Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 08:27 PM EDT

PDB ID	:	2PLY
Title	:	Structure of the mRNA binding fragment of elongation factor SelB in complex with SECIS RNA.
Authors	:	Soler, N.; Fourmy, D.; Yoshizawa, S.
Deposited on	:	2007-04-20
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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:

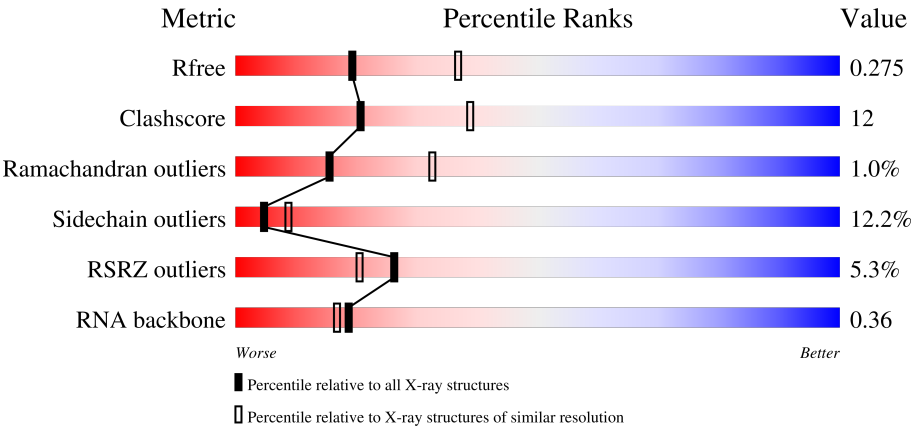
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 <=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	C	23	39% 52% 9%
1	E	23	4% · 52% 30% 13%
2	A	258	4% 58% 21% · 18%
2	B	258	5% 54% 19% · 23%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4422 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 RNA (5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP*GP*UP*CP*UP*GP*GP*CP*AP*AP*CP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			488	218	87	161	22			
1	E	23	Total	C	N	O	P	0	0	0
			488	218	87	161	22			

- Molecule 2 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	212	Total	C	N	O	0	0	0
			1696	1087	302	307			
2	B	198	Total	C	N	O	0	0	0
			1617	1038	289	290			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	TRP	SER	engineered mutation	UNP Q46455
A	536	VAL	PHE	engineered mutation	UNP Q46455
B	535	TRP	SER	engineered mutation	UNP Q46455
B	536	VAL	PHE	engineered mutation	UNP Q46455

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	5	Total	Mg	0	0
			5	5		
3	E	5	Total	Mg	0	0
			5	5		
3	A	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Cl 3 3	0	0
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	23	Total O 23 23	0	0
7	E	10	Total O 10 10	0	0
7	A	55	Total O 55 55	0	0
7	B	21	Total O 21 21	0	0

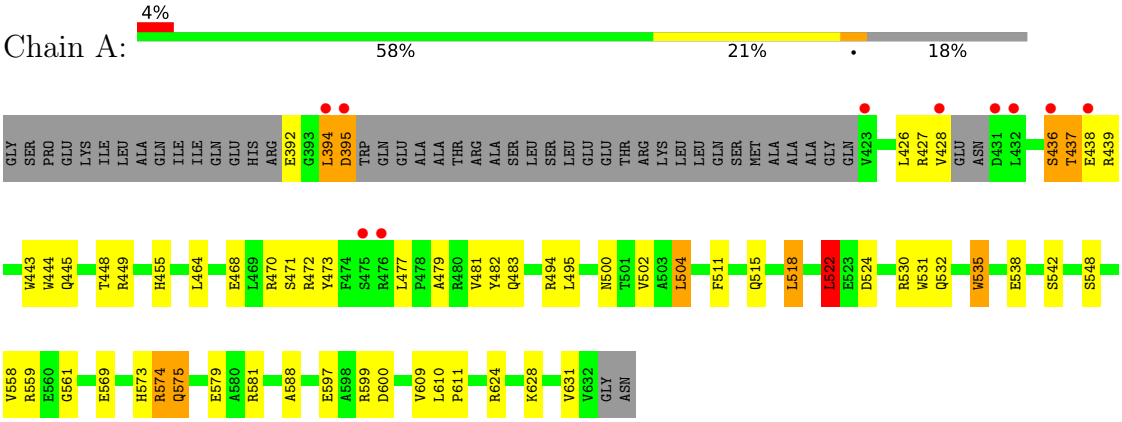
3 Residue-property plots (i)

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.

