



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:08 PM GMT

PDB ID : 3W1K  
Title : Crystal structure of the selenocysteine synthase SelA and tRNA<sup>Sec</sup> complex  
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.  
Deposited on : 2012-11-15  
Resolution : 7.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

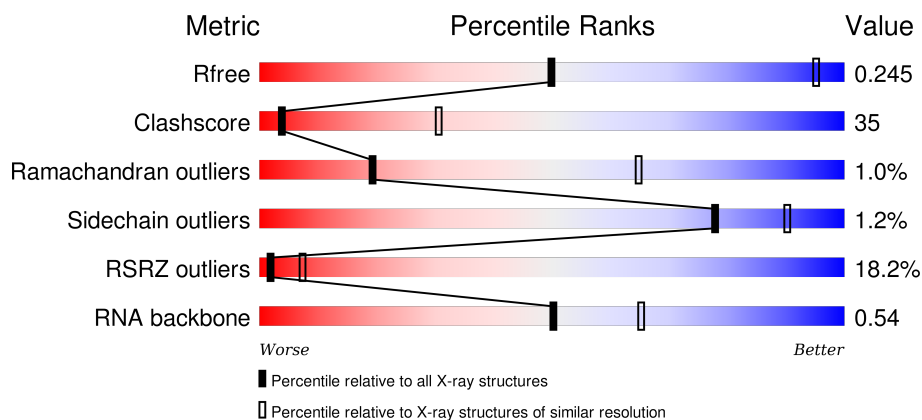
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 7.50 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))
$R_{free}$	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)
RNA backbone	2183	1106 (11.50-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	452	<div> <div>20%</div> <div> <div>44%</div> <div>54%</div> </div> </div>
1	B	452	<div> <div>14%</div> <div> <div>46%</div> <div>54%</div> </div> </div>
1	C	452	<div> <div>14%</div> <div> <div>48%</div> <div>51%</div> </div> </div>
1	D	452	<div> <div>17%</div> <div> <div>47%</div> <div>52%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	452	<div><div></div><div>23%46%53%.</div></div>
2	F	95	<div><div></div><div>6%16%78%. .</div></div>
2	G	95	<div><div></div><div>23%14%79%. .</div></div>
2	H	95	<div><div></div><div>41%17%77%. .</div></div>
2	I	95	<div><div></div><div>13%14%76%7%. .</div></div>
2	J	95	<div><div></div><div>19%14%78%5%. .</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27660 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 L-seryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	B	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	C	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	D	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	E	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140

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Chain	Residue	Modelled	Actual	Comment	Reference
E	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140

