



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2HCS  
Title : Crystal structure of RNA dependant RNA polymerase domain of West Nile virus  
Authors : Egloff, M.P.; Malet, H.; Marseilles Structural Genomics Program @ AFMB (MSGP)  
Deposited on : 2006-06-18  
Resolution : 2.50 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

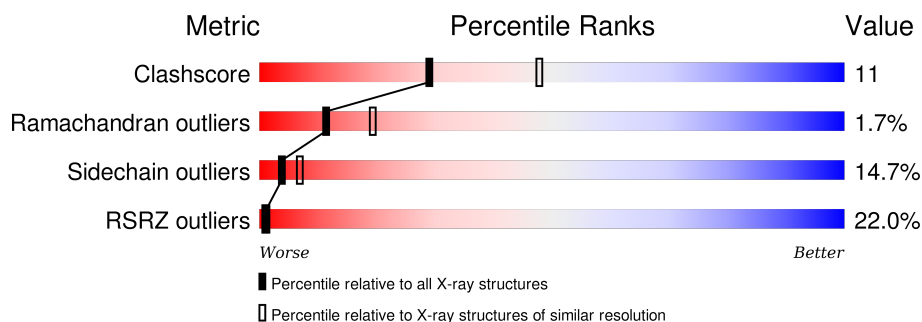
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	595	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4044 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	487	Total	C	N	O	S	0	0	0
			3936	2484	706	723	23			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	HIS	-	EXPRESSION TAG	UNP P14335
A	312	HIS	-	EXPRESSION TAG	UNP P14335
A	313	HIS	-	EXPRESSION TAG	UNP P14335
A	314	HIS	-	EXPRESSION TAG	UNP P14335
A	315	HIS	-	EXPRESSION TAG	UNP P14335
A	316	HIS	-	EXPRESSION TAG	UNP P14335
A	317	LYS	-	SEE REMARK 999	UNP P14335

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.99Å 109.99Å 69.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.88 – 2.50 34.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.88-2.50) 98.3 (34.78-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.206 , 0.243 0.244 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.8	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20157 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	0.97	14/4026 (0.3%)	0.89	12/5449 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	LYS	CE-NZ	18.57	1.95	1.49
1	A	724	LYS	CE-NZ	15.40	1.87	1.49
1	A	724	LYS	CD-CE	12.49	1.82	1.51
1	A	332	LYS	CD-CE	12.16	1.81	1.51
1	A	325	GLY	C-O	11.37	1.41	1.23
1	A	859	ARG	CZ-NH1	10.26	1.46	1.33
1	A	859	ARG	CG-CD	9.43	1.75	1.51
1	A	325	GLY	C-N	8.82	1.54	1.34
1	A	332	LYS	CG-CD	7.79	1.78	1.52
1	A	329	LEU	C-N	6.28	1.48	1.34
1	A	326	VAL	CB-CG1	5.78	1.65	1.52
1	A	332	LYS	CB-CG	5.75	1.68	1.52
1	A	436	MET	SD-CE	5.44	2.08	1.77
1	A	550	GLU	CG-CD	5.36	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	859	ARG	NE-CZ-NH2	-11.13	114.74	120.30
1	A	724	LYS	CD-CE-NZ	-10.81	86.84	111.70
1	A	436	MET	CG-SD-CE	-7.92	87.52	100.20
1	A	502	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	502	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	332	LYS	CB-CG-CD	-6.73	94.10	111.60
1	A	659	ARG	NE-CZ-NH2	-6.25	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	744	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	659	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	555	VAL	CB-CA-C	-5.31	101.32	111.40
1	A	500	LEU	CB-CG-CD1	-5.17	102.21	111.00

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	3936	0	3844	89	0
2	A	2	0	0	0	0
3	A	106	0	0	2	0
All	All	4044	0	3844	89	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 11.

