



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2016 – 04:05 PM EDT

PDB ID : 5ITY  
Title : Crystal Structure of Human NEIL1(P2G) bound to duplex DNA containing Thymine Glycol  
Authors : Zhu, C.; Lu, L.; Zhang, J.; Yue, Z.; Song, J.; Zong, S.; Liu, M.; Stovicek, O.; Gao, Y.; Yi, C.  
Deposited on : 2016-03-17  
Resolution : 2.48 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

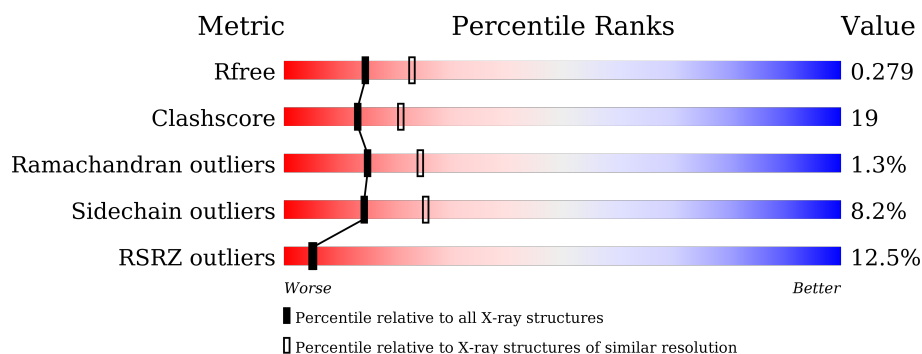
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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))
$R_{free}$	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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. 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	400	<div> <div>4%</div> <div> <div>53%</div> <div>12%</div> <div>•</div> <div>34%</div> </div> </div>
1	B	400	<div> <div>4%</div> <div> <div>46%</div> <div>16%</div> <div>•</div> <div>35%</div> </div> </div>
1	C	400	<div> <div>17%</div> <div> <div>40%</div> <div>21%</div> <div>5%</div> <div>35%</div> </div> </div>
2	D	26	<div> <div>8%</div> <div> <div>50%</div> <div>46%</div> <div>•</div> </div> </div>
2	E	26	<div> <div>15%</div> <div> <div>38%</div> <div>58%</div> <div>•</div> </div> </div>
2	F	26	<div> <div>19%</div> <div> <div>31%</div> <div>69%</div> </div> </div>

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
3	GOL	B	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8239 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 Endonuclease 8-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	5	0
			2148	1370	398	370	10			
1	B	262	Total	C	N	O	S	0	0	0
			2078	1327	381	360	10			
1	C	261	Total	C	N	O	S	0	0	0
			2066	1319	380	357	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	PRO	engineered mutation	UNP Q96FI4
A	242	ARG	LYS	engineered mutation	UNP Q96FI4
A	391	ALA	-	expression tag	UNP Q96FI4
A	392	ALA	-	expression tag	UNP Q96FI4
A	393	LEU	-	expression tag	UNP Q96FI4
A	394	GLY	-	expression tag	UNP Q96FI4
A	395	HIS	-	expression tag	UNP Q96FI4
A	396	HIS	-	expression tag	UNP Q96FI4
A	397	HIS	-	expression tag	UNP Q96FI4
A	398	HIS	-	expression tag	UNP Q96FI4
A	399	HIS	-	expression tag	UNP Q96FI4
A	400	HIS	-	expression tag	UNP Q96FI4
B	2	GLY	PRO	engineered mutation	UNP Q96FI4
B	242	ARG	LYS	engineered mutation	UNP Q96FI4
B	391	ALA	-	expression tag	UNP Q96FI4
B	392	ALA	-	expression tag	UNP Q96FI4
B	393	LEU	-	expression tag	UNP Q96FI4
B	394	GLY	-	expression tag	UNP Q96FI4
B	395	HIS	-	expression tag	UNP Q96FI4
B	396	HIS	-	expression tag	UNP Q96FI4
B	397	HIS	-	expression tag	UNP Q96FI4
B	398	HIS	-	expression tag	UNP Q96FI4
B	399	HIS	-	expression tag	UNP Q96FI4

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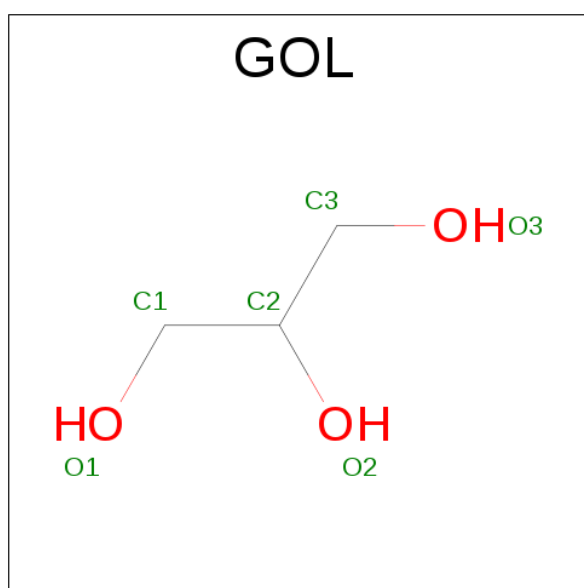
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Chain	Residue	Modelled	Actual	Comment	Reference
B	400	HIS	-	expression tag	UNP Q96FI4
C	2	GLY	PRO	engineered mutation	UNP Q96FI4
C	242	ARG	LYS	engineered mutation	UNP Q96FI4
C	391	ALA	-	expression tag	UNP Q96FI4
C	392	ALA	-	expression tag	UNP Q96FI4
C	393	LEU	-	expression tag	UNP Q96FI4
C	394	GLY	-	expression tag	UNP Q96FI4
C	395	HIS	-	expression tag	UNP Q96FI4
