



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:46 pm GMT

PDB ID : 3GOD  
Title : Structural basis for DNase activity of a conserved protein implicated in CRISPR-mediated antiviral defense  
Authors : Wiedenheft, B.  
Deposited on : 2009-03-18  
Resolution : 2.17 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

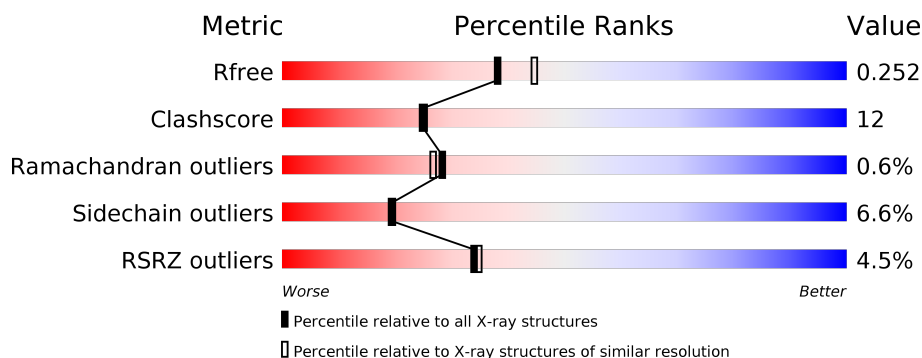
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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))
$R_{free}$	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	328	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	328	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>5%</div> <div>11%</div> </div> </div>
1	D	328	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10442 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 Cas1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	Se	0	5	0
			2556	1608	473	469	3	3			
1	B	319	Total	C	N	O	S	Se	0	2	0
			2528	1592	468	462	3	3			
1	C	293	Total	C	N	O	S	Se	0	1	0
			2305	1448	431	420	3	3			
1	D	299	Total	C	N	O	S	Se	0	1	0
			2359	1485	442	426	3	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q02ML7
A	-2	SER	-	EXPRESSION TAG	UNP Q02ML7
A	-1	PHE	-	EXPRESSION TAG	UNP Q02ML7
A	0	THR	-	EXPRESSION TAG	UNP Q02ML7
B	-3	GLY	-	EXPRESSION TAG	UNP Q02ML7
B	-2	SER	-	EXPRESSION TAG	UNP Q02ML7
B	-1	PHE	-	EXPRESSION TAG	UNP Q02ML7
B	0	THR	-	EXPRESSION TAG	UNP Q02ML7
C	-3	GLY	-	EXPRESSION TAG	UNP Q02ML7
C	-2	SER	-	EXPRESSION TAG	UNP Q02ML7
C	-1	PHE	-	EXPRESSION TAG	UNP Q02ML7
C	0	THR	-	EXPRESSION TAG	UNP Q02ML7
D	-3	GLY	-	EXPRESSION TAG	UNP Q02ML7
D	-2	SER	-	EXPRESSION TAG	UNP Q02ML7
D	-1	PHE	-	EXPRESSION TAG	UNP Q02ML7
D	0	THR	-	EXPRESSION TAG	UNP Q02ML7

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	A	1	Total 1	Na 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

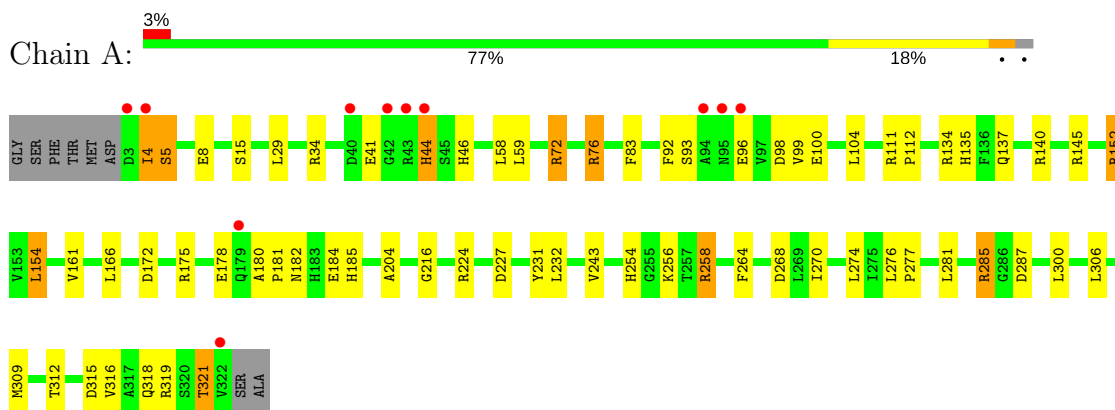
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total 214	O 214	0	0
5	B	198	Total 198	O 198	0	0
5	C	126	Total 126	O 126	0	0
5	D	148	Total 148	O 148	0	0

