



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:21 AM EDT

PDB ID : 1OE6 / pdb_00001oe6
Title : Xenopus SMUG1, an anti-mutator uracil-DNA Glycosylase
Authors : Wibley, J.E.A.; Pearl, L.H.
Deposited on : 2003-03-19
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

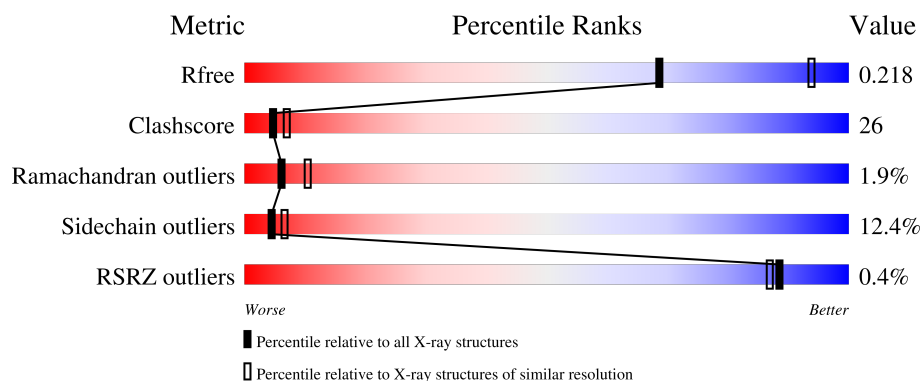
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

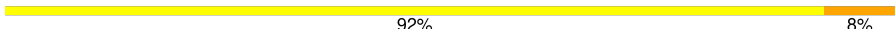
The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	
2	E	12	
3	F	12	

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
4	HMU	A	1282	-	X	-	-
4	HMU	A	1283	-	X	-	-
5	GOL	A	1284	-	X	-	-
6	IPA	A	1285[A]	-	X	X	-
6	IPA	A	1285[B]	-	X	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4499 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 SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL DNA GLYCOSYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	2	0
			1938	1243	339	343	13			
1	B	245	Total	C	N	O	S	0	0	0
			1939	1244	339	344	12			

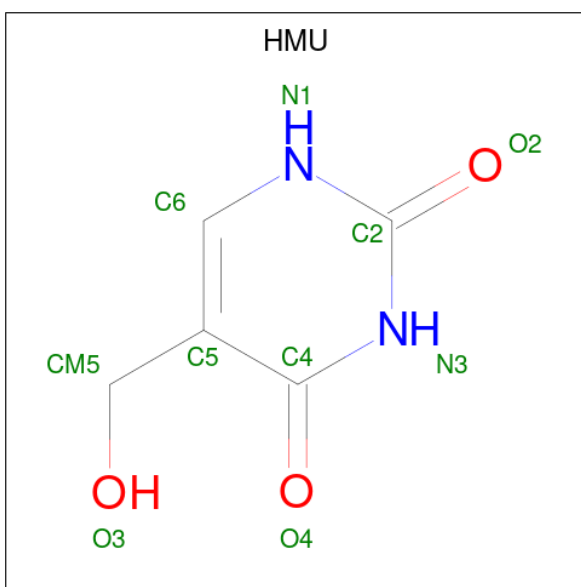
- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	0
			241	115	44	71	11			

- Molecule 3 is a DNA chain called 5'-D(*CP*GP*GP*AP*CP*TP*3DRP*AP*CP*GP*GP*G)-3'.

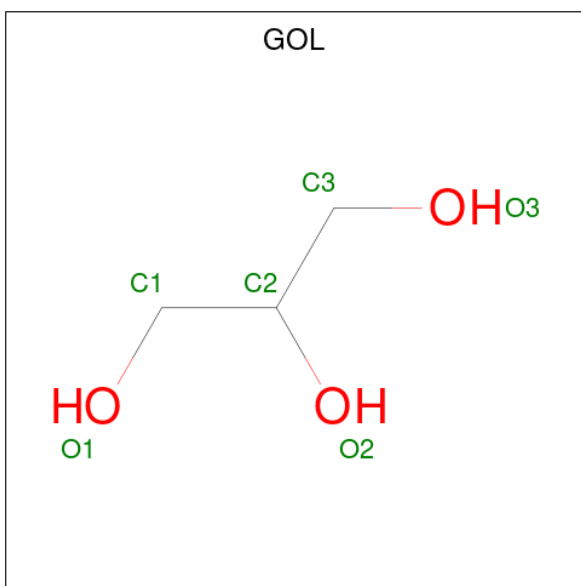
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			237	112	46	68	11			

- Molecule 4 is 5-HYDROXYMETHYL URACIL (CCD ID: HMU) (formula: C₅H₆N₂O₃).



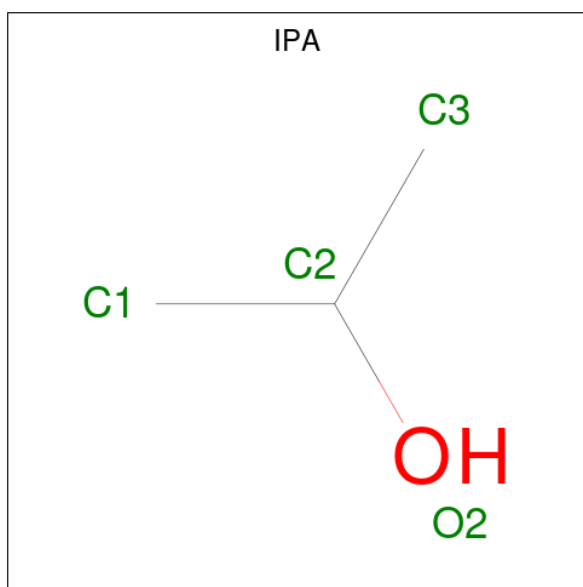
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	2	3		
4	A	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			8	6	2		

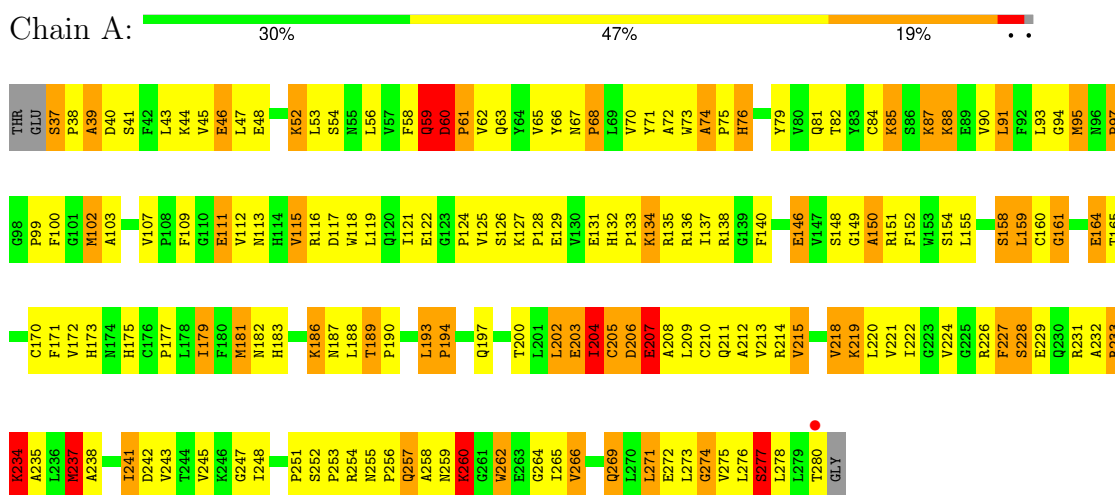
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	45	Total	O	0	0
			45	45		
7	E	6	Total	O	0	0
			6	6		
7	F	6	Total	O	0	0
			6	6		

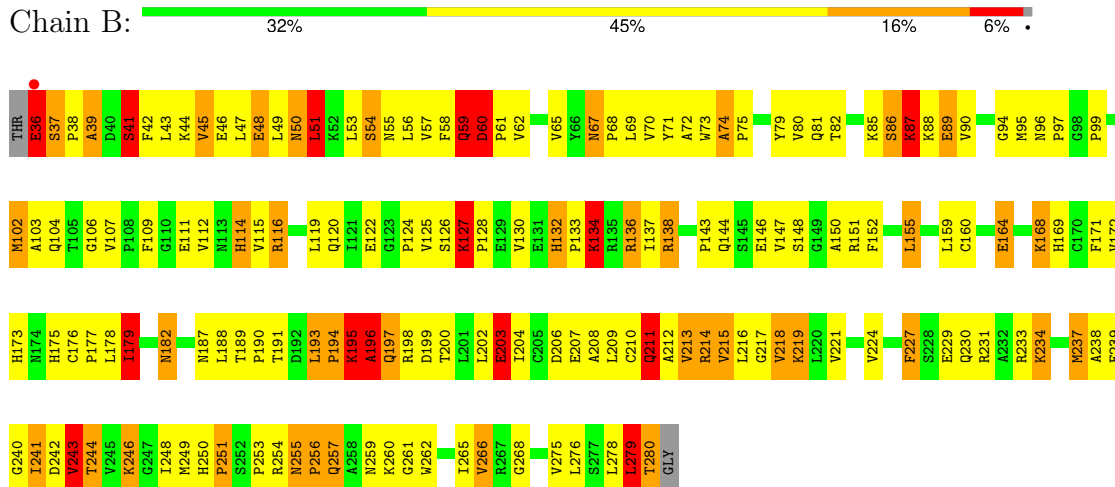
3 Residue-property plots

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 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: SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL DNA GLYCOSYLASE



• Molecule 1: SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL DNA GLYCOSYLASE

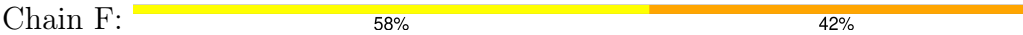


• Molecule 2: 5'-D(*CP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*G)-3'



C281
C282
C283
G284
T285
G286
A287
G288
T289
C290
C291
G292

● Molecule 3: 5'-D(*CP*GP*GP*AP*CP*TP*3DRP*AP*CP*GP*GP*G)-3'



