



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:36 AM UTC

PDB ID : 1LCB / pdb_00001lcb
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

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

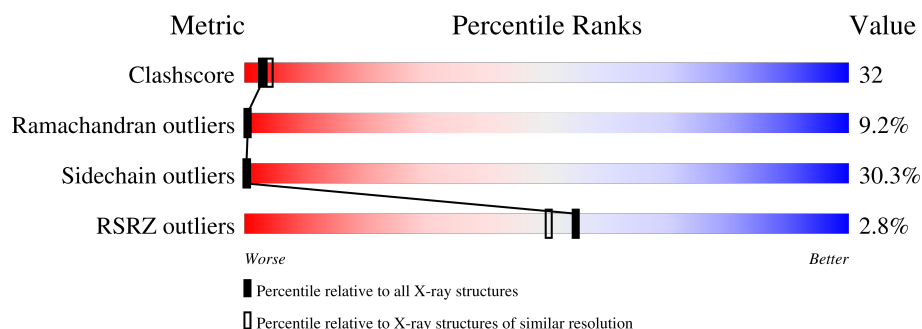
1 Overall quality at a glance

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

2 Entry composition [i](#)

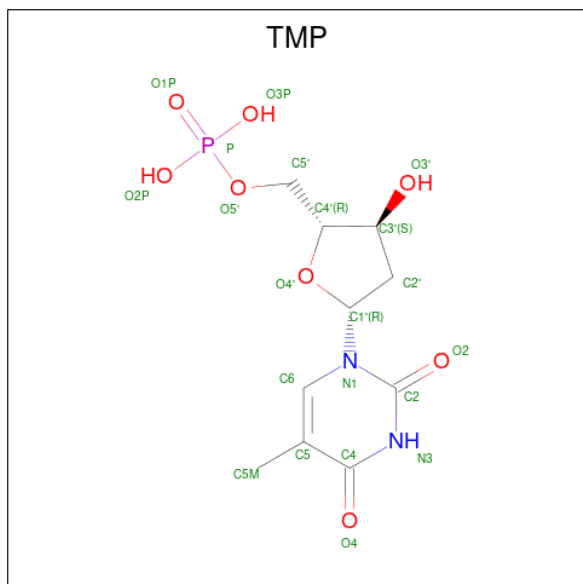
There are 4 unique types of molecules in this entry. The entry contains 3315 atoms, of which 633 are hydrogens and 0 are deuteriums.

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.

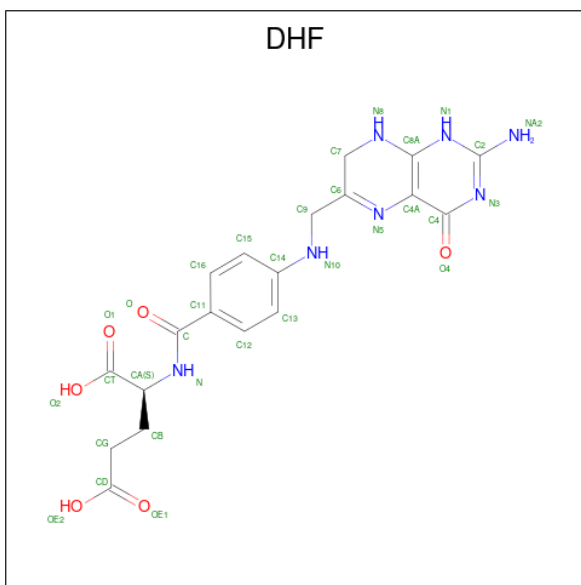
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	0	0
			3139	1677	549	438	467	8			

- Molecule 2 is THYMIDINE-5'-PHOSPHATE (CCD ID: 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 (CCD ID: 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		

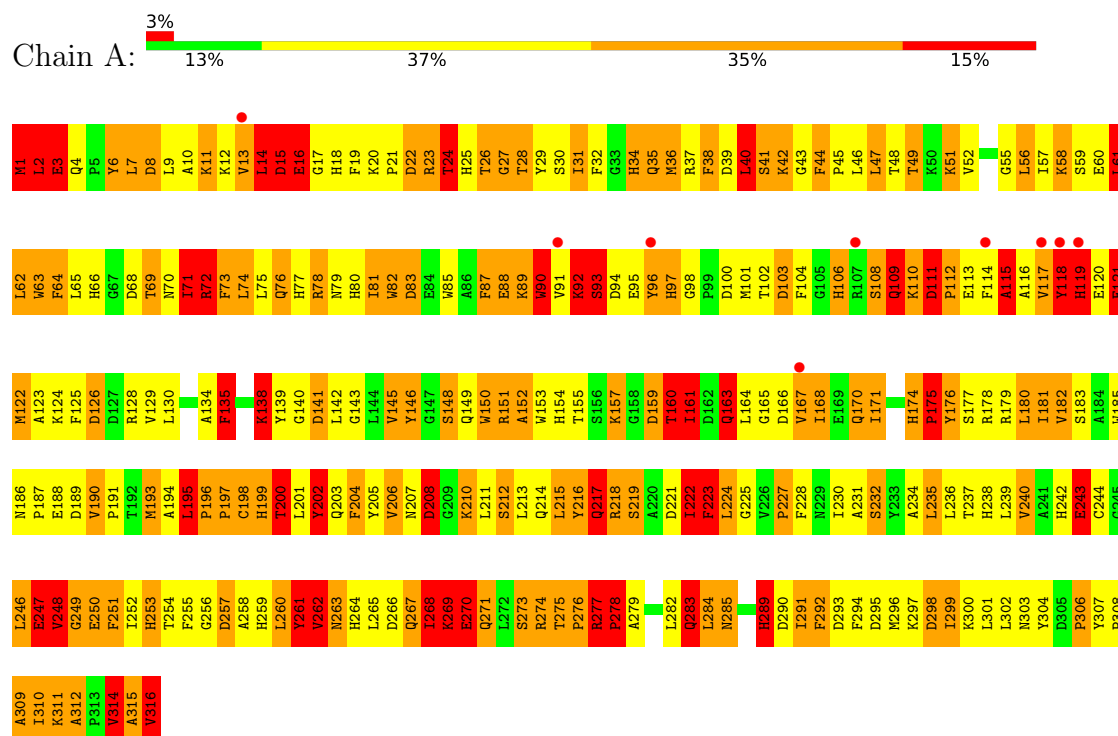
- Molecule 4 is water.

