Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:18 PM GMT

PDB ID	:	1OE6
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

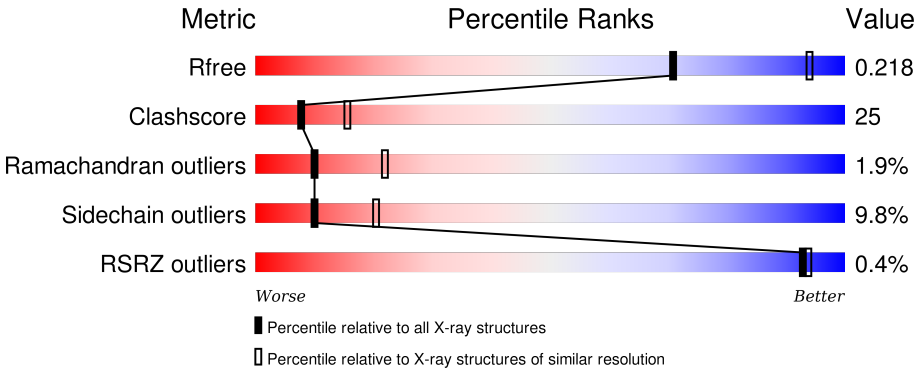
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 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	46% 39% 11%
1	B	247	% 49% 34% 11% 5%
2	E	12	92% 8%
3	F	12	67% 33%

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	-	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			

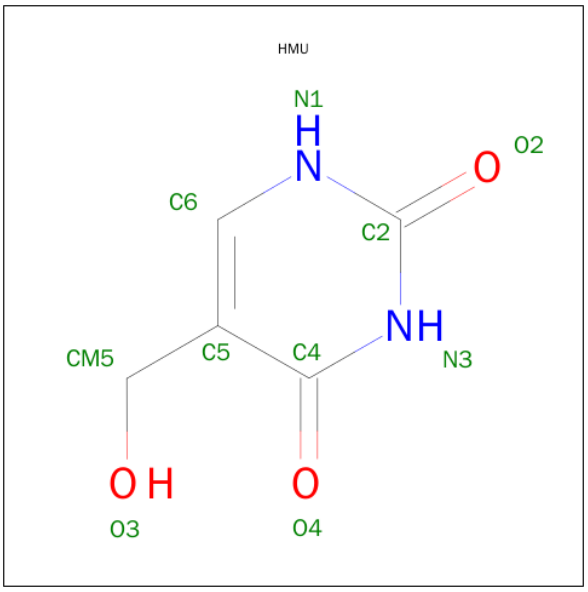
- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*G)-3'.

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'.

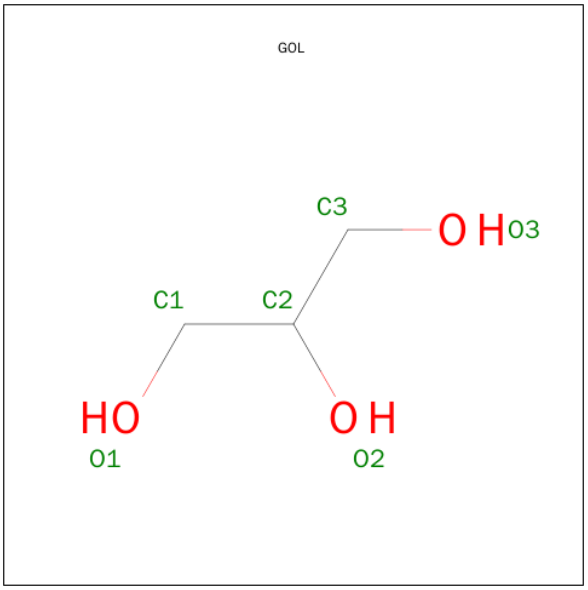
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			237	112	46	68	11			

- Molecule 4 is 5-HYDROXYMETHYL URACIL (three-letter code: HMU) (formula: $C_5H_6N_2O_3$).



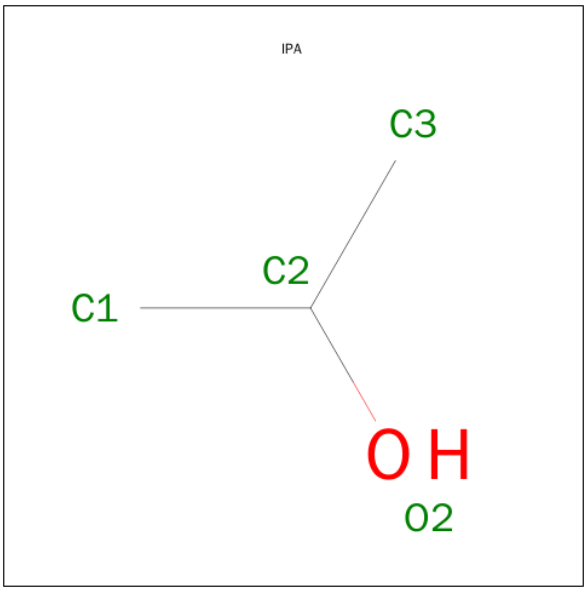
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	2	3		
4	A	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 5 is GLYCEROL (three-letter code: 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 (three-letter code: IPA) (formula: C_3H_8O).



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

- Molecule 7 is water.

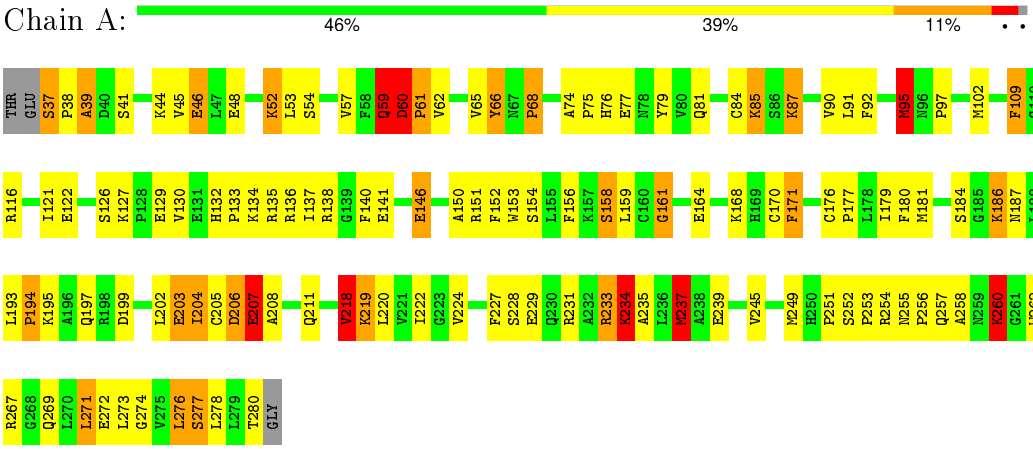
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	53	Total O 53 53	0	0
7	B	45	Total O 45 45	0	0
7	E	6	Total O 6 6	0	0
7	F	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

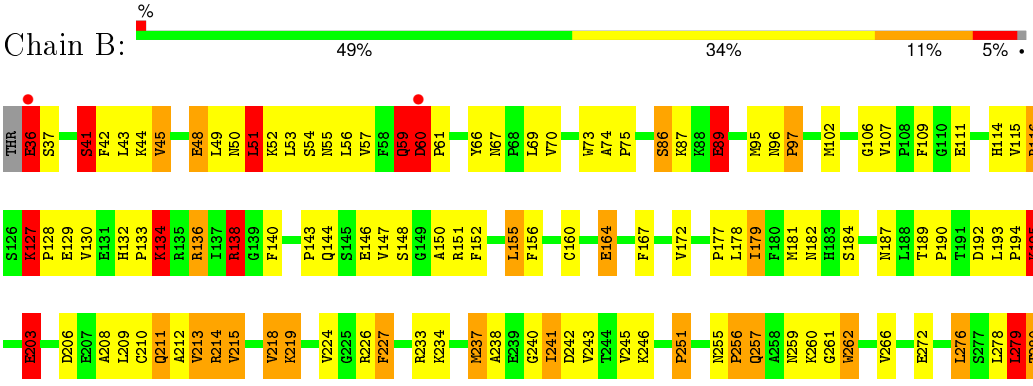
• Molecule 1: SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL DNA GLYCOSYLASE

Chain A:



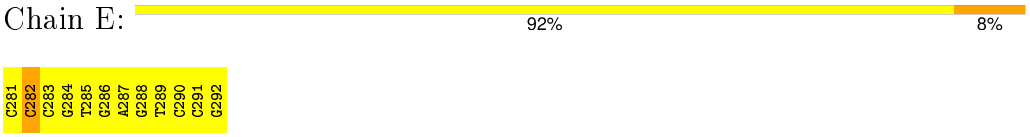
• Molecule 1: SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL DNA GLYCOSYLASE

