



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 AM UTC

PDB ID : 2HCS / pdb_00002hcs
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

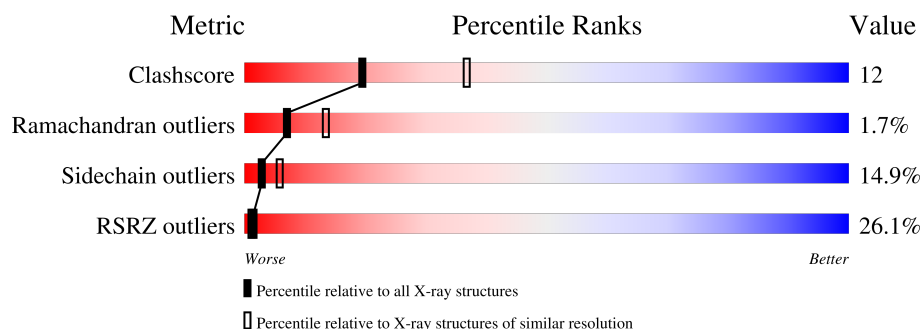
1 Overall quality at a glance

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	595	21% 58% 18% 5% 18%

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 (CCD ID: ZN) (formula: Zn).

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

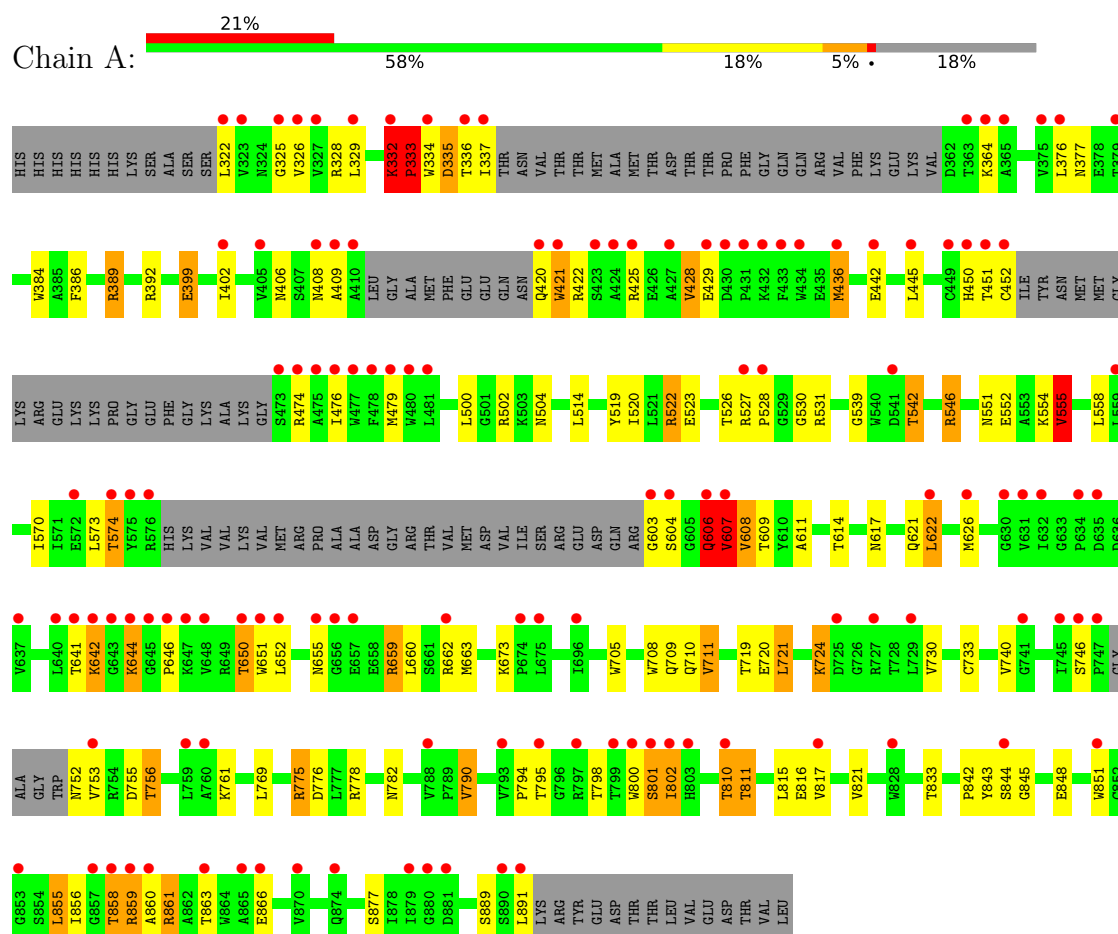
- Molecule 3 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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	P 43	Depositor
Cell constants a, b, c, α , β , γ	109.99Å 109.99Å 69.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.88 – 2.50 33.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.88-2.50) 98.2 (33.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.243 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4044	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.10	16/4026 (0.4%)	1.10	19/5449 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	GLY	C-N	15.99	1.54	1.33
1	A	332	LYS	CE-NZ	15.37	1.95	1.49
1	A	325	GLY	C-O	14.57	1.41	1.23
1	A	724	LYS	CE-NZ	12.74	1.87	1.49
1	A	436	MET	SD-CE	11.50	2.08	1.79
1	A	724	LYS	CD-CE	10.01	1.82	1.52
1	A	329	LEU	C-N	9.87	1.48	1.33
1	A	859	ARG	CZ-NH1	9.74	1.46	1.32
1	A	332	LYS	CD-CE	9.73	1.81	1.52
1	A	332	LYS	CG-CD	8.83	1.78	1.52
1	A	859	ARG	CG-CD	7.69	1.75	1.52
1	A	326	VAL	N-CA	-6.88	1.38	1.46
1	A	607	VAL	CA-CB	5.89	1.62	1.54
1	A	329	LEU	C-O	-5.50	1.16	1.24
1	A	333	PRO	N-CA	5.29	1.54	1.47
1	A	332	LYS	CB-CG	5.21	1.68	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	LYS	CD-CE-NZ	-7.83	86.84	111.90
1	A	332	LYS	CB-CG-CD	-7.48	94.10	111.30
1	A	555	VAL	CB-CA-C	-7.35	101.32	112.05
1	A	329	LEU	CA-C-O	7.06	128.14	119.11
1	A	711	VAL	CB-CA-C	6.63	117.10	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	811	THR	N-CA-C	-6.40	105.23	114.12
1	A	810	THR	CB-CA-C	-6.11	99.20	111.17
1	A	436	MET	CG-SD-CE	-6.08	87.52	100.90
1	A	790	VAL	CB-CA-C	-6.05	104.11	112.04
1	A	800	TRP	N-CA-C	-5.80	101.10	110.32
1	A	724	LYS	CG-CD-CE	-5.76	98.05	111.30
1	A	364	LYS	N-CA-C	5.69	119.18	108.65
1	A	711	VAL	N-CA-CB	5.63	116.26	110.23
1	A	798	THR	N-CA-C	-5.53	107.19	114.04
1	A	428	VAL	N-CA-C	5.17	115.39	110.53
1	A	833	THR	CA-C-N	5.08	125.36	119.92
1	A	833	THR	C-N-CA	5.08	125.36	119.92
1	A	326	VAL	N-CA-C	-5.03	105.94	110.82
1	A	333	PRO	CA-CB-CG	-5.02	94.96	104.50

