



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:58 PM UTC

PDB ID : 5B2Q / pdb_00005b2q
Title : Crystal structure of Francisella novicida Cas9 RHA in complex with sgRNA and target DNA (TGG PAM)
Authors : Hirano, H.; Nishimasu, H.; Nakane, T.; Ishitani, R.; Nureki, O.
Deposited on : 2016-02-01
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

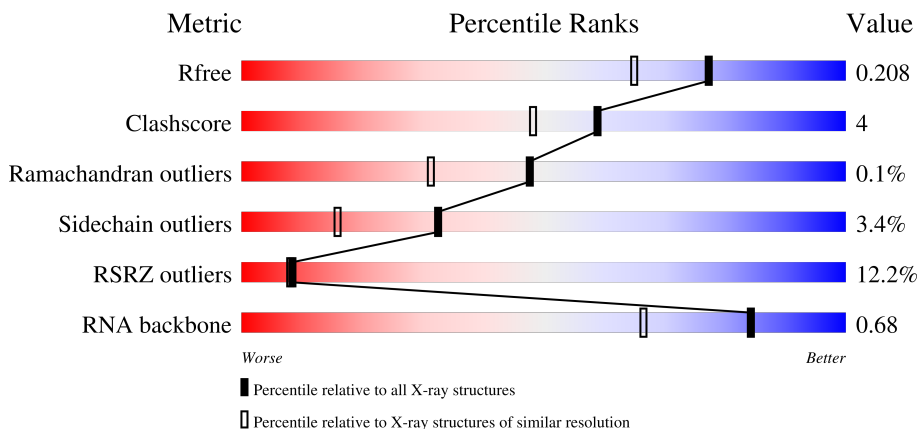
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)
RNA backbone	3983	1094 (2.20-1.20)

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 $\leq 5\%$. 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	1632	12% 78% 10% • 11%
2	B	94	79% 18% •
3	C	30	70% 30%
4	D	9	78% 22%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15694 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	1455	Total	C	N	O	S	0	16	0
			11802	7550	2027	2194	31			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0Q5Y3
A	-1	SER	-	expression tag	UNP A0Q5Y3
A	0	HIS	-	expression tag	UNP A0Q5Y3
A	995	ALA	ASN	engineered mutation	UNP A0Q5Y3
A	1369	ARG	GLU	conflict	UNP A0Q5Y3
A	1449	HIS	GLU	conflict	UNP A0Q5Y3
A	1556	ALA	ARG	conflict	UNP A0Q5Y3

- Molecule 2 is a RNA chain called Guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	P	0	0	0
			1991	886	350	661	94			

- Molecule 3 is a DNA chain called Target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			595	285	105	176	29			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*GP*GP*TP*AP*TP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total	C	N	O	P	0	0	0
			185	89	34	54	8			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		
6	B	2	Total	Na	0	0
			2	2		

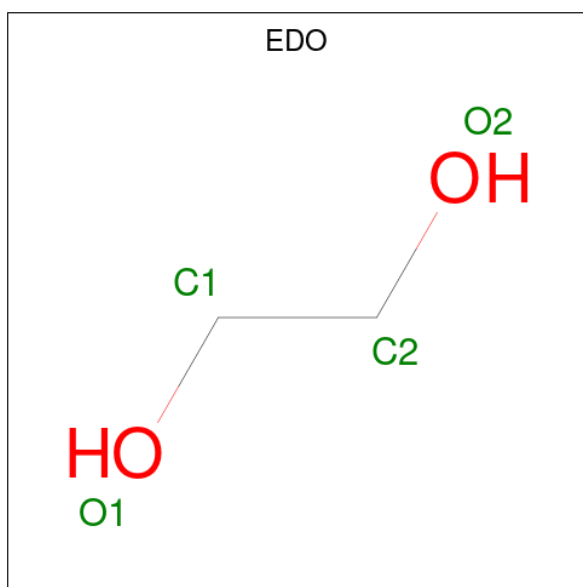
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	10	Total	Ca	0	0
			10	10		
8	B	7	Total	Ca	0	0
			7	7		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



