wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2024 – 04:06 PM JST

PDB ID	:	5B2O
Title	:	Crystal structure of Francisella novicida Cas9 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 (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 (i)) were used in the production of this report:

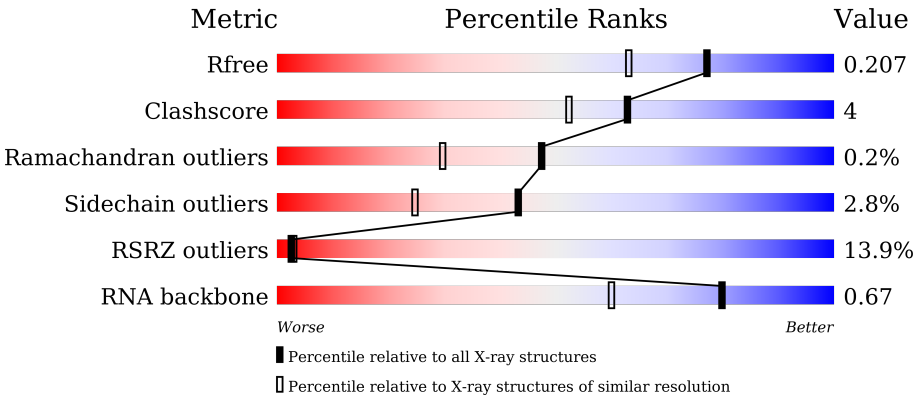
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)
RNA backbone	3102	1007 (2.38-1.02)

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
1	A	1632	13% 79% 9% • 11%
2	B	94	49% 43% 6% •
3	C	30	3% 47% 47% 7%
4	D	9	78% 22%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15717 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	19	0
			11791	7536	2025	2199	31			

There are 4 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

- 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

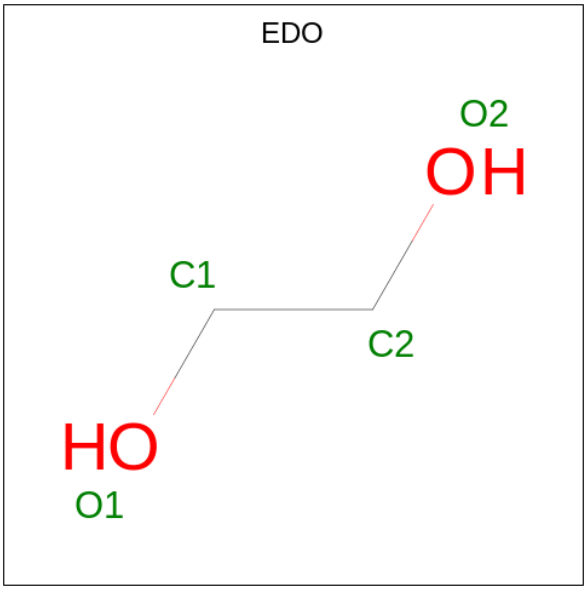
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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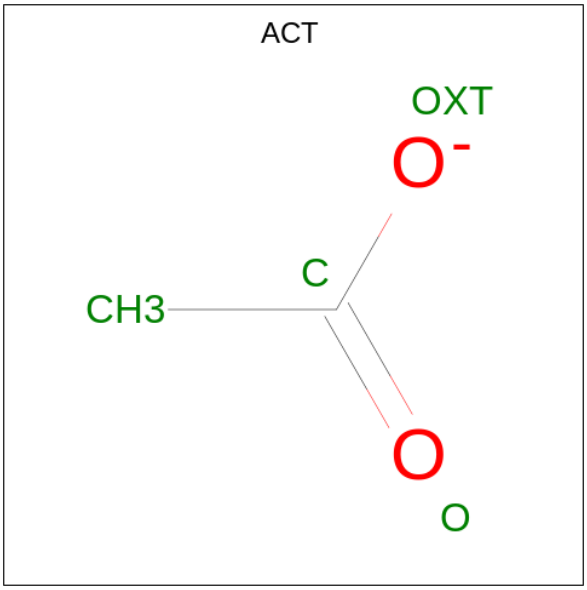
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 4 2 2	0	0

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 11 is water.

