



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:15 PM GMT

PDB ID : 1WSU
Title : C-terminal domain of elongation factor selB complexed with SECIS RNA
Authors : Yoshizawa, S.; Rasubala, L.; Ose, T.; Kohda, D.; Fourmy, D.; Maenaka, K.
Deposited on : 2004-11-11
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

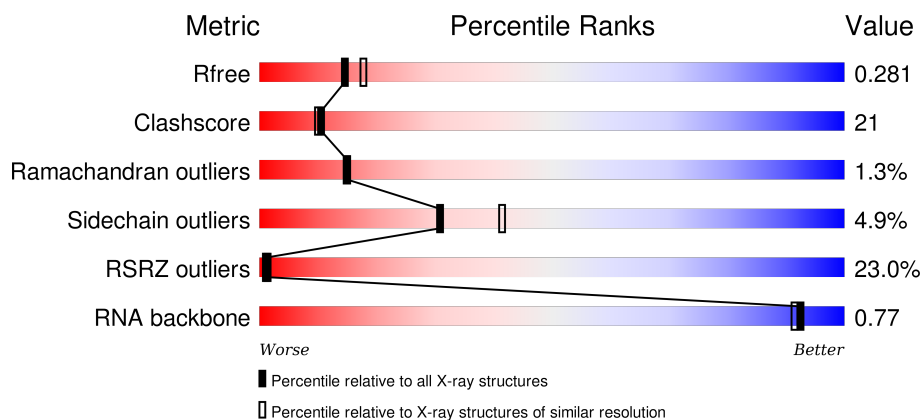
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)
RNA backbone	2183	1011 (2.84-1.76)

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. 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	E	23	<div> <div>48%</div> <div>35%</div> <div>13%</div> <div>•</div> </div>
1	F	23	<div> <div>4%</div> <div>52%</div> <div>30%</div> <div>13%</div> <div>•</div> </div>
1	G	23	<div> <div>70%</div> <div>30%</div> <div>52%</div> <div>9%</div> <div>9%</div> </div>
2	A	124	<div> <div>4%</div> <div>75%</div> <div>23%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	124	<p>2% 74% 22% ...</p>
2	C	124	<p>35% 42% 37% 18%</p>
2	D	124	<p>44% 45% 49% ..</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5484 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 5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP*GP*UP*CP*U*GP*GP*CP*AP*AP*CP*GP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	22	Total	C	N	O	P	0	0	0
			465	209	85	151	20			
1	F	22	Total	C	N	O	P	0	0	0
			465	209	85	151	20			
1	G	21	Total	C	N	O	P	0	0	0
			445	200	82	144	19			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	124	Total	C	N	O	0	0	0
			1007	642	178	187			
2	B	122	Total	C	N	O	0	0	0
			994	636	175	183			
2	C	102	Total	C	N	O	0	0	0
			845	547	149	149			
2	D	121	Total	C	N	O	0	0	0
			990	633	175	182			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	511	GLY	-	CLONING ARTIFACT	UNP Q46455
B	511	GLY	-	CLONING ARTIFACT	UNP Q46455
C	511	GLY	-	CLONING ARTIFACT	UNP Q46455
D	511	GLY	-	CLONING ARTIFACT	UNP Q46455

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total 114	O 114	0	0
3	B	75	Total 75	O 75	0	0
3	C	21	Total 21	O 21	0	0
3	D	11	Total 11	O 11	0	0
3	E	22	Total 22	O 22	0	0
3	F	16	Total 16	O 16	0	0
3	G	14	Total 14	O 14	0	0

3 Residue-property plots [i](#)

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.