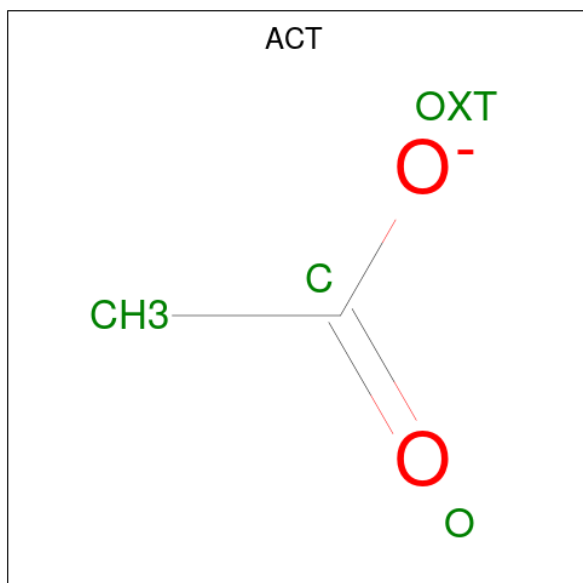
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total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

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

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		

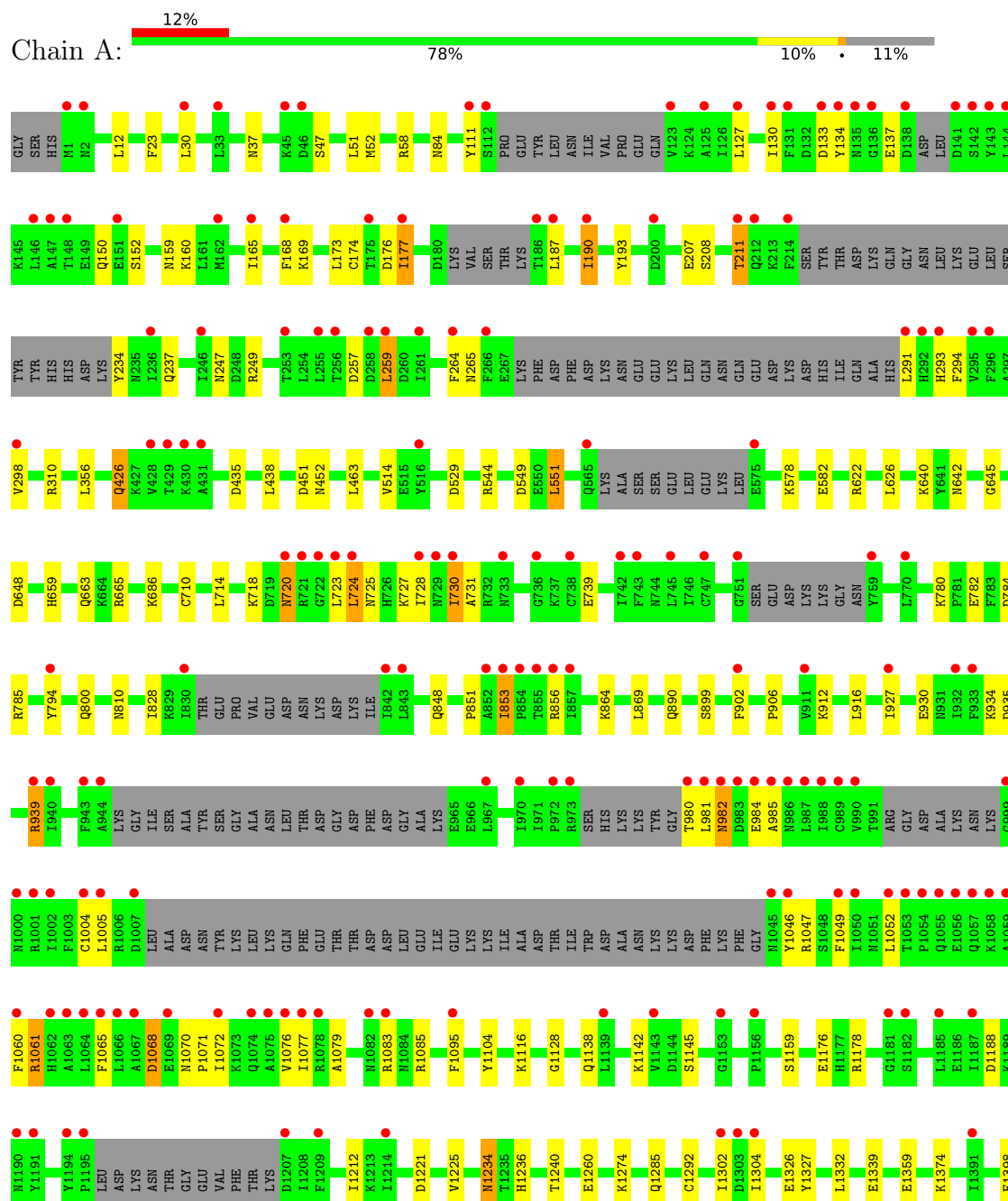
- Molecule 11 is water.