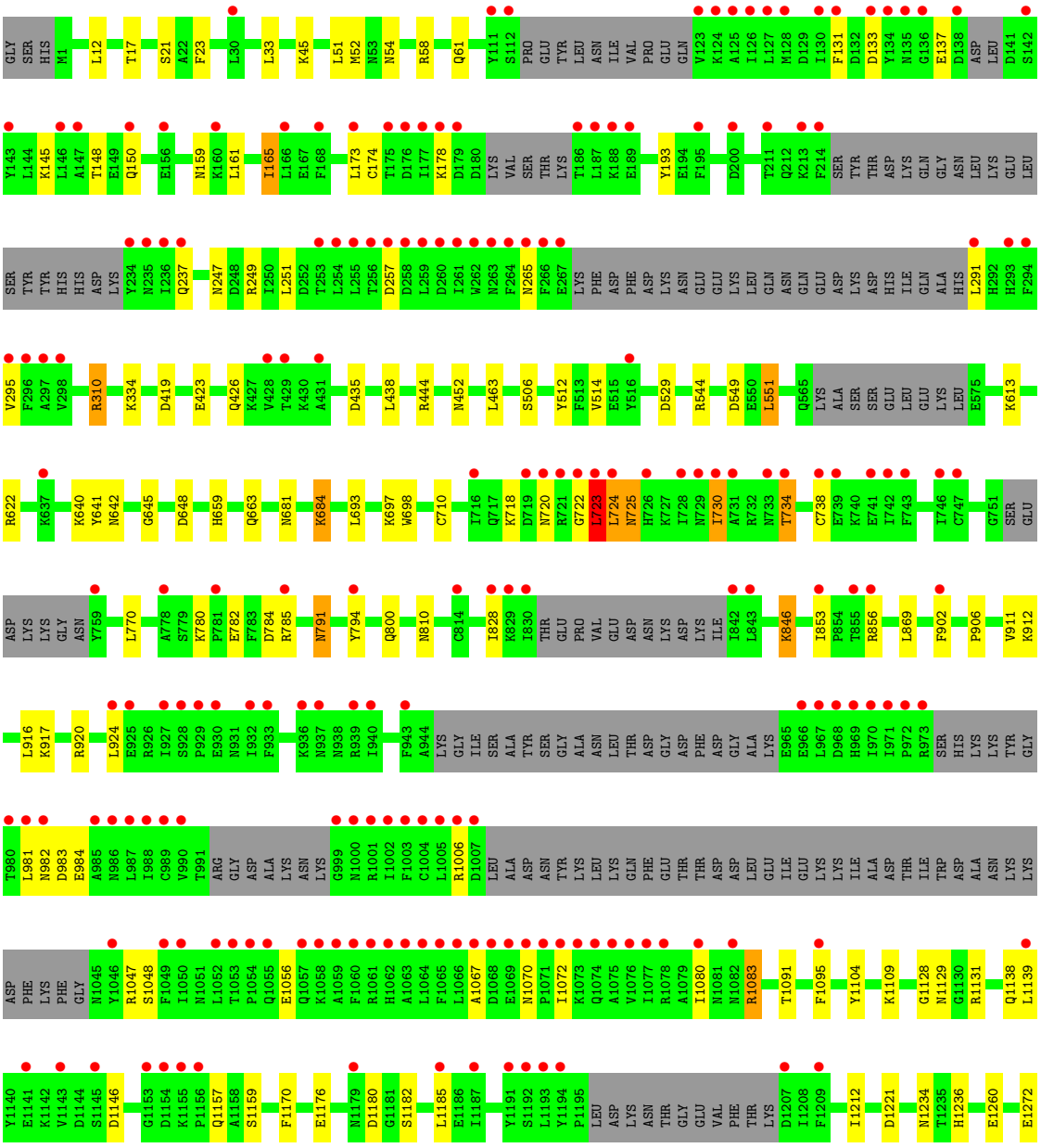
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	618	Total O 618 618	0	0
11	B	334	Total O 334 334	0	0
11	C	71	Total O 71 71	0	0
11	D	8	Total O 8 8	0	0

