wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 01:23 PM EDT

PDB ID	:	2ZM6
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit
Authors	:	Kaminishi, T.; Wang, H.; Kawazoe, M.; Ishii, R.; Schluenzen, F.; Hanawa-Suetsugu, K.; Wilson, D.N.; Nomura, M.; Takemoto, C.; Shirouzu, M.; Fucini, P.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2008-04-11
Resolution	:	3.30 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 (1)) were used in the production of this report:

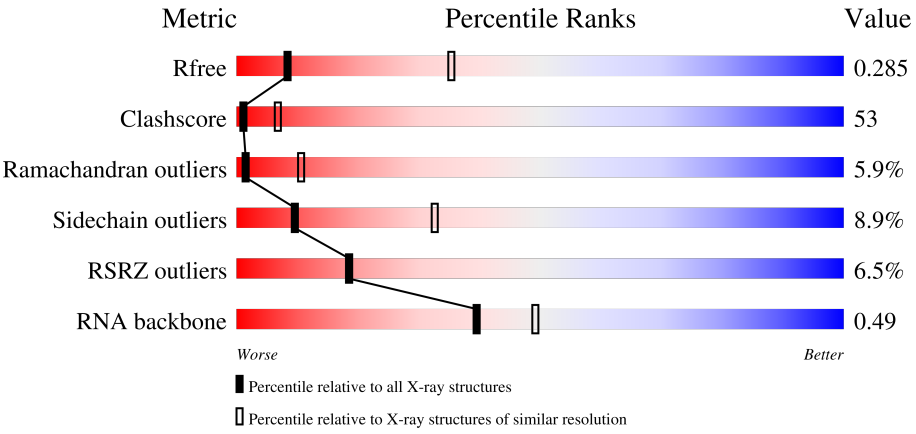
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	1509	9% 59% 21% 10%
2	B	255	39% 39% 9% 13%
3	C	238	6% 33% 42% 11% 13%
4	D	208	4% 43% 47% 9%

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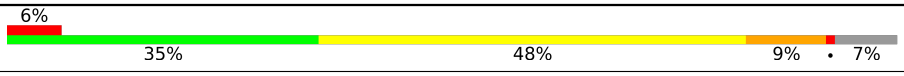
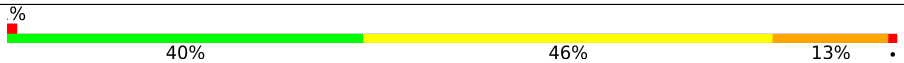
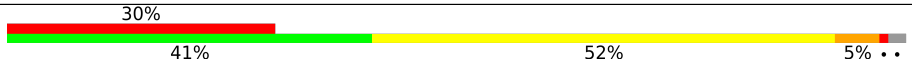
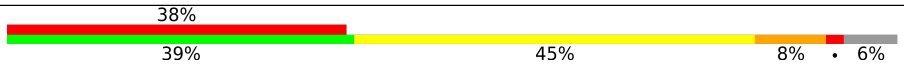
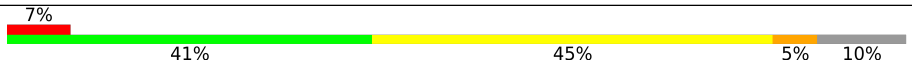
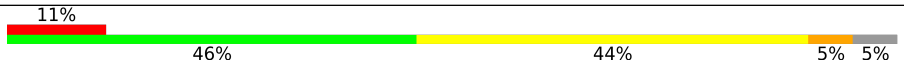
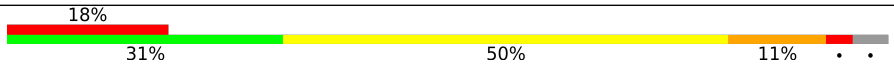
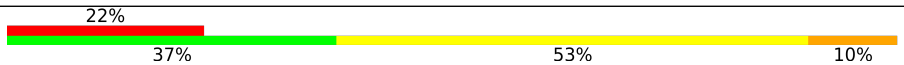
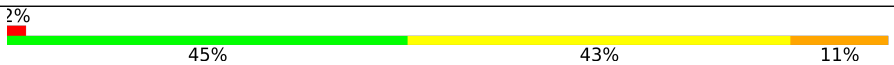
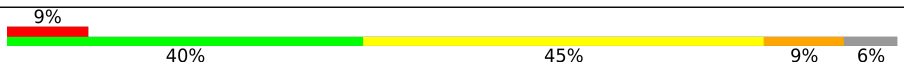
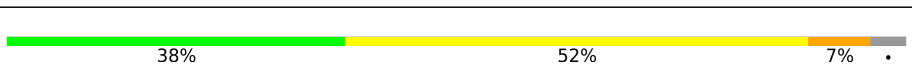
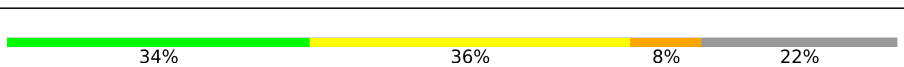
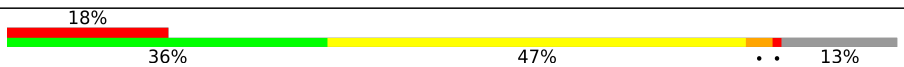
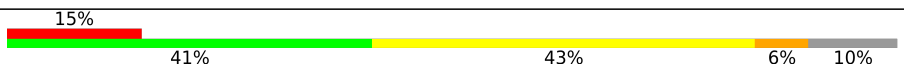
Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	128	
12	L	131	
13	M	125	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	87	
19	S	92	
20	T	105	
21	V	26	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 51308 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1506	32372	14408	5996	10462	1506	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	222	1810	1154	328	323	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	206	1612	1016	314	281	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	150	1146	724	217	201	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	101	843	531	155	154	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	153	Total	C	N	O	S	0	0	0
			1231	764	246	215	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	125	Total	C	N	O	0	0	0
			993	629	195	169			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			853	531	160	159	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			559	357	109	93			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	94	Total	C	N	O	S	0	0	0
			734	453	157	122	2			

