



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:50 PM UTC

PDB ID : 1LCE / pdb_00001lce
Title : LACTOBACILLUS CASEI THYMIDYLATE SYNTHASE TERNARY COM-
PLEX WITH DUMP AND CH2THF
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

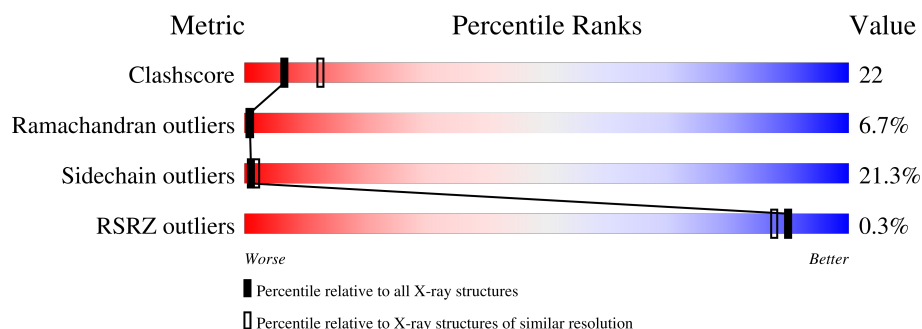
1 Overall quality at a glance

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	UMP	A	317	X	-	-	-
3	TMF	A	318	X	-	X	-

2 Entry composition [i](#)

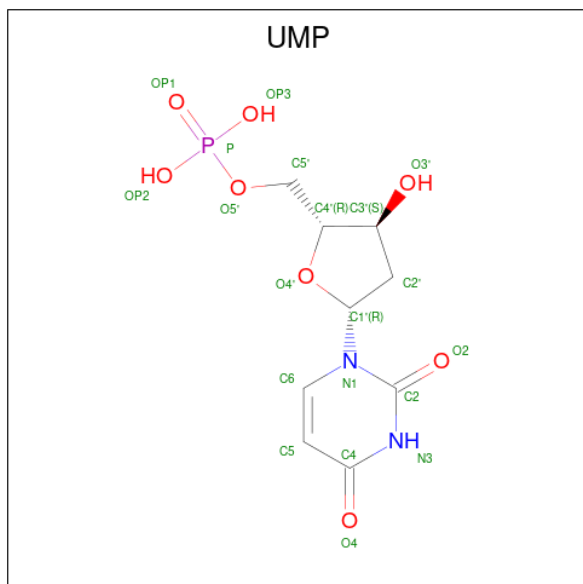
There are 4 unique types of molecules in this entry. The entry contains 3283 atoms, of which 610 are hydrogens and 0 are deuteriums.

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.

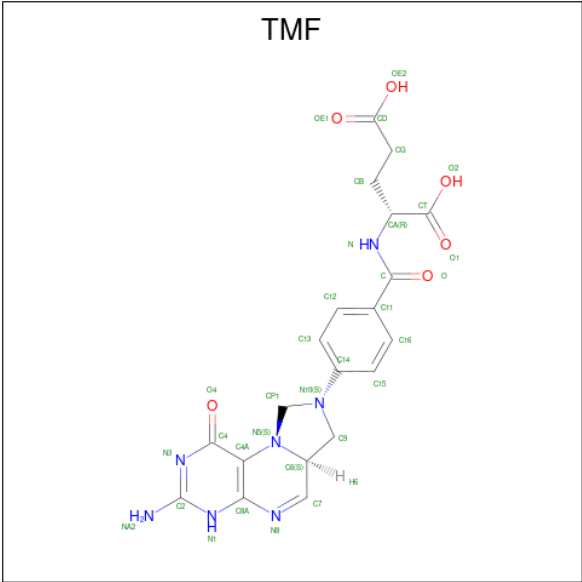
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	316	3139	1677	549	438	467	8	0	0	0

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



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

- Molecule 3 is 5,10-METHYLENE-6-HYDROFOLIC ACID (CCD ID: TMF) (formula: $C_{20}H_{21}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	7	6		

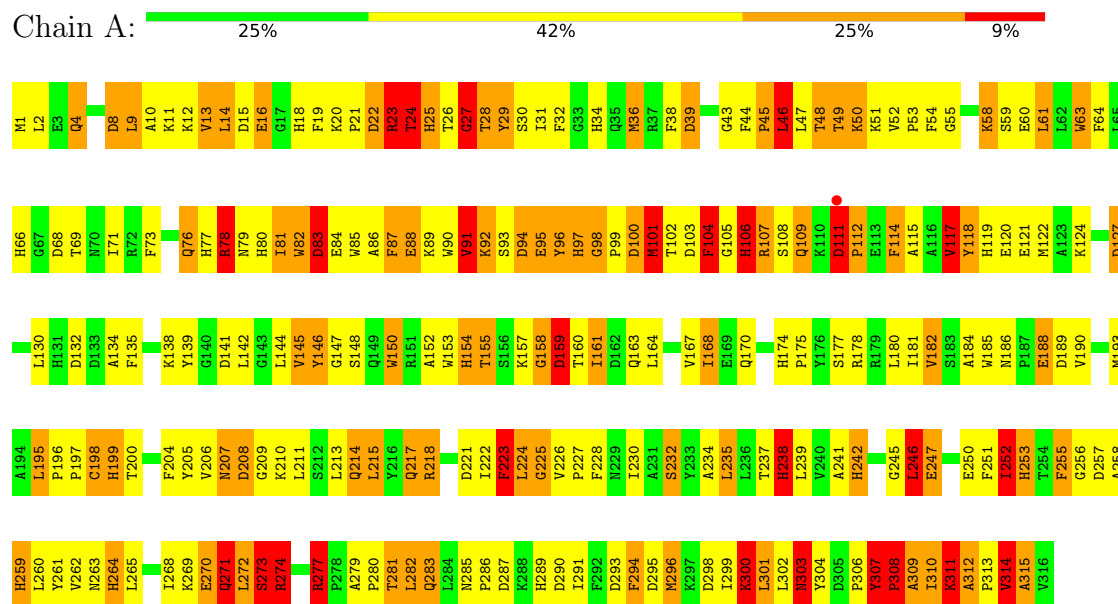
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	30	Total	H	O	0	0
			90	60	30		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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, α , β , γ	78.90Å 78.90Å 229.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	58.5 (15.00-2.50) 58.5 (15.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.42Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.204 , (Not available) 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3283	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.62	37/2674 (1.4%)	2.66	251/3634 (6.9%)

