



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:00 PM GMT

PDB ID : 3V28  
Title : Crystal structure of HPF bound to the 70S ribosome. This PDB entry contains coordinates for the 30S subunit with bound HPF of the 2nd ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-11  
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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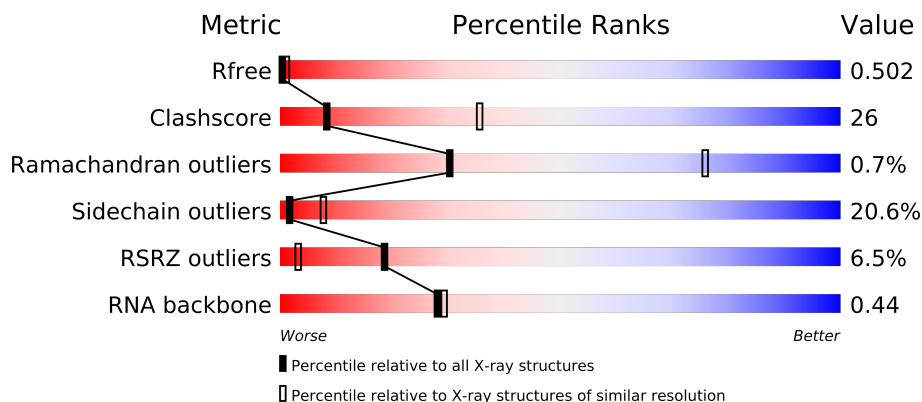
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	

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Mol	Chain	Length	Quality of chain
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	X	101	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 50808 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	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			777	493	137	144	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	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
			1045	665	188	190	2			

- 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
			852	533	163	156			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	96	Total	C	N	O	0	0	0
			663	410	132	121			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			828	516	155	154	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
			905	567	178	159	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	114	Total	C	N	O	S	0	0	0
			804	497	164	142	1			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			478	303	99	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
			724	453	143	126	2			

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	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
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a protein called Probable sigma(54) modulation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	95	Total	C	N	O	S	0	0	0
			601	378	108	114	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	96	HIS	-	EXPRESSION TAG	UNP P0AFX0
X	97	HIS	-	EXPRESSION TAG	UNP P0AFX0
X	98	HIS	-	EXPRESSION TAG	UNP P0AFX0
X	99	HIS	-	EXPRESSION TAG	UNP P0AFX0
X	100	HIS	-	EXPRESSION TAG	UNP P0AFX0
X	101	HIS	-	EXPRESSION TAG	UNP P0AFX0

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	Q	1	Total	Mg	0	0
			1	1		
23	A	168	Total	Mg	0	0
			168	168		
23	E	1	Total	Mg	0	0
			1	1		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	282	Total	O	0	0
			282	282		

