



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 PM UTC

PDB ID : 1VZD / pdb_00001vzd
Title : L. CASEI THYMIDYLATE SYNTHASE MUTANT E60Q TERNARY COMPLEX WITH FDUMP AND CB3717
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

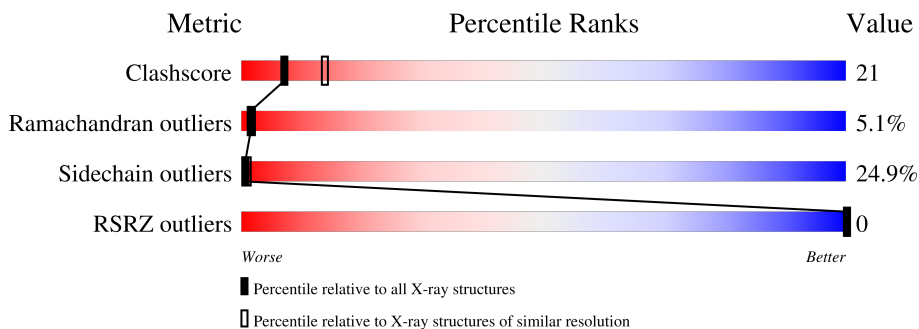
1 Overall quality at a glance

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3561 atoms, of which 789 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.

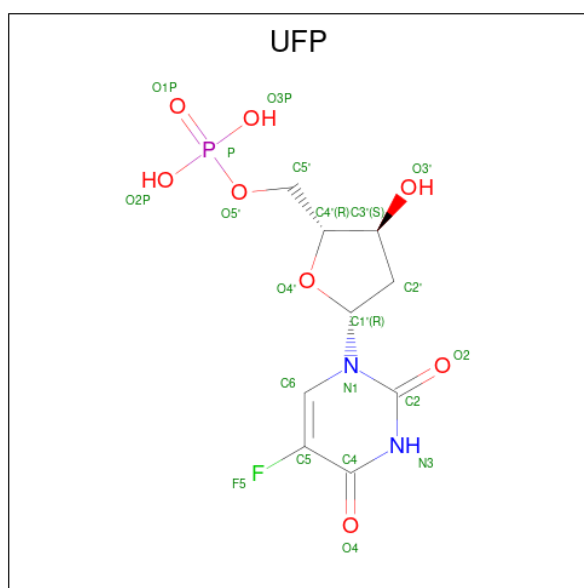
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

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

There are 2 discrepancies between the modelled and reference sequences:

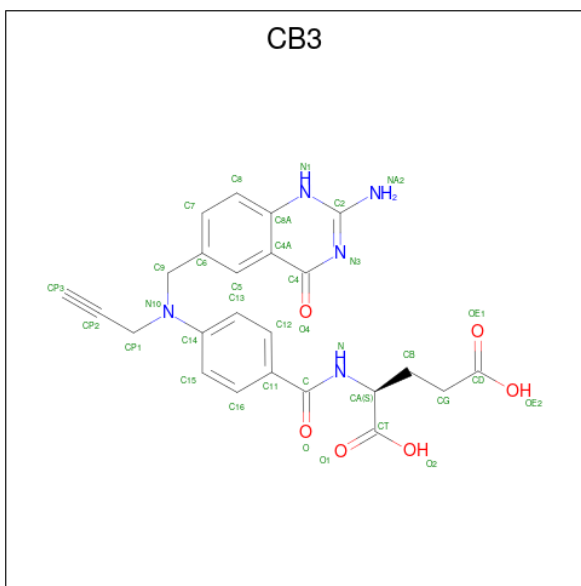
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	engineered mutation	UNP P00469
A	111	ALA	ASP	conflict	UNP P00469

- Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: $C_9H_{12}FN_2O_8P$).



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

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula:

$$\text{C}_{24}\text{H}_{23}\text{N}_5\text{O}_6).$$


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 39	C 24	H 4	N 5	O 6	0	0

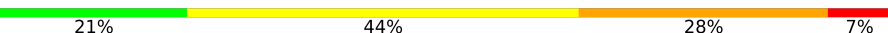
- Molecule 4 is water.

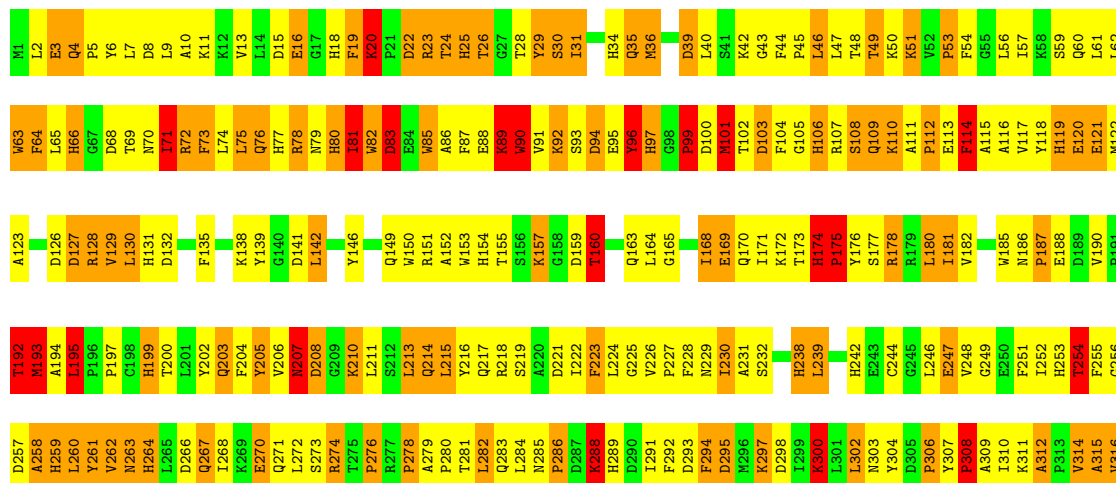
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	126	Total	H	O	0	0
			378	252	126		

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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.50Å 78.50Å 230.60Å 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) 60.3 (15.00-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.18Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , (Not available) 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3561	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: UFP, CB3