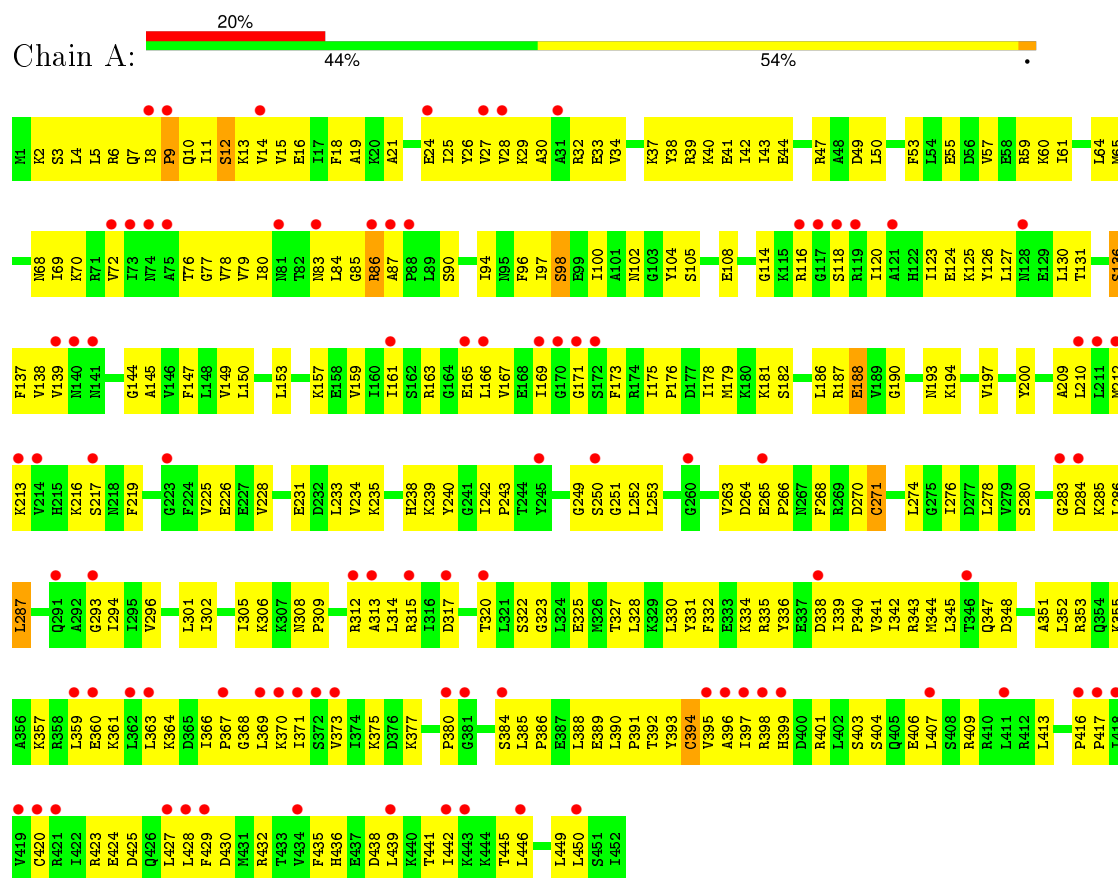
- Molecule 2 is a RNA chain called selenocysteine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	G	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	H	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	I	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	J	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			

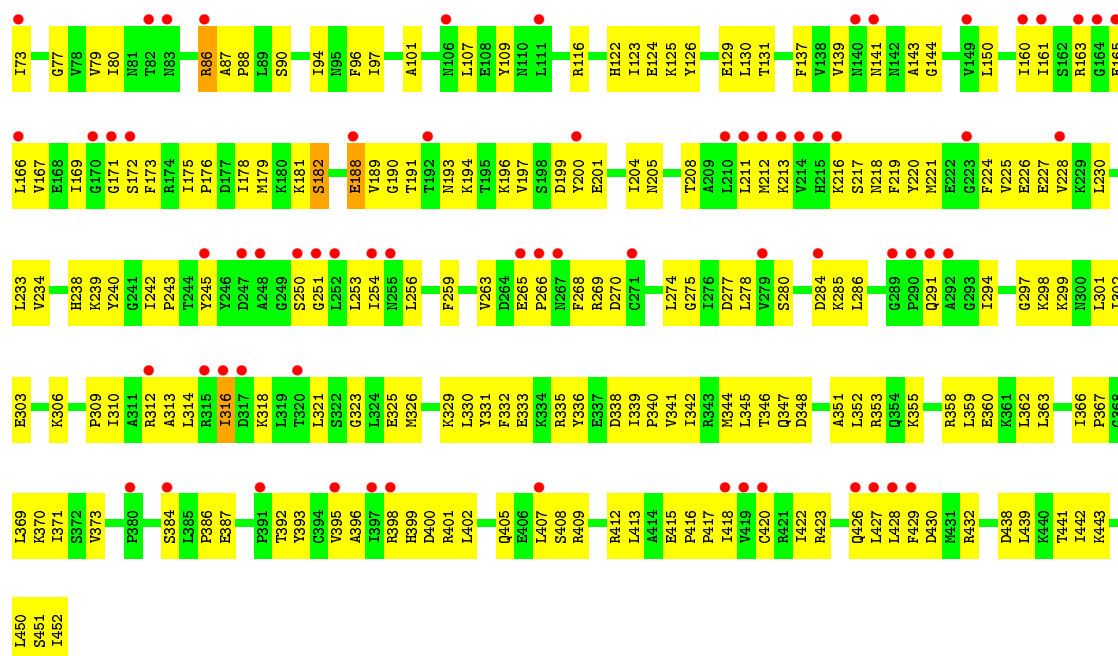
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

