



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:29 AM GMT

PDB ID : 2HCN
Title : Crystal structure of RNA dependent RNA polymerase domain from west nile virus
Authors : Egloff, M.P.; Malet, H.; Marseilles Structural Genomics Program @ AFMB (MSGP)
Deposited on : 2006-06-17
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

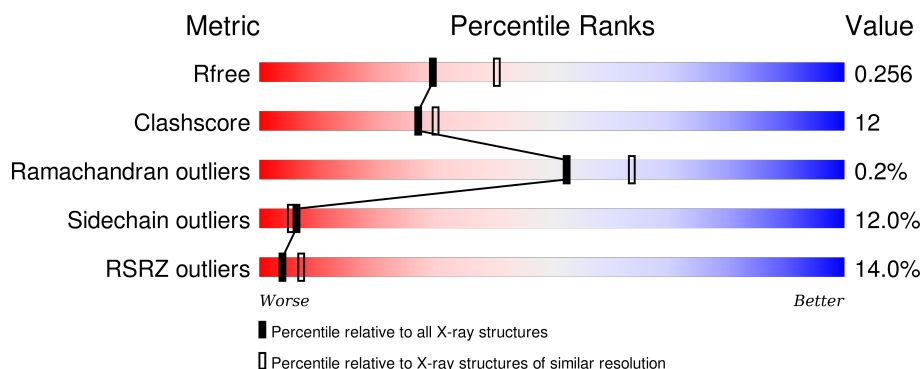
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 ≥ 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	<div> <div>11%</div> <div>59%</div> <div>18%</div> <div>• •</div> <div>18%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4107 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	486	Total	C	N	O	S	0	0	0
			3931	2482	705	721	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	110.06Å 110.06Å 68.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.82 – 2.35 34.81 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.82-2.35) 99.9 (34.81-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.259 0.204 , 0.256	Depositor DCC
R_{free} test set	1734 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.2	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34317 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4107	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.93	13/4021 (0.3%)	0.90	18/5444 (0.3%)

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	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	LYS	CE-NZ	22.71	2.05	1.49
1	A	332	LYS	CD-CE	14.58	1.87	1.51
1	A	432	LYS	CD-CE	12.92	1.83	1.51
1	A	329	LEU	CG-CD1	10.07	1.89	1.51
1	A	325	GLY	C-N	8.39	1.53	1.34
1	A	432	LYS	CE-NZ	7.39	1.67	1.49
1	A	326	VAL	CB-CG1	7.05	1.67	1.52
1	A	432	LYS	CG-CD	7.01	1.76	1.52
1	A	329	LEU	CG-CD2	6.91	1.77	1.51
1	A	326	VAL	CB-CG2	6.71	1.67	1.52
1	A	327	VAL	C-O	5.70	1.34	1.23
1	A	859	ARG	CD-NE	5.23	1.55	1.46
1	A	859	ARG	CZ-NH1	5.21	1.39	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	859	ARG	NE-CZ-NH2	-13.69	113.46	120.30
1	A	332	LYS	CD-CE-NZ	-9.41	90.05	111.70
1	A	502	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	502	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	659	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	659	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	555	VAL	CB-CA-C	-6.32	99.38	111.40
1	A	859	ARG	NH1-CZ-NH2	6.25	126.27	119.40
1	A	755	ASP	N-CA-C	-5.86	95.17	111.00
1	A	432	LYS	CG-CD-CE	-5.84	94.37	111.90
1	A	756	THR	N-CA-C	5.70	126.39	111.00
1	A	500	LEU	CA-CB-CG	-5.32	103.07	115.30
1	A	555	VAL	CG1-CB-CG2	5.32	119.40	110.90
1	A	515	GLN	CB-CA-C	-5.29	99.83	110.40
1	A	622	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	849	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	535	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	432	LYS	CD-CE-NZ	-5.02	100.16	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	327	VAL	Mainchain
1	A	755	ASP	Peptide

