Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 04:21 PM JST

PDB ID	:	5CZZ
Title	:	Crystal structure of Staphylococcus aureus Cas9 in complex with sgRNA and target DNA (TTGAAT PAM)
Authors	:	Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2015-08-01
Resolution	:	2.60 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:

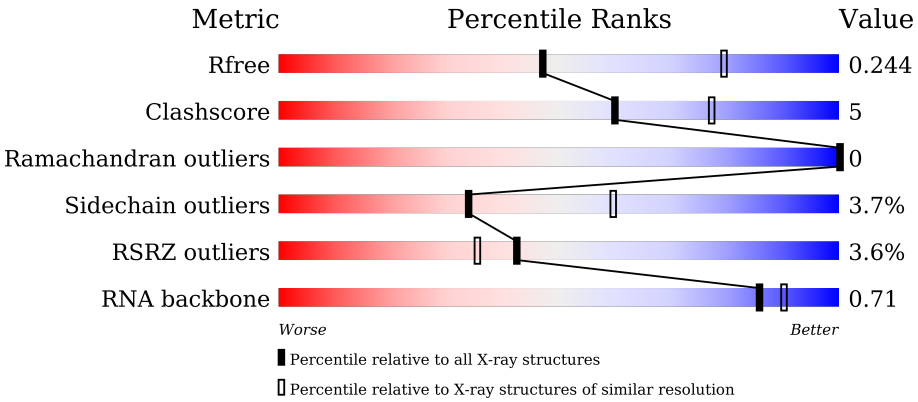
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	1056	4% 84% 13% ••
2	B	73	5% 74% 22% •
3	C	28	68% 32%
4	D	8	75% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10834 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	1043	Total	C	N	O	S	0	0	0
			8419	5344	1461	1600	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP J7RUA5
A	-1	SER	-	expression tag	UNP J7RUA5
A	0	HIS	-	expression tag	UNP J7RUA5
A	580	ALA	ASN	engineered mutation	UNP J7RUA5
A	946	ALA	CYS	engineered mutation	UNP J7RUA5

- Molecule 2 is a RNA chain called RNA (73-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	P	0	0	0
			1545	689	279	504	73			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	2	0
			603	290	109	175	29			

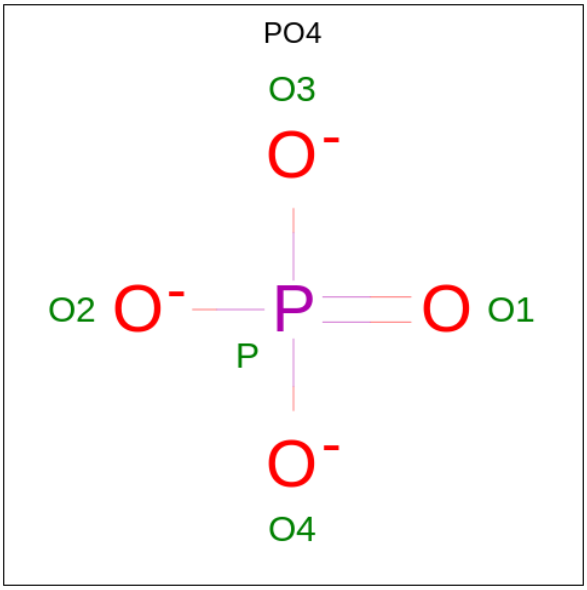
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*GP*AP*AP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			164	80	31	46	7			

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

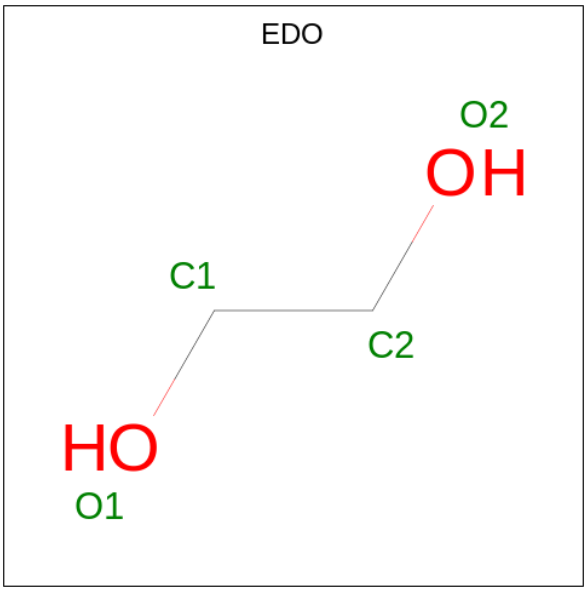
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Na 3 3	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O P 5 4 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	B	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

