Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 03:01 PM JST

PDB ID	:	5XH7
Title	:	Crystal structure of the Acidaminococcus sp. BV3L6 Cpf1 RR variant in complex with crRNA and target DNA (TCCA PAM)
Authors	:	Nishimasu, H.; Yamano, T.; Ishitani, R.; Nureki, O.
Deposited on	:	2017-04-19
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*
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:

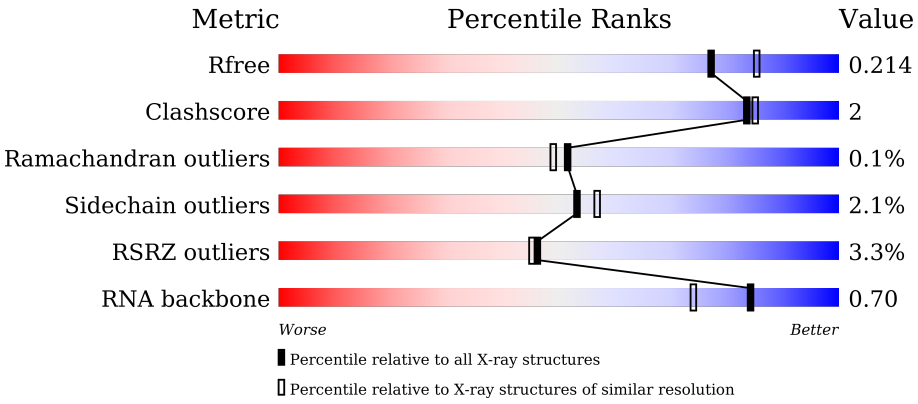
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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 >=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	1310	3% 90% 7% .
2	B	43	79% 14% 7%
3	C	34	3% 65% 24% 12%
4	D	10	10% 80% 20%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12823 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 Cpf1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1283	Total	C	N	O	S	0	12	0
			10431	6688	1772	1943	28			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP U2UMQ6
A	-1	SER	-	expression tag	UNP U2UMQ6
A	0	HIS	-	expression tag	UNP U2UMQ6
A	542	ARG	SER	engineered mutation	UNP U2UMQ6
A	607	ARG	LYS	engineered mutation	UNP U2UMQ6

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	P	0	0	0
			829	370	141	279	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			614	291	114	179	30			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			196	95	34	58	9			

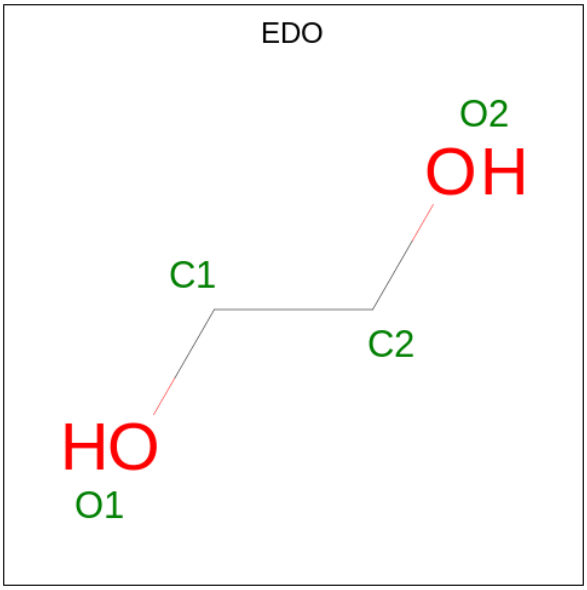
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	3	Total Na 3 3	0	0
5	C	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 8 is water.

