WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 02:43 PM JST

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)

The following versions of software and data (see references (i)) were used in the production of this report:

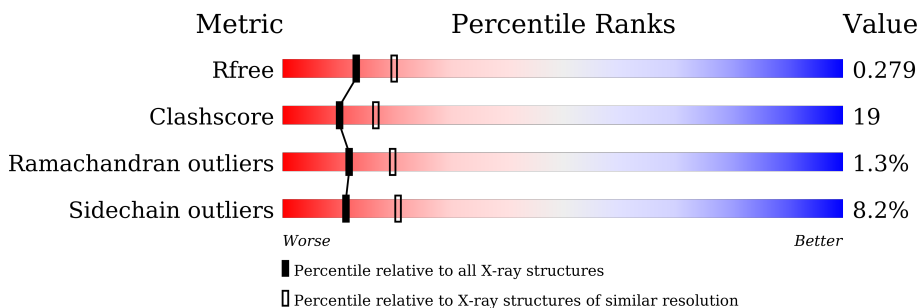|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.48 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	Percentile Ranks	Value
Rfree		0.279
Clashscore		19
Ramachandran outliers		1.3%
Sidechain outliers		8.2%

Worse — *Better*

▌ Percentile relative to all X-ray structures

◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	400	53% 12% • 34%
1	B	400	46% 16% • 34%
1	C	400	40% 21% 5% 35%
2	D	26	50% 42% 8%
2	E	26	38% 54% 8%
2	F	26	31% 65% •

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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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 527	C 252	N 96	O 155	P 24	0	0	0
2	E	26	Total 527	C 252	N 96	O 155	P 24	0	0	0
2	F	26	Total 527	C 252	N 96	O 155	P 24	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
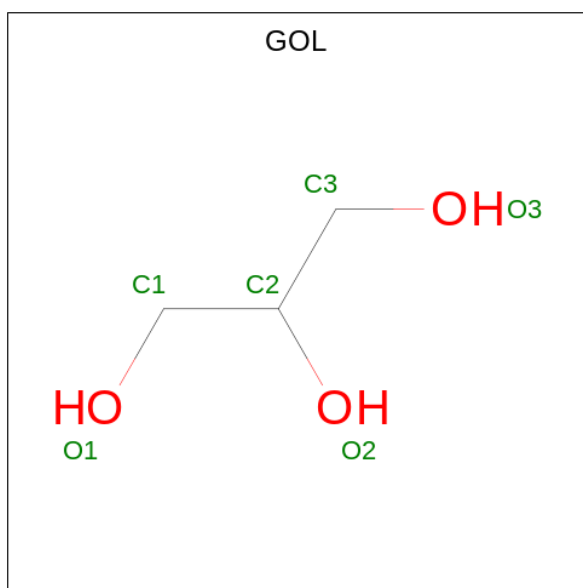
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

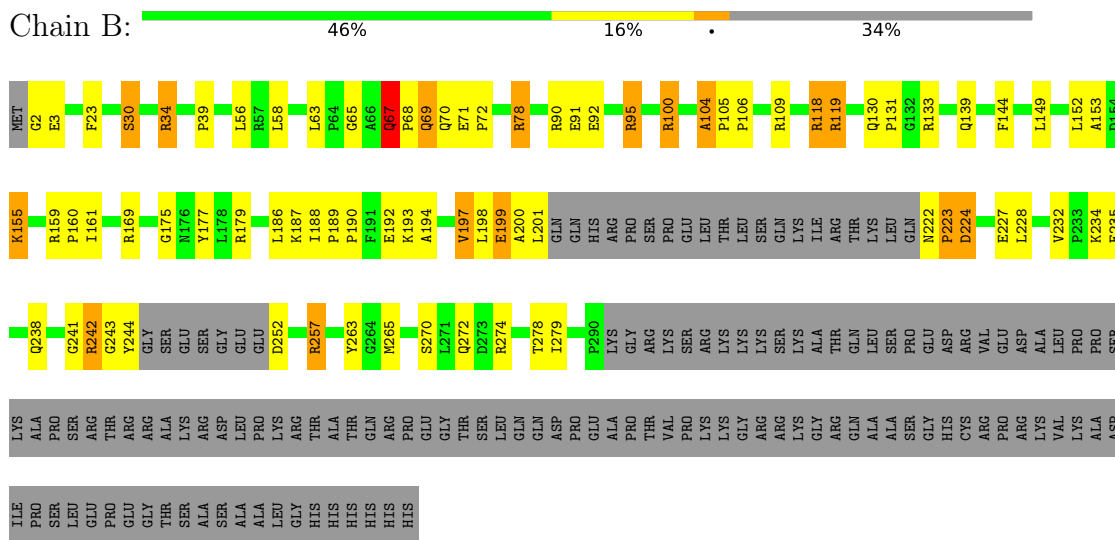These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.
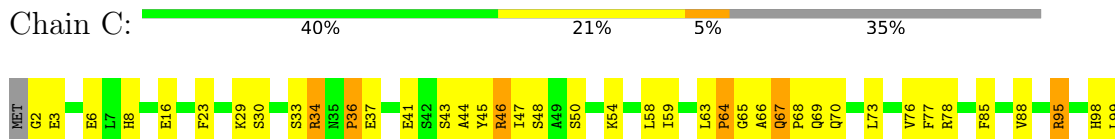
- Molecule 1: Endonuclease 8-like 1