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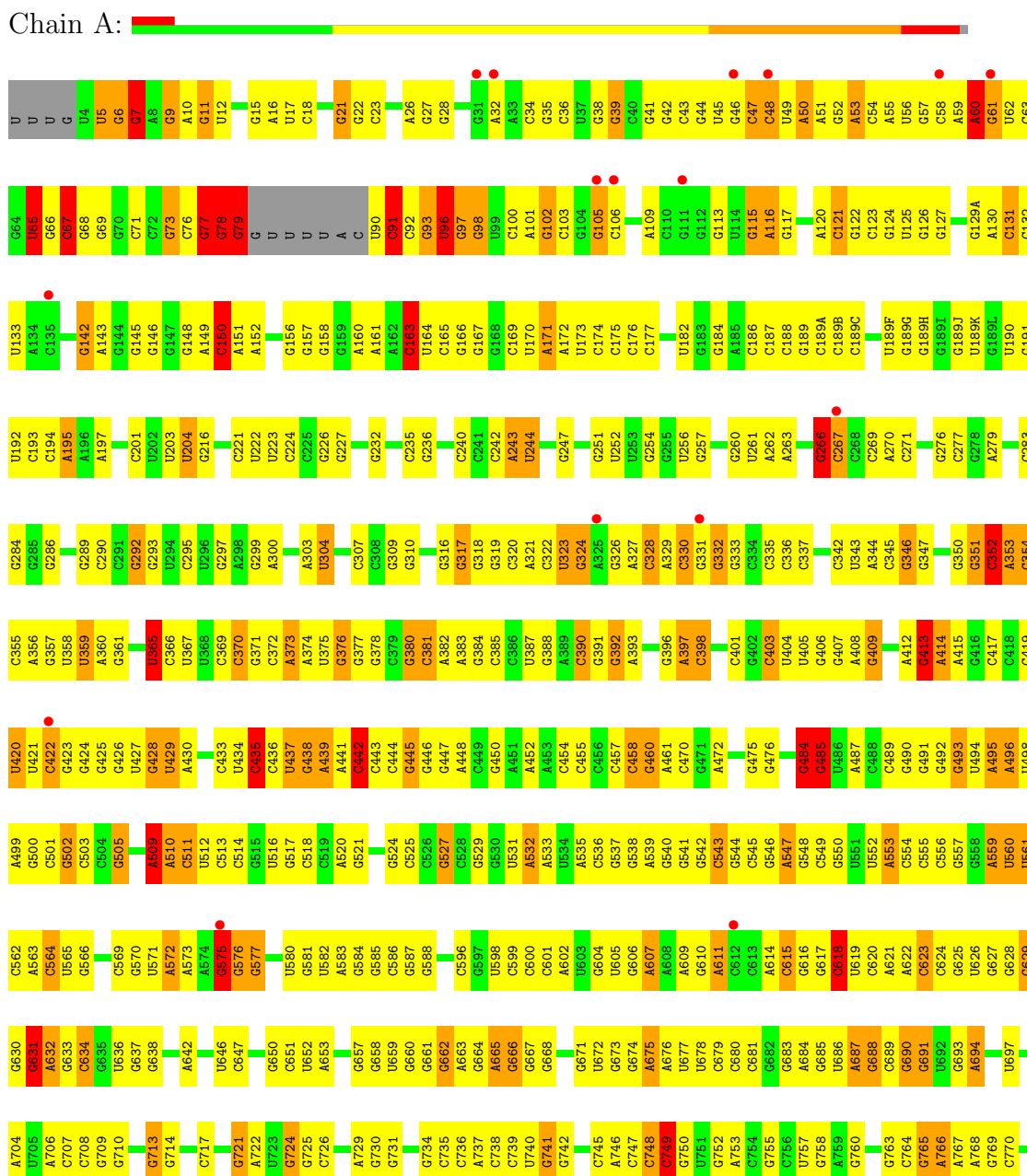
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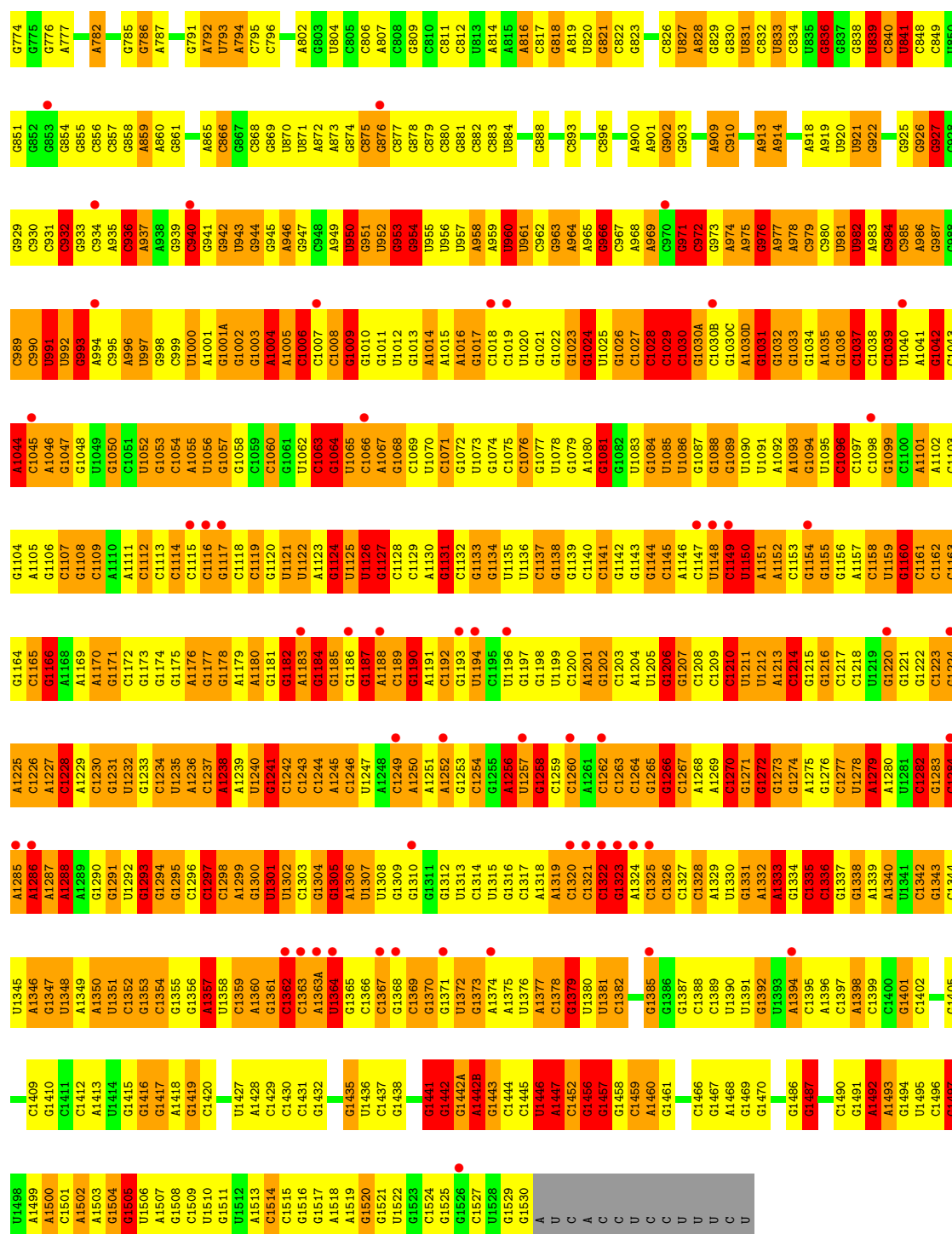
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	C	1	Total 1	O 1	0	0
25	D	1	Total 1	O 1	0	0
25	E	2	Total 2	O 2	0	0
25	K	1	Total 1	O 1	0	0
25	L	2	Total 2	O 2	0	0
25	N	1	Total 1	O 1	0	0
25	Q	1	Total 1	O 1	0	0
25	T	2	Total 2	O 2	0	0
25	X	1	Total 1	O 1	0	0

