



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 4, 2024 – 04:10 PM JST

PDB ID : 8X5V  
Title : BICas9-sgRNA-target DNA complex  
Authors : Nakane, T.; Nakagawa, R.; Yamashita, K.; Nishimasu, H.; Nureki, O.  
Deposited on : 2023-11-19  
Resolution : 2.00 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

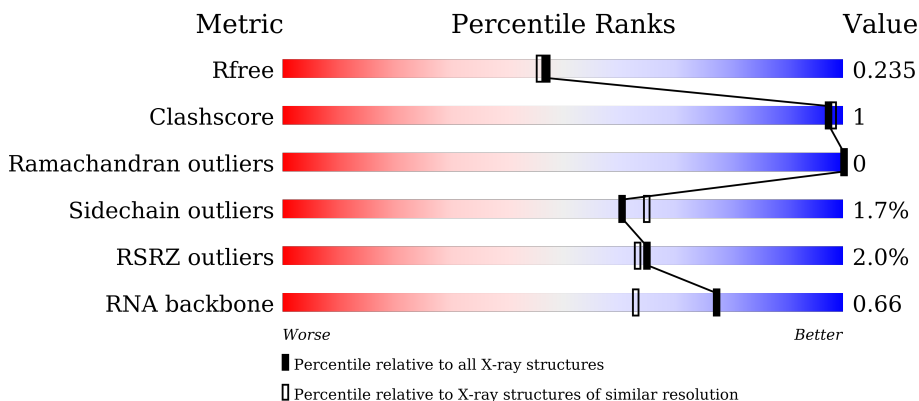
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

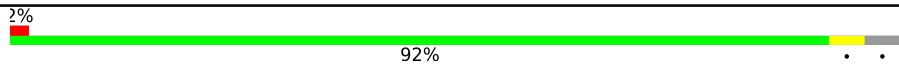



The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)
RNA backbone	3102	1079 (2.50-1.50)

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  $\geq 3$ , 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	933	 2% 92%
2	B	110	 67% 26%
3	C	28	 61% 39%
4	D	8	 75% 25%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10610 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 BICas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	892	7172	4549	1269	1334	20	0	5	0

- Molecule 2 is a RNA chain called RNA (110-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	106	2258	1007	396	749	106	0	0	0

- Molecule 3 is a DNA chain called DNA (28-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	28	567	272	103	165	27	0	0	0

- Molecule 4 is a DNA chain called DNA (8-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	8	158	78	27	46	7	0	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

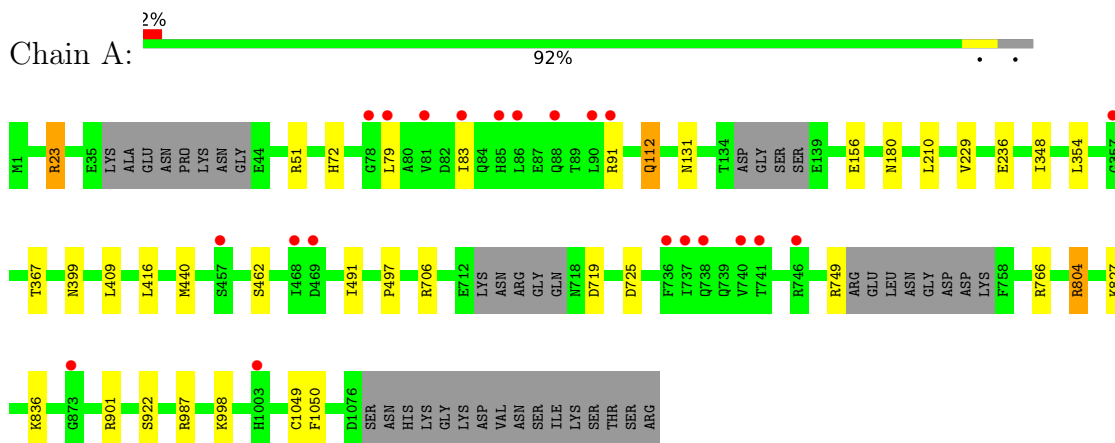
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	171	Total O 171 171	0	0
8	B	105	Total O 105 105	0	0
8	C	40	Total O 40 40	0	0
8	D	9	Total O 9 9	0	0