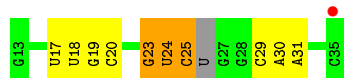
- Molecule 1: 5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP*GP*UP*CP*U*GP*GP*CP*AP*AP*CP*GP*CP*C)-3'

Chain E: 



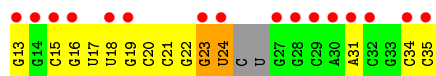
- Molecule 1: 5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP*GP*UP*CP*U*GP*GP*CP*AP*AP*CP*GP*CP*C)-3'

Chain F: 




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

Chain G: 




- Molecule 2: Selenocysteine-specific elongation factor

Chain A: 

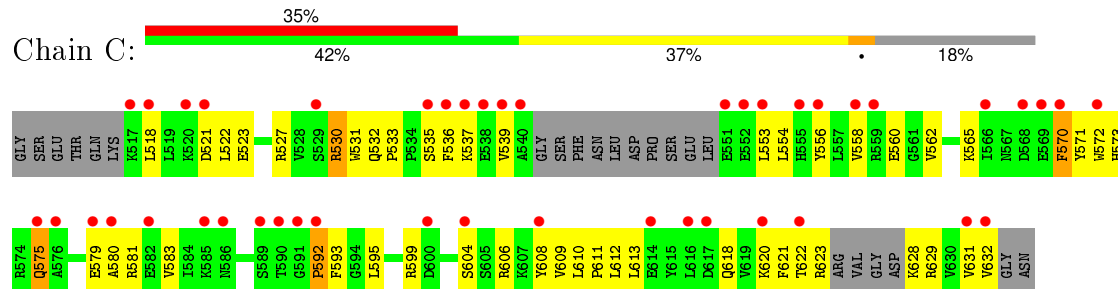


- Molecule 2: Selenocysteine-specific elongation factor

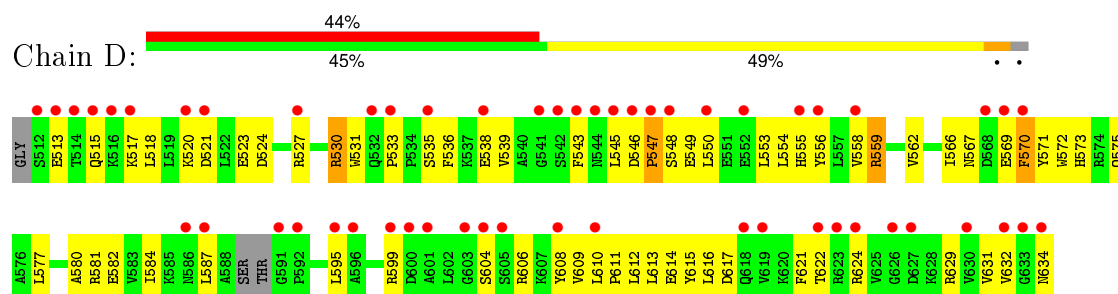
Chain B: 



- Molecule 2: Selenocysteine-specific elongation factor



- Molecule 2: Selenocysteine-specific elongation factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	81.86Å 169.81Å 71.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 9.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (10.00-2.30) 93.2 (9.99-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.279 0.227 , 0.281	Depositor DCC
R_{free} test set	4099 reflections (10.91%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 86.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 41657 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5484	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.57 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3220e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	E	0.43	0/518	0.74	0/805
1	F	0.35	0/518	0.67	0/805
1	G	0.23	0/496	0.65	0/771
2	A	0.46	0/1027	0.66	0/1383
2	B	0.44	0/1014	0.65	0/1367
2	C	0.29	0/861	0.50	0/1158
2	D	0.30	0/1009	0.54	0/1357
All	All	0.37	0/5443	0.63	0/7646

There are no bond length outliers.

There are no bond angle outliers.

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	E	465	0	243	13	0
1	F	465	0	243	14	0
1	G	445	0	232	23	0
2	A	1007	0	1014	24	0
2	B	994	0	1005	24	0
2	C	845	0	865	51	0
2	D	990	0	998	71	0
3	A	114	0	0	10	0
3	B	75	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	21	0	0	3	0
3	D	11	0	0	2	0
3	E	22	0	0	0	0
3	F	16	0	0	0	0
3	G	14	0	0	3	0
All	All	5484	0	4600	207	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 21.

