



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:25 AM UTC

PDB ID : 2TDD / pdb_00002tdd
Title : STRUCTURES OF THYMIDYLATE SYNTHASE WITH A C-TERMINAL DELETION: ROLE OF THE C-TERMINUS IN ALIGNMENT OF D/UMP AND CH₂H₄FOLATE
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Deposited on : 1993-04-05
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

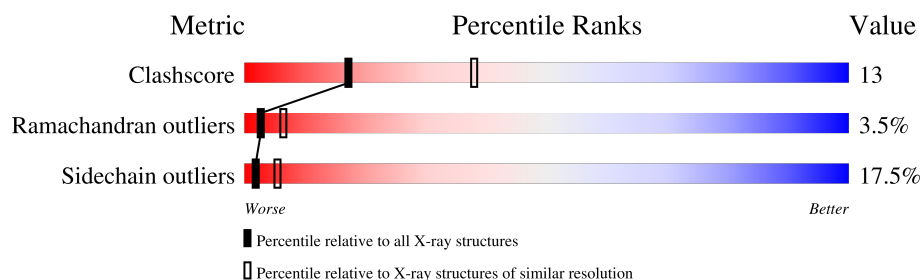
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UFP	A	529	X	-	-	-

2 Entry composition [i](#)

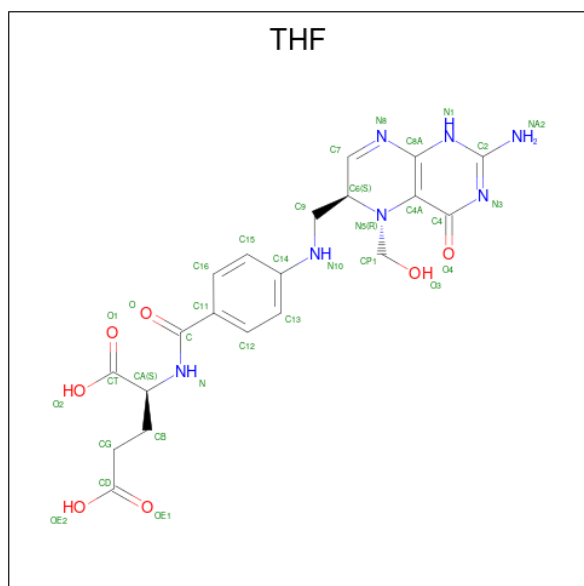
There are 4 unique types of molecules in this entry. The entry contains 2644 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

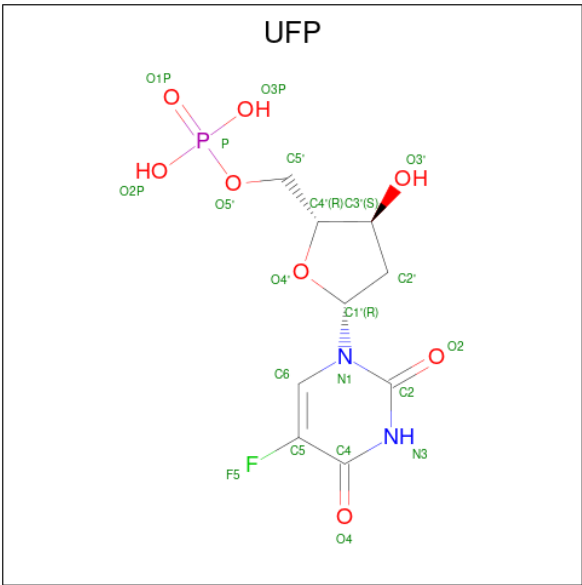
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2580	1669	437	466	8			

- Molecule 2 is 5-HYDROXYMETHYLENE-6-HYDROFOLIC ACID (CCD ID: THF) (formula: C₂₀H₂₃N₇O₇).



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

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: C₉H₁₂FN₂O₈P).



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

- Molecule 4 is water.