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	3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	VAL	CA-CB	8.85	1.59	1.53
1	A	199	HIS	CD2-NE2	-8.13	1.28	1.37
1	A	238	HIS	CD2-NE2	-7.67	1.29	1.37
1	A	259	HIS	CD2-NE2	-7.41	1.29	1.37
1	A	124	LYS	CA-CB	7.02	1.64	1.53
1	A	80	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	154	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	161	ILE	CA-CB	6.83	1.62	1.54
1	A	182	VAL	CA-CB	-6.80	1.45	1.54
1	A	259	HIS	CG-ND1	-6.70	1.30	1.38
1	A	253	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	77	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	66	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	107	ARG	NE-CZ	6.33	1.40	1.33
1	A	253	HIS	CG-ND1	-6.31	1.31	1.38
1	A	281	THR	CA-C	6.22	1.60	1.52
1	A	8	ASP	CA-CB	6.11	1.64	1.53
1	A	69	THR	CA-CB	5.99	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	264	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	15	ASP	CA-CB	5.90	1.63	1.53
1	A	199	HIS	CG-ND1	-5.89	1.31	1.38
1	A	81	ILE	CA-CB	5.81	1.62	1.54
1	A	289	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	242	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	4	GLN	CA-CB	5.46	1.62	1.53
1	A	109	GLN	CA-CB	5.44	1.62	1.53
1	A	34	HIS	CD2-NE2	-5.43	1.31	1.37
1	A	18	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	167	VAL	CA-CB	-5.39	1.47	1.54
1	A	247	GLU	CA-CB	5.38	1.60	1.53
1	A	119	HIS	CB-CG	5.37	1.57	1.50
1	A	25	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	97	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	238	HIS	CG-ND1	-5.14	1.32	1.38
1	A	107	ARG	CA-C	5.07	1.59	1.52
1	A	91	VAL	CA-CB	5.06	1.60	1.54

