



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 5XUS / pdb_00005xus
Title : Crystal structure of Lachnospiraceae bacterium ND2006 Cpf1 in complex with crRNA and target DNA (TTTA 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

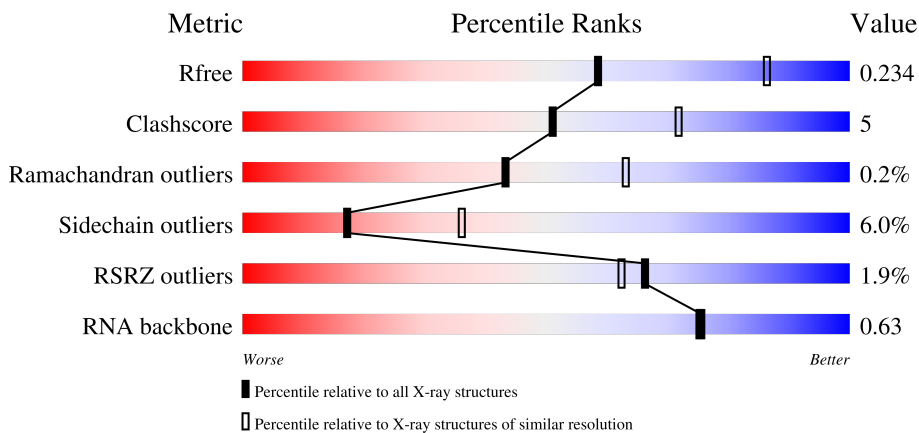
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

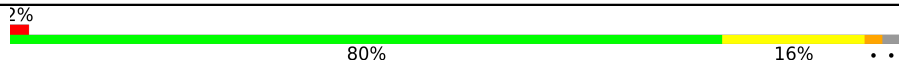



The reported resolution of this entry is 2.50 Å.

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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 $\leq 5\%$. 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	1231	 2% 80% 16%
2	B	40	 72% 25%
3	C	29	 86% 14%
4	D	9	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11542 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	1206	9776	6291	1593	1863	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	589	281	112	168	28	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	9	177	87	27	55	8	0	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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 (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	3	Total Na 3 3	0	0

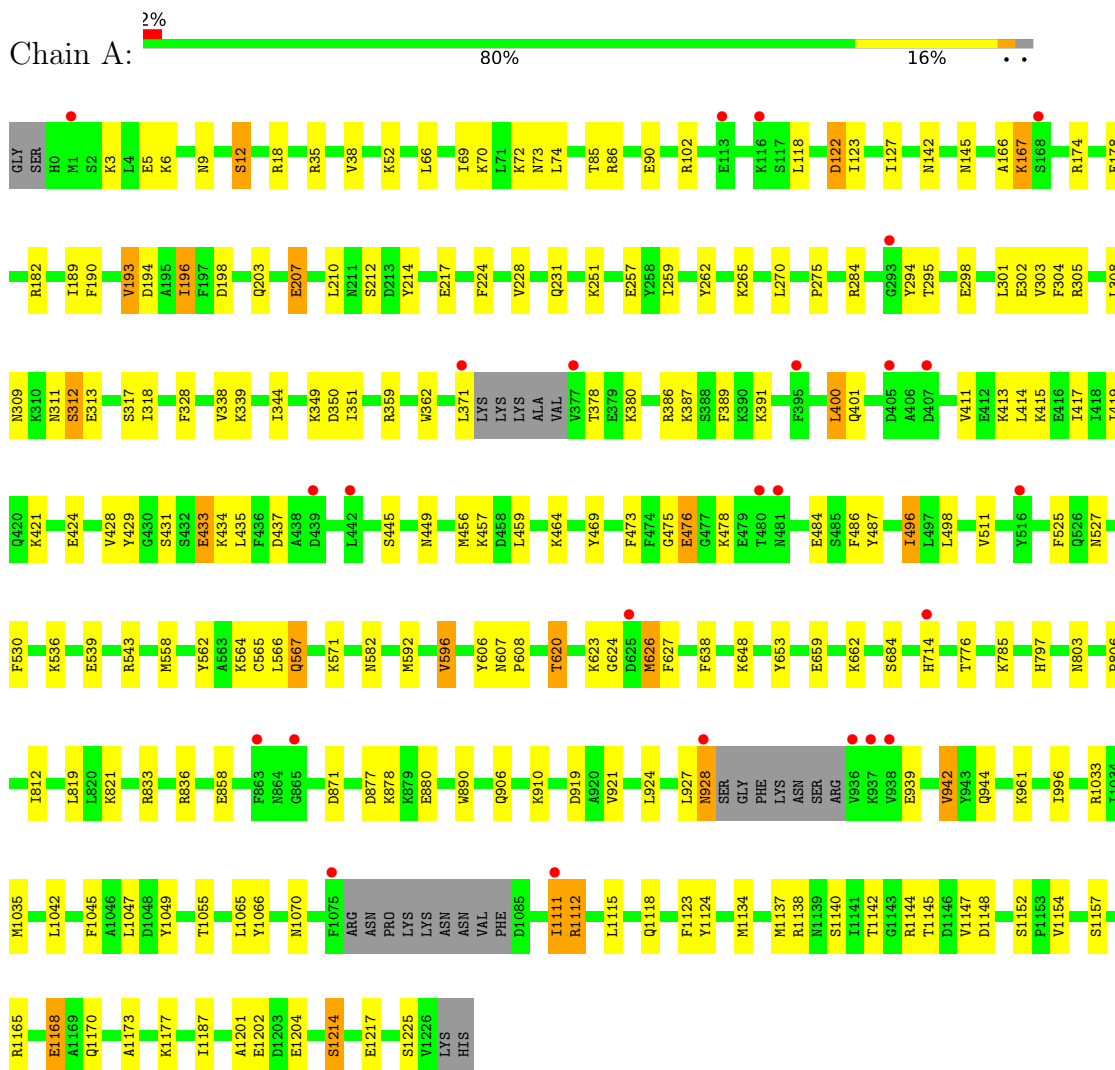
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	70	Total O 70 70	0	0
8	B	47	Total O 47 47	0	0
8	C	18	Total O 18 18	0	0

