



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:39 am GMT

PDB ID : 1LCB  
Title : LACTOBACILLUS CASEI THYMIDYLATE SYNTHASE TERNARY COM-  
PLEX WITH DTMP AND H2FOLATE  
Authors : Birdsall, D.L.; Finer-Moore, J.; Stroud, R.M.  
Deposited on : 1995-06-22  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

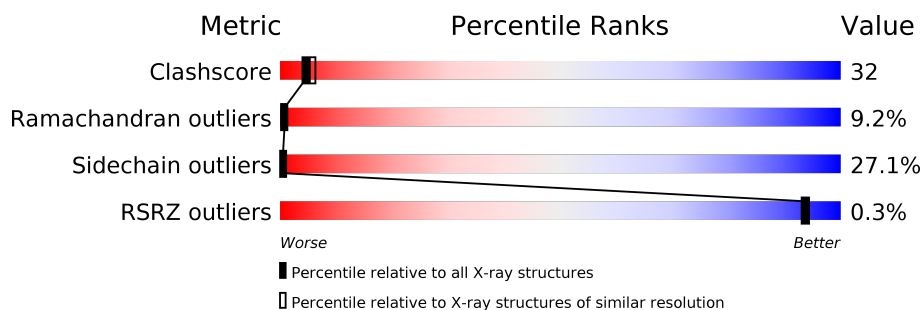
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	316	

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	TMP	A	317	X	-	-	-
3	DHF	A	318	-	-	X	X

## 2 Entry composition [i](#)

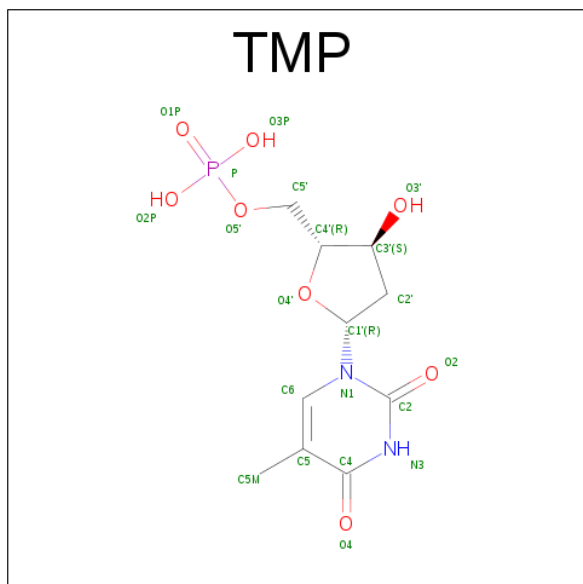
There are 4 unique types of molecules in this entry. The entry contains 3315 atoms, of which 633 are hydrogens and 0 are deuteriums.

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.

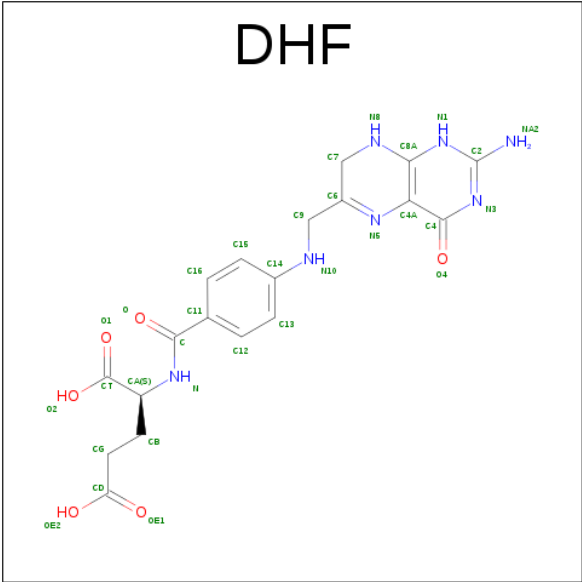
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	0	0
			3139	1677	549	438	467	8			

- Molecule 2 is THYMIDINE-5'-PHOSPHATE (three-letter code: TMP) (formula:  $C_{10}H_{15}N_2O_8P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			23	10	2	2	8	1		

- Molecule 3 is DIHYDROFOLIC ACID (three-letter code: DHF) (formula:  $C_{19}H_{21}N_7O_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			36	19	4	7	6		

