



# wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:55 PM BST

PDB ID : 3D5A  
Title : Structural basis for translation termination on the 70S ribosome. This file contains the 30S subunit, release factor 1 (RF1), two tRNA, and mRNA molecules of one 70S ribosome. The entire crystal structure contains two 70S ribosomes as described in remark 400.  
Authors : Laurberg, M.; Asahara, H.; Korostelev, A.; Zhu, J.; Trakhanov, S.; Noller, H.F.  
Deposited on : 2008-05-16  
Resolution : 3.21 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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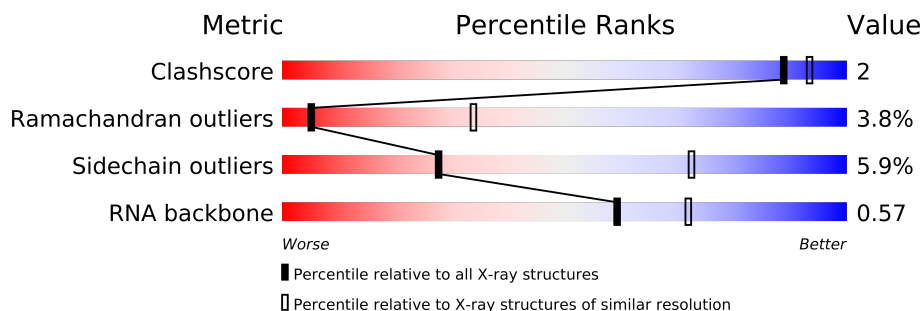
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 3.21 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))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RNA backbone	1838	1002 (3.72-2.68)







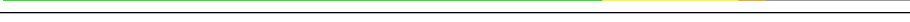

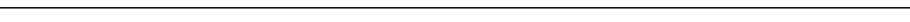

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1525	
2	Y	77	
2	Z	77	
3	V	27	
4	B	256	
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	
13	K	129	
14	L	134	

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Mol	Chain	Length	Quality of chain
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	U	27	
24	X	354	

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 58167 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	G	C	CONFLICT	GB 155076

- Molecule 2 is a RNA chain called P and E-site tRNA(fMet).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	Y	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	12	Total	C	N	O	P	0	0	0
			258	118	54	75	11			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ALA	-	INSERTION	UNP P61941
L	3	LEU	-	INSERTION	UNP P61941

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	70	Total	C	N	O	S	0	0	0
			574	367	112	95				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	24	Total	C	N	O	S	0	0	0
			208	128	50	30				

- Molecule 24 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	P	1	Total 1	Mg 1	0	0
26	G	1	Total 1	Mg 1	0	0
26	Q	1	Total 1	Mg 1	0	0
26	D	7	Total 7	Mg 7	0	0
26	K	1	Total 1	Mg 1	0	0
26	E	1	Total 1	Mg 1	0	0
26	H	2	Total 2	Mg 2	0	0
26	B	2	Total 2	Mg 2	0	0
26	I	2	Total 2	Mg 2	0	0
26	C	6	Total 6	Mg 6	0	0
26	V	1	Total 1	Mg 1	0	0
26	Z	6	Total 6	Mg 6	0	0
26	A	310	Total 310	Mg 310	0	0
26	X	6	Total 6	Mg 6	0	0
26	O	3	Total 3	Mg 3	0	0
26	Y	26	Total 26	Mg 26	0	0
26	L	2	Total 2	Mg 2	0	0
26	F	2	Total 2	Mg 2	0	0

