Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 07:26 PM JST

PDB ID	:	5XUU
Title	:	Crystal structure of Lachnospiraceae bacterium ND2006 Cpf1 in complex with crRNA and target DNA (TCCA PAM)
Authors	:	Yamano, T.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2017-06-26
Resolution	:	2.50 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:

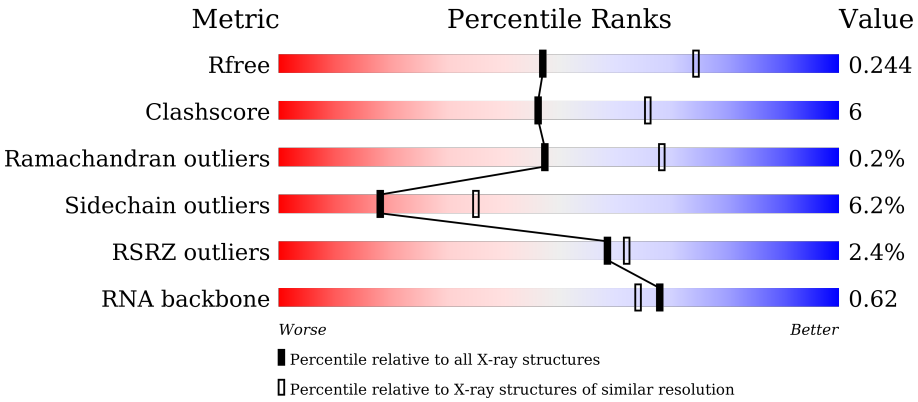
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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	1231	3% 79% 18%
2	B	40	70% 28%
3	C	29	72% 28%
4	D	9	78% 22%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11396 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 LbCpf1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1213	9749	6272	1581	1867	29	0	2	0

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	40	852	382	151	280	39	0	0	0

- Molecule 3 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	29	591	281	112	170	28	0	0	0

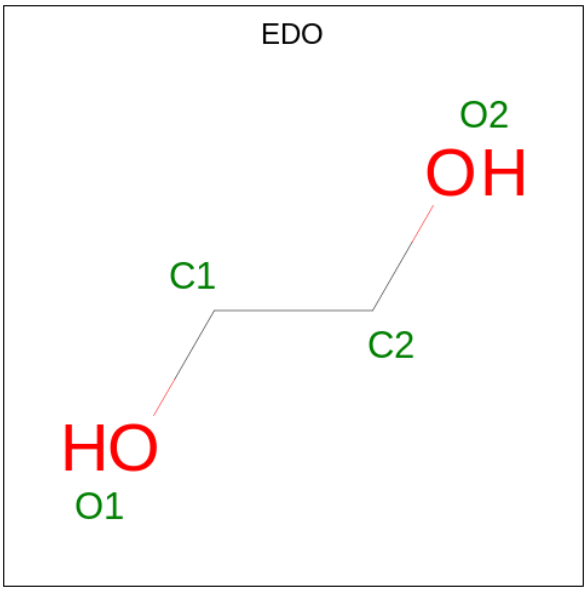
- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*TP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	9	175	85	29	53	8	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0

- Molecule 8 is water.