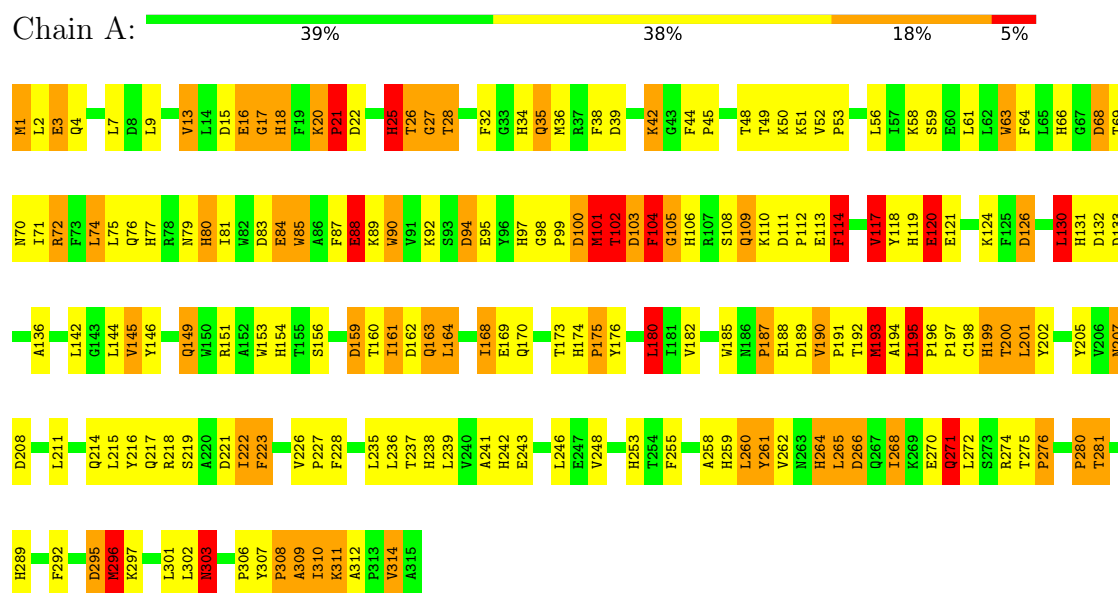
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.40Å 78.40Å 242.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2644	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.83	56/2664 (2.1%)	2.51	200/3619 (5.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	HIS	CD2-NE2	-7.56	1.29	1.37
1	A	34	HIS	CD2-NE2	-7.42	1.29	1.37
1	A	77	HIS	CD2-NE2	-7.41	1.29	1.37
1	A	276	PRO	CA-CB	-7.20	1.44	1.53
1	A	199	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	63	TRP	CA-CB	-7.06	1.42	1.53
1	A	199	HIS	CG-ND1	-6.97	1.30	1.38
1	A	109	GLN	CA-CB	-6.93	1.44	1.54
1	A	253	HIS	CG-ND1	-6.93	1.30	1.38
1	A	259	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	131	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	144	LEU	CA-CB	-6.67	1.44	1.53
1	A	264	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	130	LEU	CA-CB	-6.49	1.43	1.53
1	A	175	PRO	CA-CB	-6.46	1.44	1.53
1	A	130	LEU	CB-CG	-6.45	1.40	1.53
1	A	227	PRO	CA-CB	-6.40	1.44	1.53
1	A	253	HIS	CA-CB	-6.32	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	PRO	CA-CB	-6.30	1.45	1.53
1	A	308	PRO	CA-CB	-6.28	1.44	1.53
1	A	253	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	174	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	66	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	264	HIS	CG-ND1	-6.13	1.31	1.38
1	A	87	PHE	CA-CB	-6.05	1.43	1.53
1	A	18	HIS	CB-CG	5.92	1.58	1.50
1	A	25	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	102	THR	CA-CB	5.86	1.63	1.53
1	A	80	HIS	CG-ND1	-5.84	1.31	1.38
1	A	161	ILE	CA-CB	5.84	1.60	1.53
1	A	185	TRP	CA-CB	-5.78	1.45	1.52
1	A	39	ASP	CA-CB	-5.74	1.45	1.53
1	A	306	PRO	CA-CB	-5.69	1.44	1.53
1	A	53	PRO	CA-CB	-5.66	1.45	1.53
1	A	154	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	280	PRO	CA-CB	-5.58	1.46	1.53
1	A	106	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	21	PRO	CA-CB	-5.52	1.45	1.53
1	A	15	ASP	CA-CB	-5.46	1.44	1.53
1	A	296	MET	CA-CB	-5.45	1.44	1.53
1	A	97	HIS	CD2-NE2	-5.43	1.31	1.37
1	A	3	GLU	CA-CB	-5.38	1.47	1.53
1	A	64	PHE	CA-CB	-5.35	1.45	1.53
1	A	238	HIS	CD2-NE2	-5.32	1.32	1.37
1	A	113	GLU	C-N	5.25	1.41	1.33
1	A	83	ASP	CA-CB	-5.24	1.45	1.53
1	A	163	GLN	CA-CB	-5.23	1.44	1.53
1	A	119	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	259	HIS	CG-ND1	-5.20	1.32	1.38
1	A	310	ILE	CA-CB	5.17	1.61	1.54
1	A	289	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	146	TYR	CA-CB	-5.11	1.45	1.53
1	A	18	HIS	CG-CD2	5.08	1.41	1.35
1	A	132	ASP	CA-CB	-5.04	1.46	1.53
1	A	79	ASN	CA-CB	-5.01	1.45	1.53
1	A	198	CYS	CA-CB	-5.00	1.45	1.53