### 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.

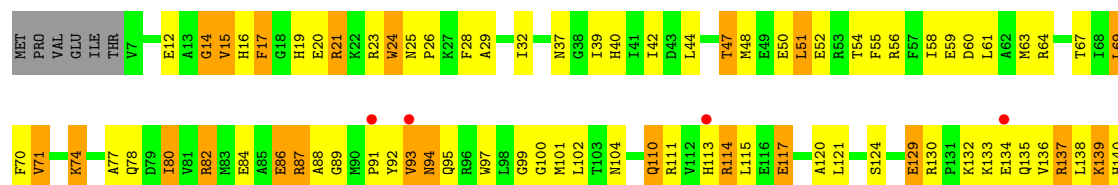
#### • Molecule 1: 16S Ribosomal RNA

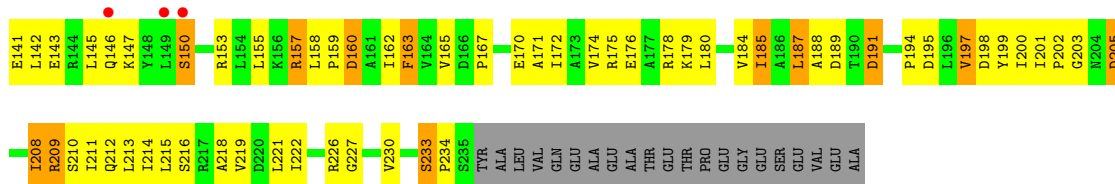




## • Molecule 2: 30S Ribosomal Protein S2

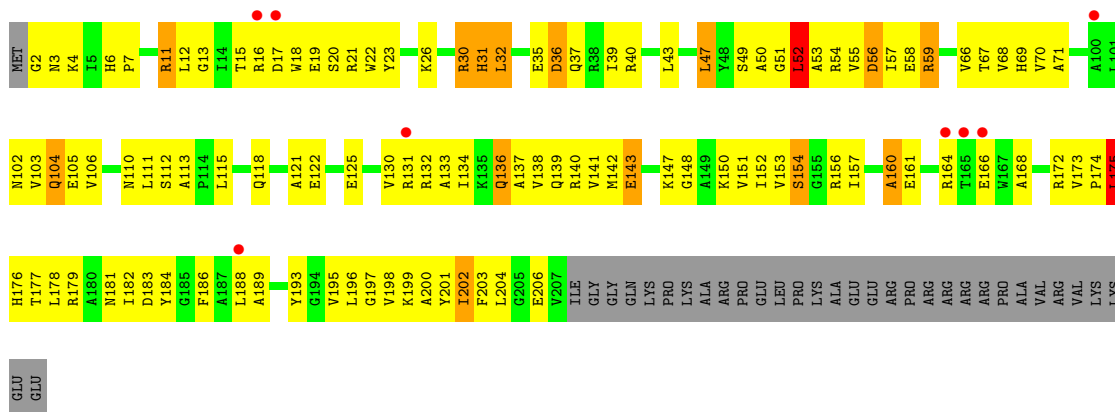
Chain B:





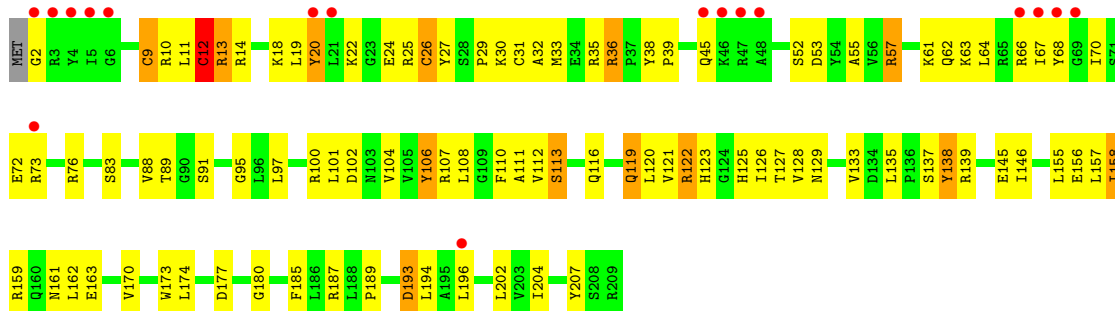
• Molecule 3: 30S Ribosomal Protein S3

Chain C:



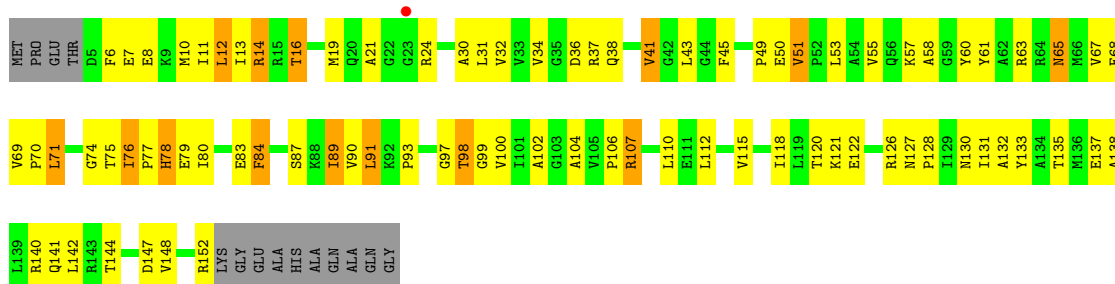
• Molecule 4: 30S Ribosomal Protein S4

Chain D:



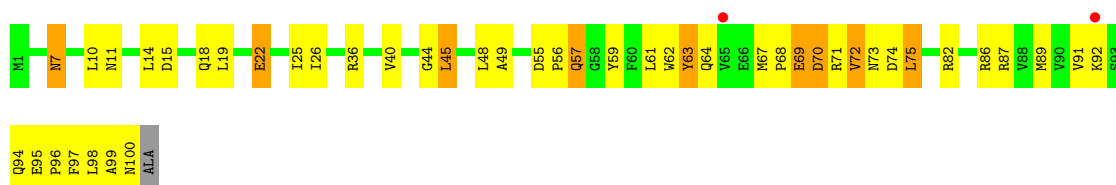
• Molecule 5: 30S Ribosomal Protein S5

Chain E:



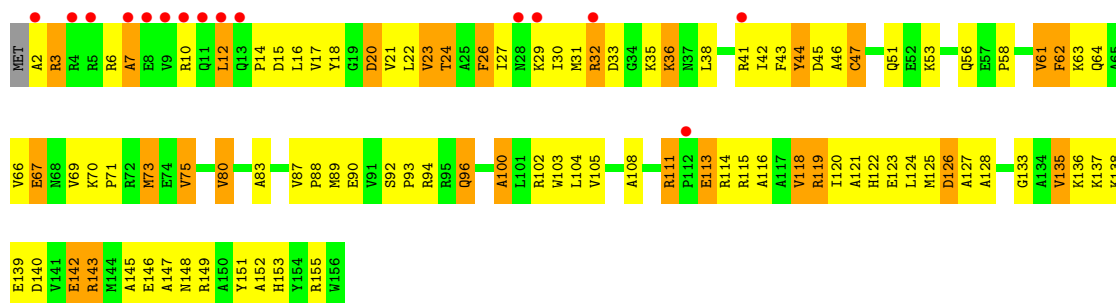
• Molecule 6: 30S Ribosomal Protein S6

Chain F:



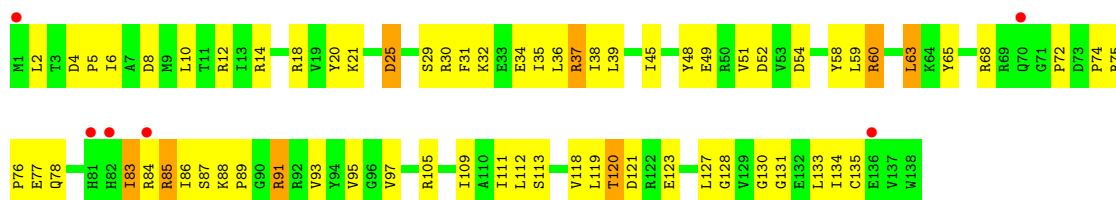
• Molecule 7: 30S Ribosomal Protein S7

Chain G:



