



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:31 pm BST

PDB ID : 5GVU
Title : crystal structure of BVDV NS3 helicase domain
Authors : Li, S.; Mao, X.
Deposited on : 2016-09-06
Resolution : 2.82 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

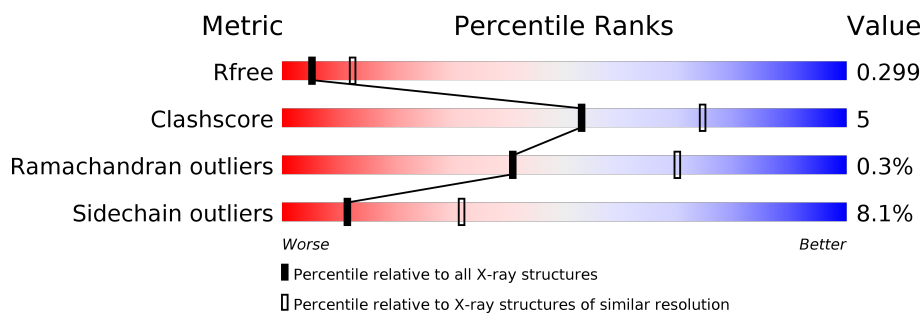
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)

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	476	
1	B	476	
1	C	476	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9452 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 NS3 helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3596	2289	609	680	18			
1	B	355	Total	C	N	O	S	0	0	0
			2824	1792	481	537	14			
1	C	377	Total	C	N	O	S	0	0	0
			2994	1902	512	565	15			

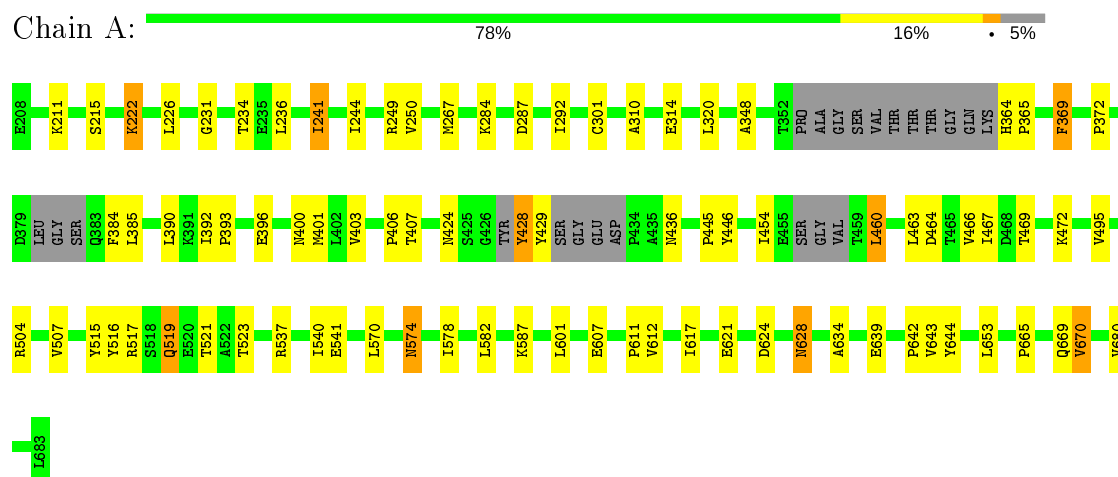
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	13	Total	O	0	0
			13	13		
2	C	10	Total	O	0	0
			10	10		