C	396	HIS	-	expression tag	UNP Q96FI4
C	397	HIS	-	expression tag	UNP Q96FI4
C	398	HIS	-	expression tag	UNP Q96FI4
C	399	HIS	-	expression tag	UNP Q96FI4
C	400	HIS	-	expression tag	UNP Q96FI4

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	26	Total	C	N	O	P	0	0	0
			527	252	96	155	24			
2	E	26	Total	C	N	O	P	0	0	0
			527	252	96	155	24			
2	F	26	Total	C	N	O	P	0	0	0
			527	252	96	155	24			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		
4	B	121	Total	O	0	0
			121	121		
4	C	8	Total	O	0	0
			8	8		
4	D	29	Total	O	0	0
			29	29		
4	E	13	Total	O	0	0
			13	13		
4	F	3	Total	O	0	0
			3	3		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.62Å 108.71Å 169.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.58 – 2.48 30.48 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.0 (91.58-2.48) 98.1 (30.48-2.48)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.176 , 0.225 0.239 , 0.279	Depositor DCC
$R_{free}$ test set	2383 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CTG

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	0.90	0/2215	1.02	9/2992 (0.3%)
1	B	0.84	0/2134	1.02	14/2886 (0.5%)
1	C	0.55	0/2122	0.73	0/2870
2	D	0.52	0/564	1.01	3/864 (0.3%)
2	E	0.62	0/564	1.17	3/864 (0.3%)
2	F	0.40	0/564	0.76	0/864
All	All	0.74	0/8163	0.95	29/11340 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	298	DG	O5'-P-OP1	-17.39	89.84	110.70
2	E	298	DG	O5'-P-OP2	12.48	125.68	110.70
1	B	119	ARG	NE-CZ-NH2	-10.05	115.27	120.30
2	D	313	DG	O5'-P-OP1	-8.26	98.26	105.70
1	A	78	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	100	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	179	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	30	SER	CB-CA-C	-7.08	96.65	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	CG-CD-NE	-6.97	97.16	111.80
1	B	119	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	100	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	224	ASP	CB-CA-C	-6.51	97.38	110.40
2	D	312	DT	O5'-P-OP2	-6.46	99.88	105.70
1	B	58	LEU	CA-CB-CG	6.20	129.55	115.30
1	A	78	ARG	CG-CD-NE	-5.94	99.32	111.80
1	A	71	GLU	C-N-CD	5.84	140.66	128.40
1	A	106	PRO	N-CA-C	-5.83	96.94	112.10
1	B	118	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	B	118	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	A	224	ASP	CB-CG-OD1	5.46	123.21	118.30
2	D	298	DG	O5'-P-OP1	-5.28	100.95	105.70
1	B	119	ARG	CG-CD-NE	-5.26	100.76	111.80
1	B	67	GLN	C-N-CD	5.22	139.36	128.40
1	B	223	PRO	C-N-CA	5.20	134.69	121.70
2	E	299	DT	O5'-P-OP1	-5.09	101.12	105.70
1	A	179	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	78	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	187	LYS	CD-CE-NZ	5.03	123.28	111.70
1	A	58	LEU	CB-CG-CD1	-5.00	102.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	PRO	Peptide
1	B	104	ALA	Peptide

## 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	2148	0	2128	66	1
1	B	2078	0	2057	79	1
1	C	2066	0	2042	107	0
2	D	527	0	298	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	527	0	298	12	0
2	F	527	0	298	22	0
3	B	6	0	8	0	0
4	A	186	0	0	10	0
4	B	121	0	0	14	0
4	C	8	0	0	0	0
4	D	29	0	0	2	0
4	E	13	0	0	0	0
4	F	3	0	0	0	0
All	All	8239	0	7129	283	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 19.

