



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2020 – 10:23 AM EDT

PDB ID : 6ASO  
Title : Structure of yeast U6 snRNP with 3'-phosphate terminated U6 RNA  
Authors : Montemayor, E.J.; Brow, D.A.; Butcher, S.E.  
Deposited on : 2017-08-25  
Resolution : 2.71 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

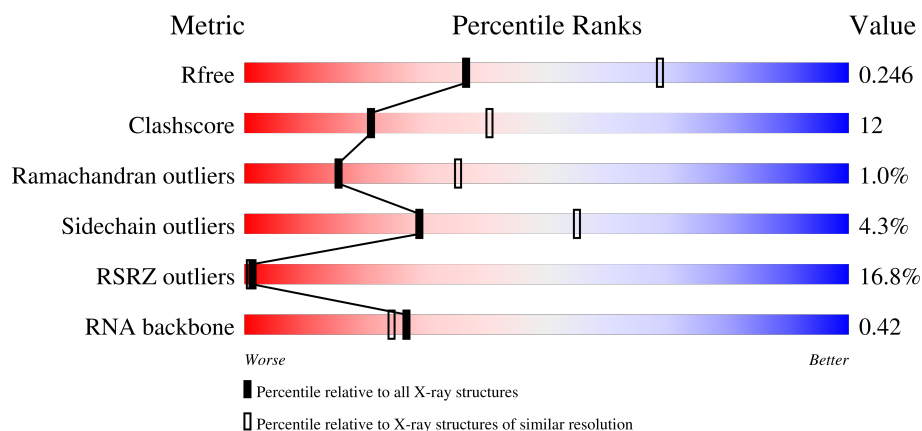
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)
RNA backbone	3102	1067 (3.00-2.44)

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 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	424	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	95	<div> <div>31%</div> <div> <div></div> <div>63%</div> <div>35%</div> <div>•</div> </div> </div>
3	C	97	<div> <div>11%</div> <div> <div></div> <div>53%</div> <div>23%</div> <div>• •</div> <div>19%</div> </div> </div>
4	D	93	<div> <div>22%</div> <div> <div></div> <div>41%</div> <div>22%</div> <div>•</div> <div>37%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	93	<div><div></div><div>23%70%15%15%</div></div>
6	F	88	<div><div></div><div>2%61%23%15%</div></div>
7	G	115	<div><div></div><div>25%42%16%42%</div></div>
8	H	115	<div><div></div><div>30%35%30%6%28%</div></div>
9	I	84	<div><div></div><div>12%25%42%14%17%</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 8863 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 U4/U6 snRNA-associated-splicing factor PRP24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2974	1879	530	551	14			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP P49960
A	445	HIS	-	expression tag	UNP P49960
A	446	HIS	-	expression tag	UNP P49960
A	447	HIS	-	expression tag	UNP P49960
A	448	HIS	-	expression tag	UNP P49960
A	449	HIS	-	expression tag	UNP P49960
A	450	HIS	-	expression tag	UNP P49960

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	95	Total	C	N	O	S	0	0	0
			770	491	130	145	4			

- Molecule 3 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	79	Total	C	N	O	S	0	0	0
			628	392	107	125	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	TRP	-	expression tag	UNP P57743
C	91	SER	-	expression tag	UNP P57743
C	92	HIS	-	expression tag	UNP P57743

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Chain	Residue	Modelled	Actual	Comment	Reference
C	93	PRO	-	expression tag	UNP P57743
C	94	GLN	-	expression tag	UNP P57743
C	95	PHE	-	expression tag	UNP P57743
C	96	GLU	-	expression tag	UNP P57743
C	97	LYS	-	expression tag	UNP P57743

- Molecule 4 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	59	Total	C	N	O	S	0	0	0
			477	309	79	87	2			

- Molecule 5 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	79	Total	C	N	O	S	0	0	0
			624	396	105	121	2			

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	75	Total	C	N	O	S	0	0	0
			583	367	96	118	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP A6ZYG7
F	0	SER	-	expression tag	UNP A6ZYG7

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	67	Total	C	N	O	S	0	0	0
			510	328	86	93	3			

- Molecule 8 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	83	Total	C	N	O		0	0	0
			663	424	114	125				

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	110	HIS	-	expression tag	UNP P47093
H	111	HIS	-	expression tag	UNP P47093
H	112	HIS	-	expression tag	UNP P47093
H	113	HIS	-	expression tag	UNP P47093
H	114	HIS	-	expression tag	UNP P47093
H	115	HIS	-	expression tag	UNP P47093

