Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:27 PM EDT

PDB ID	:	1DCT
Title	:	DNA (CYTOSINE-5) METHYLASE FROM HAEIII COVALENTLY BOUND TO DNA
Authors	:	Reinisch, K.M.; Chen, L.; Verdine, G.L.; Lipscomb, W.N.
Deposited on	:	1995-05-17
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

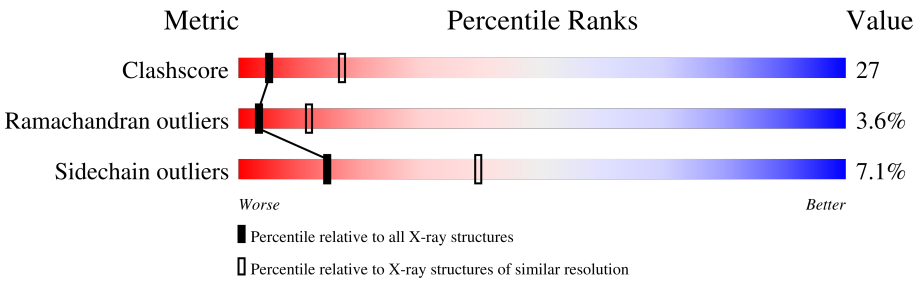
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	F	18	17% 78% 6%
1	G	18	33% 56% 11%
2	M	18	33% 61% 6%
2	N	18	50% 44% 6%
3	A	324	52% 42% 6%
3	B	324	48% 44% 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	C49	F	10	X	-	-	-
1	C49	G	10	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6908 atoms, of which 268 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 DNA chain called DNA (5'-D(*AP*CP*CP*AP*GP*CP*AP*GP*GP*(C49)P*CP*AP*CP*CP*AP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P			
1	F	18	367	174	1	73	102	17	0	0	0
1	G	16	327	155	1	65	91	15	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*AP*CP*TP*GP*GP*TP*GP*GP*(C5M)P*CP*TP*GP*CP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	M	18	368	176	65	110	17	0	0	0
2	N	17	346	166	60	104	16	0	0	0

- Molecule 3 is a protein called PROTEIN (MODIFICATION METHYLASE HAEIII).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	A	324	2749	1680	134	455	468	12	0	0	0
3	B	324	2749	1680	134	455	468	12	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: DNA (5'-D(*AP*CP*CP*AP*GP*CP*AP*GP*GP*(C49)P*CP*AP*CP*CP*AP*GP*TP*G)-3')

Chain F: 17% 78% 6%

• Molecule 1: DNA (5'-D(*AP*CP*CP*AP*GP*CP*AP*GP*GP*(C49)P*CP*AP*CP*CP*AP*GP*TP*G)-3')

Chain G: 33% 56% 11%

• Molecule 2: DNA (5'-D(*TP*CP*AP*CP*TP*GP*GP*TP*GP*GP*(C5M)P*CP*TP*GP*CP*TP*GP*G)-3')

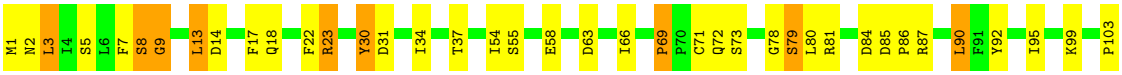
Chain M: 33% 61% 6%

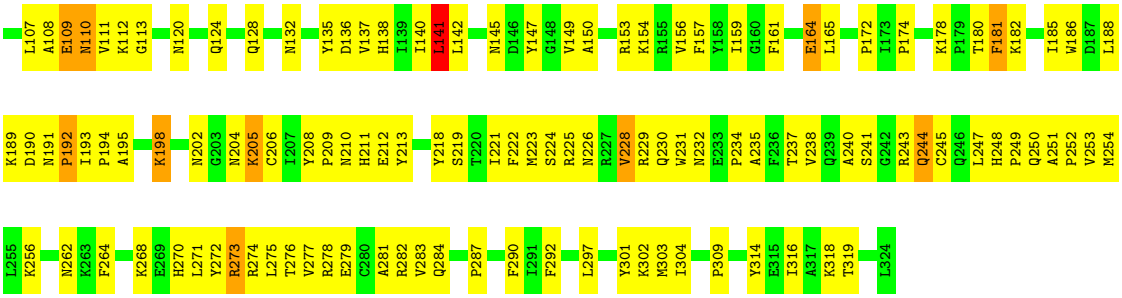
• Molecule 2: DNA (5'-D(*TP*CP*AP*CP*TP*GP*GP*TP*GP*GP*(C5M)P*CP*TP*GP*CP*TP*GP*G)-3')

Chain N: 50% 44% 6%

• Molecule 3: PROTEIN (MODIFICATION METHYLASE HAEIII)

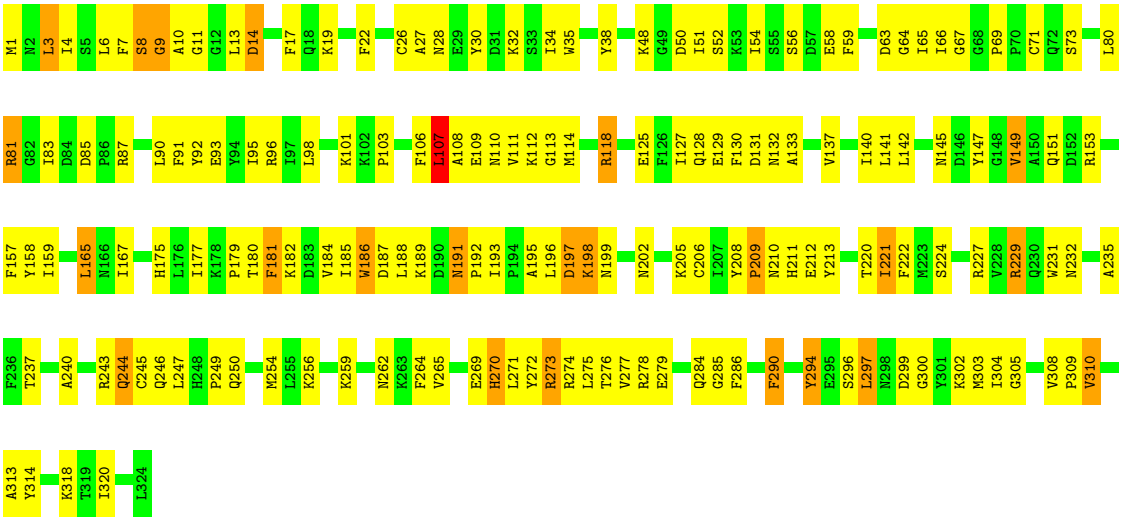
Chain A: 52% 42% 6%





- Molecule 3: PROTEIN (MODIFICATION METHYLASE HAEIII)

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.57Å 108.04Å 155.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6908	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

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: C49, 5CM, CA

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	F	1.54	2/388 (0.5%)	2.60	46/594 (7.7%)
1	G	1.57	5/343 (1.5%)	2.38	30/525 (5.7%)
2	M	1.73	5/388 (1.3%)	2.43	42/596 (7.0%)
2	N	1.75	6/363 (1.7%)	2.44	38/557 (6.8%)
3	A	0.52	0/2681	0.74	2/3615 (0.1%)
3	B	0.51	0/2681	0.76	3/3615 (0.1%)
All	All	0.89	18/6844 (0.3%)	1.37	161/9502 (1.7%)

