Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:22 PM GMT

PDB ID	:	1TDB
Title	:	STRUCTURES OF THYMIDYLATE SYNTHASE WITH A C-TERMINAL DELETION: ROLE OF THE C-TERMINUS IN ALIGNMENT OF D/UMP AND CH2H4FOLATE
Authors	:	Perry, K.M.; Carreras, C.W.; Chang, L.C.; Santi, D.V.; Stroud, R.M.
Deposited on	:	1993-02-15
Resolution	:	2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

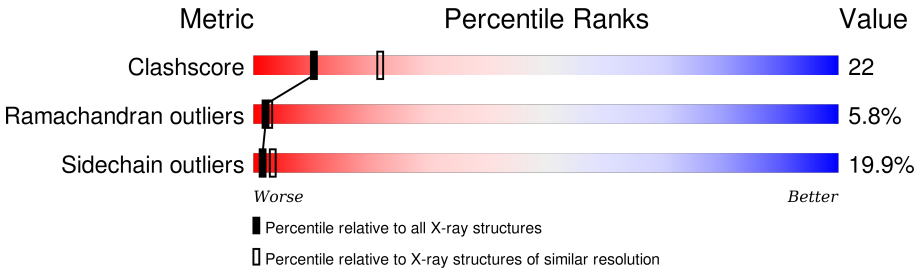
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	37% 37% 21% 5%

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	UFP	A	529	X	-	-	-

2 Entry composition

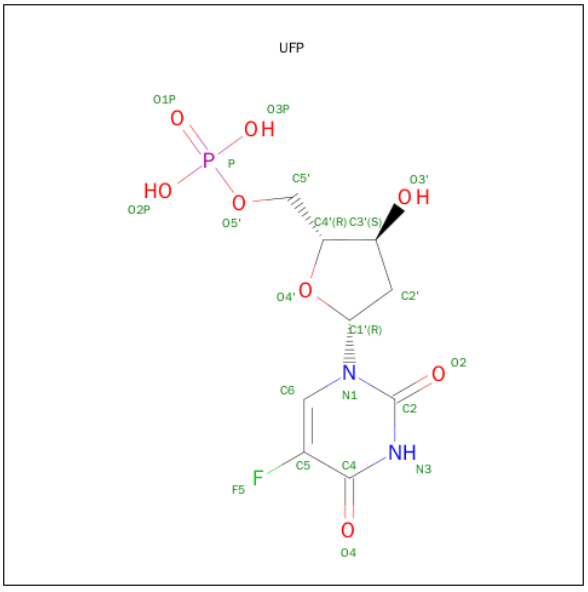
There are 3 unique types of molecules in this entry. The entry contains 2645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	315	2583	1672	437	466	8	0	0	0

- Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
2	A	1	21	9	1	2	8	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	41	41	41	0	0

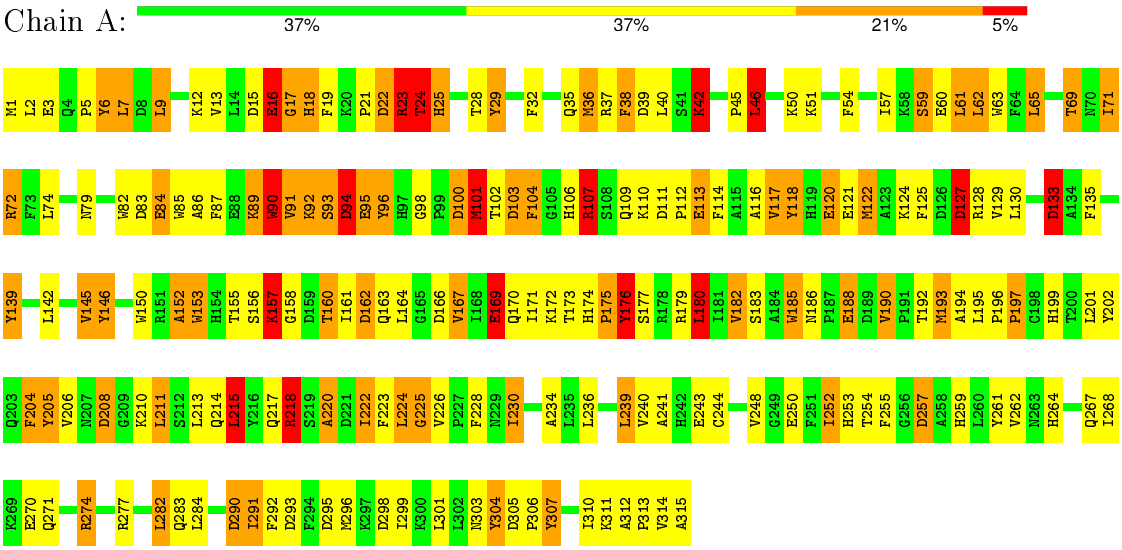
3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: THYMIDYLATE SYNTHASE