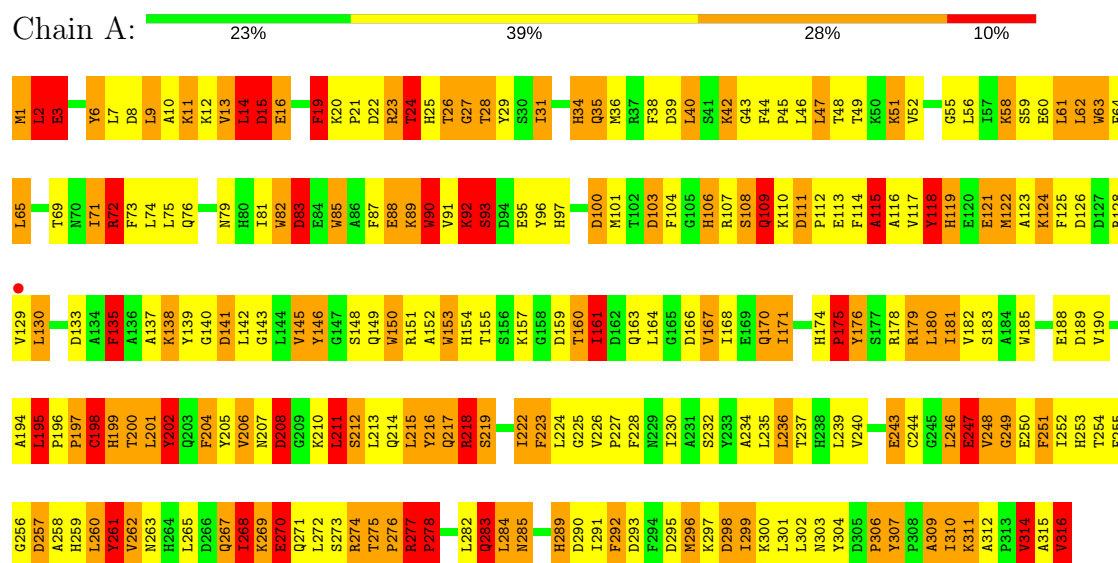
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	39	Total	H	O	0	0
			117	78	39		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

#### • Molecule 1: THYMIDYLATE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.60Å 78.60Å 229.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 58.54 – 2.47	Depositor EDS
% Data completeness (in resolution range)	52.6 (15.00-2.50) 52.0 (58.54-2.47)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.204 , (Not available) 0.224 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	4.2	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 620.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	3315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	1.35	4/2674 (0.1%)	2.41	183/3634 (5.0%)

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	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	VAL	CA-CB	5.61	1.66	1.54
1	A	161	ILE	CA-CB	5.34	1.67	1.54
1	A	268	ILE	CA-CB	5.26	1.67	1.54
1	A	26	THR	CA-CB	5.04	1.66	1.53