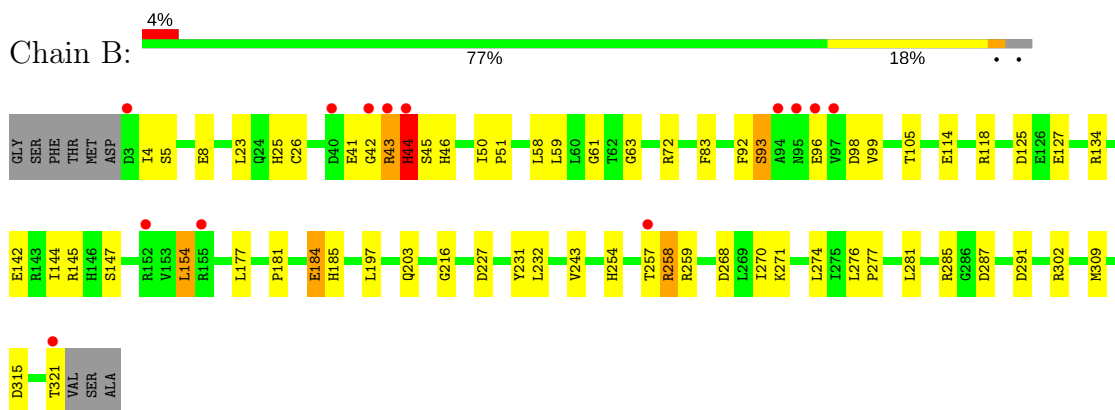
### 3 Residue-property plots

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.

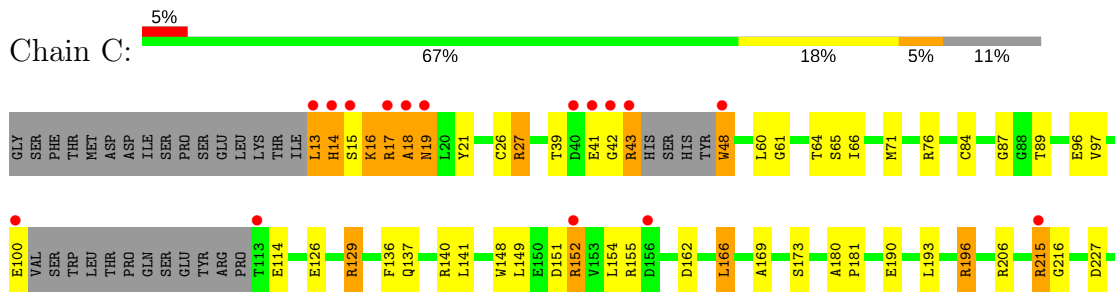
#### • Molecule 1: Cas1



#### • Molecule 1: Cas1

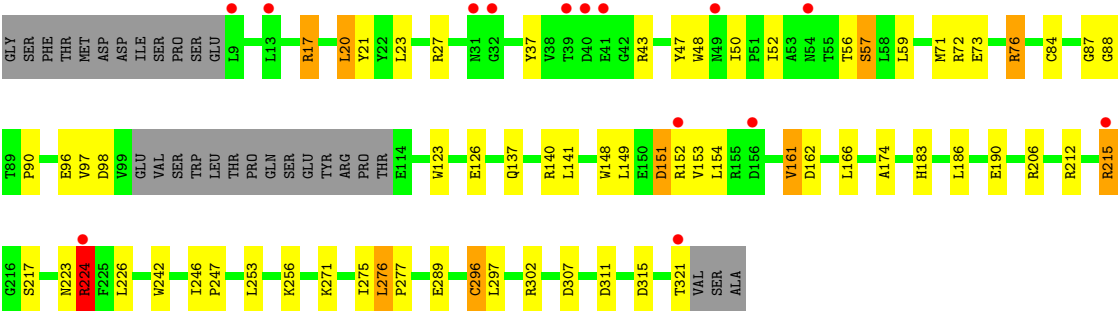


#### • Molecule 1: Cas1





● Molecule 1: Cas1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.87Å 110.96Å 130.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.17 17.97 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.7 (17.97-2.17) 100.0 (17.97-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.203 , 0.258 0.198 , 0.252	Depositor DCC
$R_{free}$ test set	8115 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8468e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, MN

