Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:39 AM GMT

PDB ID	:	3MHT
Title	:	TERNARY STRUCTURE OF HHAI METHYLTRANSFERASE WITH UNMODIFIED DNA AND ADOHCY
Authors	:	O'Gara, M.; Klimasauskas, S.; Roberts, R.J.; Cheng, X.
Deposited on	:	1996-07-24
Resolution	:	2.70 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 (i)) were used in the production of this report:

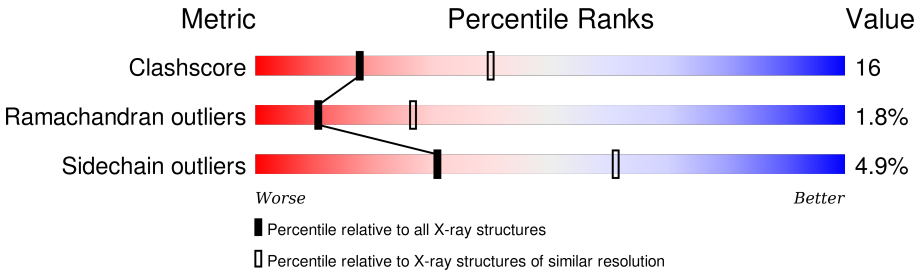
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	8% 33% 50% 8%
2	D	13	38% 62%
3	A	327	71% 27% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3211 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 DNA chain called DNA (5'-D(*GP*AP*TP*AP*GP*CP*GP*CP*TP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	12	246	117	45	72	12	0	0	0

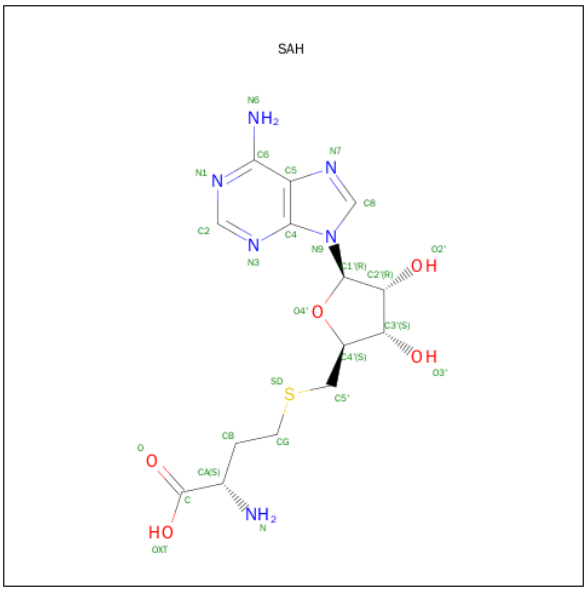
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*AP*TP*AP*GP*CP*GP*CP*TP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	13	263	127	47	77	12	0	0	0

- Molecule 3 is a protein called PROTEIN (HHAI METHYLTRANSFERASE (E.C.2.1.1.73)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	327	2606	1662	444	487	13	0	0	0

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		
5	C	2	Total	O	0	0
			2	2		
5	D	10	Total	O	0	0
			10	10		

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.

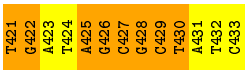
Note EDS was not executed.

- Molecule 1: DNA (5'-D(*GP*AP*TP*AP*GP*CP*GP*CP*TP*AP*TP*C)-3')

Chain C:

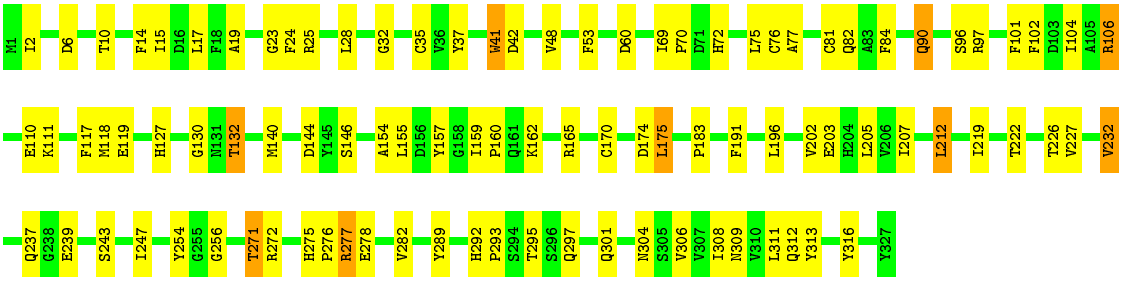
- Molecule 2: DNA (5'-D(*TP*GP*AP*TP*AP*GP*CP*GP*CP*TP*AP*TP*C)-3')

