Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 AM GMT

PDB ID	:	2TDD
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	:	1993-04-05
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 ⓘ symbol.

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

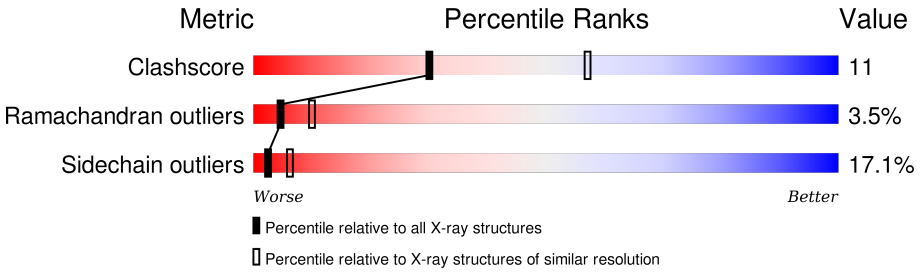
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 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	A	315	53% 35% 10% •

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
3	UFP	A	529	X	-	-	-

2 Entry composition

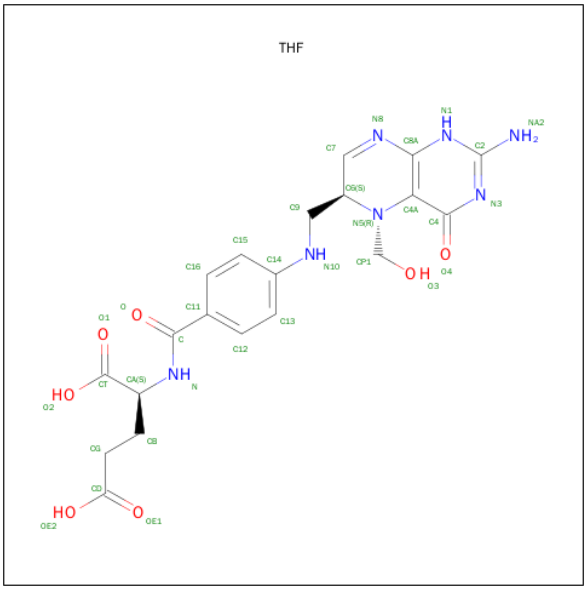
There are 4 unique types of molecules in this entry. The entry contains 2644 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

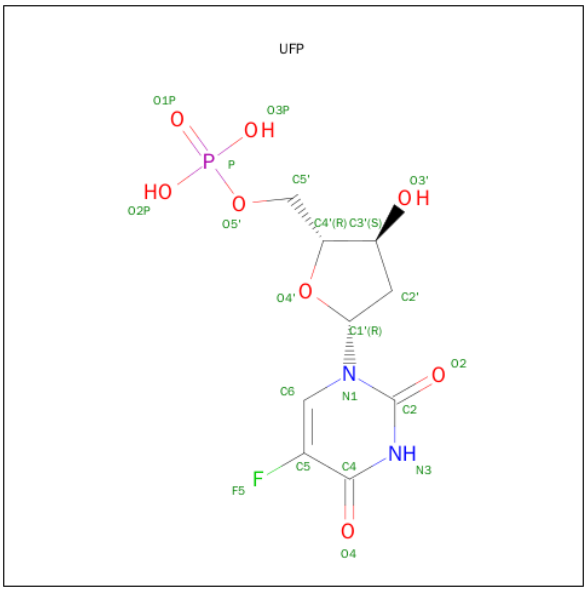
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2580	1669	437	466	8			

- Molecule 2 is 5-HYDROXYMETHYLENE-6-HYDROFOLIC ACID (three-letter code: THF) (formula: $C_{20}H_{23}N_7O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		

