



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:51 pm BST

PDB ID : 2I91  
Title : 60kDa Ro autoantigen in complex with a fragment of misfolded RNA  
Authors : Reinisch, K.M.; Stein, A.J.  
Deposited on : 2006-09-04  
Resolution : 2.65 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:

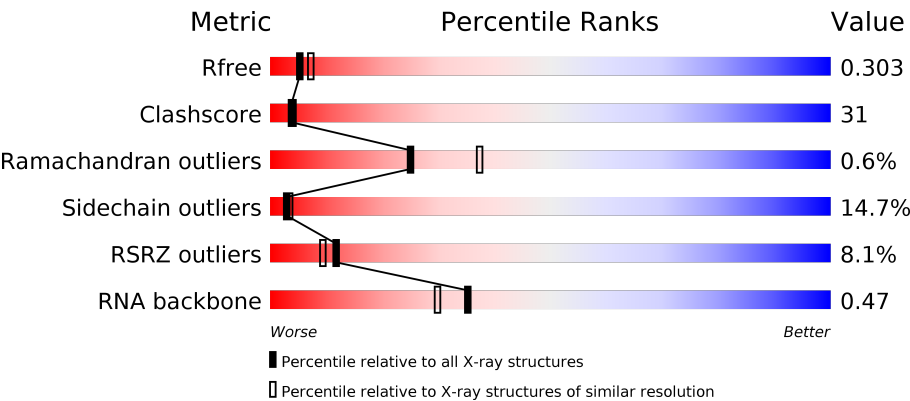
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 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 2.65 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 <sub>free</sub>	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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	C	8	<div><div>13%</div><div>100%</div></div>
1	E	8	<div><div>13%</div><div>13%</div><div>75%</div><div>13%</div></div>
2	D	15	<div><div>27%</div><div>20%</div><div>27%</div><div>40%</div><div>7%</div><div>7%</div></div>
2	F	15	<div><div>27%</div><div>13%</div><div>40%</div><div>33%</div><div>13%</div></div>

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Mol	Chain	Length	Quality of chain
3	A	538	
3	B	538	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	601	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9774 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\*CP\*CP\*UP\*AP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	8	Total	C	N	O	P	0	0	0
			162	74	27	54	7			
1	E	8	Total	C	N	O	P	0	0	0
			162	74	27	54	7			

- Molecule 2 is a RNA chain called 5'-R(\*C\*GP\*GP\*UP\*AP\*GP\*GP\*CP\*UP\*UP\*UP\*UP\*CP\*AP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	P	0	0	0
			295	133	51	98	13			
2	F	15	Total	C	N	O	P	0	0	0
			315	142	54	105	14			

- Molecule 3 is a protein called 60 kDa SS-A/Ro ribonucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	520	Total	C	N	O	S	0	0	0
			4108	2605	708	764	31			
3	B	526	Total	C	N	O	S	0	0	0
			4161	2639	717	774	31			

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	12	Total	O	0	0
			12	12		
6	D	25	Total	O	0	0
			25	25		
6	E	12	Total	O	0	0
			12	12		
6	F	20	Total	O	0	0
			20	20		
6	A	283	Total	O	0	0
			283	283		

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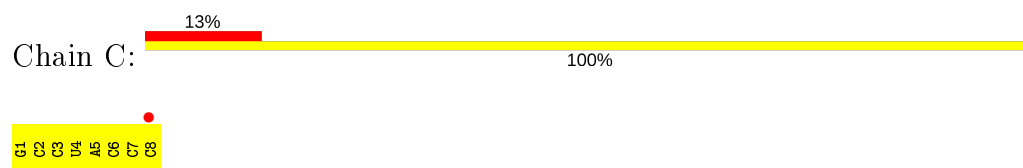
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	209	Total 209	O 209	0	0

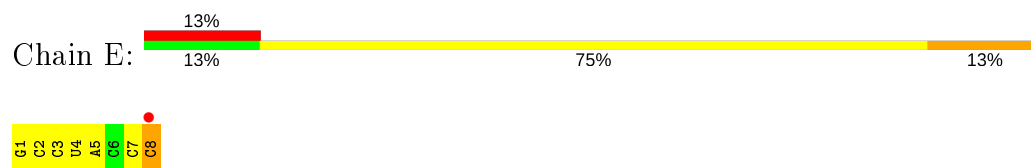
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