Chain B:



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

Chain E:



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

Chain F:


67%
33%
C293
G294
G295
A296
C297
T298
N299
A300
C301
G302
G303
G304

4 Data and refinement statistics (i)

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 43.26 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.01-2.65) 99.4 (43.26-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.43%)	DCC
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 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 20624 reflections (0.005%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, IPA, 3DR, 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	2.48	103/1997 (5.2%)	1.81	48/2707 (1.8%)
1	B	2.33	82/1990 (4.1%)	1.69	31/2698 (1.1%)
2	E	4.32	58/269 (21.6%)	5.34	124/413 (30.0%)
3	F	5.25	81/253 (32.0%)	5.51	119/387 (30.7%)
All	All	2.79	324/4509 (7.2%)	2.54	322/6205 (5.2%)

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 (324) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	298	DT	C1'-N1	18.26	1.73	1.49
3	F	296	DA	C8-N7	17.16	1.43	1.31
2	E	292	DG	C8-N7	16.76	1.41	1.30
3	F	296	DA	C6-N1	16.14	1.46	1.35
1	A	46	GLU	CD-OE2	15.73	1.43	1.25
1	A	146	GLU	CD-OE1	15.53	1.42	1.25
3	F	304	DG	P-O5'	14.78	1.74	1.59
3	F	295	DG	C6-N1	13.81	1.49	1.39
2	E	283	DC	P-OP2	13.32	1.71	1.49
3	F	298	DT	N1-C6	12.91	1.47	1.38
2	E	292	DG	N3-C4	12.89	1.44	1.35
3	F	295	DG	C2-N3	12.80	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	294	DG	C2-N3	12.64	1.42	1.32
3	F	303	DG	C6-N1	12.53	1.48	1.39
1	A	207	GLU	CD-OE1	12.52	1.39	1.25
3	F	294	DG	C6-N1	12.42	1.48	1.39
1	A	272	GLU	CD-OE2	12.35	1.39	1.25
2	E	285	DT	C1'-N1	12.25	1.65	1.49
1	A	48	GLU	CD-OE2	11.93	1.38	1.25
2	E	288	DG	C6-N1	11.91	1.47	1.39
3	F	302	DG	P-O5'	11.78	1.71	1.59
1	B	146	GLU	CD-OE1	11.74	1.38	1.25
3	F	294	DG	C3'-O3'	-11.61	1.28	1.44
3	F	293	DC	N3-C4	11.13	1.41	1.33
1	B	227	PHE	CB-CG	-11.11	1.32	1.51
3	F	296	DA	N7-C5	10.94	1.45	1.39
3	F	294	DG	N7-C5	-10.88	1.32	1.39
3	F	294	DG	N1-C2	10.63	1.46	1.37
1	B	134	LYS	CD-CE	10.53	1.77	1.51
1	B	36	GLU	CD-OE1	10.16	1.36	1.25
1	A	164	GLU	CD-OE1	10.15	1.36	1.25
1	A	115	VAL	CB-CG1	-10.15	1.31	1.52
3	F	304	DG	N7-C5	10.14	1.45	1.39
1	B	237	MET	SD-CE	10.02	2.33	1.77
2	E	282	DC	O5'-C5'	10.01	1.67	1.42
2	E	286	DG	C6-N1	9.95	1.46	1.39
3	F	296	DA	C2-N3	9.92	1.42	1.33
2	E	284	DG	P-O5'	9.83	1.69	1.59
3	F	293	DC	N1-C6	9.63	1.43	1.37
1	B	36	GLU	CD-OE2	9.62	1.36	1.25
1	A	79	TYR	CG-CD1	-9.58	1.26	1.39
1	A	207	GLU	CG-CD	9.49	1.66	1.51
1	B	57	VAL	CB-CG2	9.48	1.72	1.52
1	B	73	TRP	CZ3-CH2	-9.48	1.24	1.40
3	F	296	DA	N1-C2	9.41	1.42	1.34
2	E	290	DC	C1'-N1	9.41	1.61	1.49
3	F	303	DG	N1-C2	9.40	1.45	1.37
3	F	304	DG	C8-N7	9.27	1.36	1.30
3	F	298	DT	C2-N3	9.26	1.45	1.37
1	B	164	GLU	CD-OE1	9.20	1.35	1.25
1	B	36	GLU	CG-CD	9.16	1.65	1.51
2	E	290	DC	P-O5'	9.16	1.69	1.59
3	F	295	DG	N3-C4	9.09	1.41	1.35
2	E	282	DC	N1-C6	-8.96	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	CD-OE1	8.93	1.35	1.25
1	A	129	GLU	CD-OE2	8.92	1.35	1.25
2	E	282	DC	O4'-C1'	8.91	1.52	1.42
1	A	207	GLU	N-CA	8.80	1.64	1.46
2	E	292	DG	C2-N2	8.80	1.43	1.34
1	A	60	ASP	CB-CG	8.79	1.70	1.51
2	E	288	DG	C6-O6	8.75	1.32	1.24
2	E	283	DC	P-O5'	8.74	1.68	1.59
1	A	127	LYS	CD-CE	8.63	1.72	1.51
3	F	302	DG	C6-N1	8.47	1.45	1.39
3	F	304	DG	N9-C4	8.46	1.44	1.38
2	E	283	DC	C4-C5	8.37	1.49	1.43
1	A	87	LYS	CD-CE	8.35	1.72	1.51
2	E	292	DG	C5-C6	-8.34	1.34	1.42
3	F	293	DC	N1-C2	8.32	1.48	1.40
3	F	304	DG	C2-N3	8.28	1.39	1.32
1	B	36	GLU	CB-CG	8.24	1.67	1.52
3	F	294	DG	C8-N7	8.23	1.35	1.30
2	E	288	DG	C2-N2	8.22	1.42	1.34
2	E	288	DG	N9-C4	8.22	1.44	1.38
1	B	41	SER	C-O	8.17	1.38	1.23
1	A	66	TYR	CD2-CE2	-8.11	1.27	1.39
2	E	286	DG	N7-C5	8.10	1.44	1.39
2	E	288	DG	N3-C4	8.09	1.41	1.35
3	F	294	DG	P-O5'	8.09	1.67	1.59
3	F	302	DG	C8-N7	8.07	1.35	1.30
1	B	144	GLN	CB-CG	8.00	1.74	1.52
2	E	286	DG	C2-N3	7.94	1.39	1.32
3	F	295	DG	N1-C2	7.86	1.44	1.37
2	E	282	DC	C4'-O4'	7.83	1.52	1.45
1	B	151	ARG	C-O	7.76	1.38	1.23
1	B	122	GLU	CD-OE1	7.72	1.34	1.25
3	F	302	DG	O4'-C1'	7.63	1.51	1.42
1	B	36	GLU	C-O	7.62	1.37	1.23
1	B	262	TRP	CG-CD1	-7.61	1.26	1.36
1	A	233	ARG	NE-CZ	7.59	1.43	1.33
3	F	302	DG	N7-C5	7.58	1.43	1.39
3	F	304	DG	C5-C6	7.55	1.49	1.42
3	F	295	DG	C8-N7	7.52	1.35	1.30
1	B	195	LYS	CB-CG	7.52	1.72	1.52
3	F	302	DG	N3-C4	7.51	1.40	1.35
1	B	203	GLU	CD-OE2	7.51	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	303	DG	C2-N3	7.40	1.38	1.32
2	E	292	DG	N9-C4	7.39	1.43	1.38
3	F	302	DG	C3'-O3'	7.38	1.53	1.44
2	E	285	DT	N1-C2	7.38	1.44	1.38
1	A	237[A]	MET	CG-SD	7.37	2.00	1.81
1	A	237[B]	MET	CG-SD	7.37	2.00	1.81
3	F	303	DG	C2'-C1'	7.37	1.59	1.52
1	B	259	ASN	C-O	-7.33	1.09	1.23
1	B	130	VAL	CB-CG1	7.32	1.68	1.52
1	A	272	GLU	CD-OE1	7.30	1.33	1.25
1	B	107	VAL	CA-CB	-7.29	1.39	1.54
1	A	39	ALA	CA-CB	-7.28	1.37	1.52
1	A	218	VAL	CB-CG2	7.28	1.68	1.52
1	B	48	GLU	CD-OE2	7.27	1.33	1.25
1	B	257	GLN	CG-CD	7.24	1.67	1.51
1	A	203	GLU	CD-OE2	7.23	1.33	1.25
1	A	229	GLU	C-O	7.15	1.36	1.23
1	B	106	GLY	C-O	-7.13	1.12	1.23
1	A	211	GLN	CG-CD	7.13	1.67	1.51
1	A	112	VAL	CA-CB	-7.10	1.39	1.54
1	A	130	VAL	CB-CG2	-7.07	1.38	1.52
1	B	129	GLU	CG-CD	7.04	1.62	1.51
1	B	134	LYS	CG-CD	7.02	1.76	1.52
2	E	284	DG	N7-C5	7.02	1.43	1.39
1	B	125	VAL	C-O	-7.00	1.10	1.23
1	B	122	GLU	CG-CD	7.00	1.62	1.51
3	F	304	DG	N3-C4	6.96	1.40	1.35
1	A	90	VAL	CA-CB	-6.96	1.40	1.54
1	B	213	VAL	CB-CG2	6.95	1.67	1.52
2	E	287	DA	N3-C4	6.93	1.39	1.34
3	F	303	DG	C6-O6	6.92	1.30	1.24
1	A	116	ARG	CA-CB	-6.91	1.38	1.53
2	E	288	DG	N1-C2	6.91	1.43	1.37
1	A	79	TYR	CD2-CE2	-6.90	1.28	1.39
1	A	170	CYS	CB-SG	-6.89	1.70	1.82
1	A	141	GLU	CD-OE2	-6.89	1.18	1.25
3	F	303	DG	N9-C8	6.83	1.42	1.37
3	F	302	DG	C5-C6	6.82	1.49	1.42
3	F	300	DA	C6-N1	6.80	1.40	1.35
1	A	203	GLU	CD-OE1	6.80	1.33	1.25
1	A	62	VAL	CB-CG1	6.80	1.67	1.52
1	B	164	GLU	CG-CD	6.79	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	PRO	C-O	6.77	1.36	1.23
2	E	282	DC	C3'-C2'	6.77	1.60	1.52
1	A	48	GLU	CD-OE1	6.75	1.33	1.25
1	B	96	ASN	CG-ND2	6.72	1.49	1.32
2	E	289	DT	C2-O2	6.69	1.27	1.22
1	A	152	PHE	N-CA	-6.68	1.32	1.46
1	B	203	GLU	CG-CD	6.68	1.61	1.51
3	F	300	DA	C2-N3	6.66	1.39	1.33