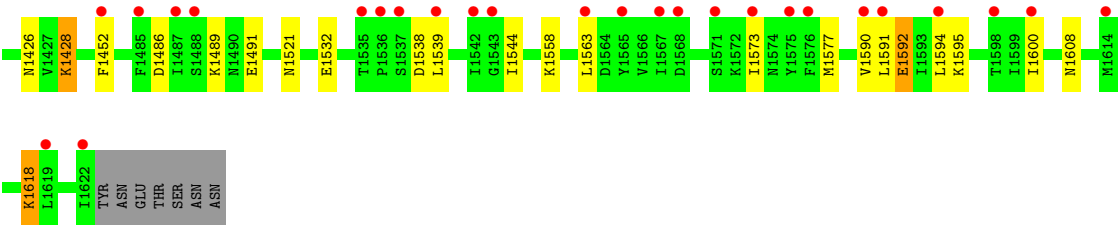
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	588	Total	O	0	0
			588	588		
11	B	334	Total	O	0	0
			334	334		
11	C	64	Total	O	0	0
			64	64		
11	D	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

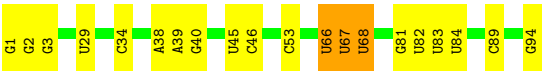
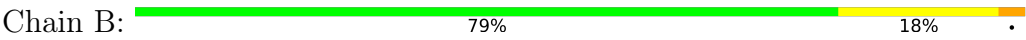
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 endonuclease Cas9

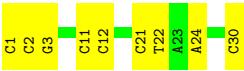




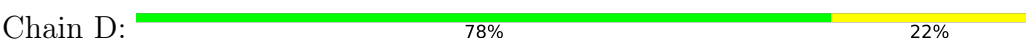
● Molecule 2: Guide RNA



● Molecule 3: Target DNA



● Molecule 4: DNA (5'-D(*TP*GP*GP*TP*AP*TP*CP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.56Å 158.98Å 96.74Å 90.00° 106.88° 90.00°	Depositor
Resolution (Å)	46.29 – 1.70 46.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.29-1.70) 98.8 (46.29-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.183 , 0.206 0.185 , 0.208	Depositor DCC
R_{free} test set	12762 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15694	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, ZN, ACT, NA, CA, CL

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	0/12077	0.51	1/16290 (0.0%)
2	B	0.50	0/2224	0.66	0/3465
3	C	0.45	0/664	0.65	0/1018
4	D	0.37	0/207	0.61	0/319
All	All	0.37	0/15172	0.55	1/21092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ARG	CG-CD-NE	-6.00	98.80	112.00

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	11802	0	11583	102	1
2	B	1991	0	997	13	0
3	C	595	0	337	11	0
4	D	185	0	104	1	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
7	A	2	0	0	0	0
8	A	10	0	0	0	0
8	B	7	0	0	0	0
9	A	48	0	72	4	0
9	B	48	0	72	3	0
10	A	8	0	6	0	0
11	A	588	0	0	9	0
11	B	334	0	0	2	0
11	C	64	0	0	1	0
11	D	7	0	0	0	0
All	All	15694	0	13171	120	1

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 4.

The worst 5 of 120 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:265:ASN:O	1:A:291:LEU:N	2.06	0.88
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.59	0.83
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.03	0.76
1:A:578:LYS:NZ	1:A:582:GLU:OE2	2.20	0.75
1:A:169:LYS:HB3	1:A:187:LEU:HD11	1.68	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:NH2	1:A:1260:GLU:OE2[2_445]	2.11	0.09

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	1444/1632 (88%)	1412 (98%)	30 (2%)	2 (0%)	48 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PHE
1	A	1128	GLY

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	1260/1483 (85%)	1218 (97%)	42 (3%)	33 17

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1061	ARG
1	A	1398	PHE
1	A	1068	ASP
1	A	1145	SER
1	A	1558	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	677	GLN
1	A	800	GLN
1	A	1234	ASN
1	A	725	ASN
1	A	877	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	91/94 (96%)	6 (6%)	2 (2%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	29	U
2	B	53	C
2	B	67	U
2	B	68	U
2	B	83	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	66	U
2	B	67	U

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 50 ligands modelled in this entry, 24 are monoatomic - leaving 26 for Mogul analysis.