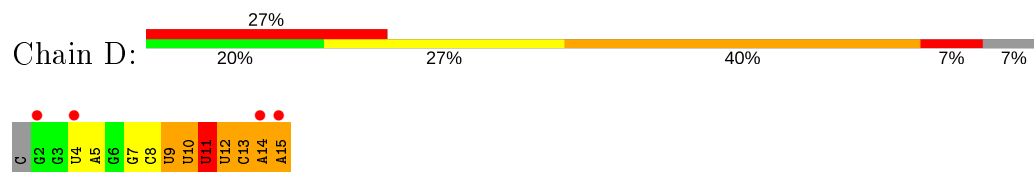
- Molecule 1: 5'-R(\*GP\*CP\*CP\*UP\*AP\*CP\*CP\*C)-3'



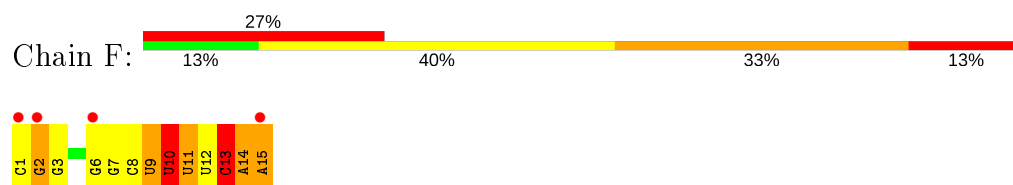
- Molecule 1: 5'-R(\*GP\*CP\*CP\*UP\*AP\*CP\*CP\*C)-3'



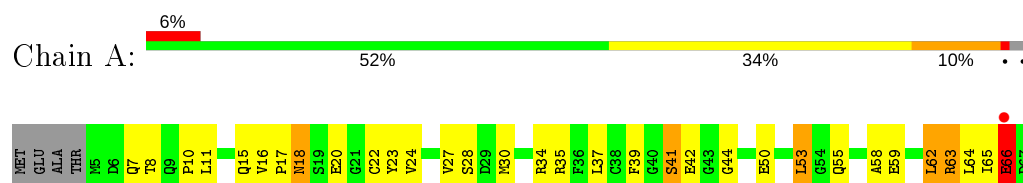
- Molecule 2: 5'-R(\*C\*GP\*GP\*UP\*AP\*GP\*GP\*CP\*UP\*UP\*UP\*UP\*CP\*AP\*A)-3'

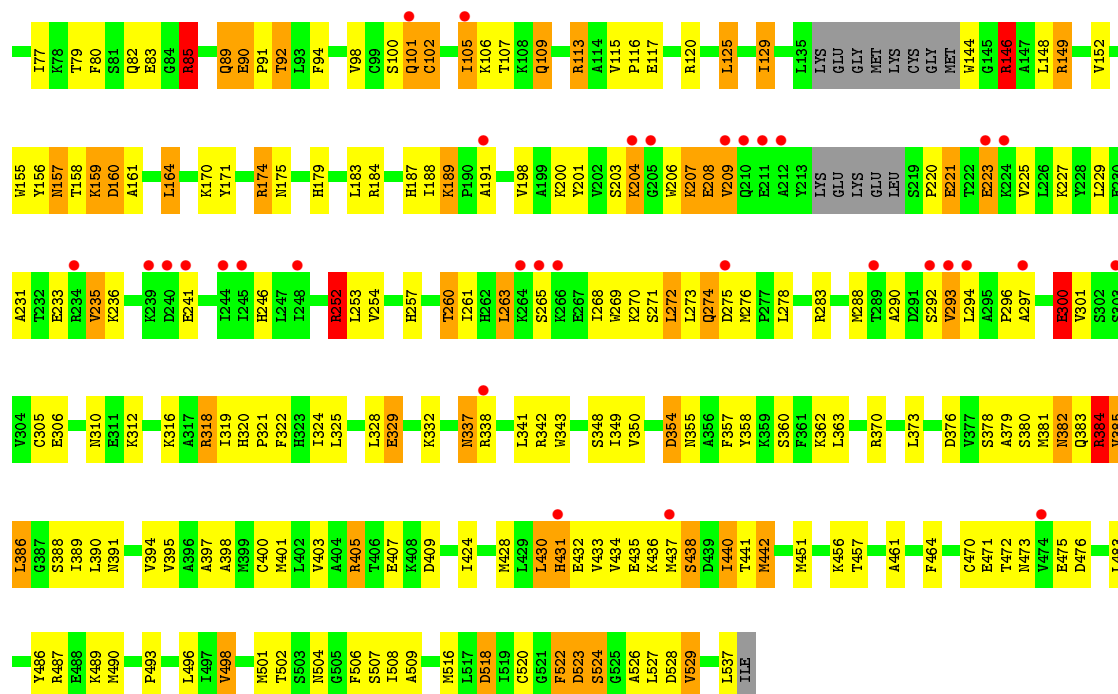


- Molecule 2: 5'-R(\*C\*GP\*GP\*UP\*AP\*GP\*GP\*CP\*UP\*UP\*UP\*UP\*CP\*AP\*A)-3'

