



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:59 am BST

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

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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

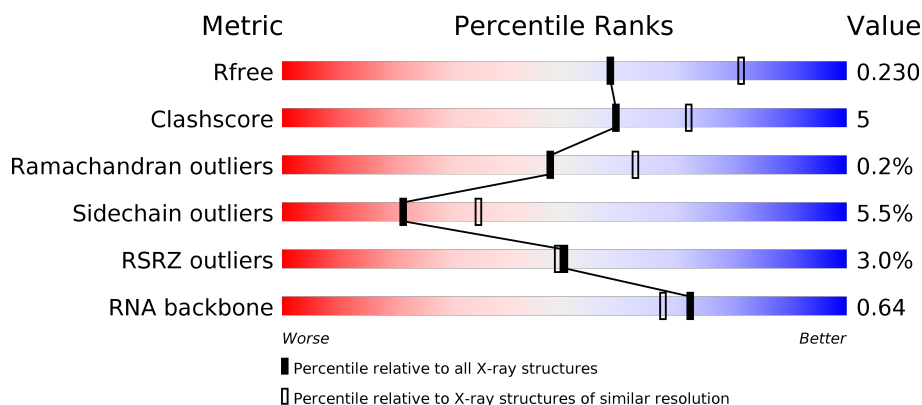
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	E	1231	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
2	B	40	<div> <div></div> <div> <div>80%</div> <div>20%</div> </div> </div>
2	F	40	<div> <div></div> <div> <div>68%</div> <div>25%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	C	29	 76%24%
3	G	29	 69%31%
4	D	9	 67%33%
4	H	9	 67%33%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 23419 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	1216	Total	C	N	O	S	0	2	0
			9897	6368	1620	1880	29			
1	E	1208	Total	C	N	O	S	0	4	0
			9810	6312	1606	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			
2	F	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
			592	281	112	171	28			
3	G	29	Total	C	N	O	P	0	0	0
			592	281	112	171	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total	C	N	O	P	0	0	0
			174	84	30	52	8			
4	H	9	Total	C	N	O	P	0	0	0
			174	84	30	52	8			

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

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	F	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
7	C	1	Total Na 1 1	0	0
7	F	1	Total Na 1 1	0	0

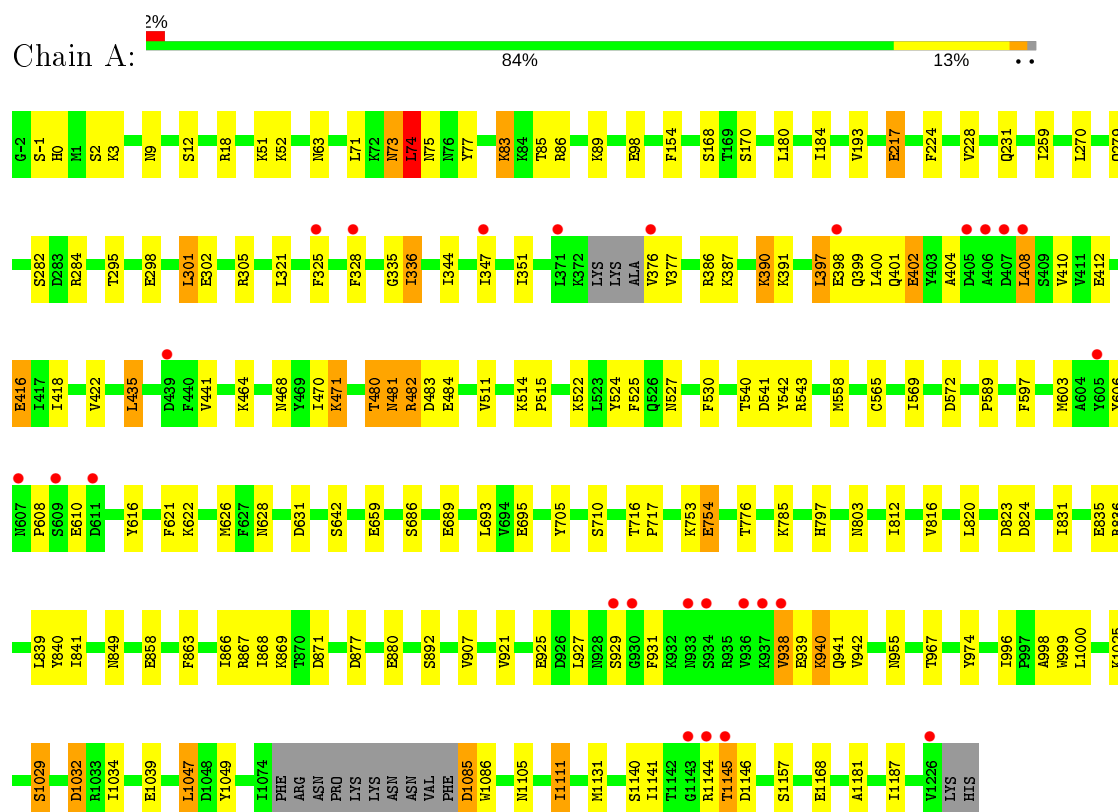
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	187	Total 187	O 187	0	0
8	B	58	Total 58	O 58	0	0
8	C	34	Total 34	O 34	0	0
8	E	120	Total 120	O 120	0	0
8	F	33	Total 33	O 33	0	0
8	G	23	Total 23	O 23	0	0

