



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:03 am GMT

PDB ID : 1HNX  
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL  
SUBUNIT IN COMPLEX WITH PACTAMYCIN  
Authors : Brodersen, D.E.; Clemons Jr., W.M.; Carter, A.P.; Morgan-Warren, R.; Wim-  
berly, B.T.; Ramakrishnan, V.  
Deposited on : 2000-12-08  
Resolution : 3.40 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.

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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	:	1.7.2 (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

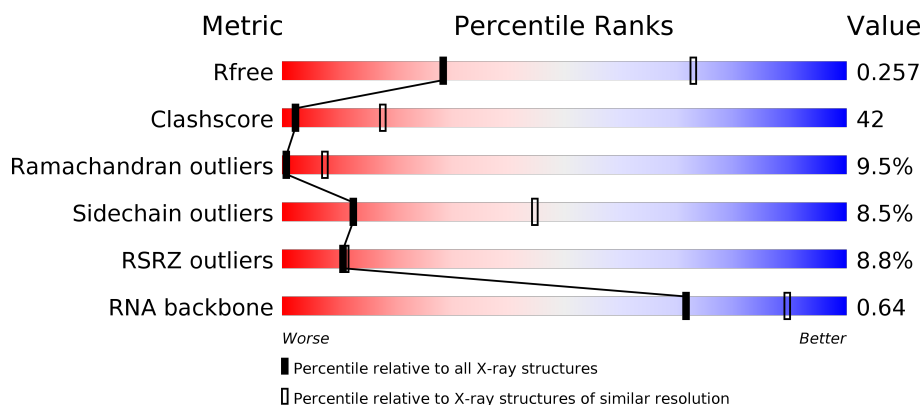
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)
RNA backbone	2435	1009 (3.96-2.84)

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	1522	<div> <div>14%</div> <div> <div>21%</div> <div>63%</div> <div>14%</div> <div>..</div> </div> </div>
2	X	6	<div> <div>17%</div> <div> <div>33%</div> <div>67%</div> </div> </div>
3	B	256	<div> <div>5%</div> <div> <div>17%</div> <div>58%</div> <div>15%</div> <div>9%</div> <div>.</div> </div> </div>
4	C	239	<div> <div>17%</div> <div> <div>51%</div> <div>17%</div> <div>14%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	D	209	
6	E	162	
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	
12	K	129	
13	L	135	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	
22	V	26	

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	1546	-	-	-	X
23	MG	A	1553	-	-	-	X
23	MG	A	1557	-	-	-	X
23	MG	A	1560	-	-	-	X
23	MG	A	1562	-	-	-	X
23	MG	A	1566	-	-	-	X
23	MG	A	1586	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1593	-	-	-	X
23	MG	A	1595	-	-	-	X
23	MG	A	1600	-	-	-	X
23	MG	A	1606	-	-	-	X
23	MG	A	1626	-	-	-	X
23	MG	A	1629	-	-	-	X

## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 51910 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
1	A	1507	Total	C	N	O	P	22	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called FRAGMENT OF MESSENGER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	P	0	0	0
			117	54	14	44	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	88	Total	C	N	O	S	0	0	0
			735	462	147	125	1			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

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

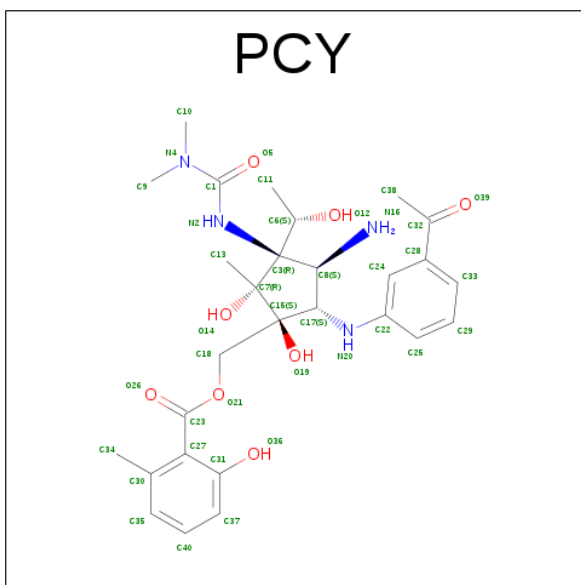
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	1	Total	Mg	0	0
			1	1		
23	A	94	Total	Mg	0	0
			94	94		
23	D	1	Total	Mg	0	0
			1	1		

- 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		

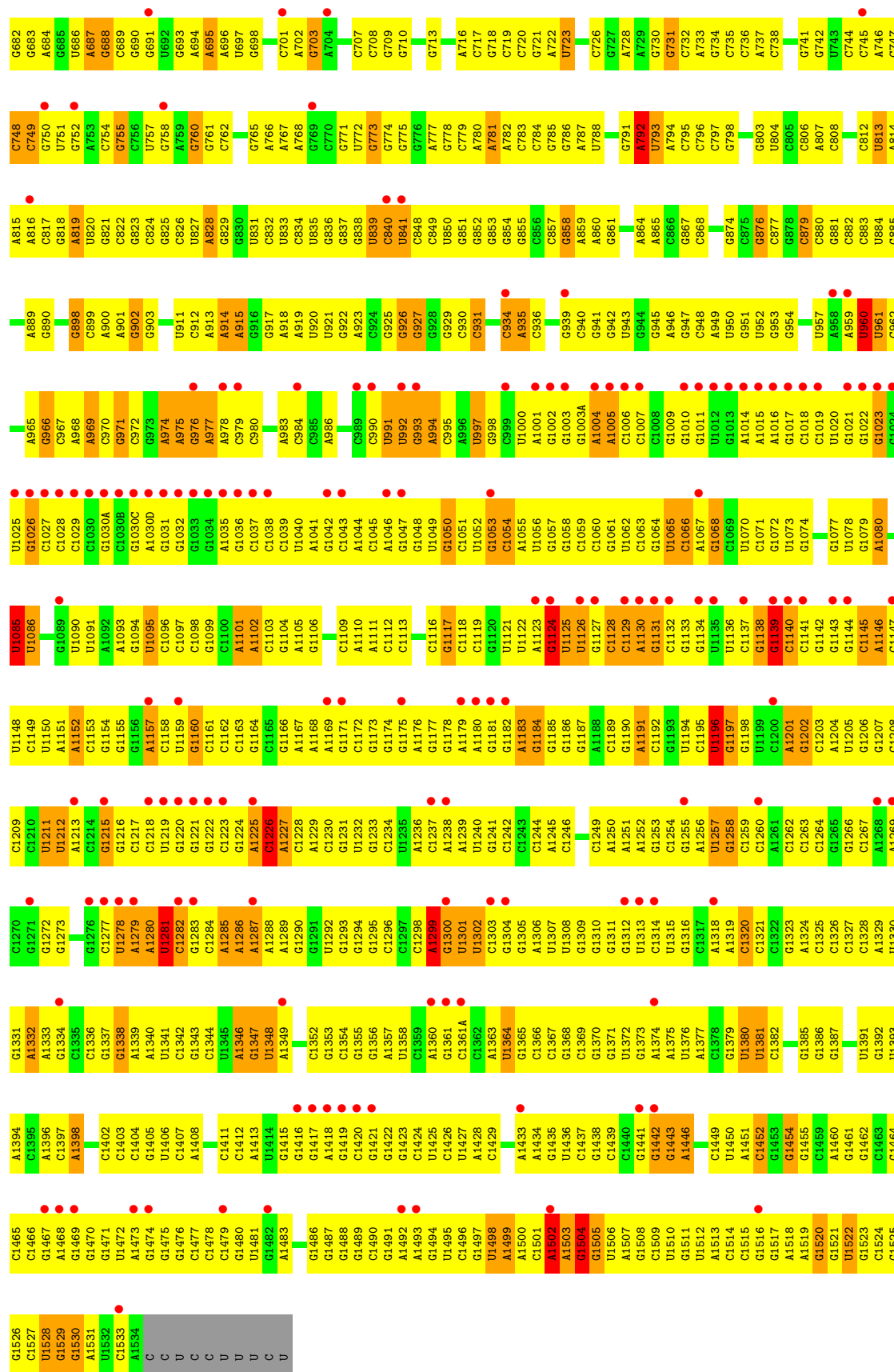
- Molecule 25 is DE-6-MSA-PACTAMYCIN (three-letter code: PCY) (formula: C<sub>28</sub>H<sub>38</sub>N<sub>4</sub>O<sub>8</sub>).