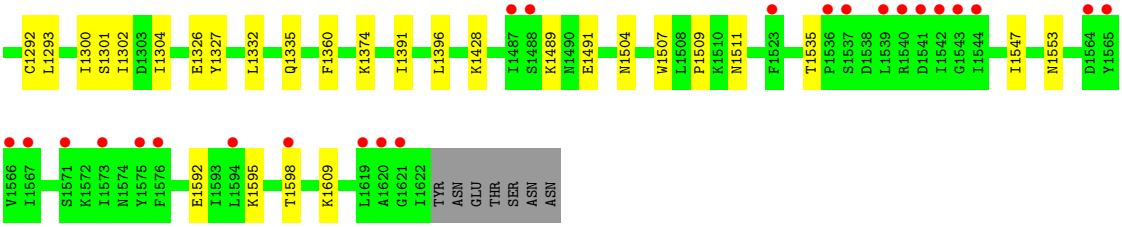
3 Residue-property plots (i)

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 endonuclease Cas9

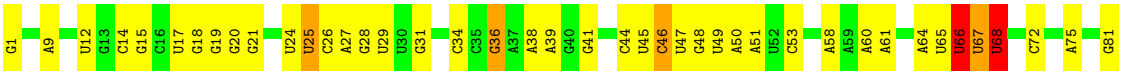
Chain A:

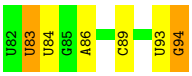




• Molecule 2: Guide RNA

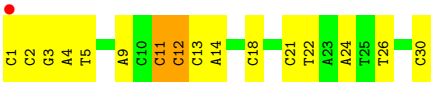
Chain B:





• Molecule 3: Target DNA

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.92Å 159.10Å 96.81Å 90.00° 107.04° 90.00°	Depositor
Resolution (Å)	46.28 – 1.70 46.28 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (46.28-1.70) 96.1 (46.28-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.184 , 0.207 0.184 , 0.207	Depositor DCC
R_{free} test set	12436 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15717	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, ACT, CA, EDO, ZN, NA

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	0.50	0/12068	0.61	2/16282 (0.0%)
2	B	1.12	5/2224 (0.2%)	1.57	48/3465 (1.4%)
3	C	1.26	3/664 (0.5%)	1.31	8/1018 (0.8%)
4	D	1.02	0/207	1.08	0/319
All	All	0.68	8/15163 (0.1%)	0.89	58/21084 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	G	N7-C5	6.32	1.43	1.39
2	B	21	G	C8-N7	6.14	1.34	1.30
3	C	26	DT	C3'-O3'	-5.87	1.36	1.44
3	C	12	DC	C3'-O3'	-5.36	1.36	1.44
2	B	44	C	C2-O2	5.24	1.29	1.24

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	11	DC	O5'-P-OP2	-12.03	94.88	105.70
3	C	12	DC	O5'-P-OP2	-10.69	96.08	105.70
2	B	50	A	N1-C2-N3	-9.66	124.47	129.30
2	B	50	A	C2-N3-C4	8.89	115.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	14	DA	O5'-P-OP2	-8.48	98.07	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	36	G	Sidechain

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	11791	0	11524	102	1
2	B	1991	0	997	16	0
3	C	595	0	337	9	0
4	D	185	0	104	2	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
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	3	0
9	B	40	0	60	6	0
9	C	4	0	6	0	0
10	A	4	0	3	0	0
10	B	4	0	3	0	0
11	A	618	0	0	12	0
11	B	334	0	0	1	0
11	C	71	0	0	0	0
11	D	8	0	0	0	0
All	All	15717	0	13106	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:54[B]:ASN:OD1	1:A:58[B]:ARG:NH1	1.99	0.96
1:A:265:ASN:O	1:A:291:LEU:N	2.08	0.87
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.64	0.80
1:A:1335[A]:GLN:NE2	11:A:1801:HOH:O	2.05	0.79
3:C:4:DA:H2"	3:C:5:DT:H5"	1.67	0.76

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:NH1	1:A:1260:GLU:OE2[2_445]	2.02	0.18

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	1446/1632 (89%)	1405 (97%)	38 (3%)	3 (0%)	47 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	722	GLY
1	A	723	LEU
1	A	1128	GLY

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	1255/1484 (85%)	1221 (97%)	34 (3%)	44 26