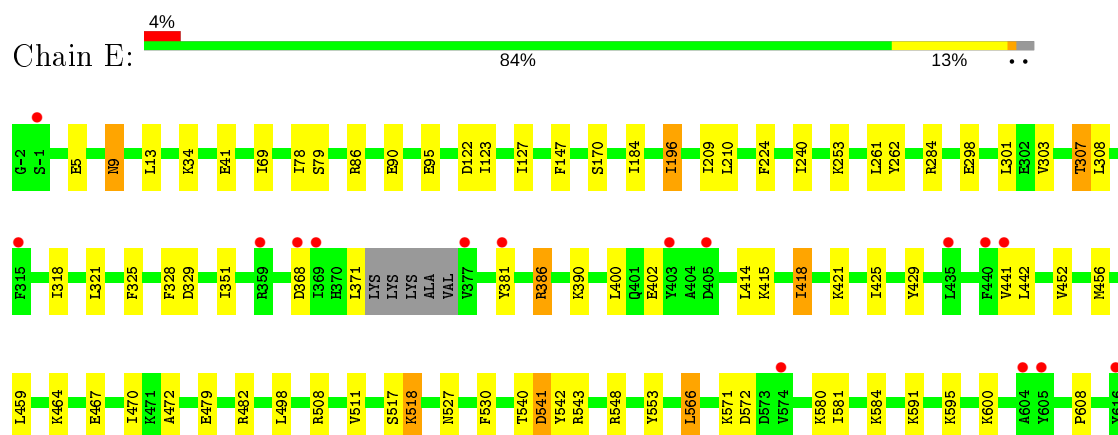
### 3 Residue-property plots [i](#)

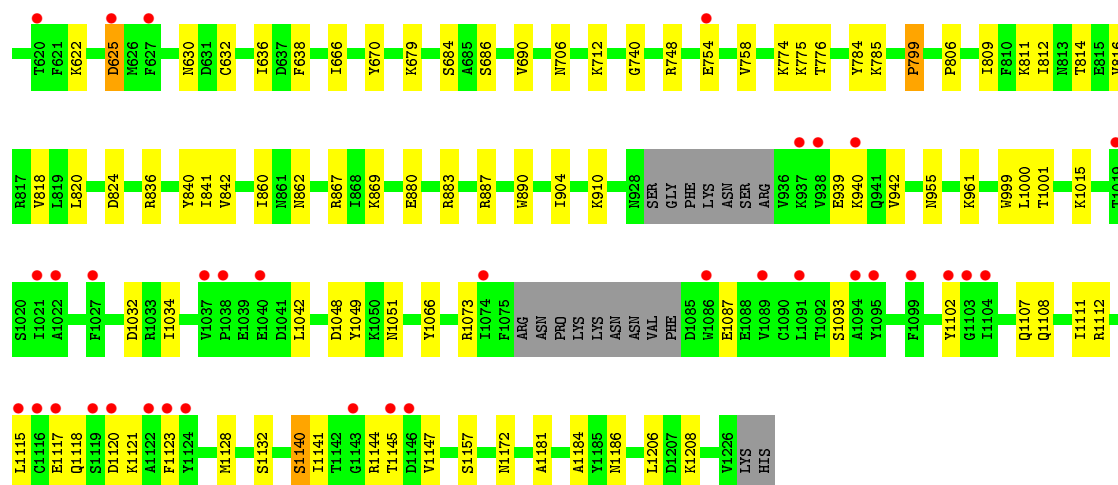
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

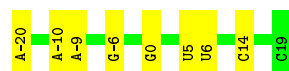


#### • Molecule 1: LbCpf1





- Molecule 2: crRNA



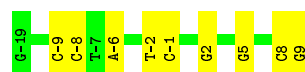
- Molecule 2: crRNA



- Molecule 3: DNA (29-MER)



- Molecule 3: DNA (29-MER)



