



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:04 PM UTC

PDB ID : 5X2H / pdb_00005x2h
Title : Crystal structure of Campylobacter jejuni Cas9 in complex with sgRNA and target DNA (AGAAACA PAM)
Authors : Yamada, M.; Watanabe, Y.; Hirano, H.; Nakane, T.; Ishitani, R.; Nishimasu, H.; Nureki, O.
Deposited on : 2017-01-31
Resolution : 2.30 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

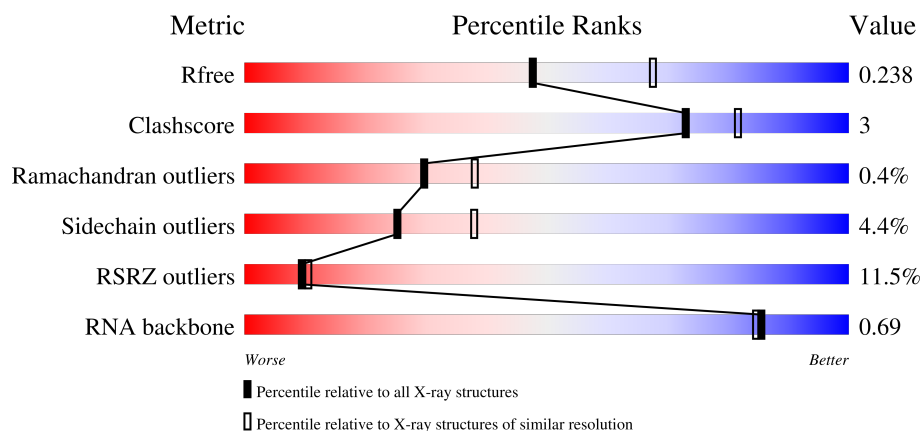
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

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	835	12% 78% 11% • 11%
2	B	93	83% 16% •
3	C	28	86% 14%
4	D	8	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8919 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 endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	0	0
			5925	3824	1006	1084	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	SER	-	expression tag	UNP Q0P897
A	-4	SER	-	expression tag	UNP Q0P897
A	-3	GLY	-	expression tag	UNP Q0P897
A	-2	SER	-	expression tag	UNP Q0P897
A	-1	GLY	-	expression tag	UNP Q0P897
A	0	HIS	-	expression tag	UNP Q0P897
A	636	GLY	-	linker	UNP Q0P897
A	637	GLY	-	linker	UNP Q0P897
A	638	GLY	-	linker	UNP Q0P897
A	639	SER	-	linker	UNP Q0P897
A	640	GLY	-	linker	UNP Q0P897
A	641	GLY	-	linker	UNP Q0P897

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	93	Total	C	N	O	P	0	0	0
			1990	889	361	647	93			

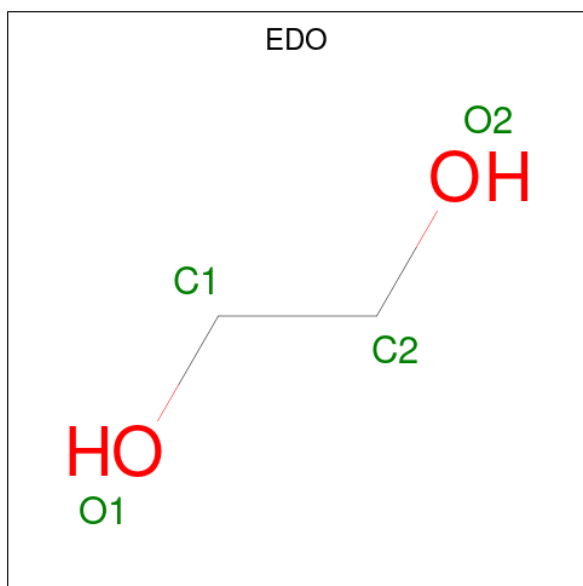
- Molecule 3 is a DNA chain called Target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			560	270	93	170	27			

- Molecule 4 is a DNA chain called Non-target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			165	79	38	41	7			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