All (200) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	PHE	N-CA-C	16.30	129.05	111.28
1	A	18	HIS	CA-CB-CG	15.86	129.66	113.80
1	A	106	HIS	CA-CB-CG	13.05	126.85	113.80
1	A	114	PHE	CA-CB-CG	12.96	126.76	113.80
1	A	26	THR	N-CA-C	-11.17	99.16	113.12
1	A	103	ASP	CA-C-N	11.04	135.07	120.28
1	A	103	ASP	C-N-CA	11.04	135.07	120.28
1	A	235	LEU	N-CA-C	-10.86	98.15	111.40
1	A	295	ASP	CA-CB-CG	10.75	123.35	112.60
1	A	228	PHE	CA-CB-CG	10.60	124.40	113.80
1	A	169	GLU	N-CA-C	-10.53	99.34	111.03
1	A	255	PHE	CA-CB-CG	10.39	124.19	113.80
1	A	77	HIS	CA-CB-CG	-10.04	103.76	113.80
1	A	242	HIS	CA-CB-CG	9.73	123.53	113.80
1	A	35	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	A	68	ASP	CA-CB-CG	9.32	121.92	112.60
1	A	77	HIS	CB-CG-CD2	-9.14	119.32	131.20
1	A	169	GLU	CB-CA-C	-9.12	96.82	110.95
1	A	22	ASP	CA-CB-CG	9.11	121.71	112.60
1	A	169	GLU	CA-CB-CG	9.06	132.22	114.10
1	A	258	ALA	O-C-N	-9.06	112.44	123.04
1	A	242	HIS	CA-C-O	-8.97	111.46	120.70
1	A	4	GLN	OE1-CD-NE2	-8.86	113.74	122.60
1	A	221	ASP	CA-CB-CG	8.78	121.38	112.60
1	A	189	ASP	CA-CB-CG	8.26	120.86	112.60
1	A	72	ARG	CA-C-O	-8.23	111.69	120.42
1	A	100	ASP	N-CA-C	8.14	128.14	110.80
1	A	174	HIS	CB-CG-CD2	-8.14	120.62	131.20
1	A	169	GLU	N-CA-CB	8.13	121.77	109.98
1	A	202	TYR	CA-CB-CG	8.00	128.31	113.90
1	A	226	VAL	N-CA-CB	-7.96	105.48	110.50
1	A	159	ASP	N-CA-C	7.96	121.33	110.35
1	A	42	LYS	CB-CG-CD	7.85	129.36	111.30
1	A	193	MET	O-C-N	7.84	133.02	122.59
1	A	237	THR	CA-C-O	-7.83	112.25	120.55
1	A	111	ASP	N-CA-C	7.75	126.94	109.81
1	A	16	GLU	CB-CG-CD	7.61	125.54	112.60
1	A	120	GLU	N-CA-C	-7.56	103.51	112.89
1	A	207	ASN	CA-CB-CG	7.52	120.12	112.60
1	A	25	HIS	N-CA-C	7.52	126.81	110.80
1	A	238	HIS	CA-CB-CG	7.46	121.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	HIS	O-C-N	-7.44	113.82	122.89
1	A	192	THR	N-CA-C	-7.34	100.33	111.56
1	A	208	ASP	CA-CB-CG	7.33	119.92	112.60
1	A	126	ASP	CA-CB-CG	-7.32	105.28	112.60
1	A	271	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	A	2	LEU	CD1-CG-CD2	-7.29	94.76	110.80
1	A	193	MET	CA-C-O	7.28	130.92	120.51
1	A	145	VAL	O-C-N	-7.26	115.06	122.75
1	A	216	TYR	O-C-N	-7.24	114.97	123.22
1	A	45	PRO	N-CA-C	7.21	127.33	112.47
1	A	88	GLU	N-CA-C	-7.10	102.59	111.11
1	A	85	TRP	CG-CD2-CE3	7.10	141.00	133.90
1	A	113	GLU	CA-C-N	7.10	132.57	120.72
1	A	113	GLU	C-N-CA	7.10	132.57	120.72
1	A	145	VAL	N-CA-C	-7.07	99.91	108.53
1	A	303	ASN	CA-CB-CG	7.05	119.65	112.60
1	A	200	THR	N-CA-C	7.02	122.96	111.37
1	A	246	LEU	N-CA-CB	-6.95	99.46	111.55
1	A	25	HIS	CB-CG-ND1	6.92	133.07	122.70
1	A	15	ASP	N-CA-C	6.89	118.68	111.03
1	A	97	HIS	CB-CG-CD2	-6.89	122.24	131.20
1	A	70	ASN	CA-CB-CG	-6.88	105.72	112.60
1	A	119	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	A	105	GLY	O-C-N	6.77	128.69	122.19
1	A	94	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	34	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	A	44	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	114	PHE	N-CA-C	6.69	120.70	112.54
1	A	85	TRP	CB-CG-CD1	-6.69	116.87	126.90
1	A	161	ILE	N-CA-CB	-6.67	103.07	111.41
1	A	25	HIS	CB-CG-CD2	-6.65	122.56	131.20
1	A	268	ILE	N-CA-C	-6.64	103.85	110.62
1	A	63	TRP	CG-CD2-CE3	6.61	140.51	133.90
1	A	131	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	170	GLN	CA-C-O	-6.58	113.52	120.63
1	A	271	GLN	CA-CB-CG	6.56	127.22	114.10
1	A	211	LEU	CA-CB-CG	6.52	139.12	116.30
1	A	25	HIS	O-C-N	6.50	131.23	122.59
1	A	193	MET	N-CA-C	6.48	124.61	110.80
1	A	35	GLN	CG-CD-NE2	6.43	126.05	116.40
1	A	174	HIS	CB-CG-ND1	6.42	132.34	122.70
1	A	151	ARG	N-CA-C	6.37	121.21	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	182	VAL	N-CA-C	-6.34	99.23	108.11
1	A	162	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	238	HIS	CB-CG-ND1	6.32	132.17	122.70
1	A	102	THR	CA-C-N	6.31	133.60	121.54
1	A	102	THR	C-N-CA	6.31	133.60	121.54
1	A	259	HIS	CA-CB-CG	6.31	120.11	113.80
1	A	303	ASN	N-CA-C	6.25	124.11	110.80
1	A	76	GLN	N-CA-C	-6.24	104.76	112.38
1	A	218	ARG	CG-CD-NE	-6.24	98.27	112.00