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	F	1	2
1	G	1	0
2	M	0	1
3	A	0	1
3	B	0	1
All	All	2	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	8	DT	C3'-O3'	-8.62	1.32	1.44
2	M	8	DT	C3'-O3'	-8.24	1.33	1.44
1	G	14	DC	C4'-O4'	-6.53	1.38	1.45
1	F	9	DG	C3'-O3'	-6.34	1.35	1.44
2	N	10	DG	C4'-O4'	-6.30	1.38	1.45
2	M	10	DG	C3'-O3'	-6.05	1.36	1.44
2	N	10	DG	C3'-O3'	-5.76	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	9	DG	C6-N1	-5.52	1.35	1.39
1	G	17	DT	C4'-O4'	-5.51	1.39	1.45
1	G	9	DG	C6-N1	-5.46	1.35	1.39
1	G	13	DC	C3'-O3'	-5.44	1.36	1.44
2	M	2	DC	C4'-O4'	-5.41	1.39	1.45
1	G	15	DA	C4'-O4'	-5.32	1.39	1.45
2	N	1	DT	C3'-O3'	-5.22	1.37	1.44
2	N	1	DT	C5-C7	5.10	1.53	1.50
2	M	1	DT	C5-C7	5.08	1.53	1.50
2	N	9	DG	C3'-O3'	-5.05	1.37	1.44
2	M	14	DG	C6-N1	-5.02	1.36	1.39