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	CA-CB-CG	14.22	126.82	112.60
1	A	8	ASP	CA-CB-CG	13.34	125.94	112.60
1	A	77	HIS	CA-CB-CG	-12.95	100.86	113.80
1	A	237	THR	N-CA-C	-11.58	98.35	110.97
1	A	141	ASP	CA-CB-CG	11.47	124.07	112.60
1	A	114	PHE	N-CA-C	10.92	126.93	113.50
1	A	106	HIS	N-CA-C	10.83	126.48	112.41
1	A	242	HIS	CA-CB-CG	10.54	124.34	113.80
1	A	308	PRO	N-CA-CB	-10.10	92.64	103.25
1	A	48	THR	N-CA-C	-9.97	101.24	113.50
1	A	4	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	A	159	ASP	N-CA-C	9.43	122.47	108.14
1	A	147	GLY	O-C-N	-9.34	112.57	122.19
1	A	39	ASP	CA-CB-CG	9.07	121.67	112.60
1	A	223	PHE	CA-CB-CG	-9.05	104.75	113.80
1	A	217	GLN	N-CA-C	-8.98	96.05	110.32
1	A	97	HIS	CA-CB-CG	-8.90	104.90	113.80
1	A	14	LEU	N-CA-C	-8.74	96.85	109.96
1	A	303	ASN	CA-C-O	8.66	132.89	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	HIS	N-CA-C	8.47	128.84	110.80
1	A	285	ASN	CA-CB-CG	-8.43	104.17	112.60
1	A	111	ASP	CA-C-N	8.42	130.36	119.84
1	A	111	ASP	C-N-CA	8.42	130.36	119.84
1	A	122	MET	CG-SD-CE	-8.29	82.67	100.90
1	A	295	ASP	N-CA-C	-8.26	98.25	110.48
1	A	66	HIS	CB-CG-CD2	-8.24	120.48	131.20
1	A	298	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	188	GLU	O-C-N	8.22	130.64	122.09
1	A	68	ASP	CA-CB-CG	8.03	120.63	112.60
1	A	122	MET	CA-CB-CG	-8.03	98.05	114.10
1	A	82	TRP	N-CA-C	7.97	123.12	113.23
1	A	101	MET	CA-CB-CG	-7.92	98.27	114.10
1	A	12	LYS	N-CA-C	-7.90	104.16	113.88
1	A	296	MET	CG-SD-CE	-7.86	83.62	100.90
1	A	18	HIS	CA-CB-CG	7.85	121.65	113.80
1	A	274	ARG	N-CA-C	7.83	121.80	109.81
1	A	104	PHE	CA-CB-CG	7.83	121.63	113.80
1	A	23	ARG	CA-CB-CG	7.83	129.75	114.10
1	A	207	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	A	153	TRP	N-CA-C	-7.76	98.32	109.96
1	A	53	PRO	N-CA-C	7.72	122.87	110.21
1	A	88	GLU	CA-CB-CG	7.72	129.54	114.10
1	A	287	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	124	LYS	CA-CB-CG	7.67	129.43	114.10
1	A	290	ASP	CA-C-O	-7.62	111.99	120.60
1	A	88	GLU	CB-CG-CD	7.62	125.55	112.60
1	A	279	ALA	N-CA-C	7.58	119.27	109.64
1	A	49	THR	CA-C-O	-7.56	112.88	122.63
1	A	105	GLY	CA-C-N	-7.53	110.66	122.49
1	A	105	GLY	C-N-CA	-7.53	110.66	122.49
1	A	13	VAL	CB-CA-C	-7.51	102.19	112.02
1	A	200	THR	N-CA-C	7.48	119.52	111.36
1	A	71	ILE	CA-CB-CG2	-7.46	97.82	110.50
1	A	84	GLU	N-CA-C	7.43	121.44	112.38
1	A	189	ASP	CA-CB-CG	7.39	119.99	112.60
1	A	22	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	61	LEU	N-CA-C	-7.33	103.23	111.14
1	A	177	SER	CA-C-O	7.33	128.61	120.70
1	A	146	TYR	CA-C-O	-7.32	112.79	120.55
1	A	79	ASN	O-C-N	-7.31	114.67	123.29
1	A	88	GLU	N-CA-CB	7.28	120.98	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	MET	O-C-N	7.28	132.19	123.24
1	A	25	HIS	CB-CG-CD2	-7.27	121.74	131.20
1	A	108	SER	N-CA-C	-7.27	100.24	110.50
1	A	87	PHE	CA-CB-CG	7.23	121.03	113.80
1	A	111	ASP	CA-C-O	-7.22	110.27	120.16
1	A	158	GLY	N-CA-C	7.18	125.56	115.43
1	A	53	PRO	O-C-N	-7.17	115.98	122.93
1	A	106	HIS	CB-CG-CD2	-7.14	121.91	131.20
1	A	224	LEU	CA-C-O	-7.12	112.82	121.36
1	A	263	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	207	ASN	CA-CB-CG	7.09	119.69	112.60
1	A	281	THR	O-C-N	-7.08	114.94	123.29
1	A	93	SER	CA-C-N	7.06	130.32	120.29
1	A	93	SER	C-N-CA	7.06	130.32	120.29
1	A	242	HIS	CB-CG-CD2	-7.06	122.02	131.20
1	A	39	ASP	N-CA-C	-7.05	97.23	108.73
1	A	135	PHE	CA-CB-CG	-7.04	106.76	113.80
1	A	89	LYS	CA-C-O	-6.96	113.73	120.90
1	A	250	GLU	N-CA-CB	-6.96	100.77	111.56
1	A	159	ASP	CA-C-N	6.94	134.80	121.54
1	A	159	ASP	C-N-CA	6.94	134.80	121.54
1	A	78	ARG	CD-NE-CZ	6.87	134.02	124.40
1	A	120	GLU	CB-CG-CD	6.87	124.28	112.60
1	A	97	HIS	CB-CG-CD2	-6.87	122.27	131.20
1	A	83	ASP	N-CA-C	6.87	125.43	110.80
1	A	96	TYR	N-CA-C	6.87	118.77	111.28
1	A	287	ASP	N-CA-C	-6.81	103.78	111.14
1	A	174	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	A	188	GLU	N-CA-CB	6.76	120.02	109.94
1	A	132	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	209	GLY	N-CA-C	-6.74	100.02	112.62
1	A	108	SER	CA-CB-OG	6.74	124.57	111.10
1	A	79	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	271	GLN	CA-C-O	6.71	128.19	120.00
1	A	64	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	198	CYS	O-C-N	-6.55	113.84	122.42
1	A	272	LEU	N-CA-C	-6.53	104.24	111.36
1	A	301	LEU	N-CA-C	6.46	121.20	107.70
1	A	141	ASP	N-CA-C	-6.45	98.01	108.52
1	A	258	ALA	N-CA-C	-6.45	98.71	108.96
1	A	29	TYR	N-CA-C	-6.44	96.74	108.02
1	A	25	HIS	N-CA-C	6.43	124.51	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	CA-C-O	6.43	129.71	120.51
1	A	112	PRO	N-CA-C	-6.43	99.23	112.47
1	A	197	PRO	CB-CA-C	6.42	119.74	111.46
1	A	94	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	251	PHE	N-CA-C	-6.41	97.35	108.69
1	A	289	HIS	CB-CG-CD2	-6.40	122.89	131.20
1	A	272	LEU	CA-C-O	-6.39	113.64	120.42
1	A	77	HIS	CB-CG-CD2	-6.39	122.90	131.20
1	A	295	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	109	GLN	CA-CB-CG	6.36	126.83	114.10
1	A	106	HIS	CA-CB-CG	-6.36	107.44	113.80
1	A	80	HIS	CB-CG-CD2	-6.36	122.94	131.20
1	A	107	ARG	N-CA-CB	-6.33	100.08	110.40
1	A	88	GLU	CB-CA-C	-6.32	99.93	110.68
1	A	188	GLU	N-CA-C	-6.30	103.54	111.11
1	A	198	CYS	CA-C-O	6.30	126.34	119.15
1	A	27	GLY	CA-C-O	6.30	131.53	120.57
1	A	18	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	A	71	ILE	CA-CB-CG1	6.23	120.99	110.40
1	A	291	ILE	CA-CB-CG2	-6.22	99.92	110.50
1	A	246	LEU	N-CA-C	6.19	119.22	110.50
1	A	138	LYS	CG-CD-CE	6.15	125.45	111.30
1	A	186	ASN	CA-CB-CG	6.15	118.75	112.60
