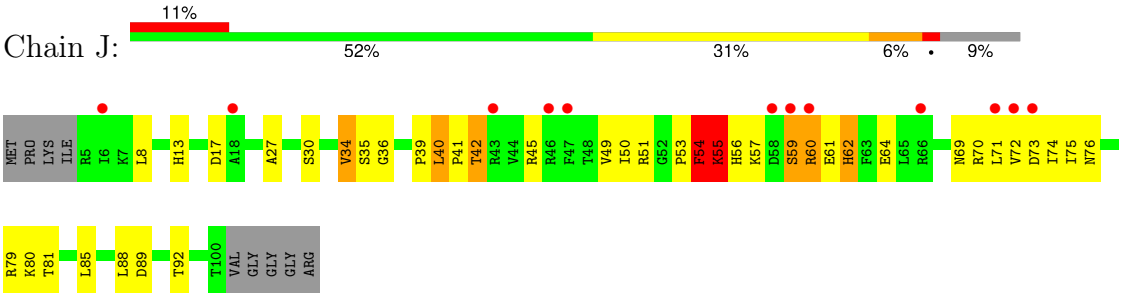
• Molecule 9: 30S ribosomal protein S9

Chain I:



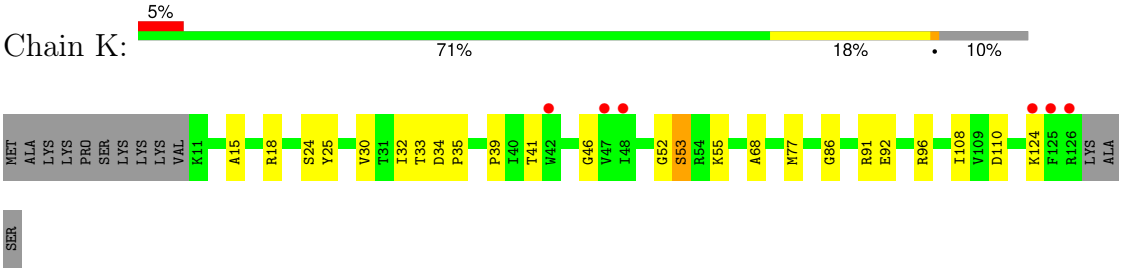
• Molecule 10: 30S ribosomal protein S10

Chain J:



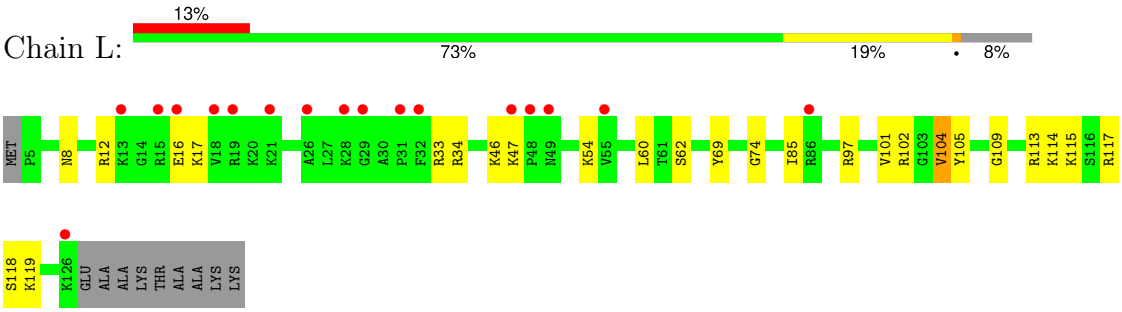
• Molecule 11: 30S ribosomal protein S11

Chain K:



• Molecule 12: 30S ribosomal protein S12

Chain L:



• Molecule 13: 30S ribosomal protein S13

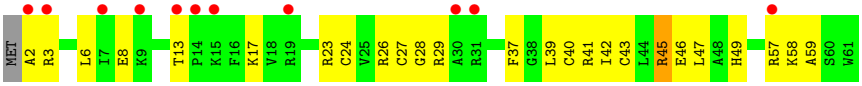
Chain M:



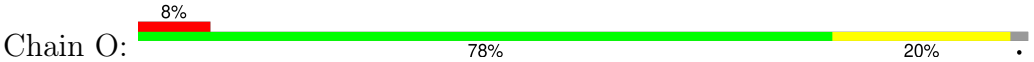


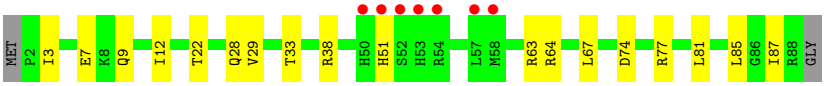
• Molecule 14: 30S ribosomal protein S14 type Z



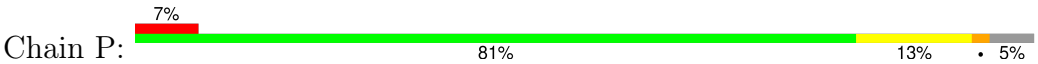


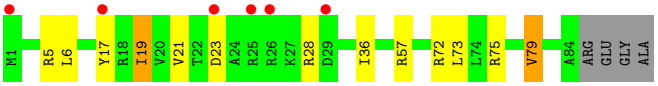
• Molecule 15: 30S ribosomal protein S15





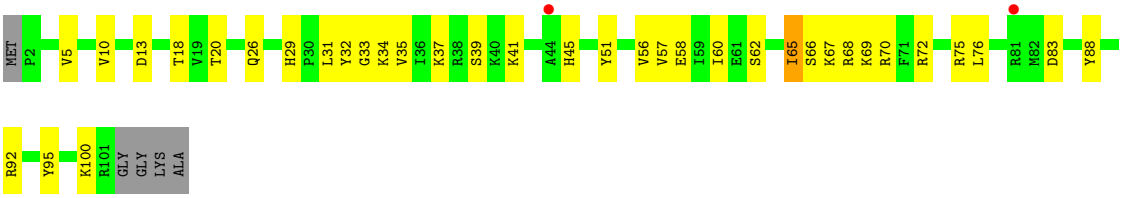
• Molecule 16: 30S ribosomal protein S16





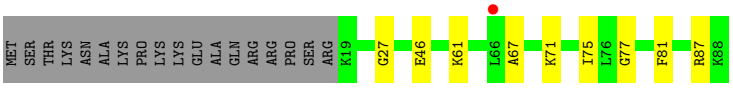
• Molecule 17: 30S ribosomal protein S17





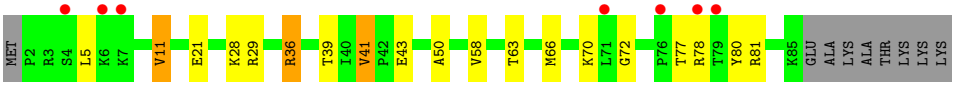
• Molecule 18: 30S ribosomal protein S18





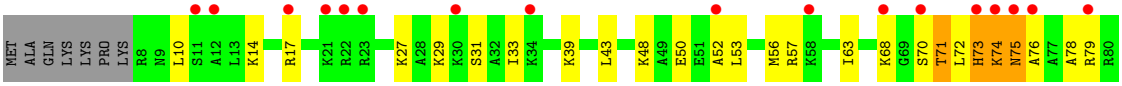
• Molecule 19: 30S ribosomal protein S19