All (89) 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:859:ARG:CD	1:A:859:ARG:CG	1.75	1.60
1:A:332:LYS:CG	1:A:332:LYS:CD	1.78	1.59
1:A:724:LYS:CE	1:A:724:LYS:CD	1.82	1.55
1:A:332:LYS:CD	1:A:332:LYS:CE	1.81	1.53
1:A:436:MET:CE	1:A:436:MET:SD	2.08	1.41
1:A:724:LYS:CE	1:A:724:LYS:NZ	1.87	1.33
1:A:332:LYS:NZ	1:A:332:LYS:CE	1.95	1.28
1:A:402:ILE:HG12	1:A:428:VAL:HG11	1.45	0.98
1:A:752:ASN:O	1:A:756:THR:HG23	1.74	0.86
1:A:332:LYS:CD	1:A:332:LYS:CB	2.53	0.84
1:A:530:GLY:O	1:A:673:LYS:HE3	1.80	0.81
1:A:724:LYS:CG	1:A:724:LYS:CE	2.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HG12	1:A:428:VAL:CG1	2.12	0.79
1:A:859:ARG:CD	1:A:859:ARG:CB	2.63	0.76
1:A:752:ASN:HD22	1:A:755:ASP:H	1.34	0.74
1:A:724:LYS:NZ	1:A:724:LYS:CD	2.54	0.71
1:A:389:ARG:NH2	1:A:504:ASN:O	2.23	0.71
1:A:384:TRP:CH2	1:A:555:VAL:HG13	2.29	0.68
1:A:859:ARG:NE	1:A:859:ARG:CG	2.56	0.67
1:A:436:MET:CE	1:A:436:MET:CG	2.74	0.66
1:A:551:ASN:HD22	1:A:554:LYS:HE3	1.59	0.65
1:A:332:LYS:HB3	1:A:333:PRO:HD3	1.78	0.65
1:A:429:GLU:HG2	3:A:1006:HOH:O	1.98	0.63
1:A:451:THR:HB	1:A:479:MET:HG2	1.80	0.63
1:A:721:LEU:HD21	1:A:843:TYR:O	1.99	0.63
1:A:546:ARG:HB3	1:A:546:ARG:NH2	2.14	0.62
1:A:500:LEU:CD1	1:A:611:ALA:HA	2.29	0.62
1:A:570:ILE:O	1:A:573:LEU:HB2	2.01	0.60
1:A:332:LYS:HB3	1:A:332:LYS:CD	2.32	0.60
1:A:539:GLY:O	1:A:542:THR:HB	2.02	0.59
1:A:782:ASN:HD22	1:A:891:LEU:HD21	1.68	0.59
1:A:752:ASN:ND2	1:A:755:ASP:H	1.99	0.59
1:A:801:SER:N	3:A:1010:HOH:O	2.36	0.58
1:A:332:LYS:CG	1:A:332:LYS:CE	2.82	0.57
1:A:502:ARG:NH2	1:A:663:MET:O	2.24	0.57
1:A:606:GLN:HA	1:A:609:THR:HB	1.87	0.56
1:A:855:LEU:O	1:A:858:THR:HB	2.05	0.56
1:A:337:ILE:CG2	1:A:337:ILE:O	2.53	0.56
1:A:607:VAL:HG13	1:A:608:VAL:H	1.71	0.55
1:A:500:LEU:HD12	1:A:611:ALA:HA	1.88	0.54
1:A:646:PRO:O	1:A:650:THR:HG23	2.09	0.53
1:A:709:GLN:HE21	1:A:719:THR:HA	1.73	0.52
1:A:337:ILE:HG22	1:A:337:ILE:O	2.10	0.50
1:A:775:ARG:NH2	1:A:845:GLY:H	2.10	0.50
1:A:500:LEU:HD11	1:A:611:ALA:O	2.12	0.50
1:A:386:PHE:O	1:A:389:ARG:HB2	2.13	0.49
1:A:500:LEU:HD13	1:A:614:THR:HB	1.94	0.49
1:A:719:THR:O	1:A:730:VAL:HA	2.13	0.49
1:A:606:GLN:N	1:A:606:GLN:CD	2.66	0.48
1:A:848:GLU:OE2	1:A:848:GLU:N	2.44	0.48
1:A:421:TRP:O	1:A:421:TRP:HD1	1.97	0.48
1:A:332:LYS:HB3	1:A:332:LYS:HD3	1.96	0.48
1:A:531:ARG:HB3	1:A:705:TRP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LEU:HD21	1:A:844:SER:HA	1.96	0.48
1:A:377:ASN:ND2	1:A:554:LYS:HZ1	2.12	0.47
1:A:721:LEU:HD13	1:A:842:PRO:HG2	1.96	0.47
1:A:408:ASN:HB3	1:A:409:ALA:HA	1.96	0.47
1:A:546:ARG:HH21	1:A:546:ARG:CG	2.29	0.47
1:A:399:GLU:H	1:A:399:GLU:CD	2.18	0.47
1:A:420:GLN:HG3	1:A:421:TRP:H	1.80	0.46
1:A:421:TRP:O	1:A:421:TRP:CD1	2.69	0.46
1:A:705:TRP:CD1	1:A:710:GLN:HG3	2.50	0.46
1:A:761:LYS:HG2	1:A:794:PRO:HG3	1.97	0.46
1:A:552:GLU:O	1:A:555:VAL:HG22	2.17	0.45
1:A:858:THR:HG22	1:A:861:ARG:H	1.81	0.45
1:A:641:THR:HB	1:A:644:LYS:HG3	1.99	0.45
1:A:604:SER:HB2	1:A:609:THR:OG1	2.16	0.45
1:A:776:ASP:OD1	1:A:861:ARG:NH1	2.47	0.44
1:A:406:ASN:O	1:A:425:ARG:NH2	2.48	0.44
1:A:333:PRO:HB2	1:A:334:TRP:CE3	2.52	0.44
1:A:606:GLN:CD	1:A:606:GLN:H	2.19	0.44
1:A:335:ASP:O	1:A:337:ILE:N	2.51	0.44
1:A:719:THR:HG22	1:A:720:GLU:O	2.18	0.44
1:A:782:ASN:ND2	1:A:891:LEU:HD21	2.32	0.43
1:A:617:ASN:HD21	1:A:621:GLN:HE21	1.64	0.43
1:A:574:THR:HB	1:A:603:GLY:N	2.34	0.43
1:A:528:PRO:O	1:A:662:ARG:NH2	2.52	0.43
1:A:617:ASN:ND2	1:A:621:GLN:HE21	2.17	0.43
1:A:651:TRP:CZ2	1:A:659:ARG:HD2	2.54	0.43
1:A:622:LEU:HD13	1:A:663:MET:HE1	2.01	0.42
1:A:622:LEU:HD13	1:A:663:MET:CE	2.49	0.42
1:A:522:ARG:HG3	1:A:708:TRP:CZ2	2.54	0.42
1:A:709:GLN:NE2	1:A:719:THR:HA	2.34	0.42
1:A:709:GLN:NE2	1:A:720:GLU:H	2.17	0.42
1:A:724:LYS:HZ3	1:A:724:LYS:CD	2.32	0.41
1:A:519:TYR:O	1:A:523:GLU:HG3	2.21	0.41
1:A:421:TRP:HE1	1:A:425:ARG:NE	2.20	0.40
1:A:626:MET:HG3	1:A:651:TRP:CE3	2.56	0.40
1:A:573:LEU:HD23	1:A:573:LEU:HA	1.94	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	475/595 (80%)	447 (94%)	20 (4%)	8 (2%)	11	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ARG
1	A	606	GLN
1	A	607	VAL
1	A	336	THR
1	A	642	LYS
1	A	801	SER
1	A	335	ASP
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	416/508 (82%)	355 (85%)	61 (15%)	4	7