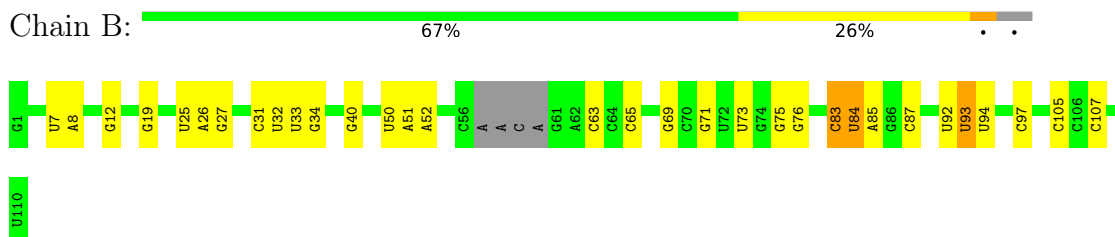
### 3 Residue-property plots [i](#)

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: BICas9



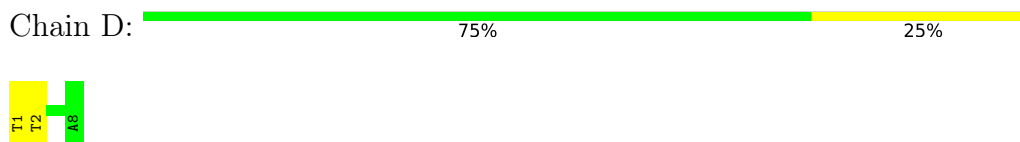
- Molecule 2: RNA (110-mer)



- Molecule 3: DNA (28-mer)



- Molecule 4: DNA (8-mer)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.75Å 99.21Å 119.30Å 90.00° 97.09° 90.00°	Depositor
Resolution (Å)	118.39 – 2.00 118.39 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.39-2.00) 99.9 (118.39-2.00)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.198 , 0.231 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	5612 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtrriage
Anisotropy	0.218	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, EDO, 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	0.39	0/7324	0.74	0/9882
2	B	0.65	0/2521	1.36	27/3925 (0.7%)
3	C	0.71	0/635	1.44	13/977 (1.3%)
4	D	0.73	0/176	1.29	0/269
All	All	0.49	0/10656	1.00	40/15053 (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
1	A	0	4

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	40	G	O5'-P-OP2	-11.40	95.44	105.70
3	C	6	DG	O5'-P-OP1	10.44	123.23	110.70
2	B	26	A	O5'-P-OP2	-9.43	97.21	105.70
2	B	71	G	O5'-P-OP2	-9.21	97.42	105.70
2	B	12	G	O5'-P-OP2	-9.03	97.57	105.70
2	B	19	G	O5'-P-OP2	-8.53	98.02	105.70
3	C	-7	DT	O5'-P-OP1	-8.41	98.13	105.70
2	B	97	C	O5'-P-OP2	-8.23	98.29	105.70
2	B	33	U	O5'-P-OP2	-7.37	99.07	105.70
2	B	40	G	O5'-P-OP1	7.12	119.24	110.70
3	C	-7	DT	O5'-P-OP2	7.04	119.15	110.70
3	C	-6	DT	O4'-C1'-N1	-7.04	103.07	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	107	C	O5'-P-OP2	-6.91	99.48	105.70
2	B	52	A	O3'-P-O5'	-6.75	91.17	104.00
2	B	69	G	O5'-P-OP2	-6.67	99.70	105.70
2	B	25	U	OP2-P-O3'	6.38	119.23	105.20
2	B	50	U	O5'-P-OP2	-6.18	100.14	105.70
2	B	7	U	OP2-P-O3'	6.08	118.57	105.20
2	B	65	C	O5'-P-OP2	6.04	117.94	110.70
3	C	-2	DA	O5'-P-OP2	-5.82	100.46	105.70
2	B	83	C	O3'-P-O5'	-5.70	93.16	104.00
3	C	7	DC	OP2-P-O3'	5.69	117.73	105.20
2	B	34	G	OP2-P-O3'	5.67	117.66	105.20
2	B	105	C	O5'-P-OP2	-5.61	100.65	105.70
3	C	1	DG	O5'-P-OP2	-5.57	100.69	105.70
3	C	6	DG	O5'-P-OP2	-5.54	100.72	105.70
3	C	2	DC	OP2-P-O3'	5.54	117.38	105.20
3	C	3	DC	O5'-P-OP2	-5.43	100.81	105.70
2	B	75	G	OP2-P-O3'	5.34	116.94	105.20
2	B	93	U	OP2-P-O3'	5.32	116.91	105.20
3	C	-4	DG	O4'-C1'-N9	5.27	111.69	108.00
2	B	73	U	OP2-P-O3'	5.27	116.79	105.20
2	B	7	U	O3'-P-O5'	-5.15	94.21	104.00
2	B	32	U	O5'-P-OP2	-5.13	101.08	105.70
2	B	8	A	OP2-P-O3'	5.09	116.40	105.20
2	B	26	A	OP2-P-O3'	5.09	116.39	105.20
2	B	69	G	O5'-P-OP1	-5.05	101.16	105.70
3	C	8	DG	OP2-P-O3'	5.04	116.28	105.20
3	C	16	DT	C4'-C3'-C2'	-5.03	98.57	103.10
2	B	27	G	O5'-P-OP2	-5.00	101.20	105.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	ARG	Sidechain
1	A	804	ARG	Sidechain
1	A	901	ARG	Sidechain
1	A	91	ARG	Peptide