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	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	78.80Å 78.80Å 243.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.65	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2645	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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: UFP

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	1.39	15/2667 (0.6%)	2.41	164/3624 (4.5%)

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	A	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	VAL	CA-CB	6.45	1.68	1.54
1	A	185	TRP	CD1-NE1	-6.10	1.27	1.38
1	A	113	GLU	CG-CD	6.02	1.60	1.51
1	A	188	GLU	CD-OE1	-5.91	1.19	1.25
1	A	185	TRP	CG-CD2	-5.81	1.33	1.43
1	A	82	TRP	CG-CD2	-5.67	1.34	1.43
1	A	150	TRP	CG-CD2	-5.57	1.34	1.43
1	A	250	GLU	CD-OE2	-5.51	1.19	1.25
1	A	169	GLU	CB-CG	5.47	1.62	1.52
1	A	60	GLU	CD-OE1	-5.42	1.19	1.25
1	A	185	TRP	NE1-CE2	-5.25	1.30	1.37
1	A	3	GLU	CG-CD	5.20	1.59	1.51
1	A	59	SER	CA-CB	5.16	1.60	1.52
1	A	183	SER	CA-CB	-5.14	1.45	1.52
1	A	127	ASP	CB-CG	5.14	1.62	1.51

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	A	274	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	A	19	PHE	CB-CG-CD2	-11.74	112.58	120.80
1	A	85	TRP	CD1-CG-CD2	11.16	115.23	106.30
1	A	314	VAL	O-C-N	10.90	140.14	122.70
1	A	277	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	A	91	VAL	CA-CB-CG2	-9.75	96.28	110.90
1	A	85	TRP	CE2-CD2-CG	-9.41	99.77	107.30
1	A	146	TYR	CB-CG-CD1	-9.28	115.43	121.00
1	A	180	LEU	CA-CB-CG	9.27	136.61	115.30
1	A	9	LEU	CA-CB-CG	9.13	136.29	115.30
1	A	205	TYR	CB-CG-CD2	-9.07	115.56	121.00
1	A	153	TRP	CD1-CG-CD2	8.91	113.42	106.30
1	A	188	GLU	CA-CB-CG	8.77	132.68	113.40
1	A	314	VAL	CA-C-N	-8.75	97.94	117.20
1	A	94	ASP	CA-C-N	-8.71	98.05	117.20
1	A	102	THR	CA-C-N	-8.62	98.23	117.20
1	A	293	ASP	N-CA-CB	-8.55	95.21	110.60
1	A	157	LYS	N-CA-C	-8.48	88.09	111.00
1	A	162	ASP	CA-CB-CG	8.41	131.90	113.40
1	A	29	TYR	CB-CG-CD1	-8.28	116.03	121.00
1	A	63	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	A	169	GLU	CA-CB-CG	8.02	131.04	113.40
1	A	23	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	248	VAL	CA-CB-CG2	-7.94	98.99	110.90
1	A	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	162	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	153	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	A	61	LEU	CA-CB-CG	7.74	133.09	115.30
1	A	218	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	277	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	63	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	A	160	THR	N-CA-CB	-7.53	96.00	110.30
1	A	185	TRP	CG-CD2-CE3	7.50	140.65	133.90
1	A	208	ASP	N-CA-C	7.49	131.23	111.00
1	A	103	ASP	CA-C-N	-7.47	100.77	117.20
1	A	6	TYR	CB-CG-CD2	-7.45	116.53	121.00
1	A	72	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	72	ARG	CB-CG-CD	7.39	130.81	111.60
