



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 4C11 / pdb_00004c11
Title : Dengue virus RNA dependent RNA polymerase with residues from the NS5 linker region
Authors : Lim, S.P.; Lescar, J.
Deposited on : 2013-08-09
Resolution : 2.60 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

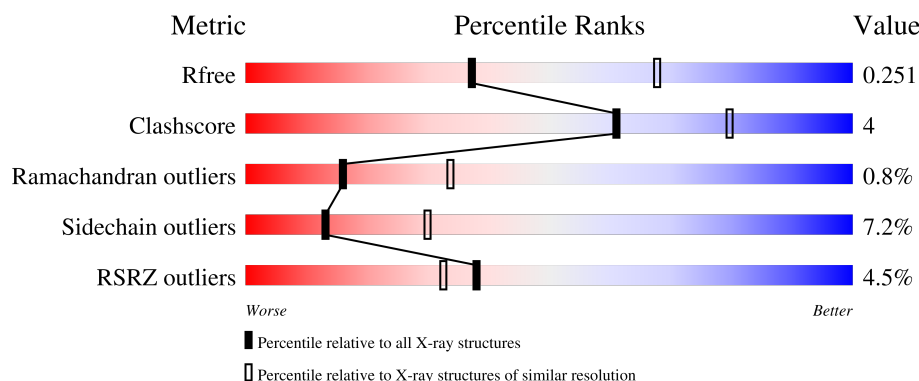
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	638	
2	B	638	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10134 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 DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	2	0
			4842	3057	872	882	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	GLU	GLY	conflict	UNP Q6DLV0
A	454	LYS	MET	conflict	UNP Q6DLV0

- Molecule 2 is a protein called DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	603	Total	C	N	O	S	0	0	0
			4864	3068	871	893	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	GLU	GLY	conflict	UNP Q6DLV0
B	409	ALA	GLY	conflict	UNP Q6DLV0
B	455	ALA	GLY	conflict	UNP Q6DLV0

- 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		
3	B	2	Total	Zn	0	0
			2	2		

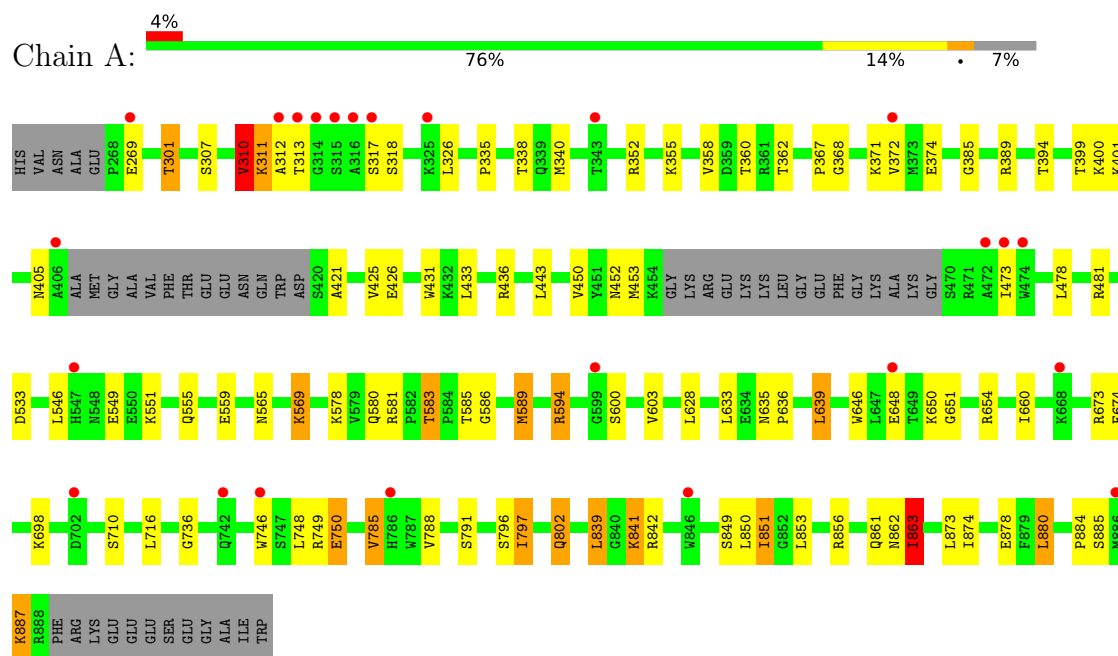
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	236	Total 236	O 236	0	0
4	B	188	Total 188	O 188	0	0

