Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2021 – 05:01 am BST

PDB ID	:	7NIO
Title	:	Crystal structure of the SARS-CoV-2 helicase APO form
Authors	:	Newman, J.A.; Yosaatmadja, Y.; Douangamath, A.; Bountra, C.; Gileadi, O.
Deposited on	:	2021-02-12
Resolution	:	2.20 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:

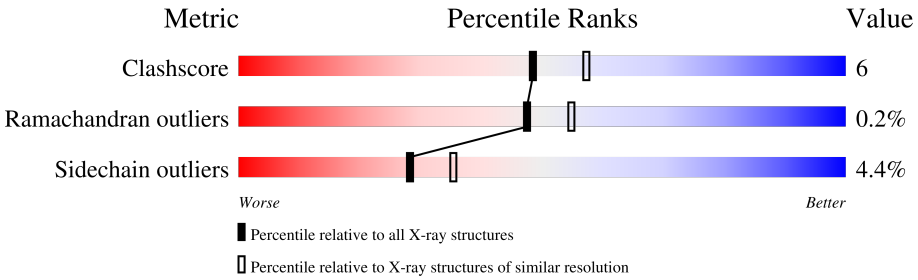
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	603	83% 14%
1	E	603	80% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9269 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 SARS-CoV-2 helicase NSP13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	1	0
			4541	2894	759	852	36			
1	E	585	Total	C	N	O	S	0	0	0
			4501	2869	750	848	34			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P0DTD1
A	0	MET	-	expression tag	UNP P0DTD1
E	-1	SER	-	expression tag	UNP P0DTD1
E	0	MET	-	expression tag	UNP P0DTD1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	E	3	Total	Zn	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	108	Total	O	0	0
			108	108		
3	E	113	Total	O	0	0
			113	113		

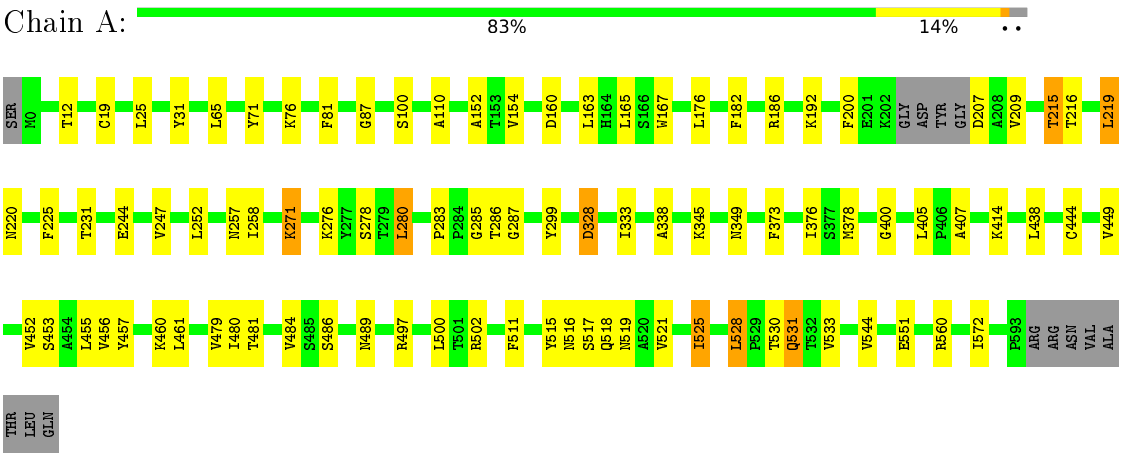
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