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1157	GLN
1	A	1234	ASN
1	A	1511	ASN
1	A	724	LEU
1	A	723	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	938	ASN
1	A	1234	ASN
1	A	1236	HIS
1	A	1157	GLN
1	A	604	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	92/94 (97%)	8 (8%)	2 (2%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	18	G
2	B	29	U
2	B	53	C
2	B	58	A
2	B	67	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 24 are monoatomic - leaving 25 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	A	1717	-	3,3,3	0.46	0	2,2,2	0.49	0
9	EDO	A	1718	-	3,3,3	0.44	0	2,2,2	0.70	0
9	EDO	A	1725	-	3,3,3	0.47	0	2,2,2	0.17	0
9	EDO	A	1724	-	3,3,3	0.54	0	2,2,2	0.04	0
9	EDO	A	1716	-	3,3,3	0.42	0	2,2,2	0.39	0
9	EDO	B	112	-	3,3,3	0.75	0	2,2,2	0.17	0
10	ACT	B	120	-	3,3,3	0.74	0	3,3,3	1.36	0
9	EDO	B	117	-	3,3,3	0.37	0	2,2,2	0.23	0
9	EDO	B	115	-	3,3,3	0.50	0	2,2,2	0.11	0
9	EDO	B	113	-	3,3,3	0.82	0	2,2,2	0.18	0
9	EDO	C	101	-	3,3,3	0.59	0	2,2,2	0.22	0
10	ACT	A	1728	-	3,3,3	0.78	0	3,3,3	0.99	0
9	EDO	B	119	-	3,3,3	0.45	0	2,2,2	0.35	0
9	EDO	A	1722	-	3,3,3	0.35	0	2,2,2	0.66	0
9	EDO	B	118	-	3,3,3	0.50	0	2,2,2	0.29	0
9	EDO	A	1727	-	3,3,3	0.38	0	2,2,2	0.60	0
9	EDO	A	1721	-	3,3,3	0.71	0	2,2,2	0.21	0
9	EDO	A	1719	-	3,3,3	0.54	0	2,2,2	0.21	0
9	EDO	A	1726	-	3,3,3	0.52	0	2,2,2	0.12	0
9	EDO	A	1720	-	3,3,3	0.61	0	2,2,2	0.37	0
9	EDO	A	1723	-	3,3,3	0.62	0	2,2,2	0.38	0
9	EDO	B	110	-	3,3,3	0.42	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	EDO	B	114	-	3,3,3	0.55	0	2,2,2	0.01	0
9	EDO	B	111	-	3,3,3	0.67	0	2,2,2	0.29	0
9	EDO	B	116	-	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	A	1717	-	-	0/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	A	1725	-	-	1/1/1/1	-
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	A	1716	-	-	0/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-
9	EDO	B	117	-	-	0/1/1/1	-
9	EDO	B	115	-	-	1/1/1/1	-
9	EDO	B	113	-	-	0/1/1/1	-
9	EDO	C	101	-	-	0/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	A	1722	-	-	1/1/1/1	-
9	EDO	B	118	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	A	1721	-	-	0/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	A	1726	-	-	1/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	A	1723	-	-	0/1/1/1	-
9	EDO	B	110	-	-	0/1/1/1	-
9	EDO	B	114	-	-	1/1/1/1	-
9	EDO	B	111	-	-	1/1/1/1	-
9	EDO	B	116	-	-	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	1722	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	A	1726	EDO	O1-C1-C2-O2
9	B	111	EDO	O1-C1-C2-O2
9	B	114	EDO	O1-C1-C2-O2
9	A	1725	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1725	EDO	2	0
9	B	117	EDO	2	0
9	B	119	EDO	1	0
9	A	1722	EDO	1	0
9	B	116	EDO	3	0

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, 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	OWAB(Å^2)	Q<0.9
1	A	1455/1632 (89%)	0.57	219 (15%) 2 2	19, 44, 98, 147	0
2	B	93/94 (98%)	-0.33	0 100 100	19, 29, 59, 84	0
3	C	30/30 (100%)	-0.12	1 (3%) 46 51	24, 50, 74, 106	0
4	D	9/9 (100%)	0.20	0 100 100	30, 52, 94, 105	0
All	All	1587/1765 (89%)	0.50	220 (13%) 2 3	19, 43, 97, 147	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1066	LEU	12.7
1	A	723	LEU	10.9
1	A	1071	PRO	10.7
1	A	131	PHE	8.7
1	A	1060	PHE	8.5

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

There are no monosaccharides in this entry.