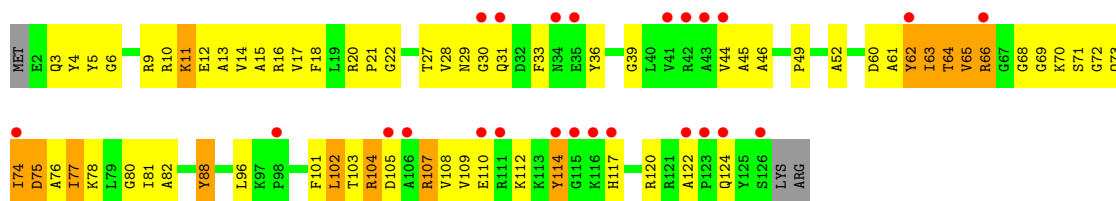
• Molecule 8: 30S Ribosomal Protein S8

Chain H:



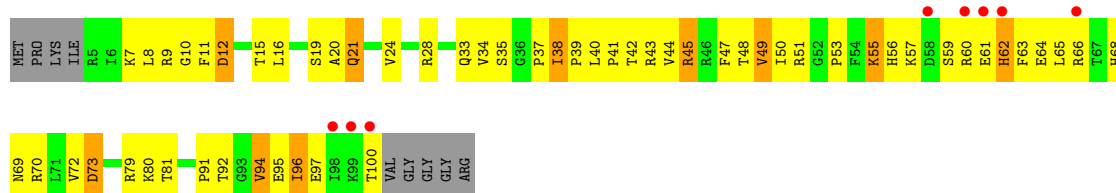
• Molecule 9: 30S Ribosomal Protein S9

Chain I:



• Molecule 10: 30S Ribosomal Protein S10

Chain J:



• Molecule 11: 30S Ribosomal Protein S11

MET	ALA	LYS	LYS	PRO	SER	LYS	LYS	LYS	VAL	LYS	ARG	Q13	V14	A15	S16	I21	E22	A23	N26	N27	T28	I29	T30	T31	I32	T33	D34	N38	P39	I40	T41	W42	S43	S44	G45	G46	W47	Y50	Y59	D67	A68	K71	A72	K73	A74	Y75	S79	D80	D81	Y86
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Sequence logo for the 100th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows amino acids: R85, G86, R91, E92, R96, Q99, L103, Q104, V105, V109, N117, G118, C119, R120, P121, R126, LYS, ALA, and SER. Red dots above G86, R91, and C119 indicate high information content.

- Chain L:

R102	D106	A107	V110	R113	K114	K115	S116	R117	S118	K119	Y120	G121	K126	GLU	ALA	ALA	LYS	THR	ALA	ALA	LYS	LYS		MET	P5	T6	Q9	L10	V11	R12	K17	V18	R19	V24	P25	A26	L27	K28	G29	F32	R33	V36	T42	V43	T44	P45	K46	L52	R53	V58	R59	L60	T61	S62	G63	Y64	E65	V66	I70	E79	H80	S81	V82	V83	L84	I85	R86	R97	Y98	H99	I100	W101
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- Chain M:

A72	E73	V74	N77	I78	L81	M82	D83	I84	G85	C86	R87	R88	G89	L90	R91	H92	R93	R94	G95	L96	P97	V98	R99	G100	Q101	R102	T103	R104	T105	N106	A107	R108	T109	R110	K111	G112	K115	THR	VAL	ALA	GLY	LYS	LYS	LYS	ALA	PRO	ARG	LYS	A72	E73	V74	N77	I78	L81	M82	D83	I84	G85	C86	R87	R88	G89	L90	R91	H92	R93	R94	G95	L96	P97	V98	R99	G100	Q101	R102	T103	R104	T105	N106	A107	R108	T109	R110	K111	G112	K115	THR	VAL	ALA	GLY	LYS	LYS	LYS	ALA	PRO	ARG	LYS	A72	E73	V74	N77	I78	L81	M82	D83	I84	G85	C86	R87	R88	G89	L90	R91	H92	R93	R94	G95	L96	P97	V98	R99	G100	Q101	R102	T103	R104	T105	N106	A107	R108	T109	R110	K111	G112	K115	THR	VAL	ALA	GLY	LYS	LYS	LYS	ALA	PRO	ARG	LYS
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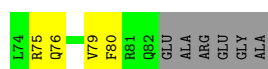
- Chain N:

Met	Met
A1	A1
A2	A2
A3	A3
K4	K4
A5	A5
L6	L6
I7	I7
E8	E8
R12	R12
T13	T13
F16	F16
K17	K17
V18	V18
R19	R19
A20	A20
V21	V21
T22	T22
C23	C23
R24	R24
V25	V25
R26	R26
C27	C27
G28	G28
R29	R29
A30	A30
R31	R31
S32	S32
V33	V33
Y34	Y34
R35	R35
F36	F36
F37	F37
C38	C38
L39	L39
C40	C40
R41	R41
I42	I42
C43	C43
L44	L44
R45	R45
E46	E46
L47	L47
A48	A48
H49	H49
K50	K50
G51	G51
O52	O52
L53	L53
P54	P54
G55	G55
V56	V56
R57	R57
K58	K58
A59	A59
S60	S60

- Chain 0:

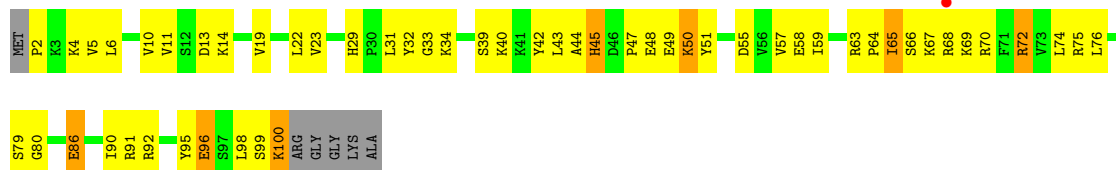
I82	E83	K84	L85	G86	I87	R88	G89																																											
MET	P2	I3	T4	E7	K8	I12	Q13	F14	F15	A16	D21	T22	G23	S24	T25	E26	R35	L39	L43	K44	V45	H46	K47	H50	H51	S52	H53	R54	G55	L56	L57	M58	M59	V60	G61	R64	R65	L66	L67	R68	Y69	L70	R71	R72	E73	D74	P75	E76	R77	Y78