Chain D:



- Molecule 3: PROTEIN (HHAI METHYLTRANSFERASE (E.C.2.1.1.73))

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	99.86Å 99.86Å 325.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	88.7 (20.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3211	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	C	2.98	27/275 (9.8%)	4.48	77/422 (18.2%)
2	D	3.52	43/294 (14.6%)	4.15	79/452 (17.5%)
3	A	0.57	0/2661	0.74	1/3586 (0.0%)
All	All	1.47	70/3230 (2.2%)	2.02	157/4460 (3.5%)

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	C	0	3
2	D	0	3
All	All	0	6

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	408	DG	N9-C4	12.81	1.48	1.38
2	D	427	DC	C5'-C4'	12.06	1.64	1.51
2	D	427	DC	N1-C6	-11.28	1.30	1.37
2	D	429	DC	P-O5'	11.23	1.71	1.59
2	D	421	DT	C5'-C4'	11.05	1.63	1.51
2	D	428	DG	P-O5'	-10.53	1.49	1.59
1	C	405	DA	N9-C4	-10.31	1.31	1.37
2	D	421	DT	C2'-C1'	-10.06	1.42	1.52
1	C	410	DT	C5-C7	9.70	1.55	1.50
1	C	413	DC	C4'-C3'	9.39	1.62	1.53
1	C	407	DC	C4'-O4'	-9.01	1.36	1.45
2	D	428	DG	N9-C8	-8.98	1.31	1.37
2	D	428	DG	C6-N1	-8.51	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	429	DC	C4'-C3'	8.17	1.61	1.53
2	D	421	DT	C5-C6	-8.09	1.28	1.34
1	C	403	DA	C6-N1	-8.01	1.29	1.35
2	D	421	DT	N1-C2	7.77	1.44	1.38
2	D	428	DG	C3'-O3'	-7.47	1.34	1.44
2	D	421	DT	O4'-C1'	7.47	1.51	1.42
2	D	433	DC	C2-N3	7.43	1.41	1.35
1	C	410	DT	C5-C6	7.26	1.39	1.34
2	D	423	DA	N9-C4	7.20	1.42	1.37
2	D	428	DG	C5-C6	-7.17	1.35	1.42
1	C	405	DA	C4'-C3'	-7.13	1.45	1.52
2	D	432	DT	O3'-P	-6.89	1.52	1.61
