Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 12:18 AM EST

PDB ID	:	4RIC
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:

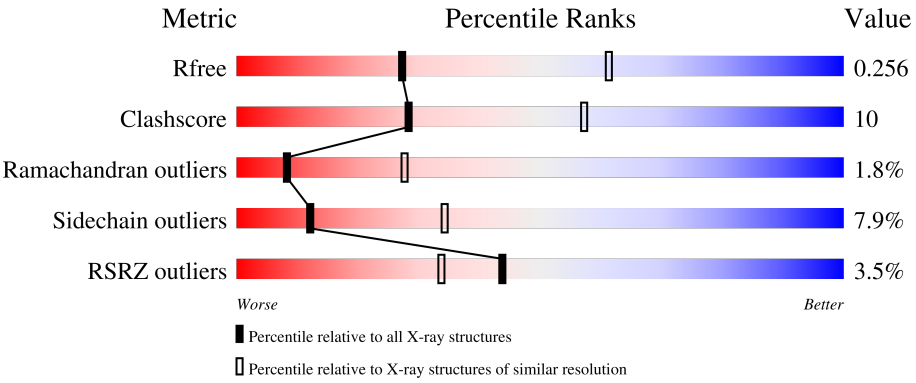
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	3% 71% 23%
1	B	631	5% 70% 27%
2	U	21	57% 38% 5%
2	X	21	67% 24% 5% 5%
3	V	12	83% 17%

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Mol	Chain	Length	Quality of chain
3	Y	12	
4	T	14	
4	W	14	

2 Entry composition (i)

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 (three-letter code: CA) (formula: Ca).

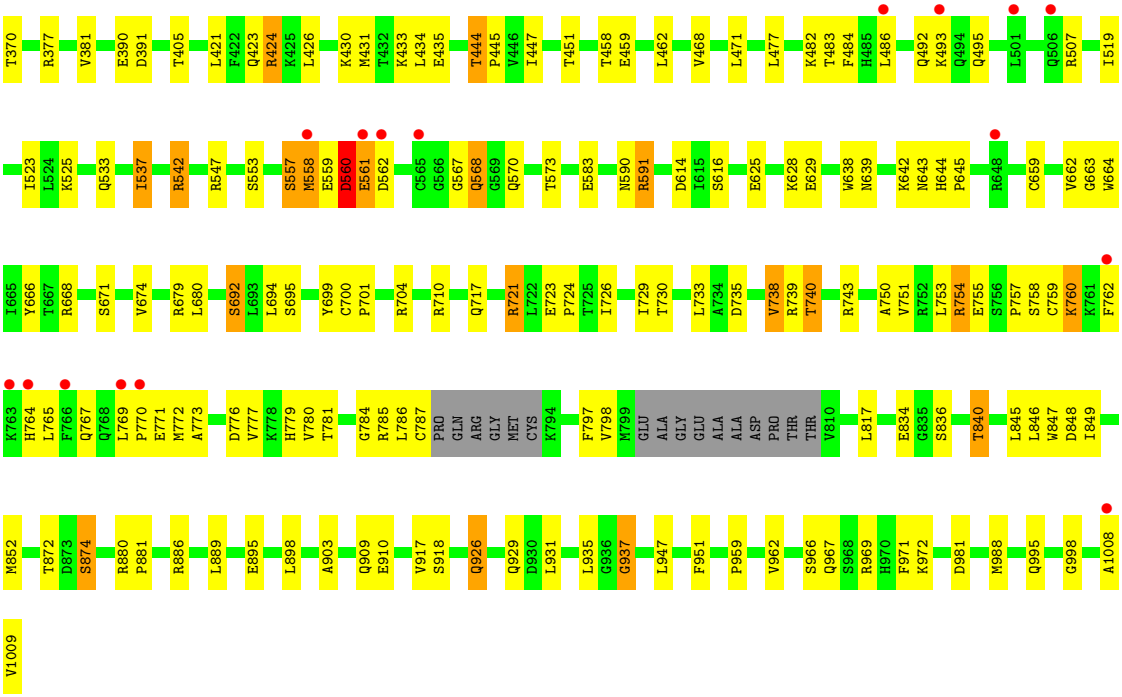
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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.