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, 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	78.60Å 78.60Å 229.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	52.6 (15.00-2.50) 52.4 (15.00-2.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	4.2	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	3315	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	1.85	45/2674 (1.7%)	2.89	304/3634 (8.4%)

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 (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	THR	CA-CB	12.87	1.66	1.53
1	A	161	ILE	CA-CB	9.93	1.67	1.54
1	A	268	ILE	CA-CB	9.72	1.67	1.54
1	A	196	PRO	CA-C	9.60	1.57	1.51
1	A	199	HIS	CD2-NE2	-9.04	1.27	1.37
1	A	97	HIS	CA-CB	8.34	1.63	1.52
1	A	289	HIS	CD2-NE2	-8.05	1.28	1.37
1	A	154	HIS	CD2-NE2	-7.90	1.29	1.37
1	A	253	HIS	CD2-NE2	-7.30	1.29	1.37
1	A	34	HIS	CD2-NE2	-7.26	1.29	1.37
1	A	199	HIS	CG-ND1	-6.90	1.30	1.38
1	A	264	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	259	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	238	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	97	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	310	ILE	CA-CB	6.58	1.62	1.54
1	A	77	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	18	HIS	CD2-NE2	-6.46	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	167	VAL	CA-CB	6.25	1.61	1.54
1	A	242	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	302	LEU	CA-CB	5.93	1.62	1.53
1	A	23	ARG	N-CA	5.91	1.53	1.46
1	A	95	GLU	CA-CB	5.91	1.64	1.53
1	A	174	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	119	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	266	ASP	CA-CB	5.78	1.63	1.53
1	A	80	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	240	VAL	CA-CB	5.68	1.60	1.54
1	A	193	MET	C-N	5.66	1.41	1.33
1	A	205	TYR	CA-CB	-5.58	1.43	1.54
1	A	102	THR	CA-C	5.44	1.59	1.52
1	A	71	ILE	CA-CB	5.40	1.61	1.54
1	A	247	GLU	CA-CB	5.39	1.61	1.53
1	A	106	HIS	CB-CG	5.39	1.57	1.50
1	A	238	HIS	CG-ND1	-5.33	1.32	1.38
1	A	106	HIS	CG-CD2	5.29	1.41	1.35
1	A	285	ASN	CA-C	5.28	1.59	1.53
1	A	157	LYS	CA-CB	5.25	1.58	1.53
1	A	271	GLN	CA-CB	-5.11	1.45	1.53
1	A	18	HIS	CG-CD2	5.10	1.41	1.35
1	A	97	HIS	CG-CD2	5.08	1.41	1.35
1	A	106	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	119	HIS	CA-CB	5.06	1.62	1.53
1	A	110	LYS	CA-CB	5.01	1.61	1.53

