



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:41 PM GMT

PDB ID : 3UN9
Title : Crystal structure of an immune receptor
Authors : Hong, M.; Yoon, S.I.; Wilson, I.A.
Deposited on : 2011-11-15
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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (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

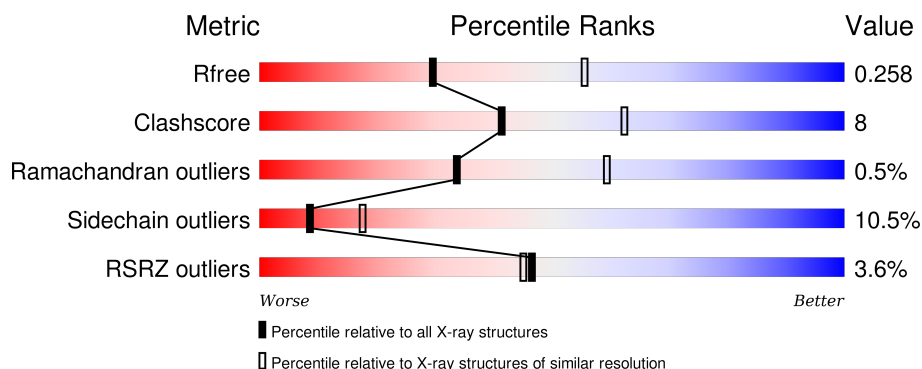
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 ≥ 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	372	<div> <div>2%</div> <div>63%</div> <div>14%</div> <div>•</div> <div>21%</div> </div>
1	B	372	<div> <div>3%</div> <div>62%</div> <div>14%</div> <div>•</div> <div>21%</div> </div>
1	C	372	<div> <div>3%</div> <div>57%</div> <div>15%</div> <div>•</div> <div>25%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6679 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 NLR family member X1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	17	0	0
			2277	1426	424	421	6			
1	B	294	Total	C	N	O	S	11	2	0
			2293	1436	425	426	6			
1	C	279	Total	C	N	O	S	0	1	0
			2097	1317	381	393	6			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	625	MET	-	EXPRESSION TAG	UNP Q86UT6
A	626	LEU	-	EXPRESSION TAG	UNP Q86UT6
A	627	LEU	-	EXPRESSION TAG	UNP Q86UT6
A	628	VAL	-	EXPRESSION TAG	UNP Q86UT6
A	976	PRO	-	EXPRESSION TAG	UNP Q86UT6
A	977	SER	-	EXPRESSION TAG	UNP Q86UT6
A	978	GLY	-	EXPRESSION TAG	UNP Q86UT6
A	979	SER	-	EXPRESSION TAG	UNP Q86UT6
A	980	TRP	-	EXPRESSION TAG	UNP Q86UT6
A	981	SER	-	EXPRESSION TAG	UNP Q86UT6
A	982	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	983	PRO	-	EXPRESSION TAG	UNP Q86UT6
A	984	GLN	-	EXPRESSION TAG	UNP Q86UT6
A	985	PHE	-	EXPRESSION TAG	UNP Q86UT6
A	986	GLU	-	EXPRESSION TAG	UNP Q86UT6
A	987	LYS	-	EXPRESSION TAG	UNP Q86UT6
A	988	GLY	-	EXPRESSION TAG	UNP Q86UT6
A	989	ALA	-	EXPRESSION TAG	UNP Q86UT6
A	990	GLY	-	EXPRESSION TAG	UNP Q86UT6
A	991	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	992	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	993	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	994	HIS	-	EXPRESSION TAG	UNP Q86UT6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	995	HIS	-	EXPRESSION TAG	UNP Q86UT6
A	996	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	625	MET	-	EXPRESSION TAG	UNP Q86UT6
B	626	LEU	-	EXPRESSION TAG	UNP Q86UT6
B	627	LEU	-	EXPRESSION TAG	UNP Q86UT6
B	628	VAL	-	EXPRESSION TAG	UNP Q86UT6
B	976	PRO	-	EXPRESSION TAG	UNP Q86UT6
B	977	SER	-	EXPRESSION TAG	UNP Q86UT6
B	978	GLY	-	EXPRESSION TAG	UNP Q86UT6
B	979	SER	-	EXPRESSION TAG	UNP Q86UT6
B	980	TRP	-	EXPRESSION TAG	UNP Q86UT6
B	981	SER	-	EXPRESSION TAG	UNP Q86UT6
B	982	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	983	PRO	-	EXPRESSION TAG	UNP Q86UT6
B	984	GLN	-	EXPRESSION TAG	UNP Q86UT6
B	985	PHE	-	EXPRESSION TAG	UNP Q86UT6
B	986	GLU	-	EXPRESSION TAG	UNP Q86UT6
B	987	LYS	-	EXPRESSION TAG	UNP Q86UT6
B	988	GLY	-	EXPRESSION TAG	UNP Q86UT6
B	989	ALA	-	EXPRESSION TAG	UNP Q86UT6
B	990	GLY	-	EXPRESSION TAG	UNP Q86UT6
B	991	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	992	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	993	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	994	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	995	HIS	-	EXPRESSION TAG	UNP Q86UT6
B	996	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	625	MET	-	EXPRESSION TAG	UNP Q86UT6
C	626	LEU	-	EXPRESSION TAG	UNP Q86UT6
C	627	LEU	-	EXPRESSION TAG	UNP Q86UT6
C	628	VAL	-	EXPRESSION TAG	UNP Q86UT6
C	976	PRO	-	EXPRESSION TAG	UNP Q86UT6
C	977	SER	-	EXPRESSION TAG	UNP Q86UT6
C	978	GLY	-	EXPRESSION TAG	UNP Q86UT6
C	979	SER	-	EXPRESSION TAG	UNP Q86UT6
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C	985	PHE	-	EXPRESSION TAG	UNP Q86UT6
C	986	GLU	-	EXPRESSION TAG	UNP Q86UT6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	987	LYS	-	EXPRESSION TAG	UNP Q86UT6
C	988	GLY	-	EXPRESSION TAG	UNP Q86UT6
C	989	ALA	-	EXPRESSION TAG	UNP Q86UT6
C	990	GLY	-	EXPRESSION TAG	UNP Q86UT6
C	991	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	992	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	993	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	994	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	995	HIS	-	EXPRESSION TAG	UNP Q86UT6
C	996	HIS	-	EXPRESSION TAG	UNP Q86UT6

- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

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

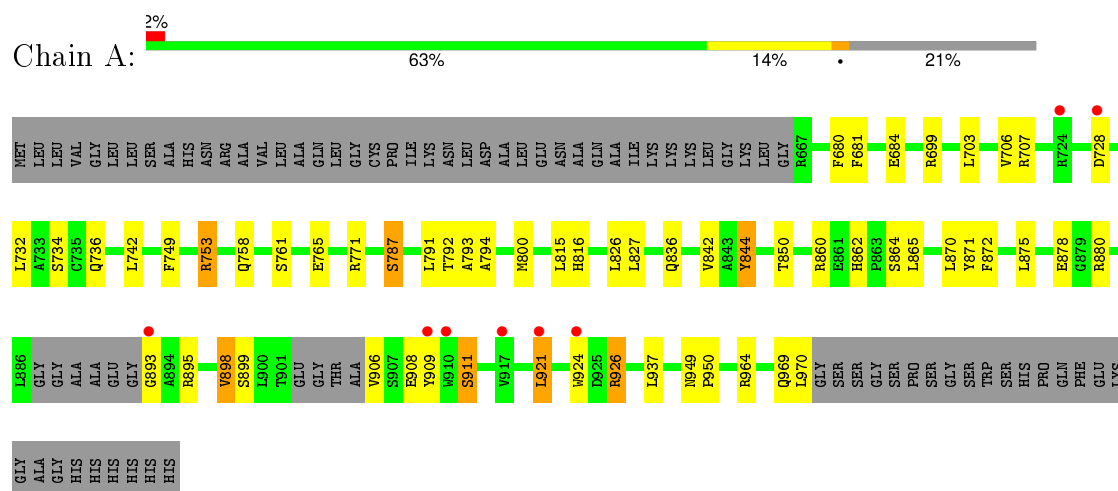
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0