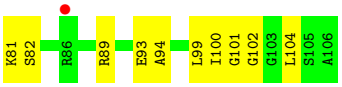




• Molecule 20: 30S ribosomal protein S20

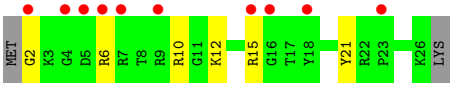






• Molecule 21: 30S ribosomal protein Thx





• Molecule 22: Toxin YoeB





• Molecule 22: Toxin YoeB





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.71Å 401.71Å 175.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 3.74 49.83 – 3.74	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.83-3.74) 90.5 (49.83-3.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.77Å)	Xtriage
Refinement program	PHENIX dev_3406	Depositor
R, R_{free}	0.206 , 0.224 0.207 , 0.225	Depositor DCC
R_{free} test set	7170 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	142.5	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 110.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53243	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SF4, ZN, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	5/36349 (0.0%)	0.49	10/56729 (0.0%)
2	B	0.48	1/1950 (0.1%)	1.03	9/2630 (0.3%)
3	C	0.35	0/1629	0.87	4/2195 (0.2%)
4	D	0.48	0/1733	0.93	8/2318 (0.3%)
5	E	0.47	0/1171	0.86	1/1576 (0.1%)
6	F	0.35	0/850	0.75	1/1147 (0.1%)
7	G	0.34	0/1276	0.83	0/1709
8	H	0.54	0/1128	0.84	4/1517 (0.3%)
9	I	0.34	0/1017	1.01	7/1365 (0.5%)
10	J	0.41	0/790	1.47	15/1063 (1.4%)
11	K	0.40	0/879	0.77	1/1187 (0.1%)
12	L	0.47	0/972	1.04	4/1301 (0.3%)
13	M	0.40	0/938	1.05	9/1258 (0.7%)
14	N	0.42	0/501	1.03	3/664 (0.5%)
15	O	0.43	0/740	0.72	0/987
16	P	0.48	0/721	0.94	3/970 (0.3%)
17	Q	0.44	0/847	0.87	3/1131 (0.3%)
18	R	0.41	0/579	0.94	3/768 (0.4%)
19	S	0.34	0/689	1.00	4/926 (0.4%)
20	T	0.38	0/765	1.08	6/1007 (0.6%)
21	U	0.32	0/221	0.85	1/288 (0.3%)
22	Y	0.30	0/742	0.89	2/1002 (0.2%)
22	Z	0.29	0/743	1.01	6/1002 (0.6%)
All	All	0.40	6/57230 (0.0%)	0.68	104/84740 (0.1%)

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
1	A	0	1
10	J	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1443	G	C6-O6	13.64	1.51	1.24
1	A	701	C	C1'-N1	12.98	1.67	1.47
1	A	1030(C)	G	C1'-N9	10.58	1.63	1.48
1	A	476	G	C1'-N9	-9.82	1.33	1.48
1	A	1443	G	C6-N1	7.97	1.55	1.39

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	G	N9-C1'-C2'	-18.79	83.81	112.00
10	J	54	PHE	CA-C-N	17.52	155.00	121.54
10	J	54	PHE	C-N-CA	17.52	155.00	121.54
22	Z	60	ILE	N-CA-C	-10.06	103.67	112.12
13	M	7	VAL	N-CA-C	-9.15	103.77	112.83

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	476	G	Sidechain
10	J	54	PHE	Peptide

5.2 Too-close contacts (i)

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	32514	0	16412	537	25
2	B	1915	0	1969	41	1
3	C	1605	0	1668	26	0
4	D	1703	0	1765	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1155	0	1213	15	0
6	F	837	0	852	15	0
7	G	1257	0	1296	18	0
8	H	1108	0	1165	26	0
9	I	998	0	1024	26	0
10	J	777	0	815	30	1
11	K	864	0	881	15	0
12	L	956	0	1046	31	0
13	M	928	0	987	21	0
14	N	492	0	530	33	0
15	O	729	0	768	15	0
16	P	705	0	725	7	0
17	Q	834	0	904	27	0
18	R	574	0	644	6	0
19	S	674	0	699	13	0
20	T	763	0	861	27	0
21	U	217	0	234	4	0
22	Y	722	0	713	17	0
22	Z	723	0	713	12	0
23	A	182	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
24	D	8	0	0	7	0
25	N	1	0	0	0	0
All	All	53243	0	37884	851	27

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 10.

The worst 5 of 851 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)
14:N:24:CYS:HB2	14:N:40:CYS:SG	1.79	1.21
14:N:24:CYS:CB	14:N:40:CYS:SG	2.35	1.15
1:A:129(A):G:N1	1:A:190(C):C:O2	1.85	1.08
12:L:8:ASN:CG	17:Q:34:LYS:HZ3	1.64	1.04
12:L:8:ASN:CG	17:Q:34:LYS:NZ	2.16	1.02

The worst 5 of 27 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:84:U:N3	1:A:1542:U:O4[3_545]	1.57	0.63
1:A:84:U:O2	1:A:1542:U:N3[3_545]	1.62	0.58
1:A:703:G:N1	1:A:1452:C:C4[4_554]	1.64	0.56
1:A:703:G:N1	1:A:1452:C:C5[4_554]	1.67	0.53
1:A:703:G:C6	1:A:1452:C:N3[4_554]	1.75	0.45

