



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:48 PM UTC

PDB ID : 2HCN / pdb_00002hcn
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

<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

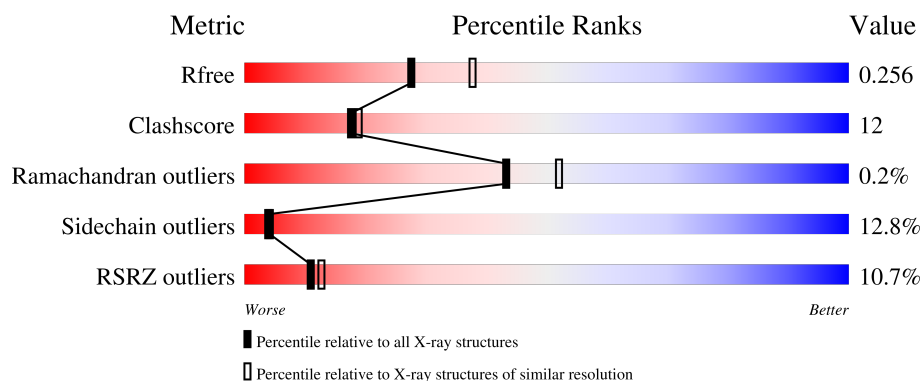
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	9% 58% 18% 5% 18%

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

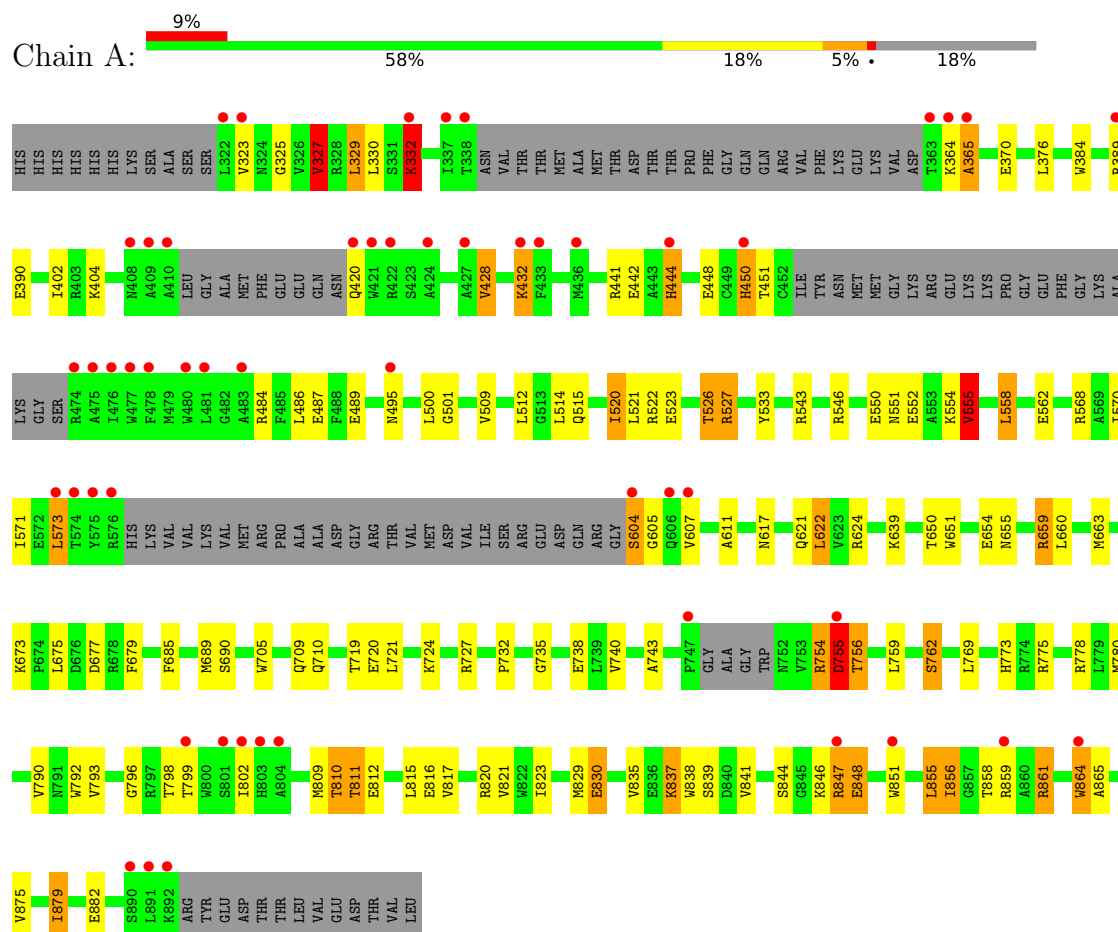
- Molecule 4 is water.

