



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 08:59 PM EST

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 Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

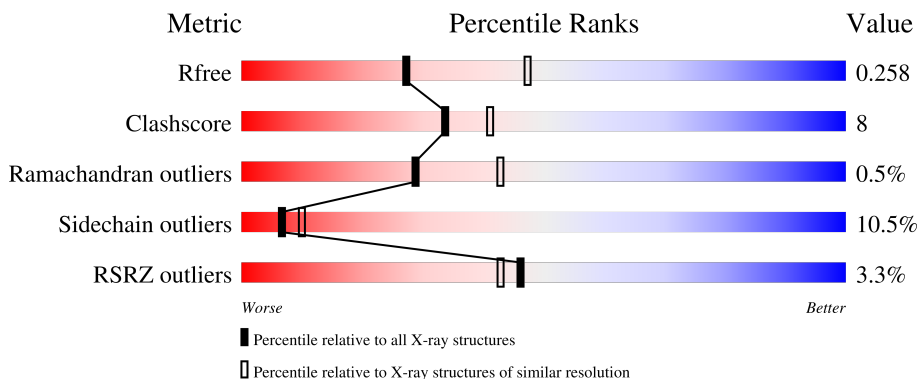
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

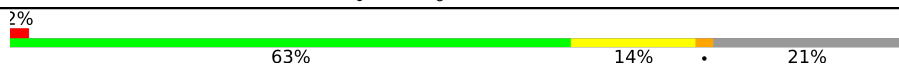
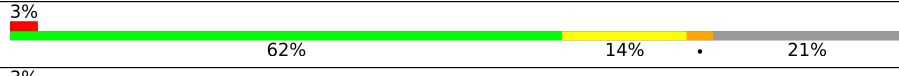

The reported resolution of this entry is 2.65 Å.

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))
$R_{free}$	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)

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 of 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	372	 2% 63% 14% 21%
1	B	372	 3% 62% 14% 21%
1	C	372	 3% 57% 15% 25%

## 2 Entry composition i

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
			Total	C	N	O	S			
1	A	294	2277	1426	424	421	6	17	0	0
1	B	294	2293	1436	425	426	6	11	2	0
1	C	279	2097	1317	381	393	6	0	1	0

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
C	980	TRP	-	expression tag	UNP Q86UT6
C	981	SER	-	expression tag	UNP Q86UT6
C	982	HIS	-	expression tag	UNP Q86UT6
C	983	PRO	-	expression tag	UNP Q86UT6
C	984	GLN	-	expression tag	UNP Q86UT6
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

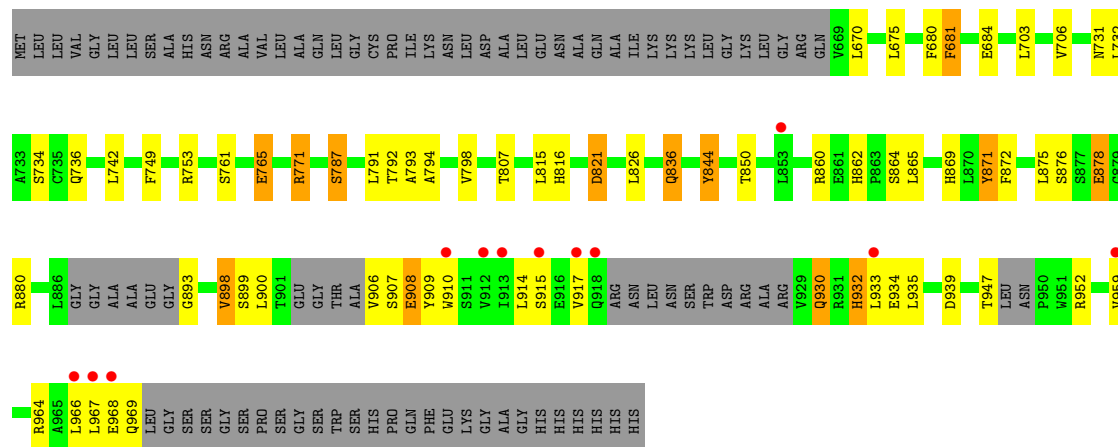
- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.65Å)	Xtrriage
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 (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage'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.*

<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: 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%)

All (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
1	C	681	PHE	CG-CD1	-7.64	1.27	1.38
1	C	681	PHE	CG-CD2	-6.94	1.28	1.38
1	C	681	PHE	CE1-CZ	-6.92	1.24	1.37
1	B	669	VAL	C-N	6.17	1.48	1.34
1	A	871	TYR	CE2-CZ	-5.82	1.30	1.38
1	C	765	GLU	CG-CD	5.35	1.59	1.51
1	B	871	TYR	CE2-CZ	-5.33	1.31	1.38
1	A	681	PHE	CE2-CZ	-5.09	1.27	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

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.

