



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:57 PM GMT

PDB ID : 1VZD  
Title : L. CASEI THYMIDYLATE SYNTHASE MUTANT E60Q TERNARY COM-  
PLEX 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

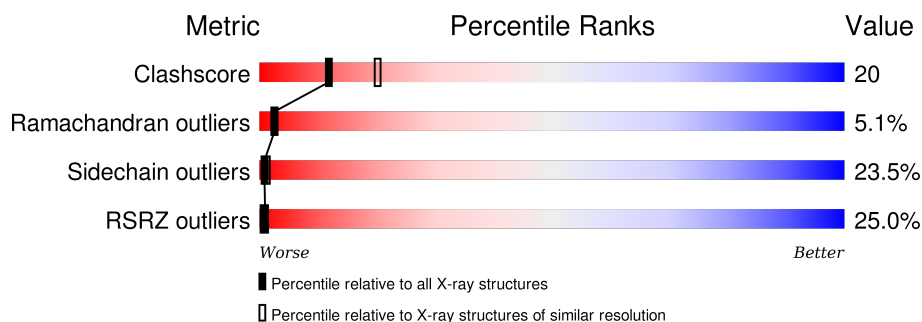
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

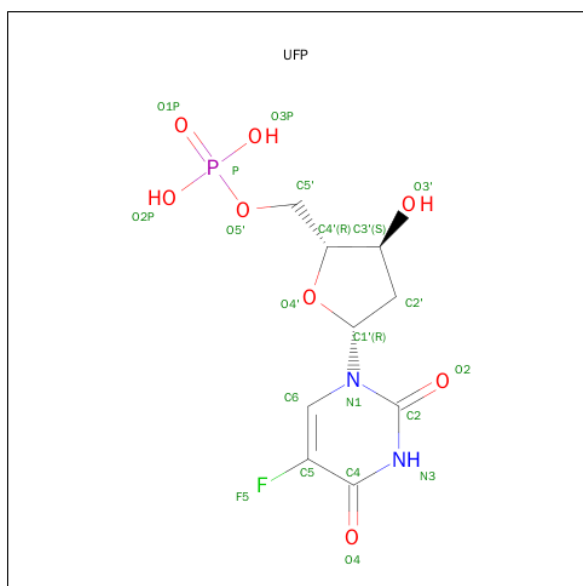
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

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

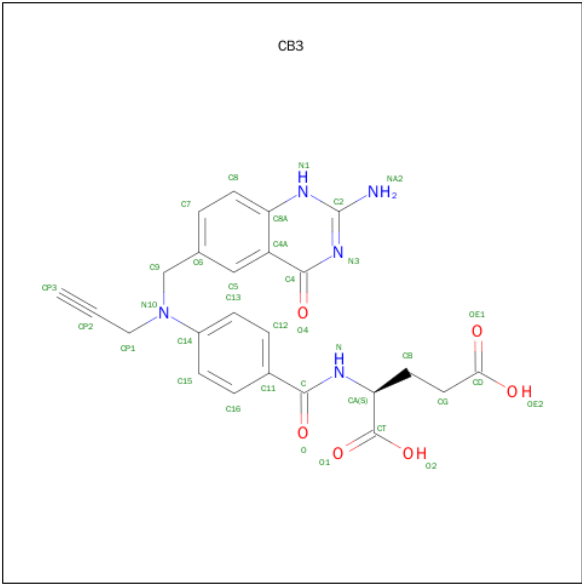
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	ENGINEERED	UNP P00469
A	111	ALA	ASP	CONFLICT	UNP P00469

- Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: C<sub>9</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>8</sub>P).



(formula: C<sub>24</sub>H<sub>23</sub>N<sub>5</sub>O<sub>6</sub>).



