



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:01 PM UTC

PDB ID : 1VZC / pdb_00001vzc
Title : L. CASEI THYMIDYLATE SYNTHASE MUTANT E60Q BINARY COM-
PLEX WITH FDUMP
Authors : Birdsall, D.L.; Finer-Moore, J.; Stroud, R.M.
Deposited on : 1996-09-18
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

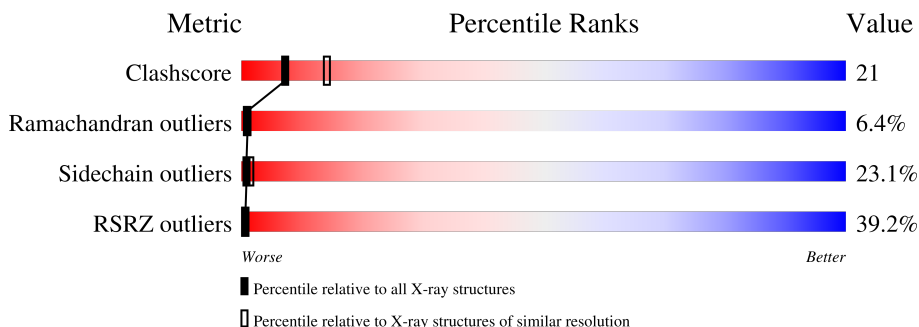
1 Overall quality at a glance

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	39% 23% 43% 26% 7%

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	UFP	A	317	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3267 atoms, of which 615 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.

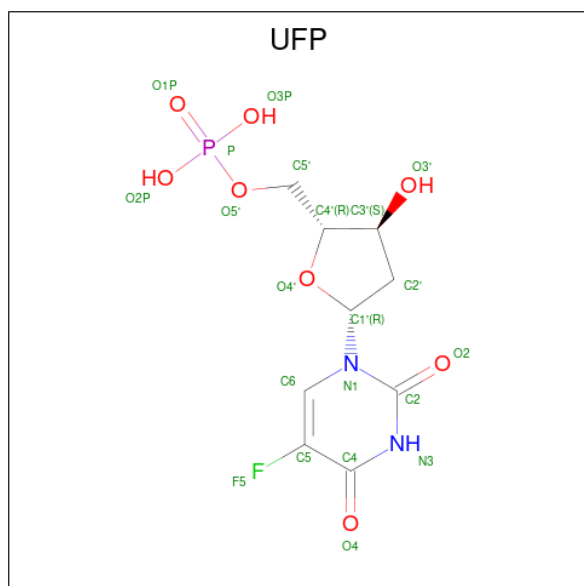
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	316	3122	1677	532	439	466	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	engineered mutation	UNP P00469
A	111	ALA	ASP	conflict	UNP P00469

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	F	H	N	O	P		
2	A	1	22	9	1	1	2	8	1	0	0

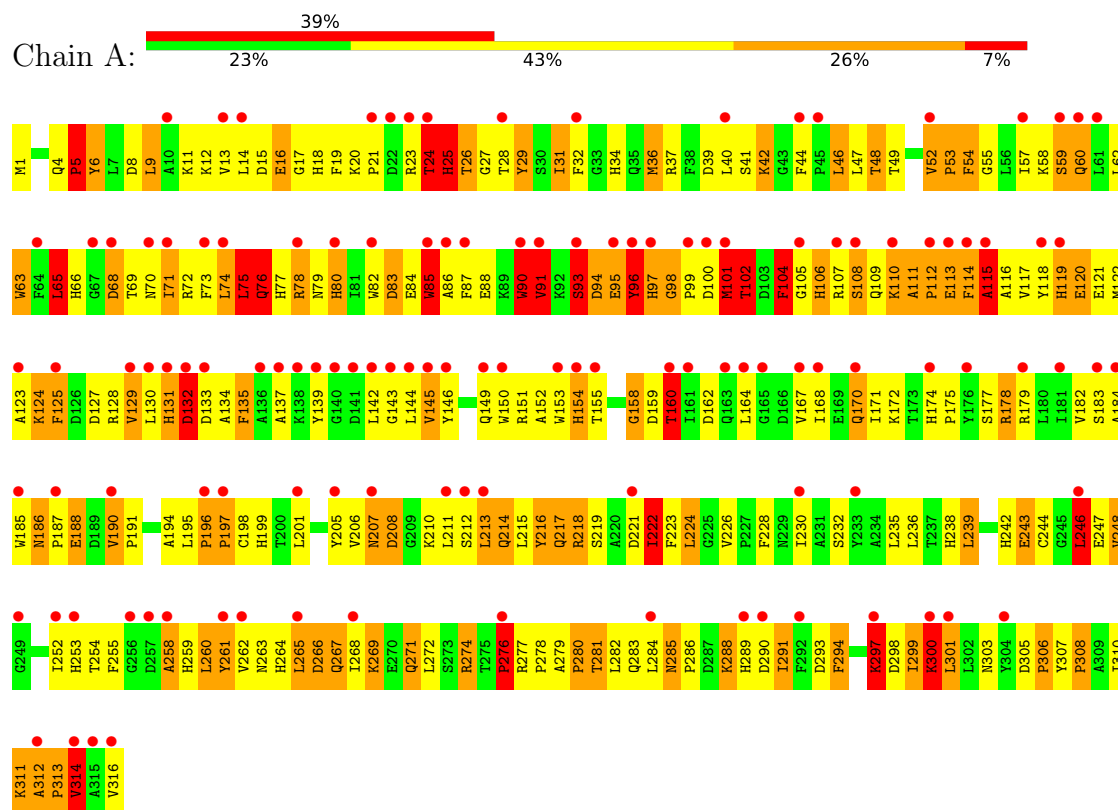
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	41	Total	H	O	0	0
			123	82	41		

3 Residue-property plots [i](#)

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	79.50Å 79.50Å 229.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 59.8 (15.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.05Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.201 , (Not available) 0.322 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	3267	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 4.62% 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: 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	1.93	76/2674 (2.8%)	2.63	247/3634 (6.8%)

