



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:26 AM UTC

PDB ID : 8OHM / pdb_00008ohm
Title : CRYSTAL STRUCTURE OF RNA HELICASE FROM GENOTYPE 1B
HEPATITIS C VIRUS: MECHANISM OF UNWINDING DUPLEX RNA
Authors : Cho, H.S.; Ha, N.C.; Kang, L.W.; Oh, B.H.
Deposited on : 1998-03-13
Resolution : 2.30 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

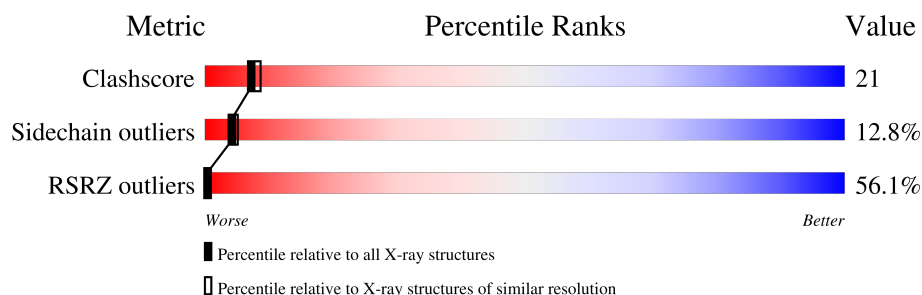
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	435	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3368 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 HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3228	2048	548	613	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	THR	SER	conflict	UNP P26663
A	240	VAL	ALA	conflict	UNP P26663
A	258	ALA	THR	conflict	UNP P26663
A	263	GLY	ALA	conflict	UNP P26663
A	265	ILE	VAL	conflict	UNP P26663
A	299	SER	THR	conflict	UNP P26663
A	358	VAL	ALA	conflict	UNP P26663
A	383	ALA	GLY	conflict	UNP P26663
A	386	LEU	ILE	conflict	UNP P26663
A	403	SER	ILE	conflict	UNP P26663
A	447	ASP	GLU	conflict	UNP P26663
A	584	SER	CYS	conflict	UNP P26663
A	586	THR	ILE	conflict	UNP P26663
A	605	LEU	VAL	conflict	UNP P26663
A	615	VAL	ILE	conflict	UNP P26663
A	618	PHE	TYR	conflict	UNP P26663

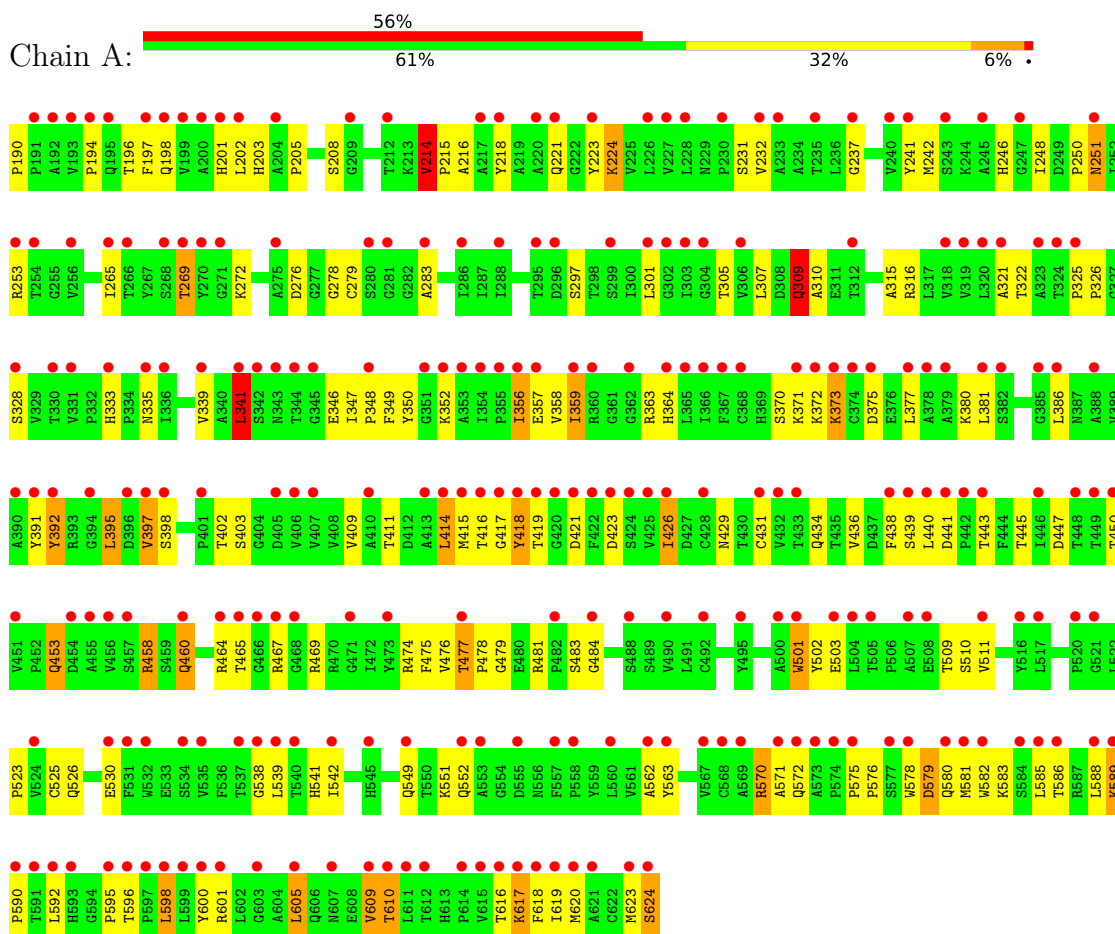
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	140	Total	O	0	0
			140	140		