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	2	DC	O4'-C4'-C3'	10.12	112.07	106.00
1	F	13	DC	C1'-O4'-C4'	-9.23	100.87	110.10
1	F	13	DC	O4'-C4'-C3'	9.15	111.49	106.00
1	F	4	DA	N1-C2-N3	-8.98	124.81	129.30
1	G	4	DA	N1-C2-N3	-8.92	124.84	129.30
2	N	3	DA	N1-C2-N3	-8.83	124.88	129.30
1	G	7	DA	N1-C2-N3	-8.82	124.89	129.30
2	M	3	DA	N1-C2-N3	-8.78	124.91	129.30
1	F	4	DA	C6-N1-C2	8.63	123.78	118.60
1	G	12	DA	N1-C2-N3	-8.62	124.99	129.30
1	F	15	DA	N1-C2-N3	-8.54	125.03	129.30
1	G	7	DA	C6-N1-C2	8.21	123.53	118.60
1	F	7	DA	N1-C2-N3	-8.19	125.20	129.30
2	M	18	DG	C1'-O4'-C4'	-8.17	101.93	110.10
1	F	12	DA	C6-N1-C2	8.17	123.50	118.60
1	F	12	DA	N1-C2-N3	-8.11	125.24	129.30
1	G	4	DA	C6-N1-C2	8.02	123.41	118.60
1	G	12	DA	C6-N1-C2	7.96	123.38	118.60
1	G	15	DA	N1-C2-N3	-7.90	125.35	129.30
2	M	3	DA	C6-N1-C2	7.89	123.33	118.60
1	F	1	DA	N1-C2-N3	-7.87	125.37	129.30
1	F	15	DA	P-O5'-C5'	-7.85	108.35	120.90
1	F	7	DA	C6-N1-C2	7.83	123.30	118.60
1	F	5	DG	O4'-C4'-C3'	7.70	110.62	106.00
2	N	3	DA	C6-N1-C2	7.67	123.20	118.60
2	N	10	DG	P-O5'-C5'	-7.49	108.92	120.90
2	M	5	DT	C2-N3-C4	-7.44	122.73	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	5	DT	C2-N3-C4	-7.43	122.74	127.20
1	F	2	DC	C1'-O4'-C4'	-7.42	102.68	110.10
1	F	1	DA	C6-N1-C2	7.38	123.03	118.60
1	G	15	DA	P-O5'-C5'	-7.21	109.37	120.90
2	M	1	DT	C2-N3-C4	-7.18	122.89	127.20
2	N	14	DG	C5-C6-N1	7.17	115.09	111.50
1	F	17	DT	C2-N3-C4	-7.16	122.90	127.20
1	F	15	DA	C6-N1-C2	7.15	122.89	118.60
1	G	17	DT	C2-N3-C4	-7.12	122.93	127.20
2	N	1	DT	C2-N3-C4	-7.12	122.93	127.20
2	N	7	DG	O4'-C4'-C3'	7.12	110.27	106.00
2	M	14	DG	C5-C6-N1	6.94	114.97	111.50
2	N	13	DT	C2-N3-C4	-6.93	123.04	127.20
2	M	10	DG	P-O5'-C5'	-6.92	109.82	120.90
2	N	8	DT	C2-N3-C4	-6.92	123.05	127.20
2	M	7	DG	P-O5'-C5'	-6.92	109.83	120.90
1	F	8	DG	C5-C6-N1	6.92	114.96	111.50
2	M	13	DT	C2-N3-C4	-6.90	123.06	127.20
2	M	7	DG	C5-C6-N1	6.86	114.93	111.50
2	N	6	DG	O4'-C1'-C2'	-6.85	100.42	105.90
2	N	16	DT	C2-N3-C4	-6.76	123.14	127.20
2	M	8	DT	C2-N3-C4	-6.75	123.15	127.20
1	F	11	DC	O4'-C4'-C3'	6.70	110.02	106.00
1	G	15	DA	C6-N1-C2	6.70	122.62	118.60
1	G	13	DC	C1'-O4'-C4'	-6.69	103.41	110.10
1	F	13	DC	C4'-C3'-C2'	-6.68	97.09	103.10
2	N	7	DG	P-O5'-C5'	-6.54	110.44	120.90
1	G	8	DG	C5-C6-N1	6.51	114.76	111.50
1	F	5	DG	C5-C6-N1	6.50	114.75	111.50
2	M	16	DT	C2-N3-C4	-6.45	123.33	127.20
1	G	17	DT	N1-C2-N3	6.45	118.47	114.60
1	F	3	DC	O4'-C4'-C3'	6.44	109.86	106.00
1	F	5	DG	C1'-O4'-C4'	-6.42	103.68	110.10
1	F	16	DG	C5-C6-N1	6.39	114.69	111.50
1	F	18	DG	C5-C6-N1	6.37	114.69	111.50
2	M	15	DC	P-O5'-C5'	-6.36	110.73	120.90
2	M	6	DG	C5-C6-N1	6.36	114.68	111.50
1	G	18	DG	C5-C6-N1	6.34	114.67	111.50
1	F	8	DG	O4'-C4'-C3'	6.34	109.80	106.00
2	M	9	DG	C5-C6-N1	6.30	114.65	111.50
1	G	14	DC	N3-C4-C5	-6.23	119.41	121.90
2	N	4	DC	O4'-C4'-C3'	6.23	109.74	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	4	DC	N3-C4-C5	-6.21	119.41	121.90
1	G	5	DG	C5-C6-N1	6.20	114.60	111.50
2	M	1	DT	N1-C2-N3	6.19	118.31	114.60
2	N	15	DC	N3-C4-C5	-6.19	119.42	121.90
1	G	9	DG	C5-C6-N1	6.19	114.59	111.50
1	F	1	DA	C5-C6-N1	-6.16	114.62	117.70
1	F	4	DA	C5-C6-N1	-6.11	114.65	117.70
3	B	107	LEU	CA-CB-CG	6.10	129.34	115.30
1	G	7	DA	C5-C6-N1	-6.08	114.66	117.70
2	M	5	DT	N1-C2-N3	6.07	118.25	114.60
2	M	7	DG	O4'-C4'-C3'	6.07	109.64	106.00
2	N	10	DG	C5-C6-N1	6.04	114.52	111.50
2	N	7	DG	C5-C6-N1	6.02	114.51	111.50
2	N	9	DG	C5-C6-N1	6.02	114.51	111.50
1	G	12	DA	P-O5'-C5'	-6.02	111.28	120.90
2	N	16	DT	O4'-C4'-C3'	6.01	109.61	106.00
1	F	17	DT	N1-C2-N3	5.98	118.19	114.60
1	F	7	DA	C5-C6-N1	-5.97	114.72	117.70
2	M	2	DC	N3-C4-C5	-5.93	119.53	121.90
2	N	4	DC	N3-C4-C5	-5.93	119.53	121.90
2	N	6	DG	C5-C6-N1	5.92	114.46	111.50
2	N	13	DT	O4'-C4'-C3'	5.92	109.55	106.00
2	N	1	DT	N1-C2-N3	5.89	118.13	114.60
1	F	3	DC	C1'-O4'-C4'	-5.88	104.22	110.10
2	M	13	DT	O4'-C4'-C3'	5.88	109.53	106.00
1	F	14	DC	N3-C4-C5	-5.87	119.55	121.90
2	N	10	DG	O4'-C4'-C3'	5.85	109.51	106.00
1	G	18	DG	O4'-C4'-C3'	5.84	109.50	106.00
2	M	10	DG	C5-C6-N1	5.84	114.42	111.50
2	N	5	DT	N1-C2-N3	5.82	118.09	114.60
2	N	17	DG	C5-C6-N1	5.82	114.41	111.50
1	G	16	DG	C5-C6-N1	5.81	114.41	111.50
1	F	11	DC	N3-C4-C5	-5.79	119.58	121.90
2	N	2	DC	N3-C4-C5	-5.79	119.58	121.90
2	M	2	DC	O4'-C4'-C3'	5.75	109.45	106.00
1	F	9	DG	C5-C6-N1	5.72	114.36	111.50
2	N	1	DT	N3-C4-C5	5.69	118.61	115.20
1	F	2	DC	N3-C4-C5	-5.68	119.63	121.90
2	M	6	DG	O4'-C1'-C2'	-5.63	101.39	105.90
2	M	13	DT	N1-C2-N3	5.61	117.96	114.60
2	N	13	DT	N1-C2-N3	5.59	117.96	114.60
2	M	16	DT	N3-C4-C5	5.58	118.55	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	11	DC	N3-C4-C5	-5.58	119.67	121.90
2	N	12	DC	N3-C4-C5	-5.57	119.67	121.90
1	G	4	DA	C5-C6-N1	-5.57	114.92	117.70
2	N	3	DA	C5-C6-N1	-5.56	114.92	117.70
1	G	12	DA	C5-C6-N1	-5.56	114.92	117.70
2	N	5	DT	O4'-C1'-C2'	-5.55	101.46	105.90
2	M	18	DG	C5-C6-N1	5.54	114.27	111.50
1	F	12	DA	C5-C6-N1	-5.54	114.93	117.70
2	M	5	DT	N3-C4-C5	5.54	118.52	115.20
3	A	136	ASP	N-CA-C	-5.53	96.07	111.00
1	F	18	DG	O4'-C4'-C3'	5.53	109.31	106.00
2	M	17	DG	C5-C6-N1	5.52	114.26	111.50
1	F	11	DC	C1'-O4'-C4'	-5.51	104.59	110.10
1	G	3	DC	N3-C4-C5	-5.49	119.70	121.90
2	M	15	DC	N3-C4-C5	-5.49	119.71	121.90
2	N	5	DT	N3-C4-C5	5.46	118.48	115.20
2	N	8	DT	N1-C2-N3	5.45	117.87	114.60
2	M	4	DC	O4'-C4'-C3'	5.44	109.26	106.00
2	M	3	DA	C5-C6-N1	-5.43	114.98	117.70
3	A	141	LEU	N-CA-C	-5.43	96.34	111.00
1	F	18	DG	C1'-O4'-C4'	-5.38	104.72	110.10
1	G	3	DC	C2-N3-C4	5.38	122.59	119.90
1	G	13	DC	N3-C4-C5	-5.34	119.76	121.90
2	M	8	DT	N1-C2-N3	5.34	117.80	114.60
1	G	14	DC	C2-N3-C4	5.34	122.57	119.90
3	B	81	ARG	N-CA-C	-5.34	96.59	111.00
2	M	1	DT	N3-C4-C5	5.33	118.39	115.20
3	B	290	PHE	N-CA-C	-5.33	96.62	111.00
2	M	14	DG	P-O3'-C3'	5.32	126.08	119.70
1	F	5	DG	P-O3'-C3'	5.29	126.05	119.70
1	F	12	DA	P-O5'-C5'	-5.28	112.45	120.90
1	F	6	DC	N3-C4-C5	-5.26	119.79	121.90
2	M	12	DC	N3-C4-C5	-5.24	119.80	121.90
2	M	16	DT	N1-C2-N3	5.24	117.75	114.60
1	G	4	DA	P-O3'-C3'	5.20	125.94	119.70
1	G	15	DA	C5-C6-N1	-5.18	115.11	117.70
1	F	13	DC	N3-C4-C5	-5.18	119.83	121.90
2	M	13	DT	N3-C4-C5	5.17	118.30	115.20
2	N	16	DT	N1-C2-N3	5.17	117.70	114.60
2	N	15	DC	C2-N3-C4	5.17	122.48	119.90
2	M	8	DT	N3-C4-C5	5.16	118.30	115.20
2	N	3	DA	O4'-C1'-N9	-5.16	104.39	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	17	DT	N3-C4-C5	5.15	118.29	115.20
1	F	2	DC	P-O3'-C3'	5.11	125.83	119.70
2	M	10	DG	O4'-C4'-C3'	5.08	109.05	106.00
2	N	16	DT	P-O3'-C3'	5.07	125.78	119.70
1	F	15	DA	C5-C6-N1	-5.06	115.17	117.70
2	N	13	DT	N3-C4-C5	5.02	118.21	115.20
2	M	9	DG	P-O5'-C5'	-5.02	112.87	120.90
2	M	5	DT	P-O3'-C3'	5.01	125.72	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	10	C49	C1'
1	G	10	C49	C1'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	147	TYR	Sidechain
3	B	38	TYR	Sidechain
1	F	1	DA	Sidechain
1	F	17	DT	Sidechain
2	M	17	DG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	367	0	200	18	0
1	G	327	0	178	10	0
2	M	368	0	207	14	0
2	N	346	0	196	5	0
3	A	2615	134	2606	153	0
3	B	2615	134	2606	160	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	6640	268	5993	343	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 27.

