



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:55 AM UTC

PDB ID : 4RIC / pdb_00004ric
Title : FAN1 Nuclease bound to 5' hydroxyl (dT-dT) single flap DNA
Authors : Pavletich, N.P.; Wang, R.
Deposited on : 2014-10-05
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

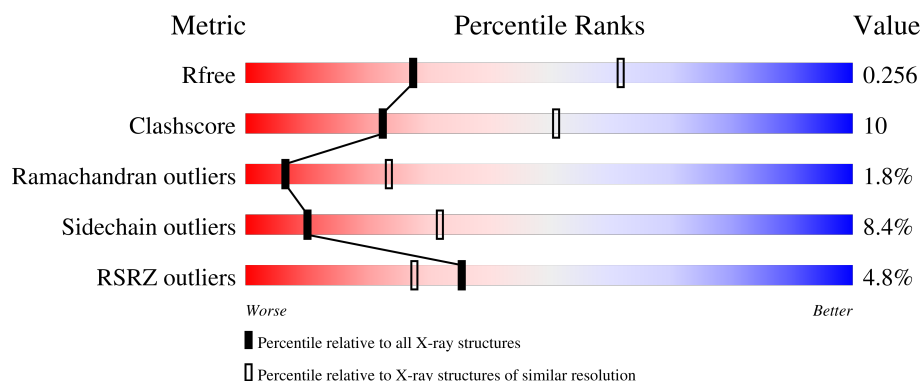
1 Overall quality at a glance

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	631	4% 68% 25% • •
1	B	631	5% 68% 28% •
2	U	21	5% 57% 38% 5%
2	X	21	5% 67% 29% 5%
3	V	12	17% 83% 17%

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Mol	Chain	Length	Quality of chain
3	Y	12	 67% 33%
4	T	14	 21% 29% 50%
4	W	14	 43% 7% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11571 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	615	Total	C	N	O	S	0	0	0
			4942	3145	880	890	27			
1	B	628	Total	C	N	O	S	0	0	0
			5035	3199	897	912	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	deletion	UNP Q9Y2M0
A	?	-	THR	deletion	UNP Q9Y2M0
A	?	-	TRP	deletion	UNP Q9Y2M0
A	?	-	GLY	deletion	UNP Q9Y2M0
A	?	-	LYS	deletion	UNP Q9Y2M0
A	?	-	ASN	deletion	UNP Q9Y2M0
A	?	-	LYS	deletion	UNP Q9Y2M0
A	?	-	PRO	deletion	UNP Q9Y2M0
A	?	-	GLY	deletion	UNP Q9Y2M0
B	?	-	CYS	deletion	UNP Q9Y2M0
B	?	-	THR	deletion	UNP Q9Y2M0
B	?	-	TRP	deletion	UNP Q9Y2M0
B	?	-	GLY	deletion	UNP Q9Y2M0
B	?	-	LYS	deletion	UNP Q9Y2M0
B	?	-	ASN	deletion	UNP Q9Y2M0
B	?	-	LYS	deletion	UNP Q9Y2M0
B	?	-	PRO	deletion	UNP Q9Y2M0
B	?	-	GLY	deletion	UNP Q9Y2M0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	20	Total	C	N	O	P	0	0	0
			401	191	70	120	20			
2	U	20	Total	C	N	O	P	0	0	0
			401	191	70	120	20			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*TP*GP*AP*GP*GP*AP*GP*TP*CP*T)-3').

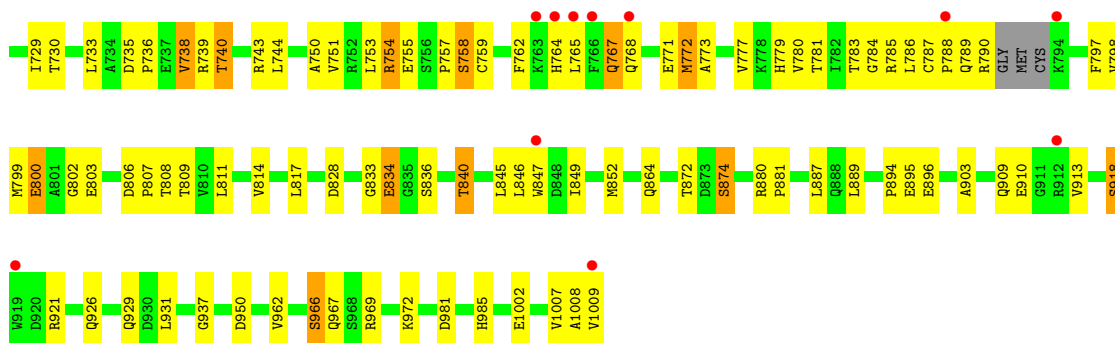
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	12	Total	C	N	O	P	0	0	0
			247	118	47	71	11			
3	V	12	Total	C	N	O	P	0	0	0
			247	118	47	71	11			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*GP*AP*GP*GP*CP*GP*TP*G)-3').