- Molecule 9 is a RNA chain called *Saccharomyces cerevisiae* strain HB\_S\_GIMBLETTRO AD\_9 chromosome XII sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	P	0	0	0
			1495	668	267	489	71			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	62	G	A	conflict	GB 1039023481
I	79	G	A	conflict	GB 1039023481

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	I	1	Total	K	0	0
			1	1		
10	A	1	Total	K	0	0
			1	1		

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	I	1	Total	Mn	0	0
			1	1		

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	2	Total	Mg	0	0
			2	2		

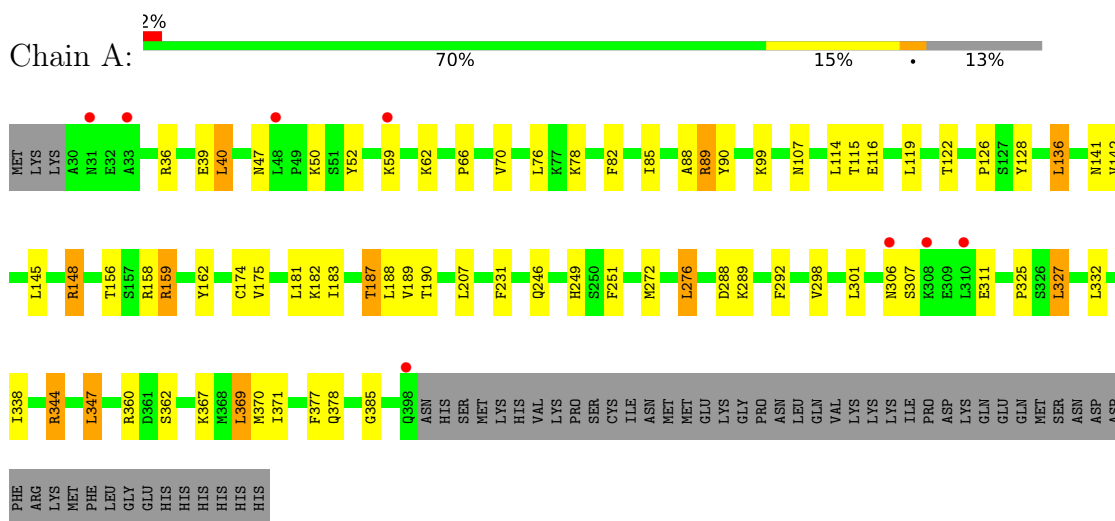
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	76	Total 76	O 76	0	0
13	B	6	Total 6	O 6	0	0
13	C	1	Total 1	O 1	0	0
13	E	1	Total 1	O 1	0	0
13	F	6	Total 6	O 6	0	0
13	H	1	Total 1	O 1	0	0
13	I	43	Total 43	O 43	0	0

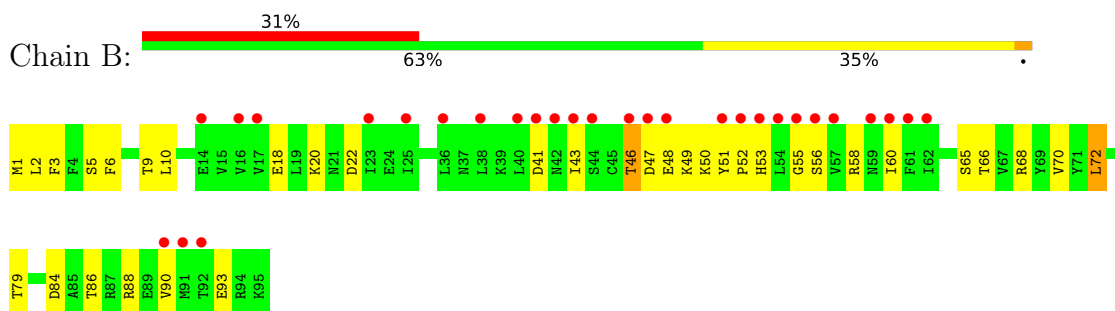
### 3 Residue-property plots

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

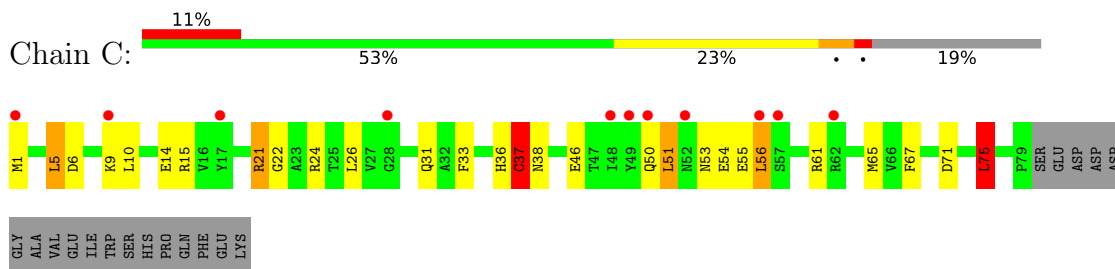
- Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



