



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:43 AM UTC

PDB ID : 4RY3 / pdb_00004ry3
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

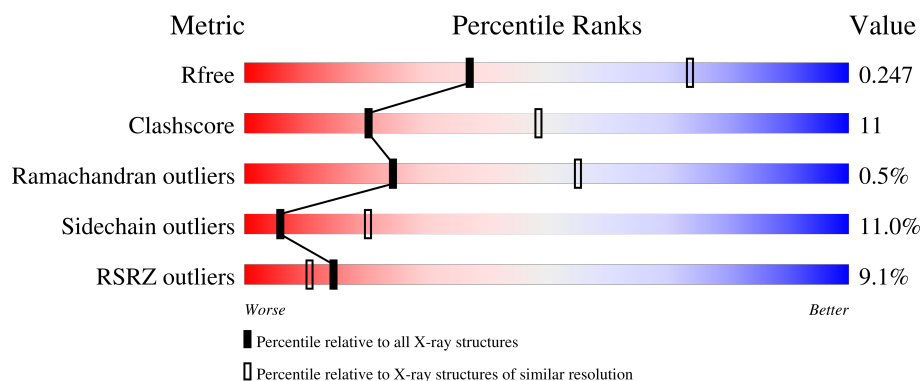
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	648	8% 68% 19% • 8%

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

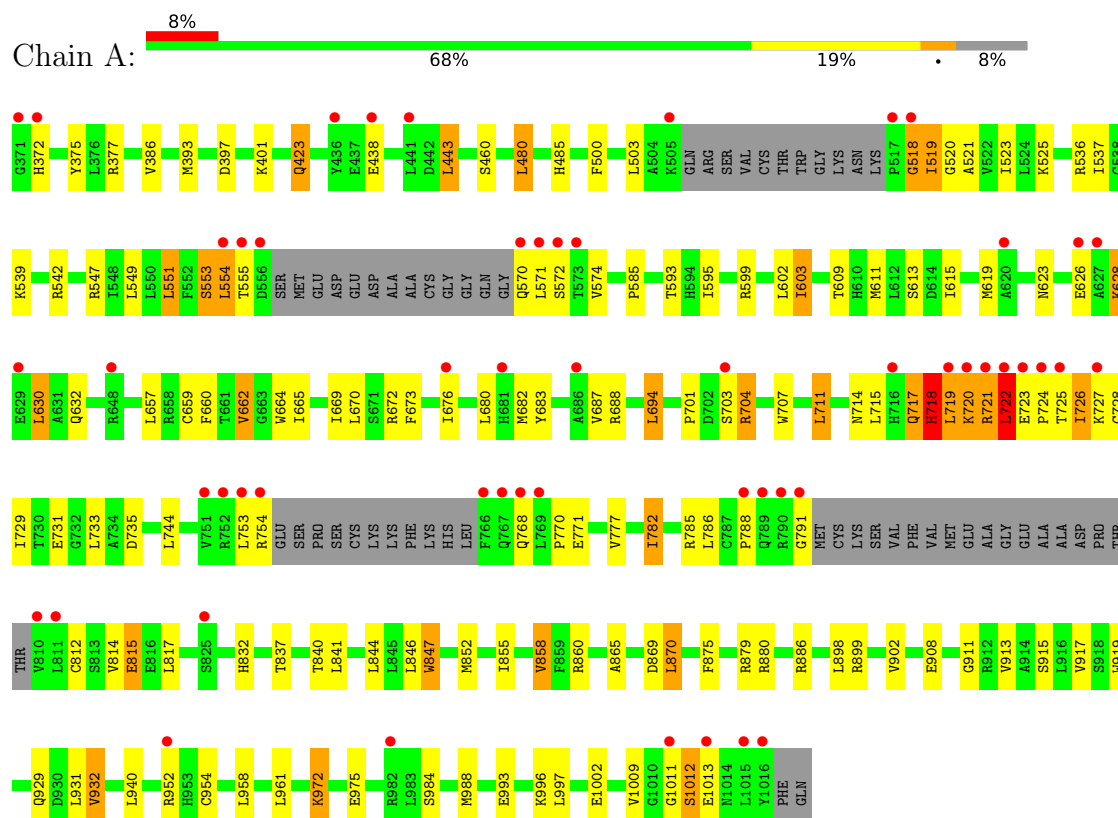
- Molecule 2 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Fanconi-associated nuclease 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	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) 96.3 (19.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.208 , 0.243 0.213 , 0.247	Depositor DCC
R_{free} test set	1727 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4775	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.54	0/4873	0.96	18/6589 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	LEU	CB-CA-C	11.30	131.56	110.10
1	A	518	GLY	N-CA-C	10.85	138.91	113.18
1	A	718	HIS	N-CA-C	9.56	121.69	110.41
1	A	719	LEU	N-CA-C	-8.43	87.39	111.00
1	A	812	CYS	N-CA-C	7.83	118.95	108.38
1	A	719	LEU	CA-C-N	7.50	131.36	120.71
1	A	719	LEU	C-N-CA	7.50	131.36	120.71
1	A	554	LEU	N-CA-C	6.35	117.86	111.07
1	A	518	GLY	CA-C-N	6.20	128.59	120.60
1	A	518	GLY	C-N-CA	6.20	128.59	120.60
1	A	662	VAL	CB-CA-C	-5.93	104.29	111.88
1	A	718	HIS	CA-C-N	5.83	132.19	121.70
1	A	718	HIS	C-N-CA	5.83	132.19	121.70
1	A	603	ILE	CB-CA-C	-5.44	104.73	111.70
1	A	662	VAL	N-CA-C	5.23	115.85	110.36
1	A	858	VAL	CB-CA-C	5.17	115.61	111.06
1	A	485	HIS	N-CA-C	5.16	118.56	111.54
1	A	553	SER	CB-CA-C	-5.16	105.04	111.43