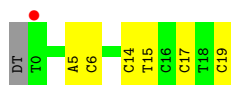
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	W	7	Total	C	N	O	P	0	0	0
			148	69	30	42	7			
4	T	7	Total	C	N	O	P	0	0	0
			148	69	30	42	7			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

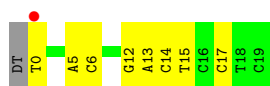
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		



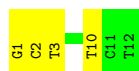
- Molecule 2: DNA (5'-D(*TP*TP*AP*GP*CP*CP*AP*CP*GP*CP*CP*TP*AP*GP*AP*CP*TP*CP*CP*TP*C)-3')



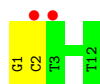
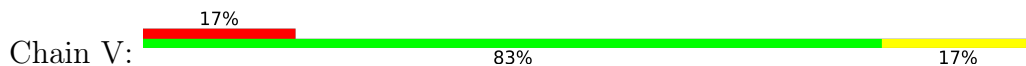
- Molecule 2: DNA (5'-D(*TP*TP*AP*GP*CP*CP*AP*CP*GP*CP*CP*TP*AP*GP*AP*CP*TP*CP*CP*TP*C)-3')



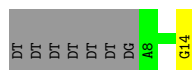
- Molecule 3: DNA (5'-D(*GP*CP*TP*GP*AP*GP*GP*AP*GP*TP*CP*T)-3')



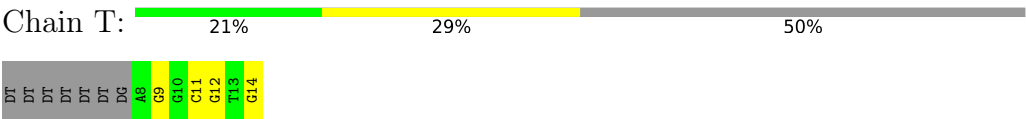
- Molecule 3: DNA (5'-D(*GP*CP*TP*GP*AP*GP*GP*AP*GP*TP*CP*T)-3')



- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*GP*AP*GP*GP*CP*GP*TP*G)-3')



- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*GP*AP*GP*GP*CP*GP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.70Å 110.99Å 105.43Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.80) 94.4 (50.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.223 , 0.257 0.226 , 0.256	Depositor DCC
R_{free} test set	2177 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11571	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: CA

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	0.63	0/5044	0.95	4/6818 (0.1%)
1	B	0.61	0/5140	0.94	6/6952 (0.1%)
2	U	0.37	0/447	0.72	0/685
2	X	0.38	0/447	0.85	0/685
3	V	0.37	0/277	0.80	0/427
3	Y	0.36	0/277	0.82	0/427
4	T	0.41	0/166	0.79	1/255 (0.4%)
4	W	0.45	0/166	0.81	0/255
All	All	0.59	0/11964	0.92	11/16504 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	570	GLN	N-CA-C	7.72	119.52	110.41
1	A	861	ASN	N-CA-C	5.99	116.15	108.24
1	B	787	CYS	CA-C-N	5.78	127.07	119.84
1	B	787	CYS	C-N-CA	5.78	127.07	119.84
1	B	674	VAL	N-CA-CB	5.67	117.19	110.55
1	B	806	ASP	N-CA-C	5.67	113.33	108.22
1	A	554	LEU	N-CA-C	-5.55	105.31	111.36
1	A	961	LEU	N-CA-C	5.38	118.01	109.50
1	A	508	SER	N-CA-C	5.19	117.61	111.33
4	T	9	DG	C2'-C3'-O3'	-5.09	103.87	111.50
1	B	562	ASP	N-CA-C	5.01	117.47	109.96

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	4942	0	4975	110	1
1	B	5035	0	5059	116	2
2	U	401	0	225	6	0
2	X	401	0	225	6	0
3	V	247	0	137	1	0
3	Y	247	0	137	3	0
4	T	148	0	79	3	0
4	W	148	0	79	0	1
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	11571	0	10916	236	2