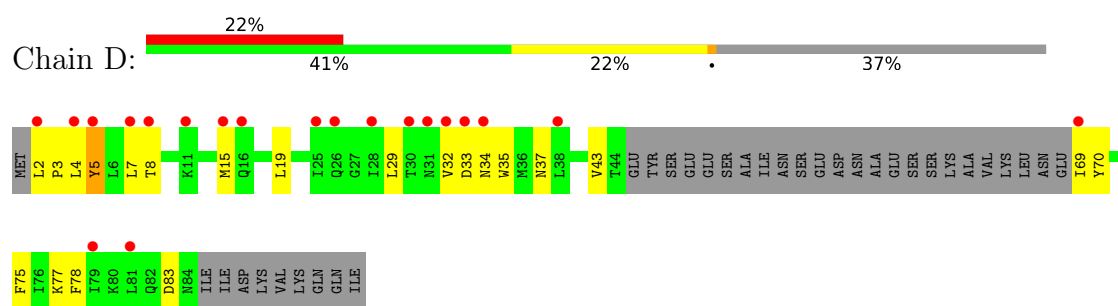
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2



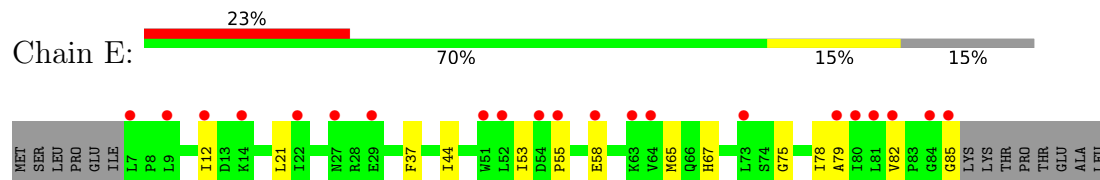
- Molecule 3: U6 snRNA-associated Sm-like protein LSm3



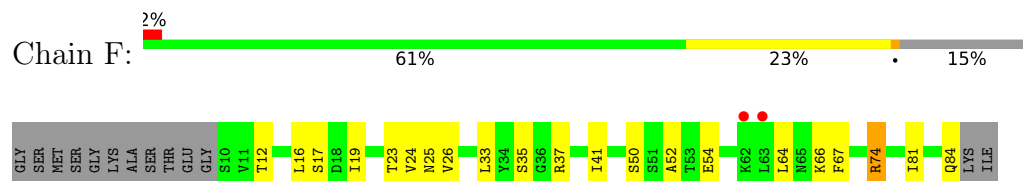
- Molecule 4: U6 snRNA-associated Sm-like protein LSm4



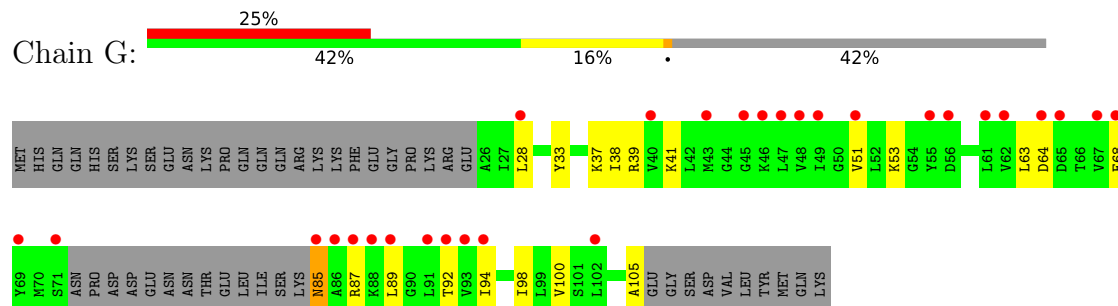
- Molecule 5: U6 snRNA-associated Sm-like protein LSm5