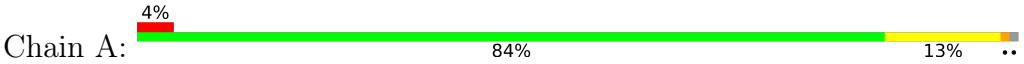
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	54	Total O 54 54	0	0
8	B	17	Total O 17 17	0	0
8	C	4	Total O 4 4	0	0
8	D	10	Total O 10 10	0	0

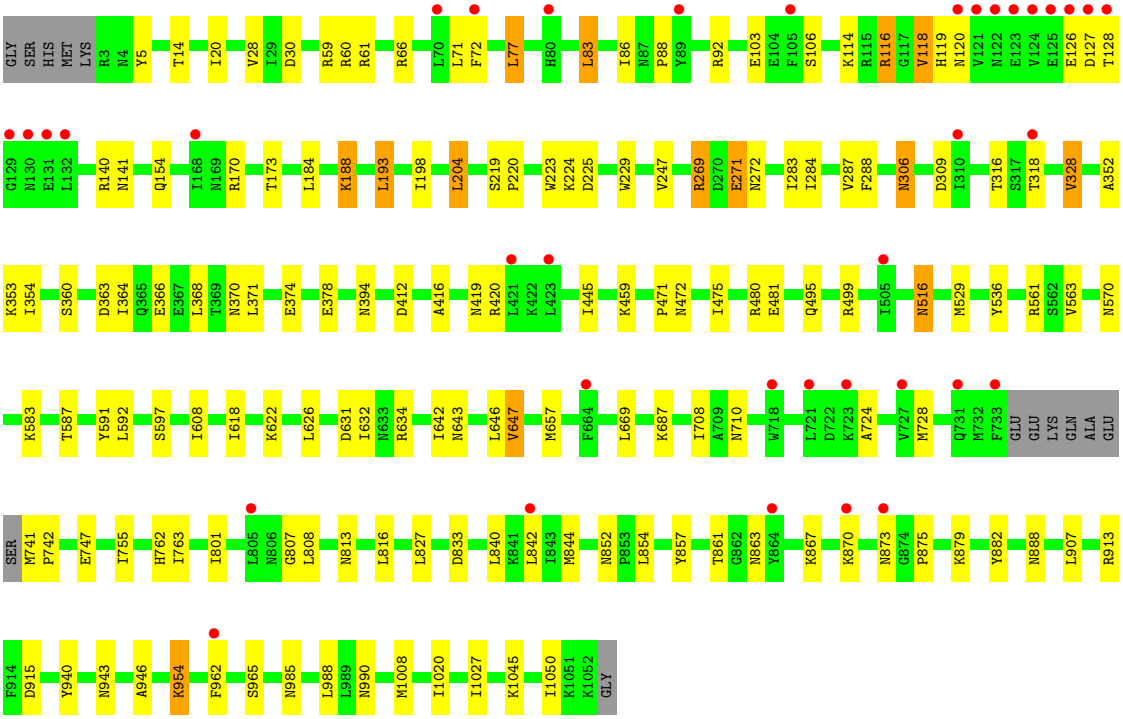
3 Residue-property plots (i)

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

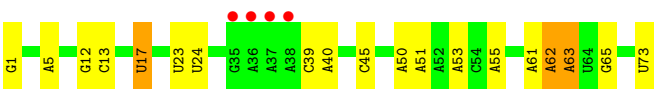
Chain A:





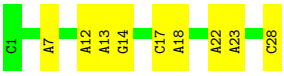
• Molecule 2: RNA (73-MER)

Chain B:



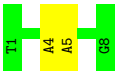
• Molecule 3: DNA (28-MER)

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	67.58Å 345.58Å 98.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.60 49.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.04-2.60) 99.3 (49.04-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.241 0.220 , 0.244	Depositor DCC
R_{free} test set	3512 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10834	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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, NA, PO4

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	0.21	0/8565	0.36	0/11562
2	B	0.29	1/1729 (0.1%)	0.67	0/2692
3	C	0.50	0/675	0.87	0/1037
4	D	0.53	0/184	1.02	0/283
All	All	0.26	1/11153 (0.0%)	0.49	0/15574

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-10.54	1.48	1.61

There are no bond angle outliers.