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 HELICASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.30Å 93.30Å 104.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (10.00-2.30) 96.1 (10.00-2.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.59 (at 1.73Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.233 , 0.303 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	3368	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

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	0.72	0/3307	1.13	21/4524 (0.5%)

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	310	ALA	N-CA-C	8.90	120.59	111.07
1	A	190	PRO	N-CA-CB	7.19	110.91	103.00
1	A	251	ASN	N-CA-C	-7.14	98.41	109.76
1	A	609	VAL	N-CA-C	6.82	118.17	108.42
1	A	224	LYS	N-CA-C	-6.62	98.44	109.24
1	A	309	GLN	N-CA-C	6.61	121.51	113.38
1	A	411	THR	N-CA-C	-6.54	100.53	109.95
1	A	356	ILE	N-CA-C	5.80	116.53	110.62
1	A	579	ASP	N-CA-C	-5.73	102.55	110.35
1	A	443	THR	N-CA-C	5.63	117.78	108.48
1	A	502	TYR	N-CA-C	5.49	120.08	113.17
1	A	616	THR	N-CA-C	-5.46	105.33	111.28
1	A	501	TRP	N-CA-C	5.45	120.30	113.43
1	A	620	MET	N-CA-C	-5.39	105.49	111.36
1	A	341	LEU	N-CA-C	-5.29	103.15	110.35
1	A	509	THR	N-CA-C	-5.25	105.46	111.07
1	A	589	LYS	CA-C-N	5.16	124.47	118.85
1	A	589	LYS	C-N-CA	5.16	124.47	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	VAL	N-CA-C	-5.14	106.18	112.35
1	A	481	ARG	N-CA-C	5.11	116.35	109.24
1	A	598	LEU	N-CA-C	5.11	117.10	109.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	TYR	Sidechain
1	A	563	TYR	Sidechain

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	3228	0	3165	132	0
2	A	140	0	0	7	1
All	All	3368	0	3165	132	1

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 21.

