Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:27 PM GMT

PDB ID	:	1TSD
Title	:	THYMIDYLATE SYNTHASE COMPLEX WITH 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (DUMP) AND FOLATE ANALOG 1843U89
Authors	:	Weichsel, A.; Montfort, W.R.
Deposited on	:	1995-08-15
Resolution	:	1.95 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 ⓘ symbol.

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

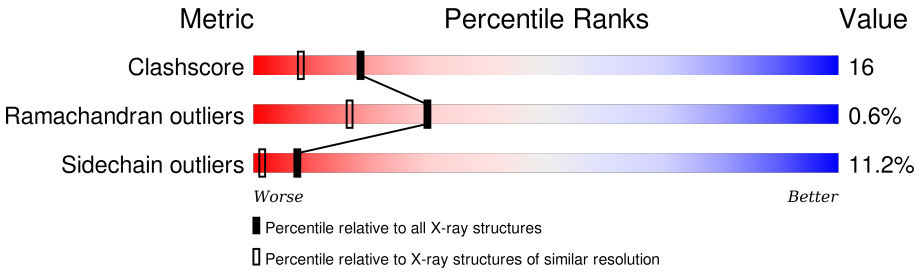
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.95 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	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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	A	265	63% 25% 9% ·
1	B	265	55% 35% 8% ·

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
2	BME	A	265	-	-	X	-
2	BME	A	266	-	-	X	-

2 Entry composition

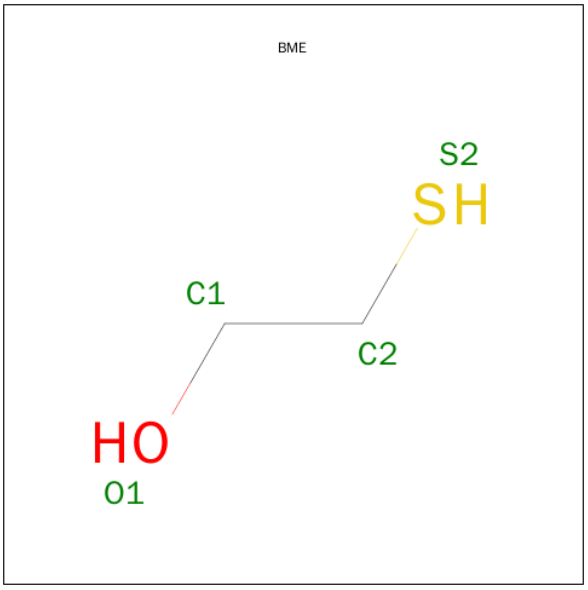
There are 5 unique types of molecules in this entry. The entry contains 4616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDYLATE SYNTHASE.

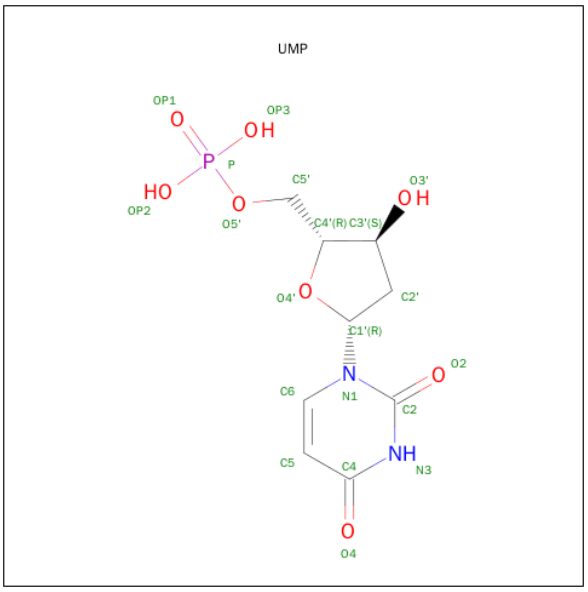
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			
1	B	265	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



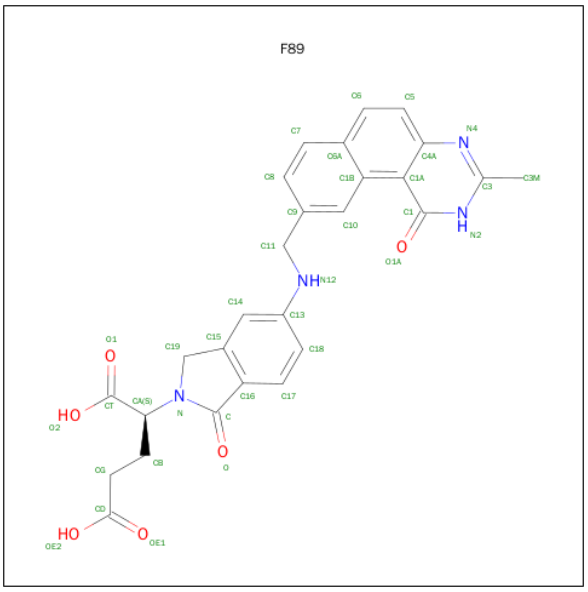
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is S)-2-(5(((1,2-DIHYDRO-3-METHYL-1-OXOBENZO(F)QUINAZOLIN-9-YL) METHYL)AMINO)1-OXO-2-ISOINDOLINYL)GLUTARIC ACID (three-letter code: F89) (formula: $C_{27}H_{24}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			37	27	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			37	27	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	80	Total	O	0	0
			80	80		

