



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:54 pm BST

PDB ID : 2HFZ  
Title : Crystal structure of RNA dependent RNA polymerase domain from West Nile virus  
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Deposited on : 2006-06-26  
Resolution : 3.00 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

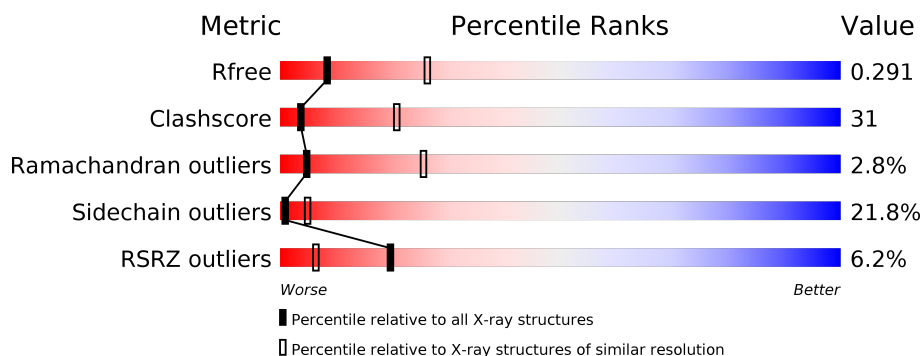
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	639	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4929 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 RNA-directed RNA polymerase(NS5).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4915	3083	888	915	29			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	HIS	-	EXPRESSION TAG	UNP P14335
A	268	HIS	-	EXPRESSION TAG	UNP P14335
A	269	HIS	-	EXPRESSION TAG	UNP P14335
A	270	HIS	-	EXPRESSION TAG	UNP P14335
A	271	HIS	-	EXPRESSION TAG	UNP P14335
A	272	HIS	-	EXPRESSION TAG	UNP P14335
A	273	LYS	-	SEE REMARK 999	UNP P14335

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

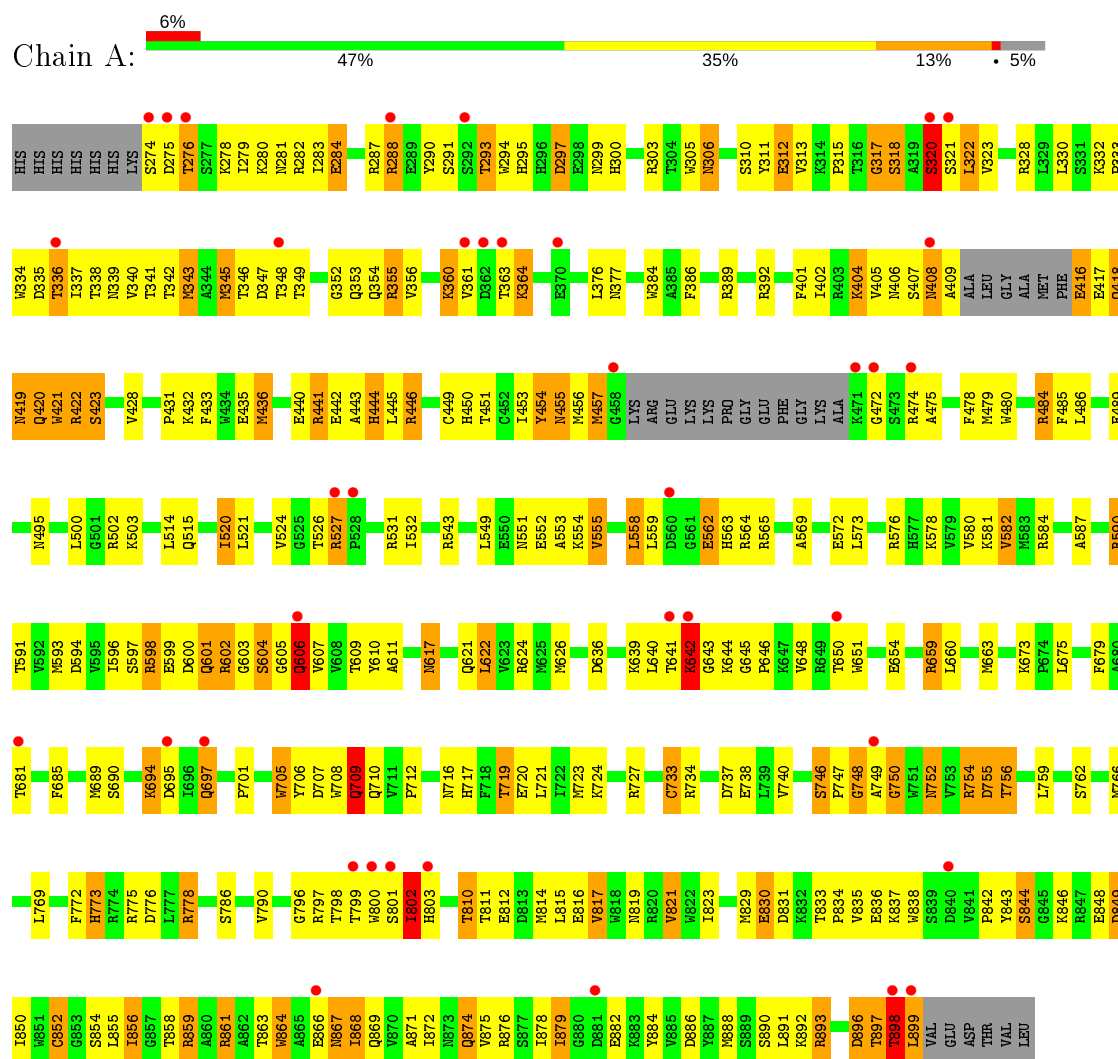
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		

