



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:55 am BST

PDB ID : 4RIB  
Title : FAN1 Nuclease bound to 5' phosphorylated p(dT) single flap DNA  
Authors : Pavletich, N.P.; Wang, R.  
Deposited on : 2014-10-05  
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

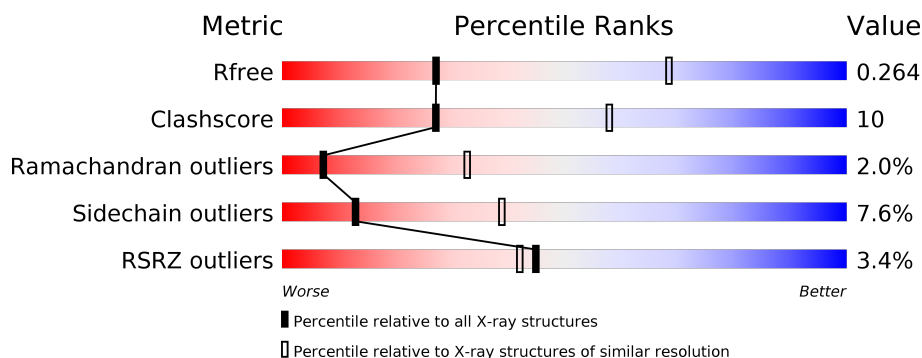
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 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	651	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>24%</div> <div>• 6%</div> </div> </div>
1	B	651	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• •</div> </div> </div>
2	U	20	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	X	20	<div> <div></div> <div> <div>75%</div> <div>25%</div> </div> </div>
3	V	12	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
3	Y	12	<div> <div></div> <div> <div>58%</div> <div>42%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	W	14	
4	Z	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 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	GLY	-	EXPRESSION TAG	UNP Q9Y2M0
A	359	ALA	-	EXPRESSION TAG	UNP Q9Y2M0
A	360	HIS	-	EXPRESSION TAG	UNP Q9Y2M0
A	361	MET	-	EXPRESSION TAG	UNP Q9Y2M0
A	362	THR	-	EXPRESSION TAG	UNP Q9Y2M0
A	363	ARG	-	EXPRESSION TAG	UNP Q9Y2M0
A	487	ALA	VAL	ENGINEERED MUTATION	UNP Q9Y2M0
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	358	GLY	-	EXPRESSION TAG	UNP Q9Y2M0
B	359	ALA	-	EXPRESSION TAG	UNP Q9Y2M0
B	360	HIS	-	EXPRESSION TAG	UNP Q9Y2M0
B	361	MET	-	EXPRESSION TAG	UNP Q9Y2M0
B	362	THR	-	EXPRESSION TAG	UNP Q9Y2M0
B	363	ARG	-	EXPRESSION TAG	UNP Q9Y2M0
B	487	ALA	VAL	ENGINEERED MUTATION	UNP Q9Y2M0
B	?	-	CYS	DELETION	UNP Q9Y2M0
B	?	-	THR	DELETION	UNP Q9Y2M0

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Chain	Residue	Modelled	Actual	Comment	Reference
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(P\*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	Z	7	Total	C	N	O	P	0	0	0
			148	69	30	42	7			
4	W	7	Total	C	N	O	P	0	0	0
			148	69	30	42	7			