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	328	ARG
1	A	332	LYS

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Mol	Chain	Res	Type
1	A	333	PRO
1	A	364	LYS
1	A	376	LEU
1	A	392	ARG
1	A	399	GLU
1	A	404	LYS
1	A	421	TRP
1	A	422	ARG
1	A	442	GLU
1	A	445	LEU
1	A	450	HIS
1	A	452	CYS
1	A	474	ARG
1	A	484	ARG
1	A	514	LEU
1	A	526	THR
1	A	527	ARG
1	A	542	THR
1	A	546	ARG
1	A	555	VAL
1	A	558	LEU
1	A	574	THR
1	A	606	GLN
1	A	608	VAL
1	A	617	ASN
1	A	622	LEU
1	A	642	LYS
1	A	650	THR
1	A	652	LEU
1	A	659	ARG
1	A	660	LEU
1	A	711	VAL
1	A	721	LEU
1	A	733	CYS
1	A	740	VAL
1	A	746	SER
1	A	754	ARG
1	A	756	THR
1	A	769	LEU
1	A	775	ARG
1	A	778	ARG
1	A	790	VAL

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Mol	Chain	Res	Type
1	A	795	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	851	TRP
1	A	855	LEU
1	A	858	THR
1	A	861	ARG
1	A	863	THR
1	A	866	GLU
1	A	877	SER
1	A	889	SER