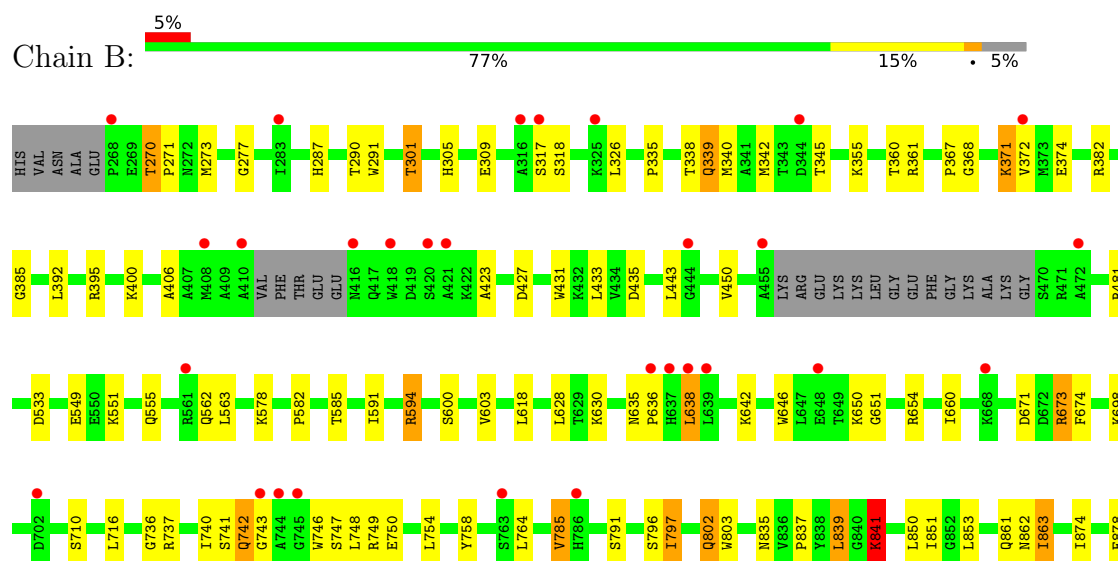
3 Residue-property plots

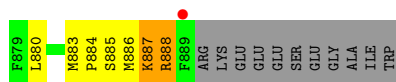
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE