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	204 (87%)	30 (13%)	0	100	100
3	C	203/239 (85%)	176 (87%)	26 (13%)	1 (0%)	24	56
4	D	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	56
5	E	149/162 (92%)	143 (96%)	6 (4%)	0	100	100
6	F	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
8	H	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
9	I	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	J	94/105 (90%)	75 (80%)	15 (16%)	4 (4%)	2	19
11	K	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	L	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	16	47
13	M	114/126 (90%)	102 (90%)	11 (10%)	1 (1%)	14	45
14	N	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	34
15	O	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	P	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	S	82/93 (88%)	70 (85%)	12 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	T	97/106 (92%)	85 (88%)	9 (9%)	3 (3%)	3 26
21	U	23/27 (85%)	21 (91%)	2 (9%)	0	100 100
22	Y	82/84 (98%)	72 (88%)	10 (12%)	0	100 100
22	Z	82/84 (98%)	76 (93%)	4 (5%)	2 (2%)	4 29
All	All	2501/2706 (92%)	2281 (91%)	206 (8%)	14 (1%)	21 52

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
20	T	74	LYS
20	T	75	ASN
3	C	12	LEU
10	J	56	HIS

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	204/220 (93%)	198 (97%)	6 (3%)	37 57
3	C	159/188 (85%)	156 (98%)	3 (2%)	50 65
4	D	180/181 (99%)	174 (97%)	6 (3%)	33 55
5	E	116/123 (94%)	115 (99%)	1 (1%)	70 74
6	F	90/90 (100%)	90 (100%)	0	100 100
7	G	126/127 (99%)	125 (99%)	1 (1%)	73 76
8	H	118/119 (99%)	117 (99%)	1 (1%)	73 76
9	I	97/99 (98%)	95 (98%)	2 (2%)	47 64
10	J	86/92 (94%)	86 (100%)	0	100 100
11	K	88/99 (89%)	85 (97%)	3 (3%)	32 55
12	L	103/109 (94%)	102 (99%)	1 (1%)	68 74
13	M	94/101 (93%)	91 (97%)	3 (3%)	34 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	49/50 (98%)	49 (100%)	0	100 100
15	O	79/80 (99%)	79 (100%)	0	100 100
16	P	72/74 (97%)	71 (99%)	1 (1%)	59 70
17	Q	95/97 (98%)	92 (97%)	3 (3%)	34 56
18	R	61/77 (79%)	61 (100%)	0	100 100
19	S	73/80 (91%)	71 (97%)	2 (3%)	39 59
20	T	76/82 (93%)	76 (100%)	0	100 100
21	U	20/22 (91%)	20 (100%)	0	100 100
22	Y	78/78 (100%)	78 (100%)	0	100 100
22	Z	78/78 (100%)	78 (100%)	0	100 100
All	All	2142/2266 (94%)	2109 (98%)	33 (2%)	57 68

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	31	LEU
17	Q	35	VAL
19	S	41	VAL
4	D	33	MET
4	D	22	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	77	ASN
17	Q	93	GLN
22	Y	64	HIS
19	S	57	HIS
9	I	31	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1523 (99%)	281 (18%)	47 (3%)

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1129	C
1	A	1300	G
1	A	1145	C
1	A	1256	A
1	A	1347	G

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	A	1541	1	18,21,22	1.28	1 (5%)	21,30,33	1.84	4 (19%)
1	PSU	A	1540	1	18,21,22	1.16	1 (5%)	21,30,33	1.89	5 (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
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1541	PSU	C6-C5	4.43	1.40	1.35
1	A	1540	PSU	C6-C5	3.84	1.39	1.35

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	C4-N3-C2	-4.75	119.83	126.37
1	A	1541	PSU	C4-N3-C2	-4.69	119.91	126.37
1	A	1540	PSU	N1-C2-N3	4.62	120.04	115.17
1	A	1541	PSU	N1-C2-N3	4.55	119.97	115.17
1	A	1540	PSU	O2-C2-N1	-2.75	119.95	122.79

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1541	PSU	C2'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 186 ligands modelled in this entry, 185 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	$\#\|Z\| > 2$
24	SF4	D	301	4	0,12,12	-	-	-		

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
24	SF4	D	301	4	-	-	0/6/5/5

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.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	301	SF4	7	0