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	TYR	CB-CG-CD2	-14.44	112.33	121.00
1	A	178	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	A	176	TYR	CB-CG-CD1	11.41	127.84	121.00
1	A	72	ARG	NE-CZ-NH2	-11.17	114.71	120.30
1	A	154	HIS	CA-C-N	-10.34	94.46	117.20
1	A	307	TYR	CB-CG-CD2	-9.88	115.07	121.00
1	A	205	TYR	CB-CG-CD1	-9.81	115.12	121.00
1	A	109	GLN	CA-CB-CG	9.63	134.60	113.40
1	A	179	ARG	NE-CZ-NH1	9.19	124.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	LYS	CA-CB-CG	-9.08	93.43	113.40
1	A	185	TRP	CD1-CG-CD2	8.97	113.47	106.30
1	A	72	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	222	ILE	CA-C-N	-8.76	97.92	117.20
1	A	176	TYR	CA-CB-CG	8.65	129.83	113.40
1	A	199	HIS	CA-C-N	-8.49	98.52	117.20
1	A	82	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	A	199	HIS	O-C-N	8.11	135.68	122.70
1	A	90	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	A	185	TRP	CE2-CD2-CG	-8.07	100.85	107.30
1	A	82	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	A	90	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	A	302	LEU	CA-CB-CG	8.03	133.76	115.30
1	A	154	HIS	O-C-N	7.96	135.44	122.70
1	A	202	TYR	CA-CB-CG	7.86	128.33	113.40
1	A	167	VAL	CG1-CB-CG2	-7.80	98.42	110.90
1	A	254	THR	CA-C-N	-7.78	100.09	117.20
1	A	257	ASP	CB-CG-OD1	7.64	125.17	118.30
1	A	275	THR	CA-CB-CG2	-7.59	101.77	112.40
1	A	201	LEU	CA-CB-CG	7.53	132.61	115.30
1	A	204	PHE	CA-C-N	-7.49	100.72	117.20
1	A	314	VAL	CA-CB-CG1	-7.38	99.83	110.90
1	A	95	GLU	CA-CB-CG	7.37	129.61	113.40
1	A	310	ILE	CB-CA-C	7.32	126.24	111.60
1	A	290	ASP	N-CA-CB	-7.25	97.55	110.60
1	A	133	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	175	PRO	N-CA-C	7.15	130.68	112.10
1	A	65	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	292	PHE	N-CA-CB	-7.06	97.89	110.60
1	A	298	ASP	N-CA-C	-7.04	91.99	111.00
1	A	47	LEU	CA-CB-CG	7.04	131.48	115.30
1	A	104	PHE	CA-C-N	7.01	130.23	116.20
1	A	247	GLU	CA-CB-CG	6.98	128.75	113.40
1	A	236	LEU	CA-CB-CG	6.94	131.26	115.30
1	A	106	HIS	CA-CB-CG	6.88	125.30	113.60
1	A	58	LYS	CA-CB-CG	6.80	128.36	113.40
1	A	88	GLU	CA-CB-CG	6.80	128.36	113.40
1	A	274	ARG	N-CA-C	-6.80	92.64	111.00
1	A	150	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	A	260	LEU	CA-C-N	-6.75	102.34	117.20
1	A	261	TYR	CA-CB-CG	6.74	126.21	113.40
1	A	270	GLU	CA-CB-CG	6.74	128.23	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	VAL	CG1-CB-CG2	-6.73	100.14	110.90
1	A	24	THR	CA-CB-CG2	6.71	121.79	112.40
1	A	14	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	310	ILE	N-CA-CB	-6.70	95.39	110.80
1	A	178	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	272	LEU	CA-CB-CG	6.68	130.65	115.30
1	A	189	ASP	CA-CB-CG	6.61	127.93	113.40
1	A	63	TRP	CE2-CD2-CG	-6.57	102.04	107.30
1	A	278	PRO	N-CA-C	6.52	129.06	112.10
1	A	295	ASP	O-C-N	6.49	133.08	122.70
1	A	183	SER	O-C-N	6.48	133.07	122.70
1	A	2	LEU	CA-C-N	6.41	131.31	117.20
1	A	277	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	63	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	A	14	LEU	N-CA-C	6.37	128.19	111.00
1	A	23	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	260	LEU	O-C-N	6.33	132.83	122.70
1	A	195	LEU	N-CA-C	-6.33	93.91	111.00
1	A	85	TRP	CD1-CG-CD2	6.32	111.35	106.30
1	A	108	SER	CA-CB-OG	6.32	128.25	111.20
1	A	83	ASP	CA-C-N	-6.31	103.31	117.20
1	A	34	HIS	CA-CB-CG	-6.26	102.95	113.60
1	A	150	TRP	CG-CD2-CE3	6.24	139.52	133.90
1	A	90	TRP	CB-CG-CD1	-6.22	118.92	127.00
1	A	153	TRP	CE2-CD2-CG	-6.22	102.32	107.30
1	A	35	GLN	O-C-N	6.21	132.64	122.70
1	A	285	ASN	N-CA-CB	-6.19	99.46	110.60
1	A	295	ASP	CA-C-N	-6.18	103.60	117.20
1	A	9	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	274	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	274	ARG	CG-CD-NE	-6.13	98.93	111.80
1	A	150	TRP	CD1-CG-CD2	6.12	111.19	106.30
1	A	283	GLN	CA-CB-CG	6.10	126.83	113.40
1	A	6	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	211	LEU	CA-CB-CG	-6.06	101.35	115.30
1	A	11	LYS	CA-CB-CG	6.06	126.73	113.40
1	A	206	VAL	N-CA-C	-6.04	94.68	111.00
1	A	160	THR	N-CA-CB	-5.97	98.96	110.30
1	A	201	LEU	CB-CG-CD1	-5.96	100.86	111.00
1	A	2	LEU	CB-CG-CD2	-5.94	100.90	111.00
1	A	24	THR	CA-CB-OG1	-5.94	96.53	109.00
1	A	314	VAL	N-CA-C	5.92	126.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	GLY	O-C-N	5.90	132.15	122.70