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 (236) 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:B:426:LEU:HD13	1:B:537:ILE:HG22	1.40	1.02
1:A:836:SER:O	1:A:840:THR:HG23	1.61	1.00
1:A:426:LEU:HD13	1:A:537:ILE:HG22	1.49	0.94
1:B:836:SER:O	1:B:840:THR:HG23	1.68	0.93
1:A:668:ARG:HH21	2:U:0:DT:H5"	1.36	0.91
1:A:391:ASP:HB2	1:A:591:ARG:HH22	1.35	0.90
1:A:784:GLY:HA3	1:A:817:LEU:HD21	1.53	0.89
1:A:872:THR:HG22	1:A:874:SER:H	1.35	0.89
1:B:872:THR:HG22	1:B:874:SER:H	1.36	0.88
1:B:802:GLY:HA2	1:B:807:PRO:HA	1.54	0.87
1:B:554:LEU:O	1:B:559:GLU:HG2	1.74	0.86
1:A:426:LEU:CD1	1:A:537:ILE:HG22	2.06	0.84
1:B:553:SER:HB2	1:B:557:SER:HB3	1.63	0.80
1:B:784:GLY:HA3	1:B:817:LEU:HD21	1.63	0.80
1:B:426:LEU:CD1	1:B:537:ILE:HG22	2.11	0.80
1:A:668:ARG:NH2	2:U:0:DT:H5"	1.97	0.80
1:B:549:LEU:HD21	1:B:571:LEU:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:LEU:HB2	1:A:1008:ALA:HB1	1.66	0.75
1:B:391:ASP:HB2	1:B:591:ARG:HH12	1.51	0.75
1:A:426:LEU:HD13	1:A:537:ILE:CG2	2.16	0.75
1:B:426:LEU:HD13	1:B:537:ILE:CG2	2.17	0.75
1:B:733:LEU:O	1:B:743:ARG:NH2	2.23	0.72
1:A:849:ILE:O	1:A:852:MET:HB2	1.89	0.72
1:A:701:PRO:O	1:A:704:ARG:HG3	1.91	0.71
1:A:659:CYS:HA	1:A:664:TRP:CD2	2.25	0.70
1:A:694:LEU:O	1:A:704:ARG:NH2	2.24	0.70
1:B:486:LEU:CD1	1:B:507:ARG:HH22	2.05	0.69
1:A:738:VAL:C	1:A:739:ARG:HG2	2.18	0.69
1:B:723:GLU:HB3	1:B:724:PRO:HD3	1.75	0.68
1:B:694:LEU:O	1:B:704:ARG:NH2	2.27	0.68
1:B:704:ARG:NH1	1:B:735:ASP:OD2	2.26	0.68
3:Y:1:DG:H2''	3:Y:2:DC:OP2	1.95	0.67
1:B:738:VAL:C	1:B:739:ARG:HG2	2.19	0.67
1:A:733:LEU:O	1:A:743:ARG:NH2	2.27	0.67
1:A:849:ILE:HG23	1:A:852:MET:CE	2.25	0.66
1:B:507:ARG:O	1:B:519:ILE:HG22	1.95	0.66
1:B:849:ILE:HG23	1:B:852:MET:CE	2.25	0.66
2:U:14:DC:H2''	2:U:15:DT:OP2	1.94	0.66
1:B:659:CYS:HA	1:B:664:TRP:CD2	2.31	0.65
1:A:553:SER:OG	1:A:557:SER:HB3	1.96	0.65
1:B:625:GLU:O	1:B:629:GLU:HG2	1.96	0.65
1:A:762:PHE:HB2	1:A:764:HIS:HD2	1.62	0.65
1:A:625:GLU:O	1:A:629:GLU:HG2	1.97	0.65
1:B:701:PRO:O	1:B:704:ARG:HG3	1.95	0.65
2:U:12:DG:H2''	2:U:13:DA:OP2	1.97	0.65
1:B:762:PHE:HB2	1:B:764:HIS:HD2	1.62	0.64
1:B:849:ILE:HG23	1:B:852:MET:HE3	1.80	0.63
1:B:845:LEU:C	1:B:846:LEU:HD12	2.24	0.63
1:A:507:ARG:O	1:A:519:ILE:HG22	1.99	0.62
1:A:926:GLN:HE21	1:A:926:GLN:HA	1.65	0.61
1:A:486:LEU:CD1	1:A:507:ARG:HH22	2.13	0.61
1:A:391:ASP:HB2	1:A:591:ARG:NH2	2.12	0.61
1:A:723:GLU:HB3	1:A:724:PRO:HD3	1.83	0.61
1:B:783:THR:HA	1:B:1007:VAL:O	1.99	0.61
1:A:704:ARG:NH1	1:A:735:ASP:OD2	2.31	0.61
1:A:558:MET:O	1:A:562:ASP:HA	2.00	0.60
1:A:845:LEU:C	1:A:846:LEU:HD12	2.27	0.60