1	B	147	VAL	CB-CG1	-6.60	1.39	1.52
3	F	300	DA	C6-N6	6.60	1.39	1.33
1	A	260	LYS	CD-CE	6.57	1.67	1.51
1	B	146	GLU	N-CA	-6.57	1.33	1.46
1	B	127	LYS	CG-CD	6.57	1.74	1.52
3	F	300	DA	N3-C4	-6.55	1.30	1.34
2	E	286	DG	C6-O6	6.51	1.30	1.24
1	A	237[A]	MET	SD-CE	6.47	2.14	1.77
1	A	237[B]	MET	SD-CE	6.47	2.14	1.77
1	A	95	MET	CG-SD	6.47	1.98	1.81
2	E	286	DG	C5-C6	6.46	1.48	1.42
1	A	129	GLU	CG-CD	6.45	1.61	1.51
1	A	68	PRO	CA-C	-6.45	1.40	1.52
1	A	180	PHE	CE2-CZ	6.44	1.49	1.37
3	F	294	DG	C3'-C2'	-6.43	1.44	1.52
1	B	210	CYS	CB-SG	6.41	1.93	1.82
1	B	156	PHE	CD2-CE2	-6.41	1.26	1.39
1	A	206	ASP	C-O	-6.40	1.11	1.23
1	B	206	ASP	CB-CG	6.37	1.65	1.51
2	E	288	DG	C3'-O3'	-6.37	1.35	1.44
2	E	281	DC	C2-O2	6.35	1.30	1.24
3	F	303	DG	C2-N2	6.35	1.41	1.34
1	B	208	ALA	CA-CB	-6.34	1.39	1.52
3	F	303	DG	C8-N7	6.32	1.34	1.30
3	F	304	DG	O5'-C5'	6.32	1.58	1.42
1	B	184	SER	CB-OG	6.31	1.50	1.42
2	E	282	DC	O3'-P	6.29	1.68	1.61
1	A	245	VAL	C-O	-6.25	1.11	1.23
1	B	134	LYS	CE-NZ	6.21	1.64	1.49
1	B	66	TYR	CE1-CZ	6.21	1.46	1.38
1	A	48	GLU	CG-CD	6.17	1.61	1.51
1	A	206	ASP	N-CA	6.17	1.58	1.46
1	A	228	SER	CB-OG	-6.16	1.34	1.42
1	A	136	ARG	C-O	-6.16	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	ARG	C-O	-6.13	1.11	1.23
1	B	36	GLU	N-CA	6.10	1.58	1.46
1	A	129	GLU	CD-OE1	6.09	1.32	1.25
2	E	291	DC	O3'-P	-6.07	1.53	1.61
1	B	59	GLN	CG-CD	6.04	1.65	1.51
1	A	146	GLU	CG-CD	6.02	1.60	1.51
2	E	290	DC	C2'-C1'	6.00	1.58	1.52
1	B	73	TRP	CD2-CE2	-6.00	1.34	1.41
2	E	291	DC	N3-C4	5.98	1.38	1.33
1	A	229	GLU	CD-OE2	5.96	1.32	1.25
1	A	122	GLU	CD-OE2	5.94	1.32	1.25
1	A	140	PHE	CE2-CZ	-5.92	1.26	1.37
1	B	42	PHE	CB-CG	-5.92	1.41	1.51
1	B	143	PRO	CA-C	5.89	1.64	1.52
1	A	207	GLU	CA-CB	5.88	1.66	1.53
3	F	296	DA	N9-C4	5.86	1.41	1.37
2	E	284	DG	C6-O6	5.84	1.29	1.24
1	A	121	ILE	C-O	-5.84	1.12	1.23
1	B	127	LYS	CD-CE	5.84	1.65	1.51
1	B	219	LYS	CG-CD	5.84	1.72	1.52
1	A	46	GLU	CD-OE1	5.82	1.32	1.25
3	F	296	DA	C5-C4	5.82	1.42	1.38
2	E	292	DG	C2'-C1'	5.80	1.58	1.52
3	F	302	DG	N9-C8	5.78	1.41	1.37
1	A	111	GLU	CD-OE2	5.77	1.31	1.25
1	A	233	ARG	CG-CD	5.74	1.66	1.51
1	B	260	LYS	CB-CG	5.74	1.68	1.52
1	A	231	ARG	CG-CD	-5.73	1.37	1.51
2	E	282	DC	C3'-O3'	5.73	1.51	1.44
3	F	301	DC	N3-C4	5.73	1.38	1.33
1	A	204	ILE	CB-CG2	-5.73	1.35	1.52
1	B	115	VAL	CA-C	5.73	1.67	1.52
2	E	289	DT	C2'-C1'	5.72	1.58	1.52
1	A	57	VAL	CB-CG2	5.72	1.64	1.52
1	B	48	GLU	C-O	5.70	1.34	1.23
3	F	296	DA	N3-C4	5.70	1.38	1.34
2	E	289	DT	N3-C4	-5.69	1.34	1.38
3	F	300	DA	N1-C2	5.69	1.39	1.34
3	F	297	DC	N3-C4	-5.69	1.29	1.33
2	E	283	DC	C3'-O3'	5.68	1.51	1.44
3	F	300	DA	C8-N7	5.68	1.35	1.31
1	A	37	SER	N-CA	5.68	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	LYS	CD-CE	5.67	1.65	1.51
1	A	116	ARG	CZ-NH1	5.67	1.40	1.33
1	B	215	VAL	CA-CB	-5.66	1.42	1.54
3	F	296	DA	O3'-P	5.66	1.68	1.61
1	B	51	LEU	C-O	5.64	1.34	1.23
1	B	146	GLU	CD-OE2	5.63	1.31	1.25
3	F	297	DC	C5-C6	5.63	1.38	1.34
3	F	304	DG	C5-C4	5.62	1.42	1.38
1	A	44	LYS	CB-CG	5.61	1.67	1.52
2	E	288	DG	C8-N7	5.60	1.34	1.30
1	B	167	PHE	CG-CD2	-5.60	1.30	1.38
2	E	287	DA	C4'-O4'	5.59	1.50	1.45
1	A	81	GLN	CB-CG	5.58	1.67	1.52
3	F	298	DT	C4-C5	5.58	1.50	1.45
1	B	140	PHE	CB-CG	-5.56	1.41	1.51
1	A	156	PHE	CD2-CE2	-5.55	1.28	1.39
1	A	273	LEU	CA-C	-5.55	1.38	1.52
1	A	54	SER	CB-OG	5.53	1.49	1.42
3	F	297	DC	O5'-C5'	5.53	1.56	1.42
1	A	57	VAL	CB-CG1	5.52	1.64	1.52
3	F	301	DC	C2-O2	5.52	1.29	1.24
1	A	184	SER	CB-OG	5.51	1.49	1.42
2	E	286	DG	N1-C2	5.51	1.42	1.37
1	A	171	PHE	CD2-CE2	-5.50	1.28	1.39
3	F	295	DG	C3'-O3'	-5.50	1.36	1.44
1	A	170	CYS	C-O	-5.49	1.12	1.23
1	A	112	VAL	CB-CG1	-5.49	1.41	1.52
2	E	284	DG	C6-N1	5.49	1.43	1.39
3	F	304	DG	C6-O6	5.48	1.29	1.24
1	A	65	VAL	CB-CG2	-5.48	1.41	1.52
1	A	186	LYS	CD-CE	5.48	1.65	1.51
1	A	195	LYS	CD-CE	5.48	1.65	1.51
2	E	288	DG	P-O5'	5.48	1.65	1.59
1	A	60	ASP	C-O	5.47	1.33	1.23
3	F	293	DC	C2-N3	5.46	1.40	1.35
3	F	293	DC	C2-O2	5.44	1.29	1.24
1	B	122	GLU	CB-CG	5.44	1.62	1.52
1	B	128	PRO	CA-C	5.43	1.63	1.52
1	A	187	ASN	CB-CG	5.43	1.63	1.51
1	B	224	VAL	CB-CG2	5.43	1.64	1.52
3	F	298	DT	N3-C4	5.41	1.43	1.38
1	B	109	PHE	CE2-CZ	5.40	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLN	CG-CD	5.40	1.63	1.51
1	B	278	LEU	C-O	-5.38	1.13	1.23
1	A	219	LYS	CB-CG	5.38	1.67	1.52
1	A	197	GLN	C-O	5.37	1.33	1.23
2	E	281	DC	C5'-C4'	5.36	1.57	1.51
1	A	206	ASP	CA-C	5.35	1.66	1.52
1	B	60	ASP	CB-CG	5.34	1.62	1.51
1	A	153	TRP	CE3-CZ3	5.33	1.47	1.38
1	B	116	ARG	NE-CZ	5.32	1.40	1.33
1	B	150	ALA	C-O	5.32	1.33	1.23
1	A	280	THR	CA-CB	5.31	1.67	1.53
1	B	260	LYS	N-CA	-5.31	1.35	1.46
1	A	92	PHE	CD2-CE2	-5.31	1.28	1.39
1	A	168	LYS	CD-CE	5.30	1.64	1.51
3	F	302	DG	C5'-C4'	5.30	1.57	1.51
1	A	134	LYS	CG-CD	5.28	1.70	1.52
1	A	176	CYS	CB-SG	5.26	1.91	1.82
3	F	294	DG	C2-N2	5.26	1.39	1.34
1	A	264	GLY	C-O	-5.26	1.15	1.23
3	F	303	DG	C3'-C2'	5.25	1.58	1.52
1	A	258	ALA	CA-CB	-5.25	1.41	1.52
3	F	298	DT	P-OP2	5.24	1.57	1.49
1	B	196	ALA	CA-C	-5.24	1.39	1.52
1	A	137	ILE	C-O	-5.23	1.13	1.23
1	A	140	PHE	CB-CG	-5.23	1.42	1.51
1	B	177	PRO	CA-C	-5.23	1.42	1.52
1	A	109	PHE	CD1-CE1	5.22	1.49	1.39
1	B	172	VAL	CA-C	-5.22	1.39	1.52
1	B	212	ALA	CA-CB	-5.22	1.41	1.52
2	E	292	DG	N1-C2	5.21	1.42	1.37
1	A	68	PRO	CA-CB	-5.20	1.43	1.53
2	E	287	DA	C5-C4	5.20	1.42	1.38
1	B	152	PHE	C-O	-5.19	1.13	1.23
2	E	289	DT	P-O5'	5.19	1.65	1.59
1	B	218	VAL	CA-CB	5.18	1.65	1.54
2	E	286	DG	C4'-O4'	5.18	1.50	1.45
3	F	302	DG	N9-C4	5.17	1.42	1.38
2	E	292	DG	C6-N1	-5.16	1.35	1.39
1	A	77	GLU	CD-OE2	5.15	1.31	1.25
1	A	245	VAL	N-CA	-5.14	1.36	1.46
2	E	289	DT	C4-C5	5.13	1.49	1.45
2	E	287	DA	P-O5'	5.13	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	LYS	CE-NZ	5.12	1.61	1.49
1	B	89	GLU	CD-OE1	5.12	1.31	1.25
3	F	303	DG	C5-C4	5.11	1.42	1.38
1	A	140	PHE	CE1-CZ	5.10	1.47	1.37
1	B	138	ARG	CG-CD	5.08	1.64	1.51
1	A	122	GLU	CG-CD	5.08	1.59	1.51
1	B	199	ASP	CB-CG	5.08	1.62	1.51
3	F	296	DA	P-O5'	5.07	1.64	1.59
1	B	95	MET	CA-CB	-5.06	1.42	1.53
3	F	303	DG	C3'-O3'	5.05	1.50	1.44
2	E	283	DC	P-OP1	5.05	1.57	1.49
1	A	260	LYS	CG-CD	5.04	1.69	1.52
3	F	300	DA	C4'-C3'	-5.03	1.47	1.52
1	B	272	GLU	CG-CD	5.03	1.59	1.51
3	F	302	DG	O5'-C5'	5.03	1.54	1.42
1	A	235	ALA	CA-CB	-5.02	1.42	1.52
1	A	220	LEU	C-O	-5.02	1.13	1.23
1	A	116	ARG	CB-CG	-5.00	1.39	1.52

