



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:05 am BST

PDB ID : 5XUS
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 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 : 2.11
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) : 2.11

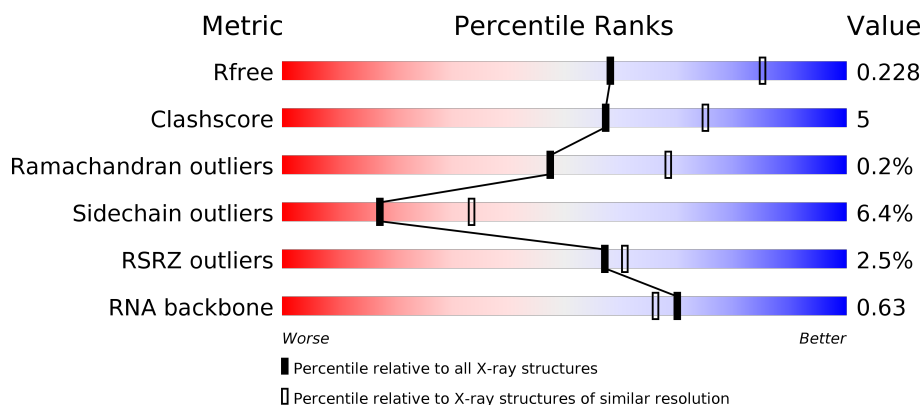
1 Overall quality at a glance

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}	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 on 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	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
2	B	40	<div> <div>70%</div> <div>23%</div> <div>8%</div> </div>
3	C	29	<div> <div>83%</div> <div>17%</div> </div>
4	D	9	<div> <div>100%</div> </div>

2 Entry composition [i](#)

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
1	A	1206	Total	C	N	O	S	0	2	0
			9776	6291	1593	1863	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
			589	281	112	168	28			

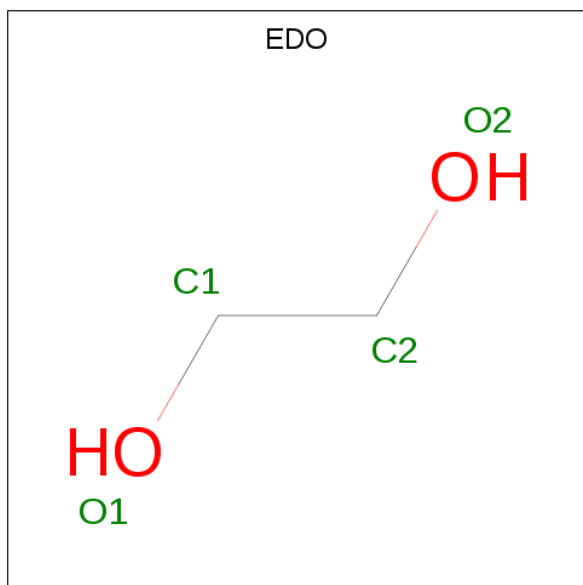
- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*A)-3').