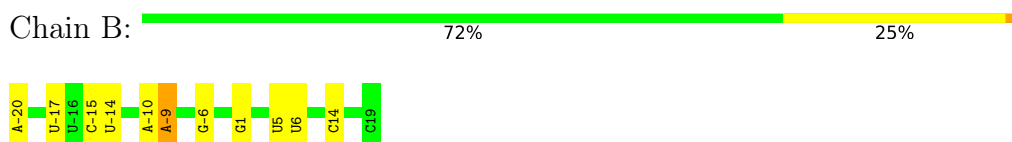
3 Residue-property plots i

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

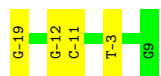


- Molecule 2: crRNA



- Molecule 3: DNA (29-MER)

Chain C:  86% 14%



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

Chain D:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.20Å 103.20Å 363.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.50 49.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.64-2.50) 99.7 (49.64-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.178 , 0.228 0.185 , 0.234	Depositor DCC
R_{free} test set	3497 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11542	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.32	0/9992	0.50	0/13478
2	B	0.40	0/953	0.60	0/1484
3	C	0.40	0/661	0.62	0/1017
4	D	0.44	0/196	0.71	0/300
All	All	0.33	0/11802	0.53	0/16279

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	9776	0	9445	110	1
2	B	852	0	429	6	0
3	C	589	0	326	3	0
4	D	177	0	105	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	12	0	0
7	B	3	0	0	0	0
8	A	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	47	0	0	0	0
8	C	18	0	0	0	0
All	All	11542	0	10317	113	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 5.