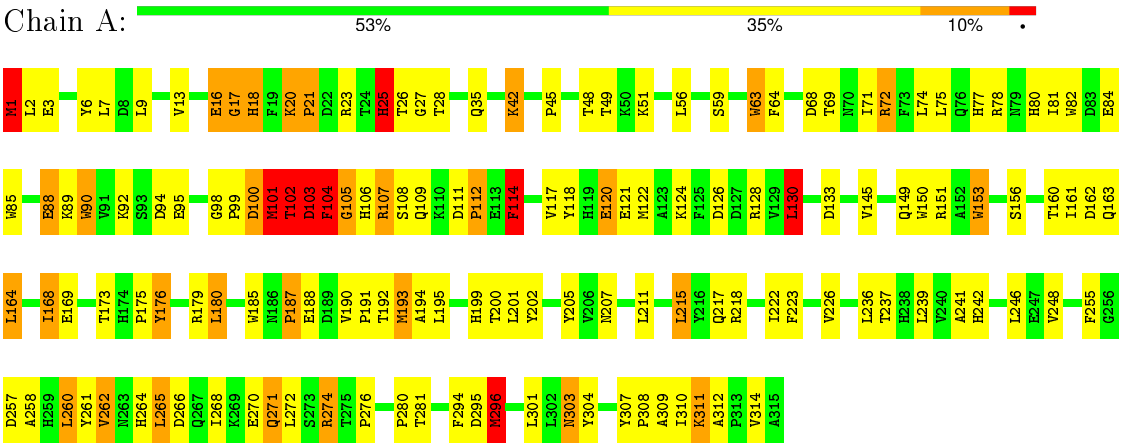
3 Residue-property plots (i)

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	78.40Å 78.40Å 242.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2644	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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, THF

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	3/2664 (0.1%)	2.08	107/3619 (3.0%)

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	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLU	CB-CG	5.76	1.63	1.52
1	A	63	TRP	CA-CB	-5.28	1.42	1.53
1	A	16	GLU	CG-CD	5.25	1.59	1.51