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	0.85	0/2618	0.85	4/3541 (0.1%)
1	B	0.83	0/2584	0.84	2/3494 (0.1%)
1	C	0.88	1/2347 (0.0%)	0.93	7/3166 (0.2%)
1	D	0.90	1/2405 (0.0%)	0.87	5/3246 (0.2%)
All	All	0.86	2/9954 (0.0%)	0.87	18/13447 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	296	CYS	CB-SG	-11.32	1.63	1.82
1	C	42	GLY	C-N	7.03	1.50	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	GLY	O-C-N	-10.55	105.83	122.70
1	C	42	GLY	C-N-CA	8.79	143.68	121.70
1	A	224	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	42	GLY	CA-C-N	6.86	132.29	117.20
1	D	224[A]	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	D	224[B]	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	76	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	72	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	D	72	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	285	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	D	43	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	C	129	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	224	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	259	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	166	LEU	CA-CB-CG	-5.19	103.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	72	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	315	ASP	CB-CG-OD1	-5.03	113.77	118.30

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	2556	0	2528	55	0
1	B	2528	0	2504	48	0
1	C	2305	0	2284	87	0
1	D	2359	0	2342	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	214	0	0	6	0
5	B	198	0	0	8	0
5	C	126	0	0	4	0
5	D	148	0	0	9	0
All	All	10442	0	9658	237	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 12.