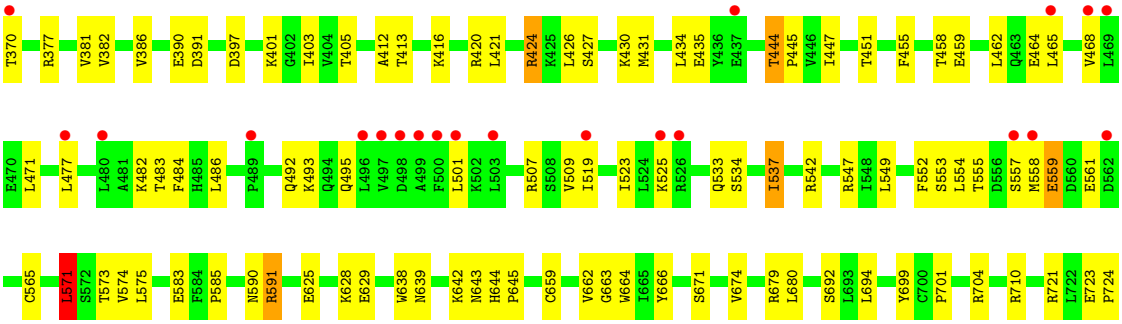
• Molecule 1: Fanconi-associated nuclease 1

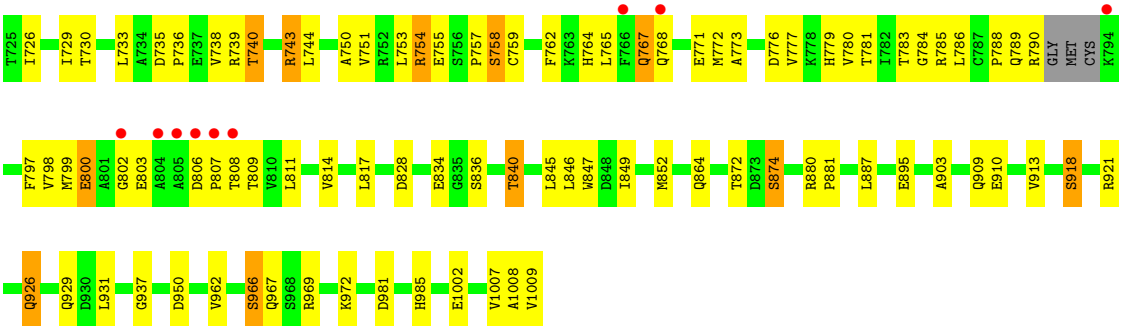
Chain A:



• Molecule 1: Fanconi-associated nuclease 1

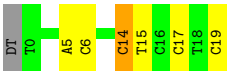
Chain B:





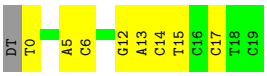
• Molecule 2: DNA (5'-D(*TP*TP*AP*GP*CP*CP*AP*CP*GP*CP*CP*TP*AP*GP*AP*CP *TP*CP*CP*TP*C)-3')

Chain X:



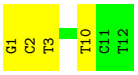
• Molecule 2: DNA (5'-D(*TP*TP*AP*GP*CP*CP*AP*CP*GP*CP*CP*TP*AP*GP*AP*CP *TP*CP*CP*TP*C)-3')

Chain U:



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

Chain Y:

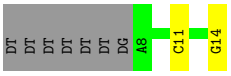


• Molecule 3: DNA (5'-D(*GP*CP*TP*GP*AP*GP*GP*AP*GP*TP*CP*T)-3')

Chain V:

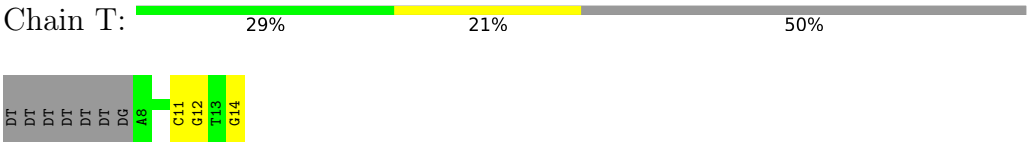
• Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*GP*AP*GP*GP*CP*GP*TP*G)-3')

Chain W:



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

Chain T:



4 Data and refinement statistics (i)

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 79.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.80) 94.2 (79.69-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.09%)	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 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.48	0/5044	0.69	0/6818
1	B	0.47	0/5140	0.68	2/6952 (0.0%)
2	U	0.35	0/447	0.77	0/685
2	X	0.41	0/447	0.84	1/685 (0.1%)
3	V	0.39	0/277	0.77	0/427
3	Y	0.37	0/277	0.75	0/427
4	T	0.47	0/166	0.80	0/255
4	W	0.54	0/166	0.89	1/255 (0.4%)
All	All	0.47	0/11964	0.70	4/16504 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	11	DC	C1'-O4'-C4'	-6.08	104.02	110.10
1	B	743	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	X	14	DC	C1'-O4'-C4'	-5.83	104.27	110.10
1	B	743	ARG	NE-CZ-NH2	-5.41	117.59	120.30

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	99	1
1	B	5035	0	5059	111	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	220	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 (220) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:849:ILE:HG23	1:B:852:MET:HE3	1.76	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
1:A:738:VAL:C	1:A:739:ARG:HG2	2.18	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:738:VAL:C	1:B:739:ARG:HG2	2.19	0.62
1:A:507:ARG:O	1:A:519:ILE:HG22	1.99	0.62
1:A:849:ILE:HG23	1:A:852:MET:HE3	1.82	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:B:486:LEU:HD11	1:B:507:ARG:HH22	1.64	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:LEU:C	1:B:846:LEU:HD12	2.24	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
2:X:14:DC:H2'	2:X:15:DT:H71	1.85	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:845:LEU:C	1:A:846:LEU:HD12	2.27	0.55
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: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:B:757:PRO:C	1:B:759:CYS:H	2.11	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:B:799:MET:HE3	1:B:817:LEU:HD12	1.91	0.53
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
1:B:459:GLU:O	1:B:462:LEU:HB3	2.09	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: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:A:757:PRO:C	1:A:759:CYS:H	2.14	0.51
1:B:391:ASP:CB	1:B:591:ARG:HH12	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD21	1:B:434:LEU:HD21	1.93	0.50
1:B:559:GLU:C	1:B:561:GLU:H	2.14	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: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:739:ARG:O	1:A:740:THR:C	2.52	0.47
1:A:777:VAL:O	1:A:779:HIS:HD2	1.97	0.47
1:A:909:GLN:O	1:A:910:GLU:C	2.53	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:B:739:ARG:O	1:B:740:THR:C	2.52	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
1:A:482:LYS:C	1:A:484:PHE:H	2.18	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: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: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:797:PHE:HE2	1:B:1008:ALA:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ASN:HA	1:A:642:LYS:HG2	2.00	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: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:909:GLN:O	1:B:910:GLU:C	2.56	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:482:LYS:C	1:B:484:PHE:H	2.21	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: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
1:A:926:GLN:HA	1:A:926:GLN:NE2	2.33	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:B:767:GLN:O	1:B:768:GLN:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:554:LEU:C	1:B:559:GLU:HG2	2.37	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
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:729:ILE:HG21	1:A:750:ALA:HB2	2.04	0.40
1:A:692:SER:O	1:A:695:SER:OG	2.34	0.40
1:A:898:LEU:HD11	1:A:937:GLY:H	1.85	0.40
1:B:798:VAL:HG22	1:B:811:LEU:HD23	2.04	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

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%)	7 23
1	B	624/631 (99%)	567 (91%)	48 (8%)	9 (1%)	11 34
All	All	1233/1262 (98%)	1129 (92%)	82 (7%)	22 (2%)	8 28

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 (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	538/550 (98%)	498 (93%)	40 (7%)	13 37
1	B	547/550 (100%)	501 (92%)	46 (8%)	11 31
All	All	1085/1100 (99%)	999 (92%)	86 (8%)	12 34

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	THR
1	A	390	GLU
1	A	405	THR
1	A	424	ARG
1	A	435	GLU
1	A	444	THR
1	A	451	THR
1	A	525	LYS
1	A	537	ILE
1	A	542	ARG
1	A	547	ARG
1	A	560	ASP
1	A	573	THR
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	710	ARG
1	A	721	ARG
1	A	730	THR
1	A	738	VAL
1	A	751	VAL
1	A	753	LEU