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

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

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

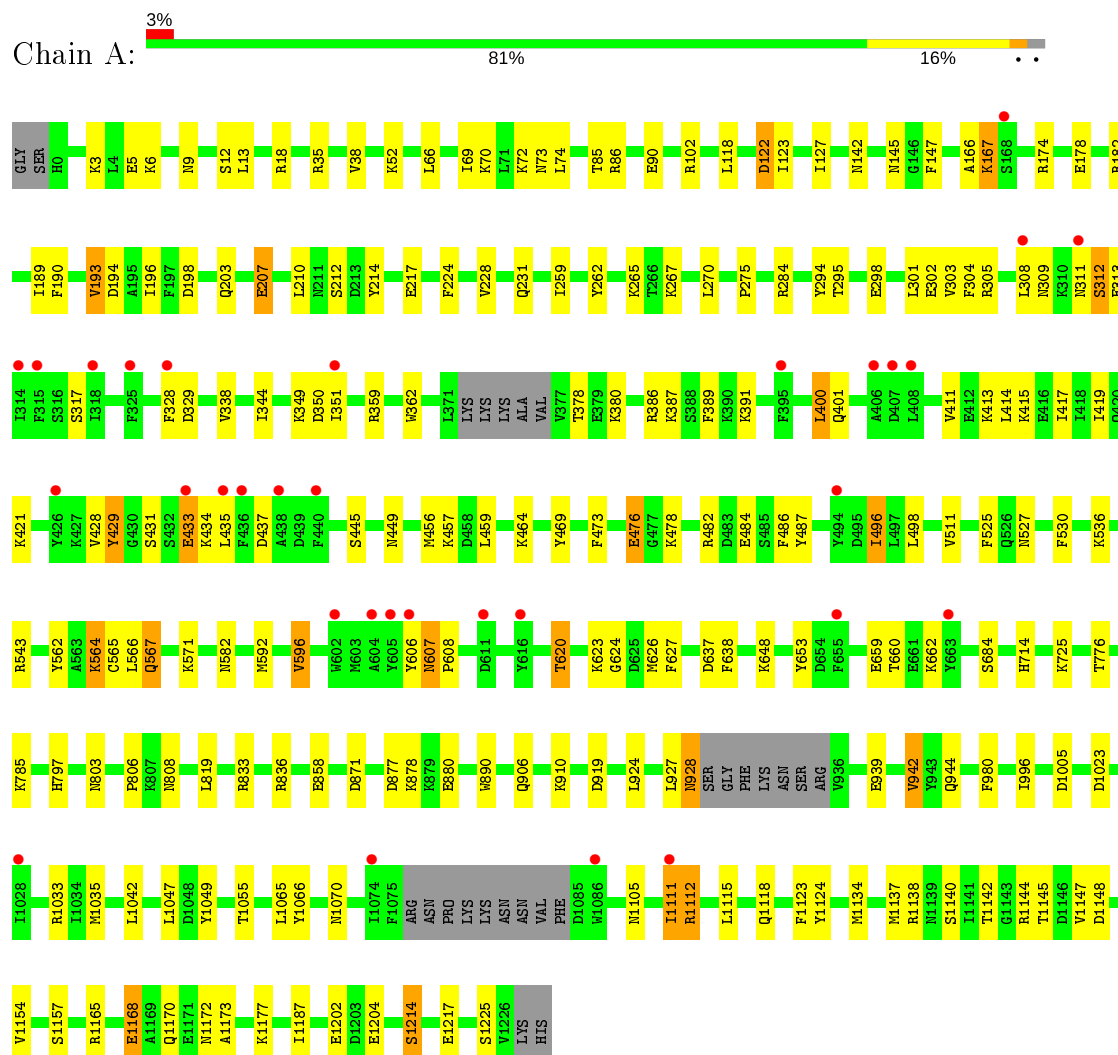
- Molecule 8 is water.

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

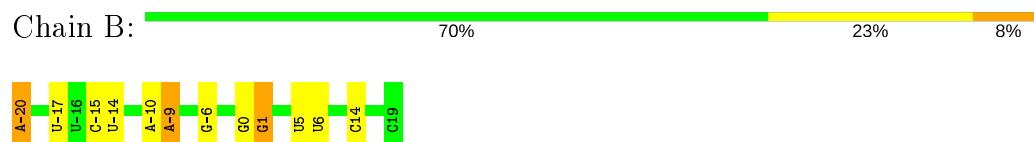
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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

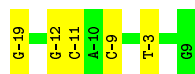


• Molecule 2: crRNA



- Molecule 3: DNA (29-MER)

Chain C:  83% 17%



- 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)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.178 , 0.228 0.178 , 0.228	Depositor DCC
R_{free} test set	3495 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.40	0/9992	0.53	0/13478
2	B	0.68	0/953	1.14	4/1484 (0.3%)
3	C	0.90	0/661	0.98	1/1017 (0.1%)
4	D	0.90	0/196	1.11	0/300
All	All	0.48	0/11802	0.66	5/16279 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	0	G	O4'-C1'-N9	7.20	113.96	108.20
2	B	1	G	O5'-P-OP2	-5.74	100.54	105.70
3	C	-9	DC	O5'-P-OP2	-5.52	100.73	105.70
2	B	-20	A	C8-N9-C4	5.06	107.83	105.80
2	B	-20	A	N9-C4-C5	-5.01	103.80	105.80