1	A	188	GLU	CB-CA-C	-6.15	100.97	110.81
1	A	73	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	277	ARG	CA-CB-CG	6.08	126.26	114.10
1	A	25	HIS	CB-CG-ND1	6.06	131.79	122.70
1	A	270	GLU	N-CA-C	6.06	118.67	111.71
1	A	300	LYS	N-CA-C	6.05	118.90	109.52
1	A	303	ASN	N-CA-C	6.03	123.64	110.80
1	A	160	THR	N-CA-CB	-5.98	100.38	110.49
1	A	184	ALA	O-C-N	-5.98	115.24	122.48
1	A	69	THR	N-CA-C	-5.97	104.65	112.41
1	A	10	ALA	O-C-N	-5.95	114.97	122.17
1	A	58	LYS	CA-CB-CG	5.94	125.98	114.10
1	A	28	THR	CA-C-O	5.93	128.46	121.58
1	A	170	GLN	CB-CG-CD	5.89	122.62	112.60
1	A	155	THR	O-C-N	5.89	129.56	122.85
1	A	207	ASN	CA-C-N	5.88	132.78	121.54
1	A	207	ASN	C-N-CA	5.88	132.78	121.54
1	A	2	LEU	N-CA-C	5.88	118.47	111.71
1	A	16	GLU	CA-CB-CG	-5.84	102.41	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	CA-CB-CG	5.82	119.62	113.80
1	A	178	ARG	N-CA-CB	-5.79	100.78	110.22
1	A	36	MET	CA-CB-CG	5.78	125.65	114.10
1	A	263	ASN	CB-CA-C	-5.78	101.77	110.90
1	A	283	GLN	CA-C-O	-5.77	114.88	121.58
1	A	274	ARG	N-CA-CB	-5.76	102.40	111.05
1	A	92	LYS	CA-CB-CG	5.75	125.61	114.10
1	A	13	VAL	CA-C-N	5.75	129.00	120.95
1	A	13	VAL	C-N-CA	5.75	129.00	120.95
1	A	182	VAL	N-CA-C	-5.70	100.28	108.48
1	A	247	GLU	CA-CB-CG	5.70	125.49	114.10
1	A	15	ASP	CA-C-O	5.68	128.63	120.51
1	A	252	ILE	N-CA-CB	-5.67	103.53	111.25
1	A	190	VAL	CB-CA-C	-5.66	108.35	114.35
1	A	245	GLY	N-CA-C	-5.62	107.79	114.48
1	A	106	HIS	O-C-N	5.58	129.48	122.22
1	A	127	ASP	CA-CB-CG	-5.58	107.02	112.60
1	A	84	GLU	CA-CB-CG	5.57	125.24	114.10
1	A	114	PHE	N-CA-CB	-5.57	102.34	110.53
1	A	106	HIS	CB-CG-ND1	5.54	131.01	122.70
1	A	159	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	279	ALA	CA-C-N	5.53	125.84	119.92
1	A	279	ALA	C-N-CA	5.53	125.84	119.92
1	A	132	ASP	N-CA-C	-5.52	100.80	109.25
1	A	309	ALA	O-C-N	-5.52	114.76	121.83
1	A	145	VAL	N-CA-C	-5.52	101.80	108.53
1	A	168	ILE	N-CA-C	-5.51	104.20	111.09
1	A	312	ALA	N-CA-C	-5.50	102.72	110.31
1	A	197	PRO	O-C-N	-5.50	116.38	123.03
1	A	124	LYS	CG-CD-CE	5.47	123.89	111.30
1	A	214	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	43	GLY	O-C-N	-5.46	118.56	123.96
1	A	46	LEU	O-C-N	5.46	129.20	123.03
1	A	224	LEU	O-C-N	-5.45	116.95	123.06
1	A	186	ASN	CB-CA-C	-5.45	103.89	110.15
1	A	314	VAL	N-CA-C	5.45	120.67	109.34
1	A	77	HIS	N-CA-C	5.42	119.16	112.54
1	A	208	ASP	N-CA-C	-5.42	99.25	110.80
1	A	96	TYR	O-C-N	5.39	127.84	122.12
1	A	145	VAL	N-CA-CB	-5.39	106.12	112.32
1	A	294	PHE	O-C-N	-5.39	116.01	123.12
1	A	13	VAL	N-CA-C	-5.39	105.47	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	N-CA-C	5.37	122.24	110.80
1	A	115	ALA	N-CA-C	5.37	118.99	112.23
1	A	48	THR	O-C-N	-5.36	115.31	122.49
1	A	76	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	63	TRP	CA-C-O	-5.35	115.20	120.82
1	A	120	GLU	CA-CB-CG	5.34	124.78	114.10
1	A	188	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	308	PRO	CB-CA-C	5.33	120.36	111.56
1	A	144	LEU	N-CA-C	5.33	118.11	107.62
1	A	157	LYS	N-CA-CB	-5.33	99.71	111.69
1	A	308	PRO	N-CA-C	5.32	123.43	112.47
1	A	124	LYS	O-C-N	-5.31	116.60	122.07
1	A	30	SER	O-C-N	5.31	129.03	123.03
1	A	264	HIS	CA-CB-CG	5.30	119.10	113.80
1	A	308	PRO	N-CD-CG	-5.30	95.25	103.20
1	A	87	PHE	CA-C-O	-5.29	114.91	120.63
1	A	112	PRO	CA-N-CD	-5.29	104.59	112.00
1	A	277	ARG	CA-C-N	5.29	125.21	119.76
1	A	277	ARG	C-N-CA	5.29	125.21	119.76
1	A	4	GLN	CB-CG-CD	5.28	121.58	112.60
1	A	117	VAL	N-CA-C	-5.27	106.67	111.67
1	A	154	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	A	97	HIS	O-C-N	5.25	129.57	122.59
1	A	45	PRO	CA-C-N	-5.23	113.22	122.74
1	A	45	PRO	C-N-CA	-5.23	113.22	122.74
1	A	199	HIS	CE1-NE2-CD2	5.22	114.22	109.00
1	A	199	HIS	CG-CD2-NE2	-5.22	101.98	107.20
1	A	273	SER	CA-CB-OG	5.21	121.53	111.10
1	A	247	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	226	VAL	N-CA-C	5.18	120.08	108.88
1	A	242	HIS	N-CA-CB	-5.18	101.79	110.39
1	A	77	HIS	CA-C-N	5.18	131.43	121.54
1	A	77	HIS	C-N-CA	5.18	131.43	121.54
1	A	89	LYS	O-C-N	-5.17	116.44	122.03
1	A	265	LEU	N-CA-C	5.17	116.72	111.14
1	A	217	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	150	TRP	N-CA-C	5.16	116.76	111.03
1	A	13	VAL	N-CA-CB	5.16	117.17	110.57
1	A	232	SER	N-CA-C	-5.15	105.56	111.07
1	A	4	GLN	CG-CD-NE2	5.15	124.12	116.40
1	A	311	LYS	O-C-N	-5.14	117.22	123.13
1	A	95	GLU	CA-CB-CG	5.13	124.36	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLU	CA-CB-CG	5.13	124.36	114.10
1	A	255	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	82	TRP	CG-CD1-NE1	-5.12	103.54	110.20
1	A	186	ASN	CB-CG-ND2	-5.12	108.72	116.40
1	A	235	LEU	CA-C-N	5.12	127.40	120.44
1	A	235	LEU	C-N-CA	5.12	127.40	120.44
1	A	77	HIS	O-C-N	5.11	129.27	122.43
1	A	225	GLY	O-C-N	-5.10	116.06	122.70
1	A	4	GLN	CA-C-O	-5.09	113.18	120.16
1	A	24	THR	CA-C-N	5.09	131.26	121.54
1	A	24	THR	C-N-CA	5.09	131.26	121.54
1	A	228	PHE	N-CA-C	5.07	117.59	111.40
1	A	282	LEU	N-CA-C	-5.07	101.13	109.40
1	A	83	ASP	CA-CB-CG	-5.07	107.53	112.60
1	A	238	HIS	N-CA-C	5.05	118.54	112.38
1	A	195	LEU	N-CA-C	-5.04	98.72	108.45
1	A	92	LYS	CA-C-O	5.03	125.52	119.43
1	A	167	VAL	N-CA-CB	-5.03	103.71	110.54
1	A	104	PHE	CA-C-N	5.02	131.25	121.41
1	A	104	PHE	C-N-CA	5.02	131.25	121.41
1	A	134	ALA	N-CA-C	-5.02	100.12	110.80
1	A	185	TRP	CE2-CD2-CG	-5.02	101.18	107.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Peptide
1	A	307	TYR	Peptide
1	A	98	GLY	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	108	0