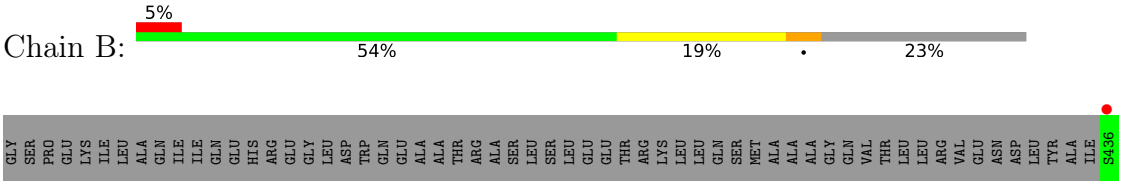
• Molecule 1: RNA (5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP*GP*UP*CP*UP*GP*GP *CP*AP*AP*CP*GP*CP*C)-3')

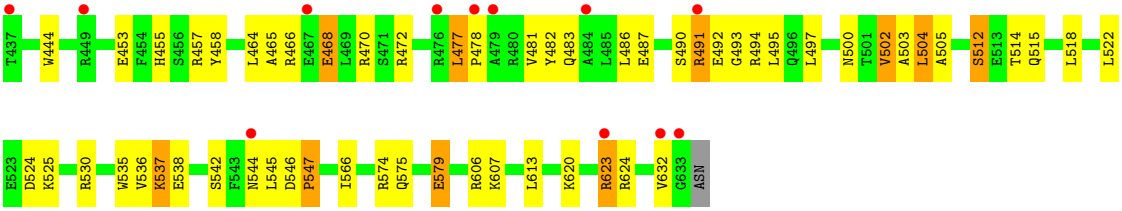
• Molecule 1: RNA (5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP*GP*UP*CP*UP*GP*GP *CP*AP*AP*CP*GP*CP*C)-3')

• Molecule 2: Selenocysteine-specific elongation factor



• Molecule 2: Selenocysteine-specific elongation factor




T437
W444
R449
E453
F454
H455
S456
R457
Y458
L464
A465
R466
E467
E468
L469
R470
S471
R472
R475
L477
P478
A479
R480
V481
Y482
Q483
A484
L485
L486
E487
S490
R491
E492
G493
R494
L495
Q496
L497
N500
T501
V502
A503
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A505
S512
E513
T514
Q515
L518
L522
E523
D524
K525
R530
W535
V536
K537
E538
S542
P543
N544
L545
D546
P547
I566
R574
Q575
E579
R606
K607
L613
K620
R623
R624
V632
G633
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.64Å 120.84Å 50.87Å 90.00° 100.18° 90.00°	Depositor
Resolution (Å)	95.35 – 2.60 17.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (95.35-2.60) 100.0 (17.56-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.287 0.227 , 0.275	Depositor DCC
R_{free} test set	1474 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4422	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, MG, NA, CL

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	C	2.69	18/544 (3.3%)	3.13	72/847 (8.5%)
1	E	1.63	4/544 (0.7%)	2.57	49/847 (5.8%)
2	A	0.98	3/1735 (0.2%)	0.96	4/2352 (0.2%)
2	B	0.89	0/1657	0.91	3/2246 (0.1%)
All	All	1.37	25/4480 (0.6%)	1.69	128/6292 (2.0%)