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	104	1
2	B	852	0	429	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
7	B	3	0	0	0	0
8	A	70	0	0	0	0
8	B	47	0	0	0	0
8	C	18	0	0	0	0
All	All	11542	0	10317	107	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 (107) 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: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: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:562:TYR:HB3	1:A:565:CYS:HB3	1.91	0.53
1:A:536:LYS:HD3	1:A:582:ASN:OD1	2.09	0.53
1:A:1070[A]:ASN:HD21	1:A:1165:ARG:HH12	1.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:N	1:A:122:ASP:OD1	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
1:A:785:LYS:HB2	2:B:-20:A:H5"	1.93	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:378:THR:HG22	1:A:380:LYS:H	1.78	0.49
1:A:304:PHE:CD1	1:A:456:MET:HG2	2.47	0.48
1:A:1214:SER:OG	1:A:1217:GLU:HG3	2.14	0.48
1:A:880:GLU:HG2	1:A:939:GLU:HG2	1.94	0.48
1:A:1140:SER:HA	1:A:1147:VAL:O	2.14	0.48
1:A:18:ARG:HD3	2:B:1:G:H5"	1.95	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:1204:GLU:H	1:A:1204:GLU:CD	2.17	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:350:ASP:HB3	1:A:417:ILE:HD13	1.96	0.47
1:A:66:LEU:O	1:A:69:ILE:HG22	2.15	0.47
1:A:102:ARG:CZ	1:A:166:ALA:HB2	2.45	0.46
1:A:564:LYS:HZ3	1:A:567:GLN:HB3	1.79	0.46
1:A:196:ILE:HG13	1:A:262:TYR:CD1	2.51	0.46
1:A:193:VAL:HG22	1:A:270:LEU:HD13	1.97	0.46
2:B:5:U:H2'	2:B:6:U:O4'	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:ILE:O	1:A:1111:ILE:HG12	2.17	0.44
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:HA	1:A:648:LYS:HD3	1.88	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:428:VAL:HG11	1:A:459:LEU:HA	2.01	0.43
1:A:1111:ILE:H	1:A:1111:ILE:HG22	1.52	0.43
1:A:309:ASN:O	1:A:312:SER:HB3	2.17	0.43
1:A:167:LYS:HG2	3:C:-3:DT:H4'	2.00	0.43
1:A:924:LEU:HA	1:A:924:LEU:HD23	1.82	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:476:GLU:HG3	1:A:478:LYS:H	1.84	0.42
1:A:86:ARG:HA	1:A:90:GLU:OE1	2.19	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: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:70:LYS:HD3	1:A:70:LYS:HA	1.88	0.42
1:A:9:ASN:ND2	1:A:806:PRO:HA	2.35	0.42
1:A:210:LEU:HD13	1:A:214:TYR:HB2	2.02	0.42
1:A:725:LYS:HZ2	6:A:1303:EDO:HO1	1.60	0.41
1:A:1005:ASP:HB2	1:A:1137:MET:HE1	2.01	0.41
2:B:-15:C:H2'	2:B:-14:U:C6	2.55	0.41
1:A:1168:GLU:HA	1:A:1177:LYS:HB3	2.03	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:72:LYS:C	1:A:74:LEU:H	2.24	0.41
1:A:1065:LEU:CB	1:A:1134:MET:HE1	2.50	0.41
1:A:1033:ARG:HA	1:A:1112:ARG:NE	2.36	0.41
1:A:359:ARG:HE	1:A:359:ARG:HB2	1.68	0.41
1:A:309:ASN:OD1	1:A:311:ASN:N	2.54	0.41
1:A:637:ASP:OD1	1:A:660:THR:OG1	2.33	0.41
1:A:1042:LEU:HD13	1:A:1066:TYR:HB3	2.03	0.41
1:A:142:ASN:HA	1:A:142:ASN:HD22	1.73	0.41
1:A:349:LYS:HE2	3:C:-19:DG:C8	2.56	0.41
1:A:415:LYS:O	1:A:419:ILE:HG12	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:HG2	1:A:433:GLU:H	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%)	47 68