### 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: RNA-directed RNA polymerase(NS5)



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.33Å 103.45Å 190.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.35 – 3.00 21.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (95.35-3.00) 96.5 (21.95-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.99Å)	Xtriage
Refinement program	BUSTER-TNT 1.3.1	Depositor
R, $R_{free}$	0.260 , 0.265 0.276 , 0.291	Depositor DCC
$R_{free}$ test set	1440 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.39	2/5029 (0.0%)	0.56	3/6807 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	733	CYS	CB-SG	10.34	1.99	1.82
1	A	852	CYS	CB-SG	8.48	1.96	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	HIS	CB-CA-C	-6.51	97.39	110.40
1	A	852	CYS	CA-CB-SG	6.26	125.27	114.00
1	A	898	THR	N-CA-C	5.64	126.23	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	898	THR	CA

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	4915	0	4784	304	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	12	0	0	1	0
All	All	4929	0	4784	304	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 31.

All (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:SER:HB3	1:A:345:MET:HA	1.21	1.12
1:A:317:GLY:HA3	1:A:349:THR:HA	1.29	1.11
1:A:867:ASN:N	1:A:867:ASN:HD22	1.56	0.99
1:A:279:ILE:HG22	1:A:283:ILE:HD11	1.46	0.97
1:A:293:THR:HG21	1:A:312:GLU:HB2	1.49	0.94
1:A:846:LYS:HZ1	1:A:899:LEU:HD22	1.32	0.93
1:A:899:LEU:H	1:A:899:LEU:HD23	1.33	0.92
1:A:334:TRP:HA	1:A:337:ILE:HD13	1.57	0.87
1:A:444:HIS:CE1	1:A:486:LEU:HD13	2.08	0.87
1:A:455:ASN:ND2	1:A:580:VAL:HG13	1.91	0.86
1:A:293:THR:CG2	1:A:312:GLU:HB2	2.06	0.84
1:A:384:TRP:CH2	1:A:555:VAL:HG13	2.13	0.84
1:A:797:ARG:HD3	1:A:800:TRP:CH2	2.14	0.83
1:A:797:ARG:HD3	1:A:800:TRP:CZ2	2.15	0.82
1:A:581:LYS:HB3	1:A:593:MET:CE	2.09	0.81
1:A:279:ILE:HG22	1:A:283:ILE:CD1	2.11	0.81
1:A:601:GLN:NE2	1:A:601:GLN:HA	1.95	0.81
1:A:355:ARG:HH11	1:A:355:ARG:HG3	1.45	0.81
1:A:867:ASN:ND2	1:A:867:ASN:N	2.28	0.81
1:A:846:LYS:NZ	1:A:899:LEU:HB3	2.00	0.77
1:A:846:LYS:HZ3	1:A:899:LEU:HD13	1.49	0.77
1:A:587:ALA:O	1:A:590:ARG:HG2	1.85	0.77
1:A:773:HIS:CD2	1:A:773:HIS:H	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:GLN:OE1	1:A:720:GLU:HB2	1.84	0.76
1:A:312:GLU:OE2	1:A:590:ARG:HB2	1.87	0.75
1:A:581:LYS:HB3	1:A:593:MET:HE2	1.68	0.75
