



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:37 AM UTC

PDB ID : 4Q2C / pdb_00004q2c
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

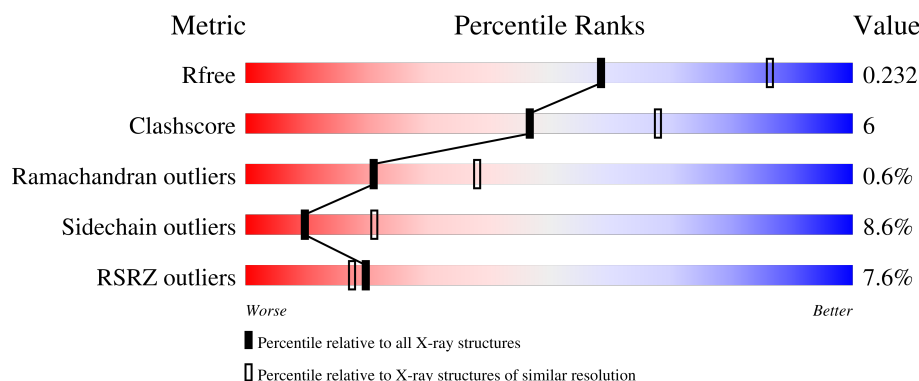
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	949	7% 79% 16% ..

2 Entry composition

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	A	926	Total	C	N	O	S	Se	0	0	0
			7202	4572	1292	1312	7	19			

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

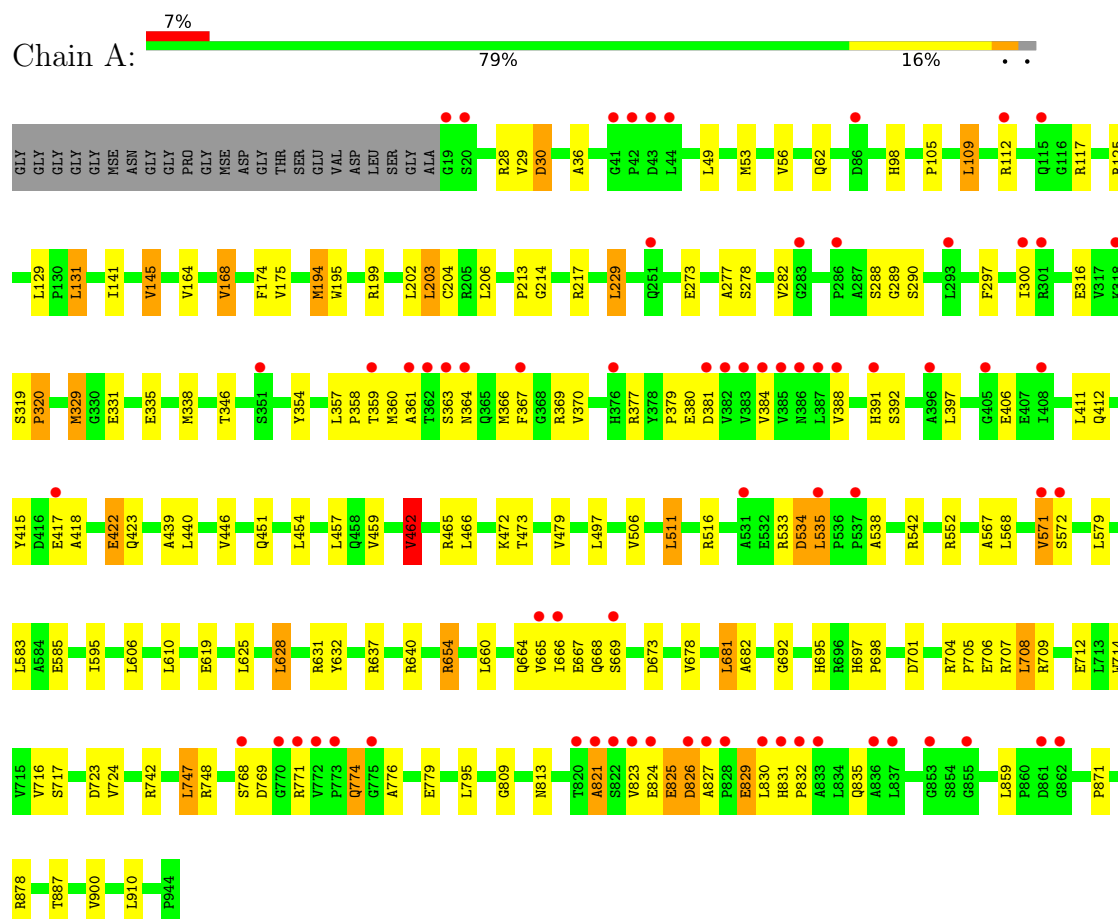
- Molecule 3 is water.

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

3 Residue-property plots

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.27Å 214.56Å 102.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.78 – 2.50 93.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.4 (93.78-2.50) 93.4 (93.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.191 , 0.229 0.194 , 0.232	Depositor 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 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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](#)

