



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 10:17 AM BST

PDB ID : 1FKA
Title : STRUCTURE OF FUNCTIONALLY ACTIVATED SMALL RIBOSOMAL
SUBUNIT AT 3.3 Å RESOLUTION
Authors : Schlutzen, F.; Tocilj, A.; Zarivach, R.; Harms, J.; Gluehmann, M.; Janell,
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Deposited on : 2000-08-09
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

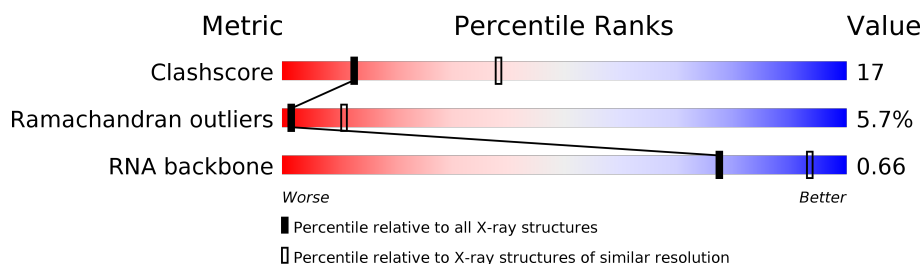
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)


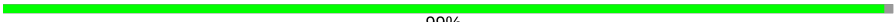







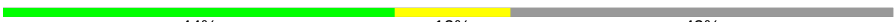


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1518	38% 49% 11% .
2	B	111	100%
3	C	176	100%
4	D	209	67% 9% . 23%
5	E	162	84% 13% .
6	F	101	89% 7% .
7	G	151	82% .. 15%
8	H	138	88% 9% ..

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Mol	Chain	Length	Quality of chain
9	I	89	 100%
10	J	71	 99% .
11	K	70	 100%
12	L	103	 100%
13	M	77	 100%
14	N	26	 100%
15	O	89	 92% 6% ..
16	P	73	 100%
17	Q	84	 80% 20%
18	R	88	 44% 13% 43%
19	S	93	 58% 19% . 22%
20	T	95	 83% 17%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 34977 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	1479	Total	C	N	O	P	0	0	0
			28902	12742	4656	10025	1479			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	C	DELETION	GB 155076
A	?	-	G	DELETION	GB 155076
A	?	-	C	DELETION	GB 155076
A	?	-	A	DELETION	GB 155076

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	111	Total	C	0	0	111
			111	111			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	176	Total	C	0	0	176
			176	176			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	161	Total	C	N	O	0	0	0
			793	471	161	161			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	157	Total	C	N	O	0	0	0
			768	454	157	157			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	97	Total	C	N	O	0	0	0
			482	288	97	97			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	128	Total	C	N	O	0	0	0
			634	378	128	128			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	136	Total	C	N	O	0	0	0
			667	395	136	136			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	ASP	GLU	CONFLICT	UNP P24319
H	37	ARG	LYS	CONFLICT	UNP P24319
H	52	ASP	GLU	CONFLICT	UNP P24319
H	61	VAL	ILE	CONFLICT	UNP P24319
H	62	TYR	HIS	CONFLICT	UNP P24319
H	81	HIS	LYS	CONFLICT	UNP P24319
H	88	LYS	ARG	CONFLICT	UNP P24319
H	115	SER	PRO	CONFLICT	UNP P24319

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	I	89	Total	C	0	0	89
			89	89			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	70	Total C 70 70	0	0	70

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	70	Total C 70 70	0	0	70

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	103	Total C 103 103	0	0	103

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	M	77	Total C 77 77	0	0	77

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	N	26	Total C 26 26	0	0	26

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	O	88	Total C N O 434 258 88 88	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	80	GLU	ALA	CONFLICT	UNP P80378
O	81	ILE	LEU	CONFLICT	UNP P80378
O	82	VAL	ILE	CONFLICT	UNP P80378
O	87	LEU	ILE	CONFLICT	UNP P80378