- Molecule 1: Endonuclease 8-like 1

- Molecule 1: Endonuclease 8-like 1

Y102 T103 A104 P105 P106 G107 A111 R122 W123 D124 L125 K128 P135 C136 V137 L138 Q139 E140 Y141 Q142 Q143 F144 R145 E146 N147 V148 D154 K155 A156 F157 D158 R159 P160 Q168 R169 F170 G175 N176 Y177 L178 K187 F191 R195 S196 E199 A200 LEU GLN

GLN HIS ARG PRO SER PRO GLU LEU THR LEU SER GLN LYS ILE ARG THR LYS LEU GLN N222 P223 E227 V232 P233 Q238 L239 R242 G243 Y244 GLY SER GLU SER GLY GLU GLU D252 R257 C262 Y263 G264 M265 M268 D273 R274 H275 G276 W280 F281 Q282 G283

D284 P285 P290 LYS GLY ARG LYS SER ARG LYS LYS SER LYS ALA THR GLN LEU SER PRO GLU ASP ARG VAL GLU ASP ALA LEU PRO PRO SER LYS ALA PRO SER ARG THR ARG ALA LYS ARG ASP LEU PRO LYS ARG THR ALA THR GLN ARG PRO GLU GLY THR SER LEU GLN

GLN ASP PRO GLU ALA PRO THR VAL PRO LYS LYS GLY ARG GLN LYS ALA SER GLY HIS CYS ARG PRO ARG LYS VAL LYS ALA ASP ILE PRO SER LEU GLU PRO GLU GLY GLY THR SER ALA SER ALA ALA LEU GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: DNA (26-MER)

Chain D: 50% 42% 8%

C291 G292 T293 A296 T297 G298 T301 A302 C303 T306 A307 G308 A309 T312 G313 G318

• Molecule 2: DNA (26-MER)

Chain E: 38% 54% 8%

C291 G292 T293 C294 A295 A296 T297 G298 T299 C300 A307 G308 C311 T312 C316 G317 G318

• Molecule 2: DNA (26-MER)

Chain F: 31% 65% ·

C291 G292 T293 C294 A295 A296 T297 G298 T299 T306 A307 G308 A309 C310 C311 T312 C316 G317 G318

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.56 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.176 , 0.225 0.240 , 0.279	Depositor DCC
R_{free} test set	2387 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	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^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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(^{o})	Ideal(^{o})
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 (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	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:HG2	1:A:34:ARG:HH11	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:HH11	1:C:95:ARG:HG3	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:67:GLN:CB	1:C:68:PRO:HD2	2.03	0.89
1:C:105:PRO:O	1:C:107:GLY:N	2.04	0.89
2:F:293:DT:H4'	2:F:293:DT:OP1	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:HH11	1:C:95:ARG:CG	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:H	1:C:125:LEU:HD12	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:H	1:B:201:LEU:HD12	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:HZ2	1:A:155:LYS:H	1.35	0.73
1:C:34:ARG:HB2	1:C:34:ARG:NH1	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:HG2	1:C:274:ARG:HH11	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:HD2	1:A:106:PRO:O	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:N	1:B:69:GLN:OE1	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:HB2	1:C:34:ARG:HH11	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:78:ARG:NH1	2:E:300:DC:OP1	2.34	0.60
1:B:159:ARG:HD2	1:B:274:ARG:NH2	2.16	0.60
1:B:201:LEU:H	1:B:201:LEU:CD1	2.13	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:O	1:A:106:PRO:CD	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:3:GLU:CD	1:C:175:GLY:HA3	2.25	0.56
1:C:155:LYS:H	1:C:155:LYS:HD3	1.70	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:C	1:C:147:ASN:HD22	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:NZ	1:A:155:LYS:HB2	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:2[B]:GLY:N	4:A:512:HOH:O	2.41	0.52
1:A:159:ARG:NH1	1:A:274:ARG:HD3	2.20	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:72:PRO:HG3	4:A:634:HOH:O	2.11	0.50
1:A:187:LYS:NZ	4:A:510:HOH:O	2.41	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:95:ARG:CG	1:C:95:ARG:NH1	2.64	0.48
1:C:154:ASP:HB3	1:C:157:PHE:HD2	1.78	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:A:242:ARG:HH22	2:D:297:CTG:C4	2.27	0.48
1:C:159:ARG:NH1	1:C:274:ARG:HG2	2.29	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:CG	1:A:275[B]:HIS:O	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:H5"	2:F:293:DT:H6	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:70:GLN:HE21	1:A:70:GLN:HA	1.80	0.47
1:A:198:LEU:HA	1:A:201:LEU:HD21	1.97	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:HH11	1:C:274:ARG:CG	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:A:274:ARG:NH2	2:D:306:DT:O5'	2.48	0.46
1:C:273:ASP:O	1:C:274:ARG:C	2.52	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:B:263:TYR:OH	2:E:297:CTG:OP1	2.22	0.45
1:C:274:ARG:HB2	1:C:274:ARG:CZ	2.46	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:OP2	2:D:302:DA:H2'	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:56:LEU:HD23	1:B:56:LEU:C	2.38	0.44
1:B:222:ASN:N	1:B:223:PRO:CD	2.81	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:H	1:C:155:LYS:CD	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:46:ARG:HG3	1:A:63:LEU:HD21	2.01	0.43
1:A:99:LEU:C	1:A:100:ARG:HG2	2.39	0.43
1:A:70:GLN:HA	1:A:70:GLN:NE2	2.34	0.43
4:A:590:HOH:O	2:D:296:DA:H4'	2.19	0.43
1:C:223:PRO:HA	1:C:227:GLU:OE1	2.18	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:54:LYS:HE3	1:C:168:GLN:OE1	2.20	0.42
1:C:147:ASN:C	1:C:147:ASN:ND2	2.72	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:HA	1:B:187:LYS:HD3	1.65	0.42
1:B:67:GLN:HA	1:B:68:PRO:O	2.18	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: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:58:LEU:HD12	1:C:77:PHE:CE1	2.55	0.41
1:C:136:CYS:C	1:C:138:LEU:N	2.73	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:29:LYS:CE	1:C:33:SER:O	2.68	0.41
1:C:262:CYS:O	1:C:265:MET:HB2	2.20	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:95:ARG:HH11	1:B:95:ARG:CB	2.33	0.41
1:B:130:GLN:HA	1:B:131:PRO:HD3	2.01	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:104:ALA:HB1	1:B:105:PRO:HD2	2.03	0.41
1:C:178:LEU:HD23	1:C:178:LEU:HA	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%)	19	33
1	B	256/400 (64%)	240 (94%)	15 (6%)	1 (0%)	34	52
1	C	255/400 (64%)	217 (85%)	31 (12%)	7 (3%)	5	6
All	All	774/1200 (64%)	709 (92%)	55 (7%)	10 (1%)	12	19