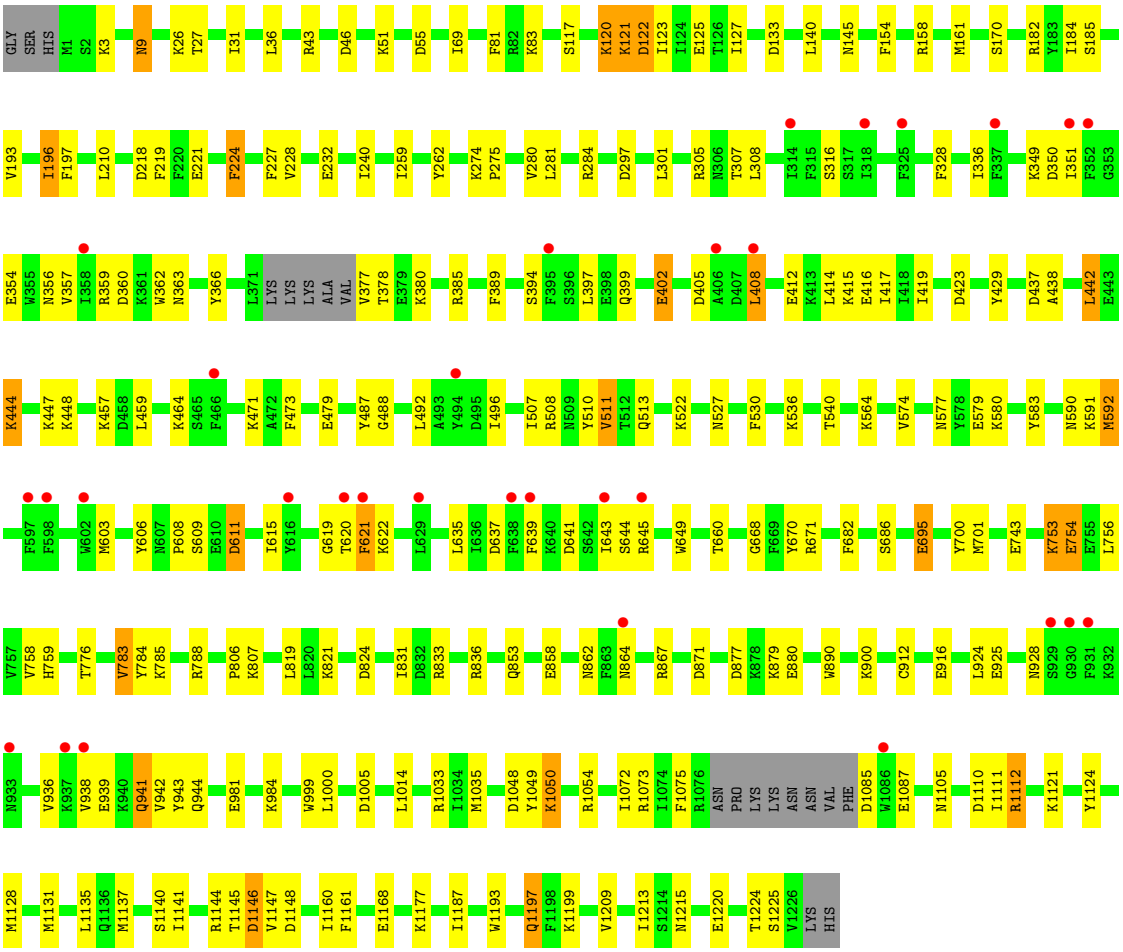
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	12	Total O 12 12	0	0
8	B	7	Total O 7 7	0	0

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.

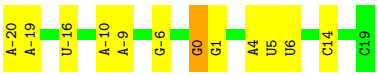
- Molecule 1: LbCpf1

Chain A:



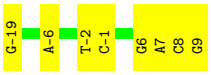
- Molecule 2: crRNA

Chain B:



• Molecule 3: DNA (29-MER)

Chain C:



• Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*CP*CP*A)-3')

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.95Å 101.95Å 372.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 2.50 49.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.17-2.50) 99.7 (49.17-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.193 , 0.244 0.193 , 0.244	Depositor DCC
R_{free} test set	3439 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	74.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11396	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, MG, 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	0.40	0/9963	0.54	0/13453
2	B	0.64	0/953	1.08	1/1484 (0.1%)
3	C	0.87	0/663	0.99	1/1021 (0.1%)
4	D	0.82	0/194	0.94	0/296
All	All	0.47	0/11773	0.65	2/16254 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	0	G	O4'-C1'-N9	6.12	113.09	108.20
3	C	-6	DA	O4'-C1'-N9	5.40	111.78	108.00

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	9749	0	9346	129	0
2	B	852	0	429	7	0
3	C	591	0	326	4	0
4	D	175	0	103	2	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	12	0	0
7	B	1	0	0	0	0
8	A	12	0	0	1	0
8	B	7	0	0	0	0
All	All	11396	0	10216	135	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 6.