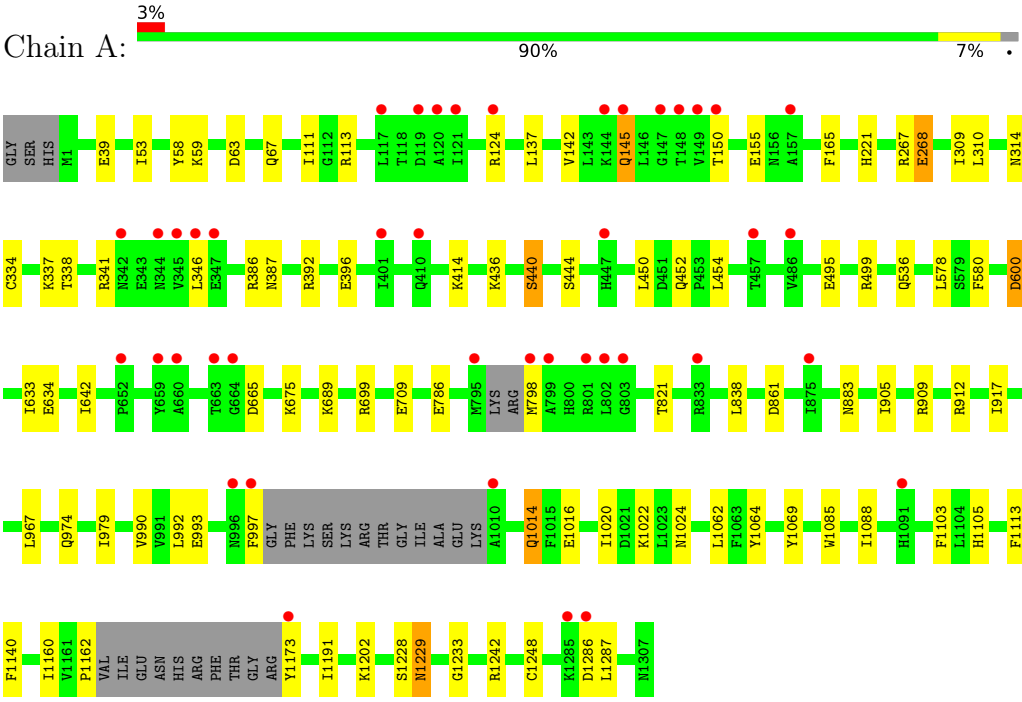
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	500	Total O 500 500	0	0
8	B	109	Total O 109 109	0	0
8	C	61	Total O 61 61	0	0
8	D	13	Total O 13 13	0	0

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.

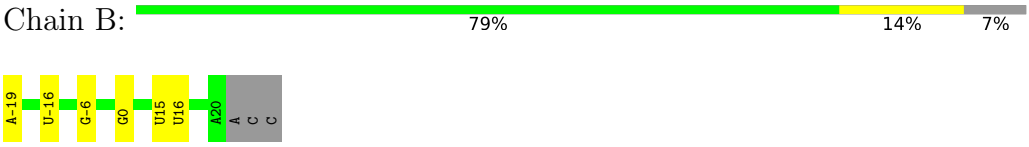
• Molecule 1: CRISPR-associated endonuclease Cpf1

Chain A:



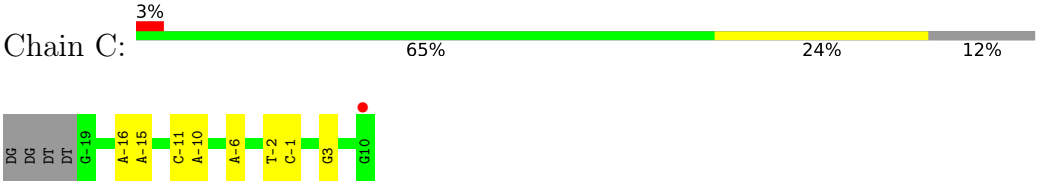
• Molecule 2: crRNA

Chain B:



• Molecule 3: Target DNA strand

Chain C:



• Molecule 4: Non-target DNA strand

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.66Å 133.30Å 200.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.00) 99.7 (40.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.183 , 0.214 0.183 , 0.214	Depositor DCC
R_{free} test set	7406 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, 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	0.36	0/10702	0.51	0/14481
2	B	0.56	0/925	1.01	1/1440 (0.1%)
3	C	0.82	0/688	0.96	0/1059
4	D	0.75	0/218	0.95	0/333
All	All	0.42	0/12533	0.62	1/17313 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	0	G	O4'-C1'-N9	6.45	113.36	108.20

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	10431	0	10287	49	0
2	B	829	0	416	2	0
3	C	614	0	337	5	0
4	D	196	0	114	1	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
6	A	1	0	0	0	0
7	A	52	0	78	0	0
7	B	12	0	18	2	0
8	A	500	0	0	2	0
8	B	109	0	0	0	0
8	C	61	0	0	0	0
8	D	13	0	0	0	0
All	All	12823	0	11250	55	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 2.