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

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

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

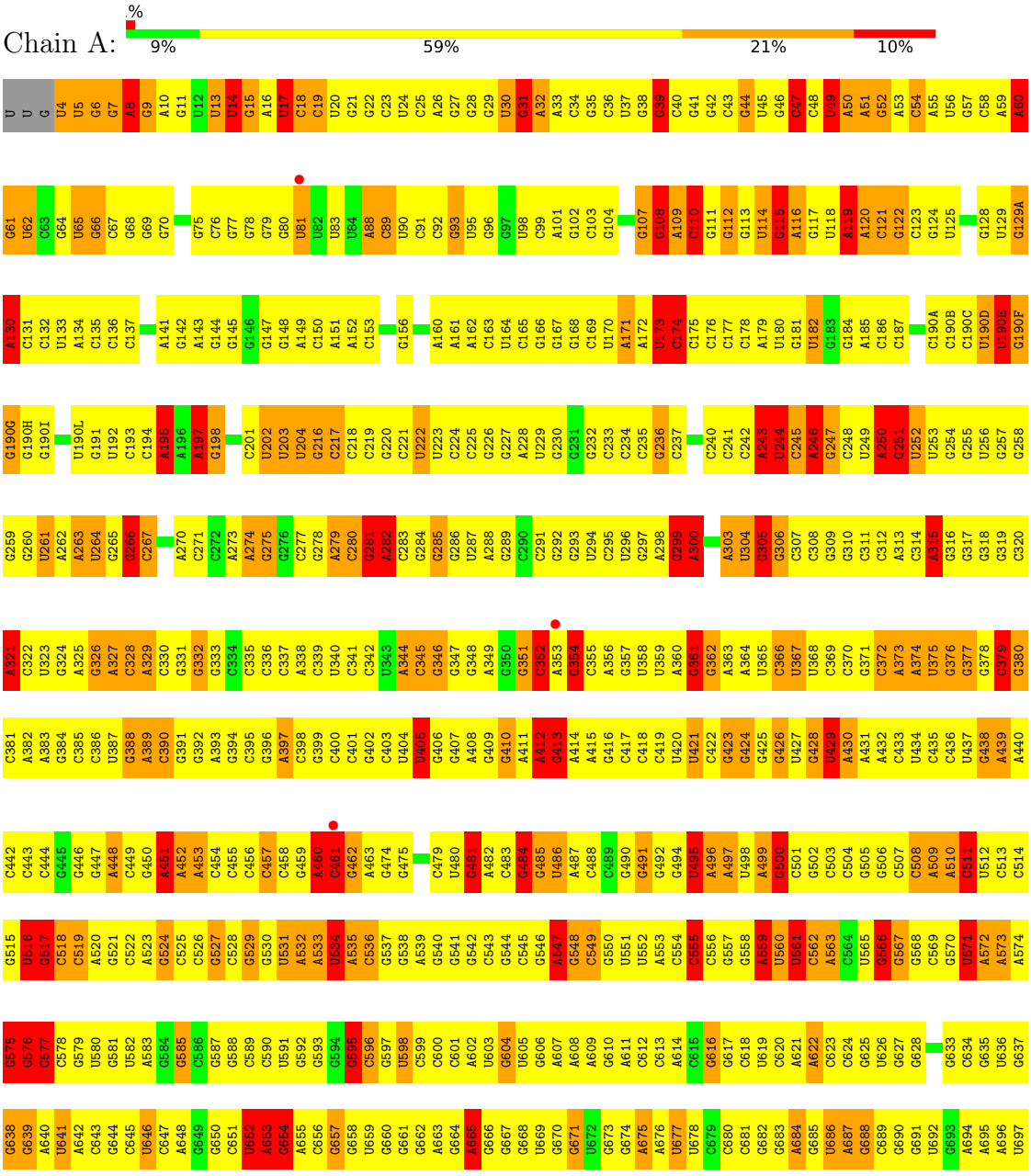
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	D	1	Total 1	Zn 1	0	0
22	N	1	Total 1	Zn 1	0	0