## 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	7172	0	7108	14	1
2	B	2258	0	1140	1	0
3	C	567	0	317	0	0
4	D	158	0	93	1	0
5	A	68	0	102	0	0
5	B	12	0	18	0	0
5	C	4	0	6	0	0
6	A	45	0	0	0	0
7	A	1	0	0	0	0
8	A	171	0	0	2	0
8	B	105	0	0	0	0
8	C	40	0	0	0	0
8	D	9	0	0	0	0
All	All	10610	0	8784	16	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 1.

All (16) 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:719:ASP:OD2	1:A:804:ARG:NH2	2.30	0.63
1:A:79:LEU:HG	1:A:210:LEU:HD13	1.82	0.61
1:A:440:MET:HE2	8:A:1371:HOH:O	2.02	0.59
1:A:72:HIS:CD2	1:A:83:ILE:HD11	2.40	0.56
1:A:23:ARG:HD2	1:A:23:ARG:O	2.10	0.52
1:A:79:LEU:HD11	1:A:210:LEU:HB3	1.96	0.48
1:A:367:THR:HG23	1:A:399:ASN:HB2	1.96	0.48
1:A:987:ARG:NH2	1:A:1049[B]:CYS:SG	2.88	0.46
1:A:491:ILE:HD12	1:A:497:PRO:HD3	1.98	0.45
1:A:112:GLN:H	1:A:112:GLN:HE21	1.66	0.42
4:D:1:DT:H2'	4:D:2:DT:C6	2.55	0.42
1:A:131:ASN:ND2	1:A:229:VAL:HG11	2.35	0.42
2:B:83:C:O3'	2:B:84:U:H4'	2.20	0.41
1:A:998:LYS:NZ	8:A:1215:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:HD12	1:A:416:LEU:HD11	2.01	0.41
1:A:706:ARG:HD3	1:A:725:ASP:OD1	2.20	0.40

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:156:GLU:OE1	1:A:156:GLU:OE1[2_656]	2.13	0.07

## 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	886/933 (95%)	869 (98%)	17 (2%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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	772/836 (92%)	759 (98%)	13 (2%)	<a href="#">60</a> <a href="#">65</a>

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	112	GLN
1	A	180	ASN
1	A	236	GLU
1	A	354	LEU
1	A	409	LEU
1	A	462	SER
1	A	749	ARG
1	A	766	ARG
1	A	827	LYS
1	A	836	LYS
1	A	922	SER
1	A	1050	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	112	GLN
1	A	182	ASN
1	A	276	GLN
1	A	477	ASN
1	A	780	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	104/110 (94%)	10 (9%)	1 (0%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	31	C
2	B	51	A
2	B	63	C
2	B	76	G
2	B	84	U
2	B	85	A
2	B	87	C
2	B	92	U
2	B	93	U