All (283) 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:C:43:SER:HB3	1:C:67:GLN:CG	1.41	1.46
1:C:43:SER:CB	1:C:67:GLN:HG2	1.49	1.42
1:C:104:ALA:HB1	1:C:105:PRO:CD	1.69	1.20
1:C:43:SER:OG	1:C:67:GLN:HG2	1.41	1.18
1:B:179:ARG:NH2	4:B:601:HOH:O	1.77	1.15
1:B:3:GLU:OE1	1:B:175:GLY:CA	1.94	1.14
1:C:43:SER:HB3	1:C:67:GLN:HG3	1.17	1.13
1:C:104:ALA:CB	1:C:105:PRO:HD2	1.79	1.12
1:A:34:ARG:HH11	1:A:34:ARG:HG2	1.11	1.10
1:B:3:GLU:OE1	1:B:175:GLY:C	1.90	1.09
1:C:43:SER:CB	1:C:67:GLN:CG	2.15	1.03
1:C:105:PRO:HB2	1:C:106:PRO:CD	1.88	1.03
1:C:275:HIS:ND1	1:C:275:HIS:O	1.91	1.02
1:C:67:GLN:HB3	1:C:68:PRO:CD	1.93	0.99
1:B:2:GLY:O	4:B:602:HOH:O	1.82	0.98
2:D:308:DG:H2''	2:D:309:DA:H5'	1.44	0.98
1:C:105:PRO:HB2	1:C:106:PRO:HD2	1.43	0.97
1:C:138:LEU:HD11	1:C:233:PRO:HB2	1.45	0.97
1:B:194:ALA:O	1:B:197:VAL:HG23	1.64	0.96
1:A:242:ARG:NH2	2:D:297:CTG:H3	1.64	0.96
2:F:317:DG:H2''	2:F:318:DG:OP2	1.61	0.95
1:A:242:ARG:HH22	2:D:297:CTG:H3	1.12	0.93
1:A:242:ARG:HD3	4:A:503:HOH:O	1.69	0.92
1:A:197:VAL:O	1:A:201:LEU:HD23	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:HG3	1:C:95:ARG:HH11	1.31	0.92
1:A:198:LEU:HD13	1:A:201:LEU:HD21	1.51	0.92
1:C:104:ALA:HB1	1:C:105:PRO:HD2	0.94	0.91
1:C:105:PRO:O	1:C:107:GLY:N	2.04	0.89
1:C:67:GLN:CB	1:C:68:PRO:HD2	2.03	0.89
2:F:293:DT:OP1	2:F:293:DT:H4'	1.69	0.89
1:B:155:LYS:H	1:B:155:LYS:HE3	1.38	0.89
1:C:67:GLN:HB3	1:C:68:PRO:HD2	1.53	0.87
1:C:43:SER:HG	1:C:67:GLN:HG2	1.39	0.87
1:A:67:GLN:HA	1:A:68:PRO:O	1.73	0.87
1:B:71:GLU:HG3	1:B:72:PRO:HD2	1.58	0.86
1:C:105:PRO:CB	1:C:106:PRO:HD2	2.07	0.85
1:C:95:ARG:CG	1:C:95:ARG:HH11	1.93	0.82
1:A:159:ARG:HH12	1:A:274:ARG:HD3	1.45	0.82
2:F:293:DT:H2''	2:F:294:DC:O5'	1.81	0.81
1:C:125:LEU:HD12	1:C:125:LEU:H	1.46	0.81
1:B:105:PRO:HG2	1:B:106:PRO:HD3	1.61	0.80
1:B:23:PHE:HB3	4:B:605:HOH:O	1.80	0.80
1:C:67:GLN:CB	1:C:68:PRO:CD	2.60	0.80
1:A:195:ARG:O	1:A:199:GLU:HB2	1.83	0.79
1:B:198:LEU:C	1:B:199:GLU:HG2	2.02	0.79
1:B:3:GLU:OE2	1:B:177:TYR:CD2	2.36	0.78
1:B:201:LEU:HD12	1:B:201:LEU:H	1.48	0.78
1:B:199:GLU:OE1	1:B:201:LEU:HD11	1.83	0.78
1:B:3:GLU:OE1	1:B:175:GLY:HA3	1.83	0.78
1:A:130:GLN:NE2	1:A:133:ARG:HE	1.84	0.75
1:B:194:ALA:O	1:B:197:VAL:CG2	2.35	0.75
2:D:307:DA:H2''	2:D:308:DG:O5'	1.86	0.74
1:A:34:ARG:HG2	1:A:34:ARG:NH1	1.87	0.74
1:B:2:GLY:N	2:E:297:CTG:O2	2.20	0.74
1:A:155:LYS:H	1:A:155:LYS:HZ2	1.35	0.73
1:C:34:ARG:NH1	1:C:34:ARG:HB2	2.03	0.73
1:C:148:VAL:HG22	1:C:170:PHE:HB3	1.70	0.73
1:C:275:HIS:NE2	2:F:299:DT:O4	2.20	0.73
1:C:141:TYR:OH	1:C:145:ARG:NH1	2.20	0.72
1:B:3:GLU:OE1	1:B:175:GLY:N	2.22	0.72
1:B:201:LEU:HD12	1:B:201:LEU:N	2.04	0.72
1:A:184:TYR:O	1:A:187:LYS:HE2	1.89	0.72
1:C:99:LEU:HB2	1:C:123:TRP:CH2	2.25	0.72
1:B:159:ARG:HD2	1:B:274:ARG:HH22	1.56	0.71
1:B:69:GLN:CD	1:B:69:GLN:H	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:PRO:CB	1:C:106:PRO:CD	2.65	0.71
1:C:105:PRO:CG	1:C:106:PRO:HD2	2.21	0.70
1:C:263:TYR:OH	2:F:297:CTG:OP1	2.08	0.70