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

3 Residue-property plots [i](#)

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	110.06Å 110.06Å 68.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.82 – 2.35 34.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.82-2.35) 99.9 (34.82-2.35)	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 (5.05%)	wwPDB-VP
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 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	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, 0.333 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: CA, 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	1.04	14/4021 (0.3%)	1.15	21/5444 (0.4%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	LYS	CE-NZ	18.82	2.05	1.49
1	A	325	GLY	C-N	14.49	1.53	1.33
1	A	332	LYS	CD-CE	11.75	1.87	1.52
1	A	329	LEU	CG-CD1	11.08	1.89	1.52
1	A	432	LYS	CD-CE	10.36	1.83	1.52
1	A	327	VAL	C-O	8.20	1.34	1.24
1	A	432	LYS	CG-CD	7.95	1.76	1.52
1	A	329	LEU	CG-CD2	7.53	1.77	1.52
1	A	325	GLY	C-O	7.03	1.31	1.24
1	A	859	ARG	CD-NE	6.49	1.55	1.46
1	A	432	LYS	CE-NZ	6.06	1.67	1.49
1	A	332	LYS	C-N	5.49	1.40	1.33
1	A	509	VAL	CA-CB	5.24	1.61	1.54
1	A	859	ARG	CZ-NH1	5.05	1.39	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	756	THR	N-CA-C	12.56	126.39	111.82
1	A	555	VAL	CB-CA-C	-8.24	99.38	112.16
1	A	432	LYS	CG-CD-CE	-7.36	94.37	111.30
1	A	444	HIS	N-CA-C	7.23	122.21	112.88
1	A	332	LYS	O-C-N	7.20	126.89	120.48
1	A	332	LYS	CD-CE-NZ	-6.83	90.05	111.90
1	A	755	ASP	CA-C-N	6.66	130.43	120.31
1	A	755	ASP	C-N-CA	6.66	130.43	120.31
1	A	859	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	A	755	ASP	N-CA-C	-6.23	95.17	107.69
1	A	841	VAL	CA-C-N	6.14	126.10	119.78
1	A	841	VAL	C-N-CA	6.14	126.10	119.78
1	A	501	GLY	N-CA-C	-5.99	105.74	112.33
1	A	811	THR	N-CA-C	-5.76	106.29	113.38
1	A	327	VAL	CA-C-O	-5.50	114.64	120.64
1	A	859	ARG	NH1-CZ-NH2	5.36	126.27	119.30
1	A	450	HIS	CB-CA-C	5.12	117.12	109.13
1	A	332	LYS	CG-CD-CE	-5.11	99.54	111.30
1	A	444	HIS	CB-CA-C	5.11	119.36	110.72
1	A	655	ASN	N-CA-C	5.11	120.51	113.97
1	A	325	GLY	O-C-N	5.02	128.67	122.84

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	96	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	96	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 (96) 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:CD	1:A:432:LYS:CG	1.76	1.63
1:A:329:LEU:CG	1:A:329:LEU:CD2	1.77	1.58
1:A:432:LYS:CD	1:A:432:LYS:CE	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:CE	1:A:332:LYS:NZ	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:CE	1:A:332:LYS:CG	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:CD	1:A:432:LYS:CB	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:727:ARG:HD2	1:A:829:MET:HE2	1.71	0.73
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:HE2	1:A:837:LYS:HA	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:562:GLU:OE1	4:A:1041:HOH:O	2.17	0.59
1:A:875:VAL:O	1:A:879:ILE:HG23	2.01	0.59
1:A:551:ASN:ND2	1:A:554:LYS:HZ1	1.99	0.59
1:A:724:LYS:HE3	4:A:1035:HOH:O	2.05	0.56
1:A:735:GLY:O	1:A:738:GLU:HG2	2.06	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:552:GLU:O	1:A:555:VAL:HG22	2.09	0.53
1:A:837:LYS:HG3	1:A:839:SER:H	1.73	0.53
1:A:762:SER:HB3	1:A:809:MET:SD	2.49	0.52
1:A:495:ASN:ND2	1:A:607:VAL:O	2.42	0.52
1:A:810:THR:HB	1:A:812:GLU:H	1.75	0.52
1:A:622:LEU:HD13	1:A:663:MET:HE1	1.92	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:571:ILE:C	1:A:573:LEU:H	2.18	0.52
1:A:617:ASN:ND2	1:A:621:GLN:HE21	2.08	0.52
1:A:332:LYS:CE	1:A:332:LYS:HG2	2.38	0.51
1:A:650:THR:O	1:A:654:GLU:HG2	2.11	0.51
1:A:861:ARG:O	1:A:864:TRP:CD1	2.52	0.51
1:A:512:LEU:CD1	1:A:520:ILE:HD13	2.41	0.50
1:A:533:TYR:OH	1:A:677:ASP:OD1	2.28	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: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:CD	1:A:332:LYS:NZ	2.78	0.47
1:A:441:ARG:HH11	1:A:489:GLU:CD	2.21	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:830:GLU:H	1:A:830:GLU:CD	2.23	0.46
1:A:329:LEU:CD2	1:A:329:LEU:CB	2.82	0.45
1:A:793:VAL:HG12	4:A:1061:HOH:O	2.16	0.45
1:A:864:TRP:CD1	1:A:865:ALA:H	2.34	0.45
1:A:823:ILE:HD11	1:A:835:VAL:HG23	1.99	0.44
1:A:432:LYS:CD	1:A:432:LYS:HB2	2.46	0.44
1:A:721:LEU:HD11	1:A:773:HIS:HB3	1.99	0.44
1:A:441:ARG:NH1	1:A:489:GLU:CD	2.75	0.43
1:A:759:LEU:HD13	1:A:796:GLY:HA3	2.01	0.43
1:A:846:LYS:H	1:A:847:ARG:NH1	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:O	1:A:365:ALA:C	2.62	0.42
1:A:837:LYS:HE2	1:A:837:LYS:CA	2.49	0.42
1:A:487:GLU:OE1	1:A:605:GLY:HA3	2.19	0.42
1:A:370:GLU:OE1	1:A:639:LYS:HG2	2.20	0.42
1:A:732:PRO:O	1:A:773:HIS:HE1	2.03	0.42
1:A:847:ARG:HD2	1:A:848:GLU:H	1.85	0.42
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:685:PHE:O	1:A:689:MET:HG3	2.20	0.41
1:A:727:ARG:HB3	1:A:829:MET:HE1	2.03	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:709:GLN:NE2	1:A:720:GLU:H	2.19	0.41
1:A:732:PRO:O	1:A:773:HIS:CE1	2.73	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

