



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:17 am GMT

PDB ID : 4OX9  
Title : Crystal structure of the aminoglycoside resistance methyltransferase NpmA bound to the 30S ribosomal subunit  
Authors : Dunkle, J.A.; Conn, G.L.; Dunham, C.M.  
Deposited on : 2014-02-04  
Resolution : 3.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949



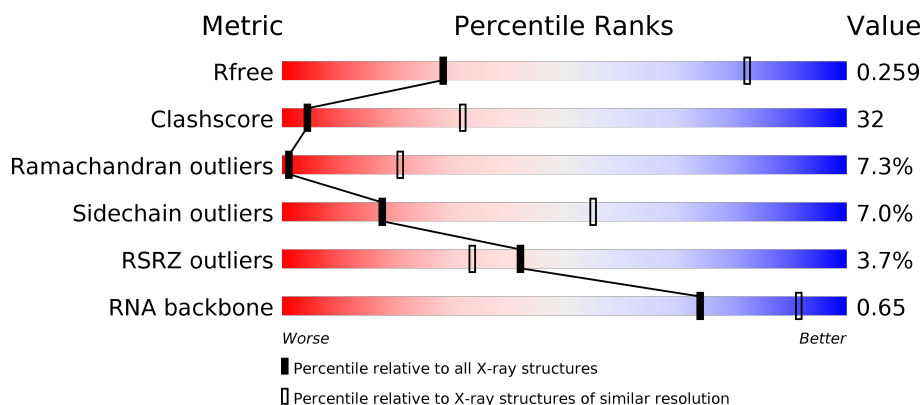
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)
RNA backbone	2435	1016 (4.70-2.90)



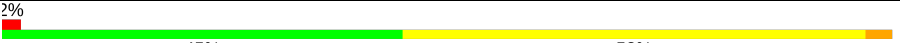

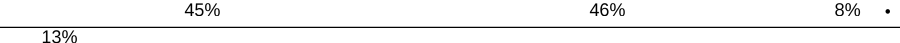


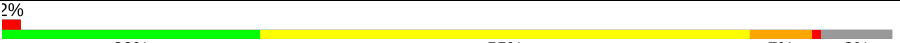

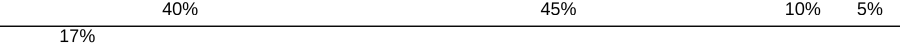
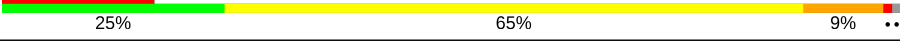

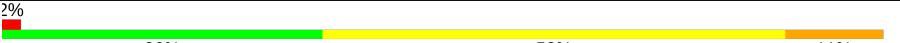


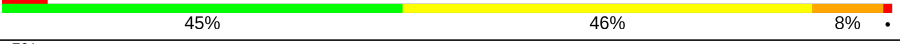
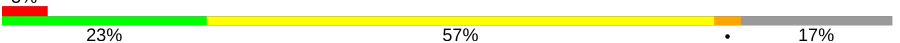
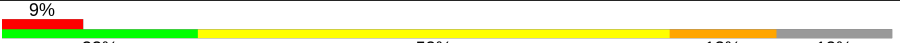
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	1513	<div> <div>2%</div> <div>32% 54% 12%</div> </div>
2	B	256	<div> <div>3%</div> <div>25% 52% 12% 9%</div> </div>
3	C	239	<div> <div>4%</div> <div>26% 46% 14%</div> </div>
4	D	208	<div> <div>0%</div> <div>43% 52%</div> </div>

*Continued on next page...*



Continued from previous page...

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	129	
12	L	131	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	
22	Y	222	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1601	-	-	-	X
23	MG	A	1607	-	-	-	X
23	MG	A	1609	-	-	-	X
23	MG	A	1611	-	-	-	X
23	MG	A	1616	-	-	-	X
23	MG	A	1624	-	-	-	X
23	MG	A	1629	-	-	-	X

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1634	-	-	-	X
23	MG	A	1637	-	-	-	X
23	MG	A	1639	-	-	-	X
23	MG	A	1645	-	-	-	X
23	MG	A	1651	-	-	-	X
23	MG	A	1655	-	-	-	X
23	MG	A	1661	-	-	-	X
23	MG	A	1663	-	-	-	X
23	MG	A	1669	-	-	-	X
23	MG	A	1670	-	-	-	X
23	MG	A	1681	-	-	-	X
23	MG	A	1700	-	-	-	X
23	MG	A	1701	-	-	-	X
23	MG	A	1702	-	-	-	X
23	MG	A	1703	-	-	-	X
23	MG	A	1704	-	-	-	X
23	MG	A	1713	-	-	-	X
23	MG	A	1715	-	-	-	X
23	MG	N	102	-	-	-	X



## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 53527 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14418	6002	10467	1507			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	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
			1612	1016	314	281	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
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	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	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			785	494	153	137	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	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	125	Total	C	N	O	S	0	0	0
			997	617	207	171	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	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- 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	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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



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

- Molecule 22 is a protein called 16S rRNA (adenine(1408)-N(1))-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	219	Total	C	N	O	S	0	0	0
			1761	1138	294	328	1			

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

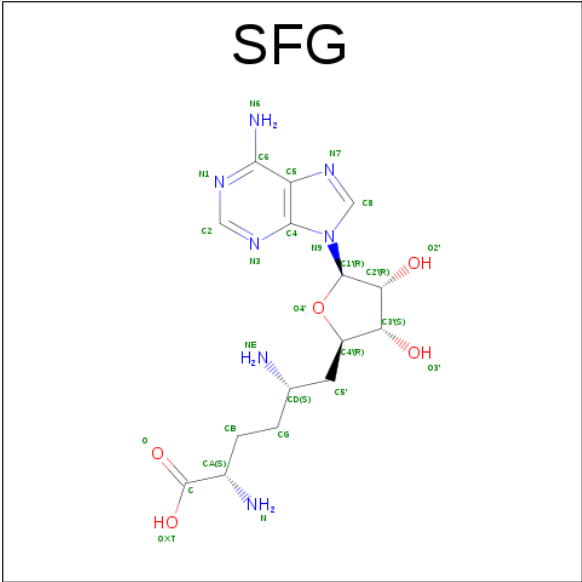
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Mg	0	0
			1	1		
23	A	117	Total	Mg	0	0
			117	117		
23	N	1	Total	Mg	0	0
			1	1		
23	E	1	Total	Mg	0	0
			1	1		

- 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 SINEFUNGIN (three-letter code: SFG) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>7</sub>O<sub>5</sub>).





