



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:46 am BST

PDB ID : 8OHM
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

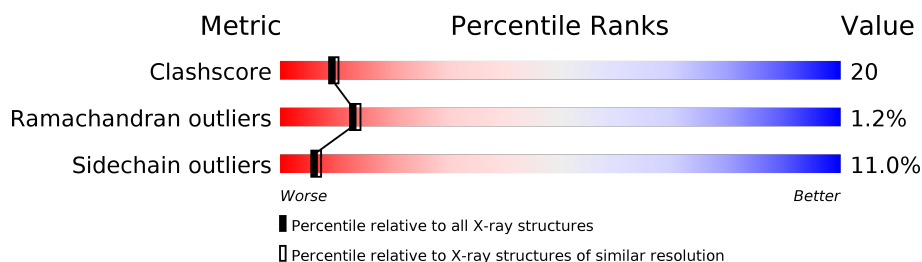
1 Overall quality at a glance

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 on 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 $\leq 5\%$.

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
			Total	C	N	O	S			
1	A	435	3228	2048	548	613	19	0	0	0

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

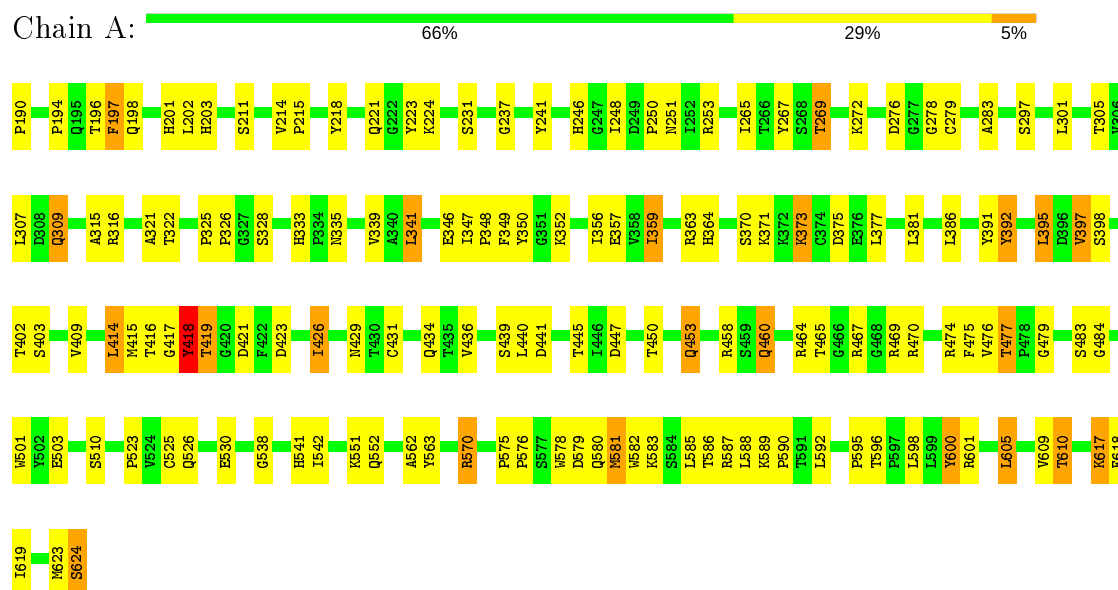
- Molecule 2 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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	93.30 Å 93.30 Å 104.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 29.32 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.0 (10.00-2.30) 43.5 (29.32-1.73)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.59 (at 1.73 Å)	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)	0.36 , 71.4	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 [i](#)

5.1 Standard geometry [i](#)

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	0.54	0/3307	0.76	1/4524 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	190	PRO	N-CA-CB	6.34	110.91	103.30

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 [i](#)

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	127	0
2	A	140	0	0	7	1
All	All	3368	0	3165	127	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 20.

All (127) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:588:LEU:C	1:A:590:PRO:HD2	2.26	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:253:ARG:HH21	1:A:276:ASP:CG	2.12	0.53
1:A:526:GLN:NE2	2:A:850:HOH:O	2.40	0.53
1:A:392:TYR:HE1	1:A:395:LEU:HD21	1.74	0.52
1:A:598:LEU:HG	1:A:609:VAL:HG21	1.91	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:579:ASP:C	1:A:581:MET:H	2.16	0.47
1:A:370:SER:O	1:A:373:LYS:HB2	2.14	0.47
1:A:202:LEU:O	1:A:321:ALA:HA	2.15	0.47
1:A:579:ASP:C	1:A:581:MET:N	2.69	0.46
1:A:586:THR:C	1:A:588:LEU:H	2.19	0.46
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:194:PRO:HG3	1:A:198:GLN:CG	2.42	0.45
1:A:605:LEU:N	1:A:605:LEU:CD2	2.69	0.45
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:434:GLN:HA	1:A:447:ASP:O	2.18	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:211:SER:O	1:A:267:TYR:OH	2.28	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:402:THR:O	1:A:402:THR:HG22	2.18	0.42
1:A:419:THR:OG1	1:A:467:ARG:NH1	2.52	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: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:617:LYS:HZ2	1:A:617:LYS:HG3	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:PRO:HG2	1:A:610:THR:OG1	2.20	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:415:MET:C	1:A:417:GLY:H	2.24	0.40
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 symmetry 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](#)

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	433/435 (100%)	406 (94%)	22 (5%)	5 (1%)	13 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	THR
1	A	197	PHE
1	A	479	GLY

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Mol	Chain	Res	Type
1	A	587	ARG
1	A	418	TYR

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	344/355 (97%)	306 (89%)	38 (11%)	6 7

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	THR
1	A	231	SER
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	359	ILE
1	A	373	LYS
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	460	GLN

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Mol	Chain	Res	Type
1	A	465	THR
1	A	470	ARG
1	A	477	THR
1	A	510	SER
1	A	530	GLU
1	A	552	GLN
1	A	570	ARG
1	A	581	MET
1	A	585	LEU
1	A	600	TYR
1	A	605	LEU
1	A	610	THR
1	A	617	LYS
1	A	624	SER

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	201	HIS
1	A	203	HIS
1	A	221	GLN
1	A	246	HIS
1	A	309	GLN
1	A	333	HIS
1	A	429	ASN
1	A	453	GLN
1	A	526	GLN
1	A	552	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

There are no ligands in this entry.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.