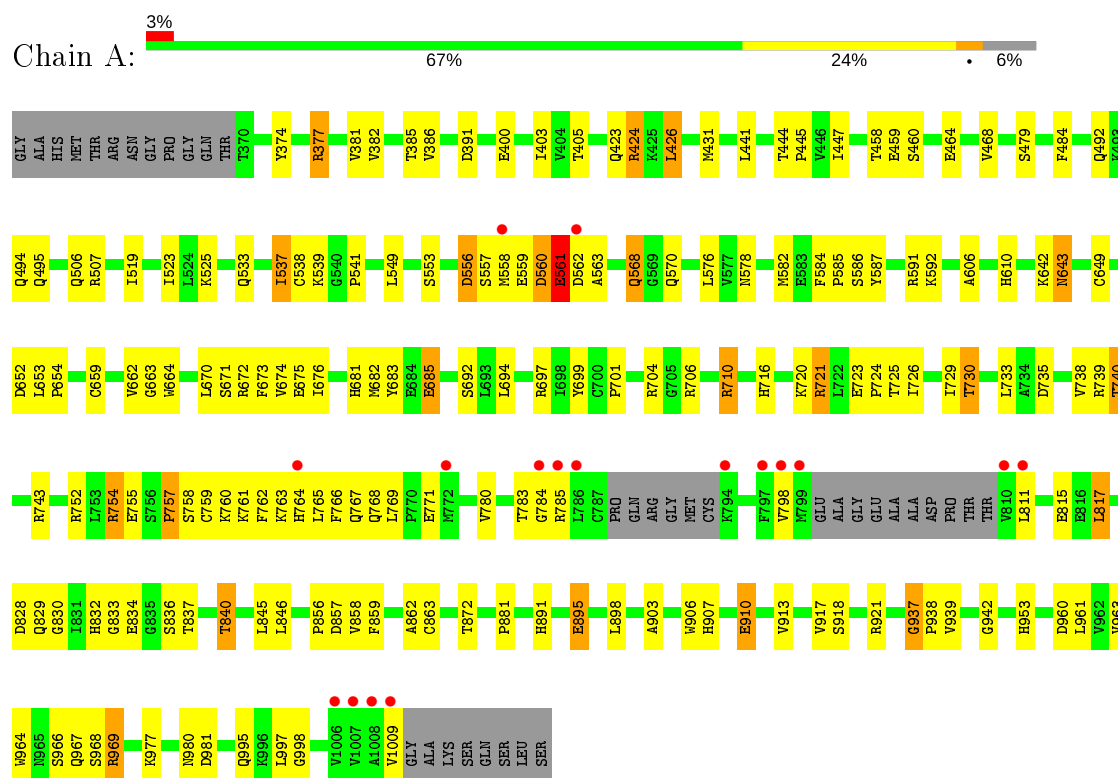
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

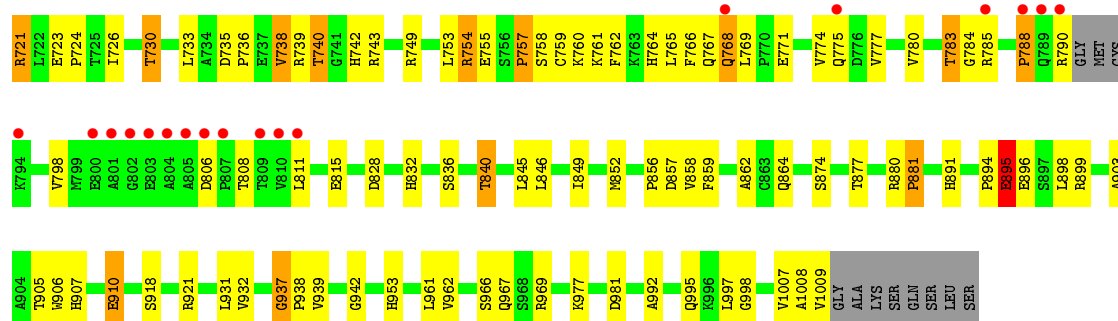
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

### 3 Residue-property plots [i](#)

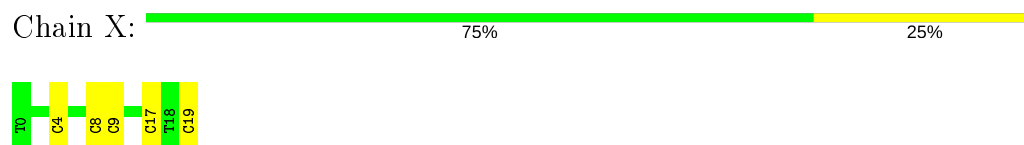
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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





- Molecule 2: DNA (5'-D(P\*TP\*AP\*GP\*CP\*CP\*AP\*CP\*GP\*CP\*CP\*TP\*AP\*GP\*AP\*CP\*T  
P\*CP\*CP\*TP\*C)-3')



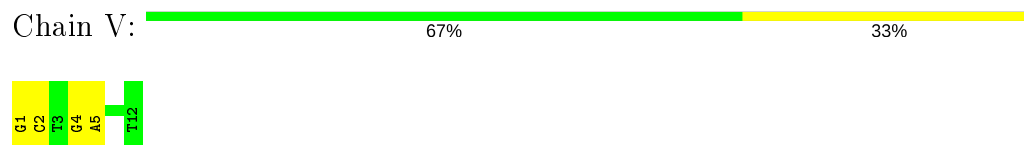
- Molecule 2: DNA (5'-D(P\*TP\*AP\*GP\*CP\*CP\*AP\*CP\*GP\*CP\*CP\*TP\*AP\*GP\*AP\*CP\*T  
P\*CP\*CP\*TP\*C)-3')



