



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:55 PM UTC

PDB ID : 3IEM / pdb_00003iem
Title : Crystal Structure of TTHA0252 from *Thermus thermophilus* HB8 complexed with RNA analog
Authors : Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.
Deposited on : 2009-07-23
Resolution : 2.50 Å (reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

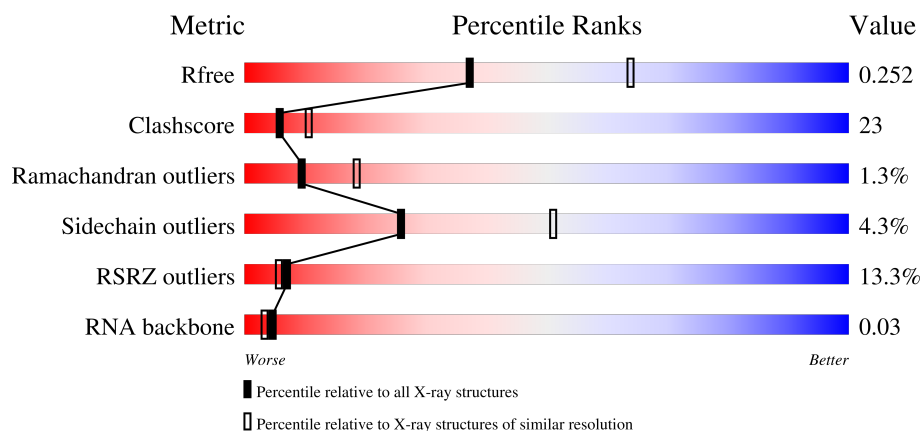
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



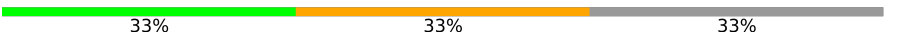
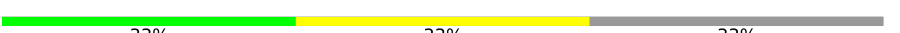
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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 of 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 $\leq 5\%$. 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	431	
1	B	431	
1	C	431	
1	D	431	

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Mol	Chain	Length	Quality of chain
2	G	6	
2	H	6	
2	I	6	
2	J	6	
2	K	6	
2	L	6	
2	M	6	
2	N	6	
2	O	6	
2	P	6	

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
2	SSU	G	3	-	-	X	-
2	SSU	M	2	-	-	X	-
3	SO4	A	446	-	-	X	-
3	SO4	B	445	-	-	X	-
3	SO4	B	448	-	-	X	-
3	SO4	C	439	-	-	X	-
3	SO4	D	436	-	-	X	-
3	SO4	D	439	-	-	X	-
5	FLC	B	450	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14354 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.

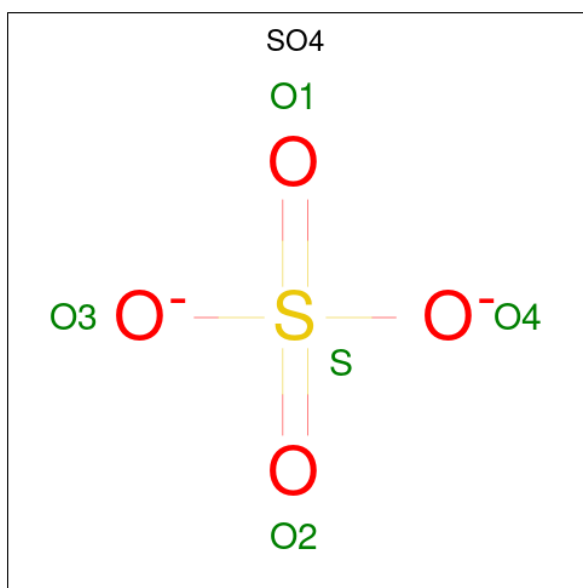
- Molecule 1 is a protein called Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			

- Molecule 2 is a RNA chain called RNA (5'-R(*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	6	Total 101	C 45	N 10	O 36	P 5	S 5	0	0	1
2	H	4	Total 61	C 27	N 6	O 22	P 3	S 3	0	0	1
2	I	6	Total 85	C 36	N 8	O 31	P 5	S 5	0	0	1
2	J	3	Total 41	C 18	N 4	O 15	P 2	S 2	0	0	1
2	K	3	Total 57	C 27	N 6	O 20	P 2	S 2	0	0	0
2	L	4	Total 45	C 18	N 4	O 17	P 3	S 3	0	0	1
2	M	2	Total 21	C 9	N 2	O 8	P 1	S 1	0	0	0
2	N	3	Total 41	C 18	N 4	O 15	P 2	S 2	0	0	1
2	O	2	Total 37	C 18	N 4	O 13	P 1	S 1	0	0	0
2	P	2	Total 21	C 9	N 2	O 8	P 1	S 1	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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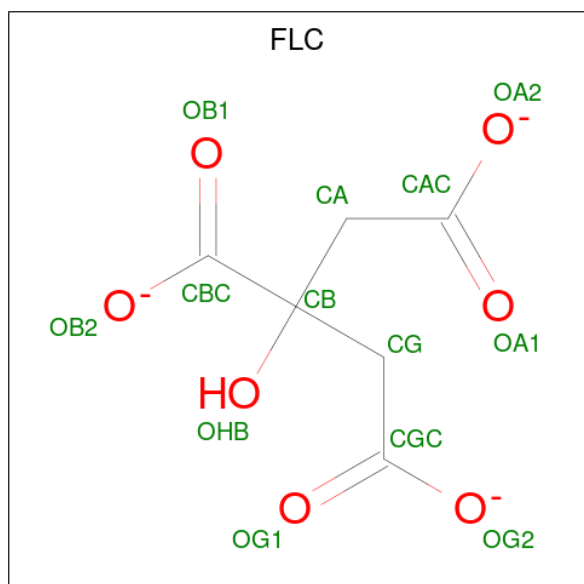
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		