1	A	103	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	29	TYR	N-CA-C	-5.88	95.12	111.00
1	A	218	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	309	ALA	N-CA-CB	-5.86	101.90	110.10
1	A	222	ILE	CA-CB-CG2	-5.84	99.22	110.90
1	A	216	TYR	CA-C-N	-5.83	104.36	117.20
1	A	178	ARG	CB-CG-CD	5.82	126.74	111.60
1	A	249	GLY	N-CA-C	-5.82	98.56	113.10
1	A	19	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	A	107	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	42	LYS	CG-CD-CE	5.75	129.16	111.90
1	A	13	VAL	CA-C-N	5.75	129.85	117.20
1	A	25	HIS	CA-CB-CG	5.74	123.35	113.60
1	A	85	TRP	CE2-CD2-CG	-5.73	102.72	107.30
1	A	293	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	185	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	A	130	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	2	LEU	N-CA-C	5.63	126.20	111.00
1	A	292	PHE	CB-CA-C	5.63	121.65	110.40
1	A	188	GLU	O-C-N	5.62	131.69	122.70
1	A	204	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	A	217	GLN	N-CA-C	-5.57	95.96	111.00
1	A	72	ARG	CA-CB-CG	5.57	125.65	113.40
1	A	259	HIS	CA-CB-CG	5.54	123.01	113.60
1	A	100	ASP	N-CA-C	5.50	125.85	111.00
1	A	137	ALA	N-CA-CB	5.49	117.79	110.10
1	A	214	GLN	CG-CD-NE2	5.48	129.85	116.70
1	A	39	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	304	TYR	CB-CG-CD1	5.45	124.27	121.00
1	A	316	VAL	CA-CB-CG2	5.45	119.07	110.90
1	A	188	GLU	N-CA-CB	-5.44	100.80	110.60
1	A	204	PHE	O-C-N	5.43	131.39	122.70
1	A	76	GLN	CB-CA-C	-5.38	99.64	110.40
1	A	252	ILE	CG1-CB-CG2	-5.38	99.56	111.40
1	A	83	ASP	O-C-N	5.38	131.31	122.70
1	A	309	ALA	CB-CA-C	5.36	118.14	110.10
1	A	135	PHE	CB-CG-CD1	-5.36	117.05	120.80
1	A	205	TYR	CD1-CG-CD2	5.36	123.79	117.90
1	A	228	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	35	GLN	CA-C-N	-5.35	105.43	117.20
1	A	284	LEU	CA-CB-CG	5.34	127.58	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	VAL	CA-CB-CG2	-5.34	102.89	110.90
1	A	15	ASP	CA-C-N	-5.34	105.46	117.20
1	A	153	TRP	CD1-CG-CD2	5.33	110.56	106.30
1	A	185	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	A	234	ALA	N-CA-CB	5.33	117.56	110.10
1	A	256	GLY	CA-C-N	-5.32	105.49	117.20
1	A	180	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	226	VAL	CA-CB-CG2	-5.32	102.93	110.90
1	A	179	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	205	TYR	CG-CD2-CE2	-5.30	117.06	121.30
1	A	217	GLN	N-CA-CB	-5.30	101.07	110.60
1	A	92	LYS	CA-CB-CG	5.29	125.03	113.40
1	A	311	LYS	N-CA-CB	-5.28	101.09	110.60
1	A	56	LEU	N-CA-CB	-5.25	99.89	110.40
1	A	108	SER	N-CA-C	-5.25	96.83	111.00
1	A	181	ILE	CA-C-N	-5.22	105.70	117.20
1	A	51	LYS	CA-C-N	-5.21	105.73	117.20
1	A	171	ILE	CA-C-N	-5.21	105.75	117.20
1	A	302	LEU	CA-C-N	-5.20	105.76	117.20
1	A	90	TRP	CA-CB-CG	5.19	123.57	113.70
1	A	205	TYR	N-CA-CB	-5.19	101.25	110.60
1	A	118	TYR	CA-C-N	5.19	128.62	117.20
1	A	194	ALA	CA-C-N	-5.19	105.78	117.20
1	A	304	TYR	CA-CB-CG	5.17	123.23	113.40
1	A	93	SER	CB-CA-C	-5.17	100.28	110.10
1	A	307	TYR	CD1-CG-CD2	5.16	123.57	117.90
1	A	115	ALA	N-CA-CB	-5.13	102.91	110.10
1	A	181	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	A	298	ASP	CA-CB-CG	5.12	124.66	113.40
1	A	91	VAL	CA-CB-CG1	-5.12	103.22	110.90
1	A	274	ARG	CB-CG-CD	5.12	124.90	111.60
1	A	47	LEU	N-CA-C	5.11	124.80	111.00
1	A	290	ASP	CB-CA-C	5.11	120.61	110.40
1	A	298	ASP	N-CA-CB	5.10	119.78	110.60
1	A	219	SER	O-C-N	5.10	130.85	122.70
1	A	284	LEU	N-CA-C	-5.10	97.24	111.00
1	A	28	THR	CB-CA-C	-5.09	97.87	111.60
1	A	188	GLU	CA-C-N	-5.09	106.01	117.20
1	A	216	TYR	CA-C-O	5.08	130.77	120.10
1	A	301	LEU	O-C-N	5.08	130.83	122.70
1	A	208	ASP	N-CA-CB	5.08	119.74	110.60
1	A	306	PRO	CA-N-CD	-5.07	104.41	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	VAL	O-C-N	-5.06	114.61	122.70
1	A	198	CYS	CA-CB-SG	5.05	123.09	114.00
1	A	137	ALA	CB-CA-C	-5.03	102.55	110.10
1	A	296	MET	CA-CB-CG	5.03	121.86	113.30
1	A	141	ASP	CA-C-N	-5.03	106.14	117.20
1	A	93	SER	CA-CB-OG	5.01	124.73	111.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Peptide
1	A	118	TYR	Sidechain
1	A	146	TYR	Sidechain
1	A	151	ARG	Sidechain
1	A	176	TYR	Sidechain
1	A	195	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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	2590	549	2496	157	0
2	A	21	2	12	4	0
3	A	32	4	19	9	0
4	A	39	78	0	10	0
All	All	2682	633	2527	163	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 32.