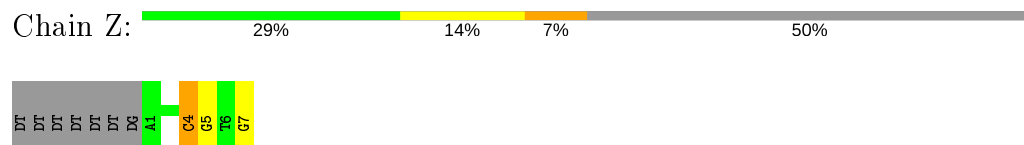
- Molecule 3: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*AP\*GP\*TP\*CP\*T)-3')



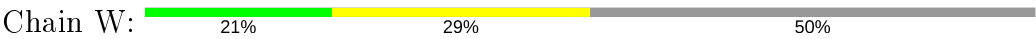
- Molecule 3: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*AP\*GP\*TP\*CP\*T)-3')



- 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')



DT	DT	DT	DT	DT	DT	DG	A1	G2	G3	C4	G5	G6	G7
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.70Å 110.99Å 105.43Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 64.73 – 3.21	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-3.25) 91.9 (64.73-3.21)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.226 , 0.265 0.223 , 0.264	Depositor DCC
$R_{free}$ test set	1381 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 73.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/5044	0.63	0/6818
1	B	0.41	0/5140	0.62	0/6952
2	U	0.30	0/447	0.82	0/685
2	X	0.36	0/447	0.79	0/685
3	V	0.27	0/277	0.72	0/427
3	Y	0.33	0/277	0.68	0/427
4	W	0.34	0/166	0.86	0/255
4	Z	0.43	0/166	0.85	1/255 (0.4%)
All	All	0.40	0/11964	0.65	1/16504 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	4	DC	C1'-O4'-C4'	-5.05	105.05	110.10