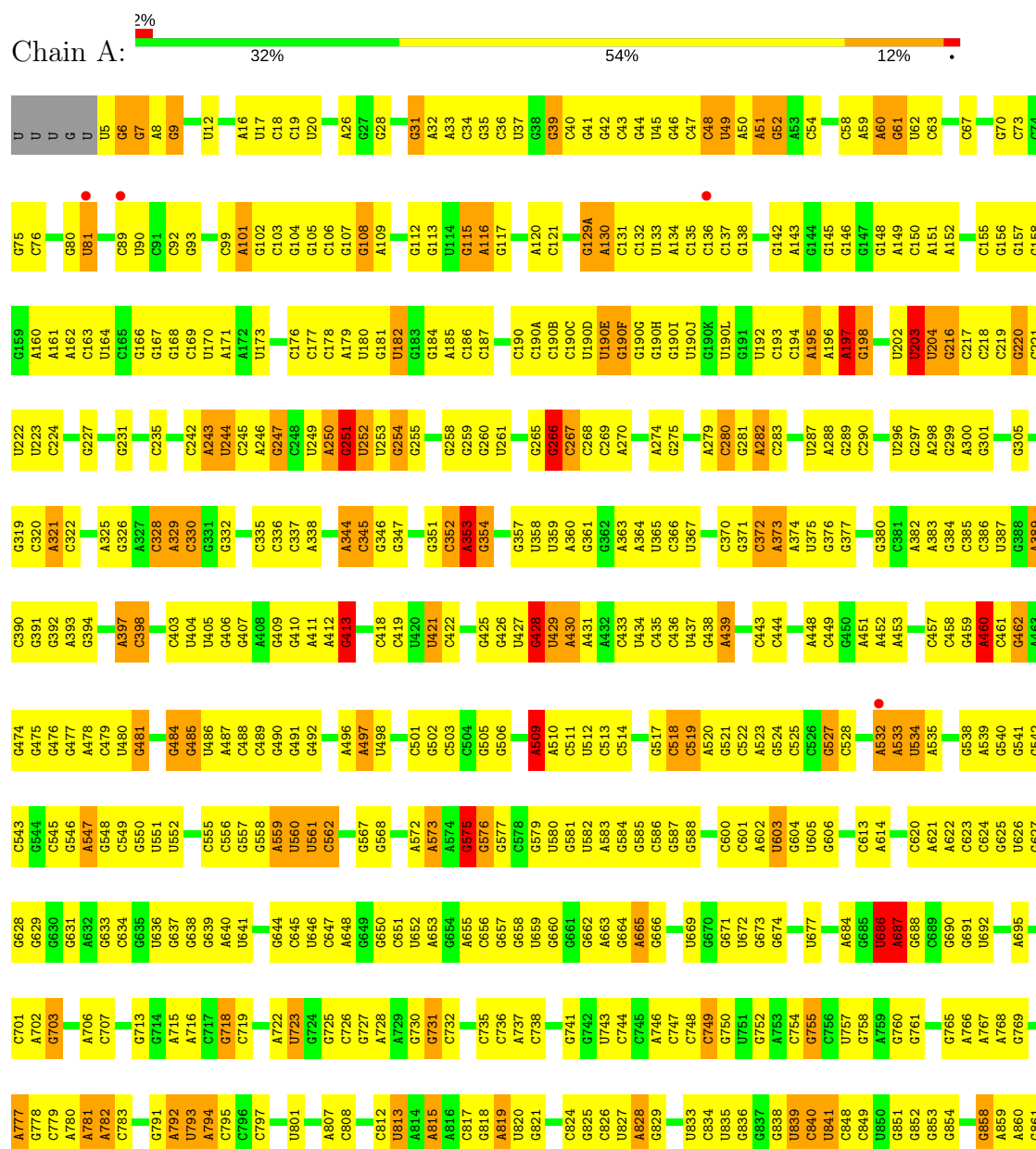
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	Y	1	Total	C	N	O	0	0
			27	15	7	5		