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASP	CA-CB-CG	15.33	127.93	112.60
1	A	57	ILE	N-CA-C	-14.33	98.06	111.67
1	A	14	LEU	N-CA-C	13.92	128.19	110.65
1	A	298	ASP	CA-CB-CG	12.06	124.66	112.60
1	A	106	HIS	CA-CB-CG	11.50	125.30	113.80
1	A	291	ILE	N-CA-C	-11.22	103.05	113.71
1	A	208	ASP	CA-CB-CG	11.19	123.79	112.60
1	A	100	ASP	N-CA-C	11.07	125.85	110.35
1	A	214	GLN	OE1-CD-NE2	-10.93	111.67	122.60
1	A	34	HIS	CA-CB-CG	-10.85	102.95	113.80
1	A	310	ILE	CB-CA-C	10.82	126.24	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASP	CA-CB-CG	10.61	123.21	112.60
1	A	269	LYS	CA-CB-CG	-10.33	93.43	114.10
1	A	274	ARG	N-CA-C	-10.28	92.64	109.40
1	A	109	GLN	CA-CB-CG	10.25	134.60	114.10
1	A	83	ASP	N-CA-C	10.17	124.36	111.24
1	A	104	PHE	N-CA-C	9.92	123.33	111.33
1	A	216	TYR	CA-C-O	9.88	130.77	120.40
1	A	154	HIS	O-C-N	9.77	135.44	123.13
1	A	310	ILE	N-CA-CB	-9.67	95.39	110.86
1	A	223	PHE	CA-CB-CG	-9.63	104.17	113.80
1	A	25	HIS	CA-CB-CG	9.55	123.35	113.80
1	A	159	ASP	CA-CB-CG	9.50	122.10	112.60
1	A	259	HIS	CA-CB-CG	9.21	123.01	113.80
1	A	15	ASP	CA-CB-CG	9.20	121.80	112.60
1	A	121	GLU	N-CA-C	-9.18	100.39	111.69
1	A	214	GLN	CG-CD-NE2	8.97	129.85	116.40
1	A	188	GLU	N-CA-C	8.89	122.89	112.93
1	A	176	TYR	CA-CB-CG	8.85	129.83	113.90
1	A	175	PRO	N-CA-C	8.84	130.68	112.47
1	A	298	ASP	N-CA-C	-8.83	91.99	110.80
1	A	24	THR	CA-CB-OG1	-8.71	96.53	109.60
1	A	199	HIS	O-C-N	8.66	135.68	122.87
1	A	295	ASP	O-C-N	8.65	133.08	123.13
1	A	154	HIS	CA-C-O	8.62	129.69	120.46
1	A	108	SER	CA-CB-OG	8.57	128.25	111.10
1	A	314	VAL	N-CA-C	8.49	126.99	109.34
1	A	109	GLN	OE1-CD-NE2	-8.40	114.20	122.60
1	A	292	PHE	N-CA-CB	-8.34	97.89	109.98
1	A	217	GLN	N-CA-C	-8.14	95.96	109.07
1	A	108	SER	N-CA-C	-8.13	96.83	109.76
1	A	70	ASN	CA-CB-CG	-8.12	104.48	112.60
1	A	194	ALA	CA-C-O	8.11	128.57	119.41
1	A	152	ALA	N-CA-C	8.09	119.96	110.41
1	A	29	TYR	N-CA-C	-8.06	95.12	108.34
1	A	278	PRO	N-CA-C	8.05	129.06	112.47
1	A	202	TYR	CA-CB-CG	8.02	128.33	113.90
1	A	95	GLU	N-CA-C	7.99	120.49	109.54
1	A	290	ASP	CA-CB-CG	7.99	120.59	112.60
1	A	83	ASP	O-C-N	7.93	131.31	122.11
1	A	266	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	183	SER	O-C-N	7.87	133.07	123.16
1	A	88	GLU	CB-CG-CD	7.85	125.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	LYS	CG-CD-CE	7.77	129.16	111.30
1	A	95	GLU	CA-CB-CG	7.75	129.61	114.10
1	A	263	ASN	CA-CB-CG	7.73	120.33	112.60
1	A	310	ILE	CA-C-O	7.70	129.77	120.84
1	A	77	HIS	CA-CB-CG	-7.67	106.12	113.80
1	A	285	ASN	N-CA-C	7.59	120.49	109.71
1	A	163	GLN	N-CA-C	7.58	121.77	112.23
1	A	13	VAL	O-C-N	-7.49	114.61	121.87
1	A	92	LYS	N-CA-C	-7.48	104.18	113.38
1	A	35	GLN	O-C-N	7.48	132.64	123.44
1	A	44	PHE	CA-CB-CG	-7.41	106.39	113.80
1	A	96	TYR	N-CA-C	-7.38	99.50	110.06
1	A	88	GLU	N-CA-C	-7.37	99.29	111.37
1	A	247	GLU	CA-CB-CG	7.33	128.75	114.10
1	A	188	GLU	O-C-N	7.29	131.69	122.37
1	A	256	GLY	O-C-N	7.27	132.15	122.70
1	A	308	PRO	CA-C-N	-7.25	113.00	123.00
1	A	308	PRO	C-N-CA	-7.25	113.00	123.00
1	A	2	LEU	N-CA-C	7.23	126.20	110.80
1	A	18	HIS	CA-CB-CG	7.21	121.01	113.80
1	A	204	PHE	O-C-N	7.21	131.39	123.10
1	A	195	LEU	N-CA-C	-7.19	93.91	109.81
1	A	194	ALA	N-CA-C	7.15	122.13	113.41
1	A	58	LYS	CA-CB-CG	7.13	128.36	114.10
1	A	88	GLU	CA-CB-CG	7.13	128.36	114.10
1	A	275	THR	CA-C-N	7.12	128.74	119.84
1	A	275	THR	C-N-CA	7.12	128.74	119.84
1	A	191	PRO	N-CA-C	7.10	122.92	113.40
1	A	223	PHE	CA-C-O	-7.07	110.40	120.51
1	A	309	ALA	CA-C-O	7.07	128.09	120.38
1	A	188	GLU	N-CA-CB	-7.07	100.80	110.56
1	A	270	GLU	CA-CB-CG	7.07	128.23	114.10
1	A	206	VAL	N-CA-C	-7.05	94.68	109.34
1	A	37	ARG	N-CA-C	7.01	120.93	109.72
1	A	80	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	A	252	ILE	O-C-N	-6.98	115.29	123.04
1	A	154	HIS	CB-CG-CD2	-6.98	122.13	131.20
1	A	284	LEU	N-CA-C	-6.95	97.24	109.06
1	A	154	HIS	CA-CB-CG	6.95	120.75	113.80
1	A	292	PHE	CB-CA-C	6.91	121.65	110.95
1	A	17	GLY	N-CA-C	-6.90	102.04	112.60
1	A	261	TYR	CA-CB-CG	6.84	126.21	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	242	HIS	CA-CB-CG	6.83	120.63	113.80
1	A	93	SER	CA-CB-OG	6.81	124.73	111.10
1	A	22	ASP	O-C-N	-6.80	115.32	122.94
1	A	196	PRO	O-C-N	6.80	124.44	121.31
1	A	41	SER	N-CA-C	-6.79	104.81	113.23
1	A	126	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	178	ARG	CB-CG-CD	6.71	126.74	111.30
1	A	315	ALA	N-CA-C	6.71	119.16	111.11
1	A	311	LYS	N-CA-C	6.69	120.31	109.40
1	A	196	PRO	CB-CA-C	6.66	117.65	111.39
1	A	160	THR	N-CA-CB	-6.65	98.96	111.00
1	A	24	THR	CA-CB-CG2	6.64	121.79	110.50
1	A	222	ILE	CA-CB-CG2	-6.64	99.22	110.50
1	A	240	VAL	CA-C-O	-6.63	114.38	121.27
1	A	98	GLY	CA-C-N	6.60	128.09	119.84
1	A	98	GLY	C-N-CA	6.60	128.09	119.84
1	A	242	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	4	GLN	O-C-N	-6.59	113.74	121.32
1	A	47	LEU	N-CA-C	6.57	124.80	110.80
1	A	104	PHE	CA-C-O	-6.57	113.54	120.63
1	A	203	GLN	N-CA-C	6.56	119.63	109.07
1	A	250	GLU	N-CA-C	6.56	119.28	108.99
1	A	16	GLU	N-CA-C	6.50	121.22	113.16
1	A	76	GLN	CB-CA-C	-6.50	99.64	110.68
1	A	222	ILE	CA-C-O	6.48	128.73	120.76
1	A	77	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	A	141	ASP	CA-C-O	6.46	127.82	120.84
1	A	279	ALA	N-CA-C	6.44	124.05	109.81
1	A	251	PHE	CA-CB-CG	6.43	120.23	113.80
1	A	289	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	A	118	TYR	CA-C-O	-6.42	114.26	121.00
1	A	183	SER	N-CA-C	-6.37	99.82	109.95
1	A	193	MET	O-C-N	6.37	130.12	122.85
1	A	294	PHE	CA-C-N	-6.37	113.70	122.30
1	A	294	PHE	C-N-CA	-6.37	113.70	122.30
1	A	203	GLN	CA-C-O	6.37	127.32	120.38
1	A	283	GLN	CA-CB-CG	6.37	126.83	114.10
1	A	11	LYS	CA-CB-CG	6.31	126.73	114.10
1	A	28	THR	CB-CA-C	-6.31	97.87	110.42
1	A	238	HIS	O-C-N	6.31	128.57	122.07
1	A	264	HIS	CB-CG-CD2	-6.30	123.01	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	THR	O-C-N	6.29	130.54	123.19
1	A	134	ALA	CA-C-N	6.28	133.08	121.52
1	A	134	ALA	C-N-CA	6.28	133.08	121.52
1	A	277	ARG	CA-C-N	6.28	127.69	119.84
1	A	277	ARG	C-N-CA	6.28	127.69	119.84
1	A	254	THR	CA-C-O	6.25	127.74	120.80
1	A	159	ASP	N-CA-C	6.24	124.09	110.80
1	A	222	ILE	O-C-N	6.23	129.47	122.68
1	A	314	VAL	CA-CB-CG1	-6.22	99.83	110.40
1	A	148	SER	N-CA-C	-6.20	105.76	113.38
1	A	275	THR	O-C-N	6.19	128.91	121.60
1	A	260	LEU	O-C-N	6.19	132.83	122.93
1	A	174	HIS	O-C-N	-6.17	114.22	121.32
1	A	174	HIS	CA-C-N	6.17	127.55	119.84
1	A	174	HIS	C-N-CA	6.17	127.55	119.84
1	A	249	GLY	N-CA-C	-6.17	98.56	113.18