All (132) 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:279:CYS:H	1:A:309:GLN:NE2	1.69	0.90
1:A:429:ASN:ND2	1:A:476:VAL:H	1.72	0.86
1:A:279:CYS:H	1:A:309:GLN:HE21	1.27	0.83
1:A:305:THR:O	1:A:309:GLN:HG3	1.80	0.82
1:A:598:LEU:HB2	1:A:609:VAL:HG21	1.62	0.81
1:A:194:PRO:HG3	1:A:198:GLN:HG2	1.63	0.80
1:A:269:THR:HG22	1:A:272:LYS:H	1.46	0.79
1:A:605:LEU:HD22	1:A:605:LEU:N	1.96	0.79
1:A:429:ASN:HA	1:A:453:GLN:NE2	2.00	0.76
1:A:347:ILE:HD13	1:A:381:LEU:CD2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:HB2	1:A:609:VAL:CG2	2.18	0.73
1:A:623:MET:O	1:A:624:SER:HB2	1.87	0.73
1:A:589:LYS:N	1:A:590:PRO:HD2	2.02	0.72
1:A:429:ASN:HD21	1:A:476:VAL:H	1.39	0.69
1:A:197:PHE:HD1	1:A:315:ALA:O	1.76	0.68
1:A:221:GLN:HE21	1:A:223:TYR:HE2	1.42	0.66
1:A:588:LEU:O	1:A:592:LEU:HG	1.95	0.66
1:A:248:ILE:O	1:A:250:PRO:HD3	1.96	0.65
1:A:418:TYR:CD2	1:A:419:THR:N	2.64	0.65
1:A:576:PRO:HB3	1:A:605:LEU:HD12	1.77	0.65
1:A:429:ASN:ND2	1:A:477:THR:H	1.96	0.64
1:A:391:TYR:HA	1:A:395:LEU:HD12	1.79	0.64
1:A:538:GLY:HA3	1:A:618:PHE:CE1	2.33	0.64
1:A:333:HIS:CD2	1:A:335:ASN:H	2.16	0.63
1:A:601:ARG:HH11	1:A:605:LEU:CD2	2.11	0.63
1:A:347:ILE:HD12	1:A:359:ILE:HD11	1.79	0.63
1:A:429:ASN:ND2	1:A:476:VAL:N	2.45	0.62
1:A:197:PHE:HA	1:A:316:ARG:O	2.00	0.62
1:A:419:THR:CB	1:A:467:ARG:NH1	2.63	0.62
1:A:341:LEU:HD13	1:A:474:ARG:HB3	1.83	0.61
1:A:605:LEU:HD22	1:A:605:LEU:H	1.63	0.61
1:A:224:LYS:HD2	1:A:283:ALA:O	2.02	0.60
1:A:588:LEU:C	1:A:590:PRO:HD2	2.26	0.60
1:A:598:LEU:CG	1:A:609:VAL:HG21	2.32	0.60
1:A:429:ASN:HD21	1:A:475:PHE:HB2	1.66	0.59
1:A:596:THR:O	1:A:609:VAL:HG23	2.01	0.59
1:A:598:LEU:CB	1:A:609:VAL:HG21	2.30	0.59
1:A:541:HIS:O	1:A:570:ARG:NH2	2.35	0.59
1:A:359:ILE:HA	1:A:364:HIS:CD2	2.37	0.59
1:A:429:ASN:HD21	1:A:476:VAL:N	2.00	0.58
1:A:580:GLN:O	1:A:583:LYS:HG2	2.02	0.58
1:A:253:ARG:HH21	1:A:276:ASP:CG	2.12	0.58
1:A:525:CYS:SG	1:A:526:GLN:N	2.77	0.58
1:A:416:THR:HA	1:A:464:ARG:NE	2.19	0.57
1:A:423:ASP:OD1	1:A:469:ARG:NH2	2.36	0.57
1:A:576:PRO:HG2	1:A:582:TRP:CZ2	2.40	0.57
1:A:419:THR:HB	1:A:467:ARG:NH1	2.19	0.57
1:A:426:ILE:HD13	1:A:474:ARG:HD2	1.87	0.57
1:A:458:ARG:NH2	1:A:477:THR:O	2.34	0.56
1:A:416:THR:HA	1:A:464:ARG:CZ	2.35	0.56
1:A:269:THR:HG21	2:A:825:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:CYS:N	1:A:309:GLN:NE2	2.49	0.56
1:A:194:PRO:CG	1:A:198:GLN:HG2	2.34	0.56
1:A:333:HIS:HD2	1:A:335:ASN:H	1.52	0.55
1:A:589:LYS:N	1:A:590:PRO:CD	2.69	0.55
1:A:347:ILE:HD13	1:A:381:LEU:HD21	1.86	0.55
1:A:460:GLN:OE1	1:A:464:ARG:NH2	2.39	0.55
1:A:201:HIS:HD2	2:A:801:HOH:O	1.90	0.55
1:A:418:TYR:O	1:A:419:THR:O	2.24	0.55
1:A:339:VAL:O	1:A:474:ARG:HA	2.07	0.54
1:A:375:ASP:OD1	1:A:392:TYR:OH	2.24	0.54
1:A:203:HIS:HE1	2:A:801:HOH:O	1.91	0.53
1:A:526:GLN:NE2	2:A:850:HOH:O	2.40	0.53
1:A:579:ASP:C	1:A:581:MET:H	2.16	0.52
1:A:392:TYR:HE1	1:A:395:LEU:HD21	1.74	0.52
1:A:205:PRO:O	1:A:208:SER:OG	2.26	0.52
1:A:598:LEU:HG	1:A:609:VAL:HG21	1.91	0.52