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/7361	0.79	17/10000 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ASN	N-CA-C	6.95	118.54	110.97
1	A	654	ARG	CA-C-N	6.38	126.36	119.78
1	A	654	ARG	C-N-CA	6.38	126.36	119.78
1	A	825	GLU	N-CA-C	6.32	117.96	111.14
1	A	462	VAL	CB-CA-C	-6.30	103.63	112.14
1	A	30	ASP	CA-C-N	6.07	125.95	119.28
1	A	30	ASP	C-N-CA	6.07	125.95	119.28
1	A	29	VAL	N-CA-C	5.95	121.72	109.34
1	A	813	ASN	N-CA-C	5.64	118.36	111.82
1	A	827	ALA	CA-C-N	5.27	125.21	119.78
1	A	827	ALA	C-N-CA	5.27	125.21	119.78
1	A	217	ARG	CA-C-N	5.24	125.15	119.85
1	A	217	ARG	C-N-CA	5.24	125.15	119.85
1	A	809	GLY	CA-C-N	5.20	125.00	119.28
1	A	809	GLY	C-N-CA	5.20	125.00	119.28
1	A	534	ASP	N-CA-C	5.08	117.66	110.50
1	A	724	VAL	N-CA-C	5.04	112.54	107.55

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	7202	0	7156	82	0
2	A	3	0	0	0	0
3	A	282	0	0	6	0
All	All	7487	0	7156	82	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 (82) 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
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: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:288:SER:OG	1:A:289:GLY:O	2.16	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:C	1:A:381:ASP:H	2.27	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

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	924/949 (97%)	889 (96%)	29 (3%)	6 (1%)	21	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	SER
1	A	769	ASP
1	A	380	GLU
1	A	821	ALA

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Mol	Chain	Res	Type
1	A	30	ASP
1	A	320	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	745/736 (101%)	681 (91%)	64 (9%)	10	21

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	109	LEU
1	A	112	ARG
1	A	125	ARG
1	A	131	LEU
1	A	145	VAL
1	A	168	VAL
1	A	175	VAL
1	A	194	MSE
1	A	203	LEU
1	A	206	LEU
1	A	229	LEU
1	A	278	SER
1	A	329	MSE
1	A	331	GLU
1	A	359	THR
1	A	360	MSE
1	A	366	MSE
1	A	384	VAL
1	A	388	VAL
1	A	397	LEU
1	A	406	GLU
1	A	411	LEU
1	A	412	GLN

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Mol	Chain	Res	Type
1	A	417	GLU
1	A	422	GLU
1	A	423	GLN
1	A	440	LEU
1	A	462	VAL
1	A	466	LEU
1	A	473	THR
1	A	497	LEU
1	A	511	LEU
1	A	533	ARG
1	A	534	ASP
1	A	535	LEU
1	A	568	LEU
1	A	571	VAL
1	A	579	LEU
1	A	583	LEU
1	A	585	GLU
1	A	610	LEU
1	A	619	GLU
1	A	625	LEU
1	A	628	LEU
1	A	631	ARG
1	A	664	GLN
1	A	665	VAL
1	A	681	LEU
1	A	707	ARG
1	A	708	LEU
1	A	747	LEU
1	A	768	SER
1	A	774	GLN
1	A	779	GLU
1	A	795	LEU
1	A	825	GLU
1	A	826	ASP
1	A	829	GLU
1	A	835	GLN
1	A	859	LEU
1	A	878	ARG
1	A	887	THR
1	A	900	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	754	GLN
1	A	801	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 oligosaccharides 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 ⓘ

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	907/949 (95%)	0.35	69 (7%) 20 17	24, 45, 100, 175	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	827	ALA	6.2
1	A	362	THR	5.9
1	A	830	LEU	5.8
1	A	826	ASP	5.8
1	A	535	LEU	5.8
1	A	828	PRO	5.8
1	A	823	VAL	5.4
1	A	821	ALA	5.1
1	A	44	LEU	4.9
1	A	833	ALA	4.9
1	A	364	ASN	4.9
1	A	387	LEU	4.8
1	A	363	SER	4.7
1	A	43	ASP	4.7
1	A	115	GLN	4.4
1	A	832	PRO	4.3
1	A	775	GLY	4.3
1	A	768	SER	4.0
1	A	386	ASN	4.0
1	A	824	GLU	3.9
1	A	382	VAL	3.9
1	A	666	ILE	3.9
1	A	361	ALA	3.7
1	A	300	ILE	3.7
1	A	385	VAL	3.5
1	A	862	GLY	3.4
1	A	405	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	773	PRO	3.4
1	A	531	ALA	3.3
1	A	831	HIS	3.3
1	A	388	VAL	3.1
1	A	665	VAL	3.1
1	A	20	SER	3.1
1	A	770	GLY	3.0
1	A	383	VAL	2.9
1	A	19	GLY	2.9
1	A	367	PHE	2.9
1	A	42	PRO	2.8
1	A	772	VAL	2.7
1	A	381	ASP	2.7
1	A	408	ILE	2.7
1	A	384	VAL	2.7
1	A	571	VAL	2.7
1	A	669	SER	2.7
1	A	822	SER	2.7
1	A	771	ARG	2.7
1	A	41	GLY	2.7
1	A	820	THR	2.6
1	A	283	GLY	2.6
1	A	351	SER	2.6
1	A	855	GLY	2.6
1	A	286	PRO	2.5
1	A	836	ALA	2.4
1	A	537	PRO	2.4
1	A	359	THR	2.4
1	A	572	SER	2.3
1	A	318	LYS	2.3
1	A	853	GLY	2.3
1	A	396	ALA	2.2
1	A	417	GLU	2.2
1	A	837	LEU	2.1
1	A	301	ARG	2.1
1	A	86	ASP	2.1
1	A	112	ARG	2.1
1	A	391	HIS	2.1
1	A	251	GLN	2.1
1	A	376	HIS	2.1
1	A	293	LEU	2.0
1	A	861	ASP	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 oligosaccharides 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, median, 95th 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	A	1003	1/1	0.97	0.11	57,57,57,57	0
2	NI	A	1001	1/1	0.99	0.04	34,34,34,34	0
2	NI	A	1002	1/1	1.00	0.05	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.