1	A	119	HIS	CB-CG-ND1	6.22	132.02	122.70
1	A	297	LYS	N-CA-C	6.19	120.55	113.19
1	A	77	HIS	CB-CG-ND1	6.17	131.96	122.70
1	A	80	HIS	N-CA-C	6.17	121.57	113.30
1	A	103	ASP	O-C-N	6.16	130.78	122.59
1	A	15	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	110	LYS	N-CA-C	-6.16	97.69	110.80
1	A	84	GLU	CB-CG-CD	6.07	122.92	112.60
1	A	238	HIS	CB-CG-CD2	-6.05	123.34	131.20
1	A	90	TRP	N-CA-C	-6.04	105.57	113.12
1	A	154	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	A	180	LEU	N-CA-CB	-5.99	100.36	110.49
1	A	214	GLN	CB-CG-CD	5.99	122.78	112.60
1	A	48	THR	O-C-N	-5.98	114.20	122.46
1	A	190	VAL	N-CA-C	5.97	121.78	108.88
1	A	296	MET	N-CA-CB	-5.95	100.43	110.49
1	A	248	VAL	CA-C-O	5.94	126.62	120.39
1	A	222	ILE	N-CA-C	5.92	121.64	109.34
1	A	142	LEU	CA-C-O	5.90	126.63	119.49
1	A	28	THR	O-C-N	-5.88	116.71	123.42
1	A	268	ILE	CA-C-O	-5.86	114.85	120.95
1	A	289	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	261	TYR	N-CA-C	-5.83	102.28	110.50
1	A	83	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	168	ILE	CA-C-O	-5.81	114.20	120.47
1	A	302	LEU	N-CA-C	-5.79	100.74	109.95
1	A	39	ASP	N-CA-C	-5.78	99.77	108.96
1	A	90	TRP	CE2-CD2-CG	-5.78	100.27	107.20
1	A	100	ASP	CA-CB-CG	-5.77	106.83	112.60
1	A	156	SER	O-C-N	-5.76	115.48	122.22
1	A	185	TRP	CE2-CD2-CG	-5.75	100.30	107.20
1	A	196	PRO	CA-C-N	5.75	126.08	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	PRO	C-N-CA	5.75	126.08	119.93
1	A	168	ILE	N-CA-C	-5.75	103.91	111.09
1	A	131	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	103	ASP	CA-C-O	5.74	128.71	120.51
1	A	42	LYS	CG-CD-CE	5.71	124.44	111.30
1	A	226	VAL	CA-C-O	-5.71	113.99	118.85
1	A	162	ASP	CA-C-O	-5.71	115.50	122.41
1	A	58	LYS	CA-C-O	-5.69	114.81	121.07
1	A	189	ASP	O-C-N	-5.68	115.28	122.27
1	A	97	HIS	CB-CG-ND1	5.67	131.21	122.70
1	A	13	VAL	N-CA-C	-5.64	105.03	110.72
1	A	242	HIS	N-CA-C	-5.62	105.07	111.14
1	A	80	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	97	HIS	N-CA-C	-5.60	99.17	108.75
1	A	281	THR	O-C-N	-5.58	115.91	123.10
1	A	266	ASP	CA-CB-CG	-5.57	107.03	112.60
1	A	52	VAL	O-C-N	-5.56	116.41	121.41
1	A	214	GLN	CA-C-O	-5.55	114.71	120.70
1	A	15	ASP	CA-C-O	-5.54	115.19	120.90
1	A	292	PHE	N-CA-C	-5.53	105.79	112.54
1	A	174	HIS	CA-CB-CG	5.53	119.33	113.80
1	A	34	HIS	CB-CG-ND1	5.52	130.98	122.70
1	A	248	VAL	O-C-N	5.50	129.20	123.26
1	A	314	VAL	O-C-N	5.49	129.44	122.57
1	A	113	GLU	N-CA-C	-5.47	106.45	113.01
1	A	16	GLU	CA-CB-CG	5.45	124.99	114.10
1	A	18	HIS	CA-C-O	-5.44	115.06	121.16
1	A	180	LEU	O-C-N	-5.44	115.35	122.59
1	A	211	LEU	N-CA-C	5.44	118.68	109.76
1	A	219	SER	O-C-N	-5.43	116.56	123.24
1	A	185	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	A	85	TRP	CE2-CD2-CG	-5.42	100.70	107.20
1	A	100	ASP	CA-C-N	5.42	131.88	121.54
1	A	100	ASP	C-N-CA	5.42	131.88	121.54
1	A	17	GLY	CA-C-O	5.40	129.96	120.57
1	A	163	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	201	LEU	O-C-N	-5.39	117.11	123.41
1	A	289	HIS	CB-CG-ND1	5.38	130.76	122.70
1	A	280	PRO	O-C-N	-5.37	116.45	123.06
1	A	292	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	66	HIS	N-CA-C	-5.36	106.78	113.38
1	A	168	ILE	CA-CB-CG1	-5.36	101.29	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	HIS	N-CA-CB	-5.35	102.20	110.65
1	A	223	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	199	HIS	CB-CA-C	-5.32	104.20	112.07
1	A	50	LYS	CG-CD-CE	-5.30	99.10	111.30
1	A	243	GLU	CA-C-O	-5.29	115.25	120.70
1	A	198	CYS	N-CA-C	-5.26	105.62	111.36
1	A	314	VAL	CA-C-N	5.26	131.16	121.70
1	A	314	VAL	C-N-CA	5.26	131.16	121.70
1	A	236	LEU	CA-C-O	-5.25	115.29	120.90
1	A	149	GLN	N-CA-C	-5.25	103.53	111.56
1	A	117	VAL	CA-CB-CG2	-5.24	101.49	110.40
1	A	149	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	195	LEU	N-CA-C	-5.21	99.15	109.10
1	A	195	LEU	CA-C-N	5.21	125.74	120.38
1	A	195	LEU	C-N-CA	5.21	125.74	120.38
1	A	25	HIS	CA-C-O	5.19	127.94	120.51
1	A	259	HIS	N-CA-C	5.18	117.86	109.06
1	A	309	ALA	CA-C-O	-5.17	115.70	121.81
1	A	4	GLN	CB-CG-CD	5.13	121.33	112.60
1	A	226	VAL	CA-C-N	5.13	124.75	119.05