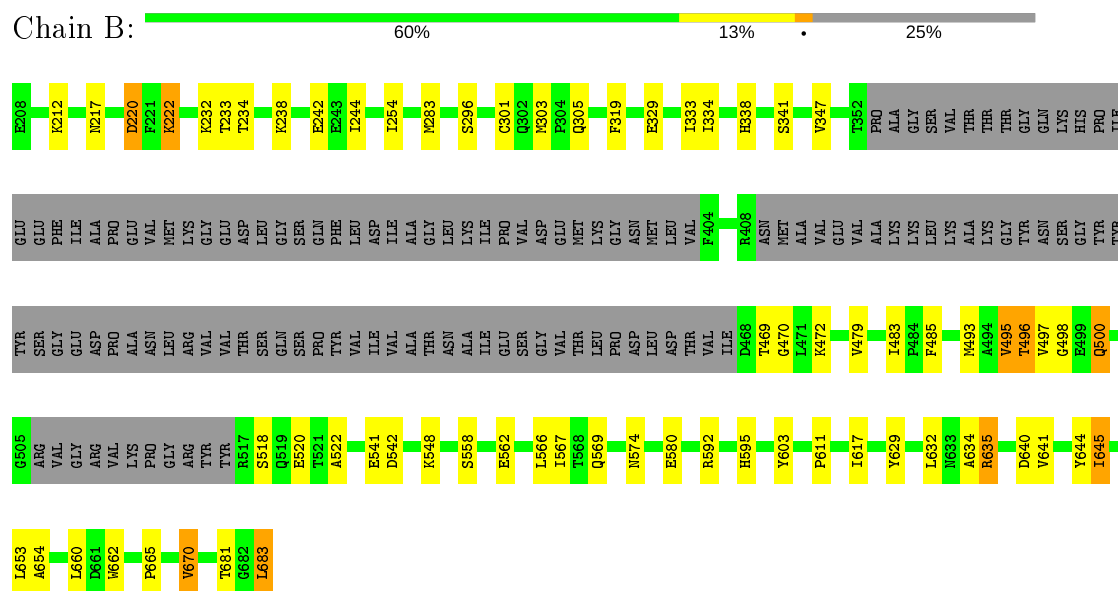
3 Residue-property plots [i](#)

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: NS3 helicase

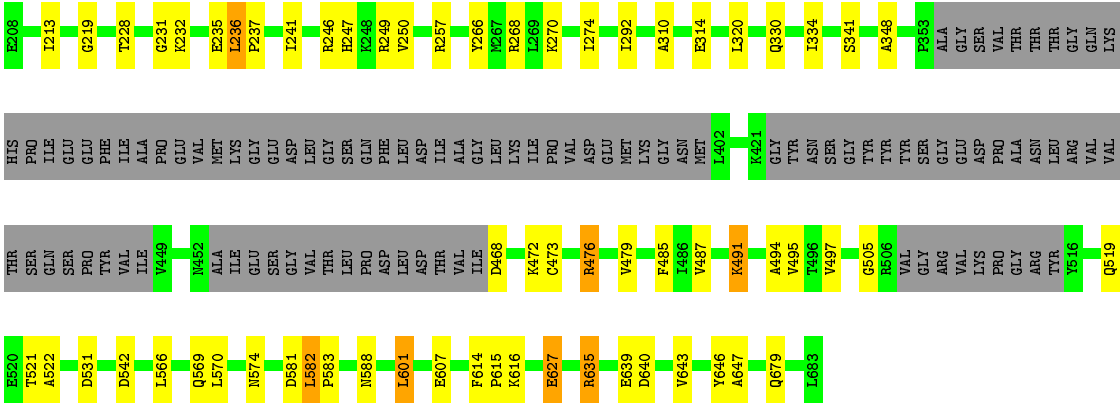


• Molecule 1: NS3 helicase



• Molecule 1: NS3 helicase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	121.10Å 121.10Å 109.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 2.82 48.61 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.01-2.82) 99.9 (48.61-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0124, REFMAC 5.8.0124	Depositor
R, R_{free}	0.272 , 0.298 0.272 , 0.299	Depositor DCC
R_{free} test set	2121 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.119 for -h,-k,l 0.119 for h,-h-k,-l 0.390 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9452	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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	0.42	0/3661	0.66	0/4949
1	B	0.41	0/2875	0.69	0/3886
1	C	0.43	0/3046	0.68	1/4115 (0.0%)
All	All	0.42	0/9582	0.68	1/12950 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	601	LEU	CA-CB-CG	5.07	126.95	115.30

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	3596	0	3626	39	0
1	B	2824	0	2833	36	0
1	C	2994	0	3025	28	0
2	A	15	0	0	0	0
2	B	13	0	0	0	0
2	C	10	0	0	0	0
All	All	9452	0	9484	102	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 5.

