



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:40 PM GMT

PDB ID : 3RNU  
Title : Structural Basis of Cytosolic DNA Sensing by Innate Immune Receptors  
Authors : Jin, T.C.; Xiao, T.  
Deposited on : 2011-04-22  
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  
<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

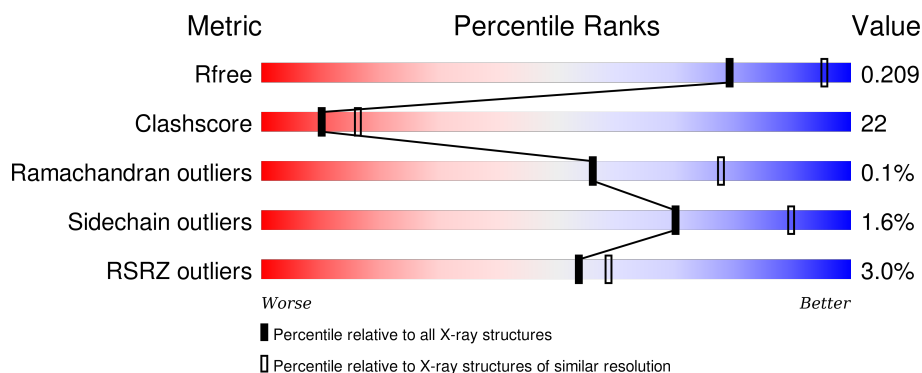
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	204	<div> <div>3%</div> <div>56%</div> <div>41%</div> <div>.</div> </div>
1	B	204	<div> <div>3%</div> <div>66%</div> <div>31%</div> <div>..</div> </div>
1	C	204	<div> <div>%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>
1	D	204	<div> <div>4%</div> <div>51%</div> <div>46%</div> <div>.</div> </div>
2	K	16	<div> <div>31%</div> <div>69%</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	16	

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	FMT	B	4	-	-	-	X
4	FMT	C	3	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7087 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 Gamma-interferon-inducible protein 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	1	1	0
			1572	997	273	294	8			
1	B	201	Total	C	N	O	S	1	1	0
			1593	1008	276	301	8			
1	C	199	Total	C	N	O	S	1	0	0
			1572	997	273	294	8			
1	D	199	Total	C	N	O	S	1	1	0
			1572	997	273	294	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	GLY	-	EXPRESSION TAG	UNP Q16666
A	568	SER	-	EXPRESSION TAG	UNP Q16666
A	569	VAL	-	EXPRESSION TAG	UNP Q16666
A	570	ASP	-	EXPRESSION TAG	UNP Q16666
A	767	ALA	-	EXPRESSION TAG	UNP Q16666
A	768	ALA	-	EXPRESSION TAG	UNP Q16666
A	769	ALA	-	EXPRESSION TAG	UNP Q16666
A	770	SER	-	EXPRESSION TAG	UNP Q16666
B	567	GLY	-	EXPRESSION TAG	UNP Q16666
B	568	SER	-	EXPRESSION TAG	UNP Q16666
B	569	VAL	-	EXPRESSION TAG	UNP Q16666
B	570	ASP	-	EXPRESSION TAG	UNP Q16666
B	767	ALA	-	EXPRESSION TAG	UNP Q16666
B	768	ALA	-	EXPRESSION TAG	UNP Q16666
B	769	ALA	-	EXPRESSION TAG	UNP Q16666
B	770	SER	-	EXPRESSION TAG	UNP Q16666
C	567	GLY	-	EXPRESSION TAG	UNP Q16666
C	568	SER	-	EXPRESSION TAG	UNP Q16666
C	569	VAL	-	EXPRESSION TAG	UNP Q16666
C	570	ASP	-	EXPRESSION TAG	UNP Q16666
C	767	ALA	-	EXPRESSION TAG	UNP Q16666

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Chain	Residue	Modelled	Actual	Comment	Reference
C	768	ALA	-	EXPRESSION TAG	UNP Q16666
C	769	ALA	-	EXPRESSION TAG	UNP Q16666
C	770	SER	-	EXPRESSION TAG	UNP Q16666
D	567	GLY	-	EXPRESSION TAG	UNP Q16666
D	568	SER	-	EXPRESSION TAG	UNP Q16666
D	569	VAL	-	EXPRESSION TAG	UNP Q16666
D	570	ASP	-	EXPRESSION TAG	UNP Q16666
D	767	ALA	-	EXPRESSION TAG	UNP Q16666
D	768	ALA	-	EXPRESSION TAG	UNP Q16666
D	769	ALA	-	EXPRESSION TAG	UNP Q16666
D	770	SER	-	EXPRESSION TAG	UNP Q16666

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*CP\*CP\*AP\*TP\*CP\*AP\*AP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	16	Total	C	N	O	P	0	0	0
			331	157	71	88	15			

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*CP\*TP\*CP\*TP\*TP\*TP\*GP\*AP\*TP\*GP\*GP\*CP\*C)-3').