1	A	226	VAL	C-N-CA	5.13	124.75	119.05
1	A	241	ALA	CB-CA-C	-5.12	101.98	110.68
1	A	32	PHE	CA-CB-CG	-5.12	108.69	113.80
1	A	136	ALA	N-CA-C	-5.12	105.70	111.28
1	A	27	GLY	CA-C-O	-5.11	118.19	122.33
1	A	218	ARG	N-CA-C	5.10	116.91	111.36
1	A	74	LEU	N-CA-C	-5.09	105.64	111.14
1	A	63	TRP	N-CA-C	-5.06	105.45	110.97
1	A	303	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	61	LEU	CA-C-O	-5.04	115.07	120.42
1	A	275	THR	CA-C-N	5.02	125.02	119.90
1	A	275	THR	C-N-CA	5.02	125.02	119.90
1	A	110	LYS	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Mainchain
1	A	20	LYS	Peptide
1	A	205	TYR	Sidechain
1	A	98	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2580	0	2479	65	0
2	A	34	0	21	6	0
3	A	21	0	9	0	0
4	A	9	0	0	0	0
All	All	2644	0	2509	65	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 13.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PRO:HB2	1:A:301:LEU:HD11	1.57	0.86
1:A:271:GLN:HA	1:A:274:ARG:HD2	1.61	0.82
1:A:262:VAL:HA	1:A:265:LEU:HD23	1.63	0.79
1:A:21:PRO:HA	1:A:25:HIS:CE1	2.21	0.75
1:A:101:MET:HE2	1:A:118:TYR:HD1	1.51	0.75
1:A:26:THR:HG1	1:A:261:TYR:HD1	1.36	0.71
1:A:223:PHE:HE2	1:A:312:ALA:HB3	1.56	0.70
1:A:13:VAL:HG11	1:A:260:LEU:HB2	1.73	0.69
1:A:175:PRO:HB2	1:A:176:TYR:HD1	1.59	0.68
1:A:84:GLU:HB3	2:A:568:THF:HN21	1.59	0.66
1:A:51:LYS:HB3	1:A:309:ALA:HB2	1.81	0.63
1:A:104:PHE:HD1	1:A:105:GLY:H	1.46	0.62
1:A:104:PHE:HD1	1:A:105:GLY:N	1.97	0.62
1:A:84:GLU:O	1:A:88:GLU:HB2	2.01	0.61
1:A:153:TRP:HB3	1:A:161:ILE:HB	1.82	0.60
1:A:13:VAL:O	1:A:17:GLY:HA3	2.00	0.60
1:A:112:PRO:HB2	1:A:114:PHE:H	1.67	0.59
1:A:21:PRO:HA	1:A:25:HIS:NE2	2.17	0.59
1:A:85:TRP:NE1	2:A:568:THF:HN1	2.01	0.59
1:A:268:ILE:O	1:A:272:LEU:HD23	2.03	0.59
1:A:262:VAL:O	1:A:265:LEU:HB2	2.03	0.58
1:A:26:THR:OG1	1:A:261:TYR:HD1	1.87	0.56
1:A:126:ASP:O	1:A:130:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:O	1:A:149:GLN:HG2	2.06	0.56
1:A:69:THR:HG22	1:A:145:VAL:HG12	1.89	0.55
1:A:311:LYS:HD3	1:A:311:LYS:H	1.72	0.55
1:A:260:LEU:HD22	1:A:265:LEU:HD22	1.88	0.55
1:A:271:GLN:HB3	1:A:310:ILE:CD1	2.37	0.55
1:A:36:MET:HE3	1:A:38:PHE:CE1	2.43	0.54
1:A:84:GLU:CD	2:A:568:THF:HN22	2.16	0.54
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.42	0.53
1:A:101:MET:HE2	1:A:118:TYR:CD1	2.38	0.53
1:A:72:ARG:HH22	1:A:133:ASP:HA	1.72	0.53
1:A:274:ARG:HB3	1:A:307:TYR:HE2	1.74	0.52
1:A:104:PHE:CD1	1:A:105:GLY:N	2.78	0.51
1:A:200:THR:HG22	1:A:201:LEU:HB2	1.91	0.51
1:A:193:MET:HE2	1:A:195:LEU:O	2.11	0.51
1:A:112:PRO:HB2	1:A:114:PHE:HB3	1.94	0.50
1:A:274:ARG:HB3	1:A:307:TYR:CE2	2.46	0.50
1:A:271:GLN:O	1:A:274:ARG:HB2	2.11	0.49
1:A:101:MET:HE1	1:A:117:VAL:HG12	1.95	0.48
1:A:1:MET:HG2	1:A:276:PRO:HB2	1.97	0.47
1:A:25:HIS:CE1	1:A:27:GLY:HA2	2.50	0.47
1:A:187:PRO:O	1:A:190:VAL:HG22	2.14	0.47
1:A:120:GLU:O	1:A:124:LYS:HG3	2.15	0.47
1:A:84:GLU:HB3	2:A:568:THF:NA2	2.30	0.44
1:A:90:TRP:CZ3	1:A:95:GLU:HB3	2.53	0.44
1:A:274:ARG:NH2	1:A:308:PRO:HD2	2.33	0.44
1:A:188:GLU:O	1:A:191:PRO:HD2	2.18	0.43
1:A:56:LEU:HB3	1:A:81:ILE:HD11	2.00	0.43
1:A:84:GLU:CD	2:A:568:THF:NA2	2.76	0.43
1:A:13:VAL:HG21	1:A:222:ILE:HG13	2.01	0.43
1:A:175:PRO:HB2	1:A:176:TYR:CD1	2.46	0.43
1:A:88:GLU:HG3	1:A:104:PHE:CZ	2.54	0.42
1:A:265:LEU:O	1:A:268:ILE:HG22	2.20	0.42
1:A:36:MET:HE3	1:A:38:PHE:CZ	2.53	0.42
1:A:271:GLN:HB3	1:A:310:ILE:HD12	2.01	0.42
1:A:223:PHE:CE2	1:A:312:ALA:HB3	2.46	0.41
1:A:27:GLY:O	1:A:28:THR:HG23	2.20	0.41
1:A:261:TYR:HB2	1:A:264:HIS:ND1	2.36	0.41
1:A:164:LEU:HD22	1:A:168:ILE:HD12	2.03	0.41
1:A:159:ASP:CG	1:A:160:THR:H	2.29	0.40
1:A:199:HIS:CD2	1:A:217:GLN:HG3	2.56	0.40
1:A:84:GLU:OE1	2:A:568:THF:NA2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD22	1:A:80:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	313/315 (99%)	266 (85%)	36 (12%)	11 (4%)	3 6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	92	LYS
1	A	99	PRO
1	A	102	THR
1	A	314	VAL
1	A	296	MET
1	A	101	MET
1	A	180	LEU
1	A	193	MET
1	A	194	ALA
1	A	303	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	275/277 (99%)	227 (82%)	48 (18%)	2 5