All (207) 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:C:613:LEU:HB3	2:C:629:ARG:HH12	0.91	1.07
2:D:535:SER:OG	2:D:538:GLU:HG3	1.58	1.02
2:D:613:LEU:HB3	2:D:629:ARG:HH12	1.23	1.02
2:C:613:LEU:HB3	2:C:629:ARG:NH1	1.74	1.01
1:G:17:U:H3	1:G:31:A:H62	1.16	0.90
1:E:17:U:H3	1:E:31:A:H62	1.13	0.89
2:C:613:LEU:CB	2:C:629:ARG:HH12	1.85	0.84
3:A:62:HOH:O	2:B:586:ASN:HB3	1.78	0.83
2:C:535:SER:HA	2:C:570:PHE:HB3	1.65	0.78
2:D:610:LEU:HB3	2:D:611:PRO:HD3	1.65	0.78
2:C:556:TYR:O	2:C:560:GLU:HG2	1.84	0.77
2:A:586:ASN:HB3	3:B:145:HOH:O	1.85	0.76
1:F:17:U:H3	1:F:31:A:H62	1.33	0.76
2:D:567:ASN:ND2	2:D:569:GLU:H	1.84	0.75
2:C:581:ARG:HG3	2:C:621:PHE:CZ	2.23	0.74
1:G:13:G:H5''	3:G:177:HOH:O	1.87	0.73
1:G:17:U:H3	1:G:31:A:N6	1.87	0.72
2:D:546:ASP:HB2	2:D:549:GLU:HB3	1.71	0.72
2:D:613:LEU:HB3	2:D:629:ARG:NH1	2.01	0.72
2:D:535:SER:OG	2:D:538:GLU:CG	2.35	0.72
2:C:623:ARG:HD3	2:C:632:VAL:HG11	1.71	0.71
2:D:535:SER:HA	2:D:570:PHE:HB3	1.74	0.70
2:C:531:TRP:HZ2	2:C:579:GLU:HG2	1.59	0.68
2:A:530:ARG:CZ	2:B:530:ARG:HG3	2.24	0.68
2:C:554:LEU:HD13	2:C:571:TYR:CE2	2.29	0.68
1:F:19:G:H2'	1:F:20:C:C6	2.29	0.67
1:G:19:G:H2'	1:G:20:C:C6	2.28	0.67
2:A:573:HIS:HD2	2:A:575:GLN:H	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:573:HIS:CD2	2:A:575:GLN:H	2.11	0.67
2:D:577:LEU:HG	2:D:581:ARG:HD2	1.76	0.66
2:B:530:ARG:HD3	3:B:154:HOH:O	1.93	0.66
2:D:556:TYR:O	2:D:559:ARG:HG2	1.95	0.66
3:A:188:HOH:O	2:B:579:GLU:HG2	1.93	0.66
1:F:24:U:H4'	1:F:25:C:O5'	1.96	0.66
2:D:629:ARG:HG3	2:D:629:ARG:HH11	1.61	0.65
2:A:527:ARG:HD3	2:B:579:GLU:OE1	1.94	0.65
2:C:527:ARG:HD3	3:C:61:HOH:O	1.96	0.65
2:A:610:LEU:HB3	2:A:611:PRO:HD3	1.81	0.63
1:E:23:G:O2'	1:E:24:U:O5'	2.16	0.63
2:D:535:SER:HB2	2:D:569:GLU:HG2	1.79	0.62
2:D:573:HIS:CD2	2:D:575:GLN:H	2.18	0.62
1:G:21:C:H2'	1:G:22:G:C8	2.35	0.62
2:C:537:LYS:NZ	2:C:537:LYS:HB2	2.14	0.62
2:C:554:LEU:O	2:C:558:VAL:HG23	2.00	0.61
2:D:527:ARG:HG2	2:D:527:ARG:HH21	1.64	0.61
2:D:577:LEU:O	2:D:581:ARG:HG3	2.00	0.61
2:C:595:LEU:HD22	2:C:610:LEU:HD13	1.84	0.60
2:D:546:ASP:HB2	2:D:549:GLU:CB	2.31	0.60
2:A:566:ILE:HG13	2:A:572:TRP:CD1	2.37	0.60
2:D:604:SER:HB3	2:D:609:VAL:CG2	2.32	0.60
1:F:23:G:O2'	1:F:24:U:O5'	2.20	0.59
1:G:22:G:OP2	2:C:606:ARG:HD2	2.02	0.59
2:C:618:GLN:HA	3:C:155:HOH:O	2.00	0.59