1:A:431:PRO:O	1:A:435:GLU:HG3	1.86	0.75
1:A:451:THR:HB	1:A:479:MET:SD	2.26	0.75
1:A:453:ILE:CD1	1:A:581:LYS:HD2	2.18	0.73
1:A:867:ASN:H	1:A:867:ASN:HD22	1.36	0.73
1:A:681:THR:HG22	1:A:701:PRO:HG3	1.70	0.73
1:A:317:GLY:O	1:A:349:THR:HG22	1.89	0.73
1:A:641:THR:HG21	1:A:642:LYS:HE2	1.71	0.73
1:A:846:LYS:HZ3	1:A:899:LEU:HB3	1.52	0.72
1:A:454:TYR:HE1	1:A:580:VAL:HG22	1.53	0.72
1:A:354:GLN:CD	1:A:584:ARG:HG3	2.10	0.72
1:A:872:ILE:O	1:A:876:ARG:HG3	1.90	0.72
1:A:598:ARG:HB3	1:A:601:GLN:HG2	1.73	0.71
1:A:293:THR:CG2	1:A:312:GLU:H	2.02	0.71
1:A:321:SER:CB	1:A:345:MET:HA	2.12	0.71
1:A:775:ARG:HD2	1:A:856:ILE:HD12	1.73	0.70
1:A:320:SER:HB3	1:A:345:MET:HG3	1.73	0.69
1:A:552:GLU:O	1:A:555:VAL:HG22	1.93	0.69
1:A:846:LYS:NZ	1:A:899:LEU:HD22	2.06	0.69
1:A:694:LYS:HE2	1:A:695:ASP:OD1	1.92	0.69
1:A:641:THR:OG1	1:A:642:LYS:HG2	1.93	0.69
1:A:800:TRP:O	1:A:802:ILE:N	2.26	0.69
1:A:569:ALA:O	1:A:573:LEU:HB2	1.94	0.68
1:A:719:THR:HG21	1:A:848:GLU:OE2	1.92	0.68
1:A:846:LYS:NZ	1:A:899:LEU:HD13	2.07	0.68
1:A:389:ARG:HH11	1:A:389:ARG:HG3	1.58	0.68
1:A:322:LEU:N	1:A:322:LEU:HD22	2.09	0.68
1:A:353:GLN:HE22	1:A:457:MET:HE2	1.59	0.67
1:A:453:ILE:HD11	1:A:581:LYS:HD2	1.75	0.67
1:A:578:LYS:HE2	1:A:602:ARG:HD3	1.75	0.67
1:A:389:ARG:CG	1:A:389:ARG:HH11	2.09	0.66
1:A:846:LYS:CE	1:A:899:LEU:HD13	2.26	0.66
1:A:386:PHE:O	1:A:389:ARG:HG2	1.95	0.66
1:A:455:ASN:HD21	1:A:580:VAL:HG13	1.60	0.66
1:A:441:ARG:NH1	1:A:489:GLU:OE1	2.29	0.66
1:A:727:ARG:HD2	1:A:829:MET:CE	2.25	0.66
1:A:624:ARG:HG2	1:A:679:PHE:CE1	2.31	0.65
1:A:355:ARG:NH1	1:A:355:ARG:HG3	2.11	0.65
1:A:863:THR:O	1:A:867:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.61	0.65
1:A:605:GLY:O	1:A:607:VAL:N	2.30	0.65
1:A:297:ASP:O	1:A:299:ASN:ND2	2.30	0.64
1:A:322:LEU:HD22	1:A:322:LEU:H	1.61	0.64
1:A:311:TYR:OH	1:A:581:LYS:HE2	1.97	0.64
1:A:776:ASP:OD1	1:A:861:ARG:NH1	2.30	0.63
1:A:282:ARG:NH2	1:A:573:LEU:O	2.29	0.63
1:A:727:ARG:HD2	1:A:829:MET:HE2	1.81	0.63
1:A:868:ILE:O	1:A:868:ILE:HD13	1.98	0.63
1:A:641:THR:O	1:A:643:GLY:N	2.30	0.63
1:A:581:LYS:HB3	1:A:593:MET:HE1	1.80	0.63
1:A:893:ARG:HG2	1:A:893:ARG:NH1	2.13	0.62
1:A:279:ILE:CG2	1:A:283:ILE:HD11	2.26	0.62
1:A:317:GLY:CA	1:A:349:THR:HA	2.17	0.62
1:A:836:GLU:O	1:A:837:LYS:HG3	2.00	0.62
1:A:837:LYS:HB2	1:A:837:LYS:NZ	2.14	0.62
1:A:754:ARG:HH11	1:A:754:ARG:HG2	1.65	0.62
1:A:899:LEU:H	1:A:899:LEU:CD2	2.11	0.61
1:A:320:SER:HB3	1:A:345:MET:CE	2.30	0.61