All (163) 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:24:THR:HG21	4:A:348:HOH:O	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:276:PRO:HB2	1.94	1.07
1:A:24:THR:CG2	4:A:348:HOH:O	2.05	1.00
1:A:69:THR:HG22	1:A:145:VAL:HG12	1.53	0.90
1:A:19:PHE:HE1	1:A:27:GLY:HA3	1.44	0.81
1:A:19:PHE:HA	1:A:28:THR:O	1.79	0.81
1:A:87:PHE:CE1	1:A:122:MET:HA	2.15	0.81
1:A:152:ALA:HA	1:A:160:THR:HG23	1.63	0.80
1:A:60:GLU:HG2	4:A:353:HOH:O	1.80	0.80
1:A:101:MET:SD	1:A:118:TYR:HB2	2.21	0.80
1:A:109:GLN:HB2	1:A:314:VAL:HG21	1.64	0.78
1:A:21:PRO:HA	1:A:27:GLY:HA2	1.67	0.77
2:A:317:TMP:H4'	3:A:318:DHF:HN1	1.50	0.76
1:A:3:GLU:HG2	1:A:47:LEU:HA	1.70	0.72
1:A:123:ALA:O	1:A:126:ASP:HB2	1.90	0.72
1:A:60:GLU:CG	4:A:353:HOH:O	2.36	0.72
1:A:90:TRP:HZ2	1:A:124:LYS:NZ	1.87	0.71
1:A:114:PHE:HA	1:A:118:TYR:HB3	1.72	0.70
2:A:317:TMP:H4'	3:A:318:DHF:N1	2.06	0.69
1:A:90:TRP:HZ2	1:A:124:LYS:HZ2	1.40	0.68
1:A:126:ASP:O	1:A:129:VAL:HB	1.94	0.68
3:A:318:DHF:H13	4:A:347:HOH:O	1.94	0.67
1:A:71:ILE:HB	1:A:140:GLY:O	1.95	0.67
1:A:13:VAL:HG11	1:A:260:LEU:HB2	1.76	0.67
1:A:224:LEU:HD23	3:A:318:DHF:HG1	1.77	0.67
1:A:210:LYS:HA	1:A:247:GLU:O	1.95	0.66
1:A:51:LYS:HB3	1:A:309:ALA:HB2	1.76	0.66
1:A:199:HIS:HB3	1:A:215:LEU:HD21	1.77	0.66
1:A:9:LEU:HD12	1:A:222:ILE:HG21	1.77	0.66
1:A:138:LYS:HE2	1:A:138:LYS:O	1.96	0.65
1:A:285:ASN:HB3	1:A:298:ASP:HB3	1.78	0.65
1:A:108:SER:HB2	1:A:314:VAL:HG11	1.77	0.65
1:A:222:ILE:HD12	1:A:260:LEU:HD12	1.77	0.65
1:A:40:LEU:HB2	1:A:248:VAL:HG13	1.78	0.65
1:A:81:ILE:HG22	1:A:82:TRP:CD1	2.32	0.64
1:A:297:LYS:HG2	1:A:300:LYS:HE3	1.78	0.64
1:A:210:LYS:HB3	1:A:249:GLY:HA3	1.78	0.63
1:A:60:GLU:HB3	4:A:353:HOH:O	1.99	0.62
1:A:190:VAL:HG22	1:A:196:PRO:HB3	1.79	0.62
1:A:180:LEU:H	1:A:181:ILE:HD12	1.65	0.61
1:A:40:LEU:HB2	1:A:248:VAL:CG1	2.30	0.60
1:A:128:ARG:HG2	1:A:135:PHE:CG	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:HG3	1:A:291:ILE:HG23	1.83	0.60
1:A:47:LEU:HB2	1:A:52:VAL:HG21	1.84	0.59
1:A:223:PHE:CD1	1:A:268:ILE:HG12	2.37	0.59
1:A:12:LYS:O	1:A:16:GLU:HB3	2.02	0.59
1:A:38:PHE:O	1:A:250:GLU:HB2	2.01	0.59
1:A:19:PHE:CE1	1:A:27:GLY:HA3	2.33	0.59
1:A:206:VAL:HG13	1:A:246:LEU:HD21	1.85	0.58
1:A:182:VAL:HB	1:A:202:TYR:CE1	2.38	0.58
1:A:114:PHE:CA	1:A:118:TYR:HB3	2.35	0.57
1:A:204:PHE:HD2	1:A:211:LEU:HD11	1.69	0.57
1:A:175:PRO:O	1:A:206:VAL:HB	2.05	0.57
1:A:61:LEU:HG	1:A:235:LEU:HD23	1.88	0.56