1	A	185	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	A	1	MET	CA-CB-CG	-7.33	100.85	113.30
1	A	190	VAL	CG1-CB-CG2	-7.14	99.47	110.90
1	A	150	TRP	CD1-CG-CD2	7.12	112.00	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	MET	CA-CB-CG	7.11	125.38	113.30
1	A	176	TYR	CB-CG-CD1	-7.08	116.75	121.00
1	A	42	LYS	CA-CB-CG	7.07	128.95	113.40
1	A	185	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	16	GLU	CA-CB-CG	-6.98	98.05	113.40
1	A	46	LEU	CA-C-N	-6.98	101.85	117.20
1	A	19	PHE	CG-CD2-CE2	-6.97	113.13	120.80
1	A	150	TRP	CG-CD2-CE3	6.97	140.18	133.90
1	A	155	THR	N-CA-CB	-6.92	97.16	110.30
1	A	91	VAL	CA-CB-CG1	6.92	121.27	110.90
1	A	150	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	A	193	MET	CA-C-N	-6.80	102.23	117.20
1	A	293	ASP	CB-CA-C	6.80	124.00	110.40
1	A	96	TYR	CD1-CE1-CZ	-6.71	113.76	119.80
1	A	6	TYR	CB-CG-CD1	6.69	125.01	121.00
1	A	248	VAL	CG1-CB-CG2	6.67	121.57	110.90
1	A	139	TYR	CA-C-N	-6.67	102.87	116.20
1	A	39	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	60	GLU	O-C-N	-6.64	112.07	122.70
1	A	101	MET	CG-SD-CE	6.62	110.80	100.20
1	A	307	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	A	107	ARG	CA-CB-CG	6.61	127.94	113.40
1	A	116	ALA	CA-C-N	6.58	131.68	117.20
1	A	179	ARG	CA-CB-CG	6.55	127.82	113.40
1	A	314	VAL	CA-CB-CG2	-6.54	101.09	110.90
1	A	305	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	23	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	94	ASP	O-C-N	6.32	132.81	122.70
1	A	153	TRP	CG-CD1-NE1	-6.31	103.79	110.10
1	A	32	PHE	CB-CG-CD2	-6.12	116.51	120.80
1	A	109	GLN	CB-CA-C	6.11	122.62	110.40
1	A	24	THR	N-CA-C	-6.10	94.53	111.00
1	A	150	TRP	NE1-CE2-CZ2	-6.08	123.71	130.40
1	A	69	THR	CA-CB-CG2	6.03	120.84	112.40
1	A	185	TRP	CE2-CD2-CG	-6.02	102.48	107.30
1	A	90	TRP	CE2-CD2-CG	-5.99	102.51	107.30
1	A	206	VAL	CA-CB-CG1	-5.96	101.97	110.90
1	A	109	GLN	N-CA-CB	-5.88	100.02	110.60
1	A	65	LEU	CB-CG-CD1	-5.87	101.02	111.00
1	A	243	GLU	CA-C-N	5.87	130.12	117.20
1	A	96	TYR	CD1-CG-CD2	5.86	124.34	117.90
1	A	96	TYR	CG-CD2-CE2	-5.86	116.61	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	ASP	CA-C-O	5.85	132.39	120.10
1	A	90	TRP	CB-CG-CD1	-5.85	119.40	127.00
1	A	116	ALA	O-C-N	-5.84	113.36	122.70
1	A	215	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	93	SER	N-CA-C	5.82	126.72	111.00
1	A	208	ASP	N-CA-CB	-5.78	100.19	110.60
1	A	211	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	305	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	37	ARG	CA-CB-CG	5.77	126.09	113.40
1	A	167	VAL	CB-CA-C	-5.76	100.45	111.40
1	A	226	VAL	CA-CB-CG2	-5.74	102.29	110.90
1	A	290	ASP	CA-C-N	-5.74	104.57	117.20
1	A	100	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	82	TRP	CE2-CD2-CG	-5.73	102.72	107.30
1	A	303	ASN	OD1-CG-ND2	-5.72	108.73	121.90
1	A	182	VAL	N-CA-C	-5.72	95.55	111.00
1	A	145	VAL	CA-CB-CG1	-5.70	102.34	110.90
1	A	146	TYR	CB-CG-CD2	5.68	124.41	121.00