1:B:486:LEU:HD11	1:B:507:ARG:HH22	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ARG:NH2	4:T:14:DG:OP1	2.34	0.60
1:B:849:ILE:O	1:B:852:MET:HB2	2.02	0.60
1:A:484:PHE:CE2	1:A:523:ILE:HG12	2.36	0.60
1:B:391:ASP:HB2	1:B:591:ARG:HH22	1.68	0.59
1:B:757:PRO:C	1:B:759:CYS:H	2.11	0.59
2:X:14:DC:H2'	2:X:15:DT:H72	1.85	0.59
1:A:759:CYS:O	1:A:762:PHE:CD1	2.56	0.59
1:A:553:SER:HB3	1:A:558:MET:HB3	1.84	0.59
1:A:458:THR:HG22	1:A:459:GLU:N	2.19	0.58
1:A:567:GLY:HA3	1:A:570:GLN:HE22	1.68	0.58
1:A:849:ILE:HG23	1:A:852:MET:HE3	1.84	0.58
1:A:486:LEU:HD11	1:A:507:ARG:HH22	1.69	0.57
1:A:560:ASP:O	1:A:561:GLU:HG2	2.04	0.57
1:A:663:GLY:HA3	1:A:699:TYR:CZ	2.39	0.57
3:V:1:DG:H2''	3:V:2:DC:OP2	2.04	0.57
1:B:931:LEU:HD11	1:B:962:VAL:HG11	1.86	0.57
1:A:721:ARG:O	1:A:724:PRO:HD2	2.05	0.57
1:B:465:LEU:HD23	1:B:501:LEU:HD23	1.87	0.56
1:B:759:CYS:O	1:B:762:PHE:CD1	2.58	0.56
1:A:738:VAL:O	1:A:739:ARG:HG2	2.05	0.56
1:A:757:PRO:C	1:A:759:CYS:H	2.14	0.56
1:B:663:GLY:HA3	1:B:699:TYR:CZ	2.41	0.55
1:A:659:CYS:HA	1:A:664:TRP:CG	2.42	0.55
1:B:559:GLU:C	1:B:561:GLU:H	2.14	0.55
1:B:391:ASP:HB2	1:B:591:ARG:NH1	2.19	0.55
1:A:735:ASP:HB3	1:A:738:VAL:HG13	1.88	0.55
1:A:931:LEU:HD11	1:A:962:VAL:HG11	1.89	0.55
1:A:787:CYS:HB2	1:A:798:VAL:HG23	1.88	0.54
1:B:555:THR:HB	1:B:864:GLN:HG2	1.89	0.54
1:A:760:LYS:HB3	1:B:790:ARG:HH22	1.72	0.54
1:B:484:PHE:CE2	1:B:523:ILE:HG12	2.43	0.54
1:B:828:ASP:OD2	1:B:966:SER:HB2	2.08	0.54
1:B:492:GLN:HB2	1:B:495:GLN:HG2	1.90	0.54
1:B:926:GLN:HE21	1:B:926:GLN:HA	1.72	0.54
1:A:759:CYS:O	1:A:762:PHE:HD1	1.90	0.53
1:A:430:LYS:HG3	1:A:471:LEU:HD11	1.91	0.53
1:B:785:ARG:HG2	1:B:1009:VAL:HB	1.89	0.53
1:B:431:MET:HG3	1:B:533:GLN:HB3	1.91	0.53
1:A:744:LEU:HA	1:A:772:MET:HE1	1.91	0.52
1:A:423:GLN:HA	1:A:570:GLN:HG2	1.91	0.52
1:B:786:LEU:HB2	1:B:1008:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:MET:HE3	1:B:817:LEU:HD12	1.91	0.52
1:B:459:GLU:O	1:B:462:LEU:HB3	2.09	0.52
1:A:739:ARG:O	1:A:740:THR:C	2.52	0.52
1:A:909:GLN:O	1:A:910:GLU:C	2.53	0.52
1:B:458:THR:HG22	1:B:459:GLU:N	2.24	0.52
1:B:659:CYS:HA	1:B:664:TRP:CG	2.45	0.52
1:B:739:ARG:O	1:B:740:THR:C	2.52	0.52
1:A:492:GLN:HB2	1:A:495:GLN:HG2	1.91	0.52
1:B:771:GLU:O	1:B:773:ALA:N	2.42	0.52
1:A:421:LEU:HD21	1:A:434:LEU:HD21	1.92	0.52
1:A:935:LEU:HA	1:A:971:PHE:CE2	2.44	0.51
1:B:744:LEU:HA	1:B:772:MET:HE1	1.91	0.51
1:A:482:LYS:C	1:A:484:PHE:H	2.18	0.51
1:B:391:ASP:CB	1:B:591:ARG:HH12	2.20	0.51
1:B:421:LEU:HD21	1:B:434:LEU:HD21	1.93	0.50
1:B:759:CYS:O	1:B:762:PHE:HD1	1.92	0.50
1:A:542:ARG:HH22	1:A:570:GLN:HG3	1.75	0.50
1:A:717:GLN:HG3	4:T:11:DC:H5''	1.93	0.50
1:A:628:LYS:HD3	1:A:680:LEU:CD1	2.42	0.50