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	3931	0	3841	93	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	173	0	0	6	0
All	All	4107	0	3841	93	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 (93) 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:432:LYS:CG	1:A:432:LYS:CD	1.76	1.63
1:A:329:LEU:CG	1:A:329:LEU:CD2	1.77	1.58
1:A:432:LYS:CE	1:A:432:LYS:CD	1.83	1.55
1:A:432:LYS:CE	1:A:432:LYS:NZ	1.67	1.51
1:A:332:LYS:CD	1:A:332:LYS:CE	1.87	1.49
1:A:329:LEU:CG	1:A:329:LEU:CD1	1.89	1.48
1:A:332:LYS:NZ	1:A:332:LYS:CE	2.05	1.19
1:A:444:HIS:HB3	1:A:448:GLU:O	1.46	1.16
1:A:861:ARG:O	1:A:864:TRP:HD1	1.60	0.84
1:A:332:LYS:CG	1:A:332:LYS:CE	2.55	0.84
1:A:792:TRP:CH2	1:A:879:ILE:HD13	2.13	0.84
1:A:837:LYS:HE2	1:A:838:TRP:H	1.50	0.76
1:A:432:LYS:CG	1:A:432:LYS:CE	2.63	0.76
1:A:432:LYS:CB	1:A:432:LYS:CD	2.64	0.76
1:A:441:ARG:NH1	1:A:489:GLU:OE1	2.18	0.76
1:A:775:ARG:HD2	1:A:856:ILE:HD12	1.67	0.74
1:A:527:ARG:O	1:A:673:LYS:HD3	1.88	0.74
1:A:330:LEU:O	1:A:864:TRP:HZ3	1.73	0.72
1:A:570:ILE:O	1:A:573:LEU:HB2	1.90	0.71
1:A:523:GLU:O	1:A:526:THR:HG22	1.93	0.68
1:A:444:HIS:CB	1:A:448:GLU:O	2.35	0.64
1:A:727:ARG:HD2	1:A:829:MET:CE	2.27	0.64
1:A:837:LYS:HA	1:A:837:LYS:HE2	1.79	0.63
1:A:487:GLU:OE1	1:A:604:SER:HA	1.98	0.63
1:A:847:ARG:H	1:A:847:ARG:HH11	1.48	0.62
1:A:820:ARG:HD3	4:A:1027:HOH:O	2.01	0.61
1:A:864:TRP:CD1	1:A:865:ALA:N	2.69	0.61
1:A:384:TRP:CH2	1:A:555:VAL:HG13	2.35	0.61
1:A:792:TRP:CH2	1:A:879:ILE:CD1	2.84	0.60
1:A:875:VAL:O	1:A:879:ILE:HG23	2.01	0.59
1:A:562:GLU:OE1	4:A:1041:HOH:O	2.17	0.59
1:A:724:LYS:HE3	4:A:1035:HOH:O	2.05	0.56
1:A:727:ARG:HD2	1:A:829:MET:HE2	1.88	0.56
1:A:735:GLY:O	1:A:738:GLU:HG2	2.06	0.55
1:A:377:ASN:ND2	1:A:554:LYS:HZ1	2.05	0.55
1:A:855:LEU:O	1:A:858:THR:HG22	2.07	0.55
1:A:402:ILE:HG12	1:A:428:VAL:HG13	1.89	0.54
1:A:512:LEU:HD13	1:A:520:ILE:CD1	2.38	0.54
1:A:512:LEU:HD13	1:A:520:ILE:HD13	1.89	0.54
1:A:432:LYS:CD	1:A:432:LYS:NZ	2.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LYS:HG3	1:A:839:SER:H	1.73	0.53
1:A:552:GLU:O	1:A:555:VAL:HG22	2.09	0.53
1:A:762:SER:HB3	1:A:809:MET:SD	2.49	0.52
1:A:810:THR:HB	1:A:812:GLU:H	1.75	0.52
1:A:495:ASN:ND2	1:A:607:VAL:O	2.42	0.52