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





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

Chain H:  67% 33%

C-9  
C-2  
A-1

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.95Å 103.54Å 342.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.40 49.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.40) 96.9 (49.85-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.177 , 0.229 0.178 , 0.230	Depositor DCC
$R_{free}$ test set	6680 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23419	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.41	0/10113	0.54	2/13622 (0.0%)
1	E	0.38	0/10029	0.51	0/13514
2	B	0.71	0/953	1.17	1/1484 (0.1%)
2	F	0.62	0/953	1.14	4/1484 (0.3%)
3	C	0.97	1/664 (0.2%)	0.96	1/1023 (0.1%)
3	G	0.88	1/664 (0.2%)	1.00	0/1023
4	D	0.91	1/193 (0.5%)	0.88	0/294
4	H	0.78	0/193	0.90	0/294
All	All	0.48	3/23762 (0.0%)	0.65	8/32738 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	DT	C3'-O3'	-6.20	1.35	1.44
4	D	-6	DC	C3'-O3'	-5.67	1.36	1.44
3	G	-6	DA	C3'-O3'	-5.21	1.37	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	G	O5'-P-OP1	8.14	120.47	110.70
2	F	0	G	O4'-C1'-N9	7.21	113.97	108.20
2	F	1	G	O5'-P-OP2	-6.41	99.93	105.70
1	A	435	LEU	CA-CB-CG	6.26	129.69	115.30
1	A	1047	LEU	CA-CB-CG	5.99	129.07	115.30
2	B	0	G	O4'-C1'-N9	5.81	112.85	108.20
3	C	-6	DA	O4'-C1'-N9	5.45	111.81	108.00
2	F	-4	A	N1-C6-N6	5.24	121.74	118.60