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	298	DT	O4'-C1'-N1	22.18	123.53	108.00
3	F	297	DC	C5-C4-N4	18.73	133.31	120.20
3	F	293	DC	N1-C2-O2	18.57	130.04	118.90
2	E	291	DC	O5'-P-OP1	-18.05	89.04	110.70
2	E	291	DC	O4'-C1'-N1	16.89	119.82	108.00
3	F	302	DG	O4'-C4'-C3'	-16.81	95.91	106.00
3	F	297	DC	N3-C4-N4	-16.65	106.34	118.00
2	E	292	DG	C5-C6-O6	-16.33	118.80	128.60
2	E	290	DC	N3-C4-N4	-15.92	106.86	118.00
3	F	295	DG	OP1-P-OP2	15.79	143.28	119.60
3	F	295	DG	C6-N1-C2	-15.44	115.84	125.10
3	F	303	DG	O4'-C1'-N9	15.20	118.64	108.00
2	E	283	DC	C6-N1-C2	14.99	126.30	120.30
2	E	285	DT	O4'-C1'-N1	14.90	118.43	108.00
3	F	304	DG	N1-C6-O6	-14.78	111.03	119.90
3	F	300	DA	O5'-P-OP2	-14.75	92.42	105.70
2	E	289	DT	O5'-P-OP1	-14.71	92.46	105.70
2	E	287	DA	O4'-C1'-N9	-14.54	97.82	108.00
3	F	295	DG	C5-C6-O6	-14.32	120.01	128.60
2	E	287	DA	O4'-C4'-C3'	-13.92	97.65	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	304	DG	C5-C6-O6	13.71	136.83	128.60
2	E	292	DG	N1-C2-N3	-13.68	115.69	123.90
3	F	298	DT	O5'-P-OP2	-13.66	93.41	105.70
2	E	289	DT	C6-C5-C7	-13.61	114.73	122.90
1	A	151	ARG	NE-CZ-NH2	-13.45	113.57	120.30
3	F	304	DG	N3-C2-N2	13.29	129.20	119.90
2	E	290	DC	N3-C4-C5	13.23	127.19	121.90
2	E	282	DC	OP1-P-O3'	-12.90	76.82	105.20
2	E	292	DG	C4-C5-N7	12.83	115.93	110.80
3	F	295	DG	N1-C2-N3	12.79	131.57	123.90
3	F	294	DG	C5-C6-O6	-12.58	121.06	128.60
2	E	289	DT	N3-C4-O4	-12.39	112.46	119.90
2	E	288	DG	P-O3'-C3'	12.36	134.53	119.70
2	E	282	DC	O4'-C1'-N1	12.34	116.64	108.00
1	A	151	ARG	NE-CZ-NH1	12.27	126.44	120.30
3	F	304	DG	N1-C2-N2	-12.27	105.16	116.20
3	F	295	DG	O5'-P-OP2	-12.21	94.71	105.70
2	E	283	DC	N3-C4-C5	12.15	126.76	121.90
2	E	281	DC	O3'-P-O5'	-11.86	81.47	104.00
2	E	283	DC	OP1-P-OP2	11.84	137.35	119.60
2	E	285	DT	O4'-C4'-C3'	-11.63	99.02	106.00
3	F	293	DC	C2-N3-C4	11.55	125.67	119.90
2	E	286	DG	C6-N1-C2	-11.53	118.18	125.10
3	F	303	DG	N1-C6-O6	11.50	126.80	119.90
2	E	282	DC	OP1-P-OP2	11.49	136.84	119.60
2	E	284	DG	N3-C2-N2	11.39	127.87	119.90
2	E	282	DC	C4-C5-C6	11.34	123.07	117.40
2	E	285	DT	C3'-C2'-C1'	-11.23	89.02	102.50
3	F	295	DG	C2-N3-C4	-11.09	106.36	111.90
3	F	298	DT	OP1-P-OP2	11.06	136.19	119.60
2	E	284	DG	C4-C5-N7	11.04	115.22	110.80
2	E	292	DG	C5-C6-N1	11.00	117.00	111.50
2	E	289	DT	C1'-O4'-C4'	-10.94	99.16	110.10
1	A	233	ARG	NE-CZ-NH2	10.87	125.73	120.30
3	F	298	DT	N1-C2-O2	-10.82	114.44	123.10
2	E	291	DC	C5'-C4'-C3'	-10.81	94.64	114.10
3	F	296	DA	N7-C8-N9	-10.73	108.44	113.80
3	F	294	DG	C6-C5-N7	-10.71	123.97	130.40
3	F	293	DC	N1-C2-N3	-10.68	111.72	119.20
1	B	198	ARG	NE-CZ-NH1	10.66	125.63	120.30
2	E	289	DT	OP1-P-OP2	10.54	135.41	119.60
3	F	294	DG	N1-C6-O6	10.38	126.13	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	290	DC	C2-N3-C4	-10.34	114.73	119.90
3	F	296	DA	C8-N9-C4	10.34	109.94	105.80
3	F	297	DC	OP1-P-O3'	-10.33	82.48	105.20
3	F	294	DG	C6-N1-C2	-10.28	118.94	125.10
2	E	284	DG	N9-C4-C5	-10.14	101.34	105.40
3	F	295	DG	N1-C2-N2	-10.06	107.14	116.20
2	E	289	DT	C5-C4-O4	10.01	131.91	124.90
3	F	301	DC	C6-N1-C2	9.94	124.28	120.30
2	E	289	DT	P-O3'-C3'	9.89	131.56	119.70
2	E	289	DT	C4-C5-C7	9.72	124.83	119.00
3	F	300	DA	N1-C2-N3	9.61	134.11	129.30
3	F	296	DA	N1-C2-N3	-9.54	124.53	129.30
3	F	304	DG	P-O5'-C5'	9.52	136.13	120.90
3	F	303	DG	C5-C6-O6	-9.41	122.95	128.60
2	E	282	DC	OP2-P-O3'	9.37	125.81	105.20
3	F	296	DA	O4'-C1'-N9	-9.20	101.56	108.00
3	F	297	DC	C2-N1-C1'	-9.20	108.68	118.80
3	F	302	DG	C2-N3-C4	9.18	116.49	111.90
1	A	60	ASP	CB-CG-OD2	9.14	126.52	118.30
3	F	295	DG	C5-N7-C8	-9.13	99.74	104.30
1	A	280	THR	CA-CB-CG2	9.11	125.16	112.40
3	F	294	DG	N3-C2-N2	9.10	126.27	119.90
1	A	192	ASP	CB-CG-OD2	9.04	126.44	118.30
2	E	291	DC	O5'-P-OP2	9.01	121.51	110.70
2	E	285	DT	N3-C2-O2	-8.99	116.91	122.30
2	E	288	DG	N1-C6-O6	8.96	125.28	119.90
2	E	282	DC	N3-C4-C5	-8.88	118.35	121.90
3	F	295	DG	O4'-C4'-C3'	-8.84	100.70	106.00
3	F	298	DT	O5'-P-OP1	8.79	121.25	110.70
2	E	288	DG	N1-C2-N2	8.73	124.06	116.20
2	E	291	DC	C2-N3-C4	-8.71	115.54	119.90
2	E	284	DG	P-O5'-C5'	8.70	134.81	120.90
3	F	302	DG	O5'-P-OP1	8.70	121.13	110.70
1	B	56	LEU	CA-CB-CG	8.69	135.28	115.30
2	E	287	DA	C1'-O4'-C4'	8.64	118.74	110.10
3	F	298	DT	O4'-C1'-C2'	-8.64	98.99	105.90
2	E	286	DG	OP1-P-OP2	8.61	132.51	119.60
3	F	302	DG	O4'-C1'-N9	8.54	113.97	108.00
2	E	283	DC	N3-C4-N4	-8.51	112.04	118.00
3	F	303	DG	C6-C5-N7	-8.47	125.32	130.40
2	E	284	DG	O5'-P-OP1	8.39	120.77	110.70
3	F	302	DG	P-O3'-C3'	8.38	129.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	292	DG	OP1-P-OP2	8.34	132.11	119.60
3	F	298	DT	O4'-C4'-C3'	-8.24	101.06	106.00
2	E	282	DC	O5'-P-OP2	8.23	120.57	110.70
2	E	281	DC	C6-N1-C2	8.22	123.59	120.30
3	F	295	DG	C4-C5-N7	8.22	114.09	110.80
1	A	95	MET	CG-SD-CE	8.19	113.30	100.20
2	E	282	DC	O4'-C4'-C3'	-8.18	101.09	106.00
1	A	52	LYS	CD-CE-NZ	-8.17	92.91	111.70
3	F	295	DG	C5-C6-N1	8.17	115.59	111.50
2	E	281	DC	C4-C5-C6	-8.15	113.32	117.40
1	A	199	ASP	CB-CG-OD2	8.14	125.62	118.30
2	E	282	DC	O5'-P-OP1	-8.12	98.39	105.70
1	A	267	ARG	NE-CZ-NH2	-8.10	116.25	120.30
2	E	288	DG	C8-N9-C4	-8.09	103.16	106.40
3	F	303	DG	C5-N7-C8	-8.09	100.25	104.30
3	F	295	DG	C6-C5-N7	-8.09	125.55	130.40
3	F	293	DC	C6-N1-C1'	-8.08	111.11	120.80
2	E	288	DG	N3-C2-N2	-8.04	114.27	119.90
2	E	290	DC	C5-C4-N4	8.02	125.81	120.20
2	E	287	DA	P-O5'-C5'	8.00	133.70	120.90
3	F	300	DA	C6-N1-C2	-7.97	113.82	118.60
3	F	293	DC	C5-C6-N1	7.90	124.95	121.00
3	F	303	DG	C4-C5-N7	7.86	113.95	110.80
3	F	296	DA	P-O3'-C3'	7.83	129.09	119.70
3	F	300	DA	C4-C5-C6	7.75	120.88	117.00
3	F	300	DA	N9-C4-C5	7.71	108.89	105.80
1	A	280	THR	CA-C-O	7.70	136.26	120.10
3	F	295	DG	P-O3'-C3'	7.68	128.92	119.70
1	A	161	GLY	N-CA-C	7.65	132.23	113.10
2	E	286	DG	C5-C6-N1	7.64	115.32	111.50
2	E	286	DG	O4'-C1'-N9	7.60	113.32	108.00
1	A	206	ASP	CB-CG-OD1	7.55	125.09	118.30
3	F	298	DT	N3-C2-O2	7.54	126.82	122.30
2	E	283	DC	C5-C6-N1	-7.54	117.23	121.00
2	E	284	DG	N1-C2-N2	-7.50	109.45	116.20
2	E	282	DC	C6-N1-C2	-7.48	117.31	120.30
3	F	300	DA	C8-N9-C4	-7.47	102.81	105.80
2	E	284	DG	N3-C4-N9	7.46	130.48	126.00
3	F	294	DG	C4-C5-C6	7.46	123.27	118.80
2	E	281	DC	N3-C4-C5	7.43	124.87	121.90
3	F	295	DG	N1-C6-O6	7.42	124.35	119.90
3	F	293	DC	C2-N1-C1'	7.42	126.96	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	283	DC	N1-C2-O2	7.39	123.33	118.90
3	F	298	DT	C6-N1-C2	-7.36	117.62	121.30
3	F	303	DG	P-O5'-C5'	7.35	132.66	120.90
3	F	297	DC	C2-N3-C4	7.29	123.55	119.90
3	F	302	DG	N1-C6-O6	-7.22	115.57	119.90
3	F	304	DG	C4-C5-N7	-7.20	107.92	110.80
2	E	292	DG	N3-C2-N2	7.19	124.94	119.90
1	A	206	ASP	C-N-CA	7.17	139.63	121.70
1	B	206	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	224	VAL	N-CA-C	-7.10	91.82	111.00
3	F	294	DG	N1-C2-N2	-7.10	109.81	116.20
2	E	282	DC	C5-C4-N4	7.08	125.16	120.20
2	E	284	DG	C8-N9-C4	7.06	109.22	106.40
2	E	283	DC	O4'-C1'-N1	7.04	112.93	108.00
3	F	303	DG	N7-C8-N9	7.02	116.61	113.10
1	B	242	ASP	CB-CG-OD2	7.00	124.60	118.30