All (343) 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:F:4:DA:H2"	1:F:5:DG:C8	2.04	0.93
3:A:202:ASN:HB3	3:A:205:LYS:HB3	1.51	0.92
3:B:240:ALA:HB1	3:B:302:LYS:HA	1.52	0.90
3:B:212:GLU:HG3	3:B:297:LEU:HD21	1.55	0.87
3:B:153:ARG:HG3	3:B:237:THR:HG23	1.60	0.83
3:A:314:TYR:CZ	3:A:318:LYS:HD2	2.14	0.81
3:A:111:VAL:HG12	3:A:113:GLY:H	1.44	0.81
3:A:153:ARG:CZ	3:A:284:GLN:HE22	1.94	0.79
3:B:80:LEU:HB2	3:B:118:ARG:NH1	1.99	0.77
1:F:4:DA:H2"	1:F:5:DG:N7	1.99	0.77
3:A:213:TYR:HB3	3:A:276:THR:HG22	1.69	0.75
3:B:80:LEU:HB2	3:B:118:ARG:HH11	1.53	0.74
3:B:210:ASN:HD22	3:B:278:ARG:HH21	1.34	0.73
2:M:16:DT:H1'	2:M:17:DG:OP2	1.88	0.73
3:B:186:TRP:O	3:B:189:LYS:HG2	1.88	0.73
3:B:3:LEU:HD21	3:B:22:PHE:HB3	1.71	0.73
2:M:15:DC:H2"	2:M:16:DT:C5	2.26	0.71
3:B:202:ASN:HB3	3:B:205:LYS:HB3	1.70	0.71
3:B:181:PHE:CD2	3:B:249:PRO:HG3	2.26	0.71
3:A:244:GLN:HE21	3:A:244:GLN:HA	1.57	0.70
3:B:198:LYS:NZ	3:B:198:LYS:H	1.89	0.70
3:A:287:PRO:HG2	3:A:290:PHE:HB2	1.72	0.70
3:A:37:THR:HG21	3:A:303:MET:SD	2.32	0.68
3:B:314:TYR:CZ	3:B:318:LYS:HD2	2.29	0.68
3:A:153:ARG:HG3	3:A:237:THR:HG23	1.73	0.68
2:N:13:DT:H2"	2:N:14:DG:C8	2.29	0.68
3:A:54:ILE:HG23	3:A:58:GLU:HG3	1.76	0.68
2:N:10:DG:C8	3:B:221:ILE:HG23	2.30	0.67
1:F:11:DC:N4	3:A:221:ILE:HD11	2.09	0.67
3:B:4:ILE:HD11	3:B:59:PHE:CD1	2.30	0.67
2:M:13:DT:H2"	2:M:14:DG:C8	2.30	0.66
3:B:63:ASP:O	3:B:103:PRO:HB2	1.96	0.66
3:A:185:ILE:HD13	3:A:279:GLU:HB3	1.77	0.65
3:A:279:GLU:O	3:A:282:ARG:HB2	1.97	0.64
3:B:210:ASN:OD1	3:B:294:TYR:HE1	1.80	0.64
3:B:208:TYR:CD1	3:B:209:PRO:HD2	2.32	0.64
3:B:264:PHE:HB3	3:B:272:TYR:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:DC:H2"	1:F:4:DA:C8	2.33	0.64
3:B:264:PHE:HD1	3:B:272:TYR:CD1	2.16	0.63
3:B:149:VAL:HG11	3:B:309:PRO:HB3	1.81	0.63
3:B:87:ARG:HA	3:B:90:LEU:HD12	1.80	0.63
3:B:198:LYS:H	3:B:198:LYS:HZ3	1.47	0.63
3:B:308:VAL:CG1	3:B:313:ALA:HB2	2.29	0.62
3:B:264:PHE:HB3	3:B:272:TYR:CE2	2.35	0.62
3:A:63:ASP:O	3:A:103:PRO:HB2	2.00	0.61
3:A:153:ARG:NH1	3:A:284:GLN:NE2	2.48	0.61
3:A:180:THR:HG21	3:A:232:ASN:O	1.99	0.61
3:B:127:ILE:HA	3:B:130:PHE:HD2	1.65	0.61
1:G:10:C49:O1P	3:B:111:VAL:HG11	1.99	0.61
3:B:300:GLY:O	3:B:304:ILE:HG13	2.01	0.61
3:A:277:VAL:HG22	3:A:301:TYR:CE1	2.37	0.60
2:M:9:DG:N7	3:A:243:ARG:NH1	2.50	0.60
3:B:294:TYR:CD2	3:B:297:LEU:HA	2.36	0.60
3:A:252:PRO:HG2	3:A:272:TYR:OH	2.02	0.59
1:F:1:DA:H2"	1:F:2:DC:C6	2.37	0.59
3:A:195:ALA:HB2	3:A:297:LEU:HD11	1.84	0.59
3:B:145:ASN:HA	3:B:149:VAL:O	2.02	0.59
3:B:198:LYS:NZ	3:B:198:LYS:N	2.49	0.59
3:B:244:GLN:HA	3:B:244:GLN:HE21	1.68	0.58
3:B:106:PHE:CZ	3:B:130:PHE:CD1	2.92	0.58
3:B:243:ARG:HH11	3:B:243:ARG:HG2	1.69	0.58
3:A:193:ILE:O	3:A:212:GLU:HA	2.04	0.58
3:B:181:PHE:CE2	3:B:229:ARG:HB3	2.39	0.58
1:F:3:DC:OP2	1:F:3:DC:H6	1.87	0.58
2:M:14:DG:H1'	2:M:15:DC:H5'	1.86	0.57
3:A:7:PHE:CE2	3:A:69:PRO:HG3	2.39	0.57
1:F:6:DC:H2"	1:F:7:DA:C8	2.39	0.57
3:A:195:ALA:HB2	3:A:297:LEU:CD1	2.34	0.57
3:A:194:PRO:HB3	3:A:213:TYR:CZ	2.39	0.57
3:B:308:VAL:HG12	3:B:313:ALA:HB2	1.86	0.57
3:A:73:SER:HB2	3:A:81:ARG:O	2.05	0.57
3:A:210:ASN:HD22	3:A:278:ARG:HH21	1.52	0.57
3:A:230:GLN:HE22	3:A:252:PRO:HA	1.70	0.57
2:M:10:DG:C8	3:A:221:ILE:HG23	2.40	0.56
3:A:182:LYS:HA	3:A:231:TRP:CE3	2.40	0.56
3:A:185:ILE:CD1	3:A:279:GLU:HB3	2.35	0.56
3:B:235:ALA:HB1	3:B:246:GLN:HE22	1.69	0.56
1:G:6:DC:H2"	1:G:7:DA:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:181:PHE:HE2	3:B:229:ARG:HB3	1.70	0.56
3:B:245:CYS:SG	3:B:275:LEU:HB2	2.46	0.56
3:B:69:PRO:HB2	3:B:91:PHE:HD1	1.70	0.56
1:F:8:DG:H2"	1:F:9:DG:C8	2.40	0.56
3:B:210:ASN:ND2	3:B:278:ARG:HH21	2.03	0.56
3:A:153:ARG:NH1	3:A:284:GLN:HE22	2.04	0.55
3:A:238:VAL:HB	3:A:284:GLN:HE21	1.69	0.55
3:B:277:VAL:HG21	3:B:297:LEU:HD23	1.88	0.55
3:A:208:TYR:CD1	3:A:209:PRO:HD2	2.42	0.55
1:F:15:DA:H2"	1:F:16:DG:C8	2.42	0.55