All (113) 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:1033:ARG:NH2	1:A:1035:MET:SD	2.52	0.82
1:A:182:ARG:NH1	1:A:275:PRO:O	2.17	0.76
1:A:308:LEU:O	1:A:429:TYR:OH	2.04	0.74
1:A:1170:GLN:HE21	1:A:1173:ALA:HA	1.53	0.74
1:A:3:LYS:HG2	1:A:819:LEU:HB3	1.71	0.73
1:A:927:LEU:O	1:A:928:ASN:ND2	2.21	0.71
1:A:996:ILE:HD11	1:A:1187:ILE:HG23	1.76	0.66
1:A:351:ILE:HD11	1:A:414:LEU:HD21	1.79	0.65
1:A:858:GLU:HG2	1:A:871:ASP:HA	1.77	0.65
1:A:265:LYS:O	1:A:386:ARG:NH2	2.31	0.63
1:A:313:GLU:HG3	1:A:496:ILE:HD11	1.79	0.62
1:A:539:GLU:HG2	1:A:558:MET:HE1	1.82	0.62
1:A:298:GLU:O	1:A:302:GLU:HG2	2.01	0.61
1:A:464:LYS:NZ	2:B:14:C:OP1	2.34	0.60
1:A:203:GLN:NE2	1:A:207:GLU:OE1	2.35	0.60
1:A:12:SER:HB3	1:A:803:ASN:O	2.01	0.59
1:A:457:LYS:HD2	1:A:890:TRP:CD2	2.37	0.59
1:A:445:SER:O	1:A:449:ASN:N	2.36	0.58
1:A:123:ILE:HA	1:A:127:ILE:HB	1.85	0.58
1:A:1111:ILE:HG12	1:A:1115:LEU:HG	1.88	0.56
1:A:1066:TYR:C	1:A:1134:MET:HE3	2.31	0.55
1:A:414:LEU:HD13	1:A:473:PHE:HE2	1.71	0.54
1:A:836:ARG:HG3	1:A:1148:ASP:HB2	1.91	0.53
1:A:1065:LEU:HB3	1:A:1134:MET:HE2	1.91	0.53
1:A:536:LYS:HD3	1:A:582:ASN:OD1	2.09	0.53
1:A:562:TYR:HB3	1:A:565:CYS:HB3	1.91	0.53
1:A:1070[A]:ASN:HD21	1:A:1165:ARG:HH12	1.57	0.53
1:A:1204:GLU:H	1:A:1204:GLU:CD	2.17	0.53
1:A:122:ASP:OD1	1:A:122:ASP:N	2.39	0.52
1:A:623:LYS:HA	1:A:627:PHE:CG	2.44	0.52
1:A:362:TRP:CZ3	1:A:389:PHE:HB2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:LYS:HB2	2:B:-20:A:H5''	1.93	0.51
1:A:1137:MET:HE3	1:A:1152:SER:HA	1.92	0.51
1:A:190:PHE:O	1:A:194:ASP:HB2	2.10	0.51
1:A:18:ARG:HG2	1:A:797:HIS:CD2	2.46	0.51
1:A:193:VAL:HG11	1:A:259:ILE:HD11	1.91	0.50
1:A:3:LYS:HE2	1:A:919:ASP:OD2	2.11	0.50
3:C:-12:DG:H2'	3:C:-11:DC:C6	2.46	0.50
1:A:620:THR:HA	1:A:626:MET:O	2.11	0.50
1:A:564:LYS:HZ3	1:A:567:GLN:HB3	1.75	0.49
1:A:378:THR:HG22	1:A:380:LYS:H	1.78	0.49
1:A:1066:TYR:O	1:A:1134:MET:HE3	2.12	0.49
1:A:251:LYS:NZ	1:A:257:GLU:OE2	2.46	0.48
1:A:304:PHE:CD1	1:A:456:MET:HG2	2.47	0.48
1:A:880:GLU:HG2	1:A:939:GLU:HG2	1.94	0.48
1:A:1214:SER:OG	1:A:1217:GLU:HG3	2.14	0.48
1:A:18:ARG:HD3	2:B:1:G:H5''	1.95	0.48
1:A:1140:SER:HA	1:A:1147:VAL:O	2.14	0.48
1:A:118:LEU:HA	1:A:123:ILE:HD12	1.95	0.48
1:A:421:LYS:HE3	1:A:469:TYR:HB2	1.96	0.47
1:A:1115:LEU:HD22	1:A:1123:PHE:HZ	1.80	0.47
1:A:301:LEU:HD21	1:A:435:LEU:HD11	1.97	0.47
1:A:906:GLN:O	1:A:910:LYS:HG2	2.14	0.47
1:A:525:PHE:O	1:A:543:ARG:NH2	2.40	0.47
1:A:66:LEU:O	1:A:69:ILE:HG22	2.15	0.47
1:A:350:ASP:HB3	1:A:417:ILE:HD13	1.96	0.47
1:A:102:ARG:CZ	1:A:166:ALA:HB2	2.45	0.46