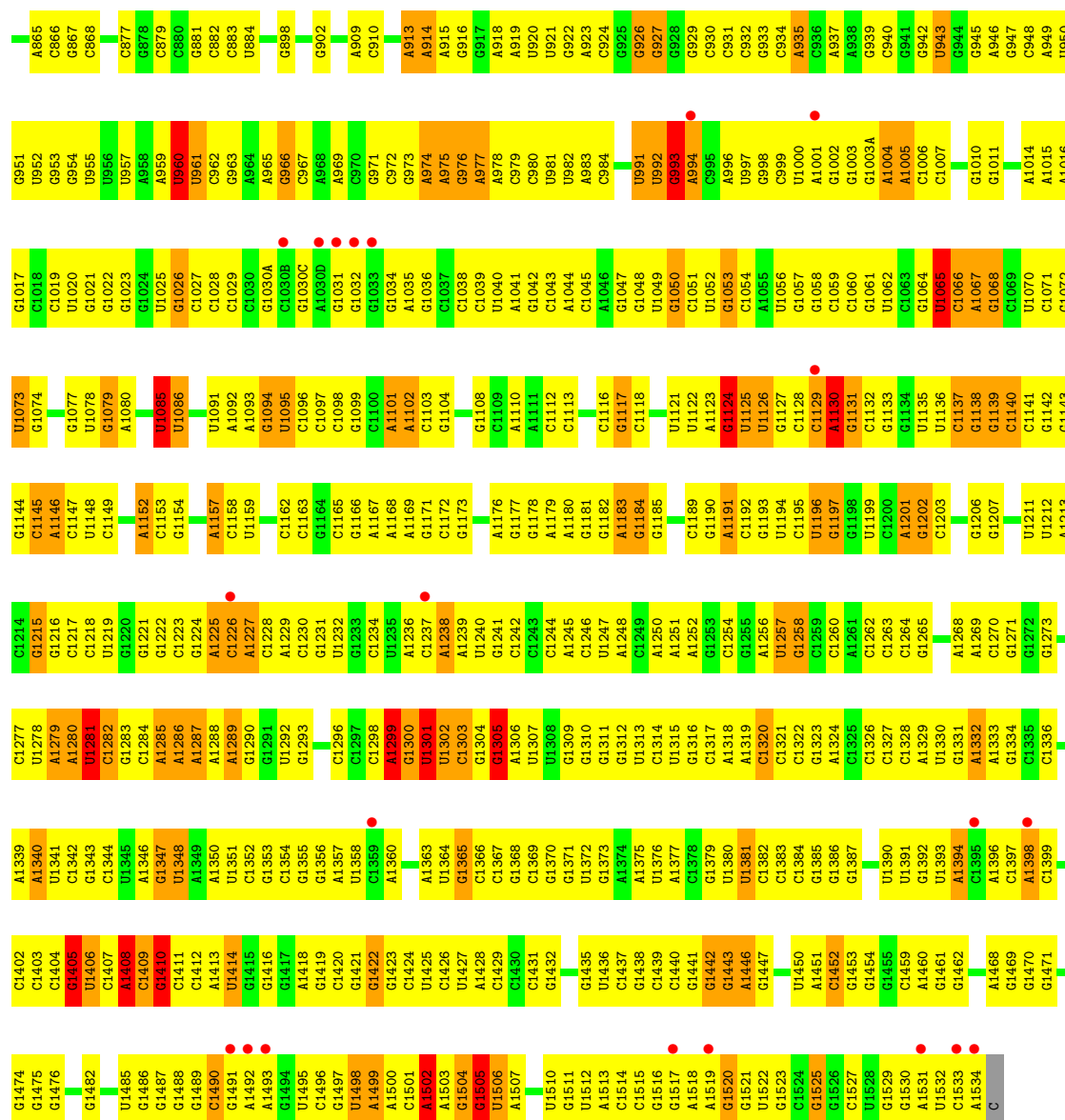
### 3 Residue-property plots

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

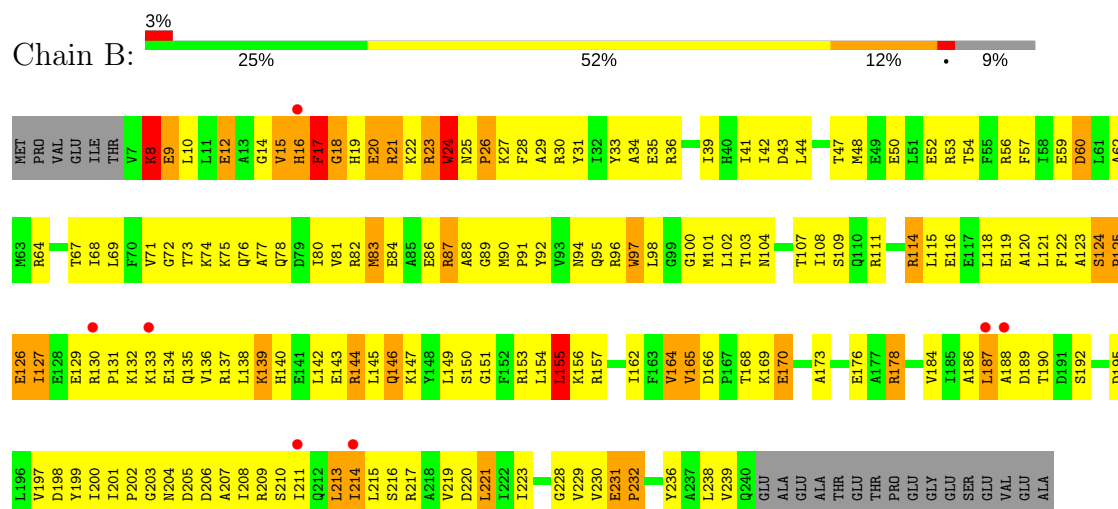
#### • Molecule 1: 16S rRNA





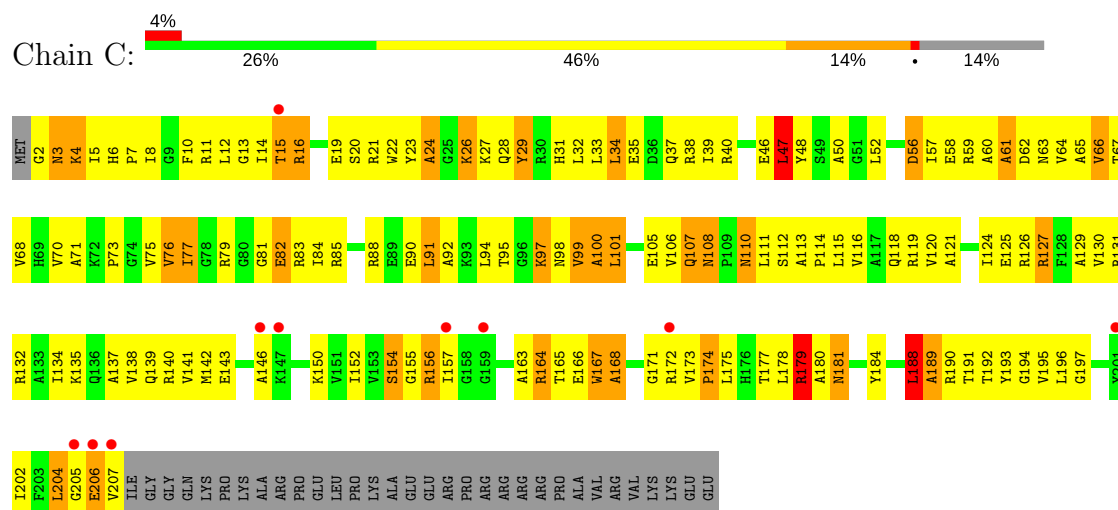


### • Molecule 2: 30S ribosomal protein S2

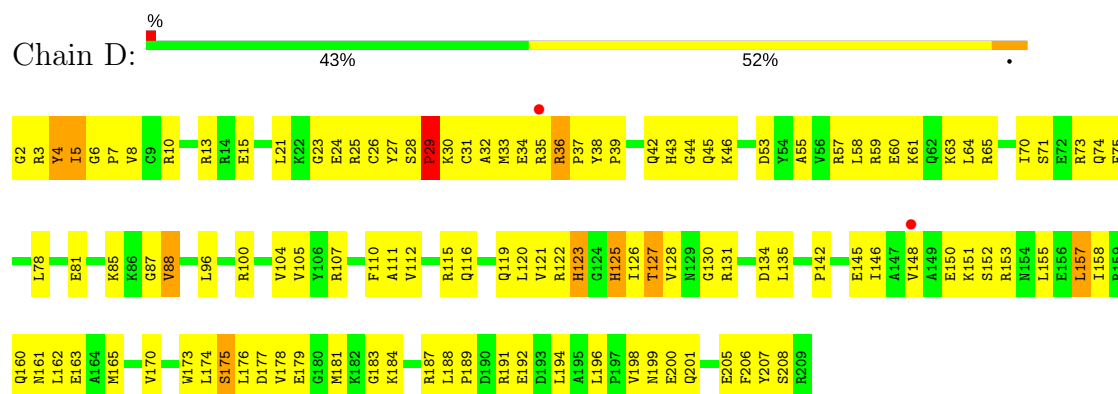




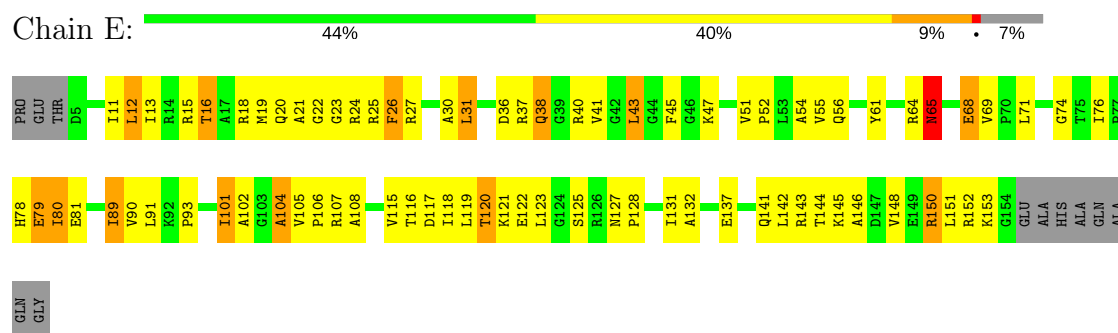
- Molecule 3: 30S ribosomal protein S3



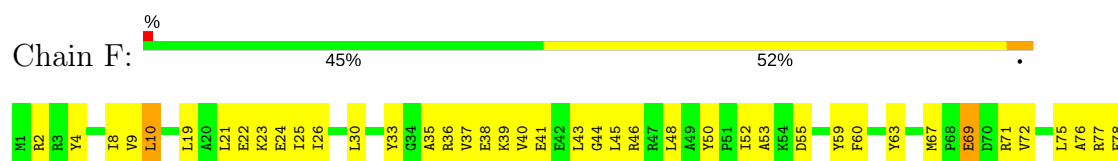
- Molecule 4: 30S ribosomal protein S4



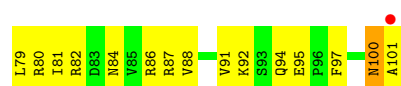
- Molecule 5: 30S ribosomal protein S5