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

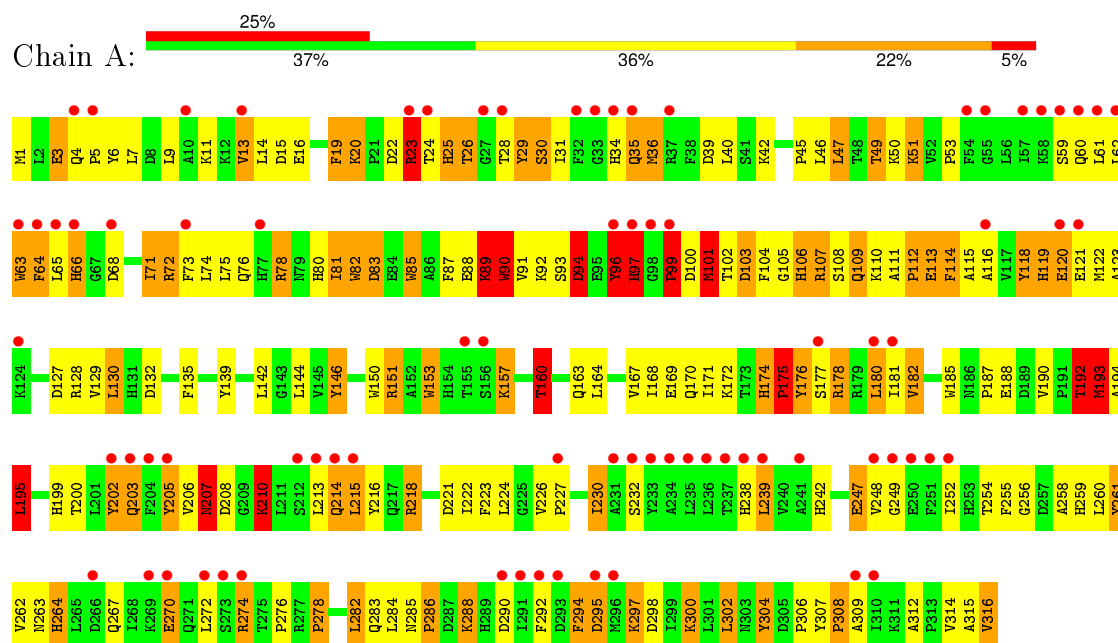
- Molecule 4 is water.

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

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	78.50 Å 78.50 Å 230.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 67.98 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 45.6 (67.98-2.19)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.18 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.188 , (Not available) 0.194 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 854.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 10269 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	3561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.39	4/2674 (0.1%)	2.24	131/3634 (3.6%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	TRP	CG-CD2	-5.44	1.34	1.43
1	A	82	TRP	CD1-NE1	-5.34	1.28	1.38
1	A	232	SER	CA-CB	-5.14	1.45	1.52
1	A	286	PRO	CA-CB	-5.08	1.43	1.53