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	8

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	HIS	CD2-NE2	-7.66	1.29	1.37
1	A	259	HIS	CD2-NE2	-7.64	1.29	1.37
1	A	63	TRP	CA-CB	-7.29	1.42	1.53
1	A	66	HIS	CD2-NE2	-7.24	1.29	1.37
1	A	264	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	77	HIS	CG-ND1	-7.03	1.30	1.38
1	A	23	ARG	NE-CZ	6.99	1.40	1.33
1	A	91	VAL	CA-CB	6.93	1.62	1.54
1	A	242	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	206	VAL	CA-CB	6.75	1.63	1.54
1	A	25	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	146	TYR	CA-CB	-6.58	1.42	1.53
1	A	230	ILE	CA-CB	-6.50	1.46	1.54
1	A	221	ASP	CA-CB	-6.40	1.45	1.53
1	A	255	PHE	CA-CB	-6.36	1.43	1.53
1	A	314	VAL	CA-CB	6.32	1.63	1.54
1	A	150	TRP	NE1-CE2	-6.28	1.30	1.37
1	A	119	HIS	CA-C	6.22	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	253	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	218	ARG	CA-CB	-6.14	1.43	1.53
1	A	26	THR	CA-CB	6.10	1.62	1.53
1	A	54	PHE	CA-CB	-6.09	1.42	1.53
1	A	197	PRO	CA-CB	-6.02	1.46	1.53
1	A	80	HIS	CG-ND1	-5.97	1.31	1.38
1	A	164	LEU	CA-CB	-5.96	1.44	1.53
1	A	127	ASP	CA-CB	-5.96	1.46	1.53
1	A	199	HIS	CG-ND1	-5.94	1.31	1.38
1	A	238	HIS	CG-ND1	-5.93	1.31	1.38
1	A	20	LYS	CA-C	5.92	1.57	1.52
1	A	299	ILE	CA-CB	5.92	1.62	1.54
1	A	135	PHE	CA-CB	-5.90	1.44	1.53
1	A	77	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	259	HIS	CG-ND1	-5.89	1.31	1.38
1	A	253	HIS	CA-CB	-5.85	1.45	1.53
1	A	82	TRP	CA-CB	-5.83	1.45	1.53
1	A	133	ASP	CA-CB	-5.79	1.44	1.53
1	A	174	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	308	PRO	CA-CB	-5.75	1.45	1.53
1	A	290	ASP	CA-CB	-5.74	1.43	1.53
1	A	150	TRP	CG-CD2	-5.73	1.33	1.43
1	A	77	HIS	CA-CB	-5.66	1.45	1.53
1	A	119	HIS	CB-CG	5.61	1.58	1.50
1	A	46	LEU	CA-CB	-5.58	1.44	1.53
1	A	306	PRO	CA-CB	-5.58	1.45	1.53
1	A	264	HIS	CG-ND1	-5.56	1.32	1.38
1	A	125	PHE	CA-CB	-5.56	1.44	1.53
1	A	253	HIS	CG-ND1	-5.54	1.32	1.38
1	A	301	LEU	CA-CB	-5.54	1.45	1.53
1	A	158	GLY	C-N	5.53	1.41	1.33
1	A	65	LEU	CA-CB	-5.52	1.43	1.53
1	A	177	SER	CA-CB	-5.50	1.44	1.53
1	A	238	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	11	LYS	CA-CB	-5.48	1.44	1.53
1	A	185	TRP	CA-CB	-5.44	1.44	1.53
1	A	36	MET	CA-CB	-5.39	1.44	1.53
1	A	74	LEU	CA-CB	-5.37	1.44	1.53
1	A	217	GLN	CA-CB	-5.34	1.46	1.53
1	A	188	GLU	CA-CB	-5.30	1.45	1.53
1	A	34	HIS	CG-ND1	-5.27	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	PHE	CA-CB	-5.25	1.44	1.53
1	A	37	ARG	CA-CB	-5.25	1.44	1.53
1	A	210	LYS	CA-CB	-5.23	1.45	1.53
1	A	212	SER	CA-CB	-5.22	1.44	1.53
1	A	110	LYS	N-CA	5.18	1.52	1.46
1	A	294	PHE	CA-CB	-5.17	1.45	1.53
1	A	102	THR	CA-CB	5.16	1.62	1.53
1	A	297	LYS	CA-CB	-5.13	1.46	1.52
1	A	34	HIS	CD2-NE2	-5.13	1.32	1.37
1	A	196	PRO	CA-CB	-5.13	1.47	1.54
1	A	280	PRO	CA-CB	-5.11	1.46	1.53
1	A	276	PRO	CA-CB	-5.10	1.46	1.53
1	A	8	ASP	CA-CB	-5.09	1.44	1.53
1	A	267	GLN	CA-CB	-5.07	1.45	1.53
1	A	32	PHE	CA-CB	-5.04	1.45	1.53
1	A	119	HIS	CD2-NE2	-5.02	1.32	1.37