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	4942	0	4978	106	0
1	B	5035	0	5062	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	401	0	225	9	0
2	X	401	0	225	4	0
3	V	247	0	137	2	0
3	Y	247	0	137	3	0
4	W	148	0	79	3	0
4	Z	148	0	79	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	11571	0	10922	227	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 (227) 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:391:ASP:HB2	1:B:591:ARG:HH12	1.21	1.02
1:A:701:PRO:O	1:A:704:ARG:HG3	1.74	0.88
1:A:553:SER:O	1:A:559:GLU:HB2	1.74	0.88
1:A:391:ASP:HB2	1:A:591:ARG:HH12	1.38	0.86
1:B:507:ARG:O	1:B:519:ILE:HG22	1.74	0.85
1:A:694:LEU:O	1:A:704:ARG:NH2	2.10	0.85
1:A:377:ARG:HH11	1:A:377:ARG:HB3	1.44	0.83
1:A:507:ARG:O	1:A:519:ILE:HG22	1.79	0.83
1:B:385:THR:HG23	1:B:862:ALA:HB3	1.61	0.81
1:B:701:PRO:O	1:B:704:ARG:HG3	1.82	0.79
1:B:694:LEU:O	1:B:704:ARG:NH2	2.18	0.77
1:B:391:ASP:CB	1:B:591:ARG:HH12	1.99	0.76
1:B:377:ARG:HB3	1:B:377:ARG:HH11	1.52	0.74
1:A:763:LYS:NZ	1:B:788:PRO:HG2	2.05	0.72
1:A:828:ASP:OD2	1:A:966:SER:HB2	1.91	0.71
1:B:836:SER:O	1:B:840:THR:HG23	1.91	0.70
1:A:391:ASP:CB	1:A:591:ARG:HH12	2.07	0.68
1:B:606:ALA:O	1:B:610:HIS:CD2	2.48	0.66
1:A:385:THR:HG23	1:A:862:ALA:HB3	1.76	0.66
1:A:765:LEU:HD22	1:A:769:LEU:HD11	1.78	0.65
1:A:798:VAL:HG22	1:A:811:LEU:HD23	1.79	0.65
1:A:759:CYS:O	1:A:761:LYS:N	2.29	0.65
1:B:659:CYS:HA	1:B:664:TRP:CD2	2.33	0.64
1:A:659:CYS:HA	1:A:664:TRP:CD2	2.33	0.63
1:B:785:ARG:HG2	1:B:1009:VAL:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:LEU:O	1:B:846:LEU:HD12	1.98	0.63
1:B:798:VAL:HG22	1:B:811:LEU:HD23	1.81	0.63
1:A:723:GLU:HB3	1:A:724:PRO:HD3	1.80	0.62
1:B:723:GLU:HB3	1:B:724:PRO:HD3	1.81	0.62
1:B:856:PRO:O	1:B:857:ASP:HB2	1.99	0.62
1:A:836:SER:O	1:A:840:THR:HG23	1.99	0.62
1:A:549:LEU:HD21	1:A:570:GLN:O	2.00	0.61
1:A:578:ASN:O	1:A:582:MET:HG3	1.99	0.61
1:A:587:TYR:CD1	1:A:859:PHE:CD1	2.89	0.60
1:A:426:LEU:HD13	1:A:537:ILE:HG22	1.83	0.60
1:B:739:ARG:HG3	1:B:953:HIS:CD2	2.37	0.60
1:B:757:PRO:C	1:B:759:CYS:H	2.05	0.60
1:B:391:ASP:HB2	1:B:591:ARG:NH1	2.05	0.60
1:B:759:CYS:O	1:B:761:LYS:N	2.33	0.59
1:B:426:LEU:HD13	1:B:537:ILE:HG22	1.84	0.59
1:A:492:GLN:HB2	1:A:495:GLN:HG2	1.85	0.59
1:B:492:GLN:HB2	1:B:495:GLN:HG2	1.84	0.59
1:B:845:LEU:C	1:B:846:LEU:HD12	2.23	0.59
1:B:765:LEU:HD22	1:B:769:LEU:HD11	1.83	0.59
1:A:704:ARG:NH1	1:A:735:ASP:OD2	2.36	0.58
1:B:659:CYS:HA	1:B:664:TRP:CG	2.38	0.58
1:A:659:CYS:HA	1:A:664:TRP:CG	2.39	0.58
1:B:555:THR:HB	1:B:864:GLN:HG2	1.84	0.58
1:A:606:ALA:O	1:A:610:HIS:CD2	2.56	0.58
1:A:754:ARG:HG3	1:A:755:GLU:N	2.17	0.58
1:B:704:ARG:NH1	1:B:735:ASP:OD2	2.36	0.57
1:B:942:GLY:HA3	1:B:997:LEU:HD21	1.86	0.57
1:A:939:VAL:HA	1:A:997:LEU:HD22	1.87	0.57
1:A:431:MET:HG3	1:A:533:GLN:HB3	1.86	0.57
1:A:757:PRO:C	1:A:759:CYS:H	2.06	0.57
1:A:906:TRP:O	1:A:910:GLU:HB2	2.05	0.57
1:A:391:ASP:HB2	1:A:591:ARG:NH1	2.16	0.57
1:A:726:ILE:O	1:A:730:THR:OG1	2.22	0.57
1:B:560:ASP:O	1:B:561:GLU:HB2	2.05	0.56
1:A:763:LYS:HZ1	1:B:788:PRO:HG2	1.70	0.56
3:Y:4:DG:H2"	3:Y:5:DA:OP2	2.05	0.56
1:B:663:GLY:HA3	1:B:699:TYR:CZ	2.40	0.56
3:V:4:DG:H2"	3:V:5:DA:OP2	2.05	0.56
1:B:898:LEU:HD11	1:B:937:GLY:H	1.71	0.56
1:A:898:LEU:HD11	1:A:937:GLY:H	1.70	0.56
1:A:845:LEU:C	1:A:846:LEU:HD12	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:12:DG:H2"	2:U:13:DA:OP2	2.06	0.56
1:A:663:GLY:HA3	1:A:699:TYR:CZ	2.41	0.55
1:A:785:ARG:HG2	1:A:1009:VAL:HB	1.88	0.55