5.3.1 Protein backbone

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%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	ALA

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	415/508 (82%)	362 (87%)	53 (13%)	4 4

All (53) 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	420	GLN
1	A	428	VAL
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	520	ILE
1	A	521	LEU
1	A	522	ARG
1	A	526	THR
1	A	527	ARG
1	A	555	VAL
1	A	558	LEU
1	A	573	LEU
1	A	604	SER
1	A	622	LEU
1	A	659	ARG
1	A	660	LEU
1	A	675	LEU
1	A	719	THR
1	A	740	VAL
1	A	754	ARG
1	A	755	ASP
1	A	756	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Sometimes 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	444	HIS
1	A	495	ASN
1	A	551	ASN
1	A	617	ASN
1	A	709	GLN
1	A	716	ASN
1	A	752	ASN
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 [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 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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.81	52 (10%)	11 13	46, 56, 77, 101	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	575	TYR	5.5
1	A	478	PHE	5.3
1	A	864	TRP	4.7
1	A	410	ALA	4.6
1	A	409	ALA	4.5
1	A	802	ILE	4.1
1	A	322	LEU	4.0
1	A	573	LEU	3.9
1	A	421	TRP	3.8
1	A	755	ASP	3.4
1	A	892	LYS	3.2
1	A	475	ALA	3.2
1	A	607	VAL	3.2
1	A	804	ALA	3.1
1	A	337	ILE	3.1
1	A	436	MET	3.1
1	A	891	LEU	3.0
1	A	576	ARG	2.9
1	A	890	SER	2.9
1	A	450	HIS	2.9
1	A	803	HIS	2.9
1	A	477	TRP	2.9
1	A	801	SER	2.9
1	A	474	ARG	2.8
1	A	424	ALA	2.8
1	A	851	TRP	2.8
1	A	338	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	422	ARG	2.8
1	A	323	VAL	2.8
1	A	364	LYS	2.7
1	A	408	ASN	2.7
1	A	480	TRP	2.6
1	A	363	THR	2.6
1	A	427	ALA	2.5
1	A	420	GLN	2.5
1	A	389	ARG	2.4
1	A	606	GLN	2.4
1	A	432	LYS	2.3
1	A	604	SER	2.3
1	A	859	ARG	2.3
1	A	476	ILE	2.3
1	A	799	THR	2.2
1	A	747	PRO	2.2
1	A	481	LEU	2.1
1	A	444	HIS	2.1
1	A	433	PHE	2.1
1	A	574	THR	2.1
1	A	483	ALA	2.1
1	A	332	LYS	2.1
1	A	495	ASN	2.1
1	A	847	ARG	2.1
1	A	365	ALA	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	ZN	A	3	1/1	0.96	0.08	56,56,56,56	0
3	ZN	A	2	1/1	0.98	0.05	65,65,65,65	0
2	CA	A	1	1/1	0.99	0.07	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.