



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 06:01 PM GMT

PDB ID : 2I2U
Title : Crystal Structure of Ribosome with messenger RNA and the Anticodon stem-loop of P-site tRNA. This file contains the 30s subunit of one 70s ribosome. The entire crystal structure contains two 70s ribosomes and is described in remark 400.
Authors : Berk, V.; Zhang, W.; Pai, R.D.; Cate, J.H.D.
Deposited on : 2006-08-16
Resolution : 3.22 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>

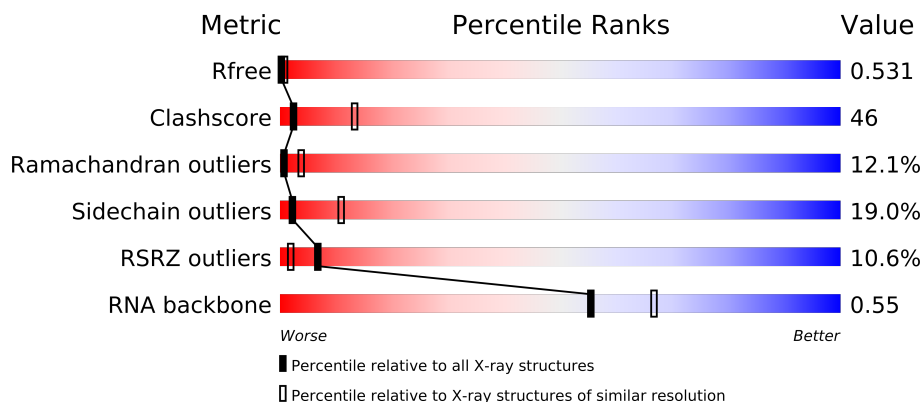
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.22 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	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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	1542	
2	W	17	
3	X	6	
4	B	240	
5	C	232	
6	D	205	
7	E	166	
8	F	135	
9	G	178	
10	H	129	
11	I	129	
12	J	103	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	K	128	
14	L	123	
15	M	117	
16	N	100	
17	O	88	
18	P	82	
19	Q	83	
20	R	74	
21	S	91	
22	T	86	
23	U	70	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
24	MG	A	1557	-	X
24	MG	A	1563	-	X
24	MG	A	1578	-	X
24	MG	A	1585	-	X
24	MG	A	1586	-	X
24	MG	A	1587	-	X
24	MG	A	1591	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52179 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	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a RNA chain called PHE TRNA (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			

- Molecule 3 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 23 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	X	1	Total	Mg	0	0
			1	1		
24	A	56	Total	Mg	0	0
			56	56		
24	N	1	Total	Mg	0	0
			1	1		

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	271	Total	O	0	0
			271	271		
25	I	2	Total	O	0	0
			2	2		
25	L	1	Total	O	0	0
			1	1		
25	N	1	Total	O	0	0
			1	1		
25	P	2	Total	O	0	0
			2	2		
25	T	2	Total	O	0	0
			2	2		
25	U	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