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	59/2674 (2.2%)	2.68	252/3634 (6.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	VAL	CA-CB	7.91	1.65	1.54
1	A	253	HIS	CD2-NE2	-7.63	1.29	1.37
1	A	24	THR	CA-CB	7.47	1.61	1.54
1	A	286	PRO	CA-CB	-7.47	1.43	1.53
1	A	66	HIS	CD2-NE2	-7.22	1.29	1.37
1	A	48	THR	CA-CB	-7.00	1.42	1.53
1	A	199	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	259	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	141	ASP	CA-CB	-6.67	1.44	1.53
1	A	264	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	253	HIS	CG-ND1	-6.58	1.31	1.38
1	A	18	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	129	VAL	CA-CB	6.28	1.61	1.54
1	A	217	GLN	CA-CB	-6.18	1.44	1.53
1	A	77	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	119	HIS	CG-CD2	6.07	1.42	1.35
1	A	261	TYR	CA-CB	-6.07	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	LEU	CA-CB	-6.03	1.45	1.53
1	A	66	HIS	CG-ND1	-6.00	1.31	1.38
1	A	127	ASP	CA-CB	-6.00	1.46	1.53
1	A	80	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	276	PRO	CA-CB	-5.78	1.46	1.53
1	A	53	PRO	CA-CB	-5.74	1.45	1.53
1	A	268	ILE	CA-CB	5.72	1.61	1.54
1	A	205	TYR	CA-CB	-5.71	1.44	1.53
1	A	280	PRO	CA-CB	-5.67	1.46	1.54
1	A	46	LEU	CA-CB	-5.65	1.45	1.53
1	A	131	HIS	CA-CB	-5.62	1.45	1.54
1	A	63	TRP	CA-CB	-5.60	1.44	1.53
1	A	97	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	251	PHE	CA-CB	-5.57	1.44	1.53
1	A	308	PRO	CA-CB	-5.54	1.46	1.53
1	A	244	CYS	CA-CB	-5.52	1.44	1.53
1	A	80	HIS	CG-CD2	5.48	1.41	1.35
1	A	174	HIS	CD2-NE2	-5.45	1.31	1.37
1	A	238	HIS	CG-ND1	-5.43	1.32	1.38
1	A	259	HIS	CG-ND1	-5.42	1.32	1.38
1	A	289	HIS	CD2-NE2	-5.42	1.31	1.37
1	A	199	HIS	CG-ND1	-5.36	1.32	1.38
1	A	229	ASN	CA-CB	-5.32	1.44	1.53
1	A	71	ILE	CA-CB	5.31	1.61	1.54
1	A	197	PRO	CA-CB	-5.29	1.47	1.53
1	A	278	PRO	CA-CB	-5.27	1.46	1.53
1	A	154	HIS	CG-CD2	5.25	1.41	1.35
1	A	232	SER	CA-CB	-5.21	1.45	1.53
1	A	63	TRP	CG-CD2	-5.20	1.34	1.43
1	A	204	PHE	CA-CB	-5.17	1.46	1.53
1	A	300	LYS	CA-CB	-5.17	1.45	1.53
1	A	75	LEU	CA-CB	-5.15	1.45	1.53
1	A	88	GLU	CA-CB	-5.14	1.45	1.53
1	A	291	ILE	CA-CB	5.12	1.63	1.54
1	A	257	ASP	CA-CB	-5.10	1.46	1.52
1	A	306	PRO	CA-CB	-5.10	1.47	1.54
1	A	262	VAL	CA-CB	5.06	1.60	1.54
1	A	260	LEU	CA-CB	-5.05	1.45	1.53
1	A	174	HIS	CA-CB	-5.04	1.45	1.53
1	A	170	GLN	CA-CB	-5.03	1.45	1.53
1	A	31	ILE	CA-CB	5.02	1.62	1.54