1:A:193:VAL:HG22	1:A:270:LEU:HD13	1.97	0.46
1:A:196:ILE:HG13	1:A:262:TYR:CD1	2.51	0.46
2:B:5:U:H2'	2:B:6:U:O4'	2.16	0.46
1:A:72:LYS:C	1:A:74:LEU:H	2.24	0.46
1:A:305:ARG:NH2	1:A:437:ASP:O	2.49	0.45
1:A:836:ARG:HD3	1:A:1144:ARG:O	2.16	0.45
1:A:608:PRO:HB3	1:A:638:PHE:CE1	2.51	0.45
1:A:659:GLU:HG3	1:A:662:LYS:HG3	1.98	0.45
1:A:571:LYS:HD2	1:A:684:SER:HB2	1.99	0.45
1:A:592:MET:O	1:A:596:VAL:HG13	2.17	0.45
1:A:606:TYR:HE1	1:A:638:PHE:CE1	2.34	0.45
1:A:304:PHE:CE1	1:A:456:MET:HG2	2.51	0.45
1:A:714[A]:HIS:NE2	2:B:-9:A:OP2	2.41	0.45
1:A:145:ASN:H	1:A:145:ASN:HD22	1.65	0.45
1:A:338:VAL:HG12	1:A:344:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ARG:HD2	1:A:1140:SER:OG	2.18	0.44
1:A:189:ILE:O	1:A:193:VAL:HB	2.17	0.44
1:A:527:ASN:HB3	1:A:530:PHE:HB2	1.98	0.44
1:A:648:LYS:HD3	1:A:648:LYS:HA	1.88	0.44
1:A:339:LYS:HB2	1:A:475:GLY:C	2.43	0.44
1:A:1118:GLN:O	1:A:1124:TYR:OH	2.27	0.44
1:A:1202:GLU:HG2	1:A:1204:GLU:OE1	2.18	0.44
1:A:231:GLN:HB3	1:A:284:ARG:HD2	1.99	0.44
1:A:1111:ILE:HG12	1:A:1111:ILE:O	2.17	0.44
1:A:821:LYS:NZ	1:A:1201:ALA:O	2.45	0.43
1:A:428:VAL:HG11	1:A:459:LEU:HA	2.01	0.43
1:A:167:LYS:HG2	3:C:-3:DT:H4'	2.00	0.43
1:A:309:ASN:O	1:A:312:SER:HB3	2.17	0.43
1:A:1111:ILE:H	1:A:1111:ILE:HG22	1.52	0.43
1:A:924:LEU:HD23	1:A:924:LEU:HA	1.82	0.43
1:A:1045:PHE:CD1	1:A:1134:MET:HE1	2.54	0.43
1:A:1111:ILE:HD11	1:A:1115:LEU:HD21	2.01	0.43
1:A:1115:LEU:HD22	1:A:1123:PHE:CZ	2.54	0.43
1:A:607:ASN:HD22	1:A:608:PRO:N	2.16	0.43
1:A:86:ARG:HA	1:A:90:GLU:OE1	2.19	0.42
1:A:476:GLU:HG3	1:A:478:LYS:H	1.84	0.42
1:A:387:LYS:O	1:A:391:LYS:HG3	2.20	0.42
1:A:486:PHE:HD1	1:A:487:TYR:CD1	2.37	0.42
1:A:1137:MET:HB3	1:A:1137:MET:HE2	1.74	0.42
1:A:9:ASN:ND2	1:A:806:PRO:HA	2.35	0.42
1:A:70:LYS:HA	1:A:70:LYS:HD3	1.88	0.42
1:A:174:ARG:NE	1:A:178:GLU:OE2	2.47	0.42
1:A:624:GLY:H	1:A:627:PHE:HB2	1.84	0.42
1:A:210:LEU:HD13	1:A:214:TYR:HB2	2.02	0.42
2:B:-15:C:H2'	2:B:-14:U:C6	2.55	0.41
1:A:294:TYR:OH	1:A:303:VAL:HG11	2.20	0.41
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.92	0.41
1:A:1168:GLU:HA	1:A:1177:LYS:HB3	2.03	0.41
1:A:309:ASN:OD1	1:A:311:ASN:N	2.54	0.41
1:A:359:ARG:HE	1:A:359:ARG:HB2	1.68	0.41
1:A:1033:ARG:HA	1:A:1112:ARG:NE	2.36	0.41
1:A:142:ASN:HD22	1:A:142:ASN:HA	1.73	0.41
1:A:349:LYS:HE2	3:C:-19:DG:C8	2.56	0.41
1:A:1042:LEU:HD13	1:A:1066:TYR:HB3	2.03	0.41
1:A:415:LYS:O	1:A:419:ILE:HG12	2.20	0.40
1:A:433:GLU:H	1:A:433:GLU:HG2	1.45	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:35:ARG:NH2	1:A:217:GLU:OE1[5_547]	2.19	0.01

