



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 04:45 am BST

PDB ID : 5JRG  
Title : Crystal structure of the nucleosome containing the DNA with tetrahydrofuran (THF)  
Authors : Osakabe, A.; Arimura, Y.; Horikoshi, N.; Kurumizaka, H.  
Deposited on : 2016-05-06  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (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

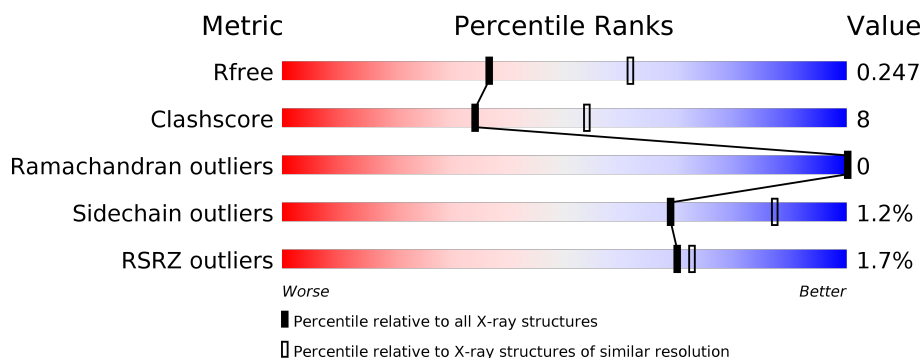
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	139	<div> <div>57%</div> <div>12%</div> <div>30%</div> </div>
1	E	139	<div> <div>62%</div> <div>9%</div> <div>29%</div> </div>
2	B	106	<div> <div>59%</div> <div>14%</div> <div>26%</div> </div>
2	F	106	<div> <div>71%</div> <div>10%</div> <div>19%</div> </div>
3	C	133	<div> <div>63%</div> <div>17%</div> <div>20%</div> </div>
3	G	133	<div> <div>72%</div> <div>10%</div> <div>18%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	129	<p>4% 60% 13% 2% 21%</p>
4	H	129	<p>1% 69% 5% 25%</p>
5	I	145	<p>2% 60% 38% 1%</p>
6	J	145	<p>1% 57% 41% 1%</p>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12282 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 Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
2	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	107	Total	C	N	O	0	0	0
			824	520	161	143			
3	G	109	Total	C	N	O	0	0	0
			840	529	166	145			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	97	Total	C	N	O	S	0	0	0
			769	483	143	141	2			
4	H	96	Total	C	N	O	S	0	0	0
			756	474	140	140	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	145	Total	C	N	O	P	0	0	0
			2939	1405	532	859	143			

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	145	Total	C	N	O	P	0	0	0
			2961	1416	533	868	144			

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	E	1	Total	Cl	0	0
			1	1		

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	6	Total	Mn	0	0
			6	6		
8	I	8	Total	Mn	0	0
			8	8		
8	E	1	Total	Mn	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	14	Total	O	0	0
			14	14		
9	C	27	Total	O	0	0
			27	27		
9	D	12	Total	O	0	0
			12	12		
9	E	35	Total	O	0	0
			35	35		
9	F	21	Total	O	0	0
			21	21		
9	G	24	Total	O	0	0
			24	24		

*Continued on next page...*

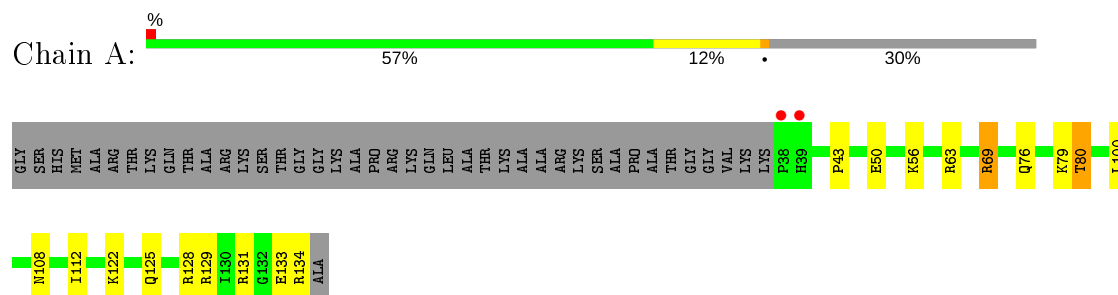
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	11	Total 11	O 11	0	0
9	I	48	Total 48	O 48	0	0
9	J	44	Total 44	O 44	0	0