All (102) 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:B:635:ARG:NH2	1:B:640:ASP:O	2.15	0.79
1:A:463:LEU:HG	1:A:507:VAL:HG12	1.64	0.78
1:C:476:ARG:HG3	1:C:476:ARG:HH11	1.53	0.72
1:A:392:ILE:HD11	1:A:467:ILE:HD13	1.72	0.72
1:A:463:LEU:HG	1:A:507:VAL:CG1	2.20	0.70
1:A:424:ASN:HB3	1:A:445:PRO:O	1.92	0.69
1:B:212:LYS:HB3	1:B:222:LYS:HE2	1.72	0.69
1:C:616:LYS:HE3	1:C:627:GLU:CD	2.13	0.69
1:B:603:TYR:HB3	1:B:645:ILE:CG2	2.22	0.69
1:A:390:LEU:HD13	1:A:467:ILE:HD11	1.77	0.66
1:B:497:VAL:HA	1:B:522:ALA:HB1	1.77	0.66
1:C:219:GLY:HA2	1:C:341:SER:O	1.99	0.62
1:A:665:PRO:HB3	1:A:670:VAL:HG22	1.82	0.61
1:A:460:LEU:HG	1:A:463:LEU:HD22	1.85	0.59
1:C:616:LYS:CE	1:C:627:GLU:OE2	2.51	0.59
1:B:603:TYR:HB3	1:B:645:ILE:HG22	1.84	0.59
1:A:372:PRO:HA	1:A:519:GLN:HE22	1.68	0.58
1:A:400:ASN:HB3	1:A:446:TYR:CE1	2.38	0.57
1:A:617:ILE:HG12	1:A:653:LEU:HD23	1.87	0.57
1:C:616:LYS:CE	1:C:627:GLU:CD	2.73	0.57
1:A:241:ILE:HD12	1:A:292:ILE:HG13	1.86	0.56
1:A:628:ASN:OD1	1:A:628:ASN:N	2.37	0.56
1:A:392:ILE:CD1	1:A:467:ILE:HD13	2.35	0.56
1:B:329:GLU:O	1:B:333:ILE:HG12	2.07	0.55
1:A:403:VAL:HA	1:A:467:ILE:HG23	1.89	0.54
1:B:496:THR:HB	1:B:498:GLY:HA3	1.90	0.54
1:B:617:ILE:HD11	1:B:654:ALA:HB2	1.89	0.53
1:A:611:PRO:HB2	1:A:634:ALA:HB2	1.90	0.53
1:C:310:ALA:O	1:C:314:GLU:HG2	2.07	0.53
1:B:472:LYS:HG3	1:B:493:MET:HB2	1.91	0.52
1:B:644:TYR:HB2	1:B:662:TRP:CZ3	2.45	0.52
1:A:222:LYS:HZ2	1:B:683:LEU:HD13	1.73	0.52
1:C:213:ILE:HD13	1:C:236:LEU:HD21	1.93	0.51
1:B:470:GLY:HA3	1:B:518:SER:OG	2.11	0.50
1:B:233:THR:HG23	1:B:234:THR:HG23	1.93	0.50
1:C:487:VAL:HA	1:C:647:ALA:O	2.12	0.50
1:B:497:VAL:N	1:B:498:GLY:HA3	2.27	0.49
1:A:515:TYR:CE2	1:A:517:ARG:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:PRO:HB3	1:C:250:VAL:HG11	1.94	0.49
1:B:254:ILE:O	1:B:296:SER:HA	2.12	0.49
1:C:228:THR:H	1:C:232:LYS:HB3	1.78	0.49
1:B:665:PRO:HB3	1:B:670:VAL:CG2	2.42	0.49
1:A:607:GLU:HB3	1:A:643:VAL:HG13	1.94	0.49
1:B:217:ASN:O	1:B:220:ASP:HB2	2.13	0.48
1:A:250:VAL:HB	1:A:292:ILE:HG12	1.96	0.48
1:C:472:LYS:HE2	1:C:494:ALA:O	2.14	0.47
1:C:566:LEU:HA	1:C:569:GLN:HE21	1.78	0.47
1:A:612:VAL:HG21	1:A:642:PRO:HG3	1.96	0.47
1:A:364:HIS:HA	1:A:365:PRO:HD3	1.83	0.46
1:A:310:ALA:O	1:A:314:GLU:HG2	2.16	0.46
1:C:231:GLY:O	1:C:235:GLU:HG2	2.16	0.46
1:A:234:THR:HB	1:A:267:MET:SD	2.56	0.46
1:C:330:GLN:O	1:C:334:ILE:HG12	2.15	0.46
1:A:401:MET:HG2	1:A:467:ILE:HG22	1.98	0.46