All (237) 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:C:18:ALA:C	1:C:19:ASN:HD22	1.45	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:HG2	1:C:27:ARG:HH11	1.18	1.04
1:C:285:ARG:HH11	1:C:285:ARG:HG2	1.20	0.99
1:D:96:GLU:HG2	5:D:545:HOH:O	1.62	0.99
1:A:254:HIS:HE1	1:A:268:ASP:OD2	1.51	0.92
1:A:76[B]:ARG:HH11	1:A:76[B]:ARG:HG3	1.34	0.92
1:B:43:ARG:HG2	1:B:44:HIS:N	1.83	0.91
1:C:100:GLU:HB3	1:C:114:GLU:HB2	1.54	0.88
1:A:72:ARG:O	1:A:76[B]:ARG:HG2	1.72	0.88
1:C:43:ARG:HD2	1:C:43:ARG:N	1.89	0.88
1:A:76[B]:ARG:NH1	1:A:76[B]:ARG:HG3	1.89	0.87
1:C:18:ALA:C	1:C:19:ASN:ND2	2.29	0.85
1:B:302:ARG:HD3	5:B:569:HOH:O	1.77	0.85
1:C:96:GLU:HG2	5:C:666:HOH:O	1.77	0.83
1:B:93:SER:OG	1:B:98:ASP:OD1	1.96	0.82
1:C:19:ASN:N	1:C:19:ASN:HD22	1.76	0.82
1:C:27:ARG:CG	1:C:27:ARG:HH11	1.90	0.81
1:D:97:VAL:HG23	5:D:551:HOH:O	1.81	0.80
1:C:27:ARG:HG2	1:C:27:ARG:NH1	1.89	0.79
1:D:151:ASP:OD2	1:D:153:VAL:HG22	1.81	0.79
1:C:14:HIS:HB2	1:C:21:TYR:CD1	2.18	0.79
1:C:152:ARG:HB2	1:C:152:ARG:NH2	1.97	0.78
1:A:4:ILE:HG23	1:A:4:ILE:O	1.83	0.78
1:D:153:VAL:HG21	1:D:302:ARG:CZ	2.14	0.78
1:D:215:ARG:HD2	5:D:396:HOH:O	1.83	0.77
1:C:285:ARG:CG	1:C:285:ARG:HH11	1.97	0.75
1:C:100:GLU:HB3	1:C:114:GLU:CB	2.16	0.74
1:C:14:HIS:HB2	1:C:21:TYR:HD1	1.52	0.74
1:C:15:SER:H	1:C:16:LYS:HD2	1.52	0.74
1:B:254:HIS:HE1	1:B:268:ASP:OD2	1.73	0.72
1:C:14:HIS:HB3	1:C:21:TYR:HB3	1.70	0.72
1:D:153:VAL:HG21	1:D:302:ARG:NH1	2.06	0.70
1:A:274:LEU:HD13	1:A:300:LEU:HD23	1.73	0.70
1:C:152:ARG:HH21	1:C:152:ARG:HB2	1.54	0.70
1:C:43:ARG:H	1:C:43:ARG:HD2	1.55	0.70
1:A:318:GLN:O	1:A:321:THR:HG22	1.93	0.69
1:C:169:ALA:CB	1:C:196:ARG:HD2	2.22	0.69
1:C:15:SER:N	1:C:16:LYS:HD2	2.08	0.68
1:B:43:ARG:CG	1:B:44:HIS:N	2.57	0.68
1:C:100:GLU:H	1:C:114:GLU:HG2	1.60	0.67
1:D:276:LEU:HB3	1:D:277:PRO:HD3	1.77	0.67
1:C:100:GLU:HG3	1:C:100:GLU:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ARG:HG2	1:C:18:ALA:H	1.58	0.67
1:C:17:ARG:HG2	1:C:18:ALA:N	2.11	0.66
1:B:203:GLN:HG3	5:B:641:HOH:O	1.95	0.66
1:C:14:HIS:HB3	1:C:21:TYR:CB	2.26	0.66
1:C:27:ARG:HG3	1:C:65:SER:OG	1.96	0.66
1:D:123:TRP:CZ2	1:D:256:LYS:HG2	2.30	0.66
1:C:13:LEU:C	1:C:14:HIS:CG	2.69	0.65
1:D:140:ARG:NH1	1:D:190:GLU:HG2	2.11	0.65
1:B:134:ARG:HG2	1:B:177:LEU:HD21	1.78	0.65
1:D:206:ARG:NH1	1:D:206:ARG:HB2	2.12	0.64
1:A:135:HIS:CE1	1:A:315[A]:ASP:OD2	2.50	0.64
1:C:43:ARG:CD	1:C:43:ARG:N	2.60	0.64
1:C:206:ARG:HB2	1:C:206:ARG:NH1	2.12	0.64
1:C:114:GLU:HG3	5:C:674:HOH:O	1.96	0.64
1:C:43:ARG:H	1:C:43:ARG:CD	2.11	0.64
1:D:20:LEU:HD11	1:D:59:LEU:HG	1.80	0.63
1:A:76[A]:ARG:HH11	1:A:76[A]:ARG:HG3	1.63	0.63
1:B:181:PRO:HD2	1:B:185:HIS:CG	2.34	0.63
1:D:271:LYS:HE3	5:D:669:HOH:O	1.99	0.63
1:D:140:ARG:HH12	1:D:190:GLU:HG2	1.63	0.63
1:D:206:ARG:HB2	1:D:206:ARG:HH11	1.63	0.62
1:A:4:ILE:CG2	1:A:4:ILE:O	2.47	0.62
1:B:270:ILE:HG12	1:B:309:MSE:HE3	1.81	0.62
1:B:274:LEU:HG	5:B:546:HOH:O	1.99	0.62
1:C:16:LYS:CD	1:C:16:LYS:N	2.61	0.62
1:A:145:ARG:NH1	1:A:145:ARG:HB3	2.14	0.62
1:A:72:ARG:NH2	5:A:679:HOH:O	2.04	0.62
1:B:315:ASP:HB3	5:B:601:HOH:O	2.00	0.61
1:D:97:VAL:CG2	5:D:551:HOH:O	2.45	0.61
1:A:216:GLY:HA2	1:A:227:ASP:OD2	2.00	0.61
1:C:89:THR:OG1	1:C:235:GLY:HA3	2.00	0.61
1:D:17:ARG:NH2	1:D:311:ASP:OD2	2.32	0.61
1:D:123:TRP:CH2	1:D:256:LYS:HG2	2.35	0.61
1:A:258:ARG:HG2	1:A:264:PHE:CD2	2.36	0.61
1:A:41:GLU:HB2	1:A:44:HIS:O	2.01	0.61
1:B:254:HIS:CE1	1:B:268:ASP:OD2	2.54	0.60
1:C:285:ARG:NH1	1:C:285:ARG:HG2	2.02	0.60
1:B:154:LEU:CD1	1:B:281:LEU:HD11	2.31	0.60
1:C:14:HIS:HB3	1:C:21:TYR:CA	2.32	0.60
1:D:21:TYR:CD1	1:D:50:ILE:HG12	2.38	0.59
