

Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2022 – 12:45 AM EDT

PDB ID	:	4Q2C
Title	:	Crystal structure of CRISPR-associated protein
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Deposited on	:	2014-04-07
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.29
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.29
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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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					
			6%					
1	А	949	80%	15%	••			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7487 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 CRISPR-associated helicase Cas3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	926	Total 7202	C 4572	N 1292	O 1312	${ m S} 7$	Se 19	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-4	GLY	-	expression tag	UNP D1CGD0
А	-3	GLY	-	expression tag	UNP D1CGD0
А	-2	GLY	-	expression tag	UNP D1CGD0
А	-1	GLY	-	expression tag	UNP D1CGD0
А	0	GLY	-	expression tag	UNP D1CGD0

• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total Ni 3 3	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	282	Total O 282 282	0	0



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 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: CRISPR-associated helicase Cas3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	104.27Å 214.56Å 102.20Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	93.78 - 2.50	Depositor
Resolution (A)	93.78 - 2.50	EDS
% Data completeness	93.4 (93.78-2.50)	Depositor
(in resolution range)	93.4(93.78-2.50)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.91 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
B B.	0.191 , 0.229	Depositor
It, Itfree	0.193 , 0.232	DCC
R_{free} test set	1871 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	41.6	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 53.7	EDS
L-test for $twinning^2$	$ < L > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7487	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/7361	0.47	0/10000	

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 (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	А	7202	0	7156	81	0
2	А	3	0	0	0	0
3	А	282	0	0	6	0
All	All	7487	0	7156	81	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 (81) 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:418:ALA:HB3	1:A:826:ASP:HB2	1.65	0.79