1:B:319:PHE:HA	1:B:347:VAL:O	2.17	0.45
1:B:603:TYR:HB3	1:B:645:ILE:HG21	1.97	0.45
1:B:483:ILE:HG21	1:B:665:PRO:HD3	1.98	0.45
1:A:284:LYS:HB3	1:A:287:ASP:HB2	1.99	0.45
1:A:384:PHE:HA	1:A:393:PRO:HA	1.97	0.45
1:B:562:GLU:HG3	1:B:567:ILE:HG13	1.98	0.45
1:B:611:PRO:HB2	1:B:634:ALA:HB2	1.97	0.45
1:C:479:VAL:HA	1:C:485:PHE:O	2.16	0.45
1:A:467:ILE:HD12	1:A:516:TYR:O	2.17	0.44
1:B:496:THR:O	1:B:500:GLN:HB3	2.18	0.44
1:B:629:TYR:HB2	1:B:632:LEU:HD12	1.99	0.44
1:A:446:TYR:OH	1:A:460:LEU:HD12	2.18	0.44
1:A:400:ASN:H	1:A:464:ASP:HB2	1.83	0.44
1:B:629:TYR:HB2	1:B:632:LEU:CD1	2.48	0.44
1:C:616:LYS:CE	1:C:627:GLU:OE1	2.65	0.44
1:A:537:ARG:HA	1:A:540:ILE:HD12	2.00	0.43
1:C:246:ARG:HD3	1:C:274:ILE:HG12	1.99	0.43
1:C:250:VAL:HB	1:C:292:ILE:HG12	2.01	0.43
1:C:320:LEU:HD12	1:C:348:ALA:HB2	2.01	0.43
1:A:446:TYR:OH	1:A:460:LEU:CD1	2.66	0.43
1:B:495:VAL:HB	1:B:500:GLN:HB2	2.01	0.43
1:C:607:GLU:HB3	1:C:643:VAL:HG13	1.99	0.43
1:C:635:ARG:NH2	1:C:640:ASP:O	2.52	0.43
1:C:266:TYR:O	1:C:270:LYS:HB2	2.19	0.43
1:C:497:VAL:HA	1:C:522:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PHE:N	1:A:369:PHE:CD1	2.87	0.42
1:A:320:LEU:HD12	1:A:348:ALA:HB2	2.01	0.42
1:A:428:TYR:OH	1:A:436:ASN:HB2	2.20	0.42
1:B:479:VAL:HA	1:B:485:PHE:O	2.20	0.42
1:C:241:ILE:HD13	1:C:292:ILE:HG13	2.01	0.42
1:B:569:GLN:OE1	1:B:681:THR:HG22	2.20	0.42
1:A:392:ILE:HD11	1:A:467:ILE:CD1	2.44	0.42
1:C:479:VAL:HG21	1:C:569:GLN:HB3	2.01	0.42
1:A:574:ASN:O	1:A:578:ILE:HG12	2.20	0.41
1:B:566:LEU:HA	1:B:569:GLN:HE21	1.85	0.41
1:C:614:PHE:HA	1:C:615:PRO:HD2	1.85	0.41
1:B:469:THR:O	1:B:518:SER:HB3	2.20	0.41
1:C:582:LEU:HA	1:C:583:PRO:HD2	1.87	0.41
1:B:645:ILE:HD11	1:B:670:VAL:HB	2.01	0.41
1:B:641:VAL:HG21	1:B:660:LEU:HB3	2.03	0.41
1:C:476:ARG:HB2	1:C:491:LYS:HG3	2.03	0.41
1:A:472:LYS:HD3	1:A:495:VAL:HG12	2.03	0.41
1:B:305:GLN:H	1:B:542:ASP:CG	2.24	0.41
1:B:595:HIS:HD2	1:B:632:LEU:HD11	1.86	0.41
1:A:390:LEU:HD11	1:A:469:THR:HA	2.04	0.40
1:B:338:HIS:HA	1:B:341:SER:HB3	2.04	0.40
1:B:283:MET:SD	1:B:303:MET:HG2	2.61	0.40
1:A:466:VAL:HG23	1:A:507:VAL:HG13	2.03	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	442/476 (93%)	426 (96%)	14 (3%)	2 (0%)	29 59
1	B	347/476 (73%)	333 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	367/476 (77%)	353 (96%)	13 (4%)	1 (0%)	41	70
All	All	1156/1428 (81%)	1112 (96%)	41 (4%)	3 (0%)	41	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	505	GLY
1	A	231	GLY
1	A	406	PRO