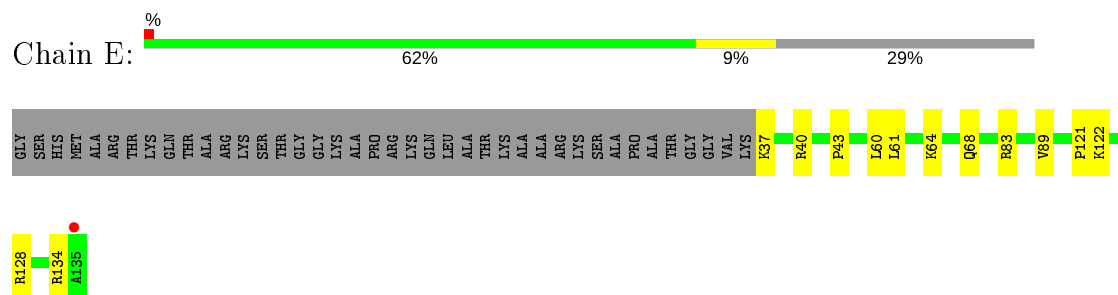
### 3 Residue-property plots [i](#)

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.

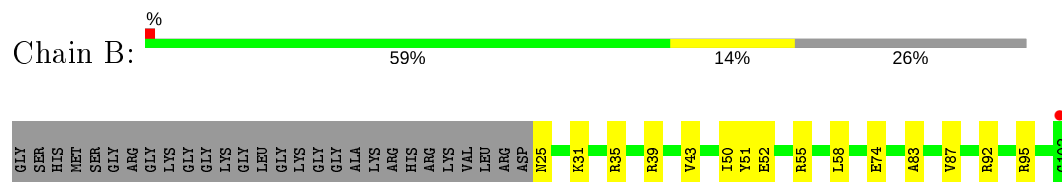
- Molecule 1: Histone H3.1



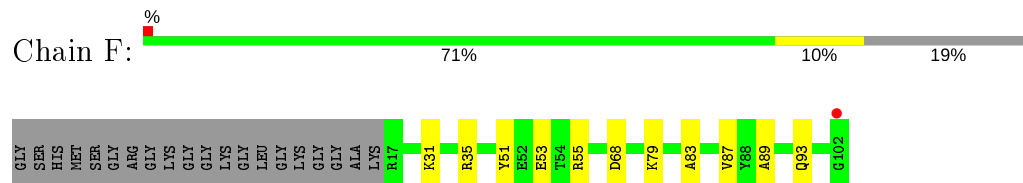
- Molecule 1: Histone H3.1



- Molecule 2: Histone H4



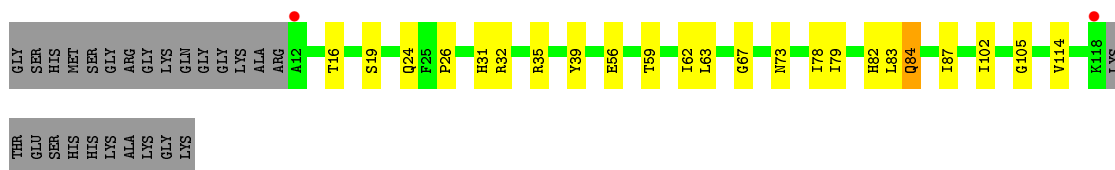
- Molecule 2: Histone H4



- Molecule 3: Histone H2A type 1-B/E



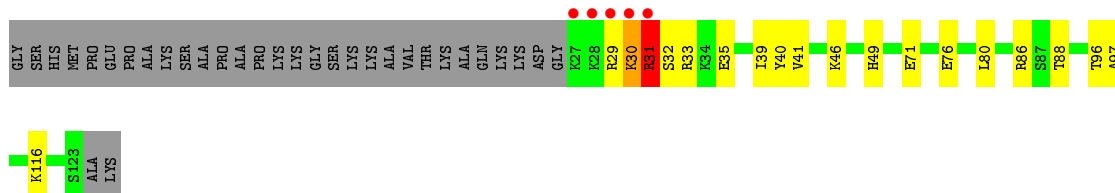




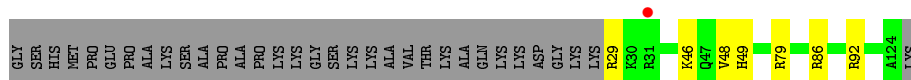
- Molecule 3: Histone H2A type 1-B/E



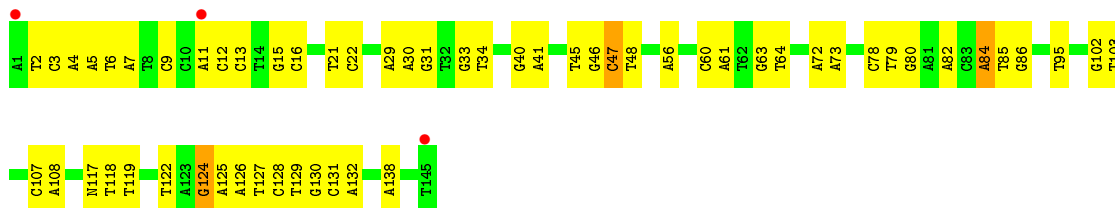
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J