1:B:587:TYR:CD1	1:B:859:PHE:CD2	2.94	0.55
3:V:1:DG:C6	3:V:2:DC:N4	2.74	0.55
1:A:856:PRO:O	1:A:857:ASP:HB2	2.07	0.55
1:A:377:ARG:O	1:A:381:VAL:HG23	2.07	0.54
1:B:738:VAL:O	1:B:743:ARG:NH1	2.40	0.54
1:B:578:ASN:O	1:B:582:MET:HG3	2.07	0.54
1:A:642:LYS:O	1:A:643:ASN:HB2	2.07	0.54
1:B:382:VAL:O	1:B:386:VAL:HG23	2.07	0.54
1:B:906:TRP:O	1:B:910:GLU:HB2	2.08	0.54
1:B:784:GLY:O	1:B:1008:ALA:HA	2.08	0.54
1:A:584:PHE:CE2	1:A:863:CYS:O	2.61	0.53
3:Y:2:DC:H2"	3:Y:3:DT:H5'	1.91	0.53
1:A:977:LYS:HD2	1:A:981:ASP:OD1	2.09	0.53
1:B:681:HIS:HA	1:B:683:TYR:CE1	2.44	0.52
1:A:506:GLN:HG3	1:A:507:ARG:HG3	1.91	0.52
1:A:374:TYR:OH	2:X:19:DC:OP2	2.24	0.52
1:B:754:ARG:HG3	1:B:755:GLU:N	2.24	0.52
1:B:858:VAL:HG23	1:B:859:PHE:CD1	2.44	0.52
1:A:377:ARG:HH11	1:A:377:ARG:CB	2.20	0.52
1:B:733:LEU:O	1:B:743:ARG:NH2	2.43	0.52
1:B:849:ILE:HG23	1:B:852:MET:HE1	1.90	0.52
1:A:716:HIS:O	1:A:720:LYS:HA	2.10	0.52
1:A:458:THR:HG22	1:A:460:SER:H	1.75	0.51
1:B:653:LEU:HD23	1:B:654:PRO:HD2	1.92	0.51
1:A:681:HIS:HA	1:A:683:TYR:CE1	2.46	0.51
2:X:4:DC:H42	4:Z:7:DG:H1	1.59	0.51
1:A:431:MET:SD	1:A:447:ILE:HD13	2.50	0.51
1:A:995:GLN:O	1:A:998:GLY:N	2.39	0.51
1:A:891:HIS:CD2	1:A:938:PRO:HA	2.46	0.50
1:B:682:MET:HB3	1:B:685:GLU:HG3	1.93	0.50
1:A:458:THR:CG2	1:A:459:GLU:N	2.74	0.50
1:B:656:PHE:CE2	1:B:858:VAL:HG12	2.47	0.50
1:A:858:VAL:HG23	1:A:859:PHE:CD2	2.47	0.50
1:B:757:PRO:O	1:B:759:CYS:N	2.45	0.50
3:Y:1:DG:H5"	4:W:7:DG:H2"	1.93	0.50
1:B:464:GLU:O	1:B:468:VAL:HG23	2.12	0.49
1:A:585:PRO:HD3	1:A:913:VAL:O	2.13	0.49
1:B:391:ASP:H	1:B:591:ARG:HH22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:4:DC:H2''	4:Z:5:DG:O5'	2.12	0.49
1:A:733:LEU:O	1:A:743:ARG:NH2	2.46	0.49
1:A:830:GLY:HA2	1:A:963:VAL:HA	1.95	0.49
1:A:721:ARG:NH2	1:A:723:GLU:H	2.11	0.49
1:B:374:TYR:OH	2:U:19:DC:OP2	2.21	0.48
1:A:784:GLY:HA3	1:A:817:LEU:HD21	1.94	0.48
1:B:891:HIS:CD2	1:B:938:PRO:HA	2.48	0.48
1:A:682:MET:HB3	1:A:685:GLU:HG3	1.95	0.48
1:B:726:ILE:O	1:B:730:THR:OG1	2.31	0.48
1:A:673:PHE:HA	1:A:676:ILE:HD12	1.96	0.48
1:A:752:ARG:NH2	4:W:3:DG:H5''	2.27	0.48
1:A:757:PRO:O	1:A:759:CYS:N	2.47	0.48
1:B:774:VAL:HG13	1:B:992:ALA:HB2	1.95	0.48
1:A:556:ASP:O	1:A:560:ASP:N	2.45	0.48
1:B:931:LEU:HD11	1:B:962:VAL:HG11	1.95	0.48
1:A:891:HIS:HD2	1:A:938:PRO:HA	1.78	0.48
1:A:980:ASN:ND2	2:U:6:DC:H2'	2.29	0.47
2:U:11:DA:H2''	2:U:12:DG:C8	2.49	0.47
1:A:484:PHE:CE2	1:A:523:ILE:HG12	2.49	0.47
1:A:762:PHE:HB2	1:A:764:HIS:HD2	1.78	0.47
1:A:815:GLU:HG2	1:A:832:HIS:CE1	2.49	0.47
1:A:942:GLY:HA3	1:A:997:LEU:HD21	1.96	0.47
1:B:377:ARG:O	1:B:381:VAL:HG23	2.13	0.47
1:B:766:PHE:O	1:B:768:GLN:N	2.48	0.47
1:B:553:SER:HB2	1:B:557:SER:HB3	1.97	0.47
1:A:382:VAL:O	1:A:386:VAL:HG23	2.15	0.46
1:A:738:VAL:O	1:A:743:ARG:NH1	2.48	0.46
1:B:444:THR:N	1:B:445:PRO:HD2	2.30	0.46
1:B:538:CYS:HB3	1:B:541:PRO:HD2	1.96	0.46
1:A:444:THR:N	1:A:445:PRO:HD2	2.30	0.46
1:A:559:GLU:C	1:A:561:GLU:H	2.19	0.46
1:B:642:LYS:O	1:B:643:ASN:HB2	2.16	0.46
1:B:977:LYS:HD2	1:B:981:ASP:OD1	2.16	0.46
1:A:710:ARG:HA	1:A:710:ARG:HD2	1.55	0.46
1:B:906:TRP:CD1	1:B:906:TRP:C	2.89	0.46
1:B:891:HIS:HD2	1:B:938:PRO:HA	1.81	0.46
1:B:716:HIS:O	1:B:720:LYS:HA	2.15	0.45
1:B:400:GLU:HA	1:B:403:ILE:HD12	1.97	0.45
1:B:815:GLU:HG2	1:B:832:HIS:CE1	2.51	0.45
2:U:8:DC:H2''	2:U:9:DC:C6	2.51	0.45
1:B:762:PHE:HB2	1:B:764:HIS:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLN:HA	1:A:568:GLN:OE1	2.17	0.45
1:A:833:GLY:HA3	1:A:837:THR:OG1	2.16	0.45