1:A:216:ALA:HB2	1:A:242:MET:HE1	1.91	0.51
1:A:586:THR:C	1:A:588:LEU:H	2.19	0.51
1:A:221:GLN:NE2	1:A:223:TYR:HE2	2.07	0.51
1:A:601:ARG:NH1	1:A:605:LEU:CD2	2.74	0.50
1:A:214:VAL:HB	1:A:215:PRO:HD3	1.93	0.50
1:A:392:TYR:CE1	1:A:395:LEU:HD21	2.47	0.50
1:A:251:ASN:HB3	2:A:920:HOH:O	2.12	0.50
1:A:414:LEU:HD21	1:A:418:TYR:CD2	2.47	0.50
1:A:194:PRO:HG2	1:A:316:ARG:O	2.12	0.50
1:A:414:LEU:HD22	1:A:418:TYR:HB3	1.94	0.49
1:A:598:LEU:HD22	1:A:600:TYR:O	2.12	0.49
1:A:503:GLU:N	2:A:898:HOH:O	2.41	0.49
1:A:386:LEU:HD12	1:A:386:LEU:N	2.29	0.48
1:A:370:SER:O	1:A:373:LYS:HB2	2.14	0.47
1:A:579:ASP:C	1:A:581:MET:N	2.69	0.47
1:A:202:LEU:O	1:A:321:ALA:HA	2.15	0.47
1:A:218:TYR:O	1:A:221:GLN:HB2	2.14	0.46
1:A:542:ILE:HD11	1:A:562:ALA:HB3	1.98	0.46
1:A:395:LEU:HD23	1:A:395:LEU:N	2.31	0.46
1:A:501:TRP:CH2	1:A:551:LYS:HB3	2.51	0.46
1:A:352:LYS:HG2	1:A:476:VAL:HG13	1.98	0.45
1:A:415:MET:C	1:A:417:GLY:H	2.24	0.45
1:A:194:PRO:HG3	1:A:198:GLN:CG	2.42	0.45
1:A:617:LYS:HZ2	1:A:617:LYS:HG3	1.65	0.45
1:A:605:LEU:N	1:A:605:LEU:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASN:CA	1:A:453:GLN:NE2	2.77	0.45
1:A:246:HIS:HB3	1:A:248:ILE:HD12	1.99	0.45
1:A:253:ARG:NH2	1:A:276:ASP:OD2	2.37	0.45
1:A:619:ILE:O	1:A:623:MET:HG2	2.17	0.45
1:A:377:LEU:HB3	1:A:409:VAL:HG11	1.99	0.44
1:A:415:MET:C	1:A:417:GLY:N	2.76	0.44
1:A:434:GLN:HA	1:A:447:ASP:O	2.18	0.44
1:A:438:PHE:HD1	1:A:623:MET:HE1	1.83	0.44
1:A:241:TYR:OH	1:A:246:HIS:CE1	2.71	0.43
1:A:346:GLU:OE1	1:A:356:ILE:HG22	2.18	0.43
1:A:325:PRO:HA	1:A:326:PRO:HD3	1.95	0.43
1:A:363:ARG:HB2	1:A:421:ASP:O	2.17	0.43
1:A:601:ARG:NH1	1:A:605:LEU:HD23	2.33	0.43
1:A:349:PHE:O	1:A:350:TYR:HB2	2.19	0.43
1:A:347:ILE:CD1	1:A:359:ILE:HD11	2.49	0.42
1:A:352:LYS:CG	1:A:476:VAL:HG13	2.49	0.42
1:A:419:THR:OG1	1:A:467:ARG:NH1	2.52	0.42
1:A:478:PRO:O	1:A:479:GLY:C	2.62	0.42
1:A:601:ARG:HH11	1:A:605:LEU:HD21	1.83	0.42
1:A:328:SER:HB2	1:A:483:SER:OG	2.19	0.42
1:A:402:THR:O	1:A:402:THR:HG22	2.18	0.42
1:A:371:LYS:HE3	1:A:392:TYR:CE1	2.55	0.42
1:A:441:ASP:O	1:A:601:ARG:NE	2.49	0.42
1:A:436:VAL:HA	1:A:445:THR:O	2.20	0.41
1:A:596:THR:O	1:A:609:VAL:HA	2.20	0.41
1:A:203:HIS:HA	1:A:322:THR:O	2.21	0.41
1:A:575:PRO:HD2	1:A:578:TRP:CZ2	2.55	0.41
1:A:595:PRO:HG2	1:A:610:THR:OG1	2.20	0.41
1:A:571:ALA:O	1:A:572:GLN:C	2.62	0.41
1:A:237:GLY:HA3	2:A:928:HOH:O	2.19	0.41
1:A:248:ILE:HG21	1:A:265:ILE:HD12	2.02	0.41
1:A:570:ARG:H	1:A:570:ARG:HG2	1.62	0.41
1:A:278:GLY:HA3	1:A:309:GLN:HE22	1.86	0.41
1:A:347:ILE:HA	1:A:348:PRO:HD3	1.90	0.41
1:A:397:VAL:HG11	1:A:418:TYR:CD1	2.56	0.41
1:A:484:GLY:O	1:A:523:PRO:HA	2.21	0.41
1:A:203:HIS:CD2	1:A:325:PRO:HG3	2.56	0.41
1:A:194:PRO:HD3	1:A:198:GLN:HG2	2.04	0.40
1:A:429:ASN:HD22	1:A:477:THR:H	1.69	0.40
1:A:579:ASP:O	1:A:581:MET:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:869:HOH:O	2:A:869:HOH:O[4_556]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	344/355 (97%)	300 (87%)	44 (13%)	4 4