	lo de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:829:GLU:HA	1:A:830:LEU:HB2	1.66	0.77
1:A:572:SER:HA	1:A:717:SER:HB3	1.70	0.74
1:A:701:ASP:OD1	1:A:704:ARG:NH1	2.21	0.72
1:A:109:LEU:O	1:A:117:ARG:NH1	2.23	0.71
1:A:129:LEU:HD23	1:A:194:MSE:HB3	1.73	0.69
1:A:415:TYR:CE2	1:A:422:GLU:HG2	2.29	0.67
1:A:98:HIS:HA	1:A:168:VAL:HG13	1.77	0.66
1:A:748:ARG:NH1	1:A:774:GLN:OE1	2.29	0.65
1:A:288:SER:OG	1:A:289:GLY:O	2.16	0.63
1:A:53:MSE:HE1	1:A:202:LEU:HB3	1.81	0.63
1:A:316:GLU:OE1	1:A:552:ARG:NH2	2.30	0.61
1:A:871:PRO:HG3	1:A:910:LEU:HD12	1.83	0.60
1:A:361:ALA:HA	1:A:669:SER:OG	2.04	0.58
1:A:62:GLN:NE2	1:A:273:GLU:OE2	2.37	0.58
1:A:567:ALA:HB3	1:A:712:GLU:HG2	1.86	0.57
1:A:701:ASP:O	1:A:709:ARG:NH1	2.36	0.57
1:A:511:LEU:O	1:A:516:ARG:NH1	2.38	0.56
1:A:821:ALA:H	1:A:823:VAL:HG23	1.70	0.56
1:A:357:LEU:HD12	1:A:363:SER:HA	1.87	0.56
1:A:654:ARG:NH2	1:A:673:ASP:O	2.39	0.56
1:A:705:PRO:HG2	1:A:708:LEU:HB2	1.87	0.56
1:A:109:LEU:HD21	1:A:131:LEU:HG	1.88	0.56
1:A:821:ALA:HA	1:A:823:VAL:H	1.71	0.55
1:A:632:TYR:HB2	1:A:637:ARG:HG2	1.87	0.55
1:A:199:ARG:NH1	3:A:1214:HOH:O	2.39	0.55
1:A:338:MSE:HE1	1:A:370:VAL:HA	1.90	0.54
1:A:535:LEU:HD13	1:A:535:LEU:H	1.74	0.53
1:A:454:LEU:HD23	1:A:457:LEU:HD12	1.89	0.53
1:A:640:ARG:NH2	3:A:1124:HOH:O	2.40	0.53
1:A:771:ARG:NH2	3:A:1157:HOH:O	2.38	0.53
1:A:289:GLY:HA3	1:A:377:ARG:HH12	1.72	0.53
1:A:742:ARG:NH1	3:A:1380:HOH:O	2.37	0.52
1:A:329:MSE:H	1:A:329:MSE:SE	2.42	0.52
1:A:538:ALA:O	1:A:542:ARG:NH1	2.44	0.51
1:A:174:PHE:HB2	1:A:824:GLU:HG3	1.92	0.51
1:A:706:GLU:HA	1:A:709:ARG:HG3	1.92	0.50
1:A:459:VAL:O	1:A:462:VAL:HG22	2.10	0.50
1:A:367:PHE:CE2	1:A:391:HIS:HA	2.47	0.50
1:A:392:SER:HB3	1:A:439:ALA:HB2	1.93	0.50
1:A:329:MSE:HG3	1:A:692:GLY:HA3	1.93	0.50
1:A:681:LEU:HD22	1:A:682:ALA:H	1.77	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:723:ASP:OD2	1:A:776:ALA:HB1	2.12	0.49
1:A:358:PRO:HG2	1:A:361:ALA:HB2	1.94	0.49
1:A:628:LEU:HD13	1:A:666:ILE:HD11	1.94	0.49
1:A:319:SER:HB2	1:A:320:PRO:HD3	1.93	0.49
1:A:667:GLU:HG2	1:A:668:GLN:HG3	1.94	0.48
1:A:204:CYS:SG	3:A:1136:HOH:O	2.60	0.48
1:A:695:HIS:HA	1:A:704:ARG:NH2	2.29	0.48
1:A:628:LEU:HB2	1:A:660:LEU:HD11	1.95	0.47
1:A:379:PRO:O	1:A:381:ASP:N	2.48	0.47
1:A:164:VAL:O	1:A:168:VAL:HB	2.16	0.46
1:A:367:PHE:CE2	1:A:446:VAL:HB	2.51	0.46
1:A:571:VAL:HG13	1:A:716:VAL:HA	1.98	0.45
1:A:354:TYR:HB2	1:A:472:LYS:HD3	1.99	0.45
1:A:213:PRO:HA	1:A:214:GLY:HA2	1.62	0.45
1:A:277:ALA:HA	1:A:282:VAL:HG22	1.98	0.45
1:A:288:SER:HA	1:A:289:GLY:HA3	1.69	0.45
1:A:451:GLN:OE1	1:A:465:ARG:NH2	2.50	0.45
1:A:678:VAL:HG22	1:A:714:TRP:HB2	1.99	0.45
1:A:829:GLU:HG2	1:A:832:PRO:HD2	1.99	0.44
1:A:297:PHE:O	1:A:300:ILE:HG22	2.17	0.44
1:A:56:VAL:HG21	1:A:98:HIS:CE1	2.53	0.43
1:A:335:GLU:OE1	1:A:369:ARG:NH1	2.52	0.43
1:A:821:ALA:HA	1:A:823:VAL:N	2.34	0.43
1:A:831:HIS:HB2	1:A:832:PRO:HD3	2.01	0.42
1:A:105:PRO:HD3	1:A:195:TRP:CE2	2.54	0.42
1:A:459:VAL:HG12	1:A:830:LEU:H	1.84	0.42
1:A:141:ILE:O	1:A:145:VAL:HG13	2.18	0.42
1:A:288:SER:HB2	1:A:346:THR:HG23	2.01	0.42
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.88	0.42
1:A:36:ALA:HB2	1:A:49:LEU:HA	2.01	0.42
1:A:595:ILE:HG21	1:A:606:LEU:HD21	2.01	0.42
1:A:701:ASP:HA	1:A:704:ARG:HH11	1.85	0.41
1:A:654:ARG:HD3	3:A:1132:HOH:O	2.20	0.41
1:A:300:ILE:HD12	1:A:300:ILE:HA	1.97	0.41
1:A:479:VAL:HG21	1:A:506:VAL:HG13	2.02	0.41
1:A:747:LEU:HD12	1:A:747:LEU:HA	1.91	0.41
1:A:229:LEU:HD12	1:A:229:LEU:HA	1.85	0.41
1:A:422:GLU:H	1:A:422:GLU:HG3	1.47	0.40
1:A:697:HIS:HA	1:A:698:PRO:HD2	1.87	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	А	924/949~(97%)	889 (96%)	29 (3%)	6 (1%)	25	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	290	SER
1	А	769	ASP
1	А	380	GLU
1	А	821	ALA
1	А	30	ASP
1	А	320	PRO