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	ASP	CA-C-N	-11.37	92.19	117.20
1	A	151	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	A	211	LEU	CA-CB-CG	10.36	139.12	115.30
1	A	114	PHE	CB-CG-CD1	10.04	127.83	120.80
1	A	151	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	A	193	MET	CA-C-N	-9.61	96.06	117.20
1	A	18	HIS	CA-CB-CG	9.45	129.66	113.60
1	A	128	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	A	218	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	90	TRP	CE2-CD2-CG	-8.79	100.27	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	TRP	CE2-CD2-CG	-8.75	100.30	107.30
1	A	63	TRP	CD1-CG-CD2	8.58	113.17	106.30
1	A	78	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	169	GLU	CA-CB-CG	8.56	132.22	113.40
1	A	274	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	85	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	A	128	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	85	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	185	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	A	114	PHE	CB-CG-CD2	-7.93	115.25	120.80
1	A	85	TRP	CG-CD2-CE3	7.89	141.00	133.90
1	A	90	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	A	202	TYR	CA-CB-CG	7.85	128.31	113.40
1	A	85	TRP	CB-CG-CD1	-7.79	116.87	127.00
1	A	106	HIS	CA-CB-CG	7.79	126.85	113.60
1	A	25	HIS	CA-C-N	-7.76	100.13	117.20
1	A	64	PHE	CB-CG-CD2	-7.59	115.48	120.80
1	A	150	TRP	CD1-CG-CD2	7.56	112.34	106.30
1	A	179	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	63	TRP	CG-CD2-CE3	7.34	140.51	133.90
1	A	63	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	A	185	TRP	NE1-CE2-CZ2	-6.86	122.85	130.40
1	A	42	LYS	CB-CG-CD	6.83	129.36	111.60
1	A	169	GLU	CB-CA-C	-6.79	96.82	110.40
1	A	304	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	A	82	TRP	CD1-CG-CD2	6.72	111.67	106.30
1	A	104	PHE	N-CA-C	6.69	129.05	111.00
1	A	248	VAL	CA-C-N	-6.55	103.10	116.20
1	A	294	PHE	CB-CG-CD1	6.50	125.35	120.80
1	A	193	MET	O-C-N	6.45	133.02	122.70
1	A	218	ARG	CG-CD-NE	-6.44	98.27	111.80
1	A	258	ALA	O-C-N	-6.41	112.44	122.70
1	A	100	ASP	N-CA-C	6.35	128.14	111.00
1	A	262	VAL	CG1-CB-CG2	6.33	121.02	110.90
1	A	18	HIS	CA-C-N	6.32	131.11	117.20
1	A	271	GLN	CA-CB-CG	6.28	127.22	113.40
1	A	72	ARG	CA-C-N	6.28	131.01	117.20
1	A	117	VAL	CA-CB-CG2	-6.27	101.49	110.90
1	A	82	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	A	169	GLU	N-CA-CB	6.21	121.77	110.60
1	A	150	TRP	CE2-CD2-CG	-6.16	102.38	107.30
1	A	130	LEU	CB-CG-CD2	-6.13	100.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	A	1	MET	CG-SD-CE	6.05	109.88	100.20
1	A	185	TRP	CG-CD2-CE3	6.03	139.32	133.90
1	A	111	ASP	N-CA-C	5.90	126.94	111.00
1	A	45	PRO	N-CA-C	5.86	127.33	112.10
1	A	25	HIS	N-CA-C	5.86	126.81	111.00
1	A	242	HIS	CA-CB-CG	5.84	123.53	113.60
1	A	90	TRP	CB-CG-CD1	-5.83	119.42	127.00
1	A	77	HIS	CA-CB-CG	-5.79	103.76	113.60
1	A	153	TRP	CE2-CD2-CG	-5.77	102.69	107.30
1	A	107	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	185	TRP	NE1-CE2-CD2	5.69	112.99	107.30
1	A	215	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	296	MET	N-CA-CB	-5.65	100.43	110.60
1	A	6	TYR	CB-CG-CD1	5.64	124.38	121.00
1	A	150	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	153	TRP	CD1-CG-CD2	5.62	110.79	106.30
1	A	176	TYR	CB-CG-CD1	5.60	124.36	121.00
1	A	237	THR	CA-C-N	5.57	129.44	117.20
1	A	18	HIS	O-C-N	-5.55	113.82	122.70
1	A	304	TYR	CB-CG-CD1	5.55	124.33	121.00
1	A	85	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	90	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	A	218	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	246	LEU	N-CA-CB	-5.47	99.46	110.40
1	A	107	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	241	ALA	CB-CA-C	-5.42	101.98	110.10
1	A	176	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	A	114	PHE	CA-CB-CG	5.36	126.76	113.90
1	A	103	ASP	C-N-CA	5.35	135.07	121.70
1	A	112	PRO	CA-C-N	-5.34	105.46	117.20
1	A	25	HIS	O-C-N	5.33	131.23	122.70
1	A	48	THR	O-C-N	-5.31	114.20	122.70
1	A	16	GLU	CA-CB-CG	5.27	124.99	113.40
1	A	2	LEU	CD1-CG-CD2	-5.25	94.76	110.50
1	A	122	MET	CA-CB-CG	5.22	122.17	113.30
1	A	160	THR	CA-C-N	-5.20	105.75	117.20
1	A	17	GLY	CA-C-O	5.20	129.96	120.60
1	A	102	THR	CA-C-N	-5.18	105.81	117.20
1	A	193	MET	CA-C-O	5.15	130.92	120.10
1	A	162	ASP	CA-C-N	5.15	128.52	117.20
1	A	226	VAL	CA-CB-CG2	-5.13	103.20	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	TRP	NE1-CE2-CD2	5.13	112.43	107.30
1	A	168	ILE	CA-CB-CG1	-5.11	101.29	111.00
1	A	236	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	257	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	255	PHE	CB-CA-C	-5.06	100.28	110.40
1	A	23	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	103	ASP	O-C-N	5.05	130.78	122.70
1	A	105	GLY	CA-C-N	-5.05	106.10	117.20
1	A	193	MET	N-CA-C	5.04	124.61	111.00
1	A	192	THR	CA-CB-CG2	-5.03	105.35	112.40
1	A	156	SER	CA-C-N	5.02	128.24	117.20
1	A	180	LEU	N-CA-CB	-5.02	100.36	110.40
1	A	179	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Mainchain
1	A	20	LYS	Peptide
1	A	205	TYR	Sidechain
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	2580	0	2479	57	0
2	A	34	0	21	4	0
3	A	21	0	9	0	0
4	A	9	0	0	0	0
All	All	2644	0	2509	57	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 11.