All (135) 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:27:THR:HG21	1:A:701:MET:H	1.33	0.90
1:A:759:HIS:HB2	1:A:783:VAL:HG23	1.62	0.80
1:A:836:ARG:NH2	1:A:1141:ILE:O	2.19	0.75
1:A:359:ARG:O	1:A:363:ASN:ND2	2.20	0.75
1:A:785:LYS:HB2	2:B:-20:A:H5"	1.68	0.74
1:A:182:ARG:NH1	1:A:275:PRO:O	2.22	0.72
1:A:363:ASN:OD1	1:A:385:ARG:NH2	2.23	0.71
1:A:1073:ARG:NH1	1:A:1087:GLU:OE1	2.22	0.71
1:A:161:MET:HE3	1:A:280:VAL:HG12	1.73	0.69
1:A:615:ILE:O	1:A:619:GLY:N	2.26	0.68
1:A:639:PHE:O	1:A:643:ILE:HG12	1.94	0.68
1:A:125[B]:GLU:OE2	1:A:145:ASN:ND2	2.28	0.67
1:A:1005:ASP:HB2	1:A:1137:MET:HE1	1.78	0.65
1:A:880:GLU:HG3	1:A:939:GLU:HB2	1.80	0.64
1:A:603:MET:HG2	1:A:608:PRO:HD3	1.81	0.63
1:A:301:LEU:HD11	1:A:442:LEU:HD21	1.79	0.62
1:A:1146:ASP:OD1	1:A:1146:ASP:N	2.22	0.61
1:A:941:GLN:HG2	1:A:943:TYR:HD1	1.66	0.60
1:A:611:ASP:O	1:A:615:ILE:HG12	2.02	0.59
1:A:464:LYS:NZ	2:B:14:C:OP1	2.37	0.58
1:A:336:ILE:HB	1:A:397:LEU:HD22	1.86	0.58
1:A:621:PHE:HD1	1:A:622:LYS:N	2.00	0.57
1:A:1140:SER:HA	1:A:1147:VAL:HG12	1.85	0.57
1:A:51:LYS:HG2	1:A:154:PHE:CE1	2.40	0.56
1:A:536:LYS:HZ1	1:A:580:LYS:HE3	1.70	0.56
1:A:412:GLU:O	1:A:416:GLU:HG3	2.06	0.56
1:A:1141:ILE:HB	1:A:1144:ARG:HG3	1.88	0.56
3:C:-2:DT:H2'	3:C:-1:DC:C6	2.41	0.55
1:A:753:LYS:HD3	1:A:754:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LYS:NZ	1:A:580:LYS:HE3	2.21	0.55
1:A:27:THR:HG22	1:A:700:TYR:HA	1.88	0.55
1:A:218:ASP:HB3	1:A:224:PHE:CE1	2.43	0.54
1:A:447:LYS:HD3	1:A:513:GLN:HB2	1.89	0.54
3:C:8:DC:H2"	3:C:9:DG:C8	2.42	0.54
1:A:429:TYR:CE1	1:A:459:LEU:HD11	2.43	0.54
1:A:641:ASP:O	1:A:644:SER:OG	2.26	0.53
2:B:0:G:H1'	2:B:1:G:C8	2.44	0.53
1:A:196:ILE:HD11	1:A:262:TYR:CZ	2.45	0.52
1:A:46:ASP:HB3	1:A:140:LEU:HD11	1.92	0.52
1:A:1075:PHE:O	1:A:1085:ASP:N	2.43	0.52
1:A:193:VAL:HG11	1:A:259:ILE:HG12	1.93	0.51
1:A:999:TRP:CH2	1:A:1000:LEU:HD12	2.45	0.51
1:A:941:GLN:HG2	1:A:943:TYR:CD1	2.46	0.51
1:A:43:ARG:NH2	8:A:1402:HOH:O	2.43	0.51
1:A:123:ILE:HA	1:A:127:ILE:HB	1.92	0.50
1:A:26:LYS:HD2	1:A:695:GLU:OE1	2.12	0.50