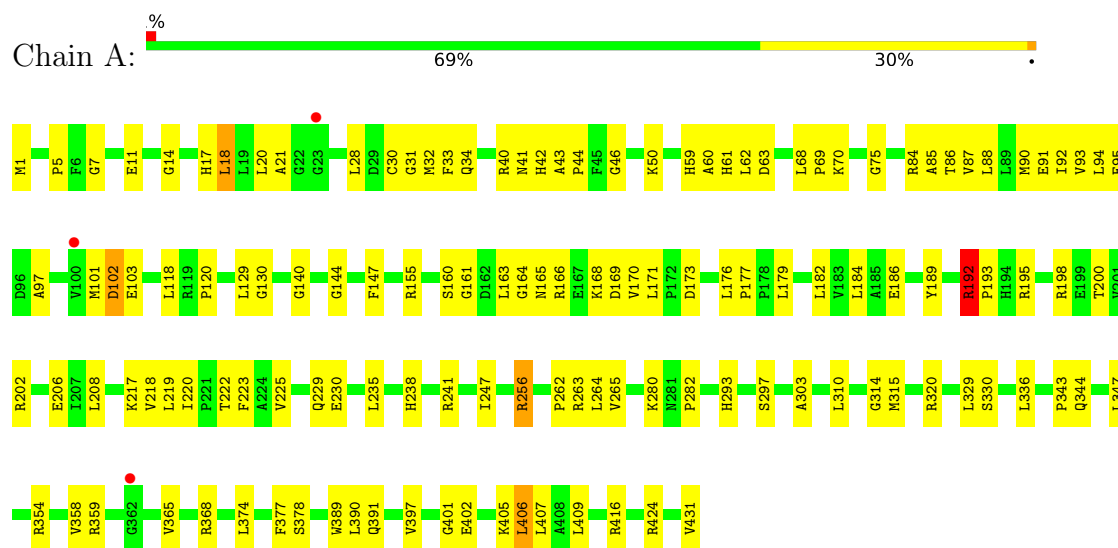
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total 84	O 84	0	0
6	B	71	Total 71	O 71	0	0
6	C	22	Total 22	O 22	0	0
6	D	37	Total 37	O 37	0	0
6	G	1	Total 1	O 1	0	0
6	J	2	Total 2	O 2	0	0
6	K	2	Total 2	O 2	0	0
6	L	2	Total 2	O 2	0	0
6	M	1	Total 1	O 1	0	0
6	O	2	Total 2	O 2	0	0

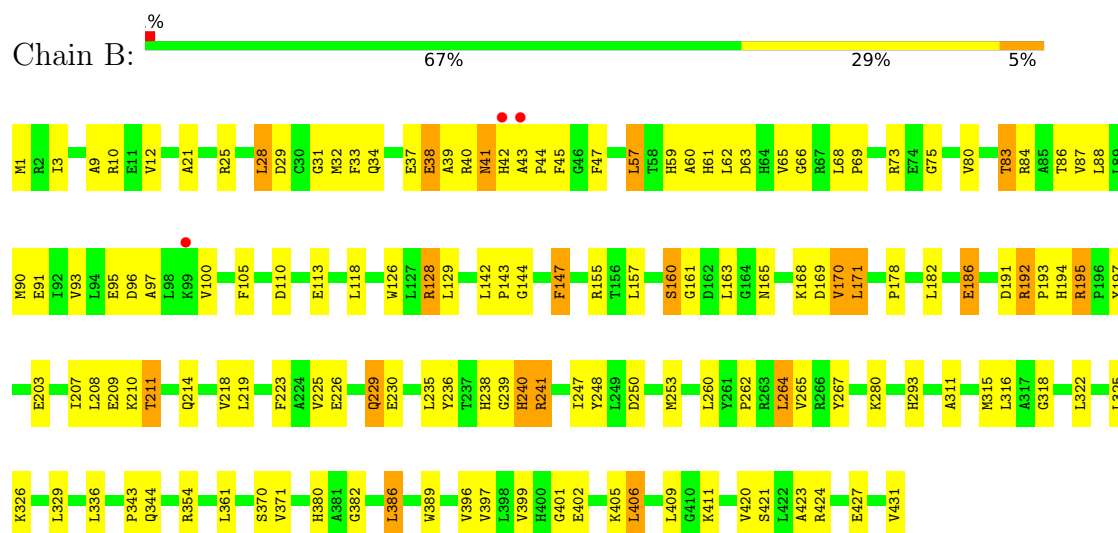
3 Residue-property plots [i](#)

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 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: Ribonuclease TTHA0252