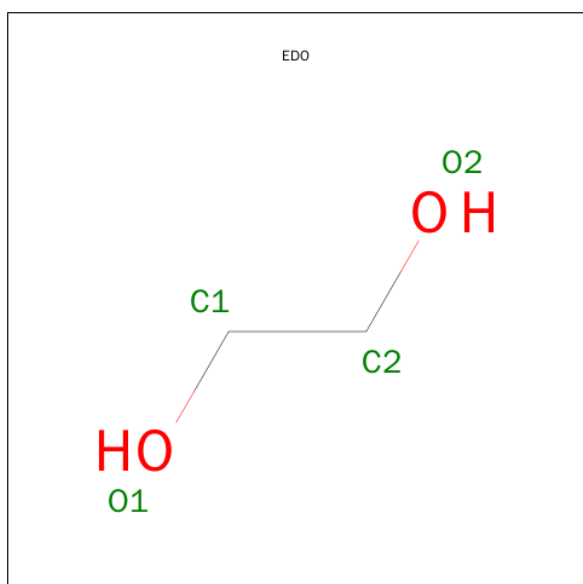
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	16	Total	C	N	O	P	0	0	0
			319	155	49	100	15			

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



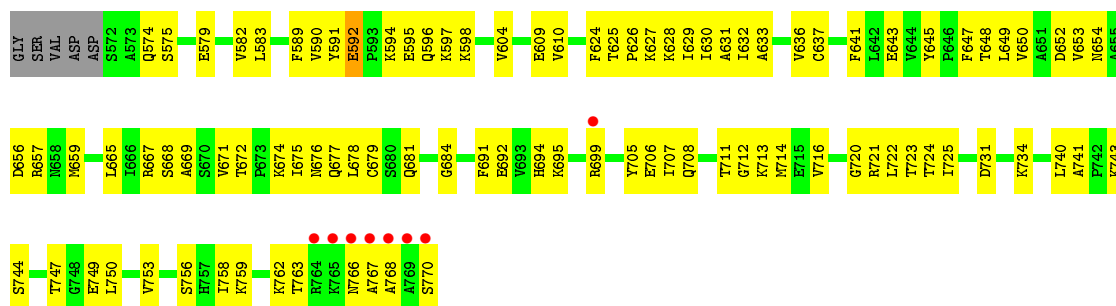
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		
6	B	26	Total	O	0	0
			26	26		
6	C	24	Total	O	0	0
			24	24		
6	D	25	Total	O	0	0
			25	25		
6	K	4	Total	O	0	0
			4	4		
6	L	2	Total	O	0	0
			2	2		

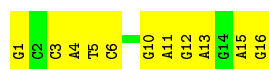






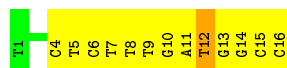
- Molecule 2: DNA (5'-D(\*GP\*CP\*CP\*AP\*TP\*CP\*AP\*AP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*G)-3')

Chain K: 31% 69%



- Molecule 3: DNA (5'-D(\*TP\*CP\*TP\*CP\*TP\*CP\*TP\*TP\*TP\*GP\*AP\*TP\*GP\*GP\*CP\*C)-3')

Chain L: 19% 75% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.84Å 126.84Å 163.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.39 – 2.50 41.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.39-2.50) 91.0 (41.39-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_736)	Depositor
R, $R_{free}$	0.176 , 0.216 0.176 , 0.209	Depositor DCC
$R_{free}$ test set	1563 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.000 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.000 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.000 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.000 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.486 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 33115 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	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 36.02 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without*

<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.

*pseudo translational symmetry is equal to  $5.3267\text{e-}04$ . The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

## 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: FMT, EDO

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	0.31	0/1598	0.50	0/2152
1	B	0.31	0/1622	0.49	0/2185
1	C	0.32	0/1598	0.53	0/2152
1	D	0.32	0/1598	0.51	0/2152
2	K	0.47	0/374	0.93	0/576
3	L	0.44	0/354	1.18	1/544 (0.2%)
All	All	0.33	0/7144	0.60	1/9761 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	L	12	DT	O4'-C1'-N1	5.24	111.67	108.00

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	A	1572	0	1603	81	0
1	B	1593	0	1618	49	0
1	C	1572	0	1604	61	0
1	D	1572	0	1603	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	331	0	179	16	0
3	L	319	0	185	9	0
4	A	3	0	1	1	0
4	B	3	0	1	0	0
4	C	3	0	1	1	0
4	D	6	0	2	0	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
6	A	24	0	0	3	0
6	B	26	0	0	1	0
6	C	24	0	0	0	0
6	D	25	0	0	3	0
6	K	4	0	0	2	0
6	L	2	0	0	0	0
All	All	7087	0	6809	299	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 22.