1:D:52:ILE:O	1:D:52:ILE:HG22	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:CD	1:C:16:LYS:H	2.15	0.59
1:A:76[B]:ARG:HH11	1:A:76[B]:ARG:CG	2.07	0.59
1:C:215:ARG:N	5:C:685:HOH:O	2.36	0.58
1:A:181:PRO:HD2	1:A:185:HIS:CG	2.39	0.58
1:D:20:LEU:HD13	1:D:57:SER:HB3	1.84	0.58
1:C:100:GLU:C	1:C:114:GLU:HB3	2.23	0.58
1:C:169:ALA:HB1	1:C:196:ARG:HD2	1.86	0.58
1:B:105:THR:HG23	5:D:545:HOH:O	2.04	0.58
1:B:114:GLU:O	1:B:118:ARG:HG3	2.04	0.58
1:B:259:ARG:HD3	1:D:98:ASP:OD2	2.05	0.57
1:C:126:GLU:OE1	1:C:129:ARG:HD3	2.05	0.56
1:B:216:GLY:HA2	1:B:227:ASP:OD2	2.06	0.56
1:A:100:GLU:OE2	1:A:258:ARG:NH2	2.38	0.55
1:B:41:GLU:HB2	1:B:44:HIS:CB	2.37	0.55
1:D:126:GLU:OE1	1:D:126:GLU:HA	2.07	0.55
1:D:97:VAL:HG21	1:D:242:TRP:O	2.07	0.55
1:C:315:ASP:HB3	1:C:319:ARG:NH1	2.21	0.54
1:A:93:SER:OG	1:A:98:ASP:OD1	2.19	0.54
1:C:148:TRP:CE3	1:C:166:LEU:HD13	2.41	0.54
1:C:100:GLU:N	1:C:114:GLU:HG2	2.21	0.54
1:D:87:GLY:HA3	1:D:297:LEU:HD13	1.90	0.53
1:B:83:PHE:CE2	1:D:71:MSE:HG3	2.43	0.53
1:C:169:ALA:HB2	1:C:196:ARG:HD2	1.89	0.53
1:B:257:THR:O	1:B:258:ARG:HD3	2.08	0.53
1:C:18:ALA:CA	1:C:19:ASN:HD22	2.19	0.53
1:B:285:ARG:NH2	5:B:609:HOH:O	2.28	0.53
1:A:135:HIS:HE1	1:A:315[A]:ASP:OD2	1.93	0.52
1:A:83:PHE:HE2	1:A:104:LEU:HD11	1.74	0.52
1:C:270:ILE:C	1:C:270:ILE:HD12	2.29	0.52
5:A:429:HOH:O	1:D:224[B]:ARG:HD3	2.08	0.52
1:B:134:ARG:HG2	1:B:177:LEU:CD2	2.38	0.52
1:D:27:ARG:HG3	5:D:426:HOH:O	2.09	0.52
1:B:41:GLU:HB2	1:B:44:HIS:HB3	1.91	0.52
1:D:73:GLU:OE2	1:D:76:ARG:NH1	2.43	0.52
1:C:141:LEU:HD21	1:C:193:LEU:HD22	1.91	0.52
1:A:285:ARG:NH2	1:A:287:ASP:OD2	2.42	0.52
1:C:293:ARG:NH1	1:C:297:LEU:HD11	2.25	0.52
1:D:17:ARG:HH11	1:D:17:ARG:HG3	1.74	0.52
1:C:97:VAL:HG21	1:C:242:TRP:O	2.10	0.51
1:C:285:ARG:CG	1:C:285:ARG:NH1	2.65	0.51
1:A:270:ILE:HG12	1:A:309:MSE:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:N	1:C:16:LYS:HD2	2.24	0.51
1:A:137:GLN:HE22	1:A:140[B]:ARG:HH11	1.57	0.51
1:A:172:ASP:OD1	1:A:175:ARG:NH2	2.40	0.51
1:C:136:PHE:HE2	1:C:316:VAL:HG21	1.75	0.51
1:C:173:SER:OG	1:C:193:LEU:HD13	2.11	0.50
1:C:216:GLY:HA2	1:C:227:ASP:OD2	2.11	0.50
1:A:76[A]:ARG:HG3	1:A:76[A]:ARG:NH1	2.26	0.50
1:C:14:HIS:HB3	1:C:21:TYR:HA	1.92	0.50
1:D:247:PRO:HA	5:D:596:HOH:O	2.10	0.50
1:A:182:ASN:HB3	5:A:436:HOH:O	2.12	0.50
1:B:271[B]:LYS:HD2	5:B:535:HOH:O	2.12	0.49
1:C:48:TRP:HA	1:C:48:TRP:CE3	2.47	0.49
1:D:17:ARG:NH1	1:D:17:ARG:HG3	2.28	0.49
1:B:41:GLU:HG3	1:B:46:HIS:CG	2.47	0.49
1:B:125:ASP:OD1	1:B:127:GLU:HG2	2.13	0.49
1:A:41:GLU:HG3	1:A:46:HIS:CG	2.48	0.48
1:A:181:PRO:HD2	1:A:185:HIS:CD2	2.49	0.48
1:A:41:GLU:HG3	1:A:46:HIS:CD2	2.48	0.48
1:A:161:VAL:HA	1:A:204:ALA:HB2	1.95	0.48
1:A:321:THR:HG23	1:A:321:THR:O	2.14	0.48
1:C:13:LEU:O	1:C:14:HIS:CG	2.66	0.48
1:D:141:LEU:HD13	1:D:174:ALA:HB2	1.95	0.48
1:A:276:LEU:HB3	1:A:277:PRO:HD3	1.96	0.48
1:A:72:ARG:NH1	5:A:415:HOH:O	2.39	0.48
1:A:154:LEU:CD1	1:A:281:LEU:HD11	2.45	0.47
1:B:41:GLU:HG3	1:B:46:HIS:CD2	2.48	0.47
1:A:154:LEU:HD12	1:A:281:LEU:HD11	1.95	0.47
1:D:21:TYR:CD2	1:D:21:TYR:N	2.83	0.47
1:B:4:ILE:HG22	1:B:8:GLU:HB2	1.95	0.47
1:C:140:ARG:NH1	1:C:190:GLU:HG2	2.30	0.47
1:A:315[A]:ASP:OD2	1:A:319:ARG:NH1	2.48	0.47
1:C:100:GLU:HB3	1:C:114:GLU:HG2	1.97	0.47
1:A:145:ARG:HH11	1:A:145:ARG:HB3	1.75	0.46
1:D:148:TRP:CE3	1:D:166:LEU:HD13	2.50	0.46
1:D:224[B]:ARG:NH1	5:D:403:HOH:O	2.48	0.46
1:A:178:GLU:OE2	1:A:178:GLU:HA	2.16	0.46
1:C:141:LEU:HD21	1:C:193:LEU:CD2	2.46	0.46
1:B:154:LEU:HD11	1:B:281:LEU:HD11	1.98	0.46
1:C:206:ARG:HB2	1:C:206:ARG:HH11	1.77	0.46
1:B:154:LEU:HD13	1:B:154:LEU:HA	1.73	0.45