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, 95^{th} 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	1511/1523 (99%)	-0.10	18 (1%) 76 51	90, 147, 260, 421	0
2	B	236/256 (92%)	0.31	7 (2%) 52 33	118, 180, 289, 354	0
3	C	205/239 (85%)	0.13	8 (3%) 43 28	151, 217, 273, 325	0
4	D	208/209 (99%)	0.21	7 (3%) 48 31	117, 162, 211, 236	0
5	E	151/162 (93%)	0.04	0 100 100	99, 137, 180, 240	0
6	F	100/101 (99%)	-0.21	0 100 100	133, 182, 222, 246	0
7	G	155/156 (99%)	0.28	13 (8%) 17 14	142, 199, 246, 274	0
8	H	137/138 (99%)	0.16	3 (2%) 62 40	87, 124, 161, 190	0
9	I	126/128 (98%)	0.65	16 (12%) 8 10	139, 212, 286, 326	0
10	J	96/105 (91%)	0.73	12 (12%) 8 10	165, 256, 318, 339	0
11	K	116/129 (89%)	0.36	6 (5%) 33 22	117, 159, 224, 272	0
12	L	122/132 (92%)	0.64	17 (13%) 6 8	100, 155, 209, 293	0
13	M	116/126 (92%)	0.36	6 (5%) 33 22	159, 191, 243, 346	0
14	N	60/61 (98%)	1.20	11 (18%) 3 5	180, 207, 257, 273	0
15	O	87/89 (97%)	0.19	7 (8%) 18 15	99, 144, 189, 201	0
16	P	84/88 (95%)	0.50	6 (7%) 22 16	117, 150, 191, 239	0
17	Q	100/105 (95%)	0.27	2 (2%) 65 42	107, 136, 182, 230	0
18	R	70/88 (79%)	0.01	1 (1%) 73 48	118, 156, 207, 220	0
19	S	84/93 (90%)	0.44	7 (8%) 17 14	173, 225, 264, 279	0
20	T	99/106 (93%)	0.96	18 (18%) 3 5	121, 164, 241, 269	0
21	U	25/27 (92%)	1.75	10 (40%) 1 1	179, 222, 254, 262	0
22	Y	84/84 (100%)	0.42	6 (7%) 22 16	184, 252, 296, 327	0
22	Z	84/84 (100%)	0.03	2 (2%) 59 38	262, 313, 356, 402	0
All	All	4056/4229 (95%)	0.18	183 (4%) 38 25	87, 166, 279, 421	0

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	T	73	HIS	8.7
9	I	105	ASP	7.0
22	Y	18	GLU	5.4
22	Z	29	GLU	5.3
7	G	33	ASP	5.2

