Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 07:25 PM JST

PDB ID	:	5XUT
Title	:	Crystal structure of Lachnospiraceae bacterium ND2006 Cpf1 in complex with crRNA and target DNA (TCTA PAM)
Authors	:	Yamano, T.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2017-06-26
Resolution	:	2.40 Å(reported)

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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.238
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		6.6%
RSRZ outliers		2.2%
RNA backbone		0.61

Worse ... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
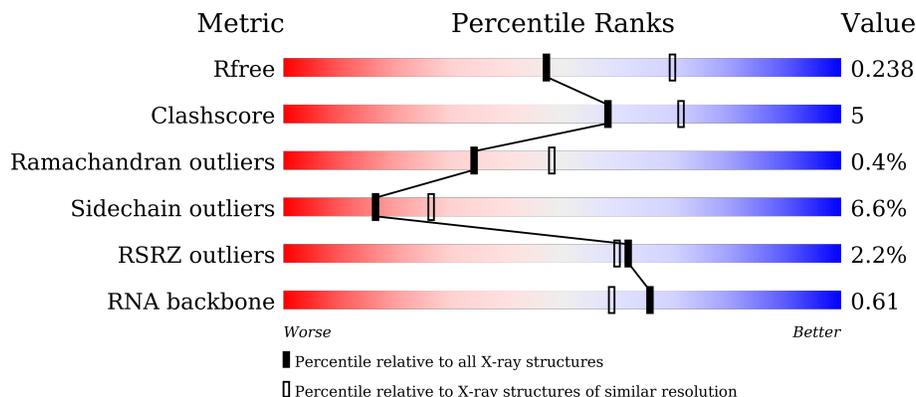
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	2% / 82% / 15% / ••
2	B	40	65% / 30% / 5%
3	C	29	59% / 41%
4	D	9	89% / 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NA	B	101	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 11467 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
1	A	1217	Total	C	N	O	S	0	1	0
			9794	6309	1590	1866	29			

- 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
			852	382	151	280	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	29	Total	C	N	O	P	0	0	0
			590	281	112	169	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total	C	N	O	P	0	0	0
			176	86	28	54	8			

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

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

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

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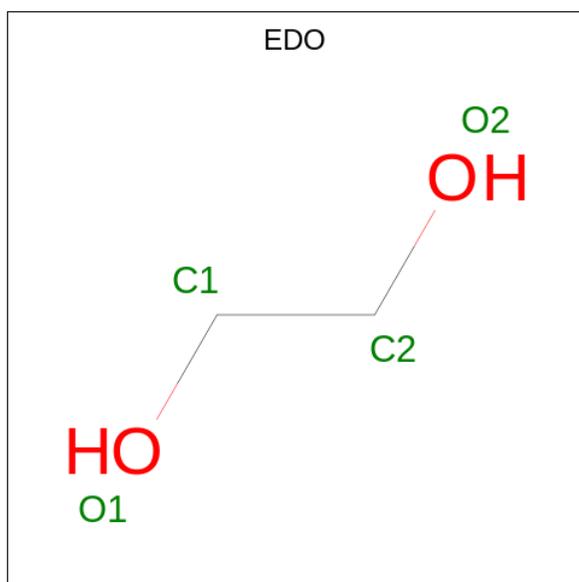
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0

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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	34	Total 34	O 34	0	0
8	B	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

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


• Molecule 2: crRNA

• Molecule 3: DNA (29-MER)