1:G:8:DG:H2"	1:G:9:DG:C8	2.42	0.55
3:A:112:LYS:HE2	3:A:141:LEU:HD21	1.87	0.55
3:A:188:LEU:O	3:A:211:HIS:HE1	1.90	0.55
3:A:229:ARG:HG2	3:A:234:PRO:O	2.07	0.55
3:B:195:ALA:HB2	3:B:297:LEU:HD13	1.89	0.55
3:A:107:LEU:HD13	3:A:108:ALA:N	2.21	0.55
3:A:186:TRP:HA	3:A:231:TRP:CH2	2.42	0.55
3:A:3:LEU:CD2	3:A:22:PHE:HB3	2.37	0.54
3:A:240:ALA:HB1	3:A:302:LYS:HA	1.88	0.54
3:B:299:ASP:O	3:B:303:MET:HG3	2.08	0.54
3:A:256:LYS:HA	3:A:262:ASN:HA	1.89	0.54
3:B:151:GLN:NE2	3:B:153:ARG:HD2	2.23	0.54
3:B:197:ASP:OD2	3:B:198:LYS:HD2	2.08	0.54
3:A:198:LYS:HA	3:A:198:LYS:NZ	2.23	0.54
3:A:181:PHE:CE2	3:A:229:ARG:HB3	2.43	0.53
3:B:151:GLN:HA	3:B:235:ALA:O	2.07	0.53
2:M:17:DG:P	2:M:17:DG:C8	3.01	0.53
3:A:13:LEU:HD23	3:A:17:PHE:CD1	2.43	0.53
3:B:256:LYS:HE3	3:B:262:ASN:HD21	1.71	0.53
3:A:230:GLN:HE21	3:A:253:VAL:HG23	1.72	0.53
3:A:14:ASP:O	3:A:18:GLN:HG3	2.09	0.53
3:A:221:ILE:HA	3:A:224:SER:OG	2.09	0.53
2:N:14:DG:H1'	2:N:15:DC:H5'	1.90	0.53
3:B:198:LYS:HZ3	3:B:198:LYS:N	2.05	0.53
3:A:226:ASN:OD1	3:A:228:VAL:HG23	2.08	0.53
1:G:15:DA:H2"	1:G:16:DG:C8	2.43	0.53
3:B:180:THR:HG21	3:B:232:ASN:O	2.09	0.53
3:B:284:GLN:OE1	3:B:309:PRO:HG3	2.08	0.52
3:A:247:LEU:HD12	3:A:254:MET:CE	2.38	0.52
3:A:290:PHE:HE1	3:A:292:PHE:CE2	2.27	0.52
3:A:145:ASN:HA	3:A:149:VAL:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:227:ARG:H	3:B:254:MET:CE	2.22	0.52
3:A:281:ALA:HB2	3:A:304:ILE:HD13	1.91	0.52
3:B:213:TYR:HB3	3:B:276:THR:HA	1.91	0.52
3:A:72:GLN:H	3:A:72:GLN:CD	2.13	0.52
1:F:5:DG:H2"	1:F:6:DC:H6	1.74	0.52
3:A:120:ASN:O	3:A:124:GLN:HB2	2.09	0.52
3:A:30:TYR:CD1	3:A:31:ASP:N	2.78	0.52
3:B:95:ILE:O	3:B:98:LEU:HB3	2.10	0.51
3:B:147:TYR:HA	3:B:175:HIS:ND1	2.26	0.51
1:G:10:C49:N4	3:B:109:GLU:OE1	2.43	0.51
3:B:107:LEU:HD22	3:B:159:ILE:HG12	1.91	0.51
3:B:69:PRO:HG2	3:B:91:PHE:CD1	2.45	0.51
3:A:112:LYS:HD2	3:A:154:LYS:HD2	1.91	0.51
3:A:13:LEU:HD23	3:A:17:PHE:CE1	2.46	0.50
3:A:1:MET:HE2	3:A:22:PHE:HE1	1.75	0.50
3:A:228:VAL:HG22	3:A:254:MET:HE3	1.93	0.50
3:A:188:LEU:O	3:A:211:HIS:CE1	2.64	0.50
3:A:245:CYS:SG	3:A:275:LEU:HB2	2.51	0.50
3:B:32:LYS:HA	3:B:35:TRP:CE2	2.47	0.50
1:F:10:C49:F	3:A:71:CYS:CB	2.46	0.50
3:A:219:SER:O	3:A:222:PHE:HB3	2.11	0.50
3:B:185:ILE:O	3:B:187:ASP:N	2.45	0.50
3:B:73:SER:HB2	3:B:81:ARG:O	2.12	0.50
3:B:196:LEU:HD11	3:B:202:ASN:OD1	2.12	0.50
3:B:4:ILE:CG2	3:B:65:ILE:HG12	2.42	0.50
3:B:181:PHE:CE1	3:B:235:ALA:HB2	2.46	0.50
3:A:248:HIS:CG	3:A:249:PRO:HD2	2.46	0.49
3:B:54:ILE:HG23	3:B:58:GLU:HG3	1.94	0.49
3:B:247:LEU:HD11	3:B:264:PHE:HE1	1.77	0.49
1:F:5:DG:H2"	1:F:6:DC:C6	2.47	0.49
3:A:142:LEU:O	3:A:154:LYS:HA	2.12	0.49
3:A:181:PHE:CD2	3:A:249:PRO:HG3	2.47	0.49
3:B:8:SER:O	3:B:9:GLY:O	2.30	0.49
3:B:165:LEU:HB2	3:B:167:ILE:HG12	1.94	0.49
3:B:284:GLN:HG3	3:B:304:ILE:HG22	1.92	0.49
3:B:294:TYR:CE2	3:B:297:LEU:HA	2.48	0.49
3:A:54:ILE:CG2	3:A:58:GLU:HG3	2.41	0.49
3:B:111:VAL:HG12	3:B:113:GLY:H	1.77	0.49
3:B:112:LYS:HE3	3:B:141:LEU:HD21	1.94	0.49
3:A:186:TRP:O	3:A:189:LYS:HG2	2.13	0.49
1:F:3:DC:H2"	1:F:4:DA:N7	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:222:PHE:HD1	3:A:223:MET:SD	2.36	0.49
3:B:13:LEU:HB3	3:B:66:ILE:HD12	1.94	0.49
2:M:17:DG:H1'	2:M:18:DG:O4'	2.12	0.48
3:A:314:TYR:O	3:A:318:LYS:HG3	2.13	0.48
3:B:240:ALA:CA	3:B:305:GLY:HA3	2.42	0.48
3:A:54:ILE:HG23	3:A:58:GLU:CG	2.43	0.48
3:A:247:LEU:HD22	3:A:273:ARG:O	2.13	0.48
1:F:12:DA:H5"	3:A:79:SER:OG	2.13	0.48
2:N:2:DC:H2"	2:N:3:DA:C8	2.48	0.48
3:A:198:LYS:HA	3:A:198:LYS:HZ2	1.78	0.48
3:B:264:PHE:CD1	3:B:272:TYR:CD1	3.00	0.48
3:A:55:SER:O	3:A:58:GLU:HB2	2.14	0.48
3:A:92:TYR:HA	3:A:95:ILE:HD12	1.96	0.48
3:A:172:PRO:N	3:A:319:THR:HG21	2.29	0.48
3:B:191:ASN:H	3:B:192:PRO:CD	2.27	0.48
3:B:28:ASN:HD21	3:B:51:ILE:HB	1.79	0.48
3:B:34:ILE:HG12	3:B:303:MET:HG2	1.96	0.48
3:A:191:ASN:N	3:A:192:PRO:HD3	2.29	0.48
3:A:224:SER:O	3:A:225:ARG:NH1	2.47	0.48