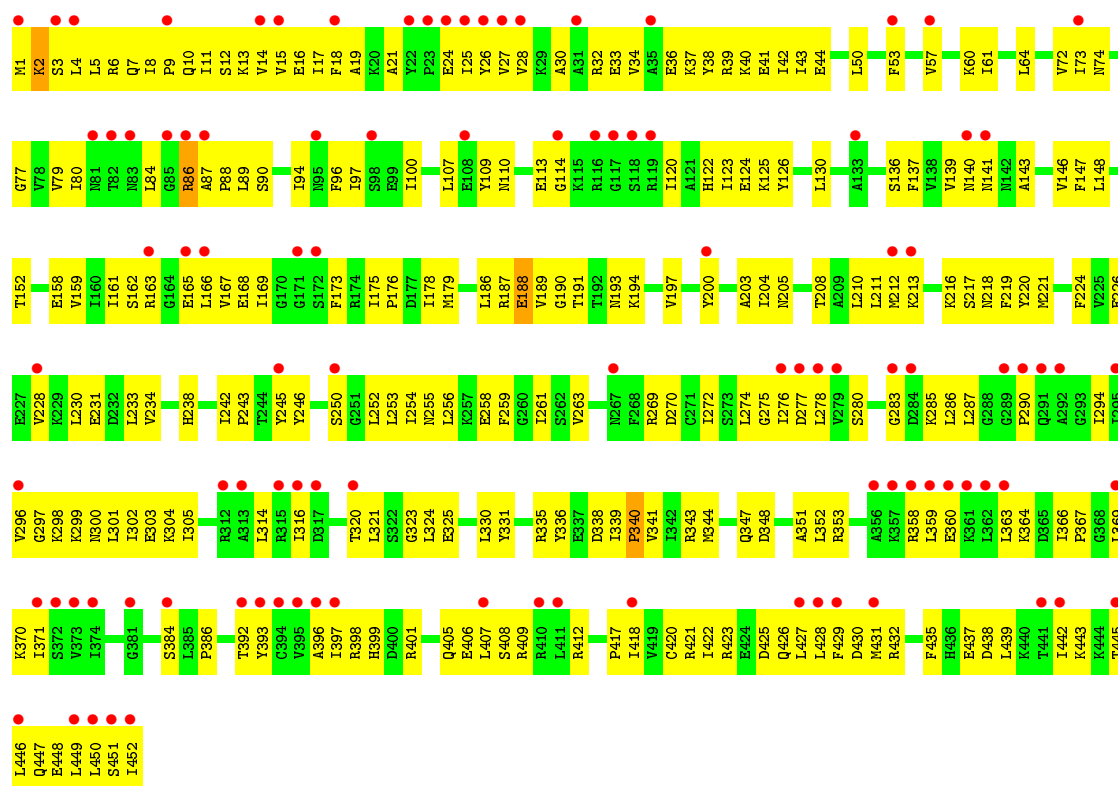
- Molecule 1: L-seryl-tRNA(Sec) selenium transferase