1	A	302	LEU	CA-C-O	6.14	128.99	121.99
1	A	301	LEU	O-C-N	6.11	130.83	123.13
1	A	181	ILE	O-C-N	6.08	129.42	123.03
1	A	39	ASP	CA-C-O	6.08	126.89	120.33
1	A	83	ASP	CA-C-N	6.08	130.41	120.63
1	A	83	ASP	C-N-CA	6.08	130.41	120.63
1	A	165	GLY	O-C-N	-6.07	116.36	122.19
1	A	273	SER	CA-CB-OG	6.07	123.23	111.10
1	A	275	THR	CA-CB-OG1	6.05	118.68	109.60
1	A	293	ASP	CB-CA-C	-6.05	100.66	110.77
1	A	217	GLN	N-CA-CB	-6.05	101.07	110.57
1	A	183	SER	CA-C-N	6.04	133.11	122.42
1	A	183	SER	C-N-CA	6.04	133.11	122.42
1	A	257	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	219	SER	O-C-N	6.01	130.85	123.10
1	A	290	ASP	N-CA-CB	-6.00	97.55	110.88
1	A	205	TYR	N-CA-CB	-6.00	101.25	111.69
1	A	23	ARG	N-CA-C	6.00	121.26	111.37
1	A	73	PHE	CA-CB-CG	5.99	119.79	113.80
1	A	56	LEU	N-CA-CB	-5.98	99.89	110.42
1	A	221	ASP	O-C-N	-5.98	115.51	122.87
1	A	120	GLU	N-CA-CB	-5.95	101.93	110.80
1	A	238	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	274	ARG	CG-CD-NE	-5.94	98.93	112.00
1	A	312	ALA	N-CA-C	5.94	119.52	110.50
1	A	109	GLN	CG-CD-NE2	5.93	125.29	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	GLN	CB-CA-C	5.92	119.96	109.72
1	A	87	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	49	THR	N-CA-C	5.92	118.51	111.71
1	A	274	ARG	CB-CG-CD	5.91	124.90	111.30
1	A	16	GLU	CA-C-O	5.88	126.40	119.28
1	A	32	PHE	N-CA-C	-5.88	98.27	110.80
1	A	193	MET	CA-C-N	5.84	132.54	122.09
1	A	193	MET	C-N-CA	5.84	132.54	122.09
1	A	259	HIS	N-CA-C	5.84	118.73	108.75
1	A	234	ALA	N-CA-C	-5.83	105.27	112.90
1	A	6	TYR	N-CA-C	-5.82	105.02	111.36
1	A	210	LYS	CA-C-N	-5.82	113.18	121.50
1	A	210	LYS	C-N-CA	-5.82	113.18	121.50
1	A	290	ASP	N-CA-C	-5.80	97.93	108.65
1	A	115	ALA	CA-C-O	5.79	128.79	120.51
1	A	72	ARG	CA-CB-CG	5.77	125.65	114.10
1	A	39	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	242	HIS	CB-CG-ND1	5.76	131.35	122.70
1	A	177	SER	O-C-N	5.76	130.22	122.96
1	A	243	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	76	GLN	N-CA-CB	5.74	118.67	110.06
1	A	78	ARG	N-CA-CB	-5.73	103.59	112.30
1	A	90	TRP	N-CA-C	5.73	123.00	110.80
1	A	285	ASN	CA-C-N	5.71	125.39	119.05
1	A	285	ASN	C-N-CA	5.71	125.39	119.05
1	A	248	VAL	N-CA-CB	-5.71	101.81	111.23
1	A	2	LEU	CA-C-O	-5.70	112.36	120.51
1	A	117	VAL	CA-C-O	-5.70	115.34	121.27
1	A	77	HIS	CA-C-N	5.69	130.65	122.40
1	A	77	HIS	C-N-CA	5.69	130.65	122.40
1	A	292	PHE	N-CA-C	5.68	117.34	111.03
1	A	30	SER	N-CA-C	5.68	118.05	109.41
1	A	232	SER	N-CA-C	-5.67	104.73	111.03
1	A	219	SER	N-CA-C	-5.67	101.36	110.14
1	A	176	TYR	CB-CG-CD2	-5.64	112.33	120.80
1	A	221	ASP	N-CA-C	5.64	118.23	107.75
1	A	167	VAL	CG1-CB-CG2	-5.62	98.42	110.80
1	A	150	TRP	CG-CD2-CE3	5.62	139.52	133.90
1	A	242	HIS	CA-C-O	-5.60	114.93	120.70
1	A	311	LYS	N-CA-CB	-5.60	101.09	110.83
1	A	111	ASP	O-C-N	-5.58	114.90	121.32
1	A	61	LEU	O-C-N	5.57	127.82	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	PHE	O-C-N	-5.56	116.23	122.12
1	A	18	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	A	103	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	149	GLN	N-CA-C	-5.53	105.66	112.90
1	A	309	ALA	N-CA-CB	-5.52	101.90	110.57
1	A	56	LEU	N-CA-C	5.52	119.76	113.19
1	A	58	LYS	N-CA-CB	5.51	118.22	110.12
1	A	298	ASP	N-CA-CB	5.50	119.78	110.49
1	A	38	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	171	ILE	CA-C-O	5.49	126.76	121.05
1	A	1	MET	CA-C-O	-5.49	111.48	120.80
1	A	251	PHE	N-CA-C	-5.48	100.77	109.59
1	A	208	ASP	N-CA-CB	5.47	119.74	110.49
1	A	92	LYS	CA-CB-CG	5.46	125.03	114.10
1	A	151	ARG	CB-CG-CD	5.44	123.80	111.30
1	A	150	TRP	N-CA-C	-5.43	104.89	112.45
1	A	306	PRO	CA-N-CD	-5.42	104.41	112.00
1	A	268	ILE	CA-C-O	-5.40	115.13	120.85
1	A	289	HIS	CB-CA-C	-5.39	103.17	111.74
1	A	97	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	A	176	TYR	CA-C-N	5.39	129.00	121.24
1	A	176	TYR	C-N-CA	5.39	129.00	121.24
1	A	82	TRP	CE2-CD2-CG	-5.39	100.74	107.20
1	A	3	GLU	O-C-N	-5.35	115.47	122.59
1	A	91	VAL	O-C-N	5.35	128.88	122.03
1	A	227	PRO	N-CA-C	5.34	121.56	113.81
1	A	160	THR	CB-CA-C	5.34	119.93	109.35
1	A	74	LEU	CA-C-O	-5.32	114.91	120.55
1	A	90	TRP	CB-CG-CD1	-5.32	118.92	126.90
1	A	26	THR	CA-C-O	5.32	126.62	121.67
1	A	231	ALA	N-CA-C	5.32	119.82	113.23
1	A	295	ASP	CA-C-N	5.31	131.69	121.54
1	A	295	ASP	C-N-CA	5.31	131.69	121.54
1	A	90	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	A	185	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	A	13	VAL	CA-C-O	-5.29	115.45	120.95
1	A	28	THR	N-CA-CB	5.28	119.41	110.49
1	A	141	ASP	N-CA-C	5.26	117.54	107.75
1	A	7	LEU	O-C-N	5.26	128.15	122.15
1	A	186	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	90	TRP	CA-CB-CG	5.25	123.57	113.60
1	A	64	PHE	CA-CB-CG	5.23	119.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	THR	CA-C-O	5.22	124.26	118.52
1	A	231	ALA	CA-C-O	-5.22	113.16	119.27
1	A	15	ASP	O-C-N	5.22	129.53	122.59
1	A	44	PHE	CA-C-N	5.22	126.36	119.84
1	A	44	PHE	C-N-CA	5.22	126.36	119.84
1	A	13	VAL	N-CA-C	5.21	115.93	110.62
1	A	227	PRO	N-CA-CB	-5.20	97.47	103.30
1	A	224	LEU	CA-C-O	5.20	126.26	120.90
1	A	4	GLN	N-CA-C	5.18	121.26	109.81
1	A	304	TYR	CA-CB-CG	5.18	123.23	113.90
1	A	40	LEU	N-CA-CB	-5.18	102.49	110.46
1	A	63	TRP	CA-C-O	-5.17	115.38	121.07
1	A	262	VAL	N-CA-C	5.17	120.08	109.34
1	A	15	ASP	CA-C-N	5.16	131.72	122.38
1	A	15	ASP	C-N-CA	5.16	131.72	122.38
1	A	108	SER	CA-C-N	5.15	131.37	121.54
1	A	108	SER	C-N-CA	5.15	131.37	121.54
1	A	178	ARG	NE-CZ-NH1	5.13	126.64	121.50
1	A	275	THR	CA-CB-CG2	-5.13	101.77	110.50
1	A	40	LEU	N-CA-C	5.12	119.24	113.15
1	A	112	PRO	O-C-N	-5.12	115.62	122.22
1	A	204	PHE	CA-C-O	5.12	127.32	121.28
1	A	4	GLN	CB-CG-CD	5.11	121.29	112.60
1	A	110	LYS	CG-CD-CE	5.11	123.05	111.30
1	A	185	TRP	CG-CD2-CE3	5.11	139.00	133.90
1	A	316	VAL	CA-CB-CG2	5.10	119.07	110.40
1	A	93	SER	CB-CA-C	-5.10	100.28	110.42
1	A	90	TRP	O-C-N	-5.09	115.81	122.59
1	A	138	LYS	CA-CB-CG	-5.09	103.91	114.10
1	A	167	VAL	N-CA-C	-5.09	105.53	110.42
1	A	200	THR	CA-C-O	-5.09	113.23	120.51
1	A	13	VAL	N-CA-CB	-5.08	103.63	110.54
1	A	283	GLN	N-CA-C	-5.07	101.61	109.72
1	A	285	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	81	ILE	N-CA-CB	-5.06	102.88	111.23
1	A	117	VAL	N-CA-CB	-5.05	104.90	110.51
1	A	68	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	135	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	58	LYS	CB-CA-C	-5.02	102.45	110.79
1	A	51	LYS	CG-CD-CE	5.01	122.83	111.30
1	A	61	LEU	N-CA-C	5.01	116.43	110.97