All (55) 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:990[B]:VAL:HG22	1:A:1062[B]:LEU:HD22	1.66	0.77
1:A:386:ARG:HH21	1:A:387:ASN:HD21	1.38	0.71
1:A:992:LEU:HD13	1:A:1016:GLU:HG2	1.74	0.69
1:A:53:ILE:HD13	1:A:155:GLU:HG2	1.75	0.67
1:A:1020:ILE:HD11	1:A:1064:TYR:OH	1.95	0.66
1:A:699:ARG:NH1	1:A:709:GLU:OE2	2.30	0.64
1:A:861:ASP:OD1	8:A:1501:HOH:O	2.15	0.64
1:A:909:ARG:NH2	1:A:993:GLU:OE1	2.34	0.61
1:A:600:ASP:HB3	1:A:603:LYS:HE2	1.86	0.58
1:A:992:LEU:HD12	1:A:1062[A]:LEU:HD21	1.85	0.58
1:A:905:ILE:HB	1:A:990[B]:VAL:HG12	1.86	0.58
1:A:346:LEU:HD22	1:A:450:LEU:HD12	1.86	0.56
1:A:327:GLU:HG3	1:A:331:GLN:HE21	1.72	0.54
1:A:997:PHE:HB2	8:A:1540:HOH:O	2.08	0.54
2:B:-19:A:N7	7:B:106:EDO:H22	2.24	0.52
1:A:786:GLU:HB2	7:B:105:EDO:H11	1.92	0.52
1:A:578:LEU:HD23	1:A:580:PHE:CZ	2.44	0.51
1:A:689:LYS:HD2	3:C:3:DG:OP1	2.11	0.50
1:A:1113:PHE:HB2	1:A:1140:PHE:HB2	1.94	0.49
4:D:-10:DC:H2"	4:D:-9:DA:C8	2.48	0.49
1:A:912:ARG:NH1	1:A:1233:GLY:O	2.43	0.49
1:A:58:TYR:OH	1:A:137:LEU:HD11	2.12	0.48
1:A:1242:ARG:HG2	1:A:1248[B]:CYS:SG	2.53	0.48
1:A:1069:TYR:OH	1:A:1127:ARG:HD3	2.14	0.48
1:A:1014:GLN:NE2	3:C:-6:DA:OP1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:ASP:OD1	1:A:1287:LEU:N	2.39	0.48
3:C:-16:DA:H2'	3:C:-15:DA:C8	2.49	0.48
1:A:436:LYS:O	1:A:440:SER:OG	2.33	0.47
1:A:495:GLU:O	1:A:499:ARG:HG3	2.14	0.47
1:A:337:LYS:NZ	1:A:452:GLN:O	2.48	0.47
1:A:268:GLU:H	1:A:268:GLU:CD	2.18	0.46
3:C:-2:DT:H2'	3:C:-1:DC:C6	2.52	0.45
1:A:142:VAL:HA	1:A:145:GLN:HG3	1.99	0.45
1:A:392:ARG:O	1:A:396:GLU:HG3	2.16	0.45
1:A:59:LYS:HD3	1:A:310:LEU:O	2.17	0.44
1:A:642:ILE:HD11	1:A:675:LYS:HE3	2.00	0.44
1:A:1191:ILE:HG23	1:A:1202:LYS:HD2	1.99	0.44
1:A:63:ASP:O	1:A:67:GLN:HG3	2.18	0.44
1:A:338:THR:HA	1:A:341:ARG:HH21	1.83	0.43
1:A:1162:PRO:HB3	1:A:1173:TYR:CZ	2.53	0.43
1:A:39:GLU:OE1	1:A:536:GLN:HG3	2.18	0.43
1:A:633:ILE:HD12	1:A:634:GLU:HG3	2.01	0.43
1:A:1085:TRP:CE3	1:A:1088:ILE:HD12	2.53	0.43
1:A:1103:PHE:CZ	1:A:1116:HIS:HB2	2.53	0.43
1:A:334:CYS:HB2	1:A:454:LEU:HD12	2.01	0.42
1:A:111:ILE:HG13	1:A:113:ARG:HG3	2.01	0.42
1:A:1160:ILE:HD13	1:A:1229:ASN:HB2	2.02	0.42
3:C:-11:DC:H2'	3:C:-10:DA:C8	2.55	0.42
1:A:917:ILE:HG21	1:A:979:ILE:HD11	2.01	0.42
1:A:992:LEU:CD1	1:A:1062[A]:LEU:HD21	2.50	0.41
2:B:15:U:H2'	2:B:16:U:C6	2.56	0.41
1:A:1229:ASN:C	1:A:1229:ASN:HD22	2.24	0.41
1:A:309:ILE:O	1:A:310:LEU:HB2	2.22	0.40
1:A:943:LYS:HG3	1:A:967:LEU:HD21	2.03	0.40
1:A:935:ILE:HG21	1:A:974:GLN:HB3	2.02	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	1287/1310 (98%)	1263 (98%)	23 (2%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	ASP