1:A:579:GLU:HB3	1:A:682:PHE:HB3	1.93	0.50
1:A:429:TYR:CD1	1:A:459:LEU:HD11	2.47	0.49
1:A:1048:ASP:OD1	1:A:1050:LYS:HG2	2.11	0.49
1:A:457:LYS:HD2	1:A:890:TRP:CD2	2.47	0.49
1:A:366:TYR:CD1	1:A:385:ARG:HG3	2.47	0.49
1:A:1193:TRP:CG	1:A:1213:ILE:HD12	2.47	0.48
1:A:1124:TYR:O	1:A:1128:MET:HG2	2.13	0.48
1:A:1197:GLN:HB3	1:A:1209:VAL:HG11	1.94	0.48
1:A:121:LYS:HE3	4:D:-4:DT:H4'	1.94	0.48
1:A:1140:SER:HB3	1:A:1148:ASP:HA	1.95	0.48
1:A:405:ASP:O	1:A:408:LEU:N	2.45	0.48
1:A:1033:ARG:NH2	1:A:1035:MET:SD	2.87	0.48
1:A:210:LEU:HD21	1:A:240:ILE:HD11	1.96	0.47
1:A:356:ASN:ND2	1:A:360:ASP:OD2	2.46	0.47
1:A:121:LYS:HD3	1:A:125[B]:GLU:OE1	2.13	0.47
1:A:1072:ILE:HG21	1:A:1141:ILE:HD13	1.97	0.47
1:A:219:PHE:HE2	1:A:227:PHE:CD2	2.33	0.47
1:A:668:GLY:HA2	1:A:671:ARG:NH2	2.30	0.47
1:A:590:ASN:HB3	1:A:670:TYR:CD2	2.50	0.47
1:A:161:MET:HE1	1:A:281:LEU:HD22	1.96	0.47
1:A:784:TYR:O	2:B:-19:A:H5'	2.15	0.46
1:A:349:LYS:HE3	3:C:-19:DG:C8	2.51	0.46
1:A:788:ARG:HD2	2:B:-16:U:OP2	2.16	0.46
1:A:350:ASP:HB2	1:A:351:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ILE:HD11	1:A:414:LEU:HD23	1.98	0.46
1:A:444:LYS:HD2	1:A:448:LYS:O	2.16	0.46
1:A:912:CYS:O	1:A:916:GLU:HG3	2.15	0.46
1:A:27:THR:HG21	1:A:701:MET:N	2.14	0.45
1:A:758:VAL:HG22	1:A:784:TYR:CD2	2.51	0.45
1:A:591:LYS:HD3	4:D:-1:DA:H1'	1.98	0.45
1:A:1110:ASP:OD2	1:A:1112:ARG:NH1	2.48	0.45
1:A:1220:GLU:O	1:A:1224:THR:OG1	2.28	0.45
1:A:307:THR:O	1:A:308:LEU:HD12	2.17	0.45
1:A:754:GLU:H	1:A:754:GLU:HG3	1.40	0.45
1:A:55:ASP:CG	1:A:158:ARG:HH21	2.20	0.45
1:A:1160:ILE:HD12	1:A:1161:PHE:H	1.82	0.45
1:A:414:LEU:HD13	1:A:473:PHE:HE2	1.82	0.45
1:A:362:TRP:CZ3	1:A:389:PHE:HB2	2.52	0.45
1:A:522:LYS:HE3	1:A:743:GLU:HG2	1.98	0.45
1:A:862:ASN:ND2	1:A:867:ARG:HG3	2.32	0.44
1:A:925:GLU:HG3	1:A:1187:ILE:HD11	1.98	0.44
1:A:1050:LYS:HG2	1:A:1050:LYS:H	1.61	0.44
1:A:508:ARG:HG3	1:A:890:TRP:CE2	2.52	0.44
1:A:3:LYS:HD2	1:A:819:LEU:HB3	1.99	0.44
1:A:399:GLN:O	1:A:402:GLU:HB3	2.18	0.44
1:A:122:ASP:OD1	1:A:122:ASP:N	2.48	0.44