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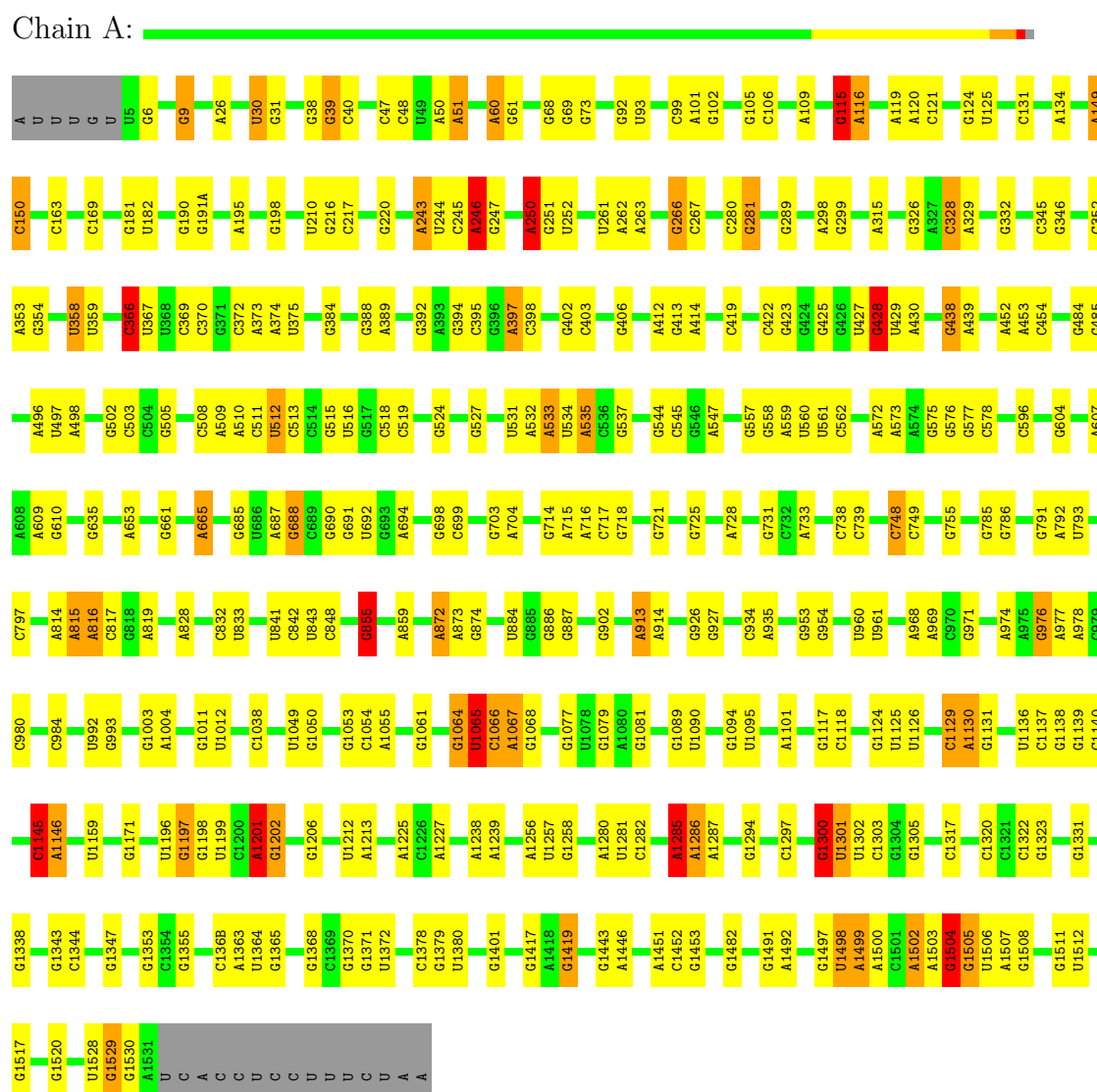
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	M	1	Total	Mg	0	0
			1	1		

### 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.

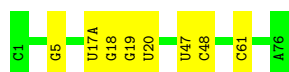
Note EDS was not executed.

#### • Molecule 1: 16S rRNA



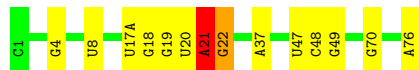
#### • Molecule 2: P and E-site tRNA(fMet)

Chain Z: 



- Molecule 2: P and E-site tRNA(fMet)

Chain Y:



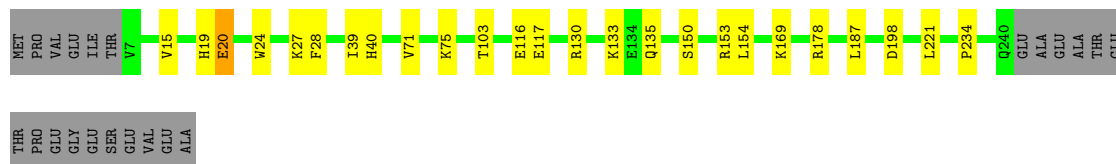
- Molecule 3: mRNA

Chain V:



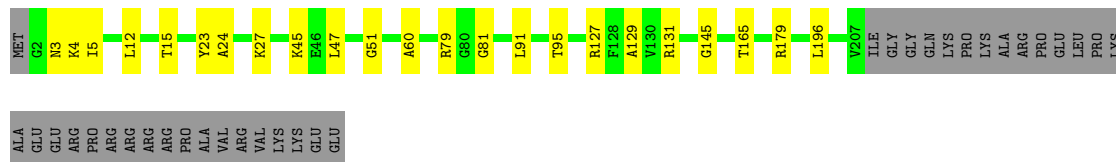
- Molecule 4: 30S ribosomal protein S2

Chain B:



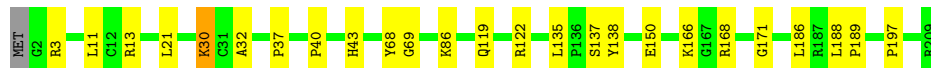
- Molecule 5: 30S ribosomal protein S3

Chain C:



- Molecule 6: 30S ribosomal protein S4

Chain D:



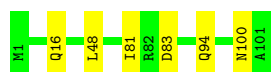
- Molecule 7: 30S ribosomal protein S5

Chain E:



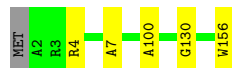
- Molecule 8: 30S ribosomal protein S6

Chain F:



- Molecule 9: 30S ribosomal protein S7

Chain G:



- Molecule 10: 30S ribosomal protein S8

Chain H:



- Molecule 11: 30S ribosomal protein S9

Chain I:



- Molecule 12: 30S ribosomal protein S10

Chain J:



- Molecule 13: 30S ribosomal protein S11

Chain K:



- Molecule 14: 30S ribosomal protein S12

Chain L:



- Molecule 15: 30S ribosomal protein S13

Chain M:



- Molecule 16: 30S ribosomal protein S14

Chain N:



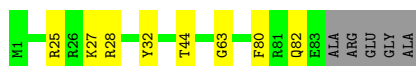
- Molecule 17: 30S ribosomal protein S15

Chain O:



- Molecule 18: 30S ribosomal protein S16

Chain P:



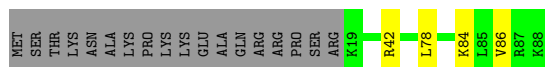
- Molecule 19: 30S ribosomal protein S17

Chain Q:



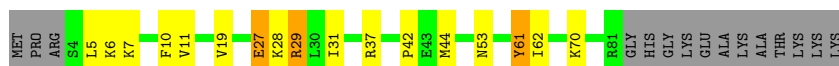
- Molecule 20: 30S ribosomal protein S18

Chain R:



- Molecule 21: 30S ribosomal protein S19

Chain S:



- Molecule 22: 30S ribosomal protein S20

Chain T:



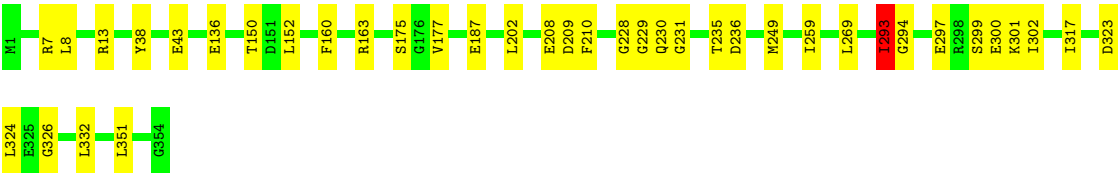
- Molecule 23: 30S ribosomal protein Thx

Chain U:



- Molecule 24: Peptide chain release factor 1

Chain X:



## 4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.13Å 454.39Å 616.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 3.21	Depositor
% Data completeness (in resolution range)	95.1 (49.90-3.21)	Depositor
$R_{merge}$	0.27	Depositor
$R_{sym}$	0.27	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.292 , 0.319	Depositor
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.069	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.26$ , $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 952768 reflections	Xtriage
Total number of atoms	58167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.17% 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	0.42	0/36194	0.85	27/56493 (0.0%)
2	Y	0.42	0/1832	0.81	1/2855 (0.0%)
2	Z	0.39	0/1832	0.80	0/2855
3	V	0.43	0/291	0.81	0/452
4	B	0.21	0/1935	0.38	0/2609
5	C	0.21	0/1636	0.36	0/2205
6	D	0.22	0/1733	0.38	0/2318
7	E	0.22	0/1171	0.39	0/1576
8	F	0.22	0/856	0.39	0/1154
9	G	0.21	0/1276	0.36	0/1709
10	H	0.22	0/1136	0.40	0/1527
11	I	0.21	0/1029	0.37	0/1378
12	J	0.21	0/807	0.39	0/1085
13	K	0.21	0/900	0.39	0/1213
14	L	0.23	0/986	0.42	0/1320
15	M	0.19	0/943	0.39	0/1265
16	N	0.22	0/501	0.36	0/664
17	O	0.22	0/745	0.36	0/992
18	P	0.22	0/716	0.40	0/963
19	Q	0.22	0/836	0.38	0/1117
20	R	0.22	0/579	0.39	0/768
21	S	0.21	0/642	0.38	0/865
22	T	0.22	0/764	0.36	0/1006
23	U	0.20	0/212	0.36	0/277
24	X	0.23	0/2850	0.40	0/3829
All	All	0.36	0/62402	0.73	28/92495 (0.0%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	G	P-O3'-C3'	7.06	128.17	119.70
1	A	1300	G	P-O3'-C3'	6.98	128.08	119.70
1	A	1201	A	P-O3'-C3'	6.72	127.77	119.70
1	A	1285	A	P-O3'-C3'	6.57	127.58	119.70
1	A	1498	U	P-O3'-C3'	6.49	127.49	119.70

There are no chirality outliers.

There are no planarity outliers.

## 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	32332	0	0	98	0
2	Y	1640	0	0	4	0
2	Z	1640	0	0	0	0
3	V	258	0	0	1	0
4	B	1900	0	0	2	0
5	C	1612	0	0	1	0
6	D	1703	0	0	3	0
7	E	1155	0	0	4	0
8	F	843	0	0	1	0
9	G	1257	0	0	0	0
10	H	1116	0	0	1	0
11	I	1011	0	0	1	0
12	J	794	0	0	1	0
13	K	885	0	0	2	0
14	L	970	0	0	3	0
15	M	933	0	0	1	0
16	N	492	0	0	1	0
17	O	734	0	0	2	0
18	P	700	0	0	2	0
19	Q	823	0	0	0	0
20	R	574	0	0	0	0
21	S	629	0	0	2	0
22	T	762	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	U	208	0	0	0	0
24	X	2813	0	0	5	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	310	0	0	0	0
26	B	2	0	0	0	0
26	C	6	0	0	0	0
26	D	7	0	0	0	0
26	E	1	0	0	0	0
26	F	2	0	0	0	0
26	G	1	0	0	0	0
26	H	2	0	0	0	0
26	I	2	0	0	0	0
26	K	1	0	0	0	0
26	L	2	0	0	0	0
26	M	1	0	0	0	0
26	O	3	0	0	0	0
26	P	1	0	0	0	0
26	Q	1	0	0	0	0
26	V	1	0	0	0	0
26	X	6	0	0	0	0
26	Y	26	0	0	0	0
26	Z	6	0	0	0	0
All	All	58167	0	0	128	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 2.