2	D	425	DA	C8-N7	-6.75	1.26	1.31
2	D	426	DG	C4'-C3'	6.70	1.60	1.53
1	C	407	DC	N1-C2	-6.62	1.33	1.40
2	D	423	DA	C3'-C2'	6.58	1.60	1.52
2	D	425	DA	C4'-O4'	-6.55	1.38	1.45
2	D	432	DT	C2-N3	6.50	1.43	1.37
2	D	423	DA	N9-C8	6.47	1.43	1.37
2	D	428	DG	N7-C5	-6.34	1.35	1.39
2	D	424	DT	O3'-P	-6.28	1.53	1.61
1	C	412	DT	O3'-P	6.13	1.68	1.61
2	D	430	DT	C2'-C1'	-6.04	1.46	1.52
1	C	404	DT	P-O5'	6.00	1.65	1.59
1	C	408	DG	C2'-C1'	-5.98	1.46	1.52
1	C	407	DC	C4-N4	5.98	1.39	1.33
1	C	404	DT	C2'-C1'	-5.97	1.46	1.52
2	D	424	DT	C4'-O4'	-5.96	1.39	1.45
2	D	427	DC	N3-C4	-5.96	1.29	1.33
2	D	427	DC	N1-C2	5.94	1.46	1.40
2	D	423	DA	C5-C6	5.91	1.46	1.41
1	C	410	DT	N3-C4	-5.87	1.33	1.38
2	D	432	DT	N1-C2	5.85	1.42	1.38
1	C	404	DT	N1-C6	-5.84	1.34	1.38
2	D	426	DG	C3'-C2'	5.80	1.59	1.52
1	C	407	DC	C5'-C4'	5.77	1.57	1.51
2	D	421	DT	N3-C4	5.72	1.43	1.38
1	C	407	DC	N3-C4	5.66	1.38	1.33
2	D	433	DC	N3-C4	5.65	1.38	1.33
2	D	425	DA	C5-C4	-5.57	1.34	1.38
2	D	429	DC	C2'-C1'	-5.46	1.46	1.52
1	C	402	DG	C5'-C4'	5.45	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	423	DA	N7-C5	5.45	1.42	1.39
2	D	431	DA	N3-C4	5.42	1.38	1.34
1	C	406	DG	N9-C4	5.41	1.42	1.38
1	C	405	DA	N3-C4	-5.41	1.31	1.34
1	C	405	DA	N7-C5	-5.39	1.36	1.39
2	D	423	DA	C3'-O3'	5.37	1.50	1.44
2	D	432	DT	C4-O4	5.33	1.28	1.23
1	C	409	DC	C5'-C4'	5.32	1.57	1.51
1	C	408	DG	C5-C6	5.32	1.47	1.42
1	C	408	DG	C3'-C2'	5.24	1.58	1.52
1	C	403	DA	N9-C8	-5.05	1.33	1.37
2	D	424	DT	C2'-C1'	5.03	1.57	1.52
2	D	425	DA	O4'-C1'	-5.03	1.36	1.42
2	D	426	DG	C2-N3	5.02	1.36	1.32
1	C	412	DT	N1-C2	5.01	1.42	1.38