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	9897	0	9658	102	0
1	E	9810	0	9544	88	0
2	B	852	0	429	3	0
2	F	852	0	429	11	0
3	C	592	0	326	4	0
3	G	592	0	326	5	0
4	D	174	0	102	1	0
4	H	174	0	102	6	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	4	0	6	0	0
6	B	4	0	6	1	0
6	E	4	0	6	0	0
6	F	4	0	6	1	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
8	A	187	0	0	8	0
8	B	58	0	0	0	0
8	C	34	0	0	1	0
8	E	120	0	0	2	0
8	F	33	0	0	0	0
8	G	23	0	0	0	0
All	All	23419	0	20940	207	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 (207) 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:336:ILE:HG12	1:A:397:LEU:HD11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:LYS:HB2	2:B:-20:A:H5''	1.56	0.88
1:A:284:ARG:NH1	8:A:1403:HOH:O	2.13	0.81
1:A:168:SER:O	8:A:1401:HOH:O	2.03	0.77
3:C:6:DG:N3	8:C:201:HOH:O	2.19	0.74
1:A:73:ASN:H	1:A:73:ASN:HD22	1.36	0.73
1:E:86:ARG:O	8:E:1401:HOH:O	2.05	0.73
1:A:231:GLN:HB2	1:A:279[B]:GLN:HG2	1.73	0.69
1:A:849:ASN:OD1	8:A:1402:HOH:O	2.10	0.68
1:E:329:ASP:OD2	1:E:415:LYS:NZ	2.27	0.67
1:A:527:ASN:ND2	1:A:541:ASP:O	2.28	0.67
1:E:1141:ILE:HG23	1:E:1144:ARG:HB2	1.76	0.66
1:A:880:GLU:OE2	1:A:940:LYS:HB3	1.97	0.65
1:E:527:ASN:ND2	1:E:541:ASP:O	2.29	0.64
1:E:591:LYS:HE2	4:H:-1:DA:H2''	1.78	0.64
1:E:527:ASN:HB3	1:E:530:PHE:HB2	1.81	0.63
1:A:279[B]:GLN:HG3	1:A:282:SER:HB3	1.81	0.63
4:D:-8:DG:H1'	4:D:-7:DT:H5'	1.81	0.63
1:A:996:ILE:HD11	1:A:1187:ILE:HG23	1.81	0.62
1:A:831:ILE:HG12	1:A:841:ILE:HD13	1.82	0.62
1:A:525:PHE:O	1:A:543:ARG:NH2	2.34	0.61
1:A:321:LEU:HD13	1:A:470:ILE:HD13	1.83	0.61
1:E:1073:ARG:NH1	1:E:1087:GLU:OE1	2.34	0.61
1:E:880:GLU:HG2	1:E:939:GLU:HB3	1.83	0.60
1:E:785:LYS:HB2	2:F:-20:A:H5''	1.84	0.60
1:A:659:GLU:HG2	1:E:824:ASP:HB2	1.83	0.60
1:E:418:ILE:HD12	1:E:470:ILE:HD11	1.83	0.60
1:E:429:TYR:CE2	1:E:459:LEU:HD11	2.36	0.60
4:H:-1:DA:H5''	4:H:-1:DA:C8	2.36	0.60
1:A:3:LYS:NZ	1:A:823:ASP:OD2	2.34	0.59
1:E:625:ASP:OD1	1:E:625:ASP:N	2.27	0.59
1:E:298:GLU:H	1:E:298:GLU:CD	2.06	0.59
1:E:774:LYS:NZ	2:F:-10:A:OP2	2.32	0.59
1:A:858:GLU:HG2	1:A:871:ASP:HA	1.84	0.58
1:E:303:VAL:O	1:E:307:THR:OG1	2.22	0.58
1:E:904:ILE:HD11	1:E:942:VAL:HG13	1.84	0.57
1:E:386:ARG:NH1	2:F:19:C:OP1	2.37	0.57
1:E:86:ARG:HA	1:E:90:GLU:OE1	2.05	0.57
1:E:1115:LEU:HD22	1:E:1123:PHE:HZ	1.70	0.57
1:E:1102:TYR:HB3	1:E:1118:GLN:HE21	1.70	0.56
1:E:196:ILE:HD11	1:E:262:TYR:CZ	2.40	0.56
1:A:835:GLU:HG2	1:A:940:LYS:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:O	1:A:484:GLU:N	2.39	0.55
1:A:836:ARG:NH2	1:A:1145:THR:HA	2.21	0.55
1:A:468:ASN:O	1:A:471:LYS:HG3	2.07	0.54
1:A:1141:ILE:HB	1:A:1144:ARG:HB2	1.89	0.54
1:A:836:ARG:NH1	1:A:1141:ILE:O	2.40	0.54
1:E:351:ILE:HD11	1:E:414:LEU:HD21	1.90	0.54
1:E:799:PRO:HG3	6:F:102:EDO:H12	1.89	0.53
1:E:1102:TYR:HB3	1:E:1118:GLN:NE2	2.22	0.53
1:A:180:LEU:O	1:A:184:ILE:HG13	2.09	0.53
1:E:548:ARG:HD3	1:E:553:TYR:CZ	2.44	0.53
1:E:812:ILE:O	1:E:816:VAL:HG23	2.09	0.53
1:A:397:LEU:O	1:A:401:GLN:N	2.37	0.52
1:E:518:LYS:HE2	1:E:748:ARG:HG3	1.91	0.52
1:E:572:ASP:HB2	1:E:686:SER:HB2	1.91	0.52
1:A:597:PHE:CE1	1:A:642:SER:HB3	2.44	0.52
2:F:-10:A:H4'	2:F:-9:A:C2	2.44	0.52
1:A:543:ARG:NH1	8:A:1409:HOH:O	2.41	0.52
1:E:608:PRO:HB3	1:E:638:PHE:CE1	2.45	0.52
1:A:754:GLU:H	1:A:754:GLU:CD	2.12	0.52
1:A:231:GLN:HG2	1:A:284:ARG:HB3	1.92	0.52