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	7	LEU
1	A	9	LEU
1	A	16	GLU
1	A	18	HIS
1	A	20	LYS
1	A	21	PRO
1	A	25	HIS
1	A	35	GLN
1	A	42	LYS
1	A	49	THR
1	A	59	SER
1	A	71	ILE
1	A	74	LEU
1	A	88	GLU
1	A	89	LYS
1	A	94	ASP
1	A	100	ASP
1	A	101	MET
1	A	102	THR
1	A	104	PHE
1	A	108	SER
1	A	109	GLN
1	A	114	PHE
1	A	117	VAL
1	A	120	GLU
1	A	121	GLU
1	A	130	LEU
1	A	163	GLN
1	A	164	LEU
1	A	173	THR
1	A	180	LEU
1	A	187	PRO
1	A	195	LEU
1	A	207	ASN
1	A	215	LEU
1	A	239	LEU

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Mol	Chain	Res	Type
1	A	260	LEU
1	A	265	LEU
1	A	266	ASP
1	A	270	GLU
1	A	271	GLN
1	A	281	THR
1	A	295	ASP
1	A	296	MET
1	A	303	ASN
1	A	311	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	217	GLN
1	A	229	ASN
1	A	253	HIS
1	A	263	ASN
1	A	271	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	UFP	A	529	-	22,22,22	2.74	7 (31%)	32,33,33	2.61	12 (37%)
2	THF	A	568	-	32,36,36	2.75	9 (28%)	37,50,50	2.83	17 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UFP	A	529	-	1/1/4/4	1/10/22/22	0/2/2/2
2	THF	A	568	-	-	10/22/37/37	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	568	THF	O4-C4	8.77	1.39	1.23
3	A	529	UFP	C6-C5	7.49	1.43	1.33
3	A	529	UFP	C4-C5	5.69	1.51	1.44
2	A	568	THF	C2-NA2	5.63	1.47	1.34
2	A	568	THF	C7-N8	5.51	1.35	1.28
2	A	568	THF	C2-N3	-5.18	1.20	1.33
3	A	529	UFP	O4'-C1'	-4.12	1.33	1.42
2	A	568	THF	CP1-N5	3.81	1.50	1.45
3	A	529	UFP	C2-N1	3.77	1.44	1.38
3	A	529	UFP	C2'-C1'	-3.18	1.43	1.52
3	A	529	UFP	O4'-C4'	2.82	1.51	1.45
2	A	568	THF	CB-CA	-2.58	1.47	1.53
3	A	529	UFP	P-O5'	2.48	1.68	1.60
2	A	568	THF	CG-CD	2.35	1.56	1.50
2	A	568	THF	C14-N10	2.30	1.45	1.38
2	A	568	THF	C8A-N1	-2.10	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	529	UFP	O4'-C1'-C2'	7.65	120.53	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	568	THF	C7-N8-C8A	6.96	121.69	115.47
2	A	568	THF	N1-C2-N3	6.87	135.90	123.32
2	A	568	THF	C8A-C4A-N5	-6.74	110.72	119.80
2	A	568	THF	NA2-C2-N3	-5.28	109.36	119.67
3	A	529	UFP	C2'-C1'-N1	5.11	126.58	113.81
2	A	568	THF	CT-CA-N	4.82	121.75	110.57
3	A	529	UFP	C1'-N1-C6	-4.76	112.75	120.74
3	A	529	UFP	O2P-P-O5'	-4.29	95.48	106.67
3	A	529	UFP	C1'-N1-C2	4.20	125.88	117.66
3	A	529	UFP	C4'-O4'-C1'	-3.83	100.41	109.51
2	A	568	THF	C12-C13-C14	-3.82	115.90	120.30
3	A	529	UFP	N3-C2-N1	3.43	119.35	114.89
2	A	568	THF	C11-C-N	3.00	122.60	117.04
3	A	529	UFP	O4'-C1'-N1	2.81	112.84	107.86
3	A	529	UFP	O2-C2-N3	-2.63	116.63	121.49
3	A	529	UFP	O3P-P-O2P	2.56	117.39	107.80
3	A	529	UFP	C4-N3-C2	-2.46	124.11	127.34
2	A	568	THF	C13-C14-N10	-2.46	115.41	120.96
2	A	568	THF	C15-C16-C11	-2.45	118.18	120.80
2	A	568	THF	O4-C4-N3	2.40	124.31	120.27
3	A	529	UFP	O4-C4-C5	2.32	127.66	125.69
2	A	568	THF	C15-C14-C13	2.27	122.06	119.04
2	A	568	THF	C6-C9-N10	-2.27	106.93	111.80
2	A	568	THF	O3-CP1-N5	2.24	118.11	112.31
2	A	568	THF	CB-CA-CT	2.16	115.47	110.35
2	A	568	THF	C13-C12-C11	2.06	123.00	120.80
2	A	568	THF	CB-CG-CD	2.02	117.88	112.49
2	A	568	THF	O-C-N	-2.01	118.64	122.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	529	UFP	C1'