1:C:19:ASN:N	1:C:19:ASN:ND2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:HIS:CB	1:C:21:TYR:HD1	2.25	0.45
1:B:59:LEU:HD13	1:B:231:TYR:HB3	1.97	0.45
1:C:16:LYS:H	1:C:16:LYS:HD3	1.82	0.45
1:C:321:THR:C	5:C:681:HOH:O	2.54	0.45
1:A:5:SER:OG	1:A:8[A]:GLU:OE2	2.32	0.45
1:B:154:LEU:HD12	1:B:281:LEU:HD11	1.99	0.45
1:C:100:GLU:HB3	1:C:114:GLU:CG	2.47	0.45
1:C:136:PHE:CE2	1:C:316:VAL:HG21	2.51	0.45
1:C:39:THR:CG2	1:C:43:ARG:HB2	2.47	0.45
1:D:56:THR:HG22	1:D:57:SER:N	2.32	0.45
1:A:166:LEU:HD13	1:A:166:LEU:C	2.38	0.44
1:C:149:LEU:HG	1:C:166:LEU:HD23	2.00	0.44
1:B:276:LEU:HB3	1:B:277:PRO:HD3	1.99	0.44
1:B:92:PHE:CZ	1:B:99:VAL:HG21	2.52	0.44
1:D:17:ARG:HB2	1:D:307:ASP:OD1	2.17	0.44
1:C:14:HIS:CB	1:C:21:TYR:CD1	2.97	0.44
1:A:285:ARG:HD3	5:A:339:HOH:O	2.18	0.44
1:B:25:HIS:HA	1:B:63:GLY:O	2.18	0.44
1:D:149:LEU:HG	1:D:166:LEU:HD23	2.00	0.44
1:B:154:LEU:CD1	1:B:281:LEU:CD1	2.95	0.43
1:C:66:ILE:HD13	1:C:71:MSE:HG2	1.98	0.43
1:B:154:LEU:HD11	1:B:281:LEU:CD1	2.48	0.43
1:C:246:ILE:HA	1:C:247:PRO:HD3	1.87	0.43
1:A:111:ARG:HB3	1:A:112:PRO:HD2	2.01	0.43
1:A:256:LYS:HA	1:A:256:LYS:HD2	1.65	0.43
1:C:27:ARG:HG3	1:C:65:SER:HG	1.83	0.43
1:C:87:GLY:HA3	1:C:297:LEU:HD13	2.01	0.43
1:B:61:GLY:HA3	5:B:366:HOH:O	2.18	0.43
1:A:258:ARG:HG2	1:A:264:PHE:CE2	2.54	0.43
1:B:23:LEU:HB3	1:B:26:CYS:SG	2.58	0.43
1:B:83:PHE:CD2	1:D:71:MSE:HG3	2.53	0.43
1:C:14:HIS:CB	1:C:21:TYR:HA	2.49	0.43
1:C:310:ILE:O	1:C:314:LYS:HG3	2.18	0.43
1:D:212:ARG:HD2	1:D:223:ASN:OD1	2.18	0.43
1:D:226:LEU:HD21	1:D:276:LEU:HD13	2.01	0.43
1:A:34:ARG:NH1	1:D:289:GLU:OE1	2.49	0.43
1:A:152:ARG:HE	1:A:152:ARG:HB2	1.62	0.42
1:A:44:HIS:CD2	1:A:46:HIS:NE2	2.87	0.42
1:B:287:ASP:HB3	1:B:291:ASP:HB2	2.01	0.42
1:D:186:LEU:HA	1:D:186:LEU:HD12	1.89	0.42
1:D:246:ILE:HA	1:D:247:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:THR:O	1:A:316:VAL:HG23	2.19	0.42
1:D:137:GLN:OE1	1:D:140:ARG:NH1	2.47	0.42
1:D:23:LEU:HD22	1:D:47:TYR:CG	2.55	0.42
1:B:285:ARG:NH1	1:B:287:ASP:OD2	2.52	0.42
1:C:149:LEU:HA	1:C:149:LEU:HD23	1.63	0.42
1:C:137:GLN:OE1	1:C:140:ARG:NH1	2.45	0.42
1:A:134:ARG:NH2	1:A:180:ALA:O	2.44	0.41
1:A:15:SER:HA	1:A:306:LEU:HD23	2.02	0.41
1:A:59:LEU:HD13	1:A:231:TYR:HB3	2.02	0.41
1:B:41:GLU:HB2	1:B:44:HIS:HB2	2.01	0.41
1:D:27:ARG:HH11	1:D:27:ARG:HG2	1.84	0.41
1:A:29:LEU:C	1:A:29:LEU:HD12	2.41	0.41
1:B:321:THR:N	5:B:663:HOH:O	2.54	0.41
1:C:100:GLU:H	1:C:114:GLU:CG	2.28	0.41
1:C:126:GLU:OE1	1:C:126:GLU:HA	2.21	0.41
1:C:26:CYS:O	1:C:64:THR:HA	2.20	0.41
1:D:148:TRP:CE3	1:D:161:VAL:HG11	2.55	0.41
1:D:37:TYR:N	1:D:37:TYR:CD2	2.88	0.41
1:D:153:VAL:HG23	1:D:154:LEU:N	2.36	0.41
1:B:50:ILE:HA	1:B:51:PRO:HD3	1.87	0.41
1:B:181:PRO:HD2	1:B:185:HIS:CD2	2.56	0.41
1:A:72:ARG:NE	5:A:679:HOH:O	2.53	0.40
1:A:92:PHE:CZ	1:A:99:VAL:HG21	2.56	0.40
1:B:184:GLU:HG2	1:B:185:HIS:N	2.35	0.40
1:C:180:ALA:HA	1:C:181:PRO:HD3	1.78	0.40
1:C:61:GLY:HA2	1:C:84:CYS:O	2.21	0.40
1:C:137:GLN:HE21	1:C:253:LEU:CD2	2.34	0.40
1:C:18:ALA:HB3	1:C:19:ASN:ND2	2.36	0.40
1:B:144:ILE:HD13	1:B:197:LEU:HD11	2.03	0.40
1:C:149:LEU:HG	1:C:166:LEU:CD2	2.52	0.40
1:D:84:CYS:SG	1:D:88:GLY:HA2	2.61	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	323/328 (98%)	316 (98%)	6 (2%)	1 (0%)	44	47
1	B	319/328 (97%)	310 (97%)	7 (2%)	2 (1%)	28	27
1	C	288/328 (88%)	275 (96%)	11 (4%)	2 (1%)	25	22
1	D	296/328 (90%)	287 (97%)	7 (2%)	2 (1%)	25	22
All	All	1226/1312 (93%)	1188 (97%)	31 (2%)	7 (1%)	28	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	HIS
1	C	162	ASP
1	D	162	ASP
1	B	42	GLY
1	C	18	ALA
1	D	48	TRP
1	A	4	ILE