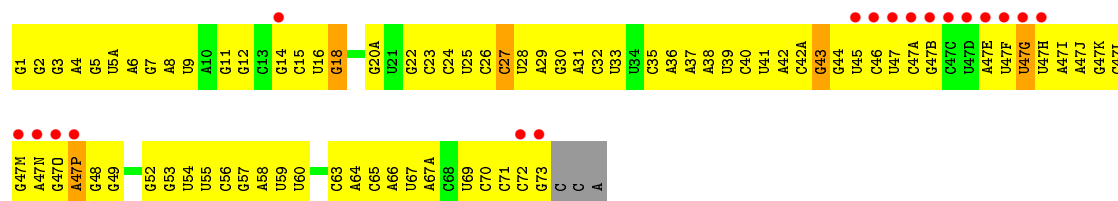


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase



• Molecule 2: selenocysteine tRNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.55Å 355.97Å 165.50Å 90.00° 115.41° 90.00°	Depositor
Resolution (Å)	49.94 – 7.50 49.94 – 7.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.94-7.50) 98.0 (49.94-7.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 7.37Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.194 , 0.240 0.200 , 0.245	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	391.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 555.7	EDS
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	1 of 9776 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	27660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	525.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.41	0/3597	0.65	0/4831
1	B	0.39	0/3597	0.65	0/4831
1	C	0.39	0/3597	0.64	0/4831
1	D	0.41	0/3597	0.65	0/4831
1	E	0.40	0/3597	0.64	0/4831
2	F	0.49	1/2185 (0.0%)	0.75	0/3401
2	G	0.44	1/2185 (0.0%)	0.73	0/3401
2	H	0.42	1/2185 (0.0%)	0.73	0/3401
2	I	0.43	1/2185 (0.0%)	0.72	0/3401
2	J	0.43	1/2185 (0.0%)	0.72	2/3401 (0.1%)
All	All	0.42	5/28910 (0.0%)	0.68	2/41160 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	G	OP3-P	-7.24	1.52	1.61
2	I	1	G	OP3-P	-7.05	1.52	1.61
2	J	1	G	OP3-P	-7.05	1.52	1.61
2	H	1	G	OP3-P	-6.86	1.52	1.61
2	G	1	G	OP3-P	-6.77	1.53	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	47(P)	A	OP2-P-O3'	6.24	118.93	105.20
2	J	27	C	OP2-P-O3'	5.73	117.81	105.20

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	3575	0	3760	295	0
1	B	3575	0	3760	291	0
1	C	3575	0	3760	282	0
1	D	3575	0	3760	298	0
1	E	3575	0	3760	255	0
2	F	1957	0	989	102	0
2	G	1957	0	989	124	0
2	H	1957	0	989	105	0
2	I	1957	0	989	112	0
2	J	1957	0	989	91	0
All	All	27660	0	23745	1783	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 35.

The worst 5 of 1783 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:C:157:LYS:HE2	1:C:209:ALA:HB2	1.27	1.14
1:B:1:MET:HG3	1:B:4:LEU:HD12	1.31	1.12
1:C:102:ASN:HB3	1:D:71:ARG:HH22	1.15	1.08
1:A:10:GLN:H	1:A:13:LYS:HD2	1.13	1.08
2:J:32:C:H2'	2:J:33:U:C6	1.93	1.02

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/452 (99%)	423 (94%)	22 (5%)	4 (1%)	21	67
1	B	449/452 (99%)	419 (93%)	25 (6%)	5 (1%)	17	63
1	C	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	21	67
1	D	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	21	67
1	E	449/452 (99%)	420 (94%)	23 (5%)	6 (1%)	15	60
All	All	2245/2260 (99%)	2104 (94%)	118 (5%)	23 (1%)	19	65

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	9	PRO
1	E	9	PRO
1	B	124	GLU
1	C	124	GLU
1	D	124	GLU

### 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	
1	A	390/390 (100%)	380 (97%)	10 (3%)	54	80
1	B	390/390 (100%)	389 (100%)	1 (0%)	94	96
1	C	390/390 (100%)	385 (99%)	5 (1%)	76	89
1	D	390/390 (100%)	384 (98%)	6 (2%)	72	88
1	E	390/390 (100%)	389 (100%)	1 (0%)	94	96
All	All	1950/1950 (100%)	1927 (99%)	23 (1%)	78	90

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	GLU

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Mol	Chain	Res	Type
1	C	188	GLU
1	D	316	ILE
1	C	3	SER
1	C	317	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	68	ASN
1	C	291	GLN
1	E	347	GLN
1	C	95	ASN
1	C	122	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	91/95 (95%)	6 (6%)	0
2	G	91/95 (95%)	6 (6%)	0
2	H	91/95 (95%)	6 (6%)	0
2	I	91/95 (95%)	9 (9%)	1 (1%)
2	J	91/95 (95%)	6 (6%)	0
All	All	455/475 (95%)	33 (7%)	1 (0%)