G-19 A-16 A-15 A-6 A-5 T-4 T-3 T-2 C-1 C0 T1 G6 A7 C8 G9
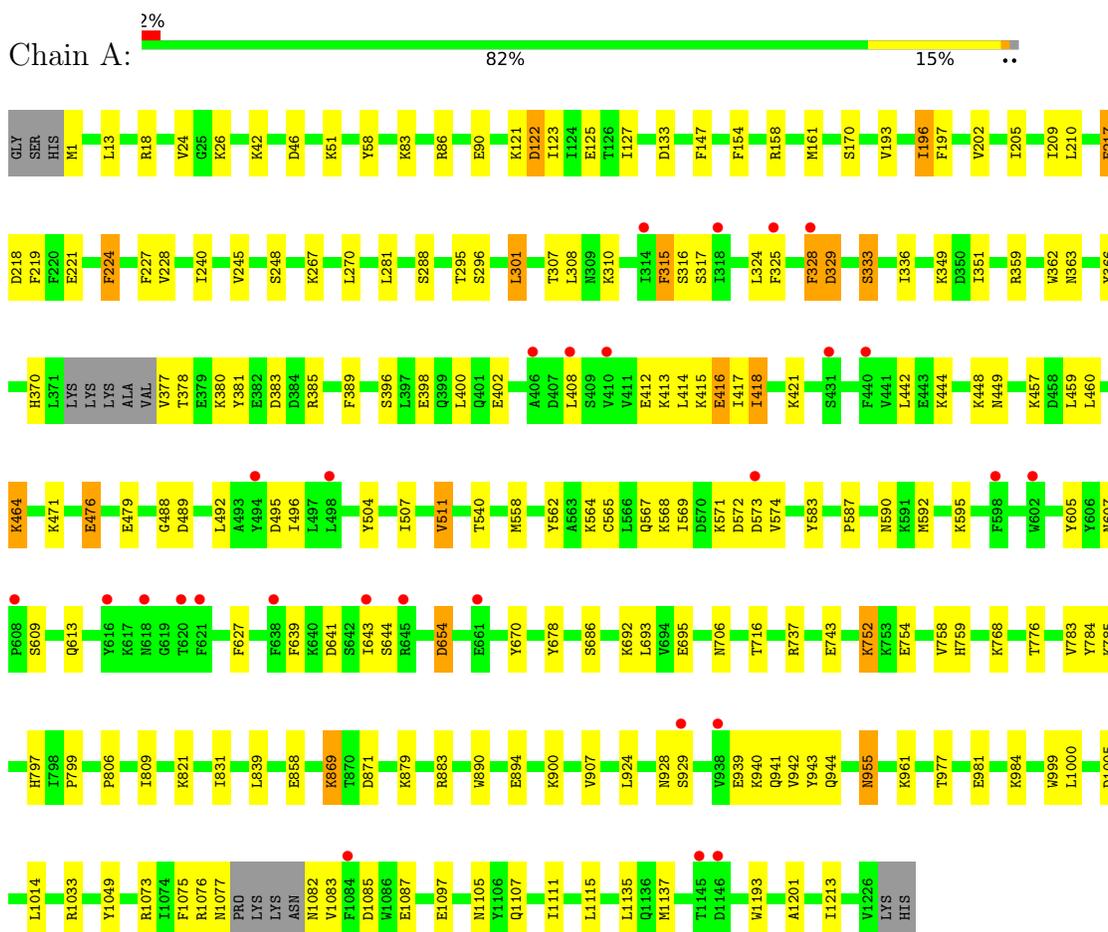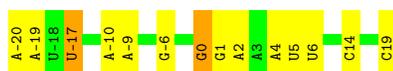
• Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*CP*TP*A)-3')

Chain D:

89%   11%

C-9 C-3 T-2 A-1

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.45Å 102.45Å 373.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.40 49.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.40-2.40) 95.4 (49.40-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.193 , 0.238 0.193 , 0.238	Depositor DCC
R_{free} test set	3781 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.0	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	11467	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NA, MG, EDO

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	0/10007	0.53	0/13504
2	B	0.69	0/953	1.12	2/1484 (0.1%)
3	C	0.88	1/662 (0.2%)	0.99	2/1019 (0.2%)
4	D	0.78	0/195	1.00	0/298
All	All	0.48	1/11817 (0.0%)	0.65	4/16305 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	-4	DT	C3'-O3'	-5.00	1.37	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	0	G	O4'-C1'-N9	7.66	114.33	108.20
3	C	-6	DA	O4'-C1'-N9	6.66	112.66	108.00
3	C	1	DT	O5'-P-OP1	-6.29	100.04	105.70
2	B	2	A	C5-C6-N6	5.34	127.97	123.70