3:A:250:GLN:HG3	3:A:271:LEU:HB3	1.96	0.48
3:B:240:ALA:HA	3:B:305:GLY:HA3	1.94	0.48
3:B:127:ILE:O	3:B:130:PHE:N	2.47	0.48
3:B:142:LEU:HD22	3:B:147:TYR:CE2	2.49	0.47
3:B:273:ARG:HH21	3:B:276:THR:HG23	1.79	0.47
3:B:247:LEU:HD22	3:B:273:ARG:O	2.14	0.47
2:M:17:DG:OP2	2:M:17:DG:C8	2.67	0.47
3:A:95:ILE:O	3:A:99:LYS:HG3	2.13	0.47
3:A:212:GLU:O	3:A:276:THR:HB	2.15	0.47
3:A:222:PHE:CD1	3:A:223:MET:SD	3.08	0.47
3:A:231:TRP:CE2	3:A:249:PRO:HB2	2.50	0.47
3:B:197:ASP:O	3:B:198:LYS:HB2	2.15	0.47
2:M:2:DC:H2"	2:M:3:DA:C8	2.49	0.47
1:G:3:DC:H2"	1:G:4:DA:OP2	2.15	0.47
3:A:188:LEU:HD11	3:A:282:ARG:HG3	1.96	0.47
3:B:235:ALA:HB1	3:B:246:GLN:NE2	2.30	0.47
3:A:111:VAL:HG12	3:A:113:GLY:N	2.22	0.47
3:A:181:PHE:HE2	3:A:229:ARG:HB3	1.79	0.47
3:A:248:HIS:CD2	3:A:249:PRO:HD2	2.50	0.46
1:G:10:C49:F	3:B:71:CYS:CB	2.53	0.46
1:G:18:DG:H2"	3:A:84:ASP:CG	2.35	0.46
3:B:191:ASN:N	3:B:192:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:212:GLU:CG	3:B:297:LEU:HD21	2.34	0.46
3:A:202:ASN:OD1	3:A:205:LYS:HD3	2.16	0.46
3:A:254:MET:SD	3:A:264:PHE:CE1	3.09	0.46
3:A:153:ARG:CZ	3:A:284:GLN:NE2	2.69	0.46
3:B:28:ASN:HB2	3:B:59:PHE:HE1	1.80	0.46
3:B:182:LYS:HA	3:B:231:TRP:CE3	2.50	0.46
3:B:256:LYS:HE3	3:B:262:ASN:ND2	2.30	0.46
1:F:11:DC:H42	3:A:221:ILE:HD11	1.78	0.46
3:A:198:LYS:HA	3:A:198:LYS:CE	2.45	0.46
3:A:185:ILE:HD11	3:A:283:VAL:HG23	1.98	0.46
3:B:3:LEU:HB2	3:B:64:GLY:O	2.16	0.46
3:B:67:GLY:O	3:B:108:ALA:HA	2.16	0.46
3:B:270:HIS:CD2	3:B:271:LEU:HG	2.50	0.46
3:A:181:PHE:CZ	3:A:235:ALA:HB2	2.51	0.46
3:B:240:ALA:HB2	3:B:305:GLY:C	2.36	0.46
3:A:5:SER:OG	3:A:8:SER:HB3	2.16	0.46
3:A:86:PRO:O	3:A:90:LEU:HD12	2.16	0.46
3:B:107:LEU:HD23	3:B:320:ILE:HD11	1.97	0.46
3:B:210:ASN:HD22	3:B:278:ARG:NH2	2.10	0.46
3:A:109:GLU:HG2	3:A:110:ASN:H	1.80	0.46
3:A:8:SER:O	3:A:9:GLY:O	2.33	0.45
3:A:81:ARG:NH1	3:A:85:ASP:OD2	2.50	0.45
3:A:204:ASN:O	3:A:206:CYS:N	2.49	0.45
3:A:314:TYR:CE2	3:A:318:LYS:HD2	2.50	0.45
3:B:229:ARG:O	3:B:249:PRO:HA	2.16	0.45
3:A:13:LEU:HD22	3:A:66:ILE:HB	1.98	0.45
3:B:26:CYS:SG	3:B:27:ALA:N	2.89	0.45
3:A:244:GLN:HE21	3:A:244:GLN:CA	2.27	0.45
3:A:87:ARG:HA	3:A:90:LEU:HD12	1.99	0.45
3:B:1:MET:CE	3:B:22:PHE:HE1	2.30	0.45
3:B:69:PRO:CB	3:B:91:PHE:HD1	2.29	0.45
3:A:3:LEU:HD21	3:A:22:PHE:HB3	1.99	0.45
3:A:37:THR:HG23	3:A:292:PHE:HA	1.99	0.45
3:B:185:ILE:HG23	3:B:279:GLU:HG2	1.97	0.45
3:B:264:PHE:CD1	3:B:272:TYR:CG	3.05	0.45
2:M:15:DC:H2"	2:M:16:DT:C7	2.46	0.45
3:A:208:TYR:HB3	3:A:211:HIS:HB2	1.99	0.45
3:A:34:ILE:O	3:A:37:THR:N	2.50	0.44
3:B:191:ASN:OD1	3:B:211:HIS:CE1	2.69	0.44
3:B:224:SER:O	3:B:262:ASN:ND2	2.50	0.44
2:N:5:DT:H1'	2:N:6:DG:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:128:GLN:HG3	3:A:132:ASN:HD21	1.82	0.44
3:A:3:LEU:HD22	3:A:22:PHE:HB3	1.99	0.44
3:A:172:PRO:CA	3:A:319:THR:HG21	2.48	0.44
3:B:196:LEU:O	3:B:197:ASP:C	2.54	0.44
2:M:15:DC:H2"	2:M:16:DT:C6	2.53	0.44
3:A:1:MET:HE2	3:A:22:PHE:CE1	2.52	0.44
3:A:87:ARG:HA	3:A:90:LEU:CD1	2.48	0.44
3:A:85:ASP:OD1	3:A:87:ARG:HB2	2.18	0.44
3:A:135:TYR:HA	3:A:161:PHE:O	2.18	0.44
3:B:6:LEU:O	3:B:7:PHE:C	2.56	0.44
3:B:199:ASN:O	3:B:297:LEU:HD12	2.18	0.44
1:F:10:C49:F	3:A:71:CYS:N	2.40	0.44
3:A:141:LEU:HD12	3:A:142:LEU:N	2.33	0.44
3:A:185:ILE:HG22	3:A:185:ILE:O	2.17	0.44
3:A:218:TYR:CE1	3:A:274:ARG:CZ	3.01	0.44
3:B:247:LEU:CD1	3:B:264:PHE:HE1	2.31	0.44
3:B:262:ASN:N	3:B:262:ASN:HD22	2.15	0.44
3:B:81:ARG:HH11	3:B:81:ARG:HB2	1.83	0.43
3:B:181:PHE:CE1	3:B:185:ILE:HD11	2.53	0.43
3:B:185:ILE:HB	3:B:231:TRP:CZ3	2.53	0.43
3:B:244:GLN:HE21	3:B:244:GLN:CA	2.30	0.43
3:A:182:LYS:HA	3:A:231:TRP:HE3	1.82	0.43
3:A:188:LEU:CD1	3:A:282:ARG:HG3	2.49	0.43
3:A:3:LEU:HD23	3:A:23:ARG:O	2.18	0.43
3:B:198:LYS:H	3:B:198:LYS:HZ2	1.65	0.43
3:B:8:SER:O	3:B:9:GLY:C	2.56	0.43
3:B:17:PHE:O	3:B:22:PHE:HB2	2.19	0.43
1:F:10:C49:O1P	3:A:111:VAL:HG11	2.18	0.43
