



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:06 am BST

PDB ID : 2VBC
Title : Crystal structure of the NS3 protease-helicase from Dengue virus
Authors : Luo, D.H.; Xu, T.; Hunke, C.; Gruber, G.; Vasudevan, S.G.; Lescar, J.
Deposited on : 2007-09-10
Resolution : 3.15 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

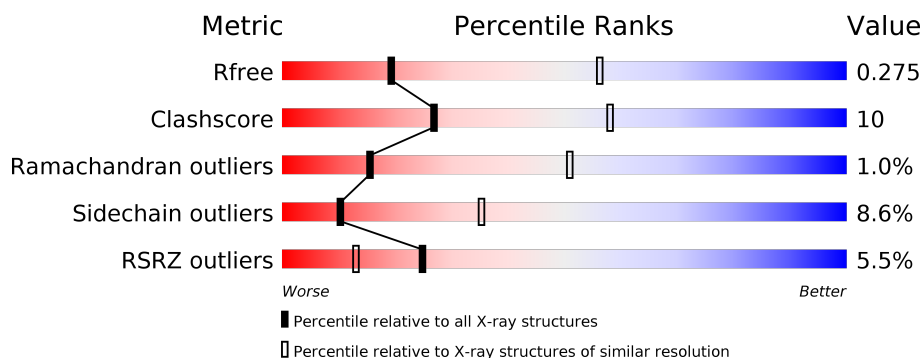
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 $\leq 5\%$. 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	618	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </div> </div>
2	B	31	<div> <div>35%</div> <div>13%</div> <div>52%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4868 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 4 NS3 FULL-LENGTH PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4720	2977	843	879	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ASP	GLU	conflict	UNP Q2TN89

- Molecule 2 is a protein called PARTIAL POLYPROTEIN FOR NS2A AND NS2B, TYPE 4 PROTOTYPE DV4 H241.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			114	71	19	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	GLY	-	expression tag	UNP Q91EQ2
B	46	SER	-	expression tag	UNP Q91EQ2
B	47	ALA	-	expression tag	UNP Q91EQ2
B	48	MET	-	expression tag	UNP Q91EQ2

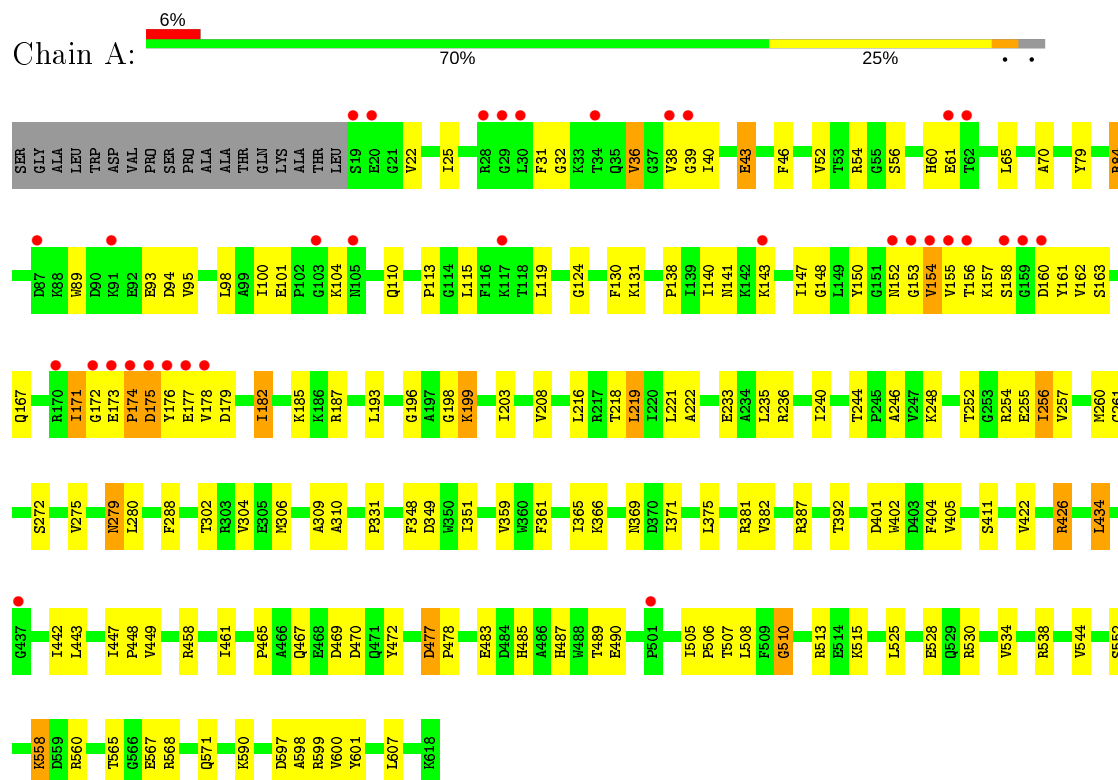
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	1	Total	O	0	0
			1	1		