1:B:198:LEU:O	1:B:199:GLU:HG2	1.92	0.69
1:A:34:ARG:HH11	1:A:34:ARG:CG	1.99	0.69
2:D:301:DT:H2'	4:D:413:HOH:O	1.91	0.68
1:B:67:GLN:HA	1:B:68:PRO:C	2.14	0.68
1:A:275[B]:HIS:HE1	2:D:308:DG:O6	1.75	0.68
2:F:316:DC:H2''	2:F:317:DG:O5'	1.94	0.68
2:F:308:DG:H2''	2:F:309:DA:H5'	1.75	0.68
1:C:43:SER:CB	1:C:67:GLN:HG3	2.05	0.68
1:C:242:ARG:HA	1:C:252:ASP:HB2	1.76	0.67
1:C:160:PRO:HB3	1:C:191:PHE:HA	1.75	0.67
1:A:198:LEU:CD1	1:A:201:LEU:HD21	2.25	0.66
1:C:274:ARG:HH11	1:C:274:ARG:HG2	1.60	0.66
1:B:105:PRO:CG	1:B:106:PRO:HD3	2.26	0.66
2:E:307:DA:H2''	2:E:308:DG:OP2	1.96	0.65
1:A:67:GLN:NE2	4:A:501:HOH:O	1.57	0.65
1:C:105:PRO:HG2	1:C:106:PRO:HD2	1.78	0.65
1:A:106:PRO:O	1:A:106:PRO:HD2	1.96	0.64
2:E:291:DC:H2''	2:E:292:DG:H5'	1.78	0.64
1:C:67:GLN:HB2	1:C:68:PRO:HD2	1.79	0.64
1:C:8:HIS:HE1	1:C:139:GLN:NE2	1.96	0.64
1:B:130:GLN:NE2	1:B:133:ARG:HE	1.96	0.63
1:A:81:MET:SD	2:D:298:DG:H5''	2.38	0.63
1:B:69:GLN:OE1	1:B:69:GLN:N	2.32	0.63
1:B:104:ALA:HB1	1:B:105:PRO:CD	2.29	0.62
1:C:8:HIS:CE1	1:C:139:GLN:NE2	2.67	0.62
1:A:88:VAL:HG21	1:A:94:PRO:HD3	1.81	0.62
1:C:34:ARG:HH11	1:C:34:ARG:HB2	1.63	0.62
1:B:161:ILE:HD13	1:B:194:ALA:HA	1.81	0.62
1:C:138:LEU:CD1	1:C:233:PRO:HB2	2.25	0.62
1:A:67:GLN:CA	1:A:68:PRO:O	2.45	0.61
1:C:273:ASP:O	1:C:276:GLY:N	2.31	0.61
2:D:301:DT:H6	4:D:413:HOH:O	1.84	0.60
1:C:29:LYS:HD3	1:C:37:GLU:OE2	2.01	0.60
1:A:275[B]:HIS:CE1	2:D:308:DG:O6	2.54	0.60
1:B:201:LEU:H	1:B:201:LEU:CD1	2.13	0.60
1:B:159:ARG:HD2	1:B:274:ARG:NH2	2.16	0.60
1:B:78:ARG:NH1	2:E:300:DC:OP1	2.34	0.60
1:C:274:ARG:HD3	1:C:275:HIS:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LEU:O	1:C:65:GLY:N	2.35	0.59
1:A:67:GLN:HA	1:A:68:PRO:C	2.23	0.59
1:C:48:SER:HB2	1:C:59:ILE:HB	1.84	0.58
1:B:155:LYS:H	1:B:155:LYS:CE	2.15	0.57
1:C:8:HIS:HE1	1:C:139:GLN:HE22	1.51	0.57
1:A:106:PRO:CD	1:A:106:PRO:O	2.52	0.57
1:C:175:GLY:HA3	2:F:298:DG:OP1	2.04	0.57
2:E:295:DC:H2''	2:E:296:DA:C8	2.39	0.57
1:B:65:GLY:HA3	1:C:239:LEU:HD23	1.87	0.57
2:E:291:DC:H2'	2:E:292:DG:C8	2.39	0.57
1:C:155:LYS:HD3	1:C:155:LYS:H	1.70	0.56
1:C:3:GLU:CD	1:C:175:GLY:HA3	2.25	0.56
1:B:224:ASP:HB2	1:B:227:GLU:CB	2.34	0.56
1:C:95:ARG:HG3	1:C:95:ARG:NH1	2.07	0.56
1:A:274:ARG:HH11	1:A:275[A]:HIS:CE1	2.23	0.56
1:A:9:LEU:HD13	1:A:242:ARG:HG2	1.87	0.56
1:C:274:ARG:O	1:C:275:HIS:HB3	2.04	0.56
1:C:2:GLY:HA2	2:F:297:CTG:O2	2.06	0.56
1:B:234:LYS:HE2	4:B:675:HOH:O	2.04	0.56
1:C:242:ARG:HA	1:C:252:ASP:CB	2.36	0.56
1:C:147:ASN:HD22	1:C:147:ASN:C	2.08	0.55
1:C:199:GLU:O	1:C:200:ALA:HB2	2.05	0.55
1:A:242:ARG:NH2	2:D:297:CTG:N3	2.43	0.55
1:B:130:GLN:HE21	1:B:133:ARG:HE	1.52	0.55
1:A:155:LYS:H	1:A:155:LYS:NZ	2.05	0.54
2:F:316:DC:C2'	2:F:317:DG:O5'	2.54	0.54
2:F:317:DG:C2'	2:F:318:DG:OP2	2.44	0.54
1:A:155:LYS:HB2	1:A:155:LYS:NZ	2.22	0.54
1:B:118:ARG:O	1:B:119:ARG:HB2	2.08	0.54
1:C:29:LYS:HE2	1:C:33:SER:O	2.08	0.54
1:C:66:ALA:O	1:C:67:GLN:O	2.25	0.53
1:A:197:VAL:O	1:A:201:LEU:CD2	2.52	0.53
1:B:278:THR:C	4:B:601:HOH:O	2.47	0.53