1:A:354:GLN:CG	1:A:584:ARG:HG3	2.30	0.61
1:A:527:ARG:O	1:A:673:LYS:HD3	2.00	0.61
1:A:578:LYS:HZ3	1:A:603:GLY:N	1.99	0.61
1:A:748:GLY:O	1:A:750:GLY:N	2.33	0.61
1:A:404:LYS:O	1:A:408:ASN:HB3	2.01	0.61
1:A:641:THR:OG1	1:A:642:LYS:HE3	2.00	0.61
1:A:719:THR:HG21	1:A:848:GLU:CD	2.21	0.60
1:A:318:SER:O	1:A:349:THR:HG23	2.01	0.60
1:A:445:LEU:CD2	1:A:562:GLU:HG3	2.32	0.60
1:A:879:ILE:C	1:A:879:ILE:HD13	2.22	0.60
1:A:418:GLN:HG3	1:A:747:PRO:HB3	1.83	0.59
1:A:454:TYR:CE1	1:A:580:VAL:HG22	2.37	0.59
1:A:355:ARG:HG3	1:A:356:VAL:N	2.17	0.59
1:A:454:TYR:HE1	1:A:580:VAL:CG2	2.15	0.59
1:A:320:SER:HB3	1:A:345:MET:CG	2.33	0.59
1:A:893:ARG:HG2	1:A:893:ARG:HH11	1.68	0.59
1:A:775:ARG:NH2	1:A:844:SER:O	2.36	0.59
1:A:861:ARG:O	1:A:864:TRP:HD1	1.84	0.59
1:A:502:ARG:NH2	1:A:663:MET:O	2.28	0.59
1:A:879:ILE:HD12	1:A:884:TYR:OH	2.03	0.58
1:A:578:LYS:NZ	1:A:603:GLY:O	2.29	0.58
1:A:293:THR:HG21	1:A:312:GLU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TRP:HE1	1:A:360:LYS:HD3	1.69	0.58
1:A:407:SER:O	1:A:409:ALA:N	2.36	0.58
1:A:353:GLN:NE2	1:A:457:MET:HE2	2.18	0.58
1:A:582:VAL:N	1:A:593:MET:HE2	2.19	0.58
1:A:707:ASP:OD1	1:A:709:GLN:HB2	2.03	0.58
1:A:453:ILE:HD12	1:A:581:LYS:HD2	1.85	0.57
1:A:817:VAL:O	1:A:821:VAL:HG13	2.04	0.57
1:A:650:THR:O	1:A:654:GLU:HG2	2.04	0.57
1:A:578:LYS:CE	1:A:602:ARG:HD3	2.35	0.57
1:A:867:ASN:H	1:A:867:ASN:ND2	1.97	0.57
1:A:343:MET:HE1	1:A:738:GLU:HA	1.88	0.56
1:A:786:SER:O	1:A:876:ARG:NH2	2.30	0.56
1:A:288:ARG:HG3	1:A:288:ARG:NH1	2.21	0.56
1:A:543:ARG:HD2	1:A:690:SER:O	2.05	0.56
1:A:651:TRP:CZ2	1:A:659:ARG:HD2	2.41	0.56
1:A:340:VAL:HG12	1:A:737:ASP:O	2.06	0.56
1:A:402:ILE:HG12	1:A:428:VAL:HB	1.86	0.55
1:A:284:GLU:O	1:A:288:ARG:HG2	2.07	0.55
1:A:276:THR:O	1:A:276:THR:HG22	2.07	0.54
1:A:752:ASN:O	1:A:756:THR:HG23	2.07	0.54
1:A:721:LEU:HD11	1:A:773:HIS:HB3	1.89	0.54
1:A:888:MET:O	1:A:891:LEU:HB3	2.08	0.54
1:A:337:ILE:O	1:A:339:ASN:N	2.40	0.54
1:A:622:LEU:HD13	1:A:663:MET:CE	2.37	0.54
1:A:636:ASP:HB3	1:A:640:LEU:HD12	1.88	0.54
1:A:689:MET:O	1:A:690:SER:HB2	2.08	0.54
1:A:293:THR:HG21	1:A:312:GLU:CB	2.31	0.54
1:A:293:THR:HG22	1:A:312:GLU:H	1.72	0.54
1:A:445:LEU:HD22	1:A:562:GLU:HG3	1.90	0.54
1:A:893:ARG:HH11	1:A:893:ARG:CG	2.21	0.54
1:A:313:VAL:HG11	1:A:593:MET:HB2	1.90	0.53
1:A:846:LYS:HZ3	1:A:899:LEU:CD1	2.20	0.53
1:A:641:THR:OG1	1:A:644:LYS:HD3	2.08	0.53
1:A:288:ARG:HH11	1:A:288:ARG:HG3	1.73	0.53