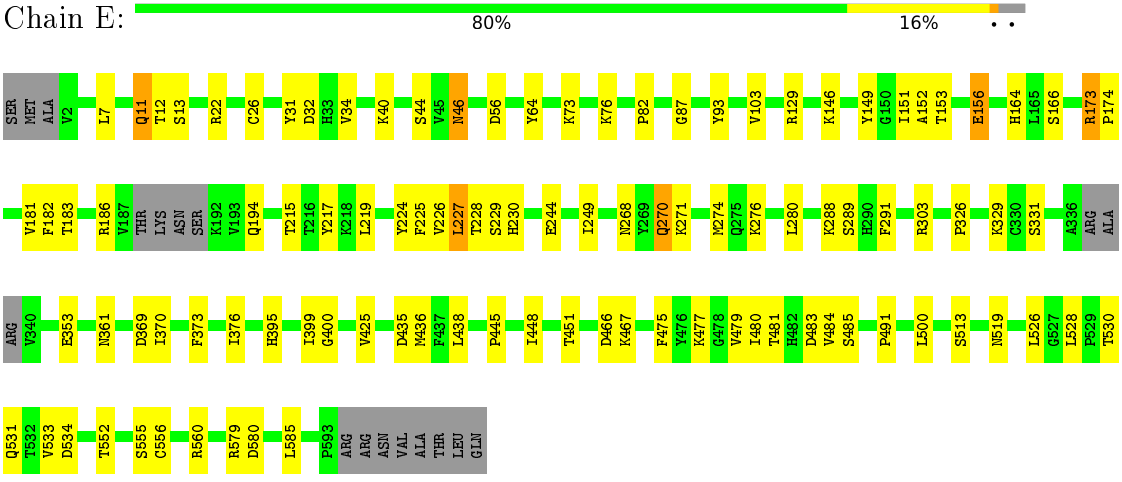
- Molecule 1: SARS-CoV-2 helicase NSP13

Chain A:



- Molecule 1: SARS-CoV-2 helicase NSP13

Chain E:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.70Å 70.12Å 84.00Å 104.31° 93.30° 112.16°	Depositor
Resolution (Å)	80.24 – 2.20	Depositor
% Data completeness (in resolution range)	91.6 (80.24-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.230 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9269	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

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	0.27	0/4644	0.45	0/6331
1	E	0.26	0/4603	0.46	0/6274
All	All	0.27	0/9247	0.45	0/12605

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	4541	0	4454	49	0
1	E	4501	0	4408	64	0
2	A	3	0	0	0	0
2	E	3	0	0	0	0
3	A	108	0	0	4	0
3	E	113	0	0	7	0
All	All	9269	0	8862	108	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 6.