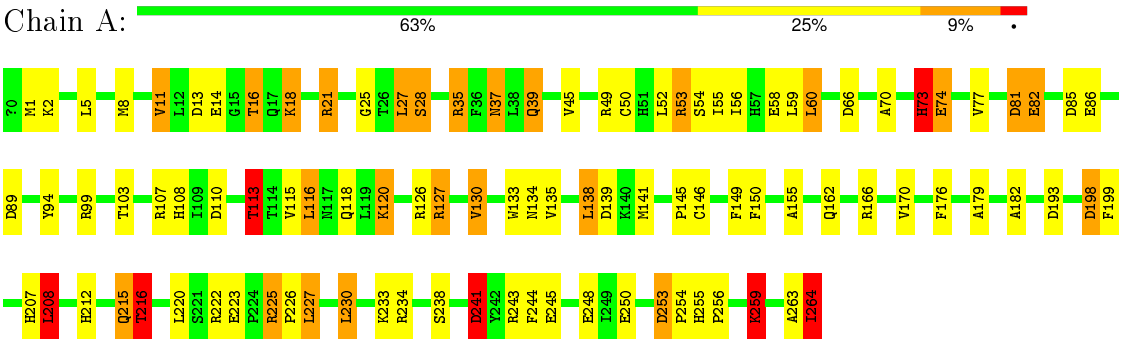
3 Residue-property plots (i)

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.

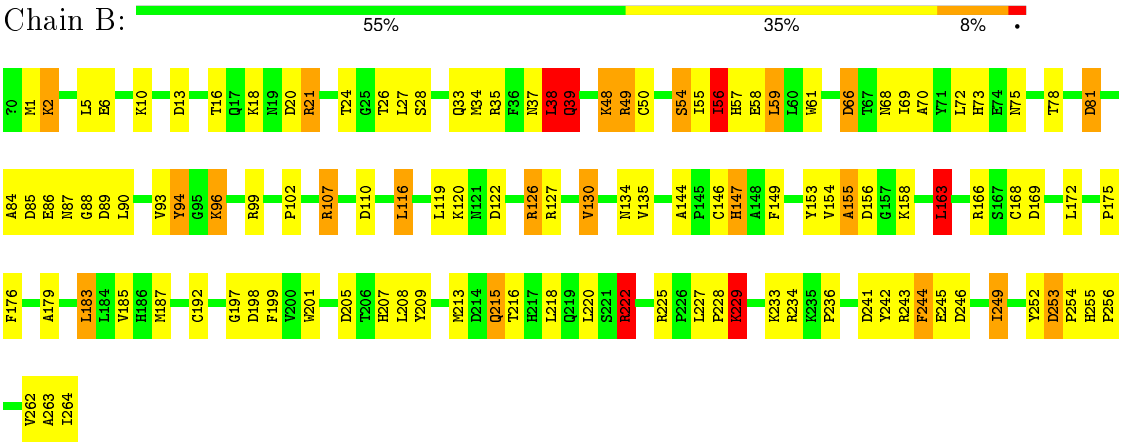
- Molecule 1: THYMIDYLATE SYNTHASE

Chain A:



- Molecule 1: THYMIDYLATE SYNTHASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	127.52Å 127.52Å 68.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 1.95	Depositor
% Data completeness (in resolution range)	98.9 (7.00-1.95)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: FMT, F89, UMP, BME

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	1.05	1/2210 (0.0%)	1.91	56/3000 (1.9%)
1	B	1.05	0/2210	2.02	80/3000 (2.7%)
All	All	1.05	1/4420 (0.0%)	1.97	136/6000 (2.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CD-OE2	-5.05	1.20	1.25