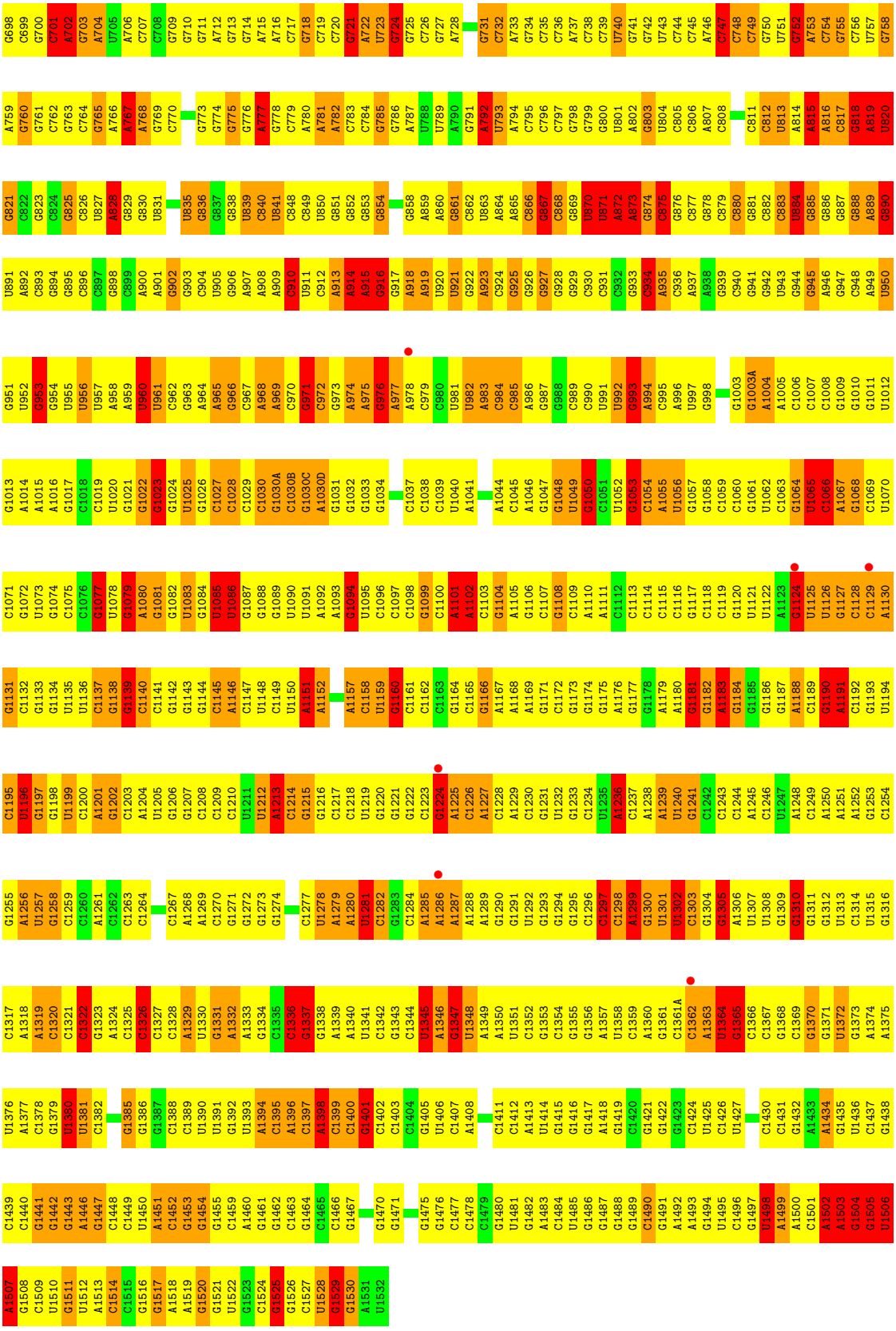
3 Residue-property plots (i)

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 ribosomal RNA

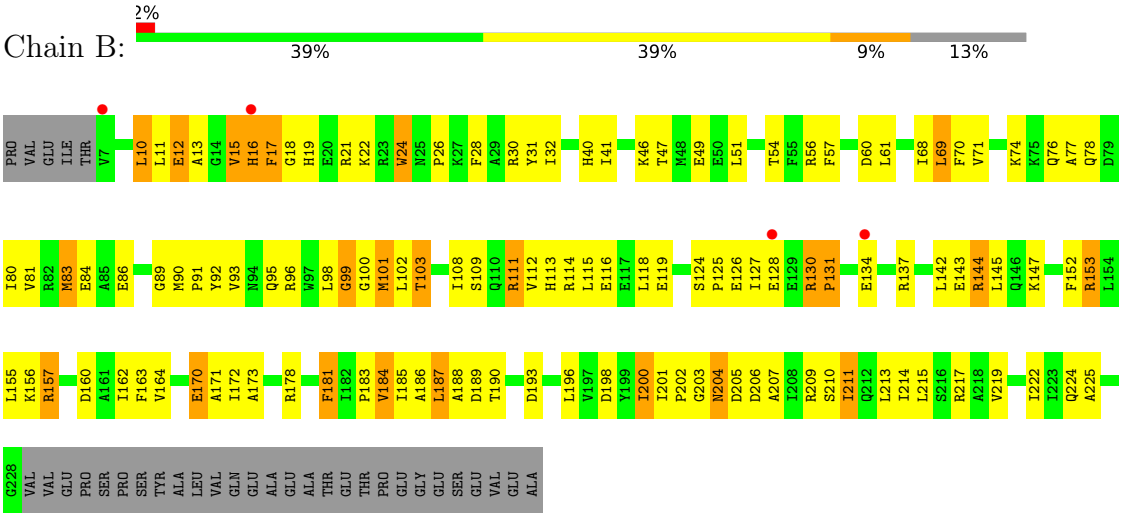
Chain A:





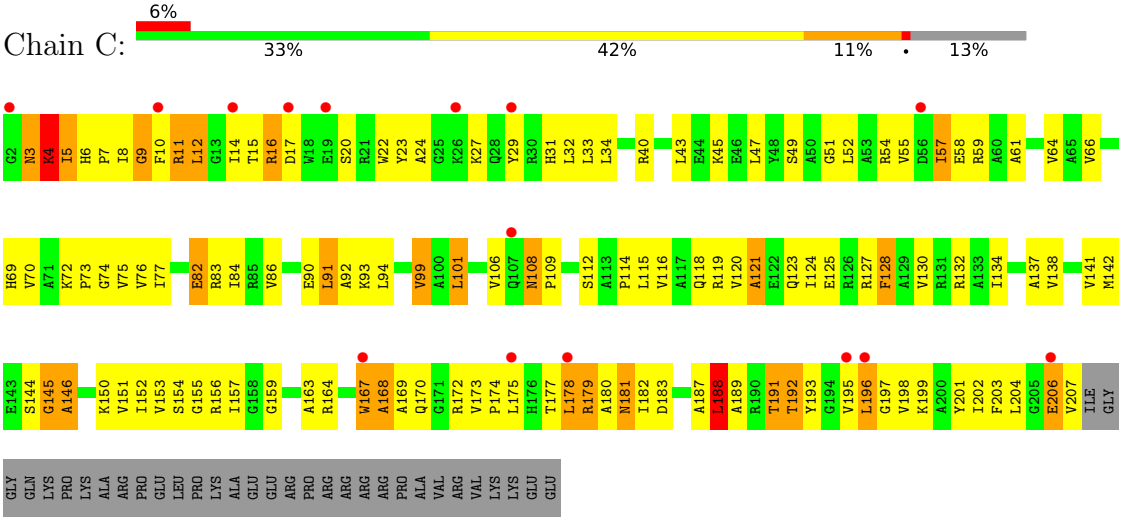
• Molecule 2: 30S ribosomal protein S2

Chain B:



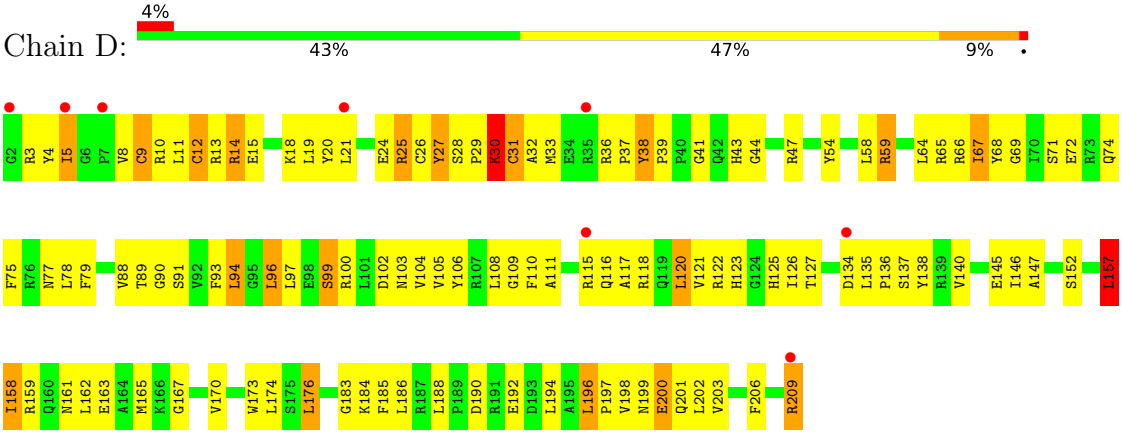
• Molecule 3: 30S ribosomal protein S3

Chain C:



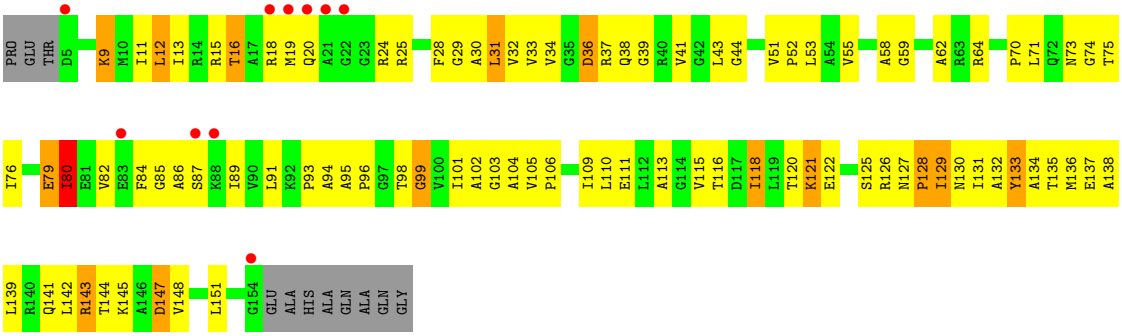
• Molecule 4: 30S ribosomal protein S4

Chain D:



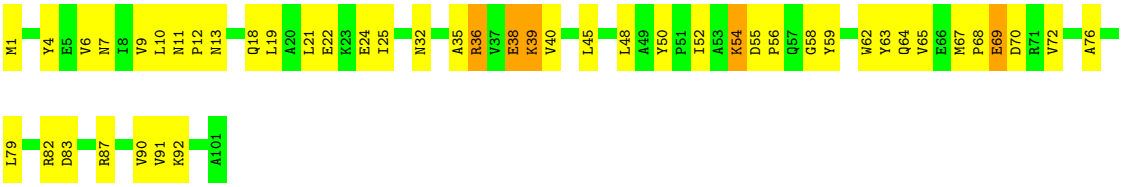
• Molecule 5: 30S ribosomal protein S5

Chain E:



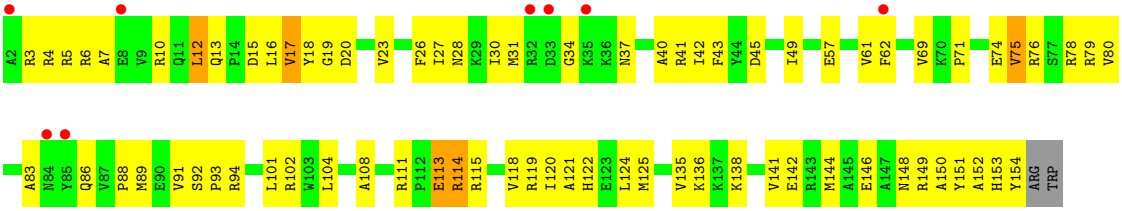
• Molecule 6: 30S ribosomal protein S6

Chain F:



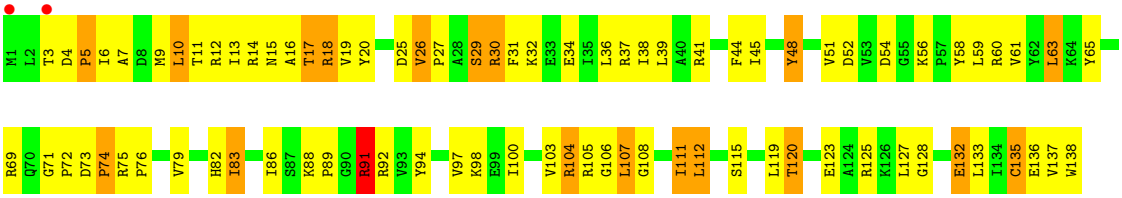
• Molecule 7: 30S ribosomal protein S7

Chain G:



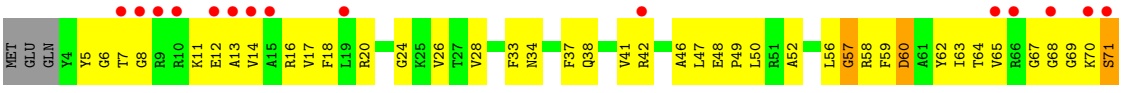
• Molecule 8: 30S ribosomal protein S8

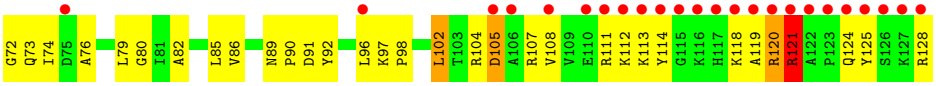
Chain H:



• Molecule 9: 30S ribosomal protein S9

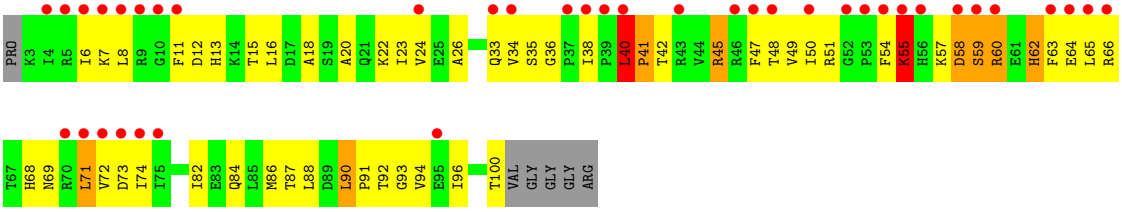
Chain I:





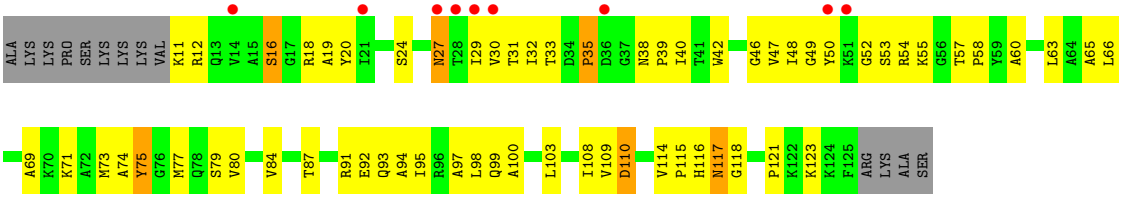
• Molecule 10: 30S ribosomal protein S10

Chain J:



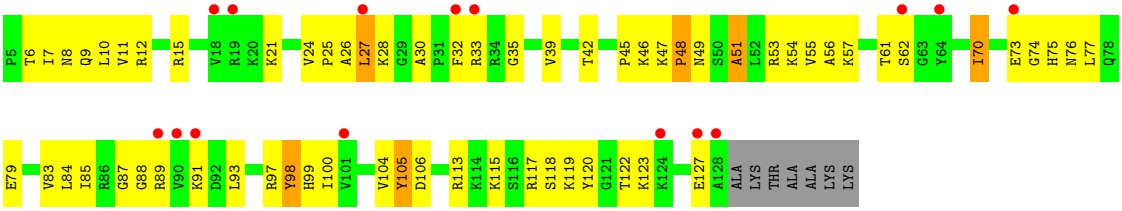
• Molecule 11: 30S ribosomal protein S11

Chain K:



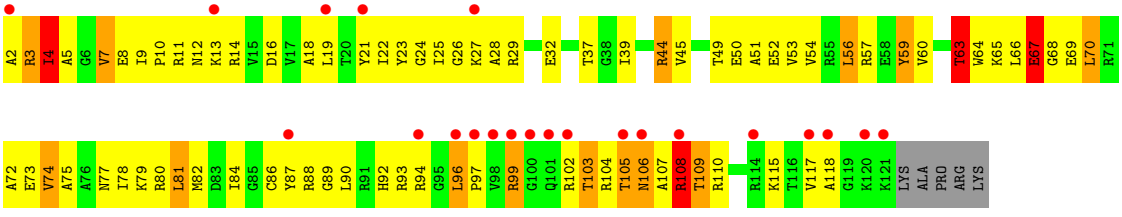
• Molecule 12: 30S ribosomal protein S12

Chain L:



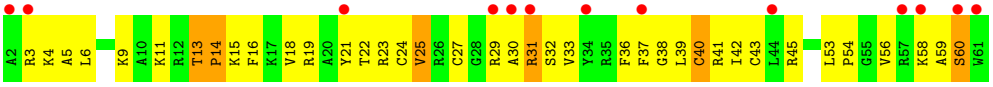
• Molecule 13: 30S ribosomal protein S13

Chain M:

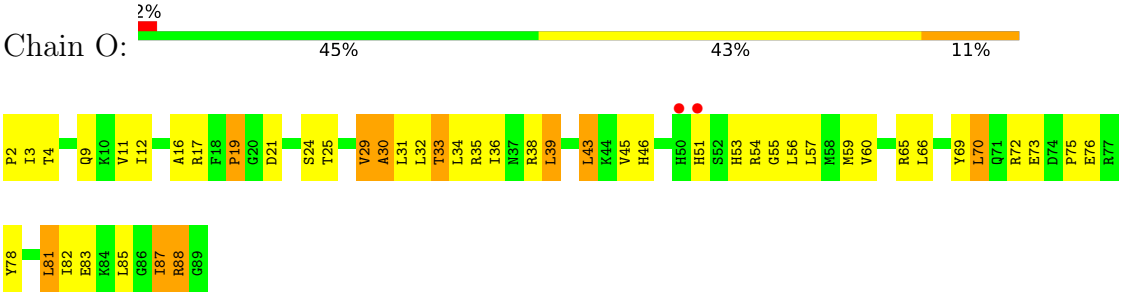


• Molecule 14: 30S ribosomal protein S14 type Z

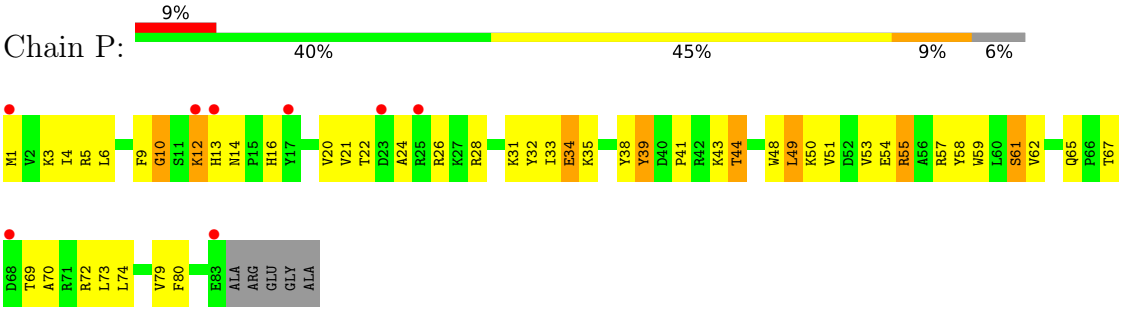
Chain N:



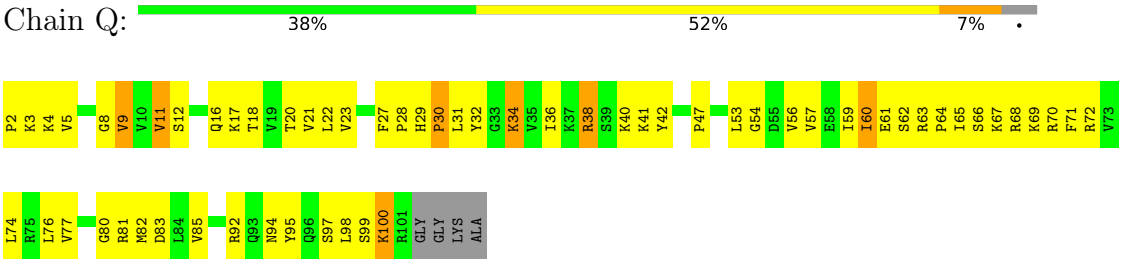
• Molecule 15: 30S ribosomal protein S15



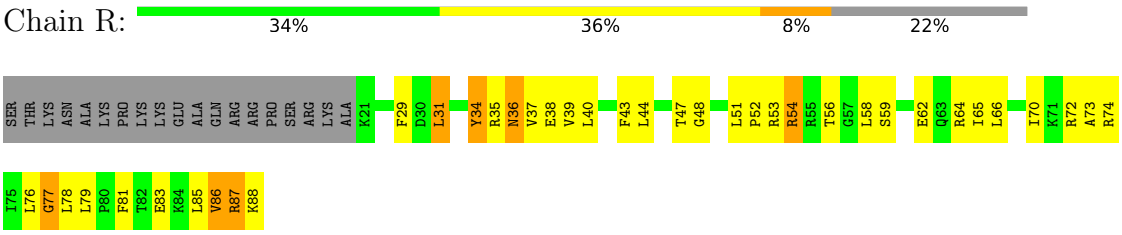
• Molecule 16: 30S ribosomal protein S16



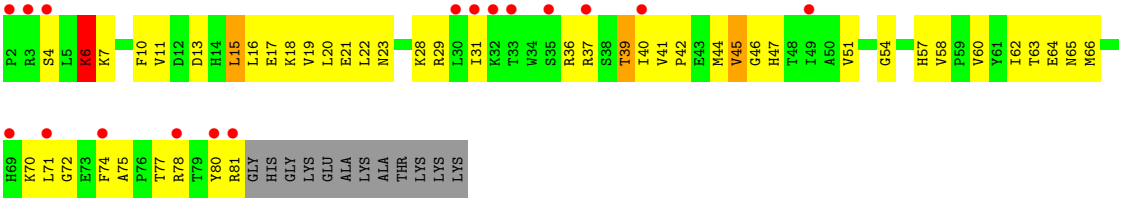
• Molecule 17: 30S ribosomal protein S17