G293
G294
G295
A296
C297
T298
I299
A300
C301
G302
G303
G304

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.97Å 86.52Å 78.46Å 90.00° 118.53° 90.00°	Depositor
Resolution (Å)	69.01 – 2.65 68.93 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.01-2.65) 99.4 (68.93-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.154 , 0.218 0.166 , 0.218	Depositor DCC
R_{free} test set	1063 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4499	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR, GOL, IPA, HMU

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	2.96	169/1997 (8.5%)	2.20	86/2707 (3.2%)
1	B	2.88	153/1990 (7.7%)	2.12	78/2698 (2.9%)
2	E	2.14	6/269 (2.2%)	3.36	54/413 (13.1%)
3	F	2.29	6/253 (2.4%)	3.14	45/387 (11.6%)
All	All	2.85	334/4509 (7.4%)	2.33	263/6205 (4.2%)

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	3
All	All	0	4

All (334) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	MET	SD-CE	21.77	2.33	1.79
1	B	125	VAL	C-O	-14.15	1.10	1.24
1	A	237[A]	MET	SD-CE	13.82	2.14	1.79
1	A	237[B]	MET	SD-CE	13.82	2.14	1.79
1	A	207	GLU	N-CA	13.77	1.64	1.46
1	B	41	SER	C-O	12.40	1.38	1.24
1	B	115	VAL	CA-C	12.29	1.67	1.52
1	A	245	VAL	C-O	-12.22	1.11	1.24
1	B	151	ARG	C-O	11.95	1.38	1.24
2	E	283	DC	P-OP2	11.57	1.71	1.48
1	B	107	VAL	CA-CB	-11.43	1.39	1.54
1	A	112	VAL	CA-CB	-11.30	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	C-O	11.18	1.36	1.24
1	A	152	PHE	N-CA	-11.16	1.32	1.46
1	A	121	ILE	C-O	-11.08	1.12	1.24
1	B	172	VAL	CA-C	-11.07	1.39	1.52
1	B	116	ARG	C-O	-10.69	1.11	1.24
1	A	273	LEU	CA-C	-10.57	1.38	1.52
1	A	206	ASP	CA-C	10.51	1.66	1.52
1	B	146	GLU	N-CA	-10.47	1.33	1.46
1	A	39	ALA	CA-CB	-10.42	1.37	1.53
1	A	206	ASP	C-O	-10.15	1.11	1.24
1	B	74	ALA	CA-CB	-10.07	1.42	1.53
1	B	196	ALA	CA-C	-10.03	1.39	1.52
1	A	136	ARG	C-O	-10.01	1.11	1.23
1	B	259	ASN	C-O	-9.94	1.09	1.24
1	B	143	PRO	C-O	9.88	1.36	1.24
1	B	194	PRO	CA-C	9.85	1.62	1.52
1	B	177	PRO	CA-C	-9.83	1.42	1.52
1	A	90	VAL	CA-CB	-9.81	1.40	1.55
1	A	245	VAL	CA-C	-9.69	1.41	1.52
1	A	206	ASP	N-CA	9.68	1.58	1.46
1	B	215	VAL	CA-CB	-9.64	1.42	1.54
1	A	68	PRO	CA-C	-9.56	1.40	1.52
1	B	224	VAL	CA-C	-9.56	1.43	1.53
1	A	74	ALA	N-CA	9.53	1.53	1.46
1	B	128	PRO	CA-C	9.36	1.63	1.52
1	A	116	ARG	CA-CB	-9.32	1.38	1.53
1	B	45	VAL	CA-C	-9.30	1.41	1.52
1	A	46	GLU	CD-OE2	9.26	1.43	1.25
1	B	152	PHE	C-O	-9.21	1.13	1.24
1	A	146	GLU	CD-OE1	9.15	1.42	1.25
1	B	172	VAL	C-O	-9.11	1.14	1.23
1	B	278	LEU	C-O	-9.05	1.13	1.24
1	B	208	ALA	CA-CB	-9.02	1.39	1.53
1	A	233	ARG	NE-CZ	8.97	1.43	1.33
1	B	67	ASN	N-CA	-8.97	1.37	1.46
1	A	137	ILE	C-O	-8.95	1.13	1.24
1	A	220	LEU	C-O	-8.90	1.13	1.24
1	B	48	GLU	C-O	8.76	1.34	1.24
1	B	265	ILE	CA-CB	-8.73	1.44	1.54
1	B	207	GLU	C-O	-8.72	1.14	1.24
1	B	106	GLY	C-O	-8.65	1.12	1.23
1	B	51	LEU	C-O	8.64	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	PRO	CA-C	8.61	1.64	1.52
1	A	170	CYS	C-O	-8.55	1.12	1.23
1	B	218	VAL	CA-CB	8.54	1.65	1.54
1	A	45	VAL	CA-C	-8.52	1.42	1.52
1	B	155	LEU	C-O	-8.51	1.14	1.24
1	A	245	VAL	N-CA	-8.50	1.36	1.46
1	A	189	THR	CA-CB	-8.47	1.41	1.53
1	B	134	LYS	CD-CE	8.38	1.77	1.52
1	B	124	PRO	C-O	8.35	1.33	1.23
1	A	52	LYS	CA-C	8.29	1.63	1.52
2	E	282	DC	O5'-C5'	8.17	1.67	1.42
1	B	260	LYS	N-CA	-8.09	1.35	1.46
1	B	224	VAL	CA-CB	-8.06	1.44	1.53
1	A	227	PHE	C-O	-7.98	1.15	1.24
1	B	250	HIS	CA-C	7.98	1.61	1.53
1	B	150	ALA	C-O	7.98	1.33	1.24
1	B	134	LYS	CG-CD	7.96	1.76	1.52
1	B	42	PHE	CA-C	-7.95	1.42	1.52
1	A	207	GLU	CA-CB	7.94	1.66	1.53
1	B	227	PHE	CB-CG	-7.90	1.32	1.50
3	F	298	DT	C1'-N1	7.85	1.73	1.49
1	A	187	ASN	C-O	-7.84	1.14	1.23
1	A	258	ALA	CA-CB	-7.83	1.41	1.53
1	A	237[A]	MET	CG-SD	7.82	2.00	1.80
1	A	237[B]	MET	CG-SD	7.82	2.00	1.80
1	B	96	ASN	CG-ND2	7.82	1.49	1.33
1	B	175	HIS	N-CA	-7.75	1.37	1.46
1	A	203	GLU	C-O	-7.73	1.14	1.24
1	B	212	ALA	CA-C	-7.70	1.42	1.52
1	A	247	GLY	C-O	-7.52	1.15	1.24
1	A	197	GLN	C-O	7.52	1.33	1.24
1	B	119	LEU	N-CA	-7.51	1.36	1.46
1	A	211	GLN	C-O	7.46	1.32	1.24
1	A	65	VAL	N-CA	-7.44	1.37	1.46
1	A	67	ASN	C-O	-7.44	1.17	1.24
1	B	127	LYS	CG-CD	7.44	1.74	1.52
1	A	60	ASP	C-O	7.43	1.33	1.24
1	A	158	SER	CA-C	-7.41	1.43	1.53
1	A	207	GLU	CD-OE1	7.41	1.39	1.25
1	A	146	GLU	CA-C	7.38	1.62	1.52
1	B	88	LYS	CA-C	-7.37	1.43	1.52
1	A	272	GLU	CD-OE2	7.31	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	THR	C-O	-7.30	1.14	1.24
1	A	60	ASP	CB-CG	7.27	1.70	1.52
1	B	254	ARG	C-O	-7.25	1.14	1.24
1	B	144	GLN	CB-CG	7.23	1.74	1.52
1	A	183	HIS	CA-C	7.22	1.62	1.52
1	B	179	ILE	N-CA	-7.21	1.37	1.46
1	B	211	GLN	C-O	7.16	1.32	1.24
1	B	36	GLU	C-O	7.14	1.37	1.23
1	B	248	ILE	N-CA	-7.14	1.37	1.46
1	A	264	GLY	C-O	-7.14	1.15	1.23
1	A	172	VAL	CA-CB	-7.13	1.44	1.54
1	A	115	VAL	CA-C	-7.13	1.44	1.52
1	B	126	SER	C-O	-7.12	1.15	1.24
1	B	212	ALA	CA-CB	-7.11	1.41	1.53
1	B	266	VAL	C-O	-7.10	1.16	1.24
1	B	65	VAL	C-O	-7.08	1.16	1.24
1	A	85	LYS	C-O	-7.08	1.15	1.24
1	B	130	VAL	C-O	-7.08	1.16	1.24
1	A	48	GLU	CD-OE2	7.07	1.38	1.25
1	A	235	ALA	CA-CB	-7.04	1.42	1.53
3	F	304	DG	P-O5'	7.04	1.74	1.60
1	A	231	ARG	N-CA	-7.00	1.37	1.46
1	B	146	GLU	CD-OE1	6.96	1.38	1.25
1	B	116	ARG	CA-C	-6.95	1.44	1.52
1	B	82	THR	CA-C	-6.93	1.43	1.52
1	B	234	LYS	CA-C	-6.90	1.43	1.52
1	A	95	MET	CG-SD	6.89	1.98	1.80
1	A	124	PRO	C-O	-6.88	1.16	1.23
1	B	74	ALA	C-O	6.87	1.31	1.24
1	A	262	TRP	C-O	6.87	1.31	1.24
1	A	212	ALA	C-O	-6.86	1.16	1.24
1	B	198	ARG	C-O	-6.83	1.16	1.24
1	A	193	LEU	CA-C	6.83	1.61	1.52
1	B	115	VAL	C-O	-6.82	1.16	1.24
1	B	197	GLN	N-CA	6.80	1.54	1.46
1	B	195	LYS	CB-CG	6.80	1.72	1.52
1	A	127	LYS	CD-CE	6.79	1.72	1.52
1	A	238	ALA	CA-CB	-6.72	1.42	1.53
1	A	213	VAL	C-O	-6.71	1.16	1.24
1	A	272	GLU	C-O	-6.68	1.15	1.24
1	A	181	MET	SD-CE	6.67	1.96	1.79
1	A	213	VAL	CA-CB	-6.64	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	VAL	CA-CB	6.63	1.61	1.53
1	A	172	VAL	CA-C	-6.62	1.44	1.52
1	B	219	LYS	CG-CD	6.62	1.72	1.52
1	A	65	VAL	C-O	-6.59	1.17	1.24
1	B	173	HIS	C-O	-6.59	1.16	1.23
1	A	87	LYS	CD-CE	6.56	1.72	1.52
1	A	95	MET	SD-CE	-6.56	1.63	1.79
1	B	176	CYS	C-O	6.54	1.32	1.24
1	A	140	PHE	CA-C	-6.53	1.41	1.52
1	A	181	MET	C-O	6.53	1.32	1.23
1	A	48	GLU	C-O	-6.52	1.16	1.24
1	B	36	GLU	N-CA	6.47	1.58	1.46
1	A	210	CYS	C-O	-6.46	1.16	1.24
1	A	54	SER	C-O	-6.41	1.16	1.24
1	A	128	PRO	C-O	6.38	1.31	1.23