2:D:517:LYS:O	2:D:521:ASP:HB2	2.02	0.59
2:C:573:HIS:CD2	2:C:575:GLN:HB2	2.38	0.59
2:B:624:ARG:HD2	2:B:626:GLY:O	2.02	0.59
2:B:565:LYS:NZ	2:B:568:ASP:HA	2.18	0.58
2:D:599:ARG:HG2	2:D:604:SER:O	2.03	0.58
1:E:17:U:H3	1:E:31:A:N6	1.94	0.58
2:D:617:ASP:HA	2:D:622:THR:O	2.04	0.58
2:D:599:ARG:HD2	2:D:606:ARG:N	2.19	0.57
2:D:554:LEU:O	2:D:558:VAL:HG23	2.04	0.57
2:C:610:LEU:HB3	2:C:611:PRO:HD3	1.86	0.57
2:C:530:ARG:HG3	2:D:530:ARG:NH2	2.20	0.57
2:D:527:ARG:HH11	2:D:573:HIS:CE1	2.23	0.57
2:D:604:SER:HB3	2:D:609:VAL:HG23	1.88	0.56
2:C:527:ARG:NH2	2:D:582:GLU:HG2	2.21	0.56
2:D:621:PHE:CD2	2:D:622:THR:HG23	2.41	0.56
2:D:632:VAL:C	2:D:634:ASN:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:608:TYR:C	2:D:611:PRO:HD2	2.26	0.55
2:D:573:HIS:HD2	2:D:575:GLN:H	1.54	0.55
2:D:536:PHE:CE1	2:D:550:LEU:HD23	2.42	0.55
1:E:23:G:H1'	1:E:24:U:C5	2.42	0.55
2:B:573:HIS:CD2	2:B:575:GLN:H	2.24	0.55
2:C:554:LEU:HD13	2:C:571:TYR:HE2	1.69	0.55
2:A:535:SER:OG	2:A:538:GLU:HG3	2.07	0.55
1:E:23:G:H4'	1:E:24:U:OP1	2.08	0.54
2:D:535:SER:O	2:D:539:VAL:HG23	2.08	0.54
2:C:531:TRP:NE1	2:C:580:ALA:HB2	2.22	0.54
2:D:566:ILE:HG23	2:D:615:TYR:HB2	1.89	0.54
1:E:16:G:H2'	1:E:17:U:C6	2.42	0.54
1:F:17:U:H3	1:F:31:A:N6	2.03	0.54
2:C:537:LYS:HZ2	2:C:537:LYS:HB2	1.72	0.54
2:D:632:VAL:HG23	2:D:632:VAL:O	2.07	0.54
2:C:592:PRO:HB2	2:C:628:LYS:HD2	1.88	0.54
2:C:573:HIS:HD2	2:C:575:GLN:HB2	1.73	0.54
2:C:530:ARG:HD3	2:D:530:ARG:NH1	2.23	0.53
1:F:24:U:O2'	1:F:25:C:OP2	2.27	0.53
2:D:580:ALA:O	2:D:584:ILE:HG12	2.08	0.53
1:E:33:G:H2'	1:E:34:C:O4'	2.09	0.53
2:D:545:LEU:HB3	2:D:549:GLU:OE1	2.08	0.53
2:A:530:ARG:NH1	2:B:530:ARG:HG3	2.24	0.53
1:F:23:G:H1'	1:F:24:U:C5	2.45	0.52
1:F:24:U:H1'	1:F:25:C:C6	2.45	0.52
1:E:24:U:O2'	1:E:25:C:OP2	2.26	0.52
2:D:567:ASN:HD21	2:D:569:GLU:CB	2.22	0.52
2:B:585:LYS:HB2	2:B:585:LYS:NZ	2.25	0.52
2:D:629:ARG:NH1	2:D:629:ARG:HG3	2.24	0.52
2:D:606:ARG:HH21	2:D:610:LEU:HD22	1.74	0.52
2:D:547:PRO:C	2:D:549:GLU:H	2.14	0.52
2:A:628:LYS:HE3	3:A:232:HOH:O	2.09	0.52
2:D:624:ARG:HA	2:D:629:ARG:HD3	1.92	0.51
2:D:611:PRO:HB2	3:D:244:HOH:O	2.09	0.51
1:G:24:U:H2'	1:G:24:U:O2	2.11	0.51
1:G:18:U:H2'	1:G:19:G:C8	2.46	0.51
2:C:532:GLN:NE2	2:C:604:SER:HA	2.25	0.51
1:G:23:G:O2'	1:G:24:U:P	2.69	0.51
2:D:523:GLU:HG3	2:D:562:VAL:CG1	2.40	0.50