1:A:846:LYS:HZ1	1:A:899:LEU:CD2	2.11	0.53
1:A:555:VAL:O	1:A:558:LEU:HB2	2.09	0.53
1:A:602:ARG:HH21	1:A:609:THR:HG21	1.74	0.53
1:A:317:GLY:HA2	1:A:348:THR:O	2.09	0.53
1:A:602:ARG:NH2	1:A:606:GLN:OE1	2.43	0.52
1:A:320:SER:HB3	1:A:345:MET:HE3	1.91	0.52
1:A:879:ILE:HD13	1:A:879:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:C	1:A:339:ASN:H	2.13	0.52
1:A:354:GLN:HG3	1:A:584:ARG:HG3	1.91	0.52
1:A:321:SER:H	1:A:345:MET:HE3	1.74	0.51
1:A:553:ALA:HB2	1:A:576:ARG:NH2	2.24	0.51
1:A:330:LEU:O	1:A:864:TRP:HZ3	1.91	0.51
1:A:856:ILE:HA	1:A:861:ARG:HD3	1.92	0.51
1:A:719:THR:HG21	1:A:848:GLU:OE1	2.11	0.51
1:A:320:SER:HA	1:A:346:THR:O	2.10	0.51
1:A:420:GLN:O	1:A:423:SER:HB2	2.10	0.51
1:A:297:ASP:OD2	1:A:584:ARG:NH2	2.44	0.51
1:A:694:LYS:HG3	1:A:695:ASP:N	2.25	0.51
1:A:766:MET:HG3	1:A:798:THR:HG21	1.93	0.51
1:A:440:GLU:OE1	1:A:450:HIS:HB2	2.12	0.50
1:A:444:HIS:HE1	1:A:486:LEU:HD13	1.70	0.50
1:A:287:ARG:O	1:A:291:SER:HB2	2.10	0.50
1:A:449:CYS:HB2	1:A:573:LEU:HD13	1.93	0.50
1:A:814:MET:HA	1:A:817:VAL:HG13	1.93	0.50
1:A:626:MET:SD	1:A:648:VAL:HG13	2.52	0.49
1:A:578:LYS:HZ3	1:A:603:GLY:H	1.58	0.49
1:A:432:LYS:NZ	1:A:474:ARG:HH22	2.10	0.49
1:A:773:HIS:HD2	1:A:773:HIS:H	1.55	0.49
1:A:823:ILE:HD11	1:A:835:VAL:HG23	1.95	0.49
1:A:899:LEU:N	1:A:899:LEU:HD23	2.14	0.49
1:A:599:GLU:HG3	1:A:600:ASP:OD2	2.13	0.49
1:A:846:LYS:HZ3	1:A:899:LEU:CB	2.25	0.49
1:A:337:ILE:O	1:A:341:THR:HG23	2.12	0.48
1:A:443:ALA:O	1:A:446:ARG:HG2	2.12	0.48
1:A:641:THR:HB	1:A:642:LYS:H	1.28	0.48
1:A:543:ARG:HG3	1:A:543:ARG:HH11	1.77	0.48
1:A:754:ARG:HH11	1:A:754:ARG:CG	2.24	0.48
1:A:759:LEU:HD13	1:A:796:GLY:HA3	1.96	0.48
1:A:830:GLU:H	1:A:830:GLU:CD	2.17	0.48
1:A:897:THR:OG1	1:A:898:THR:N	2.46	0.48
1:A:332:LYS:HB3	1:A:333:PRO:HD3	1.95	0.48
1:A:294:TRP:O	1:A:295:HIS:HB3	2.14	0.48
1:A:401:PHE:CE1	1:A:485:PHE:HA	2.49	0.48
1:A:418:GLN:CG	1:A:419:ASN:H	2.25	0.48
1:A:281:ASN:HB2	4:A:2:HOH:O	2.14	0.47
1:A:500:LEU:HD13	1:A:611:ALA:HA	1.95	0.47
1:A:875:VAL:O	1:A:879:ILE:HG23	2.14	0.47
1:A:402:ILE:HG22	1:A:406:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ASP:N	1:A:896:ASP:OD1	2.46	0.47
1:A:773:HIS:O	1:A:843:TYR:HD2	1.96	0.47
1:A:402:ILE:HG22	1:A:406:ASN:ND2	2.29	0.47
1:A:405:VAL:O	1:A:421:TRP:NE1	2.47	0.47
1:A:645:GLY:N	1:A:646:PRO:CD	2.78	0.47
1:A:716:ASN:HD21	1:A:734:ARG:HD2	1.80	0.47
1:A:747:PRO:O	1:A:748:GLY:O	2.32	0.47