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	126	ARG	NE-CZ-NH2	-21.81	109.39	120.30
1	B	205	ASP	CB-CG-OD2	14.41	131.26	118.30
1	A	166	ARG	NE-CZ-NH1	-14.18	113.21	120.30
1	A	35	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	A	35	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	B	81	ASP	CB-CG-OD2	12.35	129.42	118.30
1	B	107	ARG	NE-CZ-NH1	11.97	126.28	120.30
1	B	246	ASP	CB-CG-OD2	9.98	127.28	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	198	ASP	CB-CG-OD1	9.57	126.92	118.30
1	B	49	ARG	NE-CZ-NH2	9.49	125.04	120.30
1	B	149	PHE	N-CA-CB	-9.11	94.20	110.60
1	B	130	VAL	CA-CB-CG1	8.93	124.29	110.90
1	A	216	THR	CA-CB-CG2	8.71	124.59	112.40
1	B	35	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	208	LEU	CA-CB-CG	8.43	134.68	115.30
1	B	110	ASP	CB-CG-OD1	8.39	125.85	118.30
1	B	66	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	209	TYR	CB-CG-CD2	8.12	125.87	121.00
1	B	126	ARG	NH1-CZ-NH2	8.11	128.32	119.40
1	A	13	ASP	CB-CG-OD1	8.10	125.59	118.30
1	A	85	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	B	56	ILE	CA-CB-CG2	8.04	126.98	110.90
1	B	99	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	B	166	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	B	13	ASP	CB-CG-OD1	-7.87	111.22	118.30
1	A	149	PHE	N-CA-CB	-7.77	96.61	110.60
1	A	198	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	127	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	A	28	SER	N-CA-CB	-7.65	99.02	110.50
1	B	127	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	89	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	B	209	TYR	CB-CG-CD1	-7.51	116.50	121.00
1	A	259	LYS	N-CA-CB	7.37	123.86	110.60
1	A	130	VAL	CA-CB-CG2	7.30	121.85	110.90
1	A	166	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	225	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	81	ASP	CB-CG-OD1	6.94	124.55	118.30
1	A	227	LEU	N-CA-CB	-6.84	96.71	110.40
1	B	253	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	B	163	LEU	CB-CG-CD2	6.80	122.56	111.00
1	B	147	HIS	CA-CB-CG	6.78	125.13	113.60
1	A	253	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	B	28	SER	N-CA-CB	-6.77	100.35	110.50
1	A	155	ALA	N-CA-CB	6.73	119.52	110.10
1	B	122	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	243	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	38	LEU	CB-CA-C	6.53	122.60	110.20
1	B	107	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	B	166	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	81	ASP	CB-CG-OD1	-6.36	112.57	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	LEU	CA-CB-CG	6.36	129.94	115.30
1	A	234	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	222	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	216	THR	CA-CB-CG2	6.32	121.24	112.40
1	B	241	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	A	1	MET	CG-SD-CE	-6.28	90.16	100.20
1	A	77	VAL	CB-CA-C	6.22	123.21	111.40
1	B	205	ASP	OD1-CG-OD2	-6.20	111.52	123.30
1	B	20	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	A	27	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	139	ASP	CB-CA-C	6.17	122.73	110.40
1	B	130	VAL	N-CA-CB	6.15	125.02	111.50
1	A	208	LEU	CB-CG-CD1	6.11	121.39	111.00
1	B	48	LYS	CA-CB-CG	6.10	126.81	113.40
1	A	74	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	B	222	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	144	ALA	N-CA-CB	-6.04	101.64	110.10
1	B	169	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	156	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	1	MET	CB-CA-C	5.87	122.14	110.40
1	B	35	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	38	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	108	HIS	N-CA-CB	5.81	121.05	110.60
1	A	199	PHE	N-CA-CB	5.76	120.97	110.60
1	A	126	ARG	CB-CG-CD	5.75	126.54	111.60
1	A	73	HIS	CA-CB-CG	-5.71	103.89	113.60
1	B	34	MET	CB-CA-C	5.69	121.78	110.40
1	A	182	ALA	CB-CA-C	5.68	118.62	110.10
1	B	225	ARG	CD-NE-CZ	-5.68	115.65	123.60
1	A	54	SER	CB-CA-C	5.67	120.87	110.10
1	A	113	THR	CA-CB-CG2	5.63	120.28	112.40
1	B	244	PHE	CB-CA-C	5.61	121.61	110.40
1	B	116	LEU	O-C-N	-5.60	113.74	122.70
1	B	169	ASP	CB-CA-C	5.60	121.60	110.40
1	A	250	GLU	OE1-CD-OE2	5.60	130.02	123.30
1	A	11	VAL	CA-CB-CG1	5.55	119.23	110.90
1	B	24	THR	N-CA-CB	5.53	120.81	110.30
1	B	199	PHE	N-CA-CB	5.47	120.45	110.60
1	A	248	GLU	CA-CB-CG	5.46	125.41	113.40