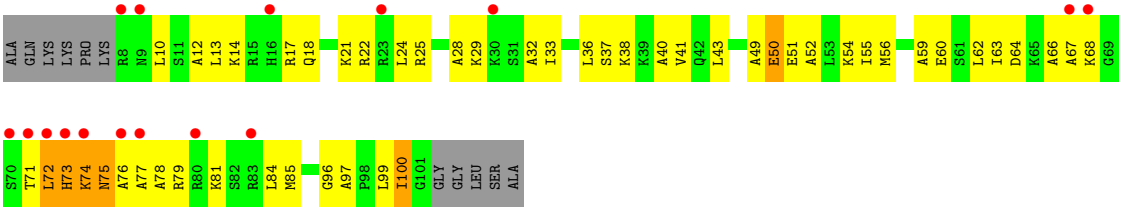
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein Thx

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	411.50Å 411.50Å 172.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	184.03 – 3.30 184.03 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (184.03-3.30) 97.7 (184.03-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.292 , 0.323 0.252 , 0.285	Depositor DCC
R_{free} test set	10942 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	95.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.12 , 20.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	51308	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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

5.1 Standard geometry

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

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	0.97	29/36237 (0.1%)	0.99	122/56558 (0.2%)
2	B	0.68	0/1842	0.91	1/2479 (0.0%)
3	C	0.62	0/1636	0.88	3/2205 (0.1%)
4	D	0.72	2/1733 (0.1%)	1.01	7/2318 (0.3%)
5	E	0.81	0/1162	1.02	0/1564
6	F	0.57	0/856	0.83	0/1154
7	G	0.48	0/1248	0.71	0/1672
8	H	0.76	0/1136	1.02	3/1527 (0.2%)
9	I	0.56	0/1011	0.80	1/1354 (0.1%)
10	J	0.53	0/807	0.87	2/1085 (0.2%)
11	K	0.53	0/868	0.82	0/1173
12	L	0.59	0/986	0.89	1/1320 (0.1%)
13	M	0.54	0/965	0.88	3/1292 (0.2%)
14	N	0.58	0/501	0.98	1/664 (0.2%)
15	O	0.66	0/745	0.90	1/992 (0.1%)
16	P	0.66	0/716	0.88	0/963
17	Q	0.69	0/847	0.92	0/1131
18	R	0.56	0/564	0.89	0/748
19	S	0.53	0/661	0.92	1/890 (0.1%)
20	T	0.50	0/736	0.83	1/970 (0.1%)
21	V	0.60	0/212	0.77	0/277
All	All	0.87	31/55469 (0.1%)	0.96	147/82336 (0.2%)

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	160
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	H	0	1
17	Q	0	1
All	All	0	164

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1077	G	C5-C6	-12.45	1.29	1.42
1	A	1511	G	N3-C4	-8.17	1.29	1.35
1	A	1108	G	C5-C6	7.17	1.49	1.42
1	A	378	G	C5-C6	-6.89	1.35	1.42
1	A	1081	G	N3-C4	-6.69	1.30	1.35

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	A	N9-C1'-C2'	10.65	127.85	114.00
1	A	934	C	N1-C1'-C2'	9.98	126.98	114.00
14	N	40	CYS	CA-CB-SG	9.68	131.43	114.00
1	A	1336	C	N1-C1'-C2'	9.27	126.05	114.00
4	D	12	CYS	CA-CB-SG	9.23	130.62	114.00

There are no chirality outliers.

5 of 164 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	U	Sidechain
1	A	15	G	Sidechain
1	A	17	U	Sidechain
1	A	19	C	Sidechain
1	A	30	U	Sidechain

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	32372	0	16335	3399	0
2	B	1810	0	1861	119	0
3	C	1612	0	1677	169	0
4	D	1703	0	1763	134	0
5	E	1146	0	1207	112	0
6	F	843	0	857	42	0
7	G	1231	0	1273	81	0
8	H	1116	0	1177	113	0
9	I	993	0	1029	103	0
10	J	794	0	840	65	0
11	K	853	0	868	52	0
12	L	970	0	1057	77	0
13	M	955	0	1021	98	0
14	N	492	0	529	62	0
15	O	734	0	771	41	0
16	P	700	0	720	65	0
17	Q	834	0	906	70	0
18	R	559	0	624	49	0
19	S	647	0	673	57	0
20	T	734	0	832	55	0
21	V	208	0	221	15	0
22	D	1	0	0	0	0
22	N	1	0	0	0	0
All	All	51308	0	36241	4584	0

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 53.

The worst 5 of 4584 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:C:C2’	1:A:1028:C:H5”	1.52	1.36
1:A:1250:A:H2’	1:A:1251:A:C8	1.72	1.25
14:N:24:CYS:SG	14:N:39:LEU:HA	1.79	1.21
1:A:1027:C:H2’	1:A:1028:C:C5’	1.72	1.19
1:A:109:A:H2’	1:A:326:G:N2	1.58	1.18

There are no symmetry-related clashes.

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	220/255 (86%)	165 (75%)	41 (19%)	14 (6%)	1 9
3	C	204/238 (86%)	140 (69%)	47 (23%)	17 (8%)	1 5
4	D	206/208 (99%)	153 (74%)	42 (20%)	11 (5%)	2 12
5	E	148/161 (92%)	113 (76%)	24 (16%)	11 (7%)	1 7
6	F	99/101 (98%)	86 (87%)	9 (9%)	4 (4%)	3 18
7	G	151/155 (97%)	126 (83%)	21 (14%)	4 (3%)	5 27
8	H	136/138 (99%)	117 (86%)	13 (10%)	6 (4%)	2 16
9	I	123/128 (96%)	98 (80%)	21 (17%)	4 (3%)	4 22
10	J	96/104 (92%)	74 (77%)	14 (15%)	8 (8%)	1 5
11	K	113/128 (88%)	88 (78%)	17 (15%)	8 (7%)	1 7
12	L	122/131 (93%)	87 (71%)	26 (21%)	9 (7%)	1 7
13	M	118/125 (94%)	75 (64%)	31 (26%)	12 (10%)	0 3
14	N	58/60 (97%)	46 (79%)	12 (21%)	0	100 100
15	O	86/88 (98%)	62 (72%)	17 (20%)	7 (8%)	1 6
16	P	81/88 (92%)	58 (72%)	19 (24%)	4 (5%)	2 14
17	Q	98/104 (94%)	77 (79%)	16 (16%)	5 (5%)	2 13
18	R	66/87 (76%)	45 (68%)	17 (26%)	4 (6%)	1 10
19	S	78/92 (85%)	62 (80%)	15 (19%)	1 (1%)	12 40
20	T	92/105 (88%)	70 (76%)	16 (17%)	6 (6%)	1 9
21	V	22/26 (85%)	17 (77%)	3 (14%)	2 (9%)	1 4
All	All	2317/2522 (92%)	1759 (76%)	421 (18%)	137 (6%)	1 10