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	407	DC	O4'-C4'-C3'	-30.79	87.52	106.00
2	D	421	DT	O4'-C4'-C3'	-25.67	90.60	106.00
1	C	407	DC	C1'-O4'-C4'	-23.60	86.50	110.10
2	D	433	DC	O4'-C4'-C3'	-19.09	94.54	106.00
1	C	405	DA	O4'-C1'-C2'	-17.01	92.29	105.90
2	D	427	DC	C4'-C3'-C2'	-16.00	88.70	103.10
1	C	402	DG	O4'-C4'-C3'	-14.87	97.08	106.00
2	D	429	DC	N1-C2-O2	13.77	127.16	118.90
1	C	407	DC	O4'-C1'-C2'	-13.44	95.15	105.90
1	C	409	DC	C1'-O4'-C4'	-13.20	96.90	110.10
2	D	425	DA	N1-C6-N6	13.11	126.47	118.60
2	D	427	DC	P-O3'-C3'	13.08	135.39	119.70
1	C	407	DC	N3-C4-N4	12.95	127.06	118.00
1	C	406	DG	C4'-C3'-C2'	-12.88	91.51	103.10
1	C	410	DT	C4-C5-C7	-12.27	111.64	119.00
1	C	413	DC	O4'-C1'-N1	12.03	116.42	108.00
1	C	409	DC	P-O3'-C3'	11.99	134.09	119.70
2	D	426	DG	C4'-C3'-C2'	-11.95	92.34	103.10
2	D	425	DA	C5-C6-N6	-11.35	114.62	123.70
2	D	429	DC	N3-C2-O2	-11.29	114.00	121.90
1	C	404	DT	C6-C5-C7	-11.15	116.21	122.90
1	C	407	DC	N3-C4-C5	-10.96	117.51	121.90
1	C	406	DG	O4'-C1'-C2'	-10.85	97.22	105.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	432	DT	C4-C5-C6	10.75	124.45	118.00
2	D	421	DT	N1-C2-O2	10.73	131.69	123.10
2	D	421	DT	C4'-C3'-C2'	10.66	112.69	103.10
2	D	427	DC	O4'-C1'-N1	-10.61	100.58	108.00
2	D	430	DT	O4'-C4'-C3'	-10.48	99.71	106.00
2	D	432	DT	C6-C5-C7	-10.30	116.72	122.90
2	D	432	DT	O4'-C1'-C2'	-10.19	97.75	105.90
1	C	404	DT	O3'-P-O5'	-10.03	84.95	104.00
2	D	433	DC	C1'-O4'-C4'	-10.03	100.08	110.10
2	D	432	DT	O4'-C1'-N1	9.39	114.57	108.00
2	D	430	DT	C3'-C2'-C1'	-9.12	91.56	102.50
1	C	412	DT	O4'-C1'-C2'	-9.01	98.69	105.90
2	D	426	DG	O4'-C1'-N9	9.01	114.31	108.00
2	D	433	DC	O4'-C1'-C2'	-8.96	98.73	105.90
1	C	406	DG	C2-N3-C4	8.90	116.35	111.90
1	C	406	DG	N3-C2-N2	8.87	126.11	119.90
1	C	404	DT	O4'-C1'-C2'	-8.85	98.82	105.90
1	C	409	DC	O4'-C4'-C3'	-8.78	100.73	106.00
1	C	407	DC	C2-N3-C4	8.64	124.22	119.90
1	C	402	DG	N3-C2-N2	-8.52	113.94	119.90
1	C	405	DA	O3'-P-O5'	-8.48	87.88	104.00
2	D	430	DT	O3'-P-O5'	-8.36	88.12	104.00
2	D	427	DC	C4-C5-C6	8.30	121.55	117.40
2	D	421	DT	N3-C2-O2	-8.27	117.34	122.30
2	D	428	DG	C2-N3-C4	-8.26	107.77	111.90
1	C	412	DT	N3-C2-O2	-8.13	117.42	122.30
2	D	428	DG	O4'-C1'-C2'	8.10	112.38	105.90
1	C	410	DT	C6-N1-C2	-8.06	117.27	121.30
1	C	412	DT	O4'-C1'-N1	7.96	113.57	108.00
2	D	423	DA	O4'-C1'-C2'	-7.93	99.55	105.90
1	C	413	DC	C1'-O4'-C4'	-7.92	102.17	110.10