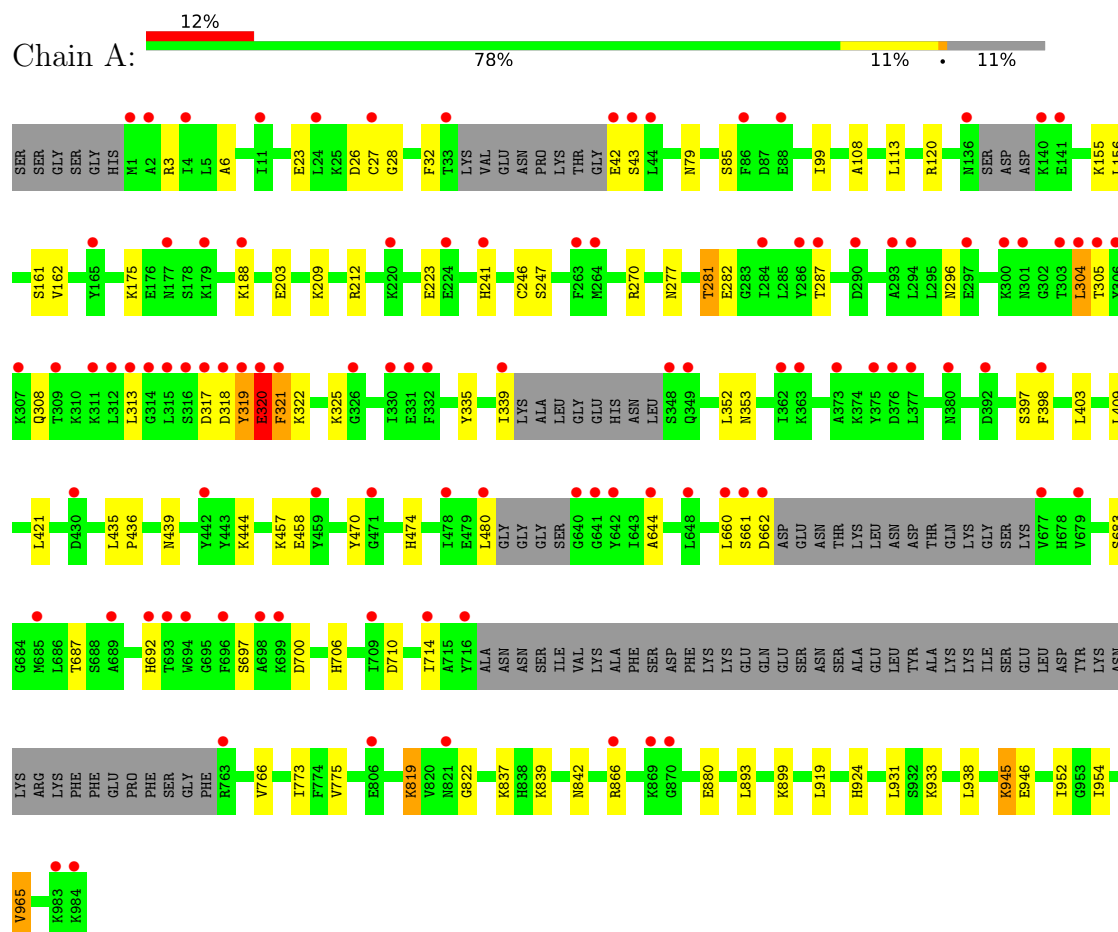
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total	O	0	0
			145	145		
6	B	99	Total	O	0	0
			99	99		
6	C	18	Total	O	0	0
			18	18		
6	D	13	Total	O	0	0
			13	13		

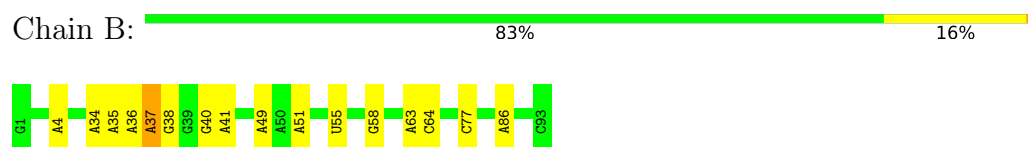
3 Residue-property plots

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 endonuclease Cas9



• Molecule 2: sgRNA



• Molecule 3: Target DNA strand





- Molecule 4: Non-target DNA strand

Chain D:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.04Å 103.91Å 134.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.81 – 2.30 72.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.81-2.30) 99.7 (72.81-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.200 , 0.231 0.207 , 0.238	Depositor DCC
R_{free} test set	3148 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.814	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8919	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 3.58% 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: EDO

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	0.11	0/6030	0.31	0/8109
2	B	0.11	0/2227	0.28	0/3470
3	C	0.21	0/624	0.39	0/959
4	D	0.25	0/187	0.47	0/287
All	All	0.13	0/9068	0.31	0/12825

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	A	5925	0	5871	46	0
2	B	1990	0	1002	4	0
3	C	560	0	319	4	0
4	D	165	0	90	0	0
5	B	4	0	6	0	0
6	A	145	0	0	1	0
6	B	99	0	0	0	0
6	C	18	0	0	0	0
6	D	13	0	0	0	0
All	All	8919	0	7288	51	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 3.