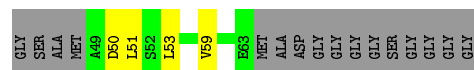
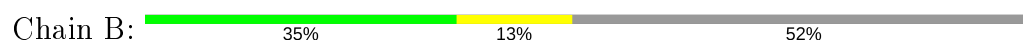
3 Residue-property plots

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 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 4 NS3 FULL-LENGTH PROTEIN



• Molecule 2: PARTIAL POLYPROTEIN FOR NS2A AND NS2B, TYPE 4 PROTOTYPE DV4 H241



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.87Å 88.24Å 76.68Å 90.00° 94.21° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15 19.91 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.15) 99.7 (19.91-3.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.277 0.201 , 0.275	Depositor DCC
R_{free} test set	583 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4868	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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	0.37	0/4826	0.55	0/6534
2	B	0.37	0/115	0.53	0/156
All	All	0.37	0/4941	0.55	0/6690

There are no bond length outliers.

There are no bond angle outliers.

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	4720	0	4688	98	0
2	B	114	0	103	3	0
3	A	33	0	0	1	0
3	B	1	0	0	0	0
All	All	4868	0	4791	98	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 10.

All (98) 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:198:GLY:CA	1:A:199:LYS:HB2	1.73	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLY:HA2	1:A:199:LYS:CB	1.69	1.17
1:A:161:TYR:CB	1:A:162:VAL:HA	1.77	1.14
1:A:177:GLU:HB3	1:A:178:VAL:HA	1.39	1.02
1:A:490:GLU:HG2	1:A:544:VAL:HB	1.46	0.96
1:A:174:PRO:HB2	1:A:175:ASP:HB2	1.49	0.94
1:A:198:GLY:HA2	1:A:199:LYS:HB2	0.90	0.90
1:A:218:THR:HG23	1:A:280:LEU:HD23	1.56	0.87
1:A:153:GLY:CA	1:A:154:VAL:HB	2.07	0.84
1:A:153:GLY:HA3	1:A:154:VAL:HB	1.59	0.83
1:A:174:PRO:CB	1:A:175:ASP:HB2	2.15	0.77
1:A:161:TYR:CB	1:A:162:VAL:CA	2.63	0.76
1:A:177:GLU:CB	1:A:178:VAL:HA	2.18	0.72
1:A:365:ILE:HD12	1:A:365:ILE:H	1.54	0.72
1:A:240:ILE:HG22	1:A:257:VAL:HB	1.70	0.71
1:A:95:VAL:HG22	1:A:113:PRO:HG3	1.73	0.69
1:A:98:LEU:HB3	1:A:138:PRO:HG2	1.74	0.68
1:A:447:ILE:HB	1:A:448:PRO:HD2	1.76	0.67
1:A:196:GLY:H	1:A:199:LYS:HD3	1.61	0.66
1:A:387:ARG:HB2	1:A:387:ARG:HH11	1.61	0.65
1:A:89:TRP:HB2	1:A:147:ILE:HD12	1.78	0.64
1:A:156:THR:HG22	1:A:162:VAL:H	1.64	0.63
1:A:401:ASP:HA	3:A:2013:HOH:O	2.00	0.62
1:A:141:ASN:HD22	1:A:147:ILE:HG21	1.66	0.61
1:A:422:VAL:HG23	1:A:461:ILE:HD13	1.82	0.60
1:A:530:ARG:O	1:A:534:VAL:HG23	2.01	0.60
1:A:598:ALA:HA	1:A:601:TYR:CE1	2.37	0.59
1:A:304:VAL:HA	1:A:309:ALA:O	2.03	0.57
1:A:193:LEU:HD11	1:A:199:LYS:HA	1.85	0.57
1:A:485:HIS:CD2	1:A:487:HIS:H	2.24	0.55
1:A:510:GLY:N	1:A:513:ARG:HH21	2.05	0.55
1:A:485:HIS:HD2	1:A:487:HIS:H	1.53	0.55
1:A:254:ARG:HG3	1:A:256:ILE:HD13	1.89	0.54
1:A:359:VAL:HB	1:A:422:VAL:HG22	1.91	0.53
1:A:65:LEU:HD22	1:A:79:TYR:HB3	1.91	0.52
1:A:221:LEU:HD23	1:A:260:MET:HG3	1.92	0.52
1:A:43:GLU:HB2	1:A:84:ARG:HD3	1.92	0.52