• Molecule 2: DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.99Å 136.05Å 103.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.60 19.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.94-2.60) 97.7 (19.94-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.192 , 0.245 0.198 , 0.251	Depositor DCC
R_{free} test set	2676 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10134	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% 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: 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	0.87	3/4974 (0.1%)	1.42	41/6737 (0.6%)
2	B	0.88	3/4987 (0.1%)	1.45	43/6760 (0.6%)
All	All	0.88	6/9961 (0.1%)	1.43	84/13497 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	MET	SD-CE	-7.35	1.61	1.79
2	B	886	MET	CA-C	6.96	1.61	1.52
1	A	863	ILE	CA-CB	5.96	1.57	1.53
2	B	660	ILE	CG1-CD1	-5.19	1.31	1.51
1	A	660	ILE	CG1-CD1	-5.19	1.31	1.51
2	B	863	ILE	CA-CB	5.05	1.57	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	886	MET	CA-C-N	11.20	138.54	122.08
2	B	886	MET	C-N-CA	11.20	138.54	122.08
2	B	887	LYS	N-CA-C	10.78	126.14	111.90
1	A	310	VAL	CA-C-N	8.94	137.79	121.70
1	A	310	VAL	C-N-CA	8.94	137.79	121.70
1	A	600	SER	N-CA-C	6.91	119.69	111.33
2	B	746	TRP	N-CA-CB	6.84	119.81	110.57
2	B	796	SER	CA-C-N	6.82	129.80	120.46
2	B	796	SER	C-N-CA	6.82	129.80	120.46
2	B	271	PRO	N-CA-C	6.78	121.04	110.80
1	A	533	ASP	CA-CB-CG	6.72	119.33	112.60
2	B	600	SER	N-CA-C	6.67	119.40	111.33
1	A	639	LEU	CA-C-N	6.39	129.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	639	LEU	C-N-CA	6.39	129.48	120.28
2	B	747	SER	N-CA-C	-6.22	98.86	109.24
2	B	533	ASP	CA-CB-CG	6.02	118.62	112.60
2	B	635	ASN	N-CA-C	5.99	118.10	109.48
1	A	884	PRO	CA-C-N	5.89	132.80	121.54
1	A	884	PRO	C-N-CA	5.89	132.80	121.54
2	B	841	LYS	CA-C-N	5.89	128.09	120.44
2	B	841	LYS	C-N-CA	5.89	128.09	120.44
2	B	603	VAL	N-CA-C	-5.88	101.99	109.58
1	A	796	SER	CA-C-N	5.80	129.64	120.47
1	A	796	SER	C-N-CA	5.80	129.64	120.47
2	B	270	THR	CB-CA-C	5.75	116.63	110.65
1	A	603	VAL	N-CA-C	-5.71	101.44	109.21
1	A	546	LEU	CA-C-N	5.67	127.81	120.44
1	A	546	LEU	C-N-CA	5.67	127.81	120.44
2	B	885	SER	N-CA-C	-5.60	105.71	112.54
2	B	673	ARG	CA-C-N	5.59	128.04	120.38
2	B	673	ARG	C-N-CA	5.59	128.04	120.38
2	B	862	ASN	CA-C-N	5.58	123.76	120.24
2	B	862	ASN	C-N-CA	5.58	123.76	120.24
1	A	549	GLU	CA-C-N	5.58	128.31	120.28
1	A	549	GLU	C-N-CA	5.58	128.31	120.28
2	B	427	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	750	GLU	CA-C-N	5.57	127.68	120.44
2	B	750	GLU	C-N-CA	5.57	127.68	120.44
2	B	674	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	673	ARG	CA-C-N	5.54	127.96	120.38
1	A	673	ARG	C-N-CA	5.54	127.96	120.38
1	A	559	GLU	CB-CG-CD	5.53	122.00	112.60
1	A	839	LEU	N-CA-C	-5.53	103.23	110.53
2	B	746	TRP	CA-C-N	5.50	131.65	122.73
2	B	746	TRP	C-N-CA	5.50	131.65	122.73
1	A	310	VAL	CA-C-O	-5.49	113.92	120.78
1	A	311	LYS	CA-C-N	5.48	131.57	121.70
1	A	311	LYS	C-N-CA	5.48	131.57	121.70
1	A	674	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	358	VAL	N-CA-C	5.38	117.28	111.58
1	A	569	LYS	N-CA-C	5.35	116.92	111.14
1	A	885	SER	CA-C-N	5.30	129.89	122.36
1	A	885	SER	C-N-CA	5.30	129.89	122.36
2	B	839	LEU	N-CA-C	-5.27	103.57	110.53
1	A	394	THR	CA-C-N	5.26	127.65	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	THR	C-N-CA	5.26	127.65	120.54
1	A	635	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	648	GLU	CB-CG-CD	5.23	121.49	112.60
2	B	423	ALA	CA-C-N	5.20	127.50	120.38
2	B	423	ALA	C-N-CA	5.20	127.50	120.38
1	A	862	ASN	CA-C-N	5.20	123.51	120.24
1	A	862	ASN	C-N-CA	5.20	123.51	120.24
2	B	339	GLN	CA-C-N	5.12	127.40	120.38
2	B	339	GLN	C-N-CA	5.12	127.40	120.38
2	B	549	GLU	CA-C-N	5.12	127.65	120.28
2	B	549	GLU	C-N-CA	5.12	127.65	120.28
2	B	835	ASN	CA-C-N	5.11	126.27	122.59
2	B	835	ASN	C-N-CA	5.11	126.27	122.59
1	A	362	THR	CB-CA-C	5.11	115.67	109.85
1	A	785	VAL	N-CA-C	5.10	116.44	110.62
2	B	741	SER	N-CA-C	-5.10	102.09	109.59
2	B	785	VAL	N-CA-C	5.09	116.43	110.62
2	B	638	LEU	N-CA-C	5.09	118.01	110.48
1	A	338	THR	CA-C-N	5.08	127.08	120.28
1	A	338	THR	C-N-CA	5.08	127.08	120.28
2	B	885	SER	CA-C-N	5.07	130.32	122.26
2	B	885	SER	C-N-CA	5.07	130.32	122.26
1	A	583	THR	CB-CA-C	5.05	116.80	109.08
1	A	750	GLU	CA-C-N	5.04	126.99	120.44
1	A	750	GLU	C-N-CA	5.04	126.99	120.44
2	B	837	PRO	N-CA-C	5.03	119.22	111.57
2	B	758	TYR	CA-C-N	5.03	127.33	120.54
2	B	758	TYR	C-N-CA	5.03	127.33	120.54
1	A	887	LYS	N-CA-C	5.02	117.83	110.30

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	4842	0	4748	44	0
2	B	4864	0	4723	38	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	236	0	0	1	0
4	B	188	0	0	1	0
All	All	10134	0	9471	81	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 4.