1	A	115	VAL	CB-CG1	-6.37	1.31	1.52
1	B	253	PRO	CA-C	-6.37	1.44	1.52
1	A	76	HIS	C-O	6.34	1.31	1.24
1	A	226	ARG	CA-C	-6.34	1.44	1.52
1	B	70	VAL	C-O	6.34	1.31	1.24
1	A	150	ALA	C-O	6.32	1.31	1.24
1	B	249	MET	N-CA	-6.32	1.38	1.46
1	A	203	GLU	N-CA	-6.31	1.38	1.46
1	A	102	MET	SD-CE	-6.31	1.63	1.79
1	B	95	MET	CA-CB	-6.30	1.42	1.53
1	B	116	ARG	NE-CZ	6.29	1.40	1.33
1	A	68	PRO	CA-CB	-6.26	1.43	1.54
1	B	257	GLN	CG-CD	6.26	1.67	1.52
1	B	182	ASN	N-CA	6.25	1.52	1.46
1	B	114	HIS	CA-C	-6.25	1.44	1.52
1	A	186	LYS	CA-C	6.24	1.61	1.52
1	B	73	TRP	CZ3-CH2	-6.23	1.24	1.40
1	B	107	VAL	C-O	-6.21	1.16	1.24
1	A	93	LEU	N-CA	6.21	1.53	1.46
1	A	160	CYS	CA-CB	-6.19	1.45	1.54
1	A	272	GLU	N-CA	6.18	1.54	1.46
1	B	191	THR	CA-CB	6.18	1.63	1.53
1	B	43	LEU	N-CA	6.17	1.54	1.46
1	B	227	PHE	C-N	-6.16	1.25	1.34
1	A	211	GLN	CG-CD	6.16	1.67	1.52
1	B	95	MET	SD-CE	-6.16	1.64	1.79
1	B	120	GLN	C-O	-6.14	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	ARG	CA-C	-6.13	1.44	1.52
1	A	111	GLU	CA-C	-6.13	1.45	1.52
1	B	57	VAL	CB-CG2	6.12	1.72	1.52
1	A	131	GLU	C-O	-6.12	1.16	1.24
1	B	132	HIS	CA-C	6.08	1.60	1.53
1	A	275	VAL	N-CA	-6.07	1.40	1.46
1	B	109	PHE	CA-C	6.05	1.60	1.52
1	B	36	GLU	CD-OE1	6.04	1.36	1.25
1	B	227	PHE	CA-CB	-6.04	1.43	1.53
1	A	164	GLU	CD-OE1	6.04	1.36	1.25
1	A	37	SER	N-CA	6.03	1.57	1.46
1	A	79	TYR	CG-CD1	-6.03	1.26	1.39
1	A	269	GLN	CA-C	-6.02	1.44	1.52
1	B	79	TYR	C-O	6.01	1.31	1.24
1	A	155	LEU	N-CA	-6.00	1.39	1.46
1	B	126	SER	CA-C	-6.00	1.44	1.52
1	A	134	LYS	CG-CD	5.99	1.70	1.52
1	B	147	VAL	C-O	-5.97	1.17	1.24
1	A	221	VAL	CA-CB	-5.96	1.47	1.54
3	F	296	DA	C8-N7	5.96	1.43	1.31
1	B	210	CYS	C-O	5.95	1.30	1.24
1	A	63	GLN	N-CA	5.93	1.53	1.46
1	B	58	PHE	CA-CB	-5.93	1.44	1.53
1	A	60	ASP	CA-C	-5.91	1.45	1.52
1	B	47	LEU	N-CA	5.91	1.53	1.46
1	B	103	ALA	C-O	-5.90	1.16	1.24
1	A	53	LEU	C-O	-5.89	1.17	1.24
1	A	266	VAL	CA-C	-5.89	1.44	1.52
1	B	221	VAL	CA-CB	-5.87	1.47	1.54
1	A	125	VAL	N-CA	-5.84	1.39	1.46
1	A	99	PRO	N-CA	-5.83	1.39	1.47
1	A	119	LEU	CB-CG	-5.82	1.41	1.53
1	A	82	THR	CA-CB	-5.80	1.44	1.53
1	A	228	SER	CA-C	-5.80	1.45	1.52
1	A	94	GLY	C-O	-5.77	1.18	1.23
1	B	36	GLU	CA-C	5.76	1.65	1.52
3	F	296	DA	C6-N1	5.75	1.46	1.35
1	B	102	MET	N-CA	-5.74	1.39	1.46
1	B	171	PHE	N-CA	-5.73	1.39	1.46
1	B	36	GLU	CD-OE2	5.73	1.36	1.25
1	A	237[A]	MET	CA-CB	5.72	1.62	1.53
1	A	237[B]	MET	CA-CB	5.72	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	THR	N-CA	-5.72	1.39	1.46
1	A	260	LYS	CG-CD	5.71	1.69	1.52
1	B	198	ARG	NE-CZ	5.71	1.39	1.33
1	B	239	GLU	C-O	-5.70	1.18	1.24
1	B	188	LEU	CA-C	-5.69	1.45	1.52
1	B	81	GLN	CD-OE1	5.68	1.34	1.23
1	A	91	LEU	C-O	-5.67	1.17	1.23
1	B	243	VAL	CA-CB	5.67	1.62	1.54
1	A	88	LYS	CA-C	5.67	1.59	1.52
1	B	237	MET	N-CA	-5.66	1.39	1.46
1	A	207	GLU	CG-CD	5.66	1.66	1.52
1	A	62	VAL	CA-C	-5.63	1.46	1.52
1	A	189	THR	CB-OG1	-5.63	1.34	1.43
1	B	65	VAL	N-CA	-5.62	1.39	1.46
1	A	235	ALA	C-O	-5.61	1.16	1.24
1	B	159	LEU	N-CA	-5.61	1.39	1.46
1	B	221	VAL	N-CA	-5.59	1.39	1.46
1	A	181	MET	CA-CB	-5.58	1.45	1.53
1	A	224	VAL	CA-C	-5.58	1.46	1.52
1	A	233	ARG	CA-CB	-5.57	1.44	1.53
1	B	195	LYS	CG-CD	5.56	1.69	1.52
1	B	168	LYS	CG-CD	5.55	1.69	1.52
2	E	282	DC	O4'-C1'	5.54	1.52	1.41
1	A	248	ILE	CA-CB	-5.54	1.45	1.54
3	F	302	DG	P-O5'	5.54	1.71	1.60
1	A	149	GLY	C-O	5.53	1.30	1.23
1	A	127	LYS	CG-CD	5.52	1.69	1.52
1	B	57	VAL	CA-CB	5.52	1.61	1.54
1	A	158	SER	C-O	-5.51	1.17	1.23
1	B	137	ILE	CA-CB	5.51	1.60	1.54
1	A	277	SER	N-CA	-5.50	1.39	1.46
1	A	118	TRP	CA-C	-5.49	1.46	1.52
1	B	164	GLU	CD-OE1	5.49	1.35	1.25
1	A	116	ARG	CZ-NH1	5.47	1.40	1.32
1	B	246	LYS	CG-CD	5.47	1.68	1.52
1	B	213	VAL	C-O	5.46	1.30	1.24
1	B	36	GLU	CG-CD	5.45	1.65	1.52
1	A	47	LEU	CA-C	5.45	1.60	1.52
1	B	159	LEU	C-O	-5.45	1.17	1.24
1	A	60	ASP	CG-OD2	5.44	1.35	1.25
1	A	107	VAL	N-CA	-5.42	1.40	1.46
1	A	274	GLY	C-O	-5.41	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	HIS	C-O	-5.41	1.17	1.24
1	B	58	PHE	C-O	-5.40	1.16	1.23
1	B	70	VAL	N-CA	5.39	1.53	1.46
1	B	87	LYS	CA-C	-5.36	1.45	1.52
1	B	124	PRO	CA-C	-5.34	1.45	1.52
1	A	232	ALA	C-O	-5.34	1.17	1.24
1	A	118	TRP	C-O	-5.34	1.16	1.23
1	B	203	GLU	CD-OE1	5.33	1.35	1.25
1	A	93	LEU	CA-C	-5.32	1.46	1.52
1	A	129	GLU	CD-OE2	5.32	1.35	1.25
1	A	61	PRO	C-O	5.32	1.30	1.24
1	A	269	GLN	CD-NE2	-5.32	1.22	1.33
1	A	137	ILE	N-CA	-5.31	1.39	1.46
1	B	72	ALA	CA-C	-5.30	1.45	1.52
1	A	275	VAL	CA-CB	5.30	1.61	1.54
1	A	205	CYS	C-N	5.30	1.41	1.33
1	A	113	ASN	CA-C	-5.29	1.46	1.52
1	A	204	ILE	CB-CG2	-5.29	1.35	1.52
1	B	39	ALA	N-CA	5.28	1.52	1.46
1	A	188	LEU	CA-C	-5.28	1.46	1.52
1	B	206	ASP	CA-C	5.27	1.59	1.52
1	B	41	SER	CA-C	5.27	1.59	1.52
1	B	246	LYS	N-CA	5.25	1.53	1.45
1	B	204	ILE	C-O	5.24	1.30	1.24
2	E	285	DT	C1'-N1	5.24	1.65	1.49
1	B	206	ASP	CB-CG	5.23	1.65	1.52
1	A	152	PHE	C-O	-5.22	1.18	1.24
1	A	257	GLN	CD-OE1	5.22	1.33	1.23
1	A	277	SER	C-O	5.21	1.30	1.24
1	B	260	LYS	CB-CG	5.20	1.68	1.52
1	A	179	ILE	CA-C	-5.19	1.46	1.52
1	A	204	ILE	C-O	5.19	1.30	1.24
1	A	135	ARG	C-O	5.18	1.28	1.23
1	A	172	VAL	C-N	-5.18	1.27	1.33
1	A	102	MET	C-O	5.18	1.30	1.24
1	B	80	VAL	CA-CB	-5.18	1.48	1.54
1	B	191	THR	CA-C	-5.18	1.45	1.52
1	B	70	VAL	CA-C	5.16	1.59	1.52
1	B	203	GLU	CA-CB	5.16	1.61	1.53
1	B	59	GLN	CG-CD	5.15	1.65	1.52
1	A	73	TRP	CA-C	-5.15	1.46	1.52
1	A	70	VAL	C-O	5.15	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	ASN	N-CA	5.13	1.51	1.45
1	A	72	ALA	N-CA	5.13	1.52	1.46
1	B	36	GLU	CB-CG	5.12	1.67	1.52
1	B	216	LEU	C-O	5.11	1.30	1.24
1	B	211	GLN	N-CA	5.10	1.52	1.46
3	F	304	DG	O5'-C5'	5.10	1.58	1.42
1	B	173	HIS	CA-C	-5.09	1.46	1.52
1	A	44	LYS	CB-CG	5.08	1.67	1.52
1	A	209	LEU	CA-C	5.08	1.59	1.52
2	E	292	DG	C8-N7	5.08	1.41	1.30
1	A	260	LYS	CD-CE	5.08	1.67	1.52
1	B	134	LYS	CE-NZ	5.07	1.64	1.49
1	A	203	GLU	CA-C	-5.05	1.45	1.52
1	A	52	LYS	CA-CB	-5.05	1.45	1.53
1	A	81	GLN	CB-CG	5.05	1.67	1.52
1	A	126	SER	C-O	-5.05	1.17	1.24
1	A	202	LEU	CB-CG	5.05	1.63	1.53
1	B	255	ASN	C-O	5.05	1.31	1.24
1	B	62	VAL	C-O	-5.03	1.18	1.24
2	E	282	DC	O3'-P	5.03	1.68	1.61
1	A	159	LEU	C-O	-5.03	1.18	1.24
1	A	243	VAL	CA-CB	5.02	1.61	1.54
1	B	254	ARG	NE-CZ	5.02	1.38	1.33
1	B	42	PHE	CA-CB	-5.01	1.45	1.53
1	B	203	GLU	N-CA	5.01	1.52	1.46
1	A	207	GLU	C-O	5.01	1.30	1.24
1	A	172	VAL	C-O	5.00	1.29	1.24
1	B	229	GLU	CA-C	5.00	1.59	1.52