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	P	73	Total C 73 73	0	0	73

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	Q	84	Total C N O 420 252 84 84	0	0	0

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	R	50	Total C N O 246 146 50 50	0	0	0

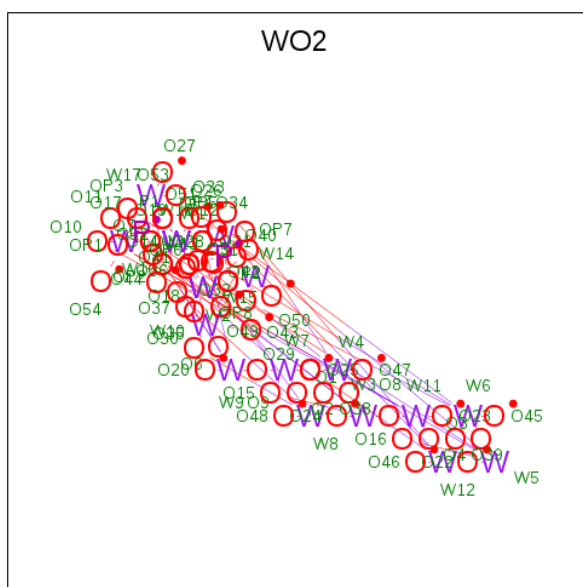
- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	S	73	Total C N O 359 213 73 73	0	0	0

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	T	95	Total C N O 470 280 95 95	0	0	0

- Molecule 21 is OCTADECATUNGSTENYL DIPHOSPHATE (three-letter code: WO2) (formula: O₆₂P₂W₁₈).



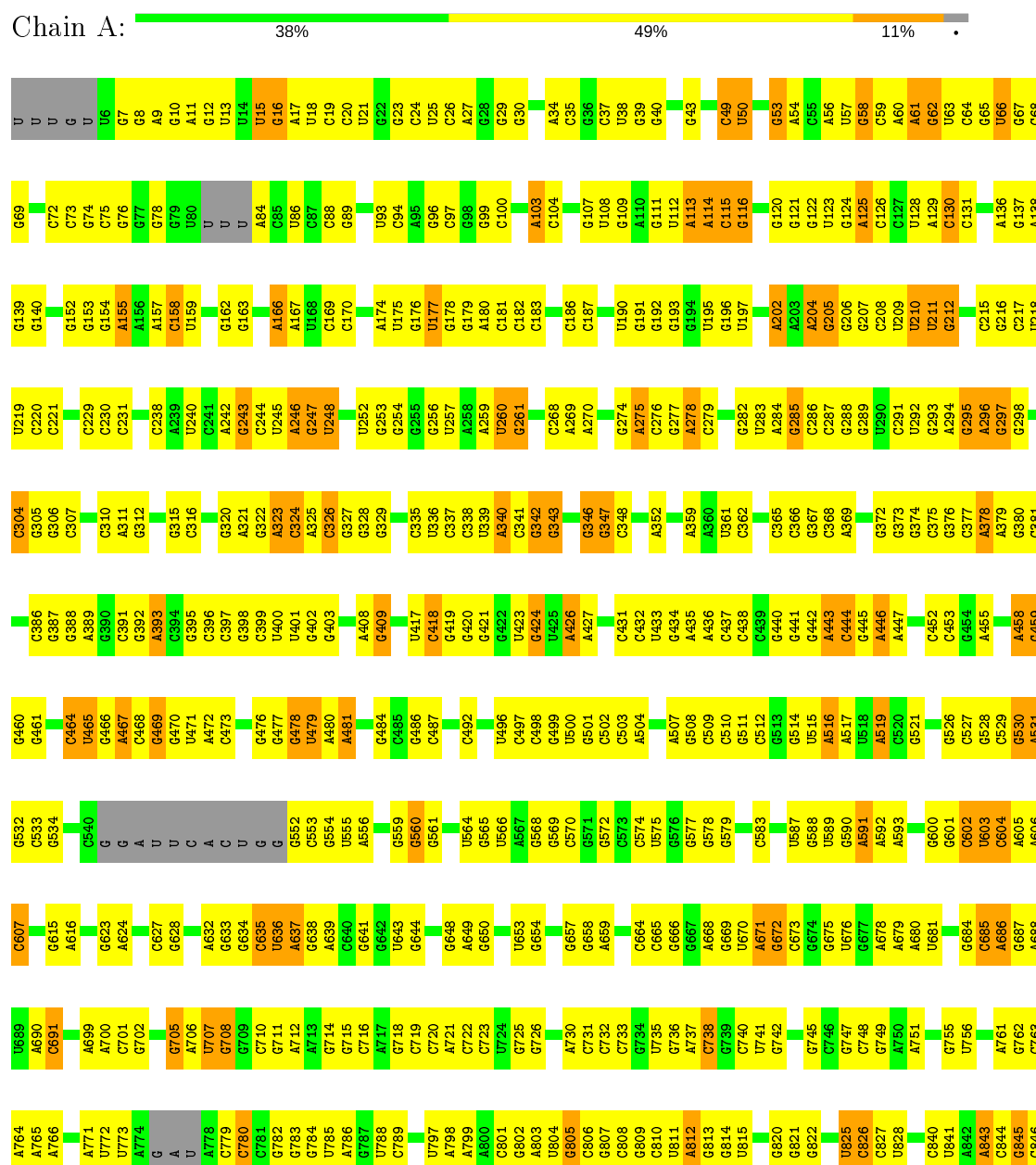
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total W 1 1	0	0
21	A	1	Total W 1 1	0	0
21	C	1	Total W 1 1	0	0
21	G	1	Total W 1 1	0	0
21	H	1	Total W 1 1	0	0
21	K	1	Total W 1 1	0	0
21	R	1	Total W 1 1	0	0