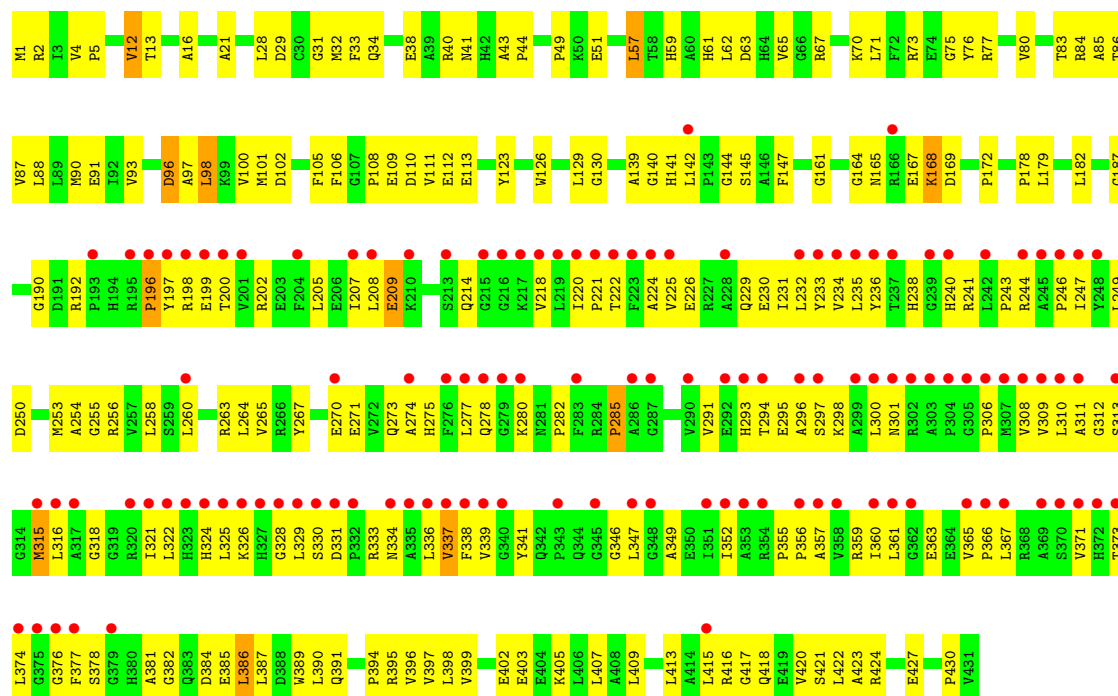


• Molecule 1: Ribonuclease TTHA0252

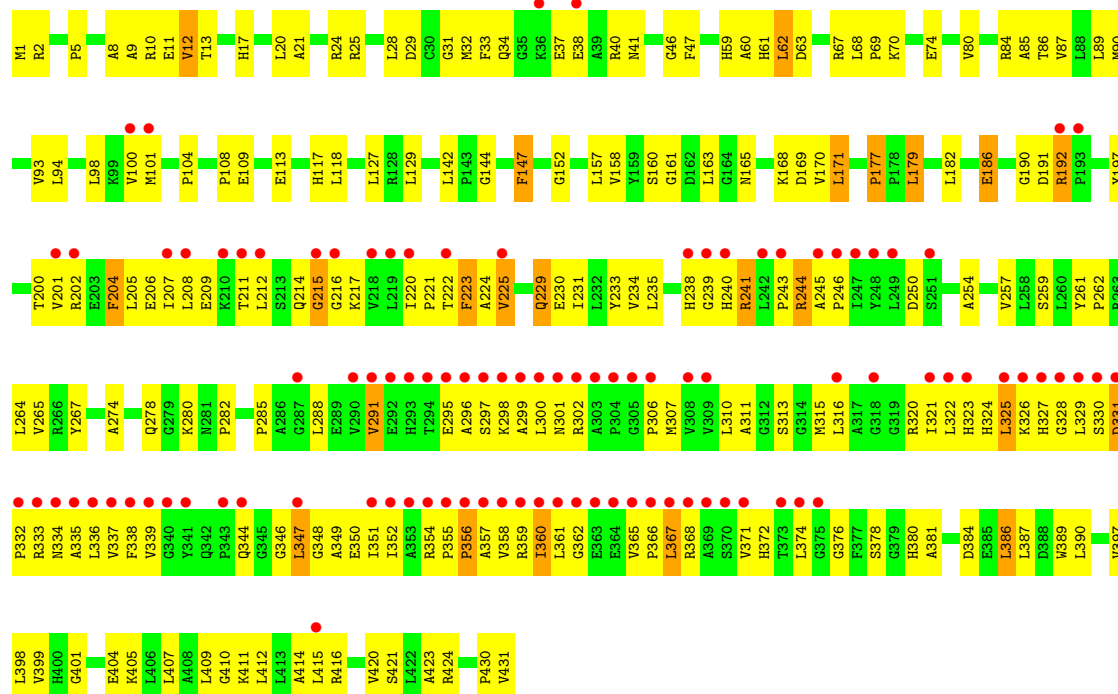


• Molecule 1: Ribonuclease TTHA0252



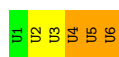


• Molecule 1: Ribonuclease TTHA0252



• Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')