- Chain P: 



- Molecule 17: 30S Ribosomal Protein S17

Chain Q:



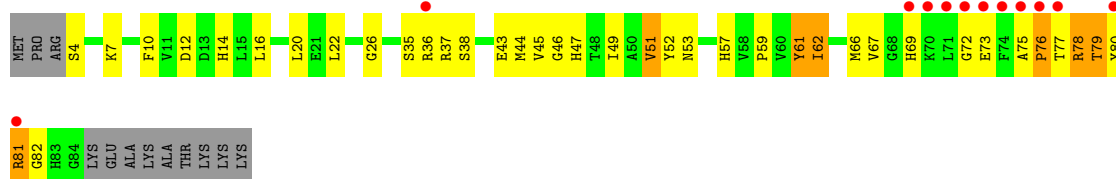
- Molecule 18: 30S Ribosomal Protein S18

Chain R:



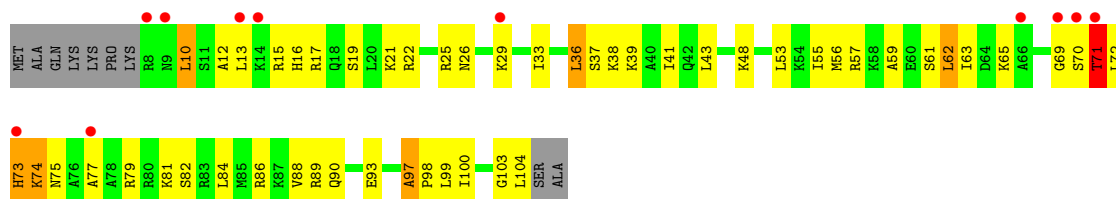
- Molecule 19: 30S Ribosomal Protein S19

Chain S:



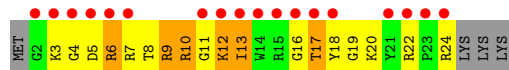
- Molecule 20: 30S Ribosomal Protein S20

Chain T:



- Molecule 21: 30S Ribosomal Protein THX

Chain U:



- Molecule 22: Probable sigma(54) modulation protein

Chain X:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.216 , 0.258 0.499 , 0.502	Depositor DCC
$R_{free}$ test set	49855 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 64.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 993194 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.47	EDS
Total number of atoms	50808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	1.11	53/36028 (0.1%)	1.55	750/56231 (1.3%)
2	B	0.75	0/1809	0.79	1/2450 (0.0%)
3	C	0.78	0/1474	0.86	2/2003 (0.1%)
4	D	0.72	2/1556 (0.1%)	0.87	3/2113 (0.1%)
5	E	0.63	0/1121	0.82	1/1517 (0.1%)
6	F	0.62	0/790	0.73	0/1077
7	G	0.96	0/1183	0.90	0/1599
8	H	0.58	0/1065	0.75	0/1445
9	I	1.00	0/867	0.91	1/1180 (0.1%)
10	J	0.90	0/676	0.97	0/924
11	K	0.61	0/843	0.75	1/1144 (0.1%)
12	L	0.64	0/921	0.80	0/1247
13	M	1.03	0/814	1.03	2/1107 (0.2%)
14	N	0.77	1/487 (0.2%)	0.87	1/649 (0.2%)
15	O	0.66	0/735	0.85	0/981
16	P	0.56	0/667	0.82	0/905
17	Q	0.69	1/836 (0.1%)	0.85	0/1117
18	R	0.63	0/519	0.76	1/699 (0.1%)
19	S	0.98	0/574	0.93	0/781
20	T	0.62	0/715	0.84	1/947 (0.1%)
21	U	0.91	0/203	0.97	0/266
22	X	0.77	0/606	0.82	0/828
All	All	1.00	57/54489 (0.1%)	1.37	764/81210 (0.9%)

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
2	B	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
4	D	0	1
7	G	0	2
9	I	0	1
10	J	0	2
13	M	0	2
15	O	0	1
17	Q	0	1
19	S	0	1
20	T	0	1
All	All	0	17

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1442(A)	G	N9-C4	17.19	1.51	1.38
1	A	1442(A)	G	C2-N3	14.30	1.44	1.32
1	A	1442(A)	G	N3-C4	12.97	1.44	1.35
4	D	12	CYS	CB-SG	11.03	2.00	1.82
1	A	1442(A)	G	C2-N2	8.08	1.42	1.34

The worst 5 of 764 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1442(A)	G	N3-C4-C5	-26.14	115.53	128.60
1	A	1442(A)	G	N3-C4-N9	25.18	141.10	126.00
1	A	1442(A)	G	N3-C2-N2	23.08	136.06	119.90
1	A	1442(A)	G	C4-N9-C1'	18.90	151.07	126.50
1	A	1149	C	N1-C2-O2	16.98	129.09	118.90

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	129	GLU	Peptide
2	B	130	ARG	Peptide
2	B	14	GLY	Peptide
2	B	71	VAL	Peptide
3	C	160	ALA	Peptide

## 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	32185	0	16244	1259	0
2	B	1775	0	1743	121	0
3	C	1450	0	1314	123	0
4	D	1526	0	1415	85	0
5	E	1105	0	1130	60	0
6	F	777	0	737	34	0
7	G	1164	0	1106	99	0
8	H	1045	0	1033	51	0
9	I	852	0	742	79	0
10	J	663	0	558	70	0
11	K	828	0	822	28	0
12	L	905	0	916	32	0
13	M	804	0	752	60	0
14	N	478	0	496	58	0
15	O	724	0	749	31	0
16	P	651	0	638	36	0
17	Q	823	0	891	47	0
18	R	514	0	530	21	0
19	S	560	0	466	40	0
20	T	713	0	766	39	0
21	U	199	0	208	23	0
22	X	601	0	485	16	0
23	A	168	0	0	0	0
23	E	1	0	0	0	0
23	Q	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	282	0	0	25	0
25	C	1	0	0	2	0
25	D	1	0	0	0	0
25	E	2	0	0	0	0
25	K	1	0	0	1	0
25	L	2	0	0	1	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	2	0	0	0	0
25	X	1	0	0	0	0
All	All	50808	0	33741	2164	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 26.