1:A:754:ARG:HG3	1:A:755:GLU:N	2.26	0.50
1:B:789:GLN:O	1:B:790:ARG:HG2	2.12	0.49
1:B:777:VAL:O	1:B:779:HIS:HD2	1.95	0.49
1:A:771:GLU:O	1:A:773:ALA:N	2.46	0.49
1:B:482:LYS:C	1:B:484:PHE:H	2.21	0.49
1:B:909:GLN:O	1:B:910:GLU:C	2.56	0.48
1:B:639:ASN:HA	1:B:642:LYS:HG2	1.94	0.48
1:B:738:VAL:O	1:B:743:ARG:NH1	2.46	0.48
1:A:431:MET:SD	1:A:447:ILE:HD13	2.53	0.48
1:A:777:VAL:O	1:A:779:HIS:HD2	1.97	0.47
1:B:382:VAL:HG11	1:B:549:LEU:HD12	1.96	0.47
1:B:880:ARG:HB3	1:B:881:PRO:HD3	1.97	0.47
1:A:458:THR:CG2	1:A:459:GLU:N	2.77	0.47
2:X:14:DC:H2''	2:X:15:DT:H5'	1.97	0.47
1:A:554:LEU:HD23	1:A:558:MET:HE1	1.96	0.47
1:A:834:GLU:HA	1:A:959:PRO:O	2.14	0.47
1:B:754:ARG:HG3	1:B:755:GLU:N	2.29	0.47
1:B:553:SER:HB2	1:B:558:MET:H	1.78	0.47
1:A:424:ARG:HD3	2:X:17:DC:H3'	1.97	0.46
1:A:644:HIS:ND1	1:A:645:PRO:HD2	2.30	0.46
1:B:559:GLU:OE2	1:B:559:GLU:HA	2.14	0.46
3:Y:2:DC:H2''	3:Y:3:DT:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:MET:HE3	1:A:817:LEU:HD12	1.98	0.46
1:B:549:LEU:HD21	1:B:571:LEU:N	2.24	0.46
1:B:739:ARG:HD2	1:B:950:ASP:OD2	2.16	0.46
1:A:780:VAL:CG1	1:A:781:THR:N	2.79	0.46
1:A:785:ARG:HG2	1:A:1009:VAL:HB	1.98	0.46
1:B:554:LEU:C	1:B:559:GLU:HG2	2.37	0.46
1:B:767:GLN:O	1:B:768:GLN:C	2.58	0.46
1:B:553:SER:CB	1:B:557:SER:HB3	2.41	0.46
1:A:642:LYS:O	1:A:643:ASN:HB2	2.17	0.45
1:B:431:MET:SD	1:B:447:ILE:HD13	2.56	0.45
1:A:840:THR:HB	1:A:917:VAL:HA	1.98	0.45
1:B:972:LYS:HD3	1:B:1002:GLU:OE1	2.17	0.45
1:A:578:ASN:HB2	1:A:582:MET:HE3	1.99	0.45
1:B:391:ASP:HB2	1:B:591:ARG:NH2	2.31	0.45
1:A:769:LEU:HA	1:A:770:PRO:HD2	1.85	0.45
1:B:894:PRO:C	1:B:896:GLU:H	2.24	0.45
1:B:797:PHE:HE2	1:B:1008:ALA:HB2	1.81	0.45
1:A:639:ASN:HA	1:A:642:LYS:HG2	2.00	0.44
1:A:757:PRO:C	1:A:759:CYS:N	2.76	0.44
1:B:757:PRO:C	1:B:759:CYS:N	2.74	0.44
1:B:780:VAL:CG1	1:B:781:THR:N	2.80	0.44
1:B:477:LEU:HD12	1:B:493:LYS:HG3	2.00	0.44
1:B:757:PRO:O	1:B:759:CYS:N	2.50	0.44
1:A:567:GLY:O	1:A:568:GLN:HB2	2.17	0.44
1:A:519:ILE:O	1:A:523:ILE:HG13	2.18	0.44
1:B:552:PHE:HE2	1:B:575:LEU:HD21	1.83	0.44
1:B:642:LYS:O	1:B:643:ASN:HB2	2.18	0.44
1:B:833:GLY:O	1:B:834:GLU:C	2.61	0.44
1:A:638:TRP:HB2	1:A:666:TYR:CG	2.52	0.43
1:A:903:ALA:HB2	1:A:929:GLN:NE2	2.33	0.43
1:B:458:THR:CG2	1:B:459:GLU:N	2.81	0.43
1:A:559:GLU:O	1:A:561:GLU:N	2.51	0.43
1:A:797:PHE:HE2	1:A:1008:ALA:HB2	1.82	0.43
1:A:762:PHE:HB2	1:A:764:HIS:CD2	2.49	0.43
1:B:800:GLU:HB3	1:B:809:THR:HA	2.00	0.43
1:A:424:ARG:NH1	2:X:17:DC:OP1	2.40	0.43
1:A:894:PRO:C	1:A:896:GLU:H	2.27	0.43
1:B:847:TRP:CE2	1:B:909:GLN:HG3	2.53	0.43
1:B:903:ALA:HB2	1:B:929:GLN:NE2	2.34	0.43