1	A	253	HIS	N-CA-C	-5.67	95.69	111.00
1	A	313	PRO	N-CA-CB	5.67	110.10	103.30
1	A	72	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
1	A	169	GLU	N-CA-CB	5.63	120.73	110.60
1	A	93	SER	CA-C-N	-5.62	104.83	117.20
1	A	220	ALA	CA-C-N	-5.62	104.84	117.20
1	A	94	ASP	C-N-CA	5.61	135.72	121.70
1	A	96	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	A	94	ASP	N-CA-C	5.57	126.05	111.00
1	A	90	TRP	CD1-CG-CD2	5.56	110.75	106.30
1	A	179	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
1	A	9	LEU	CB-CG-CD1	-5.52	101.61	111.00
1	A	24	THR	C-N-CA	5.51	135.49	121.70
1	A	82	TRP	CD2-CE2-CZ2	-5.46	115.75	122.30
1	A	90	TRP	CE3-CZ3-CH2	-5.45	115.20	121.20
1	A	3	GLU	CA-CB-CG	5.40	125.28	113.40
1	A	117	VAL	CA-CB-CG1	-5.39	102.81	110.90
1	A	96	TYR	CA-CB-CG	-5.38	103.17	113.40
1	A	167	VAL	CA-C-N	5.37	129.00	117.20
1	A	17	GLY	CA-C-N	-5.35	105.43	117.20
1	A	230	ILE	CA-CB-CG1	-5.35	100.84	111.00
1	A	179	ARG	O-C-N	-5.33	114.17	122.70
1	A	161	ILE	CB-CG1-CD1	5.32	128.78	113.90
1	A	190	VAL	CA-C-N	5.30	131.94	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	VAL	N-CA-CB	5.29	123.14	111.50
1	A	71	ILE	CB-CA-C	5.27	122.15	111.60
1	A	255	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	A	19	PHE	CD1-CG-CD2	5.25	125.13	118.30
1	A	204	PHE	CB-CG-CD1	5.25	124.48	120.80
1	A	314	VAL	C-N-CA	5.24	134.80	121.70
1	A	282	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	A	139	TYR	O-C-N	5.24	132.10	123.20
1	A	63	TRP	CB-CG-CD1	-5.20	120.25	127.00
1	A	240	VAL	CA-C-N	5.19	128.62	117.20
1	A	103	ASP	C-N-CA	5.19	134.67	121.70
1	A	128	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	252	ILE	CA-CB-CG2	-5.17	100.55	110.90
1	A	267	GLN	CG-CD-OE1	-5.16	111.28	121.60
1	A	166	ASP	CA-CB-CG	5.15	124.73	113.40
1	A	22	ASP	C-N-CA	5.15	134.56	121.70
1	A	293	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	71	ILE	N-CA-CB	-5.12	99.03	110.80
1	A	296	MET	CG-SD-CE	5.11	108.38	100.20
1	A	217	GLN	N-CA-C	-5.09	97.24	111.00
1	A	241	ALA	N-CA-CB	5.09	117.22	110.10
1	A	42	LYS	N-CA-CB	-5.08	101.45	110.60
1	A	38	PHE	CB-CA-C	-5.08	100.25	110.40
1	A	153	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	A	162	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	A	208	ASP	CA-CB-CG	-5.07	102.25	113.40
1	A	17	GLY	CA-C-O	5.07	129.72	120.60
1	A	194	ALA	N-CA-CB	-5.06	103.01	110.10
1	A	18	HIS	CB-CA-C	5.05	120.51	110.40
1	A	239	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	201	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	239	LEU	CD1-CG-CD2	-5.04	95.37	110.50
1	A	1	MET	N-CA-CB	-5.01	101.58	110.60
1	A	167	VAL	CA-C-O	-5.01	109.58	120.10
1	A	244	CYS	CA-CB-SG	-5.01	104.98	114.00
1	A	274	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	240	VAL	CA-CB-CG1	-5.00	103.40	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Peptide
1	A	176	TYR	Sidechain
1	A	304	TYR	Sidechain
1	A	312	ALA	Peptide
1	A	98	GLY	Peptide