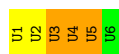
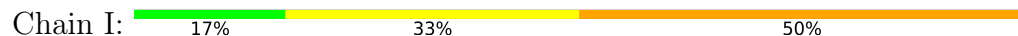




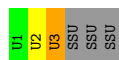
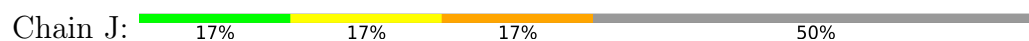
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



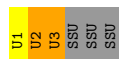
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



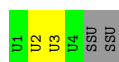
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



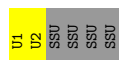
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



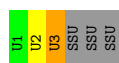
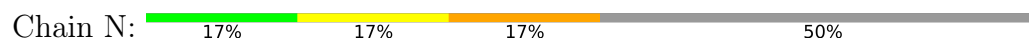
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')

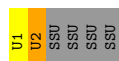


- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



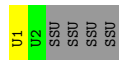
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')





- Molecule 2: RNA (5'-R(* (SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')

Chain P: 17% 17% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.69Å 146.44Å 119.97Å 90.00° 110.37° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.50) 94.0 (50.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.41 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.257 0.208 , 0.252	Depositor DCC
R_{free} test set	8060 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14354	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SSU, FLC, SO4

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	0.48	0/3407	0.98	13/4621 (0.3%)
1	B	0.47	0/3407	0.98	13/4621 (0.3%)
1	C	0.37	0/3407	0.93	11/4621 (0.2%)
1	D	0.38	0/3407	0.93	12/4621 (0.3%)
All	All	0.43	0/13628	0.95	49/18484 (0.3%)

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	ARG	N-CA-C	10.59	117.50	108.07
1	A	192	ARG	N-CA-C	10.56	117.72	108.22
1	B	170	VAL	N-CA-C	7.98	118.78	110.72
1	A	161	GLY	N-CA-C	-7.50	98.58	111.47
1	B	225	VAL	N-CA-C	7.04	120.87	111.44

There are no chirality outliers.

There are no planarity outliers.

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	3326	0	3351	98	0
1	B	3326	0	3351	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3326	0	3351	191	0
1	D	3326	0	3351	210	0
2	G	101	0	51	21	0
2	H	61	0	31	4	0
2	I	85	0	40	14	0
2	J	41	0	21	1	0
2	K	57	0	31	7	0
2	L	45	0	20	1	0
2	M	21	0	10	7	0
2	N	41	0	21	2	0
2	O	37	0	21	6	0
2	P	21	0	10	2	0
3	A	80	0	0	5	0
3	B	90	0	0	4	0
3	C	60	0	0	2	0
3	D	55	0	0	5	0
3	J	5	0	0	0	0
3	K	5	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	13	0	5	4	0
6	A	84	0	0	6	0
6	B	71	0	0	1	0
6	C	22	0	0	0	0
6	D	37	0	0	0	0
6	G	1	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
6	M	1	0	0	0	0
6	O	2	0	0	1	0
All	All	14354	0	13665	642	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 23.

The worst 5 of 642 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)
2:M:1:SSU:H1'	2:M:2:SSU:S1P	1.56	1.45
1:D:331:ASP:H	1:D:368:ARG:HB2	1.21	1.03
1:D:47:PHE:HA	2:M:2:SSU:S1P	1.99	1.03
2:M:1:SSU:C1'	2:M:2:SSU:S1P	2.47	1.03
1:C:98:LEU:HD11	1:C:108:PRO:HA	1.39	1.01

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	
1	A	429/431 (100%)	410 (96%)	17 (4%)	2 (0%)	24	43
1	B	429/431 (100%)	405 (94%)	21 (5%)	3 (1%)	18	34
1	C	429/431 (100%)	369 (86%)	50 (12%)	10 (2%)	5	8
1	D	429/431 (100%)	377 (88%)	44 (10%)	8 (2%)	6	11
All	All	1716/1724 (100%)	1561 (91%)	132 (8%)	23 (1%)	9	18

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	241	ARG
1	A	102	ASP
1	B	240	HIS
1	B	241	ARG
1	C	168	LYS

5.3.2 Protein sidechains [i](#)

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	
1	A	342/342 (100%)	326 (95%)	16 (5%)	23	47
1	B	342/342 (100%)	323 (94%)	19 (6%)	19	39
1	C	342/342 (100%)	334 (98%)	8 (2%)	44	72
1	D	342/342 (100%)	326 (95%)	16 (5%)	23	47
All	All	1368/1368 (100%)	1309 (96%)	59 (4%)	26	51

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	325	LEU
1	D	386	LEU
1	C	28	LEU
1	D	367	LEU
1	D	229	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	342	GLN
1	D	165	ASN
1	C	418	GLN
1	D	41	ASN
1	D	214	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	4/6 (66%)	3 (75%)	0
2	H	2/6 (33%)	2 (100%)	0
2	I	3/6 (50%)	3 (100%)	0
2	J	1/6 (16%)	1 (100%)	0
2	K	2/6 (33%)	2 (100%)	0
2	L	1/6 (16%)	0	0
2	M	0/6	-	-
2	N	1/6 (16%)	1 (100%)	0
2	O	1/6 (16%)	1 (100%)	0
2	P	0/6	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	15/60 (25%)	13 (86%)	0

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	4	SSU
2	G	5	SSU
2	G	6	SSU
2	H	3	SSU
2	H	4	SSU