1:B:382:VAL:O	1:B:386:VAL:HG23	2.18	0.43
1:A:726:ILE:HG23	1:A:765:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:GLN:HA	1:A:926:GLN:NE2	2.33	0.43
1:A:767:GLN:O	1:A:768:GLN:C	2.61	0.43
1:B:403:ILE:HG23	1:B:455:PHE:HE1	1.84	0.43
1:B:397:ASP:O	1:B:401:LYS:HG3	2.18	0.42
1:B:887:LEU:HD23	1:B:887:LEU:HA	1.93	0.42
1:B:430:LYS:HG3	1:B:471:LEU:HD11	2.01	0.42
1:B:444:THR:N	1:B:445:PRO:HD2	2.34	0.42
1:B:726:ILE:HG23	1:B:765:LEU:HG	2.01	0.42
1:B:426:LEU:O	1:B:427:SER:HB3	2.20	0.42
4:T:11:DC:H2''	4:T:12:DG:O5'	2.20	0.42
1:B:723:GLU:CB	1:B:724:PRO:HD3	2.48	0.42
1:A:700:CYS:N	1:A:701:PRO:HD3	2.33	0.42
1:A:780:VAL:HG12	1:A:781:THR:N	2.34	0.42
1:A:590:ASN:OD1	1:A:590:ASN:C	2.63	0.42
1:B:638:TRP:HB2	1:B:666:TYR:CG	2.55	0.42
1:A:947:LEU:O	1:A:951:PHE:HB2	2.20	0.42
1:B:918:SER:HB2	1:B:921:ARG:HB2	2.01	0.42
1:B:412:ALA:O	1:B:416:LYS:HG3	2.20	0.42
1:B:420:ARG:O	1:B:424:ARG:HG2	2.20	0.42
1:B:628:LYS:HD3	1:B:680:LEU:CD1	2.49	0.42
1:B:729:ILE:HG21	1:B:750:ALA:HB2	2.01	0.42
1:B:424:ARG:HD3	2:U:17:DC:H3'	2.00	0.42
1:B:762:PHE:CE2	1:B:765:LEU:HB2	2.54	0.42
1:A:444:THR:N	1:A:445:PRO:HD2	2.35	0.41
1:B:644:HIS:ND1	1:B:645:PRO:HD2	2.35	0.41
1:B:744:LEU:HD23	1:B:985:HIS:HB3	2.02	0.41
1:A:880:ARG:HB3	1:A:881:PRO:HD3	2.01	0.41
1:B:585:PRO:HD3	1:B:913:VAL:O	2.21	0.41
1:A:431:MET:HG3	1:A:533:GLN:HB3	2.02	0.41
1:A:847:TRP:CE2	1:A:909:GLN:HG3	2.56	0.41
2:U:5:DA:H1'	2:U:6:DC:H5'	2.03	0.41
1:A:757:PRO:O	1:A:759:CYS:N	2.54	0.41
1:A:848:ASP:OD2	1:A:886:ARG:NH2	2.51	0.41
1:A:906:TRP:CD1	1:A:906:TRP:C	2.98	0.41
1:B:552:PHE:CE2	1:B:575:LEU:HD21	2.56	0.41
1:A:377:ARG:O	1:A:381:VAL:HG23	2.21	0.41
1:B:377:ARG:O	1:B:381:VAL:HG23	2.20	0.41
1:B:462:LEU:HD11	1:B:468:VAL:HG22	2.03	0.41
1:B:471:LEU:HD21	1:B:534:SER:OG	2.20	0.41
1:B:591:ARG:H	1:B:591:ARG:HG2	1.78	0.41
1:B:735:ASP:HA	1:B:736:PRO:HD2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LYS:NZ	3:Y:10:DT:OP1	2.49	0.41
1:A:995:GLN:O	1:A:998:GLY:N	2.43	0.41
2:X:5:DA:H1'	2:X:6:DC:H5'	2.03	0.41
2:X:19:DC:H6	2:X:19:DC:H2'	1.78	0.41
1:A:462:LEU:HD11	1:A:468:VAL:HG22	2.03	0.40
1:A:692:SER:O	1:A:695:SER:OG	2.34	0.40
1:A:729:ILE:HG21	1:A:750:ALA:HB2	2.04	0.40
1:A:898:LEU:HD11	1:A:937:GLY:H	1.85	0.40
1:A:983:LEU:HB2	1:A:988:MET:HE2	2.03	0.40
1:B:798:VAL:HG22	1:B:811:LEU:HD23	2.04	0.40
1:A:397:ASP:C	1:A:397:ASP:OD1	2.65	0.40
1:A:477:LEU:HD12	1:A:493:LYS:HG3	2.04	0.40
1:B:464:GLU:O	1:B:468:VAL:HG23	2.21	0.40
1:B:772:MET:HE2	1:B:772:MET:HB3	1.99	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ASP:OD2	1:B:509:VAL:CG2[2_545]	2.13	0.07
1:B:679:ARG:NH2	4:W:14:DG:OP1[1_655]	2.16	0.04