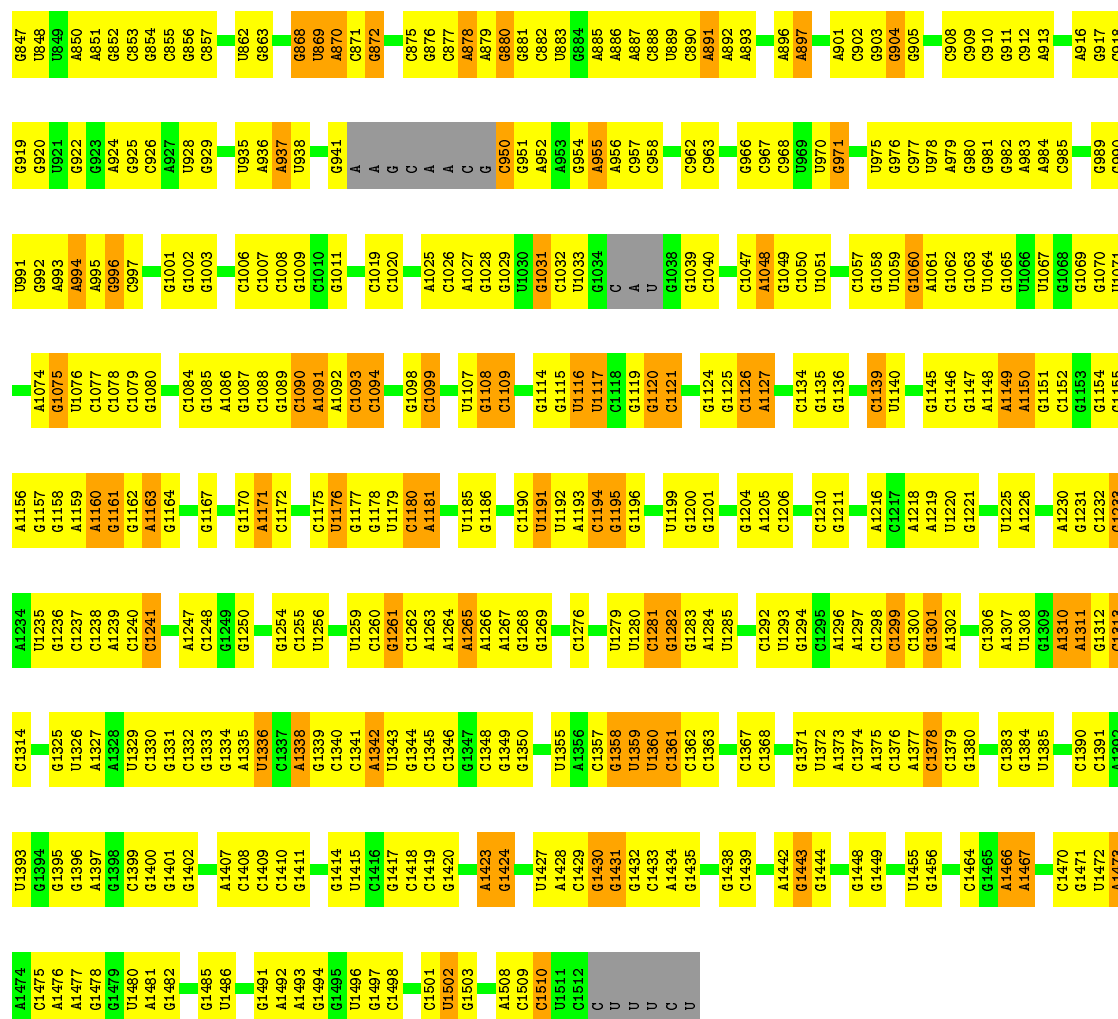
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 RIBOSOMAL RNA