3:A:137:VAL:HG12	3:A:138:HIS:N	2.33	0.43
3:A:185:ILE:O	3:A:185:ILE:CG2	2.67	0.43
3:A:268:LYS:HA	3:A:268:LYS:HD3	1.77	0.43
3:B:193:ILE:O	3:B:212:GLU:HA	2.19	0.43
3:B:222:PHE:CZ	3:B:227:ARG:HG3	2.53	0.43
3:B:286:PHE:CE2	3:B:304:ILE:HG23	2.53	0.43
3:A:229:ARG:HG2	3:A:235:ALA:HA	2.01	0.43
3:B:83:ILE:HD11	3:B:92:TYR:OH	2.19	0.43
2:M:5:DT:H1'	2:M:6:DG:C8	2.53	0.42
3:B:35:TRP:CD2	3:B:48:LYS:HG2	2.54	0.42
3:B:125:GLU:O	3:B:129:GLU:HG2	2.19	0.42
3:B:185:ILE:O	3:B:186:TRP:C	2.58	0.42
3:B:285:GLY:O	3:B:310:VAL:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:THR:OG1	3:A:182:LYS:HG2	2.20	0.42
3:B:11:GLY:O	3:B:14:ASP:HB2	2.20	0.42
3:B:93:GLU:OE1	3:B:96:ARG:NH1	2.52	0.42
3:B:153:ARG:HG3	3:B:237:THR:CG2	2.41	0.42
2:M:10:DG:C6	3:A:221:ILE:HG12	2.55	0.42
3:A:157:PHE:CE2	3:A:316:ILE:HD11	2.54	0.42
3:A:228:VAL:HG22	3:A:254:MET:CE	2.49	0.42
3:A:284:GLN:O	3:A:309:PRO:HA	2.20	0.42
3:B:85:ASP:OD1	3:B:87:ARG:N	2.50	0.42
3:B:294:TYR:CD1	3:B:294:TYR:N	2.87	0.42
3:B:114:MET:SD	3:B:158:TYR:OH	2.68	0.42
3:B:277:VAL:CG2	3:B:297:LEU:HD23	2.49	0.42
3:B:188:LEU:HB3	3:B:211:HIS:NE2	2.35	0.42
3:B:202:ASN:HB2	3:B:206:CYS:SG	2.59	0.42
3:B:50:ASP:OD1	3:B:52:SER:N	2.53	0.42
3:A:228:VAL:HG11	3:A:251:ALA:O	2.20	0.42
3:A:221:ILE:HD12	3:A:221:ILE:C	2.41	0.41
3:B:127:ILE:O	3:B:128:GLN:C	2.59	0.41
3:B:157:PHE:N	3:B:157:PHE:CD1	2.88	0.41
3:B:132:ASN:N	3:B:132:ASN:ND2	2.69	0.41
3:B:140:ILE:O	3:B:140:ILE:HG13	2.20	0.41
3:B:191:ASN:H	3:B:192:PRO:HD3	1.85	0.41
3:B:198:LYS:HZ2	3:B:198:LYS:HA	1.85	0.41
3:B:101:LYS:HD3	3:B:101:LYS:HA	1.83	0.41
3:B:17:PHE:HB3	3:B:22:PHE:HB2	2.03	0.41
3:B:112:LYS:HG3	3:B:141:LEU:HD11	2.02	0.41
3:A:164:GLU:HG2	3:A:165:LEU:N	2.35	0.41
1:G:13:DC:OP2	3:B:81:ARG:NH2	2.54	0.41
3:A:78:GLY:O	3:A:79:SER:C	2.58	0.41
1:G:10:C49:F	3:B:71:CYS:HB3	2.11	0.41
3:A:3:LEU:HD23	3:A:3:LEU:N	2.36	0.41
3:A:141:LEU:HD12	3:A:142:LEU:H	1.86	0.41
3:A:164:GLU:HG2	3:A:165:LEU:H	1.85	0.41
3:A:193:ILE:CD1	3:A:206:CYS:HA	2.50	0.41
3:A:248:HIS:CG	3:A:249:PRO:CD	3.04	0.41
3:A:297:LEU:O	3:A:301:TYR:HD1	2.04	0.41
3:B:4:ILE:CD1	3:B:59:PHE:CD1	3.03	0.41
3:B:128:GLN:HE21	3:B:132:ASN:HD21	1.69	0.41
3:B:181:PHE:CD1	3:B:185:ILE:HD11	2.56	0.41
3:B:243:ARG:HG2	3:B:243:ARG:NH1	2.34	0.41
3:A:85:ASP:OD1	3:A:87:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:229:ARG:CG	3:A:234:PRO:O	2.69	0.41
3:A:2:ASN:O	3:A:63:ASP:HB2	2.21	0.40
3:A:142:LEU:HD23	3:A:142:LEU:HA	1.87	0.40
3:B:302:LYS:O	3:B:303:MET:C	2.59	0.40
3:A:141:LEU:HD11	3:A:154:LYS:HB3	2.03	0.40
3:B:10:ALA:HB1	3:B:290:PHE:CZ	2.56	0.40
3:B:19:LYS:HD2	3:B:314:TYR:CG	2.55	0.40
3:B:83:ILE:HD11	3:B:92:TYR:CE2	2.56	0.40
3:B:130:PHE:O	3:B:133:ALA:HB3	2.21	0.40
1:F:10:C49:F	3:A:71:CYS:HB3	2.09	0.40
3:A:72:GLN:OE1	3:A:72:GLN:N	2.51	0.40
3:A:138:HIS:N	3:A:159:ILE:O	2.53	0.40
3:B:80:LEU:CB	3:B:118:ARG:HH11	2.29	0.40
3:B:130:PHE:HB2	3:B:137:VAL:CG2	2.51	0.40
3:B:180:THR:O	3:B:184:VAL:HG22	2.21	0.40
3:A:247:LEU:HD12	3:A:254:MET:HE1	2.03	0.40
3:B:128:GLN:O	3:B:131:ASP:HB3	2.21	0.40
3:B:167:ILE:HA	3:B:167:ILE:HD13	1.83	0.40
3:B:256:LYS:CE	3:B:262:ASN:HD21	2.34	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
3	A	322/324 (99%)	273 (85%)	39 (12%)	10 (3%)	4 14
3	B	322/324 (99%)	283 (88%)	26 (8%)	13 (4%)	3 9
All	All	644/648 (99%)	556 (86%)	65 (10%)	23 (4%)	3 11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	9	GLY
3	A	80	LEU
3	A	241	SER
3	B	9	GLY
3	B	186	TRP
3	A	79	SER
3	A	205	LYS
3	B	250	GLN
3	B	259	LYS
3	B	269	GLU
3	A	270	HIS
3	B	191	ASN
3	B	270	HIS
3	A	150	ALA
3	B	118	ARG
3	B	197	ASP
3	A	174	PRO
3	B	209	PRO
3	B	310	VAL
3	A	192	PRO
3	B	265	VAL
3	A	69	PRO
3	B	179	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	281/281 (100%)	262 (93%)	19 (7%)	16	42
3	B	281/281 (100%)	260 (92%)	21 (8%)	13	37
All	All	562/562 (100%)	522 (93%)	40 (7%)	14	39