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	1130/1172 (96%)	1104 (98%)	26 (2%)	50 53

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	145	GLN
1	A	150	THR
1	A	165	PHE
1	A	221[A]	HIS
1	A	221[B]	HIS
1	A	267	ARG
1	A	268	GLU
1	A	314	ASN
1	A	414	LYS
1	A	440	SER
1	A	444	SER
1	A	620	GLN
1	A	665	ASP
1	A	798	MET
1	A	821	THR
1	A	838	LEU
1	A	883[A]	ASN

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Mol	Chain	Res	Type
1	A	883[B]	ASN
1	A	941	GLN
1	A	1014	GLN
1	A	1022	LYS
1	A	1024	ASN
1	A	1105	HIS
1	A	1228	SER
1	A	1229	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	70	GLN
1	A	145	GLN
1	A	224	ASN
1	A	331	GLN
1	A	387	ASN
1	A	560	ASN
1	A	620	GLN
1	A	856	HIS
1	A	890	GLN
1	A	941	GLN
1	A	974	GLN
1	A	1014	GLN
1	A	1105	HIS
1	A	1229	ASN
1	A	1275	GLN
1	A	1291	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	38/43 (88%)	2 (5%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-16	U
2	B	-6	G

There are no RNA pucker outliers to report.

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 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
7	EDO	A	1405	-	3,3,3	0.44	0	2,2,2	0.22	0
7	EDO	A	1408	-	3,3,3	0.50	0	2,2,2	0.41	0
7	EDO	A	1412	-	3,3,3	0.54	0	2,2,2	0.16	0
7	EDO	B	104	-	3,3,3	0.56	0	2,2,2	0.15	0
7	EDO	A	1407	-	3,3,3	0.68	0	2,2,2	0.29	0
7	EDO	A	1410	-	3,3,3	0.37	0	2,2,2	0.57	0
7	EDO	B	106	-	3,3,3	0.50	0	2,2,2	0.28	0
7	EDO	A	1413	-	3,3,3	0.45	0	2,2,2	0.20	0
7	EDO	A	1404	-	3,3,3	0.50	0	2,2,2	0.28	0
7	EDO	A	1411	-	3,3,3	0.46	0	2,2,2	0.44	0
7	EDO	B	105	-	3,3,3	0.45	0	2,2,2	0.43	0
7	EDO	A	1409	-	3,3,3	0.45	0	2,2,2	0.43	0
7	EDO	A	1415	-	3,3,3	0.49	0	2,2,2	0.29	0
7	EDO	A	1414	-	3,3,3	0.49	0	2,2,2	0.15	0
7	EDO	A	1403	-	3,3,3	0.46	0	2,2,2	0.29	0
7	EDO	A	1406	-	3,3,3	0.42	0	2,2,2	0.40	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
7	EDO	A	1405	-	-	0/1/1/1	-
7	EDO	A	1408	-	-	0/1/1/1	-
7	EDO	A	1412	-	-	0/1/1/1	-
7	EDO	B	104	-	-	0/1/1/1	-
7	EDO	A	1407	-	-	0/1/1/1	-
7	EDO	A	1410	-	-	0/1/1/1	-
7	EDO	B	106	-	-	0/1/1/1	-
7	EDO	A	1413	-	-	0/1/1/1	-
7	EDO	A	1404	-	-	0/1/1/1	-
7	EDO	A	1411	-	-	1/1/1/1	-
7	EDO	B	105	-	-	0/1/1/1	-
7	EDO	A	1409	-	-	0/1/1/1	-
7	EDO	A	1415	-	-	0/1/1/1	-
7	EDO	A	1414	-	-	0/1/1/1	-
7	EDO	A	1403	-	-	0/1/1/1	-
7	EDO	A	1406	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1411	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	106	EDO	1	0