1	B	185	VAL	CA-CB-CG1	5.45	119.08	110.90
1	B	213	MET	N-CA-CB	5.45	120.41	110.60
1	B	86	GLU	N-CA-CB	5.43	120.38	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	THR	OG1-CB-CG2	5.43	122.49	110.00
1	B	229	LYS	N-CA-CB	5.42	120.36	110.60
1	B	130	VAL	CB-CA-C	5.42	121.70	111.40
1	B	20	ASP	OD1-CG-OD2	5.41	133.59	123.30
1	B	168	CYS	CA-C-O	5.41	131.46	120.10
1	B	59	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	B	153	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	A	21	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	66	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	39	GLN	CA-CB-CG	-5.28	101.79	113.40
1	B	27	LEU	N-CA-C	-5.28	96.75	111.00
1	B	20	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	241	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	14	GLU	CG-CD-OE1	-5.25	107.81	118.30
1	A	216	THR	N-CA-CB	5.24	120.26	110.30
1	B	249	ILE	CA-CB-CG2	5.23	121.36	110.90
1	A	133	TRP	CB-CA-C	5.23	120.86	110.40
1	A	21	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	66	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	175	PRO	N-CD-CG	-5.18	95.43	103.20
1	A	230	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	119	LEU	CB-CG-CD1	5.17	119.79	111.00
1	B	199	PHE	CB-CG-CD1	-5.17	117.18	120.80
1	B	39	GLN	CA-CB-CG	5.15	124.73	113.40
1	B	126	ARG	CB-CG-CD	-5.15	98.21	111.60
1	B	86	GLU	CG-CD-OE1	5.12	128.54	118.30
1	B	56	ILE	CB-CA-C	5.11	121.81	111.60
1	A	25	GLY	O-C-N	5.10	130.86	122.70
1	A	107	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	264	ILE	CA-CB-CG2	5.08	121.07	110.90
1	B	225	ARG	N-CA-CB	-5.08	101.45	110.60
1	B	241	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	127	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	B	135	VAL	C-N-CA	5.06	132.93	122.30
1	A	52	LEU	CB-CA-C	5.05	119.81	110.20
1	A	99	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	245	GLU	CG-CD-OE2	-5.05	108.20	118.30
1	A	207	HIS	CA-C-O	5.05	130.71	120.10
1	B	155	ALA	N-CA-CB	5.05	117.17	110.10
1	A	193	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	68	ASN	CA-CB-CG	-5.04	102.32	113.40
1	A	21	ARG	NH1-CZ-NH2	-5.03	113.87	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	CYS	CA-CB-SG	-5.03	104.95	114.00
1	B	222	ARG	CD-NE-CZ	-5.00	116.59	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	B	21	ARG	Sidechain
1	B	222	ARG	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	A	2153	0	2078	65	0
1	B	2153	0	2080	67	0
2	A	8	0	10	11	0
3	A	20	0	9	2	0
3	B	20	0	11	4	0
4	A	37	0	23	6	0
4	B	37	0	22	3	0
5	A	108	0	0	0	0
5	B	80	0	0	3	0
All	All	4616	0	4233	135	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 (135) 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:A:215:GLN:NE2	1:A:215:GLN:H	1.66	0.91
1:A:215:GLN:HE21	1:A:215:GLN:H	0.93	0.91
1:B:183:LEU:HD22	1:B:187:MET:HE2	1.53	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:HD2	2:A:266:BME:H11	1.57	0.87
1:B:215:GLN:HE21	1:B:215:GLN:H	1.22	0.85
1:B:234:ARG:O	1:B:236:PRO:HD3	1.77	0.84
1:B:218:LEU:HD11	1:B:222:ARG:HH21	1.42	0.84
1:A:50:CYS:HB3	2:A:265:BME:H11	1.62	0.81
1:B:10:LYS:HE2	5:B:454:HOH:O	1.83	0.79
1:B:183:LEU:HD22	1:B:187:MET:CE	2.12	0.79
1:A:215:GLN:N	1:A:215:GLN:HE21	1.78	0.76
1:A:110:ASP:OD2	1:A:113:THR:HG23	1.85	0.76
1:A:127:ARG:NH2	3:B:265:UMP:OP2	2.20	0.75
1:A:146:CYS:SG	3:A:267:UMP:C6	2.85	0.69
1:B:49:ARG:HH12	1:B:256:PRO:HA	1.57	0.68
1:A:176:PHE:CE1	2:A:265:BME:H21	2.30	0.67
1:B:146:CYS:SG	3:B:265:UMP:C6	2.88	0.66
4:B:266:F89:O	4:B:266:F89:CT	2.44	0.66
1:A:243:ARG:NH1	1:A:245:GLU:HB2	2.12	0.64
1:B:37:ASN:OD1	1:B:39:GLN:HB2	1.98	0.64
1:A:255:HIS:HB3	1:A:256:PRO:HD2	1.78	0.64
1:B:228:PRO:O	1:B:229:LYS:HD2	1.98	0.64
1:B:49:ARG:NH1	1:B:256:PRO:HA	2.11	0.64
1:A:243:ARG:HH12	1:A:245:GLU:HB2	1.63	0.64
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.29	0.62
1:A:120:LYS:HB2	2:A:266:BME:H11	1.81	0.62
1:A:176:PHE:CZ	2:A:265:BME:H21	2.34	0.61
1:A:120:LYS:HB2	2:A:266:BME:S2	2.40	0.61
1:A:176:PHE:HZ	4:A:268:F89:O1	1.83	0.61
1:B:55:ILE:HD13	1:B:179:ALA:HB3	1.84	0.60
1:A:8:MET:HE3	1:A:220:LEU:HD13	1.84	0.60
1:B:39:GLN:OE1	1:B:39:GLN:HA	2.02	0.59
1:A:50:CYS:CB	2:A:265:BME:H11	2.32	0.59
1:A:35:ARG:HD3	1:A:198:ASP:OD2	2.03	0.59
1:A:120:LYS:CD	2:A:266:BME:H11	2.32	0.58
1:A:73:HIS:CE1	1:A:81:ASP:OD1	2.56	0.57
1:A:238:SER:O	1:A:241:ASP:HB2	2.04	0.57
1:B:61:TRP:CE3	1:B:72:LEU:HD11	2.40	0.57
1:B:69:ILE:HG23	1:B:90:LEU:HD11	1.87	0.56