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	PHE	CA-CB-CG	14.94	128.74	113.80
1	A	174	HIS	CA-CB-CG	12.74	126.54	113.80
1	A	25	HIS	N-CA-C	12.21	136.81	110.80
1	A	207	ASN	CA-CB-CG	11.15	123.75	112.60
1	A	66	HIS	CA-CB-CG	10.78	124.58	113.80
1	A	27	GLY	N-CA-C	-10.66	101.82	111.95
1	A	109	GLN	OE1-CD-NE2	-10.55	112.05	122.60
1	A	97	HIS	N-CA-C	-10.27	95.23	109.71
1	A	94	ASP	N-CA-C	-10.12	100.08	111.82
1	A	199	HIS	ND1-CG-CD2	10.09	116.19	106.10
1	A	15	ASP	N-CA-C	9.61	121.70	111.03
1	A	66	HIS	CB-CA-C	-9.46	93.95	109.56
1	A	97	HIS	CA-CB-CG	9.45	123.25	113.80
1	A	109	GLN	CB-CG-CD	9.41	128.59	112.60
1	A	57	ILE	N-CA-C	-9.19	101.39	110.30
1	A	208	ASP	CA-CB-CG	9.14	121.75	112.60
1	A	210	LYS	N-CA-C	9.12	124.72	109.76
1	A	289	HIS	ND1-CG-CD2	9.11	115.21	106.10
1	A	111	ALA	N-CA-C	9.03	129.76	109.81
1	A	281	THR	CA-CB-OG1	-8.94	96.19	109.60
1	A	110	LYS	N-CA-C	8.92	129.80	110.80
1	A	68	ASP	CA-CB-CG	8.78	121.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLN	OE1-CD-NE2	-8.77	113.83	122.60
1	A	77	HIS	ND1-CG-CD2	8.70	114.80	106.10
1	A	25	HIS	ND1-CG-CD2	8.65	114.75	106.10
1	A	19	PHE	CA-CB-CG	8.62	122.42	113.80
1	A	100	ASP	CA-CB-CG	8.58	121.18	112.60
1	A	66	HIS	ND1-CG-CD2	8.46	114.56	106.10
1	A	269	LYS	N-CA-C	-8.45	102.01	111.14
1	A	114	PHE	N-CA-C	-8.35	101.71	112.23
1	A	120	GLU	CB-CG-CD	8.31	126.73	112.60
1	A	145	VAL	N-CA-C	-8.29	96.63	108.65
1	A	85	TRP	CB-CG-CD1	-8.16	114.66	126.90
1	A	66	HIS	CB-CG-CD2	-8.10	120.67	131.20
1	A	69	THR	N-CA-C	-8.05	103.48	113.38
1	A	101	MET	N-CA-C	8.05	122.77	113.19
1	A	242	HIS	CA-CB-CG	7.98	121.78	113.80
1	A	186	ASN	OD1-CG-ND2	-7.81	114.79	122.60
1	A	160	THR	CA-CB-OG1	-7.75	97.97	109.60
1	A	298	ASP	N-CA-C	-7.62	102.50	112.41
1	A	106	HIS	ND1-CG-CD2	7.61	113.71	106.10
1	A	300	LYS	CB-CG-CD	7.60	128.78	111.30
1	A	98	GLY	CA-C-N	7.54	129.27	119.84
1	A	98	GLY	C-N-CA	7.54	129.27	119.84
1	A	174	HIS	CA-C-N	7.53	127.41	119.05
1	A	174	HIS	C-N-CA	7.53	127.41	119.05
1	A	175	PRO	N-CA-C	7.42	123.84	113.53
1	A	85	TRP	CG-CD2-CE3	7.39	141.29	133.90
1	A	286	PRO	N-CA-C	7.38	123.11	114.03
1	A	96	TYR	O-C-N	7.36	131.76	122.93
1	A	218	ARG	N-CA-C	7.32	122.62	112.45
1	A	34	HIS	ND1-CG-CD2	7.30	113.40	106.10
1	A	12	LYS	CA-C-O	-7.27	113.07	121.07
1	A	104	PHE	N-CA-C	7.27	126.29	110.80
1	A	48	THR	O-C-N	-7.25	113.89	122.15
1	A	109	GLN	CG-CD-NE2	7.23	127.25	116.40
1	A	70	ASN	CA-C-O	7.22	128.70	120.54
1	A	254	THR	CA-C-O	7.21	128.24	120.38
1	A	101	MET	CA-CB-CG	-7.21	99.69	114.10
1	A	242	HIS	CA-C-O	-7.20	110.52	119.38
1	A	303	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	A	154	HIS	CA-CB-CG	7.12	120.92	113.80
1	A	5	PRO	CA-N-CD	-7.10	102.06	112.00
1	A	39	ASP	CA-CB-CG	7.07	119.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	LYS	CA-C-O	-6.98	113.05	120.80
1	A	300	LYS	CG-CD-CE	6.95	127.28	111.30
1	A	96	TYR	N-CA-CB	6.91	121.20	110.21
1	A	266	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	98	GLY	O-C-N	6.89	128.66	121.77
1	A	66	HIS	N-CA-CB	6.86	120.92	110.42
1	A	253	HIS	ND1-CG-CD2	6.84	112.94	106.10
1	A	190	VAL	CA-C-O	-6.76	113.11	118.85
1	A	199	HIS	CG-CD2-NE2	-6.76	100.44	107.20
1	A	6	TYR	O-C-N	-6.75	114.96	122.12
1	A	259	HIS	N-CA-C	6.73	120.37	109.40
1	A	264	HIS	ND1-CG-CD2	6.73	112.83	106.10
1	A	172	LYS	CB-CG-CD	6.71	126.73	111.30
1	A	129	VAL	CB-CA-C	-6.64	100.39	111.29
1	A	179	ARG	NE-CZ-NH1	6.64	128.14	121.50
1	A	80	HIS	ND1-CG-CD2	6.61	112.71	106.10
1	A	281	THR	CA-CB-CG2	6.59	121.70	110.50
1	A	88	GLU	N-CA-C	-6.58	103.60	111.69
1	A	106	HIS	CG-CD2-NE2	-6.54	100.66	107.20
1	A	9	LEU	N-CA-C	-6.53	103.37	112.45
1	A	162	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	297	LYS	CA-CB-CG	-6.51	101.09	114.10
1	A	18	HIS	ND1-CG-CD2	6.50	112.61	106.10
1	A	90	TRP	CB-CA-C	-6.45	100.95	110.95
1	A	24	THR	N-CA-CB	-6.44	99.61	110.49
1	A	207	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	A	84	GLU	CA-C-N	6.38	131.48	120.58
1	A	84	GLU	C-N-CA	6.38	131.48	120.58
1	A	259	HIS	ND1-CG-CD2	6.38	112.48	106.10
1	A	91	VAL	CA-C-O	-6.37	114.43	121.05
1	A	78	ARG	CA-CB-CG	6.35	126.81	114.10
1	A	93	SER	N-CA-C	6.31	124.24	110.80
1	A	222	ILE	CB-CA-C	-6.28	102.42	112.16
1	A	310	ILE	N-CA-C	-6.28	99.47	109.20
1	A	289	HIS	CA-CB-CG	-6.27	107.53	113.80
1	A	27	GLY	CA-C-O	-6.27	118.14	122.22
1	A	174	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	A	109	GLN	N-CA-C	-6.26	105.61	113.18
1	A	182	VAL	N-CA-C	-6.26	99.11	108.12
1	A	142	LEU	N-CA-C	6.24	121.68	113.20
1	A	90	TRP	N-CA-CB	6.22	118.99	109.98
1	A	101	MET	CA-C-N	6.20	133.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	MET	C-N-CA	6.20	133.38	121.54
1	A	73	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	57	ILE	O-C-N	6.15	128.28	121.94
1	A	53	PRO	N-CA-C	6.12	125.08	112.47
1	A	108	SER	N-CA-C	-6.08	105.86	113.28
1	A	242	HIS	ND1-CG-CD2	6.06	112.16	106.10
1	A	77	HIS	CA-CB-CG	-6.06	107.74	113.80
1	A	228	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	146	TYR	CA-CB-CG	-6.03	103.05	113.90
1	A	96	TYR	CA-C-N	6.02	130.42	122.06
1	A	96	TYR	C-N-CA	6.02	130.42	122.06
1	A	72	ARG	CA-C-O	-5.99	114.49	120.90
1	A	260	LEU	O-C-N	-5.98	116.03	122.85
1	A	308	PRO	N-CD-CG	-5.97	94.24	103.20
1	A	271	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	59	SER	CA-C-O	-5.95	114.24	120.55
1	A	16	GLU	CB-CG-CD	5.95	122.71	112.60
1	A	124	LYS	N-CA-C	-5.94	104.38	111.69
1	A	70	ASN	N-CA-C	5.92	119.30	109.46