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	2583	0	2487	110	0
2	A	21	0	9	2	0
3	A	41	0	0	2	0
All	All	2645	0	2496	110	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 22.

All (110) 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:65:LEU:HD13	1:A:291:ILE:HG12	1.51	0.90
1:A:29:TYR:HE1	1:A:262:VAL:HG23	1.39	0.86
1:A:91:VAL:HG21	1:A:101:MET:HB2	1.61	0.81
1:A:90:TRP:CH2	1:A:95:GLU:HB3	2.15	0.81
1:A:90:TRP:HA	1:A:90:TRP:CE3	2.18	0.76
1:A:86:ALA:HB2	1:A:142:LEU:HD21	1.69	0.73
1:A:40:LEU:HD21	1:A:234:ALA:HB1	1.70	0.72
1:A:127:ASP:HA	1:A:130:LEU:HD12	1.71	0.72
1:A:74:LEU:HB3	1:A:79:ASN:HB3	1.72	0.71
1:A:65:LEU:HB3	1:A:292:PHE:HD1	1.55	0.71
1:A:90:TRP:HA	1:A:90:TRP:HE3	1.57	0.70
1:A:120:GLU:O	1:A:124:LYS:HG3	1.91	0.69
1:A:12:LYS:O	1:A:16:GLU:HB2	1.93	0.69
1:A:87:PHE:CE1	1:A:122:MET:HA	2.27	0.69
1:A:177:SER:HB3	1:A:180:LEU:HD13	1.74	0.68
1:A:23:ARG:HG3	1:A:261:TYR:HE1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:HE1	1:A:315:ALA:HA	1.60	0.66
1:A:264:HIS:CE1	1:A:315:ALA:HA	2.32	0.65
1:A:28:THR:CG2	1:A:259:HIS:HB2	2.29	0.63
1:A:51:LYS:HZ3	1:A:304:TYR:HE2	1.47	0.62
1:A:72:ARG:HG3	1:A:129:VAL:O	2.01	0.60
1:A:46:LEU:HD12	1:A:301:LEU:HD21	1.84	0.60
1:A:122:MET:O	1:A:125:PHE:HB3	2.03	0.59
1:A:72:ARG:HH22	1:A:133:ASP:HA	1.67	0.59
1:A:204:PHE:CD2	1:A:213:LEU:HD12	2.38	0.58
1:A:223:PHE:CE2	1:A:224:LEU:HD23	2.38	0.58
1:A:6:TYR:HD1	1:A:7:LEU:HD12	1.68	0.58
1:A:90:TRP:CH2	1:A:135:PHE:HE2	2.22	0.58
1:A:54:PHE:HA	1:A:57:ILE:HD12	1.86	0.57
1:A:65:LEU:CD1	1:A:291:ILE:HG12	2.30	0.57
1:A:92:LYS:HD2	1:A:93:SER:H	1.70	0.57
1:A:222:ILE:HB	1:A:259:HIS:O	2.04	0.57
1:A:21:PRO:HB2	1:A:25:HIS:ND1	2.20	0.56
1:A:59:SER:HB2	1:A:79:ASN:ND2	2.21	0.56
1:A:218:ARG:HH22	2:A:529:UFP:P	2.29	0.56
1:A:193:MET:HB2	1:A:196:PRO:HD3	1.88	0.56
1:A:107:ARG:HB2	1:A:114:PHE:CE2	2.41	0.56
1:A:156:SER:O	1:A:157:LYS:HB2	2.06	0.56
1:A:284:LEU:HD23	1:A:299:ILE:HG23	1.88	0.56
1:A:220:ALA:HA	2:A:529:UFP:O2	2.05	0.55
1:A:101:MET:SD	1:A:101:MET:N	2.79	0.55
1:A:177:SER:HB3	1:A:180:LEU:CD1	2.36	0.55
1:A:13:VAL:HG21	1:A:222:ILE:HD13	1.90	0.54
1:A:224:LEU:HG	1:A:264:HIS:NE2	2.23	0.54
1:A:38:PHE:HZ	1:A:230:ILE:HD13	1.71	0.54
1:A:163:GLN:O	1:A:167:VAL:HG22	2.07	0.53
1:A:271:GLN:HA	1:A:274:ARG:HG3	1.91	0.53
1:A:114:PHE:HA	1:A:117:VAL:HG22	1.91	0.52
1:A:84:GLU:HA	1:A:87:PHE:HB3	1.94	0.50
1:A:38:PHE:CZ	1:A:230:ILE:HD13	2.47	0.49
1:A:2:LEU:HD12	1:A:42:LYS:HB3	1.93	0.49
1:A:271:GLN:HB3	1:A:310:ILE:HD11	1.94	0.49
1:A:180:LEU:HD23	1:A:204:PHE:HB2	1.95	0.49
1:A:163:GLN:CB	1:A:182:VAL:HG13	2.42	0.49
1:A:202:TYR:HA	1:A:214:GLN:O	2.13	0.48