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	391/407 (96%)	356 (91%)	35 (9%)	9	27
1	B	307/407 (75%)	284 (92%)	23 (8%)	13	35
1	C	325/407 (80%)	300 (92%)	25 (8%)	13	34
All	All	1023/1221 (84%)	940 (92%)	83 (8%)	11	32

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	A	215	SER
1	A	222	LYS
1	A	226	LEU
1	A	236	LEU
1	A	241	ILE
1	A	244	ILE
1	A	249	ARG
1	A	301	CYS
1	A	369	PHE
1	A	385	LEU
1	A	396	GLU

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Mol	Chain	Res	Type
1	A	407	THR
1	A	428	TYR
1	A	429	TYR
1	A	454	ILE
1	A	460	LEU
1	A	504	ARG
1	A	519	GLN
1	A	521	THR
1	A	523	THR
1	A	541	GLU
1	A	570	LEU
1	A	574	ASN
1	A	582	LEU
1	A	587	LYS
1	A	601	LEU
1	A	621	GLU
1	A	624	ASP
1	A	628	ASN
1	A	639	GLU
1	A	644	TYR
1	A	669	GLN
1	A	670	VAL
1	A	680	VAL
1	B	220	ASP
1	B	222	LYS
1	B	232	LYS
1	B	238	LYS
1	B	242	GLU
1	B	244	ILE
1	B	301	CYS
1	B	334	ILE
1	B	495	VAL
1	B	496	THR
1	B	500	GLN
1	B	520	GLU
1	B	541	GLU
1	B	548	LYS
1	B	558	SER
1	B	574	ASN
1	B	580	GLU
1	B	592	ARG
1	B	635	ARG

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Mol	Chain	Res	Type
1	B	645	ILE
1	B	653	LEU
1	B	670	VAL
1	B	683	LEU
1	C	236	LEU
1	C	247	HIS
1	C	249	ARG
1	C	257	ARG
1	C	268	ARG
1	C	468	ASP
1	C	473	CYS
1	C	476	ARG
1	C	491	LYS
1	C	495	VAL
1	C	519	GLN
1	C	521	THR
1	C	531	ASP
1	C	542	ASP
1	C	570	LEU
1	C	574	ASN
1	C	581	ASP
1	C	582	LEU
1	C	588	ASN
1	C	601	LEU
1	C	627	GLU
1	C	635	ARG
1	C	639	GLU
1	C	646	TYR
1	C	679	GLN

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

Mol	Chain	Res	Type
1	A	324	HIS
1	A	519	GLN
1	A	569	GLN
1	A	633	ASN
1	A	669	GLN
1	B	223	GLN
1	B	277	ASN
1	C	265	GLN
1	C	324	HIS

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Mol	Chain	Res	Type
1	C	569	GLN
1	C	575	ASN
1	C	669	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 carbohydrates 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 ⓘ

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.