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, 95^{th} 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	0.84	0.22	192,201,210,210	0
1	PSU	A	1540	20/21	0.90	0.23	260,288,300,318	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, 95^{th} 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
23	MG	A	1677	1/1	-0.10	0.31	180,180,180,180	0
23	MG	A	1615	1/1	0.08	0.40	164,164,164,164	0
23	MG	A	1735	1/1	0.08	0.29	134,134,134,134	0
23	MG	A	1717	1/1	0.15	0.19	153,153,153,153	0
23	MG	A	1779	1/1	0.19	0.30	160,160,160,160	0
23	MG	A	1758	1/1	0.24	0.27	146,146,146,146	0
23	MG	A	1679	1/1	0.24	0.28	156,156,156,156	0
23	MG	A	1778	1/1	0.25	0.46	141,141,141,141	0
23	MG	A	1764	1/1	0.25	0.39	138,138,138,138	0
23	MG	A	1613	1/1	0.28	0.27	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1617	1/1	0.28	0.38	145,145,145,145	0
23	MG	A	1682	1/1	0.30	0.17	182,182,182,182	0
23	MG	A	1776	1/1	0.32	0.28	153,153,153,153	0
23	MG	A	1772	1/1	0.35	0.16	167,167,167,167	0
23	MG	A	1622	1/1	0.35	0.41	133,133,133,133	0
23	MG	A	1755	1/1	0.36	0.20	134,134,134,134	0
23	MG	A	1744	1/1	0.37	0.27	153,153,153,153	0
23	MG	A	1719	1/1	0.37	0.27	173,173,173,173	0
23	MG	A	1602	1/1	0.39	0.39	196,196,196,196	0
23	MG	A	1724	1/1	0.42	0.22	100,100,100,100	0
23	MG	A	1692	1/1	0.42	0.46	171,171,171,171	0
23	MG	A	1708	1/1	0.45	0.46	134,134,134,134	0
23	MG	A	1711	1/1	0.45	0.16	158,158,158,158	0
23	MG	A	1736	1/1	0.46	0.20	179,179,179,179	0
23	MG	A	1672	1/1	0.47	0.38	110,110,110,110	0
23	MG	A	1762	1/1	0.48	0.25	144,144,144,144	0
23	MG	A	1781	1/1	0.48	0.21	156,156,156,156	0
23	MG	A	1705	1/1	0.50	0.30	144,144,144,144	0
23	MG	A	1665	1/1	0.50	0.32	129,129,129,129	0
23	MG	E	201	1/1	0.50	0.25	85,85,85,85	0
23	MG	A	1678	1/1	0.51	0.38	143,143,143,143	0
23	MG	A	1610	1/1	0.52	0.13	143,143,143,143	0
23	MG	A	1673	1/1	0.52	0.14	188,188,188,188	0
23	MG	A	1695	1/1	0.53	0.17	115,115,115,115	0
23	MG	A	1618	1/1	0.55	0.19	169,169,169,169	0
23	MG	A	1757	1/1	0.56	0.13	105,105,105,105	0
23	MG	A	1707	1/1	0.59	0.42	146,146,146,146	0
23	MG	A	1693	1/1	0.59	0.48	128,128,128,128	0
23	MG	A	1770	1/1	0.59	0.23	184,184,184,184	0
23	MG	A	1680	1/1	0.60	0.15	138,138,138,138	0
23	MG	A	1628	1/1	0.60	0.28	132,132,132,132	0
23	MG	A	1729	1/1	0.60	0.21	124,124,124,124	0
23	MG	A	1625	1/1	0.61	0.41	171,171,171,171	0
23	MG	A	1741	1/1	0.61	0.44	136,136,136,136	0
23	MG	A	1604	1/1	0.61	0.92	145,145,145,145	0
23	MG	A	1740	1/1	0.62	0.23	146,146,146,146	0
23	MG	A	1723	1/1	0.63	0.17	157,157,157,157	0
23	MG	A	1634	1/1	0.64	0.39	154,154,154,154	0
23	MG	A	1640	1/1	0.64	0.21	157,157,157,157	0
23	MG	A	1658	1/1	0.64	0.16	185,185,185,185	0
23	MG	A	1620	1/1	0.64	0.36	168,168,168,168	0
23	MG	A	1771	1/1	0.65	0.38	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1612	1/1	0.65	0.69	179,179,179,179	0
23	MG	A	1722	1/1	0.65	0.18	204,204,204,204	0
23	MG	A	1660	1/1	0.65	0.24	100,100,100,100	0
23	MG	A	1712	1/1	0.65	0.47	157,157,157,157	0