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ASP	CA-CB-CG	14.98	127.58	112.60
1	A	66	HIS	CA-CB-CG	12.65	126.45	113.80
1	A	68	ASP	N-CA-C	12.28	128.29	110.24
1	A	294	PHE	CA-C-O	11.96	132.91	120.95
1	A	114	PHE	CA-CB-CG	-11.83	101.97	113.80
1	A	266	ASP	CA-CB-CG	11.65	124.25	112.60
1	A	22	ASP	CA-CB-CG	11.37	123.97	112.60
1	A	83	ASP	CA-CB-CG	11.09	123.69	112.60
1	A	96	TYR	O-C-N	10.90	135.87	123.01
1	A	25	HIS	CA-CB-CG	10.79	124.58	113.80
1	A	278	PRO	O-C-N	10.54	135.12	123.01
1	A	120	GLU	N-CA-C	9.80	122.04	111.36
1	A	295	ASP	N-CA-C	-9.68	95.55	110.17
1	A	264	HIS	CA-CB-CG	9.65	123.45	113.80
1	A	106	HIS	CA-CB-CG	9.62	123.42	113.80
1	A	35	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	A	26	THR	CA-C-O	9.34	129.66	120.88
1	A	64	PHE	CA-CB-CG	9.21	123.01	113.80
1	A	242	HIS	CA-CB-CG	9.16	122.96	113.80
1	A	93	SER	N-CA-C	9.13	123.19	108.76
1	A	127	ASP	CA-CB-CG	-9.08	103.52	112.60
1	A	29	TYR	N-CA-C	-8.90	93.75	108.34
1	A	160	THR	N-CA-CB	-8.85	95.82	110.68
1	A	110	LYS	N-CA-C	-8.73	93.53	107.93
1	A	157	LYS	N-CA-CB	-8.72	100.59	110.35
1	A	263	ASN	CA-CB-CG	8.65	121.25	112.60
1	A	228	PHE	CA-CB-CG	8.53	122.33	113.80
1	A	288	LYS	CA-C-O	8.48	130.55	120.20
1	A	208	ASP	CA-CB-CG	8.38	120.98	112.60
1	A	96	TYR	CA-C-O	8.24	130.44	121.05
1	A	264	HIS	CA-C-N	8.19	135.77	121.52
1	A	264	HIS	C-N-CA	8.19	135.77	121.52
1	A	192	THR	CA-CB-OG1	-8.15	97.37	109.60
1	A	97	HIS	N-CA-C	-8.03	94.68	107.93
1	A	253	HIS	CA-CB-CG	8.01	121.81	113.80
1	A	160	THR	CB-CA-C	8.00	124.35	109.71
1	A	267	GLN	OE1-CD-NE2	-7.92	114.69	122.60
1	A	186	ASN	CA-CB-CG	7.91	120.51	112.60
1	A	97	HIS	CA-CB-CG	7.86	121.66	113.80
1	A	192	THR	CA-CB-CG2	7.83	123.81	110.50
1	A	25	HIS	CB-CG-CD2	-7.81	121.05	131.20
1	A	69	THR	N-CA-C	-7.79	103.09	112.59
1	A	267	GLN	CG-CD-NE2	7.73	128.00	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ALA	N-CA-C	-7.67	94.46	110.80
1	A	70	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	316	VAL	CB-CA-C	7.47	125.58	111.40
1	A	97	HIS	CB-CG-CD2	-7.44	121.53	131.20
1	A	270	GLU	CB-CG-CD	7.42	125.21	112.60
1	A	178	ARG	NE-CZ-NH1	7.40	128.90	121.50
1	A	35	GLN	N-CA-C	-7.36	97.23	109.07
1	A	102	THR	O-C-N	7.30	131.95	122.68
1	A	19	PHE	CA-CB-CG	7.25	121.05	113.80
1	A	44	PHE	CA-CB-CG	-7.25	106.55	113.80
1	A	31	ILE	N-CA-C	-7.23	98.00	109.20
1	A	109	GLN	OE1-CD-NE2	-7.21	115.39	122.60
1	A	188	GLU	CA-CB-CG	7.06	128.22	114.10
1	A	24	THR	N-CA-C	-7.05	100.38	108.49
1	A	152	ALA	N-CA-C	6.99	118.66	110.41
1	A	238	HIS	O-C-N	6.99	130.12	122.15
1	A	247	GLU	CA-CB-CG	6.98	128.06	114.10
1	A	3	GLU	N-CA-C	6.97	121.10	112.59
1	A	89	LYS	CG-CD-CE	6.93	127.23	111.30
1	A	73	PHE	CA-CB-CG	6.91	120.71	113.80
1	A	266	ASP	N-CA-C	-6.88	103.86	111.36
1	A	177	SER	CA-C-O	6.87	128.12	120.70
1	A	43	GLY	N-CA-C	6.86	120.14	110.74
1	A	130	LEU	N-CA-CB	-6.83	98.44	110.39
1	A	51	LYS	O-C-N	6.83	131.33	122.93
1	A	149	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	260	LEU	CA-C-N	-6.80	112.51	122.65
1	A	260	LEU	C-N-CA	-6.80	112.51	122.65
1	A	159	ASP	N-CA-C	6.80	120.70	109.96
1	A	26	THR	N-CA-C	6.70	120.56	110.64
1	A	102	THR	CA-C-O	6.69	127.88	120.92
1	A	163	GLN	CB-CA-C	-6.60	99.84	110.79
1	A	95	GLU	N-CA-C	-6.59	103.36	111.40
1	A	294	PHE	N-CA-C	6.58	120.02	110.42
1	A	3	GLU	CA-CB-CG	6.57	127.25	114.10
1	A	77	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	A	295	ASP	CA-C-N	6.55	129.36	120.38
1	A	295	ASP	C-N-CA	6.55	129.36	120.38
1	A	188	GLU	CA-C-O	6.53	127.48	119.97
1	A	239	LEU	CA-C-O	-6.53	113.97	120.82
1	A	316	VAL	N-CA-C	-6.52	92.73	111.00
1	A	93	SER	O-C-N	6.45	130.71	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	262	VAL	N-CA-CB	-6.43	101.79	110.54
1	A	157	LYS	CB-CG-CD	6.38	125.98	111.30
1	A	163	GLN	CA-CB-CG	6.36	126.82	114.10
1	A	231	ALA	CA-C-O	-6.34	114.17	120.70
1	A	310	ILE	N-CA-CB	-6.33	103.70	111.67
1	A	207	ASN	N-CA-C	-6.32	97.35	110.80
1	A	90	TRP	CB-CG-CD1	-6.31	117.43	126.90
1	A	289	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	A	120	GLU	O-C-N	-6.29	114.98	122.15
1	A	88	GLU	CA-CB-CG	6.27	126.64	114.10
1	A	149	GLN	O-C-N	-6.23	115.30	122.03
1	A	46	LEU	N-CA-C	-6.23	99.08	109.24
1	A	109	GLN	CA-CB-CG	6.22	126.54	114.10
1	A	86	ALA	CA-C-O	6.21	127.11	120.10
1	A	270	GLU	CA-CB-CG	6.21	126.51	114.10
1	A	251	PHE	N-CA-C	-6.18	98.20	108.34
1	A	16	GLU	N-CA-C	6.15	119.88	112.38
1	A	271	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	108	SER	CA-CB-OG	6.12	123.33	111.10
1	A	106	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	A	126	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	95	GLU	CB-CG-CD	6.08	122.93	112.60
1	A	51	LYS	CA-CB-CG	6.07	126.25	114.10
1	A	242	HIS	CA-C-O	-6.07	114.08	120.63
1	A	197	PRO	CB-CA-C	6.05	118.16	111.56
1	A	79	ASN	O-C-N	-6.03	116.18	123.29
1	A	80	HIS	CB-CG-CD2	-6.02	123.37	131.20
1	A	174	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	A	149	GLN	CB-CG-CD	6.00	122.81	112.60
1	A	174	HIS	CA-C-N	5.96	127.30	119.84
1	A	174	HIS	C-N-CA	5.96	127.30	119.84
1	A	109	GLN	N-CA-C	-5.96	104.91	111.82
1	A	217	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	279	ALA	CA-C-O	-5.93	113.99	120.69
1	A	316	VAL	CA-CB-CG1	5.93	120.48	110.40
1	A	266	ASP	CA-C-N	5.92	128.69	120.29
1	A	266	ASP	C-N-CA	5.92	128.69	120.29
1	A	102	THR	CA-C-N	5.91	132.83	121.54
1	A	102	THR	C-N-CA	5.91	132.83	121.54
1	A	207	ASN	CB-CG-ND2	5.90	125.25	116.40