1:E:1032:ASP:O	1:E:1112:ARG:NH1	2.44	0.51
1:A:73:ASN:N	1:A:73:ASN:HD22	2.06	0.51
1:E:41:GLU:OE1	1:E:518:LYS:NZ	2.33	0.51
1:E:806:PRO:HG2	1:E:809:ILE:HD11	1.92	0.50
1:E:1120:ASP:OD1	1:E:1121:LYS:N	2.44	0.50
1:A:820:LEU:HD11	1:A:921:VAL:HG11	1.93	0.50
1:E:1042:LEU:HD13	1:E:1066:TYR:HB3	1.92	0.50
3:C:6:DG:H2''	3:C:7:DA:C8	2.47	0.50
1:A:621:PHE:CZ	1:A:622:LYS:HE3	2.47	0.49
1:E:571:LYS:HD3	1:E:684:SER:HB2	1.93	0.49
1:E:999:TRP:CH2	1:E:1000:LEU:HD12	2.47	0.49
1:A:376:VAL:HG22	1:A:377:VAL:H	1.76	0.49
1:A:0:HIS:ND1	1:A:824:ASP:HB3	2.28	0.49
1:E:9:ASN:ND2	1:E:806:PRO:HA	2.28	0.49
1:E:1034:ILE:O	1:E:1111:ILE:HG22	2.13	0.49
2:B:5:U:H2'	2:B:6:U:O4'	2.13	0.49
1:A:927:LEU:HD22	1:A:931:PHE:HD2	1.77	0.49
1:A:938:VAL:O	1:A:940:LYS:N	2.46	0.48
1:E:467:GLU:OE2	1:E:498:LEU:HD23	2.13	0.48
1:A:1039:GLU:CD	1:A:1039:GLU:H	2.16	0.48
1:A:616:TYR:HD1	1:A:621:PHE:CE2	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:860:ILE:O	1:E:910:LYS:NZ	2.34	0.48
1:E:321:LEU:O	1:E:325:PHE:HD2	1.97	0.48
1:E:580:LYS:NZ	1:E:581:ILE:O	2.39	0.48
1:A:823:ASP:OD1	1:A:824:ASP:N	2.47	0.48
1:E:464:LYS:NZ	2:F:14:C:OP1	2.47	0.47
1:A:831:ILE:HG12	1:A:841:ILE:CD1	2.44	0.47
1:E:1172:ASN:N	1:E:1172:ASN:OD1	2.46	0.47
4:H:-9:DC:H5'	4:H:-9:DC:C6	2.49	0.47
1:E:210:LEU:HD21	1:E:240:ILE:HD11	1.97	0.47
8:A:1448:HOH:O	6:B:102:EDO:H22	2.14	0.47
1:A:193:VAL:HG13	1:A:270:LEU:HD13	1.95	0.47
3:C:-12:DG:H2'	3:C:-11:DC:C6	2.50	0.47
1:A:927:LEU:HD22	1:A:931:PHE:CD2	2.50	0.47
1:E:472:ALA:O	8:E:1402:HOH:O	2.21	0.47
1:A:858:GLU:OE2	1:A:869:LYS:HD3	2.14	0.46
1:A:967:THR:HG22	1:A:974:TYR:CE1	2.50	0.46
1:E:842:VAL:HG23	1:E:1184:ALA:HB3	1.96	0.46
1:A:522:LYS:HD3	1:A:524:TYR:CZ	2.50	0.46
1:A:603:MET:HG2	1:A:608:PRO:HG3	1.98	0.46
1:A:399:GLN:O	1:A:402:GLU:HG3	2.15	0.46
1:A:412:GLU:O	1:A:416:GLU:HG2	2.15	0.46
1:E:123:ILE:HA	1:E:127:ILE:HB	1.97	0.46
1:E:940:LYS:O	1:E:942:VAL:HG23	2.16	0.46
1:A:480:THR:O	1:A:482:ARG:N	2.45	0.46
1:A:967:THR:HG22	1:A:974:TYR:HE1	1.81	0.46
1:A:397:LEU:HA	1:A:400:LEU:HB2	1.97	0.46
1:A:572:ASP:HB2	1:A:686:SER:HB2	1.96	0.46
1:A:514:LYS:HG3	1:A:515:PRO:HD2	1.98	0.46
1:A:569:ILE:HD12	1:A:689:GLU:HB3	1.97	0.46
1:A:193:VAL:HG11	1:A:259:ILE:HG12	1.98	0.45
1:E:527:ASN:HB2	1:E:543:ARG:NH1	2.30	0.45
1:E:542:TYR:HE2	3:G:2:DG:OP2	2.00	0.45
1:A:347:ILE:O	1:A:351:ILE:HG13	2.17	0.45
3:G:8:DC:H2''	3:G:9:DG:C8	2.51	0.45
1:E:308:LEU:O	1:E:429:TYR:OH	2.18	0.45
1:A:776:THR:HG22	8:A:1564:HOH:O	2.16	0.45
1:A:1146:ASP:N	1:A:1146:ASP:OD1	2.50	0.44
1:E:479:GLU:HB2	1:E:482[A]:ARG:HG3	1.98	0.44
1:E:706:ASN:HB2	2:F:-17:U:OP1	2.17	0.44
2:F:-10:A:H4'	2:F:-9:A:N3	2.33	0.44
1:A:416:GLU:HG2	1:A:416:GLU:H	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:-2:DT:H2'	3:G:-1:DC:C6	2.52	0.44
1:E:34:LYS:HE3	1:E:34:LYS:HB2	1.84	0.44
1:A:217:GLU:HB3	8:A:1560:HOH:O	2.18	0.44
1:A:1032:ASP:OD1	1:A:1032:ASP:N	2.51	0.44
1:E:860:ILE:HD13	1:E:869:LYS:HB2	2.00	0.44
1:A:301:LEU:HB3	1:A:305:ARG:NH1	2.33	0.44
1:A:464:LYS:NZ	2:B:14:C:OP1	2.51	0.44
1:A:279[B]:GLN:CG	1:A:282:SER:HB3	2.45	0.44
1:A:335:GLY:HA2	1:A:481:ASN:O	2.17	0.44
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.67	0.44
1:A:840:TYR:CZ	1:A:1181:ALA:HB2	2.53	0.43
1:A:628:ASN:HB3	1:A:631:ASP:HB2	2.00	0.43
1:A:77:TYR:HE1	1:A:98:GLU:HB2	1.83	0.43
3:G:-9:DC:H2'	3:G:-8:DC:C6	2.52	0.43