1:A:267:GLN:O	1:A:270:GLU:HB3	2.07	0.55
1:A:72:ARG:HA	1:A:129:VAL:HG12	1.88	0.55
1:A:223:PHE:HZ	1:A:310:ILE:HG22	1.72	0.55
1:A:217:GLN:HG3	1:A:219:SER:O	2.07	0.55
1:A:115:ALA:CB	4:A:351:HOH:O	2.55	0.54
1:A:69:THR:HG21	1:A:143:GLY:O	2.07	0.54
1:A:153:TRP:O	1:A:160:THR:HA	2.08	0.54
1:A:182:VAL:HB	1:A:202:TYR:HE1	1.73	0.54
1:A:27:GLY:O	1:A:28:THR:HG23	2.08	0.53
1:A:61:LEU:HD23	1:A:232:SER:HB3	1.90	0.53
1:A:90:TRP:HA	1:A:93:SER:OG	2.07	0.53
1:A:108:SER:O	1:A:109:GLN:HB2	2.09	0.53
1:A:277:ARG:HB2	1:A:307:TYR:HE1	1.73	0.53
1:A:34:HIS:HB3	1:A:255:PHE:HD2	1.74	0.53
1:A:71:ILE:HD13	1:A:74:LEU:HB2	1.91	0.52
1:A:48:THR:HG21	1:A:278:PRO:O	2.09	0.52
1:A:89:LYS:O	1:A:92:LYS:HD3	2.09	0.52
1:A:93:SER:HB2	1:A:96:TYR:HB3	1.90	0.52
1:A:90:TRP:CE3	1:A:135:PHE:HZ	2.27	0.52
1:A:34:HIS:HB3	1:A:255:PHE:CD2	2.44	0.52
1:A:90:TRP:CE3	1:A:96:TYR:HB2	2.44	0.52
1:A:167:VAL:HG12	1:A:168:ILE:CD1	2.40	0.52
1:A:291:ILE:HG13	1:A:292:PHE:CD1	2.45	0.51
1:A:224:LEU:HD21	1:A:312:ALA:HB3	1.92	0.51
1:A:167:VAL:HG12	1:A:168:ILE:HD12	1.91	0.51
1:A:223:PHE:HE1	1:A:271:GLN:NE2	2.08	0.51
1:A:224:LEU:HB3	3:A:318:DHF:CT	2.41	0.51
1:A:64:PHE:CD1	1:A:146:TYR:HB2	2.46	0.51
1:A:207:ASN:HB3	1:A:210:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD11	1:A:239:LEU:CD2	2.41	0.51
1:A:202:TYR:HB3	1:A:215:LEU:HD23	1.93	0.51
1:A:48:THR:O	1:A:307:TYR:HD1	1.93	0.50
1:A:51:LYS:HE3	1:A:306:PRO:HG2	1.93	0.50
1:A:224:LEU:HD23	3:A:318:DHF:CG	2.41	0.50
1:A:9:LEU:CD1	1:A:222:ILE:HG21	2.41	0.50
1:A:10:ALA:HA	1:A:222:ILE:CD1	2.42	0.50
1:A:282:LEU:HD11	1:A:299:ILE:HG22	1.94	0.49
1:A:148:SER:HA	1:A:152:ALA:HB3	1.94	0.49
1:A:274:ARG:HH21	1:A:307:TYR:HB3	1.77	0.48
1:A:36:MET:HB3	1:A:253:HIS:HB3	1.95	0.48
1:A:168:ILE:HD11	1:A:240:VAL:HG22	1.95	0.48
1:A:166:ASP:O	1:A:170:GLN:HB2	2.14	0.48
1:A:69:THR:O	1:A:141:ASP:HA	2.14	0.48
1:A:2:LEU:HG	1:A:45:PRO:HB3	1.94	0.48
1:A:110:LYS:O	1:A:112:PRO:HD3	2.14	0.48
1:A:122:MET:O	1:A:125:PHE:HB3	2.14	0.48
1:A:60:GLU:O	1:A:63:TRP:HB3	2.14	0.48
1:A:195:LEU:HD21	2:A:317:TMP:H51	1.95	0.48
1:A:9:LEU:HD13	1:A:222:ILE:HD13	1.95	0.48
1:A:62:LEU:HD11	1:A:299:ILE:HD11	1.96	0.48
1:A:210:LYS:HB3	1:A:249:GLY:CA	2.44	0.47
1:A:211:LEU:HD23	1:A:237:THR:HG23	1.95	0.47
1:A:175:PRO:HB3	1:A:206:VAL:HG11	1.97	0.47
1:A:2:LEU:HD21	1:A:43:GLY:O	2.14	0.47
3:A:318:DHF:O2	3:A:318:DHF:H12	2.15	0.47
1:A:90:TRP:O	1:A:90:TRP:CG	2.67	0.47