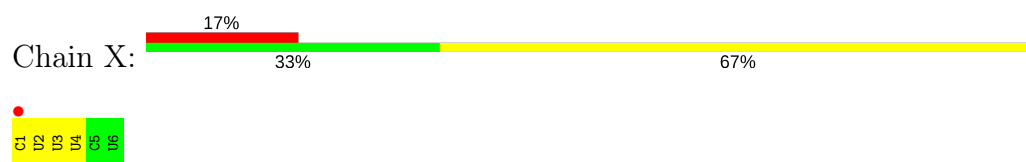




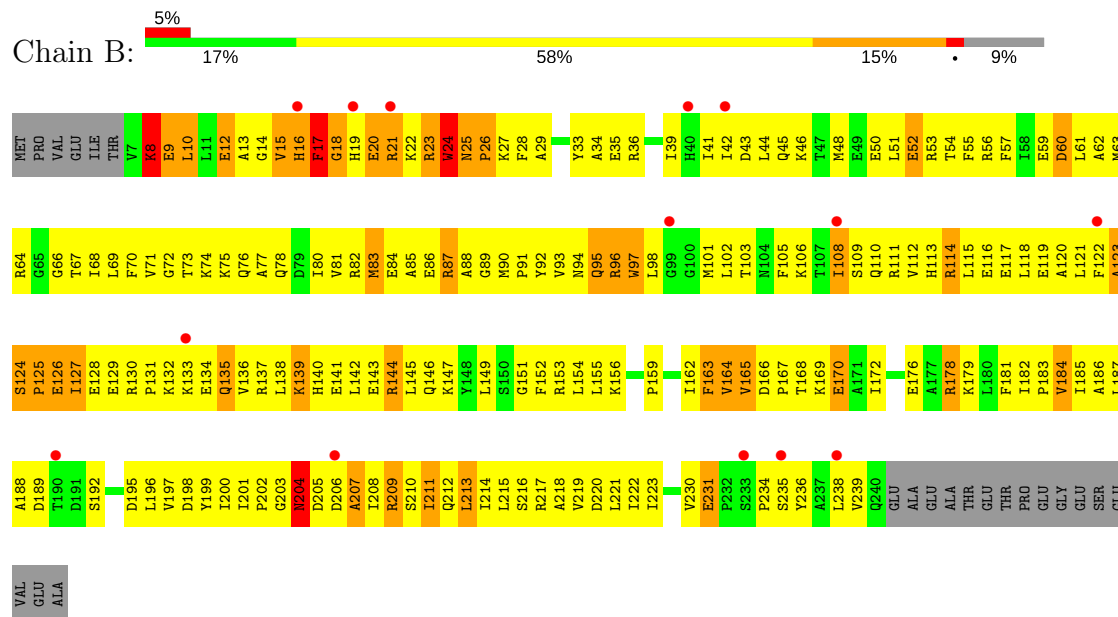
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			40	28	4	8		