2	A	20	1	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	33	0	19	17	0
4	A	30	60	0	1	0
All	All	2673	610	2525	112	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 (112) 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:8:ASP:HA	1:A:11:LYS:HE3	1.54	0.90
1:A:81:ILE:HG21	3:A:318:TMF:H92	1.57	0.86
1:A:199:HIS:HB3	1:A:215:LEU:HD21	1.60	0.82
1:A:211:LEU:HB2	1:A:246:LEU:HD13	1.61	0.80
1:A:85:TRP:HA	1:A:88:GLU:HG2	1.65	0.77
1:A:59:SER:HB3	1:A:296:MET:HE1	1.69	0.74
1:A:101:MET:SD	1:A:104:PHE:HB3	2.30	0.72
1:A:195:LEU:HG	3:A:318:TMF:NA2	2.06	0.71
1:A:54:PHE:CD2	1:A:301:LEU:HD22	2.29	0.68
1:A:101:MET:HE3	1:A:117:VAL:HG12	1.76	0.68
1:A:51:LYS:HD2	1:A:306:PRO:HG3	1.76	0.66
1:A:104:PHE:HB2	1:A:118:TYR:CD1	2.31	0.66
1:A:175:PRO:HB3	1:A:206:VAL:HG11	1.77	0.65
1:A:82:TRP:CZ2	3:A:318:TMF:H6	2.32	0.65
1:A:195:LEU:HG	3:A:318:TMF:HN21	1.61	0.65
1:A:20:LYS:HB3	1:A:28:THR:OG1	1.96	0.65
1:A:95:GLU:HB2	1:A:139:TYR:OH	1.96	0.64
1:A:55:GLY:HA2	1:A:58:LYS:HD2	1.78	0.64
1:A:274:ARG:HB2	1:A:307:TYR:CE2	2.33	0.64
2:A:317:UMP:O4	3:A:318:TMF:HCP1	1.97	0.64
1:A:204:PHE:CD2	1:A:211:LEU:HD21	2.34	0.63
1:A:90:TRP:HZ3	1:A:95:GLU:HB3	1.62	0.62
1:A:100:ASP:O	1:A:101:MET:HE2	1.99	0.61
1:A:195:LEU:CG	3:A:318:TMF:HN21	2.14	0.60
1:A:235:LEU:HD11	1:A:299:ILE:HG21	1.84	0.59
1:A:270:GLU:O	1:A:273:SER:HB3	2.02	0.58
1:A:48:THR:HB	1:A:277:ARG:HG3	1.86	0.58
1:A:48:THR:O	1:A:306:PRO:HA	2.04	0.58
1:A:49:THR:O	1:A:50:LYS:HB3	2.05	0.57
1:A:205:TYR:HE2	1:A:207:ASN:OD1	1.87	0.57
1:A:81:ILE:CG2	3:A:318:TMF:H92	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HA	3:A:318:TMF:CT	2.37	0.55
1:A:309:ALA:O	1:A:310:ILE:HG13	2.07	0.54
1:A:19:PHE:HA	1:A:28:THR:O	2.09	0.53
1:A:85:TRP:O	1:A:88:GLU:HB2	2.09	0.53
1:A:46:LEU:HD12	1:A:280:PRO:HG3	1.91	0.53
1:A:164:LEU:O	1:A:168:ILE:HG12	2.10	0.52
1:A:224:LEU:HD21	1:A:312:ALA:HB3	1.91	0.52
3:A:318:TMF:H15	3:A:318:TMF:N8	2.24	0.52
1:A:283:GLN:HE21	1:A:300:LYS:NZ	2.08	0.51
1:A:281:THR:HB	1:A:302:LEU:HB2	1.92	0.51
1:A:224:LEU:HA	3:A:318:TMF:O2	2.11	0.50
1:A:230:ILE:HG12	1:A:253:HIS:ND1	2.25	0.50
1:A:83:ASP:O	1:A:86:ALA:HB3	2.11	0.50
3:A:318:TMF:H15	3:A:318:TMF:C7	2.42	0.50
1:A:38:PHE:CE2	1:A:230:ILE:HD13	2.46	0.49
1:A:198:CYS:O	1:A:217:GLN:HA	2.11	0.49
1:A:20:LYS:O	1:A:27:GLY:HA2	2.13	0.49
1:A:90:TRP:CZ3	1:A:95:GLU:HB3	2.45	0.48
1:A:204:PHE:HB3	1:A:211:LEU:HD11	1.94	0.48
1:A:195:LEU:HD12	1:A:196:PRO:HD2	1.94	0.48
1:A:23:ARG:NH1	2:A:317:UMP:H5'	2.28	0.48
1:A:307:TYR:HB3	1:A:308:PRO:HB2	1.95	0.48
1:A:224:LEU:HD22	3:A:318:TMF:HG2	1.95	0.47
1:A:283:GLN:NE2	1:A:300:LYS:HZ3	2.12	0.47
1:A:205:TYR:CE2	1:A:207:ASN:HA	2.49	0.47
1:A:101:MET:HE2	1:A:101:MET:HA	1.96	0.47
1:A:29:TYR:O	1:A:259:HIS:HA	2.14	0.47
1:A:44:PHE:HB3	1:A:280:PRO:HG2	1.97	0.47
1:A:47:LEU:HD22	1:A:227:PRO:HB3	1.97	0.47
1:A:32:PHE:HA	1:A:256:GLY:O	2.15	0.47
1:A:264:HIS:CD2	1:A:312:ALA:HB1	2.50	0.47
1:A:36:MET:HE3	1:A:255:PHE:HZ	1.80	0.46
1:A:47:LEU:O	1:A:304:TYR:HE1	1.98	0.46
1:A:223:PHE:CE2	1:A:312:ALA:HB2	2.51	0.46
1:A:274:ARG:HB2	1:A:307:TYR:CZ	2.50	0.46
1:A:60:GLU:O	1:A:63:TRP:HB3	2.16	0.46
1:A:9:LEU:HG	1:A:36:MET:HE2	1.98	0.46
1:A:54:PHE:CG	1:A:301:LEU:HD22	2.51	0.45
1:A:198:CYS:SG	1:A:218:ARG:NH2	2.83	0.45
1:A:222:ILE:HD12	1:A:259:HIS:C	2.41	0.45
1:A:204:PHE:CE2	1:A:213:LEU:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLN:HG3	1:A:252:ILE:HG22	1.99	0.45
1:A:98:GLY:HA3	1:A:99:PRO:HD3	1.52	0.45
1:A:221:ASP:HB2	2:A:317:UMP:H2"	1.97	0.45
1:A:104:PHE:HA	1:A:114:PHE:CD2	2.52	0.45
1:A:257:ASP:OD1	1:A:259:HIS:ND1	2.50	0.45
1:A:106:HIS:NE2	1:A:314:VAL:HB	2.32	0.45
1:A:195:LEU:CG	3:A:318:TMF:NA2	2.76	0.45
1:A:24:THR:O	1:A:26:THR:N	2.50	0.45
1:A:85:TRP:CH2	1:A:195:LEU:HB3	2.51	0.45
1:A:91:VAL:HA	1:A:96:TYR:CD1	2.52	0.45
1:A:106:HIS:HE1	1:A:315:ALA:O	2.00	0.45
1:A:224:LEU:HD22	3:A:318:TMF:CG	2.47	0.45
1:A:242:HIS:HE1	1:A:286:PRO:HA	1.82	0.45
1:A:44:PHE:CD1	1:A:45:PRO:HD2	2.52	0.44
1:A:234:ALA:O	1:A:238:HIS:HB2	2.18	0.44
1:A:274:ARG:CB	1:A:307:TYR:CE2	3.00	0.44
1:A:46:LEU:HA	4:A:355:HOH:O	2.17	0.44
1:A:311:LYS:NZ	1:A:313:PRO:HD3	2.33	0.44
1:A:181:ILE:HD13	1:A:181:ILE:HG21	1.84	0.43
1:A:158:GLY:O	1:A:159:ASP:HB3	2.18	0.43
1:A:14:LEU:HD22	1:A:268:ILE:HG23	2.01	0.43
1:A:81:ILE:HG21	1:A:81:ILE:HD13	1.82	0.43
1:A:204:PHE:HD2	1:A:211:LEU:HD21	1.78	0.43
1:A:283:GLN:HE21	1:A:300:LYS:HZ3	1.66	0.43
1:A:271:GLN:HA	1:A:274:ARG:HD3	2.00	0.43
1:A:225:GLY:N	3:A:318:TMF:O1	2.52	0.42
1:A:163:GLN:HB3	1:A:182:VAL:HG13	2.00	0.42
1:A:306:PRO:HG2	1:A:307:TYR:O	2.19	0.42
1:A:90:TRP:CH2	1:A:96:TYR:HA	2.55	0.42
1:A:260:LEU:HD21	1:A:268:ILE:HG21	2.01	0.42
1:A:241:ALA:HA	1:A:246:LEU:HD12	2.02	0.41
1:A:146:TYR:O	1:A:150:TRP:HB2	2.20	0.41
1:A:224:LEU:HD22	3:A:318:TMF:CB	2.51	0.41
1:A:87:PHE:HD2	1:A:104:PHE:CE2	2.39	0.41
1:A:103:ASP:O	1:A:104:PHE:C	2.64	0.41
1:A:261:TYR:HB2	1:A:264:HIS:ND1	2.36	0.41
1:A:36:MET:HE3	1:A:255:PHE:CZ	2.55	0.41
1:A:101:MET:HA	1:A:101:MET:CE	2.42	0.41
1:A:198:CYS:O	1:A:217:GLN:HG3	2.21	0.40
2:A:317:UMP:C4	3:A:318:TMF:HCP1	2.56	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	314/316 (99%)	255 (81%)	38 (12%)	21 (7%)	1 1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	25	HIS
1	A	50	LYS
1	A	78	ARG
1	A	97	HIS
1	A	104	PHE
1	A	111	ASP
1	A	112	PRO
1	A	208	ASP
1	A	223	PHE
1	A	303	ASN
1	A	308	PRO
1	A	314	VAL
1	A	27	GLY
1	A	100	ASP
1	A	273	SER
1	A	315	ALA
1	A	152	ALA
1	A	210	LYS
1	A	180	LEU
1	A	307	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	277/278 (100%)	218 (79%)	59 (21%)	1 2