1:A:83:ASP:HB3	1:A:122:MET:CE	2.45	0.47
1:A:115:ALA:HB3	4:A:351:HOH:O	2.14	0.47
1:A:146:TYR:HD1	1:A:150:TRP:HE1	1.63	0.47
1:A:87:PHE:CG	1:A:122:MET:HG2	2.51	0.46
1:A:204:PHE:CD2	1:A:211:LEU:HD11	2.50	0.46
1:A:8:ASP:O	1:A:11:LYS:HG2	2.15	0.46
1:A:315:ALA:O	1:A:316:VAL:HG23	2.17	0.45
2:A:317:TMP:H2'1	3:A:318:DHF:C2	2.47	0.45
1:A:6:TYR:CE2	1:A:222:ILE:HG22	2.52	0.45
3:A:318:DHF:C13	4:A:347:HOH:O	2.56	0.45
1:A:235:LEU:HG	1:A:239:LEU:HD13	1.98	0.45
1:A:14:LEU:HD21	1:A:269:LYS:HG3	1.97	0.45
1:A:274:ARG:HH12	1:A:310:ILE:HG13	1.81	0.45
1:A:196:PRO:HA	1:A:197:PRO:HD2	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:HD11	1:A:204:PHE:CD2	2.51	0.45
1:A:261:TYR:HE1	4:A:348:HOH:O	1.99	0.44
1:A:87:PHE:HZ	1:A:121:GLU:HB3	1.83	0.44
1:A:2:LEU:HD22	1:A:42:LYS:O	2.18	0.44
1:A:71:ILE:O	1:A:75:LEU:HG	2.17	0.44
1:A:224:LEU:HD21	1:A:312:ALA:CB	2.47	0.44
1:A:7:LEU:CD1	1:A:276:PRO:HG3	2.48	0.44
1:A:212:SER:HA	1:A:250:GLU:O	2.17	0.44
1:A:222:ILE:O	1:A:260:LEU:HG	2.17	0.44
1:A:289:HIS:N	1:A:289:HIS:CD2	2.86	0.44
1:A:74:LEU:HD22	1:A:79:ASN:ND2	2.33	0.43
1:A:230:ILE:HG23	1:A:251:PHE:HE2	1.84	0.43
1:A:49:THR:HB	1:A:271:GLN:HG2	2.00	0.43
1:A:275:THR:HA	1:A:276:PRO:HD3	1.76	0.43
1:A:87:PHE:HB2	1:A:122:MET:HE3	2.01	0.43
1:A:200:THR:OG1	1:A:218:ARG:HG2	2.19	0.43
1:A:274:ARG:NH2	1:A:307:TYR:HB3	2.34	0.43
1:A:63:TRP:HB2	1:A:73:PHE:CE1	2.54	0.43
1:A:47:LEU:HB2	1:A:52:VAL:CG2	2.48	0.43
1:A:7:LEU:HD11	1:A:276:PRO:HG3	2.01	0.43
1:A:116:ALA:O	1:A:119:HIS:N	2.52	0.42
1:A:198:CYS:O	1:A:217:GLN:HA	2.19	0.42
1:A:65:LEU:HD22	1:A:291:ILE:HD12	2.02	0.42
1:A:55:GLY:HA2	1:A:58:LYS:HD3	2.02	0.42
1:A:283:GLN:OE1	1:A:300:LYS:HB2	2.20	0.42
1:A:155:THR:C	1:A:157:LYS:H	2.23	0.42
1:A:125:PHE:CE1	1:A:139:TYR:HB3	2.55	0.41
1:A:153:TRP:HB3	1:A:161:ILE:HG23	2.01	0.41
1:A:215:LEU:HD22	1:A:216:TYR:N	2.35	0.41
1:A:10:ALA:HA	1:A:222:ILE:HD13	2.03	0.41
1:A:31:ILE:HG13	1:A:258:ALA:HB3	2.03	0.41
1:A:117:VAL:O	1:A:121:GLU:N	2.54	0.41
1:A:206:VAL:HG22	1:A:246:LEU:HD21	2.02	0.40
1:A:277:ARG:HB2	1:A:307:TYR:CE1	2.54	0.40
1:A:298:ASP:O	1:A:300:LYS:HG3	2.21	0.40
1:A:64:PHE:HZ	1:A:82:TRP:CZ2	2.39	0.40
1:A:63:TRP:HB2	1:A:73:PHE:HE1	1.85	0.40
1:A:85:TRP:HH2	1:A:195:LEU:HD22	1.85	0.40
1:A:277:ARG:NH2	1:A:307:TYR:HA	2.37	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	314/316 (99%)	227 (72%)	58 (18%)	29 (9%)	<b>1</b> <b>1</b>