1:A:727:ARG:HB3	1:A:829:MET:HE1	1.96	0.47
1:A:772:PHE:O	1:A:778:ARG:HD3	2.15	0.47
1:A:330:LEU:CD2	1:A:868:ILE:HD11	2.45	0.47
1:A:801:SER:OG	1:A:802:ILE:N	2.48	0.47
1:A:337:ILE:HG22	1:A:337:ILE:O	2.14	0.46
1:A:524:VAL:C	1:A:526:THR:H	2.18	0.46
1:A:578:LYS:O	1:A:597:SER:HB2	2.15	0.46
1:A:610:TYR:CE1	1:A:803:HIS:CE1	3.03	0.46
1:A:300:HIS:O	1:A:300:HIS:ND1	2.49	0.46
1:A:622:LEU:HD13	1:A:663:MET:HE1	1.95	0.46
1:A:416:GLU:OE1	1:A:416:GLU:HA	2.15	0.46
1:A:810:THR:HB	1:A:812:GLU:H	1.79	0.46
1:A:293:THR:HG21	1:A:312:GLU:N	2.30	0.46
1:A:402:ILE:CG2	1:A:406:ASN:ND2	2.79	0.46
1:A:377:ASN:ND2	1:A:554:LYS:HZ1	2.13	0.46
1:A:874:GLN:O	1:A:878:ILE:HG13	2.15	0.46
1:A:332:LYS:O	1:A:335:ASP:HB2	2.15	0.46
1:A:617:ASN:ND2	1:A:621:GLN:HE21	2.14	0.46
1:A:456:MET:HE3	1:A:480:TRP:HB2	1.98	0.46
1:A:578:LYS:HG3	1:A:601:GLN:CB	2.46	0.46
1:A:551:ASN:ND2	1:A:554:LYS:HZ1	2.13	0.45
1:A:814:MET:CE	1:A:817:VAL:HG11	2.46	0.45
1:A:355:ARG:CG	1:A:356:VAL:N	2.79	0.45
1:A:532:ILE:O	1:A:705:TRP:HE3	1.98	0.45
1:A:322:LEU:HB2	1:A:746:SER:O	2.16	0.45
1:A:315:PRO:HG3	1:A:591:THR:OG1	2.15	0.45
1:A:754:ARG:NH1	1:A:754:ARG:CG	2.80	0.45
1:A:278:LYS:HB3	1:A:573:LEU:CD2	2.46	0.45
1:A:814:MET:HE1	1:A:817:VAL:HG11	1.99	0.45
1:A:888:MET:O	1:A:891:LEU:N	2.44	0.45
1:A:419:ASN:O	1:A:422:ARG:HG2	2.17	0.45
1:A:436:MET:HE3	1:A:475:ALA:HB1	1.99	0.45
1:A:723:MET:HG2	1:A:842:PRO:HG3	1.99	0.45
1:A:549:LEU:O	1:A:576:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:ARG:NE	1:A:849:ASP:OD2	2.46	0.45
1:A:306:ASN:O	1:A:596:ILE:HA	2.17	0.45
1:A:846:LYS:NZ	1:A:899:LEU:CB	2.76	0.45
1:A:712:PRO:HG3	1:A:717:HIS:HE1	1.81	0.44
1:A:727:ARG:HD2	1:A:829:MET:HE1	1.98	0.44
1:A:866:GLU:OE2	1:A:866:GLU:HA	2.17	0.44
1:A:893:ARG:NH1	1:A:893:ARG:CG	2.78	0.44
1:A:290:TYR:O	1:A:294:TRP:N	2.47	0.44
1:A:343:MET:O	1:A:343:MET:HG2	2.18	0.44
1:A:321:SER:HB3	1:A:345:MET:CA	2.15	0.44
1:A:456:MET:HE3	1:A:480:TRP:CB	2.47	0.44
1:A:697:GLN:OE1	1:A:697:GLN:HA	2.09	0.44
1:A:330:LEU:HD22	1:A:868:ILE:HD11	2.00	0.44
1:A:681:THR:HG22	1:A:701:PRO:CG	2.45	0.44
1:A:348:THR:O	1:A:348:THR:HG22	2.16	0.44
1:A:418:GLN:HG3	1:A:747:PRO:CB	2.46	0.44
1:A:606:GLN:HA	1:A:609:THR:HB	2.00	0.44
1:A:531:ARG:HG2	1:A:706:TYR:CE1	2.52	0.44
1:A:562:GLU:OE2	1:A:565:ARG:NH2	2.51	0.44
1:A:858:THR:HG22	1:A:859:ARG:N	2.32	0.44
1:A:311:TYR:O	1:A:313:VAL:HG13	2.17	0.43
1:A:330:LEU:O	1:A:864:TRP:CZ3	2.71	0.43