1:B:61:TRP:CD2	1:B:72:LEU:HD11	2.41	0.55
1:A:212:HIS:O	1:A:216:THR:HG23	2.06	0.55
1:A:49:ARG:HH21	1:A:254:PRO:HG2	1.70	0.55
1:B:2:LYS:HE2	1:B:2:LYS:H	1.69	0.55
1:B:56:ILE:HD12	1:B:244:PHE:CD1	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:MET:CE	1:A:220:LEU:HD13	2.37	0.54
1:B:222:ARG:HB3	1:B:255:HIS:CE1	2.42	0.54
1:B:215:GLN:NE2	1:B:215:GLN:H	2.00	0.54
1:A:11:VAL:HG22	1:A:208:LEU:HD22	1.90	0.54
1:A:55:ILE:HD13	1:A:179:ALA:HB3	1.91	0.53
1:B:263:ALA:HB2	5:B:305:HOH:O	2.07	0.53
1:B:69:ILE:HD13	1:B:81:ASP:OD2	2.08	0.53
1:B:228:PRO:C	1:B:229:LYS:HD2	2.29	0.53
1:A:53:ARG:HA	1:A:244:PHE:HE1	1.73	0.53
1:B:93:VAL:O	1:B:94:TYR:C	2.47	0.53
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.74	0.53
1:B:58:GLU:O	1:B:61:TRP:HB3	2.09	0.52
1:B:59:LEU:HD21	1:B:187:MET:HE3	1.91	0.52
1:B:56:ILE:C	1:B:56:ILE:HD13	2.30	0.52
1:A:56:ILE:HG22	1:A:60:LEU:HD22	1.92	0.52
1:A:53:ARG:HH11	1:A:53:ARG:HG3	1.75	0.52
1:A:70:ALA:O	1:A:73:HIS:HB2	2.10	0.51
4:A:268:F89:C9	4:A:268:F89:H14	2.40	0.51
4:B:266:F89:H10	4:B:266:F89:O1A	2.11	0.51
1:B:2:LYS:H	1:B:2:LYS:CD	2.23	0.51
1:A:73:HIS:HE1	1:A:81:ASP:OD1	1.93	0.50
1:B:48:LYS:HG3	5:B:306:HOH:O	2.11	0.50
1:A:225:ARG:HD2	1:A:253:ASP:O	2.12	0.49
1:B:57:HIS:CD2	1:B:75:ASN:ND2	2.81	0.49
1:B:147:HIS:HB2	1:B:163:LEU:HD21	1.95	0.49
1:B:228:PRO:HG2	1:B:249:ILE:HD11	1.94	0.48
1:B:96:LYS:NZ	1:B:102:PRO:HG3	2.28	0.48
1:A:120:LYS:HB2	2:A:266:BME:C1	2.44	0.48
1:B:215:GLN:HE21	1:B:215:GLN:N	2.02	0.48
1:B:172:LEU:HD21	1:B:262:VAL:HG22	1.96	0.48
1:A:37:ASN:HD21	1:A:39:GLN:HB2	1.79	0.48
1:B:26:THR:HB	1:B:207:HIS:HB2	1.96	0.48
1:A:49:ARG:HE	1:A:49:ARG:HB2	1.37	0.47
1:B:2:LYS:CE	1:B:2:LYS:H	2.27	0.47
1:A:45:VAL:HG22	1:A:50:CYS:SG	2.54	0.47
1:B:33:GLN:HA	1:B:201:TRP:O	2.14	0.47
1:A:170:VAL:HB	1:A:208:LEU:HD13	1.97	0.47
1:B:78:THR:HA	1:B:81:ASP:OD1	2.16	0.46
1:B:183:LEU:CD2	1:B:187:MET:HE2	2.36	0.46
1:A:53:ARG:HA	1:A:244:PHE:CE1	2.49	0.46
1:A:141:MET:SD	1:A:145:PRO:HD3	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:CE2	2:A:265:BME:H12	2.51	0.46
1:A:127:ARG:HH21	3:B:265:UMP:P	2.38	0.46
1:A:212:HIS:O	1:A:216:THR:CG2	2.64	0.45
1:A:150:PHE:HA	1:A:162:GLN:O	2.16	0.45
1:A:18:LYS:HE3	1:B:154:VAL:O	2.16	0.45
1:B:179:ALA:O	1:B:183:LEU:HB2	2.16	0.45
1:A:176:PHE:CE1	4:A:268:F89:H192	2.52	0.45
1:A:259:LYS:HB3	1:A:259:LYS:HE2	1.63	0.44
1:B:2:LYS:O	1:B:6:GLU:HG3	2.18	0.44
1:B:73:HIS:C	1:B:75:ASN:H	2.21	0.44
1:A:135:VAL:HA	1:A:138:LEU:HD22	1.98	0.44
1:B:56:ILE:HD12	1:B:244:PHE:HD1	1.81	0.44
1:B:39:GLN:HE21	1:B:158:LYS:CE	2.30	0.44
1:B:187:MET:HG2	1:B:242:TYR:CE2	2.52	0.44
1:A:16:THR:HG21	1:B:155:ALA:HB1	1.99	0.44
1:B:49:ARG:NH1	1:B:49:ARG:HB2	2.33	0.43
1:B:55:ILE:HG12	1:B:176:PHE:HD2	1.82	0.43
1:A:215:GLN:NE2	1:A:215:GLN:N	2.50	0.43
1:B:39:GLN:HE21	1:B:158:LYS:HE3	1.82	0.43
3:A:267:UMP:OP2	1:B:126:ARG:HD3	2.18	0.43
1:A:82:GLU:HG3	1:A:264:ILE:HD11	1.99	0.43
1:B:84:ALA:HB1	1:B:88:GLY:C	2.39	0.43
1:B:57:HIS:NE2	1:B:75:ASN:ND2	2.64	0.43
1:A:49:ARG:NH2	1:A:254:PRO:HG2	2.34	0.43
1:A:116:LEU:O	2:A:266:BME:H22	2.19	0.42
1:A:82:GLU:CG	1:A:264:ILE:HD11	2.47	0.42
4:B:266:F89:HG2	4:B:266:F89:H191	2.01	0.42
1:B:228:PRO:HB2	1:B:249:ILE:HG13	2.00	0.42
1:A:56:ILE:HD12	1:A:244:PHE:CE1	2.54	0.42
1:A:5:LEU:HD23	1:A:8:MET:CE	2.50	0.42
1:B:85:ASP:OD1	1:B:87:ASN:HB2	2.19	0.42
1:A:49:ARG:NH2	1:A:254:PRO:HD2	2.34	0.41
1:B:55:ILE:HG12	1:B:176:PHE:CD2	2.55	0.41
1:B:54:SER:HB2	1:B:176:PHE:HE2	1.85	0.41
1:B:252:TYR:CE2	1:B:254:PRO:HG3	2.55	0.41
1:B:146:CYS:SG	3:B:265:UMP:C5	3.13	0.41
1:A:86:GLU:H	1:A:86:GLU:CD	2.24	0.41
1:B:70:ALA:O	1:B:73:HIS:N	2.51	0.41
1:B:252:TYR:CZ	1:B:254:PRO:HG3	2.56	0.41
1:B:38:LEU:HB2	1:B:197:GLY:O	2.21	0.41
1:A:176:PHE:CZ	4:A:268:F89:H192	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASN:ND2	1:A:39:GLN:H	2.19	0.41
1:B:228:PRO:HB2	1:B:249:ILE:CG1	2.51	0.40
1:B:61:TRP:CD1	1:B:66:ASP:HB3	2.57	0.40
1:A:115:VAL:HG21	1:A:130:VAL:HG23	2.02	0.40
1:A:225:ARG:HB3	1:A:226:PRO:CD	2.51	0.40
4:A:268:F89:O1A	4:A:268:F89:H10	2.21	0.40
1:A:263:ALA:O	4:A:268:F89:H3M1	2.21	0.40
1:B:228:PRO:HB2	1:B:249:ILE:HD11	2.03	0.40
1:B:102:PRO:HA	1:B:107:ARG: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	263/265 (99%)	256 (97%)	5 (2%)	2 (1%)	24	11
1	B	263/265 (99%)	250 (95%)	12 (5%)	1 (0%)	39	27
All	All	526/530 (99%)	506 (96%)	17 (3%)	3 (1%)	30	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	TYR
1	A	74	GLU
1	A	94	TYR