1:A:6:TYR:CD1	1:A:7:LEU:HD12	2.49	0.48
1:A:224:LEU:HD12	1:A:315:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASP:O	1:A:298:ASP:HB2	2.14	0.48
1:A:163:GLN:HB2	1:A:182:VAL:HG13	1.95	0.48
1:A:264:HIS:HE1	1:A:315:ALA:O	1.96	0.47
1:A:239:LEU:HD23	1:A:291:ILE:HB	1.97	0.47
1:A:90:TRP:HH2	1:A:95:GLU:HB3	1.72	0.47
1:A:107:ARG:HA	1:A:110:LYS:HG2	1.97	0.47
1:A:35:GLN:HA	1:A:254:THR:HA	1.97	0.47
1:A:50:LYS:HE3	3:A:321:HOH:O	2.14	0.47
1:A:72:ARG:NH2	1:A:133:ASP:HA	2.29	0.47
1:A:86:ALA:HB2	1:A:142:LEU:CD2	2.44	0.46
1:A:152:ALA:CB	1:A:160:THR:HG23	2.45	0.46
1:A:29:TYR:CE1	1:A:262:VAL:HG23	2.31	0.46
1:A:96:TYR:OH	1:A:101:MET:SD	2.74	0.46
1:A:185:TRP:CE2	1:A:190:VAL:HG21	2.51	0.46
1:A:121:GLU:HA	1:A:124:LYS:HD2	1.97	0.46
1:A:257:ASP:OD1	1:A:259:HIS:ND1	2.48	0.46
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.81	0.46
1:A:205:TYR:O	1:A:211:LEU:HA	2.16	0.45
1:A:174:HIS:O	1:A:176:TYR:N	2.49	0.45
1:A:28:THR:HG22	1:A:259:HIS:HB2	1.96	0.45
1:A:193:MET:CB	1:A:196:PRO:HD3	2.46	0.45
1:A:186:ASN:O	1:A:190:VAL:HG23	2.16	0.45
1:A:214:GLN:OE1	1:A:252:ILE:HB	2.17	0.45
1:A:23:ARG:HG3	1:A:261:TYR:CE1	2.45	0.44
1:A:107:ARG:HB2	1:A:114:PHE:CD2	2.53	0.44
1:A:222:ILE:HD12	1:A:259:HIS:C	2.37	0.44
1:A:23:ARG:HB3	1:A:24:THR:H	1.64	0.44
1:A:106:HIS:HB2	3:A:356:HOH:O	2.17	0.44
1:A:89:LYS:HA	1:A:92:LYS:HB2	2.00	0.43
1:A:274:ARG:CZ	1:A:307:TYR:HB3	2.48	0.43
1:A:152:ALA:HB1	1:A:160:THR:HG23	2.00	0.43
1:A:171:ILE:O	1:A:175:PRO:HD3	2.18	0.43
1:A:225:GLY:O	1:A:228:PHE:HB2	2.18	0.43
1:A:13:VAL:HG21	1:A:222:ILE:CD1	2.49	0.43
1:A:121:GLU:HA	1:A:124:LYS:CD	2.48	0.42
1:A:291:ILE:HD13	1:A:292:PHE:N	2.33	0.42
1:A:146:TYR:CD1	1:A:146:TYR:N	2.85	0.42
1:A:35:GLN:NE2	1:A:214:GLN:HE22	2.18	0.42
1:A:89:LYS:NZ	1:A:139:TYR:O	2.52	0.42
1:A:12:LYS:HB3	1:A:12:LYS:HE3	1.88	0.42
1:A:118:TYR:O	1:A:122:MET:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD11	1:A:299:ILE:HG21	2.01	0.42
1:A:62:LEU:HA	1:A:62:LEU:HD13	1.74	0.42
1:A:65:LEU:HB3	1:A:292:PHE:CD1	2.44	0.41
1:A:223:PHE:CD2	1:A:224:LEU:HD23	2.56	0.41
1:A:169:GLU:O	1:A:173:THR:HG23	2.21	0.41
1:A:199:HIS:HB3	1:A:215:LEU:HD21	2.02	0.41
1:A:18:HIS:O	1:A:29:TYR:HA	2.22	0.40
1:A:153:TRP:CH2	1:A:186:ASN:HB2	2.55	0.40
1:A:224:LEU:HA	1:A:224:LEU:HD22	1.91	0.40
1:A:186:ASN:OD1	1:A:188:GLU:HB3	2.21	0.40
1:A:91:VAL:HG21	1:A:101:MET:CB	2.42	0.40
1:A:86:ALA:HA	1:A:89:LYS:NZ	2.36	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	313/315 (99%)	259 (83%)	36 (12%)	18 (6%)	2 3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	112	PRO
1	A	133	ASP
1	A	157	LYS
1	A	158	GLY
1	A	175	PRO
1	A	208	ASP
1	A	23	ARG
1	A	84	GLU