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLN
1	A	9	LEU
1	A	13	VAL
1	A	21	PRO
1	A	22	ASP
1	A	23	ARG
1	A	24	THR
1	A	31	ILE
1	A	39	ASP
1	A	46	LEU
1	A	52	VAL
1	A	61	LEU
1	A	76	GLN
1	A	78	ARG
1	A	83	ASP
1	A	91	VAL
1	A	92	LYS
1	A	94	ASP
1	A	101	MET
1	A	102	THR
1	A	106	HIS
1	A	107	ARG
1	A	109	GLN
1	A	117	VAL
1	A	118	TYR
1	A	127	ASP
1	A	130	LEU
1	A	142	LEU
1	A	145	VAL
1	A	148	SER
1	A	154	HIS
1	A	155	THR
1	A	159	ASP
1	A	161	ILE

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Mol	Chain	Res	Type
1	A	188	GLU
1	A	215	LEU
1	A	218	ARG
1	A	232	SER
1	A	238	HIS
1	A	239	LEU
1	A	246	LEU
1	A	247	GLU
1	A	252	ILE
1	A	262	VAL
1	A	269	LYS
1	A	271	GLN
1	A	272	LEU
1	A	274	ARG
1	A	277	ARG
1	A	282	LEU
1	A	293	ASP
1	A	294	PHE
1	A	300	LYS
1	A	303	ASN
1	A	308	PRO
1	A	310	ILE
1	A	311	LYS
1	A	314	VAL