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	$\# Z > 2$
9	EDO	B	116	-	3,3,3	0.50	0	2,2,2	0.15	0
9	EDO	A	1722	-	3,3,3	0.48	0	2,2,2	0.28	0
9	EDO	A	1723	-	3,3,3	0.47	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	B	115	-	3,3,3	0.49	0	2,2,2	0.16	0
9	EDO	A	1720	-	3,3,3	0.52	0	2,2,2	0.23	0
9	EDO	B	120	-	3,3,3	0.34	0	2,2,2	0.35	0
9	EDO	A	1716	-	3,3,3	0.38	0	2,2,2	0.44	0
9	EDO	A	1719	-	3,3,3	0.59	0	2,2,2	0.32	0
9	EDO	B	119	-	3,3,3	0.46	0	2,2,2	0.04	0
10	ACT	A	1728	-	3,3,3	0.77	0	3,3,3	1.38	0
9	EDO	B	110	-	3,3,3	0.41	0	2,2,2	0.41	0
9	EDO	B	121	-	3,3,3	0.46	0	2,2,2	0.35	0
9	EDO	A	1725	-	3,3,3	0.45	0	2,2,2	0.40	0
9	EDO	B	111	-	3,3,3	0.49	0	2,2,2	0.44	0
9	EDO	A	1717	-	3,3,3	0.41	0	2,2,2	0.48	0
9	EDO	B	118	-	3,3,3	0.41	0	2,2,2	0.58	0
9	EDO	A	1721	-	3,3,3	0.34	0	2,2,2	0.56	0
9	EDO	B	113	-	3,3,3	0.64	0	2,2,2	0.11	0
9	EDO	A	1727	-	3,3,3	0.33	0	2,2,2	0.62	0
9	EDO	B	114	-	3,3,3	0.47	0	2,2,2	0.37	0
10	ACT	A	1729	-	3,3,3	0.75	0	3,3,3	1.12	0
9	EDO	B	112	-	3,3,3	0.60	0	2,2,2	0.06	0
9	EDO	A	1726	-	3,3,3	0.46	0	2,2,2	0.21	0
9	EDO	A	1718	-	3,3,3	0.46	0	2,2,2	0.06	0
9	EDO	A	1724	-	3,3,3	0.50	0	2,2,2	0.14	0
9	EDO	B	117	-	3,3,3	0.40	0	2,2,2	0.56	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
9	EDO	B	116	-	-	1/1/1/1	-
9	EDO	A	1722	-	-	0/1/1/1	-
9	EDO	A	1723	-	-	0/1/1/1	-
9	EDO	B	115	-	-	0/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	B	120	-	-	0/1/1/1	-
9	EDO	A	1716	-	-	0/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	B	110	-	-	0/1/1/1	-
9	EDO	B	121	-	-	0/1/1/1	-
9	EDO	A	1725	-	-	1/1/1/1	-
9	EDO	B	111	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1717	-	-	0/1/1/1	-
9	EDO	B	118	-	-	1/1/1/1	-
9	EDO	A	1721	-	-	1/1/1/1	-
9	EDO	B	113	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	B	114	-	-	0/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-
9	EDO	A	1726	-	-	1/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	B	117	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1726	EDO	O1-C1-C2-O2
9	A	1721	EDO	O1-C1-C2-O2
9	B	116	EDO	O1-C1-C2-O2
9	A	1725	EDO	O1-C1-C2-O2
9	B	111	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	120	EDO	1	0
9	B	119	EDO	1	0
9	B	121	EDO	1	0
9	A	1725	EDO	2	0
9	A	1721	EDO	1	0
9	A	1727	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	1455/1632 (89%)	0.69	194 (13%) 7 6	12, 45, 101, 143	16 (1%)
2	B	93/94 (98%)	-0.56	0 100 100	19, 29, 58, 79	0
3	C	30/30 (100%)	-0.01	0 100 100	24, 51, 79, 115	0
4	D	9/9 (100%)	0.33	0 100 100	36, 52, 110, 111	0
All	All	1587/1765 (89%)	0.60	194 (12%) 8 8	12, 44, 101, 143	16 (1%)