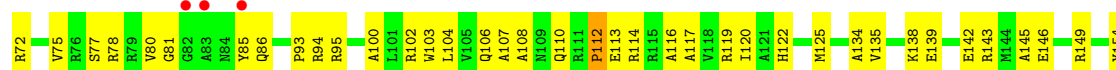
- Molecule 6: 30S ribosomal protein S6







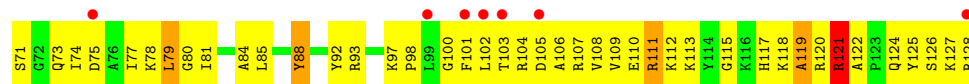
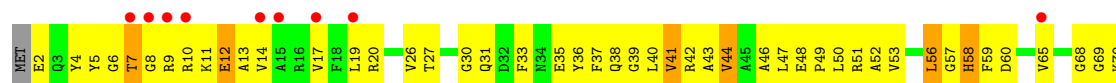
• Molecule 7: 30S ribosomal protein S7



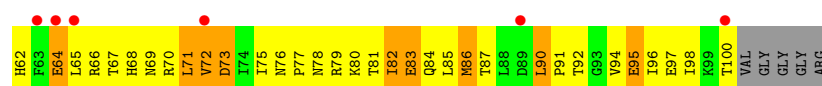
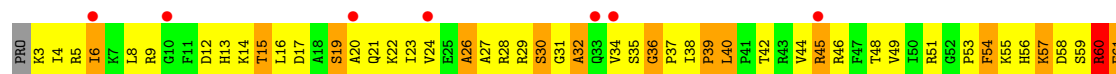
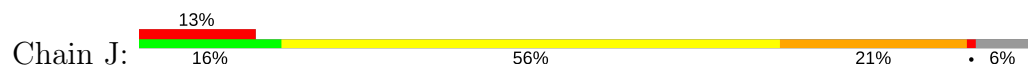
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11



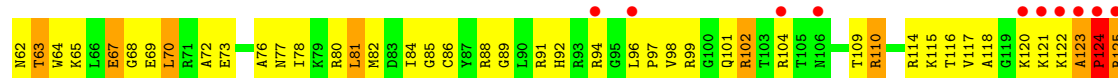




• Molecule 12: 30S ribosomal protein S12



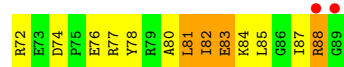
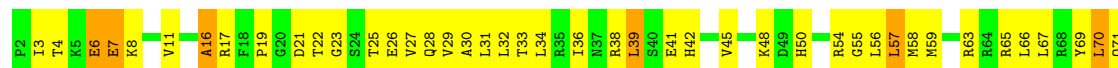
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z