2:C:565:LYS:HG3	2:C:571:TYR:HE1	1.76	0.50
1:E:23:G:O2'	1:E:24:U:P	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:550:LEU:HD12	2:D:553:LEU:HD12	1.93	0.50
2:C:581:ARG:HB2	3:C:49:HOH:O	2.11	0.50
2:C:533:PRO:HG3	2:C:572:TRP:CD1	2.46	0.50
1:E:19:G:H2'	1:E:20:C:C6	2.46	0.50
2:D:572:TRP:CH2	2:D:612:LEU:HD22	2.46	0.50
2:D:555:HIS:HA	2:D:558:VAL:HB	1.94	0.50
2:D:612:LEU:O	2:D:616:LEU:HG	2.12	0.50
1:G:18:U:H2'	1:G:19:G:H8	1.77	0.49
2:A:575:GLN:HG2	3:A:188:HOH:O	2.10	0.49
2:D:621:PHE:O	2:D:632:VAL:HG22	2.12	0.49
2:C:622:THR:HG22	2:C:631:VAL:HA	1.94	0.49
2:C:527:ARG:HH22	2:D:582:GLU:HG2	1.77	0.49
2:D:527:ARG:HG2	2:D:527:ARG:NH2	2.27	0.49
2:A:513:GLU:OE2	2:A:516:LYS:HD2	2.11	0.49
1:G:13:G:H8	3:G:177:HOH:O	1.96	0.49
2:C:565:LYS:HA	2:C:571:TYR:CD1	2.48	0.48
2:A:574:ARG:HD2	3:A:64:HOH:O	2.12	0.48
2:D:608:TYR:O	2:D:611:PRO:HD2	2.13	0.48
1:F:23:G:H4'	1:F:24:U:OP1	2.13	0.48
1:F:23:G:O2'	1:F:24:U:P	2.71	0.48
2:D:595:LEU:HD13	2:D:613:LEU:HD12	1.96	0.48
1:G:15:C:H2'	1:G:16:G:C8	2.48	0.48
2:A:520:LYS:HG3	2:B:586:ASN:OD1	2.14	0.48
2:C:629:ARG:HH11	2:C:629:ARG:HG3	1.79	0.48
1:G:23:G:O2'	1:G:24:U:O5'	2.24	0.48
2:A:592:PRO:HG3	2:A:630:VAL:HG23	1.95	0.48
2:D:566:ILE:N	2:D:566:ILE:HD12	2.28	0.47
2:C:535:SER:O	2:C:539:VAL:HG22	2.14	0.47
2:D:555:HIS:O	2:D:558:VAL:HB	2.14	0.47
1:G:24:U:H2'	3:G:250:HOH:O	2.13	0.47
1:G:19:G:H2'	1:G:20:C:H6	1.78	0.47
2:C:618:GLN:C	2:C:620:LYS:H	2.18	0.47
2:C:530:ARG:HB3	2:C:531:TRP:H	1.48	0.47
2:D:524:ASP:HA	2:D:527:ARG:HB3	1.97	0.47
2:C:553:LEU:O	2:C:556:TYR:HB3	2.14	0.47
2:B:573:HIS:HD2	2:B:575:GLN:H	1.61	0.47
2:C:523:GLU:HG3	2:C:562:VAL:CG1	2.45	0.47
2:C:623:ARG:HD3	2:C:632:VAL:CG1	2.43	0.47
2:B:555:HIS:HB3	2:B:559:ARG:NH1	2.30	0.47
1:G:23:G:H4'	1:G:24:U:OP1	2.14	0.46
2:B:550:LEU:O	2:B:554:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:624:ARG:HD3	2:D:629:ARG:HE	1.80	0.46
2:A:537:LYS:HG3	3:A:68:HOH:O	2.16	0.46
2:B:586:ASN:ND2	3:B:107:HOH:O	2.49	0.46
1:G:21:C:OP1	2:C:599:ARG:HD3	2.16	0.46
2:D:595:LEU:CD1	2:D:613:LEU:HD12	2.46	0.46
1:E:16:G:H2'	1:E:17:U:H6	1.80	0.46
1:E:24:U:H4'	1:E:25:C:O5'	2.16	0.46
2:A:517:LYS:NZ	3:A:193:HOH:O	2.49	0.46
2:A:632:VAL:HA	3:A:58:HOH:O	2.15	0.46
2:D:533:PRO:HG3	2:D:572:TRP:CD1	2.51	0.45
2:B:595:LEU:HD23	2:B:606:ARG:NH1	2.31	0.45