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

Of 35 non-standard protein/DNA/RNA residues modelled in this entry, 6 are modelled with single atom - leaving 29 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	$\# Z > 2$
2	SSU	K	1	2	18,18,22	0.31	0	26,26,33	0.39	0
2	SSU	M	2	2	0,3,22	-	-	0,3,33	-	-
2	SSU	G	2	2	18,21,22	0.26	0	25,30,33	0.40	0
2	SSU	I	6	2	0,3,22	-	-	0,3,33	-	-
2	SSU	K	3	2	18,21,22	0.27	0	25,30,33	0.29	0
2	SSU	N	2	2	18,21,22	0.28	0	25,30,33	0.36	0
2	SSU	P	1	2	18,18,22	0.22	0	26,26,33	0.37	0
2	SSU	G	4	2	18,21,22	0.30	0	25,30,33	0.32	0
2	SSU	I	2	2	18,21,22	0.23	0	25,30,33	0.34	0
2	SSU	G	5	2	18,21,22	0.27	0	25,30,33	0.32	0
2	SSU	N	3	2	18,21,22	0.27	0	25,30,33	0.29	0
2	SSU	O	1	2	18,18,22	0.27	0	26,26,33	0.30	0
2	SSU	P	2	2	0,3,22	-	-	0,3,33	-	-
2	SSU	I	5	2	18,21,22	0.31	0	25,30,33	0.42	0
2	SSU	L	3	2	18,21,22	0.28	0	25,30,33	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SSU	H	4	2	18,21,22	0.26	0	25,30,33	0.30	0
2	SSU	M	1	2	18,18,22	0.31	0	26,26,33	0.60	0
2	SSU	I	4	2	18,21,22	0.28	0	25,30,33	0.37	0
2	SSU	J	3	2	18,21,22	0.28	0	25,30,33	0.37	0
2	SSU	I	3	2	18,21,22	0.24	0	25,30,33	0.60	0
2	SSU	G	3	2	18,21,22	0.29	0	25,30,33	0.48	0
2	SSU	K	2	2	18,21,22	0.29	0	25,30,33	0.28	0
2	SSU	J	2	2	18,21,22	0.34	0	25,30,33	0.35	0
2	SSU	L	4	2	0,3,22	-	-	0,3,33	-	-
2	SSU	L	2	2	18,21,22	0.32	0	25,30,33	0.43	0
2	SSU	H	2	2	18,21,22	0.25	0	25,30,33	0.25	0
2	SSU	G	6	2	18,21,22	0.25	0	25,30,33	0.37	0
2	SSU	H	3	2	18,21,22	0.23	0	25,30,33	0.28	0
2	SSU	O	2	2	18,21,22	0.24	0	25,30,33	0.33	0

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
2	SSU	K	1	2	-	2/6/22/26	0/2/2/2
2	SSU	G	2	2	-	4/7/25/26	0/2/2/2
2	SSU	K	3	2	-	5/7/25/26	0/2/2/2
2	SSU	N	2	2	-	2/7/25/26	0/2/2/2
2	SSU	P	1	2	-	2/6/22/26	0/2/2/2
2	SSU	G	4	2	-	5/7/25/26	0/2/2/2
2	SSU	I	2	2	-	7/7/25/26	0/2/2/2
2	SSU	G	5	2	-	0/7/25/26	0/2/2/2
2	SSU	N	3	2	-	1/7/25/26	0/2/2/2
2	SSU	O	1	2	-	3/6/22/26	0/2/2/2
2	SSU	I	5	2	-	4/7/25/26	0/2/2/2
2	SSU	L	3	2	-	0/7/25/26	0/2/2/2
2	SSU	H	4	2	-	3/7/25/26	0/2/2/2
2	SSU	M	1	2	-	2/6/22/26	0/2/2/2
2	SSU	I	4	2	-	6/7/25/26	0/2/2/2
2	SSU	J	3	2	-	2/7/25/26	0/2/2/2
2	SSU	I	3	2	-	3/7/25/26	0/2/2/2
2	SSU	G	3	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SSU	K	2	2	-	1/7/25/26	0/2/2/2
2	SSU	J	2	2	-	2/7/25/26	0/2/2/2
2	SSU	L	2	2	-	0/7/25/26	0/2/2/2
2	SSU	H	2	2	-	0/7/25/26	0/2/2/2
2	SSU	G	6	2	-	2/7/25/26	0/2/2/2
2	SSU	H	3	2	-	1/7/25/26	0/2/2/2
2	SSU	O	2	2	-	2/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	6	SSU	C4'-C5'-O5'-P
2	I	4	SSU	C2'-C1'-N1-C6
2	I	4	SSU	C2'-C1'-N1-C2
2	I	5	SSU	O4'-C1'-N1-C6
2	I	5	SSU	O4'-C1'-N1-C2

There are no ring outliers.