1:A:148:GLY:HA2	1:A:167:GLN:HB3	1.92	0.51
1:A:70:ALA:HB3	1:A:465:PRO:HB3	1.91	0.51
1:A:46:PHE:HB3	1:A:79:TYR:HB2	1.93	0.51
1:A:222:ALA:O	1:A:261:CYS:HA	2.10	0.51
1:A:38:VAL:HG21	1:A:100:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:HG21	1:A:235:LEU:HD21	1.94	0.50
1:A:571:GLN:OE1	1:A:590:LYS:HB3	2.11	0.50
1:A:56:SER:HB2	2:B:51:LEU:HD11	1.94	0.49
1:A:140:ILE:HD12	2:B:59:VAL:HG13	1.94	0.49
1:A:244:THR:HG22	1:A:246:ALA:H	1.78	0.49
1:A:101:GLU:HB2	1:A:104:LYS:HB2	1.93	0.48
1:A:153:GLY:HA2	1:A:154:VAL:HB	1.92	0.48
1:A:382:VAL:HA	1:A:404:PHE:O	2.14	0.48
1:A:178:VAL:HG22	1:A:179:ASP:H	1.77	0.48
1:A:434:LEU:HD21	1:A:442:ILE:HG12	1.94	0.48
1:A:152:ASN:HA	1:A:153:GLY:HA2	1.64	0.47
1:A:248:LYS:HB3	1:A:272:SER:HB2	1.96	0.47
1:A:185:LYS:HA	1:A:310:ALA:HB2	1.96	0.47
1:A:36:VAL:HB	1:A:52:VAL:HG13	1.95	0.47
1:A:280:LEU:HA	1:A:310:ALA:O	2.14	0.47
1:A:25:ILE:HD11	1:A:46:PHE:HZ	1.79	0.47
1:A:182:ILE:HD13	1:A:182:ILE:H	1.80	0.47
1:A:387:ARG:HB2	1:A:387:ARG:NH1	2.29	0.46
1:A:458:ARG:HG3	1:A:472:TYR:CG	2.51	0.46
1:A:371:ILE:O	1:A:375:LEU:HG	2.16	0.46
1:A:40:ILE:HD11	1:A:138:PRO:HD3	1.98	0.46
1:A:153:GLY:HA3	1:A:154:VAL:CB	2.34	0.46
1:A:558:LYS:O	1:A:560:ARG:HG2	2.16	0.45
1:A:348:PHE:HB3	1:A:351:ILE:HD12	1.98	0.45
1:A:216:LEU:HB3	1:A:279:ASN:ND2	2.31	0.45
1:A:477:ASP:HA	1:A:478:PRO:HD3	1.87	0.45
1:A:331:PRO:HG2	1:A:469:ASP:OD1	2.17	0.45
1:A:597:ASP:O	1:A:600:VAL:HG22	2.17	0.45
1:A:505:ILE:HA	1:A:506:PRO:HD3	1.87	0.44
1:A:93:GLU:HG2	1:A:94:ASP:H	1.81	0.44
1:A:525:LEU:O	1:A:530:ARG:HB2	2.17	0.44
1:A:84:ARG:HH11	1:A:84:ARG:HB2	1.82	0.44
1:A:130:PHE:HD1	1:A:150:TYR:CZ	2.35	0.44
1:A:22:VAL:HG11	1:A:100:ILE:HG13	1.99	0.44
1:A:84:ARG:HH22	1:A:175:ASP:HB3	1.83	0.43
1:A:193:LEU:HD13	1:A:203:ILE:HD12	1.99	0.43
1:A:60:HIS:CG	1:A:61:GLU:N	2.87	0.43
1:A:525:LEU:HD11	1:A:552:SER:HB3	2.00	0.42
1:A:171:ILE:HA	1:A:172:GLY:HA3	1.73	0.42
1:A:39:GLY:HA3	1:A:46:PHE:CZ	2.55	0.42
1:A:60:HIS:HB3	2:B:53:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HA	1:A:124:GLY:HA2	2.02	0.42
1:A:426:ARG:HG3	1:A:449:VAL:HG22	2.00	0.42
1:A:426:ARG:NH1	1:A:472:TYR:OH	2.46	0.42
1:A:366:LYS:HA	1:A:369:ASN:HD22	1.85	0.42
1:A:198:GLY:CA	1:A:199:LYS:CB	2.54	0.41
1:A:219:LEU:HD22	1:A:221:LEU:HG	2.02	0.41
1:A:157:LYS:HA	1:A:158:SER:HA	1.83	0.41
1:A:175:ASP:HA	1:A:176:TYR:HA	1.93	0.41
1:A:381:ARG:HB2	1:A:402:TRP:HA	2.03	0.41
1:A:31:PHE:HA	1:A:32:GLY:HA3	1.63	0.40
1:A:490:GLU:CD	1:A:599:ARG:HH12	2.23	0.40
1:A:154:VAL:HA	1:A:155:VAL:HA	1.57	0.40
1:A:94:ASP:HB2	1:A:110:GLN:HE21	1.87	0.40
1:A:534:VAL:HG12	1:A:538:ARG:HH11	1.86	0.40
1:A:361:PHE:CE2	1:A:411:SER:HB2	2.57	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	598/618 (97%)	534 (89%)	58 (10%)	6 (1%)	15	51
2	B	13/31 (42%)	11 (85%)	2 (15%)	0	100	100
All	All	611/649 (94%)	545 (89%)	60 (10%)	6 (1%)	15	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	LYS
1	A	510	GLY
1	A	160	ASP