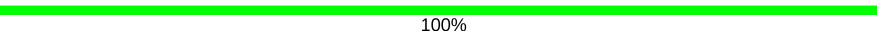


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B: 

There are no outlier residues recorded for this chain.

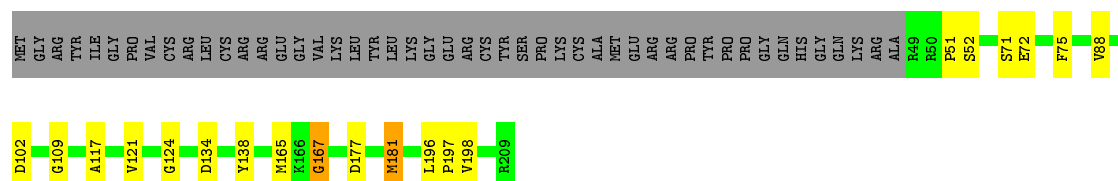
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C: 


There are no outlier residues recorded for this chain.

- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D: 




- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:  84% 13% .



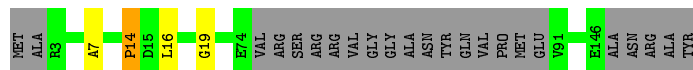
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:  89% 7% .




- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:  82% 15% ..



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:  88% 9% ..



- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:  99% .



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:  92% 6% ..




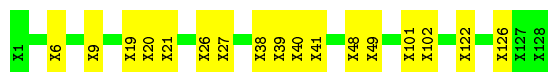
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:  100%

There are no outlier residues recorded for this chain.

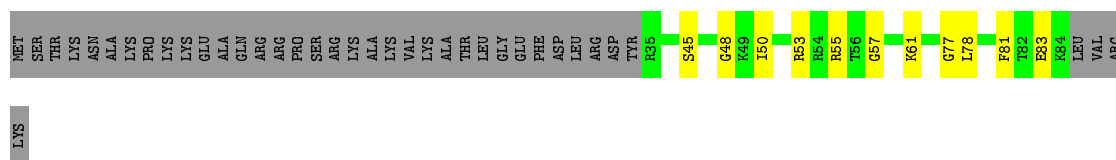
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:  80% 20%