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	9794	0	9435	97	0
2	B	852	0	429	7	0
3	C	590	0	326	5	0
4	D	176	0	104	1	0
5	A	1	0	0	0	0
6	A	4	0	6	0	0
6	B	4	0	6	2	0
7	B	1	0	0	0	0
8	A	34	0	0	0	0
8	B	11	0	0	0	0
All	All	11467	0	10306	104	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 (104) 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:333:SER:HB3	1:A:398:GLU:HB2	1.67	0.76
1:A:1073:ARG:NH1	1:A:1087:GLU:OE1	2.23	0.71
1:A:941:GLN:HG2	1:A:943:TYR:HD1	1.57	0.70
1:A:193:VAL:O	1:A:196:ILE:HG22	1.93	0.68
1:A:716:THR:OG1	1:A:961:LYS:NZ	2.19	0.67
1:A:1005:ASP:HB2	1:A:1137:MET:HE1	1.77	0.66
1:A:351:ILE:HD11	1:A:414:LEU:HD23	1.79	0.65
1:A:569:ILE:HD11	1:A:693:LEU:HD11	1.78	0.65
1:A:799:PRO:HG3	6:B:102:EDO:H21	1.81	0.63
1:A:759:HIS:HB2	1:A:783:VAL:HG23	1.82	0.61
1:A:572:ASP:HB2	1:A:686:SER:HB2	1.83	0.60
1:A:785:LYS:HB2	2:B:-20:A:H5"	1.83	0.60
1:A:941:GLN:HG2	1:A:943:TYR:CD1	2.37	0.59
1:A:161:MET:HE1	1:A:281:LEU:HB2	1.83	0.59
1:A:639:PHE:O	1:A:643:ILE:HG12	2.03	0.59
1:A:349:LYS:HE3	3:C:-19:DG:C8	2.39	0.58
1:A:743:GLU:OE1	6:B:102:EDO:O1	2.16	0.57
1:A:377:VAL:HB	1:A:380:LYS:HE2	1.88	0.56
1:A:325:PHE:CD2	1:A:418:ILE:HD12	2.39	0.56
1:A:1193:TRP:CG	1:A:1213:ILE:HD12	2.41	0.56
3:C:8:DC:H2"	3:C:9:DG:C8	2.42	0.54
1:A:362:TRP:CZ3	1:A:389:PHE:HB2	2.43	0.54
1:A:641:ASP:O	1:A:644:SER:OG	2.27	0.53
2:B:0:G:H1'	2:B:1:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:PRO:HD2	1:A:592:MET:CE	2.39	0.52
1:A:363:ASN:OD1	1:A:385:ARG:HD3	2.09	0.52
1:A:219:PHE:HE2	1:A:227:PHE:CD2	2.28	0.51
1:A:562:TYR:HB3	1:A:565:CYS:HB3	1.92	0.51
1:A:1075:PHE:O	1:A:1085:ASP:N	2.40	0.51
1:A:464:LYS:NZ	2:B:14:C:OP1	2.44	0.50
1:A:218:ASP:HB3	1:A:224:PHE:CE1	2.47	0.49
1:A:858:GLU:OE1	1:A:869:LYS:HD3	2.12	0.49
1:A:609:SER:O	1:A:613:GLN:N	2.42	0.49
1:A:366:TYR:CZ	1:A:370:HIS:CD2	3.00	0.49
1:A:123:ILE:HA	1:A:127:ILE:HB	1.95	0.49
1:A:413:LYS:O	1:A:417:ILE:HG12	2.13	0.48
1:A:821:LYS:HE3	1:A:1201:ALA:O	2.13	0.48
1:A:784:TYR:O	2:B:-19:A:H5'	2.14	0.48
1:A:301:LEU:HD11	1:A:442:LEU:HD11	1.96	0.48
1:A:1014:LEU:HD12	1:A:1135:LEU:HD11	1.96	0.48
1:A:193:VAL:HG12	1:A:270:LEU:HD23	1.96	0.48
1:A:328:PHE:HB2	1:A:415:LYS:HE2	1.95	0.48
1:A:488:GLY:O	1:A:492:LEU:HD13	2.14	0.48
1:A:366:TYR:CD1	1:A:385:ARG:HG3	2.49	0.48
1:A:507:ILE:O	1:A:511:VAL:HB	2.15	0.47
1:A:564:LYS:O	1:A:567:GLN:HG2	2.14	0.47
1:A:51:LYS:HG2	1:A:154:PHE:CE1	2.49	0.47
1:A:831:ILE:HB	1:A:924:LEU:HD23	1.97	0.47
1:A:444:LYS:HB3	1:A:449:ASN:HB2	1.98	0.46
1:A:758:VAL:HG22	1:A:784:TYR:CD2	2.50	0.46