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	8419	0	8294	82	0
2	B	1545	0	773	11	0
3	C	603	0	339	7	0
4	D	164	0	93	2	0
5	A	3	0	0	0	0
5	B	1	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	B	5	0	0	0	0
7	B	4	0	6	0	0
7	D	4	0	6	0	0
8	A	54	0	0	0	0
8	B	17	0	0	0	0
8	C	4	0	0	0	0
8	D	10	0	0	0	0
All	All	10834	0	9511	93	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 5.

All (93) 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:269:ARG:HG3	1:A:271:GLU:HG2	1.68	0.75
1:A:861:THR:HG23	1:A:863:ASN:H	1.57	0.70
1:A:366:GLU:O	1:A:370:ASN:ND2	2.31	0.62
1:A:882:TYR:OH	3:C:7:DA:OP1	2.18	0.61
1:A:954:LYS:NZ	1:A:990:ASN:OD1	2.33	0.61
1:A:92:ARG:NH1	1:A:154:GLN:OE1	2.28	0.61
1:A:60:ARG:NH1	1:A:114:LYS:O	2.33	0.61
1:A:247:VAL:HG21	1:A:353:LYS:HA	1.84	0.60
1:A:867:LYS:NZ	2:B:45:C:O2	2.33	0.60
1:A:184:LEU:HD13	1:A:198:ILE:HG13	1.83	0.60
1:A:459:LYS:NZ	2:B:73:U:OP1	2.31	0.60
1:A:808:LEU:HD11	1:A:879:LYS:HA	1.84	0.60
2:B:62:A:H4'	2:B:63:A:O5'	2.02	0.59
1:A:643:ASN:HA	1:A:647:VAL:HG12	1.86	0.57
1:A:394:ASN:ND2	2:B:5:A:OP2	2.37	0.57
1:A:419:ASN:ND2	3:C:28:DC:O3'	2.38	0.57
1:A:66:ARG:HE	1:A:204:LEU:HD11	1.68	0.57
1:A:587:THR:HG23	1:A:632:ILE:HD11	1.87	0.56
1:A:807:GLY:O	1:A:813:ASN:ND2	2.35	0.56
1:A:269:ARG:NH1	1:A:272:ASN:O	2.35	0.55
1:A:360:SER:OG	1:A:363:ASP:OD2	2.25	0.55
3:C:12[A]:DA:H2'	3:C:13[A]:DA:H8	1.72	0.54
1:A:328:VAL:HG11	1:A:352:ALA:HB2	1.90	0.54
1:A:306:ASN:ND2	1:A:309:ASP:OD2	2.42	0.53
1:A:867:LYS:HB3	1:A:875:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:NH1	2:B:17:U:OP2	2.43	0.51
1:A:316:THR:HG23	1:A:318:THR:H	1.76	0.51
1:A:378:GLU:OE1	1:A:378:GLU:N	2.45	0.50
2:B:12:G:H2'	2:B:13:C:C6	2.47	0.50
1:A:224:LYS:NZ	1:A:225:ASP:OD2	2.42	0.50
1:A:412:ASP:OD2	1:A:420:ARG:NH2	2.42	0.50
1:A:840:LEU:HD11	1:A:854:LEU:HD21	1.94	0.50
1:A:28:VAL:HG12	1:A:762:HIS:HD2	1.76	0.49
1:A:128:THR:HB	1:A:140:ARG:HH21	1.76	0.49
1:A:5:TYR:CE2	1:A:471:PRO:HB3	2.48	0.49
1:A:915:ASP:HB3	1:A:962:PHE:HE1	1.77	0.49
1:A:72:PHE:HE1	1:A:77:LEU:HD12	1.77	0.49
1:A:631:ASP:HB3	1:A:634:ARG:HD3	1.95	0.49
1:A:985:ASN:ND2	4:D:4:DA:N7	2.57	0.48
1:A:360:SER:O	1:A:364:ILE:HG12	2.14	0.48
1:A:687:LYS:HB3	1:A:755:ILE:HG23	1.96	0.48
1:A:61:ARG:NH1	2:B:53:A:OP1	2.46	0.48