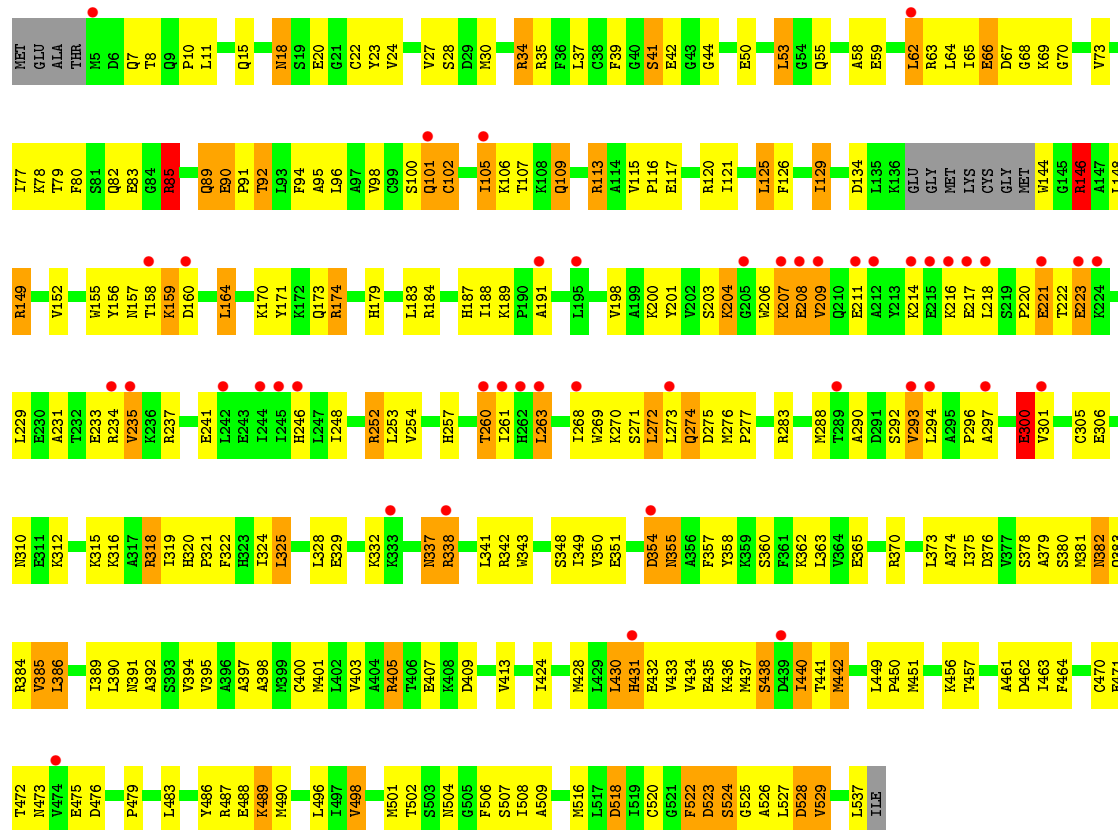
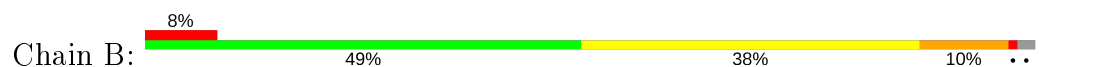


- Molecule 3: 60 kDa SS-A/Ro ribonucleoprotein





• Molecule 3: 60 kDa SS-A/Ro ribonucleoprotein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.68Å 119.98Å 73.54Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 37.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.65) 94.9 (37.25-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.285 0.264 , 0.303	Depositor DCC
$R_{free}$ test set	4252 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	9774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 21.54 % 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 6.8704e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.44	0/179	0.80	0/276
1	E	0.36	0/179	0.66	0/276
2	D	0.63	0/329	1.17	2/511 (0.4%)
2	F	0.51	0/351	1.07	3/545 (0.6%)
3	A	0.53	4/4181 (0.1%)	1.24	47/5643 (0.8%)
3	B	0.55	5/4235 (0.1%)	1.22	47/5714 (0.8%)
All	All	0.54	9/9454 (0.1%)	1.20	99/12965 (0.8%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	42	GLU	CD-OE1	-13.70	1.10	1.25
3	A	42	GLU	CD-OE1	-13.28	1.11	1.25
3	A	42	GLU	CD-OE2	-9.74	1.15	1.25
3	B	42	GLU	CD-OE2	-9.43	1.15	1.25
3	B	208	GLU	CD-OE1	-6.72	1.18	1.25