All (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
1:A:791:LEU:O	1:A:792:THR:HB	1.70	0.91
1:B:791:LEU:O	1:B:792:THR:HB	1.70	0.90
1:B:938:ARG:HH11	1:B:938:ARG:CG	1.89	0.84
1:B:949:ASN:HB3	1:B:952:ARG:HB2	1.62	0.82
1:C:742:LEU:HD23	1:C:749:PHE:HE2	1.45	0.81
1:C:934:GLU:HA	1:C:967:LEU:HD21	1.63	0.81
1:C:880:ARG:NH1	1:C:898:VAL:O	2.13	0.80
1:A:742:LEU:HD23	1:A:749:PHE:HE2	1.48	0.79
1:B:742:LEU:HD23	1:B:749:PHE:HE2	1.46	0.79
1:B:926:ARG:HG2	1:B:970:LEU:HD22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:871:TYR:CE2	1:C:900:LEU:HD13	2.21	0.76
1:A:862:HIS:HD2	1:A:864:SER:H	1.34	0.74
1:C:670:LEU:HD23	1:C:675:LEU:HA	1.70	0.74
1:B:938:ARG:HG3	1:B:938:ARG:NH1	2.02	0.71
1:B:931:ARG:HB2	1:B:931:ARG:HH11	1.56	0.70
1:C:860:ARG:HH21	1:C:893:GLY:HA2	1.58	0.67
1:A:800:MET:CE	1:A:827:LEU:HD23	2.24	0.67
1:B:862:HIS:HD2	1:B:864:SER:H	1.43	0.67
1:A:862:HIS:CD2	1:A:864:SER:H	2.13	0.67
1:B:862:HIS:CD2	1:B:864:SER:H	2.15	0.65
1:A:880:ARG:NH1	1:A:898:VAL:O	2.30	0.65
1:B:792:THR:HG22	1:B:794:ALA:N	2.14	0.63
1:A:753:ARG:CG	1:A:753:ARG:HH11	2.12	0.62
1:B:880:ARG:NH1	1:B:898:VAL:O	2.33	0.62
1:A:792:THR:CG2	1:A:793:ALA:N	2.63	0.62
1:C:862:HIS:HD2	1:C:864:SER:H	1.48	0.61
1:A:921:LEU:HD22	1:A:970:LEU:HD21	1.84	0.60
1:C:966:LEU:HA	1:C:969:GLN:HB3	1.83	0.59
1:A:921:LEU:HD12	1:A:969:GLN:HG2	1.85	0.59
1:B:960:GLU:O	1:B:964:ARG:HG3	2.01	0.58
1:B:862:HIS:HD2	1:B:865:LEU:H	1.52	0.58
1:C:907:SER:HB3	1:C:959:VAL:HG22	1.85	0.58
1:B:703:LEU:HB2	1:B:732:LEU:HD22	1.85	0.57
1:B:944:ARG:NH2	1:B:960:GLU:OE2	2.35	0.57
1:C:703:LEU:HB2	1:C:732:LEU:HD22	1.87	0.57
1:A:800:MET:HE3	1:A:827:LEU:HD23	1.86	0.57
1:C:792:THR:HG22	1:C:794:ALA:N	2.19	0.57
1:C:871:TYR:CD2	1:C:900:LEU:HD13	2.40	0.56
1:B:684:GLU:HG3	1:C:681:PHE:CD2	2.42	0.55
1:C:862:HIS:CD2	1:C:864:SER:H	2.24	0.55
1:A:926:ARG:HH21	1:C:736:GLN:HE22	1.55	0.55
1:B:792:THR:CG2	1:B:793:ALA:N	2.72	0.53
1:C:731:ASN:O	1:C:732:LEU:HD23	2.08	0.52
1:C:792:THR:CG2	1:C:793:ALA:N	2.72	0.52
1:A:703:LEU:HB2	1:A:732:LEU:HD22	1.91	0.52
1:C:910:TRP:O	1:C:914:LEU:N	2.37	0.51
1:B:862:HIS:CD2	1:B:865:LEU:H	2.29	0.51
1:C:871:TYR:OH	1:C:908:GLU:HB3	2.10	0.51
1:C:935:LEU:O	1:C:939:ASP:HB2	2.11	0.51
1:C:871:TYR:H	1:C:871:TYR:HD1	1.59	0.50
1:C:909:TYR:N	1:C:909:TYR:CD1	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:932:HIS:ND1	1:C:932:HIS:N	2.59	0.50