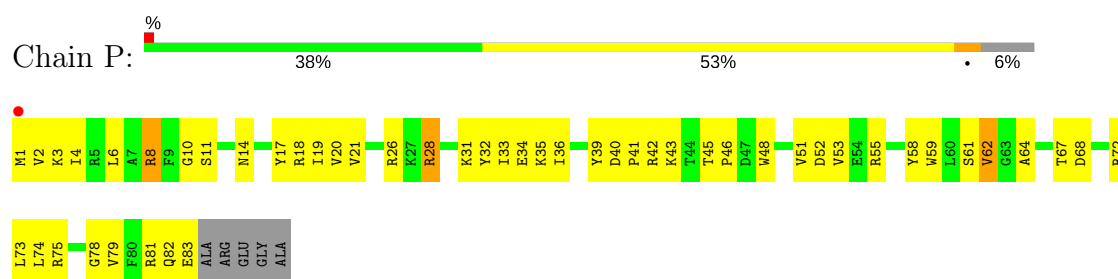


• Molecule 15: 30S ribosomal protein S15

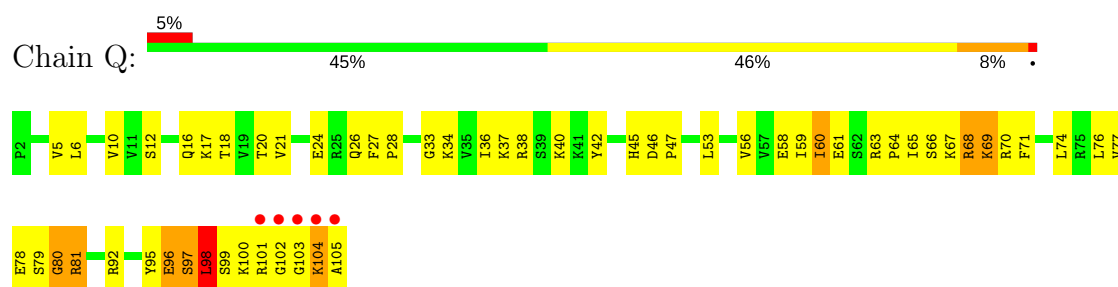


• Molecule 16: 30S ribosomal protein S16

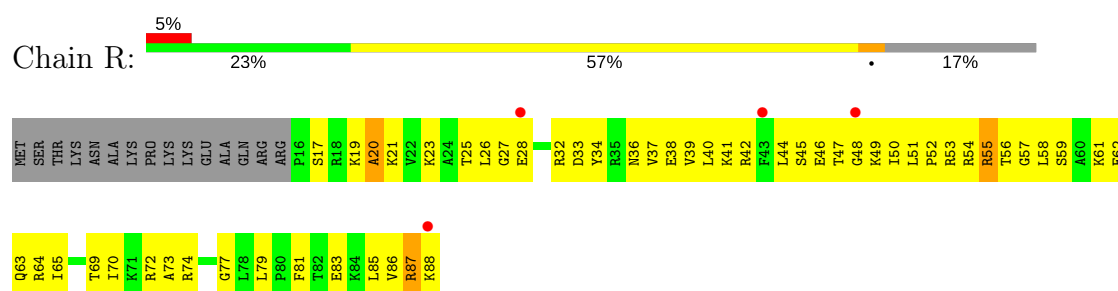




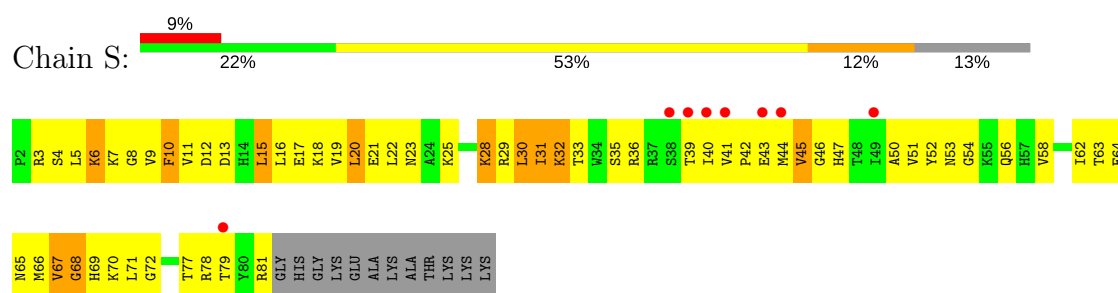
- Molecule 17: 30S ribosomal protein S17



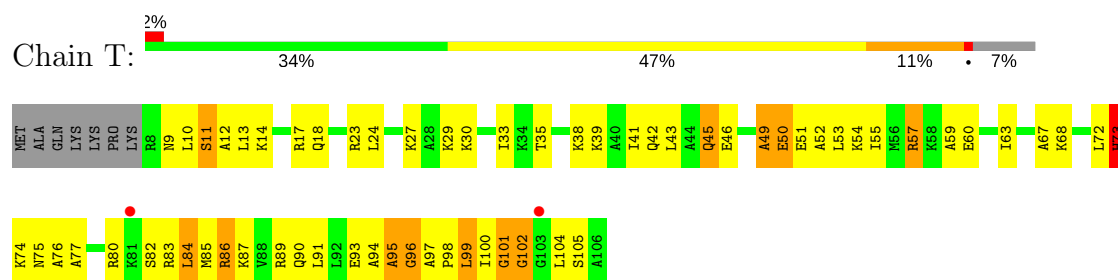
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

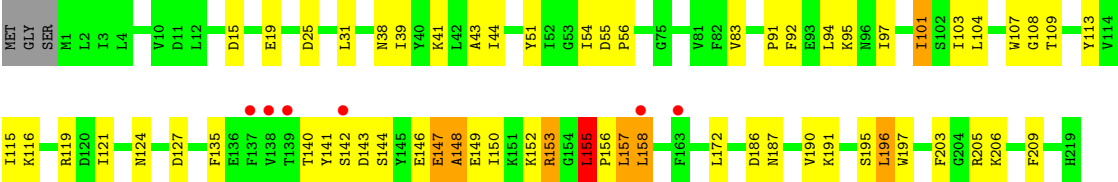


- Molecule 21: 30S ribosomal protein Thx





● Molecule 22: 16S rRNA (adenine(1408)-N(1))-methyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	403.52Å 403.52Å 176.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.80 49.71 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.72-3.80) 94.1 (49.71-3.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.233 , 0.257 0.234 , 0.259	Depositor DCC
$R_{free}$ test set	7030 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	135.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 81.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	53527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SFG, 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	0.49	4/36262 (0.0%)	0.77	54/56597 (0.1%)
2	B	0.42	0/1935	0.69	1/2609 (0.0%)
3	C	0.43	0/1636	0.67	0/2205
4	D	0.44	0/1733	0.65	0/2318
5	E	0.69	2/1162 (0.2%)	0.83	2/1564 (0.1%)
6	F	0.43	0/856	0.64	0/1154
7	G	0.38	0/1276	0.62	0/1709
8	H	0.44	0/1136	0.74	0/1527
9	I	0.36	0/1029	0.62	0/1379
10	J	0.47	0/798	0.73	0/1073
11	K	0.39	0/900	0.70	0/1213
12	L	0.42	0/986	0.72	0/1320
13	M	0.40	0/1008	0.67	0/1347
14	N	0.40	0/501	0.78	0/664
15	O	0.36	0/745	0.63	1/992 (0.1%)
16	P	0.43	0/716	0.76	0/963
17	Q	0.48	0/870	0.75	0/1159
18	R	0.43	0/604	0.64	0/801
19	S	0.35	0/661	0.72	1/890 (0.1%)
20	T	0.45	0/765	0.74	0/1007
21	V	0.43	0/212	0.64	0/277
22	Y	0.49	0/1796	0.83	3/2418 (0.1%)
All	All	0.47	6/57587 (0.0%)	0.75	62/85186 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	41