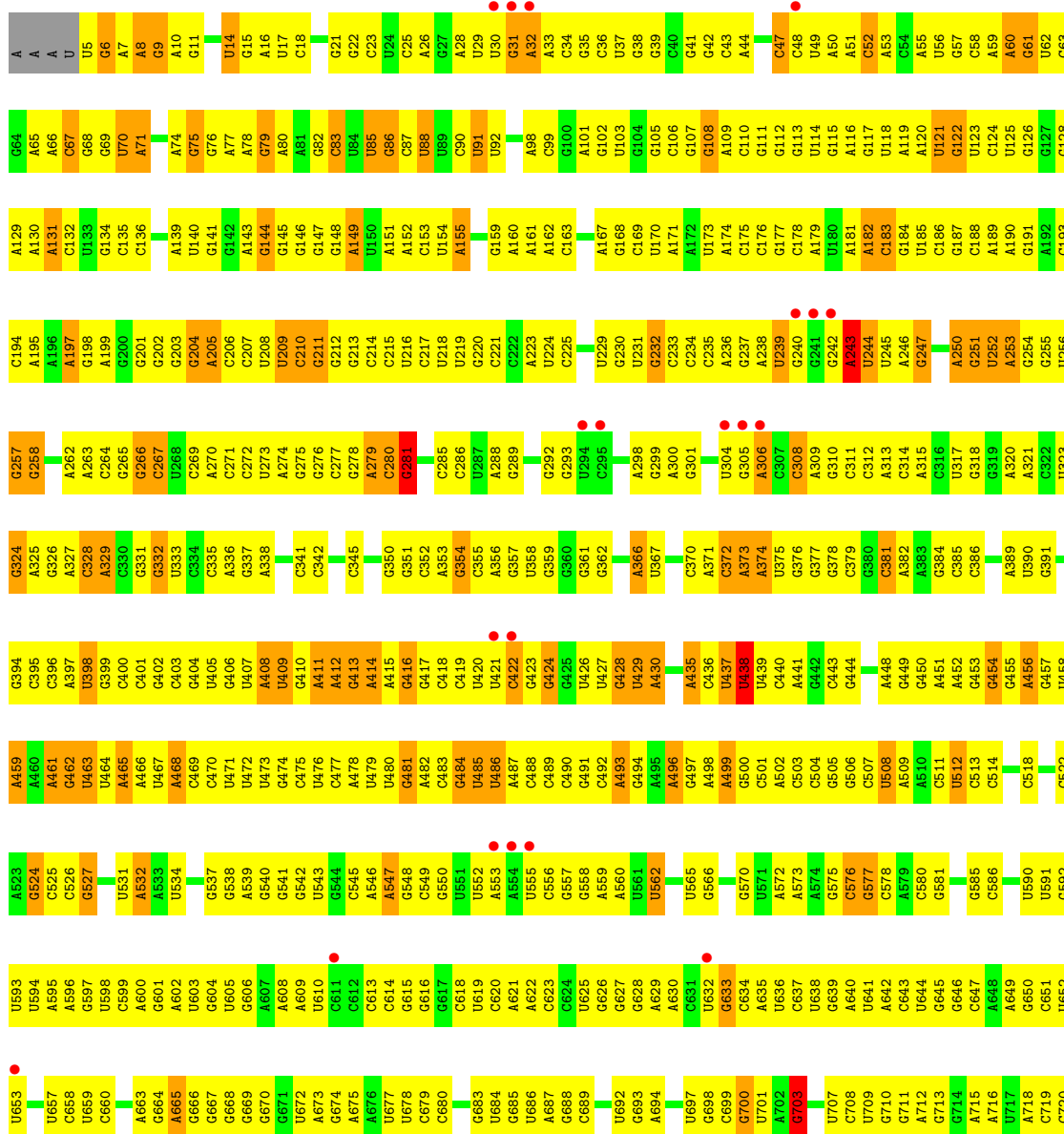
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	5	Total	O	0	0
			5	5		

3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

Chain A: 





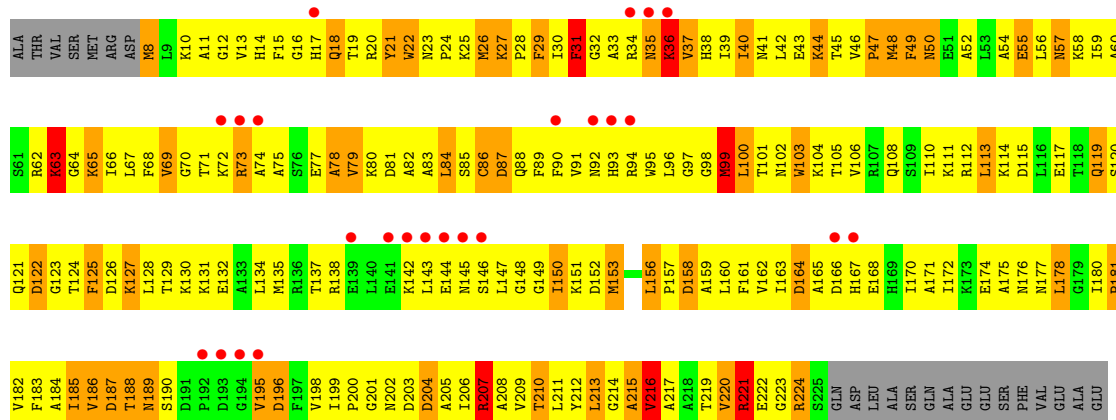
- Molecule 3: MRNA

Chain X:



- Molecule 4: 30S ribosomal protein S2

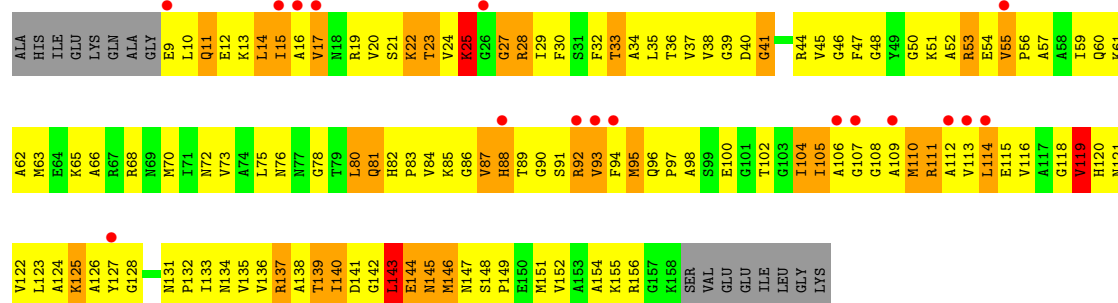
Chain B:





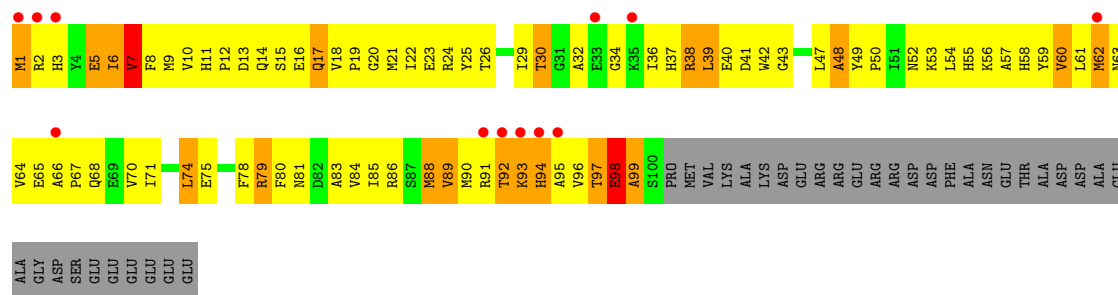
• Molecule 7: 30S ribosomal protein S5

Chain E:



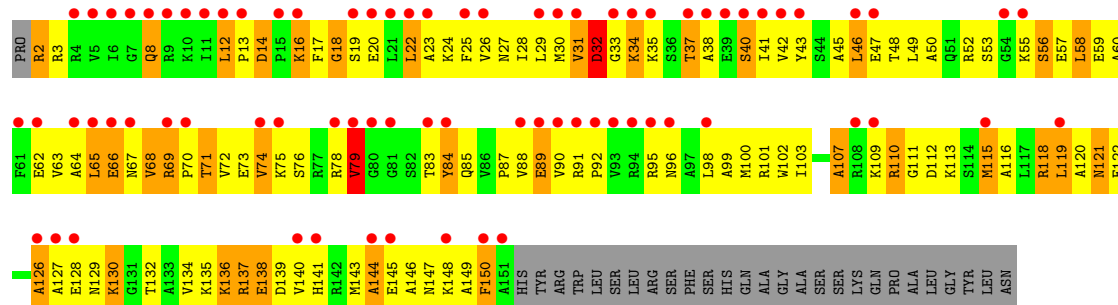
• Molecule 8: 30S ribosomal protein S6

Chain F:



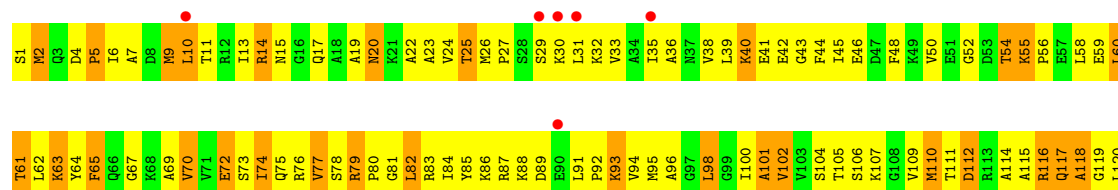
• Molecule 9: 30S ribosomal protein S7

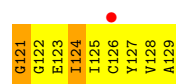
Chain G:



• Molecule 10: 30S ribosomal protein S8

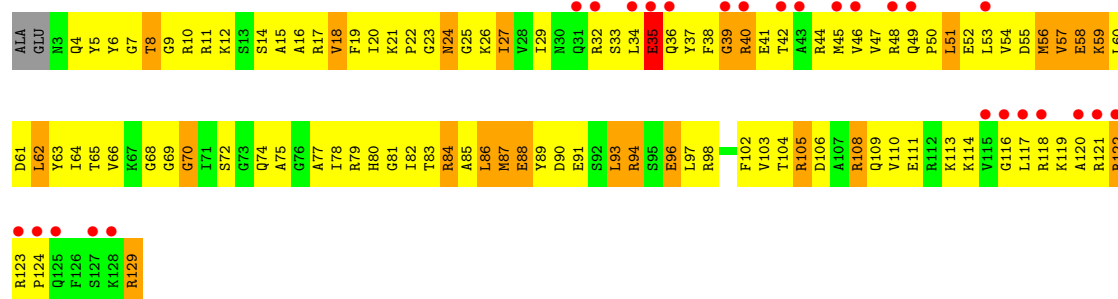
Chain H:





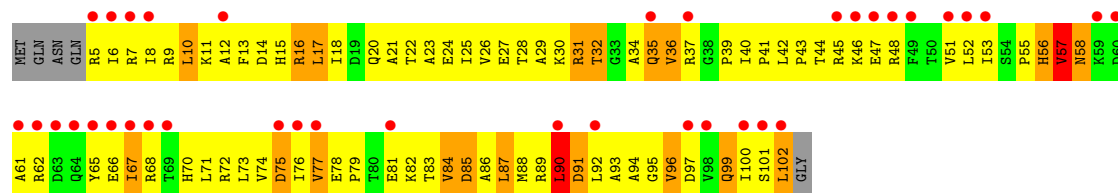
• Molecule 11: 30S ribosomal protein S9

Chain I:



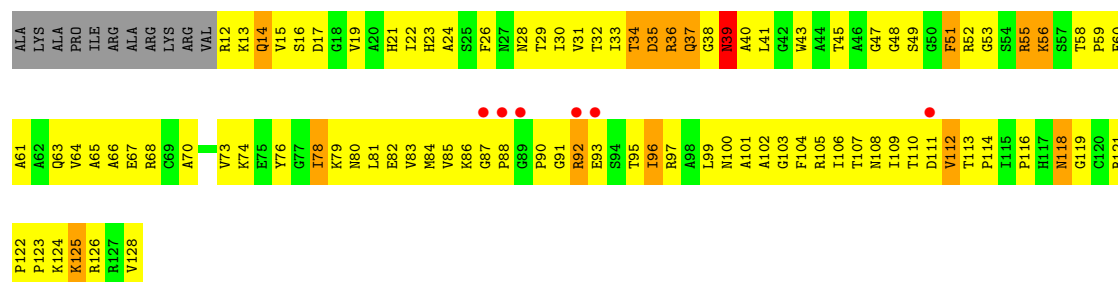
• Molecule 12: 30S ribosomal protein S10

Chain J:



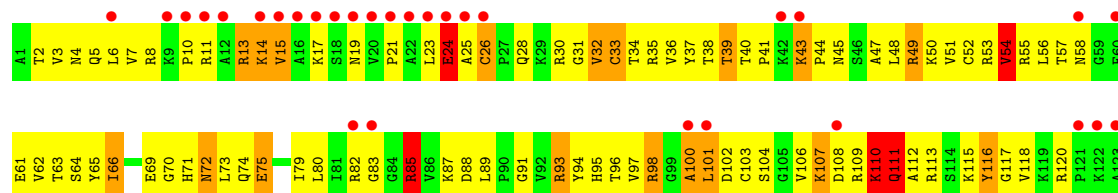
• Molecule 13: 30S ribosomal protein S11

Chain K:



• Molecule 14: 30S ribosomal protein S12

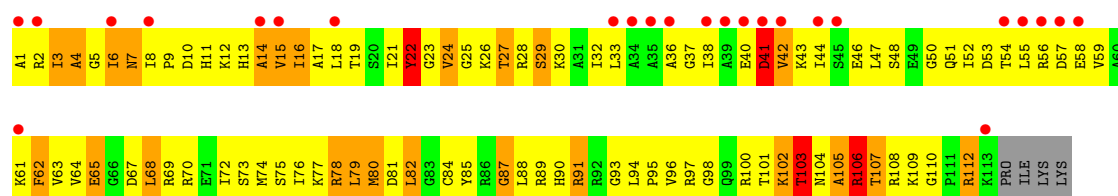
Chain L:



• Molecule 15: 30S ribosomal protein S13

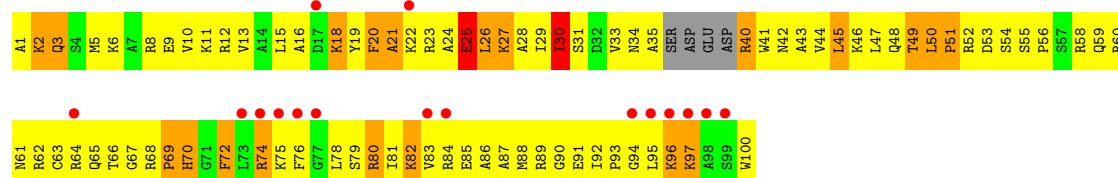
Chain M:





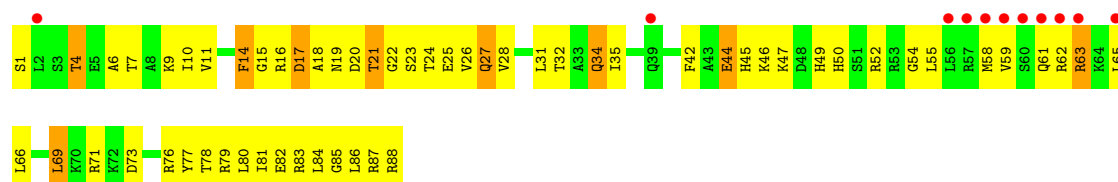
• Molecule 16: 30S ribosomal protein S14

Chain N:



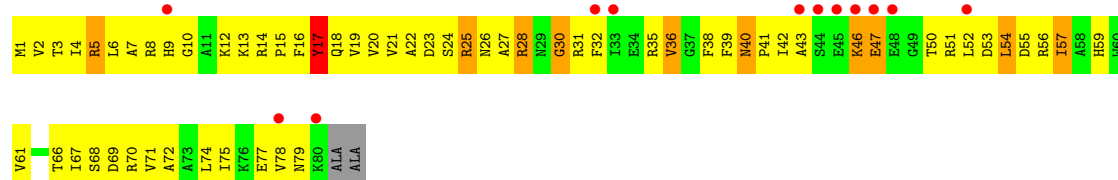
• Molecule 17: 30S ribosomal protein S15

Chain O:



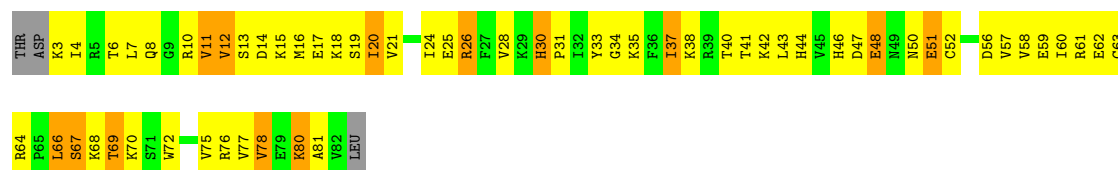
• Molecule 18: 30S ribosomal protein S16

Chain P:



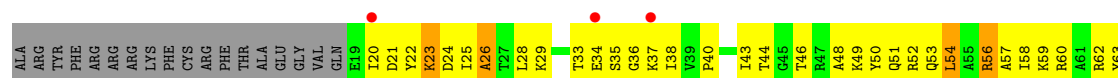
• Molecule 19: 30S ribosomal protein S17

Chain Q:



• Molecule 20: 30S ribosomal protein S18

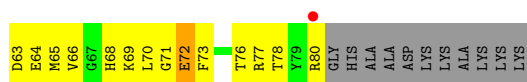
Chain R:





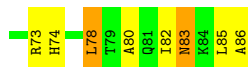
- Molecule 21: 30S ribosomal protein S19

Chain S:



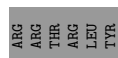
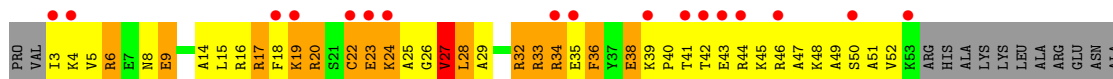
- Molecule 22: 30S ribosomal protein S20

Chain T:



- Molecule 23: 30S ribosomal protein S21

Chain U:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.78Å 395.22Å 744.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.22 184.07 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.22) 75.7 (184.07-3.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.287 , 0.320 0.528 , 0.531	Depositor DCC
R_{free} test set	37268 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 753156 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.56	EDS
Total number of atoms	52179	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: MG

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	0.25	0/36762	0.73	7/57350 (0.0%)
2	W	0.31	0/401	0.74	0/622
3	X	0.49	0/138	0.88	0/212
4	B	0.25	0/1735	0.45	0/2338
5	C	0.23	0/1651	0.44	0/2225
6	D	0.23	0/1665	0.45	0/2227
7	E	0.23	0/1118	0.47	0/1504
8	F	0.24	0/835	0.45	0/1128
9	G	0.23	0/1187	0.44	0/1591
10	H	0.23	0/989	0.46	0/1326
11	I	0.24	0/1034	0.44	0/1375
12	J	0.22	0/796	0.47	0/1077
13	K	0.24	0/893	0.45	0/1205
14	L	0.22	0/969	0.46	0/1300
15	M	0.22	0/884	0.46	0/1181
16	N	0.24	0/786	0.44	0/1046
17	O	0.23	0/724	0.44	0/966
18	P	0.25	0/648	0.43	0/870
19	Q	0.24	0/657	0.46	0/881
20	R	0.23	0/462	0.46	0/621
21	S	0.25	0/652	0.45	0/877
22	T	0.23	0/671	0.41	0/888
23	U	0.26	0/430	0.44	0/570
All	All	0.24	0/56087	0.66	7/83380 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	U	N1-C1'-C2'	-6.97	104.33	112.00
1	A	243	A	C2'-C3'-O3'	6.77	124.53	113.70
1	A	765	G	N9-C1'-C2'	-6.69	104.64	112.00
1	A	232	G	C5'-C4'-C3'	-5.41	107.35	116.00
1	A	281	G	N9-C1'-C2'	-5.37	106.09	112.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	281	G	Sidechain
1	A	324	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain

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	32831	0	16521	1465	0
2	W	360	0	185	9	0
3	X	125	0	63	5	0
4	B	1704	0	1732	320	0
5	C	1624	0	1699	251	0
6	D	1643	0	1710	255	0
7	E	1105	0	1148	217	0
8	F	817	0	808	123	0
9	G	1174	0	1230	167	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	979	0	1034	166	0
11	I	1022	0	1070	193	0
12	J	786	0	828	121	0
13	K	877	0	887	141	0
14	L	955	0	1019	119	0
15	M	876	0	937	165	0
16	N	774	0	828	133	0
17	O	716	0	742	70	0
18	P	638	0	656	103	0
19	Q	648	0	691	75	0
20	R	455	0	478	54	0
21	S	637	0	665	109	0
22	T	665	0	714	60	0
23	U	425	0	449	88	0
24	A	56	0	0	0	0
24	N	1	0	0	0	0
24	X	1	0	0	0	0
25	A	271	0	0	4	0
25	I	2	0	0	1	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	P	2	0	0	0	0
25	T	2	0	0	0	0
25	U	1	0	0	0	0
25	X	5	0	0	1	0
All	All	52179	0	36094	4054	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 46.

The worst 5 of 4054 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:E:47:PHE:H	7:E:66:ALA:HA	1.11	1.08
8:F:29:ILE:HG21	8:F:64:VAL:HG11	1.36	1.07
1:A:842:U:H3'	1:A:843:U:H4'	1.41	1.03
11:I:27:ILE:HA	11:I:62:LEU:HD21	1.39	1.03
1:A:1348:U:H4'	11:I:121:ARG:HD2	1.37	1.02

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	
4	B	216/240 (90%)	106 (49%)	71 (33%)	39 (18%)	0	1
5	C	204/232 (88%)	119 (58%)	57 (28%)	28 (14%)	0	2
6	D	203/205 (99%)	122 (60%)	54 (27%)	27 (13%)	0	2
7	E	148/166 (89%)	78 (53%)	50 (34%)	20 (14%)	0	2
8	F	98/135 (73%)	52 (53%)	30 (31%)	16 (16%)	0	1
9	G	148/178 (83%)	89 (60%)	40 (27%)	19 (13%)	0	3
10	H	127/129 (98%)	78 (61%)	35 (28%)	14 (11%)	1	5
11	I	125/129 (97%)	74 (59%)	44 (35%)	7 (6%)	3	23
12	J	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	2
13	K	115/128 (90%)	82 (71%)	25 (22%)	8 (7%)	2	14
14	L	121/123 (98%)	80 (66%)	24 (20%)	17 (14%)	0	2
15	M	111/117 (95%)	66 (60%)	29 (26%)	16 (14%)	0	2
16	N	94/100 (94%)	46 (49%)	29 (31%)	19 (20%)	0	0
17	O	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	10	52
18	P	78/82 (95%)	53 (68%)	17 (22%)	8 (10%)	1	6
19	Q	78/83 (94%)	51 (65%)	20 (26%)	7 (9%)	1	8
20	R	53/74 (72%)	37 (70%)	12 (23%)	4 (8%)	2	12
21	S	77/91 (85%)	55 (71%)	18 (23%)	4 (5%)	3	25
22	T	83/86 (96%)	59 (71%)	20 (24%)	4 (5%)	4	27
23	U	49/70 (70%)	27 (55%)	16 (33%)	6 (12%)	1	3
All	All	2310/2559 (90%)	1404 (61%)	627 (27%)	279 (12%)	1	4

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	17	HIS
4	B	26	MET
4	B	125	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	186	VAL
4	B	187	ASP