2:D:308:DG:C2'	2:D:309:DA:H5'	2.28	0.53
1:C:45:TYR:HE2	1:C:47:ILE:HD11	1.73	0.53
1:C:78:ARG:NH1	1:C:122:ARG:HB2	2.23	0.53
1:C:140:GLU:O	1:C:144:PHE:HB3	2.09	0.53
1:B:91:GLU:HA	1:B:91:GLU:OE1	2.09	0.53
1:A:130:GLN:HE21	1:A:133:ARG:HE	1.55	0.53
1:C:265:MET:O	1:C:268:MET:HB2	2.09	0.52
1:C:46:ARG:HH11	1:C:63:LEU:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:NH1	1:A:274:ARG:HD3	2.20	0.52
1:A:2[B]:GLY:N	4:A:512:HOH:O	2.41	0.52
1:C:30:SER:HB3	1:C:98:HIS:HA	1.92	0.52
1:A:159:ARG:HH12	1:A:274:ARG:CD	2.18	0.52
1:C:232:VAL:HB	1:C:233:PRO:CD	2.39	0.52
1:B:71:GLU:CG	1:B:72:PRO:HD2	2.35	0.51
1:A:167:ASP:OD1	1:A:169[B]:ARG:HG2	2.10	0.51
1:B:224:ASP:HB2	1:B:227:GLU:HB2	1.92	0.51
1:C:23:PHE:HB3	1:C:45:TYR:CZ	2.46	0.51
1:A:70:GLN:O	4:A:502:HOH:O	2.19	0.51
1:A:2[A]:GLY:HA3	2:D:297:CTG:H2"	1.94	0.50
1:B:159:ARG:HB3	1:B:160:PRO:HD2	1.94	0.50
2:F:291:DC:H2'	2:F:292:DG:C8	2.47	0.50
1:A:187:LYS:NZ	4:A:510:HOH:O	2.41	0.50
1:A:72:PRO:HG3	4:A:634:HOH:O	2.11	0.50
1:B:161:ILE:HD13	1:B:197:VAL:HG21	1.94	0.49
1:B:234:LYS:NZ	4:B:604:HOH:O	2.35	0.49
2:E:293:DT:H2"	2:E:294:DC:C6	2.46	0.49
1:B:105:PRO:CD	1:B:106:PRO:HD3	2.43	0.49
1:A:198:LEU:HA	1:A:201:LEU:CD2	2.43	0.48
1:C:154:ASP:HB3	1:C:157:PHE:HD2	1.78	0.48
1:C:95:ARG:CG	1:C:95:ARG:NH1	2.64	0.48
1:A:89:PRO:HD3	4:A:617:HOH:O	2.12	0.48
1:C:99:LEU:HD22	1:C:123:TRP:CE2	2.49	0.48
1:C:104:ALA:CB	1:C:105:PRO:CD	2.47	0.48
1:B:194:ALA:HA	1:B:197:VAL:CG2	2.43	0.48
1:C:159:ARG:NH1	1:C:274:ARG:HG2	2.29	0.48
1:A:242:ARG:HH22	2:D:297:CTG:C4	2.27	0.48
1:B:270:SER:HA	1:B:279:ILE:O	2.14	0.48
2:F:308:DG:C2'	2:F:309:DA:H5'	2.44	0.47
1:B:224:ASP:HB2	1:B:227:GLU:HB3	1.96	0.47
1:A:275[B]:HIS:O	1:A:275[B]:HIS:CG	2.67	0.47
1:B:169:ARG:HD2	4:B:638:HOH:O	2.13	0.47
1:C:36:PRO:HG3	1:C:125:LEU:HD11	1.97	0.47
2:F:293:DT:H6	2:F:293:DT:H5"	1.79	0.47
1:C:154:ASP:H	1:C:195:ARG:HH21	1.61	0.47
2:F:308:DG:H2"	2:F:309:DA:H8	1.79	0.47
1:A:198:LEU:HA	1:A:201:LEU:HD21	1.97	0.47
1:A:70:GLN:HE21	1:A:70:GLN:HA	1.80	0.47
1:C:154:ASP:HB3	1:C:157:PHE:CD2	2.50	0.47
2:F:311:DC:H2'	2:F:312:DT:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD11	1:B:198:LEU:O	2.14	0.47
1:C:196:SER:HA	1:C:199:GLU:OE1	2.15	0.47
2:F:292:DG:H2''	2:F:293:DT:H5''	1.96	0.47
1:B:39:PRO:HB3	4:B:706:HOH:O	2.14	0.46
1:A:241:GLY:O	1:A:244:TYR:HB2	2.16	0.46
1:C:274:ARG:CG	1:C:274:ARG:HH11	2.24	0.46
1:C:23:PHE:CD2	1:C:102:TYR:O	2.67	0.46
1:C:141:TYR:OH	1:C:145:ARG:HD2	2.16	0.46
1:C:275:HIS:NE2	2:F:299:DT:H73	2.31	0.46
1:B:222:ASN:N	1:B:223:PRO:HD2	2.31	0.46
1:A:23:PHE:CE1	1:A:47:ILE:HD12	2.51	0.46
1:C:273:ASP:O	1:C:274:ARG:C	2.52	0.46
1:A:274:ARG:NH2	2:D:306:DT:O5'	2.48	0.46
1:C:99:LEU:HB2	1:C:123:TRP:CZ3	2.50	0.46
1:A:274:ARG:HH12	2:D:306:DT:H6	1.63	0.46
1:A:270:SER:HA	1:A:279:ILE:O	2.16	0.46
1:A:70:GLN:HE21	1:A:70:GLN:CA	2.26	0.45
1:C:274:ARG:CZ	1:C:274:ARG:HB2	2.46	0.45
1:B:263:TYR:OH	2:E:297:CTG:OP1	2.22	0.45
1:C:263:TYR:CD1	1:C:280:TRP:CD1	3.04	0.45
1:B:3:GLU:HG2	2:E:298:DG:OP1	2.16	0.45