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%)	977 (94%)	67 (6%)	17 33

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6	LYS
1	A	13	LEU
1	A	38	VAL
1	A	52	LYS
1	A	85	THR
1	A	122	ASP
1	A	147	PHE
1	A	167	LYS
1	A	193	VAL
1	A	198	ASP
1	A	207	GLU
1	A	212	SER
1	A	224	PHE
1	A	228	VAL
1	A	267	LYS
1	A	295	THR
1	A	312	SER
1	A	317	SER
1	A	328	PHE
1	A	329	ASP
1	A	400	LEU
1	A	401	GLN
1	A	411	VAL
1	A	413	LYS
1	A	429	TYR
1	A	431	SER
1	A	433	GLU
1	A	434	LYS
1	A	476	GLU
1	A	482	ARG
1	A	484	GLU
1	A	496	ILE
1	A	498	LEU
1	A	511	VAL
1	A	564	LYS
1	A	566	LEU
1	A	567	GLN
1	A	596	VAL
1	A	607	ASN
1	A	620	THR
1	A	653	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	776	THR
1	A	808	ASN
1	A	833	ARG
1	A	877	ASP
1	A	878	LYS
1	A	928	ASN
1	A	942	VAL
1	A	944	GLN
1	A	980	PHE
1	A	1023	ASP
1	A	1047	LEU
1	A	1049	TYR
1	A	1055	THR
1	A	1105	ASN
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	1172	ASN
1	A	1214	SER
1	A	1225	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
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	370	HIS
1	A	529	GLN
1	A	567	GLN
1	A	607	ASN
1	A	703	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	759	HIS
1	A	862	ASN
1	A	864	ASN
1	A	873	HIS
1	A	1051	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%)	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 carbohydrates 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	0.45	0	2,2,2	0.52	0
6	EDO	A	1302	-	3,3,3	0.40	0	2,2,2	0.54	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1303	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, 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%)	0.19	32 (2%) 54 58	49, 81, 121, 156	0
2	B	40/40 (100%)	0.00	0 100 100	54, 61, 80, 87	0
3	C	29/29 (100%)	-0.04	0 100 100	55, 65, 117, 135	0
4	D	9/9 (100%)	0.04	0 100 100	74, 77, 121, 135	0
All	All	1284/1309 (98%)	0.18	32 (2%) 57 61	49, 80, 121, 156	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	TYR	3.4
1	A	1111	ILE	3.3
1	A	435	LEU	3.2
1	A	1028	ILE	3.0
1	A	426	TYR	3.0
1	A	408	LEU	2.9
1	A	395	PHE	2.9
1	A	315	PHE	2.8
1	A	407	ASP	2.8
1	A	318	ILE	2.7
1	A	1086	TRP	2.6
1	A	602	TRP	2.6
1	A	168	SER	2.6
1	A	325	PHE	2.5
1	A	605	TYR	2.4
1	A	433	GLU	2.3
1	A	611	ASP	2.3
1	A	438	ALA	2.3
1	A	328	PHE	2.3
1	A	351	ILE	2.3
1	A	616	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	604	ALA	2.2
1	A	663	TYR	2.2
1	A	406	ALA	2.1
1	A	308	LEU	2.1
1	A	440	PHE	2.1
1	A	311	ASN	2.1
1	A	1074	ILE	2.1
1	A	436	PHE	2.1
1	A	314	ILE	2.0
1	A	655	PHE	2.0
1	A	606	TYR	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 carbohydrates 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(\AA^2)	Q<0.9
7	NA	B	102	1/1	0.70	0.11	86,86,86,86	0
6	EDO	A	1303	4/4	0.90	0.30	75,81,83,84	0
7	NA	B	104	1/1	0.90	0.37	83,83,83,83	0
7	NA	B	103	1/1	0.92	0.12	81,81,81,81	0
5	MG	B	101	1/1	0.96	0.20	56,56,56,56	0
6	EDO	A	1302	4/4	0.98	0.26	68,72,74,75	0
5	MG	A	1301	1/1	0.98	0.27	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.