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	281	DC	O3'-P-O5'	-15.02	81.47	104.00
2	E	291	DC	C5'-C4'-C3'	-13.51	94.64	114.90
1	A	215	VAL	N-CA-C	12.19	123.05	110.62
2	E	288	DG	C4'-C3'-O3'	-11.13	93.30	110.00
3	F	304	DG	P-O5'-C5'	10.76	136.13	120.00
1	A	273	LEU	N-CA-C	-10.51	100.46	113.38
2	E	282	DC	OP1-P-O3'	-10.39	76.82	108.00
1	B	279	LEU	N-CA-C	-10.36	93.48	110.17
3	F	298	DT	O4'-C1'-N1	10.08	123.53	108.40
3	F	293	DC	O5'-C5'-C4'	-10.00	95.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	284	DG	P-O5'-C5'	9.88	134.81	120.00
1	B	45	VAL	CB-CA-C	-9.87	98.82	112.14
1	A	45	VAL	CB-CA-C	-9.78	98.94	112.14
2	E	288	DG	P-O3'-C3'	9.55	134.53	120.20
1	A	206	ASP	CA-C-N	9.47	139.63	121.54
1	A	206	ASP	C-N-CA	9.47	139.63	121.54
1	A	280	THR	CB-CA-C	9.46	129.92	109.10
1	A	224	VAL	N-CA-C	-9.37	91.82	106.72
1	B	169	HIS	N-CA-C	9.37	124.44	112.92
1	A	122	GLU	N-CA-C	-9.23	95.38	109.14
2	E	287	DA	P-O5'-C5'	9.13	133.70	120.00
1	B	73	TRP	N-CA-C	-9.11	101.30	111.14
1	A	280	THR	CA-C-O	9.09	136.26	120.80
1	B	56	LEU	CA-C-N	-8.92	111.46	123.14
1	B	56	LEU	C-N-CA	-8.92	111.46	123.14
3	F	297	DC	C5-C4-N4	8.67	133.31	120.30
2	E	282	DC	C5'-C4'-C3'	-8.65	101.93	114.90
2	E	283	DC	O3'-P-O5'	-8.64	91.04	104.00
1	A	280	THR	CA-CB-CG2	8.62	125.16	110.50
1	B	81	GLN	N-CA-C	8.58	121.71	111.33
2	E	287	DA	C4'-C3'-O3'	-8.51	97.23	110.00
3	F	297	DC	OP1-P-O3'	-8.51	82.48	108.00
3	F	303	DG	P-O5'-C5'	8.44	132.66	120.00
1	B	55	ASN	N-CA-C	8.39	124.95	113.37
2	E	285	DT	C3'-C2'-C1'	-8.39	89.02	101.60
1	B	57	VAL	CB-CA-C	8.38	123.03	110.63
1	B	85	LYS	N-CA-C	-8.31	103.24	112.72
1	B	268	GLY	N-CA-C	8.25	122.47	112.49
1	B	112	VAL	N-CA-C	8.24	119.01	110.36
1	B	197	GLN	N-CA-CB	8.23	122.41	110.06
1	A	148	SER	N-CA-C	8.18	120.92	111.11
1	A	161	GLY	N-CA-C	8.04	132.23	113.18
1	B	46	GLU	N-CA-C	8.04	120.12	111.36
1	A	237[A]	MET	N-CA-C	-7.91	102.60	111.14
1	A	237[B]	MET	N-CA-C	-7.91	102.60	111.14
1	A	53	LEU	N-CA-C	7.90	119.89	111.28
3	F	294	DG	C4'-C3'-O3'	-7.84	98.24	110.00
1	A	203	GLU	N-CA-C	-7.79	101.62	112.45
1	A	43	LEU	N-CA-C	7.78	119.77	111.28
3	F	295	DG	OP1-P-OP2	7.76	143.28	120.00
1	B	234	LYS	N-CA-C	-7.71	101.74	112.45
3	F	297	DC	N3-C4-N4	-7.70	106.34	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	DC	O3'-P-O5'	-7.67	92.50	104.00
2	E	291	DC	O4'-C1'-N1	7.62	119.82	108.40
1	A	205	CYS	N-CA-C	7.61	120.68	111.40
2	E	289	DT	P-O3'-C3'	7.58	131.56	120.20
1	B	116	ARG	N-CA-C	-7.54	103.00	111.14
1	B	250	HIS	N-CA-C	7.53	118.26	109.60
3	F	294	DG	O3'-P-O5'	-7.53	92.70	104.00
1	B	191	THR	CA-C-O	-7.52	111.78	120.20
2	E	290	DC	O3'-P-O5'	-7.45	92.83	104.00
1	A	203	GLU	CA-C-O	-7.44	110.93	120.00
3	F	304	DG	N1-C2-N2	-7.43	105.16	116.30
1	A	159	LEU	N-CA-C	7.40	119.99	111.11
2	E	290	DC	N3-C4-N4	-7.36	106.86	117.90
3	F	297	DC	C2-N1-C1'	-7.35	108.68	119.70
2	E	283	DC	C5'-C4'-O4'	7.34	120.40	109.40
3	F	300	DA	C4'-C3'-O3'	-7.32	99.02	110.00
2	E	282	DC	C5'-C4'-O4'	7.31	120.36	109.40
1	A	233	ARG	NE-CZ-NH2	7.26	125.73	119.20
3	F	293	DC	N1-C2-O2	7.23	130.04	119.20
2	E	289	DT	P-O5'-C5'	7.18	130.78	120.00
3	F	302	DG	P-O5'-C5'	7.13	130.69	120.00
2	E	291	DC	C2'-C3'-O3'	7.11	122.17	111.50
2	E	287	DA	O4'-C1'-N9	-7.05	97.82	108.40
2	E	289	DT	C1'-O4'-C4'	-7.03	99.16	109.70
1	A	207	GLU	CA-CB-CG	6.97	128.04	114.10
2	E	283	DC	P-O5'-C5'	6.92	130.37	120.00
1	B	251	PRO	N-CD-CG	6.91	113.56	103.20
3	F	303	DG	O4'-C1'-N9	6.82	118.64	108.40
1	B	51	LEU	N-CA-C	6.80	119.32	111.02
1	A	272	GLU	CA-CB-CG	-6.80	100.51	114.10
1	A	94	GLY	O-C-N	-6.77	116.45	122.88
1	A	112	VAL	CB-CA-C	-6.76	102.89	112.22
2	E	289	DT	N3-C4-O4	-6.76	112.46	122.60
1	A	259	ASN	N-CA-C	6.75	121.22	113.19
1	B	132	HIS	N-CA-C	-6.75	101.56	109.93
1	A	194	PRO	CA-C-O	-6.74	113.66	121.34
3	F	295	DG	C5'-C4'-O4'	6.73	119.50	109.40
1	B	202	LEU	N-CA-C	6.71	118.68	111.36
1	A	242	ASP	N-CA-C	6.71	120.58	108.17
1	A	215	VAL	N-CA-CB	6.70	119.65	110.54
2	E	285	DT	O4'-C1'-N1	6.69	118.43	108.40
2	E	291	DC	O5'-P-OP1	-6.65	89.04	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	302	DG	C5'-C4'-O4'	6.64	119.36	109.40
1	A	206	ASP	O-C-N	-6.59	113.82	122.59
2	E	286	DG	P-O5'-C5'	6.53	129.79	120.00
2	E	290	DC	C4'-C3'-O3'	-6.52	100.21	110.00
1	B	37	SER	CA-C-O	6.50	126.61	119.32
1	A	134	LYS	CB-CA-C	6.49	121.52	110.56
2	E	283	DC	O5'-C5'-C4'	-6.49	101.07	110.80
1	A	158	SER	CB-CA-C	-6.46	98.73	110.56
1	A	146	GLU	CA-CB-CG	6.46	127.02	114.10
1	B	68	PRO	CB-CA-C	-6.42	100.96	111.56
1	A	206	ASP	N-CA-C	6.40	124.42	110.80
3	F	302	DG	P-O3'-C3'	6.38	129.76	120.20
1	B	213	VAL	CB-CA-C	-6.37	103.54	112.14
2	E	285	DT	O5'-C5'-C4'	-6.36	101.25	110.80
1	B	71	TYR	N-CA-C	6.35	120.13	112.38
1	B	215	VAL	CB-CA-C	-6.35	103.72	112.04
2	E	282	DC	O3'-P-O5'	-6.34	94.48	104.00
3	F	304	DG	N3-C2-N2	6.33	129.20	119.70
2	E	292	DG	C5-C6-O6	-6.33	118.80	128.30
3	F	302	DG	O4'-C4'-C3'	-6.32	95.91	105.40
1	A	126	SER	CB-CA-C	6.31	122.98	110.42
2	E	287	DA	N9-C1'-C2'	6.31	122.96	113.50
1	B	195	LYS	CA-C-N	-6.30	109.50	121.54
1	B	195	LYS	C-N-CA	-6.30	109.50	121.54
1	B	82	THR	N-CA-C	-6.30	105.42	113.23
1	A	151	ARG	NE-CZ-NH2	-6.25	113.57	119.20
1	B	203	GLU	CA-CB-CG	6.25	126.60	114.10
1	A	61	PRO	N-CD-CG	6.24	112.56	103.20
2	E	289	DT	C5-C4-O4	6.21	131.91	122.60
1	B	239	GLU	N-CA-C	-6.21	103.90	112.03
1	A	68	PRO	N-CD-CG	-6.20	93.89	103.20
1	B	255	ASN	CA-C-O	6.19	124.72	119.71
1	A	48	GLU	N-CA-CB	6.18	119.21	110.12
2	E	289	DT	C6-C5-C7	-6.18	114.73	124.00
1	B	255	ASN	N-CA-C	6.17	120.68	108.59
1	A	214	ARG	CA-C-O	-6.16	114.36	120.82
1	B	255	ASN	CB-CA-C	-6.14	104.91	110.44
1	B	124	PRO	CA-C-O	-6.13	114.38	121.86
3	F	295	DG	N1-C2-N2	-6.10	107.14	116.30
1	B	79	TYR	N-CA-C	-6.08	104.58	111.14
3	F	295	DG	C6-N1-C2	-6.04	115.84	124.90
2	E	287	DA	C1'-O4'-C4'	6.03	118.74	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	ASN	N-CA-CB	6.02	118.97	110.12