1:B:149:LEU:HD22	1:B:201:LEU:HA	1.99	0.45
1:C:141:TYR:O	1:C:142:GLN:C	2.55	0.45
1:C:155:LYS:HA	1:C:158:ASP:OD2	2.17	0.45
2:D:302:DA:H2'	2:D:302:DA:OP2	2.17	0.45
2:F:306:DT:H2''	2:F:307:DA:C8	2.51	0.45
1:C:88:VAL:O	1:C:111:ALA:N	2.39	0.45
1:B:186:LEU:HB2	1:B:188:ILE:HD12	1.98	0.44
2:F:295:DC:H2''	2:F:296:DA:C8	2.53	0.44
1:A:46:ARG:NH1	4:A:508:HOH:O	2.40	0.44
1:A:88:VAL:HB	1:A:89:PRO:HD2	2.00	0.44
1:B:222:ASN:N	1:B:223:PRO:CD	2.81	0.44
1:B:56:LEU:HD23	1:B:56:LEU:C	2.38	0.44
1:B:242:ARG:NH2	2:E:297:CTG:O4	2.51	0.44
1:C:23:PHE:O	1:C:44:ALA:HA	2.17	0.44
2:E:311:DC:H2'	2:E:312:DT:C6	2.52	0.44
1:B:189:PRO:HB2	1:B:192:GLU:HG2	2.00	0.44
1:C:274:ARG:CG	1:C:274:ARG:NH1	2.80	0.44
1:B:90:ARG:HD3	1:B:109:ARG:NH2	2.32	0.44
1:C:155:LYS:CD	1:C:155:LYS:H	2.30	0.44
1:B:189:PRO:HA	1:B:190:PRO:HD2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:PRO:HD3	1:C:147:ASN:OD1	2.18	0.43
2:F:316:DC:H2'	2:F:317:DG:C8	2.54	0.43
1:A:222:ASN:N	1:A:223:PRO:HD3	2.33	0.43
1:C:29:LYS:HG2	1:C:30:SER:O	2.18	0.43
1:B:222:ASN:ND2	4:B:614:HOH:O	2.50	0.43
2:F:293:DT:H2'	2:F:294:DC:C6	2.54	0.43
1:A:99:LEU:C	1:A:100:ARG:HG2	2.39	0.43
1:A:46:ARG:HG3	1:A:63:LEU:HD21	2.01	0.43
1:A:70:GLN:NE2	1:A:70:GLN:HA	2.34	0.43
1:C:223:PRO:HA	1:C:227:GLU:OE1	2.18	0.43
4:A:590:HOH:O	2:D:296:DA:H4'	2.19	0.43
1:B:153:ALA:N	4:B:606:HOH:O	2.37	0.43
1:B:232:VAL:O	1:B:235:GLU:HB2	2.19	0.43
1:B:272:GLN:HG2	4:B:677:HOH:O	2.18	0.43
1:B:193:LYS:O	1:B:197:VAL:HG22	2.18	0.43
1:C:136:CYS:O	1:C:138:LEU:N	2.52	0.43
1:B:186:LEU:HG	1:B:228:LEU:HD12	2.01	0.42
1:C:187:LYS:HZ1	1:C:282:GLN:HB3	1.84	0.42
1:A:2[A]:GLY:N	4:A:523:HOH:O	2.52	0.42
1:C:41:GLU:O	1:C:68:PRO:CG	2.67	0.42
1:C:63:LEU:HB3	1:C:64:PRO:HD2	2.01	0.42
2:D:292:DG:H2''	2:D:293:DT:H5'	2.01	0.42
1:A:56:LEU:C	1:A:56:LEU:HD23	2.40	0.42
1:A:63:LEU:HB3	1:A:64:PRO:CD	2.49	0.42
1:C:147:ASN:ND2	1:C:147:ASN:C	2.72	0.42
1:C:54:LYS:HE3	1:C:168:GLN:OE1	2.20	0.42
1:A:155:LYS:H	1:A:155:LYS:CE	2.33	0.42
1:B:104:ALA:HB1	1:B:105:PRO:HD3	1.98	0.42
1:C:6:GLU:CD	1:C:6:GLU:H	2.22	0.42
1:B:187:LYS:HD3	1:B:187:LYS:HA	1.65	0.42
1:B:199:GLU:HA	1:B:200:ALA:C	2.38	0.42
1:B:257:ARG:O	4:B:603:HOH:O	2.21	0.42
1:B:67:GLN:HA	1:B:68:PRO:O	2.18	0.42
1:B:92:GLU:HA	4:B:610:HOH:O	2.19	0.42
1:A:195:ARG:O	1:A:199:GLU:N	2.53	0.41
1:C:136:CYS:C	1:C:138:LEU:N	2.73	0.41
1:C:58:LEU:HD12	1:C:77:PHE:CE1	2.55	0.41
1:C:284:ASP:HA	1:C:285:PRO:HD3	1.78	0.41
1:A:2[B]:GLY:HA2	2:D:297:CTG:H2''	2.02	0.41
1:B:241:GLY:C	1:B:243:GLY:N	2.73	0.41
1:A:184:TYR:O	1:A:187:LYS:CE	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:CYS:O	1:C:265:MET:HB2	2.20	0.41
1:C:29:LYS:CE	1:C:33:SER:O	2.68	0.41
2:E:316:DC:H2"	2:E:317:DG:C8	2.56	0.41
1:A:155:LYS:HB2	1:A:155:LYS:HZ3	1.86	0.41
1:A:63:LEU:HB3	1:A:64:PRO:HD2	2.03	0.41
1:B:241:GLY:O	1:B:243:GLY:N	2.53	0.41
1:C:148:VAL:CG2	1:C:170:PHE:HB3	2.45	0.41
1:B:130:GLN:HA	1:B:131:PRO:HD3	2.01	0.41
1:B:95:ARG:CB	1:B:95:ARG:HH11	2.33	0.41
1:B:104:ALA:HB1	1:B:105:PRO:HD2	2.03	0.41