1	A	213	LEU	CD1-CG-CD2	-5.85	97.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	N-CA-C	5.84	118.28	107.99
1	A	286	PRO	N-CA-C	5.84	121.23	113.57
1	A	82	TRP	CE2-CD2-CG	-5.84	100.19	107.20
1	A	285	ASN	O-C-N	-5.84	114.61	121.32
1	A	293	ASP	N-CA-C	5.83	119.58	112.23
1	A	4	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	30	SER	N-CA-C	5.82	118.95	109.06
1	A	316	VAL	CA-CB-CG2	-5.82	100.51	110.40
1	A	186	ASN	CA-C-N	5.80	127.09	119.84
1	A	186	ASN	C-N-CA	5.80	127.09	119.84
1	A	117	VAL	N-CA-CB	5.80	120.79	111.23
1	A	308	PRO	N-CA-C	5.79	124.41	112.47
1	A	109	GLN	CA-C-N	5.79	130.96	121.58
1	A	109	GLN	C-N-CA	5.79	130.96	121.58
1	A	292	PHE	N-CA-CB	-5.78	100.79	110.39
1	A	82	TRP	CG-CD2-CE3	5.71	139.61	133.90
1	A	103	ASP	N-CA-C	-5.71	98.65	110.80
1	A	258	ALA	N-CA-C	-5.71	99.89	108.96
1	A	97	HIS	CB-CA-C	5.70	118.31	110.34
1	A	223	PHE	N-CA-C	5.69	120.24	112.04
1	A	18	HIS	CA-CB-CG	5.69	119.49	113.80
1	A	121	GLU	CB-CG-CD	5.69	122.27	112.60
1	A	199	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	282	LEU	CA-C-O	5.66	128.40	121.72
1	A	174	HIS	CA-CB-CG	5.66	119.46	113.80
1	A	142	LEU	N-CA-C	5.65	119.43	112.54
1	A	163	GLN	N-CA-C	5.65	117.44	111.28
1	A	77	HIS	CA-CB-CG	-5.64	108.16	113.80
1	A	68	ASP	CA-C-O	5.62	127.08	120.96
1	A	150	TRP	CA-CB-CG	5.61	124.26	113.60
1	A	271	GLN	CG-CD-NE2	5.59	124.79	116.40
1	A	119	HIS	O-C-N	-5.58	115.41	122.17
1	A	187	PRO	N-CA-C	5.57	123.94	112.47
1	A	225	GLY	CA-C-O	-5.57	115.02	120.75
1	A	178	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	A	81	ILE	CB-CG1-CD1	5.55	125.46	113.80
1	A	54	PHE	CA-C-N	5.54	126.25	119.99
1	A	54	PHE	C-N-CA	5.54	126.25	119.99
1	A	80	HIS	CA-CB-CG	5.53	119.33	113.80
1	A	316	VAL	N-CA-CB	-5.52	102.12	111.50
1	A	130	LEU	O-C-N	-5.51	114.85	122.46
1	A	90	TRP	CE2-CD2-CG	-5.51	100.59	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	O-C-N	5.51	129.92	122.59
1	A	25	HIS	CB-CG-ND1	5.51	130.97	122.70
1	A	185	TRP	CE2-CD2-CE3	5.50	124.30	118.80
1	A	170	GLN	CA-CB-CG	5.50	125.09	114.10
1	A	207	ASN	OD1-CG-ND2	-5.50	117.11	122.60
1	A	63	TRP	CE2-CD2-CG	-5.49	100.61	107.20
1	A	256	GLY	N-CA-C	-5.49	100.17	113.18
1	A	57	ILE	N-CA-CB	-5.48	101.40	110.56
1	A	101	MET	CA-CB-CG	5.48	125.06	114.10
1	A	2	LEU	CA-C-N	-5.45	114.01	122.67
1	A	2	LEU	C-N-CA	-5.45	114.01	122.67
1	A	259	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	A	194	ALA	CB-CA-C	-5.43	102.28	110.92
1	A	99	PRO	O-C-N	5.43	129.97	122.64
1	A	174	HIS	CA-C-O	-5.42	112.73	120.16
1	A	99	PRO	N-CA-C	5.42	123.63	112.47
1	A	254	THR	CA-CB-OG1	-5.40	101.51	109.60
1	A	297	LYS	CA-CB-CG	5.38	124.86	114.10
1	A	102	THR	N-CA-C	-5.38	98.52	107.99
1	A	262	VAL	CB-CA-C	5.37	119.39	112.14
1	A	273	SER	N-CA-C	-5.37	106.71	113.20
1	A	66	HIS	ND1-CG-CD2	5.36	111.46	106.10
1	A	246	LEU	O-C-N	-5.36	116.94	122.94
1	A	281	THR	N-CA-C	5.35	117.80	108.76
1	A	193	MET	N-CA-C	5.34	122.19	110.80
1	A	4	GLN	CA-C-N	5.33	126.51	119.84
1	A	4	GLN	C-N-CA	5.33	126.51	119.84
1	A	157	LYS	CB-CA-C	5.33	119.96	112.07
1	A	76	GLN	CB-CG-CD	-5.33	103.54	112.60
1	A	100	ASP	O-C-N	5.33	129.68	122.59
1	A	92	LYS	N-CA-C	5.33	118.88	112.38
1	A	85	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	A	312	ALA	N-CA-C	5.32	121.80	108.40
1	A	72	ARG	CA-C-O	-5.32	114.09	120.10
1	A	85	TRP	CA-C-N	5.31	127.93	120.28
1	A	85	TRP	C-N-CA	5.31	127.93	120.28
1	A	311	LYS	CB-CG-CD	5.31	123.51	111.30
1	A	117	VAL	CB-CA-C	-5.30	102.59	111.29
1	A	20	LYS	CB-CG-CD	-5.30	99.11	111.30
1	A	238	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	302	LEU	N-CA-C	5.30	118.13	109.59
1	A	120	GLU	CB-CA-C	-5.30	101.84	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	GLN	CB-CG-CD	5.29	121.59	112.60
1	A	226	VAL	CA-CB-CG2	-5.29	101.41	110.40
1	A	300	LYS	CA-C-O	5.29	126.15	120.38
1	A	181	ILE	O-C-N	5.29	128.66	123.00
1	A	128	ARG	CA-C-N	5.29	127.22	120.56
1	A	128	ARG	C-N-CA	5.29	127.22	120.56
1	A	101	MET	N-CA-C	5.27	122.02	110.80
1	A	219	SER	O-C-N	5.26	129.78	123.36
1	A	278	PRO	CA-C-N	5.25	128.63	120.60
1	A	278	PRO	C-N-CA	5.25	128.63	120.60
1	A	23	ARG	O-C-N	5.25	129.61	121.63
1	A	221	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	291	ILE	CA-C-O	5.24	126.37	120.03
1	A	297	LYS	CG-CD-CE	5.23	123.33	111.30
1	A	221	ASP	CA-C-O	5.22	126.28	120.43
1	A	90	TRP	CG-CD2-CE3	5.22	139.12	133.90
1	A	168	ILE	CB-CG1-CD1	5.22	124.76	113.80
1	A	210	LYS	CA-CB-CG	5.21	124.53	114.10
1	A	303	ASN	CB-CG-ND2	5.16	124.14	116.40
1	A	8	ASP	O-C-N	-5.15	115.41	122.46
1	A	97	HIS	CB-CG-ND1	5.13	130.40	122.70
1	A	165	GLY	N-CA-C	-5.13	106.55	112.50
1	A	229	ASN	CB-CG-ND2	5.13	124.09	116.40
1	A	24	THR	CA-C-O	5.13	123.88	120.19
1	A	315	ALA	CA-C-N	5.13	130.93	121.70
1	A	315	ALA	C-N-CA	5.13	130.93	121.70
1	A	263	ASN	CB-CG-ND2	5.12	124.08	116.40
1	A	208	ASP	O-C-N	-5.11	114.89	122.04
1	A	280	PRO	CA-C-O	-5.10	115.85	122.13
1	A	130	LEU	CB-CA-C	5.10	120.58	110.17
1	A	103	ASP	CA-C-O	5.10	127.80	120.51
1	A	43	GLY	CA-C-O	5.09	126.11	120.97
1	A	155	THR	N-CA-C	5.09	118.11	109.76
1	A	205	TYR	CA-CB-CG	5.09	123.05	113.90
1	A	257	ASP	CA-C-O	5.08	126.21	120.92
1	A	63	TRP	CD1-CG-CD2	5.07	114.42	106.30
1	A	169	GLU	CB-CG-CD	5.07	121.22	112.60
1	A	10	ALA	CA-C-O	-5.05	115.07	120.42
1	A	264	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	A	66	HIS	N-CA-C	5.03	118.75	109.24
1	A	39	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	LEU	Peptide
1	A	20	LYS	Peptide
1	A	205	TYR	Sidechain
1	A	216	TYR	Sidechain
1	A	4	GLN	Peptide
1	A	96	TYR	Sidechain