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	377	ASN
1	A	495	ASN
1	A	551	ASN
1	A	617	ASN
1	A	687	ASN
1	A	697	GLN
1	A	709	GLN
1	A	752	ASN
1	A	782	ASN
1	A	874	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 [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	487/595 (81%)	1.39	107 (21%) 1 1	38, 52, 76, 94	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	PHE	9.8
1	A	477	TRP	8.6
1	A	747	PRO	8.1
1	A	433	PHE	7.2
1	A	473	SER	6.9
1	A	645	GLY	6.1
1	A	363	THR	5.6
1	A	802	ILE	5.6
1	A	434	TRP	5.4
1	A	427	ALA	5.3
1	A	800	TRP	5.0
1	A	431	PRO	4.6
1	A	326	VAL	4.6
1	A	476	ILE	4.5
1	A	429	GLU	4.5
1	A	891	LEU	4.4
1	A	430	ASP	4.4
1	A	436	MET	4.3
1	A	860	ALA	4.2
1	A	474	ARG	4.2
1	A	480	TRP	4.2
1	A	481	LEU	4.1
1	A	830	GLU	4.1
1	A	831	ASP	4.1
1	A	362	ASP	4.0
1	A	421	TRP	4.0
1	A	322	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	420	GLN	3.9
1	A	642	LYS	3.8
1	A	410	ALA	3.8
1	A	424	ALA	3.7
1	A	425	ARG	3.5
1	A	479	MET	3.5
1	A	803	HIS	3.5
1	A	656	GLY	3.5
1	A	745	ILE	3.4
1	A	746	SER	3.4
1	A	644	LYS	3.4
1	A	475	ALA	3.4
1	A	890	SER	3.3
1	A	336	THR	3.3
1	A	879	ILE	3.3
1	A	428	VAL	3.2
1	A	323	VAL	3.2
1	A	695	ASP	3.1
1	A	754	ARG	2.9
1	A	450	HIS	2.9
1	A	541	ASP	2.9
1	A	665	VAL	2.9
1	A	788	VAL	2.9
1	A	399	GLU	2.9
1	A	725	ASP	2.8
1	A	801	SER	2.8
1	A	392	ARG	2.8
1	A	403	ARG	2.7
1	A	422	ARG	2.7
1	A	575	TYR	2.7
1	A	647	LYS	2.7
1	A	753	VAL	2.7
1	A	871	ALA	2.6
1	A	426	GLU	2.6
1	A	451	THR	2.5
1	A	697	GLN	2.5
1	A	851	TRP	2.5
1	A	432	LYS	2.5
1	A	437	VAL	2.5
1	A	828	TRP	2.5
1	A	614	THR	2.5
1	A	643	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	836	GLU	2.5
1	A	435	GLU	2.4
1	A	542	THR	2.4
1	A	635	ASP	2.4
1	A	449	CYS	2.4
1	A	722	ILE	2.4
1	A	514	LEU	2.3
1	A	835	VAL	2.3
1	A	641	THR	2.3
1	A	733	CYS	2.3
1	A	559	LEU	2.3
1	A	752	ASN	2.3
1	A	771	TYR	2.3
1	A	880	GLY	2.3
1	A	408	ASN	2.3
1	A	804	ALA	2.2
1	A	364	LYS	2.2
1	A	619	ALA	2.2
1	A	327	VAL	2.2
1	A	648	VAL	2.2
1	A	732	PRO	2.2
1	A	331	SER	2.2
1	A	324	ASN	2.2
1	A	866	GLU	2.2
1	A	829	MET	2.1
1	A	566	LEU	2.1
1	A	651	TRP	2.1
1	A	649	ARG	2.1
1	A	618	LEU	2.1
1	A	799	THR	2.1
1	A	790	VAL	2.1
1	A	606	GLN	2.1
1	A	657	GLU	2.1
1	A	539	GLY	2.0
1	A	675	LEU	2.0
1	A	844	SER	2.0
1	A	376	LEU	2.0
1	A	452	CYS	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 [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
2	ZN	A	1	1/1	0.68	0.08	-2.71	63,63,63,63	0
2	ZN	A	2	1/1	0.96	0.06	-	63,63,63,63	0

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

There are no such residues in this entry.