1:A:121:LYS:HD2	1:A:125:GLU:OE1	2.15	0.46
2:B:4:A:H2'	2:B:5:U:O4'	2.16	0.46
1:A:307:THR:O	1:A:308:LEU:HD12	2.16	0.45
1:A:412:GLU:O	1:A:416:GLU:HG2	2.16	0.45
1:A:210:LEU:HD21	1:A:240:ILE:HD11	1.97	0.45
1:A:471:LYS:HG2	1:A:471:LYS:O	2.15	0.45
1:A:329:ASP:N	1:A:329:ASP:OD1	2.50	0.45
1:A:58:TYR:CE2	1:A:158:ARG:HG3	2.52	0.45
1:A:205:ILE:HG23	1:A:209:ILE:HD12	1.99	0.45
1:A:457:LYS:HD2	1:A:890:TRP:CD2	2.52	0.44
1:A:900:LYS:NZ	1:A:941:GLN:O	2.33	0.44
1:A:678:TYR:CE2	1:A:737:ARG:HG2	2.52	0.44
1:A:366:TYR:CE1	1:A:370:HIS:HD2	2.36	0.44
1:A:42:LYS:HE2	1:A:46:ASP:OD2	2.18	0.44
1:A:839:LEU:HD13	1:A:907:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HA	1:A:90:GLU:OE1	2.17	0.44
1:A:444:LYS:HD2	1:A:448:LYS:O	2.17	0.44
3:C:-16:DA:H2'	3:C:-15:DA:C8	2.53	0.44
1:A:122:ASP:OD1	1:A:122:ASP:N	2.51	0.43
2:B:5:U:H2'	2:B:6:U:O4'	2.19	0.43
1:A:706:ASN:HB2	2:B:-17:U:OP1	2.19	0.43
1:A:196:ILE:HG23	1:A:197:PHE:CD1	2.53	0.43
1:A:1077:ASN:C	1:A:1082:ASN:HA	2.39	0.43
1:A:26:LYS:HE2	1:A:695:GLU:O	2.18	0.43
1:A:217:GLU:H	1:A:217:GLU:HG3	1.41	0.43
1:A:571:LYS:HE2	1:A:573:ASP:HA	2.01	0.43
3:C:6:DG:H2"	3:C:7:DA:C8	2.54	0.43
1:A:245:VAL:HB	1:A:288:SER:HB3	2.00	0.43
1:A:564:LYS:HD2	1:A:567:GLN:NE2	2.33	0.43
1:A:1076:ARG:HA	1:A:1083:VAL:O	2.19	0.42
1:A:13:LEU:HD23	1:A:13:LEU:N	2.34	0.42
1:A:752:LYS:H	1:A:752:LYS:HG2	1.55	0.42
1:A:219:PHE:HE2	1:A:227:PHE:CE2	2.37	0.42
1:A:752:LYS:HE3	1:A:752:LYS:HB3	1.86	0.42
1:A:806:PRO:HG2	1:A:809:ILE:HD11	2.02	0.42
1:A:121:LYS:HG2	4:D:-3:DC:OP1	2.20	0.42
1:A:759:HIS:HB2	1:A:783:VAL:CG2	2.48	0.42
1:A:366:TYR:CE1	1:A:370:HIS:CD2	3.08	0.42
1:A:999:TRP:CH2	1:A:1000:LEU:HD12	2.55	0.42
3:C:-2:DT:H2'	3:C:-1:DC:C6	2.55	0.42
1:A:858:GLU:HG2	1:A:871:ASP:HA	2.01	0.41
1:A:460:LEU:HB3	1:A:504:TYR:CD1	2.54	0.41
1:A:18:ARG:HG2	1:A:797:HIS:CD2	2.55	0.41
1:A:476:GLU:O	1:A:476:GLU:HG3	2.20	0.41
1:A:590:ASN:HB3	1:A:670:TYR:CD2	2.56	0.41
1:A:83:LYS:HE2	1:A:83:LYS:HB3	1.92	0.41
1:A:460:LEU:HB3	1:A:504:TYR:HD1	1.86	0.41
1:A:590:ASN:HA	1:A:670:TYR:CZ	2.56	0.41
1:A:928:ASN:ND2	1:A:928:ASN:H	2.19	0.41
1:A:955:ASN:ND2	1:A:977:THR:OG1	2.53	0.40
1:A:310:LYS:HA	1:A:315:PHE:CD2	2.56	0.40
1:A:336:ILE:O	1:A:396:SER:HA	2.21	0.40
1:A:1111:ILE:O	1:A:1115:LEU:HG	2.22	0.40
1:A:883:ARG:NH1	1:A:939:GLU:OE1	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1212/1231 (98%)	1159 (96%)	48 (4%)	5 (0%)	34	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	TYR
1	A	381	TYR
1	A	984	LYS
1	A	654	ASP
1	A	574	VAL