1	C	402	DG	C1'-O4'-C4'	7.91	118.01	110.10
2	D	421	DT	C6-C5-C7	-7.82	118.21	122.90
2	D	425	DA	O4'-C1'-C2'	-7.80	99.66	105.90
2	D	427	DC	O4'-C4'-C3'	-7.79	101.33	106.00
2	D	427	DC	N3-C2-O2	-7.76	116.47	121.90
1	C	402	DG	C5-C6-O6	-7.66	124.00	128.60
1	C	404	DT	C4-C5-C6	7.58	122.55	118.00
2	D	424	DT	C4-C5-C6	7.46	122.48	118.00
2	D	424	DT	C4-C5-C7	-7.40	114.56	119.00
1	C	402	DG	O4'-C1'-C2'	-7.37	100.00	105.90
1	C	407	DC	C3'-C2'-C1'	-7.37	93.66	102.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	405	DA	OP2-P-O3'	7.36	121.40	105.20
2	D	432	DT	C6-N1-C2	-7.34	117.63	121.30
2	D	422	DG	O4'-C4'-C3'	-7.33	101.57	104.50
1	C	410	DT	C6-N1-C1'	7.27	131.31	120.40
1	C	406	DG	C5-C6-N1	7.23	115.11	111.50
1	C	409	DC	N3-C4-C5	-7.21	119.01	121.90
2	D	422	DG	C6-C5-N7	-7.08	126.15	130.40
1	C	404	DT	C1'-O4'-C4'	-7.06	103.04	110.10
1	C	410	DT	N1-C2-N3	7.06	118.84	114.60
2	D	421	DT	C6-N1-C1'	-7.04	109.83	120.40
1	C	402	DG	N1-C6-O6	7.03	124.12	119.90
1	C	412	DT	C4-C5-C6	6.99	122.19	118.00
1	C	407	DC	P-O3'-C3'	-6.95	111.36	119.70
1	C	407	DC	C5-C4-N4	-6.86	115.39	120.20
2	D	422	DG	N7-C8-N9	6.86	116.53	113.10
2	D	431	DA	C4'-C3'-C2'	-6.82	96.96	103.10
2	D	431	DA	N1-C2-N3	-6.79	125.91	129.30
1	C	402	DG	C8-N9-C4	-6.77	103.69	106.40
2	D	427	DC	O4'-C1'-C2'	-6.73	100.51	105.90
2	D	423	DA	O3'-P-O5'	-6.72	91.23	104.00
2	D	426	DG	C2-N3-C4	6.71	115.26	111.90
2	D	425	DA	P-O5'-C5'	-6.71	110.16	120.90
1	C	410	DT	C4-C5-C6	6.66	122.00	118.00
1	C	410	DT	C5'-C4'-C3'	-6.66	102.11	114.10
2	D	426	DG	N3-C2-N2	6.63	124.54	119.90
1	C	413	DC	C3'-C2'-C1'	-6.63	94.54	102.50
1	C	408	DG	C2-N3-C4	6.61	115.20	111.90
2	D	424	DT	N3-C2-O2	-6.58	118.35	122.30
1	C	404	DT	C4'-C3'-C2'	-6.58	97.17	103.10
1	C	407	DC	C5-C6-N1	6.58	124.29	121.00
1	C	406	DG	N3-C4-C5	-6.52	125.34	128.60
2	D	424	DT	O4'-C1'-C2'	-6.50	100.70	105.90
1	C	409	DC	O4'-C1'-N1	6.47	112.53	108.00
2	D	430	DT	C5-C6-N1	-6.43	119.84	123.70
1	C	409	DC	O5'-P-OP2	-6.40	99.94	105.70
2	D	421	DT	N1-C2-N3	-6.36	110.78	114.60
2	D	422	DG	C2-N3-C4	-6.35	108.72	111.90
1	C	409	DC	C4'-C3'-C2'	-6.32	97.41	103.10
1	C	403	DA	C5'-C4'-C3'	-6.32	102.73	114.10
2	D	422	DG	C5-N7-C8	-6.25	101.18	104.30
2	D	427	DC	N3-C4-C5	-6.24	119.41	121.90
2	D	426	DG	C8-N9-C4	-6.22	103.91	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	403	DA	O4'-C1'-C2'	-6.20	100.94	105.90
1	C	402	DG	P-O3'-C3'	6.19	127.13	119.70
1	C	406	DG	P-O3'-C3'	6.14	127.07	119.70