All (108) 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:E:73:LYS:HZ3	1:E:76:LYS:HE2	1.54	0.71
1:A:444:CYS:SG	3:A:803:HOH:O	2.51	0.69
1:E:556:CYS:SG	3:E:802:HOH:O	2.50	0.68
1:A:333:ILE:HD13	1:A:349:ASN:HA	1.75	0.67
1:E:268:ASN:HB3	1:E:291:PHE:HE1	1.60	0.66
1:A:405:LEU:HD11	1:A:533:VAL:HG12	1.80	0.64
1:A:328:ASP:OD1	1:A:328:ASP:N	2.25	0.63
1:E:182:PHE:HA	1:E:227:LEU:HA	1.82	0.62
1:E:152:ALA:HB3	1:E:225:PHE:HB2	1.84	0.59
1:A:460:LYS:NZ	3:A:819:HOH:O	2.36	0.59
1:A:511:PHE:HB3	1:A:530:THR:HG22	1.85	0.58
1:A:453:SER:HA	1:A:457:TYR:HB2	1.84	0.58
1:E:271:LYS:HD3	1:E:435:ASP:HB3	1.85	0.58
1:E:445:PRO:HD2	1:E:448:ILE:HD12	1.84	0.58
1:A:285:GLY:O	1:A:287:GLY:N	2.35	0.57
1:E:22:ARG:NH1	3:E:816:HOH:O	2.36	0.57
1:A:497:ARG:HD2	1:A:525:ILE:HG22	1.86	0.57
1:A:479:VAL:HG13	1:E:481:THR:HG22	1.87	0.56
1:A:480:ILE:HB	1:E:480:ILE:HB	1.88	0.56
1:E:326:PRO:HG2	1:E:329:LYS:HE2	1.88	0.55
1:A:215:THR:OG1	1:A:216:THR:N	2.39	0.55
1:A:12:THR:HG21	1:A:25:LEU:O	2.06	0.55
1:E:146:LYS:HB3	1:E:227:LEU:HD13	1.88	0.55
1:A:551:GLU:HB2	1:E:552:THR:HG22	1.89	0.54
1:E:226:VAL:HG13	1:E:227:LEU:H	1.73	0.54
1:A:182:PHE:HB3	1:A:225:PHE:HB3	1.88	0.53
1:E:182:PHE:HB3	1:E:225:PHE:HB3	1.89	0.53
1:A:533:VAL:HG11	1:A:560:ARG:HG3	1.91	0.53
1:E:534:ASP:OD2	3:E:801:HOH:O	2.18	0.53
1:E:331:SER:HB2	1:E:353:GLU:HG3	1.91	0.53
1:A:280:LEU:HD21	1:A:438:LEU:HG	1.90	0.53
1:E:12:THR:HB	1:E:26:CYS:HA	1.92	0.52
1:E:500:LEU:HD11	1:E:528:LEU:HD11	1.91	0.52
1:E:555:SER:OG	3:E:802:HOH:O	2.19	0.51
1:A:533:VAL:HG23	3:A:816:HOH:O	2.09	0.51
1:E:560:ARG:NE	3:E:801:HOH:O	2.28	0.51
1:A:452:VAL:HA	1:A:455:LEU:HB3	1.92	0.51
1:A:455:LEU:HG	1:A:456:VAL:HG13	1.93	0.50
1:A:65:LEU:HD23	1:A:81:PHE:CZ	2.46	0.50
1:E:466:ASP:OD2	1:E:467:LYS:N	2.44	0.50
1:E:249:ILE:HD11	1:E:270:GLN:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG23	1:A:438:LEU:HB2	1.94	0.49
1:A:481:THR:HG22	1:E:479:VAL:HG13	1.94	0.49
1:E:46:ASN:N	1:E:46:ASN:OD1	2.45	0.49
1:A:152:ALA:HB1	1:A:165:LEU:HD22	1.96	0.48
1:A:244:GLU:HB2	1:A:276:LYS:HB2	1.95	0.48
1:E:32:ASP:HB2	1:E:103:VAL:HG11	1.95	0.48
1:A:444:CYS:HB2	1:A:449:VAL:HG22	1.95	0.48
1:E:146:LYS:HZ3	1:E:227:LEU:HB3	1.77	0.48
1:A:152:ALA:HB2	1:A:167:TRP:CH2	2.49	0.47
1:E:244:GLU:HB2	1:E:276:LYS:HB2	1.97	0.47
1:A:519:ASN:ND2	1:A:531:GLN:O	2.39	0.47
1:E:451:THR:HG21	1:E:585:LEU:HD23	1.97	0.47
1:A:283:PRO:HG2	1:A:461:LEU:HD13	1.97	0.47
1:A:31:TYR:CE2	1:A:87:GLY:HA2	2.50	0.46
1:E:513:SER:OG	1:E:519:ASN:OD1	2.23	0.46
1:A:517:SER:O	1:A:521:VAL:HG23	2.15	0.46
1:E:153:THR:HB	1:E:166:SER:HB2	1.98	0.46
1:A:252:LEU:HB3	1:A:299:TYR:CD1	2.50	0.46
1:E:533:VAL:HG11	1:E:560:ARG:HG3	1.98	0.45
1:A:378:MET:O	1:A:407:ALA:HB2	2.16	0.45
1:E:31:TYR:CE2	1:E:87:GLY:HA2	2.51	0.45
1:E:376:ILE:HG22	1:E:400:GLY:HA3	1.97	0.45
1:E:181:VAL:O	1:E:228:THR:N	2.40	0.45
1:E:303:ARG:NH1	1:E:353:GLU:O	2.49	0.45
1:E:353:GLU:OE1	3:E:804:HOH:O	2.21	0.45
1:A:154:VAL:HG22	1:A:163:LEU:HD13	1.99	0.45
1:E:11:GLN:HG2	1:E:93:TYR:CE2	2.52	0.45
1:E:129:ARG:HA	1:E:129:ARG:HD2	1.82	0.45
1:A:176:LEU:HD22	1:A:200:PHE:HB2	2.00	0.45
1:A:489:ASN:N	1:A:518:GLN:OE1	2.34	0.44
1:E:11:GLN:HG2	1:E:93:TYR:HE2	1.83	0.44
1:E:173:ARG:HH12	1:E:485:SER:HB3	1.83	0.44
1:E:13:SER:O	1:E:44:SER:HA	2.18	0.44
1:E:226:VAL:HG13	1:E:227:LEU:N	2.33	0.44
1:E:64:TYR:HA	1:E:82:PRO:HA	2.00	0.43
1:E:173:ARG:NH1	1:E:484:VAL:O	2.46	0.43
1:A:414:LYS:HG2	1:E:580:ASP:HA	2.01	0.43
1:E:186:ARG:HH21	1:E:219:LEU:HA	1.84	0.43
1:A:152:ALA:HB2	1:A:167:TRP:CZ3	2.54	0.43
1:E:156:GLU:HB3	1:E:164:HIS:HB2	2.00	0.43
1:A:500:LEU:HD23	1:A:500:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:VAL:O	1:A:572:ILE:HA	2.19	0.42
1:E:34:VAL:O	1:E:40:LYS:NZ	2.37	0.42
1:E:479:VAL:HB	1:E:491:PRO:HG2	2.02	0.42
1:A:486:SER:HB3	1:A:515:TYR:HB3	2.02	0.42
1:E:270:GLN:O	1:E:274:MET:HG3	2.19	0.42
1:E:519:ASN:O	1:E:530:THR:HG21	2.19	0.42
1:E:475:PHE:CZ	1:E:477:LYS:HE2	2.55	0.42
1:A:186:ARG:NH1	1:A:219:LEU:HA	2.34	0.42
1:A:405:LEU:HD21	1:A:560:ARG:HA	2.02	0.42
1:E:149:TYR:HB3	1:E:174:PRO:HG3	2.01	0.42
1:E:500:LEU:HD12	1:E:526:LEU:HD22	2.01	0.42
1:E:146:LYS:NZ	1:E:227:LEU:HB3	2.36	0.41
1:E:173:ARG:NH2	1:E:485:SER:OG	2.53	0.41
1:E:280:LEU:HD12	1:E:436:MET:HB2	2.02	0.41
1:A:71:TYR:OH	3:A:801:HOH:O	2.16	0.41
1:E:280:LEU:HD11	1:E:438:LEU:HD21	2.01	0.41
1:E:370:ILE:HG12	1:E:395:HIS:HB2	2.02	0.41
1:A:376:ILE:HG22	1:A:400:GLY:HA3	2.02	0.41
1:A:176:LEU:HD13	1:A:209:VAL:HG11	2.03	0.41
1:E:151:ILE:HG22	1:E:224:TYR:HB2	2.03	0.41
1:A:19:CYS:SG	1:A:110:ALA:HB1	2.61	0.41
1:A:528:LEU:H	1:A:528:LEU:HG	1.62	0.40
1:E:151:ILE:O	3:E:803:HOH:O	2.21	0.40
1:E:288:LYS:HD2	1:E:399:ILE:HG22	2.03	0.40
1:A:271:LYS:HD3	1:A:271:LYS:HA	1.61	0.40
1:E:376:ILE:HG12	1:E:425:VAL:HG11	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	587/603 (97%)	546 (93%)	40 (7%)	1 (0%)	47	55
1	E	579/603 (96%)	550 (95%)	28 (5%)	1 (0%)	47	55
All	All	1166/1206 (97%)	1096 (94%)	68 (6%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	227	LEU
1	A	338	ALA