All (51) 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:320:GLU:HG3	3:C:17:DT:H5'	1.70	0.72
1:A:305:THR:HA	1:A:325:LYS:HA	1.75	0.68
1:A:480:LEU:HG	1:A:644:ALA:HB2	1.74	0.67
1:A:893:LEU:HD22	1:A:965:VAL:HG22	1.76	0.66
1:A:212:ARG:NH2	1:A:223:GLU:OE2	2.27	0.66
1:A:866:ARG:NH2	3:C:-6:DT:O4	2.30	0.64
1:A:775:VAL:H	1:A:924:HIS:HD2	1.47	0.62
1:A:277:ASN:O	1:A:281:THR:OG1	2.18	0.61
1:A:247:SER:OG	2:B:4:A:OP1	2.16	0.59
1:A:839:LYS:NZ	1:A:880:GLU:O	2.36	0.58
1:A:661:SER:OG	1:A:662:ASP:N	2.37	0.58
1:A:317:ASP:OD1	1:A:318:ASP:N	2.36	0.57
1:A:27:CYS:HB3	1:A:773:ILE:HD11	1.85	0.56
1:A:99:ILE:O	1:A:120:ARG:NH2	2.28	0.56
1:A:305:THR:HG22	1:A:308:GLN:HG3	1.87	0.56
1:A:710:ASP:O	1:A:714:ILE:HG12	2.07	0.55
1:A:819:LYS:HD3	1:A:822:GLY:HA2	1.90	0.54
1:A:85:SER:OG	6:A:1001:HOH:O	2.18	0.54
1:A:3:ARG:H	1:A:474:HIS:HD2	1.56	0.53
1:A:6:ALA:HB1	1:A:714:ILE:HB	1.92	0.52
1:A:775:VAL:H	1:A:924:HIS:CD2	2.28	0.50
1:A:246:CYS:HB2	1:A:397:SER:HB3	1.95	0.48
1:A:320:GLU:H	1:A:320:GLU:CD	2.22	0.48
1:A:108:ALA:HB2	1:A:113:LEU:HD11	1.96	0.47
1:A:42:GLU:HG2	1:A:43:SER:H	1.80	0.47
1:A:353:ASN:HB3	1:A:398:PHE:CZ	2.50	0.47
1:A:919:LEU:HG	1:A:954:ILE:HG22	1.97	0.47
1:A:318:ASP:HA	1:A:321:PHE:CE2	2.49	0.47
2:B:36:A:H5'	2:B:37:A:OP2	2.15	0.46
1:A:161:SER:HB2	1:A:203:GLU:HG3	1.97	0.46
1:A:32:PHE:CG	1:A:458:GLU:HG3	2.52	0.45
1:A:700:ASP:O	1:A:706:HIS:HB3	2.17	0.45
1:A:837:LYS:NZ	1:A:842:ASN:OD1	2.42	0.45
2:B:40:G:H2'	2:B:41:A:C8	2.51	0.45
2:B:34:A:H2'	2:B:35:A:O4'	2.16	0.45
1:A:26:ASP:OD2	1:A:470:TYR:OH	2.34	0.45
1:A:403:LEU:HB3	1:A:421:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:HIS:HA	1:A:697:SER:HB2	2.00	0.44
1:A:945:LYS:HG3	1:A:946:GLU:HG2	2.01	0.43
3:C:9:DC:H2'	3:C:10:DA:C8	2.53	0.43
1:A:439:ASN:HA	1:A:444:LYS:HD3	1.99	0.43
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.90	0.43
1:A:938:LEU:HD11	1:A:952:ILE:HD13	2.01	0.43
1:A:435:LEU:HD12	1:A:436:PRO:HD2	2.01	0.42
1:A:319:TYR:O	1:A:320:GLU:C	2.62	0.41
1:A:683:SER:O	1:A:687:THR:HG23	2.20	0.41
3:C:9:DC:H2'	3:C:10:DA:H8	1.86	0.41
1:A:321:PHE:HD1	1:A:321:PHE:HA	1.70	0.41
1:A:335:TYR:O	1:A:339:ILE:HG13	2.20	0.41
1:A:28:GLY:HA2	1:A:773:ILE:HG23	2.02	0.41
1:A:156:LEU:HD21	1:A:162:VAL:HG22	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	732/835 (88%)	707 (97%)	22 (3%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLU
1	A	322	LYS
1	A	188	LYS

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	610/740 (82%)	583 (96%)	27 (4%)	25	38