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1060	PHE	6.3
1	A	1077	ILE	6.3
1	A	1054	PRO	5.7
1	A	1052	LEU	5.7
1	A	1059	ALA	5.6

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
6	NA	A	1703	1/1	0.81	0.14	63,63,63,63	0
9	EDO	B	119	4/4	0.82	0.22	63,65,69,70	0
9	EDO	A	1726	4/4	0.84	0.23	83,85,85,85	0
9	EDO	B	120	4/4	0.85	0.18	50,51,55,57	0
9	EDO	A	1727	4/4	0.86	0.32	81,81,82,83	0
9	EDO	B	121	4/4	0.86	0.24	56,59,61,62	0
9	EDO	B	118	4/4	0.88	0.16	45,54,58,58	0
9	EDO	A	1724	4/4	0.89	0.14	45,47,48,50	0
9	EDO	A	1725	4/4	0.90	0.11	42,45,51,57	0
9	EDO	B	117	4/4	0.90	0.16	34,46,52,55	0
10	ACT	A	1728	4/4	0.91	0.22	82,84,84,85	0
9	EDO	B	114	4/4	0.92	0.12	34,40,42,44	0
9	EDO	B	115	4/4	0.92	0.15	47,51,52,56	0
8	CA	A	1713	1/1	0.92	0.08	82,82,82,82	0
9	EDO	A	1721	4/4	0.92	0.12	45,46,47,49	0
9	EDO	A	1720	4/4	0.93	0.14	33,34,36,38	0
9	EDO	A	1723	4/4	0.94	0.11	45,45,49,52	0
9	EDO	A	1719	4/4	0.94	0.10	30,36,37,38	0
6	NA	A	1702	1/1	0.94	0.09	47,47,47,47	0
9	EDO	B	116	4/4	0.94	0.10	39,43,48,50	0
9	EDO	A	1716	4/4	0.94	0.12	39,45,45,47	0
8	CA	B	108	1/1	0.95	0.10	69,69,69,69	0
8	CA	B	109	1/1	0.95	0.12	70,70,70,70	0
8	CA	A	1712	1/1	0.95	0.12	72,72,72,72	0
8	CA	B	104	1/1	0.95	0.09	67,67,67,67	0
8	CA	B	107	1/1	0.95	0.10	64,64,64,64	0
9	EDO	A	1717	4/4	0.96	0.08	37,42,46,48	0
9	EDO	B	111	4/4	0.96	0.08	30,32,32,36	0
9	EDO	A	1718	4/4	0.96	0.07	32,37,38,38	0
7	CL	A	1704	1/1	0.96	0.09	43,43,43,43	0
8	CA	A	1714	1/1	0.96	0.10	69,69,69,69	0
8	CA	A	1706	1/1	0.96	0.10	67,67,67,67	0
9	EDO	A	1722	4/4	0.96	0.10	28,34,39,43	0
8	CA	A	1709	1/1	0.96	0.09	49,49,49,49	0
8	CA	A	1710	1/1	0.96	0.12	47,47,47,47	0
8	CA	A	1711	1/1	0.96	0.06	75,75,75,75	0
6	NA	B	102	1/1	0.96	0.10	59,59,59,59	0
10	ACT	A	1729	4/4	0.96	0.10	35,35,36,37	0
8	CA	B	106	1/1	0.97	0.12	44,44,44,44	0
9	EDO	B	113	4/4	0.97	0.07	29,29,31,33	0
8	CA	A	1715	1/1	0.97	0.15	54,54,54,54	0
9	EDO	B	110	4/4	0.97	0.06	31,32,35,37	0
9	EDO	B	112	4/4	0.99	0.04	23,24,24,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	A	1708	1/1	0.99	0.07	47,47,47,47	0
8	CA	B	105	1/1	0.99	0.03	35,35,35,35	0
7	CL	A	1705	1/1	0.99	0.08	28,28,28,28	0
6	NA	B	101	1/1	0.99	0.03	28,28,28,28	0
8	CA	A	1707	1/1	0.99	0.10	36,36,36,36	0
5	ZN	A	1701	1/1	1.00	0.01	25,25,25,25	0
8	CA	B	103	1/1	1.00	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.