25 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	SSU	2	0
2	M	2	SSU	7	0
2	G	2	SSU	4	0
2	K	3	SSU	3	0
2	N	2	SSU	2	0
2	P	1	SSU	2	0
2	G	4	SSU	5	0
2	I	2	SSU	4	0
2	G	5	SSU	3	0
2	N	3	SSU	2	0
2	O	1	SSU	3	0
2	I	5	SSU	3	0
2	L	3	SSU	1	0
2	H	4	SSU	2	0
2	M	1	SSU	4	0
2	I	4	SSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	3	SSU	1	0
2	I	3	SSU	5	0
2	G	3	SSU	7	0
2	K	2	SSU	3	0
2	J	2	SSU	1	0
2	L	2	SSU	1	0
2	G	6	SSU	5	0
2	H	3	SSU	2	0
2	O	2	SSU	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 8 are monoatomic - leaving 60 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	$\# Z > 2$
3	SO4	A	443	-	4,4,4	1.05	0	6,6,6	0.59	0
3	SO4	A	437	-	4,4,4	1.02	0	6,6,6	0.58	0
3	SO4	C	436	-	4,4,4	1.07	0	6,6,6	0.57	0
3	SO4	C	433	-	4,4,4	1.07	0	6,6,6	0.58	0
3	SO4	A	440	-	4,4,4	1.08	0	6,6,6	0.57	0
3	SO4	C	437	-	4,4,4	1.07	0	6,6,6	0.57	0
3	SO4	B	433	-	4,4,4	1.07	0	6,6,6	0.58	0
3	SO4	C	440	-	4,4,4	1.08	0	6,6,6	0.58	0
3	SO4	D	438	-	4,4,4	1.10	0	6,6,6	0.58	0
3	SO4	B	448	-	4,4,4	1.09	0	6,6,6	0.57	0
3	SO4	D	436	-	4,4,4	1.09	0	6,6,6	0.55	0
3	SO4	A	446	-	4,4,4	1.05	0	6,6,6	0.59	0
3	SO4	J	40	-	4,4,4	1.06	0	6,6,6	0.57	0
3	SO4	A	447	-	4,4,4	1.06	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	444	-	4,4,4	1.07	0	6,6,6	0.57	0
3	SO4	K	36	-	4,4,4	1.08	0	6,6,6	0.57	0
3	SO4	D	435	-	4,4,4	1.05	0	6,6,6	0.58	0
3	SO4	C	432	-	4,4,4	1.06	0	6,6,6	0.58	0
5	FLC	B	450	-	12,12,12	1.61	4 (33%)	17,17,17	1.41	1 (5%)
3	SO4	D	437	-	4,4,4	1.06	0	6,6,6	0.57	0
3	SO4	D	441	-	4,4,4	1.07	0	6,6,6	0.56	0
3	SO4	A	436	-	4,4,4	1.09	0	6,6,6	0.59	0
3	SO4	A	435	-	4,4,4	1.10	0	6,6,6	0.57	0
3	SO4	B	442	-	4,4,4	1.06	0	6,6,6	0.58	0
3	SO4	A	441	-	4,4,4	1.06	0	6,6,6	0.57	0
3	SO4	B	439	-	4,4,4	1.08	0	6,6,6	0.56	0
3	SO4	D	433	-	4,4,4	1.08	0	6,6,6	0.58	0
3	SO4	D	432	-	4,4,4	1.07	0	6,6,6	0.57	0
3	SO4	C	442	-	4,4,4	1.04	0	6,6,6	0.56	0
3	SO4	D	440	-	4,4,4	1.07	0	6,6,6	0.58	0
3	SO4	A	432	-	4,4,4	1.07	0	6,6,6	0.56	0
3	SO4	A	434	-	4,4,4	1.07	0	6,6,6	0.58	0
3	SO4	C	441	-	4,4,4	1.09	0	6,6,6	0.56	0
3	SO4	C	439	-	4,4,4	1.09	0	6,6,6	0.57	0
3	SO4	B	447	-	4,4,4	1.00	0	6,6,6	0.61	0
3	SO4	C	435	-	4,4,4	1.08	0	6,6,6	0.58	0
3	SO4	B	436	-	4,4,4	1.05	0	6,6,6	0.58	0
3	SO4	B	441	-	4,4,4	1.08	0	6,6,6	0.57	0
3	SO4	C	434	-	4,4,4	1.06	0	6,6,6	0.58	0
3	SO4	A	439	-	4,4,4	1.08	0	6,6,6	0.56	0
3	SO4	D	439	-	4,4,4	1.08	0	6,6,6	0.57	0
3	SO4	C	443	-	4,4,4	1.08	0	6,6,6	0.59	0
3	SO4	B	445	-	4,4,4	1.11	0	6,6,6	0.54	0
3	SO4	B	435	-	4,4,4	1.08	0	6,6,6	0.57	0
3	SO4	D	442	-	4,4,4	1.07	0	6,6,6	0.57	0
3	SO4	B	437	-	4,4,4	1.07	0	6,6,6	0.56	0
3	SO4	B	443	-	4,4,4	1.09	0	6,6,6	0.57	0
3	SO4	D	434	-	4,4,4	1.05	0	6,6,6	0.57	0
3	SO4	A	433	-	4,4,4	1.08	0	6,6,6	0.58	0
3	SO4	A	438	-	4,4,4	1.08	0	6,6,6	0.57	0
3	SO4	B	432	-	4,4,4	1.11	0	6,6,6	0.55	0
3	SO4	B	440	-	4,4,4	1.06	0	6,6,6	0.58	0
3	SO4	A	444	-	4,4,4	1.05	0	6,6,6	0.59	0
3	SO4	A	442	-	4,4,4	1.05	0	6,6,6	0.58	0
3	SO4	B	446	-	4,4,4	1.09	0	6,6,6	0.56	0
3	SO4	B	434	-	4,4,4	1.08	0	6,6,6	0.58	0
3	SO4	A	445	-	4,4,4	1.07	0	6,6,6	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	438	-	4,4,4	1.07	0	6,6,6	0.57	0
3	SO4	B	449	-	4,4,4	1.00	0	6,6,6	0.61	0
3	SO4	B	438	-	4,4,4	1.09	0	6,6,6	0.56	0