1:A:475:ILE:HG23	1:A:708:ILE:HG22	1.96	0.47
1:A:284:ILE:HA	1:A:288:PHE:HB2	1.96	0.47
1:A:642:ILE:HG23	1:A:646:LEU:HD23	1.96	0.47
1:A:188:LYS:HA	1:A:193:LEU:HD21	1.97	0.47
1:A:223:TRP:CD1	1:A:229:TRP:HB2	2.50	0.47
1:A:608:ILE:HD12	1:A:626:LEU:HD13	1.97	0.47
1:A:563:VAL:HG21	1:A:632:ILE:HG23	1.98	0.46
1:A:940:TYR:HB2	1:A:1050:ILE:HB	1.98	0.46
1:A:570:ASN:O	1:A:622:LYS:HG2	2.16	0.46
1:A:516:ASN:N	1:A:516:ASN:OD1	2.47	0.46
1:A:801:ILE:HD13	1:A:907:LEU:HD11	1.97	0.46
3:C:12[A]:DA:H2'	3:C:13[A]:DA:C8	2.51	0.45
3:C:13[B]:DA:H2'	3:C:14:DG:H8	1.81	0.45
1:A:591:TYR:O	1:A:597:SER:OG	2.35	0.45
1:A:219:SER:HA	1:A:220:PRO:HD3	1.88	0.45
2:B:23:U:H2'	2:B:24:U:C6	2.52	0.45
1:A:710:ASN:ND2	1:A:763:ILE:HD11	2.32	0.44
3:C:17:DC:H2'	3:C:18:DA:C8	2.53	0.44
1:A:71:LEU:HD13	1:A:106:SER:HB3	2.00	0.44
1:A:618:ILE:HG13	1:A:622:LYS:HD2	2.00	0.44
1:A:88:PRO:HG2	2:B:50:A:H4'	2.00	0.44
1:A:141:ASN:ND2	1:A:170:ARG:O	2.47	0.44
1:A:827:LEU:HD23	1:A:882:TYR:HB3	1.99	0.44
1:A:77:LEU:HD21	1:A:83:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:LEU:O	1:A:852:ASN:ND2	2.38	0.43
1:A:116:ARG:H	1:A:116:ARG:HG3	1.66	0.43
1:A:445:ILE:HD12	1:A:445:ILE:HA	1.89	0.43
1:A:561:ARG:NH2	1:A:747:GLU:OE1	2.50	0.43
1:A:913:ARG:HD2	1:A:965:SER:HB3	2.00	0.43
1:A:1045:LYS:HB2	1:A:1045:LYS:NZ	2.34	0.43
1:A:119:HIS:CE1	1:A:120:ASN:HD22	2.37	0.42
1:A:592:LEU:HA	1:A:597:SER:OG	2.20	0.42
1:A:857:TYR:O	1:A:861:THR:HG22	2.19	0.42
1:A:5:TYR:CD2	1:A:20:ILE:HG23	2.54	0.42
2:B:50:A:H2'	2:B:51:A:C8	2.54	0.42
1:A:833:ASP:OD2	1:A:867:LYS:NZ	2.38	0.42
1:A:412:ASP:HB3	1:A:416:ALA:HB3	2.01	0.42
1:A:536:TYR:OH	1:A:583:LYS:NZ	2.42	0.42
1:A:741:MET:HA	1:A:742:PRO:HD3	1.91	0.42
3:C:22:DA:H2'	3:C:23:DA:C8	2.55	0.42
1:A:86:ILE:H	1:A:86:ILE:HG13	1.54	0.42
1:A:118:VAL:O	1:A:173:THR:N	2.45	0.41
1:A:495:GLN:O	1:A:499:ARG:HG3	2.20	0.41
1:A:888:ASN:HD21	1:A:988:LEU:HD22	1.85	0.41
1:A:283:ILE:O	1:A:287:VAL:HG22	2.20	0.41
1:A:724:ALA:O	1:A:728:MET:HG3	2.20	0.41
1:A:354:ILE:HD12	1:A:368:LEU:HD23	2.03	0.41
4:D:4:DA:H1'	4:D:5:DA:C8	2.56	0.41
1:A:1020:ILE:HD12	1:A:1027:ILE:HD11	2.03	0.41
2:B:39:C:H2'	2:B:40:A:C8	2.55	0.41
1:A:943:ASN:HB3	1:A:946:ALA: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	1039/1056 (98%)	1007 (97%)	32 (3%)	0	100	100