1:E:421:LYS:O	1:E:425:ILE:HG13	2.18	0.43
1:E:566:LEU:HD22	1:E:566:LEU:HA	1.88	0.43
1:A:12:SER:HB3	1:A:803:ASN:O	2.18	0.43
1:E:840:TYR:CZ	1:E:1181:ALA:HB2	2.53	0.43
1:E:666:ILE:HG13	1:E:670:TYR:CE2	2.52	0.43
1:A:716:THR:HA	1:A:717:PRO:HD3	1.90	0.43
1:A:83:LYS:HG2	1:A:86:ARG:HG2	2.01	0.43
1:E:452:VAL:O	1:E:456:MET:HG3	2.19	0.43
2:F:0:G:H1'	2:F:1:G:C8	2.54	0.43
1:E:686:SER:O	1:E:690:VAL:HG23	2.19	0.43
1:E:78:ILE:HG12	1:E:184:ILE:HD11	2.01	0.43
1:A:527:ASN:HB3	1:A:530:PHE:HB2	2.01	0.42
1:A:840:TYR:CE1	1:A:1181:ALA:HB2	2.53	0.42
1:A:404:ALA:HB2	1:A:410:VAL:HG23	2.01	0.42
1:A:52:LYS:HD2	1:A:52:LYS:HA	1.88	0.42
1:A:863:PHE:O	1:A:866:ILE:HB	2.19	0.42
2:F:-10:A:H5'	2:F:-9:A:C4	2.54	0.42
1:A:404:ALA:HB1	1:A:408:LEU:HB3	2.01	0.42
1:A:839:LEU:HD13	1:A:907:VAL:HG11	2.01	0.42
1:E:1111:ILE:HG12	1:E:1111:ILE:O	2.18	0.42
1:A:344:ILE:HD13	1:A:344:ILE:HA	1.86	0.42
1:A:565:CYS:SG	1:A:693:LEU:HD13	2.59	0.42
1:A:418:ILE:O	1:A:422:VAL:HG23	2.18	0.42
1:A:999:TRP:CH2	1:A:1000:LEU:HD12	2.55	0.42
1:E:632:CYS:O	1:E:636:ILE:HG13	2.19	0.42
1:E:600:LYS:HG3	3:G:5:DG:OP1	2.20	0.42
1:A:325:PHE:CD2	1:A:418:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:GLU:OE1	1:A:754:GLU:N	2.51	0.42
1:E:253:LYS:HE2	1:E:261:LEU:HD11	2.02	0.42
1:A:1034:ILE:O	1:A:1111:ILE:HB	2.20	0.41
1:A:589:PRO:HD2	8:A:1461:HOH:O	2.20	0.41
1:A:542:TYR:HE2	3:C:2:DG:OP2	2.03	0.41
4:H:-2:DC:H2"	4:H:-1:DA:C4	2.54	0.41
1:A:1025:LYS:O	1:A:1029:SER:OG	2.36	0.41
1:A:51:LYS:HG2	1:A:154:PHE:CE1	2.55	0.41
1:A:705:TYR:OH	1:A:710:SER:HB2	2.20	0.41
1:E:1001:THR:O	1:E:1186:ASN:ND2	2.48	0.41
1:E:1048:ASP:HB3	1:E:1051:ASN:ND2	2.36	0.41
1:A:63:ASN:HD22	1:A:63:ASN:HA	1.62	0.41
1:E:13:LEU:N	1:E:13:LEU:HD23	2.35	0.41
1:E:508:ARG:HG3	1:E:890:TRP:CE2	2.55	0.41
1:E:636:ILE:HG12	1:E:666:ILE:HD13	2.01	0.41
1:A:1085:ASP:HB3	1:A:1086:TRP:H	1.58	0.41
1:E:961:LYS:H	1:E:961:LYS:HG2	1.75	0.41
4:H:-2:DC:H2"	4:H:-1:DA:C8	2.55	0.41
1:A:1039:GLU:OE2	1:A:1039:GLU:N	2.34	0.41
1:A:925:GLU:HG2	1:A:998:ALA:HB2	2.01	0.41
1:E:820:LEU:HA	1:E:820:LEU:HD23	1.90	0.41
1:E:883:ARG:O	1:E:887:ARG:HG3	2.21	0.41
1:A:347:ILE:HD13	1:A:347:ILE:HA	1.90	0.41
1:A:73:ASN:N	1:A:73:ASN:ND2	2.68	0.41
1:E:1140:SER:HA	1:E:1147:VAL:O	2.20	0.41
1:E:712:LYS:HD2	2:F:-7:U:OP1	2.21	0.41
1:E:860:ILE:HD11	1:E:869:LYS:HD3	2.02	0.41
1:E:318:ILE:HD13	1:E:425:ILE:HD13	2.01	0.41
1:E:595:LYS:NZ	4:H:-1:DA:N3	2.67	0.41
1:E:814:THR:O	1:E:818:VAL:HG23	2.21	0.41
2:F:5:U:H2'	2:F:6:U:O4'	2.21	0.41
1:A:390:LYS:O	1:A:390:LYS:HG3	2.21	0.41
1:E:371:LEU:HD13	1:E:381:TYR:CZ	2.55	0.41
1:E:1206:LEU:HA	1:E:1206:LEU:HD23	1.88	0.40
1:E:758:VAL:HG22	1:E:784:TYR:CD2	2.57	0.40
1:E:740:GLY:O	1:E:799:PRO:HG2	2.21	0.40
1:A:18:ARG:HG2	1:A:797:HIS:CD2	2.56	0.40
1:A:812:ILE:O	1:A:816:VAL:HG23	2.22	0.40
1:E:1208:LYS:N	1:E:1208:LYS:HD2	2.35	0.40
1:E:584:LYS:HE3	1:E:584:LYS:HB3	1.87	0.40
1:A:336:ILE:CG1	1:A:397:LEU:HD11	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:TYR:O	1:A:608:PRO:HD3	2.21	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	1212/1231 (98%)	1173 (97%)	35 (3%)	4 (0%)	41	55
1	E	1204/1231 (98%)	1160 (96%)	43 (4%)	1 (0%)	51	68
All	All	2416/2462 (98%)	2333 (97%)	78 (3%)	5 (0%)	47	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	ASP
1	A	74	LEU
1	A	939	GLU
1	A	481	ASN
1	E	1108	GLN