1:A:475:ALA:O	1:A:479:MET:HG3	2.17	0.43
1:A:605:GLY:C	1:A:607:VAL:H	2.21	0.43
1:A:347:ASP:CG	1:A:352:GLY:HA3	2.38	0.43
1:A:281:ASN:HB3	1:A:449:CYS:O	2.19	0.43
1:A:602:ARG:HB2	1:A:602:ARG:HE	1.64	0.43
1:A:310:SER:HA	1:A:593:MET:O	2.18	0.43
1:A:445:LEU:HD21	1:A:562:GLU:HG3	1.98	0.43
1:A:708:TRP:C	1:A:710:GLN:H	2.22	0.43
1:A:419:ASN:OD1	1:A:755:ASP:OD2	2.37	0.43
1:A:685:PHE:O	1:A:689:MET:HG3	2.19	0.43
1:A:602:ARG:H	1:A:602:ARG:HG3	1.50	0.42
1:A:802:ILE:HG12	1:A:803:HIS:H	1.83	0.42
1:A:433:PHE:HB2	1:A:478:PHE:CE2	2.54	0.42
1:A:645:GLY:N	1:A:646:PRO:HD2	2.34	0.42
1:A:419:ASN:C	1:A:421:TRP:H	2.17	0.42
1:A:778:ARG:NH2	1:A:838:TRP:O	2.53	0.42
1:A:797:ARG:HG2	1:A:800:TRP:CE2	2.54	0.42
1:A:849:ASP:O	1:A:854:SER:HB2	2.19	0.42
1:A:389:ARG:CG	1:A:389:ARG:NH1	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ASN:HD22	1:A:752:ASN:C	2.22	0.42
1:A:819:ASN:OD1	1:A:823:ILE:HD12	2.20	0.42
1:A:868:ILE:HD13	1:A:871:ALA:HB3	2.02	0.42
1:A:474:ARG:HG2	1:A:474:ARG:NH1	2.28	0.42
1:A:456:MET:CE	1:A:480:TRP:HB2	2.49	0.42
1:A:310:SER:HB3	1:A:594:ASP:HA	2.01	0.42
1:A:526:THR:HG22	1:A:526:THR:O	2.20	0.42
1:A:384:TRP:CZ2	1:A:555:VAL:HG13	2.52	0.42
1:A:520:ILE:HD13	1:A:520:ILE:N	2.34	0.42
1:A:766:MET:CE	1:A:798:THR:CG2	2.98	0.42
1:A:833:THR:HA	1:A:834:PRO:HD3	1.80	0.41
1:A:727:ARG:HD3	1:A:831:ASP:HB3	2.01	0.41
1:A:484:ARG:HA	1:A:484:ARG:HD3	1.74	0.41
1:A:293:THR:HB	1:A:311:TYR:HB2	2.02	0.41
1:A:858:THR:CG2	1:A:859:ARG:N	2.83	0.41
1:A:559:LEU:HD22	1:A:563:HIS:CE1	2.56	0.41
1:A:584:ARG:HE	1:A:584:ARG:HB3	1.55	0.41
1:A:347:ASP:OD1	1:A:349:THR:OG1	2.30	0.41
1:A:347:ASP:HB3	1:A:352:GLY:HA3	2.03	0.41
1:A:846:LYS:O	1:A:850:ILE:HD12	2.21	0.41
1:A:622:LEU:HD13	1:A:663:MET:HE3	2.02	0.41
1:A:846:LYS:NZ	1:A:899:LEU:CG	2.84	0.41
1:A:846:LYS:NZ	1:A:899:LEU:CD1	2.80	0.41
1:A:886:ASP:OD1	1:A:888:MET:HB2	2.20	0.41
1:A:551:ASN:HD22	1:A:554:LYS:HE3	1.85	0.40
1:A:879:ILE:HD11	1:A:882:GLU:HG3	2.02	0.40
1:A:336:THR:O	1:A:336:THR:OG1	2.33	0.40
1:A:495:ASN:ND2	1:A:607:VAL:O	2.54	0.40
1:A:606:GLN:HE21	1:A:606:GLN:H	1.67	0.40
1:A:766:MET:HG3	1:A:798:THR:CG2	2.51	0.40
1:A:444:HIS:C	1:A:446:ARG:N	2.74	0.40
1:A:641:THR:CB	1:A:642:LYS:HG2	2.52	0.40
1:A:456:MET:CE	1:A:480:TRP:CB	2.99	0.40
1:A:551:ASN:ND2	1:A:554:LYS:NZ	2.69	0.40
1:A:712:PRO:HG3	1:A:717:HIS:CE1	2.56	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	602/639 (94%)	546 (91%)	39 (6%)	17 (3%)	5	25