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
22	Y	0	2
All	All	0	43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	69	VAL	C-N	11.28	1.55	1.34
5	E	101	ILE	C-N	10.62	1.58	1.34
1	A	669	U	O3'-P	6.03	1.68	1.61
1	A	604	G	O3'-P	-5.28	1.54	1.61
1	A	1405	G	O3'-P	5.17	1.67	1.61

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1406	U	O5'-P-OP2	-11.47	95.38	105.70
1	A	1498	U	C2'-C3'-O3'	9.91	131.29	109.50
1	A	1405	G	P-O3'-C3'	-9.56	108.22	119.70
1	A	243	A	C2'-C3'-O3'	9.46	130.32	109.50
1	A	559	A	C2'-C3'-O3'	9.15	129.63	109.50

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	U	Sidechain
1	A	197	A	Sidechain
1	A	203	U	Sidechain
1	A	220	G	Sidechain
1	A	231	G	Sidechain

## 5.2 Too-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 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	32394	0	16349	1169	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1900	0	1951	206	0
3	C	1612	0	1677	212	0
4	D	1703	0	1764	134	0
5	E	1146	0	1207	101	0
6	F	843	0	857	65	0
7	G	1257	0	1296	91	0
8	H	1116	0	1177	66	0
9	I	1010	0	1037	114	0
10	J	785	0	823	123	0
11	K	885	0	904	82	0
12	L	970	0	1057	106	0
13	M	997	0	1072	119	0
14	N	492	0	529	74	0
15	O	734	0	771	58	0
16	P	700	0	720	56	0
17	Q	857	0	928	85	0
18	R	598	0	670	61	0
19	S	647	0	673	83	0
20	T	763	0	860	88	0
21	V	208	0	221	26	0
22	Y	1761	0	1792	47	0
23	A	117	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
23	N	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	Y	27	0	22	3	0
All	All	53527	0	38357	2882	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 32.

The worst 5 of 2882 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)
9:I:57:GLY:O	9:I:58:HIS:HD2	1.22	1.18
20:T:54:LYS:HG3	20:T:100:ILE:CD1	1.73	1.18
12:L:41:ARG:HG2	12:L:42:THR:H	1.03	1.15
9:I:57:GLY:O	9:I:58:HIS:CD2	2.00	1.14
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.22	1.14



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	232/256 (91%)	174 (75%)	34 (15%)	24 (10%)	0	11
3	C	204/239 (85%)	135 (66%)	41 (20%)	28 (14%)	0	5
4	D	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	3	32
5	E	148/161 (92%)	130 (88%)	13 (9%)	5 (3%)	4	38
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	18	61
7	G	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1	24
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	5	41
9	I	125/128 (98%)	88 (70%)	27 (22%)	10 (8%)	1	18
10	J	96/104 (92%)	59 (62%)	20 (21%)	17 (18%)	0	3
11	K	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	19
12	L	122/131 (93%)	97 (80%)	16 (13%)	9 (7%)	1	20
13	M	123/126 (98%)	88 (72%)	27 (22%)	8 (6%)	1	24
14	N	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	7
15	O	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	2	27
16	P	81/88 (92%)	65 (80%)	15 (18%)	1 (1%)	15	58
17	Q	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	19
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	6	42
19	S	78/92 (85%)	49 (63%)	18 (23%)	11 (14%)	0	5
20	T	97/106 (92%)	63 (65%)	21 (22%)	13 (13%)	0	5
21	V	22/26 (85%)	19 (86%)	2 (9%)	1 (4%)	3	31
22	Y	217/222 (98%)	206 (95%)	6 (3%)	5 (2%)	7	46
All	All	2573/2750 (94%)	2014 (78%)	372 (14%)	187 (7%)	1	21



5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG

### 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	202/220 (92%)	182 (90%)	20 (10%)	9	40
3	C	160/188 (85%)	142 (89%)	18 (11%)	7	34
4	D	180/180 (100%)	173 (96%)	7 (4%)	37	70
5	E	115/122 (94%)	101 (88%)	14 (12%)	6	30
6	F	90/90 (100%)	87 (97%)	3 (3%)	43	74
7	G	126/126 (100%)	123 (98%)	3 (2%)	54	80
8	H	119/119 (100%)	109 (92%)	10 (8%)	13	49
9	I	98/99 (99%)	92 (94%)	6 (6%)	22	60
10	J	86/91 (94%)	77 (90%)	9 (10%)	8	37
11	K	90/99 (91%)	84 (93%)	6 (7%)	19	57
12	L	104/108 (96%)	96 (92%)	8 (8%)	15	52
13	M	100/101 (99%)	90 (90%)	10 (10%)	9	39
14	N	49/49 (100%)	47 (96%)	2 (4%)	35	69
15	O	79/79 (100%)	72 (91%)	7 (9%)	11	45
16	P	72/74 (97%)	67 (93%)	5 (7%)	18	56
17	Q	96/96 (100%)	90 (94%)	6 (6%)	21	58
18	R	64/77 (83%)	62 (97%)	2 (3%)	45	75
19	S	71/79 (90%)	68 (96%)	3 (4%)	34	68
20	T	76/82 (93%)	70 (92%)	6 (8%)	14	51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	V	19/21 (90%)	19 (100%)	0	100	100
22	Y	193/195 (99%)	185 (96%)	8 (4%)	35	69
All	All	2189/2295 (95%)	2036 (93%)	153 (7%)	18	55

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	85	ARG
10	J	64	GLU
20	T	73	HIS
8	H	92	ARG
9	I	53	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	58	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1513 (99%)	229 (15%)	0

5 of 229 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

There are no RNA pucker outliers to report.