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	162	0
2	A	21	2	12	3	0
3	A	32	4	19	9	0
4	A	39	78	0	10	0
All	All	2682	633	2527	168	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 (168) 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
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:60:GLU:HG2	4:A:353:HOH:O	1.80	0.80
1:A:152:ALA:HA	1:A:160:THR:HG23	1.63	0.80
1:A:101:MET:HE3	1:A:121:GLU:HG2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:60:GLU:CG	4:A:353:HOH:O	2.36	0.72
1:A:123:ALA:O	1:A:126:ASP:HB2	1.90	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	1.39	0.69
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:13:VAL:HG11	1:A:260:LEU:HB2	1.76	0.67
1:A:71:ILE:HB	1:A:140:GLY:O	1.95	0.67
1:A:224:LEU:HD23	3:A:318:DHF:HG1	1.77	0.67
1:A:51:LYS:HB3	1:A:309:ALA:HB2	1.76	0.66
1:A:210:LYS:HA	1:A:247:GLU:O	1.95	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:108:SER:HB2	1:A:314:VAL:HG11	1.77	0.65
1:A:285:ASN:HB3	1:A:298:ASP:HB3	1.78	0.65
1:A:40:LEU:HB2	1:A:248:VAL:HG13	1.78	0.65
1:A:222:ILE:HD12	1:A:260:LEU:HD12	1.77	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
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:19:PHE:CE1	1:A:27:GLY:HA3	2.33	0.59
1:A:38:PHE:O	1:A:250:GLU:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:ARG:HA	1:A:129:VAL:HG12	1.88	0.55
1:A:267:GLN:O	1:A:270:GLU:HB3	2.07	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:87:PHE:HB2	1:A:122:MET:HE3	1.90	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:34:HIS:HB3	1:A:255:PHE:CD2	2.44	0.52
1:A:90:TRP:CE3	1:A:135:PHE:HZ	2.27	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:224:LEU:HD21	1:A:312:ALA:HB3	1.92	0.51
1:A:291:ILE:HG13	1:A:292:PHE:CD1	2.45	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:101:MET:HE3	1:A:121:GLU:CG	2.37	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
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:9:LEU:CD1	1:A:222:ILE:HG21	2.41	0.50
1:A:224:LEU:HD23	3:A:318:DHF:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:HA	1:A:152:ALA:HB3	1.94	0.49
1:A:36:MET:HB3	1:A:253:HIS:HB3	1.95	0.48
1:A:274:ARG:HH21	1:A:307:TYR:HB3	1.77	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:2:LEU:HG	1:A:45:PRO:HB3	1.94	0.48
1:A:69:THR:O	1:A:141:ASP:HA	2.14	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: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:2:LEU:HD21	1:A:43:GLY:O	2.14	0.47
1:A:175:PRO:HB3	1:A:206:VAL:HG11	1.97	0.47
1:A:90:TRP:O	1:A:90:TRP:CG	2.67	0.47
3:A:318:DHF:O2	3:A:318:DHF:H12	2.15	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:155:THR:C	1:A:157:LYS:H	2.23	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
1:A:171:ILE:HD11	1:A:204:PHE:CD2	2.51	0.45
1:A:87:PHE:HZ	1:A:121:GLU:HB3	1.83	0.44
1:A:261:TYR:HE1	4:A:348:HOH:O	1.99	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:7:LEU:CD1	1:A:276:PRO:HG3	2.48	0.44
1:A:224:LEU:HD21	1:A:312:ALA:CB	2.47	0.44
1:A:212:SER:HA	1:A:250:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:O	1:A:260:LEU:HG	2.17	0.44
1:A:289:HIS:CD2	1:A:289:HIS:N	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: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:7:LEU:HD11	1:A:276:PRO:HG3	2.01	0.43
1:A:47:LEU:HB2	1:A:52:VAL:CG2	2.48	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:76:GLN:C	1:A:78:ARG:H	2.28	0.42
1:A:74:LEU:HD22	1:A:79:ASN:CG	2.45	0.41
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:163:GLN:CD	1:A:182:VAL:HG13	2.46	0.41
1:A:41:SER:C	1:A:43:GLY:H	2.29	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:64:PHE:HZ	1:A:82:TRP:CZ2	2.39	0.40
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: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%)	0 0

