



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:31 PM GMT

PDB ID : 4RY3  
Title : Crystal structure of human Fanconi-associated nuclease 1  
Authors : Yan, P.X.; Huo, Y.G.; Jiang, T.  
Deposited on : 2014-12-13  
Resolution : 2.80 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  
<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

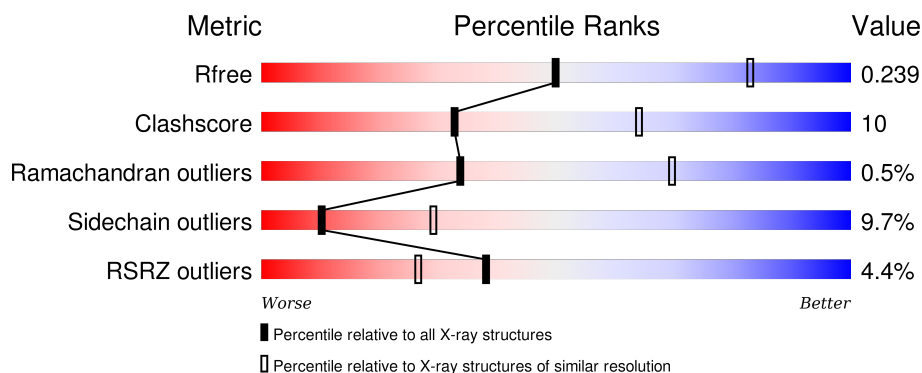
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	648	<div> <div>4%</div> <div>70%</div> <div>18%</div> <div>8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4775 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 Fanconi-associated nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4774	3043	852	856	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1011	GLY	-	EXPRESSION TAG	UNP Q9Y2M0
A	1012	SER	-	EXPRESSION TAG	UNP Q9Y2M0
A	1013	GLU	-	EXPRESSION TAG	UNP Q9Y2M0
A	1014	ASN	-	EXPRESSION TAG	UNP Q9Y2M0
A	1015	LEU	-	EXPRESSION TAG	UNP Q9Y2M0
A	1016	TYR	-	EXPRESSION TAG	UNP Q9Y2M0
A	1017	PHE	-	EXPRESSION TAG	UNP Q9Y2M0
A	1018	GLN	-	EXPRESSION TAG	UNP Q9Y2M0

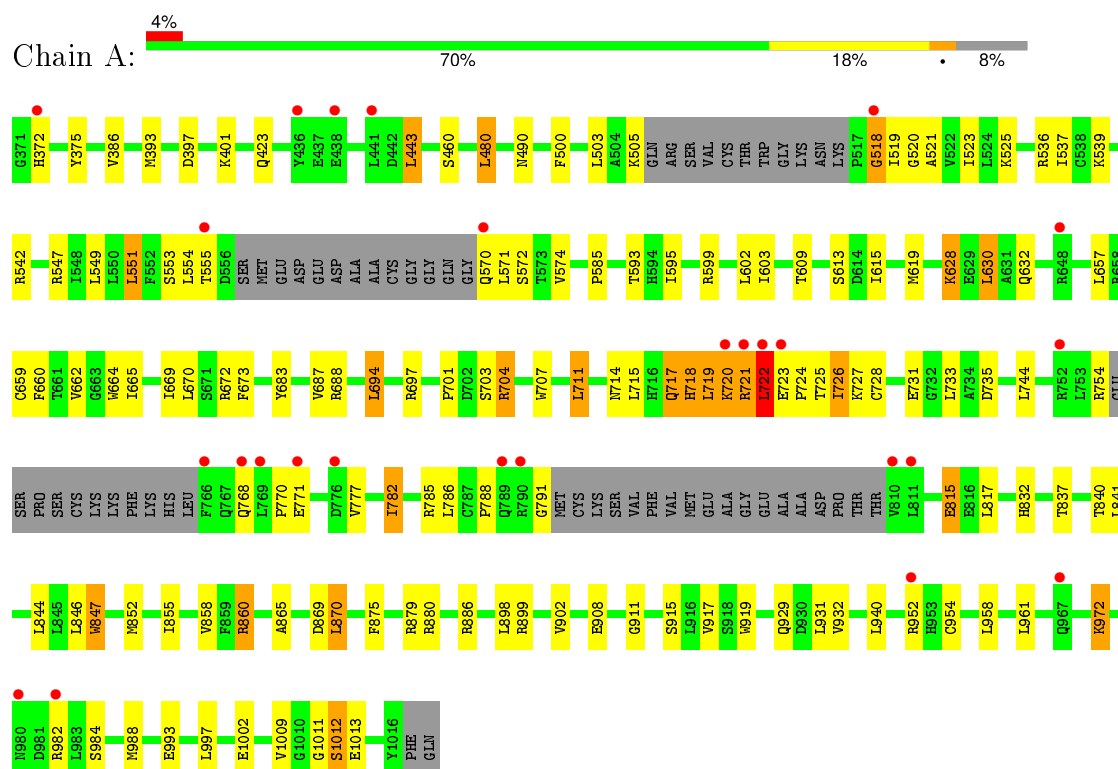
- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