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	233/233 (100%)	206 (88%)	27 (12%)	7 1
1	B	233/233 (100%)	208 (89%)	25 (11%)	8 2
All	All	466/466 (100%)	414 (89%)	52 (11%)	7 1

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	16	THR
1	A	18	LYS
1	A	27	LEU
1	A	28	SER
1	A	37	ASN
1	A	53	ARG
1	A	59	LEU
1	A	60	LEU
1	A	73	HIS
1	A	82	GLU
1	A	103	THR
1	A	113	THR
1	A	116	LEU
1	A	120	LYS
1	A	134	ASN
1	A	138	LEU
1	A	208	LEU
1	A	215	GLN
1	A	216	THR
1	A	223	GLU
1	A	227	LEU
1	A	230	LEU
1	A	233	LYS
1	A	241	ASP
1	A	259	LYS
1	A	264	ILE
1	B	2	LYS
1	B	5	LEU
1	B	16	THR
1	B	18	LYS
1	B	21	ARG
1	B	38	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	39	GLN
1	B	50	CYS
1	B	54	SER
1	B	56	ILE
1	B	89	ASP
1	B	96	LYS
1	B	116	LEU
1	B	120	LYS
1	B	130	VAL
1	B	134	ASN
1	B	163	LEU
1	B	183	LEU
1	B	215	GLN
1	B	220	LEU
1	B	227	LEU
1	B	229	LYS
1	B	233	LYS
1	B	253	ASP
1	B	264	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	39	GLN
1	A	73	HIS
1	A	75	ASN
1	A	87	ASN
1	A	97	GLN
1	A	108	HIS
1	A	117	ASN
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	215	GLN
1	A	217	HIS
1	B	87	ASN
1	B	117	ASN
1	B	118	GLN
1	B	121	ASN
1	B	134	ASN
1	B	151	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	162	GLN
1	B	215	GLN
1	B	217	HIS