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	А	745/736~(101%)	684 (92%)	61 (8%)	11 22	

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	28	ARG
1	А	109	LEU
1	А	112	ARG
1	А	163	TRP
1	А	168	VAL



Mol	Chain	Res	Type
1	А	194	MSE
1	А	203	LEU
1	А	206	LEU
1	А	217	ARG
1	А	228	MSE
1	А	229	LEU
1	А	278	SER
1	А	329	MSE
1	А	331	GLU
1	А	355	PHE
1	А	359	THR
1	А	360	MSE
1	А	366	MSE
1	А	384	VAL
1	А	388	VAL
1	А	397	LEU
1	А	406	GLU
1	А	412	GLN
1	А	417	GLU
1	А	422	GLU
1	А	423	GLN
1	А	440	LEU
1	А	450	ASP
1	А	462	VAL
1	А	466	LEU
1	А	473	THR
1	А	497	LEU
1	А	511	LEU
1	А	533	ARG
1	А	534	ASP
1	A	535	LEU
1	А	542	ARG
1	A	568	LEU
1	A	571	VAL
1	А	579	LEU
1	A	583	LEU
1	А	585	GLU
1	A	610	LEU
1	А	625	LEU
1	A	628	LEU
1	A	631	ARG
1	А	664	GLN



Mol	Chain	Res	Type
1	А	681	LEU
1	А	707	ARG
1	А	708	LEU
1	А	747	LEU
1	А	768	SER
1	А	774	GLN
1	А	779	GLU
1	А	795	LEU
1	А	825	GLU
1	А	826	ASP
1	А	829	GLU
1	А	835	GLN
1	А	859	LEU
1	А	887	THR

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	907/949~(95%)	0.54	55 (6%) 21 22	24, 45, 100, 175	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ
1	А	828	PRO	14.8
1	А	827	ALA	13.8
1	А	826	ASP	12.8
1	А	831	HIS	9.4
1	А	832	PRO	8.4
1	А	364	ASN	7.7
1	А	830	LEU	7.4
1	А	829	GLU	5.9
1	А	822	SER	5.8
1	А	823	VAL	4.9
1	А	406	GLU	4.9
1	А	824	GLU	4.7
1	А	41	GLY	4.7
1	А	363	SER	4.5
1	А	43	ASP	4.5
1	А	772	VAL	4.4
1	А	387	LEU	4.0
1	А	362	THR	3.8
1	А	855	GLY	3.8
1	А	825	GLU	3.6
1	А	833	ALA	3.5
1	А	405	GLY	3.5
1	A	361	ALA	3.4
1	A	821	ALA	3.2
1	А	365	GLN	3.1
1	А	420	GLY	3.1
1	А	383	VAL	3.1



Mol	Chain	Res Type		RSRZ
1	А	115	GLN	3.0
1	А	359	THR	3.0
1	А	302	GLN	2.9
1	А	574	PRO	2.9
1	А	42	PRO	2.7
1	А	666	ILE	2.7
1	А	407	GLU	2.6
1	А	768	SER	2.6
1	А	367	PHE	2.5
1	А	286	PRO	2.5
1	А	319	SER	2.4
1	А	294	THR	2.4
1	А	298	PRO	2.4
1	А	288	SER	2.3
1	А	388	VAL	2.3
1	А	300	ILE	2.3
1	А	308	ALA	2.3
1	А	578	ALA	2.3
1	А	386	ASN	2.3
1	А	44	LEU	2.2
1	А	556	PHE	2.2
1	А	559	SER	2.2
1	А	192	TRP	2.1
1	А	874	ALA	2.1
1	А	404	LYS	2.1
1	А	293	LEU	2.1
1	А	20	SER	2.0
1	А	771	ARG	2.0

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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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	NI	А	1003	1/1	0.95	0.22	$57,\!57,\!57,\!57$	0
2	NI	А	1002	1/1	0.99	0.21	30,30,30,30	0
2	NI	А	1001	1/1	0.99	0.16	34,34,34,34	0

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

6.5 Other polymers (i)

There are no such residues in this entry.