The worst 5 of 2164 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1441:G:H2'	1:A:1459:C:N4	1.50	1.25
1:A:1441:G:C2'	1:A:1459:C:H41	1.54	1.19
1:A:989:C:N4	1:A:1216:G:H1	1.46	1.14
1:A:1441:G:C2'	1:A:1459:C:N4	2.17	1.01
1:A:949:A:H61	1:A:1232:U:H3	1.05	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	227/256 (89%)	197 (87%)	29 (13%)	1 (0%)	43	84
3	C	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	E	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	30	76
6	F	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	30	76
8	H	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
9	I	123/128 (96%)	111 (90%)	11 (9%)	1 (1%)	27	74
10	J	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	11	48
11	K	112/129 (87%)	106 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	27	74
13	M	112/126 (89%)	87 (78%)	21 (19%)	4 (4%)	5	31
14	N	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	O	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	10	45
16	P	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	18	60
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
19	S	79/93 (85%)	65 (82%)	13 (16%)	1 (1%)	18	60
20	T	95/106 (90%)	84 (88%)	8 (8%)	3 (3%)	6	35
21	U	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
22	X	93/101 (92%)	84 (90%)	9 (10%)	0	100	100
All	All	2406/2639 (91%)	2153 (90%)	235 (10%)	18 (1%)	30	76

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	T	100	ILE
12	L	28	LYS
16	P	79	VAL
9	I	102	LEU
10	J	80	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	177/220 (80%)	133 (75%)	44 (25%)	1	3
3	C	114/188 (61%)	92 (81%)	22 (19%)	2	8
4	D	141/181 (78%)	119 (84%)	22 (16%)	4	14
5	E	108/123 (88%)	87 (81%)	21 (19%)	2	8
6	F	76/90 (84%)	58 (76%)	18 (24%)	1	4
7	G	103/127 (81%)	68 (66%)	35 (34%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	103/119 (87%)	83 (81%)	20 (19%)	2	8
9	I	62/99 (63%)	47 (76%)	15 (24%)	1	4
10	J	53/92 (58%)	39 (74%)	14 (26%)	1	2
11	K	81/99 (82%)	70 (86%)	11 (14%)	5	21
12	L	91/109 (84%)	81 (89%)	10 (11%)	9	34
13	M	64/101 (63%)	49 (77%)	15 (23%)	1	5
14	N	46/50 (92%)	32 (70%)	14 (30%)	0	1
15	O	77/80 (96%)	68 (88%)	9 (12%)	8	29
16	P	63/74 (85%)	44 (70%)	19 (30%)	0	1
17	Q	94/97 (97%)	81 (86%)	13 (14%)	5	21
18	R	49/77 (64%)	44 (90%)	5 (10%)	11	37
19	S	43/80 (54%)	32 (74%)	11 (26%)	1	2
20	T	65/82 (79%)	55 (85%)	10 (15%)	4	15
21	U	18/22 (82%)	11 (61%)	7 (39%)	0	0
22	X	38/87 (44%)	29 (76%)	9 (24%)	1	4
All	All	1666/2197 (76%)	1322 (79%)	344 (21%)	2	8

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	126	ASP
9	I	88	TYR
19	S	81	ARG
7	G	153	HIS
8	H	84	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	64	GLN
7	G	96	GLN
18	R	36	ASN
6	F	73	ASN
2	B	212	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1495/1522 (98%)	396 (26%)	34 (2%)

5 of 396 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	793	U
1	A	1064	G
1	A	1442	G
1	A	991	U
1	A	428	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 172 ligands modelled in this entry, 172 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1497/1522 (98%)	0.29	71 (4%) 30 4	50, 96, 158, 171	0
2	B	229/256 (89%)	0.24	7 (3%) 47 7	92, 116, 136, 149	0
3	C	206/239 (86%)	0.22	8 (3%) 37 5	94, 120, 143, 158	0
4	D	208/209 (99%)	0.28	17 (8%) 12 2	76, 93, 114, 124	0
5	E	148/162 (91%)	-0.06	1 (0%) 84 32	69, 88, 104, 127	0
6	F	100/101 (99%)	-0.06	2 (2%) 62 12	70, 86, 103, 117	0
7	G	155/156 (99%)	0.55	15 (9%) 8 2	122, 137, 149, 159	0
8	H	138/138 (100%)	0.36	6 (4%) 34 5	71, 92, 103, 113	0
9	I	125/128 (97%)	0.93	24 (19%) 2 0	115, 139, 152, 163	0
10	J	96/105 (91%)	0.52	8 (8%) 11 2	108, 134, 150, 160	0
11	K	114/129 (88%)	0.14	3 (2%) 53 8	63, 89, 107, 126	0
12	L	122/132 (92%)	0.28	6 (4%) 28 4	63, 77, 96, 109	0
13	M	114/126 (90%)	0.98	18 (15%) 3 1	116, 140, 151, 160	0
14	N	60/61 (98%)	1.09	11 (18%) 2 0	103, 122, 134, 139	0
15	O	88/89 (98%)	0.28	4 (4%) 32 5	63, 85, 105, 111	0
16	P	82/88 (93%)	0.39	2 (2%) 56 9	73, 85, 105, 117	0
17	Q	99/105 (94%)	0.16	1 (1%) 79 23	69, 83, 101, 108	0
18	R	68/88 (77%)	0.03	0 100 100	75, 85, 105, 117	0
19	S	81/93 (87%)	0.81	12 (14%) 3 1	114, 140, 150, 153	0
20	T	97/106 (91%)	0.63	11 (11%) 6 1	72, 86, 105, 115	0
21	U	23/27 (85%)	3.74	18 (78%) 0 0	129, 137, 148, 150	0
22	X	95/101 (94%)	0.57	10 (10%) 7 1	88, 106, 129, 145	0
All	All	3945/4161 (94%)	0.37	255 (6%) 18 3	50, 101, 152, 171	0

The worst 5 of 255 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	86	CYS	16.4
21	U	24	ARG	10.1
21	U	16	GLY	9.2
13	M	87	TYR	8.8
19	S	74	PHE	8.3