1	A	65	VAL	CB-CA-C	-6.01	101.94	110.12
1	A	241	ILE	CA-C-N	-6.00	111.76	122.32
1	A	241	ILE	C-N-CA	-6.00	111.76	122.32
3	F	295	DG	O3'-P-O5'	-5.99	95.01	104.00
1	A	88	LYS	N-CA-C	5.99	118.96	109.50
1	A	214	ARG	CA-C-N	-5.99	112.26	120.46
1	A	214	ARG	C-N-CA	-5.99	112.26	120.46
1	A	207	GLU	N-CA-CB	5.98	120.60	110.49
3	F	304	DG	N1-C6-O6	-5.98	111.03	120.00
1	A	237[A]	MET	CB-CA-C	5.95	120.31	110.90
1	A	237[B]	MET	CB-CA-C	5.95	120.31	110.90
3	F	303	DG	C2'-C3'-O3'	5.95	120.43	111.50
2	E	282	DC	OP2-P-O3'	5.94	125.81	108.00
1	A	52	LYS	CD-CE-NZ	-5.94	92.91	111.90
3	F	296	DA	P-O3'-C3'	5.93	129.09	120.20
1	A	60	ASP	O-C-N	5.91	128.12	121.32
1	B	99	PRO	CA-C-N	-5.91	113.27	122.37
1	B	99	PRO	C-N-CA	-5.91	113.27	122.37
1	A	146	GLU	CG-CD-OE1	5.89	131.94	118.40
1	A	200	THR	N-CA-C	-5.87	104.80	111.14
1	B	136	ARG	N-CA-C	-5.87	100.99	110.32
1	A	234	LYS	N-CA-C	-5.86	104.08	111.11
1	B	151	ARG	O-C-N	5.85	128.32	122.12
3	F	298	DT	N1-C2-O2	-5.84	114.44	123.20
1	B	94	GLY	N-CA-C	-5.83	101.49	112.10
3	F	294	DG	N9-C1'-C2'	5.82	122.23	113.50
3	F	295	DG	P-O3'-C3'	5.81	128.92	120.20
2	E	283	DC	OP1-P-OP2	5.78	137.35	120.00
3	F	297	DC	C6-N1-C1'	5.78	128.37	119.70
1	B	39	ALA	N-CA-C	5.77	118.03	111.11
1	A	274	GLY	N-CA-C	5.76	124.89	114.46
3	F	300	DA	C2'-C3'-O3'	5.75	120.13	111.50
1	B	60	ASP	CA-C-O	-5.74	112.29	120.16
1	B	280	THR	CA-CB-CG2	5.73	120.25	110.50
3	F	293	DC	C6-N1-C1'	-5.73	111.11	119.70
1	B	60	ASP	O-C-N	5.72	127.90	121.32
2	E	286	DG	C2'-C3'-O3'	-5.71	102.93	111.50
1	A	40	ASP	N-CA-C	5.69	118.42	111.82
3	F	304	DG	C5-C6-O6	5.69	136.83	128.30
1	A	71	TYR	N-CA-C	5.68	119.48	112.54
1	A	97	PRO	CA-C-N	-5.66	112.99	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	PRO	C-N-CA	-5.66	112.99	121.87
2	E	281	DC	C4'-C3'-O3'	5.65	118.47	110.00
1	A	95	MET	CG-SD-CE	5.64	113.30	100.90
1	B	191	THR	N-CA-CB	5.63	119.03	110.14
2	E	282	DC	OP1-P-OP2	5.61	136.84	120.00
2	E	290	DC	P-O5'-C5'	5.58	128.36	120.00
3	F	304	DG	O5'-C5'-C4'	5.55	119.13	110.80
2	E	292	DG	N1-C2-N3	-5.54	115.69	124.00
1	B	107	VAL	N-CA-CB	-5.54	103.46	111.21
1	A	194	PRO	N-CD-CG	-5.53	94.90	103.20
3	F	295	DG	C5-C6-O6	-5.53	120.01	128.30
1	A	146	GLU	CG-CD-OE2	-5.53	105.69	118.40
3	F	300	DA	N9-C1'-C2'	5.53	121.79	113.50
1	A	113	ASN	N-CA-C	5.52	117.37	111.36
2	E	289	DT	O5'-P-OP1	-5.51	92.46	109.00
1	A	259	ASN	CA-C-N	-5.50	115.03	122.95
1	A	259	ASN	C-N-CA	-5.50	115.03	122.95
1	B	217	GLY	CA-C-N	-5.50	113.70	122.50
1	B	217	GLY	C-N-CA	-5.50	113.70	122.50
2	E	282	DC	O4'-C1'-N1	5.49	116.64	108.40
2	E	281	DC	C2'-C3'-O3'	-5.49	103.27	111.50
1	B	104	GLN	N-CA-C	-5.49	106.64	113.55
3	F	296	DA	P-O5'-C5'	5.48	128.22	120.00
1	B	147	VAL	CA-C-O	-5.47	115.26	120.95
1	A	277	SER	CA-CB-OG	-5.46	100.17	111.10
1	B	198	ARG	CG-CD-NE	5.46	124.00	112.00
2	E	284	DG	N3-C2-N2	5.45	127.87	119.70
1	A	121	ILE	O-C-N	-5.44	117.38	123.26
1	A	136	ARG	CG-CD-NE	-5.43	100.05	112.00
1	B	56	LEU	CA-CB-CG	5.42	135.28	116.30
2	E	285	DT	C4'-C3'-O3'	-5.42	101.87	110.00
1	A	228	SER	CB-CA-C	-5.41	101.65	110.85
1	B	246	LYS	CB-CG-CD	5.40	123.72	111.30
1	B	242	ASP	N-CA-CB	5.40	118.43	110.49
3	F	298	DT	OP1-P-OP2	5.40	136.19	120.00
1	B	125	VAL	O-C-N	-5.39	117.33	123.10
1	B	36	GLU	CB-CA-C	5.39	120.34	110.10
1	B	179	ILE	CB-CA-C	5.38	118.78	110.50
1	A	134	LYS	CA-CB-CG	5.37	124.83	114.10
1	A	175	HIS	N-CA-C	-5.37	105.51	111.36
1	A	58	PHE	CA-C-O	-5.37	115.11	121.60
1	A	116	ARG	CB-CA-C	-5.36	101.89	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	289	DT	C4'-C3'-O3'	-5.35	101.97	110.00
1	A	165	THR	OG1-CB-CG2	-5.33	98.64	109.30
1	B	150	ALA	CA-C-N	-5.32	113.16	120.28
1	B	150	ALA	C-N-CA	-5.32	113.16	120.28
1	A	203	GLU	N-CA-CB	5.30	118.15	110.26
3	F	298	DT	O5'-C5'-C4'	-5.29	102.87	110.80
1	A	117	ASP	N-CA-CB	5.26	118.47	110.42
1	A	219	LYS	N-CA-C	-5.26	107.00	113.41
2	E	292	DG	C4'-C3'-O3'	-5.25	102.12	110.00
1	B	55	ASN	CA-C-N	-5.23	114.03	122.81
1	B	55	ASN	C-N-CA	-5.23	114.03	122.81
1	B	255	ASN	N-CA-CB	-5.22	102.28	110.11
3	F	301	DC	P-O3'-C3'	5.22	128.03	120.20
1	A	37	SER	CA-CB-OG	-5.20	100.71	111.10
3	F	300	DA	O5'-P-OP2	-5.19	92.42	108.00
1	B	90	VAL	N-CA-C	5.18	116.05	108.53
2	E	288	DG	N1-C2-N2	5.17	124.06	116.30
1	B	227	PHE	O-C-N	-5.17	116.64	122.12
2	E	287	DA	O4'-C4'-C3'	-5.17	97.65	105.40
1	A	138	ARG	CG-CD-NE	-5.17	100.63	112.00
2	E	289	DT	C2'-C3'-O3'	5.17	119.25	111.50
1	A	103	ALA	N-CA-C	5.15	118.34	111.75
2	E	289	DT	OP1-P-OP2	5.14	135.41	120.00
1	A	100	PHE	CB-CA-C	-5.13	102.70	111.02
1	B	179	ILE	CA-CB-CG2	5.12	119.21	110.50
1	A	159	LEU	CB-CA-C	-5.12	102.62	110.81
1	B	215	VAL	N-CA-C	5.11	116.45	110.62
2	E	291	DC	O5'-C5'-C4'	5.11	118.47	110.80
1	A	173	HIS	N-CA-CB	-5.11	103.65	111.56
1	B	195	LYS	CB-CG-CD	5.09	123.01	111.30
1	B	197	GLN	N-CA-C	5.09	117.49	111.33
1	B	147	VAL	N-CA-C	5.07	115.79	110.62
1	B	280	THR	CB-CA-C	5.07	120.25	109.10
1	B	244	THR	OG1-CB-CG2	-5.07	99.16	109.30
1	A	160	CYS	CB-CA-C	-5.06	100.88	109.38
1	A	224	VAL	O-C-N	5.06	128.83	122.66
1	B	127	LYS	CB-CA-C	5.06	116.88	110.16
1	B	200	THR	N-CA-CB	5.05	117.33	110.01
1	B	246	LYS	CG-CD-CE	5.05	122.92	111.30
3	F	295	DG	N1-C2-N3	5.05	131.57	124.00
1	A	207	GLU	CG-CD-OE1	5.04	129.98	118.40
1	B	124	PRO	O-C-N	5.01	129.44	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	293	DC	N1-C1'-C2'	-5.00	105.99	113.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	GLN	Peptide
1	B	196	ALA	Peptide
1	B	279	LEU	Peptide
1	B	59	GLN	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	1938	0	1943	127	0
1	B	1939	0	1942	68	0
2	E	241	0	136	8	0
3	F	237	0	132	12	0
4	A	20	0	12	4	0
5	A	6	0	5	0	0
6	A	8	0	13	63	0
7	A	53	0	0	13	0
7	B	45	0	0	11	0
7	E	6	0	0	2	0
7	F	6	0	0	2	0
All	All	4499	0	4183	217	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 26.