2	E	290	DC	O4'-C1'-C2'	6.99	111.49	105.90
1	B	192	ASP	CB-CG-OD2	6.96	124.57	118.30
3	F	301	DC	P-O3'-C3'	6.94	128.03	119.70
1	B	251	PRO	N-CD-CG	6.91	113.56	103.20
2	E	281	DC	C5-C4-N4	-6.89	115.38	120.20
2	E	282	DC	N3-C2-O2	-6.87	117.09	121.90
3	F	298	DT	N1-C2-N3	6.87	118.72	114.60
1	B	52	LYS	CD-CE-NZ	-6.83	95.98	111.70
1	A	146	GLU	CG-CD-OE1	6.82	131.94	118.30
2	E	283	DC	O3'-P-O5'	-6.82	91.04	104.00
1	A	234	LYS	CD-CE-NZ	6.78	127.30	111.70
1	A	280	THR	CB-CA-C	6.78	129.92	111.60
1	A	126	SER	CB-CA-C	6.78	122.98	110.10
2	E	282	DC	C5'-C4'-C3'	-6.76	101.93	114.10
2	E	288	DG	N9-C4-C5	6.75	108.10	105.40
2	E	285	DT	C4-C5-C6	6.73	122.04	118.00
1	A	46	GLU	OE1-CD-OE2	6.73	131.38	123.30
1	A	207	GLU	CA-CB-CG	6.66	128.04	113.40
1	B	45	VAL	CB-CA-C	-6.62	98.82	111.40
1	B	155	LEU	CA-CB-CG	6.61	130.50	115.30
1	B	138	ARG	NE-CZ-NH1	6.61	123.60	120.30
2	E	287	DA	N7-C8-N9	6.60	117.10	113.80
2	E	290	DC	C5-C6-N1	-6.57	117.71	121.00
2	E	288	DG	C4'-C3'-O3'	-6.56	93.30	109.70
1	A	45	VAL	CB-CA-C	-6.56	98.94	111.40
1	B	197	GLN	N-CA-CB	6.56	122.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	288	DG	C4-C5-N7	-6.56	108.18	110.80
1	A	77	GLU	OE1-CD-OE2	6.49	131.09	123.30
1	B	279	LEU	N-CA-C	-6.49	93.48	111.00
2	E	292	DG	C6-N1-C2	6.47	128.98	125.10
3	F	293	DC	C4-C5-C6	-6.46	114.17	117.40
1	B	60	ASP	CB-CG-OD2	6.46	124.11	118.30
2	E	283	DC	P-O3'-C3'	6.42	127.40	119.70
3	F	298	DT	C4-C5-C7	6.39	122.83	119.00
2	E	286	DG	C8-N9-C4	6.36	108.94	106.40
2	E	283	DC	C2-N3-C4	-6.33	116.73	119.90
3	F	300	DA	P-O3'-C3'	6.31	127.27	119.70
3	F	297	DC	C6-N1-C1'	6.31	128.37	120.80
1	A	146	GLU	CG-CD-OE2	-6.30	105.69	118.30
2	E	292	DG	N1-C6-O6	6.29	123.67	119.90
2	E	288	DG	C5-C6-O6	-6.28	124.83	128.60
1	A	249	MET	CG-SD-CE	-6.26	90.18	100.20
1	B	226	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	61	PRO	N-CD-CG	6.24	112.56	103.20
3	F	298	DT	C2-N3-C4	-6.24	123.46	127.20
2	E	284	DG	C3'-C2'-C1'	-6.23	95.02	102.50
3	F	296	DA	N3-C4-N9	-6.23	122.42	127.40
1	A	68	PRO	N-CD-CG	-6.20	93.89	103.20
2	E	290	DC	N3-C2-O2	-6.20	117.56	121.90
1	A	146	GLU	CA-CB-CG	6.19	127.02	113.40
2	E	289	DT	P-O5'-C5'	6.17	130.78	120.90
2	E	290	DC	C4'-C3'-C2'	6.16	108.64	103.10
3	F	297	DC	C6-N1-C2	6.15	122.76	120.30
2	E	287	DA	O4'-C1'-C2'	-6.14	100.99	105.90
1	B	57	VAL	CB-CA-C	6.12	123.03	111.40
1	B	130	VAL	CG1-CB-CG2	6.12	120.69	110.90
3	F	302	DG	P-O5'-C5'	6.12	130.69	120.90
2	E	284	DG	C4'-C3'-C2'	6.11	108.60	103.10
2	E	284	DG	C6-C5-N7	-6.11	126.73	130.40
2	E	289	DT	N3-C2-O2	-6.09	118.64	122.30
3	F	297	DC	O4'-C4'-C3'	-6.09	102.06	104.50
3	F	293	DC	O5'-C5'-C4'	-6.08	95.80	111.00
2	E	281	DC	N3-C2-O2	6.08	126.15	121.90
3	F	301	DC	O3'-P-O5'	-6.05	92.50	104.00
2	E	287	DA	C5-N7-C8	-6.04	100.88	103.90
3	F	300	DA	C2-N3-C4	-6.02	107.59	110.60
1	B	203	GLU	CA-CB-CG	6.00	126.60	113.40
2	E	286	DG	C5-C6-O6	-6.00	125.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	287	DA	C4'-C3'-C2'	6.00	108.50	103.10
1	A	204	ILE	CG1-CB-CG2	-6.00	98.21	111.40
3	F	295	DG	C4'-C3'-C2'	5.99	108.49	103.10
1	A	158	SER	CB-CA-C	-5.98	98.73	110.10
1	B	198	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
3	F	293	DC	O4'-C4'-C3'	5.95	109.57	106.00
3	F	294	DG	O3'-P-O5'	-5.95	92.70	104.00
3	F	302	DG	N9-C4-C5	5.94	107.78	105.40
2	E	286	DG	O4'-C1'-C2'	-5.93	101.15	105.90
1	A	135	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	E	283	DC	P-O5'-C5'	5.92	130.37	120.90
3	F	301	DC	N1-C2-N3	-5.91	115.06	119.20
3	F	300	DA	O4'-C1'-N9	-5.89	103.88	108.00
1	A	138	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	E	290	DC	O3'-P-O5'	-5.88	92.83	104.00
1	A	272	GLU	CA-CB-CG	-5.86	100.51	113.40
3	F	300	DA	N1-C6-N6	5.86	122.11	118.60
3	F	302	DG	C5-C6-N1	5.85	114.43	111.50
2	E	283	DC	C5'-C4'-O4'	5.84	120.40	109.30
3	F	293	DC	O4'-C1'-N1	5.84	112.09	108.00
1	A	207	GLU	CG-CD-OE1	5.84	129.98	118.30
2	E	283	DC	O4'-C1'-C2'	-5.84	101.23	105.90
2	E	292	DG	C4-C5-C6	-5.83	115.30	118.80
2	E	282	DC	C5'-C4'-O4'	5.82	120.36	109.30
3	F	303	DG	C8-N9-C4	-5.82	104.07	106.40
1	B	198	ARG	CG-CD-NE	5.81	124.00	111.80
1	A	122	GLU	N-CA-C	-5.79	95.38	111.00
3	F	301	DC	N3-C4-C5	5.78	124.21	121.90
3	F	298	DT	C6-C5-C7	-5.77	119.44	122.90
2	E	287	DA	N1-C6-N6	5.68	122.00	118.60
3	F	301	DC	C3'-C2'-C1'	-5.67	95.70	102.50
3	F	296	DA	C4-C5-N7	-5.64	107.88	110.70
1	B	276	LEU	CB-CG-CD1	-5.62	101.44	111.00
1	B	280	THR	CA-CB-CG2	5.61	120.25	112.40
1	A	136	ARG	CG-CD-NE	-5.59	100.05	111.80
1	B	138	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	134	LYS	CB-CA-C	5.56	121.52	110.40
1	A	207	GLU	N-CA-CB	5.56	120.60	110.60
2	E	286	DG	P-O5'-C5'	5.55	129.79	120.90
1	A	206	ASP	O-C-N	-5.55	113.82	122.70
1	A	194	PRO	N-CD-CG	-5.53	94.90	103.20
1	B	181	MET	CG-SD-CE	-5.53	91.35	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	292	DG	C2-N3-C4	5.51	114.66	111.90
2	E	291	DC	OP1-P-OP2	5.49	127.84	119.60
3	F	295	DG	N7-C8-N9	5.49	115.84	113.10
3	F	297	DC	C4'-C3'-C2'	5.48	108.03	103.10
2	E	287	DA	P-O3'-C3'	5.46	126.25	119.70
1	A	276	LEU	CB-CG-CD2	-5.46	101.73	111.00
2	E	287	DA	N9-C1'-C2'	5.45	122.96	112.60
2	E	292	DG	O4'-C1'-N9	5.45	111.81	108.00
3	F	297	DC	N1-C2-O2	5.40	122.14	118.90
3	F	301	DC	N3-C2-O2	5.39	125.67	121.90
2	E	285	DT	OP1-P-O3'	-5.38	93.37	105.20
3	F	295	DG	C5'-C4'-O4'	5.37	119.50	109.30
3	F	297	DC	OP1-P-OP2	5.34	127.61	119.60
1	A	138	ARG	CG-CD-NE	-5.32	100.63	111.80
1	B	36	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	B	136	ARG	NE-CZ-NH1	5.29	122.95	120.30
3	F	302	DG	C5'-C4'-O4'	5.29	119.36	109.30
3	F	300	DA	C6-C5-N7	-5.29	128.60	132.30
3	F	304	DG	C8-N9-C4	5.26	108.51	106.40
3	F	293	DC	N3-C2-O2	-5.24	118.23	121.90
3	F	300	DA	O4'-C1'-C2'	-5.23	101.72	105.90
3	F	304	DG	C5-N7-C8	5.21	106.91	104.30
2	E	292	DG	C8-N9-C1'	5.21	133.77	127.00
3	F	297	DC	P-O5'-C5'	-5.21	112.57	120.90
2	E	289	DT	C5-C6-N1	-5.20	120.58	123.70
1	B	43	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	115	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	A	134	LYS	CA-CB-CG	5.20	124.83	113.40
1	A	53	LEU	CB-CG-CD2	5.18	119.80	111.00
1	B	55	ASN	N-CA-C	5.17	124.95	111.00
2	E	284	DG	C5-N7-C8	-5.17	101.72	104.30
2	E	288	DG	OP1-P-OP2	5.16	127.35	119.60
2	E	289	DT	O4'-C1'-C2'	5.11	109.99	105.90
1	B	245	VAL	CG1-CB-CG2	-5.11	102.73	110.90
1	A	272	GLU	OE1-CD-OE2	5.10	129.43	123.30
1	B	44	LYS	CD-CE-NZ	5.07	123.37	111.70
1	A	66	TYR	CG-CD1-CE1	-5.07	117.25	121.30
3	F	294	DG	N9-C1'-C2'	5.07	122.23	112.60
3	F	295	DG	C8-N9-C1'	5.07	133.59	127.00
2	E	285	DT	C4'-C3'-C2'	5.05	107.65	103.10
1	A	239	GLU	OE1-CD-OE2	-5.05	117.24	123.30
3	F	302	DG	C6-C5-N7	5.05	133.43	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	296	DA	N3-C4-C5	5.05	130.33	126.80
1	B	70	VAL	CA-CB-CG1	5.03	118.45	110.90
2	E	282	DC	C3'-C2'-C1'	-5.03	96.47	102.50
3	F	294	DG	O4'-C4'-C3'	5.03	109.02	106.00
2	E	287	DA	C6-C5-N7	-5.02	128.79	132.30
2	E	282	DC	O3'-P-O5'	-5.01	94.48	104.00
1	A	266	VAL	CG1-CB-CG2	-5.00	102.89	110.90
2	E	288	DG	C5-N7-C8	5.00	106.80	104.30