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

### 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 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: Fanconi-associated nuclease 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.08Å 161.08Å 161.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.98-2.80) 96.6 (19.98-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.208 , 0.243 0.204 , 0.239	Depositor DCC
$R_{free}$ test set	1669 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34263 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, 0.375 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	0.45	0/4873	0.66	3/6589 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	719	LEU	CB-CA-C	11.24	131.56	110.20
1	A	518	GLY	N-CA-C	10.32	138.91	113.10
1	A	719	LEU	N-CA-C	-8.74	87.39	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	4774	0	4809	100	0
2	A	1	0	0	0	0
All	All	4775	0	4809	100	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 10.

All (100) 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:A:721:ARG:O	1:A:724:PRO:HD2	1.17	1.32
1:A:717:GLN:O	1:A:718:HIS:ND1	1.72	1.19
1:A:717:GLN:C	1:A:718:HIS:ND1	1.99	1.16
1:A:683:TYR:CG	1:A:718:HIS:HD2	1.77	1.02
1:A:721:ARG:O	1:A:724:PRO:CD	2.11	0.98
1:A:683:TYR:CD1	1:A:718:HIS:HD2	1.86	0.94
1:A:683:TYR:CG	1:A:718:HIS:CD2	2.63	0.87
1:A:715:LEU:HB3	1:A:725:THR:HG22	1.56	0.86
1:A:715:LEU:O	1:A:719:LEU:O	1.95	0.83
1:A:932:VAL:HG22	1:A:940:LEU:HD11	1.64	0.79
1:A:683:TYR:CD2	1:A:718:HIS:CD2	2.73	0.76
1:A:628:LYS:HE3	1:A:632:GLN:HE22	1.51	0.75
1:A:683:TYR:CD1	1:A:718:HIS:CD2	2.75	0.73
1:A:785:ARG:HD2	1:A:1011:GLY:HA3	1.71	0.72
1:A:714:ASN:O	1:A:718:HIS:HB2	1.90	0.70
1:A:549:LEU:HD21	1:A:572:SER:HB2	1.77	0.66
1:A:721:ARG:HG2	1:A:724:PRO:HD3	1.77	0.65
1:A:722:LEU:HD23	1:A:722:LEU:H	1.61	0.65
1:A:704:ARG:NH1	1:A:735:ASP:OD2	2.33	0.62
1:A:375:TYR:CE1	1:A:423:GLN:HG2	2.35	0.62
1:A:480:LEU:HB3	1:A:500:PHE:CZ	2.35	0.62
1:A:865:ALA:HB1	1:A:915:SER:HA	1.83	0.60
1:A:555:THR:HG22	1:A:660:PHE:HE1	1.67	0.59
1:A:630:LEU:HD12	1:A:630:LEU:H	1.67	0.59
1:A:701:PRO:O	1:A:704:ARG:HG2	2.03	0.58
1:A:537:ILE:HD11	1:A:542:ARG:HH11	1.68	0.58
1:A:723:GLU:N	1:A:724:PRO:CD	2.67	0.57
1:A:815:GLU:HG3	1:A:832:HIS:CE1	2.40	0.57
1:A:704:ARG:HH11	1:A:704:ARG:HB3	1.71	0.55
1:A:844:LEU:HD13	1:A:902:VAL:HG13	1.87	0.55
1:A:659:CYS:HA	1:A:664:TRP:CD2	2.41	0.55
1:A:972:LYS:NZ	1:A:1002:GLU:OE2	2.39	0.55
1:A:519:ILE:HG23	1:A:520:GLY:N	2.22	0.54
1:A:721:ARG:C	1:A:723:GLU:H	2.10	0.53
1:A:683:TYR:CE2	1:A:718:HIS:CD2	2.96	0.53
1:A:683:TYR:CE1	1:A:718:HIS:CD2	2.98	0.52
1:A:553:SER:O	1:A:553:SER:OG	2.26	0.51
1:A:721:ARG:N	1:A:721:ARG:HD3	2.25	0.51
1:A:659:CYS:HA	1:A:664:TRP:CG	2.46	0.51
1:A:595:ILE:HD11	1:A:657:LEU:HD22	1.93	0.51