- Molecule 5: DNA (145-MER)



- Molecule 6: DNA (145-MER)



T105	C106	C107	T116	N117	T118	T122	A123	G124	A125	A126	T127	C128	T129	G130	C131	A132	G133	G134	T135	G136	G137	A144	T145
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.49Å 108.77Å 169.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.50 49.15 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-2.50) 99.5 (49.15-2.49)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.193 , 0.245 0.195 , 0.247	Depositor DCC
$R_{free}$ test set	3297 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.0	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	0.94	EDS
Total number of atoms	12282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 3DR, 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	A	0.53	0/813	0.62	0/1090
1	E	0.61	0/828	0.67	0/1109
2	B	0.52	0/626	0.70	0/837
2	F	0.59	0/702	0.75	0/937
3	C	0.57	0/834	0.69	0/1125
3	G	0.49	0/850	0.64	0/1146
4	D	0.59	0/780	0.81	2/1044 (0.2%)
4	H	0.56	0/767	0.70	0/1029
5	I	0.97	4/3283 (0.1%)	1.05	3/5062 (0.1%)
6	J	1.02	5/3308 (0.2%)	1.06	2/5102 (0.0%)
All	All	0.81	9/12791 (0.1%)	0.91	7/18481 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	47	DC	C3'-O3'	-6.93	1.34	1.44
6	J	130	DG	C3'-O3'	-6.05	1.36	1.44
5	I	80	DG	C3'-O3'	-5.76	1.36	1.44
6	J	100	DC	C3'-O3'	-5.48	1.36	1.44
6	J	46	DG	C3'-O3'	-5.48	1.36	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	138	DA	O5'-P-OP1	-10.21	96.51	105.70
4	D	31	ARG	NE-CZ-NH1	-9.98	115.31	120.30
4	D	31	ARG	NE-CZ-NH2	9.19	124.89	120.30
6	J	40	DG	O5'-P-OP1	-6.34	100.00	105.70
5	I	84	DA	O4'-C1'-N9	5.76	112.03	108.00

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	801	0	839	19	0
1	E	816	0	856	12	0
2	B	619	0	659	14	0
2	F	694	0	742	8	0
3	C	824	0	884	19	0
3	G	840	0	902	11	0
4	D	769	0	805	22	0
4	H	756	0	784	13	0
5	I	2939	0	1622	51	0
6	J	2961	0	1637	51	0
7	A	1	0	0	1	0
7	C	1	0	0	0	0
7	E	1	0	0	1	0
7	G	1	0	0	0	0
8	E	1	0	0	0	0
8	I	8	0	0	0	0
8	J	6	0	0	0	0
9	A	8	0	0	0	0
9	B	14	0	0	0	0
9	C	27	0	0	1	0
9	D	12	0	0	0	0
9	E	35	0	0	0	0
9	F	21	0	0	0	0
9	G	24	0	0	0	0
9	H	11	0	0	2	0
9	I	48	0	0	2	0
9	J	44	0	0	0	0
All	All	12282	0	9730	182	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 8.

The worst 5 of 182 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)
3:G:71:ARG:HH12	4:H:49:HIS:CE1	1.68	1.11
4:D:31:ARG:HH12	6:J:124:DG:P	1.87	0.97
1:A:128:ARG:HD3	1:A:134:ARG:HH21	1.38	0.88
3:G:75:LYS:HD3	5:I:130:DG:H5'	1.62	0.81
5:I:12:DC:H2''	5:I:13:DC:H5''	1.66	0.78