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	LEU

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Mol	Chain	Res	Type
3	A	8	SER
3	A	13	LEU
3	A	23	ARG
3	A	30	TYR
3	A	90	LEU
3	A	109	GLU
3	A	110	ASN
3	A	140	ILE
3	A	141	LEU
3	A	156	VAL
3	A	164	GLU
3	A	178	LYS
3	A	181	PHE
3	A	190	ASP
3	A	198	LYS
3	A	228	VAL
3	A	244	GLN
3	A	273	ARG
3	B	3	LEU
3	B	8	SER
3	B	14	ASP
3	B	30	TYR
3	B	56	SER
3	B	107	LEU
3	B	110	ASN
3	B	149	VAL
3	B	165	LEU
3	B	177	ILE
3	B	181	PHE
3	B	198	LYS
3	B	220	THR
3	B	221	ILE
3	B	229	ARG
3	B	244	GLN
3	B	273	ARG
3	B	274	ARG
3	B	294	TYR
3	B	296	SER
3	B	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	145	ASN
3	A	210	ASN
3	A	211	HIS
3	A	230	GLN
3	A	244	GLN
3	A	262	ASN
3	A	284	GLN
3	B	28	ASN
3	B	132	ASN
3	B	210	ASN
3	B	211	HIS
3	B	244	GLN
3	B	262	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5CM	M	11	1,2	17,21,22	0.52	0	24,30,33	0.77	1 (4%)
1	C49	G	10	1,3	18,22,24	2.14	5 (27%)	19,33,38	4.05	7 (36%)
2	5CM	N	11	1,2	17,21,22	0.47	0	24,30,33	0.78	1 (4%)
1	C49	F	10	1,3	18,22,24	2.11	6 (33%)	19,33,38	4.24	7 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5CM	M	11	1,2	-	4/7/21/22	0/2/2/2
1	C49	G	10	1,3	1/1/8/10	6/7/40/46	0/2/2/2
2	5CM	N	11	1,2	-	4/7/21/22	0/2/2/2
1	C49	F	10	1,3	1/1/8/10	6/7/40/46	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	10	C49	F-C5	-5.36	1.32	1.42
1	F	10	C49	F-C5	-4.89	1.33	1.42
1	F	10	C49	C6-C5	-4.69	1.42	1.54
1	G	10	C49	C6-C5	-4.38	1.43	1.54
1	F	10	C49	CM5-C5	-3.43	1.43	1.51
1	G	10	C49	CM5-C5	-3.39	1.43	1.51
1	G	10	C49	O4'-C1'	2.69	1.48	1.42
1	G	10	C49	C4-N4	2.35	1.33	1.27
1	F	10	C49	O4'-C1'	2.27	1.47	1.42
1	F	10	C49	O3'-C3'	-2.20	1.38	1.43
1	F	10	C49	C4-N4	2.01	1.32	1.27

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	10	C49	O4'-C1'-N1	15.04	127.58	108.41
1	G	10	C49	O4'-C1'-N1	14.48	126.86	108.41
1	F	10	C49	C2'-C1'-N1	5.42	122.24	115.61
1	G	10	C49	C4'-O4'-C1'	-5.06	97.21	109.45
1	F	10	C49	C4'-O4'-C1'	-5.01	97.34	109.45
1	F	10	C49	O4'-C4'-C3'	4.90	117.09	105.67
1	G	10	C49	O4'-C4'-C3'	4.36	115.86	105.67
1	G	10	C49	C1'-N1-C2	3.95	123.74	118.50
1	G	10	C49	C2'-C1'-N1	3.77	120.22	115.61
1	F	10	C49	C1'-N1-C2	3.52	123.17	118.50
1	G	10	C49	O4'-C1'-C2'	3.31	112.51	106.25
1	G	10	C49	C6-N1-C1'	-2.97	115.10	120.94
1	F	10	C49	C2'-C3'-C4'	-2.92	96.68	102.76
1	F	10	C49	C6-N1-C1'	-2.09	116.83	120.94
2	M	11	5CM	C5-C4-N3	-2.08	119.43	121.67
2	N	11	5CM	C5-C4-N3	-2.07	119.44	121.67

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	10	C49	C1'
1	G	10	C49	C1'

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	10	C49	O4'-C1'-N1-C2
1	F	10	C49	O4'-C1'-N1-C6
1	G	10	C49	O4'-C1'-N1-C2
1	G	10	C49	O4'-C1'-N1-C6
1	F	10	C49	O4'-C4'-C5'-O5'
1	G	10	C49	O4'-C4'-C5'-O5'
2	M	11	5CM	C2'-C1'-N1-C6
2	N	11	5CM	C2'-C1'-N1-C6
2	M	11	5CM	C2'-C1'-N1-C2
2	N	11	5CM	C2'-C1'-N1-C2
1	F	10	C49	C2'-C1'-N1-C6
1	G	10	C49	C2'-C1'-N1-C6
2	M	11	5CM	O4'-C1'-N1-C6
2	N	11	5CM	O4'-C1'-N1-C6
1	G	10	C49	C3'-C4'-C5'-O5'
2	N	11	5CM	O4'-C1'-N1-C2
2	M	11	5CM	O4'-C1'-N1-C2
1	F	10	C49	C2'-C1'-N1-C2
1	G	10	C49	C2'-C1'-N1-C2
1	F	10	C49	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	10	C49	4	0
1	F	10	C49	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.