## 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 123 ligands modelled in this entry, 122 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
25	SFG	Y	301	-	21,29,29	1.00	2 (9%)	18,42,42	2.08	4 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SFG	Y	301	-	-	0/9/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	301	SFG	C8-N7	-2.13	1.30	1.34
25	Y	301	SFG	O4'-C1'	2.67	1.45	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	301	SFG	N3-C2-N1	-7.37	122.44	128.86
25	Y	301	SFG	C4'-O4'-C1'	-2.65	106.95	109.77
25	Y	301	SFG	C4-C5-N7	-2.38	107.11	109.41
25	Y	301	SFG	C4'-C5'-CD	-2.27	109.49	113.51

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	301	SFG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	1507/1513 (99%)	0.03	25 (1%) 70 61	18, 71, 170, 260	0
2	B	234/256 (91%)	0.13	7 (2%) 51 40	29, 94, 152, 190	0
3	C	206/239 (86%)	0.05	10 (4%) 30 24	44, 104, 145, 171	0
4	D	208/208 (100%)	0.03	2 (0%) 82 75	25, 79, 127, 182	0
5	E	150/161 (93%)	-0.18	0 100 100	18, 56, 106, 148	0
6	F	101/101 (100%)	-0.10	1 (0%) 82 75	48, 103, 142, 156	0
7	G	155/155 (100%)	-0.18	3 (1%) 67 58	40, 96, 148, 172	0
8	H	138/138 (100%)	-0.02	1 (0%) 87 82	11, 41, 81, 116	0
9	I	127/128 (99%)	0.59	16 (12%) 4 5	40, 105, 144, 165	0
10	J	98/104 (94%)	0.82	13 (13%) 4 4	55, 123, 165, 188	0
11	K	119/129 (92%)	0.14	3 (2%) 58 47	36, 81, 129, 171	0
12	L	124/131 (94%)	0.28	4 (3%) 48 38	18, 74, 120, 165	0
13	M	125/126 (99%)	1.09	22 (17%) 2 2	56, 97, 137, 185	0
14	N	60/60 (100%)	0.34	2 (3%) 47 37	44, 102, 136, 160	0
15	O	88/88 (100%)	0.14	2 (2%) 61 51	17, 63, 122, 167	0
16	P	83/88 (94%)	0.37	1 (1%) 79 71	21, 56, 95, 122	0
17	Q	104/104 (100%)	0.40	5 (4%) 31 25	13, 56, 119, 198	0
18	R	73/88 (82%)	0.25	4 (5%) 26 19	35, 82, 143, 191	0
19	S	80/92 (86%)	0.49	8 (10%) 8 7	73, 124, 155, 197	0
20	T	99/106 (93%)	0.12	2 (2%) 65 56	38, 80, 118, 156	0
21	V	24/26 (92%)	0.67	4 (16%) 2 2	51, 88, 137, 141	0
22	Y	219/222 (98%)	0.32	19 (8%) 11 9	64, 119, 160, 196	0
All	All	4122/4263 (96%)	0.15	154 (3%) 42 34	11, 82, 153, 260	0

The worst 5 of 154 RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
13	M	124	PRO	17.2
13	M	123	ALA	12.9
15	O	89	GLY	10.4
10	J	64	GLU	7.6
13	M	125	ARG	7.2