1:A:543:ARG:HD2	1:A:690:SER:O	2.10	0.52
1:A:330:LEU:O	1:A:864:TRP:CZ3	2.59	0.52
1:A:617:ASN:ND2	1:A:621:GLN:HE21	2.08	0.52
1:A:332:LYS:HG2	1:A:332:LYS:CE	2.38	0.51
1:A:861:ARG:O	1:A:864:TRP:CD1	2.52	0.51
1:A:650:THR:O	1:A:654:GLU:HG2	2.11	0.51
1:A:512:LEU:CD1	1:A:520:ILE:HD13	2.41	0.50
1:A:780:MET:HB2	1:A:864:TRP:HH2	1.76	0.50
1:A:837:LYS:HE2	1:A:838:TRP:N	2.24	0.50
1:A:327:VAL:HG11	1:A:743:ALA:CB	2.43	0.48
1:A:727:ARG:HB3	1:A:829:MET:HE1	1.96	0.48
1:A:555:VAL:O	1:A:558:LEU:HB2	2.14	0.48
1:A:551:ASN:HD22	1:A:554:LYS:HE3	1.79	0.47
1:A:402:ILE:HG12	1:A:428:VAL:CG1	2.45	0.47
1:A:762:SER:HB2	1:A:798:THR:HG21	1.96	0.47
1:A:332:LYS:NZ	1:A:332:LYS:CD	2.78	0.47
1:A:571:ILE:C	1:A:573:LEU:H	2.18	0.47
1:A:444:HIS:CE1	1:A:486:LEU:HD13	2.51	0.46
1:A:879:ILE:HD11	1:A:882:GLU:HG3	1.97	0.46
1:A:329:LEU:CB	1:A:329:LEU:CD2	2.82	0.45
1:A:793:VAL:HG12	4:A:1061:HOH:O	2.16	0.45
1:A:823:ILE:HD11	1:A:835:VAL:HG23	1.99	0.44
1:A:432:LYS:HB2	1:A:432:LYS:CD	2.46	0.44
1:A:721:LEU:HD11	1:A:773:HIS:HB3	1.99	0.44
1:A:846:LYS:H	1:A:847:ARG:NH1	2.16	0.43
1:A:759:LEU:HD13	1:A:796:GLY:HA3	2.01	0.43
1:A:727:ARG:HD2	1:A:829:MET:HE1	1.99	0.43
1:A:377:ASN:HD22	1:A:554:LYS:HZ1	1.65	0.43
1:A:546:ARG:O	1:A:550:GLU:HG3	2.18	0.42
1:A:500:LEU:HD13	1:A:611:ALA:HA	2.00	0.42
1:A:441:ARG:HH11	1:A:489:GLU:CD	2.21	0.42
1:A:837:LYS:CA	1:A:837:LYS:HE2	2.49	0.42
1:A:487:GLU:OE1	1:A:605:GLY:HA3	2.19	0.42
1:A:847:ARG:HD2	1:A:848:GLU:H	1.85	0.42
1:A:732:PRO:O	1:A:773:HIS:HE1	2.03	0.42
1:A:370:GLU:OE1	1:A:639:LYS:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:TRP:CD1	1:A:710:GLN:HG3	2.56	0.41
1:A:624:ARG:HG2	1:A:679:PHE:CE1	2.55	0.41
1:A:651:TRP:CZ2	1:A:659:ARG:HD2	2.54	0.41
1:A:830:GLU:CD	1:A:830:GLU:H	2.23	0.41
1:A:685:PHE:O	1:A:689:MET:HG3	2.20	0.41
1:A:568:ARG:NH1	4:A:1076:HOH:O	2.53	0.41
1:A:792:TRP:CZ3	1:A:879:ILE:HD13	2.55	0.41
1:A:617:ASN:HD21	1:A:621:GLN:HE21	1.67	0.41
1:A:732:PRO:O	1:A:773:HIS:CE1	2.73	0.41
1:A:709:GLN:NE2	1:A:720:GLU:H	2.19	0.41
1:A:389:ARG:HG3	1:A:390:GLU:HG3	2.02	0.40
1:A:754:ARG:NH1	4:A:1061:HOH:O	2.41	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	474/595 (80%)	452 (95%)	21 (4%)	1 (0%)	52	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	ALA