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Mol	Chain	Res	Type
1	A	95	GLU
1	A	83	ASP
1	A	104	PHE
1	A	152	ALA
1	A	197	PRO
1	A	17	GLY
1	A	25	HIS
1	A	45	PRO
1	A	225	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	276/277 (100%)	221 (80%)	55 (20%)	1 3

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	7	LEU
1	A	9	LEU
1	A	15	ASP
1	A	16	GLU
1	A	22	ASP
1	A	23	ARG
1	A	24	THR
1	A	36	MET
1	A	42	LYS
1	A	46	LEU
1	A	61	LEU
1	A	62	LEU
1	A	69	THR
1	A	71	ILE
1	A	89	LYS
1	A	90	TRP

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Mol	Chain	Res	Type
1	A	92	LYS
1	A	94	ASP
1	A	100	ASP
1	A	101	MET
1	A	103	ASP
1	A	104	PHE
1	A	107	ARG
1	A	113	GLU
1	A	118	TYR
1	A	120	GLU
1	A	122	MET
1	A	127	ASP
1	A	133	ASP
1	A	145	VAL
1	A	157	LYS
1	A	162	ASP
1	A	164	LEU
1	A	169	GLU
1	A	170	GLN
1	A	172	LYS
1	A	180	LEU
1	A	192	THR
1	A	195	LEU
1	A	197	PRO
1	A	210	LYS
1	A	215	LEU
1	A	218	ARG
1	A	222	ILE
1	A	224	LEU
1	A	236	LEU
1	A	257	ASP
1	A	268	ILE
1	A	270	GLU
1	A	283	GLN
1	A	290	ASP
1	A	291	ILE
1	A	306	PRO
1	A	311	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	149	GLN
1	A	170	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	UFP	A	529	-	18,22,22	2.65	9 (50%)	21,33,33	3.65	7 (33%)

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	UFP	A	529	-	1/1/4/4	0/6/22/22	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	529	UFP	P-O2P	-3.56	1.41	1.54
2	A	529	UFP	P-O5'	-3.45	1.48	1.60
2	A	529	UFP	F5-C5	-3.42	1.29	1.35
2	A	529	UFP	P-O1P	-3.30	1.40	1.51
2	A	529	UFP	P-O3P	-2.86	1.44	1.54
2	A	529	UFP	O4'-C4'	2.13	1.49	1.45
2	A	529	UFP	C3'-C4'	2.67	1.60	1.53
2	A	529	UFP	C4-N3	3.55	1.39	1.33
2	A	529	UFP	C4-C5	6.55	1.46	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	529	UFP	C5-C4-N3	-6.17	115.46	122.34
2	A	529	UFP	O3P-P-O5'	-2.32	99.89	106.56
2	A	529	UFP	C3'-C2'-C1'	2.56	108.56	102.40
2	A	529	UFP	O3P-P-O1P	2.70	119.26	110.58
2	A	529	UFP	C2'-C1'-N1	4.74	125.69	114.16
2	A	529	UFP	O4'-C1'-N1	8.69	122.76	107.72
2	A	529	UFP	C4-N3-C2	10.47	124.30	115.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	529	UFP	C1'

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
2	A	529	UFP	2	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.