7	B	105	EDO	1	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	1283/1310 (97%)	0.17	43 (3%) 45 44	27, 47, 77, 103	0
2	B	40/43 (93%)	-0.72	0 100 100	29, 36, 51, 88	0
3	C	30/34 (88%)	-0.15	1 (3%) 46 45	33, 42, 98, 132	0
4	D	10/10 (100%)	0.04	1 (10%) 7 6	42, 51, 117, 129	0
All	All	1363/1397 (97%)	0.14	45 (3%) 46 45	27, 47, 78, 132	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	802	LEU	5.8
1	A	1173	TYR	5.5
1	A	148	THR	5.2
1	A	147	GLY	5.1
1	A	663	THR	4.4
1	A	997	PHE	4.2
1	A	799	ALA	3.9
1	A	486	VAL	3.9
4	D	-10	DC	3.8
1	A	798	MET	3.7
1	A	1010	ALA	3.6
1	A	117	LEU	3.6
1	A	621	THR	3.6
1	A	660	ALA	3.5
1	A	149	VAL	3.5
1	A	120	ALA	3.4
1	A	659	TYR	3.4
3	C	10	DG	3.1
1	A	1286	ASP	3.1
1	A	144	LYS	3.0
1	A	652	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	801	ARG	2.9
1	A	119	ASP	2.9
1	A	795	MET	2.8
1	A	344	ASN	2.8
1	A	996	ASN	2.7
1	A	145	GLN	2.7
1	A	342	ASN	2.5
1	A	346	LEU	2.5
1	A	401	ILE	2.5
1	A	803	GLY	2.5
1	A	1285	LYS	2.3
1	A	150	THR	2.3
1	A	457	THR	2.3
1	A	345	VAL	2.3
1	A	121	ILE	2.3
1	A	447	HIS	2.2
1	A	124	ARG	2.2
1	A	157	ALA	2.1
1	A	664	GLY	2.1
1	A	875	ILE	2.1
1	A	1091	HIS	2.1
1	A	347	GLU	2.1
1	A	833	ARG	2.1
1	A	410	GLN	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 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^{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
7	EDO	A	1412	4/4	0.61	0.18	64,65,67,70	0
7	EDO	A	1407	4/4	0.81	0.18	36,47,51,60	0
7	EDO	B	106	4/4	0.82	0.19	58,61,62,63	0
7	EDO	A	1414	4/4	0.84	0.26	62,64,67,76	0
7	EDO	A	1404	4/4	0.88	0.28	28,43,48,60	0
5	NA	B	103	1/1	0.88	0.15	48,48,48,48	0
7	EDO	A	1408	4/4	0.88	0.19	60,60,61,62	0
7	EDO	A	1409	4/4	0.89	0.20	54,62,63,68	0
5	NA	C	101	1/1	0.91	0.21	51,51,51,51	0
7	EDO	B	104	4/4	0.92	0.22	47,50,52,54	0
7	EDO	A	1413	4/4	0.94	0.17	55,55,60,62	0
7	EDO	A	1410	4/4	0.94	0.28	42,53,58,61	0
7	EDO	A	1411	4/4	0.94	0.24	47,50,53,57	0
7	EDO	A	1406	4/4	0.94	0.19	47,51,52,60	0
7	EDO	A	1415	4/4	0.95	0.18	55,56,60,64	0
6	CL	A	1402	1/1	0.96	0.09	49,49,49,49	0
7	EDO	B	105	4/4	0.96	0.25	39,45,50,58	0
7	EDO	A	1405	4/4	0.96	0.14	45,46,47,49	0
5	NA	B	102	1/1	0.97	0.08	50,50,50,50	0
5	NA	B	101	1/1	0.97	0.21	47,47,47,47	0
7	EDO	A	1403	4/4	0.97	0.25	33,33,35,35	0
5	NA	A	1401	1/1	0.99	0.22	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.