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	
4	B	180/198 (91%)	143 (79%)	37 (21%)	2	8
5	C	170/189 (90%)	138 (81%)	32 (19%)	2	11
6	D	172/172 (100%)	130 (76%)	42 (24%)	1	3
7	E	113/125 (90%)	87 (77%)	26 (23%)	1	5
8	F	87/116 (75%)	76 (87%)	11 (13%)	7	30
9	G	123/146 (84%)	100 (81%)	23 (19%)	2	11
10	H	104/104 (100%)	81 (78%)	23 (22%)	1	6
11	I	105/106 (99%)	83 (79%)	22 (21%)	1	8
12	J	86/90 (96%)	71 (83%)	15 (17%)	3	13
13	K	90/98 (92%)	77 (86%)	13 (14%)	5	22
14	L	103/103 (100%)	80 (78%)	23 (22%)	1	6
15	M	91/95 (96%)	71 (78%)	20 (22%)	1	6
16	N	79/83 (95%)	66 (84%)	13 (16%)	3	14
17	O	76/76 (100%)	67 (88%)	9 (12%)	8	34
18	P	65/65 (100%)	58 (89%)	7 (11%)	9	37
19	Q	74/77 (96%)	66 (89%)	8 (11%)	9	37
20	R	48/64 (75%)	43 (90%)	5 (10%)	10	39
21	S	70/78 (90%)	51 (73%)	19 (27%)	1	2
22	T	65/65 (100%)	55 (85%)	10 (15%)	4	18
23	U	44/60 (73%)	32 (73%)	12 (27%)	0	2
All	All	1945/2110 (92%)	1575 (81%)	370 (19%)	2	11

5 of 370 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	G	130	LYS
11	I	87	MET
21	S	28	LYS
10	H	9	MET
10	H	89	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
9	G	67	ASN
11	I	24	ASN
22	T	2	ASN
9	G	121	ASN
10	H	17	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1529/1542 (99%)	272 (17%)	19 (1%)
2	W	16/17 (94%)	0	0
3	X	5/6 (83%)	3 (60%)	0
All	All	1550/1565 (99%)	275 (17%)	19 (1%)

5 of 275 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	14	U
1	A	15	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	429	U
1	A	960	U
1	A	1226	C
1	A	428	G
1	A	1300	G

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 58 ligands modelled in this entry, 58 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	1530/1542 (99%)	-0.09	50 (3%) 44 10	41, 109, 167, 180	0
2	W	17/17 (100%)	-0.12	0 100 100	63, 86, 126, 150	0
3	X	6/6 (100%)	-0.21	0 100 100	76, 83, 113, 115	0
4	B	218/240 (90%)	0.50	24 (11%) 6 2	67, 141, 180, 180	0
5	C	206/232 (88%)	0.92	39 (18%) 2 1	69, 121, 161, 180	0
6	D	205/205 (100%)	-0.17	7 (3%) 43 9	67, 120, 164, 180	0
7	E	150/166 (90%)	0.53	17 (11%) 6 2	46, 129, 180, 180	0
8	F	100/135 (74%)	0.31	12 (12%) 5 2	33, 101, 144, 165	0
9	G	150/178 (84%)	2.58	76 (50%) 0 0	71, 122, 165, 180	0
10	H	129/129 (100%)	0.08	7 (5%) 25 5	37, 106, 149, 176	0
11	I	127/129 (98%)	0.79	26 (20%) 1 1	68, 128, 167, 180	0
12	J	98/103 (95%)	2.01	37 (37%) 1 0	76, 131, 164, 180	0
13	K	117/128 (91%)	-0.11	6 (5%) 27 5	48, 91, 131, 159	0
14	L	123/123 (100%)	1.31	30 (24%) 1 1	42, 91, 138, 172	0
15	M	113/117 (96%)	0.73	25 (22%) 1 1	58, 121, 165, 176	0
16	N	96/100 (96%)	0.46	16 (16%) 2 1	65, 124, 154, 180	0
17	O	88/88 (100%)	0.75	11 (12%) 5 1	37, 96, 143, 160	0
18	P	80/82 (97%)	0.78	12 (15%) 3 1	68, 113, 155, 180	0
19	Q	80/83 (96%)	-0.18	0 100 100	50, 104, 145, 155	0
20	R	55/74 (74%)	0.35	4 (7%) 15 4	46, 101, 144, 157	0
21	S	79/91 (86%)	-0.34	1 (1%) 74 26	75, 128, 160, 180	0
22	T	85/86 (98%)	-0.35	0 100 100	65, 104, 154, 180	0
23	U	51/70 (72%)	1.62	17 (33%) 1 0	63, 125, 169, 180	0
All	All	3903/4124 (94%)	0.35	417 (10%) 7 2	33, 114, 167, 180	0

The worst 5 of 417 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	G	4	ARG	15.9
4	B	142	LYS	13.0
5	C	189	HIS	13.0
12	J	66	GLU	12.5
9	G	5	VAL	11.2