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
2	A	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	G	C8-N7	36.25	1.52	1.30
1	C	14	G	N9-C4	17.54	1.51	1.38
1	C	13	G	C6-O6	15.06	1.37	1.24
1	C	14	G	C4'-O4'	9.63	1.58	1.45
2	A	532	GLN	C-O	-9.30	1.05	1.23
1	E	13	G	C8-N7	8.49	1.36	1.30
1	C	14	G	C3'-O3'	8.36	1.53	1.42
1	C	15	C	P-OP2	8.35	1.63	1.49
1	C	14	G	C5'-C4'	7.40	1.60	1.51
2	A	532	GLN	CG-CD	-7.35	1.34	1.51
2	A	532	GLN	N-CA	-7.16	1.32	1.46
1	C	15	C	C1'-N1	7.11	1.59	1.48
1	E	33	G	C8-N7	6.69	1.34	1.30
1	C	35	C	N3-C4	6.55	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	26	U	C3'-O3'	6.45	1.51	1.42
1	C	14	G	C3'-C2'	6.36	1.59	1.52
1	C	34	C	C5-C6	6.15	1.39	1.34
1	C	33	G	C8-N7	5.89	1.34	1.30
1	C	15	C	C5-C6	5.80	1.39	1.34
1	C	34	C	C3'-O3'	-5.45	1.34	1.42
1	C	33	G	C6-O6	5.35	1.28	1.24
1	C	18	U	C4-O4	5.26	1.27	1.23
1	E	14	G	C8-N7	5.12	1.34	1.30
1	C	14	G	N7-C5	-5.08	1.36	1.39
1	C	14	G	O3'-P	5.01	1.67	1.61