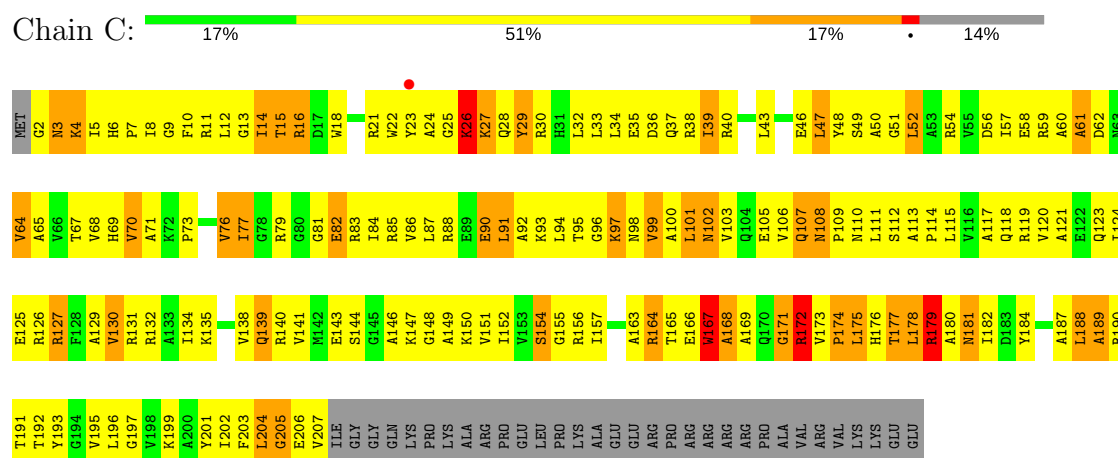




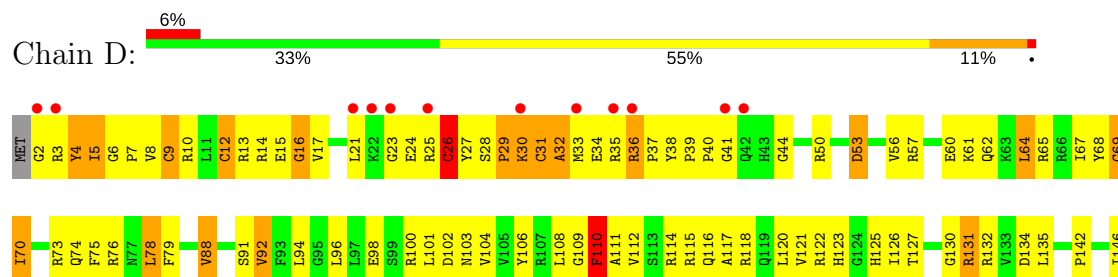
• Molecule 3: 30S RIBOSOMAL PROTEIN S2

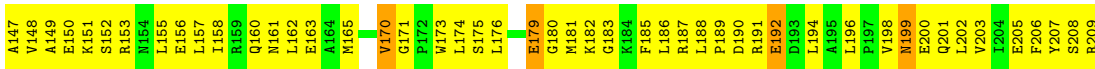


• Molecule 4: 30S RIBOSOMAL PROTEIN S3

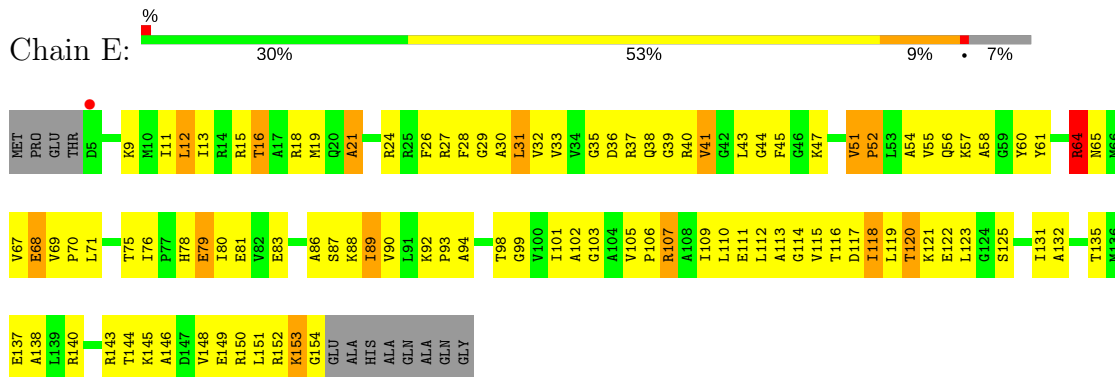


• Molecule 5: 30S RIBOSOMAL PROTEIN S4

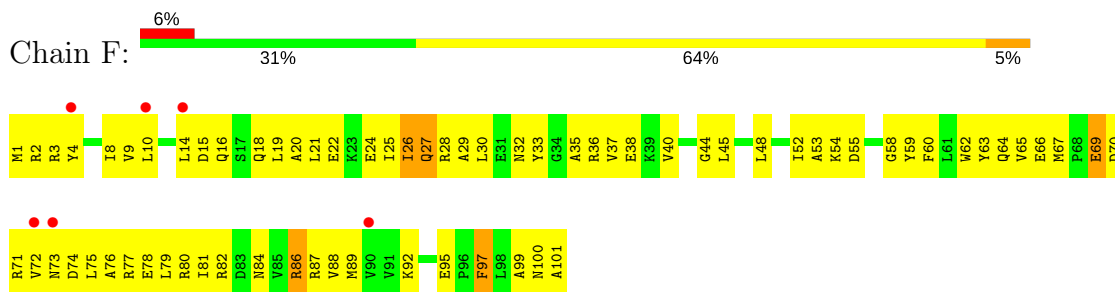




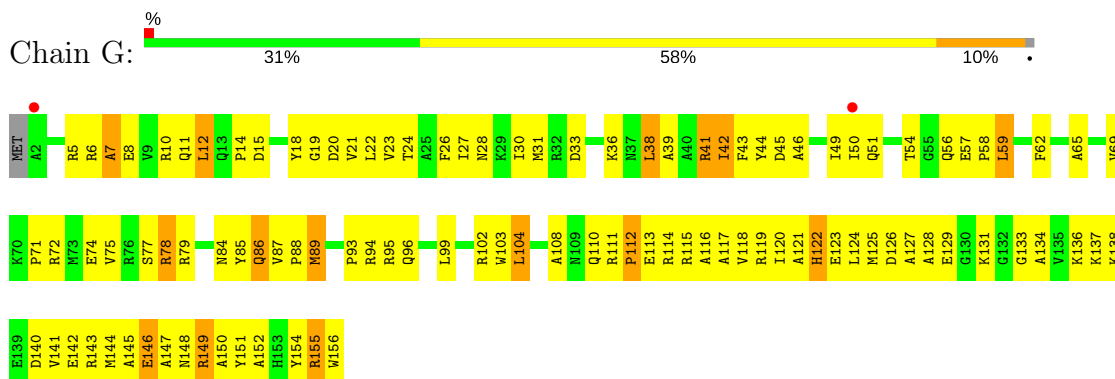
- Molecule 6: 30S RIBOSOMAL PROTEIN S5



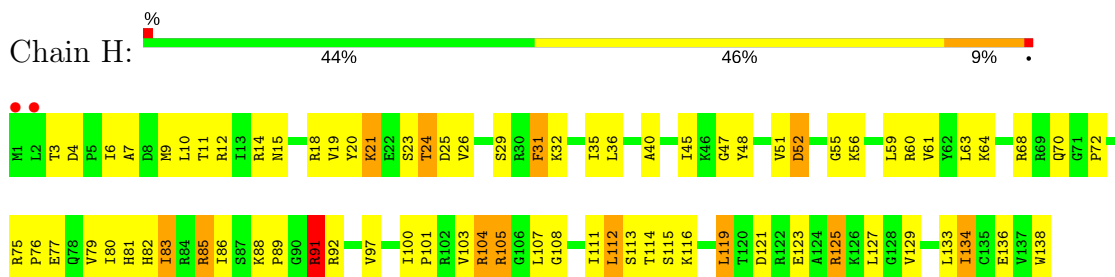
- Molecule 7: 30S RIBOSOMAL PROTEIN S6