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Mol	Chain	Res	Type
2	B	94	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	84	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 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\# Z  > 2$
5	EDO	C	201	-	3,3,3	0.12	0	2,2,2	0.51	0
5	EDO	A	1117	-	3,3,3	0.10	0	2,2,2	0.24	0
5	EDO	A	1109	-	3,3,3	0.45	0	2,2,2	0.72	0
5	EDO	A	1105	-	3,3,3	0.15	0	2,2,2	0.32	0
6	SO4	A	1122	-	4,4,4	0.36	0	6,6,6	0.16	0
6	SO4	A	1126	-	4,4,4	0.34	0	6,6,6	0.13	0
5	EDO	A	1113	-	3,3,3	0.08	0	2,2,2	0.25	0
5	EDO	A	1116	-	3,3,3	0.19	0	2,2,2	0.37	0
6	SO4	A	1118	-	4,4,4	0.38	0	6,6,6	0.13	0
5	EDO	A	1114	-	3,3,3	0.15	0	2,2,2	0.45	0
5	EDO	A	1110	-	3,3,3	0.27	0	2,2,2	0.66	0
5	EDO	B	201	-	3,3,3	0.03	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	1102	-	3,3,3	0.25	0	2,2,2	0.17	0
5	EDO	A	1115	-	3,3,3	0.11	0	2,2,2	0.26	0
5	EDO	A	1107	-	3,3,3	0.13	0	2,2,2	0.20	0
6	SO4	A	1121	-	4,4,4	0.29	0	6,6,6	0.07	0
5	EDO	B	202	-	3,3,3	0.15	0	2,2,2	0.45	0
5	EDO	A	1108	-	3,3,3	0.27	0	2,2,2	0.22	0
5	EDO	A	1112	-	3,3,3	0.23	0	2,2,2	0.57	0
5	EDO	A	1106	-	3,3,3	0.17	0	2,2,2	0.34	0
6	SO4	A	1120	-	4,4,4	0.33	0	6,6,6	0.12	0
6	SO4	A	1119	-	4,4,4	0.35	0	6,6,6	0.06	0
6	SO4	A	1124	-	4,4,4	0.36	0	6,6,6	0.06	0
5	EDO	A	1111	-	3,3,3	0.03	0	2,2,2	0.15	0
6	SO4	A	1125	-	4,4,4	0.20	0	6,6,6	0.24	0
5	EDO	A	1103	-	3,3,3	0.17	0	2,2,2	0.48	0
5	EDO	A	1104	-	3,3,3	0.37	0	2,2,2	0.43	0
5	EDO	A	1101	-	3,3,3	0.20	0	2,2,2	0.08	0
5	EDO	B	203	-	3,3,3	0.09	0	2,2,2	0.36	0
6	SO4	A	1123	-	4,4,4	0.35	0	6,6,6	0.07	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	C	201	-	-	0/1/1/1	-
5	EDO	A	1117	-	-	1/1/1/1	-
5	EDO	A	1109	-	-	1/1/1/1	-
5	EDO	A	1105	-	-	0/1/1/1	-
5	EDO	A	1113	-	-	1/1/1/1	-
5	EDO	A	1116	-	-	1/1/1/1	-
5	EDO	A	1114	-	-	0/1/1/1	-
5	EDO	A	1110	-	-	0/1/1/1	-
5	EDO	B	201	-	-	1/1/1/1	-
5	EDO	A	1102	-	-	0/1/1/1	-
5	EDO	A	1115	-	-	0/1/1/1	-
5	EDO	A	1107	-	-	1/1/1/1	-
5	EDO	B	202	-	-	0/1/1/1	-
5	EDO	A	1108	-	-	1/1/1/1	-
5	EDO	A	1112	-	-	1/1/1/1	-
5	EDO	A	1106	-	-	1/1/1/1	-
5	EDO	A	1111	-	-	0/1/1/1	-
5	EDO	A	1103	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1104	-	-	0/1/1/1	-
5	EDO	A	1101	-	-	0/1/1/1	-
5	EDO	B	203	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1107	EDO	O1-C1-C2-O2
5	A	1103	EDO	O1-C1-C2-O2
5	A	1108	EDO	O1-C1-C2-O2
5	A	1116	EDO	O1-C1-C2-O2
5	B	201	EDO	O1-C1-C2-O2
5	A	1113	EDO	O1-C1-C2-O2
5	A	1109	EDO	O1-C1-C2-O2
5	A	1106	EDO	O1-C1-C2-O2
5	A	1112	EDO	O1-C1-C2-O2
5	A	1117	EDO	O1-C1-C2-O2
5	B	203	EDO	O1-C1-C2-O2