1:C:178:LEU:HA	1:C:178:LEU:HD23	1.85	0.40
1:B:279:ILE:N	4:B:601:HOH:O	2.54	0.40
1:C:274:ARG:O	1:C:275:HIS:CB	2.70	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:199:GLU:OE1	1:B:34:ARG:NE[3_644]	2.03	0.17

## 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	263/400 (66%)	252 (96%)	9 (3%)	2 (1%)	24	39
1	B	256/400 (64%)	240 (94%)	15 (6%)	1 (0%)	39	59
1	C	255/400 (64%)	217 (85%)	31 (12%)	7 (3%)	6	8
All	All	774/1200 (64%)	709 (92%)	55 (7%)	10 (1%)	15	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	C	67	GLN
1	C	105	PRO
1	C	64	PRO
1	C	36	PRO
1	C	106	PRO
1	C	199	GLU
1	B	242	ARG
1	C	104	ALA
1	A	68	PRO

### 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	224/334 (67%)	215 (96%)	9 (4%)	38	63
1	B	216/334 (65%)	198 (92%)	18 (8%)	14	25
1	C	214/334 (64%)	188 (88%)	26 (12%)	6	10
All	All	654/1002 (65%)	601 (92%)	53 (8%)	14	26

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	34	ARG
1	A	70	GLN
1	A	155	LYS
1	A	242	ARG
1	A	251	GLU
1	A	253	PHE
1	A	257	ARG
1	A	272	GLN
1	B	30	SER
1	B	34	ARG
1	B	63	LEU
1	B	67	GLN

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Mol	Chain	Res	Type
1	B	69	GLN
1	B	70	GLN
1	B	95	ARG
1	B	100	ARG
1	B	139	GLN
1	B	144	PHE
1	B	155	LYS
1	B	197	VAL
1	B	199	GLU
1	B	238	GLN
1	B	244	TYR
1	B	252	ASP
1	B	257	ARG
1	B	265	MET
1	C	16	GLU
1	C	34	ARG
1	C	46	ARG
1	C	50	SER
1	C	69	GLN
1	C	70	GLN
1	C	73	LEU
1	C	76	VAL
1	C	85	PHE
1	C	95	ARG
1	C	103	THR
1	C	123	TRP
1	C	124	ASP
1	C	125	LEU
1	C	128	LYS
1	C	139	GLN
1	C	144	PHE
1	C	147	ASN
1	C	155	LYS
1	C	177	TYR
1	C	187	LYS
1	C	222	ASN
1	C	238	GLN
1	C	252	ASP
1	C	257	ARG
1	C	274	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	147	ASN
1	A	272	GLN
1	B	70	GLN
1	B	130	GLN
1	C	8	HIS
1	C	70	GLN
1	C	130	GLN
1	C	139	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
2	CTG	D	297	2	16,23,24	1.02	1 (6%)	18,35,38	1.55	5 (27%)
2	CTG	E	297	2	16,23,24	0.91	0	18,35,38	1.62	5 (27%)
2	CTG	F	297	2	16,23,24	1.07	2 (12%)	18,35,38	1.16	4 (22%)

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
2	CTG	D	297	2	-	0/7/45/46	0/2/2/2
2	CTG	E	297	2	-	0/7/45/46	0/2/2/2
2	CTG	F	297	2	-	0/7/45/46	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	297	CTG	C4-N3	-2.15	1.34	1.37
2	D	297	CTG	C2-N3	-2.05	1.34	1.38
2	F	297	CTG	O6-C6	2.23	1.44	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	297	CTG	C3'-C2'-C1'	-3.10	94.88	102.40
2	E	297	CTG	O5-C5-C5M	-2.92	103.24	109.09
2	E	297	CTG	C2'-C1'-N1	-2.87	111.71	115.64
2	D	297	CTG	O3'-C3'-C4'	-2.74	98.78	110.10
2	F	297	CTG	O5-C5-C5M	-2.24	104.60	109.09
2	E	297	CTG	O3'-C3'-C4'	-2.24	100.87	110.10
2	E	297	CTG	C3'-C2'-C1'	-2.21	97.05	102.40
2	D	297	CTG	O2-C2-N1	-2.10	120.23	123.35
2	F	297	CTG	C4-N3-C2	-2.10	123.19	126.83
2	E	297	CTG	C4-N3-C2	-2.04	123.30	126.83
2	F	297	CTG	O3'-C3'-C4'	-2.02	101.77	110.10
2	F	297	CTG	N3-C2-N1	2.07	118.85	116.82
2	D	297	CTG	O4'-C1'-C2'	2.13	110.46	106.28
2	D	297	CTG	C2'-C3'-C4'	2.41	107.66	102.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	297	CTG	6	0