2:A:534:PRO:HA	2:A:538:GLU:OE1	2.16	0.45
2:C:629:ARG:HG3	2:C:629:ARG:NH1	2.31	0.45
2:A:550:LEU:O	2:A:554:LEU:HG	2.17	0.45
2:D:513:GLU:C	2:D:515:GLN:H	2.19	0.45
2:D:518:LEU:HD21	2:D:545:LEU:HD11	1.99	0.45
2:B:585:LYS:HB2	2:B:585:LYS:HZ2	1.82	0.45
2:C:575:GLN:O	2:C:579:GLU:OE1	2.34	0.44
1:F:18:U:H2'	1:F:19:G:C8	2.51	0.44
1:G:21:C:OP1	2:C:599:ARG:CD	2.65	0.44
2:C:518:LEU:O	2:C:522:LEU:HG	2.18	0.44
1:F:29:C:O2'	1:F:30:A:H5'	2.17	0.44
1:E:31:A:H2'	1:E:32:C:O4'	2.17	0.44
2:C:579:GLU:O	2:C:583:VAL:HG23	2.17	0.44
2:D:570:PHE:HA	3:D:45:HOH:O	2.17	0.43
1:G:23:G:O2'	1:G:24:U:C6	2.71	0.43
2:D:530:ARG:HD2	2:D:531:TRP:CD1	2.54	0.43
2:D:571:TYR:N	2:D:571:TYR:CD1	2.87	0.43
2:B:621:PHE:HD2	2:B:622:THR:HG23	1.84	0.43
2:A:629:ARG:HG3	3:A:42:HOH:O	2.18	0.42
2:B:592:PRO:HA	2:B:629:ARG:O	2.19	0.42
2:C:572:TRP:CH2	2:C:612:LEU:HD22	2.54	0.42
2:B:599:ARG:HA	2:B:609:VAL:HG21	2.01	0.42
1:F:18:U:H2'	1:F:19:G:H8	1.85	0.42
2:D:520:LYS:HA	2:D:520:LYS:HD2	1.90	0.42
2:C:530:ARG:HG3	2:D:530:ARG:HH22	1.82	0.42
2:D:518:LEU:HD11	2:D:543:PHE:HD2	1.83	0.42
1:F:19:G:H2'	1:F:20:C:H6	1.82	0.42
2:C:599:ARG:HA	2:C:609:VAL:HG21	2.01	0.42
1:G:24:U:C2'	1:G:24:U:O2	2.68	0.42
2:C:565:LYS:HA	2:C:571:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:G:H1'	1:G:24:U:C5	2.55	0.41
2:B:610:LEU:HB3	2:B:611:PRO:HD3	2.02	0.41
2:A:595:LEU:HD23	2:A:606:ARG:NH2	2.35	0.41
1:G:15:C:H2'	1:G:16:G:H8	1.86	0.41
2:D:535:SER:HG	2:D:538:GLU:HG3	1.76	0.41
2:D:632:VAL:C	2:D:634:ASN:N	2.74	0.41
2:C:533:PRO:O	2:C:608:TYR:HE2	2.03	0.41
2:A:579:GLU:OE2	2:B:527:ARG:HD3	2.20	0.41
2:B:546:ASP:CG	2:B:547:PRO:HD2	2.42	0.41
2:C:593:PHE:O	2:C:628:LYS:HB3	2.20	0.40
2:B:599:ARG:HH11	2:B:599:ARG:HG3	1.86	0.40
2:D:535:SER:HB2	2:D:569:GLU:CG	2.50	0.40
2:A:527:ARG:NH2	3:A:188:HOH:O	2.54	0.40
1:G:34:C:H2'	1:G:35:C:O4'	2.22	0.40
2:D:527:ARG:HE	2:D:573:HIS:CD2	2.39	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	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
2	B	120/124 (97%)	116 (97%)	3 (2%)	1 (1%)	24	27
2	C	96/124 (77%)	86 (90%)	9 (9%)	1 (1%)	19	21
2	D	117/124 (94%)	104 (89%)	9 (8%)	4 (3%)	5	2
All	All	455/496 (92%)	423 (93%)	26 (6%)	6 (1%)	15	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	547	PRO
2	D	548	SER
2	B	530	ARG
2	D	587	LEU
2	D	631	VAL
2	C	592	PRO