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	146	ARG	NE-CZ-NH1	20.63	130.62	120.30
3	B	318	ARG	NE-CZ-NH1	-19.11	110.75	120.30
3	B	146	ARG	NE-CZ-NH1	-18.92	110.84	120.30
3	A	146	ARG	NE-CZ-NH2	-18.36	111.12	120.30
3	B	318	ARG	NE-CZ-NH2	17.80	129.20	120.30

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	C	162	0	89	9	0
1	E	162	0	89	6	0
2	D	295	0	151	24	0
2	F	315	0	162	22	0
3	A	4108	0	4171	263	0
3	B	4161	0	4234	275	0
4	A	4	0	3	2	0
4	B	4	0	3	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	283	0	0	13	0
6	B	209	0	0	18	0
6	C	12	0	0	0	0
6	D	25	0	0	0	0
6	E	12	0	0	0	0
6	F	20	0	0	0	0
All	All	9774	0	8902	559	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 31.

The worst 5 of 559 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:D:14:A:H3'	2:D:15:A:C5'	1.60	1.29
3:B:337:ASN:OD1	3:B:389:ILE:HD11	1.47	1.13
3:B:146:ARG:HE	3:B:146:ARG:HA	1.11	1.11
2:D:14:A:H3'	2:D:15:A:H5'	1.18	1.09
3:B:157:ASN:ND2	3:B:188:ILE:HD11	1.70	1.07

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	
3	A	514/538 (96%)	473 (92%)	38 (7%)	3 (1%)	25	37
3	B	522/538 (97%)	480 (92%)	39 (8%)	3 (1%)	25	37
All	All	1036/1076 (96%)	953 (92%)	77 (7%)	6 (1%)	25	37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	102	CYS
3	B	102	CYS
3	A	442	MET
3	B	442	MET
3	A	69	LYS

### 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	
3	A	452/467 (97%)	384 (85%)	68 (15%)	3	3
3	B	458/467 (98%)	392 (86%)	66 (14%)	3	3
All	All	910/934 (97%)	776 (85%)	134 (15%)	3	3

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	489	LYS

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Mol	Chain	Res	Type
3	B	89	GLN
3	B	440	ILE
3	A	518	ASP
3	B	30	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	485	GLN
3	B	9	GLN
3	B	355	ASN
3	A	504	ASN
3	B	26	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	7/8 (87%)	0	0
1	E	7/8 (87%)	1 (14%)	0
2	D	13/15 (86%)	7 (53%)	5 (38%)
2	F	14/15 (93%)	8 (57%)	5 (35%)
All	All	41/46 (89%)	16 (39%)	10 (24%)

5 of 16 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	9	U
2	D	10	U
2	D	11	U
2	D	12	U
2	D	13	C

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	13	C
2	F	9	U
2	F	11	U
2	D	12	U
2	F	10	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ACT	B	602	5	1,3,3	3.61	1 (100%)	0,3,3	0.00	-
4	ACT	A	601	5	1,3,3	4.37	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	ACT	CH3-C	4.37	1.54	1.48
4	B	602	ACT	CH3-C	3.61	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	ACT	1	0
4	A	601	ACT	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	8/8 (100%)	0.87	1 (12%) 3 2	32, 37, 57, 62	0
1	E	8/8 (100%)	1.22	1 (12%) 3 2	31, 39, 54, 67	0
2	D	14/15 (93%)	1.23	4 (28%) 0 0	26, 38, 55, 69	0
2	F	15/15 (100%)	1.62	4 (26%) 0 0	27, 38, 63, 63	0
3	A	520/538 (96%)	0.57	33 (6%) 20 17	11, 30, 47, 59	0
3	B	526/538 (97%)	0.59	45 (8%) 10 8	14, 31, 49, 62	0
All	All	1091/1122 (97%)	0.61	88 (8%) 12 9	11, 31, 50, 69	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	431	HIS	6.7
2	D	15	A	5.1
3	B	215	GLU	4.8
3	A	338	ARG	4.8
2	F	15	A	4.0

### 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](#)

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(Å <sup>2</sup> )	Q<0.9
4	ACT	A	601	4/4	0.64	0.32	22,23,24,26	0
5	MG	A	701	1/1	0.79	0.07	40,40,40,40	0
5	MG	B	702	1/1	0.83	0.09	29,29,29,29	0
4	ACT	B	602	4/4	0.84	0.27	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.