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	4774	0	4809	107	0
2	A	1	0	0	0	0
All	All	4775	0	4809	107	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 11.

All (107) 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:C	1:A:718:HIS:ND1	1.99	1.21
1:A:717:GLN:O	1:A:718:HIS:ND1	1.72	1.19
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:619:MET:HE1	1:A:672:ARG:HB3	1.63	0.80
1:A:932:VAL:HG22	1:A:940:LEU:HD11	1.64	0.79
1:A:615:ILE:HG22	1:A:619:MET:HE3	1.68	0.76
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:386:VAL:HG12	1:A:393:MET:HE3	1.80	0.61
1:A:865:ALA:HB1	1:A:915:SER:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:THR:HG22	1:A:660:PHE:HE1	1.67	0.59
1:A:630:LEU:H	1:A:630:LEU:HD12	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:721:ARG:C	1:A:723:GLU:H	2.10	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:HB3	1:A:704:ARG:HH11	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: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:721:ARG:N	1:A:721:ARG:HD3	2.25	0.51
1:A:595:ILE:HD11	1:A:657:LEU:HD22	1.93	0.51
1:A:659:CYS:HA	1:A:664:TRP:CG	2.46	0.51
1:A:703:SER:O	1:A:707:TRP:CD2	2.63	0.50
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:599:ARG:O	1:A:603:ILE:HG12	2.13	0.49
1:A:721:ARG:HG2	1:A:724:PRO:CD	2.41	0.49
1:A:984:SER:O	1:A:988:MET:HG3	2.13	0.48
1:A:619:MET:HE2	1:A:676:ILE:HD11	1.95	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:768:GLN:H	1:A:768:GLN:CD	2.22	0.47
1:A:547:ARG:HD2	1:A:602:LEU:HG	1.95	0.47
1:A:571:LEU:HD11	1:A:613:SER:OG	2.14	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:553:SER:O	1:A:553:SER:OG	2.26	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:680:LEU:HB3	1:A:682:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:ARG:C	1:A:723:GLU:N	2.73	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:H	1:A:726:ILE:HD13	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:665:ILE:O	1:A:669:ILE:HG12	2.18	0.44
1:A:899:ARG:HG2	1:A:929:GLN:HB3	1.98	0.44
1:A:386:VAL:HG12	1:A:393:MET:CE	2.45	0.44
1:A:694:LEU:HD12	1:A:694:LEU:HA	1.82	0.43
1:A:619:MET:HE2	1:A:676:ILE:HG12	2.00	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: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
1:A:623:ASN:HB3	1:A:626:GLU:CD	2.43	0.43
1:A:870:LEU:HD23	1:A:870:LEU:HA	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:HD12	1:A:443:LEU:HA	1.77	0.42
1:A:619:MET:HE2	1:A:676:ILE:CG1	2.50	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:HD3	1:A:721:ARG:H	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:585:PRO:HB3	1:A:847:TRP:CH2	2.55	0.41
1:A:727:LYS:O	1:A:731:GLU:HG2	2.19	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:HD23	1:A:940:LEU:HA	1.89	0.40
1:A:687:VAL:HG13	1:A:711:LEU:HD21	2.04	0.40
1:A:551:LEU:HD12	1:A:551:LEU:HA	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%)	24 55