All (217) 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:B:127:LYS:CD	1:B:127:LYS:CG	1.74	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LYS:CD	1:B:134:LYS:CE	1.77	1.57
1:B:134:LYS:CD	1:B:134:LYS:CG	1.76	1.56
3:F:298:DT:C1'	3:F:298:DT:N1	1.73	1.48
1:A:237[B]:MET:SD	1:A:237[B]:MET:CG	2.06	1.44
1:A:206:ASP:N	6:A:1285[A]:IPA:H11	1.28	1.44
1:A:253:PRO:CB	1:A:253:PRO:CG	1.74	1.43
2:E:282:DC:C5'	2:E:282:DC:O5'	1.67	1.43
1:A:206:ASP:N	6:A:1285[B]:IPA:H11	1.29	1.41
1:A:237[A]:MET:SD	1:A:237[A]:MET:CE	2.14	1.35
1:A:237[B]:MET:SD	1:A:237[B]:MET:CE	2.16	1.34
1:A:205:CYS:C	6:A:1285[A]:IPA:H11	1.67	1.20
1:B:116:ARG:HD3	7:B:2014:HOH:O	1.38	1.20
1:A:206:ASP:CA	6:A:1285[A]:IPA:H11	1.72	1.18
1:A:205:CYS:C	6:A:1285[B]:IPA:H11	1.69	1.18
1:A:206:ASP:CA	6:A:1285[B]:IPA:H11	1.73	1.17
1:A:205:CYS:C	6:A:1285[A]:IPA:C1	2.18	1.16
1:B:237:MET:SD	1:B:237:MET:CE	2.34	1.16
1:A:205:CYS:C	6:A:1285[B]:IPA:C1	2.21	1.14
1:A:206:ASP:N	6:A:1285[A]:IPA:C1	2.11	1.13
1:A:60:ASP:HB3	1:A:61:PRO:HD2	1.16	1.12
1:B:195:LYS:O	1:B:196:ALA:CB	1.97	1.10
1:A:204:ILE:O	6:A:1285[A]:IPA:H32	1.49	1.09
1:A:204:ILE:O	6:A:1285[B]:IPA:H32	1.50	1.08
1:A:60:ASP:HB3	1:A:61:PRO:CD	1.85	1.06
1:B:195:LYS:O	1:B:196:ALA:HB2	1.52	1.05
1:B:241:ILE:HG22	1:B:243:VAL:HG23	1.38	1.04
1:A:204:ILE:C	6:A:1285[B]:IPA:H13	1.82	1.02
1:A:204:ILE:C	6:A:1285[A]:IPA:H13	1.85	1.01
1:A:37:SER:HB2	1:A:38:PRO:HA	1.45	0.98
1:B:60:ASP:HB3	1:B:61:PRO:CD	1.97	0.94
1:A:207:GLU:HB2	6:A:1285[B]:IPA:H31	1.49	0.93
1:A:207:GLU:HB2	6:A:1285[B]:IPA:O2	1.67	0.93
1:A:37:SER:N	7:A:2001:HOH:O	2.02	0.92
1:A:207:GLU:HB2	6:A:1285[A]:IPA:H31	1.50	0.92
1:A:205:CYS:CA	6:A:1285[A]:IPA:H13	2.00	0.92
1:A:205:CYS:CA	6:A:1285[B]:IPA:H13	2.01	0.90
1:A:206:ASP:N	6:A:1285[B]:IPA:C1	2.12	0.90
1:A:203:GLU:O	6:A:1285[A]:IPA:H33	1.72	0.89
1:A:203:GLU:O	6:A:1285[B]:IPA:H33	1.72	0.89
1:A:205:CYS:C	6:A:1285[A]:IPA:H13	1.96	0.87
1:A:60:ASP:CB	1:A:61:PRO:CD	2.51	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:CYS:N	6:A:1285[B]:IPA:H13	1.89	0.86
1:A:46:GLU:OE1	1:A:76:HIS:HE1	1.59	0.86
1:B:60:ASP:HB3	1:B:61:PRO:HD3	1.57	0.85
1:A:205:CYS:N	6:A:1285[A]:IPA:H13	1.91	0.85
1:A:60:ASP:CB	1:A:61:PRO:HD2	2.04	0.84
1:B:209:LEU:O	1:B:213:VAL:HG23	1.77	0.84
1:A:204:ILE:O	6:A:1285[A]:IPA:H13	1.79	0.82
1:A:204:ILE:C	6:A:1285[B]:IPA:C1	2.51	0.82
1:A:204:ILE:O	6:A:1285[B]:IPA:H13	1.79	0.82
1:A:205:CYS:C	6:A:1285[B]:IPA:H13	1.98	0.81
1:B:241:ILE:CG2	1:B:243:VAL:HG23	2.11	0.81
1:A:204:ILE:C	6:A:1285[A]:IPA:H32	2.06	0.81
1:A:204:ILE:C	6:A:1285[B]:IPA:H32	2.05	0.81
1:A:237[A]:MET:HE1	7:A:2045:HOH:O	1.82	0.80
1:A:146:GLU:CG	7:A:2024:HOH:O	2.29	0.79
1:B:233:ARG:HD2	7:B:2032:HOH:O	1.84	0.78
3:F:298:DT:C1'	3:F:298:DT:C2	2.66	0.77
1:B:89:GLU:HG2	7:B:2011:HOH:O	1.86	0.75
1:A:146:GLU:HG3	7:A:2024:HOH:O	1.84	0.75
1:A:205:CYS:N	6:A:1285[A]:IPA:C1	2.49	0.75
1:A:204:ILE:C	6:A:1285[A]:IPA:C1	2.51	0.74
1:A:207:GLU:CB	6:A:1285[B]:IPA:H31	2.17	0.74
1:A:206:ASP:CA	6:A:1285[A]:IPA:C1	2.61	0.74
1:A:205:CYS:N	6:A:1285[B]:IPA:C1	2.49	0.73
1:A:207:GLU:CB	6:A:1285[A]:IPA:H31	2.18	0.73
3:F:298:DT:N1	3:F:298:DT:H1'	1.99	0.73
1:B:50:ASN:ND2	1:B:67:ASN:HD21	1.87	0.72
1:A:203:GLU:O	6:A:1285[B]:IPA:H12	1.89	0.72
1:A:37:SER:HB2	1:A:38:PRO:CA	2.20	0.72
1:A:208:ALA:N	6:A:1285[A]:IPA:O2	2.24	0.71
1:A:205:CYS:CA	6:A:1285[A]:IPA:C1	2.64	0.71
1:B:187:ASN:HB2	7:B:2020:HOH:O	1.91	0.70
1:A:205:CYS:CA	6:A:1285[B]:IPA:C1	2.66	0.69
2:E:282:DC:C5'	2:E:282:DC:P	2.81	0.68
1:B:164:GLU:HG2	7:B:2026:HOH:O	1.94	0.68
1:B:227:PHE:C	1:B:227:PHE:CD1	2.72	0.68
1:A:262:TRP:CE2	1:A:266:VAL:HG21	2.30	0.67
1:B:51:LEU:O	1:B:54:SER:OG	2.13	0.67
1:A:203:GLU:O	6:A:1285[A]:IPA:H12	1.93	0.67
1:B:41:SER:O	1:B:45:VAL:HG23	1.94	0.67
1:A:204:ILE:C	6:A:1285[A]:IPA:C3	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:295:DG:N7	7:F:2004:HOH:O	2.28	0.66
1:B:211:GLN:O	1:B:215:VAL:HG23	1.96	0.65
1:A:204:ILE:C	6:A:1285[B]:IPA:C3	2.69	0.65
1:A:91:LEU:HB2	1:A:218:VAL:HG21	1.80	0.63
1:A:95:MET:HG3	1:A:227:PHE:CE2	2.34	0.63
1:B:190:PRO:O	1:B:193:LEU:HB2	1.97	0.62
1:B:219:LYS:C	1:B:243:VAL:HG13	2.24	0.62
4:A:1283:HMU:C6	7:A:2053:HOH:O	2.46	0.62
1:A:207:GLU:HB2	6:A:1285[B]:IPA:C3	2.14	0.62
1:A:207:GLU:HB2	6:A:1285[A]:IPA:C3	2.15	0.61
1:A:207:GLU:CB	6:A:1285[B]:IPA:C3	2.78	0.61
2:E:282:DC:H5	7:E:2001:HOH:O	1.84	0.61
1:A:207:GLU:CB	6:A:1285[B]:IPA:O2	2.35	0.60
1:A:206:ASP:CA	6:A:1285[B]:IPA:C1	2.62	0.60
1:A:207:GLU:CB	6:A:1285[A]:IPA:C3	2.79	0.60
1:A:189:THR:HB	1:A:190:PRO:CD	2.32	0.59
1:A:204:ILE:HA	6:A:1285[A]:IPA:C3	2.33	0.59
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.85	0.59
1:B:138:ARG:HD3	7:B:2023:HOH:O	2.03	0.59
1:A:274:GLY:HA2	7:A:2049:HOH:O	2.04	0.58
1:A:60:ASP:CG	1:A:61:PRO:HD3	2.28	0.58
1:A:204:ILE:HA	6:A:1285[B]:IPA:C3	2.34	0.58
1:B:59:GLN:O	1:B:61:PRO:HD2	2.04	0.57
1:A:95:MET:HG3	1:A:227:PHE:CD2	2.40	0.56
1:A:204:ILE:HA	6:A:1285[A]:IPA:H33	1.88	0.55
1:B:194:PRO:HA	1:B:195:LYS:HE2	1.89	0.55
1:A:46:GLU:OE1	1:A:76:HIS:CE1	2.50	0.55