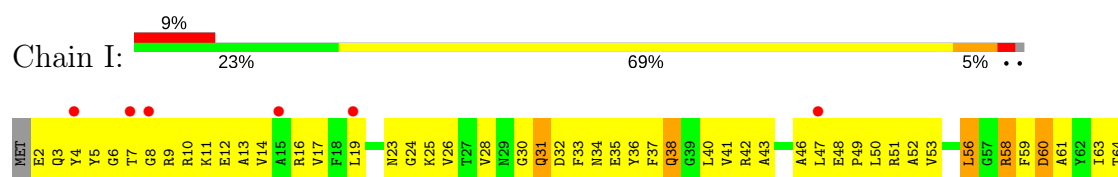
- Molecule 8: 30S RIBOSOMAL PROTEIN S7



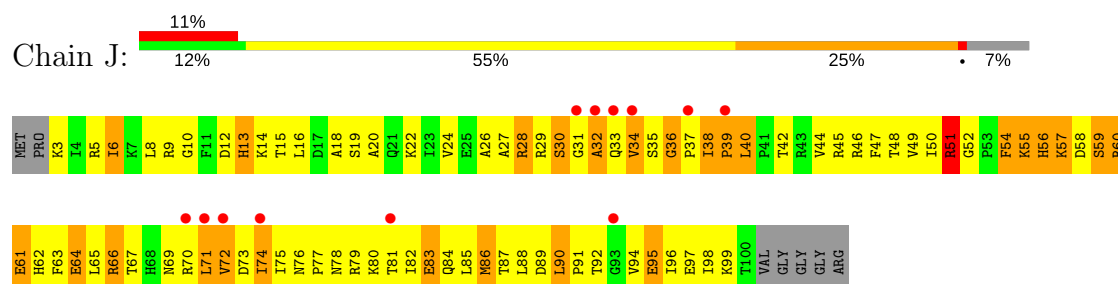
- Molecule 9: 30S RIBOSOMAL PROTEIN S8



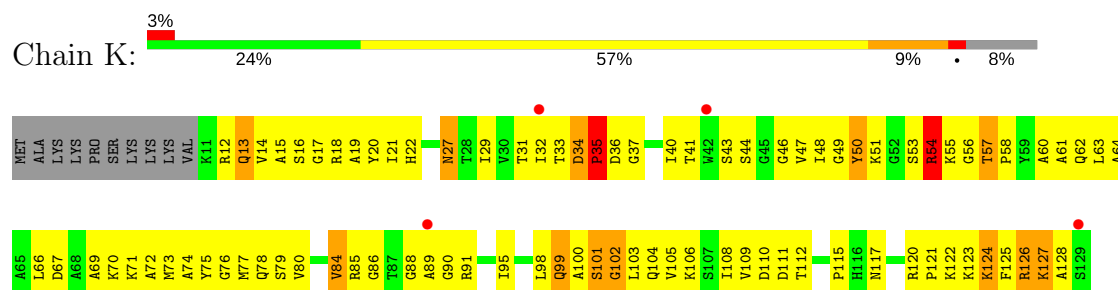
- Molecule 10: 30S RIBOSOMAL PROTEIN S9



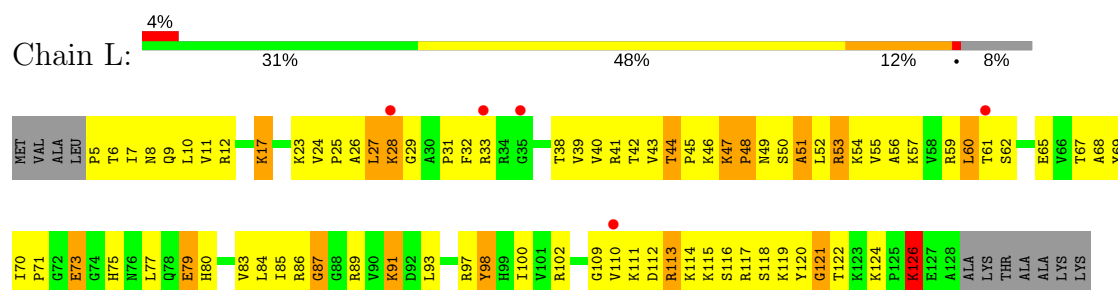
• Molecule 11: 30S RIBOSOMAL PROTEIN S10



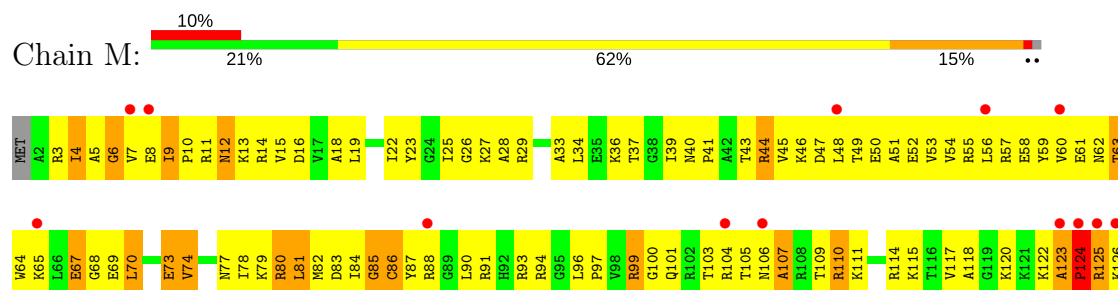
• Molecule 12: 30S RIBOSOMAL PROTEIN S11



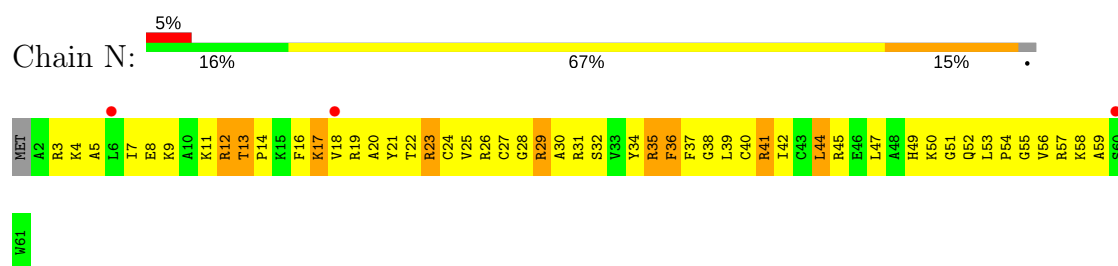
• Molecule 13: 30S RIBOSOMAL PROTEIN S12