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

Mol	Chain	Res	Type
1	A	217	GLN
1	A	229	ASN
1	A	242	HIS
1	A	283	GLN

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 [i](#)

There are no oligosaccharides 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	TMF	A	318	-	33,36,36	4.12	12 (36%)	34,52,52	3.10	14 (41%)
2	UMP	A	317	-	21,21,21	1.61	5 (23%)	30,31,31	3.19	10 (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
3	TMF	A	318	-	1/1/7/9	11/21/42/42	0/3/4/4
2	UMP	A	317	-	1/1/4/4	5/10/22/22	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	318	TMF	C7-N8	14.29	1.46	1.28
3	A	318	TMF	O4-C4	13.42	1.48	1.23
3	A	318	TMF	CP1-N5	8.20	1.51	1.45
3	A	318	TMF	C6-N5	4.40	1.52	1.48
3	A	318	TMF	CA-N	3.72	1.53	1.45
2	A	317	UMP	C2-N1	3.38	1.43	1.38
2	A	317	UMP	O4'-C1'	3.34	1.49	1.42
3	A	318	TMF	C-N	3.34	1.42	1.34
3	A	318	TMF	C8A-N1	-3.24	1.31	1.37
2	A	317	UMP	C6-N1	-2.54	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	318	TMF	C2-N3	2.43	1.39	1.33
3	A	318	TMF	O2-CT	-2.43	1.22	1.30
3	A	318	TMF	C14-N10	-2.31	1.32	1.38
2	A	317	UMP	C4-N3	2.27	1.42	1.38
3	A	318	TMF	CA-CT	2.24	1.58	1.52
3	A	318	TMF	C4A-N5	-2.17	1.31	1.37
2	A	317	UMP	P-OP2	-2.09	1.47	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	318	TMF	C7-N8-C8A	-10.67	105.94	115.47
2	A	317	UMP	O4'-C1'-N1	9.22	124.23	107.86
2	A	317	UMP	C1'-N1-C6	-7.29	107.19	121.53
2	A	317	UMP	C2'-C1'-N1	6.67	130.48	113.81
2	A	317	UMP	C1'-N1-C2	6.38	130.14	117.66
3	A	318	TMF	C15-C16-C11	-5.29	115.15	120.80
3	A	318	TMF	NA2-C2-N1	5.24	127.83	116.76
2	A	317	UMP	O4-C4-N3	4.81	126.25	119.27
3	A	318	TMF	CA-N-C	4.74	132.94	121.56
2	A	317	UMP	O4-C4-C5	-4.22	117.88	125.16
3	A	318	TMF	C13-C14-N10	-4.18	115.59	121.39
3	A	318	TMF	C12-C13-C14	-3.91	115.35	120.30
3	A	318	TMF	C8A-C4A-N5	3.70	124.80	119.80
3	A	318	TMF	CT-CA-N	3.41	118.48	110.57
3	A	318	TMF	O2-CT-O1	-3.36	116.46	124.08
3	A	318	TMF	NA2-C2-N3	-3.25	113.33	119.67
2	A	317	UMP	O2-C2-N1	3.07	126.80	122.80
3	A	318	TMF	C13-C12-C11	2.89	123.89	120.80
3	A	318	TMF	O2-CT-CA	2.60	122.32	113.51
3	A	318	TMF	N1-C2-N3	-2.47	118.79	123.32
2	A	317	UMP	O5'-C5'-C4'	2.47	117.42	108.99
3	A	318	TMF	OE1-CD-CG	-2.46	115.30	123.09
2	A	317	UMP	O4'-C1'-C2'	-2.28	101.99	106.25
2	A	317	UMP	O2-C2-N3	-2.00	117.80	121.49

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	317	UMP	C1'
3	A	318	TMF	CA

All (16) torsion outliers are listed below:

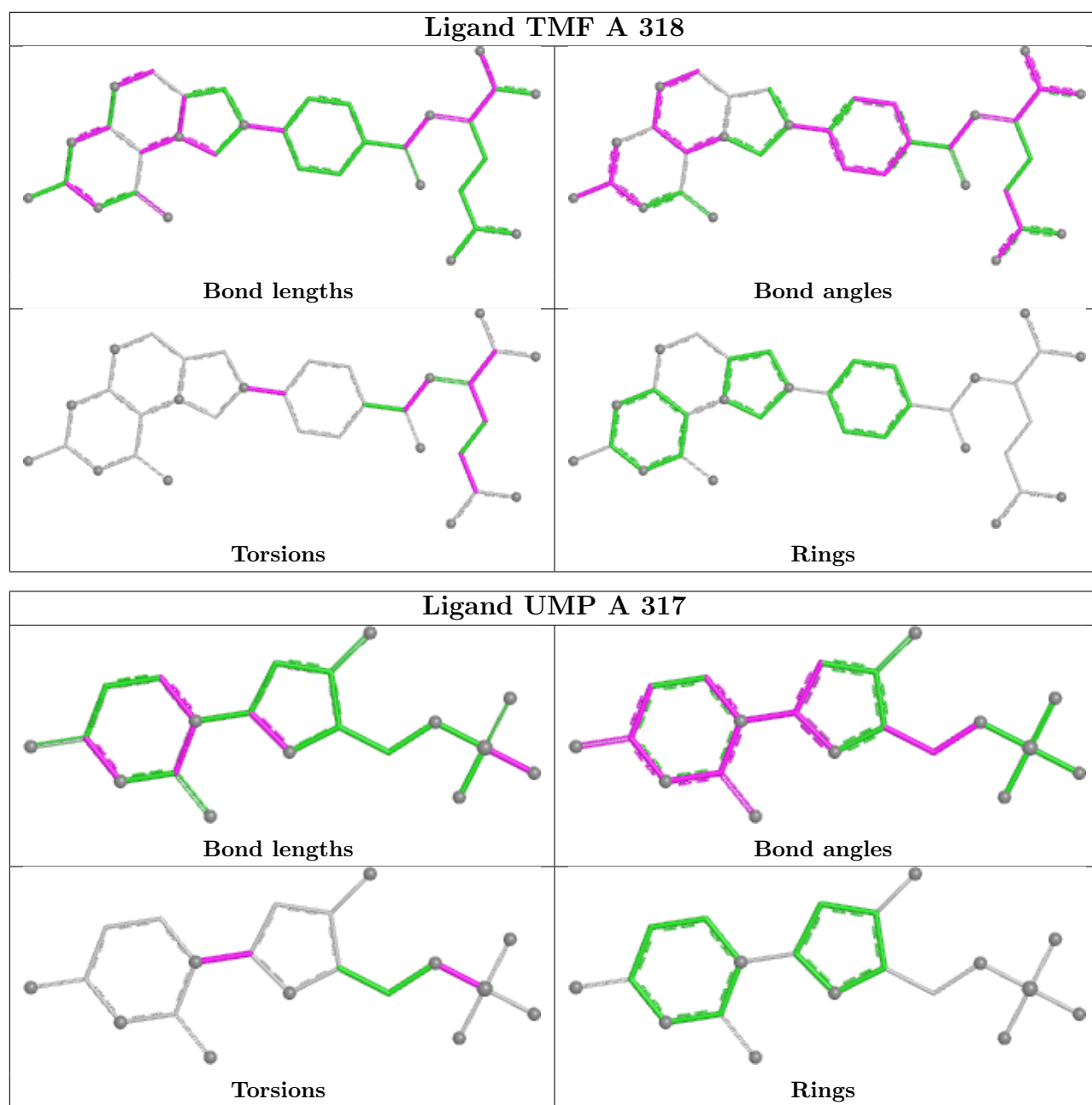
Mol	Chain	Res	Type	Atoms
2	A	317	UMP	C5'-O5'-P-OP1
2	A	317	UMP	C5'-O5'-P-OP2
2	A	317	UMP	C5'-O5'-P-OP3
3	A	318	TMF	C13-C14-N10-C9
3	A	318	TMF	C15-C14-N10-C9
3	A	318	TMF	C11-C-N-CA
3	A	318	TMF	O-C-N-CA
3	A	318	TMF	CT-CA-CB-CG
2	A	317	UMP	C2'-C1'-N1-C2
3	A	318	TMF	CB-CA-CT-O1
3	A	318	TMF	CB-CA-CT-O2
3	A	318	TMF	C13-C14-N10-CP1
3	A	318	TMF	C15-C14-N10-CP1
2	A	317	UMP	C2'-C1'-N1-C6
3	A	318	TMF	OE1-CD-CG-CB
3	A	318	TMF	OE2-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	318	TMF	17	0
2	A	317	UMP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th 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 ²)	Q<0.9
1	A	316/316 (100%)	-0.35	1 (0%) 90 87	4, 12, 22, 34	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	ASP	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

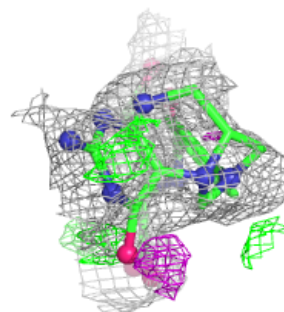
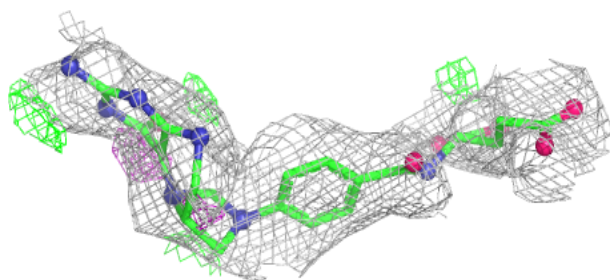
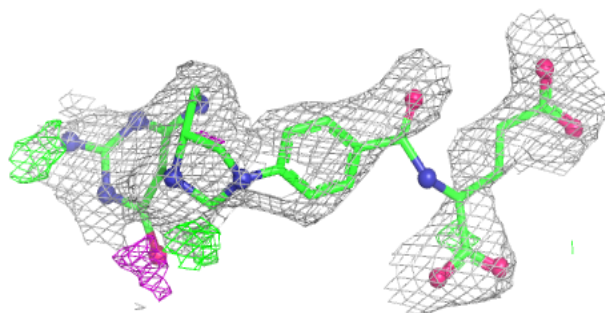
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TMF	A	318	33/33	0.80	0.14	26,26,58,58	0
2	UMP	A	317	20/20	0.93	0.11	11,18,18,18	0

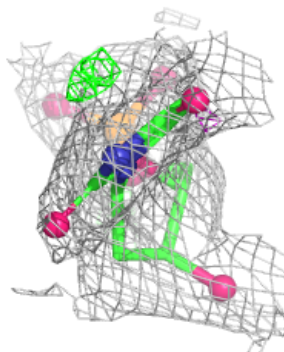
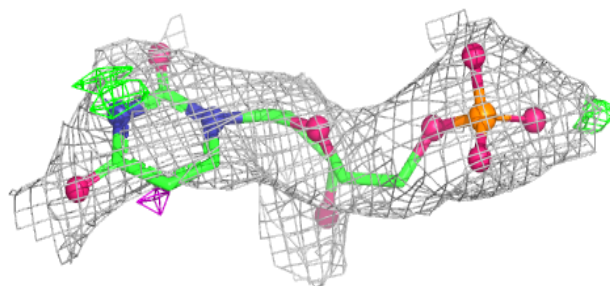
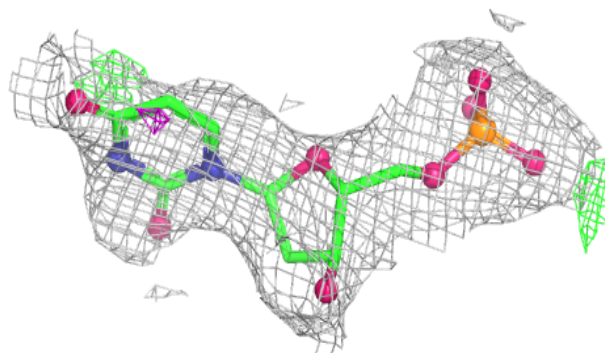
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TMF A 318:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around UMP A 317:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.