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	14	G	C8-N9-C4	-22.28	97.49	106.40
1	C	14	G	N9-C4-C5	21.06	113.82	105.40
1	C	14	G	C3'-C2'-C1'	14.25	112.90	101.50
1	E	22	G	O4'-C1'-N9	12.89	118.51	108.20
1	C	15	C	O4'-C1'-N1	12.69	118.35	108.20
1	C	14	G	N3-C4-C5	-12.15	122.53	128.60
1	C	14	G	C5-C6-O6	-11.84	121.50	128.60
1	C	14	G	C2-N3-C4	11.36	117.58	111.90
1	C	35	C	N1-C2-O2	-11.24	112.15	118.90
1	C	14	G	O3'-P-O5'	-11.21	82.70	104.00
1	E	14	G	C5-C6-O6	-11.06	121.97	128.60
1	C	26	U	O4'-C1'-N1	10.76	116.81	108.20
1	C	25	C	P-O3'-C3'	10.01	131.71	119.70
1	C	20	C	O4'-C1'-N1	9.84	116.07	108.20
1	C	35	C	C5-C4-N4	-9.79	113.35	120.20
1	E	16	G	C5-C6-N1	9.71	116.36	111.50
1	C	15	C	C6-N1-C2	-9.66	116.44	120.30
1	E	33	G	N9-C4-C5	9.28	109.11	105.40
1	E	14	G	C6-N1-C2	-9.26	119.54	125.10
1	E	35	C	O4'-C4'-C3'	-9.02	94.98	104.00
1	E	27	G	C5-C6-N1	8.98	115.99	111.50
1	C	24	U	P-O3'-C3'	8.93	130.41	119.70
1	E	21	C	C6-N1-C2	-8.87	116.75	120.30
1	C	13	G	P-O3'-C3'	-8.74	109.21	119.70
1	C	14	G	O5'-P-OP2	-8.65	97.92	105.70
1	C	15	C	N3-C4-N4	-8.62	111.97	118.00
1	E	33	G	C5-C6-O6	8.50	133.70	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	34	C	O4'-C1'-N1	8.46	114.96	108.20
1	E	21	C	N3-C4-C5	-8.42	118.53	121.90
1	C	15	C	O5'-P-OP1	8.40	120.78	110.70
1	C	14	G	C6-N1-C2	-8.37	120.08	125.10
1	C	35	C	C2-N3-C4	-8.35	115.72	119.90
1	E	27	G	C5-C6-O6	-8.04	123.78	128.60
1	E	28	G	O4'-C1'-N9	8.03	114.62	108.20
1	E	33	G	C4-C5-N7	-7.97	107.61	110.80
1	E	26	U	P-O3'-C3'	7.97	129.26	119.70
1	E	16	G	C4'-C3'-C2'	-7.86	94.74	102.60
1	C	14	G	C5'-C4'-C3'	7.77	128.43	116.00
1	C	34	C	C2-N3-C4	-7.63	116.08	119.90
1	C	14	G	OP1-P-O3'	-7.61	88.45	105.20
1	C	15	C	C5-C4-N4	7.55	125.48	120.20
1	C	14	G	O4'-C1'-N9	7.50	114.20	108.20
1	C	14	G	C4-N9-C1'	7.25	135.93	126.50
1	C	14	G	O4'-C4'-C3'	7.22	111.88	106.10
1	C	18	U	O4'-C1'-N1	7.14	113.91	108.20
2	A	600	ASP	CB-CG-OD1	7.06	124.66	118.30
1	C	20	C	P-O3'-C3'	7.03	128.13	119.70
1	C	35	C	N3-C2-O2	7.00	126.80	121.90
1	C	14	G	OP1-P-OP2	6.99	130.09	119.60
2	B	505	ALA	CB-CA-C	-6.98	99.62	110.10
1	C	15	C	P-O5'-C5'	-6.92	109.83	120.90
1	E	22	G	C5-C6-O6	6.87	132.72	128.60
1	C	13	G	C5-N7-C8	6.85	107.72	104.30
1	E	14	G	C5-C6-N1	6.81	114.91	111.50
1	C	21	C	O4'-C1'-N1	6.73	113.58	108.20
1	C	14	G	N1-C6-O6	6.70	123.92	119.90
1	C	13	G	C4-C5-C6	6.70	122.82	118.80
1	E	16	G	C6-N1-C2	-6.67	121.10	125.10
1	C	35	C	N3-C4-N4	6.66	122.66	118.00
1	E	34	C	N1-C2-O2	-6.64	114.91	118.90
1	C	34	C	C5-C6-N1	-6.59	117.70	121.00
1	C	33	G	C5-N7-C8	6.54	107.57	104.30
1	E	25	C	C1'-O4'-C4'	-6.53	104.68	109.90
1	E	13	G	N9-C4-C5	6.50	108.00	105.40
1	C	32	C	O4'-C1'-N1	6.45	113.36	108.20