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Mol	Chain	Res	Type
1	A	43	GLU
1	A	154	VAL
1	A	174	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	502/524 (96%)	459 (91%)	43 (9%)	10	35
2	B	11/17 (65%)	10 (91%)	1 (9%)	9	32
All	All	513/541 (95%)	469 (91%)	44 (9%)	10	35

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

Mol	Chain	Res	Type
1	A	36	VAL
1	A	54	ARG
1	A	84	ARG
1	A	119	LEU
1	A	131	LYS
1	A	143	LYS
1	A	163	SER
1	A	171	ILE
1	A	173	GLU
1	A	175	ASP
1	A	182	ILE
1	A	187	ARG
1	A	219	LEU
1	A	233	GLU
1	A	236	ARG
1	A	252	THR
1	A	255	GLU
1	A	256	ILE
1	A	275	VAL
1	A	279	ASN

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Mol	Chain	Res	Type
1	A	288	PHE
1	A	302	THR
1	A	306	MET
1	A	349	ASP
1	A	392	THR
1	A	405	VAL
1	A	426	ARG
1	A	434	LEU
1	A	443	LEU
1	A	467	GLN
1	A	470	ASP
1	A	477	ASP
1	A	483	GLU
1	A	489	THR
1	A	507	THR
1	A	508	LEU
1	A	515	LYS
1	A	528	GLU
1	A	558	LYS
1	A	565	THR
1	A	567	GLU
1	A	568	ARG
1	A	607	LEU
2	B	50	ASP

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	110	GLN
1	A	152	ASN
1	A	194	HIS
1	A	262	HIS
1	A	277	ASN
1	A	279	ASN
1	A	287	HIS
1	A	369	ASN
1	A	384	GLN
1	A	456	GLN
1	A	467	GLN
1	A	485	HIS

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 ⓘ

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	600/618 (97%)	0.13	34 (5%) 23 12	49, 60, 73, 79	0
2	B	15/31 (48%)	0.58	0 100 100	60, 60, 61, 61	0
All	All	615/649 (94%)	0.14	34 (5%) 25 13	49, 60, 73, 79	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	THR	4.5
1	A	30	LEU	4.2
1	A	154	VAL	4.0
1	A	177	GLU	3.9
1	A	155	VAL	3.4
1	A	160	ASP	3.2
1	A	20	GLU	3.2
1	A	34	THR	3.1
1	A	159	GLY	3.1
1	A	153	GLY	3.1
1	A	158	SER	3.0
1	A	105	ASN	3.0
1	A	103	GLY	3.0
1	A	117	LYS	2.9
1	A	61	GLU	2.8
1	A	87	ASP	2.8
1	A	29	GLY	2.8
1	A	39	GLY	2.7
1	A	170	ARG	2.5
1	A	174	PRO	2.5
1	A	501	PRO	2.4
1	A	178	VAL	2.4
1	A	437	GLY	2.4
1	A	28	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	91	LYS	2.3
1	A	173	GLU	2.3
1	A	172	GLY	2.3
1	A	175	ASP	2.3
1	A	156	THR	2.3
1	A	19	SER	2.2
1	A	176	TYR	2.2
1	A	143	LYS	2.1
1	A	152	ASN	2.1
1	A	38	VAL	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 carbohydrates 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.