1:A:703:SER:O	1:A:707:TRP:CD2	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:GLY:HA2	1:A:919:TRP:CE3	2.46	0.50
1:A:503:LEU:HD23	1:A:523:ILE:HD11	1.94	0.50
1:A:593:THR:O	1:A:860:ARG:NH2	2.45	0.50
1:A:721:ARG:HG2	1:A:724:PRO:CD	2.41	0.49
1:A:599:ARG:O	1:A:603:ILE:HG12	2.13	0.49
1:A:619:MET:HE3	1:A:672:ARG:HB3	1.95	0.49
1:A:984:SER:O	1:A:988:MET:HG3	2.13	0.48
1:A:615:ILE:HG12	1:A:630:LEU:HD13	1.95	0.48
1:A:869:ASP:O	1:A:875:PHE:HB2	2.14	0.48
1:A:571:LEU:HD11	1:A:613:SER:OG	2.14	0.47
1:A:547:ARG:HD2	1:A:602:LEU:HG	1.95	0.47
1:A:386:VAL:HG12	1:A:393:MET:CE	2.45	0.47
1:A:518:GLY:O	1:A:521:ALA:HB3	2.15	0.46
1:A:397:ASP:O	1:A:401:LYS:HG3	2.15	0.46
1:A:386:VAL:HG12	1:A:393:MET:HE3	1.98	0.45
1:A:519:ILE:CG2	1:A:520:GLY:N	2.79	0.45
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.71	0.45
1:A:782:ILE:HD12	1:A:782:ILE:HA	1.79	0.45
1:A:846:LEU:HD13	1:A:886:ARG:HG2	1.98	0.45
1:A:869:ASP:OD2	1:A:879:ARG:NH2	2.49	0.45
1:A:480:LEU:HB3	1:A:500:PHE:HZ	1.82	0.45
1:A:694:LEU:HD13	1:A:707:TRP:HE3	1.82	0.45
1:A:898:LEU:HB3	1:A:932:VAL:HG13	1.99	0.44
1:A:1012:SER:O	1:A:1012:SER:OG	2.33	0.44
1:A:723:GLU:N	1:A:724:PRO:HD2	2.32	0.44
1:A:726:ILE:HD13	1:A:726:ILE:H	1.83	0.44
1:A:717:GLN:O	1:A:718:HIS:CE1	2.60	0.44
1:A:898:LEU:HB3	1:A:932:VAL:CG1	2.47	0.44
1:A:554:LEU:HB3	1:A:660:PHE:CD1	2.53	0.44
1:A:714:ASN:O	1:A:718:HIS:CB	2.64	0.44
1:A:899:ARG:HG2	1:A:929:GLN:HB3	1.98	0.44
1:A:665:ILE:O	1:A:669:ILE:HG12	2.18	0.44
1:A:694:LEU:HA	1:A:694:LEU:HD12	1.82	0.43
1:A:723:GLU:HB3	1:A:724:PRO:HD3	1.99	0.43
1:A:852:MET:SD	1:A:879:ARG:HG2	2.58	0.43
1:A:518:GLY:O	1:A:521:ALA:N	2.43	0.43
1:A:768:GLN:CD	1:A:768:GLN:H	2.22	0.43
1:A:554:LEU:HD13	1:A:554:LEU:HA	1.85	0.43
1:A:720:LYS:HA	1:A:721:ARG:HA	1.56	0.43
1:A:840:THR:HG23	1:A:917:VAL:HG13	2.00	0.43
1:A:718:HIS:ND1	1:A:718:HIS:N	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:LEU:HA	1:A:870:LEU:HD23	1.86	0.43
1:A:549:LEU:HD11	1:A:574:VAL:HG11	2.01	0.43
1:A:717:GLN:HB2	1:A:718:HIS:CE1	2.53	0.42
1:A:788:PRO:HG2	1:A:791:GLY:O	2.19	0.42
1:A:443:LEU:HA	1:A:443:LEU:HD12	1.77	0.42
1:A:683:TYR:CZ	1:A:718:HIS:CD2	3.08	0.42
1:A:714:ASN:O	1:A:718:HIS:N	2.53	0.42
1:A:721:ARG:H	1:A:721:ARG:HD3	1.84	0.42
1:A:952:ARG:HD3	1:A:952:ARG:HA	1.92	0.42
1:A:954:CYS:O	1:A:958:LEU:HG	2.20	0.42
1:A:727:LYS:O	1:A:731:GLU:HG2	2.19	0.41
1:A:585:PRO:HB3	1:A:847:TRP:CH2	2.55	0.41
1:A:670:LEU:O	1:A:673:PHE:HB3	2.20	0.41
1:A:721:ARG:O	1:A:723:GLU:N	2.54	0.41
1:A:993:GLU:O	1:A:997:LEU:HG	2.21	0.41
1:A:940:LEU:HA	1:A:940:LEU:HD23	1.89	0.40
1:A:687:VAL:HG13	1:A:711:LEU:HD21	2.04	0.40
1:A:551:LEU:HA	1:A:551:LEU:HD12	1.95	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	583/648 (90%)	552 (95%)	28 (5%)	3 (0%)	34 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	722	LEU
1	A	770	PRO
1	A	372	HIS