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	
1	A	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
1	E	97/139 (70%)	96 (99%)	1 (1%)	0	100	100
2	B	76/106 (72%)	76 (100%)	0	0	100	100
2	F	84/106 (79%)	83 (99%)	1 (1%)	0	100	100
3	C	105/133 (79%)	102 (97%)	3 (3%)	0	100	100
3	G	107/133 (80%)	105 (98%)	2 (2%)	0	100	100
4	D	95/129 (74%)	93 (98%)	2 (2%)	0	100	100
4	H	94/129 (73%)	93 (99%)	1 (1%)	0	100	100
All	All	753/1014 (74%)	742 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	A	85/113 (75%)	83 (98%)	2 (2%)	49	74
1	E	86/113 (76%)	85 (99%)	1 (1%)	71	88
2	B	63/81 (78%)	63 (100%)	0	100	100
2	F	71/81 (88%)	71 (100%)	0	100	100
3	C	84/102 (82%)	82 (98%)	2 (2%)	49	74
3	G	85/102 (83%)	85 (100%)	0	100	100
4	D	84/107 (78%)	81 (96%)	3 (4%)	35	61
4	H	82/107 (77%)	82 (100%)	0	100	100
All	All	640/806 (79%)	632 (99%)	8 (1%)	69	87

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	114	VAL
1	E	83	ARG
4	D	30	LYS
3	C	84	GLN
4	D	29	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	108	ASN
3	C	73	ASN
4	H	49	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
6	3DR	J	117	6	8,11,12	0.48	0	9,14,17	1.47	2 (22%)
5	3DR	I	117	5	8,11,12	0.45	0	9,14,17	1.34	1 (11%)

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
6	3DR	J	117	6	-	1/3/15/16	0/1/1/1
5	3DR	I	117	5	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	J	117	3DR	O4'-C4'-C3'	2.73	107.75	103.73
6	J	117	3DR	C1'-C2'-C3'	2.63	106.17	103.20
5	I	117	3DR	O4'-C4'-C3'	2.24	107.02	103.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	117	3DR	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	117	3DR	1	0
5	I	117	3DR	1	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 19 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 [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	97/139 (69%)	-0.14	2 (2%) 63 66	24, 34, 57, 68	0
1	E	99/139 (71%)	-0.23	1 (1%) 82 84	16, 25, 41, 74	0
2	B	78/106 (73%)	-0.24	1 (1%) 77 79	24, 32, 40, 50	0
2	F	86/106 (81%)	-0.10	1 (1%) 79 80	16, 22, 32, 63	0
3	C	107/133 (80%)	-0.06	2 (1%) 66 69	17, 27, 46, 68	0
3	G	109/133 (81%)	-0.17	1 (0%) 84 86	21, 32, 62, 74	0
4	D	97/129 (75%)	0.15	5 (5%) 27 29	18, 27, 57, 78	0
4	H	96/129 (74%)	-0.05	1 (1%) 82 84	19, 30, 53, 75	0
5	I	144/145 (99%)	-0.37	3 (2%) 63 66	29, 56, 90, 110	0
6	J	144/145 (99%)	-0.41	1 (0%) 87 89	27, 55, 93, 110	0
All	All	1057/1304 (81%)	-0.18	18 (1%) 70 72	16, 33, 71, 110	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	27	LYS	6.6
4	D	29	ARG	6.6
4	D	31	ARG	6.3
1	A	38	PRO	3.8
3	C	12	ALA	3.8

### 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. 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
6	3DR	J	117	11/12	0.86	0.30	79,82,86,88	0
5	3DR	I	117	11/12	0.94	0.11	54,59,70,72	0

### 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( $\text{\AA}^2$ )	Q<0.9
8	MN	I	207	1/1	0.50	0.10	91,91,91,91	0
8	MN	J	205	1/1	0.88	0.07	82,82,82,82	0
8	MN	J	204	1/1	0.88	0.10	82,82,82,82	0
8	MN	I	206	1/1	0.91	0.06	69,69,69,69	0
8	MN	I	205	1/1	0.94	0.06	65,65,65,65	0
7	CL	A	201	1/1	0.94	0.13	47,47,47,47	0
8	MN	I	208	1/1	0.95	0.15	67,67,67,67	0
8	MN	J	201	1/1	0.96	0.09	55,55,55,55	0
8	MN	J	202	1/1	0.97	0.10	57,57,57,57	0
7	CL	E	3002	1/1	0.98	0.09	43,43,43,43	0
8	MN	J	203	1/1	0.98	0.17	67,67,67,67	0
8	MN	I	201	1/1	0.98	0.14	46,46,46,46	0
8	MN	J	206	1/1	0.98	0.11	63,63,63,63	0
8	MN	I	203	1/1	0.98	0.15	54,54,54,54	0
8	MN	I	204	1/1	0.99	0.06	50,50,50,50	0
8	MN	I	202	1/1	0.99	0.15	55,55,55,55	0
7	CL	G	2001	1/1	0.99	0.04	30,30,30,30	0
8	MN	E	3001	1/1	0.99	0.13	26,26,26,26	0
7	CL	C	201	1/1	0.99	0.04	35,35,35,35	0

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

There are no such residues in this entry.