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	892/933 (95%)	0.03	21 (2%) 59 57	37, 55, 92, 135	0
2	B	106/110 (96%)	-0.72	0 100 100	38, 55, 131, 147	0
3	C	28/28 (100%)	-0.45	0 100 100	39, 46, 60, 62	0
4	D	8/8 (100%)	-0.36	0 100 100	42, 48, 61, 71	0
All	All	1034/1079 (95%)	-0.06	21 (2%) 65 63	37, 55, 96, 147	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	6.8
1	A	81	VAL	6.4
1	A	90	LEU	6.2
1	A	457	SER	5.4
1	A	85	HIS	5.1
1	A	86	LEU	4.8
1	A	1003	HIS	4.8
1	A	737	ILE	3.7
1	A	78	GLY	3.6
1	A	83	ILE	3.4
1	A	357	GLY	3.0
1	A	740	VAL	2.9
1	A	469	ASP	2.5
1	A	738	GLN	2.4
1	A	468	ILE	2.3
1	A	91	ARG	2.2
1	A	873	GLY	2.2
1	A	736	PHE	2.2
1	A	88	GLN	2.2
1	A	746	ARG	2.2
1	A	741	THR	2.1

## 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, median, 95<sup>th</sup> 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	A	1105	4/4	0.34	0.18	85,88,93,96	0
5	EDO	A	1115	4/4	0.62	0.24	81,84,88,93	0
5	EDO	A	1107	4/4	0.74	0.16	65,73,74,77	0
5	EDO	B	203	4/4	0.77	0.16	73,73,75,80	0
5	EDO	A	1116	4/4	0.83	0.14	70,79,81,84	0
5	EDO	C	201	4/4	0.83	0.28	68,69,70,81	0
5	EDO	A	1108	4/4	0.85	0.16	48,53,58,58	0
6	SO4	A	1123	5/5	0.86	0.28	115,119,122,125	0
5	EDO	A	1101	4/4	0.87	0.17	58,60,61,63	0
5	EDO	A	1117	4/4	0.89	0.10	55,68,73,79	0
5	EDO	B	202	4/4	0.90	0.27	56,67,74,79	0
6	SO4	A	1121	5/5	0.90	0.13	88,89,111,119	0
5	EDO	A	1104	4/4	0.90	0.25	60,63,63,63	0
5	EDO	A	1103	4/4	0.91	0.12	56,58,58,64	0
5	EDO	A	1111	4/4	0.91	0.23	77,77,81,85	0
5	EDO	A	1113	4/4	0.92	0.17	71,77,77,78	0
6	SO4	A	1120	5/5	0.92	0.16	86,86,93,106	0
6	SO4	A	1125	5/5	0.92	0.23	68,69,90,96	0
5	EDO	B	201	4/4	0.93	0.27	58,60,61,63	0
5	EDO	A	1114	4/4	0.93	0.13	66,68,69,69	0
6	SO4	A	1124	5/5	0.94	0.19	112,115,120,126	0
5	EDO	A	1112	4/4	0.94	0.23	52,62,64,72	0
5	EDO	A	1102	4/4	0.95	0.13	53,54,55,55	0
5	EDO	A	1106	4/4	0.95	0.10	53,53,56,59	0
6	SO4	A	1126	5/5	0.95	0.28	62,73,82,82	0
7	CL	A	1127	1/1	0.95	0.10	68,68,68,68	0
5	EDO	A	1110	4/4	0.96	0.13	41,60,62,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	1109	4/4	0.96	0.23	53,59,64,66	0
6	SO4	A	1122	5/5	0.96	0.11	77,81,99,107	0
6	SO4	A	1119	5/5	0.96	0.05	78,96,102,108	0
6	SO4	A	1118	5/5	1.00	0.13	44,46,48,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.