1	A	88	GLU	CA-CB-CG	5.91	125.92	114.10
1	A	84	GLU	CA-CB-CG	5.88	125.86	114.10
1	A	66	HIS	CG-CD2-NE2	-5.88	101.32	107.20
1	A	248	VAL	N-CA-CB	-5.87	101.64	112.43
1	A	274	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	A	186	ASN	CB-CA-C	-5.82	104.41	110.17
1	A	125	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	285	ASN	CA-C-N	5.77	125.87	119.87
1	A	285	ASN	C-N-CA	5.77	125.87	119.87
1	A	23	ARG	CB-CG-CD	5.76	124.55	111.30
1	A	145	VAL	O-C-N	5.74	129.32	122.95
1	A	185	TRP	O-C-N	5.72	130.44	123.01
1	A	248	VAL	CG1-CB-CG2	-5.72	98.22	110.80
1	A	14	LEU	N-CA-C	-5.71	104.43	111.40
1	A	116	ALA	N-CA-C	5.68	119.68	112.87
1	A	131	HIS	ND1-CG-CD2	5.66	111.76	106.10
1	A	90	TRP	CE2-CD2-CG	-5.66	100.41	107.20
1	A	199	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	311	LYS	CG-CD-CE	5.64	124.27	111.30
1	A	95	GLU	CB-CG-CD	5.64	122.18	112.60
1	A	93	SER	CA-C-O	5.59	128.50	120.51
1	A	201	LEU	N-CA-CB	-5.58	102.34	111.66
1	A	117	VAL	CA-C-N	5.58	128.07	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	VAL	C-N-CA	5.58	128.07	120.54
1	A	151	ARG	N-CA-C	5.57	120.73	113.88
1	A	36	MET	CB-CG-SD	-5.55	96.04	112.70
1	A	85	TRP	CE2-CD2-CG	-5.55	100.54	107.20
1	A	269	LYS	CA-C-O	-5.54	114.99	120.70
1	A	44	PHE	CA-CB-CG	-5.53	108.27	113.80
1	A	170	GLN	CB-CG-CD	5.53	122.00	112.60
1	A	55	GLY	N-CA-C	5.52	118.91	112.50
1	A	21	PRO	N-CA-CB	5.52	109.04	103.25
1	A	123	ALA	N-CA-C	-5.51	105.82	112.54
1	A	207	ASN	CB-CG-ND2	5.50	124.65	116.40
1	A	29	TYR	CA-CB-CG	-5.48	104.03	113.90
1	A	65	LEU	N-CA-CB	-5.48	100.34	110.32
1	A	90	TRP	CG-CD2-CE3	5.48	139.38	133.90
1	A	214	GLN	CB-CG-CD	5.48	121.92	112.60
1	A	242	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	A	183	SER	CA-C-N	5.46	130.50	121.99
1	A	183	SER	C-N-CA	5.46	130.50	121.99
1	A	77	HIS	CG-CD2-NE2	-5.45	101.75	107.20
1	A	160	THR	CA-CB-CG2	5.45	119.76	110.50
1	A	258	ALA	N-CA-C	-5.44	99.86	108.73
1	A	84	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	63	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	A	119	HIS	O-C-N	-5.43	116.48	122.07
1	A	76	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	34	HIS	CG-CD2-NE2	-5.41	101.79	107.20
1	A	211	LEU	CB-CA-C	-5.41	101.89	110.81
1	A	79	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	238	HIS	ND1-CG-CD2	5.40	111.50	106.10
1	A	186	ASN	CA-C-N	5.40	126.58	119.84
1	A	186	ASN	C-N-CA	5.40	126.58	119.84
1	A	82	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	A	106	HIS	CA-C-O	-5.39	112.80	120.51
1	A	131	HIS	CB-CA-C	-5.38	104.39	112.09
1	A	149	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	A	4	GLN	CA-C-O	-5.33	112.86	120.16
1	A	178	ARG	N-CA-C	-5.32	106.63	113.02
1	A	25	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	279	ALA	CA-C-N	5.31	125.31	120.21
1	A	279	ALA	C-N-CA	5.31	125.31	120.21
1	A	60	GLN	CG-CD-NE2	5.30	124.35	116.40
1	A	18	HIS	CG-CD2-NE2	-5.28	101.92	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LYS	CA-C-N	5.28	134.69	121.80
1	A	110	LYS	C-N-CA	5.28	134.69	121.80
1	A	155	THR	N-CA-CB	-5.28	102.89	110.44
1	A	4	GLN	CA-C-N	5.27	126.43	119.84
1	A	4	GLN	C-N-CA	5.27	126.43	119.84
1	A	267	GLN	CB-CA-C	-5.26	101.95	110.79
1	A	246	LEU	CA-C-O	5.25	127.59	121.44
1	A	11	LYS	CB-CG-CD	-5.25	99.22	111.30
1	A	69	THR	O-C-N	-5.25	115.54	122.42
1	A	289	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	A	194	ALA	N-CA-C	-5.25	105.21	111.03
1	A	78	ARG	N-CA-CB	-5.23	104.77	112.78
1	A	21	PRO	CA-C-N	-5.23	113.59	123.27
1	A	21	PRO	C-N-CA	-5.23	113.59	123.27
1	A	216	TYR	CA-C-O	5.22	126.65	120.70
1	A	238	HIS	CA-CB-CG	5.22	119.02	113.80
1	A	75	LEU	CD1-CG-CD2	-5.22	99.32	110.80
1	A	226	VAL	CA-C-N	5.21	125.26	119.32
1	A	226	VAL	C-N-CA	5.21	125.26	119.32
1	A	23	ARG	CA-CB-CG	5.20	124.51	114.10
1	A	132	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	4	GLN	CB-CG-CD	5.19	121.43	112.60
1	A	37	ARG	N-CA-C	5.18	117.34	108.90
1	A	102	THR	N-CA-CB	-5.17	101.75	110.49
1	A	85	TRP	N-CA-C	5.17	118.05	111.69
1	A	71	ILE	CA-CB-CG2	5.17	119.29	110.50
1	A	264	HIS	CA-CB-CG	5.16	118.96	113.80
1	A	213	LEU	CD1-CG-CD2	-5.15	99.47	110.80
1	A	70	ASN	CA-C-N	5.14	127.51	120.46
1	A	70	ASN	C-N-CA	5.14	127.51	120.46
1	A	115	ALA	O-C-N	-5.14	115.75	122.59
1	A	291	ILE	CA-C-O	5.14	126.23	119.85
1	A	172	LYS	O-C-N	-5.13	115.56	122.23
1	A	34	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	253	HIS	CG-CD2-NE2	-5.09	102.11	107.20
1	A	208	ASP	N-CA-C	5.09	121.64	110.80
1	A	274	ARG	CG-CD-NE	5.09	123.19	112.00
1	A	281	THR	O-C-N	-5.08	116.76	123.16
1	A	278	PRO	CB-CA-C	5.07	118.03	111.64
1	A	179	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	A	101	MET	O-C-N	5.05	130.50	122.41
1	A	31	ILE	CB-CA-C	-5.05	102.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ILE	CA-C-N	-5.05	110.89	121.80
1	A	222	ILE	C-N-CA	-5.05	110.89	121.80
1	A	283	GLN	CG-CD-NE2	-5.04	108.84	116.40
1	A	100	ASP	N-CA-C	5.03	120.32	113.37
1	A	31	ILE	N-CA-CB	5.03	119.85	112.35
1	A	96	TYR	CA-C-O	5.03	125.96	120.58
1	A	174	HIS	ND1-CG-CD2	5.03	111.13	106.10
1	A	183	SER	N-CA-C	-5.03	102.34	110.14
1	A	282	LEU	N-CA-C	-5.03	100.26	108.76
1	A	47	LEU	N-CA-C	5.03	116.46	108.67
1	A	25	HIS	CG-CD2-NE2	-5.03	102.17	107.20
1	A	78	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	A	226	VAL	CA-C-O	-5.02	113.23	119.95
1	A	63	TRP	CD1-CG-CD2	5.00	114.31	106.30
1	A	207	ASN	CA-C-O	-5.00	114.91	120.66