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	NE-CZ-NH1	17.20	128.90	120.30
1	A	178	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	A	96	TYR	CA-C-N	-10.74	93.58	117.20
1	A	63	TRP	CD1-CG-CD2	10.15	114.42	106.30
1	A	82	TRP	CD1-CG-CD2	9.60	113.98	106.30
1	A	90	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	A	82	TRP	CE2-CD2-CG	-8.88	100.19	107.30
1	A	150	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	A	102	THR	CA-C-N	-8.45	98.62	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	TRP	CE2-CD2-CG	-8.39	100.59	107.30
1	A	63	TRP	CE2-CD2-CG	-8.36	100.61	107.30
1	A	96	TYR	O-C-N	8.23	135.87	122.70
1	A	23	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	192	THR	CA-CB-CG2	8.15	123.81	112.40
1	A	304	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	A	93	SER	CA-C-N	-7.96	99.68	117.20
1	A	278	PRO	O-C-N	7.77	135.12	122.70
1	A	278	PRO	CA-C-N	-7.72	100.22	117.20
1	A	160	THR	N-CA-CB	-7.62	95.82	110.30
1	A	66	HIS	CA-CB-CG	7.56	126.45	113.60
1	A	288	LYS	CA-C-N	-7.52	100.66	117.20
1	A	261	TYR	CB-CG-CD1	-7.49	116.50	121.00
1	A	316	VAL	CB-CA-C	7.47	125.58	111.40
1	A	23	ARG	CA-C-N	-7.38	100.97	117.20
1	A	90	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	A	302	LEU	CA-CB-CG	7.19	131.83	115.30
1	A	118	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	A	185	TRP	CD1-CG-CD2	6.97	111.87	106.30
1	A	205	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	A	316	VAL	CA-CB-CG2	-6.92	100.51	110.90
1	A	101	MET	CA-CB-CG	6.92	125.06	113.30
1	A	99	PRO	CA-C-N	-6.90	102.02	117.20
1	A	150	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	A	103	ASP	CA-C-N	-6.79	102.25	117.20
1	A	316	VAL	N-CA-C	-6.77	92.73	111.00
1	A	221	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	188	GLU	CA-CB-CG	6.74	128.22	113.40
1	A	202	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	A	247	GLU	CA-CB-CG	6.66	128.06	113.40
1	A	153	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	A	130	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	185	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	A	64	PHE	CB-CG-CD2	-6.48	116.26	120.80
1	A	110	LYS	N-CA-C	-6.47	93.53	111.00
1	A	25	HIS	CA-CB-CG	6.46	124.58	113.60
1	A	72	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	100	ASP	CA-CB-CG	6.44	127.58	113.40
1	A	68	ASP	N-CA-C	6.41	128.29	111.00
1	A	29	TYR	N-CA-C	-6.39	93.75	111.00
1	A	153	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	A	316	VAL	CA-CB-CG1	6.39	120.48	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	TRP	CG-CD2-CE3	6.35	139.61	133.90
1	A	226	VAL	CA-CB-CG2	-6.33	101.41	110.90
1	A	3	GLU	CA-CB-CG	6.29	127.25	113.40
1	A	218	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	96	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	A	123	ALA	N-CA-C	-6.12	94.46	111.00
1	A	294	PHE	CA-C-O	6.10	132.91	120.10
1	A	163	GLN	CA-CB-CG	6.10	126.82	113.40
1	A	151	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	97	HIS	N-CA-C	-6.04	94.68	111.00
1	A	88	GLU	CA-CB-CG	6.02	126.64	113.40
1	A	100	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	130	LEU	N-CA-CB	-5.98	98.44	110.40
1	A	118	TYR	CB-CG-CD1	5.98	124.59	121.00
1	A	109	GLN	CA-CB-CG	5.97	126.54	113.40
1	A	270	GLU	CA-CB-CG	5.96	126.51	113.40
1	A	146	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	85	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	A	23	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	51	LYS	CA-CB-CG	5.84	126.25	113.40
1	A	90	TRP	CG-CD2-CE3	5.80	139.12	133.90
1	A	264	HIS	CA-CB-CG	5.80	123.45	113.60
1	A	102	THR	O-C-N	5.78	131.95	122.70
1	A	106	HIS	CA-CB-CG	5.78	123.42	113.60
1	A	221	ASP	CA-C-N	-5.77	104.51	117.20
1	A	295	ASP	N-CA-C	-5.72	95.55	111.00
1	A	51	LYS	CA-C-N	-5.71	104.63	117.20
1	A	290	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	264	HIS	C-N-CA	5.63	135.77	121.70
1	A	167	VAL	CA-CB-CG2	-5.58	102.52	110.90
1	A	85	TRP	CE2-CD2-CG	-5.57	102.85	107.30
1	A	157	LYS	N-CA-CB	-5.56	100.59	110.60
1	A	150	TRP	CA-CB-CG	5.56	124.26	113.70
1	A	144	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	A	192	THR	CA-CB-OG1	-5.54	97.37	109.00
1	A	157	LYS	CB-CG-CD	5.53	125.98	111.60
1	A	150	TRP	CG-CD1-NE1	-5.53	104.57	110.10
1	A	242	HIS	CA-CB-CG	5.51	122.96	113.60
1	A	94	ASP	CA-C-N	5.50	129.30	117.20
1	A	130	LEU	CB-CA-C	5.46	120.58	110.20
1	A	47	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	82	TRP	CG-CD1-NE1	-5.45	104.65	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	PHE	N-CA-CB	-5.45	100.79	110.60
1	A	107	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	119	HIS	CA-C-N	5.41	129.10	117.20
1	A	129	VAL	CG1-CB-CG2	-5.40	102.27	110.90
1	A	51	LYS	O-C-N	5.39	131.33	122.70
1	A	1	MET	CG-SD-CE	-5.38	91.59	100.20
1	A	207	ASN	CA-C-N	5.37	129.01	117.20
1	A	91	VAL	CA-CB-CG2	-5.33	102.90	110.90
1	A	78	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	170	GLN	CA-CB-CG	5.32	125.09	113.40
1	A	242	HIS	CA-C-N	5.31	128.88	117.20
1	A	188	GLU	CA-C-N	-5.30	105.55	117.20
1	A	13	VAL	CG1-CB-CG2	-5.29	102.43	110.90
1	A	163	GLN	CB-CA-C	-5.28	99.84	110.40
1	A	226	VAL	CA-CB-CG1	5.26	118.79	110.90
1	A	63	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	A	176	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	A	120	GLU	CA-C-N	5.21	128.67	117.20
1	A	194	ALA	CB-CA-C	-5.21	102.28	110.10
1	A	297	LYS	CA-CB-CG	5.21	124.86	113.40
1	A	177	SER	CA-C-N	-5.20	105.77	117.20
1	A	285	ASN	CA-C-N	5.19	131.64	117.10
1	A	256	GLY	N-CA-C	-5.17	100.17	113.10
1	A	85	TRP	CD1-CG-CD2	5.12	110.40	106.30
1	A	282	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	89	LYS	CG-CD-CE	5.11	127.23	111.90
1	A	14	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	35	GLN	N-CA-C	-5.10	97.23	111.00
1	A	205	TYR	CA-CB-CG	5.08	123.05	113.40
1	A	239	LEU	CA-C-N	5.08	128.37	117.20
1	A	182	VAL	CA-CB-CG1	-5.08	103.29	110.90
1	A	26	THR	CA-C-N	-5.07	106.05	116.20
1	A	101	MET	CA-C-N	5.06	128.34	117.20
1	A	210	LYS	CA-CB-CG	5.06	124.53	113.40
1	A	207	ASN	N-CA-C	-5.06	97.35	111.00
1	A	30	SER	CA-C-N	-5.02	106.16	117.20
1	A	193	MET	CA-CB-CG	5.00	121.81	113.30
1	A	93	SER	O-C-N	5.00	130.71	122.70