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	125	0
1	B	1939	0	1942	65	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	64	0
7	A	53	0	0	12	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	212	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 25.

All (212) 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
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:N1	3:F:298:DT:C1'	1.73	1.48
1:A:237[B]:MET:CG	1:A:237[B]:MET:SD	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:CE	1:A:237[B]:MET:SD	2.16	1.34
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:206:ASP:CA	6:A:1285[B]:IPA:H11	1.73	1.17
1:B:237:MET:CE	1:B:237:MET:SD	2.34	1.16
1:A:205:CYS:C	6:A:1285[A]:IPA:H11	1.67	1.15
1:A:205:CYS:C	6:A:1285[B]:IPA:H11	1.69	1.13
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:A:205:CYS:C	6:A:1285[A]:IPA:C1	2.18	1.11
1:B:195:LYS:O	1:B:196:ALA:CB	1.97	1.10
1:A:205:CYS:C	6:A:1285[B]:IPA:C1	2.21	1.09
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:37:SER:HB2	1:A:38:PRO:HA	1.45	0.98
1:A:204:ILE:C	6:A:1285[B]:IPA:H13	1.82	0.98
1:A:204:ILE:C	6:A:1285[A]:IPA:H13	1.85	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:CB	1:A:61:PRO:CD	2.51	0.87
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:205:CYS:C	6:A:1285[A]:IPA:H13	1.96	0.83
1:A:204:ILE:O	6:A:1285[A]:IPA:H13	1.79	0.82
1:A:204:ILE:O	6:A:1285[B]:IPA:H13	1.79	0.82
1:B:241:ILE:CG2	1:B:243:VAL:HG23	2.11	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
1:A:204:ILE:C	6:A:1285[B]:IPA:C1	2.51	0.78
3:F:298:DT:C2	3:F:298:DT:C1'	2.66	0.77
1:A:205:CYS:C	6:A:1285[B]:IPA:H13	1.98	0.76
1:A:204:ILE:C	6:A:1285[A]:IPA:H32	2.06	0.76
1:A:204:ILE:C	6:A:1285[B]:IPA:H32	2.05	0.76
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: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:H1'	3:F:298:DT:N1	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:204:ILE:C	6:A:1285[A]:IPA:C1	2.51	0.69
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: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