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	216	TYR	Sidechain
1	A	261	TYR	Sidechain
1	A	29	TYR	Sidechain
1	A	312	ALA	Peptide
1	A	6	TYR	Sidechain
1	A	96	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	2590	532	2501	106	3
2	A	21	1	10	0	0
3	A	41	82	0	2	0
All	All	2652	615	2511	106	3

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 21.

All (106) 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:243:GLU:HG3	1:A:291:ILE:HG23	1.53	0.89
1:A:76:GLN:HB3	1:A:130:LEU:HD11	1.64	0.79
1:A:195:LEU:CD1	3:A:359:HOH:O	2.30	0.79
1:A:101:MET:HE3	1:A:101:MET:HA	1.66	0.78
1:A:288:LYS:HZ1	1:A:293:ASP:HB3	1.51	0.76
1:A:104:PHE:HB2	1:A:118:TYR:CD2	2.22	0.74
1:A:195:LEU:HD11	3:A:359:HOH:O	1.87	0.73
1:A:244:CYS:HB2	1:A:246:LEU:HD22	1.72	0.70
1:A:108:SER:HB2	1:A:119:HIS:HE1	1.57	0.70
1:A:152:ALA:HA	1:A:160:THR:HG23	1.73	0.70
1:A:223:PHE:HD1	1:A:268:ILE:HD13	1.57	0.69
1:A:71:ILE:HG22	1:A:129:VAL:HG11	1.75	0.69
1:A:265:LEU:O	1:A:269:LYS:HG3	1.94	0.67
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.30	0.67
1:A:87:PHE:HE1	1:A:91:VAL:HG23	1.60	0.66
1:A:101:MET:HE2	1:A:104:PHE:HA	1.77	0.66
1:A:87:PHE:CE1	1:A:91:VAL:HG23	2.31	0.66
1:A:101:MET:HA	1:A:101:MET:CE	2.24	0.65
1:A:205:TYR:CE2	1:A:207:ASN:HB3	2.32	0.65
1:A:90:TRP:O	1:A:93:SER:HB2	1.97	0.63
1:A:288:LYS:HZ3	1:A:288:LYS:HB3	1.64	0.63
1:A:65:LEU:HD21	1:A:291:ILE:HD12	1.80	0.63
1:A:71:ILE:HG13	1:A:86:ALA:HB2	1.80	0.63
1:A:105:GLY:HA2	1:A:108:SER:OG	1.99	0.62
1:A:125:PHE:O	1:A:129:VAL:HG23	1.98	0.62
1:A:1:MET:HG3	1:A:276:PRO:HB2	1.83	0.61
1:A:288:LYS:NZ	1:A:293:ASP:HB3	2.16	0.60
1:A:90:TRP:HA	1:A:90:TRP:CE3	2.35	0.60
1:A:101:MET:SD	1:A:118:TYR:HA	2.42	0.60
1:A:297:LYS:NZ	1:A:300:LYS:HB2	2.18	0.58
1:A:85:TRP:HZ2	1:A:195:LEU:HB2	1.68	0.57
1:A:87:PHE:CD2	1:A:122:MET:SD	2.98	0.57
1:A:274:ARG:HG2	1:A:307:TYR:CD2	2.40	0.56
1:A:48:THR:HB	1:A:277:ARG:HB2	1.86	0.56
1:A:153:TRP:O	1:A:160:THR:HA	2.04	0.56
1:A:13:VAL:O	1:A:17:GLY:HA3	2.06	0.55
1:A:265:LEU:O	1:A:268:ILE:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:HG2	1:A:218:ARG:HH22	1.72	0.54
1:A:104:PHE:HD2	1:A:118:TYR:HE2	1.56	0.53
1:A:184:ALA:O	1:A:197:PRO:HG2	2.08	0.53
1:A:128:ARG:HB3	1:A:135:PHE:CG	2.43	0.53
1:A:284:LEU:HD22	1:A:299:ILE:HG13	1.89	0.53
1:A:86:ALA:HB3	1:A:125:PHE:HE2	1.73	0.52
1:A:101:MET:CE	1:A:118:TYR:HB2	2.39	0.52
1:A:224:LEU:HD11	1:A:312:ALA:HB2	1.92	0.52
1:A:223:PHE:HD2	1:A:224:LEU:HD13	1.75	0.51
1:A:277:ARG:HD2	1:A:305:ASP:O	2.10	0.51
1:A:213:LEU:O	1:A:252:ILE:HG12	2.10	0.51
1:A:108:SER:HB2	1:A:119:HIS:CE1	2.42	0.51
1:A:104:PHE:HB2	1:A:118:TYR:CE2	2.45	0.51
1:A:24:THR:HG22	1:A:316:VAL:HA	1.92	0.51
1:A:46:LEU:HG	1:A:52:VAL:HG13	1.92	0.51
1:A:281:THR:O	1:A:301:LEU:HD22	2.11	0.51
1:A:243:GLU:HG3	1:A:291:ILE:CG2	2.34	0.51
1:A:85:TRP:CZ2	1:A:195:LEU:HB2	2.46	0.50
1:A:104:PHE:O	1:A:108:SER:HB3	2.11	0.50
1:A:110:LYS:O	1:A:112:PRO:HD2	2.12	0.50
1:A:223:PHE:CD1	1:A:268:ILE:HD13	2.43	0.50
1:A:90:TRP:HA	1:A:90:TRP:HE3	1.77	0.50
1:A:5:PRO:HB3	1:A:36:MET:HG3	1.94	0.49
1:A:40:LEU:HB2	1:A:248:VAL:CG1	2.43	0.49