### 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	263/261 (101%)	250 (95%)	13 (5%)	29	32
1	B	259/261 (99%)	245 (95%)	14 (5%)	26	28
1	C	232/261 (89%)	210 (90%)	22 (10%)	10	8
1	D	238/261 (91%)	220 (92%)	18 (8%)	15	14
All	All	992/1044 (95%)	925 (93%)	67 (7%)	19	18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER

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Mol	Chain	Res	Type
1	A	44	HIS
1	A	58	LEU
1	A	76[A]	ARG
1	A	76[B]	ARG
1	A	96	GLU
1	A	152	ARG
1	A	154	LEU
1	A	184	GLU
1	A	232	LEU
1	A	243	VAL
1	A	258	ARG
1	A	321	THR
1	B	5	SER
1	B	43	ARG
1	B	44	HIS
1	B	45	SER
1	B	58	LEU
1	B	93	SER
1	B	96	GLU
1	B	142	GLU
1	B	145	ARG
1	B	147	SER
1	B	154	LEU
1	B	184	GLU
1	B	232	LEU
1	B	243	VAL
1	C	13	LEU
1	C	14	HIS
1	C	16	LYS
1	C	17	ARG
1	C	19	ASN
1	C	27	ARG
1	C	41	GLU
1	C	43	ARG
1	C	48	TRP
1	C	60	LEU
1	C	151	ASP
1	C	152	ARG
1	C	154	LEU
1	C	155	ARG
1	C	196	ARG
1	C	215	ARG