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	LEU

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Mol	Chain	Res	Type
2	B	12	GLU
2	B	21	ARG
2	B	24	TRP
2	B	95	GLN

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	191/219 (87%)	166 (87%)	25 (13%)	4 17
3	C	160/187 (86%)	141 (88%)	19 (12%)	5 21
4	D	180/180 (100%)	166 (92%)	14 (8%)	12 38
5	E	115/122 (94%)	103 (90%)	12 (10%)	7 25
6	F	90/90 (100%)	85 (94%)	5 (6%)	21 52
7	G	124/126 (98%)	120 (97%)	4 (3%)	39 67
8	H	119/119 (100%)	107 (90%)	12 (10%)	7 27
9	I	96/99 (97%)	90 (94%)	6 (6%)	18 47
10	J	88/91 (97%)	78 (89%)	10 (11%)	5 22
11	K	87/98 (89%)	82 (94%)	5 (6%)	20 51
12	L	104/108 (96%)	100 (96%)	4 (4%)	33 62
13	M	96/100 (96%)	83 (86%)	13 (14%)	4 16
14	N	49/49 (100%)	41 (84%)	8 (16%)	2 10
15	O	79/79 (100%)	69 (87%)	10 (13%)	4 19
16	P	72/74 (97%)	65 (90%)	7 (10%)	8 29
17	Q	95/96 (99%)	87 (92%)	8 (8%)	11 35
18	R	60/76 (79%)	57 (95%)	3 (5%)	24 55
19	S	71/79 (90%)	65 (92%)	6 (8%)	10 35
20	T	74/81 (91%)	70 (95%)	4 (5%)	22 53
21	V	19/21 (90%)	19 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1969/2094 (94%)	1794 (91%)	175 (9%)	9 32

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	98	TYR
15	O	65	ARG
13	M	56	LEU
14	N	14	PRO
16	P	44	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	46	HIS
17	Q	16	GLN
20	T	75	ASN
6	F	100	ASN
6	F	27	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1509 (99%)	332 (22%)	181 (12%)

5 of 332 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G

5 of 181 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	993	G
1	A	1240	U
1	A	1065	U

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Mol	Chain	Res	Type
1	A	1157	A
1	A	1297	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1506/1509 (99%)	-0.33	9 (0%) 89 90	29, 94, 180, 218	0
2	B	222/255 (87%)	0.09	4 (1%) 68 67	43, 111, 195, 218	0
3	C	206/238 (86%)	0.24	15 (7%) 15 15	49, 123, 192, 215	0
4	D	208/208 (100%)	0.26	8 (3%) 40 37	25, 101, 171, 218	0
5	E	150/161 (93%)	0.30	10 (6%) 17 17	42, 85, 151, 185	0
6	F	101/101 (100%)	-0.05	0 100 100	53, 122, 186, 211	0
7	G	153/155 (98%)	0.12	8 (5%) 27 25	74, 136, 196, 218	0
8	H	138/138 (100%)	0.02	2 (1%) 75 75	30, 83, 156, 193	0
9	I	125/128 (97%)	1.36	39 (31%) 0 0	69, 144, 201, 218	0
10	J	98/104 (94%)	1.56	39 (39%) 0 0	61, 150, 210, 218	0
11	K	115/128 (89%)	0.19	9 (7%) 13 12	60, 118, 181, 209	0
12	L	124/131 (94%)	0.57	15 (12%) 4 3	41, 108, 169, 204	0
13	M	120/125 (96%)	0.69	22 (18%) 1 1	66, 133, 198, 218	0
14	N	60/60 (100%)	1.18	13 (21%) 0 1	56, 110, 174, 203	0
15	O	88/88 (100%)	0.16	2 (2%) 60 59	50, 103, 167, 203	0
16	P	83/88 (94%)	0.44	8 (9%) 8 8	36, 91, 152, 216	0
17	Q	100/104 (96%)	0.11	0 100 100	43, 95, 166, 211	0
18	R	68/87 (78%)	-0.03	0 100 100	49, 102, 184, 196	0
19	S	80/92 (86%)	0.78	17 (21%) 0 1	66, 143, 208, 218	0
20	T	94/105 (89%)	0.80	16 (17%) 1 1	64, 126, 190, 218	0
21	V	24/26 (92%)	3.16	16 (66%) 0 0	93, 129, 158, 188	0
All	All	3863/4031 (95%)	0.14	252 (6%) 18 18	25, 104, 188, 218	0

The worst 5 of 252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	33	GLN	9.9
9	I	128	ARG	9.7
19	S	2	PRO	9.3
13	M	121	LYS	8.0
21	V	6	ARG	7.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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
22	ZN	D	210	1/1	0.99	0.33	90,90,90,90	0
22	ZN	N	62	1/1	0.99	0.11	101,101,101,101	0

6.5 Other polymers (i)

There are no such residues in this entry.