1:A:214:GLN:HA	1:A:252:ILE:HB	1.94	0.49
1:A:297:LYS:HZ3	1:A:300:LYS:HB2	1.77	0.49
1:A:167:VAL:O	1:A:171:ILE:HG13	2.13	0.48
1:A:134:ALA:O	1:A:137:ALA:HB3	2.13	0.48
1:A:285:ASN:ND2	1:A:288:LYS:HG3	2.28	0.48
1:A:26:THR:HG22	1:A:262:VAL:HB	1.96	0.48
1:A:107:ARG:HB2	1:A:114:PHE:CD2	2.49	0.47
1:A:187:PRO:O	1:A:191:PRO:HD2	2.14	0.47
1:A:153:TRP:CZ2	1:A:186:ASN:HB2	2.50	0.46
1:A:222:ILE:HD11	1:A:258:ALA:C	2.39	0.46
1:A:186:ASN:O	1:A:190:VAL:HG23	2.14	0.46
1:A:198:CYS:O	1:A:217:GLN:HG3	2.15	0.46
1:A:54:PHE:CE2	1:A:301:LEU:HB2	2.50	0.46
1:A:26:THR:HG21	1:A:263:ASN:H	1.80	0.46
1:A:314:VAL:HB	1:A:316:VAL:HG22	1.96	0.46
1:A:291:ILE:HA	1:A:294:PHE:CD1	2.51	0.45
1:A:40:LEU:HB2	1:A:248:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:SER:HA	1:A:115:ALA:HA	1.98	0.45
1:A:260:LEU:HD21	1:A:268:ILE:HG21	1.98	0.45
1:A:63:TRP:CZ2	1:A:74:LEU:HD11	2.52	0.45
1:A:118:TYR:HD1	1:A:119:HIS:ND1	2.15	0.44
1:A:131:HIS:O	1:A:132:ASP:HB2	2.18	0.44
1:A:260:LEU:CD2	1:A:265:LEU:HD12	2.48	0.44
1:A:80:HIS:O	1:A:83:ASP:HB2	2.18	0.44
1:A:284:LEU:HD22	1:A:299:ILE:CG1	2.47	0.44
1:A:235:LEU:HG	1:A:239:LEU:CD2	2.48	0.43
1:A:101:MET:SD	1:A:118:TYR:HB2	2.59	0.42
1:A:168:ILE:HA	1:A:171:ILE:HD12	2.00	0.42
1:A:87:PHE:HZ	1:A:101:MET:HG2	1.84	0.42
1:A:267:GLN:OE1	1:A:267:GLN:N	2.50	0.42
1:A:26:THR:CG2	1:A:262:VAL:HB	2.50	0.42
1:A:41:SER:OG	1:A:42:LYS:NZ	2.52	0.42
1:A:239:LEU:O	1:A:291:ILE:HG21	2.20	0.42
1:A:101:MET:HE2	1:A:118:TYR:HB2	2.01	0.41
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.89	0.41
1:A:104:PHE:HD2	1:A:118:TYR:CE2	2.37	0.41
1:A:71:ILE:HA	1:A:71:ILE:HD13	1.69	0.41
1:A:154:HIS:HE1	1:A:188:GLU:OE2	2.04	0.41
1:A:90:TRP:HH2	1:A:128:ARG:NH2	2.19	0.41
1:A:153:TRP:CH2	1:A:186:ASN:HB2	2.56	0.41
1:A:268:ILE:O	1:A:272:LEU:HD12	2.21	0.41
1:A:28:THR:HG22	1:A:261:TYR:HA	2.03	0.40
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.91	0.40
1:A:205:TYR:HE2	1:A:207:ASN:HB3	1.79	0.40
1:A:269:LYS:O	1:A:272:LEU:HB2	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HH21	1:A:107:ARG:HH21[11_654]	0.98	0.62
1:A:178:ARG:HH11	1:A:219:SER:HG[11_554]	1.35	0.25
1:A:107:ARG:NH2	1:A:107:ARG:NH2[11_654]	2.16	0.04

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%)	248 (79%)	46 (15%)	20 (6%)	1 1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	25	HIS
1	A	102	THR
1	A	104	PHE
1	A	111	ALA
1	A	112	PRO
1	A	113	GLU
1	A	115	ALA
1	A	132	ASP
1	A	208	ASP
1	A	313	PRO
1	A	99	PRO
1	A	143	GLY
1	A	308	PRO
1	A	5	PRO
1	A	53	PRO
1	A	106	HIS
1	A	159	ASP
1	A	49	THR
1	A	158	GLY

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	242/277 (87%)	186 (77%)	56 (23%)	1 1

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	16	GLU
1	A	24	THR
1	A	25	HIS
1	A	31	ILE
1	A	42	LYS
1	A	52	VAL
1	A	58	LYS
1	A	59	SER
1	A	60	GLN
1	A	62	LEU
1	A	65	LEU
1	A	75	LEU
1	A	76	GLN
1	A	78	ARG
1	A	83	ASP
1	A	85	TRP
1	A	90	TRP
1	A	91	VAL
1	A	93	SER
1	A	94	ASP
1	A	95	GLU
1	A	96	TYR
1	A	97	HIS
1	A	101	MET
1	A	102	THR
1	A	104	PHE
1	A	113	GLU
1	A	120	GLU
1	A	121	GLU
1	A	124	LYS
1	A	144	LEU
1	A	145	VAL
1	A	160	THR
1	A	170	GLN
1	A	215	LEU