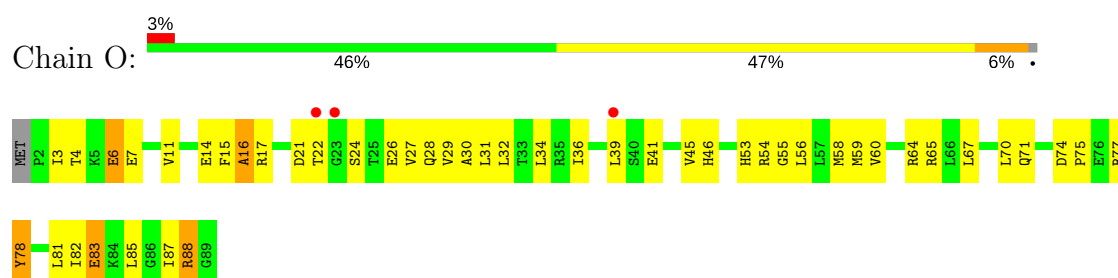
• Molecule 14: 30S RIBOSOMAL PROTEIN S13



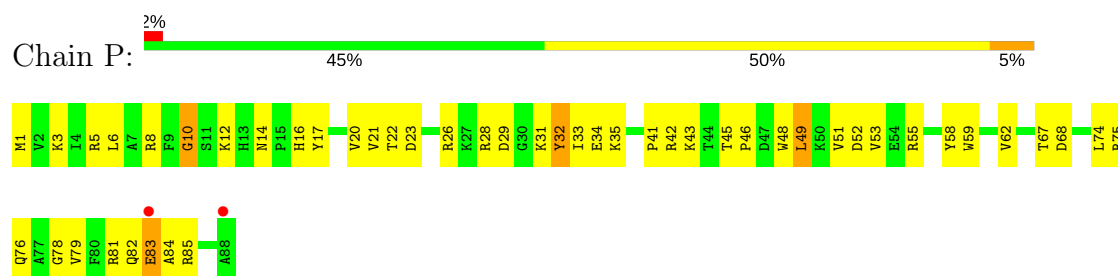
• Molecule 15: 30S RIBOSOMAL PROTEIN S14



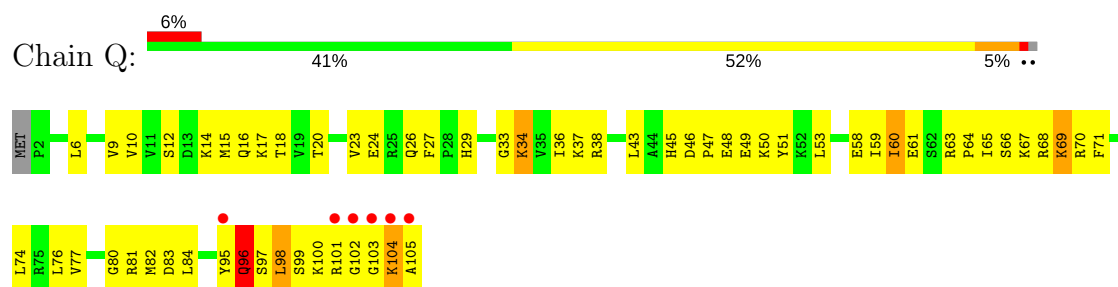
• Molecule 16: 30S RIBOSOMAL PROTEIN S15



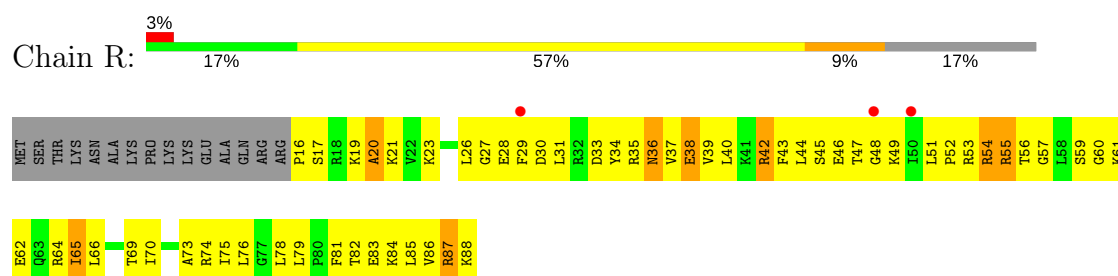
• Molecule 17: 30S RIBOSOMAL PROTEIN S16



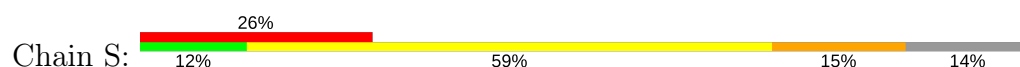
• Molecule 18: 30S RIBOSOMAL PROTEIN S17