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 [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	518/563 (92%)	461 (89%)	57 (11%)	6 20

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	ARG
1	A	423	GLN
1	A	438	GLU
1	A	443	LEU
1	A	460	SER

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Mol	Chain	Res	Type
1	A	480	LEU
1	A	519	ILE
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	611	MET
1	A	628	LYS
1	A	630	LEU
1	A	662	VAL
1	A	688	ARG
1	A	694	LEU
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	729	ILE
1	A	733	LEU
1	A	744	LEU
1	A	753	LEU
1	A	754	ARG
1	A	771	GLU
1	A	777	VAL
1	A	782	ILE
1	A	786	LEU
1	A	814	VAL
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	870	LEU
1	A	880	ARG
1	A	908	GLU

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Mol	Chain	Res	Type
1	A	913	VAL
1	A	931	LEU
1	A	932	VAL
1	A	961	LEU
1	A	972	LYS
1	A	975	GLU
1	A	996	LYS
1	A	1009	VAL
1	A	1012	SER
1	A	1013	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	A	623	ASN
1	A	717	GLN
1	A	718	HIS
1	A	742	HIS
1	A	995	GLN

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 oligosaccharides 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, 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	593/648 (91%)	0.06	54 (9%) 15 11	13, 43, 95, 129	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	570	GLN	8.5
1	A	571	LEU	7.1
1	A	720	LYS	6.6
1	A	555	THR	5.4
1	A	719	LEU	5.2
1	A	517	PRO	5.2
1	A	769	LEU	5.0
1	A	441	LEU	4.7
1	A	766	PHE	4.5
1	A	722	LEU	4.5
1	A	721	ARG	4.5
1	A	767	GLN	4.5
1	A	518	GLY	4.4
1	A	754	ARG	4.4
1	A	753	LEU	4.1
1	A	811	LEU	4.0
1	A	810	VAL	3.9
1	A	372	HIS	3.9
1	A	572	SER	3.8
1	A	723	GLU	3.7
1	A	1015	LEU	3.6
1	A	791	GLY	3.5
1	A	727	LYS	3.4
1	A	371	GLY	3.3
1	A	790	ARG	3.2
1	A	825	SER	3.1
1	A	626	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	752	ARG	2.9
1	A	648	ARG	2.8
1	A	952	ARG	2.8
1	A	982	ARG	2.8
1	A	436	TYR	2.8
1	A	629	GLU	2.7
1	A	768	GLN	2.7
1	A	1016	TYR	2.7
1	A	627	ALA	2.6
1	A	716	HIS	2.6
1	A	505	LYS	2.6
1	A	620	ALA	2.6
1	A	686	ALA	2.6
1	A	573	THR	2.5
1	A	554	LEU	2.5
1	A	1013	GLU	2.5
1	A	1011	GLY	2.4
1	A	724	PRO	2.4
1	A	789	GLN	2.4
1	A	751	VAL	2.3
1	A	788	PRO	2.3
1	A	438	GLU	2.2
1	A	556	ASP	2.2
1	A	703	SER	2.2
1	A	676	ILE	2.1
1	A	725	THR	2.0
1	A	681	HIS	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PT	A	1101	1/1	0.99	0.08	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.