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Mol	Chain	Res	Type
1	A	222	ILE
1	A	224	LEU
1	A	232	SER
1	A	236	LEU
1	A	239	LEU
1	A	243	GLU
1	A	246	LEU
1	A	247	GLU
1	A	265	LEU
1	A	266	ASP
1	A	271	GLN
1	A	276	PRO
1	A	280	PRO
1	A	288	LYS
1	A	297	LYS
1	A	300	LYS
1	A	306	PRO
1	A	311	LYS
1	A	313	PRO
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	76	GLN
1	A	97	HIS
1	A	154	HIS
1	A	229	ASN

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UFP	A	317	-	22,22,22	2.14	4 (18%)	32,33,33	2.41	11 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UFP	A	317	-	1/1/4/4	2/10/22/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	UFP	C6-C5	5.08	1.40	1.33
2	A	317	UFP	C2-N1	4.32	1.45	1.38
2	A	317	UFP	O4'-C1'	3.61	1.50	1.42
2	A	317	UFP	C4-C5	2.55	1.47	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	UFP	O4'-C1'-N1	6.06	118.62	107.86
2	A	317	UFP	F5-C5-C4	5.11	120.95	116.47
2	A	317	UFP	C1'-N1-C6	-5.01	112.34	120.74
2	A	317	UFP	O2-C2-N1	3.83	127.78	122.80
2	A	317	UFP	C2'-C3'-C4'	-3.44	95.83	102.80
2	A	317	UFP	C6-C5-C4	-3.27	119.58	122.57
2	A	317	UFP	C1'-N1-C2	3.00	123.53	117.66
2	A	317	UFP	O4'-C4'-C3'	-2.88	99.08	105.65
2	A	317	UFP	C5-C4-N3	2.61	115.03	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	UFP	O5'-P-O1P	-2.44	99.84	106.44
2	A	317	UFP	C6-N1-C2	2.26	123.56	121.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	317	UFP	C1'

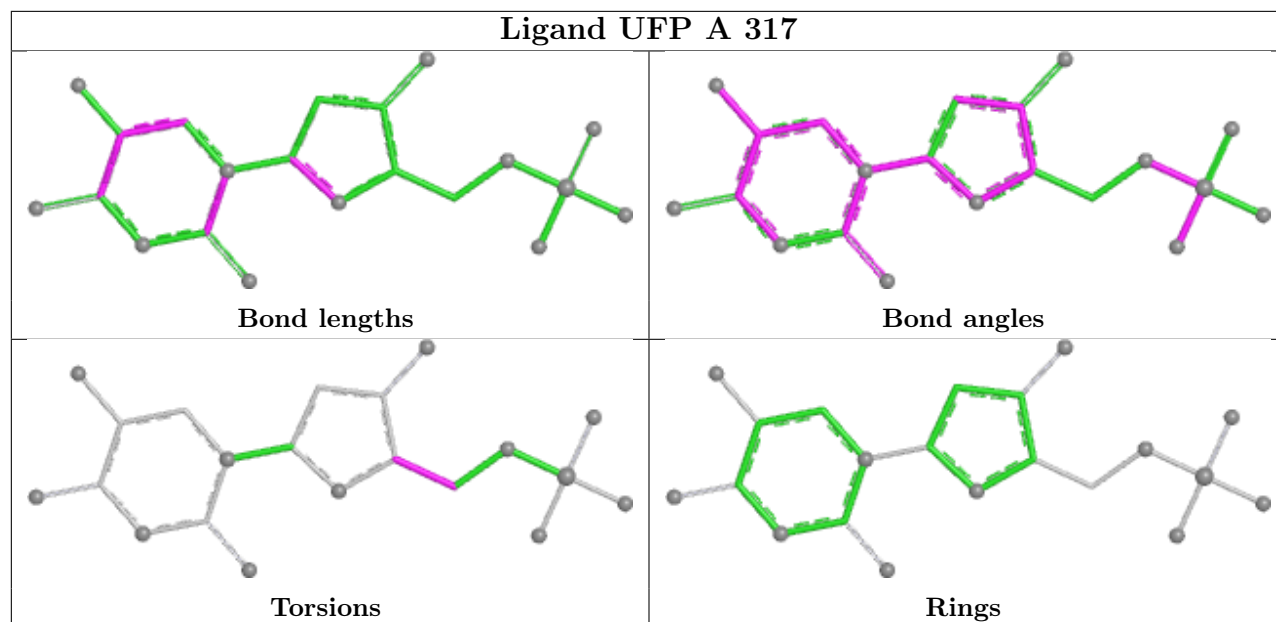
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	317	UFP	O4'-C4'-C5'-O5'
2	A	317	UFP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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%)	1.99	124 (39%) 1 0	3, 12, 23, 29	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ALA	8.1
1	A	115	ALA	7.9
1	A	315	ALA	6.4
1	A	24	THR	6.4
1	A	22	ASP	6.1
1	A	91	VAL	5.9
1	A	114	PHE	5.7
1	A	133	ASP	5.6
1	A	125	PHE	5.6
1	A	95	GLU	5.3
1	A	129	VAL	5.2
1	A	101	MET	4.9
1	A	97	HIS	4.8
1	A	90	TRP	4.7
1	A	142	LEU	4.7
1	A	86	ALA	4.4
1	A	170	GLN	4.3
1	A	21	PRO	4.2
1	A	131	HIS	4.2
1	A	312	ALA	4.1
1	A	314	VAL	4.1
1	A	23	ARG	4.0
1	A	74	LEU	4.0
1	A	196	PRO	3.9
1	A	107	ARG	3.9
1	A	316	VAL	3.9
1	A	118	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	45	PRO	3.8
1	A	85	TRP	3.8
1	A	87	PHE	3.7
1	A	113	GLU	3.7
1	A	265	LEU	3.6
1	A	201	LEU	3.6
1	A	289	HIS	3.5
1	A	262	VAL	3.5
1	A	153	TRP	3.5
1	A	160	THR	3.5
1	A	163	GLN	3.5
1	A	60	GLN	3.4
1	A	61	LEU	3.3
1	A	99	PRO	3.3
1	A	130	LEU	3.2
1	A	138	LYS	3.1
1	A	146	TYR	3.1
1	A	155	THR	3.1
1	A	10	ALA	3.1
1	A	164	LEU	3.1
1	A	96	TYR	3.0
1	A	154	HIS	3.0
1	A	137	ALA	3.0
1	A	284	LEU	3.0
1	A	93	SER	3.0
1	A	297	LYS	3.0
1	A	71	ILE	2.9
1	A	161	ILE	2.9
1	A	143	GLY	2.9
1	A	57	ILE	2.9
1	A	179	ARG	2.9
1	A	139	TYR	2.9
1	A	183	SER	2.9
1	A	252	ILE	2.9
1	A	119	HIS	2.9
1	A	184	ALA	2.9
1	A	52	VAL	2.8
1	A	123	ALA	2.8
1	A	181	ILE	2.7
1	A	212	SER	2.7
1	A	132	ASP	2.7
1	A	28	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	2.7
1	A	190	VAL	2.7
1	A	261	TYR	2.7
1	A	44	PHE	2.7
1	A	140	GLY	2.6
1	A	213	LEU	2.6
1	A	100	ASP	2.6
1	A	205	TYR	2.6
1	A	185	TRP	2.6
1	A	141	ASP	2.6
1	A	211	LEU	2.5
1	A	233	TYR	2.5
1	A	187	PRO	2.5
1	A	290	ASP	2.5
1	A	207	ASN	2.5
1	A	150	TRP	2.5
1	A	78	ARG	2.5
1	A	82	TRP	2.4
1	A	246	LEU	2.4
1	A	64	PHE	2.4
1	A	257	ASP	2.3
1	A	32	PHE	2.3
1	A	105	GLY	2.3
1	A	301	LEU	2.3
1	A	292	PHE	2.3
1	A	67	GLY	2.3
1	A	14	LEU	2.3
1	A	110	LYS	2.3
1	A	165	GLY	2.3
1	A	249	GLY	2.3
1	A	253	HIS	2.3
1	A	70	ASN	2.2
1	A	144	LEU	2.2
1	A	221	ASP	2.2
1	A	276	PRO	2.2
1	A	230	ILE	2.2
1	A	304	TYR	2.2
1	A	73	PHE	2.2
1	A	256	GLY	2.2
1	A	300	LYS	2.2
1	A	174	HIS	2.1
1	A	197	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	40	LEU	2.1
1	A	268	ILE	2.1
1	A	59	SER	2.1
1	A	145	VAL	2.1
1	A	167	VAL	2.1
1	A	258	ALA	2.1
1	A	168	ILE	2.1
1	A	108	SER	2.1
1	A	149	GLN	2.1
1	A	80	HIS	2.1
1	A	13	VAL	2.0
1	A	176	TYR	2.0
1	A	112	PRO	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](#)