1:A:354:GLU:HB2	1:A:357:VAL:HG23	1.99	0.44
1:A:936:VAL:HG22	1:A:941:GLN:NE2	2.33	0.44
1:A:488:GLY:O	1:A:492:LEU:HD13	2.18	0.43
1:A:637:ASP:OD1	1:A:660:THR:HG21	2.18	0.43
1:A:377:VAL:O	1:A:380:LYS:HG2	2.18	0.43
1:A:821:LYS:O	1:A:1199:LYS:NZ	2.49	0.43
1:A:831:ILE:HB	1:A:924:LEU:HD23	2.01	0.43
2:B:4:A:H2'	2:B:5:U:O4'	2.19	0.43
1:A:9:ASN:ND2	1:A:806:PRO:HA	2.34	0.43
1:A:117:SER:HA	1:A:120:LYS:HG3	2.01	0.43
1:A:507:ILE:O	1:A:511:VAL:HB	2.19	0.43
1:A:928:ASN:ND2	1:A:928:ASN:H	2.16	0.43
1:A:1014:LEU:HD12	1:A:1135:LEU:HD11	2.01	0.43
1:A:31:ILE:HG12	1:A:36:LEU:HD12	2.00	0.43
1:A:527:ASN:HB3	1:A:530:PHE:HB2	2.01	0.43
1:A:858:GLU:HG2	1:A:871:ASP:HA	2.00	0.43
1:A:756:LEU:O	1:A:758:VAL:HG23	2.19	0.43
1:A:1197:GLN:HB3	1:A:1209:VAL:CG1	2.49	0.43
2:B:5:U:H2'	2:B:6:U:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:PHE:HD2	1:A:635:LEU:CD2	2.32	0.42
1:A:305:ARG:NH1	1:A:437:ASP:O	2.52	0.42
1:A:1131:MET:HE3	1:A:1131:MET:HB2	1.92	0.42
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.76	0.42
1:A:807:LYS:HA	1:A:807:LYS:HD3	1.77	0.42
1:A:81:PHE:CD1	1:A:184:ILE:HG21	2.55	0.42
1:A:756:LEU:HD23	1:A:756:LEU:HA	1.89	0.42
1:A:900:LYS:NZ	1:A:941:GLN:O	2.29	0.41
1:A:938:VAL:O	1:A:941:GLN:HB2	2.20	0.41
1:A:196:ILE:HG22	1:A:197:PHE:CD1	2.54	0.41
1:A:415:LYS:O	1:A:419:ILE:HG12	2.21	0.41
1:A:479:GLU:N	1:A:479:GLU:OE1	2.53	0.41
1:A:437:ASP:OD1	1:A:438:ALA:N	2.54	0.41
1:A:577:ASN:OD1	1:A:686:SER:HA	2.20	0.41
1:A:853:GLN:OE1	1:A:1177:LYS:HG3	2.21	0.41
3:C:6:DG:H2"	3:C:7:DA:C8	2.55	0.41
1:A:925:GLU:HG3	1:A:1187:ILE:CD1	2.50	0.41
1:A:297:ASP:OD1	1:A:510:TYR:OH	2.29	0.41
1:A:363:ASN:H	1:A:363:ASN:HD22	1.69	0.41
1:A:641:ASP:CG	1:A:645:ARG:HH21	2.25	0.41
1:A:1144:ARG:HH21	1:A:1146:ASP:CG	2.25	0.41
1:A:592:MET:HE3	1:A:649:TRP:CZ2	2.57	0.40
1:A:471:LYS:O	1:A:471:LYS:HG2	2.21	0.40
1:A:999:TRP:CH2	1:A:1215:ASN:HB3	2.56	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	1209/1231 (98%)	1160 (96%)	47 (4%)	2 (0%)	47 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	984	LYS
1	A	574	VAL