2	D	432	DT	N3-C4-O4	6.14	123.58	119.90
2	D	432	DT	P-O5'-C5'	-6.13	111.09	120.90
2	D	422	DG	C8-N9-C4	-6.09	103.96	106.40
1	C	406	DG	P-O5'-C5'	6.09	130.64	120.90
2	D	421	DT	O3'-P-O5'	6.07	115.53	104.00
2	D	431	DA	P-O5'-C5'	-6.02	111.27	120.90
1	C	410	DT	C5-C4-O4	6.00	129.10	124.90
1	C	408	DG	C8-N9-C4	-5.98	104.01	106.40
2	D	423	DA	C4'-C3'-C2'	-5.97	97.72	103.10
2	D	421	DT	O4'-C1'-C2'	5.96	110.67	105.90
1	C	409	DC	N1-C2-O2	5.94	122.47	118.90
1	C	410	DT	N3-C2-O2	-5.91	118.76	122.30
2	D	423	DA	N1-C2-N3	5.88	132.24	129.30
2	D	424	DT	O4'-C4'-C3'	5.87	109.52	106.00
1	C	412	DT	C5'-C4'-C3'	-5.84	103.58	114.10
2	D	423	DA	C8-N9-C4	-5.84	103.47	105.80
2	D	428	DG	C1'-O4'-C4'	-5.83	104.27	110.10
2	D	425	DA	C2-N3-C4	5.82	113.51	110.60
1	C	406	DG	O5'-P-OP2	-5.82	100.46	105.70
1	C	403	DA	O3'-P-O5'	-5.80	92.98	104.00
1	C	406	DG	N3-C4-N9	5.80	129.48	126.00
1	C	410	DT	C6-C5-C7	5.75	126.35	122.90
2	D	429	DC	O4'-C1'-N1	-5.75	103.98	108.00
1	C	408	DG	N3-C4-C5	-5.74	125.73	128.60
2	D	426	DG	N1-C2-N3	-5.73	120.46	123.90
2	D	431	DA	O4'-C4'-C3'	5.72	109.43	106.00
1	C	402	DG	N1-C2-N2	5.70	121.33	116.20
2	D	428	DG	C5-C6-O6	-5.63	125.22	128.60
2	D	427	DC	N1-C2-O2	5.56	122.24	118.90
2	D	421	DT	C3'-C2'-C1'	-5.49	95.91	102.50
2	D	424	DT	C6-N1-C2	-5.49	118.56	121.30
2	D	432	DT	C4'-C3'-C2'	-5.48	98.17	103.10
2	D	432	DT	N3-C4-C5	-5.47	111.92	115.20
1	C	404	DT	C5'-C4'-C3'	-5.44	104.31	114.10
1	C	404	DT	N1-C2-N3	5.42	117.85	114.60
2	D	423	DA	C2-N3-C4	-5.39	107.91	110.60
1	C	405	DA	N9-C4-C5	5.37	107.95	105.80
2	D	429	DC	C4'-C3'-C2'	-5.36	98.28	103.10
1	C	410	DT	N3-C4-C5	-5.31	112.01	115.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	409	DC	P-O5'-C5'	-5.29	112.44	120.90
2	D	421	DT	C2-N1-C1'	5.24	126.59	118.20
1	C	408	DG	C4-C5-N7	-5.24	108.70	110.80
2	D	427	DC	N1-C1'-C2'	5.15	122.39	112.60
2	D	429	DC	C1'-O4'-C4'	-5.10	105.00	110.10
1	C	408	DG	C5-N7-C8	5.05	106.83	104.30
1	C	412	DT	C6-N1-C2	-5.02	118.79	121.30
3	A	212	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	403	DA	Sidechain
1	C	409	DC	Sidechain
1	C	413	DC	Sidechain
2	D	421	DT	Sidechain
2	D	428	DG	Sidechain
2	D	430	DT	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	C	246	0	135	6	0
2	D	263	0	149	11	0
3	A	2606	0	2587	87	0
4	A	26	0	19	2	0
5	A	58	0	0	8	0
5	C	2	0	0	0	0
5	D	10	0	0	0	0
All	All	3211	0	2890	95	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 16.