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	90	0
2	A	2	0	0	0	0
3	A	106	0	0	2	0
All	All	4044	0	3844	90	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 (90) 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:CD	1:A:332:LYS:CG	1.78	1.59
1:A:724:LYS:CD	1:A:724:LYS:CE	1.82	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:A:332:LYS:NZ	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:CE	1:A:724:LYS:CG	2.60	0.80
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:CD	1:A:724:LYS:NZ	2.54	0.71
1:A:389:ARG:NH2	1:A:504:ASN:O	2.23	0.71
1:A:622:LEU:HD13	1:A:663:MET:HE1	1.74	0.69
1:A:384:TRP:CH2	1:A:555:VAL:HG13	2.29	0.68
1:A:859:ARG:CG	1:A:859:ARG:NE	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:CD	1:A:332:LYS:HB3	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:606:GLN:N	1:A:606:GLN:CD	2.66	0.54
1:A:646:PRO:O	1:A:650:THR:HG23	2.09	0.53
1:A:399:GLU:H	1:A:399:GLU:CD	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:GLN:HE21	1:A:719:THR:HA	1.73	0.52
1:A:337:ILE:O	1:A:337:ILE:HG22	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:651:TRP:CD1	1:A:655:ASN:HD22	2.30	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:848:GLU:OE2	1:A:848:GLU:N	2.44	0.48
1:A:421:TRP:HD1	1:A:421:TRP:O	1.97	0.48
1:A:606:GLN:CD	1:A:606:GLN:H	2.19	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
1:A:721:LEU:HD21	1:A:844:SER:HA	1.96	0.48
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: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:377:ASN:ND2	1:A:554:LYS:HZ1	2.15	0.45
1:A:552:GLU:O	1:A:555:VAL:HG22	2.17	0.45
1:A:641:THR:HB	1:A:644:LYS:HG3	1.99	0.45
1:A:858:THR:HG22	1:A:861:ARG:H	1.81	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: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:617:ASN:HD21	1:A:621:GLN:HE21	1.64	0.43
1:A:782:ASN:ND2	1:A:891:LEU:HD21	2.32	0.43
1:A:859:ARG:O	1:A:860:ALA:C	2.61	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:421:TRP:CD1	1:A:421:TRP:C	2.97	0.43
1:A:651:TRP:CZ2	1:A:659:ARG:HD2	2.54	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:GLN:NE2	1:A:720:GLU:H	2.17	0.42
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%)	7 13

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%)	354 (85%)	62 (15%)	3 6

All (62) 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
1	A	333	PRO
1	A	376	LEU
1	A	392	ARG
1	A	399	GLU
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	476	ILE
1	A	514	LEU
1	A	520	ILE
1	A	522	ARG
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	622	LEU
1	A	642	LYS
1	A	644	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