All (81) 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:311:LYS:HB2	1:A:312:ALA:HA	1.44	0.95
2:B:802:GLN:HE21	2:B:802:GLN:H	1.19	0.89
2:B:301:THR:CG2	2:B:594:ARG:HH12	1.88	0.87
1:A:802:GLN:HE21	1:A:802:GLN:H	1.19	0.87
1:A:301:THR:CG2	1:A:594:ARG:HH12	1.88	0.85
2:B:301:THR:HG23	2:B:594:ARG:HH12	1.49	0.77
1:A:313:THR:HB	1:A:580:GLN:HE22	1.49	0.76
1:A:301:THR:HG23	1:A:594:ARG:HH12	1.52	0.75
2:B:385:GLY:HA3	2:B:555:GLN:HE22	1.52	0.74
1:A:385:GLY:HA3	1:A:555:GLN:HE22	1.52	0.74
2:B:883:MET:HB3	2:B:888:ARG:HD3	1.68	0.74
2:B:716:LEU:HD21	2:B:839:LEU:HD23	1.71	0.73
1:A:452:ASN:HB3	1:A:578:LYS:HG2	1.78	0.66
1:A:310:VAL:HB	1:A:311:LYS:HA	1.79	0.65
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.79	0.65
1:A:311:LYS:CB	1:A:312:ALA:HA	2.25	0.62
1:A:797:ILE:H	1:A:797:ILE:HD12	1.66	0.61
2:B:301:THR:HG23	2:B:594:ARG:NH1	2.15	0.60
2:B:797:ILE:HD12	2:B:797:ILE:H	1.67	0.59
1:A:301:THR:HG23	1:A:594:ARG:NH1	2.16	0.59
2:B:368:GLY:O	2:B:372:VAL:HG23	2.03	0.59
2:B:737:ARG:HA	2:B:740:ILE:HD12	1.85	0.58
2:B:841:LYS:HG2	2:B:851:ILE:HD12	1.84	0.58
2:B:372:VAL:HG11	2:B:628:LEU:HD11	1.88	0.56
1:A:269:GLU:HG3	1:A:594:ARG:HA	1.87	0.55
1:A:335:PRO:HG3	2:B:335:PRO:HG3	1.89	0.54
1:A:421:ALA:O	1:A:425:VAL:HG23	2.07	0.54
1:A:372:VAL:HG11	1:A:628:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:VAL:HG11	1:A:880:LEU:HD13	1.89	0.54
1:A:802:GLN:H	1:A:802:GLN:NE2	1.99	0.52
1:A:849:SER:OG	1:A:851:ILE:HG13	2.09	0.52
2:B:340:MET:HG3	2:B:736:GLY:HA3	1.91	0.52
1:A:785:VAL:CG1	1:A:880:LEU:HB2	2.40	0.52
2:B:802:GLN:H	2:B:802:GLN:NE2	1.99	0.51
1:A:425:VAL:HG13	1:A:431:TRP:HZ2	1.76	0.51
1:A:583:THR:HG23	1:A:586:GLY:H	1.77	0.50
2:B:290:THR:HG21	2:B:309:GLU:HG2	1.94	0.50
2:B:371:LYS:HG2	2:B:638:LEU:HB3	1.94	0.50
2:B:785:VAL:HG11	2:B:880:LEU:HB2	1.93	0.49
2:B:748:LEU:HD21	2:B:874:ILE:HA	1.93	0.48
1:A:841:LYS:HD3	1:A:851:ILE:HD13	1.95	0.48
2:B:742:GLN:HG3	2:B:754:LEU:HD21	1.94	0.48
1:A:797:ILE:H	1:A:797:ILE:CD1	2.26	0.48