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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:B:227:PHE:CD1	1:B:227:PHE:C	2.72	0.63
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:A:204:ILE:C	6:A:1285[A]:IPA:C3	2.68	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:204:ILE:C	6:A:1285[B]:IPA:C3	2.69	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:138:ARG:HD3	7:B:2023:HOH:O	2.03	0.59
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.85	0.59
1:A:204:ILE:O	6:A:1285[A]:IPA:C3	2.38	0.58
1:A:274:GLY:HA2	7:A:2049:HOH:O	2.04	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:B:219:LYS:C	1:B:243:VAL:HG13	2.24	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: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:46:GLU:OE1	1:A:76:HIS:CE1	2.50	0.55
1:A:271:LEU:HG	1:A:276:LEU:HD12	1.89	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
3:F:298:DT:C6	3:F:298:DT:C1'	2.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:CG	1:A:61:PRO:HD3	2.28	0.53
1:A:146:GLU:HG2	7:A:2024:HOH:O	1.99	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: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
2:E:282:DC:H2'	2:E:282:DC:O5'	2.11	0.50
1:B:213:VAL:HG13	1:B:218:VAL:CG2	2.41	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
1:B:219:LYS:C	1:B:243:VAL:CG1	2.80	0.49
1:A:233:ARG:O	1:A:234:LYS:C	2.48	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
3:F:298:DT:O2	3:F:298:DT:H1'	2.14	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:C2	2.43	0.48
1:B:136:ARG:NH2	7:B:2021:HOH:O	2.46	0.48
1:B:122:GLU:HG2	7:B:2017:HOH:O	2.13	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:B:87:LYS:HE2	7:B:2009:HOH:O	2.13	0.47
2:E:282:DC:C5'	2:E:282:DC:OP1	2.63	0.47
1:B:59:GLN:HB3	1:B:60:ASP:HB2	1.97	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:A:203:GLU:C	6:A:1285[B]:IPA:H12	2.35	0.46
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
1:B:49:LEU:HG	1:B:53:LEU:HD11	1.97	0.45
1:A:207:GLU:HB2	6:A:1285[B]:IPA:HO2	1.77	0.45
1:A:255:ASN:HA	1:A:256:PRO:HD3	1.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:SER:OG	1:A:278:LEU:N	2.46	0.44
1:A:150:ALA:O	1:A:154:SER:HB2	2.18	0.44
1:A:204:ILE:CA	6:A:1285[B]:IPA:H32	2.46	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:260:LYS:HB3	1:A:260:LYS:HE3	1.72	0.43
3:F:298:DT:O5'	3:F:298:DT:H2'	2.19	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
1:A:203:GLU:C	6:A:1285[A]:IPA:H12	2.39	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:C2'	3:F:303:DG:O5'	2.67	0.43
1:B:182:ASN:C	1:B:182:ASN:OD1	2.57	0.43
1:B:199:ASP:O	1:B:203:GLU:HB2	2.19	0.42
1:A:254:ARG:NH1	1:A:254:ARG:HG3	2.34	0.42
3:F:299:3DR:C1'	7:F:2006:HOH:O	2.67	0.42
1:A:251:PRO:O	1:A:252:SER:C	2.57	0.42
1:A:265:ILE:O	1:A:269:GLN:HG3	2.19	0.42
1:A:193:LEU:O	1:A:194:PRO:C	2.57	0.42
1:A:204:ILE:CA	6:A:1285[A]:IPA:H32	2.47	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:B:195:LYS:O	1:B:196:ALA:HB3	2.08	0.41
1:A:222:ILE:HD13	1:A:222:ILE:HG21	1.85	0.41
1:B:195:LYS:O	1:B:195:LYS:HG2	2.21	0.41
1:B:255:ASN:HA	1:B:256:PRO:HD3	1.91	0.41
1:A:262:TRP:O	1:A:266:VAL:HG23	2.21	0.41
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.81	0.41
1:B:148:SER:HB3	1:B:251:PRO:HG2	2.02	0.41
1:A:179:ILE:HD13	1:A:179:ILE:HG21	1.80	0.41
1:A:74:ALA:N	1:A:75:PRO:HD2	2.36	0.41
1:A:37:SER:CB	1:A:38:PRO:HA	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HA	1:B:276:LEU:HD23	1.83	0.41
1:B:179:ILE:HG21	1:B:179:ILE:HD13	1.75	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:B:209:LEU:HG	1:B:209:LEU:O	2.19	0.40
1:A:68:PRO:HD2	1:A:177:PRO:O	2.21	0.40
1:B:87:LYS:HG3	7:B:2001:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	244/247 (99%)	223 (91%)	18 (7%)	3 (1%)	16 35
1	B	243/247 (98%)	218 (90%)	19 (8%)	6 (2%)	7 15
All	All	487/494 (99%)	441 (91%)	37 (8%)	9 (2%)	10 23