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	79	ASN
1	A	155	LYS
1	A	175	LYS
1	A	209	LYS
1	A	241	HIS
1	A	270	ARG
1	A	281	THR
1	A	282	GLU
1	A	287	THR
1	A	296	ASN
1	A	304	LEU
1	A	313	LEU
1	A	319	TYR
1	A	320	GLU
1	A	321	PHE
1	A	352	LEU
1	A	409	LEU
1	A	457	LYS
1	A	660	LEU
1	A	766	VAL
1	A	819	LYS
1	A	899	LYS
1	A	931	LEU
1	A	933	LYS
1	A	945	LYS
1	A	965	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	474	HIS
1	A	707	HIS
1	A	764	GLN
1	A	910	ASN
1	A	924	HIS
1	A	934	ASN
1	A	955	GLN
1	A	978	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	92/93 (98%)	9 (9%)	1 (1%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	37	A
2	B	38	G
2	B	49	A
2	B	51	A
2	B	55	U
2	B	58	G
2	B	64	C
2	B	77	C
2	B	86	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	63	A

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	B	101	-	3,3,3	0.43	0	2,2,2	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	101	-	-	0/1/1/1	-

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	746/835 (89%)	0.82	101 (13%) 7 8	28, 62, 108, 132	0
2	B	93/93 (100%)	-0.53	0 100 100	35, 51, 80, 140	0
3	C	28/28 (100%)	-0.41	0 100 100	41, 48, 73, 77	0
4	D	8/8 (100%)	-0.42	0 100 100	33, 40, 55, 64	0
All	All	875/964 (90%)	0.63	101 (11%) 9 10	28, 60, 108, 140	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	662	ASP	8.0
1	A	136	ASN	7.7
1	A	316	SER	5.8
1	A	301	ASN	5.3
1	A	27	CYS	5.0
1	A	314	GLY	5.0
1	A	315	LEU	4.8
1	A	480	LEU	4.7
1	A	694	TRP	4.7
1	A	983	LYS	4.3
1	A	677	VAL	4.2
1	A	321	PHE	4.2
1	A	661	SER	4.2
1	A	1	MET	4.1
1	A	33	THR	4.1
1	A	319	TYR	4.1
1	A	640	GLY	4.1
1	A	140	LYS	4.0
1	A	642	TYR	4.0
1	A	376	ASP	3.8
1	A	696	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	24	LEU	3.7
1	A	88	GLU	3.6
1	A	442	TYR	3.5
1	A	313	LEU	3.5
1	A	305	THR	3.5
1	A	644	ALA	3.4
1	A	11	ILE	3.4
1	A	2	ALA	3.4
1	A	320	GLU	3.3
1	A	763	ARG	3.2
1	A	317	ASP	3.2
1	A	311	LYS	3.1
1	A	348	SER	3.1
1	A	44	LEU	3.1
1	A	330	ILE	3.1
1	A	309	THR	3.0
1	A	821	ASN	3.0
1	A	698	ALA	3.0
1	A	714	ILE	2.9
1	A	641	GLY	2.9
1	A	660	LEU	2.9
1	A	699	LYS	2.9
1	A	869	LYS	2.9
1	A	984	LYS	2.9
1	A	685	MET	2.9
1	A	716	TYR	2.9
1	A	380	ASN	2.9
1	A	300	LYS	2.8
1	A	377	LEU	2.8
1	A	339	ILE	2.8
1	A	287	THR	2.8
1	A	177	ASN	2.8
1	A	188	LYS	2.8
1	A	312	LEU	2.7
1	A	648	LEU	2.7
1	A	290	ASP	2.7
1	A	42	GLU	2.6
1	A	471	GLY	2.6
1	A	307	LYS	2.6
1	A	304	LEU	2.6
1	A	286	TYR	2.6
1	A	692	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	318	ASP	2.5
1	A	86	PHE	2.5
1	A	263	PHE	2.5
1	A	679	VAL	2.5
1	A	220	LYS	2.5
1	A	284	ILE	2.5
1	A	293	ALA	2.5
1	A	303	THR	2.4
1	A	693	THR	2.4
1	A	294	LEU	2.4
1	A	306	TYR	2.4
1	A	459	TYR	2.4
1	A	331	GLU	2.4
1	A	326	GLY	2.4
1	A	375	TYR	2.4
1	A	870	GLY	2.4
1	A	709	ILE	2.3
1	A	373	ALA	2.3
1	A	241	HIS	2.3
1	A	430	ASP	2.3
1	A	363	LYS	2.3
1	A	349	GLN	2.3
1	A	398	PHE	2.2
1	A	392	ASP	2.2
1	A	264	MET	2.2
1	A	141	GLU	2.2
1	A	224	GLU	2.1
1	A	866	ARG	2.1
1	A	297	GLU	2.1
1	A	806	GLU	2.1
1	A	332	PHE	2.1
1	A	165	TYR	2.1
1	A	478	ILE	2.0
1	A	179	LYS	2.0
1	A	43	SER	2.0
1	A	689	ALA	2.0
1	A	4	ILE	2.0
1	A	362	ILE	2.0

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

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
5	EDO	B	101	4/4	0.97	0.07	28,30,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.