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	THR
1	A	214	VAL
1	A	231	SER
1	A	232	VAL
1	A	269	THR
1	A	297	SER
1	A	301	LEU
1	A	307	LEU
1	A	309	GLN
1	A	341	LEU
1	A	357	GLU
1	A	358	VAL
1	A	359	ILE
1	A	372	LYS
1	A	373	LYS
1	A	380	LYS

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Mol	Chain	Res	Type
1	A	392	TYR
1	A	395	LEU
1	A	397	VAL
1	A	398	SER
1	A	403	SER
1	A	414	LEU
1	A	426	ILE
1	A	431	CYS
1	A	439	SER
1	A	440	LEU
1	A	450	THR
1	A	453	GLN
1	A	458	ARG
1	A	460	GLN
1	A	465	THR
1	A	477	THR
1	A	510	SER
1	A	511	VAL
1	A	530	GLU
1	A	539	LEU
1	A	549	GLN
1	A	552	GLN
1	A	570	ARG
1	A	585	LEU
1	A	605	LEU
1	A	610	THR
1	A	617	LYS
1	A	624	SER

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	201	HIS
1	A	221	GLN
1	A	246	HIS
1	A	309	GLN
1	A	333	HIS
1	A	343	ASN
1	A	429	ASN
1	A	453	GLN
1	A	526	GLN
1	A	552	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](#)

There are no ligands in this entry.