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	1563	1/1	0.20	6.18	161,161,161,161	0
24	MG	A	1557	1/1	0.57	5.76	156,156,156,156	0
24	MG	A	1587	1/1	0.12	5.50	119,119,119,119	0
24	MG	A	1585	1/1	0.22	4.39	138,138,138,138	0
24	MG	A	1578	1/1	0.93	3.28	127,127,127,127	0
24	MG	A	1586	1/1	0.22	3.07	131,131,131,131	0
24	MG	A	1591	1/1	0.35	2.90	100,100,100,100	0
24	MG	A	1546	1/1	0.20	1.90	58,58,58,58	0
24	MG	A	1588	1/1	0.23	1.62	155,155,155,155	0
24	MG	A	1594	1/1	0.17	1.24	117,117,117,117	0
24	MG	A	1597	1/1	0.13	0.89	153,153,153,153	0
24	MG	A	1568	1/1	0.21	0.63	154,154,154,154	0
24	MG	A	1562	1/1	0.22	0.62	103,103,103,103	0
24	MG	A	1581	1/1	0.25	0.24	99,99,99,99	0
24	MG	A	1596	1/1	0.12	0.22	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1551	1/1	0.18	0.05	60,60,60,60	0
24	MG	A	1574	1/1	0.19	-0.02	154,154,154,154	0
24	MG	A	1559	1/1	0.31	-0.04	149,149,149,149	0
24	MG	A	1560	1/1	0.18	-0.11	87,87,87,87	0
24	MG	A	1552	1/1	0.19	-0.14	130,130,130,130	0
24	MG	A	1553	1/1	0.25	-0.14	102,102,102,102	0
24	MG	A	1592	1/1	0.20	-0.22	103,103,103,103	0
24	MG	A	1570	1/1	0.16	-0.32	106,106,106,106	0
24	MG	A	1544	1/1	0.16	-0.35	87,87,87,87	0
24	MG	A	1566	1/1	0.17	-0.45	103,103,103,103	0
24	MG	A	1547	1/1	0.18	-0.51	98,98,98,98	0
24	MG	A	1589	1/1	0.14	-0.56	109,109,109,109	0
24	MG	A	1548	1/1	0.13	-0.69	139,139,139,139	0
24	MG	A	1577	1/1	0.12	-0.80	129,129,129,129	0
24	MG	A	1598	1/1	0.10	-0.92	97,97,97,97	0
24	MG	A	1593	1/1	0.11	-1.19	66,66,66,66	0
24	MG	A	1545	1/1	0.09	-1.20	124,124,124,124	0
24	MG	A	1549	1/1	0.09	-1.36	108,108,108,108	0
24	MG	A	1572	1/1	0.13	-1.43	97,97,97,97	0
24	MG	A	1595	1/1	0.08	-1.57	149,149,149,149	0
24	MG	A	1565	1/1	0.09	-1.58	136,136,136,136	0
24	MG	A	1555	1/1	0.09	-1.63	140,140,140,140	0
24	MG	A	1590	1/1	0.10	-1.83	119,119,119,119	0
24	MG	N	340	1/1	0.10	-1.93	104,104,104,104	0
24	MG	A	1575	1/1	0.16	-2.06	136,136,136,136	0
24	MG	A	1550	1/1	0.04	-2.09	82,82,82,82	0
24	MG	A	1579	1/1	0.07	-2.19	81,81,81,81	0
24	MG	A	1564	1/1	0.09	-2.30	98,98,98,98	0
24	MG	A	1569	1/1	0.08	-2.37	122,122,122,122	0
24	MG	A	1543	1/1	0.05	-2.68	48,48,48,48	0
24	MG	A	1573	1/1	0.10	-2.88	91,91,91,91	0
24	MG	A	1580	1/1	0.11	-2.93	102,102,102,102	0
24	MG	A	1561	1/1	0.04	-3.53	79,79,79,79	0
24	MG	X	358	1/1	0.07	-3.61	73,73,73,73	0
24	MG	A	1558	1/1	0.07	-4.44	80,80,80,80	0
24	MG	A	1571	1/1	0.06	-4.57	94,94,94,94	0
24	MG	A	1583	1/1	0.08	-4.91	123,123,123,123	0
24	MG	A	1554	1/1	0.04	-5.76	95,95,95,95	0
24	MG	A	1584	1/1	0.07	-5.96	110,110,110,110	0
24	MG	A	1576	1/1	0.07	-7.04	80,80,80,80	0
24	MG	A	1567	1/1	0.03	-7.37	54,54,54,54	0
24	MG	A	1556	1/1	0.08	-18.02	171,171,171,171	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1582	1/1	0.13	-211.00	138,138,138,138	0

6.5 Other polymers ⓘ

There are no such residues in this entry.