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%)	193 (70%)	84 (30%)	0 0

All (84) 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	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	36	MET
1	A	40	LEU
1	A	44	PHE
1	A	46	LEU
1	A	56	LEU
1	A	59	SER
1	A	61	LEU
1	A	62	LEU
1	A	71	ILE
1	A	72	ARG
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	103	ASP
1	A	106	HIS
1	A	113	GLU
1	A	118	TYR
1	A	121	GLU
1	A	122	MET
1	A	130	LEU
1	A	135	PHE
1	A	138	LYS
1	A	142	LEU
1	A	145	VAL
1	A	160	THR
1	A	161	ILE
1	A	163	GLN
1	A	164	LEU
1	A	168	ILE
1	A	170	GLN
1	A	175	PRO
1	A	179	ARG
1	A	180	LEU
1	A	182	VAL
1	A	187	PRO
1	A	190	VAL
1	A	193	MET
1	A	198	CYS
1	A	200	THR
1	A	201	LEU
1	A	202	TYR
1	A	208	ASP
1	A	212	SER
1	A	213	LEU
1	A	215	LEU
1	A	217	GLN
1	A	218	ARG
1	A	222	ILE
1	A	227	PRO
1	A	228	PHE
1	A	235	LEU
1	A	236	LEU
1	A	243	GLU
1	A	244	CYS

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	247	GLU
1	A	248	VAL
1	A	261	TYR
1	A	262	VAL
1	A	263	ASN
1	A	265	LEU
1	A	267	GLN
1	A	268	ILE
1	A	269	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	97	HIS
1	A	163	GLN
1	A	170	GLN
1	A	242	HIS
1	A	263	ASN
1	A	289	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	DHF	A	318	-	32,34,34	2.77	14 (43%)	38,47,47	2.66	9 (23%)
2	TMP	A	317	-	22,22,22	1.72	5 (22%)	32,33,33	2.35	9 (28%)

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	DHF	A	318	-	-	12/20/31/31	0/3/3/3
2	TMP	A	317	-	1/1/4/4	2/10/22/22	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	318	DHF	O4-C4	8.76	1.39	1.23
3	A	318	DHF	CB-CA	5.13	1.65	1.53
3	A	318	DHF	C8A-N8	5.09	1.37	1.32
2	A	317	TMP	C6-C5	4.71	1.42	1.34
3	A	318	DHF	CG-CD	3.87	1.59	1.50
3	A	318	DHF	CB-CG	3.61	1.63	1.52
3	A	318	DHF	C9-N10	3.44	1.50	1.45
3	A	318	DHF	C16-C11	3.42	1.44	1.39
2	A	317	TMP	C2-N1	3.18	1.43	1.38
3	A	318	DHF	CA-N	3.09	1.52	1.45
3	A	318	DHF	C15-C14	2.98	1.44	1.39
3	A	318	DHF	C7-N8	2.50	1.49	1.45
2	A	317	TMP	C2-N3	2.48	1.42	1.38
3	A	318	DHF	C8A-N1	-2.34	1.33	1.37
2	A	317	TMP	C4-N3	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	318	DHF	C12-C11	2.28	1.42	1.39
3	A	318	DHF	O2-CT	-2.20	1.23	1.30
3	A	318	DHF	CA-CT	2.20	1.58	1.52
2	A	317	TMP	O4'-C1'	2.16	1.47	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	318	DHF	CG-CB-CA	10.47	132.46	113.16
2	A	317	TMP	O4'-C1'-N1	8.52	122.99	107.86
3	A	318	DHF	C9-N10-C14	-7.84	107.23	122.42
2	A	317	TMP	C2'-C1'-N1	6.46	129.97	113.81
3	A	318	DHF	C7-N8-C8A	-5.30	112.10	123.81
2	A	317	TMP	C1'-N1-C6	-3.11	115.52	120.74
3	A	318	DHF	C4A-C8A-N8	2.74	121.51	115.89
2	A	317	TMP	O4-C4-C5	-2.71	121.81	124.92
2	A	317	TMP	C1'-N1-C2	2.58	122.71	117.66
2	A	317	TMP	C5M-C5-C4	-2.56	116.05	118.78
3	A	318	DHF	O2-CT-O1	-2.48	118.45	124.08
2	A	317	TMP	O3P-P-O2P	2.34	116.57	107.80
2	A	317	TMP	O2-C2-N1	2.33	125.83	122.80
3	A	318	DHF	O-C-N	-2.29	118.12	122.47
3	A	318	DHF	CB-CA-CT	2.25	115.69	110.35
3	A	318	DHF	C11-C-N	2.17	121.06	117.04
3	A	318	DHF	C13-C14-N10	-2.04	116.34	120.96
2	A	317	TMP	O3'-C3'-C2'	2.00	117.83	110.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	317	TMP	C1'