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

6 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	$\#\|Z\| > 2$
2	BME	A	265	-	3,3,3	0.48	0	2,2,2	1.01	0
2	BME	A	266	-	3,3,3	0.48	0	2,2,2	1.28	0
3	UMP	A	267	-	16,21,21	1.76	6 (37%)	23,31,31	3.48	8 (34%)
4	F89	A	268	-	35,41,41	2.95	9 (25%)	44,60,60	3.73	14 (31%)
3	UMP	B	265	-	16,21,21	1.81	5 (31%)	23,31,31	2.97	8 (34%)
4	F89	B	266	-	35,41,41	2.87	11 (31%)	44,60,60	4.82	27 (61%)

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	BME	A	265	-	-	0/1/1/1	0/0/0/0
2	BME	A	266	-	-	0/1/1/1	0/0/0/0
3	UMP	A	267	-	-	0/6/22/22	0/2/2/2
4	F89	A	268	-	-	0/12/30/30	0/5/5/5
3	UMP	B	265	-	-	0/6/22/22	0/2/2/2
4	F89	B	266	-	-	0/12/30/30	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	265	UMP	O5'-C5'	-3.55	1.30	1.44
4	B	266	F89	C3-N4	-3.18	1.27	1.34
3	A	267	UMP	C5'-C4'	-2.74	1.42	1.51
4	A	268	F89	C-N	-2.68	1.33	1.36
3	A	267	UMP	O5'-C5'	-2.62	1.34	1.44
3	B	265	UMP	C5'-C4'	-2.55	1.43	1.51
4	B	266	F89	C5-C4A	-2.53	1.37	1.41
4	A	268	F89	C3-N4	-2.51	1.29	1.34
4	A	268	F89	C13-N12	2.40	1.45	1.38
4	B	266	F89	C13-N12	2.48	1.46	1.38
3	A	267	UMP	C4-N3	2.53	1.37	1.33
3	B	265	UMP	C4-N3	2.59	1.37	1.33
3	A	267	UMP	C2'-C1'	2.60	1.59	1.52
3	A	267	UMP	O4'-C1'	2.73	1.48	1.42
3	A	267	UMP	P-OP2	2.76	1.64	1.54
3	B	265	UMP	C2'-C1'	2.81	1.60	1.52
4	B	266	F89	C7-C8	2.93	1.42	1.36
3	B	265	UMP	O4'-C1'	2.94	1.49	1.42
4	B	266	F89	C17-C16	3.10	1.45	1.39
4	B	266	F89	C4A-N4	3.44	1.43	1.37
4	A	268	F89	C4A-N4	4.38	1.45	1.37
4	B	266	F89	C19-N	4.43	1.50	1.46
4	A	268	F89	CA-N	4.65	1.54	1.47
4	A	268	F89	CB-CA	4.74	1.59	1.53
4	B	266	F89	CA-N	5.20	1.55	1.47
4	B	266	F89	CB-CA	5.22	1.59	1.53
4	A	268	F89	C19-N	5.57	1.51	1.46
4	A	268	F89	C3-N2	6.06	1.45	1.34
4	B	266	F89	C3-N2	6.48	1.46	1.34
4	B	266	F89	C1-C1A	9.66	1.57	1.41
4	A	268	F89	C1-C1A	11.38	1.60	1.41