All (95) 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)
3:A:82:GLN:NE2	5:A:376:HOH:O	1.82	1.04
3:A:15:ILE:HD12	3:A:37:TYR:HB3	1.42	0.99
3:A:202:VAL:HG13	3:A:205:LEU:HD12	1.46	0.96
2:D:427:DC:C6	3:A:81:CYS:SG	2.60	0.94
2:D:427:DC:H2'	3:A:304:ASN:HB3	1.58	0.85
3:A:254:TYR:HA	5:A:331:HOH:O	1.87	0.74
1:C:405:DA:H2"	1:C:406:DG:C8	2.23	0.74
3:A:15:ILE:CD1	3:A:37:TYR:HB3	2.18	0.73
3:A:202:VAL:HG11	3:A:272:ARG:CZ	2.23	0.69
1:C:406:DG:O6	3:A:256:GLY:HA3	1.94	0.67
3:A:207:ILE:O	3:A:271:THR:HG23	1.96	0.65
2:D:427:DC:C5	3:A:81:CYS:SG	2.90	0.62
3:A:306:VAL:CG2	3:A:311:LEU:HD11	2.29	0.61
3:A:226:THR:HA	5:A:351:HOH:O	1.99	0.61
3:A:162:LYS:O	3:A:162:LYS:HG2	2.00	0.61
3:A:202:VAL:HG11	3:A:272:ARG:NE	2.15	0.61
3:A:297:GLN:O	3:A:301:GLN:HG3	2.02	0.60
3:A:289:TYR:HA	5:A:361:HOH:O	2.02	0.59
3:A:6:ASP:HB2	3:A:316:TYR:HE1	1.68	0.58
3:A:219:ILE:HD13	3:A:227:VAL:HG11	1.86	0.58
3:A:202:VAL:HG11	3:A:272:ARG:HD2	1.85	0.57
3:A:202:VAL:HG11	3:A:272:ARG:CD	2.35	0.56
3:A:275:HIS:CD2	3:A:277:ARG:H	2.23	0.56
3:A:15:ILE:HG22	3:A:17:LEU:HG	1.89	0.55
3:A:41:TRP:HD1	3:A:42:ASP:N	2.03	0.55
3:A:25:ARG:HD2	3:A:53:PHE:CE1	2.43	0.54
3:A:155:LEU:HD12	3:A:155:LEU:O	2.08	0.54
3:A:23:GLY:HA2	3:A:308:ILE:HD11	1.89	0.54
3:A:311:LEU:HD12	3:A:311:LEU:N	2.23	0.53
3:A:24:PHE:CD2	3:A:76:CYS:HB3	2.43	0.53
3:A:155:LEU:HD12	3:A:155:LEU:C	2.29	0.53
3:A:75:LEU:C	3:A:75:LEU:HD23	2.28	0.53
3:A:41:TRP:CD1	3:A:42:ASP:N	2.75	0.53
3:A:202:VAL:CG1	3:A:272:ARG:HD2	2.39	0.53
2:D:427:DC:H1'	3:A:304:ASN:HA	1.90	0.53
4:A:328:SAH:HG1	5:A:374:HOH:O	2.10	0.52
3:A:275:HIS:HD2	3:A:277:ARG:HB3	1.75	0.51
3:A:306:VAL:HG21	3:A:311:LEU:HD11	1.91	0.51
3:A:232:VAL:HG12	3:A:239:GLU:HB3	1.92	0.51
1:C:406:DG:H2'	1:C:406:DG:O5'	2.11	0.51
3:A:146:SER:O	3:A:170:CYS:HA	2.10	0.51
3:A:306:VAL:HG22	3:A:311:LEU:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:140:MET:HG2	3:A:170:CYS:SG	2.51	0.51
3:A:41:TRP:HD1	3:A:42:ASP:H	1.59	0.50
3:A:10:THR:HA	3:A:32:GLY:O	2.11	0.50
2:D:427:DC:C6	3:A:304:ASN:HB2	2.47	0.50
3:A:227:VAL:HG22	3:A:243:SER:HB3	1.92	0.50
3:A:309:ASN:O	3:A:312:GLN:HB2	2.10	0.50
3:A:84:PHE:HE2	3:A:132:THR:HG21	1.76	0.50
3:A:101:PHE:O	3:A:104:ILE:HB	2.12	0.49
3:A:311:LEU:HD12	3:A:311:LEU:H	1.78	0.49
2:D:427:DC:C2'	3:A:304:ASN:HB3	2.37	0.48
3:A:15:ILE:HG12	3:A:72:HIS:CG	2.48	0.48
3:A:90:GLN:O	3:A:127:HIS:HE1	1.95	0.48
1:C:402:DG:O5'	1:C:402:DG:H2'	2.13	0.48
3:A:276:PRO:HG2	3:A:295:THR:HG22	1.94	0.47
3:A:119:GLU:OE2	3:A:165:ARG:HD2	2.14	0.47
3:A:202:VAL:CG1	3:A:205:LEU:HD12	2.31	0.47
3:A:155:LEU:HA	3:A:159:ILE:O	2.15	0.47
3:A:162:LYS:HB2	3:A:247:ILE:CD1	2.45	0.47
3:A:127:HIS:HD2	3:A:132:THR:OG1	1.98	0.47