2	E	297	CTG	3	0
2	F	297	CTG	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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	$\# Z  > 2$
3	GOL	B	501	-	5,5,5	1.02	0	5,5,5	1.07	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
3	GOL	B	501	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	265/400 (66%)	0.33	15 (5%) 27 31	16, 24, 52, 98	0
1	B	262/400 (65%)	0.56	14 (5%) 30 34	16, 32, 59, 122	0
1	C	261/400 (65%)	1.52	68 (26%) 1 1	39, 67, 93, 151	0
2	D	25/26 (96%)	0.42	2 (8%) 15 16	35, 55, 81, 101	0
2	E	25/26 (96%)	0.62	4 (16%) 3 2	32, 55, 70, 74	0
2	F	25/26 (96%)	1.04	5 (20%) 1 1	64, 81, 105, 110	0
All	All	863/1278 (67%)	0.79	108 (12%) 5 5	16, 40, 86, 151	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	PRO	12.2
1	C	66	ALA	10.6
1	C	65	GLY	9.3
1	C	22	VAL	8.4
1	C	67	GLN	8.1
1	C	64	PRO	7.9
1	C	243	GLY	7.2
1	C	105	PRO	7.0
1	C	241	GLY	6.8
1	C	21	LEU	6.7
1	C	44	ALA	6.6
1	B	243	GLY	6.5
1	C	19	ARG	6.2
1	B	240	GLY	5.9
1	C	107	GLY	5.8
1	C	110	LEU	5.8
1	B	242	ARG	5.6
1	C	244	TYR	5.3
1	C	108	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	75	LEU	5.2
1	C	63	LEU	5.1
1	C	46	ARG	5.1
1	C	266	PRO	4.8
1	B	241	GLY	4.8
1	A	2[A]	GLY	4.7
1	C	69	GLN	4.4
1	C	109	ARG	4.4
1	C	104	ALA	4.3
1	A	200	ALA	4.2
1	C	91	GLU	4.1
1	C	20	ALA	4.1
1	C	43	SER	4.0
1	C	242	ARG	4.0
2	E	318	DG	4.0
1	C	155	LYS	4.0
1	C	125	LEU	3.9
1	C	89	PRO	3.9
1	B	2	GLY	3.8
1	C	150	ARG	3.6
1	C	129	TRP	3.5
1	B	267	GLY	3.5
1	A	7	LEU	3.4
2	D	303	DC	3.3
1	C	41	GLU	3.3
1	C	25	GLY	3.3
1	C	26	CYS	3.2
1	C	92	GLU	3.2
2	F	316	DC	3.1
1	C	153	ALA	3.1
1	C	71	GLU	3.1
1	B	69	GLN	3.0
2	F	318	DG	3.0
1	C	70	GLN	2.9
1	C	78	ARG	2.9
1	B	266	PRO	2.9
1	C	271	LEU	2.9
1	C	79	PHE	2.8
2	E	291	DC	2.8
1	C	60	LEU	2.8
1	C	147	ASN	2.8
1	C	281	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	282	GLN	2.7
1	C	34	ARG	2.7
1	C	200	ALA	2.7
1	C	85	PHE	2.6
1	C	62	PRO	2.6
1	C	280	TRP	2.6
1	A	54	LYS	2.5
1	C	24	GLY	2.5
1	B	65	GLY	2.5
1	A	250	GLU	2.5
1	C	173	GLY	2.5
1	C	90	ARG	2.5
2	F	303	DC	2.5
1	C	9	LEU	2.5
1	A	274	ARG	2.4
1	C	159	ARG	2.4
1	B	255	ALA	2.4
1	A	11	SER	2.4
1	A	10	ALA	2.4
1	C	170	PHE	2.4
1	A	5	PRO	2.4
2	D	302	DA	2.4
2	F	317	DG	2.3
1	C	38	VAL	2.3
1	C	272	GLN	2.3
1	C	264	GLY	2.3
1	C	287	PRO	2.3
1	B	244	TYR	2.2
1	A	253	PHE	2.2
1	C	289	ALA	2.2
1	C	114	PHE	2.2
1	A	175	GLY	2.2
1	C	240	GLY	2.2
1	A	4	GLY	2.2
1	C	149	LEU	2.2
1	A	3	GLU	2.2
2	E	303	DC	2.1
1	C	152	LEU	2.1
1	B	254	ALA	2.1
1	B	34	ARG	2.1
2	E	317	DG	2.0
1	C	61	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	84	SER	2.0
1	B	274	ARG	2.0
1	C	120	PHE	2.0
1	A	56	LEU	2.0
2	F	306	DT	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CTG	E	297	22/23	0.93	0.20	-	40,56,61,64	0
2	CTG	D	297	22/23	0.94	0.24	-	34,47,57,58	0
2	CTG	F	297	22/23	0.91	0.19	-	63,78,85,87	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	501	6/6	0.54	0.54	8.63	57,80,85,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.