1	E	20	C	O4'-C1'-N1	6.39	113.31	108.20
1	C	33	G	C4-C5-N7	-6.39	108.25	110.80
1	E	27	G	C4-C5-N7	6.32	113.33	110.80
1	C	17	U	C5-C4-O4	6.29	129.67	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	13	G	C4-C5-N7	-6.24	108.30	110.80
1	E	16	G	P-O3'-C3'	6.22	127.17	119.70
1	C	14	G	C4'-C3'-C2'	-6.22	96.38	102.60
1	E	27	G	C5-N7-C8	-6.20	101.20	104.30
1	C	14	G	C5-C6-N1	6.16	114.58	111.50
1	E	14	G	N9-C1'-C2'	6.08	121.91	114.00
1	C	22	G	N3-C2-N2	-6.05	115.66	119.90
1	E	27	G	O4'-C1'-N9	6.05	113.04	108.20
1	E	30	A	C5'-C4'-O4'	6.05	116.36	109.10
1	E	33	G	N1-C6-O6	-6.04	116.28	119.90
1	C	15	C	O4'-C1'-C2'	-5.99	99.81	105.80
2	A	600	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	C	22	G	O4'-C1'-N9	5.90	112.92	108.20
1	C	17	U	O4'-C1'-N1	5.88	112.90	108.20
1	E	14	G	O4'-C1'-N9	5.87	112.89	108.20
1	C	16	G	N3-C2-N2	-5.86	115.80	119.90
1	E	13	G	N3-C4-N9	-5.85	122.49	126.00
1	E	18	U	C4-C5-C6	-5.82	116.20	119.70
1	C	26	U	C4-C5-C6	-5.79	116.23	119.70
1	E	28	G	C5-C6-O6	-5.78	125.13	128.60
1	C	22	G	N9-C1'-C2'	-5.77	105.65	112.00
1	E	18	U	N3-C2-O2	-5.73	118.19	122.20
1	C	25	C	O4'-C1'-N1	5.72	112.78	108.20
1	C	22	G	C8-N9-C4	-5.61	104.16	106.40
1	C	33	G	N7-C8-N9	-5.58	110.31	113.10
1	C	22	G	P-O5'-C5'	5.58	129.82	120.90
1	C	31	A	O5'-P-OP2	-5.56	100.70	105.70
1	E	18	U	O4'-C4'-C3'	-5.50	98.50	104.00
2	B	505	ALA	N-CA-C	-5.49	96.17	111.00
1	E	22	G	C3'-C2'-C1'	-5.48	97.12	101.50
1	E	24	U	P-O5'-C5'	-5.42	112.22	120.90
1	C	35	C	C5'-C4'-O4'	5.42	115.61	109.10
1	C	20	C	N3-C4-N4	-5.42	114.21	118.00
1	C	29	C	O4'-C1'-N1	5.40	112.52	108.20
1	C	33	G	C5-C6-O6	5.38	131.83	128.60
1	E	14	G	N1-C6-O6	5.38	123.12	119.90
1	E	33	G	C8-N9-C4	-5.35	104.26	106.40
1	C	32	C	C4'-C3'-C2'	-5.34	97.26	102.60
1	E	23	G	N3-C2-N2	-5.33	116.17	119.90
1	E	21	C	C4-C5-C6	5.33	120.06	117.40
2	A	531	TRP	O-C-N	-5.29	114.24	122.70
1	E	23	G	O4'-C1'-C2'	-5.28	100.52	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	23	G	C4'-C3'-O3'	-5.28	98.32	109.40
1	C	22	G	N9-C4-C5	5.27	107.51	105.40
1	C	23	G	N3-C2-N2	-5.27	116.21	119.90
1	C	35	C	O4'-C4'-C3'	-5.26	98.74	104.00
2	A	522	LEU	CA-CB-CG	5.24	127.34	115.30
1	C	35	C	N3-C4-C5	5.22	123.99	121.90
2	B	502	VAL	CB-CA-C	-5.21	101.49	111.40
1	C	21	C	P-O3'-C3'	5.21	125.95	119.70
1	E	28	G	C8-N9-C4	-5.19	104.32	106.40
1	E	30	A	C4'-C3'-C2'	-5.15	97.45	102.60
1	C	19	G	N9-C1'-C2'	-5.11	106.37	112.00
1	C	14	G	C4-C5-C6	5.11	121.87	118.80
1	E	26	U	C3'-C2'-C1'	5.05	105.54	101.50
1	E	18	U	C5-C6-N1	5.03	125.22	122.70
1	E	22	G	C6-N1-C2	5.03	128.12	125.10
1	C	16	G	C5-C6-O6	-5.02	125.59	128.60
1	C	17	U	N3-C4-O4	-5.01	115.89	119.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	394	LEU	Peptide
2	A	426	LEU	Peptide