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	317	TMP	C2'-C1'-N1-C2
2	A	317	TMP	C2'-C1'-N1-C6
3	A	318	DHF	C11-C-N-CA
3	A	318	DHF	O-C-N-CA
3	A	318	DHF	C15-C14-N10-C9
3	A	318	DHF	C13-C14-N10-C9
3	A	318	DHF	CT-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	A	318	DHF	N-CA-CB-CG
3	A	318	DHF	N-CA-CT-O1
3	A	318	DHF	N-CA-CT-O2
3	A	318	DHF	CB-CA-CT-O1
3	A	318	DHF	CB-CA-CT-O2
3	A	318	DHF	OE1-CD-CG-CB
3	A	318	DHF	OE2-CD-CG-CB

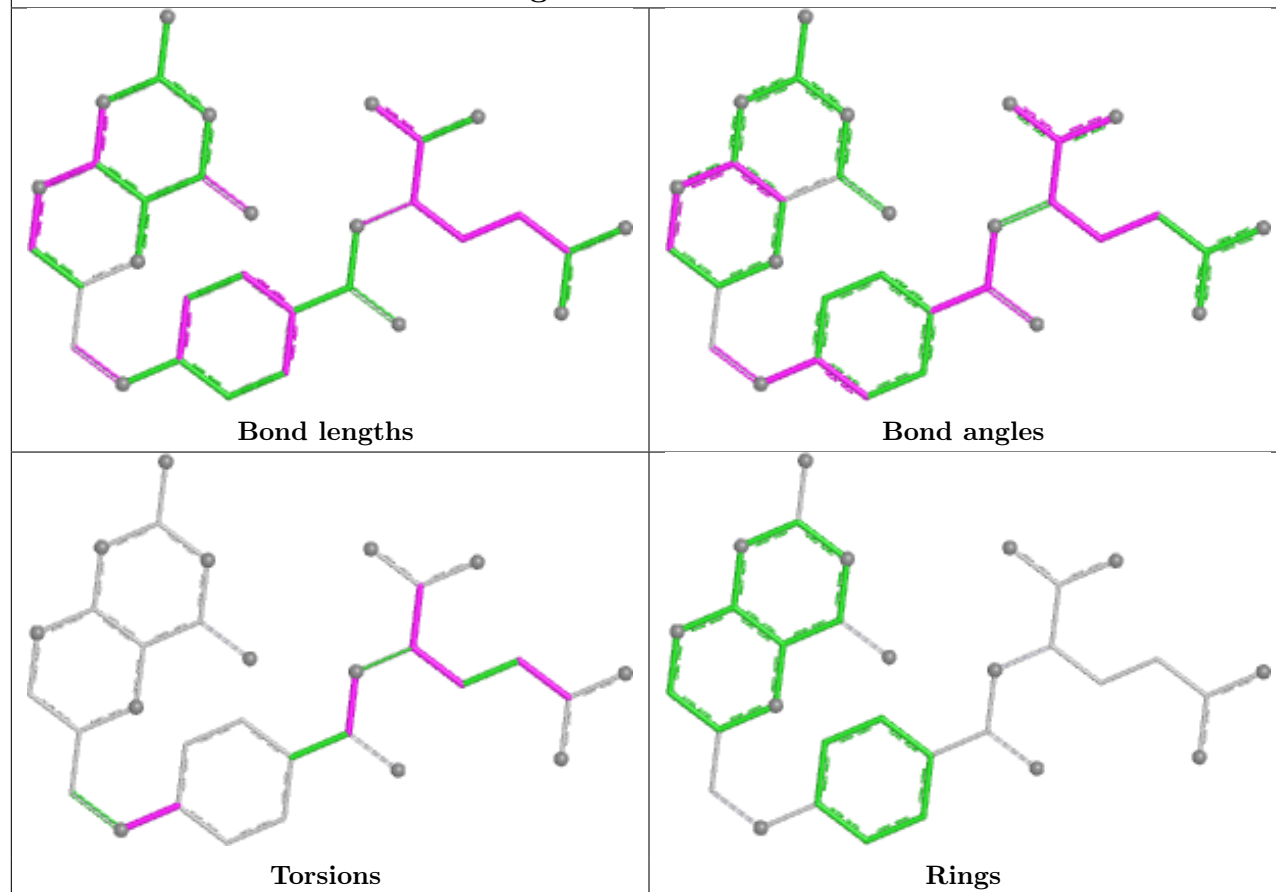
There are no ring outliers.

2 monomers are involved in 9 short contacts:

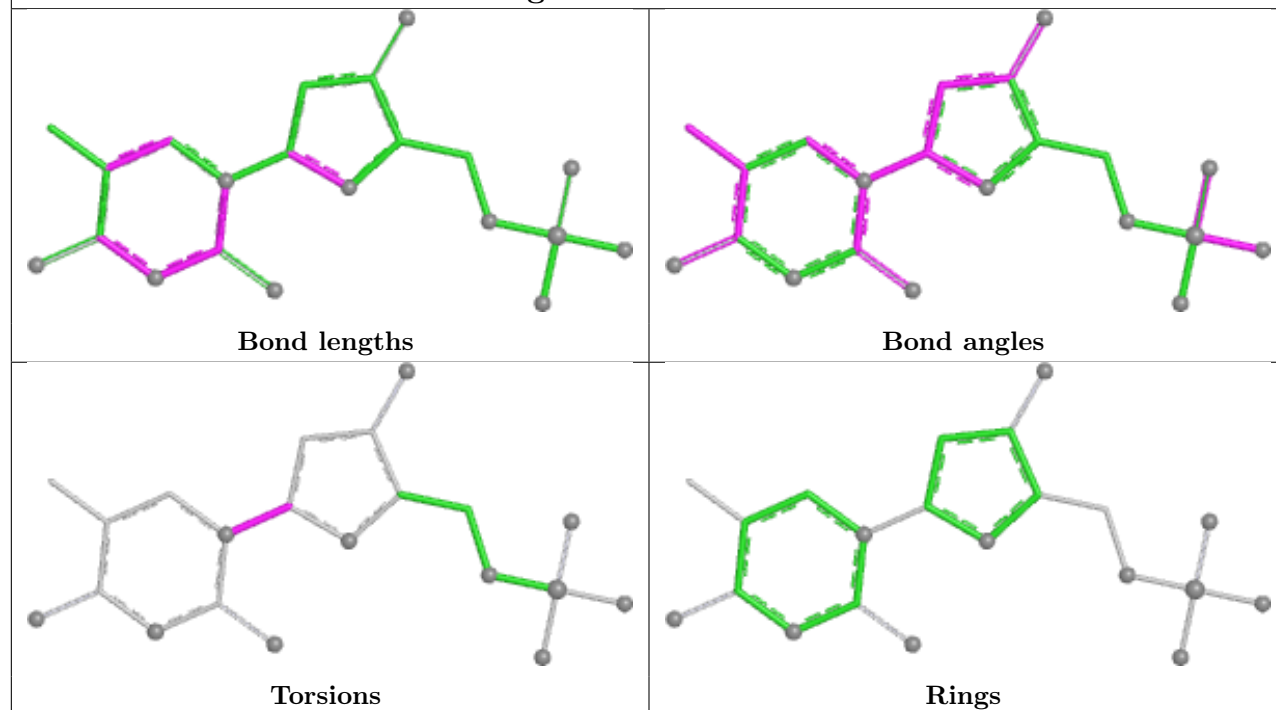
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	318	DHF	9	0
2	A	317	TMP	3	0

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.