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	
2	A	108/108 (100%)	103 (95%)	5 (5%)	33	44
2	B	107/108 (99%)	101 (94%)	6 (6%)	26	35
2	C	90/108 (83%)	85 (94%)	5 (6%)	26	35
2	D	106/108 (98%)	102 (96%)	4 (4%)	40	54
All	All	411/432 (95%)	391 (95%)	20 (5%)	31	41

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	527	ARG
2	A	546	ASP
2	A	568	ASP
2	A	597	GLU
2	A	630	VAL
2	B	530	ARG
2	B	551	GLU
2	B	566	ILE
2	B	575	GLN
2	B	623	ARG
2	B	624	ARG
2	C	521	ASP
2	C	530	ARG
2	C	536	PHE
2	C	570	PHE
2	C	575	GLN

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Mol	Chain	Res	Type
2	D	530	ARG
2	D	559	ARG
2	D	570	PHE
2	D	614	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	544	ASN
2	A	573	HIS
2	A	575	GLN
2	A	586	ASN
2	B	515	GLN
2	B	544	ASN
2	B	573	HIS
2	B	586	ASN
2	C	532	GLN
2	C	573	HIS
2	D	544	ASN
2	D	567	ASN
2	D	573	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	20/23 (86%)	3 (15%)	2 (10%)
1	F	20/23 (86%)	3 (15%)	2 (10%)
1	G	19/23 (82%)	2 (10%)	1 (5%)
All	All	59/69 (85%)	8 (13%)	5 (8%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	23	G
1	E	24	U
1	E	25	C
1	F	23	G
1	F	24	U
1	F	25	C
1	G	23	G