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	901/972 (93%)	868 (96%)	33 (4%)	34	60

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	30	ASP
1	A	77	LEU
1	A	83	LEU
1	A	103	GLU
1	A	116	ARG
1	A	118	VAL
1	A	126	GLU
1	A	127	ASP
1	A	188	LYS
1	A	193	LEU
1	A	204	LEU
1	A	269	ARG
1	A	271	GLU
1	A	306	ASN
1	A	328	VAL
1	A	371	LEU
1	A	374	GLU
1	A	472	ASN
1	A	480	ARG
1	A	481	GLU
1	A	516	ASN
1	A	529	MET

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Mol	Chain	Res	Type
1	A	647	VAL
1	A	657	MET
1	A	669	LEU
1	A	816	LEU
1	A	842	LEU
1	A	844	MET
1	A	870	LYS
1	A	873	ASN
1	A	954	LYS
1	A	1008	MET

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	120	ASN
1	A	137	GLN
1	A	306	ASN
1	A	325	ASN
1	A	377	GLN
1	A	382	GLN
1	A	419	ASN
1	A	433	GLN
1	A	472	ASN
1	A	500	GLN
1	A	570	ASN
1	A	577	GLN
1	A	762	HIS
1	A	831	HIS
1	A	832	HIS
1	A	838	GLN
1	A	873	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	71/73 (97%)	6 (8%)	1 (1%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	17	U
2	B	55	A
2	B	61	A
2	B	62	A
2	B	63	A
2	B	65	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	62	A

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
6	PO4	B	102	-	4,4,4	0.92	0	6,6,6	0.43	0
7	EDO	B	103	-	3,3,3	0.44	0	2,2,2	0.33	0
7	EDO	D	101	-	3,3,3	0.46	0	2,2,2	0.34	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	B	103	-	-	0/1/1/1	-
7	EDO	D	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, 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	1043/1056 (98%)	0.23	37 (3%) 44 36	43, 90, 136, 172	0
2	B	73/73 (100%)	-0.11	4 (5%) 25 19	53, 84, 206, 243	0
3	C	28/28 (100%)	-0.33	0 100 100	53, 68, 99, 121	0
4	D	8/8 (100%)	-0.07	0 100 100	48, 50, 61, 62	0
All	All	1152/1165 (98%)	0.20	41 (3%) 42 35	43, 89, 138, 243	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ASN	9.2
1	A	123	GLU	5.5
2	B	36	A	5.3
1	A	124	VAL	5.3
1	A	733	PHE	4.3
1	A	130	ASN	4.2
1	A	125	GLU	4.1
1	A	72	PHE	3.9
1	A	126	GLU	3.9
1	A	723	LYS	3.8
1	A	129	GLY	3.8
1	A	127	ASP	3.6
2	B	38	A	3.4
1	A	128	THR	3.3
1	A	805	LEU	3.1
1	A	310	ILE	3.0
1	A	105	PHE	2.9
1	A	121	VAL	2.9
1	A	423	LEU	2.9
1	A	168	ILE	2.8
2	B	37	A	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	505	ILE	2.7
1	A	873	ASN	2.6
1	A	89	TYR	2.5
1	A	731	GLN	2.5
1	A	120	ASN	2.4
1	A	80	HIS	2.4
1	A	131	GLU	2.4
1	A	870	LYS	2.3
1	A	132	LEU	2.3
2	B	35	G	2.3
1	A	962	PHE	2.3
1	A	70	LEU	2.3
1	A	727	VAL	2.2
1	A	864	TYR	2.2
1	A	664	PHE	2.2
1	A	721	LEU	2.1
1	A	842	LEU	2.1
1	A	421	LEU	2.1
1	A	318	THR	2.1
1	A	718	TRP	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	B	103	4/4	0.80	0.49	100,101,102,102	0
6	PO4	B	102	5/5	0.87	0.22	149,149,150,151	0
5	NA	B	101	1/1	0.88	0.10	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	A	1103	1/1	0.90	0.14	86,86,86,86	0
5	NA	A	1102	1/1	0.90	0.23	88,88,88,88	0
7	EDO	D	101	4/4	0.93	0.27	66,67,68,70	0
5	NA	C	101	1/1	0.95	0.09	62,62,62,62	0
5	NA	A	1101	1/1	0.95	0.15	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.