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1065/1117 (95%)	1000 (94%)	65 (6%)	18	30
1	E	1051/1117 (94%)	998 (95%)	53 (5%)	24	40
All	All	2116/2234 (95%)	1998 (94%)	118 (6%)	21	34

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	2	SER
1	A	9	ASN
1	A	71	LEU
1	A	73	ASN
1	A	74	LEU
1	A	75[A]	ASN
1	A	75[B]	ASN
1	A	83	LYS
1	A	85	THR
1	A	89	LYS
1	A	170	SER
1	A	217	GLU
1	A	224	PHE
1	A	228	VAL
1	A	295	THR
1	A	298	GLU
1	A	301	LEU
1	A	302	GLU
1	A	328	PHE
1	A	336	ILE
1	A	386	ARG
1	A	387	LYS
1	A	390	LYS
1	A	391	LYS
1	A	397	LEU
1	A	398	GLU
1	A	402	GLU
1	A	408	LEU
1	A	416	GLU
1	A	435	LEU
1	A	441	VAL

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Mol	Chain	Res	Type
1	A	471	LYS
1	A	480	THR
1	A	482	ARG
1	A	511	VAL
1	A	540	THR
1	A	558	MET
1	A	610	GLU
1	A	626	MET
1	A	695	GLU
1	A	753	LYS
1	A	754	GLU
1	A	867	ARG
1	A	868	ILE
1	A	877	ASP
1	A	892	SER
1	A	929	SER
1	A	938	VAL
1	A	940	LYS
1	A	941	GLN
1	A	942	VAL
1	A	955	ASN
1	A	1029	SER
1	A	1032	ASP
1	A	1047	LEU
1	A	1049	TYR
1	A	1085	ASP
1	A	1105	ASN
1	A	1111	ILE
1	A	1131	MET
1	A	1140	SER
1	A	1145	THR
1	A	1157	SER
1	A	1168	GLU
1	E	5	GLU
1	E	9	ASN
1	E	69	ILE
1	E	79	SER
1	E	95	GLU
1	E	122	ASP
1	E	147	PHE
1	E	170	SER
1	E	196	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	209	ILE
1	E	224	PHE
1	E	284	ARG
1	E	301	LEU
1	E	307	THR
1	E	328	PHE
1	E	368	ASP
1	E	386	ARG
1	E	390	LYS
1	E	400	LEU
1	E	402	GLU
1	E	418	ILE
1	E	441	VAL
1	E	442	LEU
1	E	511	VAL
1	E	517	SER
1	E	518	LYS
1	E	540	THR
1	E	541	ASP
1	E	566	LEU
1	E	622	LYS
1	E	625	ASP
1	E	630	ASN
1	E	679	LYS
1	E	754	GLU
1	E	775	LYS
1	E	776	THR
1	E	799	PRO
1	E	811	LYS
1	E	836	ARG
1	E	841	ILE
1	E	862	ASN
1	E	867	ARG
1	E	955	ASN
1	E	1015	LYS
1	E	1049	TYR
1	E	1093	SER
1	E	1107	GLN
1	E	1117	GLU
1	E	1128	MET
1	E	1132	SER
1	E	1140	SER