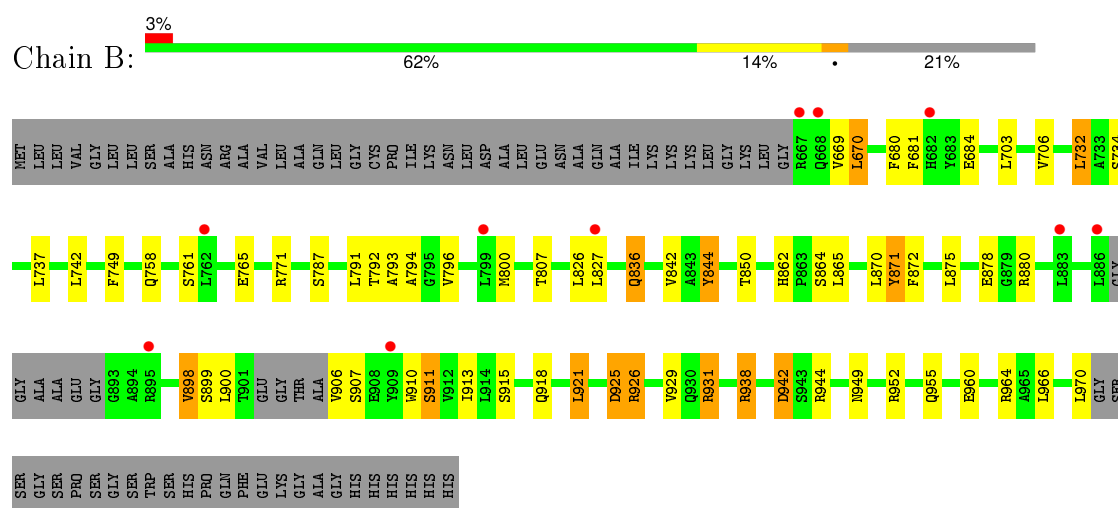
3 Residue-property plots

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 ($RSRZ > 2$). 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.