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	107	0
2	A	21	1	10	2	0
3	A	35	4	21	3	0
4	A	126	252	0	2	0
All	All	2772	789	2532	108	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 21.

All (108) 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:239:LEU:HD23	1:A:284:LEU:HD21	1.39	1.00
1:A:108:SER:HA	1:A:111:ALA:HB2	1.46	0.95
1:A:99:PRO:HB2	1:A:101:MET:HG2	1.55	0.86
1:A:222:ILE:HD11	1:A:258:ALA:HB1	1.66	0.77
1:A:175:PRO:HB3	1:A:206:VAL:HG21	1.67	0.75
1:A:34:HIS:HB3	1:A:255:PHE:HD2	1.51	0.75
1:A:85:TRP:CH2	1:A:195:LEU:HB2	2.23	0.74
1:A:34:HIS:HB3	1:A:255:PHE:CD2	2.24	0.72
1:A:314:VAL:HG13	3:A:318:CB3:H8	1.72	0.70
1:A:181:ILE:HG12	1:A:203:GLN:HB2	1.72	0.69
1:A:223:PHE:HE2	1:A:312:ALA:HB2	1.57	0.68
1:A:71:ILE:HG22	1:A:74:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:HB1	1:A:114:PHE:CB	2.27	0.65
1:A:111:ALA:HB1	1:A:114:PHE:HB2	1.82	0.61
1:A:90:TRP:HB2	1:A:139:TYR:CD1	2.36	0.60
1:A:264:HIS:HA	1:A:267:GLN:OE1	2.00	0.60
1:A:6:TYR:HA	1:A:36:MET:HE3	1.85	0.58
1:A:101:MET:HE1	1:A:118:TYR:HA	1.85	0.58
1:A:115:ALA:O	1:A:119:HIS:HB2	2.04	0.57
1:A:116:ALA:O	1:A:120:GLU:HB2	2.06	0.56
1:A:210:LYS:HB3	1:A:247:GLU:HB2	1.87	0.56
1:A:128:ARG:HB3	1:A:135:PHE:CD2	2.41	0.56
1:A:202:TYR:HB3	1:A:215:LEU:HD23	1.86	0.56
1:A:19:PHE:HD1	1:A:20:LYS:N	2.05	0.55
1:A:171:ILE:O	1:A:175:PRO:HG3	2.05	0.55
1:A:132:ASP:OD2	1:A:135:PHE:HB2	2.07	0.55
1:A:80:HIS:O	1:A:83:ASP:HB2	2.07	0.55
1:A:87:PHE:CZ	1:A:122:MET:HB2	2.41	0.54
1:A:107:ARG:NH2	1:A:114:PHE:CE1	2.75	0.53
1:A:274:ARG:HH21	1:A:307:TYR:HB3	1.72	0.53
1:A:284:LEU:HG	1:A:294:PHE:HE2	1.74	0.53
1:A:71:ILE:HB	1:A:75:LEU:HD13	1.89	0.53
1:A:49:THR:HG22	1:A:274:ARG:HB2	1.90	0.53
1:A:28:THR:HA	1:A:260:LEU:O	2.08	0.52
1:A:261:TYR:HB3	1:A:263:ASN:OD1	2.09	0.52
1:A:34:HIS:O	1:A:254:THR:HA	2.10	0.52
1:A:85:TRP:CZ2	1:A:195:LEU:HB2	2.45	0.52
1:A:223:PHE:HE2	1:A:312:ALA:CB	2.21	0.51
1:A:82:TRP:CZ2	3:A:318:CB3:CP3	2.94	0.51
1:A:87:PHE:HD2	1:A:104:PHE:CE2	2.28	0.51
1:A:283:GLN:O	1:A:284:LEU:HD12	2.11	0.51
1:A:112:PRO:HD2	1:A:114:PHE:HB2	1.93	0.50
1:A:19:PHE:CD1	1:A:20:LYS:N	2.80	0.50
1:A:192:THR:HG22	1:A:193:MET:N	2.26	0.49
1:A:23:ARG:NH2	2:A:317:UFP:O3P	2.46	0.49
1:A:111:ALA:HB1	1:A:114:PHE:HB3	1.95	0.49
1:A:288:LYS:HB3	1:A:294:PHE:CE1	2.48	0.49
1:A:51:LYS:HB3	1:A:309:ALA:HB2	1.94	0.48
1:A:76:GLN:HB3	1:A:130:LEU:HD11	1.96	0.48
1:A:122:MET:SD	1:A:122:MET:O	2.73	0.47
1:A:180:LEU:O	1:A:203:GLN:HA	2.15	0.47
1:A:40:LEU:HB2	1:A:249:GLY:O	2.15	0.47
1:A:122:MET:HE3	1:A:122:MET:HB3	1.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ILE:HG22	1:A:82:TRP:CD1	2.50	0.46
1:A:223:PHE:CE2	1:A:312:ALA:HB2	2.45	0.46
1:A:96:TYR:OH	1:A:99:PRO:HG2	2.15	0.46
1:A:115:ALA:HA	1:A:119:HIS:ND1	2.31	0.46
1:A:82:TRP:HA	4:A:442:HOH:O	2.15	0.46
1:A:6:TYR:CA	1:A:36:MET:HE3	2.46	0.46
1:A:315:ALA:O	1:A:316:VAL:HB	2.16	0.45
1:A:30:SER:OG	1:A:259:HIS:HB3	2.16	0.45
1:A:3:GLU:OE2	1:A:276:PRO:HB3	2.17	0.45
1:A:50:LYS:HG2	1:A:51:LYS:O	2.17	0.45
1:A:72:ARG:HG2	1:A:76:GLN:HE21	1.82	0.45
1:A:153:TRP:O	1:A:160:THR:HA	2.16	0.44
1:A:168:ILE:HA	1:A:171:ILE:HD12	1.99	0.44
1:A:295:ASP:O	1:A:298:ASP:HB2	2.17	0.44
1:A:314:VAL:HG13	3:A:318:CB3:C8	2.43	0.44
1:A:213:LEU:O	1:A:252:ILE:HD12	2.18	0.43
1:A:294:PHE:CD2	1:A:298:ASP:HB3	2.53	0.43
1:A:39:ASP:OD2	1:A:42:LYS:HD2	2.18	0.43
1:A:45:PRO:O	1:A:230:ILE:HD12	2.19	0.43
1:A:7:LEU:HD22	1:A:272:LEU:HD23	2.01	0.43
2:A:317:UFP:H1'	4:A:443:HOH:O	2.18	0.43
1:A:283:GLN:HE22	1:A:300:LYS:HD2	1.84	0.42
1:A:6:TYR:CE2	1:A:47:LEU:HD11	2.53	0.42
1:A:192:THR:HG22	1:A:193:MET:H	1.84	0.42
1:A:87:PHE:CE1	1:A:122:MET:HB2	2.54	0.42
1:A:87:PHE:CE2	1:A:101:MET:HE2	2.55	0.42
1:A:304:TYR:O	1:A:306:PRO:HD3	2.19	0.42
1:A:182:VAL:HB	1:A:202:TYR:CE1	2.54	0.42
1:A:210:LYS:CB	1:A:247:GLU:HB2	2.48	0.42
1:A:72:ARG:HG2	1:A:76:GLN:NE2	2.35	0.42
1:A:76:GLN:HB3	1:A:130:LEU:CD1	2.50	0.42
1:A:214:GLN:HG3	1:A:252:ILE:HB	2.02	0.41
1:A:104:PHE:HD2	1:A:118:TYR:CD1	2.39	0.41
1:A:66:HIS:HA	1:A:151:ARG:NH1	2.35	0.41
1:A:238:HIS:CE1	1:A:282:LEU:HD21	2.55	0.41
1:A:73:PHE:HA	1:A:76:GLN:HG2	2.03	0.41
1:A:101:MET:CE	1:A:118:TYR:HA	2.50	0.41
1:A:112:PRO:HB2	1:A:113:GLU:H	1.55	0.41
1:A:61:LEU:O	1:A:64:PHE:HB2	2.20	0.41
1:A:173:THR:C	1:A:175:PRO:HD3	2.46	0.41
1:A:182:VAL:HB	1:A:202:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:O	1:A:168:ILE:HG12	2.20	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.87	0.41
1:A:60:GLN:O	1:A:63:TRP:HB3	2.21	0.41
1:A:71:ILE:HD12	1:A:75:LEU:HD11	2.03	0.41
1:A:89:LYS:HA	1:A:92:LYS:HE2	2.03	0.41
1:A:146:TYR:CE1	1:A:199:HIS:HB2	2.56	0.41
1:A:168:ILE:O	1:A:172:LYS:HG3	2.21	0.41
1:A:214:GLN:HA	1:A:252:ILE:O	2.21	0.40
1:A:71:ILE:HB	1:A:75:LEU:CD1	2.51	0.40
1:A:71:ILE:O	1:A:75:LEU:HD13	2.20	0.40
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.99	0.40
1:A:13:VAL:HG22	1:A:31:ILE:HG23	2.02	0.40
1:A:72:ARG:HG2	1:A:72:ARG:O	2.21	0.40
1:A:87:PHE:CG	1:A:122:MET:HG3	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	314/316 (99%)	242 (77%)	56 (18%)	16 (5%)	1 2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	94	ASP
1	A	101	MET
1	A	112	PRO
1	A	174	HIS
1	A	176	TYR
1	A	53	PRO