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	435/435 (100%)	2.36	244 (56%) 0 0	4, 16, 28, 36	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	VAL	7.5
1	A	417	GLY	6.8
1	A	455	ALA	6.4
1	A	415	MET	6.2
1	A	588	LEU	5.9
1	A	345	GLY	5.8
1	A	396	ASP	5.5
1	A	503	GLU	5.5
1	A	592	LEU	5.4
1	A	192	ALA	5.3
1	A	398	SER	5.2
1	A	607	ASN	5.2
1	A	419	THR	5.1
1	A	624	SER	5.0
1	A	590	PRO	4.9
1	A	194	PRO	4.9
1	A	265	ILE	4.9
1	A	416	THR	4.9
1	A	573	ALA	4.8
1	A	421	ASP	4.8
1	A	571	ALA	4.8
1	A	200	ALA	4.6
1	A	247	GLY	4.4
1	A	457	SER	4.3
1	A	362	GLY	4.3
1	A	542	ILE	4.3
1	A	508	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	331	VAL	4.1
1	A	209	GLY	4.0
1	A	448	THR	4.0
1	A	397	VAL	4.0
1	A	586	THR	4.0
1	A	388	ALA	4.0
1	A	582	TRP	3.9
1	A	414	LEU	3.9
1	A	217	ALA	3.9
1	A	275	ALA	3.9
1	A	567	VAL	3.9
1	A	368	CYS	3.8
1	A	339	VAL	3.8
1	A	407	VAL	3.8
1	A	484	GLY	3.8
1	A	473	TYR	3.7
1	A	335	ASN	3.7
1	A	603	GLY	3.7
1	A	569	ALA	3.7
1	A	360	ARG	3.7
1	A	351	GLY	3.7
1	A	372	LYS	3.7
1	A	193	VAL	3.7
1	A	295	THR	3.7
1	A	355	PRO	3.7
1	A	240	VAL	3.7
1	A	256	VAL	3.7
1	A	382	SER	3.6
1	A	577	SER	3.6
1	A	357	GLU	3.6
1	A	611	LEU	3.6
1	A	428	CYS	3.6
1	A	492	CYS	3.6
1	A	454	ASP	3.6
1	A	241	TYR	3.6
1	A	366	ILE	3.6
1	A	610	THR	3.6
1	A	245	ALA	3.5
1	A	303	ILE	3.5
1	A	354	ILE	3.5
1	A	423	ASP	3.4
1	A	612	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	342	SER	3.4
1	A	391	TYR	3.4
1	A	549	GLN	3.4
1	A	344	THR	3.3
1	A	538	GLY	3.3
1	A	426	ILE	3.3
1	A	614	PRO	3.3
1	A	390	ALA	3.3
1	A	553	ALA	3.3
1	A	336	ILE	3.2
1	A	466	GLY	3.2
1	A	530	GLU	3.2
1	A	593	HIS	3.2
1	A	504	LEU	3.2
1	A	312	THR	3.2
1	A	443	THR	3.2
1	A	413	ALA	3.2
1	A	495	TYR	3.2
1	A	501	TRP	3.2
1	A	591	THR	3.2
1	A	374	CYS	3.1
1	A	281	GLY	3.1
1	A	432	VAL	3.1
1	A	328	SER	3.1
1	A	378	ALA	3.1
1	A	227	VAL	3.1
1	A	364	HIS	3.1
1	A	488	SER	3.1
1	A	440	LEU	3.1
1	A	616	THR	3.1
1	A	467	ARG	3.1
1	A	320	LEU	3.0
1	A	235	THR	3.0
1	A	521	GLY	3.0
1	A	353	ALA	3.0
1	A	517	LEU	3.0
1	A	280	SER	3.0
1	A	304	GLY	3.0
1	A	323	ALA	3.0
1	A	584	SER	3.0
1	A	418	TYR	2.9
1	A	424	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	589	LYS	2.9
1	A	441	ASP	2.9
1	A	471	GLY	2.9
1	A	507	ALA	2.9
1	A	605	LEU	2.9
1	A	597	PRO	2.9
1	A	386	LEU	2.9
1	A	578	TRP	2.9