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	111	ASP
1	A	175	PRO
1	A	223	PHE
1	A	248	VAL
1	A	257	ASP
1	A	262	VAL
1	A	277	ARG
1	A	278	PRO
1	A	296	MET
1	A	314	VAL
1	A	90	TRP
1	A	115	ALA
1	A	208	ASP
1	A	276	PRO
1	A	303	ASN
1	A	2	LEU
1	A	15	ASP
1	A	89	LYS
1	A	197	PRO
1	A	261	TYR
1	A	3	GLU
1	A	119	HIS
1	A	159	ASP
1	A	270	GLU
1	A	273	SER
1	A	174	HIS
1	A	225	GLY

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Mol	Chain	Res	Type
1	A	27	GLY

### 5.3.2 Protein sidechains ⓘ

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	277/278 (100%)	202 (73%)	75 (27%)	<b>0</b> <b>0</b>

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	14	LEU
1	A	15	ASP
1	A	16	GLU
1	A	19	PHE
1	A	20	LYS
1	A	22	ASP
1	A	23	ARG
1	A	24	THR
1	A	26	THR
1	A	31	ILE
1	A	35	GLN
1	A	40	LEU
1	A	44	PHE
1	A	46	LEU
1	A	59	SER
1	A	61	LEU
1	A	62	LEU
1	A	71	ILE
1	A	72	ARG
1	A	83	ASP
1	A	88	GLU
1	A	92	LYS
1	A	93	SER

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Mol	Chain	Res	Type
1	A	97	HIS
1	A	100	ASP
1	A	103	ASP
1	A	106	HIS
1	A	113	GLU
1	A	118	TYR
1	A	121	GLU
1	A	122	MET
1	A	124	LYS
1	A	130	LEU
1	A	135	PHE
1	A	138	LYS
1	A	142	LEU
1	A	149	GLN
1	A	161	ILE
1	A	163	GLN
1	A	164	LEU
1	A	170	GLN
1	A	175	PRO
1	A	179	ARG
1	A	198	CYS
1	A	200	THR
1	A	201	LEU
1	A	202	TYR
1	A	208	ASP
1	A	211	LEU
1	A	212	SER
1	A	213	LEU
1	A	215	LEU
1	A	218	ARG
1	A	227	PRO
1	A	236	LEU
1	A	243	GLU
1	A	244	CYS
1	A	246	LEU
1	A	247	GLU
1	A	251	PHE
1	A	261	TYR
1	A	262	VAL
1	A	263	ASN
1	A	265	LEU
1	A	267	GLN

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Mol	Chain	Res	Type
1	A	268	ILE
1	A	283	GLN
1	A	284	LEU
1	A	289	HIS
1	A	299	ILE
1	A	311	LYS
1	A	314	VAL
1	A	316	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	242	HIS
1	A	271	GLN
1	A	289	HIS

### 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](#)

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
2	TMP	A	317	-	16,22,22	1.54	2 (12%)	23,33,33	2.92	6 (26%)
3	DHF	A	318	-	24,34,34	3.02	10 (41%)	28,47,47	3.15	13 (46%)

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	TMP	A	317	-	1/1/4/4	0/6/22/22	0/2/2/2
3	DHF	A	318	-	-	0/14/31/31	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	TMP	O4'-C1'	2.12	1.47	1.42
3	A	318	DHF	C12-C11	2.16	1.42	1.39
3	A	318	DHF	CB-CG	2.29	1.63	1.53
3	A	318	DHF	C15-C14	2.99	1.44	1.39
3	A	318	DHF	C9-N10	3.08	1.50	1.45
3	A	318	DHF	C4-N3	3.20	1.38	1.33
3	A	318	DHF	C16-C11	3.21	1.44	1.39
3	A	318	DHF	CA-N	4.03	1.52	1.46
3	A	318	DHF	C6-N5	4.03	1.33	1.28
2	A	317	TMP	C4-N3	4.61	1.43	1.36
3	A	318	DHF	O4-C4	6.01	1.39	1.24
3	A	318	DHF	CB-CA	9.15	1.65	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	318	DHF	C9-N10-C14	-7.46	107.23	122.63
2	A	317	TMP	C5M-C5-C4	-4.75	116.05	121.08
3	A	318	DHF	C4A-C4-N3	-3.76	118.14	123.48
3	A	318	DHF	N3-C2-N1	-3.56	119.67	125.45
3	A	318	DHF	O-C-N	-2.38	118.12	122.46
3	A	318	DHF	C13-C14-N10	-2.33	116.34	121.03
3	A	318	DHF	CB-CA-N	-2.00	107.18	110.22
3	A	318	DHF	C11-C-N	2.22	121.06	116.97
2	A	317	TMP	O3P-P-O2P	2.22	116.57	107.61
3	A	318	DHF	CB-CA-CT	2.35	115.69	112.28
3	A	318	DHF	CA-N-C	2.70	125.85	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	TMP	C5M-C5-C6	2.97	124.59	118.67
3	A	318	DHF	C4-N3-C2	3.99	121.80	116.06
2	A	317	TMP	P-O5'-C5'	4.08	129.53	118.30
3	A	318	DHF	C2-N1-C8A	4.08	123.70	114.51
3	A	318	DHF	C4-C4A-C8A	4.70	117.66	114.52
2	A	317	TMP	C2'-C1'-N1	6.66	129.97	114.23
2	A	317	TMP	O4'-C1'-N1	9.02	122.99	107.78
3	A	318	DHF	CG-CB-CA	9.65	132.46	113.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	317	TMP	C1'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	TMP	4	0
3	A	318	DHF	9	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	316/316 (100%)	-0.56	1 (0%) 93 94	2, 4, 12, 51	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	VAL	2.4

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DHF	A	318	32/32	0.92	0.19	4.83	2,2,15,15	0
2	TMP	A	317	21/21	0.96	0.11	0.14	2,2,12,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.