1:A:204:ILE:CA	6:A:1285[A]:IPA:C3	2.85	0.55
1:B:219:LYS:O	1:B:243:VAL:CG1	2.55	0.55
1:A:271:LEU:HG	1:A:276:LEU:HD12	1.89	0.54
1:B:219:LYS:C	1:B:243:VAL:CG1	2.80	0.54
1:B:219:LYS:O	1:B:243:VAL:HG13	2.07	0.54
1:A:204:ILE:CA	6:A:1285[A]:IPA:H33	2.38	0.54
1:A:59:GLN:O	1:A:60:ASP:HB3	2.07	0.54
1:A:204:ILE:CA	6:A:1285[B]:IPA:C3	2.86	0.54
1:B:97:PRO:HB3	1:B:102:MET:HB3	1.90	0.54
3:F:298:DT:C1'	3:F:298:DT:C6	2.84	0.54
1:B:262:TRP:CE2	1:B:266:VAL:HG21	2.43	0.54
1:A:204:ILE:HA	6:A:1285[B]:IPA:H33	1.89	0.53
1:B:214:ARG:NH1	1:B:241:ILE:HD11	2.23	0.53
1:A:146:GLU:HG2	7:A:2024:HOH:O	1.99	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:O	1:A:234:LYS:C	2.48	0.53
1:A:204:ILE:O	6:A:1285[A]:IPA:C3	2.38	0.53
2:E:282:DC:C5	7:E:2001:HOH:O	2.54	0.52
1:B:60:ASP:CB	1:B:61:PRO:CD	2.82	0.52
1:A:204:ILE:CA	6:A:1285[B]:IPA:H33	2.40	0.52
4:A:1282:HMU:CM5	7:A:2024:HOH:O	2.58	0.52
1:A:37:SER:HA	1:A:39:ALA:N	2.25	0.52
1:A:59:GLN:O	1:A:60:ASP:CB	2.58	0.51
1:A:203:GLU:C	6:A:1285[B]:IPA:H12	2.35	0.51
1:A:254:ARG:HH11	1:A:254:ARG:HG3	1.76	0.51
4:A:1282:HMU:HM51	7:A:2024:HOH:O	2.11	0.51
1:B:213:VAL:HG13	1:B:218:VAL:CG2	2.41	0.50
2:E:282:DC:O5'	2:E:282:DC:H2'	2.11	0.50
1:A:109:PHE:HA	4:A:1282:HMU:HM52	1.93	0.50
1:A:207:GLU:HG2	7:A:2039:HOH:O	2.11	0.49
1:B:160:CYS:SG	1:B:279:LEU:HB3	2.52	0.49
1:B:237:MET:HG3	1:B:238:ALA:N	2.27	0.49
3:F:303:DG:H2''	3:F:304:DG:OP2	2.13	0.49
1:B:238:ALA:HB2	7:B:2034:HOH:O	2.12	0.48
1:A:132:HIS:CE1	1:A:133:PRO:HD2	2.48	0.48
1:B:67:ASN:OD1	1:B:69:LEU:HB2	2.14	0.48
3:F:298:DT:H1'	3:F:298:DT:O2	2.14	0.48
1:A:203:GLU:C	6:A:1285[A]:IPA:H12	2.39	0.48
1:B:136:ARG:NH2	7:B:2021:HOH:O	2.46	0.48
3:F:298:DT:C2	3:F:298:DT:H1'	2.43	0.48
1:B:122:GLU:HG2	7:B:2017:HOH:O	2.13	0.47
1:B:182:ASN:C	1:B:182:ASN:OD1	2.57	0.47
1:A:66:TYR:HB2	1:A:179:ILE:HG23	1.95	0.47
1:A:207:GLU:CG	7:A:2039:HOH:O	2.63	0.47
1:A:251:PRO:O	1:A:252:SER:C	2.57	0.47
1:A:88:LYS:NZ	7:A:2012:HOH:O	2.48	0.47
1:A:193:LEU:O	1:A:194:PRO:C	2.57	0.47
1:B:87:LYS:HE2	7:B:2009:HOH:O	2.13	0.47
1:B:59:GLN:HB3	1:B:60:ASP:HB2	1.97	0.47
2:E:282:DC:C5'	2:E:282:DC:OP1	2.63	0.47
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.96	0.47
1:B:49:LEU:O	1:B:53:LEU:HD12	2.15	0.47
1:B:189:THR:HB	1:B:190:PRO:HD2	1.97	0.46
1:A:37:SER:CB	1:A:38:PRO:CA	2.90	0.46
1:B:36:GLU:OE2	1:B:36:GLU:HA	2.13	0.46
1:B:251:PRO:HB3	1:B:262:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HG	1:B:53:LEU:HD11	1.97	0.45
1:A:255:ASN:HA	1:A:256:PRO:HD3	1.89	0.45
1:A:97:PRO:HB3	1:A:102:MET:HB3	1.99	0.44
1:A:74:ALA:HB3	1:A:75:PRO:CD	2.48	0.44
1:A:84:CYS:HB2	1:A:171:PHE:CE1	2.52	0.44
2:E:282:DC:OP1	2:E:282:DC:H5''	2.18	0.44
1:A:111:GLU:O	1:A:115:VAL:HG23	2.17	0.44
1:A:150:ALA:O	1:A:154:SER:HB2	2.18	0.44
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.47	0.43
3:F:303:DG:O5'	3:F:303:DG:H2'	2.17	0.43
1:A:37:SER:CA	7:A:2001:HOH:O	2.58	0.43
1:A:60:ASP:CG	1:A:61:PRO:CD	2.89	0.43
1:A:260:LYS:HE3	1:A:260:LYS:HB3	1.72	0.43
1:A:164:GLU:H	1:A:164:GLU:CD	2.26	0.43
1:A:257:GLN:OE1	2:E:282:DC:H4'	2.18	0.43
1:B:60:ASP:HB3	1:B:61:PRO:HD2	1.90	0.43
3:F:298:DT:H2'	3:F:298:DT:O5'	2.19	0.43
1:A:60:ASP:OD1	1:A:61:PRO:HD3	2.19	0.43
1:B:89:GLU:OE1	1:B:219:LYS:HG2	2.18	0.43
1:B:276:LEU:O	1:B:279:LEU:O	2.37	0.43
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.69	0.43
3:F:303:DG:O5'	3:F:303:DG:C2'	2.67	0.43
1:A:204:ILE:CA	6:A:1285[B]:IPA:H32	2.46	0.43
1:B:199:ASP:O	1:B:203:GLU:HB2	2.19	0.42
1:A:254:ARG:HG3	1:A:254:ARG:NH1	2.34	0.42
3:F:299:3DR:C1'	7:F:2006:HOH:O	2.67	0.42
1:A:265:ILE:O	1:A:269:GLN:HG3	2.19	0.42
1:A:204:ILE:CA	6:A:1285[A]:IPA:H32	2.47	0.42
1:B:230:GLN:O	1:B:231:ARG:C	2.59	0.42
1:B:111:GLU:OE1	1:B:114:HIS:ND1	2.38	0.42
1:A:204:ILE:O	6:A:1285[B]:IPA:C1	2.60	0.41
1:A:222:ILE:HD13	1:A:222:ILE:HG21	1.85	0.41
1:B:195:LYS:O	1:B:196:ALA:HB3	2.08	0.41
1:B:195:LYS:O	1:B:195:LYS:HG2	2.21	0.41
1:B:38:PRO:O	1:B:39:ALA:C	2.62	0.41
1:B:255:ASN:HA	1:B:256:PRO:HD3	1.91	0.41
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.81	0.41
1:A:262:TRP:O	1:A:266:VAL:HG23	2.21	0.41
1:A:74:ALA:N	1:A:75:PRO:HD2	2.36	0.41
1:A:179:ILE:HD13	1:A:179:ILE:HG21	1.80	0.41
1:B:148:SER:HB3	1:B:251:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:CB	1:A:38:PRO:HA	2.31	0.41
1:A:277:SER:OG	1:A:278:LEU:N	2.46	0.41
1:B:179:ILE:HG21	1:B:179:ILE:HD13	1.75	0.41
1:B:276:LEU:HA	1:B:276:LEU:HD23	1.83	0.41
1:B:67:ASN:HB2	1:B:178:LEU:CD2	2.51	0.41
1:B:132:HIS:CG	1:B:133:PRO:HD2	2.56	0.41
1:A:37:SER:HB3	1:A:41:SER:H	1.86	0.40
1:A:68:PRO:HD2	1:A:177:PRO:O	2.21	0.40
1:B:209:LEU:O	1:B:209:LEU:HG	2.19	0.40
1:B:87:LYS:HG3	7:B:2001:HOH:O	2.21	0.40
1:B:275:VAL:O	1:B:276:LEU:C	2.61	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	244/247 (99%)	223 (91%)	18 (7%)	3 (1%)	10	17
1	B	243/247 (98%)	218 (90%)	19 (8%)	6 (2%)	4	7
All	All	487/494 (99%)	441 (91%)	37 (8%)	9 (2%)	6	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	B	60	ASP
1	B	196	ALA
1	B	195	LYS
1	B	240	GLY
1	A	207	GLU
1	B	86	SER