Ligand DHF A 318



Ligand TMP A 317



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%)	0.32	9 (2%)	55 50	2, 6, 12, 38	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	TYR	3.3
1	A	107	ARG	3.2
1	A	91	VAL	2.8
1	A	114	PHE	2.6
1	A	13	VAL	2.3
1	A	117	VAL	2.2
1	A	167	VAL	2.2
1	A	118	TYR	2.0
1	A	119	HIS	2.0

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](#)

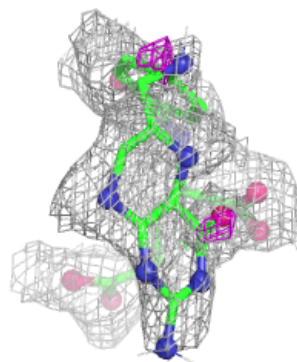
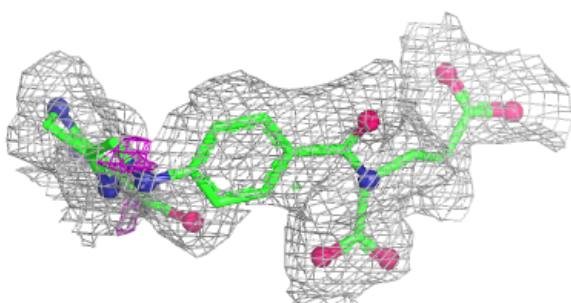
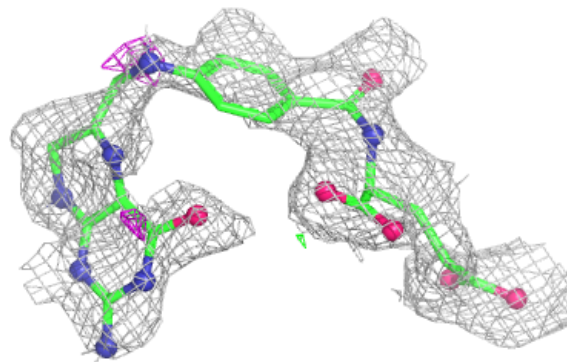
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

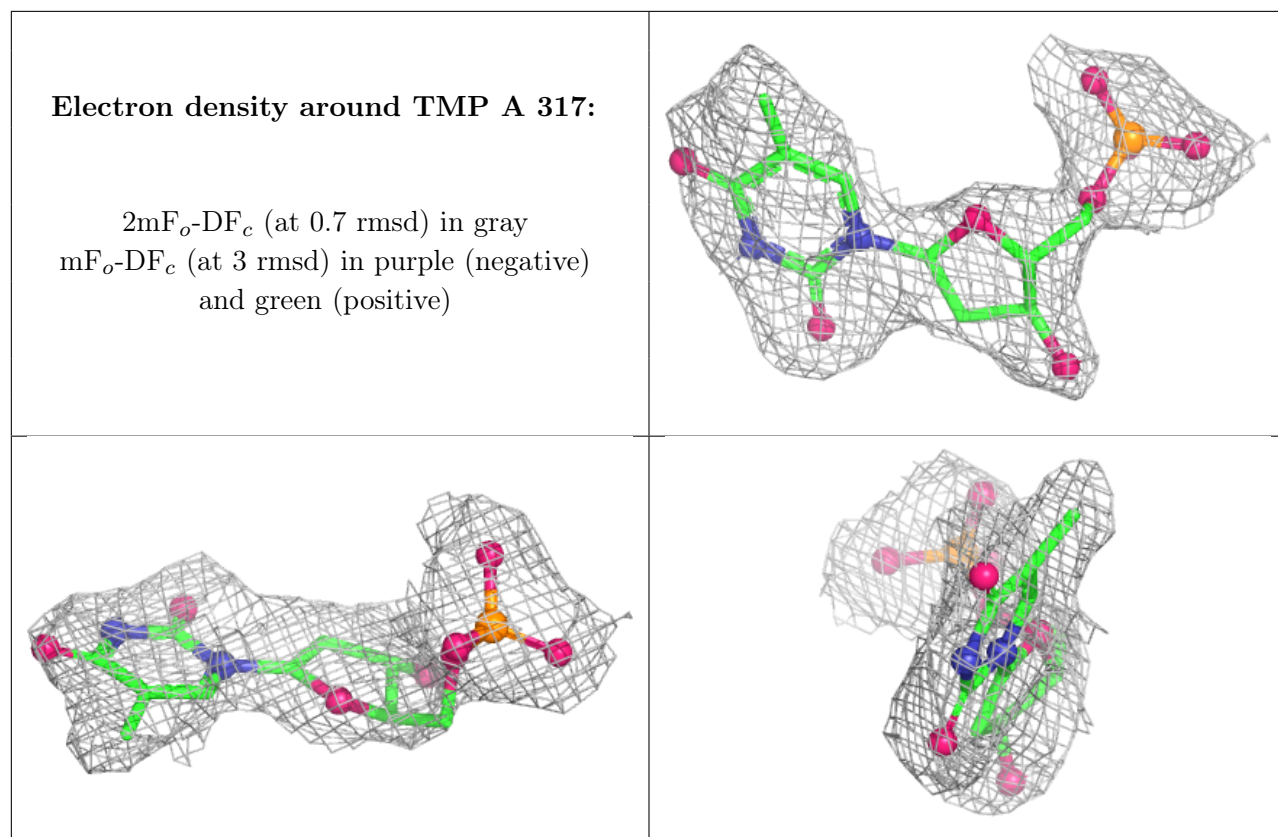
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DHF	A	318	32/32	0.83	0.12	2,2,15,15	0
2	TMP	A	317	21/21	0.94	0.09	2,2,12,15	0

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 DHF 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.