All (57) 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:280:PRO:HB2	1:A:301:LEU:HD11	1.57	0.86
1:A:271:GLN:HA	1:A:274:ARG:HD2	1.61	0.82
1:A:262:VAL:HA	1:A:265:LEU:HD23	1.63	0.79
1:A:21:PRO:HA	1:A:25:HIS:CE1	2.21	0.75
1:A:26:THR:HG1	1:A:261:TYR:HD1	1.36	0.71
1:A:223:PHE:HE2	1:A:312:ALA:HB3	1.56	0.70
1:A:13:VAL:HG11	1:A:260:LEU:HB2	1.73	0.69
1:A:175:PRO:HB2	1:A:176:TYR:HD1	1.59	0.68
1:A:84:GLU:HB3	2:A:568:THF:HN21	1.59	0.66
1:A:51:LYS:HB3	1:A:309:ALA:HB2	1.81	0.63
1:A:104:PHE:HD1	1:A:105:GLY:H	1.46	0.62
1:A:104:PHE:HD1	1:A:105:GLY:N	1.97	0.62
1:A:84:GLU:O	1:A:88:GLU:HB2	2.01	0.61
1:A:153:TRP:HB3	1:A:161:ILE:HB	1.82	0.60
1:A:13:VAL:O	1:A:17:GLY:HA3	2.00	0.60
1:A:112:PRO:HB2	1:A:114:PHE:H	1.67	0.59
1:A:21:PRO:HA	1:A:25:HIS:NE2	2.17	0.59
1:A:268:ILE:O	1:A:272:LEU:HD23	2.03	0.59
1:A:262:VAL:O	1:A:265:LEU:HB2	2.03	0.58
1:A:101:MET:HE1	1:A:118:TYR:HA	1.85	0.58
1:A:26:THR:OG1	1:A:261:TYR:HD1	1.87	0.56
1:A:126:ASP:O	1:A:130:LEU:HG	2.05	0.56
1:A:145:VAL:O	1:A:149:GLN:HG2	2.06	0.56
1:A:69:THR:HG22	1:A:145:VAL:HG12	1.89	0.55
1:A:311:LYS:H	1:A:311:LYS:HD3	1.72	0.55
1:A:260:LEU:HD22	1:A:265:LEU:HD22	1.88	0.55
1:A:271:GLN:HB3	1:A:310:ILE:CD1	2.37	0.55
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.42	0.53
1:A:72:ARG:HH22	1:A:133:ASP:HA	1.72	0.53
1:A:274:ARG:HB3	1:A:307:TYR:HE2	1.74	0.52
1:A:104:PHE:CD1	1:A:105:GLY:N	2.78	0.51
1:A:200:THR:HG22	1:A:201:LEU:HB2	1.91	0.51
1:A:112:PRO:HB2	1:A:114:PHE:HB3	1.94	0.50
1:A:274:ARG:HB3	1:A:307:TYR:CE2	2.46	0.50
1:A:271:GLN:O	1:A:274:ARG:HB2	2.11	0.49
1:A:84:GLU:CD	2:A:568:THF:HN22	2.16	0.49
1:A:25:HIS:CE1	1:A:27:GLY:HA2	2.50	0.47
1:A:1:MET:HG2	1:A:276:PRO:HB2	1.97	0.47
1:A:187:PRO:O	1:A:190:VAL:HG22	2.14	0.47
1:A:120:GLU:O	1:A:124:LYS:HG3	2.15	0.47
1:A:84:GLU:HB3	2:A:568:THF:NA2	2.30	0.44
1:A:274:ARG:NH2	1:A:308:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TRP:CZ3	1:A:95:GLU:HB3	2.53	0.44
1:A:188:GLU:O	1:A:191:PRO:HD2	2.18	0.43
1:A:56:LEU:HB3	1:A:81:ILE:HD11	2.00	0.43
1:A:13:VAL:HG21	1:A:222:ILE:HG13	2.01	0.43
1:A:175:PRO:HB2	1:A:176:TYR:CD1	2.46	0.43
1:A:88:GLU:HG3	1:A:104:PHE:CZ	2.54	0.42
1:A:265:LEU:O	1:A:268:ILE:HG22	2.20	0.42
1:A:271:GLN:HB3	1:A:310:ILE:HD12	2.01	0.42
1:A:223:PHE:CE2	1:A:312:ALA:HB3	2.46	0.41
1:A:27:GLY:O	1:A:28:THR:HG23	2.20	0.41
1:A:261:TYR:HB2	1:A:264:HIS:ND1	2.36	0.41
1:A:164:LEU:HD22	1:A:168:ILE:HD12	2.03	0.41
1:A:199:HIS:CD2	1:A:217:GLN:HG3	2.56	0.40
1:A:84:GLU:OE1	2:A:568:THF:NA2	2.54	0.40
1:A:75:LEU:HD22	1:A:80:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	266 (85%)	36 (12%)	11 (4%)	4 10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	92	LYS
1	A	99	PRO
1	A	102	THR
1	A	314	VAL
1	A	296	MET