3:A:102:PHE:O	3:A:106:ARG:HG2	2.14	0.46
3:A:275:HIS:CD2	3:A:277:ARG:HB3	2.50	0.46
3:A:306:VAL:HG23	5:A:352:HOH:O	2.16	0.46
3:A:70:PRO:O	3:A:111:LYS:HE2	2.15	0.46
3:A:219:ILE:CD1	3:A:227:VAL:HG11	2.46	0.46
3:A:130:GLY:HA2	5:A:356:HOH:O	2.16	0.46
3:A:19:ALA:O	4:A:328:SAH:HA	2.17	0.45
1:C:413:DC:H42	2:D:422:DG:H1	1.64	0.45
3:A:48:VAL:HG13	3:A:292:HIS:HD2	1.82	0.45
3:A:275:HIS:HB3	3:A:278:GLU:HG3	1.98	0.44
3:A:237:GLN:NE2	5:A:337:HOH:O	2.50	0.44
3:A:157:TYR:CE2	3:A:183:PRO:HB2	2.53	0.44
3:A:14:PHE:CZ	3:A:35:CYS:HB2	2.53	0.44
3:A:77:ALA:O	3:A:118:MET:HA	2.18	0.43
3:A:191:PHE:CZ	3:A:222:THR:HB	2.53	0.43
3:A:157:TYR:HE2	3:A:183:PRO:HB2	1.82	0.43
3:A:196:LEU:HA	3:A:278:GLU:OE2	2.18	0.43
3:A:226:THR:HG22	3:A:247:ILE:O	2.19	0.42
1:C:407:DC:N4	3:A:237:GLN:HB2	2.35	0.42
3:A:175:LEU:H	3:A:175:LEU:HG	1.59	0.42
3:A:227:VAL:HG22	3:A:227:VAL:O	2.20	0.42
3:A:292:HIS:CG	3:A:293:PRO:HD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:DG:O5'	2:D:422:DG:H2'	2.21	0.41
2:D:429:DC:O5'	2:D:429:DC:H2'	2.20	0.41
3:A:69:ILE:HA	3:A:70:PRO:HD3	1.82	0.41
3:A:311:LEU:H	3:A:311:LEU:CD1	2.32	0.41
3:A:275:HIS:O	3:A:276:PRO:C	2.60	0.41
3:A:23:GLY:HA2	3:A:308:ILE:CD1	2.51	0.41
3:A:2:ILE:N	3:A:312:GLN:OE1	2.45	0.41
3:A:183:PRO:CG	3:A:313:TYR:HB3	2.50	0.41
3:A:70:PRO:O	3:A:72:HIS:HD2	2.04	0.41
2:D:426:DG:P	3:A:162:LYS:HZ1	2.44	0.40
2:D:425:DA:H2"	2:D:426:DG:O5'	2.20	0.40
3:A:160:PRO:HB3	3:A:191:PHE:HA	2.04	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	325/327 (99%)	299 (92%)	20 (6%)	6 (2%)	11 27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	90	GLN
3	A	154	ALA
3	A	174	ASP
3	A	203	GLU
3	A	60	ASP
3	A	144	ASP

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	283/283 (100%)	269 (95%)	14 (5%)	31 61

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	28	LEU
3	A	41	TRP
3	A	96	SER
3	A	97	ARG
3	A	106	ARG
3	A	110	GLU
3	A	117	PHE
3	A	132	THR
3	A	175	LEU
3	A	212	LEU
3	A	232	VAL
3	A	271	THR
3	A	277	ARG
3	A	282	VAL

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

Mol	Chain	Res	Type
3	A	8	GLN
3	A	63	GLN
3	A	72	HIS
3	A	123	ASN
3	A	127	HIS
3	A	141	ASN
3	A	268	ASN
3	A	275	HIS
3	A	323	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SAH	A	328	-	20,28,28	0.99	1 (5%)	19,40,40	1.26	2 (10%)

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	SAH	A	328	-	-	0/7/31/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	328	SAH	C8-N7	-2.62	1.29	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	328	SAH	C2'-C1'-N9	-3.30	109.24	114.29
4	A	328	SAH	CB-CA-N	2.40	117.35	110.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	328	SAH	2	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.