## 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1651	1/1	0.86	1.11	47.91	8,8,8,8	0
23	MG	A	1703	1/1	0.92	1.06	44.92	70,70,70,70	0
23	MG	A	1713	1/1	0.72	0.81	39.84	39,39,39,39	0
23	MG	A	1637	1/1	0.87	0.97	38.21	70,70,70,70	0
23	MG	A	1629	1/1	0.85	0.94	30.64	70,70,70,70	0
23	MG	A	1700	1/1	0.85	0.94	25.44	10,10,10,10	0
23	MG	A	1607	1/1	0.76	0.57	24.79	61,61,61,61	0
23	MG	A	1669	1/1	0.40	0.81	20.22	33,33,33,33	0
23	MG	A	1616	1/1	0.78	0.71	20.16	19,19,19,19	0
23	MG	A	1624	1/1	0.65	0.88	16.98	70,70,70,70	0
23	MG	A	1634	1/1	0.96	0.56	15.44	3,3,3,3	0
23	MG	A	1702	1/1	0.91	0.46	12.62	32,32,32,32	0
23	MG	A	1609	1/1	0.89	0.53	12.22	33,33,33,33	0
23	MG	A	1663	1/1	0.95	0.42	11.49	16,16,16,16	0
23	MG	A	1601	1/1	0.24	0.59	10.95	42,42,42,42	0
23	MG	N	102	1/1	0.56	1.19	10.30	24,24,24,24	0
23	MG	A	1670	1/1	0.91	0.40	7.96	34,34,34,34	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1681	1/1	0.95	0.38	7.26	41,41,41,41	0
23	MG	A	1645	1/1	0.66	0.35	6.84	12,12,12,12	0
23	MG	A	1655	1/1	0.91	0.20	5.25	47,47,47,47	0
23	MG	A	1611	1/1	0.76	0.38	4.91	57,57,57,57	0
23	MG	A	1704	1/1	0.89	0.37	3.73	29,29,29,29	0
23	MG	A	1639	1/1	0.94	0.28	3.28	15,15,15,15	0
23	MG	A	1701	1/1	0.97	0.28	3.14	6,6,6,6	0
23	MG	A	1661	1/1	0.59	0.40	2.93	93,93,93,93	0
23	MG	A	1715	1/1	0.93	0.45	2.47	9,9,9,9	0
23	MG	A	1710	1/1	0.92	0.36	1.93	20,20,20,20	0
23	MG	A	1689	1/1	0.68	0.34	1.66	58,58,58,58	0
25	SFG	Y	301	27/27	0.87	0.36	0.45	110,110,110,110	0
23	MG	A	1659	1/1	0.98	0.23	0.25	12,12,12,12	0
23	MG	B	301	1/1	0.66	0.23	-0.30	59,59,59,59	0
24	ZN	N	101	1/1	0.97	0.16	-0.75	108,108,108,108	0
23	MG	A	1638	1/1	0.97	0.16	-1.75	47,47,47,47	0
23	MG	A	1641	1/1	0.91	0.30	-	0,0,0,0	0
23	MG	A	1652	1/1	0.48	1.17	-	42,42,42,42	0
23	MG	A	1630	1/1	0.74	0.78	-	7,7,7,7	0
23	MG	A	1696	1/1	0.62	0.73	-	27,27,27,27	0
23	MG	A	1642	1/1	0.97	0.38	-	33,33,33,33	0
23	MG	A	1605	1/1	0.83	1.19	-	8,8,8,8	0
23	MG	A	1690	1/1	0.86	1.17	-	33,33,33,33	0
23	MG	A	1677	1/1	0.67	0.71	-	63,63,63,63	0
23	MG	A	1644	1/1	0.84	0.36	-	54,54,54,54	0
23	MG	A	1678	1/1	0.83	0.98	-	27,27,27,27	0
23	MG	A	1625	1/1	0.96	0.78	-	0,0,0,0	0
23	MG	A	1654	1/1	0.77	0.83	-	16,16,16,16	0
23	MG	A	1693	1/1	0.70	1.39	-	18,18,18,18	0
23	MG	A	1646	1/1	0.38	0.68	-	18,18,18,18	0
23	MG	A	1687	1/1	0.98	0.69	-	17,17,17,17	0
23	MG	A	1648	1/1	0.96	0.52	-	4,4,4,4	0
23	MG	A	1708	1/1	0.68	0.75	-	21,21,21,21	0
23	MG	A	1658	1/1	0.59	0.59	-	40,40,40,40	0
23	MG	A	1627	1/1	0.43	0.46	-	52,52,52,52	0
23	MG	A	1674	1/1	0.77	0.77	-	8,8,8,8	0
23	MG	A	1695	1/1	0.71	1.55	-	52,52,52,52	0
23	MG	A	1667	1/1	0.73	0.46	-	76,76,76,76	0
23	MG	A	1628	1/1	0.97	0.30	-	54,54,54,54	0
23	MG	A	1619	1/1	0.93	0.35	-	40,40,40,40	0
23	MG	A	1643	1/1	0.81	0.45	-	10,10,10,10	0
23	MG	A	1640	1/1	0.80	0.31	-	33,33,33,33	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1686	1/1	0.89	0.30	-	62,62,62,62	0
23	MG	A	1603	1/1	0.49	0.79	-	36,36,36,36	0
23	MG	A	1712	1/1	0.91	0.51	-	36,36,36,36	0
23	MG	A	1632	1/1	0.82	0.79	-	27,27,27,27	0
23	MG	A	1675	1/1	0.52	0.36	-	43,43,43,43	0
23	MG	A	1613	1/1	0.79	0.91	-	63,63,63,63	0
23	MG	A	1673	1/1	0.91	0.34	-	3,3,3,3	0
23	MG	A	1610	1/1	0.98	0.24	-	63,63,63,63	0
23	MG	A	1623	1/1	0.92	1.39	-	30,30,30,30	0
23	MG	A	1662	1/1	0.51	0.49	-	67,67,67,67	0
23	MG	A	1709	1/1	0.86	0.35	-	34,34,34,34	0
23	MG	A	1660	1/1	0.94	0.29	-	4,4,4,4	0
23	MG	A	1617	1/1	0.90	0.20	-	76,76,76,76	0
23	MG	A	1664	1/1	0.98	0.26	-	7,7,7,7	0
23	MG	A	1716	1/1	0.72	0.32	-	42,42,42,42	0
23	MG	A	1691	1/1	0.96	0.22	-	2,2,2,2	0
23	MG	A	1614	1/1	0.84	0.78	-	59,59,59,59	0
23	MG	A	1622	1/1	0.90	0.35	-	29,29,29,29	0
23	MG	A	1647	1/1	0.72	0.73	-	70,70,70,70	0
23	MG	A	1688	1/1	0.53	0.85	-	28,28,28,28	0
23	MG	A	1679	1/1	0.96	0.19	-	27,27,27,27	0
23	MG	A	1705	1/1	0.77	0.81	-	16,16,16,16	0
23	MG	A	1620	1/1	0.65	1.90	-	15,15,15,15	0
23	MG	A	1676	1/1	0.91	0.41	-	5,5,5,5	0
23	MG	E	201	1/1	0.96	1.23	-	21,21,21,21	0
23	MG	A	1671	1/1	0.81	1.29	-	10,10,10,10	0
23	MG	A	1606	1/1	0.70	0.61	-	37,37,37,37	0
24	ZN	D	301	1/1	0.99	0.35	-	34,34,34,34	0
23	MG	A	1602	1/1	0.75	1.14	-	22,22,22,22	0
23	MG	A	1698	1/1	0.74	0.49	-	23,23,23,23	0
23	MG	A	1626	1/1	0.21	1.00	-	70,70,70,70	0
23	MG	A	1668	1/1	0.86	0.38	-	15,15,15,15	0
23	MG	A	1631	1/1	0.58	0.22	-	46,46,46,46	0
23	MG	A	1656	1/1	0.66	0.80	-	33,33,33,33	0
23	MG	A	1653	1/1	0.91	1.26	-	11,11,11,11	0
23	MG	A	1680	1/1	0.88	0.69	-	22,22,22,22	0
23	MG	A	1618	1/1	0.91	0.37	-	69,69,69,69	0
23	MG	A	1682	1/1	0.97	0.87	-	36,36,36,36	0
23	MG	A	1711	1/1	0.57	0.62	-	9,9,9,9	0
23	MG	A	1685	1/1	0.96	0.90	-	36,36,36,36	0
23	MG	A	1615	1/1	0.98	0.57	-	27,27,27,27	0
23	MG	A	1684	1/1	0.54	0.52	-	17,17,17,17	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1649	1/1	0.75	0.81	-	15,15,15,15	0
23	MG	A	1635	1/1	0.81	0.55	-	25,25,25,25	0
23	MG	A	1608	1/1	0.96	0.09	-	56,56,56,56	0
23	MG	A	1706	1/1	0.91	0.46	-	30,30,30,30	0
23	MG	A	1621	1/1	0.56	0.58	-	59,59,59,59	0
23	MG	A	1666	1/1	0.70	0.24	-	26,26,26,26	0
23	MG	A	1665	1/1	0.24	0.84	-	107,107,107,107	0
23	MG	A	1697	1/1	0.79	0.73	-	38,38,38,38	0
23	MG	A	1604	1/1	0.60	1.96	-	70,70,70,70	0
23	MG	A	1694	1/1	0.68	0.94	-	14,14,14,14	0
23	MG	A	1650	1/1	0.79	0.91	-	57,57,57,57	0
23	MG	A	1633	1/1	0.99	0.52	-	27,27,27,27	0
23	MG	A	1707	1/1	0.83	0.83	-	42,42,42,42	0
23	MG	A	1657	1/1	0.98	0.73	-	0,0,0,0	0
23	MG	A	1692	1/1	0.88	0.41	-	23,23,23,23	0
23	MG	A	1672	1/1	0.97	0.08	-	15,15,15,15	0
23	MG	A	1714	1/1	0.91	0.88	-	19,19,19,19	0
23	MG	A	1612	1/1	0.36	0.33	-	46,46,46,46	0
23	MG	A	1699	1/1	0.72	0.58	-	43,43,43,43	0
23	MG	A	1600	1/1	0.87	0.11	-	63,63,63,63	0
23	MG	A	1683	1/1	0.95	0.39	-	38,38,38,38	0
23	MG	A	1636	1/1	0.98	0.47	-	1,1,1,1	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.