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Mol	Chain	Res	Type
1	C	236	LEU
1	C	253	LEU
1	C	258	ARG
1	C	271	LYS
1	C	275	ILE
1	C	285	ARG
1	D	17	ARG
1	D	20	LEU
1	D	57	SER
1	D	76	ARG
1	D	90	PRO
1	D	151	ASP
1	D	152	ARG
1	D	161	VAL
1	D	183	HIS
1	D	215	ARG
1	D	217	SER
1	D	224[A]	ARG
1	D	224[B]	ARG
1	D	253	LEU
1	D	275	ILE
1	D	276	LEU
1	D	296	CYS
1	D	321	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	137	GLN
1	A	182	ASN
1	A	185	HIS
1	A	254	HIS
1	B	137	GLN
1	B	203	GLN
1	B	254	HIS
1	C	19	ASN
1	D	19	ASN

### 5.3.3 RNA [i](#)

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 8 ligands modelled in this entry, 8 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	317/328 (96%)	-0.13	11 (3%) 44 45	16, 25, 51, 72	0
1	B	316/328 (96%)	-0.06	13 (4%) 38 38	16, 27, 48, 86	0
1	C	290/328 (88%)	0.15	17 (5%) 23 24	19, 31, 54, 69	0
1	D	296/328 (90%)	0.10	14 (4%) 32 33	20, 33, 50, 67	0
All	All	1219/1312 (92%)	0.01	55 (4%) 34 35	16, 29, 51, 86	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	TRP	13.3
1	C	18	ALA	7.7
1	C	13	LEU	7.5
1	C	113	THR	7.1
1	C	100	GLU	7.0
1	B	42	GLY	6.5
1	C	152	ARG	5.7
1	B	43	ARG	5.7
1	B	95	ASN	5.6
1	C	42	GLY	5.5
1	A	3	ASP	5.3
1	D	215	ARG	5.0
1	C	43	ARG	5.0
1	C	14	HIS	4.6
1	A	4	ILE	4.3
1	A	96	GLU	4.0
1	D	41	GLU	4.0
1	D	9	LEU	3.9
1	A	43	ARG	3.9
1	A	95	ASN	3.8
1	A	322	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	321	THR	3.7
1	B	44	HIS	3.6
1	D	321	THR	3.6
1	B	94	ALA	3.5
1	D	32	GLY	3.5
1	D	152	ARG	3.4
1	A	94	ALA	3.3
1	B	40	ASP	3.3
1	A	42	GLY	3.1
1	C	156	ASP	2.9
1	C	15	SER	2.7
1	D	40	ASP	2.7
1	A	44	HIS	2.7
1	C	41	GLU	2.6
1	A	179	GLN	2.6
1	D	31	ASN	2.6
1	C	321	THR	2.5
1	C	215	ARG	2.5
1	B	96	GLU	2.4
1	C	40	ASP	2.4
1	B	3	ASP	2.4
1	D	54	ASN	2.3
1	D	13	LEU	2.3
1	D	49	ASN	2.3
1	D	39	THR	2.3
1	D	156	ASP	2.2
1	B	152	ARG	2.2
1	A	40	ASP	2.2
1	D	224[A]	ARG	2.2
1	B	155	ARG	2.1
1	C	19	ASN	2.1
1	B	97	VAL	2.1
1	C	17	ARG	2.1
1	B	257	THR	2.1

## 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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	A	326	1/1	0.98	0.09	0.27	38,38,38,38	0
3	NA	B	327	1/1	0.82	0.07	-1.33	32,32,32,32	0
2	MN	D	325	1/1	0.88	0.06	-	73,73,73,73	0
2	MN	B	325	1/1	0.97	0.04	-	48,48,48,48	0
2	MN	A	325	1/1	0.96	0.09	-	51,51,51,51	0
4	CA	A	327	1/1	0.96	0.10	-	51,51,51,51	0
4	CA	B	326	1/1	0.98	0.04	-	50,50,50,50	0
2	MN	C	325	1/1	0.94	0.03	-	69,69,69,69	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.