The worst 5 of 299 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:D:667:ARG:CZ	3:L:16:DC:H4'	1.94	0.96
1:A:587:GLU:HB3	1:D:767:ALA:HA	1.50	0.93
1:D:763:THR:HG22	1:D:766:ASN:ND2	1.84	0.93
1:D:770:SER:HA	2:K:10:DG:H5''	1.51	0.90
2:K:1:DG:H3'	6:K:104:HOH:O	1.69	0.90

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	197/204 (97%)	188 (95%)	9 (5%)	0	100	100
1	B	200/204 (98%)	192 (96%)	8 (4%)	0	100	100
1	C	197/204 (97%)	186 (94%)	10 (5%)	1 (0%)	34	55
1	D	197/204 (97%)	186 (94%)	11 (6%)	0	100	100
All	All	791/816 (97%)	752 (95%)	38 (5%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	764	ARG

### 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	176/180 (98%)	174 (99%)	2 (1%)	80	94
1	B	179/180 (99%)	175 (98%)	4 (2%)	60	84
1	C	176/180 (98%)	173 (98%)	3 (2%)	68	89
1	D	176/180 (98%)	174 (99%)	2 (1%)	80	94
All	All	707/720 (98%)	696 (98%)	11 (2%)	70	90

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	621	LYS
1	B	743	LYS
1	C	667	ARG
1	B	592	GLU
1	C	663	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	574	GLN
1	C	574	GLN
1	C	681	GLN
1	D	694	HIS
1	D	766	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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](#)

7 ligands 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	$\# Z  > 2$
4	FMT	A	6	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	B	2	-	3,3,3	0.46	0	2,2,2	0.44	0
4	FMT	B	4	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	3	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	D	1	-	3,3,3	0.43	0	2,2,2	0.65	0
4	FMT	D	5	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	7	-	0,2,2	0.00	-	0,1,1	0.00	-

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
4	FMT	A	6	-	-	0/0/0/0	0/0/0/0
5	EDO	B	2	-	-	0/1/1/1	0/0/0/0
4	FMT	B	4	-	-	0/0/0/0	0/0/0/0
4	FMT	C	3	-	-	0/0/0/0	0/0/0/0
5	EDO	D	1	-	-	0/1/1/1	0/0/0/0
4	FMT	D	5	-	-	0/0/0/0	0/0/0/0
4	FMT	D	7	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6	FMT	1	0
4	C	3	FMT	1	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	A	199/204 (97%)	-0.22	7 (3%) 48 53	39, 82, 150, 194	1 (0%)
1	B	201/204 (98%)	-0.16	7 (3%) 48 53	47, 85, 144, 216	1 (0%)
1	C	199/204 (97%)	-0.35	3 (1%) 76 79	36, 75, 136, 165	1 (0%)
1	D	199/204 (97%)	-0.12	8 (4%) 42 47	34, 80, 161, 212	1 (0%)
2	K	16/16 (100%)	-0.96	0 100 100	113, 146, 166, 181	0
3	L	16/16 (100%)	-0.76	0 100 100	104, 155, 200, 236	0
All	All	830/848 (97%)	-0.24	25 (3%) 54 59	34, 83, 155, 236	4 (0%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	GLY	10.3
1	D	769	ALA	7.9
1	B	749	GLU	7.4
1	A	572	SER	7.3
1	D	770	SER	6.4

### 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. 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(Å <sup>2</sup> )	Q<0.9
4	FMT	B	4	3/3	0.91	0.18	3.37	84,84,86,86	0
4	FMT	C	3	3/3	0.91	0.16	2.79	74,74,78,81	0
4	FMT	A	6	3/3	0.96	0.10	-0.63	53,53,56,60	0
4	FMT	D	5	3/3	0.97	0.08	-1.90	57,57,60,60	0
4	FMT	D	7	3/3	0.93	0.14	-	75,75,77,78	0
5	EDO	B	2	4/4	0.96	0.10	-	68,69,71,74	0
5	EDO	D	1	4/4	0.99	0.11	-	32,35,36,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.