1:C:862:HIS:HD2	1:C:865:LEU:H	1.60	0.49
1:A:787:SER:HB3	1:A:815:LEU:HB3	1.95	0.49
1:C:907:SER:C	1:C:909:TYR:H	2.15	0.49
1:A:792:THR:HG22	1:A:794:ALA:N	2.27	0.49
1:A:684:GLU:HG3	1:B:681:PHE:CD1	2.48	0.48
1:C:791:LEU:O	1:C:792:THR:CB	2.43	0.48
1:C:906:VAL:HG13	1:C:959:VAL:HG21	1.95	0.48
1:A:908:GLU:HA	1:A:911:SER:HB3	1.96	0.48
1:B:842:VAL:HG23	1:B:870:LEU:HD23	1.95	0.48
1:A:792:THR:HG22	1:A:793:ALA:N	2.29	0.48
1:C:844:TYR:HA	1:C:872:PHE:O	2.13	0.47
1:B:910:TRP:O	1:B:911:SER:C	2.52	0.47
1:B:938:ARG:CG	1:B:938:ARG:NH1	2.59	0.47
1:C:909:TYR:N	1:C:909:TYR:HD1	2.13	0.47
1:A:860:ARG:HH21	1:A:893:GLY:HA2	1.79	0.47
1:B:907:SER:HB3	1:B:955:GLN:HB3	1.96	0.47
1:A:753:ARG:HH11	1:A:753:ARG:HG2	1.80	0.47
1:B:800:MET:CE	1:B:827:LEU:HD23	2.45	0.47
1:A:736:GLN:HE22	1:B:926:ARG:NH2	2.13	0.46
1:C:862:HIS:CD2	1:C:865:LEU:H	2.34	0.46
1:C:816:HIS:HA	1:C:844:TYR:O	2.16	0.46
1:B:871:TYR:CD1	1:B:900:LEU:HD11	2.50	0.46
1:C:907:SER:HB3	1:C:959:VAL:HG13	1.98	0.45
1:C:964:ARG:HA	1:C:967:LEU:HD12	1.99	0.45
1:A:842:VAL:HG23	1:A:870:LEU:HD23	1.99	0.45
1:A:862:HIS:HD2	1:A:865:LEU:H	1.65	0.45
1:A:736:GLN:NE2	1:B:926:ARG:NH2	2.64	0.44
1:B:844:TYR:HA	1:B:872:PHE:O	2.17	0.44
1:B:906:VAL:O	1:B:910:TRP:HD1	2.00	0.44
1:A:800:MET:CE	1:A:827:LEU:CD2	2.94	0.44
1:B:793:ALA:O	1:B:796:VAL:HG12	2.17	0.44
1:C:807:THR:O	1:C:836:GLN:HG3	2.17	0.44
1:C:869:HIS:HB3	1:C:871:TYR:HE1	1.83	0.44
1:A:862:HIS:CD2	1:A:865:LEU:H	2.35	0.44
1:B:807:THR:O	1:B:836:GLN:HG3	2.18	0.43
1:A:844:TYR:HA	1:A:872:PHE:O	2.17	0.43
1:A:937:LEU:HD11	1:A:964:ARG:NH1	2.33	0.43
1:C:907:SER:CB	1:C:959:VAL:HG13	2.49	0.43
1:A:753:ARG:HG2	1:A:753:ARG:NH1	2.34	0.43
1:B:921:LEU:HD22	1:B:970:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:ASN:HA	1:A:950:PRO:HD3	1.90	0.42
1:A:753:ARG:CG	1:A:753:ARG:NH1	2.77	0.42
1:C:876:SER:OG	1:C:878:GLU:HG2	2.19	0.42
1:B:792:THR:HG22	1:B:794:ALA:H	1.85	0.42
1:A:792:THR:HG23	1:A:793:ALA:N	2.34	0.41
1:C:771:ARG:HG3	1:C:798:VAL:O	2.21	0.41
1:A:707:ARG:HD2	1:B:926:ARG:NH2	2.36	0.41
1:B:942:ASP:N	1:B:942:ASP:OD1	2.54	0.41
1:B:681:PHE:CD1	1:B:681:PHE:C	2.95	0.41
1:B:918:GLN:HB2	1:B:966:LEU:HD21	2.04	0.40
1:A:816:HIS:HA	1:A:844:TYR:O	2.21	0.40
1:C:871:TYR:OH	1:C:908:GLU:CB	2.70	0.40
1:C:906:VAL:HG22	1:C:906:VAL:O	2.21	0.40
1:C:787:SER:HB3	1:C:815:LEU:HB3	2.03	0.40
1:A:699:ARG:O	1:A:728:ASP:N	2.55	0.40