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	568	THF	N5-C6-C9-N10
2	A	568	THF	C7-C6-C9-N10
2	A	568	THF	N-CA-CB-CG
2	A	568	THF	CT-CA-CB-CG
2	A	568	THF	N-CA-CT-O2

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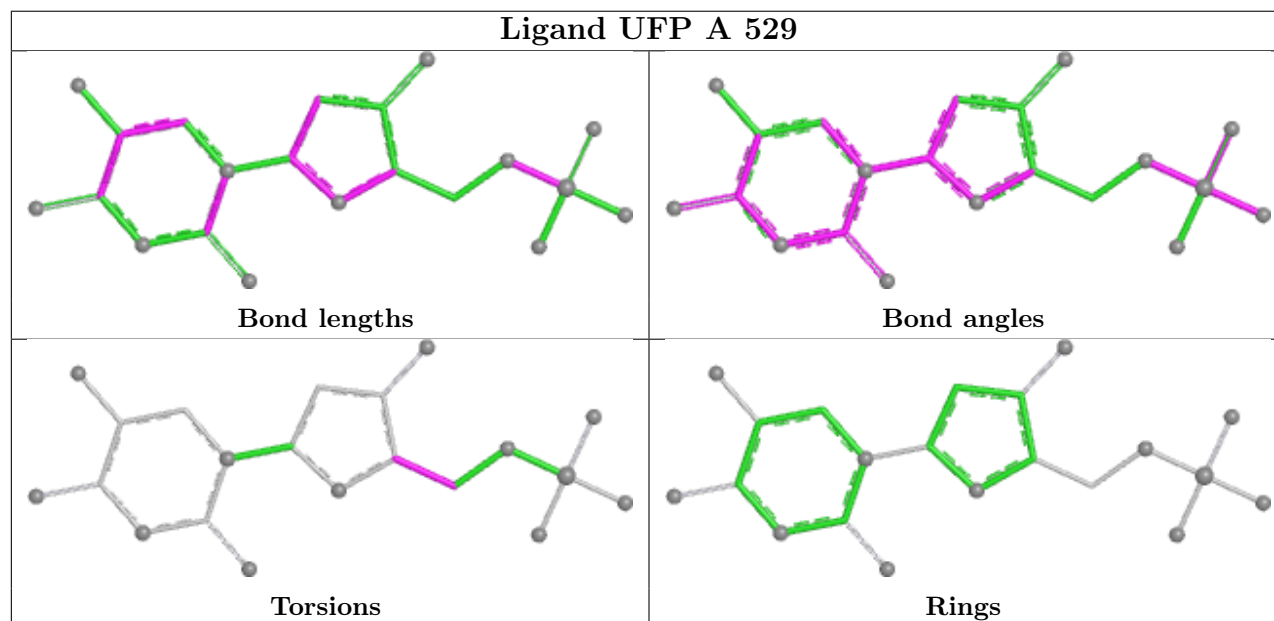
Mol	Chain	Res	Type	Atoms
2	A	568	THF	O-C-N-CA
2	A	568	THF	C11-C-N-CA
2	A	568	THF	N-CA-CT-O1
2	A	568	THF	CA-CB-CG-CD
3	A	529	UFP	O4'-C4'-C5'-O5'
2	A	568	THF	OE2-CD-CG-CB