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	C	488	0	251	10	0
1	E	488	0	251	6	0
2	A	1696	0	1643	39	0
2	B	1617	0	1601	47	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	A	2	0	0	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
7	A	55	0	0	0	0
7	B	21	0	0	0	0
7	C	23	0	0	3	0
7	E	10	0	0	0	0
All	All	4422	0	3746	99	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 12.

All (99) 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:B:623:ARG:HB2	2:B:632:VAL:HG13	1.38	1.02
2:A:392:GLU:CB	2:A:443:TRP:HZ2	1.74	1.00
2:A:428:VAL:HG12	2:A:428:VAL:O	1.68	0.93
2:B:623:ARG:HG3	2:B:632:VAL:HG11	1.50	0.91
2:B:623:ARG:HG3	2:B:632:VAL:CG1	2.02	0.90
2:A:392:GLU:CB	2:A:443:TRP:CZ2	2.58	0.87
2:B:537:LYS:H	2:B:537:LYS:HE2	1.42	0.84
2:B:512:SER:H	2:B:515:GLN:HE21	1.29	0.77
2:B:455:HIS:HE1	2:B:504:LEU:H	1.35	0.75
2:B:623:ARG:CG	2:B:632:VAL:CG1	2.66	0.74
2:A:468:GLU:HG2	2:A:472:ARG:HH12	1.53	0.73
2:B:623:ARG:CB	2:B:632:VAL:HG13	2.18	0.73
2:B:457:ARG:HD2	2:B:458:TYR:CZ	2.23	0.72
2:A:436:SER:O	2:A:438:GLU:N	2.23	0.71
2:B:535:TRP:HD1	2:B:538:GLU:OE1	1.74	0.70
2:A:428:VAL:O	2:A:428:VAL:CG1	2.40	0.70
2:A:535:TRP:HD1	2:A:538:GLU:HG3	1.59	0.68
2:B:535:TRP:HB3	2:B:537:LYS:CE	2.24	0.68
2:B:535:TRP:CD1	2:B:538:GLU:OE1	2.46	0.68
2:B:468:GLU:O	2:B:472:ARG:HB2	1.95	0.66
2:B:537:LYS:H	2:B:537:LYS:CE	2.09	0.65
2:B:623:ARG:HB2	2:B:632:VAL:CG1	2.23	0.65
2:A:395:ASP:N	2:A:395:ASP:OD1	2.30	0.64
2:B:535:TRP:HB3	2:B:537:LYS:HE3	1.81	0.63
2:B:477:LEU:HD13	2:B:481:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:LEU:HD22	2:B:478:PRO:HD2	1.82	0.62
2:B:544:ASN:O	2:B:545:LEU:HD23	2.00	0.61
1:C:15:C:P	7:C:3:HOH:O	2.58	0.60
2:B:495:LEU:HD13	2:B:502:VAL:HG11	1.83	0.60
2:A:573:HIS:HD2	2:A:575:GLN:H	1.50	0.60
2:A:394:LEU:HA	2:A:395:ASP:OD1	2.01	0.59
2:A:468:GLU:HG2	2:A:472:ARG:NH1	2.16	0.59
2:A:455:HIS:HE1	2:A:504:LEU:H	1.49	0.58
2:A:535:TRP:CD1	2:A:538:GLU:HG3	2.37	0.58
2:B:457:ARG:HD2	2:B:458:TYR:CE1	2.39	0.58
2:A:427:ARG:O	2:A:428:VAL:C	2.41	0.58
2:A:436:SER:O	2:A:437:THR:C	2.42	0.57
2:B:478:PRO:O	2:B:481:VAL:HG22	2.04	0.57
2:A:479:ALA:O	2:A:483:GLN:HG2	2.06	0.56
2:B:490:SER:HB2	2:B:497:LEU:HD12	1.88	0.56
1:C:22:G:OP2	2:B:606:ARG:NH1	2.35	0.56
2:B:535:TRP:HB3	2:B:537:LYS:HE2	1.89	0.55
2:B:478:PRO:HG2	2:B:481:VAL:CG2	2.37	0.55
2:A:470:ARG:HD3	2:A:482:TYR:CD2	2.41	0.54