1:B:702:ASP:OD1	1:B:702:ASP:N	2.48	0.44
1:A:706:ARG:HE	2:U:0:DT:H5'	1.83	0.44
1:A:424:ARG:HD2	2:X:17:DC:OP1	2.17	0.44
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.68	0.44
1:A:725:THR:O	1:A:729:ILE:HG13	2.17	0.44
1:B:484:PHE:CE2	1:B:523:ILE:HG12	2.52	0.44
1:A:400:GLU:HA	1:A:403:ILE:HD12	1.98	0.44
1:A:538:CYS:HB3	1:A:541:PRO:HD2	1.99	0.44
1:A:672:ARG:O	1:A:675:GLU:HB2	2.18	0.44
1:B:735:ASP:HA	1:B:736:PRO:HD2	1.90	0.44
1:A:739:ARG:O	1:A:740:THR:C	2.56	0.44
1:B:421:LEU:HD21	1:B:434:LEU:HD21	2.00	0.43
1:B:424:ARG:HD2	2:U:17:DC:OP1	2.17	0.43
1:B:739:ARG:O	1:B:740:THR:C	2.56	0.43
1:A:903:ALA:O	1:A:907:HIS:ND1	2.52	0.43
2:U:5:DA:H1'	2:U:6:DC:H5'	1.99	0.43
1:B:685:GLU:HG2	1:B:685:GLU:H	1.20	0.43
1:B:783:THR:HA	1:B:1007:VAL:O	2.18	0.43
1:B:441:LEU:HA	1:B:441:LEU:HD12	1.90	0.43
1:B:895:GLU:O	1:B:899:ARG:HG3	2.19	0.43
1:B:939:VAL:HA	1:B:997:LEU:HD22	2.01	0.43
1:B:420:ARG:O	1:B:424:ARG:HG2	2.18	0.43
1:B:506:GLN:HG3	1:B:507:ARG:HG3	1.99	0.43
1:B:551:LEU:O	1:B:554:LEU:HB2	2.18	0.43
1:B:673:PHE:HA	1:B:676:ILE:HD12	2.00	0.43
1:A:494:GLN:OE1	1:A:494:GLN:HA	2.18	0.42
1:A:759:CYS:C	1:A:761:LYS:H	2.22	0.42
1:A:423:GLN:HE21	1:A:576:LEU:HD22	1.83	0.42
1:B:477:LEU:HA	1:B:477:LEU:HD23	1.88	0.42
1:B:378:SER:HB3	1:B:579:LEU:HB3	2.01	0.42
1:B:894:PRO:C	1:B:896:GLU:H	2.23	0.42
1:B:431:MET:SD	1:B:447:ILE:HD13	2.59	0.42
1:B:715:LEU:HD13	1:B:724:PRO:HB2	2.01	0.42
1:B:894:PRO:O	1:B:896:GLU:N	2.51	0.42
4:W:4:DC:H2''	4:W:5:DG:O5'	2.19	0.42
1:A:642:LYS:O	1:A:643:ASN:CB	2.67	0.42
1:B:721:ARG:HG3	1:B:724:PRO:HG2	2.00	0.42
1:B:721:ARG:NH2	1:B:723:GLU:H	2.17	0.42
1:B:995:GLN:O	1:B:998:GLY:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD12	1:A:441:LEU:HA	1.87	0.42
1:B:849:ILE:HG23	1:B:852:MET:CE	2.49	0.42
1:A:464:GLU:O	1:A:468:VAL:HG23	2.20	0.42
1:B:849:ILE:HA	1:B:852:MET:HE3	2.02	0.42
2:U:11:DA:H2"	2:U:12:DG:OP2	2.20	0.42
1:A:829:GLN:HB2	1:A:964:TRP:O	2.19	0.42
1:B:903:ALA:O	1:B:907:HIS:ND1	2.53	0.42
1:A:653:LEU:HD23	1:A:654:PRO:HD2	2.02	0.42
1:A:766:PHE:O	1:A:768:GLN:N	2.53	0.42
1:A:762:PHE:HB2	1:A:764:HIS:CD2	2.54	0.41
1:B:418:TYR:CE1	1:B:537:ILE:HD11	2.55	0.41
1:B:494:GLN:HA	1:B:494:GLN:OE1	2.19	0.41
1:A:834:GLU:HG2	1:A:960:ASP:HA	2.01	0.41
1:B:759:CYS:C	1:B:761:LYS:H	2.23	0.41
1:B:777:VAL:HG22	1:B:995:GLN:NE2	2.35	0.41
1:B:749:ARG:O	1:B:753:LEU:HB2	2.20	0.41
1:A:670:LEU:O	1:A:673:PHE:HB3	2.20	0.41
2:X:8:DC:H2"	2:X:9:DC:C6	2.54	0.41
1:A:557:SER:O	1:A:563:ALA:HB2	2.20	0.41
1:A:553:SER:HB3	1:A:558:MET:HB3	2.01	0.41
1:A:840:THR:HB	1:A:917:VAL:HA	2.02	0.41
1:A:968:SER:O	1:A:969:ARG:HB2	2.21	0.41
1:A:553:SER:O	1:A:559:GLU:CB	2.58	0.41
1:B:828:ASP:OD2	1:B:966:SER:HB2	2.21	0.41
1:A:757:PRO:C	1:A:759:CYS:N	2.74	0.41
1:B:706:ARG:HA	1:B:742:HIS:CE1	2.56	0.41
1:A:721:ARG:NH1	1:A:721:ARG:HA	2.36	0.40
1:A:739:ARG:HG3	1:A:953:HIS:CD2	2.56	0.40
1:B:757:PRO:C	1:B:759:CYS:N	2.73	0.40
1:A:977:LYS:HD3	1:A:977:LYS:HA	1.90	0.40
1:B:874:SER:HA	1:B:877:THR:OG1	2.21	0.40
1:B:880:ARG:HB3	1:B:881:PRO:HD3	2.02	0.40
1:A:721:ARG:HG3	1:A:724:PRO:HG2	2.01	0.40
1:B:775:GLN:H	1:B:775:GLN:HG3	1.72	0.40
1:A:685:GLU:HG2	1:A:685:GLU:H	1.21	0.40
1:B:458:THR:CG2	1:B:459:GLU:N	2.85	0.40
1:B:762:PHE:HB2	1:B:764:HIS:CD2	2.56	0.40
1:B:880:ARG:N	1:B:881:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	609/651 (94%)	537 (88%)	60 (10%)	12 (2%)	7	33
1	B	624/651 (96%)	545 (87%)	66 (11%)	13 (2%)	7	32
All	All	1233/1302 (95%)	1082 (88%)	126 (10%)	25 (2%)	7	33