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
1	A	161	GLY
1	B	261	GLY

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	215/215 (100%)	198 (92%)	17 (8%)	15 32
1	B	214/215 (100%)	188 (88%)	26 (12%)	6 12
All	All	429/430 (100%)	386 (90%)	43 (10%)	10 19

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	59	GLN
1	A	85	LYS
1	A	87	LYS
1	A	95	MET
1	A	158	SER
1	A	159	LEU
1	A	181	MET
1	A	186	LYS
1	A	218	VAL
1	A	219	LYS
1	A	234	LYS
1	A	237[A]	MET
1	A	237[B]	MET
1	A	260	LYS
1	A	271	LEU
1	A	277	SER
1	B	36	GLU
1	B	37	SER
1	B	41	SER
1	B	48	GLU
1	B	51	LEU
1	B	59	GLN
1	B	86	SER
1	B	89	GLU
1	B	97	PRO
1	B	127	LYS

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Mol	Chain	Res	Type
1	B	134	LYS
1	B	138	ARG
1	B	155	LEU
1	B	179	ILE
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	246	LYS
1	B	256	PRO
1	B	257	GLN
1	B	279	LEU
1	B	280	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	175	HIS
1	A	230	GLN
1	B	50	ASN
1	B	78	ASN
1	B	230	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	7,11,12	2.53	2 (28%)	8,14,17	2.27	4 (50%)

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	-	1/3/15/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	299	3DR	O4'-C4'	2.62	1.49	1.44
3	F	299	3DR	O3'-C3'	5.67	1.56	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	299	3DR	C2'-C3'-C4'	-3.33	95.91	102.77
3	F	299	3DR	O4'-C4'-C5'	-3.14	102.66	109.53
3	F	299	3DR	O4'-C1'-C2'	-2.91	100.65	106.64
3	F	299	3DR	O3'-C3'-C4'	2.68	120.88	110.05

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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 carbohydrates 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	-	6,10,10	2.84	4 (66%)	8,13,13	10.56	4 (50%)
4	HMU	A	1283	-	6,10,10	1.67	1 (16%)	8,13,13	5.60	6 (75%)
5	GOL	A	1284	-	5,5,5	19.16	3 (60%)	5,5,5	10.59	4 (80%)
6	IPA	A	1285[A]	-	3,3,3	1.31	0	3,3,3	3.20	3 (100%)
6	IPA	A	1285[B]	-	3,3,3	1.26	0	3,3,3	2.88	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	-	-	0/2/2/2	0/1/1/1
4	HMU	A	1283	-	-	0/2/2/2	0/1/1/1
5	GOL	A	1284	-	-	0/4/4/4	0/0/0/0
6	IPA	A	1285[A]	-	-	0/0/0/0	0/0/0/0
6	IPA	A	1285[B]	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1282	HMU	CM5-C5	2.07	1.57	1.51
4	A	1282	HMU	C6-C5	2.57	1.43	1.37
4	A	1282	HMU	C6-N1	2.79	1.40	1.34
4	A	1283	HMU	C4-N3	3.00	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1284	GOL	C1-C2	3.59	1.66	1.52
4	A	1282	HMU	C4-N3	5.33	1.43	1.33
5	A	1284	GOL	O3-C3	24.75	2.49	1.42
5	A	1284	GOL	O2-C2	34.70	2.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1282	HMU	N1-C2-N3	-26.51	111.42	128.33
5	A	1284	GOL	O2-C2-C3	-16.58	32.62	108.65
5	A	1284	GOL	O3-C3-C2	-15.51	34.97	110.18
4	A	1283	HMU	N1-C2-N3	-8.94	122.63	128.33
4	A	1283	HMU	C5-C4-N3	-8.89	114.97	125.04
5	A	1284	GOL	O2-C2-C1	-6.00	81.12	108.65
6	A	1285[A]	IPA	O2-C2-C1	-4.11	80.54	110.42
4	A	1282	HMU	C5-C4-N3	-3.58	120.98	125.04
6	A	1285[B]	IPA	O2-C2-C3	-3.19	87.21	110.42
4	A	1283	HMU	CM5-C5-C6	-2.97	113.70	119.31
6	A	1285[B]	IPA	C3-C2-C1	-2.57	92.70	113.70
6	A	1285[A]	IPA	C3-C2-C1	-2.53	93.06	113.70
4	A	1283	HMU	CM5-C5-C4	2.42	129.10	123.23
6	A	1285[A]	IPA	O2-C2-C3	2.71	130.14	110.42
6	A	1285[B]	IPA	O2-C2-C1	2.84	131.04	110.42
5	A	1284	GOL	O1-C1-C2	2.98	124.65	110.18
4	A	1283	HMU	C6-N1-C2	3.05	120.38	115.47
4	A	1282	HMU	C6-N1-C2	7.21	127.06	115.47
4	A	1283	HMU	C4-N3-C2	8.06	122.22	115.25
4	A	1282	HMU	C4-N3-C2	10.96	124.72	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1282	HMU	3	0
4	A	1283	HMU	1	0
6	A	1285[A]	IPA	31	0
6	A	1285[B]	IPA	33	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

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^{th} 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%)	-0.50	0 100 100	20, 40, 61, 72	0
1	B	245/247 (99%)	-0.42	2 (0%) 87 87	22, 48, 68, 76	0
2	E	12/12 (100%)	-0.18	0 100 100	40, 61, 75, 82	0
3	F	11/12 (91%)	0.20	0 100 100	38, 60, 85, 87	0
All	All	512/518 (98%)	-0.44	2 (0%) 93 94	20, 45, 68, 87	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ASP	4.0
1	B	36	GLU	2.7

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

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^{th} 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^2)	Q<0.9
3	3DR	F	299	11/12	0.97	0.14	-	67,75,80,83	0

6.3 Carbohydrates

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^{th} 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^2)	Q<0.9
5	GOL	A	1284	6/6	0.52	0.36	9.33	73,84,87,90	0
4	HMU	A	1283	10/10	0.81	0.29	5.72	80,97,101,103	0
4	HMU	A	1282	10/10	0.87	0.23	5.07	46,62,75,80	0
6	IPA	A	1285[A]	4/4	0.97	0.24	1.84	124,125,126,126	4
6	IPA	A	1285[B]	4/4	0.97	0.24	1.78	125,125,126,129	4

6.5 Other polymers (i)

There are no such residues in this entry.