2:A:428:VAL:HG21	2:A:481:VAL:HG22	1.90	0.53
2:A:610:LEU:HB3	2:A:611:PRO:HD3	1.89	0.53
2:B:466:ARG:HD2	2:B:500:ASN:HA	1.91	0.52
2:A:561:GLY:O	2:A:574:ARG:HD2	2.11	0.51
1:E:17:U:H2'	1:E:18:U:O4'	2.10	0.51
2:A:445:GLN:HG3	2:A:449:ARG:HH22	1.75	0.50
2:A:518:LEU:O	2:A:522:LEU:HD22	2.12	0.50
2:B:535:TRP:CZ2	2:B:607:LYS:HE3	2.46	0.50
2:A:392:GLU:N	2:A:439:ARG:HH21	2.11	0.49
2:A:472:ARG:HG2	2:A:473:TYR:CE1	2.48	0.48
2:B:623:ARG:CB	2:B:632:VAL:CG1	2.84	0.48
2:B:477:LEU:HD13	2:B:481:VAL:CG2	2.43	0.48
1:C:25:C:P	7:C:42:HOH:O	2.71	0.48
2:B:478:PRO:HG2	2:B:481:VAL:HG21	1.96	0.48
2:B:470:ARG:HD3	2:B:482:TYR:CD2	2.50	0.47
2:B:538:GLU:O	2:B:542:SER:HB2	2.14	0.47
1:E:31:A:H2'	1:E:32:C:O4'	2.14	0.47
1:C:26:U:H5'	2:A:558:VAL:HG11	1.96	0.47
2:B:491:ARG:C	2:B:493:GLY:H	2.18	0.47
2:B:444:TRP:CH2	2:B:494:ARG:HB3	2.51	0.46
2:A:495:LEU:HD13	2:A:502:VAL:HG11	1.97	0.46
2:B:502:VAL:HG12	2:B:503:ALA:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:394:LEU:CA	2:A:395:ASP:OD1	2.64	0.45
2:B:623:ARG:HH11	2:B:632:VAL:HG11	1.82	0.45
2:A:511:PHE:HB3	2:A:515:GLN:HB2	1.99	0.45
2:A:535:TRP:CD1	2:A:538:GLU:OE2	2.71	0.44
2:B:465:ALA:HB3	2:B:468:GLU:HB2	1.98	0.44
1:E:31:A:H2'	1:E:32:C:C6	2.53	0.44
2:B:478:PRO:HG2	2:B:481:VAL:HG22	1.99	0.44
2:A:573:HIS:CD2	2:A:575:GLN:H	2.32	0.43
2:B:623:ARG:HG3	2:B:623:ARG:HH11	1.83	0.43
2:A:530:ARG:HH21	2:A:579:GLU:CD	2.21	0.43
2:A:535:TRP:HB3	2:A:569:GLU:HB2	2.01	0.43
1:C:30:A:H2'	1:C:31:A:C8	2.53	0.43
1:E:28:G:C2'	1:E:29:C:H5'	2.49	0.43
2:B:470:ARG:HB2	2:B:482:TYR:CZ	2.54	0.43
2:B:512:SER:H	2:B:515:GLN:NE2	2.06	0.42
1:C:19:G:O2'	1:C:20:C:H5'	2.19	0.42
2:B:546:ASP:HA	2:B:547:PRO:HD2	1.89	0.42
2:A:436:SER:O	2:A:439:ARG:N	2.47	0.42
2:B:537:LYS:HE2	2:B:537:LYS:N	2.22	0.42
1:C:26:U:H5'	2:A:558:VAL:CG1	2.50	0.42
2:A:599:ARG:HA	2:A:609:VAL:HG21	2.02	0.42
2:B:575:GLN:O	2:B:579:GLU:HG2	2.20	0.42
2:A:444:TRP:CZ2	2:A:494:ARG:HG2	2.54	0.41
2:A:436:SER:C	2:A:438:GLU:N	2.73	0.41
1:E:23:G:H1'	1:E:24:U:C5	2.56	0.41
2:B:613:LEU:HD23	2:B:613:LEU:HA	1.85	0.41
1:E:19:G:H2'	1:E:20:C:C6	2.56	0.41
2:A:500:ASN:OD1	2:A:559:ARG:O	2.39	0.41
1:C:28:G:H2'	1:C:29:C:C6	2.56	0.40
1:C:27:G:H8	7:C:93:HOH:O	2.04	0.40
2:A:588:ALA:CB	2:A:631:VAL:HG23	2.52	0.40
2:B:482:TYR:CZ	2:B:486:LEU:HD11	2.57	0.40
1:C:19:G:H2'	1:C:20:C:C6	2.57	0.40