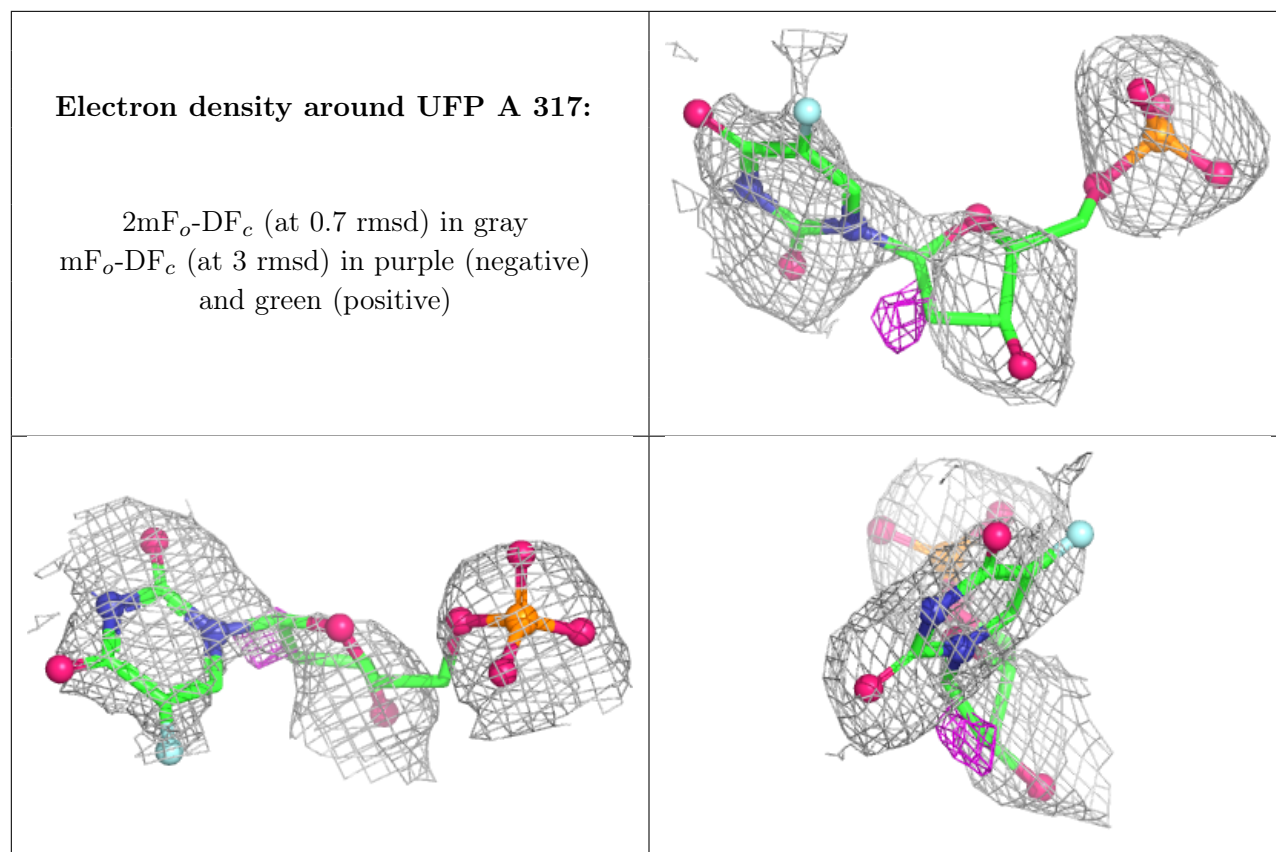
There are no oligosaccharides in this entry.

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
2	UFP	A	317	21/21	0.81	0.17	13,24,27,28	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.