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Mol	Chain	Res	Type
1	A	754	ARG
1	A	776	ASP
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	969	ARG
1	A	972	LYS
1	A	981	ASP
1	A	988	MET
1	B	370	THR
1	B	390	GLU
1	B	405	THR
1	B	413	THR
1	B	424	ARG
1	B	435	GLU
1	B	444	THR
1	B	451	THR
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	583	GLU
1	B	590	ASN
1	B	591	ARG
1	B	662	VAL
1	B	671	SER
1	B	674	VAL
1	B	692	SER
1	B	710	ARG
1	B	721	ARG
1	B	730	THR
1	B	751	VAL
1	B	753	LEU

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Mol	Chain	Res	Type
1	B	754	ARG
1	B	758	SER
1	B	776	ASP
1	B	800	GLU
1	B	803	GLU
1	B	806	ASP
1	B	808	THR
1	B	814	VAL
1	B	834	GLU
1	B	840	THR
1	B	874	SER
1	B	918	SER
1	B	926	GLN
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	ASN
1	A	764	HIS
1	A	775	GLN
1	A	926	GLN
1	A	953	HIS
1	B	389	ASN
1	B	570	GLN
1	B	610	HIS
1	B	681	HIS
1	B	718	HIS
1	B	764	HIS
1	B	829	GLN
1	B	832	HIS
1	B	926	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 monosaccharides in this entry.

5.6 Ligand geometry

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

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^{th} 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%)	0.05	16 (2%) 56 46	50, 78, 144, 179	0
1	B	628/631 (99%)	0.13	30 (4%) 30 21	54, 85, 147, 176	0
2	U	20/21 (95%)	-0.53	0 100 100	93, 110, 135, 153	0
2	X	20/21 (95%)	-0.46	0 100 100	61, 79, 126, 143	0
3	V	12/12 (100%)	-0.45	0 100 100	105, 111, 121, 122	0
3	Y	12/12 (100%)	-0.74	0 100 100	74, 88, 116, 117	0
4	T	7/14 (50%)	-0.61	0 100 100	80, 88, 110, 120	0
4	W	7/14 (50%)	-0.27	0 100 100	60, 63, 79, 92	0
All	All	1321/1356 (97%)	0.05	46 (3%) 44 34	50, 82, 145, 179	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	805	ALA	11.9
1	B	804	ALA	8.5
1	B	806	ASP	8.4
1	B	370	THR	7.5
1	A	766	PHE	6.4
1	B	807	PRO	6.2
1	B	501	LEU	5.0
1	A	770	PRO	4.9
1	B	489	PRO	4.8
1	B	497	VAL	4.6
1	A	562	ASP	4.3
1	B	768	GLN	4.2
1	B	468	VAL	3.8
1	A	769	LEU	3.6
1	B	802	GLY	3.5
1	B	503	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	565	CYS	3.1
1	A	561	GLU	3.1
1	B	469	LEU	3.0
1	B	558	MET	3.0
1	B	526	ARG	3.0
1	A	558	MET	2.9
1	A	486	LEU	2.8
1	B	525	LYS	2.8
1	B	437	GLU	2.7
1	A	648	ARG	2.7
1	B	794	LYS	2.6
1	A	762	PHE	2.6
1	B	500	PHE	2.6
1	A	501	LEU	2.6
1	A	763	LYS	2.5
1	A	764	HIS	2.5
1	B	562	ASP	2.5
1	B	465	LEU	2.5
1	A	1008	ALA	2.5
1	A	493	LYS	2.5
1	B	499	ALA	2.4
1	B	766	PHE	2.4
1	B	519	ILE	2.3
1	B	498	ASP	2.3
1	B	480	LEU	2.2
1	B	557	SER	2.2
1	B	808	THR	2.2
1	B	496	LEU	2.1
1	A	506	GLN	2.1
1	B	477	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

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^{th} 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^2)	Q<0.9
5	CA	B	1101	1/1	0.87	0.26	67,67,67,67	0
5	CA	A	1101	1/1	0.89	0.25	88,88,88,88	0

6.5 Other polymers

There are no such residues in this entry.