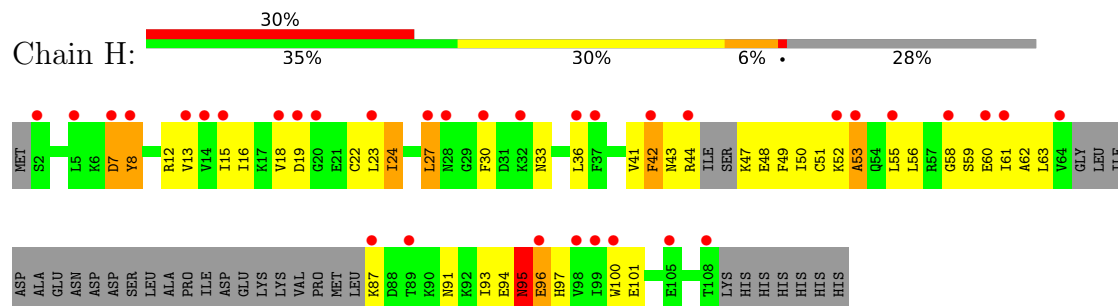
- Molecule 6: U6 snRNA-associated Sm-like protein LSm6



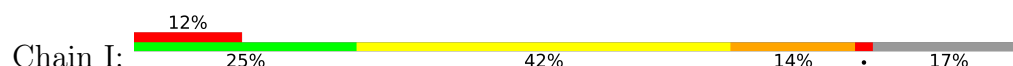
- Molecule 7: U6 snRNA-associated Sm-like protein LSm7



- Molecule 8: U6 snRNA-associated Sm-like protein LSm8



- Molecule 9: *Saccharomyces cerevisiae* strain HB\_S\_GIMBLETTROAD\_9 chromosome XII sequence





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.20Å 77.39Å 118.61Å 90.00° 105.91° 90.00°	Depositor
Resolution (Å)	55.63 – 2.71 90.59 – 2.71	Depositor EDS
% Data completeness (in resolution range)	73.6 (55.63-2.71) 73.6 (90.59-2.71)	Depositor EDS
$R_{merge}$	0.45	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.195 , 0.247 0.196 , 0.246	Depositor DCC
$R_{free}$ test set	2603 reflections (7.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 87.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: UBD, K, MN, MG

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	0.64	0/3023	1.04	12/4069 (0.3%)
2	B	0.47	0/780	0.88	0/1051
3	C	0.52	1/634 (0.2%)	0.93	2/858 (0.2%)
4	D	0.38	0/482	0.59	0/650
5	E	0.39	0/633	0.73	0/858
6	F	0.55	0/590	0.86	1/795 (0.1%)
7	G	0.37	0/511	0.78	0/683
8	H	0.44	0/669	0.81	0/897
9	I	0.84	0/1644	1.43	23/2554 (0.9%)
All	All	0.61	1/8966 (0.0%)	1.04	38/12415 (0.3%)

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
8	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	37	CYS	CB-SG	-5.79	1.72	1.81

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LEU	CB-CG-CD1	-13.34	88.33	111.00
9	I	48	C	C6-N1-C2	-9.13	116.65	120.30
1	A	136	LEU	CB-CG-CD2	-8.48	96.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	56	A	N1-C6-N6	8.37	123.62	118.60
1	A	276	LEU	CB-CG-CD2	-7.91	97.55	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	95	ASN	Peptide

## 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	2974	0	3036	48	1
2	B	770	0	779	35	0
3	C	628	0	638	33	0
4	D	477	0	498	15	0
5	E	624	0	624	10	0
6	F	583	0	577	15	0
7	G	510	0	562	14	0
8	H	663	0	671	43	0
9	I	1495	0	753	40	1
10	A	1	0	0	0	0
10	I	1	0	0	0	0
11	I	1	0	0	0	0
12	I	2	0	0	0	0
13	A	76	0	0	1	0
13	B	6	0	0	0	0
13	C	1	0	0	0	0
13	E	1	0	0	0	0
13	F	6	0	0	0	0
13	H	1	0	0	0	0
13	I	43	0	0	1	0
All	All	8863	0	8138	204	1

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.