The worst 5 of 128 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1504:G:O2'	1:A:1505:G:OP2	2.24	0.56
1:A:366:C:O2'	1:A:394:G:N2	2.39	0.55
1:A:262:A:C6	1:A:263:A:C6	2.94	0.55
1:A:1419:G:C6	1:A:1482:G:C2	2.96	0.54
1:A:394:G:C4	1:A:395:C:C5	2.97	0.52

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	232/256 (91%)	186 (80%)	37 (16%)	9 (4%)	5	33
5	C	204/239 (85%)	156 (76%)	36 (18%)	12 (6%)	2	20
6	D	206/209 (99%)	163 (79%)	31 (15%)	12 (6%)	3	21
7	E	149/162 (92%)	122 (82%)	24 (16%)	3 (2%)	11	56
8	F	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	22	74
9	G	153/156 (98%)	125 (82%)	24 (16%)	4 (3%)	8	47
10	H	136/138 (99%)	118 (87%)	17 (12%)	1 (1%)	30	80
11	I	125/128 (98%)	100 (80%)	23 (18%)	2 (2%)	14	63
12	J	96/105 (91%)	73 (76%)	18 (19%)	5 (5%)	3	25
13	K	117/129 (91%)	97 (83%)	18 (15%)	2 (2%)	14	62
14	L	122/134 (91%)	88 (72%)	26 (21%)	8 (7%)	2	16
15	M	115/126 (91%)	92 (80%)	16 (14%)	7 (6%)	2	19
16	N	58/61 (95%)	45 (78%)	8 (14%)	5 (9%)	1	8
17	O	86/89 (97%)	70 (81%)	15 (17%)	1 (1%)	19	70
18	P	81/88 (92%)	65 (80%)	14 (17%)	2 (2%)	9	49
19	Q	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	11	55
20	R	68/88 (77%)	53 (78%)	13 (19%)	2 (3%)	7	43
21	S	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	8
22	T	97/106 (92%)	79 (81%)	14 (14%)	4 (4%)	4	32
23	U	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	4	29
24	X	352/354 (99%)	297 (84%)	44 (12%)	11 (3%)	7	41
All	All	2691/2894 (93%)	2172 (81%)	418 (16%)	101 (4%)	5	34

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	47	LEU

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Mol	Chain	Res	Type
12	J	75	ILE
15	M	4	ILE
15	M	106	ASN
15	M	117	VAL

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	202/220 (92%)	189 (94%)	13 (6%)	25	69
5	C	160/188 (85%)	151 (94%)	9 (6%)	30	75
6	D	180/181 (99%)	171 (95%)	9 (5%)	34	78
7	E	116/123 (94%)	105 (90%)	11 (10%)	12	45
8	F	90/90 (100%)	86 (96%)	4 (4%)	39	81
9	G	126/127 (99%)	125 (99%)	1 (1%)	89	98
10	H	119/119 (100%)	114 (96%)	5 (4%)	40	82
11	I	98/99 (99%)	92 (94%)	6 (6%)	26	71
12	J	88/92 (96%)	80 (91%)	8 (9%)	14	47
13	K	90/99 (91%)	86 (96%)	4 (4%)	39	81
14	L	104/110 (94%)	98 (94%)	6 (6%)	28	73
15	M	94/101 (93%)	87 (93%)	7 (7%)	20	62
16	N	49/50 (98%)	47 (96%)	2 (4%)	41	82
17	O	79/80 (99%)	74 (94%)	5 (6%)	25	69
18	P	72/74 (97%)	68 (94%)	4 (6%)	30	75
19	Q	94/97 (97%)	91 (97%)	3 (3%)	51	87
20	R	61/77 (79%)	59 (97%)	2 (3%)	50	87
21	S	69/80 (86%)	59 (86%)	10 (14%)	5	22
22	T	76/82 (93%)	71 (93%)	5 (7%)	24	67
23	U	19/22 (86%)	19 (100%)	0	100	100
24	X	299/299 (100%)	278 (93%)	21 (7%)	21	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2285/2410 (95%)	2150 (94%)	135 (6%)	28 72

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	73	ASP
14	L	64	GLU
24	X	187	GLU
12	J	74	ILE
13	K	92	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1525 (98%)	211 (14%)	56 (3%)
2	Y	76/77 (98%)	11 (14%)	2 (2%)
2	Z	76/77 (98%)	8 (10%)	1 (1%)
3	V	11/27 (40%)	2 (18%)	1 (9%)
All	All	1666/1706 (97%)	232 (13%)	60 (3%)

5 of 232 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	31	G
1	A	39	G
1	A	47	C

5 of 60 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	561	U
1	A	884	U
1	A	1507	A
1	A	815	A
1	A	968	A

## 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 383 ligands modelled in this entry, 383 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

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.