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Mol	Chain	Res	Type
1	A	207	ASN
1	A	308	PRO
1	A	78	ARG
1	A	99	PRO
1	A	192	THR
1	A	103	ASP
1	A	193	MET
1	A	105	GLY
1	A	175	PRO

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	277/277 (100%)	208 (75%)	69 (25%)	0 1

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	LYS
1	A	15	ASP
1	A	16	GLU
1	A	22	ASP
1	A	24	THR
1	A	25	HIS
1	A	26	THR
1	A	29	TYR
1	A	35	GLN
1	A	36	MET
1	A	46	LEU
1	A	49	THR
1	A	56	LEU
1	A	59	SER
1	A	62	LEU
1	A	65	LEU

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Mol	Chain	Res	Type
1	A	71	ILE
1	A	78	ARG
1	A	81	ILE
1	A	83	ASP
1	A	89	LYS
1	A	90	TRP
1	A	91	VAL
1	A	94	ASP
1	A	97	HIS
1	A	106	HIS
1	A	109	GLN
1	A	110	LYS
1	A	114	PHE
1	A	121	GLU
1	A	127	ASP
1	A	129	VAL
1	A	138	LYS
1	A	142	LEU
1	A	157	LYS
1	A	160	THR
1	A	169	GLU
1	A	174	HIS
1	A	175	PRO
1	A	178	ARG
1	A	180	LEU
1	A	187	PRO
1	A	190	VAL
1	A	192	THR
1	A	193	MET
1	A	195	LEU
1	A	200	THR
1	A	203	GLN
1	A	207	ASN
1	A	208	ASP
1	A	214	GLN
1	A	215	LEU
1	A	218	ARG
1	A	224	LEU
1	A	227	PRO
1	A	230	ILE
1	A	248	VAL
1	A	254	THR

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Mol	Chain	Res	Type
1	A	262	VAL
1	A	270	GLU
1	A	274	ARG
1	A	278	PRO
1	A	286	PRO
1	A	288	LYS
1	A	297	LYS
1	A	300	LYS
1	A	302	LEU
1	A	308	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	76	GLN
1	A	77	HIS
1	A	80	HIS
1	A	186	ASN
1	A	207	ASN
1	A	283	GLN
1	A	285	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 ⓘ

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	CB3	A	318	-	37,37,37	2.81	14 (37%)	50,51,51	1.91	13 (26%)
2	UFP	A	317	-	22,22,22	2.12	7 (31%)	32,33,33	2.16	10 (31%)

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	CB3	A	318	-	-	20/27/28/28	0/3/3/3
2	UFP	A	317	-	-	9/10/22/22	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	318	CB3	O4-C4	9.48	1.39	1.23
2	A	317	UFP	C6-C5	6.06	1.41	1.33
3	A	318	CB3	CP1-N10	5.65	1.51	1.46
3	A	318	CB3	C9-N10	5.34	1.54	1.46
3	A	318	CB3	C12-C11	5.00	1.47	1.39
2	A	317	UFP	C4-C5	4.09	1.49	1.44
3	A	318	CB3	C13-C14	3.86	1.46	1.39
3	A	318	CB3	C13-C12	3.42	1.44	1.38
3	A	318	CB3	C4A-C4	-3.31	1.42	1.48
3	A	318	CB3	C16-C11	3.09	1.44	1.39
2	A	317	UFP	C2-N1	2.99	1.43	1.38
3	A	318	CB3	C8-C7	2.86	1.43	1.38
2	A	317	UFP	O4'-C1'	2.73	1.48	1.42
3	A	318	CB3	C5-C6	2.73	1.43	1.39
3	A	318	CB3	CA-N	2.37	1.50	1.45
2	A	317	UFP	P-O3P	-2.24	1.46	1.54
3	A	318	CB3	C8-C8A	2.23	1.43	1.39
2	A	317	UFP	C6-N1	-2.17	1.34	1.38
3	A	318	CB3	C8A-N1	-2.16	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	UFP	C2'-C3'	-2.09	1.47	1.52
3	A	318	CB3	OE2-CD	-2.07	1.24	1.30

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	UFP	O4'-C1'-N1	6.10	118.70	107.86
3	A	318	CB3	CP1-N10-C14	5.35	129.08	119.03
2	A	317	UFP	F5-C5-C4	4.75	120.63	116.47
3	A	318	CB3	C9-N10-C14	-4.66	112.64	120.72
3	A	318	CB3	C15-C14-N10	-4.27	115.46	121.39
3	A	318	CB3	CP2-CP1-N10	3.56	116.73	113.45
2	A	317	UFP	C2'-C1'-N1	3.50	122.56	113.81
2	A	317	UFP	C1'-N1-C6	-3.40	115.04	120.74
2	A	317	UFP	C6-C5-C4	-3.32	119.54	122.57
3	A	318	CB3	O2-CT-CA	3.25	124.51	113.51
2	A	317	UFP	C5-C4-N3	3.10	115.48	112.64
3	A	318	CB3	CG-CB-CA	2.94	118.58	113.16
3	A	318	CB3	C6-C9-N10	2.88	118.78	114.13
3	A	318	CB3	CA-N-C	2.76	128.19	121.56
2	A	317	UFP	O2P-P-O5'	-2.75	99.49	106.67
3	A	318	CB3	C13-C14-N10	2.63	125.04	121.39
3	A	318	CB3	OE2-CD-CG	2.34	121.39	114.00
3	A	318	CB3	C8A-C4A-C4	-2.19	117.74	120.11
2	A	317	UFP	C2'-C3'-C4'	-2.17	98.40	102.80
2	A	317	UFP	C4-N3-C2	-2.14	124.53	127.34
3	A	318	CB3	O2-CT-O1	-2.07	119.39	124.08
2	A	317	UFP	O2-C2-N3	-2.06	117.69	121.49
3	A	318	CB3	C12-C11-C	2.05	127.25	120.60

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	317	UFP	C3'-C4'-C5'-O5'
2	A	317	UFP	O4'-C4'-C5'-O5'
2	A	317	UFP	C5'-O5'-P-O1P
2	A	317	UFP	C5'-O5'-P-O2P
2	A	317	UFP	C5'-O5'-P-O3P
3	A	318	CB3	CP2-CP1-N10-C14
3	A	318	CB3	O-C-C11-C12
3	A	318	CB3	O-C-C11-C16