The worst 5 of 204 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:53:HIS:HE1	8:H:16:ILE:HG12	1.31	0.95
2:B:66:THR:HG21	8:H:62:ALA:HA	1.52	0.92
8:H:42:PHE:HB3	8:H:49:PHE:HA	1.60	0.82
2:B:48:GLU:HG3	2:B:50:LYS:HD2	1.63	0.80
1:A:36:ARG:O	1:A:40:LEU:HB2	1.84	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LYS:NZ	9:I:74:U:OP1[2_555]	2.12	0.08

## 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	368/424 (87%)	360 (98%)	8 (2%)	0	100	100
2	B	93/95 (98%)	82 (88%)	8 (9%)	3 (3%)	4	8
3	C	77/97 (79%)	72 (94%)	4 (5%)	1 (1%)	12	28
4	D	55/93 (59%)	47 (86%)	7 (13%)	1 (2%)	8	20
5	E	77/93 (83%)	75 (97%)	2 (3%)	0	100	100
6	F	73/88 (83%)	72 (99%)	1 (1%)	0	100	100
7	G	63/115 (55%)	63 (100%)	0	0	100	100
8	H	77/115 (67%)	66 (86%)	7 (9%)	4 (5%)	2	3
All	All	883/1120 (79%)	837 (95%)	37 (4%)	9 (1%)	15	35

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	56	LEU
4	D	83	ASP
8	H	94	GLU
8	H	96	GLU
2	B	55	GLY

### 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	333/387 (86%)	325 (98%)	8 (2%)	49	76
2	B	88/91 (97%)	85 (97%)	3 (3%)	37	65
3	C	73/89 (82%)	66 (90%)	7 (10%)	8	19
4	D	54/85 (64%)	51 (94%)	3 (6%)	21	43
5	E	71/84 (84%)	70 (99%)	1 (1%)	67	85
6	F	67/76 (88%)	65 (97%)	2 (3%)	41	69
7	G	57/103 (55%)	54 (95%)	3 (5%)	22	46
8	H	72/105 (69%)	64 (89%)	8 (11%)	6	13
All	All	815/1020 (80%)	780 (96%)	35 (4%)	29	55

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	50	GLN
4	D	15	MET
8	H	27	LEU
3	C	51	LEU
3	C	75	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	HIS

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Mol	Chain	Res	Type
6	F	84	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	I	66/84 (78%)	13 (19%)	0

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	I	36	U
9	I	46	U
9	I	50	G
9	I	51	A
9	I	52	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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
9	UBD	I	113	9	19,25,26	1.09	2 (10%)	19,37,40	1.81	7 (36%)

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
9	UBD	I	113	9	-	7/10/30/31	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	113	UBD	C4-N3	3.21	1.38	1.33
9	I	113	UBD	C6-C5	-2.09	1.33	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	113	UBD	C5-C4-N3	-3.65	115.29	123.31
9	I	113	UBD	O6P-P2-O5P	-3.02	98.87	110.68
9	I	113	UBD	O4P-P2-O5P	-2.80	99.73	110.68
9	I	113	UBD	O4P-P2-O3'	2.74	118.28	105.99
9	I	113	UBD	O6P-P2-O3'	2.73	118.22	105.99

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	113	UBD	O4'-C1'-N1-C6
9	I	113	UBD	C2'-C1'-N1-C6
9	I	113	UBD	C3'-C4'-C5'-O5'
9	I	113	UBD	O4'-C4'-C5'-O5'
9	I	113	UBD	C3'-O3'-P2-O5P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	113	UBD	1	0

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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<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	369/424 (87%)	0.47	8 (2%) 62 63	13, 43, 78, 114	0
2	B	95/95 (100%)	1.67	29 (30%) 0 0	41, 89, 159, 174	0
3	C	79/97 (81%)	0.92	11 (13%) 2 2	36, 67, 146, 182	0
4	D	59/93 (63%)	1.58	20 (33%) 0 0	105, 121, 148, 153	0
5	E	79/93 (84%)	1.25	21 (26%) 0 0	64, 97, 156, 185	0
6	F	75/88 (85%)	0.35	2 (2%) 54 55	37, 62, 96, 108	0
7	G	67/115 (58%)	1.96	29 (43%) 0 0	84, 117, 144, 151	0
8	H	83/115 (72%)	1.89	34 (40%) 0 0	88, 113, 159, 179	0
9	I	69/84 (82%)	0.84	10 (14%) 2 1	21, 76, 195, 247	0
All	All	975/1204 (80%)	1.00	164 (16%) 1 1	13, 73, 143, 247	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	54	LEU	12.6
2	B	53	HIS	9.5
2	B	55	GLY	8.4
7	G	68	GLU	8.4
2	B	52	PRO	7.4

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

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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
9	UBD	I	113	24/25	0.94	0.16	37,84,118,129	0

### 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
12	MG	I	203	1/1	0.82	0.12	70,70,70,70	0
12	MG	I	204	1/1	0.91	0.10	58,58,58,58	0
10	K	A	501	1/1	0.91	0.21	76,76,76,76	0
11	MN	I	201	1/1	0.93	0.19	102,102,102,102	0
10	K	I	202	1/1	0.96	0.11	65,65,65,65	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.