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
5	FLC	B	450	-	-	0/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	450	FLC	OG2-CGC	-2.57	1.22	1.30
5	B	450	FLC	OA2-CAC	-2.55	1.22	1.30
5	B	450	FLC	CG-CB	2.08	1.56	1.54
5	B	450	FLC	CA-CB	2.07	1.56	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	450	FLC	OB2-CBC-CB	3.97	120.76	113.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	443	SO4	1	0
3	B	448	SO4	2	0
3	D	436	SO4	2	0
3	A	446	SO4	3	0
3	K	36	SO4	1	0
5	B	450	FLC	4	0
3	D	433	SO4	1	0
3	C	439	SO4	2	0
3	D	439	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	445	SO4	2	0
3	A	444	SO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	431/431 (100%)	-0.19	3 (0%) 84 81	14, 29, 51, 67	0
1	B	431/431 (100%)	-0.14	3 (0%) 84 81	14, 29, 52, 69	0
1	C	431/431 (100%)	1.33	123 (28%) 1 1	21, 63, 117, 137	0
1	D	431/431 (100%)	1.02	101 (23%) 2 1	22, 51, 111, 134	0
2	G	0/6	-	-	-	-
2	H	0/6	-	-	-	-
2	I	0/6	-	-	-	-
2	J	0/6	-	-	-	-
2	K	0/6	-	-	-	-
2	L	0/6	-	-	-	-
2	M	0/6	-	-	-	-
2	N	0/6	-	-	-	-
2	O	0/6	-	-	-	-
2	P	0/6	-	-	-	-
All	All	1724/1784 (96%)	0.50	230 (13%) 7 6	14, 39, 111, 137	0