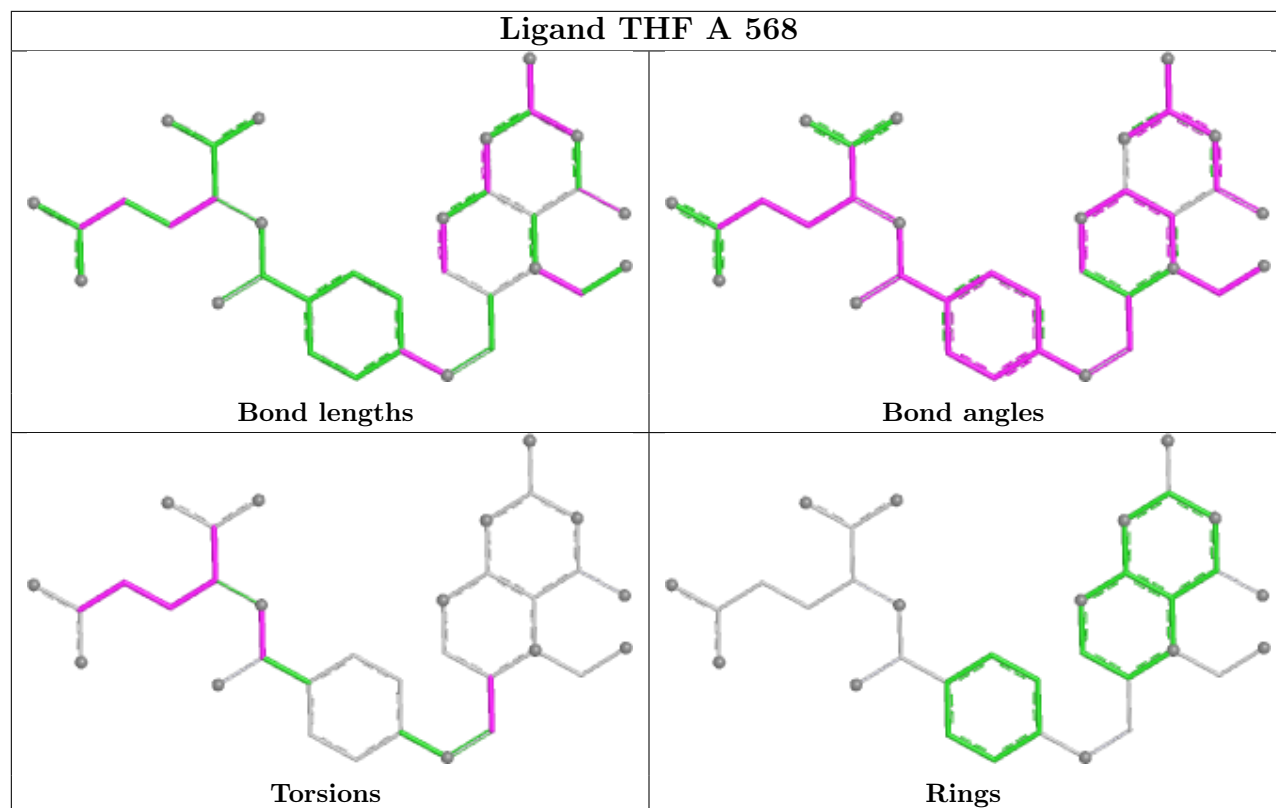
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	568	THF	6	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.