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Mol	Chain	Res	Type
1	A	733	CYS
1	A	740	VAL
1	A	746	SER
1	A	753	VAL
1	A	756	THR
1	A	769	LEU
1	A	775	ARG
1	A	778	ARG
1	A	790	VAL
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	856	ILE
1	A	858	THR
1	A	861	ARG
1	A	863	THR
1	A	866	GLU
1	A	877	SER
1	A	889	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	450	HIS
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	716	ASN
1	A	752	ASN
1	A	782	ASN
1	A	874	GLN

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 oligosaccharides 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, 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	487/595 (81%)	1.50	127 (26%) 1 1	38, 52, 76, 94	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	PHE	6.4
1	A	322	LEU	6.2
1	A	410	ALA	6.1
1	A	802	ILE	6.0
1	A	477	TRP	5.6
1	A	326	VAL	5.4
1	A	645	GLY	5.4
1	A	433	PHE	5.2
1	A	405	VAL	4.8
1	A	603	GLY	4.4
1	A	799	THR	4.3
1	A	859	ARG	4.2
1	A	336	THR	4.1
1	A	656	GLY	4.1
1	A	747	PRO	4.0
1	A	891	LEU	4.0
1	A	630	GLY	3.9
1	A	800	TRP	3.8
1	A	860	ALA	3.8
1	A	473	SER	3.8
1	A	427	ALA	3.8
1	A	420	GLN	3.8
1	A	449	CYS	3.8
1	A	480	TRP	3.8
1	A	434	TRP	3.7
1	A	745	ILE	3.7
1	A	803	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	644	LYS	3.7
1	A	890	SER	3.6
1	A	337	ILE	3.6
1	A	575	TYR	3.5
1	A	475	ALA	3.5
1	A	375	VAL	3.5
1	A	481	LEU	3.5
1	A	635	ASP	3.5
1	A	753	VAL	3.5
1	A	409	ALA	3.5
1	A	801	SER	3.5
1	A	880	GLY	3.5
1	A	643	GLY	3.4
1	A	851	TRP	3.4
1	A	329	LEU	3.4
1	A	640	LEU	3.3
1	A	647	LYS	3.3
1	A	541	ASP	3.3
1	A	651	TRP	3.3
1	A	634	PRO	3.2
1	A	450	HIS	3.2
1	A	746	SER	3.1
1	A	844	SER	3.1
1	A	436	MET	3.1
1	A	445	LEU	3.1
1	A	408	ASN	3.1
1	A	332	LYS	3.1
1	A	606	GLN	3.0
1	A	452	CYS	3.0
1	A	376	LEU	3.0
1	A	729	LEU	3.0
1	A	604	SER	2.9
1	A	870	VAL	2.9
1	A	637	VAL	2.8
1	A	574	THR	2.8
1	A	657	GLU	2.8
1	A	795	THR	2.8
1	A	675	LEU	2.8
1	A	650	THR	2.8
1	A	442	GLU	2.8
1	A	323	VAL	2.7
1	A	424	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	874	GLN	2.7
1	A	325	GLY	2.7
1	A	632	ILE	2.7
1	A	863	THR	2.6
1	A	474	ARG	2.6
1	A	379	THR	2.6
1	A	421	TRP	2.6
1	A	828	TRP	2.6
1	A	741	GLY	2.6
1	A	655	ASN	2.6
1	A	476	ILE	2.6
1	A	622	LEU	2.6
1	A	607	VAL	2.5
1	A	626	MET	2.5
1	A	759	LEU	2.5
1	A	631	VAL	2.5
1	A	648	VAL	2.5
1	A	430	ASP	2.5
1	A	425	ARG	2.5
1	A	879	ILE	2.5
1	A	479	MET	2.5
1	A	858	THR	2.4
1	A	857	GLY	2.4
1	A	788	VAL	2.4
1	A	576	ARG	2.4
1	A	451	THR	2.4
1	A	572	GLU	2.4
1	A	797	ARG	2.3
1	A	431	PRO	2.3
1	A	527	ARG	2.3
1	A	364	LYS	2.3
1	A	327	VAL	2.3
1	A	760	ALA	2.2
1	A	402	ILE	2.2
1	A	559	LEU	2.2
1	A	793	VAL	2.2
1	A	881	ASP	2.2
1	A	866	GLU	2.2
1	A	662	ARG	2.2
1	A	853	GLY	2.2
1	A	528	PRO	2.2
1	A	432	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	641	THR	2.1
1	A	652	LEU	2.1
1	A	674	PRO	2.1
1	A	429	GLU	2.1
1	A	423	SER	2.1
1	A	365	ALA	2.1
1	A	334	TRP	2.1
1	A	363	THR	2.1
1	A	696	ILE	2.1
1	A	646	PRO	2.1
1	A	865	ALA	2.0
1	A	810	THR	2.0
1	A	727	ARG	2.0
1	A	817	VAL	2.0
1	A	642	LYS	2.0
1	A	725	ASP	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	1	1/1	0.92	0.10	63,63,63,63	0
2	ZN	A	2	1/1	0.97	0.07	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.