23	MG	A	1623	1/1	0.65	0.18	186,186,186,186	0
23	MG	A	1753	1/1	0.65	0.19	115,115,115,115	0
23	MG	A	1759	1/1	0.66	0.18	134,134,134,134	0
23	MG	A	1627	1/1	0.67	0.40	196,196,196,196	0
23	MG	A	1765	1/1	0.67	0.13	101,101,101,101	0
23	MG	A	1601	1/1	0.68	0.15	148,148,148,148	0
23	MG	A	1752	1/1	0.68	0.40	120,120,120,120	0
23	MG	A	1653	1/1	0.68	0.22	115,115,115,115	0
23	MG	A	1761	1/1	0.68	0.29	139,139,139,139	0
23	MG	A	1710	1/1	0.68	0.70	104,104,104,104	0
23	MG	A	1696	1/1	0.69	0.27	157,157,157,157	0
23	MG	A	1732	1/1	0.69	0.37	134,134,134,134	0
23	MG	A	1666	1/1	0.69	0.30	110,110,110,110	0
23	MG	A	1754	1/1	0.69	0.14	150,150,150,150	0
23	MG	A	1648	1/1	0.70	0.18	123,123,123,123	0
23	MG	A	1718	1/1	0.70	0.24	168,168,168,168	0
23	MG	A	1699	1/1	0.70	0.35	163,163,163,163	0
23	MG	A	1767	1/1	0.70	0.22	137,137,137,137	0
23	MG	A	1706	1/1	0.71	0.29	136,136,136,136	0
23	MG	A	1614	1/1	0.71	0.12	84,84,84,84	0
23	MG	A	1716	1/1	0.71	0.13	87,87,87,87	0
23	MG	A	1606	1/1	0.72	0.15	148,148,148,148	0
23	MG	A	1652	1/1	0.72	0.26	146,146,146,146	0
23	MG	A	1734	1/1	0.72	0.27	107,107,107,107	0
23	MG	A	1742	1/1	0.72	0.40	123,123,123,123	0
23	MG	A	1698	1/1	0.72	0.17	95,95,95,95	0
23	MG	A	1688	1/1	0.73	0.25	77,77,77,77	0
23	MG	A	1694	1/1	0.73	0.25	96,96,96,96	0
23	MG	A	1638	1/1	0.73	0.26	133,133,133,133	0
23	MG	A	1731	1/1	0.73	0.23	124,124,124,124	0
23	MG	A	1657	1/1	0.74	0.21	71,71,71,71	0
23	MG	A	1743	1/1	0.74	0.29	165,165,165,165	0
23	MG	A	1683	1/1	0.74	0.12	149,149,149,149	0
23	MG	A	1751	1/1	0.74	0.22	98,98,98,98	0
23	MG	A	1659	1/1	0.75	0.37	154,154,154,154	0
23	MG	A	1637	1/1	0.75	0.36	87,87,87,87	0
23	MG	A	1726	1/1	0.75	0.35	143,143,143,143	0
23	MG	A	1727	1/1	0.75	0.31	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1697	1/1	0.76	0.21	137,137,137,137	0
23	MG	A	1643	1/1	0.77	0.40	84,84,84,84	0
23	MG	A	1691	1/1	0.77	0.24	95,95,95,95	0
23	MG	A	1749	1/1	0.77	0.15	96,96,96,96	0
23	MG	A	1676	1/1	0.77	0.11	188,188,188,188	0
23	MG	A	1649	1/1	0.77	0.27	116,116,116,116	0
23	MG	A	1663	1/1	0.77	0.10	123,123,123,123	0
23	MG	A	1651	1/1	0.78	0.23	118,118,118,118	0
23	MG	A	1721	1/1	0.78	0.21	94,94,94,94	0
23	MG	A	1619	1/1	0.78	0.35	141,141,141,141	0
23	MG	A	1621	1/1	0.78	0.22	73,73,73,73	0
23	MG	A	1730	1/1	0.79	0.12	96,96,96,96	0
23	MG	A	1616	1/1	0.79	0.33	136,136,136,136	0
23	MG	A	1737	1/1	0.79	0.13	87,87,87,87	0
23	MG	A	1756	1/1	0.79	0.23	137,137,137,137	0
23	MG	A	1738	1/1	0.79	0.20	100,100,100,100	0
23	MG	A	1671	1/1	0.80	0.14	185,185,185,185	0
23	MG	A	1611	1/1	0.80	0.35	154,154,154,154	0
23	MG	A	1609	1/1	0.81	0.40	84,84,84,84	0
23	MG	A	1603	1/1	0.81	0.17	159,159,159,159	0
23	MG	A	1654	1/1	0.81	0.15	84,84,84,84	0
23	MG	A	1763	1/1	0.82	0.12	112,112,112,112	0
23	MG	A	1685	1/1	0.82	0.11	73,73,73,73	0
23	MG	A	1745	1/1	0.82	0.33	110,110,110,110	0
23	MG	A	1725	1/1	0.83	0.11	76,76,76,76	0
23	MG	A	1650	1/1	0.83	0.10	81,81,81,81	0
23	MG	A	1607	1/1	0.83	0.40	124,124,124,124	0