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	499/525 (95%)	475 (95%)	24 (5%)	25	32
1	E	496/525 (94%)	476 (96%)	20 (4%)	31	40
All	All	995/1050 (95%)	951 (96%)	44 (4%)	28	35

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

Mol	Chain	Res	Type
1	A	76	LYS
1	A	100	SER
1	A	160	ASP
1	A	192	LYS
1	A	207	ASP
1	A	215	THR
1	A	219	LEU
1	A	220	ASN
1	A	231	THR
1	A	247	VAL
1	A	257	ASN
1	A	258	ILE
1	A	271	LYS
1	A	278	SER

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Mol	Chain	Res	Type
1	A	280	LEU
1	A	328	ASP
1	A	345	LYS
1	A	373	PHE
1	A	484	VAL
1	A	502	ARG
1	A	516	ASN
1	A	525	ILE
1	A	528	LEU
1	A	531	GLN
1	E	7	LEU
1	E	11	GLN
1	E	46	ASN
1	E	56	ASP
1	E	156	GLU
1	E	173	ARG
1	E	183	THR
1	E	194	GLN
1	E	215	THR
1	E	217	TYR
1	E	229	SER
1	E	230	HIS
1	E	270	GLN
1	E	289	SER
1	E	361	ASN
1	E	369	ASP
1	E	373	PHE
1	E	483	ASP
1	E	531	GLN
1	E	579	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.