### 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	518/563 (92%)	468 (90%)	50 (10%)	10	29

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	LEU
1	A	460	SER
1	A	480	LEU
1	A	490	ASN
1	A	505	LYS
1	A	525	LYS
1	A	536	ARG
1	A	539	LYS
1	A	551	LEU
1	A	570	GLN
1	A	609	THR
1	A	628	LYS
1	A	630	LEU
1	A	662	VAL
1	A	688	ARG
1	A	694	LEU
1	A	697	ARG
1	A	704	ARG
1	A	711	LEU
1	A	717	GLN
1	A	718	HIS
1	A	720	LYS
1	A	721	ARG
1	A	722	LEU
1	A	726	ILE
1	A	728	CYS
1	A	733	LEU
1	A	744	LEU
1	A	754	ARG
1	A	771	GLU

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Mol	Chain	Res	Type
1	A	777	VAL
1	A	782	ILE
1	A	786	LEU
1	A	815	GLU
1	A	817	LEU
1	A	837	THR
1	A	847	TRP
1	A	855	ILE
1	A	858	VAL
1	A	860	ARG
1	A	870	LEU
1	A	880	ARG
1	A	908	GLU
1	A	931	LEU
1	A	961	LEU
1	A	972	LYS
1	A	982	ARG
1	A	1009	VAL
1	A	1012	SER
1	A	1013	GLU

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	621	ASN
1	A	717	GLN
1	A	718	HIS
1	A	832	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 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 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	593/648 (91%)	-0.26	26 (4%) 38 26	13, 43, 95, 129	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	HIS	5.1
1	A	790	ARG	4.9
1	A	570	GLN	4.4
1	A	811	LEU	4.2
1	A	721	ARG	4.1
1	A	766	PHE	4.0
1	A	436	TYR	4.0
1	A	982	ARG	3.6
1	A	720	LYS	3.5
1	A	980	ASN	3.2
1	A	722	LEU	3.1
1	A	789	GLN	2.8
1	A	771	GLU	2.7
1	A	441	LEU	2.7
1	A	723	GLU	2.7
1	A	555	THR	2.4
1	A	967	GLN	2.3
1	A	952	ARG	2.3
1	A	768	GLN	2.2
1	A	776	ASP	2.1
1	A	518	GLY	2.1
1	A	648	ARG	2.1
1	A	810	VAL	2.1
1	A	752	ARG	2.1
1	A	438	GLU	2.0
1	A	769	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 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( $\text{\AA}^2$ )	Q<0.9
2	PT	A	1101	1/1	0.99	0.05	-1.18	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.