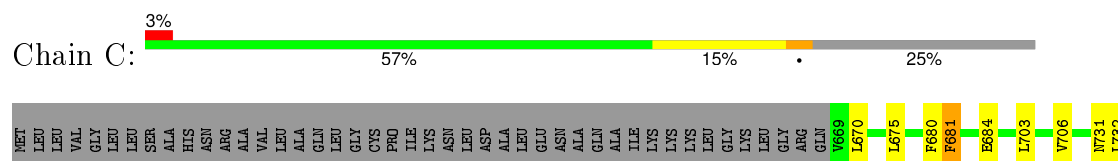
• Molecule 1: NLR family member X1

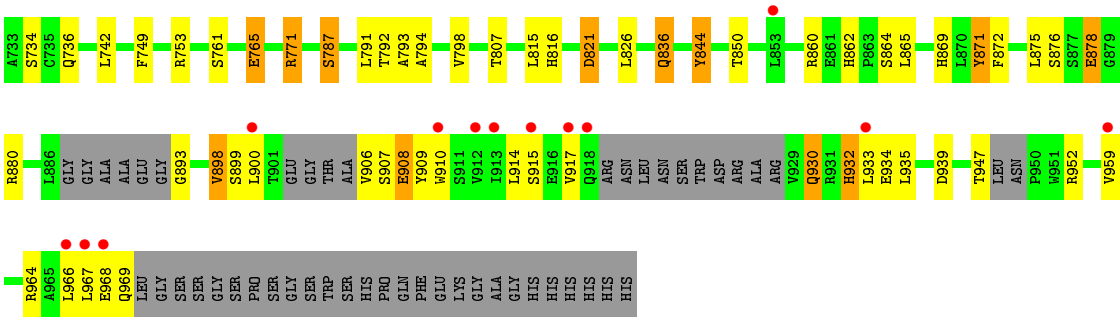


• Molecule 1: NLR family member X1



• Molecule 1: NLR family member X1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.01Å 123.47Å 145.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.24 – 2.65 77.24 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.8 (77.24-2.65) 97.9 (77.24-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.267 0.217 , 0.258	Depositor DCC
R_{free} test set	1311 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25759 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.80	2/2308 (0.1%)	0.85	1/3131 (0.0%)
1	B	0.73	2/2330 (0.1%)	0.76	2/3160 (0.1%)
1	C	0.93	9/2127 (0.4%)	0.80	0/2889
All	All	0.82	13/6765 (0.2%)	0.80	3/9180 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	871	TYR	CE2-CZ	-11.47	1.23	1.38
1	C	871	TYR	CE1-CZ	-9.55	1.26	1.38
1	C	871	TYR	CG-CD1	-9.39	1.26	1.39
1	C	871	TYR	CG-CD2	-9.20	1.27	1.39
1	C	681	PHE	CE2-CZ	-8.96	1.20	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	895	ARG	N-CA-CB	-6.57	98.77	110.60
1	B	670	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	737	LEU	CB-CG-CD2	-5.20	102.16	111.00

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	2277	0	2311	35	0
1	B	2293	0	2329	39	0
1	C	2097	0	2075	45	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	6679	0	6715	113	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 113 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:791:LEU:O	1:C:792:THR:HB	1.58	1.03
1:B:938:ARG:HH11	1:B:938:ARG:HG3	1.25	1.00
1:C:731:ASN:ND2	1:C:969:GLN:HG2	1.79	0.96
1:C:731:ASN:HD21	1:C:969:GLN:HG2	1.32	0.95
1:B:925:ASP:O	1:B:929:VAL:HG23	1.67	0.94

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	288/372 (77%)	275 (96%)	13 (4%)	0	100	100
1	B	290/372 (78%)	280 (97%)	9 (3%)	1 (0%)	46	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	270/372 (73%)	251 (93%)	16 (6%)	3 (1%)	17	38
All	All	848/1116 (76%)	806 (95%)	38 (4%)	4 (0%)	34	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	930	GLN
1	B	925	ASP
1	C	908	GLU
1	C	933	LEU

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	244/303 (80%)	221 (91%)	23 (9%)	11	22
1	B	247/303 (82%)	221 (90%)	26 (10%)	8	17
1	C	217/303 (72%)	191 (88%)	26 (12%)	6	13
All	All	708/909 (78%)	633 (89%)	75 (11%)	8	17

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	826	LEU
1	B	911	SER
1	C	917	VAL
1	B	836	GLN
1	B	878	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	838	GLN

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Mol	Chain	Res	Type
1	B	862	HIS
1	C	838	GLN
1	A	969	GLN
1	C	780	GLN

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](#)

Of 4 ligands modelled in this entry, 4 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, 95th 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 ²)	Q<0.9
1	A	294/372 (79%)	-0.05	8 (2%) 58 56	40, 68, 105, 128	4 (1%)
1	B	294/372 (79%)	0.14	10 (3%) 49 47	50, 83, 123, 144	3 (1%)
1	C	279/372 (75%)	0.10	13 (4%) 35 33	44, 68, 144, 217	0
All	All	867/1116 (77%)	0.06	31 (3%) 46 45	40, 72, 128, 217	7 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	913	ILE	5.8
1	B	667	ARG	5.5
1	C	912	VAL	4.9
1	B	668	GLN	3.9
1	A	909	TYR	3.7

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, 95th 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(\AA^2)	Q<0.9
2	PT	A	1002	1/1	0.84	0.43	-	45,45,45,45	1
2	PT	B	1001	1/1	0.89	0.34	-	82,82,82,82	1
2	PT	C	1001	1/1	0.87	0.23	-	69,69,69,69	1
2	PT	A	1001	1/1	0.91	0.24	-	85,85,85,85	1

6.5 Other polymers [i](#)

There are no such residues in this entry.