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	A	320	SER
1	A	338	THR
1	A	363	THR
1	A	408	ASN
1	A	606	GLN
1	A	642	LYS
1	A	748	GLY
1	A	749	ALA
1	A	750	GLY
1	A	898	THR
1	A	364	LYS
1	A	472	GLY
1	A	604	SER
1	A	317	GLY
1	A	709	GLN
1	A	802	ILE

### 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	523/550 (95%)	409 (78%)	114 (22%)	<b>1</b> <b>5</b>

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	SER
1	A	275	ASP
1	A	280	LYS
1	A	284	GLU
1	A	288	ARG
1	A	293	THR
1	A	297	ASP
1	A	303	ARG
1	A	306	ASN
1	A	312	GLU
1	A	318	SER
1	A	320	SER
1	A	322	LEU
1	A	323	VAL
1	A	328	ARG
1	A	336	THR
1	A	342	THR
1	A	343	MET
1	A	345	MET
1	A	355	ARG
1	A	360	LYS
1	A	361	VAL
1	A	364	LYS
1	A	376	LEU
1	A	392	ARG
1	A	404	LYS
1	A	416	GLU
1	A	417	GLU
1	A	418	GLN
1	A	419	ASN
1	A	420	GLN
1	A	421	TRP
1	A	422	ARG
1	A	423	SER
1	A	436	MET
1	A	441	ARG
1	A	442	GLU
1	A	446	ARG

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Mol	Chain	Res	Type
1	A	454	TYR
1	A	455	ASN
1	A	457	MET
1	A	484	ARG
1	A	503	LYS
1	A	514	LEU
1	A	515	GLN
1	A	520	ILE
1	A	521	LEU
1	A	527	ARG
1	A	555	VAL
1	A	558	LEU
1	A	562	GLU
1	A	564	ARG
1	A	572	GLU
1	A	582	VAL
1	A	590	ARG
1	A	598	ARG
1	A	601	GLN
1	A	602	ARG
1	A	604	SER
1	A	606	GLN
1	A	617	ASN
1	A	622	LEU
1	A	639	LYS
1	A	642	LYS
1	A	659	ARG
1	A	660	LEU
1	A	675	LEU
1	A	694	LYS
1	A	697	GLN
1	A	705	TRP
1	A	709	GLN
1	A	719	THR
1	A	724	LYS
1	A	733	CYS
1	A	740	VAL
1	A	746	SER
1	A	752	ASN
1	A	754	ARG
1	A	755	ASP
1	A	756	THR

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Mol	Chain	Res	Type
1	A	762	SER
1	A	769	LEU
1	A	773	HIS
1	A	778	ARG
1	A	790	VAL
1	A	799	THR
1	A	802	ILE
1	A	810	THR
1	A	811	THR
1	A	815	LEU
1	A	816	GLU
1	A	817	VAL
1	A	821	VAL
1	A	830	GLU
1	A	844	SER
1	A	849	ASP
1	A	852	CYS
1	A	855	LEU
1	A	856	ILE
1	A	859	ARG
1	A	861	ARG
1	A	864	TRP
1	A	867	ASN
1	A	868	ILE
1	A	869	GLN
1	A	874	GLN
1	A	879	ILE
1	A	890	SER
1	A	892	LYS
1	A	893	ARG
1	A	896	ASP
1	A	897	THR
1	A	898	THR
1	A	899	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	419	ASN
1	A	455	ASN
1	A	495	ASN

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Mol	Chain	Res	Type
1	A	551	ASN
1	A	601	GLN
1	A	617	ASN
1	A	687	ASN
1	A	716	ASN
1	A	717	HIS
1	A	752	ASN
1	A	773	HIS
1	A	803	HIS
1	A	867	ASN
1	A	869	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 carbohydrates 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<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	608/639 (95%)	0.53	38 (6%) 20 6	67, 89, 111, 133	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	SER	6.2
1	A	642	LYS	5.8
1	A	321	SER	5.7
1	A	275	ASP	5.0
1	A	641	THR	4.7
1	A	799	THR	4.5
1	A	361	VAL	4.2
1	A	898	THR	3.9
1	A	274	SER	3.6
1	A	801	SER	3.6
1	A	471	LYS	3.6
1	A	276	THR	3.6
1	A	362	ASP	3.4
1	A	749	ALA	3.3
1	A	681	THR	3.2
1	A	292	SER	3.0
1	A	472	GLY	2.8
1	A	800	TRP	2.8
1	A	881	ASP	2.6
1	A	695	ASP	2.6
1	A	866	GLU	2.5
1	A	458	GLY	2.5
1	A	528	PRO	2.5
1	A	899	LEU	2.4
1	A	840	ASP	2.4
1	A	363	THR	2.2
1	A	803	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	560	ASP	2.2
1	A	370	GLU	2.2
1	A	408	ASN	2.1
1	A	336	THR	2.1
1	A	606	GLN	2.1
1	A	348	THR	2.1
1	A	474	ARG	2.1
1	A	527	ARG	2.0
1	A	650	THR	2.0
1	A	697	GLN	2.0
1	A	288	ARG	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 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
2	MG	A	906	1/1	0.89	0.42	79,79,79,79	0
3	ZN	A	907	1/1	0.97	0.11	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.