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%)	41	56
1	C	270/372 (73%)	251 (93%)	16 (6%)	3 (1%)	14	21
All	All	848/1116 (76%)	806 (95%)	38 (4%)	4 (0%)	29	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	930	GLN
1	B	925	ASP

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Mol	Chain	Res	Type
1	C	908	GLU
1	C	933	LEU

### 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	244/303 (80%)	221 (91%)	23 (9%)	8	13
1	B	247/303 (82%)	221 (90%)	26 (10%)	7	10
1	C	217/303 (72%)	191 (88%)	26 (12%)	5	7
All	All	708/909 (78%)	633 (89%)	75 (11%)	7	10

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	680	PHE
1	A	706	VAL
1	A	734	SER
1	A	753	ARG
1	A	758	GLN
1	A	761	SER
1	A	765	GLU
1	A	771	ARG
1	A	787	SER
1	A	826	LEU
1	A	836	GLN
1	A	844	TYR
1	A	850	THR
1	A	875	LEU
1	A	878	GLU
1	A	898	VAL
1	A	899	SER
1	A	906	VAL
1	A	909	TYR
1	A	911	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	921	LEU
1	A	924	TRP
1	A	926	ARG
1	B	670	LEU
1	B	680	PHE
1	B	706	VAL
1	B	732	LEU
1	B	734	SER
1	B	758	GLN
1	B	761	SER
1	B	765	GLU
1	B	771	ARG
1	B	787	SER
1	B	826	LEU
1	B	836	GLN
1	B	844	TYR
1	B	850	THR
1	B	875	LEU
1	B	878	GLU
1	B	898	VAL
1	B	899	SER
1	B	911	SER
1	B	913	ILE
1	B	915	SER
1	B	921	LEU
1	B	926	ARG
1	B	931	ARG
1	B	938	ARG
1	B	942	ASP
1	C	680	PHE
1	C	684	GLU
1	C	706	VAL
1	C	734	SER
1	C	753	ARG
1	C	761	SER
1	C	765	GLU
1	C	771	ARG
1	C	787	SER
1	C	821[A]	ASP
1	C	821[B]	ASP
1	C	826	LEU
1	C	836	GLN

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Mol	Chain	Res	Type
1	C	844	TYR
1	C	850	THR
1	C	875	LEU
1	C	878	GLU
1	C	898	VAL
1	C	899	SER
1	C	915	SER
1	C	917	VAL
1	C	930	GLN
1	C	932	HIS
1	C	947	THR
1	C	952	ARG
1	C	968	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	736	GLN
1	A	780	GLN
1	A	838	GLN
1	A	862	HIS
1	A	918	GLN
1	A	969	GLN
1	B	838	GLN
1	B	862	HIS
1	B	918	GLN
1	B	969	GLN
1	C	736	GLN
1	C	780	GLN
1	C	838	GLN
1	C	862	HIS
1	C	930	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 monosaccharides 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

### 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	294/372 (79%)	-0.09	7 (2%) 59 54	40, 68, 105, 128	4 (1%)
1	B	294/372 (79%)	0.11	10 (3%) 45 41	50, 83, 123, 144	3 (1%)
1	C	279/372 (75%)	0.05	12 (4%) 35 31	44, 68, 144, 217	0
All	All	867/1116 (77%)	0.02	29 (3%) 46 43	40, 72, 128, 217	7 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	913	ILE	5.6
1	B	667	ARG	5.3
1	C	912	VAL	4.7
1	B	668	GLN	3.8
1	A	909	TYR	3.6
1	C	966	LEU	3.3
1	C	959	VAL	3.3
1	C	910	TRP	3.2
1	B	762	LEU	2.8
1	B	909	TYR	2.6
1	B	883	LEU	2.5
1	A	921	LEU	2.5
1	A	910	TRP	2.5
1	C	918	GLN	2.5
1	A	917	VAL	2.5
1	B	827	LEU	2.4
1	B	799	LEU	2.4
1	C	933	LEU	2.4
1	B	895	ARG	2.4
1	B	886	LEU	2.4
1	A	724	ARG	2.3
1	A	893	GLY	2.2
1	C	917	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	968	GLU	2.1
1	A	924	TRP	2.1
1	C	915	SER	2.1
1	B	682	HIS	2.0
1	C	967	LEU	2.0
1	C	853	LEU	2.0

## 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 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(Å <sup>2</sup> )	Q<0.9
2	PT	A	1002	1/1	0.84	0.43	45,45,45,45	1
2	PT	C	1001	1/1	0.87	0.23	69,69,69,69	1
2	PT	B	1001	1/1	0.89	0.34	82,82,82,82	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.