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	609/631 (96%)	562 (92%)	34 (6%)	13 (2%)	5	20
1	B	624/631 (99%)	567 (91%)	48 (8%)	9 (1%)	9	30
All	All	1233/1262 (98%)	1129 (92%)	82 (7%)	22 (2%)	6	23

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	557	SER
1	A	568	GLN
1	A	767	GLN
1	A	772	MET
1	B	767	GLN
1	B	772	MET
1	B	788	PRO
1	A	560	ASP
1	A	740	THR
1	A	937	GLY
1	B	571	LEU
1	B	740	THR
1	B	937	GLY
1	A	483	THR
1	A	558	MET
1	A	758	SER
1	A	895	GLU
1	B	483	THR
1	B	758	SER
1	B	895	GLU
1	A	561	GLU
1	A	760	LYS

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	538/550 (98%)	496 (92%)	42 (8%)	11	35
1	B	547/550 (100%)	498 (91%)	49 (9%)	9	28
All	All	1085/1100 (99%)	994 (92%)	91 (8%)	10	32

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	THR
1	A	390	GLU

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Mol	Chain	Res	Type
1	A	405	THR
1	A	424	ARG
1	A	441	LEU
1	A	444	THR
1	A	446	VAL
1	A	451	THR
1	A	488	ASN
1	A	522	VAL
1	A	525	LYS
1	A	537	ILE
1	A	542	ARG
1	A	547	ARG
1	A	573	THR
1	A	574	VAL
1	A	575	LEU
1	A	583	GLU
1	A	590	ASN
1	A	591	ARG
1	A	616	SER
1	A	662	VAL
1	A	671	SER
1	A	674	VAL
1	A	692	SER
1	A	721	ARG
1	A	730	THR
1	A	738	VAL
1	A	751	VAL
1	A	753	LEU
1	A	754	ARG
1	A	758	SER
1	A	814	VAL
1	A	834	GLU
1	A	840	THR
1	A	874	SER
1	A	889	LEU
1	A	918	SER
1	A	926	GLN
1	A	966	SER
1	A	967	GLN
1	A	981	ASP
1	B	370	THR
1	B	390	GLU