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	415/508 (82%)	365 (88%)	50 (12%)	6 5

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	VAL
1	A	332	LYS
1	A	376	LEU
1	A	404	LYS
1	A	441	ARG
1	A	442	GLU
1	A	450	HIS
1	A	451	THR
1	A	484	ARG
1	A	514	LEU
1	A	515	GLN
1	A	521	LEU
1	A	526	THR
1	A	555	VAL
1	A	558	LEU
1	A	604	SER
1	A	617	ASN
1	A	622	LEU
1	A	634	PRO
1	A	659	ARG
1	A	660	LEU
1	A	719	THR
1	A	740	VAL
1	A	747	PRO
1	A	754	ARG
1	A	755	ASP
1	A	756	THR
1	A	762	SER
1	A	769	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	816	GLU
1	A	817	VAL
1	A	821	VAL
1	A	830	GLU
1	A	837	LYS
1	A	844	SER
1	A	847	ARG
1	A	848	GLU
1	A	851	TRP
1	A	855	LEU
1	A	856	ILE
1	A	861	ARG
1	A	864	TRP
1	A	879	ILE

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	420	GLN
1	A	444	HIS
1	A	495	ASN
1	A	551	ASN
1	A	617	ASN
1	A	687	ASN
1	A	709	GLN
1	A	773	HIS
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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	486/595 (81%)	0.78	68 (13%) 4 7	46, 56, 77, 101	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	PHE	8.7
1	A	422	ARG	7.4
1	A	338	THR	7.1
1	A	475	ALA	6.1
1	A	421	TRP	5.2
1	A	476	ILE	5.0
1	A	802	ILE	5.0
1	A	801	SER	4.8
1	A	477	TRP	4.7
1	A	474	ARG	4.6
1	A	426	GLU	4.3
1	A	433	PHE	4.3
1	A	363	THR	4.0
1	A	746	SER	4.0
1	A	402	ILE	3.9
1	A	575	TYR	3.8
1	A	859	ARG	3.8
1	A	427	ALA	3.7
1	A	436	MET	3.6
1	A	479	MET	3.6
1	A	428	VAL	3.5
1	A	890	SER	3.4
1	A	420	GLN	3.4
1	A	892	LYS	3.4
1	A	430	ASP	3.4
1	A	866	GLU	3.4
1	A	864	TRP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	805	GLY	3.3
1	A	804	ALA	3.3
1	A	747	PRO	3.2
1	A	891	LEU	3.2
1	A	429	GLU	3.1
1	A	322	LEU	3.1
1	A	863	THR	3.1
1	A	435	GLU	3.0
1	A	336	THR	3.0
1	A	432	LYS	2.9
1	A	642	LYS	2.8
1	A	409	ALA	2.7
1	A	514	LEU	2.7
1	A	410	ALA	2.7
1	A	755	ASP	2.6
1	A	664	ALA	2.6
1	A	364	LYS	2.6
1	A	323	VAL	2.5
1	A	831	ASP	2.5
1	A	670	CYS	2.5
1	A	480	TRP	2.4
1	A	614	THR	2.4
1	A	671	VAL	2.3
1	A	666	SER	2.3
1	A	450	HIS	2.3
1	A	431	PRO	2.3
1	A	423	SER	2.3
1	A	618	LEU	2.3
1	A	646	PRO	2.3
1	A	424	ALA	2.3
1	A	434	TRP	2.3
1	A	616	THR	2.1
1	A	611	ALA	2.1
1	A	521	LEU	2.1
1	A	619	ALA	2.1
1	A	830	GLU	2.1
1	A	851	TRP	2.1
1	A	620	VAL	2.1
1	A	665	VAL	2.1
1	A	337	ILE	2.0
1	A	392	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. 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, 95th 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(\AA^2)	Q<0.9
2	CA	A	1	1/1	0.97	0.06	-2.51	55,55,55,55	0
3	ZN	A	2	1/1	0.98	0.05	-2.88	65,65,65,65	0
3	ZN	A	3	1/1	0.97	0.07	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.