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Mol	Chain	Res	Type	Atoms
3	A	318	CB3	N-C-C11-C16
3	A	318	CB3	C13-C14-N10-C9
3	A	318	CB3	N-C-C11-C12
3	A	318	CB3	C13-C14-N10-CP1
3	A	318	CB3	C15-C14-N10-CP1
3	A	318	CB3	C15-C14-N10-C9
3	A	318	CB3	N-CA-CB-CG
3	A	318	CB3	CT-CA-CB-CG
2	A	317	UFP	C2'-C1'-N1-C2
2	A	317	UFP	C2'-C1'-N1-C6
3	A	318	CB3	N-CA-CT-O1
3	A	318	CB3	CP2-CP1-N10-C9
3	A	318	CB3	N-CA-CT-O2
2	A	317	UFP	C4'-C5'-O5'-P
3	A	318	CB3	CT-CA-N-C
3	A	318	CB3	CB-CA-CT-O2
3	A	318	CB3	OE1-CD-CG-CB
3	A	318	CB3	CA-CB-CG-CD
3	A	318	CB3	OE2-CD-CG-CB
2	A	317	UFP	O4'-C1'-N1-C2
3	A	318	CB3	CB-CA-CT-O1

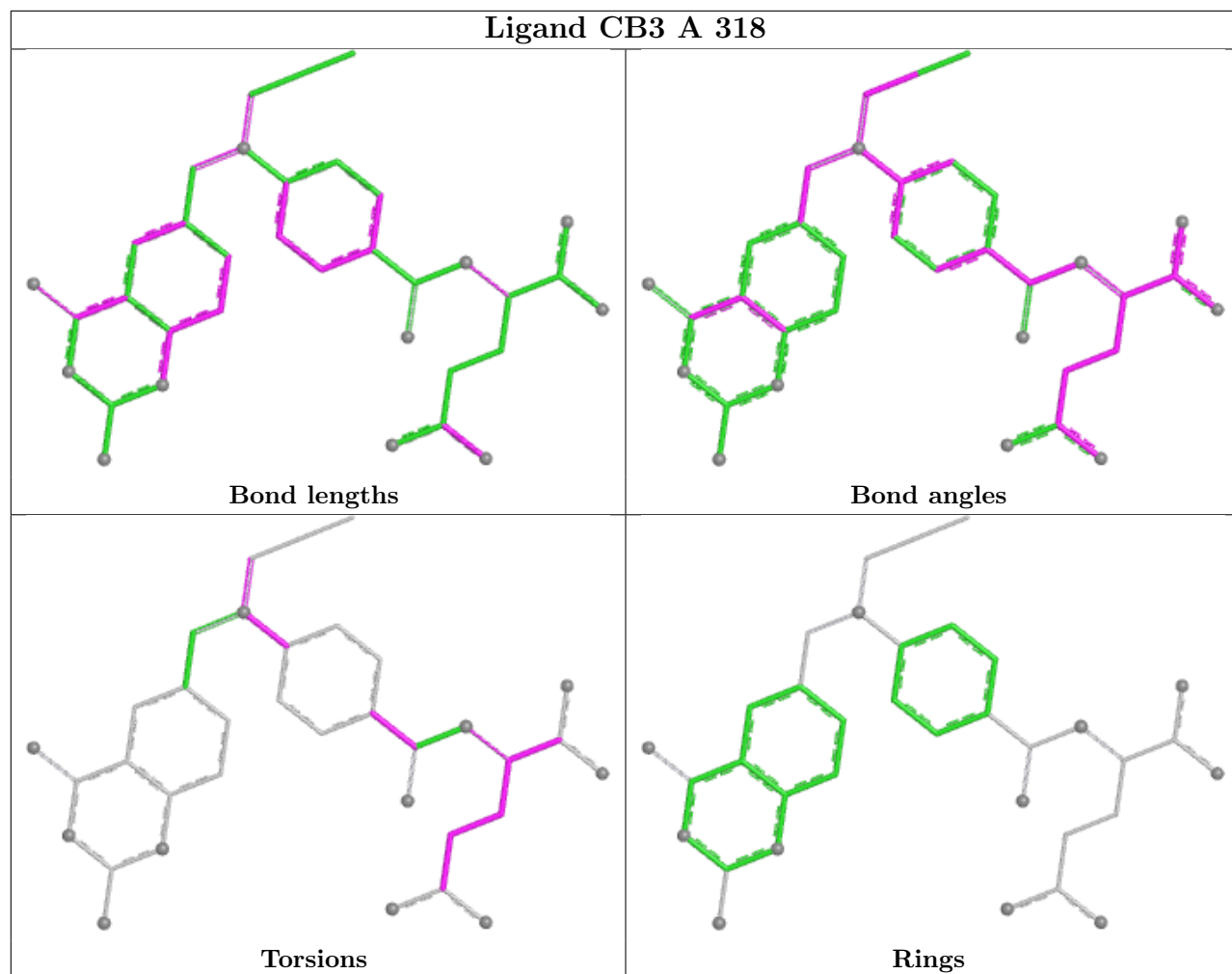
There are no ring outliers.

2 monomers are involved in 5 short contacts:

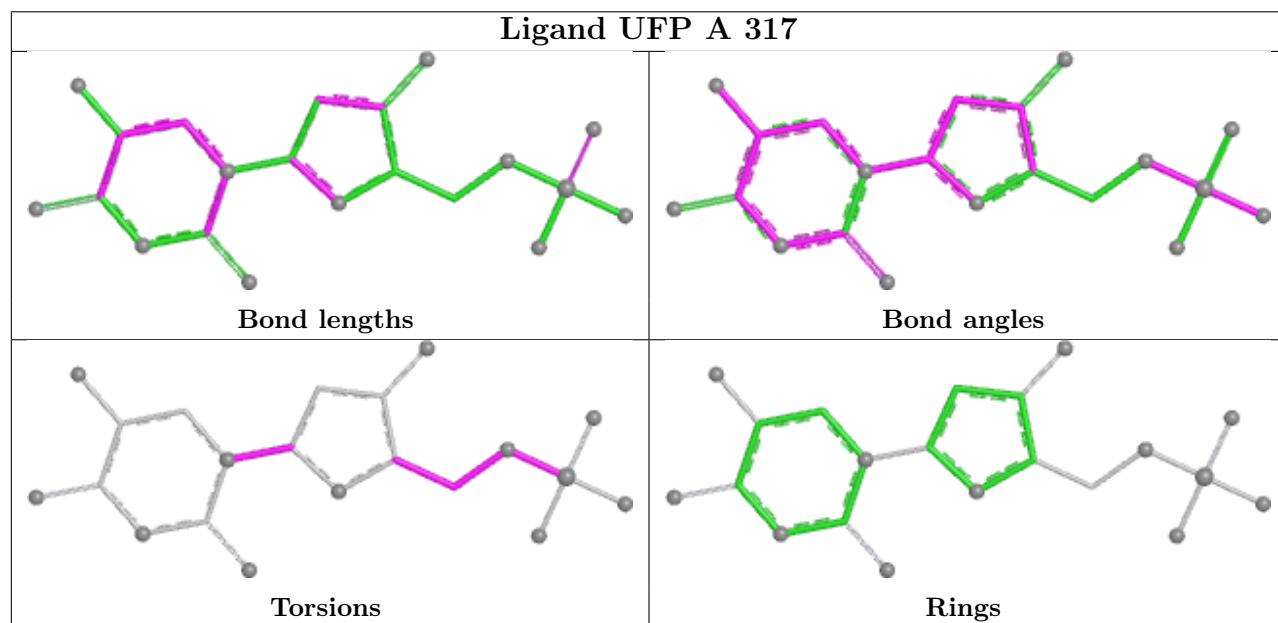
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	318	CB3	3	0
2	A	317	UFP	2	0