4:A:2231:HOH:O	2:B:582:PRO:HD2	2.14	0.47
2:B:392:LEU:HD21	2:B:563:LEU:HD12	1.96	0.47
1:A:583:THR:CG2	1:A:586:GLY:H	2.27	0.47
1:A:748:LEU:HD21	1:A:874:ILE:HA	1.96	0.47
2:B:287:HIS:O	2:B:291:TRP:HB2	2.15	0.47
2:B:273:MET:HE3	2:B:277:GLY:HA2	1.97	0.47
1:A:367:PRO:HB2	1:A:636:PRO:HA	1.96	0.47
1:A:340:MET:HG3	1:A:736:GLY:HA3	1.97	0.47
1:A:399:THR:HA	1:A:425:VAL:HG11	1.97	0.47
1:A:746:TRP:HE3	1:A:750:GLU:HB3	1.79	0.47
2:B:841:LYS:HG2	2:B:851:ILE:CD1	2.46	0.46
2:B:367:PRO:HB2	2:B:636:PRO:HA	1.97	0.46
2:B:305:HIS:HB2	2:B:591:ILE:HG22	1.98	0.46
1:A:628:LEU:HD13	1:A:633:LEU:HD21	1.97	0.46
2:B:887:LYS:N	2:B:888:ARG:HA	2.31	0.46
2:B:797:ILE:H	2:B:797:ILE:CD1	2.28	0.45
1:A:565:ASN:O	1:A:569:LYS:HB2	2.16	0.45
1:A:785:VAL:HG11	1:A:880:LEU:HB2	1.97	0.45
2:B:850:LEU:O	2:B:853:LEU:HB2	2.16	0.44
1:A:850:LEU:O	1:A:853:LEU:HB2	2.16	0.44
1:A:401:LYS:O	1:A:405:ASN:HB2	2.17	0.43
1:A:310:VAL:HB	1:A:311:LYS:CA	2.48	0.43
2:B:301:THR:HG21	2:B:360:THR:C	2.43	0.43
2:B:764:LEU:HD12	2:B:803:TRP:HB3	2.01	0.43
2:B:395:ARG:HG3	2:B:431:TRP:CZ2	2.54	0.42
1:A:301:THR:CG2	1:A:594:ARG:NH1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:PRO:HA	2:B:887:LYS:HA	2.01	0.42
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.55	0.41
2:B:618:LEU:HD23	2:B:618:LEU:HA	1.96	0.41
1:A:301:THR:HG21	1:A:360:THR:C	2.45	0.41
1:A:307:SER:HA	1:A:589:MET:O	2.20	0.41
1:A:368:GLY:O	1:A:372:VAL:HG23	2.21	0.41
1:A:433:LEU:HD23	1:A:436:ARG:HE	1.86	0.41
1:A:863:ILE:HD13	1:A:863:ILE:HA	2.00	0.41
1:A:851:ILE:HG23	1:A:856:ARG:CZ	2.51	0.41
2:B:646:TRP:CZ2	2:B:654:ARG:HG3	2.56	0.41
2:B:562:GLN:HG3	4:B:2030:HOH:O	2.22	0.40
2:B:671:ASP:CG	2:B:673:ARG:HE	2.29	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	590/638 (92%)	564 (96%)	22 (4%)	4 (1%)	18	38
2	B	597/638 (94%)	576 (96%)	15 (2%)	6 (1%)	12	28
All	All	1187/1276 (93%)	1140 (96%)	37 (3%)	10 (1%)	16	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	742	GLN
1	A	310	VAL
1	A	651	GLY
2	B	651	GLY
2	B	743	GLY
1	A	551	LYS