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Mol	Chain	Res	Type
1	G	24	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	23	G
1	E	24	U
1	F	23	G
1	F	24	U
1	G	23	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	E	22/23 (95%)	0.21	0 100 100	38, 57, 70, 73	0
1	F	22/23 (95%)	0.60	1 (4%) 37 46	50, 72, 88, 101	0
1	G	21/23 (91%)	2.72	16 (76%) 0 0	89, 110, 143, 161	0
2	A	124/124 (100%)	0.11	5 (4%) 42 51	17, 36, 69, 102	0
2	B	122/124 (98%)	0.14	3 (2%) 61 70	21, 40, 63, 100	0
2	C	102/124 (82%)	1.87	44 (43%) 0 0	60, 94, 113, 136	0
2	D	121/124 (97%)	2.33	54 (44%) 0 0	62, 90, 127, 137	0
All	All	534/565 (94%)	1.09	123 (23%) 1 1	17, 68, 118, 161	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	633	GLY	10.6
2	C	590	THR	9.4
2	D	514	THR	8.7
2	D	627	ASP	7.4
1	G	27	G	7.4
2	D	512	SER	6.8
2	D	596	ALA	6.6
2	D	544	ASN	6.5
2	D	592	PRO	6.3
2	D	634	ASN	6.2
2	D	587	LEU	6.0
2	C	552	GLU	5.8
2	C	586	ASN	5.7
2	D	623	ARG	5.3
2	C	568	ASP	5.2
2	D	591	GLY	5.2
2	D	515	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
2	D	548	SER	5.1
2	C	535	SER	5.1
2	A	634	ASN	4.9
2	C	555	HIS	4.9
1	G	35	C	4.9
2	D	600	ASP	4.7
2	B	512	SER	4.7
2	B	511	GLY	4.7
2	A	513	GLU	4.6
2	D	542	SER	4.6
2	D	610	LEU	4.5
2	D	546	ASP	4.4
2	D	555	HIS	4.4
2	D	516	LYS	4.4
2	D	624	ARG	4.3
2	C	536	PHE	4.3
2	D	619	VAL	4.3
2	C	614	GLU	4.3
2	D	541	GLY	4.3
2	C	570	PHE	4.2
2	A	633	GLY	4.2
2	D	552	GLU	4.2
2	D	543	PHE	4.1
1	G	24	U	4.1
2	D	570	PHE	4.1
2	C	617	ASP	4.0
2	D	626	GLY	4.0
2	C	631	VAL	3.9
2	C	622	THR	3.9
2	A	511	GLY	3.8
2	C	591	GLY	3.7
2	D	603	GLY	3.7
2	C	585	LYS	3.6
2	C	539	VAL	3.6
2	C	566	ILE	3.5
2	C	576	ALA	3.5
2	D	538	GLU	3.5
2	D	604	SER	3.4
2	D	520	LYS	3.4
2	C	582	GLU	3.3
2	D	550	LEU	3.3
2	D	517	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	599	ARG	3.3
2	D	513	GLU	3.2
2	D	586	ASN	3.2
2	D	568	ASP	3.2
2	D	601	ALA	3.2
1	G	31	A	3.1
1	G	28	G	3.1
2	C	521	ASP	3.1
2	B	569	GLU	3.1
2	C	559	ARG	3.1
2	D	521	ASP	3.0
1	G	34	C	3.0
2	C	616	LEU	3.0
2	D	547	PRO	2.9
2	C	632	VAL	2.9
2	D	630	VAL	2.9
2	C	575	GLN	2.9
1	G	29	C	2.9
1	G	23	G	2.8
1	G	14	G	2.8
2	C	553	LEU	2.8
2	A	512	SER	2.8
2	D	622	THR	2.8
2	D	532	GLN	2.7
2	D	618	GLN	2.7
2	D	527	ARG	2.6
2	C	540	ALA	2.6
2	D	545	LEU	2.6
2	C	529	SER	2.6
2	C	569	GLU	2.6
1	G	16	G	2.6
2	C	551	GLU	2.6
2	D	632	VAL	2.6
1	G	30	A	2.5
2	C	538	GLU	2.5
1	G	19	G	2.5
2	C	556	TYR	2.5
2	C	572	TRP	2.5
2	C	592	PRO	2.5
2	C	579	GLU	2.4
1	G	13	G	2.4
2	C	600	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	604	SER	2.4
2	C	517	LYS	2.4
2	D	558	VAL	2.4
2	D	569	GLU	2.4
2	D	605	SER	2.4
2	D	556	TYR	2.3
1	G	18	U	2.2
2	C	608	TYR	2.2
2	C	580	ALA	2.2
2	C	520	LYS	2.1
2	D	535	SER	2.1
2	D	608	TYR	2.1
1	G	15	C	2.1
2	C	620	LYS	2.1
2	C	518	LEU	2.1
2	C	537	LYS	2.1
2	C	589	SER	2.1
2	C	558	VAL	2.0
1	F	35	C	2.0
2	D	595	LEU	2.0
2	D	533	PRO	2.0
1	G	32	C	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.