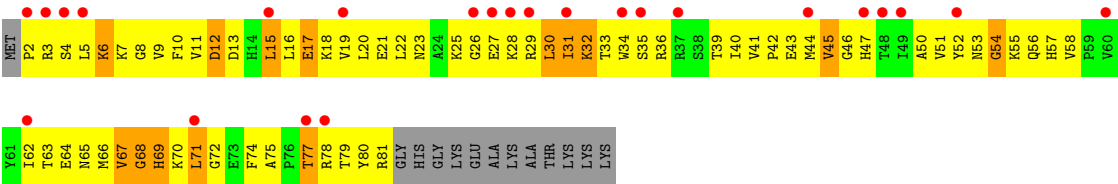


• Molecule 19: 30S RIBOSOMAL PROTEIN S18

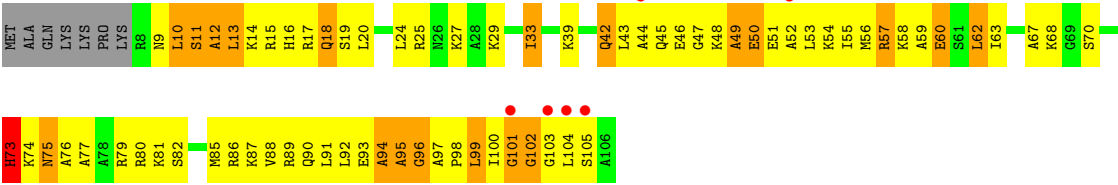


• Molecule 20: 30S RIBOSOMAL PROTEIN S19





• Molecule 21: 30S RIBOSOMAL PROTEIN S20



• Molecule 22: 30S RIBOSOMAL PROTEIN THX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.72Å 401.72Å 177.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.34 – 3.40 94.29 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.9 (95.34-3.40) 83.7 (94.29-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.13Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.280 0.213 , 0.257	Depositor DCC
$R_{free}$ test set	8780 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 105.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	51910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: ZN, PCY, 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	0.53	0/36259	0.75	42/56593 (0.1%)
2	X	0.56	0/128	0.71	0/196
3	B	0.39	0/1935	0.69	0/2609
4	C	0.38	0/1636	0.65	0/2205
5	D	0.43	0/1733	0.71	1/2318 (0.0%)
6	E	0.49	0/1162	0.80	2/1564 (0.1%)
7	F	0.35	0/856	0.65	0/1154
8	G	0.36	0/1276	0.64	0/1709
9	H	0.47	0/1136	0.78	0/1527
10	I	0.35	0/1029	0.66	0/1378
11	J	0.37	0/805	0.68	0/1082
12	K	0.40	0/900	0.75	0/1213
13	L	0.43	0/986	0.75	0/1320
14	M	0.35	0/1008	0.68	0/1347
15	N	0.41	0/501	0.78	0/664
16	O	0.39	0/745	0.64	0/992
17	P	0.46	0/751	0.76	0/1008
18	Q	0.50	0/870	0.78	0/1159
19	R	0.38	0/603	0.65	0/799
20	S	0.35	0/661	0.68	1/890 (0.1%)
21	T	0.38	0/764	0.73	0/1006
22	V	0.50	0/212	0.64	0/277
All	All	0.49	0/55956	0.74	46/83010 (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	2	47

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.79	131.03	109.50
1	A	1085	U	C2'-C3'-O3'	9.22	129.78	109.50
1	A	60	A	C2'-C3'-O3'	8.05	127.22	109.50
1	A	484	G	C2'-C3'-O3'	7.86	126.78	109.50
1	A	181	G	C2'-C3'-O3'	7.65	126.34	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1085	U	C3'
1	A	1498	U	C3'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	A	Sidechain
1	A	126	G	Sidechain
1	A	47	C	Sidechain
1	A	5	U	Sidechain
1	A	77	G	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	32391	0	16349	1512	0
2	X	117	0	64	3	0
3	B	1900	0	1951	289	0
4	C	1612	0	1677	276	0
5	D	1703	0	1764	182	0
6	E	1146	0	1207	120	0
7	F	843	0	857	83	0
8	G	1257	0	1296	113	0
9	H	1116	0	1177	96	0
10	I	1011	0	1043	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	792	0	835	158	0
12	K	885	0	904	100	0
13	L	970	0	1057	125	0
14	M	997	0	1072	142	0
15	N	492	0	529	87	0
16	O	734	0	771	63	0
17	P	735	0	752	67	0
18	Q	857	0	930	104	0
19	R	597	0	668	106	0
20	S	647	0	673	105	0
21	T	762	0	859	106	0
22	V	208	0	221	20	0
23	A	94	0	0	0	0
23	D	1	0	0	0	0
23	H	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	40	0	38	10	0
All	All	51910	0	36694	3662	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 42.

The worst 5 of 3662 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)
25:A:1632:PCY:C3	25:A:1632:PCY:N2	1.69	1.49
13:L:28:LYS:HD2	13:L:33:ARG:HH22	1.01	1.16
12:K:110:ASP:HB2	19:R:88:LYS:HD2	1.28	1.15
6:E:110:LEU:HD13	6:E:118:ILE:HD12	1.28	1.15
4:C:58:GLU:HB3	11:J:92:THR:HG21	1.29	1.15

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	
3	B	232/256 (91%)	155 (67%)	49 (21%)	28 (12%)	0	4
4	C	204/239 (85%)	120 (59%)	52 (26%)	32 (16%)	0	2
5	D	206/209 (99%)	146 (71%)	41 (20%)	19 (9%)	1	8
6	E	148/162 (91%)	126 (85%)	18 (12%)	4 (3%)	6	37
7	F	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	2	17
8	G	153/156 (98%)	114 (74%)	24 (16%)	15 (10%)	1	7
9	H	136/138 (99%)	122 (90%)	10 (7%)	4 (3%)	5	36
10	I	125/128 (98%)	90 (72%)	28 (22%)	7 (6%)	2	19
11	J	96/105 (91%)	58 (60%)	20 (21%)	18 (19%)	0	1
12	K	117/129 (91%)	87 (74%)	16 (14%)	14 (12%)	0	4
13	L	122/135 (90%)	91 (75%)	19 (16%)	12 (10%)	1	7
14	M	123/126 (98%)	84 (68%)	23 (19%)	16 (13%)	0	3
15	N	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	3
16	O	86/89 (97%)	63 (73%)	20 (23%)	3 (4%)	4	32
17	P	86/88 (98%)	66 (77%)	17 (20%)	3 (4%)	4	32
18	Q	102/105 (97%)	84 (82%)	13 (13%)	5 (5%)	2	22
19	R	71/88 (81%)	51 (72%)	18 (25%)	2 (3%)	6	37
20	S	78/93 (84%)	52 (67%)	15 (19%)	11 (14%)	0	3
21	T	97/106 (92%)	61 (63%)	19 (20%)	17 (18%)	0	1
22	V	22/26 (85%)	17 (77%)	4 (18%)	1 (4%)	3	24
All	All	2361/2540 (93%)	1702 (72%)	434 (18%)	225 (10%)	1	7

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	8	LYS
3	B	9	GLU
3	B	15	VAL
3	B	16	HIS
3	B	17	PHE

### 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	
3	B	202/220 (92%)	181 (90%)	21 (10%)	8	34
4	C	160/188 (85%)	136 (85%)	24 (15%)	3	18
5	D	180/181 (99%)	168 (93%)	12 (7%)	19	57
6	E	115/123 (94%)	102 (89%)	13 (11%)	7	29
7	F	90/90 (100%)	87 (97%)	3 (3%)	43	76
8	G	126/127 (99%)	119 (94%)	7 (6%)	25	62
9	H	119/119 (100%)	105 (88%)	14 (12%)	6	27
10	I	98/99 (99%)	86 (88%)	12 (12%)	6	26
11	J	87/92 (95%)	76 (87%)	11 (13%)	5	25
12	K	90/99 (91%)	85 (94%)	5 (6%)	25	62
13	L	104/111 (94%)	96 (92%)	8 (8%)	15	49
14	M	100/101 (99%)	93 (93%)	7 (7%)	18	55
15	N	49/50 (98%)	45 (92%)	4 (8%)	13	47
16	O	79/80 (99%)	77 (98%)	2 (2%)	53	81
17	P	74/74 (100%)	70 (95%)	4 (5%)	26	63
18	Q	96/97 (99%)	92 (96%)	4 (4%)	34	70
19	R	64/77 (83%)	57 (89%)	7 (11%)	7	32
20	S	71/80 (89%)	67 (94%)	4 (6%)	25	62
21	T	76/82 (93%)	68 (90%)	8 (10%)	8	34
22	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1999/2111 (95%)	1829 (92%)	170 (8%)	12	45