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:  44% 13% 43%




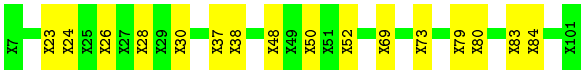
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:  58% 19% . 22%



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:  83% 17%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	406.30 Å 406.30 Å 173.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.30	Depositor
% Data completeness (in resolution range)	74.5 (35.00-3.30)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.304 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34977	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: WO2

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	0.26	1/32200 (0.0%)	0.68	4/50167 (0.0%)
4	D	0.20	0/792	0.39	0/1100
5	E	0.19	0/767	0.43	0/1062
6	F	0.19	0/481	0.42	0/670
7	G	0.19	0/632	0.37	0/878
8	H	0.19	0/666	0.41	0/923
15	O	0.19	0/433	0.40	0/601
18	R	0.22	0/245	0.41	0/339
19	S	0.27	0/358	0.49	0/496
All	All	0.26	1/36574 (0.0%)	0.66	4/56236 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	A	P-O5'	-27.68	1.32	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	950	C	O5'-P-OP2	22.27	137.42	110.70
1	A	84	A	O5'-P-OP1	14.69	128.32	110.70
1	A	84	A	P-O5'-C5'	6.46	131.23	120.90
1	A	950	C	P-O5'-C5'	6.08	130.63	120.90

There are no chirality outliers.

There are no planarity outliers.

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	28902	0	14582	812	0
2	B	111	0	0	0	0
3	C	176	0	0	0	0
4	D	793	0	351	9	0
5	E	768	0	381	8	0
6	F	482	0	212	5	0
7	G	634	0	303	1	0
8	H	667	0	293	6	0
9	I	89	0	0	0	0
10	J	70	0	0	0	0
11	K	70	0	0	0	0
12	L	103	0	0	0	0
13	M	77	0	0	0	0
14	N	26	0	0	0	0
15	O	434	0	185	3	0
16	P	73	0	0	0	0
17	Q	420	0	112	11	0
18	R	246	0	107	4	0
19	S	359	0	157	7	0
20	T	470	0	99	9	0
21	A	2	0	0	0	0
21	C	1	0	0	0	0
21	G	1	0	0	0	0
21	H	1	0	0	0	0
21	K	1	0	0	0	0
21	R	1	0	0	0	0
All	All	34977	0	16782	861	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 17.

The worst 5 of 861 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:A:H3'	1:A:607:C:H5''	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:G:H5''	1:A:1076:U:H5'	1.34	1.10
1:A:1442:A:H2'	1:A:1443:G:H5''	1.35	1.08
1:A:1501:C:H2'	1:A:1502:U:H5''	1.36	1.07
1:A:1264:A:H3'	1:A:1265:A:H5'	1.38	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	159/209 (76%)	122 (77%)	27 (17%)	10 (6%)	1	9
5	E	155/162 (96%)	124 (80%)	24 (16%)	7 (4%)	2	15
6	F	95/101 (94%)	79 (83%)	14 (15%)	2 (2%)	7	31
7	G	124/151 (82%)	110 (89%)	11 (9%)	3 (2%)	6	28
8	H	134/138 (97%)	109 (81%)	19 (14%)	6 (4%)	2	15
15	O	86/89 (97%)	74 (86%)	8 (9%)	4 (5%)	2	14
18	R	48/88 (54%)	26 (54%)	15 (31%)	7 (15%)	0	1
19	S	71/93 (76%)	46 (65%)	14 (20%)	11 (16%)	0	1
All	All	872/1031 (85%)	690 (79%)	132 (15%)	50 (6%)	1	11

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	51	PRO
4	D	198	VAL
7	G	14	PRO
8	H	74	PRO
8	H	83	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1473/1518 (97%)	228 (15%)	8 (0%)

5 of 228 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	15	U
1	A	16	G
1	A	17	A
1	A	40	G
1	A	49	C

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	346	G
1	A	903	G
1	A	636	U
1	A	296	A
1	A	478	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	56:UNK	C	101:UNK	N	3.74

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.