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	266	F89	C19-N-C	-11.89	109.16	113.05
4	B	266	F89	C19-C15-C16	-9.95	103.32	109.66
4	A	268	F89	CB-CA-N	-9.76	104.90	112.85
4	B	266	F89	C1A-C1-N2	-9.39	117.08	124.19
4	A	268	F89	C1A-C1-N2	-6.63	119.17	124.19
4	A	268	F89	O-C-C16	-5.89	116.94	128.68
4	B	266	F89	C11-C9-C10	-5.84	112.70	121.98
4	B	266	F89	C17-C16-C	-5.40	121.32	129.67
4	B	266	F89	C18-C17-C16	-4.76	113.60	121.06
3	A	267	UMP	C6-N1-C2	-4.61	113.82	121.28
4	B	266	F89	O-C-C16	-4.39	119.94	128.68
4	A	268	F89	C14-C13-N12	-4.18	113.08	120.74
3	A	267	UMP	C5-C4-N3	-3.98	112.90	123.12
4	B	266	F89	CB-CA-N	-3.92	109.66	112.85
3	B	265	UMP	C6-N1-C2	-3.89	114.97	121.28
4	A	268	F89	C19-C15-C16	-3.88	107.19	109.66
3	B	265	UMP	C5-C4-N3	-3.66	113.74	123.12
4	A	268	F89	C15-C19-N	-3.63	100.91	102.19
4	A	268	F89	C11-C9-C10	-3.63	116.21	121.98
4	B	266	F89	C13-C14-C15	-3.19	116.28	120.98
4	B	266	F89	C11-N12-C13	-3.17	113.55	122.15
4	A	268	F89	CG-CB-CA	-3.07	107.83	112.96
4	B	266	F89	CB-CG-CD	-3.04	100.61	113.02
4	B	266	F89	N4-C3-N2	-3.01	119.66	125.58
3	A	267	UMP	OP2-P-O5'	-2.71	98.77	106.56
4	A	268	F89	C15-C16-C	-2.44	107.53	108.81
4	A	268	F89	C18-C17-C16	-2.38	117.33	121.06
4	B	266	F89	CG-CB-CA	-2.34	109.05	112.96
4	A	268	F89	N4-C3-N2	-2.33	121.00	125.58
4	B	266	F89	C9-C11-N12	-2.30	108.40	113.73
4	B	266	F89	C14-C13-N12	-2.27	116.58	120.74
3	B	265	UMP	O5'-P-OP1	-2.26	101.38	107.14
4	B	266	F89	C10-C1B-C1A	-2.20	120.10	122.72
4	B	266	F89	C14-C15-C16	-2.19	117.80	120.68
4	B	266	F89	C5-C4A-N4	2.07	122.01	118.73
3	B	265	UMP	O5'-C5'-C4'	2.42	118.04	109.12
3	B	265	UMP	C5-C6-N1	2.45	126.59	120.58
4	B	266	F89	C11-C9-C8	2.46	126.36	120.90
3	A	267	UMP	O5'-C5'-C4'	2.97	120.08	109.12
3	B	265	UMP	O4'-C1'-N1	2.99	112.90	107.72
3	A	267	UMP	C5-C6-N1	3.00	127.94	120.58
4	A	268	F89	C18-C13-N12	3.06	126.91	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	265	UMP	C2'-C1'-N1	3.88	123.60	114.16
4	B	266	F89	C3M-C3-N4	4.04	124.07	117.21
3	A	267	UMP	C2'-C1'-N1	4.08	124.08	114.16
4	B	266	F89	C18-C13-C14	4.29	124.81	119.69
3	A	267	UMP	O4'-C1'-N1	4.35	115.25	107.72
4	B	266	F89	C17-C16-C15	4.41	126.42	120.64
4	B	266	F89	C19-C15-C14	5.31	137.94	129.43
4	B	266	F89	C15-C16-C	6.48	112.22	108.81
4	A	268	F89	C3-N4-C4A	7.89	124.76	115.86
4	B	266	F89	C3-N4-C4A	8.65	125.62	115.86
4	B	266	F89	O-C-N	10.79	132.98	125.22
3	B	265	UMP	C4-N3-C2	11.04	125.08	114.14
3	A	267	UMP	C4-N3-C2	12.88	126.89	114.14
4	B	266	F89	C15-C19-N	13.04	106.79	102.19
4	A	268	F89	O-C-N	15.90	136.66	125.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	265	BME	5	0
2	A	266	BME	6	0
3	A	267	UMP	2	0
4	A	268	F89	6	0
3	B	265	UMP	4	0
4	B	266	F89	3	0

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

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.