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	1031/1117 (92%)	967 (94%)	64 (6%)	18 35

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	69	ILE
1	A	83	LYS
1	A	120	LYS
1	A	121	LYS
1	A	122	ASP
1	A	133	ASP
1	A	170	SER
1	A	185	SER
1	A	196	ILE
1	A	221	GLU
1	A	224	PHE
1	A	228	VAL
1	A	232	GLU
1	A	274	LYS
1	A	284	ARG
1	A	316	SER
1	A	328	PHE
1	A	378	THR
1	A	394	SER
1	A	402	GLU
1	A	408	LEU
1	A	417	ILE

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Mol	Chain	Res	Type
1	A	423	ASP
1	A	442	LEU
1	A	444	LYS
1	A	487	TYR
1	A	496	ILE
1	A	511	VAL
1	A	540	THR
1	A	564	LYS
1	A	583	TYR
1	A	592	MET
1	A	606	TYR
1	A	609	SER
1	A	611	ASP
1	A	620	THR
1	A	621	PHE
1	A	695	GLU
1	A	753	LYS
1	A	754	GLU
1	A	776	THR
1	A	783	VAL
1	A	824	ASP
1	A	833	ARG
1	A	864	ASN
1	A	877	ASP
1	A	879	LYS
1	A	941	GLN
1	A	942	VAL
1	A	944	GLN
1	A	981	GLU
1	A	1049	TYR
1	A	1050	LYS
1	A	1054	ARG
1	A	1105	ASN
1	A	1111	ILE
1	A	1112	ARG
1	A	1121	LYS
1	A	1145	THR
1	A	1146	ASP
1	A	1168	GLU
1	A	1197	GLN
1	A	1225	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	33	ASN
1	A	268	GLN
1	A	370	HIS
1	A	529	GLN
1	A	703	GLN
1	A	862	ASN
1	A	928	ASN
1	A	1070	ASN
1	A	1100	ASN
1	A	1105	ASN
1	A	1170	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	39/40 (97%)	3 (7%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-10	A
2	B	-9	A
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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	EDO	A	1303	-	3,3,3	0.37	0	2,2,2	0.69	0
6	EDO	A	1302	-	3,3,3	0.43	0	2,2,2	0.47	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
6	EDO	A	1303	-	-	0/1/1/1	-
6	EDO	A	1302	-	-	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	1213/1231 (98%)	0.15	31 (2%) 56 59	53, 84, 134, 176	0
2	B	40/40 (100%)	-0.02	0 100 100	60, 72, 97, 116	0
3	C	29/29 (100%)	-0.06	0 100 100	62, 77, 140, 156	0
4	D	9/9 (100%)	-0.12	0 100 100	83, 92, 147, 167	0
All	All	1291/1309 (98%)	0.14	31 (2%) 59 62	53, 83, 134, 176	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	930	GLY	4.5
1	A	408	LEU	4.5
1	A	620	THR	4.4
1	A	929	SER	4.1
1	A	314	ILE	4.1
1	A	325	PHE	3.4
1	A	621	PHE	3.3
1	A	602	TRP	3.2
1	A	638	PHE	3.1
1	A	395	PHE	3.1
1	A	351	ILE	3.0
1	A	406	ALA	3.0
1	A	352	PHE	3.0
1	A	931	PHE	3.0
1	A	337	PHE	2.9
1	A	318	ILE	2.9
1	A	937	LYS	2.8
1	A	643	ILE	2.8
1	A	938	VAL	2.6
1	A	598	PHE	2.6
1	A	466	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	645	ARG	2.3
1	A	933	ASN	2.3
1	A	494	TYR	2.2
1	A	639	PHE	2.2
1	A	616	TYR	2.1
1	A	597	PHE	2.1
1	A	1086	TRP	2.1
1	A	358	ILE	2.1
1	A	629	LEU	2.0
1	A	864	ASN	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
6	EDO	A	1303	4/4	0.88	0.31	77,78,82,85	0
7	NA	B	101	1/1	0.92	0.47	94,94,94,94	0
6	EDO	A	1302	4/4	0.94	0.20	72,73,74,75	0
5	MG	A	1301	1/1	0.98	0.27	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.