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	361	LEU	6.0
1	D	365	VAL	5.7
1	D	358	VAL	5.6
1	D	366	PRO	5.4
1	D	347	LEU	5.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SSU	J	1	1/21	0.27	0.16	73,73,73,73	0
2	SSU	H	1	1/21	0.48	0.16	77,77,77,77	0
2	SSU	M	2	4/21	0.53	0.28	86,88,88,93	0
2	SSU	M	1	17/21	0.61	0.28	84,91,92,92	0
2	SSU	N	3	20/21	0.67	0.22	107,112,114,114	0
2	SSU	O	2	20/21	0.67	0.21	136,137,137,138	0
2	SSU	N	1	1/21	0.73	0.10	106,106,106,106	0
2	SSU	H	4	20/21	0.73	0.17	88,92,95,96	0
2	SSU	G	6	20/21	0.73	0.23	104,111,112,112	0
2	SSU	N	2	20/21	0.76	0.21	91,99,107,107	0
2	SSU	K	1	17/21	0.76	0.25	87,90,95,95	0
2	SSU	J	3	20/21	0.76	0.20	72,77,79,79	0
2	SSU	P	1	17/21	0.76	0.23	131,132,133,133	0
2	SSU	P	2	4/21	0.76	0.23	131,131,132,132	0
2	SSU	O	1	17/21	0.77	0.23	136,136,137,137	0
2	SSU	K	2	20/21	0.78	0.20	93,95,98,99	0
2	SSU	I	3	20/21	0.78	0.19	101,102,106,107	0
2	SSU	I	5	20/21	0.79	0.16	102,104,106,107	0
2	SSU	I	1	1/21	0.79	0.28	97,97,97,97	0
2	SSU	I	2	20/21	0.80	0.26	96,108,113,113	0
2	SSU	G	5	20/21	0.84	0.18	93,95,100,103	0
2	SSU	K	3	20/21	0.84	0.18	96,98,100,101	0
2	SSU	L	4	4/21	0.84	0.12	61,62,63,67	0
2	SSU	G	3	20/21	0.85	0.18	77,81,84,85	0
2	SSU	G	4	20/21	0.87	0.17	86,90,91,93	0
2	SSU	L	1	1/21	0.87	0.16	53,53,53,53	0
2	SSU	I	6	4/21	0.87	0.14	108,108,108,108	0
2	SSU	I	4	20/21	0.87	0.16	98,99,100,101	0
2	SSU	J	2	20/21	0.89	0.13	56,66,73,73	0
2	SSU	H	3	20/21	0.89	0.12	76,88,91,91	0
2	SSU	H	2	20/21	0.90	0.12	64,69,76,79	0
2	SSU	G	1	1/21	0.92	0.17	36,36,36,36	0
2	SSU	L	3	20/21	0.92	0.12	46,60,68,69	0
2	SSU	G	2	20/21	0.93	0.14	33,63,67,73	0
2	SSU	L	2	20/21	0.94	0.09	39,44,56,56	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
3	SO4	J	40	5/5	0.41	0.17	133,133,133,134	0
3	SO4	C	433	5/5	0.45	0.13	130,131,131,131	0
3	SO4	A	447	5/5	0.53	0.16	133,133,133,134	0
3	SO4	D	437	5/5	0.55	0.14	126,126,127,127	0
3	SO4	D	433	5/5	0.55	0.15	103,103,103,104	0
3	SO4	A	440	5/5	0.56	0.17	106,106,107,107	0
3	SO4	D	432	5/5	0.58	0.13	138,138,138,138	0
3	SO4	B	433	5/5	0.60	0.14	122,122,122,122	0
3	SO4	C	441	5/5	0.62	0.18	122,122,123,123	0
3	SO4	C	440	5/5	0.63	0.13	120,120,120,121	0
3	SO4	D	442	5/5	0.64	0.16	100,101,101,101	0
3	SO4	C	437	5/5	0.65	0.13	118,118,118,119	0
3	SO4	D	441	5/5	0.65	0.14	136,136,136,136	0
3	SO4	A	439	5/5	0.66	0.23	173,173,173,173	0
3	SO4	B	443	5/5	0.66	0.21	131,131,131,132	0
3	SO4	D	439	5/5	0.68	0.13	135,136,136,136	0
3	SO4	D	434	5/5	0.69	0.13	117,117,117,117	0
3	SO4	C	436	5/5	0.70	0.11	114,114,115,115	0
3	SO4	C	432	5/5	0.75	0.13	121,121,121,122	0
3	SO4	C	438	5/5	0.75	0.14	112,112,113,113	0
3	SO4	A	433	5/5	0.76	0.23	134,134,135,135	0
3	SO4	B	434	5/5	0.76	0.15	117,117,118,118	0
3	SO4	B	432	5/5	0.76	0.16	99,99,100,100	0
5	FLC	B	450	13/13	0.76	0.30	86,91,93,93	0
3	SO4	B	437	5/5	0.77	0.20	168,168,169,169	0
3	SO4	C	435	5/5	0.77	0.14	92,93,94,94	0
3	SO4	B	445	5/5	0.78	0.25	121,121,122,122	0
3	SO4	A	445	5/5	0.78	0.17	150,150,150,150	0
3	SO4	B	435	5/5	0.78	0.13	111,111,111,111	0
3	SO4	B	446	5/5	0.79	0.20	122,122,122,122	0
3	SO4	D	440	5/5	0.79	0.15	121,121,122,122	0
3	SO4	A	446	5/5	0.80	0.33	115,115,115,116	0
3	SO4	B	444	5/5	0.80	0.15	122,122,122,122	0
3	SO4	B	440	5/5	0.81	0.12	99,99,100,100	0
3	SO4	C	439	5/5	0.81	0.12	99,99,100,100	0
3	SO4	B	439	5/5	0.83	0.20	113,113,114,114	0
3	SO4	C	443	5/5	0.83	0.12	87,87,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	432	5/5	0.84	0.16	123,123,123,123	0
3	SO4	B	441	5/5	0.84	0.23	134,134,134,134	0
3	SO4	B	447	5/5	0.84	0.21	162,162,162,162	5
3	SO4	B	448	5/5	0.84	0.15	111,111,111,111	0
3	SO4	A	435	5/5	0.84	0.17	100,100,101,101	0
3	SO4	A	441	5/5	0.84	0.29	144,144,144,144	0
3	SO4	A	443	5/5	0.85	0.23	126,126,126,127	0
3	SO4	D	436	5/5	0.87	0.16	105,105,105,106	0
3	SO4	A	444	5/5	0.87	0.18	85,85,85,86	0
3	SO4	K	36	5/5	0.88	0.17	112,112,112,113	0
3	SO4	A	436	5/5	0.89	0.18	84,84,85,85	0
3	SO4	C	442	5/5	0.89	0.12	75,77,77,78	0
3	SO4	D	435	5/5	0.89	0.09	76,76,76,77	0
3	SO4	A	434	5/5	0.91	0.10	83,83,83,83	0
3	SO4	B	438	5/5	0.92	0.09	73,73,73,74	0
3	SO4	B	442	5/5	0.92	0.13	61,62,63,64	0
3	SO4	A	438	5/5	0.93	0.09	73,74,74,75	0
3	SO4	C	434	5/5	0.93	0.09	77,77,78,78	0
3	SO4	A	437	5/5	0.95	0.10	49,50,51,52	0
3	SO4	D	438	5/5	0.96	0.10	60,61,62,63	0
4	ZN	A	449	1/1	0.96	0.07	73,73,73,73	0
3	SO4	B	449	5/5	0.96	0.07	43,43,45,45	0
4	ZN	B	452	1/1	0.97	0.10	64,64,64,64	0
4	ZN	B	451	1/1	0.97	0.12	56,56,56,56	0
4	ZN	C	444	1/1	0.98	0.05	75,75,75,75	0
4	ZN	C	445	1/1	0.98	0.03	81,81,81,81	0
4	ZN	D	443	1/1	0.98	0.04	70,70,70,70	0
4	ZN	D	444	1/1	0.98	0.03	69,69,69,69	0
3	SO4	B	436	5/5	0.98	0.06	35,35,37,37	0
3	SO4	A	442	5/5	0.99	0.04	32,33,33,35	0
4	ZN	A	448	1/1	0.99	0.09	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.