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Mol	Chain	Res	Type
1	E	1145	THR
1	E	1157	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	33	ASN
1	A	63	ASN
1	A	73	ASN
1	A	112	ASN
1	A	145	ASN
1	A	370	HIS
1	A	703	GLN
1	A	759	HIS
1	A	822	HIS
1	A	862	ASN
1	A	889	ASN
1	A	1070	ASN
1	A	1100	ASN
1	A	1105	ASN
1	A	1170	GLN
1	E	9	ASN
1	E	33	ASN
1	E	112	ASN
1	E	142	ASN
1	E	268	GLN
1	E	370	HIS
1	E	607	ASN
1	E	703	GLN
1	E	889	ASN
1	E	1051	ASN
1	E	1100	ASN
1	E	1166	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	39/40 (97%)	3 (7%)	0
2	F	39/40 (97%)	2 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	78/80 (97%)	5 (6%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-10	A
2	B	-9	A
2	B	-6	G
2	F	-9	A
2	F	-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 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	E	1302	-	3,3,3	0.50	0	2,2,2	0.39	0
6	EDO	F	102	-	3,3,3	0.52	0	2,2,2	0.10	0
6	EDO	A	1302	-	3,3,3	0.42	0	2,2,2	0.59	0
6	EDO	B	102	-	3,3,3	0.44	0	2,2,2	0.29	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	E	1302	-	-	1/1/1/1	-
6	EDO	F	102	-	-	0/1/1/1	-
6	EDO	A	1302	-	-	0/1/1/1	-
6	EDO	B	102	-	-	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	E	1302	EDO	O1-C1-C2-O2
6	B	102	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	102	EDO	1	0
6	B	102	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1216/1231 (98%)	-0.05	26 (2%) 63 61	27, 54, 92, 132	0
1	E	1208/1231 (98%)	0.03	51 (4%) 36 35	32, 59, 105, 145	0
2	B	40/40 (100%)	-0.35	0 100 100	31, 39, 54, 60	0
2	F	40/40 (100%)	-0.49	0 100 100	34, 45, 68, 98	0
3	C	29/29 (100%)	-0.25	0 100 100	37, 43, 86, 107	0
3	G	29/29 (100%)	-0.41	0 100 100	42, 48, 91, 116	0
4	D	9/9 (100%)	-0.17	0 100 100	50, 65, 85, 103	0
4	H	9/9 (100%)	-0.03	0 100 100	54, 76, 113, 119	0
All	All	2580/2618 (98%)	-0.03	77 (2%) 50 49	27, 56, 99, 145	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1021	ILE	5.6
1	E	1143	GLY	4.5
1	E	1145	THR	4.4
1	E	938	VAL	4.4
1	A	1145	THR	4.4
1	E	1099	PHE	4.4
1	E	1074	ILE	3.9
1	A	405	ASP	3.9
1	A	408	LEU	3.9
1	A	328	PHE	3.8
1	E	1040	GLU	3.7
1	E	1146	ASP	3.5
1	E	1124	TYR	3.3
1	E	937	LYS	3.3
1	A	930	GLY	3.3
1	A	439	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	1102	TYR	3.2
1	E	1117	GLU	3.1
1	E	940	LYS	3.0
1	E	403	TYR	3.0
1	A	406	ALA	2.9
1	E	-1	SER	2.9
1	E	435	LEU	2.9
1	E	369	ILE	2.9
1	E	377	VAL	2.8
1	A	933	ASN	2.8
1	E	1038	PRO	2.8
1	E	574	VAL	2.7
1	A	371	LEU	2.7
1	E	1120	ASP	2.7
1	A	936	VAL	2.7
1	E	625	ASP	2.7
1	A	325	PHE	2.7
1	A	611	ASP	2.7
1	E	627	PHE	2.7
1	E	620	THR	2.7
1	A	937	LYS	2.6
1	E	441	VAL	2.6
1	E	440	PHE	2.6
1	A	376	VAL	2.5
1	E	1123	PHE	2.5
1	E	1094	ALA	2.5
1	A	1143	GLY	2.5
1	E	1103	GLY	2.4
1	E	1089	VAL	2.4
1	E	1095	TYR	2.4
1	A	407	ASP	2.4
1	E	315	PHE	2.4
1	A	1144	ARG	2.4
1	A	1226	VAL	2.4
1	A	347	ILE	2.4
1	E	604	ALA	2.3
1	E	1019	THR	2.3
1	E	1091	LEU	2.3
1	E	1122	ALA	2.3
1	E	381	TYR	2.3
1	A	605	TYR	2.3
1	A	938	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	1022	ALA	2.2
1	E	405	ASP	2.2
1	E	1027	PHE	2.2
1	E	359	ARG	2.2
1	E	368	ASP	2.2
1	E	1119	SER	2.2
1	E	1116	CYS	2.2
1	E	1086	TRP	2.2
1	A	398	GLU	2.2
1	A	929	SER	2.1
1	E	1104	ILE	2.1
1	A	609	SER	2.1
1	E	616	TYR	2.1
1	A	607	ASN	2.1
1	E	605	TYR	2.0
1	E	754	GLU	2.0
1	A	934	SER	2.0
1	E	1037	VAL	2.0
1	E	1115	LEU	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	NA	C	101	1/1	0.84	0.16	48,48,48,48	0
7	NA	F	101	1/1	0.86	0.09	54,54,54,54	0
7	NA	B	101	1/1	0.87	0.10	48,48,48,48	0
6	EDO	E	1302	4/4	0.93	0.24	50,58,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	F	102	4/4	0.95	0.29	48,55,56,59	0
5	MG	E	1301	1/1	0.97	0.22	25,25,25,25	0
6	EDO	B	102	4/4	0.97	0.25	49,50,52,53	0
6	EDO	A	1302	4/4	0.97	0.23	38,42,45,46	0
5	MG	A	1301	1/1	0.99	0.22	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.