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	GLU
1	A	760	LYS
1	A	767	GLN
1	B	561	GLU
1	B	760	LYS
1	B	767	GLN
1	A	740	THR
1	A	758	SER
1	A	937	GLY
1	B	758	SER
1	B	937	GLY
1	A	568	GLN
1	B	459	GLU
1	B	740	THR
1	B	895	GLU
1	A	643	ASN
1	A	895	GLU
1	B	566	GLY
1	A	556	ASP
1	B	643	ASN
1	A	881	PRO
1	B	881	PRO
1	B	788	PRO
1	A	757	PRO
1	B	757	PRO

### 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	538/563 (96%)	500 (93%)	38 (7%)	14	42
1	B	547/563 (97%)	503 (92%)	44 (8%)	12	37
All	All	1085/1126 (96%)	1003 (92%)	82 (8%)	13	39

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	ARG
1	A	405	THR
1	A	424	ARG
1	A	426	LEU
1	A	479	SER
1	A	525	LYS
1	A	537	ILE
1	A	539	LYS
1	A	560	ASP
1	A	561	GLU
1	A	562	ASP
1	A	586	SER
1	A	592	LYS
1	A	649	CYS
1	A	652	ASP
1	A	662	VAL
1	A	671	SER
1	A	674	VAL
1	A	685	GLU
1	A	692	SER
1	A	697	ARG
1	A	710	ARG
1	A	721	ARG
1	A	730	THR
1	A	754	ARG
1	A	771	GLU
1	A	780	VAL