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Mol	Chain	Res	Type
1	A	101	MET
1	A	180	LEU
1	A	193	MET
1	A	194	ALA
1	A	303	ASN

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	275/277 (99%)	228 (83%)	47 (17%)	2 6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	7	LEU
1	A	9	LEU
1	A	16	GLU
1	A	18	HIS
1	A	20	LYS
1	A	21	PRO
1	A	25	HIS
1	A	35	GLN
1	A	42	LYS
1	A	49	THR
1	A	59	SER
1	A	71	ILE
1	A	74	LEU
1	A	88	GLU
1	A	89	LYS
1	A	94	ASP
1	A	100	ASP
1	A	101	MET
1	A	102	THR

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Mol	Chain	Res	Type
1	A	103	ASP
1	A	104	PHE
1	A	107	ARG
1	A	108	SER
1	A	109	GLN
1	A	114	PHE
1	A	120	GLU
1	A	121	GLU
1	A	130	LEU
1	A	163	GLN
1	A	164	LEU
1	A	173	THR
1	A	187	PRO
1	A	195	LEU
1	A	207	ASN
1	A	215	LEU
1	A	239	LEU
1	A	260	LEU
1	A	265	LEU
1	A	266	ASP
1	A	270	GLU
1	A	281	THR
1	A	295	ASP
1	A	296	MET
1	A	303	ASN
1	A	311	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	207	ASN
1	A	217	GLN
1	A	229	ASN
1	A	263	ASN

5.3.3 RNA

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)

2 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	$\#\|Z\| > 2$
3	UFP	A	529	-	18,22,22	3.29	8 (44%)	21,33,33	3.75	8 (38%)
2	THF	A	568	-	25,36,36	3.13	6 (24%)	23,50,50	3.01	10 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UFP	A	529	-	1/1/4/4	0/6/22/22	0/2/2/2
2	THF	A	568	-	-	0/14/37/37	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	568	THF	C2-N3	-8.35	1.20	1.35
2	A	568	THF	CB-CA	-4.06	1.47	1.53
3	A	529	UFP	O4'-C1'	-3.96	1.33	1.42
3	A	529	UFP	C2'-C1'	-3.05	1.43	1.52
3	A	529	UFP	F5-C5	-2.32	1.31	1.35
2	A	568	THF	C14-N10	2.22	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	529	UFP	P-O5'	2.35	1.68	1.60
3	A	529	UFP	O4'-C4'	2.71	1.51	1.45
3	A	529	UFP	C6-C5	3.27	1.43	1.38
3	A	529	UFP	C4-N3	4.10	1.40	1.33
2	A	568	THF	O4-C4	6.25	1.39	1.24
2	A	568	THF	C2-NA2	6.48	1.47	1.34
2	A	568	THF	C7-N8	6.57	1.35	1.27
3	A	529	UFP	C4-C5	10.57	1.51	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	529	UFP	C5-C4-N3	-7.70	113.77	122.34
2	A	568	THF	NA2-C2-N3	-4.73	109.36	117.20
2	A	568	THF	C4A-C4-N3	-4.17	117.05	123.46
2	A	568	THF	C12-C13-C14	-3.90	115.90	120.28
3	A	529	UFP	O2P-P-O5'	-3.85	95.48	106.56
3	A	529	UFP	C4'-O4'-C1'	-3.58	100.41	109.47
2	A	568	THF	C13-C14-N10	-2.95	115.41	121.06
2	A	568	THF	C15-C16-C11	-2.22	118.18	120.76
2	A	568	THF	O-C-N	-2.10	118.64	122.44
2	A	568	THF	C15-C14-C13	2.15	122.06	119.06
3	A	529	UFP	O3P-P-O2P	2.63	117.39	107.38
3	A	529	UFP	O4'-C1'-N1	2.96	112.84	107.72
2	A	568	THF	C11-C-N	3.18	122.60	116.93
3	A	529	UFP	C2'-C1'-N1	5.11	126.58	114.16
2	A	568	THF	N3-C2-N1	6.32	135.90	125.53
3	A	529	UFP	O4'-C1'-C2'	7.15	120.53	106.27
2	A	568	THF	C4-C4A-C8A	7.61	120.55	114.42
3	A	529	UFP	C4-N3-C2	10.26	124.11	115.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	529	UFP	C1'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	568	THF	4	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.