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Mol	Chain	Res	Type
1	A	161	GLY
1	B	261	GLY

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	215/215 (100%)	193 (90%)	22 (10%)	7	10
1	B	214/215 (100%)	182 (85%)	32 (15%)	3	4
All	All	429/430 (100%)	375 (87%)	54 (13%)	4	6

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	56	LEU
1	A	59	GLN
1	A	85	LYS
1	A	87	LYS
1	A	134	LYS
1	A	158	SER
1	A	159	LEU
1	A	181	MET
1	A	186	LYS
1	A	204	ILE
1	A	215	VAL
1	A	218	VAL
1	A	219	LYS
1	A	228	SER
1	A	234	LYS
1	A	237[A]	MET
1	A	237[B]	MET
1	A	241	ILE
1	A	260	LYS
1	A	271	LEU

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Mol	Chain	Res	Type
1	A	277	SER
1	B	36	GLU
1	B	37	SER
1	B	41	SER
1	B	44	LYS
1	B	48	GLU
1	B	51	LEU
1	B	54	SER
1	B	59	GLN
1	B	86	SER
1	B	87	LYS
1	B	89	GLU
1	B	127	LYS
1	B	134	LYS
1	B	138	ARG
1	B	155	LEU
1	B	168	LYS
1	B	179	ILE
1	B	193	LEU
1	B	195	LYS
1	B	197	GLN
1	B	203	GLU
1	B	211	GLN
1	B	214	ARG
1	B	234	LYS
1	B	241	ILE
1	B	243	VAL
1	B	244	THR
1	B	246	LYS
1	B	256	PRO
1	B	257	GLN
1	B	279	LEU
1	B	280	THR

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	59	GLN
1	A	76	HIS
1	A	96	ASN
1	A	175	HIS
1	A	230	GLN

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Mol	Chain	Res	Type
1	B	50	ASN
1	B	78	ASN
1	B	169	HIS
1	B	230	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	3DR	F	299	3	8,11,12	2.83	3 (37%)	7,14,17	2.13	4 (57%)

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	3DR	F	299	3	-	3/3/15/16	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	299	3DR	O3'-C3'	6.09	1.56	1.43
3	F	299	3DR	O5'-C5'	3.60	1.54	1.44
3	F	299	3DR	O4'-C4'	2.89	1.49	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	299	3DR	O4'-C1'-C2'	-2.89	100.65	106.34
3	F	299	3DR	O3'-C3'-C4'	2.85	120.88	110.07
3	F	299	3DR	O4'-C4'-C3'	2.79	107.84	103.73
3	F	299	3DR	C1'-C2'-C3'	-2.19	100.92	103.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	299	3DR	C4'-C5'-O5'-P
3	F	299	3DR	C3'-C4'-C5'-O5'
3	F	299	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	299	3DR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands 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$
4	HMU	A	1282	-	10,10,10	3.84	8 (80%)	11,13,13	3.25	7 (63%)
6	IPA	A	1285[A]	-	3,3,3	1.40	0	3,3,3	3.58	3 (100%)
5	GOL	A	1284	-	5,5,5	19.76	3 (60%)	5,5,5	11.65	4 (80%)
4	HMU	A	1283	-	10,10,10	2.16	4 (40%)	11,13,13	3.94	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	IPA	A	1285[B]	-	3,3,3	1.34	0	3,3,3	3.21	3 (100%)

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
4	HMU	A	1282	-	-	2/2/2/2	0/1/1/1
4	HMU	A	1283	-	-	2/2/2/2	0/1/1/1
5	GOL	A	1284	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1284	GOL	O2-C2	35.86	2.47	1.43
5	A	1284	GOL	O3-C3	25.42	2.49	1.42
4	A	1282	HMU	O2-C2	6.71	1.37	1.23
4	A	1282	HMU	C2-N1	5.72	1.44	1.36
4	A	1282	HMU	C6-C5	4.77	1.43	1.36
4	A	1282	HMU	C2-N3	4.30	1.44	1.37
4	A	1283	HMU	C4-C5	3.84	1.54	1.45
5	A	1284	GOL	C1-C2	3.73	1.66	1.51
4	A	1283	HMU	C6-C5	3.44	1.41	1.36
4	A	1282	HMU	CM5-C5	2.91	1.57	1.51
4	A	1283	HMU	O4-C4	2.88	1.29	1.23
4	A	1282	HMU	C6-N1	2.53	1.40	1.36
4	A	1283	HMU	C2-N1	-2.50	1.33	1.36
4	A	1282	HMU	C4-N3	2.22	1.43	1.38
4	A	1282	HMU	C4-C5	2.12	1.50	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1284	GOL	O2-C2-C3	-18.49	32.62	109.18
5	A	1284	GOL	O3-C3-C2	-16.75	34.97	110.38
4	A	1283	HMU	O2-C2-N1	-8.59	113.93	122.79
4	A	1283	HMU	N1-C2-N3	7.07	122.63	115.17
5	A	1284	GOL	O2-C2-C1	-6.78	81.12	109.18
4	A	1282	HMU	O4-C4-C5	-6.12	114.42	124.71
4	A	1283	HMU	CM5-C5-C6	-5.10	113.70	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1282	HMU	C6-N1-C2	4.70	127.06	122.69
6	A	1285[A]	IPA	O2-C2-C1	-4.63	80.54	110.28
4	A	1282	HMU	C5-C4-N3	3.78	120.98	115.21
6	A	1285[B]	IPA	O2-C2-C3	-3.59	87.21	110.28
4	A	1282	HMU	N1-C2-N3	-3.55	111.42	115.17
4	A	1282	HMU	O2-C2-N3	3.53	128.13	121.86
6	A	1285[B]	IPA	O2-C2-C1	3.23	131.04	110.28
5	A	1284	GOL	O1-C1-C2	3.17	124.65	110.38
6	A	1285[A]	IPA	O2-C2-C3	3.09	130.14	110.28
4	A	1283	HMU	C4-N3-C2	-3.02	122.22	126.37
6	A	1285[B]	IPA	C3-C2-C1	-2.77	92.70	113.38
6	A	1285[A]	IPA	C3-C2-C1	-2.72	93.06	113.38
4	A	1283	HMU	C6-N1-C2	-2.49	120.38	122.69
4	A	1282	HMU	O4-C4-N3	2.34	124.51	120.11
4	A	1282	HMU	O2-C2-N1	-2.26	120.45	122.79

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1284	GOL	C1-C2-C3-O3
5	A	1284	GOL	O2-C2-C3-O3
4	A	1282	HMU	C6-C5-CM5-O3
4	A	1282	HMU	C4-C5-CM5-O3
4	A	1283	HMU	C6-C5-CM5-O3
4	A	1283	HMU	C4-C5-CM5-O3

There are no ring outliers.

4 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1282	HMU	3	0
6	A	1285[A]	IPA	31	0
4	A	1283	HMU	1	0
6	A	1285[B]	IPA	32	0

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	244/247 (98%)	-0.61	1 (0%) 88 87	17, 40, 61, 72	2 (0%)
1	B	245/247 (99%)	-0.42	1 (0%) 88 87	22, 48, 68, 76	0
2	E	12/12 (100%)	-0.20	0 100 100	40, 61, 75, 82	0
3	F	11/12 (91%)	-0.35	0 100 100	38, 60, 85, 87	0
All	All	512/518 (98%)	-0.50	2 (0%) 88 87	17, 45, 68, 87	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	GLU	3.2
1	A	280	THR	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	3DR	F	299	11/12	0.94	0.10	67,75,80,83	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	1284	6/6	0.85	0.20	73,84,87,90	0
4	HMU	A	1283	10/10	0.86	0.16	80,97,101,103	0
4	HMU	A	1282	10/10	0.90	0.12	46,62,75,80	0
6	IPA	A	1285[A]	4/4	0.93	0.11	124,125,126,126	4
6	IPA	A	1285[B]	4/4	0.93	0.11	125,125,126,129	4

6.5 Other polymers

There are no such residues in this entry.