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 (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	224/334 (67%)	215 (96%)	9 (4%)	31	53
1	B	216/334 (65%)	198 (92%)	18 (8%)	11	20
1	C	214/334 (64%)	188 (88%)	26 (12%)	5	8
All	All	654/1002 (65%)	601 (92%)	53 (8%)	11	21

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

Sometimes 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	F	297	2	19,23,24	0.98	1 (5%)	21,35,38	1.16	4 (19%)
2	CTG	D	297	2	19,23,24	1.02	1 (5%)	21,35,38	1.82	8 (38%)
2	CTG	E	297	2	19,23,24	0.94	0	21,35,38	1.78	7 (33%)

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	F	297	2	-	1/7/45/46	0/2/2/2
2	CTG	D	297	2	-	2/7/45/46	0/2/2/2
2	CTG	E	297	2	-	2/7/45/46	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	297	CTG	C2-N3	-2.14	1.34	1.38
2	F	297	CTG	C4-N3	-2.07	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	297	CTG	O4'-C1'-N1	-4.14	103.75	108.65
2	E	297	CTG	O5-C5-C4	3.49	115.29	109.87
2	D	297	CTG	C3'-C2'-C1'	-3.05	94.88	102.54
2	E	297	CTG	O5-C5-C5M	-3.01	103.24	109.09
2	D	297	CTG	O3'-C3'-C4'	-2.96	98.78	110.10
2	E	297	CTG	C2'-C1'-N1	-2.87	111.71	115.59
2	E	297	CTG	O3'-C3'-C4'	-2.41	100.87	110.10
2	D	297	CTG	C2'-C3'-C4'	2.35	107.66	102.76
2	F	297	CTG	O5-C5-C5M	-2.31	104.60	109.09
2	F	297	CTG	C4-N3-C2	-2.26	123.19	126.67
2	D	297	CTG	O5-C5-C4	2.24	113.35	109.87
2	D	297	CTG	O4'-C1'-C2'	2.22	110.46	106.25
2	E	297	CTG	C4-N3-C2	-2.19	123.30	126.67
2	E	297	CTG	C3'-C2'-C1'	-2.19	97.05	102.54
2	F	297	CTG	O3'-C3'-C4'	-2.18	101.77	110.10
2	D	297	CTG	O2-C2-N1	-2.10	120.23	123.49
2	F	297	CTG	N3-C2-N1	2.08	118.85	116.69
2	E	297	CTG	O4'-C1'-C2'	2.04	110.11	106.25
2	D	297	CTG	O5'-C5'-C4'	-2.03	102.10	108.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	297	CTG	O4'-C4'-C5'-O5'
2	E	297	CTG	O4'-C4'-C5'-O5'
2	D	297	CTG	C3'-C4'-C5'-O5'
2	E	297	CTG	C3'-C4'-C5'-O5'
2	F	297	CTG	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	1.05	0	5,5,5	1.06	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	-	-	2/4/4/4	-

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
3	B	501	GOL	O1-C1-C2-C3
3	B	501	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.