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G	24	THR
10	I	23	ASN
19	R	65	ILE

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Mol	Chain	Res	Type
8	G	126	ASP
9	H	91	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
7	F	57	GLN
8	G	56	GLN
20	S	53	ASN
7	F	94	GLN
8	G	106	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	220 (14%)	0
2	X	5/6 (83%)	1 (20%)	0
All	All	1511/1528 (98%)	221 (14%)	0

5 of 221 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 99 ligands modelled in this entry, 98 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	PCY	A	1632	-	37,42,42	7.63	37 (100%)	40,65,65	1.53	7 (17%)

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	PCY	A	1632	-	-	0/33/67/67	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1632	PCY	C38-C32	2.29	1.56	1.49
25	A	1632	PCY	C15-C17	3.20	1.65	1.54
25	A	1632	PCY	C27-C23	3.53	1.59	1.50
25	A	1632	PCY	C17-C8	4.11	1.64	1.51
25	A	1632	PCY	C10-N4	4.67	1.62	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1632	PCY	C22-N20-C17	-5.14	112.19	123.18
25	A	1632	PCY	O5-C1-N4	-2.11	118.48	122.09
25	A	1632	PCY	C38-C32-C28	-2.06	115.03	119.27
25	A	1632	PCY	O39-C32-C28	2.41	124.84	119.72
25	A	1632	PCY	C3-N2-C1	3.01	132.93	124.50

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1632	PCY	10	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	1506/1522 (98%)	1.16	210 (13%) 3 4	37, 70, 161, 199	0
2	X	6/6 (100%)	1.00	1 (16%) 2 2	62, 79, 117, 151	0
3	B	234/256 (91%)	0.23	14 (5%) 23 22	34, 87, 162, 199	0
4	C	206/239 (86%)	0.07	1 (0%) 90 88	41, 91, 153, 179	0
5	D	208/209 (99%)	0.28	12 (5%) 24 23	35, 71, 128, 191	0
6	E	150/162 (92%)	0.10	1 (0%) 87 85	34, 58, 111, 168	0
7	F	101/101 (100%)	0.46	6 (5%) 23 22	56, 95, 147, 167	0
8	G	155/156 (99%)	0.03	2 (1%) 77 73	47, 85, 147, 175	0
9	H	138/138 (100%)	0.05	2 (1%) 75 71	21, 52, 92, 139	0
10	I	127/128 (99%)	0.44	12 (9%) 9 10	37, 96, 140, 181	0
11	J	98/105 (93%)	0.67	12 (12%) 5 5	50, 119, 184, 199	0
12	K	119/129 (92%)	0.30	4 (3%) 46 41	41, 73, 137, 178	0
13	L	124/135 (91%)	0.34	5 (4%) 39 35	30, 72, 131, 180	0
14	M	125/126 (99%)	0.66	13 (10%) 7 7	56, 89, 153, 188	0
15	N	60/61 (98%)	0.45	3 (5%) 30 27	50, 86, 157, 170	0
16	O	88/89 (98%)	0.25	3 (3%) 46 41	38, 70, 136, 186	0
17	P	88/88 (100%)	0.28	2 (2%) 61 56	35, 63, 164, 198	0
18	Q	104/105 (99%)	0.62	6 (5%) 24 23	35, 62, 137, 199	0
19	R	73/88 (82%)	0.25	3 (4%) 38 34	43, 75, 154, 194	0
20	S	80/93 (86%)	1.65	24 (30%) 1 1	66, 110, 158, 199	0
21	T	99/106 (93%)	0.36	6 (6%) 22 21	44, 72, 133, 194	0
22	V	24/26 (92%)	0.58	2 (8%) 12 13	44, 79, 128, 149	0
All	All	3913/4068 (96%)	0.66	344 (8%) 11 11	21, 75, 155, 199	0

The worst 5 of 344 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Q	105	ALA	15.8
20	S	3	ARG	15.2
18	Q	103	GLY	13.2
14	M	124	PRO	13.0
18	Q	102	GLY	10.7