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Mol	Chain	Res	Type
1	A	783	THR
1	A	817	LEU
1	A	840	THR
1	A	872	THR
1	A	895	GLU
1	A	910	GLU
1	A	918	SER
1	A	921	ARG
1	A	961	LEU
1	A	967	GLN
1	A	969	ARG
1	B	377	ARG
1	B	405	THR
1	B	424	ARG
1	B	426	LEU
1	B	460	SER
1	B	479	SER
1	B	525	LYS
1	B	537	ILE
1	B	539	LYS
1	B	554	LEU
1	B	571	LEU
1	B	586	SER
1	B	592	LYS
1	B	649	CYS
1	B	652	ASP
1	B	662	VAL
1	B	671	SER
1	B	672	ARG
1	B	674	VAL
1	B	685	GLU
1	B	692	SER
1	B	697	ARG
1	B	710	ARG
1	B	721	ARG
1	B	730	THR
1	B	738	VAL
1	B	754	ARG
1	B	768	GLN
1	B	771	GLU
1	B	780	VAL
1	B	783	THR

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Mol	Chain	Res	Type
1	B	790	ARG
1	B	806	ASP
1	B	808	THR
1	B	840	THR
1	B	895	GLU
1	B	905	THR
1	B	910	GLU
1	B	918	SER
1	B	921	ARG
1	B	932	VAL
1	B	961	LEU
1	B	967	GLN
1	B	969	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	GLN
1	A	597	GLN
1	A	610	HIS
1	A	764	HIS
1	A	832	HIS
1	A	891	HIS
1	A	953	HIS
1	B	423	GLN
1	B	452	ASN
1	B	488	ASN
1	B	492	GLN
1	B	597	GLN
1	B	610	HIS
1	B	764	HIS
1	B	832	HIS
1	B	891	HIS
1	B	953	HIS
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 carbohydrates 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, 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	615/651 (94%)	0.02	17 (2%) 53 50	58, 96, 149, 178	0
1	B	628/651 (96%)	0.13	28 (4%) 33 31	67, 101, 153, 183	0
2	U	20/20 (100%)	-0.91	0 100 100	103, 111, 118, 120	0
2	X	20/20 (100%)	-0.50	0 100 100	79, 97, 130, 138	0
3	V	12/12 (100%)	-0.63	0 100 100	106, 122, 140, 144	0
3	Y	12/12 (100%)	-0.72	0 100 100	88, 105, 117, 119	0
4	W	7/14 (50%)	-0.78	0 100 100	75, 82, 111, 114	0
4	Z	7/14 (50%)	-0.21	0 100 100	70, 77, 98, 120	0
All	All	1321/1394 (94%)	0.03	45 (3%) 45 42	58, 98, 150, 183	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	370	THR	4.8
1	B	804	ALA	4.7
1	B	558	MET	4.5
1	B	801	ALA	4.5
1	B	806	ASP	4.2
1	A	558	MET	4.0
1	A	764	HIS	3.9
1	B	805	ALA	3.5
1	A	1009	VAL	3.5
1	A	772	MET	3.5
1	B	790	ARG	3.4
1	A	784	GLY	3.3
1	B	488	ASN	3.3
1	B	802	GLY	3.0
1	A	810	VAL	2.9
1	A	1008	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	807	PRO	2.9
1	A	1007	VAL	2.9
1	A	811	LEU	2.8
1	B	455	PHE	2.7
1	B	396	PHE	2.7
1	A	799	MET	2.7
1	B	803	GLU	2.6
1	A	562	ASP	2.4
1	B	800	GLU	2.4
1	A	1006	VAL	2.4
1	B	768	GLN	2.4
1	A	797	PHE	2.3
1	B	811	LEU	2.3
1	B	379	PHE	2.3
1	A	798	VAL	2.3
1	B	456	LEU	2.3
1	B	810	VAL	2.3
1	B	775	GLN	2.2
1	B	785	ARG	2.2
1	B	809	THR	2.2
1	A	785	ARG	2.2
1	B	788	PRO	2.1
1	B	537	ILE	2.1
1	A	786	LEU	2.1
1	A	794	LYS	2.1
1	B	794	LYS	2.0
1	B	789	GLN	2.0
1	B	563	ALA	2.0
1	B	440	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	A	1101	1/1	0.93	0.10	105,105,105,105	0
5	CA	B	1101	1/1	0.94	0.14	85,85,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.