5 of 33 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	18	G
2	F	20(A)	G
2	F	33	U
2	F	42(A)	C
2	F	43	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	I	44	G

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	LLP	A	285	1	23,24,25	1.17	1 (4%)	28,32,34	1.01	1 (3%)
1	LLP	B	285	1	23,24,25	1.29	2 (8%)	28,32,34	1.10	2 (7%)
1	LLP	C	285	1	23,24,25	1.14	2 (8%)	28,32,34	1.01	2 (7%)
1	LLP	D	285	1	23,24,25	1.15	1 (4%)	28,32,34	0.99	2 (7%)
1	LLP	E	285	1	23,24,25	1.18	1 (4%)	28,32,34	1.13	3 (10%)

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
1	LLP	A	285	1	-	0/15/17/19	0/1/1/1
1	LLP	B	285	1	-	0/15/17/19	0/1/1/1
1	LLP	C	285	1	-	0/15/17/19	0/1/1/1
1	LLP	D	285	1	-	0/15/17/19	0/1/1/1
1	LLP	E	285	1	-	0/15/17/19	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LLP	C4-C4'	-3.45	1.40	1.46
1	E	285	LLP	C4-C4'	-3.18	1.41	1.46
1	A	285	LLP	C4-C4'	-3.05	1.41	1.46
1	C	285	LLP	C4-C4'	-2.77	1.41	1.46
1	D	285	LLP	C4-C4'	-2.68	1.42	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LLP	O-C-CA	-2.24	119.66	125.49
1	E	285	LLP	O-C-CA	-2.13	119.94	125.49
1	D	285	LLP	O-C-CA	-2.10	120.03	125.49
1	E	285	LLP	OP4-C5'-C5	2.14	112.54	108.99
1	C	285	LLP	OP4-P-OP1	2.18	112.69	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	LLP	3	0
1	B	285	LLP	7	0
1	C	285	LLP	5	0
1	D	285	LLP	1	0
1	E	285	LLP	2	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	451/452 (99%)	1.06	89 (19%) <b>1</b> <b>7</b>	363, 478, 546, 629	0
1	B	451/452 (99%)	0.95	64 (14%) <b>4</b> <b>9</b>	371, 474, 554, 648	0
1	C	451/452 (99%)	0.78	65 (14%) <b>3</b> <b>9</b>	364, 474, 549, 625	0
1	D	451/452 (99%)	0.98	77 (17%) <b>2</b> <b>8</b>	356, 463, 536, 601	0
1	E	451/452 (99%)	1.17	103 (22%) <b>1</b> <b>6</b>	330, 466, 539, 617	0
2	F	92/95 (96%)	0.31	6 (6%) <b>22</b> <b>23</b>	505, 594, 716, 786	0
2	G	92/95 (96%)	0.92	22 (23%) <b>1</b> <b>6</b>	505, 594, 744, 870	0
2	H	92/95 (96%)	1.69	39 (42%) <b>0</b> <b>4</b>	506, 596, 753, 853	0
2	I	92/95 (96%)	0.60	12 (13%) <b>5</b> <b>10</b>	506, 596, 746, 774	0
2	J	92/95 (96%)	0.88	18 (19%) <b>1</b> <b>7</b>	506, 595, 744, 791	0
All	All	2715/2735 (99%)	0.97	495 (18%) <b>2</b> <b>7</b>	330, 482, 656, 870	0

The worst 5 of 495 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	47(O)	G	6.9
1	E	291	GLN	6.9
2	G	47(O)	G	6.1
1	E	228	VAL	6.0
2	J	47(O)	G	6.0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	B	285	24/25	0.75	0.61	-	429,446,491,495	0
1	LLP	E	285	24/25	0.70	0.67	-	290,384,467,493	0
1	LLP	D	285	24/25	0.57	0.70	-	310,432,455,471	0
1	LLP	A	285	24/25	0.65	0.69	-	384,433,449,452	0
1	LLP	C	285	24/25	0.64	0.65	-	416,449,487,497	0

### 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.