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Mol	Chain	Res	Type
2	B	551	LYS
2	B	791	SER
1	A	791	SER
2	B	406	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	520/555 (94%)	481 (92%)	39 (8%)	12	28
2	B	516/555 (93%)	480 (93%)	36 (7%)	14	31
All	All	1036/1110 (93%)	961 (93%)	75 (7%)	13	30

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	THR
1	A	310	VAL
1	A	317	SER
1	A	318	SER
1	A	326	LEU
1	A	352	ARG
1	A	355	LYS
1	A	371	LYS
1	A	374	GLU
1	A	389[A]	ARG
1	A	389[B]	ARG
1	A	400	LYS
1	A	426	GLU
1	A	443	LEU
1	A	450	VAL
1	A	453	MET
1	A	473	ILE
1	A	478	LEU
1	A	481	ARG

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Mol	Chain	Res	Type
1	A	581	ARG
1	A	585	THR
1	A	594	ARG
1	A	639	LEU
1	A	650	LYS
1	A	698	LYS
1	A	710	SER
1	A	749	ARG
1	A	788	VAL
1	A	797	ILE
1	A	802	GLN
1	A	841	LYS
1	A	842	ARG
1	A	851	ILE
1	A	861	GLN
1	A	863	ILE
1	A	873	LEU
1	A	878	GLU
1	A	880	LEU
1	A	887	LYS
2	B	270	THR
2	B	301	THR
2	B	317	SER
2	B	318	SER
2	B	326	LEU
2	B	338	THR
2	B	339	GLN
2	B	342	MET
2	B	345	THR
2	B	355	LYS
2	B	361	ARG
2	B	371	LYS
2	B	374	GLU
2	B	382	ARG
2	B	400	LYS
2	B	433	LEU
2	B	435	ASP
2	B	443	LEU
2	B	450	VAL
2	B	481	ARG
2	B	578	LYS
2	B	585	THR

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Mol	Chain	Res	Type
2	B	594	ARG
2	B	630	LYS
2	B	642	LYS
2	B	650	LYS
2	B	698	LYS
2	B	710	SER
2	B	749	ARG
2	B	797	ILE
2	B	802	GLN
2	B	841	LYS
2	B	861	GLN
2	B	863	ILE
2	B	878	GLU
2	B	888	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	387	ASN
1	A	548	ASN
1	A	555	GLN
1	A	562	GLN
1	A	617	GLN
1	A	621	GLN
1	A	635	ASN
1	A	676	ASN
1	A	682	ASN
1	A	704	GLN
1	A	760	GLN
1	A	768	HIS
1	A	801	HIS
1	A	802	GLN
1	A	835	ASN
2	B	339	GLN
2	B	387	ASN
2	B	417	GLN
2	B	452	ASN
2	B	548	ASN
2	B	554	GLN
2	B	555	GLN
2	B	573	GLN

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Mol	Chain	Res	Type
2	B	621	GLN
2	B	676	ASN
2	B	682	ASN
2	B	704	GLN
2	B	742	GLN
2	B	760	GLN
2	B	768	HIS
2	B	802	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 4 ligands modelled in this entry, 4 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 ⓘ

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	593/638 (92%)	-0.09	24 (4%)	42 37	18, 55, 98, 152	13 (2%)
2	B	603/638 (94%)	0.17	30 (4%)	34 28	24, 66, 118, 155	11 (1%)
All	All	1196/1276 (93%)	0.04	54 (4%)	38 32	18, 60, 111, 155	24 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	455	ALA	6.1
1	A	316	ALA	4.5
2	B	744	ALA	4.1
1	A	317	SER	4.0
2	B	763	SER	3.8
2	B	561	ARG	3.8
2	B	316	ALA	3.8
2	B	638	LEU	3.7
2	B	317	SER	3.7
1	A	313	THR	3.6
1	A	474	TRP	3.6
1	A	473	ILE	3.5
2	B	639	LEU	3.4
1	A	702	ASP	3.4
1	A	786	HIS	3.2
1	A	269	GLU	3.1
1	A	746	TRP	3.1
1	A	314	GLY	3.1
2	B	410	ALA	3.1
2	B	786	HIS	3.1
2	B	372	VAL	3.1
2	B	889	PHE	3.0
1	A	472	ALA	3.0
2	B	418	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	315	SER	2.9
1	A	668	LYS	2.9
2	B	745	GLY	2.8
1	A	312	ALA	2.8
1	A	406	ALA	2.7
1	A	547	HIS	2.7
2	B	648	GLU	2.7
2	B	743	GLY	2.7
2	B	268	PRO	2.7
2	B	408	MET	2.6
2	B	636	PRO	2.6
1	A	343	THR	2.5
1	A	648	GLU	2.5
1	A	372	VAL	2.5
1	A	846	TRP	2.4
1	A	325	LYS	2.4
2	B	325	LYS	2.4
2	B	472	ALA	2.4
2	B	420	SER	2.3
2	B	637	HIS	2.3
1	A	599	GLY	2.3
1	A	742	GLN	2.3
2	B	668	LYS	2.2
2	B	702	ASP	2.2
2	B	416	ASN	2.2
2	B	283	ILE	2.2
2	B	444	GLY	2.1
2	B	421	ALA	2.1
2	B	344	ASP	2.0
1	A	886	MET	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 [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
3	ZN	A	1889	1/1	0.99	0.02	53,53,53,53	0
3	ZN	B	1890	1/1	0.99	0.03	50,50,50,50	0
3	ZN	B	1891	1/1	0.99	0.03	73,73,73,73	0
3	ZN	A	1890	1/1	1.00	0.05	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.