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Mol	Chain	Res	Type
1	B	405	THR
1	B	413	THR
1	B	424	ARG
1	B	444	THR
1	B	446	VAL
1	B	451	THR
1	B	486	LEU
1	B	488	ASN
1	B	522	VAL
1	B	525	LYS
1	B	537	ILE
1	B	542	ARG
1	B	547	ARG
1	B	559	GLU
1	B	565	CYS
1	B	571	LEU
1	B	573	THR
1	B	574	VAL
1	B	575	LEU
1	B	583	GLU
1	B	590	ASN
1	B	591	ARG
1	B	603	ILE
1	B	662	VAL
1	B	671	SER
1	B	674	VAL
1	B	692	SER
1	B	721	ARG
1	B	730	THR
1	B	738	VAL
1	B	751	VAL
1	B	753	LEU
1	B	754	ARG
1	B	758	SER
1	B	800	GLU
1	B	803	GLU
1	B	808	THR
1	B	814	VAL
1	B	834	GLU
1	B	840	THR
1	B	874	SER
1	B	889	LEU

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Mol	Chain	Res	Type
1	B	918	SER
1	B	966	SER
1	B	967	GLN
1	B	969	ARG
1	B	981	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	ASN
1	A	399	GLN
1	A	488	ASN
1	A	610	HIS
1	A	764	HIS
1	A	775	GLN
1	A	832	HIS
1	A	926	GLN
1	A	929	GLN
1	A	995	GLN
1	B	389	ASN
1	B	399	GLN
1	B	533	GLN
1	B	570	GLN
1	B	610	HIS
1	B	681	HIS
1	B	714	ASN
1	B	718	HIS
1	B	764	HIS
1	B	832	HIS
1	B	891	HIS
1	B	909	GLN
1	B	926	GLN
1	B	929	GLN
1	B	995	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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, 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	615/631 (97%)	0.10	26 (4%) 40 32	50, 78, 144, 179	0
1	B	628/631 (99%)	0.27	34 (5%) 31 24	54, 85, 147, 176	0
2	U	20/21 (95%)	0.24	1 (5%) 34 26	93, 110, 135, 153	0
2	X	20/21 (95%)	-0.13	1 (5%) 34 26	61, 79, 126, 143	0
3	V	12/12 (100%)	0.47	2 (16%) 4 3	105, 111, 121, 122	0
3	Y	12/12 (100%)	-0.17	0 100 100	74, 88, 116, 117	0
4	T	7/14 (50%)	-0.39	0 100 100	80, 88, 110, 120	0
4	W	7/14 (50%)	-0.54	0 100 100	60, 63, 79, 92	0
All	All	1321/1356 (97%)	0.17	64 (4%) 35 28	50, 82, 145, 179	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	563	ALA	6.6
1	B	564	ALA	5.4
1	A	564	ALA	5.4
1	A	563	ALA	4.4
1	A	567	GLY	4.3
1	B	497	VAL	3.9
1	A	1008	ALA	3.7
1	A	1009	VAL	3.6
1	B	558	MET	3.6
1	A	489	PRO	3.5
1	B	559	GLU	3.3
1	A	559	GLU	3.2
1	B	501	LEU	3.2
1	B	565	CYS	3.2
1	B	912	ARG	3.1
1	A	558	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	557	SER	3.0
1	A	765	LEU	2.9
1	B	500	PHE	2.9
1	A	766	PHE	2.9
2	X	0	DT	2.9
1	A	565	CYS	2.9
1	B	468	VAL	2.9
1	A	556	ASP	2.8
1	A	810	VAL	2.8
1	A	557	SER	2.8
1	B	507	ARG	2.8
1	B	794	LYS	2.8
1	A	486	LEU	2.7
1	B	499	ALA	2.7
1	B	766	PHE	2.6
1	B	371	GLY	2.6
1	B	503	LEU	2.5
1	A	370	THR	2.5
1	B	370	THR	2.5
1	B	509	VAL	2.4
2	U	0	DT	2.4
1	B	919	TRP	2.4
1	B	562	ASP	2.4
1	B	764	HIS	2.4
1	A	560	ASP	2.4
1	B	763	LYS	2.3
1	A	794	LYS	2.3
1	B	465	LEU	2.3
1	A	1006	VAL	2.3
1	B	404	VAL	2.3
1	B	765	LEU	2.3
1	B	768	GLN	2.3
1	A	676	ILE	2.3
1	B	519	ILE	2.3
1	B	847	TRP	2.2
1	A	554	LEU	2.2
1	A	764	HIS	2.1
1	B	496	LEU	2.1
1	A	799	MET	2.1
1	B	788	PRO	2.1
1	B	525	LYS	2.1
1	A	769	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	V	3	DT	2.1
3	V	2	DC	2.1
1	B	460	SER	2.0
1	A	562	ASP	2.0
1	A	394	LEU	2.0
1	B	1009	VAL	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
5	CA	B	1101	1/1	0.92	0.12	67,67,67,67	0
5	CA	A	1101	1/1	0.94	0.08	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.