23	MG	A	1748	1/1	0.83	0.20	83,83,83,83	0
23	MG	A	1605	1/1	0.84	0.29	205,205,205,205	0
25	ZN	N	101	1/1	0.84	0.12	165,165,165,165	0
23	MG	A	1632	1/1	0.85	0.22	58,58,58,58	0
23	MG	A	1636	1/1	0.85	0.25	61,61,61,61	0
23	MG	A	1768	1/1	0.85	0.21	106,106,106,106	0
23	MG	A	1667	1/1	0.85	0.20	88,88,88,88	0
23	MG	A	1739	1/1	0.85	0.23	118,118,118,118	0
23	MG	A	1664	1/1	0.85	0.19	100,100,100,100	0
23	MG	A	1714	1/1	0.86	0.23	101,101,101,101	0
23	MG	A	1670	1/1	0.86	0.08	95,95,95,95	0
23	MG	A	1780	1/1	0.86	0.35	156,156,156,156	0
23	MG	A	1703	1/1	0.87	0.31	74,74,74,74	0
23	MG	A	1656	1/1	0.87	0.15	84,84,84,84	0
23	MG	A	1760	1/1	0.87	0.14	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1728	1/1	0.87	0.11	140,140,140,140	0
23	MG	A	1629	1/1	0.87	0.17	117,117,117,117	0
23	MG	A	1668	1/1	0.88	0.35	176,176,176,176	0
23	MG	A	1686	1/1	0.89	0.10	101,101,101,101	0
23	MG	A	1662	1/1	0.89	0.31	83,83,83,83	0
23	MG	A	1626	1/1	0.89	0.28	83,83,83,83	0
23	MG	A	1702	1/1	0.89	0.11	90,90,90,90	0
23	MG	A	1681	1/1	0.89	0.28	100,100,100,100	0
23	MG	A	1655	1/1	0.90	0.31	88,88,88,88	0
23	MG	A	1715	1/1	0.90	0.57	106,106,106,106	0
23	MG	A	1774	1/1	0.90	0.40	102,102,102,102	0
23	MG	A	1624	1/1	0.90	0.53	121,121,121,121	0
23	MG	A	1720	1/1	0.90	0.25	86,86,86,86	0
23	MG	A	1777	1/1	0.91	0.18	71,71,71,71	0
23	MG	A	1689	1/1	0.91	0.26	126,126,126,126	0
23	MG	A	1684	1/1	0.91	0.12	80,80,80,80	0
23	MG	A	1675	1/1	0.91	0.12	79,79,79,79	0
23	MG	A	1642	1/1	0.91	0.21	67,67,67,67	0
23	MG	B	301	1/1	0.91	0.07	150,150,150,150	0
23	MG	A	1635	1/1	0.91	0.34	103,103,103,103	0
23	MG	A	1746	1/1	0.91	0.14	171,171,171,171	0
23	MG	A	1630	1/1	0.92	0.22	82,82,82,82	0
23	MG	A	1645	1/1	0.92	0.29	76,76,76,76	0
23	MG	A	1690	1/1	0.92	0.08	82,82,82,82	0
23	MG	A	1674	1/1	0.92	0.09	89,89,89,89	0
23	MG	A	1687	1/1	0.92	0.06	57,57,57,57	0
23	MG	A	1669	1/1	0.93	0.19	165,165,165,165	0
23	MG	A	1641	1/1	0.93	0.14	73,73,73,73	0
23	MG	A	1766	1/1	0.93	0.17	128,128,128,128	0
23	MG	A	1639	1/1	0.93	0.21	125,125,125,125	0
23	MG	A	1704	1/1	0.93	0.18	98,98,98,98	0
23	MG	A	1709	1/1	0.93	0.22	122,122,122,122	0
23	MG	A	1700	1/1	0.94	0.17	94,94,94,94	0
23	MG	A	1631	1/1	0.94	0.12	55,55,55,55	0
23	MG	A	1747	1/1	0.94	0.19	140,140,140,140	0
23	MG	A	1661	1/1	0.94	0.18	75,75,75,75	0
23	MG	A	1644	1/1	0.95	0.23	67,67,67,67	0
23	MG	A	1750	1/1	0.95	0.24	93,93,93,93	0
23	MG	A	1769	1/1	0.95	0.25	99,99,99,99	0
23	MG	A	1608	1/1	0.95	0.26	56,56,56,56	0
23	MG	A	1647	1/1	0.95	0.07	84,84,84,84	0
23	MG	A	1633	1/1	0.95	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1773	1/1	0.95	0.06	82,82,82,82	0
23	MG	A	1701	1/1	0.95	0.13	147,147,147,147	0
23	MG	A	1775	1/1	0.95	0.10	114,114,114,114	0
23	MG	A	1733	1/1	0.96	0.11	156,156,156,156	0
23	MG	A	1782	1/1	0.97	0.07	87,87,87,87	0
23	MG	A	1646	1/1	0.97	0.07	68,68,68,68	0
24	SF4	D	301	8/8	0.98	0.05	114,138,170,287	0
23	MG	A	1713	1/1	0.99	0.02	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.