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	ZN	N	101	1/1	0.04	-	107,107,107,107	0
23	MG	A	1631	1/1	0.82	-	48,48,48,48	0
23	MG	A	1629	1/1	0.13	-	87,87,87,87	0
23	MG	A	1757	1/1	0.18	-	71,71,71,71	0
23	MG	A	1690	1/1	0.24	-	64,64,64,64	0
23	MG	A	1709	1/1	0.53	-	103,103,103,103	0
23	MG	A	1738	1/1	0.14	-	69,69,69,69	0
23	MG	A	1693	1/1	0.87	-	59,59,59,59	0
23	MG	A	1739	1/1	0.10	-	70,70,70,70	0
23	MG	A	1747	1/1	0.12	-	83,83,83,83	0
23	MG	A	1706	1/1	0.13	-	56,56,56,56	0
23	MG	A	1633	1/1	2.26	-	77,77,77,77	0
23	MG	A	1678	1/1	0.18	-	55,55,55,55	0
23	MG	A	1740	1/1	0.12	-	89,89,89,89	0
23	MG	A	1668	1/1	0.29	-	87,87,87,87	0
23	MG	A	1704	1/1	0.27	-	72,72,72,72	0
23	MG	A	1694	1/1	0.21	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1713	1/1	0.20	-	48,48,48,48	0
23	MG	A	1654	1/1	0.23	-	65,65,65,65	0
23	MG	A	1612	1/1	0.10	-	65,65,65,65	0
23	MG	A	1697	1/1	0.62	-	57,57,57,57	0
23	MG	A	1746	1/1	0.15	-	61,61,61,61	0
23	MG	A	1642	1/1	0.40	-	87,87,87,87	0
23	MG	A	1767	1/1	0.18	-	156,156,156,156	0
23	MG	A	1608	1/1	0.61	-	93,93,93,93	0
23	MG	A	1733	1/1	0.25	-	62,62,62,62	0
23	MG	A	1744	1/1	0.55	-	79,79,79,79	0
23	MG	A	1639	1/1	0.21	-	76,76,76,76	0
23	MG	A	1765	1/1	0.17	-	87,87,87,87	0
23	MG	A	1677	1/1	0.31	-	64,64,64,64	0
23	MG	A	1646	1/1	0.18	-	59,59,59,59	0
23	MG	A	1685	1/1	0.21	-	71,71,71,71	0
23	MG	A	1736	1/1	0.38	-	82,82,82,82	0
23	MG	A	1681	1/1	0.28	-	82,82,82,82	0
23	MG	A	1725	1/1	0.14	-	71,71,71,71	0
23	MG	A	1670	1/1	0.85	-	73,73,73,73	0
23	MG	A	1634	1/1	0.41	-	64,64,64,64	0
23	MG	A	1623	1/1	0.52	-	43,43,43,43	0
23	MG	A	1742	1/1	0.11	-	87,87,87,87	0
23	MG	A	1619	1/1	0.12	-	50,50,50,50	0
23	MG	A	1657	1/1	2.06	-	61,61,61,61	0
23	MG	A	1756	1/1	0.45	-	120,120,120,120	0
23	MG	A	1711	1/1	0.06	-	80,80,80,80	0
23	MG	A	1720	1/1	0.19	-	110,110,110,110	0
23	MG	A	1603	1/1	1.26	-	56,56,56,56	0
23	MG	A	1674	1/1	0.13	-	74,74,74,74	0
23	MG	A	1734	1/1	0.17	-	74,74,74,74	0
23	MG	A	1659	1/1	0.13	-	48,48,48,48	0
23	MG	A	1727	1/1	0.18	-	49,49,49,49	0
23	MG	A	1699	1/1	1.63	-	48,48,48,48	0
23	MG	A	1679	1/1	0.77	-	59,59,59,59	0
23	MG	A	1761	1/1	0.21	-	80,80,80,80	0
24	ZN	D	301	1/1	0.05	-	71,71,71,71	0
23	MG	A	1601	1/1	0.29	-	45,45,45,45	0
23	MG	A	1643	1/1	0.35	-	70,70,70,70	0
23	MG	A	1606	1/1	0.52	-	59,59,59,59	0
23	MG	A	1696	1/1	0.38	-	61,61,61,61	0
23	MG	A	1705	1/1	0.09	-	64,64,64,64	0
23	MG	A	1762	1/1	0.35	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1718	1/1	0.14	-	103,103,103,103	0
23	MG	A	1766	1/1	0.12	-	65,65,65,65	0
23	MG	A	1723	1/1	0.06	-	89,89,89,89	0
23	MG	A	1641	1/1	0.67	-	52,52,52,52	0
23	MG	A	1630	1/1	1.62	-	72,72,72,72	0
23	MG	A	1760	1/1	0.36	-	129,129,129,129	0
23	MG	A	1624	1/1	0.34	-	63,63,63,63	0
23	MG	A	1662	1/1	0.91	-	75,75,75,75	0
23	MG	A	1745	1/1	0.28	-	113,113,113,113	0
23	MG	A	1702	1/1	1.13	-	83,83,83,83	0
23	MG	A	1701	1/1	0.87	-	46,46,46,46	0
23	MG	A	1614	1/1	0.53	-	85,85,85,85	0
23	MG	A	1689	1/1	0.36	-	61,61,61,61	0
23	MG	A	1648	1/1	0.63	-	60,60,60,60	0
23	MG	A	1687	1/1	0.40	-	62,62,62,62	0
23	MG	A	1617	1/1	0.10	-	87,87,87,87	0
23	MG	A	1660	1/1	0.40	-	70,70,70,70	0
23	MG	A	1651	1/1	0.47	-	46,46,46,46	0
23	MG	A	1715	1/1	0.21	-	87,87,87,87	0
23	MG	A	1620	1/1	0.25	-	58,58,58,58	0
23	MG	A	1611	1/1	0.18	-	43,43,43,43	0
23	MG	Q	201	1/1	0.50	-	62,62,62,62	0
23	MG	A	1628	1/1	0.22	-	75,75,75,75	0
23	MG	A	1656	1/1	0.33	-	86,86,86,86	0
23	MG	A	1691	1/1	0.69	-	51,51,51,51	0
23	MG	A	1683	1/1	0.37	-	100,100,100,100	0
23	MG	A	1609	1/1	0.14	-	70,70,70,70	0