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	1200/1231 (98%)	1161 (97%)	37 (3%)	2 (0%)	43 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	942	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	1044/1117 (94%)	981 (94%)	63 (6%)	17 36

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU

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Mol	Chain	Res	Type
1	A	6	LYS
1	A	12	SER
1	A	38	VAL
1	A	52	LYS
1	A	85	THR
1	A	122	ASP
1	A	167	LYS
1	A	193	VAL
1	A	196	ILE
1	A	198	ASP
1	A	207	GLU
1	A	212	SER
1	A	224	PHE
1	A	228	VAL
1	A	295	THR
1	A	312	SER
1	A	317	SER
1	A	318	ILE
1	A	328	PHE
1	A	371	LEU
1	A	400	LEU
1	A	401	GLN
1	A	411	VAL
1	A	413	LYS
1	A	424	GLU
1	A	431	SER
1	A	433	GLU
1	A	434	LYS
1	A	476	GLU
1	A	484	GLU
1	A	496	ILE
1	A	498	LEU
1	A	511	VAL
1	A	566	LEU
1	A	567	GLN
1	A	596	VAL
1	A	620	THR
1	A	626	MET
1	A	653	TYR
1	A	776	THR
1	A	812	ILE
1	A	833	ARG

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Mol	Chain	Res	Type
1	A	877	ASP
1	A	878	LYS
1	A	921	VAL
1	A	928	ASN
1	A	942	VAL
1	A	944	GLN
1	A	961	LYS
1	A	1047	LEU
1	A	1049	TYR
1	A	1055	THR
1	A	1111	ILE
1	A	1112	ARG
1	A	1138	ARG
1	A	1142	THR
1	A	1145	THR
1	A	1154	VAL
1	A	1157	SER
1	A	1168	GLU
1	A	1214	SER
1	A	1225	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	28	GLN
1	A	30	ASN
1	A	33	ASN
1	A	63	ASN
1	A	73	ASN
1	A	112	ASN
1	A	142	ASN
1	A	145	ASN
1	A	200	HIS
1	A	260	ASN
1	A	363	ASN
1	A	529	GLN
1	A	607	ASN
1	A	703	GLN
1	A	759	HIS
1	A	862	ASN
1	A	873	HIS

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Mol	Chain	Res	Type
1	A	909	HIS
1	A	955	ASN
1	A	963	ASN
1	A	1051	ASN
1	A	1100	ASN
1	A	1105	ASN
1	A	1118	GLN
1	A	1170	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	39/40 (97%)	4 (10%)	0

All (4) 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

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 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	0.42	0	2,2,2	0.55	0
6	EDO	A	1302	-	3,3,3	0.37	0	2,2,2	0.57	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	-	-	1/1/1/1	-
6	EDO	A	1302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1302	EDO	O1-C1-C2-O2
6	A	1303	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å ²)	Q<0.9
1	A	1206/1231 (97%)	0.00	25 (2%) 63 59	42, 81, 121, 156	2 (0%)
2	B	40/40 (100%)	-1.03	0 100 100	54, 61, 80, 87	0
3	C	29/29 (100%)	-0.73	0 100 100	55, 65, 117, 135	0
4	D	9/9 (100%)	-0.60	0 100 100	74, 77, 121, 135	0
All	All	1284/1309 (98%)	-0.05	25 (1%) 66 62	42, 80, 121, 156	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	936	VAL	4.6
1	A	377	VAL	3.8
1	A	395	PHE	3.4
1	A	625	ASP	3.0
1	A	928	ASN	2.8
1	A	439	ASP	2.8
1	A	714[A]	HIS	2.8
1	A	937	LYS	2.6
1	A	113	GLU	2.6
1	A	442	LEU	2.5
1	A	863	PHE	2.5
1	A	405	ASP	2.3
1	A	516	TYR	2.3
1	A	481	ASN	2.3
1	A	293	GLY	2.3
1	A	1075	PHE	2.3
1	A	938	VAL	2.2
1	A	1111	ILE	2.2
1	A	1	MET	2.1
1	A	168	SER	2.1
1	A	407	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	371	LEU	2.0
1	A	865	GLY	2.0
1	A	116	LYS	2.0
1	A	480	THR	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 oligosaccharides 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, 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(Å ²)	Q<0.9
6	EDO	A	1303	4/4	0.90	0.13	75,81,83,84	0
7	NA	B	104	1/1	0.91	0.14	83,83,83,83	0
7	NA	B	103	1/1	0.94	0.07	81,81,81,81	0
7	NA	B	102	1/1	0.94	0.06	86,86,86,86	0
6	EDO	A	1302	4/4	0.95	0.10	68,72,74,75	0
5	MG	B	101	1/1	0.99	0.05	56,56,56,56	0
5	MG	A	1301	1/1	0.99	0.09	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.