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
2	A	206/258 (80%)	190 (92%)	14 (7%)	2 (1%)	15 32
2	B	196/258 (76%)	180 (92%)	14 (7%)	2 (1%)	15 32
All	All	402/516 (78%)	370 (92%)	28 (7%)	4 (1%)	15 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	437	THR
2	B	547	PRO
2	A	436	SER
2	B	492	GLU

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
2	A	169/219 (77%)	151 (89%)	18 (11%)	6 12
2	B	166/219 (76%)	143 (86%)	23 (14%)	3 6
All	All	335/438 (76%)	294 (88%)	41 (12%)	5 9

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	395	ASP
2	A	448	THR

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Mol	Chain	Res	Type
2	A	464	LEU
2	A	471	SER
2	A	477	LEU
2	A	504	LEU
2	A	518	LEU
2	A	522	LEU
2	A	524	ASP
2	A	535	TRP
2	A	542	SER
2	A	548	SER
2	A	574	ARG
2	A	575	GLN
2	A	581	ARG
2	A	597	GLU
2	A	624	ARG
2	A	628	LYS
2	B	453	GLU
2	B	464	LEU
2	B	468	GLU
2	B	477	LEU
2	B	483	GLN
2	B	487	GLU
2	B	491	ARG
2	B	504	LEU
2	B	512	SER
2	B	514	THR
2	B	518	LEU
2	B	522	LEU
2	B	524	ASP
2	B	525	LYS
2	B	530	ARG
2	B	536	VAL
2	B	537	LYS
2	B	566	ILE
2	B	574	ARG
2	B	579	GLU
2	B	620	LYS
2	B	623	ARG
2	B	624	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	455	HIS
2	A	496	GLN
2	A	573	HIS
2	A	586	ASN
2	A	618	GLN
2	B	455	HIS
2	B	483	GLN
2	B	515	GLN
2	B	532	GLN
2	B	573	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	23/23 (100%)	7 (30%)	1 (4%)
1	E	22/23 (95%)	7 (31%)	3 (13%)
All	All	45/46 (97%)	14 (31%)	4 (8%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	14	G
1	C	23	G
1	C	24	U
1	C	25	C
1	C	26	U
1	C	27	G
1	C	28	G
1	E	23	G
1	E	24	U
1	E	26	U
1	E	27	G
1	E	29	C
1	E	30	A
1	E	31	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	13	G
1	E	18	U
1	E	23	G

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Mol	Chain	Res	Type
1	E	26	U

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 24 ligands modelled in this entry, 24 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.

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)

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^{th} 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	C	23/23 (100%)	-0.37	0 100 100	8, 18, 30, 41	0
1	E	23/23 (100%)	0.03	1 (4%) 35 28	14, 20, 42, 60	0
2	A	212/258 (82%)	0.06	10 (4%) 31 25	3, 17, 59, 70	0
2	B	198/258 (76%)	0.25	13 (6%) 18 13	6, 27, 65, 68	0
All	All	456/562 (81%)	0.12	24 (5%) 26 20	3, 22, 61, 70	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	436	SER	6.3
2	A	423	VAL	4.7
2	B	633	GLY	3.6
2	B	449	ARG	3.5
2	B	544	ASN	3.5
2	B	491	ARG	3.2
1	E	26	U	3.2
2	A	436	SER	3.0
2	A	432	LEU	2.6
2	B	437	THR	2.6
2	A	475	SER	2.4
2	A	431	ASP	2.4
2	A	395	ASP	2.4
2	B	479	ALA	2.3
2	B	478	PRO	2.2
2	B	484	ALA	2.2
2	A	476	ARG	2.2
2	B	623	ARG	2.2
2	A	438	GLU	2.2
2	B	632	VAL	2.1
2	A	394	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	428	VAL	2.0
2	B	467	GLU	2.0
2	B	476	ARG	2.0

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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
5	CA	A	161	1/1	0.22	0.32	64,64,64,64	0
3	MG	C	151	1/1	0.67	0.27	57,57,57,57	0
3	MG	C	145	1/1	0.77	0.28	53,53,53,53	0
6	CL	A	168	1/1	0.78	0.13	40,40,40,40	0
3	MG	E	155	1/1	0.81	0.18	45,45,45,45	0
3	MG	C	152	1/1	0.83	0.23	49,49,49,49	0
3	MG	C	148	1/1	0.83	0.18	38,38,38,38	0
3	MG	B	146	1/1	0.87	0.30	61,61,61,61	0
3	MG	A	140	1/1	0.89	0.14	42,42,42,42	0
3	MG	E	141	1/1	0.89	0.28	41,41,41,41	0
6	CL	A	165	1/1	0.91	0.31	55,55,55,55	0
6	CL	A	167	1/1	0.91	0.42	51,51,51,51	0
3	MG	A	154	1/1	0.91	0.20	51,51,51,51	0
3	MG	A	158	1/1	0.92	0.17	28,28,28,28	0
3	MG	E	159	1/1	0.92	0.25	40,40,40,40	0
5	CA	A	162	1/1	0.93	0.16	65,65,65,65	0
3	MG	E	144	1/1	0.93	0.30	32,32,32,32	0
6	CL	B	166	1/1	0.93	0.09	53,53,53,53	0
3	MG	A	149	1/1	0.94	0.19	32,32,32,32	0
3	MG	B	157	1/1	0.94	0.38	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	C	163	1/1	0.94	0.18	24,24,24,24	0
3	MG	E	156	1/1	0.95	0.15	38,38,38,38	0
3	MG	C	147	1/1	0.97	0.16	24,24,24,24	0
3	MG	A	142	1/1	0.98	0.06	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.