23	MG	A	1764	1/1	0.40	-	69,69,69,69	0
23	MG	A	1649	1/1	1.19	-	66,66,66,66	0
23	MG	A	1755	1/1	0.10	-	61,61,61,61	0
23	MG	A	1675	1/1	0.29	-	61,61,61,61	0
23	MG	A	1632	1/1	0.75	-	69,69,69,69	0
23	MG	A	1652	1/1	0.32	-	76,76,76,76	0
23	MG	A	1613	1/1	0.52	-	66,66,66,66	0
23	MG	A	1673	1/1	0.82	-	57,57,57,57	0
23	MG	A	1664	1/1	0.20	-	80,80,80,80	0
23	MG	A	1708	1/1	0.33	-	96,96,96,96	0
23	MG	A	1625	1/1	1.32	-	63,63,63,63	0
23	MG	A	1751	1/1	0.16	-	95,95,95,95	0
23	MG	A	1640	1/1	0.46	-	82,82,82,82	0
23	MG	A	1732	1/1	0.18	-	81,81,81,81	0
23	MG	A	1663	1/1	0.46	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1627	1/1	0.29	-	55,55,55,55	0
23	MG	A	1658	1/1	0.20	-	58,58,58,58	0
23	MG	A	1698	1/1	0.51	-	47,47,47,47	0
23	MG	A	1665	1/1	0.68	-	84,84,84,84	0
23	MG	A	1729	1/1	0.27	-	52,52,52,52	0
23	MG	A	1688	1/1	0.63	-	54,54,54,54	0
23	MG	A	1647	1/1	0.38	-	86,86,86,86	0
23	MG	A	1737	1/1	0.09	-	66,66,66,66	0
23	MG	A	1644	1/1	0.67	-	53,53,53,53	0
23	MG	A	1667	1/1	0.37	-	77,77,77,77	0
23	MG	A	1669	1/1	1.09	-	76,76,76,76	0
23	MG	A	1682	1/1	0.17	-	58,58,58,58	0
23	MG	A	1750	1/1	0.08	-	88,88,88,88	0
23	MG	A	1749	1/1	0.69	-	97,97,97,97	0
23	MG	A	1638	1/1	0.27	-	52,52,52,52	0
23	MG	A	1636	1/1	1.12	-	59,59,59,59	0
23	MG	A	1758	1/1	0.34	-	86,86,86,86	0
23	MG	A	1763	1/1	0.18	-	84,84,84,84	0
23	MG	A	1716	1/1	0.41	-	73,73,73,73	0
23	MG	A	1602	1/1	0.44	-	62,62,62,62	0
23	MG	A	1700	1/1	0.58	-	69,69,69,69	0
23	MG	A	1661	1/1	0.51	-	67,67,67,67	0
23	MG	A	1676	1/1	0.49	-	73,73,73,73	0
23	MG	A	1714	1/1	0.19	-	103,103,103,103	0
23	MG	A	1752	1/1	0.11	-	58,58,58,58	0
23	MG	A	1759	1/1	0.81	-	74,74,74,74	0
23	MG	A	1653	1/1	0.25	-	57,57,57,57	0
23	MG	A	1607	1/1	0.23	-	50,50,50,50	0
23	MG	A	1712	1/1	0.19	-	63,63,63,63	0
23	MG	A	1724	1/1	0.11	-	64,64,64,64	0
23	MG	A	1695	1/1	0.57	-	50,50,50,50	0
23	MG	A	1728	1/1	0.09	-	65,65,65,65	0
23	MG	A	1655	1/1	0.42	-	98,98,98,98	0
23	MG	A	1726	1/1	0.18	-	55,55,55,55	0
23	MG	A	1710	1/1	0.23	-	94,94,94,94	0
23	MG	A	1692	1/1	0.29	-	86,86,86,86	0
23	MG	A	1721	1/1	0.07	-	83,83,83,83	0
23	MG	A	1626	1/1	0.57	-	62,62,62,62	0
23	MG	A	1615	1/1	0.37	-	65,65,65,65	0
23	MG	A	1686	1/1	0.13	-	61,61,61,61	0
23	MG	A	1722	1/1	0.08	-	54,54,54,54	0
23	MG	E	201	1/1	1.14	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1672	1/1	0.40	-	66,66,66,66	0
23	MG	A	1735	1/1	0.20	-	110,110,110,110	0
23	MG	A	1707	1/1	0.17	-	92,92,92,92	0
23	MG	A	1741	1/1	0.28	-	112,112,112,112	0
23	MG	A	1666	1/1	0.29	-	64,64,64,64	0
23	MG	A	1621	1/1	0.41	-	64,64,64,64	0
23	MG	A	1730	1/1	0.35	-	46,46,46,46	0
23	MG	A	1610	1/1	0.52	-	60,60,60,60	0
23	MG	A	1622	1/1	0.23	-	47,47,47,47	0
23	MG	A	1719	1/1	0.22	-	102,102,102,102	0
23	MG	A	1604	1/1	0.56	-	81,81,81,81	0
23	MG	A	1768	1/1	0.25	-	77,77,77,77	0
23	MG	A	1743	1/1	0.23	-	68,68,68,68	0
23	MG	A	1684	1/1	0.46	-	91,91,91,91	0
23	MG	A	1754	1/1	0.15	-	78,78,78,78	0
23	MG	A	1616	1/1	0.28	-	58,58,58,58	0
23	MG	A	1618	1/1	1.29	-	64,64,64,64	0
23	MG	A	1703	1/1	0.23	-	70,70,70,70	0
23	MG	A	1748	1/1	0.22	-	116,116,116,116	0
23	MG	A	1635	1/1	0.31	-	60,60,60,60	0
23	MG	A	1753	1/1	0.19	-	61,61,61,61	0
23	MG	A	1717	1/1	0.10	-	87,87,87,87	0
23	MG	A	1645	1/1	0.77	-	60,60,60,60	0
23	MG	A	1605	1/1	0.68	-	67,67,67,67	0
23	MG	A	1680	1/1	0.80	-	78,78,78,78	0
23	MG	A	1650	1/1	0.21	-	60,60,60,60	0
23	MG	A	1637	1/1	0.61	-	73,73,73,73	0
23	MG	A	1671	1/1	0.81	-	49,49,49,49	0
23	MG	A	1731	1/1	0.08	-	60,60,60,60	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.