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 CB3 A 318



Ligand UFP 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	0 100 100	3, 11, 18, 22	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

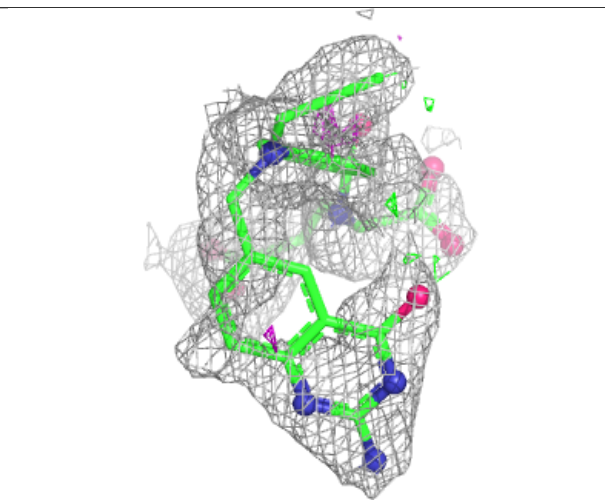
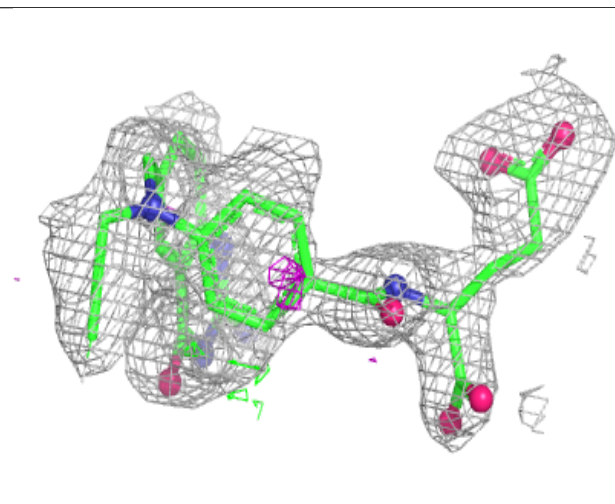
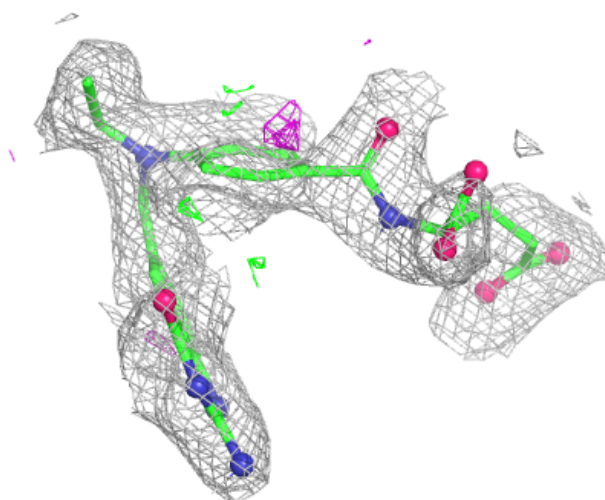
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

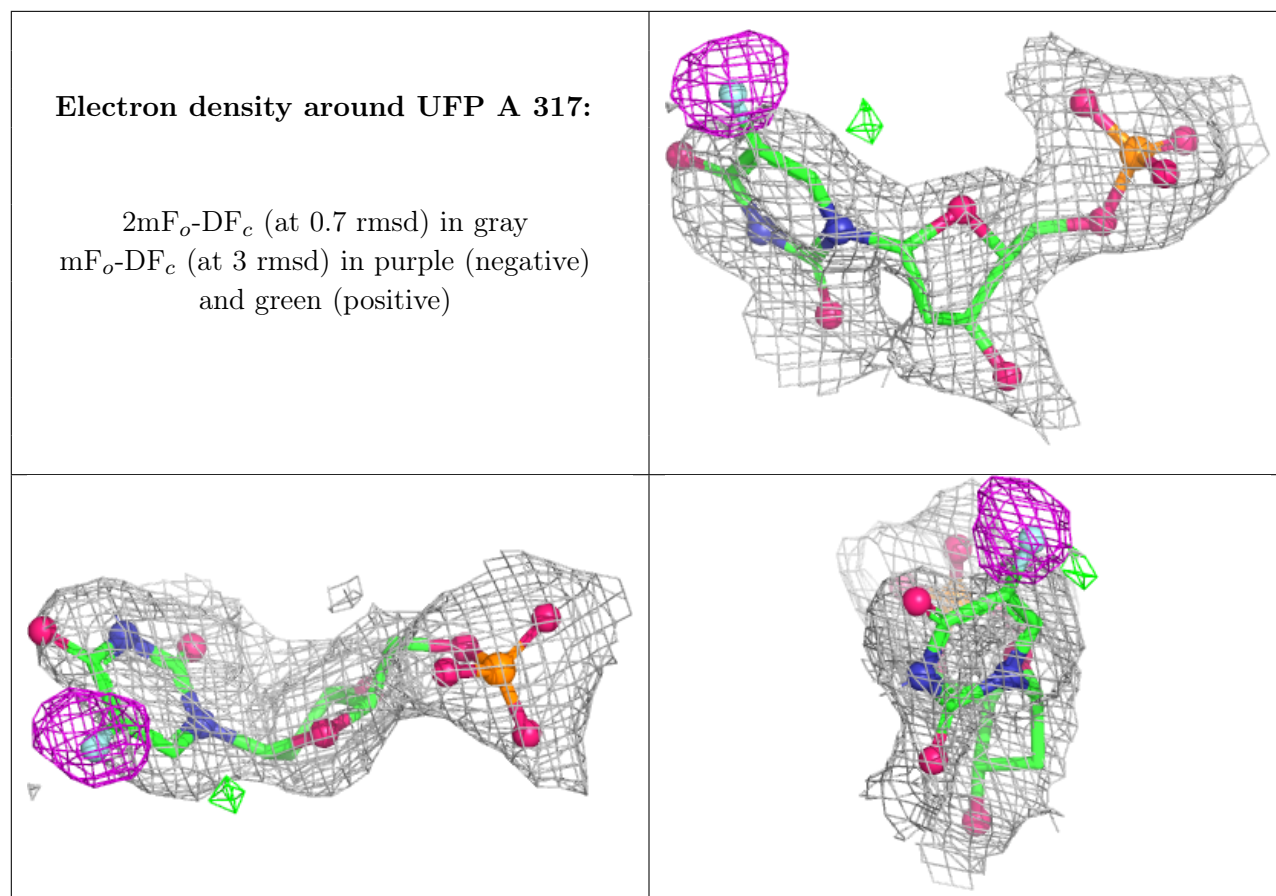
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CB3	A	318	35/35	0.84	0.10	12,20,22,24	0
2	UFP	A	317	21/21	0.89	0.11	12,15,18,22	0

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 CB3 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 ⓘ

There are no such residues in this entry.