5.3.2 Protein sidechains ⓘ

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	1038/1117 (93%)	970 (93%)	68 (7%)	16	26

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	VAL
1	A	122	ASP
1	A	133	ASP
1	A	147	PHE
1	A	170	SER

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Mol	Chain	Res	Type
1	A	196	ILE
1	A	202	VAL
1	A	217	GLU
1	A	221	GLU
1	A	224	PHE
1	A	228	VAL
1	A	248	SER
1	A	267	LYS
1	A	295	THR
1	A	296	SER
1	A	301	LEU
1	A	315	PHE
1	A	316	SER
1	A	317	SER
1	A	324	LEU
1	A	328	PHE
1	A	329	ASP
1	A	333	SER
1	A	359	ARG
1	A	378	THR
1	A	383	ASP
1	A	400	LEU
1	A	402	GLU
1	A	408	LEU
1	A	416	GLU
1	A	418	ILE
1	A	421	LYS
1	A	459	LEU
1	A	464	LYS
1	A	476	GLU
1	A	479	GLU
1	A	489	ASP
1	A	495	ASP
1	A	496	ILE
1	A	511	VAL
1	A	540	THR
1	A	558	MET
1	A	568	LYS
1	A	583	TYR
1	A	595	LYS
1	A	607	ASN
1	A	627	PHE

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Mol	Chain	Res	Type
1	A	654	ASP
1	A	692	LYS
1	A	752	LYS
1	A	754	GLU
1	A	768	LYS
1	A	776	THR
1	A	869	LYS
1	A	879	LYS
1	A	894	GLU
1	A	929	SER
1	A	940	LYS
1	A	942	VAL
1	A	944	GLN
1	A	955	ASN
1	A	981	GLU
1	A	1033	ARG
1	A	1049	TYR
1	A	1097	GLU
1	A	1105	ASN
1	A	1107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	91	ASN
1	A	145	ASN
1	A	268	GLN
1	A	370	HIS
1	A	567	GLN
1	A	607	ASN
1	A	703	GLN
1	A	889	ASN
1	A	928	ASN
1	A	941	GLN
1	A	1070	ASN
1	A	1100	ASN
1	A	1105	ASN
1	A	1170	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	39/40 (97%)	5 (12%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-17	U
2	B	-10	A
2	B	-9	A
2	B	-6	G
2	B	19	C

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	1302	-	3,3,3	0.39	0	2,2,2	0.50	0
6	EDO	B	102	-	3,3,3	0.45	0	2,2,2	0.42	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	1302	-	-	0/1/1/1	-
6	EDO	B	102	-	-	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	102	EDO	2	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, 95th 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(Å²)	Q<0.9
1	A	1217/1231 (98%)	-0.12	28 (2%)	60	58	47, 76, 130, 168	0
2	B	40/40 (100%)	-0.34	0	100	100	51, 65, 86, 105	0
3	C	29/29 (100%)	-0.34	0	100	100	57, 70, 132, 143	0
4	D	9/9 (100%)	-0.35	0	100	100	76, 96, 129, 145	0
All	All	1295/1309 (98%)	-0.14	28 (2%)	62	60	47, 75, 130, 168	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	ILE	3.9
1	A	645	ARG	3.9
1	A	620	THR	3.8
1	A	1146	ASP	3.5
1	A	408	LEU	3.4
1	A	938	VAL	3.4
1	A	616	TYR	3.3
1	A	618	ASN	3.2
1	A	314	ILE	3.1
1	A	621	PHE	3.1
1	A	929	SER	3.0
1	A	602	TRP	2.8
1	A	661	GLU	2.8
1	A	1145	THR	2.6
1	A	573	ASP	2.6
1	A	638	PHE	2.6
1	A	440	PHE	2.5
1	A	608	PRO	2.5
1	A	598	PHE	2.5
1	A	406	ALA	2.5
1	A	643	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	494	TYR	2.2
1	A	325	PHE	2.2
1	A	498	LEU	2.1
1	A	410	VAL	2.1
1	A	431	SER	2.0
1	A	328	PHE	2.0
1	A	1084	PHE	2.0

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, 95th 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(Å²)	Q<0.9
7	NA	B	101	1/1	0.55	0.75	115,115,115,115	0
6	EDO	B	102	4/4	0.94	0.23	62,67,68,70	0
6	EDO	A	1302	4/4	0.96	0.20	62,65,68,69	0
5	MG	A	1301	1/1	0.99	0.18	40,40,40,40	0

6.5   Other polymers ⓘ

There are no such residues in this entry.

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