6.4 Ligands

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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	A	1726	4/4	0.68	0.15	72,74,76,77	0
9	EDO	A	1727	4/4	0.76	0.30	76,76,76,77	0
9	EDO	B	118	4/4	0.82	0.20	44,50,52,53	0
9	EDO	B	119	4/4	0.83	0.18	57,58,58,59	0
6	NA	A	1703	1/1	0.86	0.06	64,64,64,64	0
9	EDO	A	1725	4/4	0.89	0.16	53,57,62,66	0
8	CA	A	1713	1/1	0.90	0.06	87,87,87,87	0
9	EDO	B	115	4/4	0.90	0.17	41,46,52,56	0
9	EDO	B	117	4/4	0.91	0.15	54,56,57,57	0
8	CA	B	106	1/1	0.92	0.09	63,63,63,63	0
9	EDO	A	1717	4/4	0.92	0.12	35,38,39,39	0
9	EDO	B	116	4/4	0.92	0.15	34,43,48,49	0
9	EDO	A	1722	4/4	0.93	0.16	51,52,53,54	0
9	EDO	C	101	4/4	0.93	0.11	42,43,43,43	0
8	CA	B	109	1/1	0.94	0.05	70,70,70,70	0
6	NA	A	1702	1/1	0.94	0.05	45,45,45,45	0
10	ACT	B	120	4/4	0.94	0.15	57,59,60,60	0
9	EDO	A	1721	4/4	0.95	0.08	33,34,35,35	0
8	CA	B	107	1/1	0.95	0.09	63,63,63,63	0
9	EDO	A	1724	4/4	0.95	0.11	42,42,43,43	0
8	CA	A	1710	1/1	0.95	0.05	52,52,52,52	0
9	EDO	A	1716	4/4	0.95	0.10	37,41,43,44	0
8	CA	A	1712	1/1	0.95	0.12	72,72,72,72	0
9	EDO	B	114	4/4	0.95	0.10	40,43,43,46	0
9	EDO	A	1720	4/4	0.96	0.13	31,34,36,37	0
8	CA	B	104	1/1	0.96	0.04	68,68,68,68	0
6	NA	B	102	1/1	0.96	0.12	53,53,53,53	0
8	CA	A	1714	1/1	0.96	0.14	62,62,62,62	0
9	EDO	A	1719	4/4	0.96	0.06	34,36,37,37	0
8	CA	A	1711	1/1	0.97	0.04	66,66,66,66	0
9	EDO	A	1723	4/4	0.97	0.10	30,35,38,42	0
8	CA	B	108	1/1	0.97	0.10	71,71,71,71	0
9	EDO	B	111	4/4	0.97	0.07	29,30,31,33	0
8	CA	A	1715	1/1	0.98	0.05	45,45,45,45	0
8	CA	A	1709	1/1	0.98	0.04	42,42,42,42	0
7	CL	A	1704	1/1	0.98	0.05	42,42,42,42	0
8	CA	A	1706	1/1	0.98	0.05	67,67,67,67	0
9	EDO	B	110	4/4	0.98	0.07	28,30,32,34	0
9	EDO	A	1718	4/4	0.98	0.07	35,38,41,43	0
9	EDO	B	112	4/4	0.98	0.12	22,23,23,24	0
10	ACT	A	1728	4/4	0.98	0.06	33,35,35,36	0
9	EDO	B	113	4/4	0.98	0.08	27,28,28,29	0
7	CL	A	1705	1/1	0.99	0.04	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	CA	A	1707	1/1	0.99	0.03	34,34,34,34	0
8	CA	B	105	1/1	0.99	0.03	34,34,34,34	0
8	CA	A	1708	1/1	0.99	0.06	57,57,57,57	0
5	ZN	A	1701	1/1	1.00	0.11	26,26,26,26	0
8	CA	B	103	1/1	1.00	0.04	32,32,32,32	0
6	NA	B	101	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.