## 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(Å <sup>2</sup> )	Q<0.9
23	MG	A	1562	1/1	0.96	0.65	44.99	45,45,45,45	0
23	MG	A	1557	1/1	0.98	0.43	9.85	45,45,45,45	0
23	MG	A	1553	1/1	0.96	0.40	8.11	45,45,45,45	0
23	MG	A	1626	1/1	0.91	0.30	6.57	45,45,45,45	1
23	MG	A	1629	1/1	0.95	0.71	6.53	45,45,45,45	1
23	MG	A	1606	1/1	0.94	0.52	5.73	45,45,45,45	0
23	MG	A	1586	1/1	0.93	0.38	5.41	45,45,45,45	0
23	MG	A	1566	1/1	0.75	0.40	4.98	45,45,45,45	0
23	MG	A	1600	1/1	0.95	0.38	4.87	45,45,45,45	0
23	MG	A	1595	1/1	0.97	0.35	4.49	45,45,45,45	0
23	MG	A	1593	1/1	0.95	0.32	3.61	45,45,45,45	0
23	MG	A	1560	1/1	0.93	0.30	2.39	45,45,45,45	0
23	MG	A	1546	1/1	0.95	0.38	2.32	45,45,45,45	0
23	MG	A	1614	1/1	0.72	0.28	1.91	45,45,45,45	0
25	PCY	A	1632	40/40	0.91	0.34	1.43	28,28,28,28	0
23	MG	A	1619	1/1	0.71	0.23	1.29	45,45,45,45	1
23	MG	D	215	1/1	0.92	0.31	1.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	211	1/1	0.91	0.33	1.10	45,45,45,45	0
23	MG	A	1579	1/1	0.97	0.28	0.46	45,45,45,45	0
23	MG	A	1588	1/1	0.95	0.29	0.32	45,45,45,45	0
23	MG	A	1607	1/1	0.94	0.29	-0.08	45,45,45,45	0
24	ZN	D	300	1/1	0.99	0.34	-0.23	53,53,53,53	0
24	ZN	N	190	1/1	1.00	0.22	-0.27	53,53,53,53	1
23	MG	A	1599	1/1	0.91	0.28	-0.54	45,45,45,45	0
23	MG	A	1577	1/1	0.96	0.25	-0.68	45,45,45,45	0
23	MG	A	1613	1/1	0.71	0.27	-0.81	45,45,45,45	1
23	MG	A	1604	1/1	0.90	0.21	-1.14	45,45,45,45	1
23	MG	A	1576	1/1	0.93	0.20	-1.21	45,45,45,45	0
23	MG	A	1611	1/1	0.84	0.20	-1.23	45,45,45,45	1
23	MG	A	1625	1/1	0.99	0.19	-1.24	45,45,45,45	1
23	MG	A	1620	1/1	0.88	0.19	-1.27	45,45,45,45	0
23	MG	A	1581	1/1	0.83	0.23	-1.29	45,45,45,45	1
23	MG	A	1601	1/1	0.93	0.17	-1.64	45,45,45,45	0
23	MG	A	1603	1/1	0.95	0.20	-1.83	45,45,45,45	0
23	MG	A	1575	1/1	0.89	0.13	-1.94	45,45,45,45	1
23	MG	A	1609	1/1	0.88	0.16	-2.49	45,45,45,45	0
23	MG	A	1605	1/1	0.83	0.11	-3.51	45,45,45,45	0
23	MG	A	1592	1/1	0.89	0.12	-6.39	45,45,45,45	0
23	MG	A	1627	1/1	0.99	0.39	-	45,45,45,45	1
23	MG	A	1612	1/1	0.89	0.31	-	45,45,45,45	0
23	MG	A	1621	1/1	0.95	0.57	-	45,45,45,45	1
23	MG	A	1584	1/1	0.98	0.47	-	45,45,45,45	0
23	MG	A	86	1/1	0.92	0.40	-	45,45,45,45	0
23	MG	A	1608	1/1	0.98	0.07	-	45,45,45,45	0
23	MG	A	1563	1/1	0.94	0.22	-	45,45,45,45	0
23	MG	A	1616	1/1	0.92	0.18	-	45,45,45,45	0
23	MG	A	1618	1/1	0.68	0.80	-	45,45,45,45	1
23	MG	A	1552	1/1	0.97	0.20	-	45,45,45,45	0
23	MG	A	1610	1/1	0.92	0.18	-	45,45,45,45	0
23	MG	A	1550	1/1	0.53	0.74	-	45,45,45,45	1
23	MG	A	1578	1/1	0.87	0.33	-	45,45,45,45	0
23	MG	A	1590	1/1	0.79	0.34	-	45,45,45,45	0
23	MG	A	1565	1/1	0.93	0.67	-	45,45,45,45	0
23	MG	A	1561	1/1	0.95	0.73	-	45,45,45,45	0
23	MG	A	1547	1/1	0.97	0.50	-	45,45,45,45	0
23	MG	A	1574	1/1	0.90	0.29	-	45,45,45,45	0
23	MG	A	1598	1/1	0.96	0.23	-	45,45,45,45	1
23	MG	A	1558	1/1	0.82	0.30	-	45,45,45,45	0
23	MG	A	1597	1/1	0.89	0.12	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1567	1/1	0.88	0.59	-	45,45,45,45	0
23	MG	A	1594	1/1	0.94	0.35	-	45,45,45,45	0
23	MG	A	1549	1/1	0.83	0.17	-	45,45,45,45	1
23	MG	A	1628	1/1	0.99	0.26	-	45,45,45,45	1
23	MG	A	1568	1/1	0.78	0.57	-	45,45,45,45	0
23	MG	A	71	1/1	0.86	0.47	-	45,45,45,45	0
23	MG	A	1596	1/1	0.93	0.40	-	45,45,45,45	1
23	MG	A	1623	1/1	0.87	0.43	-	45,45,45,45	1
23	MG	A	1569	1/1	0.95	1.06	-	45,45,45,45	1
23	MG	A	1571	1/1	0.91	0.24	-	45,45,45,45	0
23	MG	A	1624	1/1	0.95	0.50	-	45,45,45,45	1
23	MG	A	1572	1/1	0.96	0.61	-	45,45,45,45	0
23	MG	A	1622	1/1	0.97	0.51	-	45,45,45,45	1
23	MG	A	1591	1/1	0.90	0.51	-	45,45,45,45	0
23	MG	A	1573	1/1	0.97	0.47	-	45,45,45,45	0
23	MG	A	1570	1/1	0.90	0.31	-	45,45,45,45	1
23	MG	A	1617	1/1	0.97	0.40	-	45,45,45,45	1
23	MG	A	1582	1/1	0.92	0.32	-	45,45,45,45	1
23	MG	A	1585	1/1	0.77	0.42	-	45,45,45,45	1
23	MG	A	1564	1/1	0.77	0.22	-	45,45,45,45	0
23	MG	A	1551	1/1	0.93	0.36	-	45,45,45,45	0
23	MG	A	1631	1/1	0.99	0.55	-	45,45,45,45	1
23	MG	A	210	1/1	0.64	0.37	-	45,45,45,45	1
23	MG	A	1587	1/1	0.90	0.36	-	45,45,45,45	0
23	MG	A	214	1/1	0.90	0.16	-	45,45,45,45	0
23	MG	A	212	1/1	0.77	0.95	-	45,45,45,45	1
23	MG	A	1630	1/1	0.96	1.31	-	45,45,45,45	1
23	MG	A	1559	1/1	0.93	0.42	-	45,45,45,45	0
23	MG	A	87	1/1	0.92	0.24	-	45,45,45,45	1
23	MG	A	1545	1/1	0.83	0.11	-	45,45,45,45	0
23	MG	A	1589	1/1	0.98	0.32	-	45,45,45,45	0
23	MG	H	213	1/1	0.64	1.00	-	45,45,45,45	1
23	MG	A	1555	1/1	0.97	0.32	-	45,45,45,45	0
23	MG	A	1554	1/1	0.98	0.51	-	45,45,45,45	0
23	MG	A	1615	1/1	0.78	0.96	-	45,45,45,45	1
23	MG	A	1548	1/1	0.73	0.30	-	45,45,45,45	0
23	MG	A	1580	1/1	0.90	0.17	-	45,45,45,45	0
23	MG	A	1602	1/1	0.95	0.37	-	45,45,45,45	0
23	MG	A	1583	1/1	0.94	0.12	-	45,45,45,45	0
23	MG	A	1556	1/1	0.67	0.27	-	45,45,45,45	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.