1	A	319	VAL	2.8
1	A	540	THR	2.8
1	A	202	LEU	2.8
1	A	199	VAL	2.8
1	A	490	VAL	2.8
1	A	270	TYR	2.8
1	A	197	PHE	2.8
1	A	545	HIS	2.8
1	A	343	ASN	2.8
1	A	552	GLN	2.8
1	A	233	ALA	2.8
1	A	464	ARG	2.8
1	A	563	TYR	2.7
1	A	422	PHE	2.7
1	A	449	THR	2.7
1	A	237	GLY	2.7
1	A	204	ALA	2.7
1	A	392	TYR	2.7
1	A	574	PRO	2.7
1	A	617	LYS	2.7
1	A	377	LEU	2.7
1	A	516	TYR	2.7
1	A	254	THR	2.7
1	A	220	ALA	2.6
1	A	451	VAL	2.6
1	A	420	GLY	2.6
1	A	442	PRO	2.6
1	A	341	LEU	2.6
1	A	379	ALA	2.6
1	A	621	ALA	2.6
1	A	500	ALA	2.6
1	A	212	THR	2.6
1	A	268	SER	2.6
1	A	410	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	405	ASP	2.6
1	A	615	VAL	2.6
1	A	560	LEU	2.5
1	A	333	HIS	2.5
1	A	371	LYS	2.5
1	A	223	TYR	2.5
1	A	620	MET	2.5
1	A	375	ASP	2.5
1	A	394	GLY	2.5
1	A	195	GLN	2.5
1	A	359	ILE	2.5
1	A	228	LEU	2.5
1	A	555	ASP	2.5
1	A	302	GLY	2.5
1	A	367	PHE	2.5
1	A	439	SER	2.5
1	A	218	TYR	2.5
1	A	381	LEU	2.5
1	A	572	GLN	2.5
1	A	446	ILE	2.4
1	A	232	VAL	2.4
1	A	425	VAL	2.4
1	A	580	GLN	2.4
1	A	520	PRO	2.4
1	A	595	PRO	2.4
1	A	460	GLN	2.4
1	A	330	THR	2.4
1	A	438	PHE	2.4
1	A	618	PHE	2.4
1	A	373	LYS	2.3
1	A	537	THR	2.3
1	A	243	SER	2.3
1	A	318	VAL	2.3
1	A	557	PHE	2.3
1	A	558	PRO	2.3
1	A	385	GLY	2.3
1	A	266	THR	2.3
1	A	477	THR	2.3
1	A	531	PHE	2.3
1	A	598	LEU	2.3
1	A	191	PRO	2.3
1	A	623	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	596	THR	2.3
1	A	226	LEU	2.3
1	A	365	LEU	2.3
1	A	431	CYS	2.3
1	A	465	THR	2.3
1	A	599	LEU	2.2
1	A	230	PRO	2.2
1	A	575	PRO	2.2
1	A	532	TRP	2.2
1	A	325	PRO	2.2
1	A	283	ALA	2.2
1	A	321	ALA	2.2
1	A	286	ILE	2.2
1	A	288	ILE	2.2
1	A	348	PRO	2.2
1	A	568	CYS	2.2
1	A	539	LEU	2.2
1	A	406	VAL	2.2
1	A	581	MET	2.2
1	A	269	THR	2.2
1	A	534	SER	2.2
1	A	619	ILE	2.1
1	A	251	ASN	2.1
1	A	482	PRO	2.1
1	A	201	HIS	2.1
1	A	299	SER	2.1
1	A	306	VAL	2.1
1	A	198	GLN	2.1
1	A	401	PRO	2.1
1	A	562	ALA	2.1
1	A	352	LYS	2.1
1	A	356	ILE	2.1
1	A	524	VAL	2.1
1	A	535	VAL	2.1
1	A	271	GLY	2.1
1	A	253	ARG	2.1
1	A	324	THR	2.1
1	A	585	LEU	2.1
1	A	456	VAL	2.1
1	A	468	GLY	2.1
1	A	433	THR	2.0
1	A	450	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	600	TYR	2.0
1	A	511	VAL	2.0
1	A	601	ARG	2.0
1	A	505	THR	2.0
1	A	221	GLN	2.0
1	A	296	ASP	2.0
1	A	301	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.