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	103	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	104	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 20.

All (104) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:171:ILE:O	1:A:175:PRO:HG3	2.05	0.55
1:A:19:PHE:HD1	1:A:20:LYS:N	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:288:LYS:HB3	1:A:294:PHE:CE1	2.48	0.49
1:A:111:ALA:HB1	1:A:114:PHE:HB3	1.95	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:O	1:A:122:MET:SD	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:ILE:HA	1:A:171:ILE:HD12	1.99	0.44
1:A:153:TRP:O	1:A:160:THR:HA	2.16	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
2:A:317:UFP:H1'	4:A:443:HOH:O	2.18	0.43
1:A:7:LEU:HD22	1:A:272:LEU:HD23	2.01	0.43
1:A:283:GLN:HE22	1:A:300:LYS:HD2	1.84	0.42
1:A:192:THR:HG22	1:A:193:MET:H	1.84	0.42
1:A:6:TYR:CE2	1:A:47:LEU:HD11	2.53	0.42
1:A:6:TYR:HA	1:A:36:MET:HE1	2.01	0.42
1:A:87:PHE:CE1	1:A:122:MET:HB2	2.54	0.42
1:A:304:TYR:O	1:A:306:PRO:HD3	2.19	0.42
1:A:210:LYS:CB	1:A:247:GLU:HB2	2.48	0.42
1:A:182:VAL:HB	1:A:202:TYR:CE1	2.54	0.42
1:A:76:GLN:HB3	1:A:130:LEU:CD1	2.50	0.42
1:A:72:ARG:HG2	1:A:76:GLN:NE2	2.35	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:101:MET:CE	1:A:118:TYR:HA	2.50	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:112:PRO:HB2	1:A:113:GLU:H	1.55	0.41
1:A:73:PHE:HA	1:A:76:GLN:HG2	2.03	0.41
1:A:182:VAL:HB	1:A:202:TYR:CZ	2.55	0.41
1:A:61:LEU:O	1:A:64:PHE:HB2	2.20	0.41
1:A:164:LEU:O	1:A:168:ILE:HG12	2.20	0.41
1:A:96:TYR:CG	1:A:97:HIS:N	2.88	0.41
1:A:71:ILE:HD12	1:A:75:LEU:HD11	2.03	0.41
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.87	0.41
1:A:146:TYR:CE1	1:A:199:HIS:HB2	2.56	0.41
1:A:60:GLN:O	1:A:63:TRP:HB3	2.21	0.41
1:A:89:LYS:HA	1:A:92:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:LEU:HA	1:A:180:LEU:HD12	1.99	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:72:ARG:HG2	1:A:72:ARG:O	2.21	0.40
1:A:13:VAL:HG22	1:A:31:ILE:HG23	2.02	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%)	<b>2</b> <b>2</b>

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
1	A	207	ASN
1	A	308	PRO
1	A	78	ARG
1	A	99	PRO
1	A	192	THR
1	A	103	ASP

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Mol	Chain	Res	Type
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%)	212 (76%)	65 (24%)	<b>1</b> <b>1</b>

All (65) 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	19	PHE
1	A	22	ASP
1	A	23	ARG
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	59	SER
1	A	62	LEU
1	A	65	LEU
1	A	71	ILE
1	A	81	ILE
1	A	83	ASP
1	A	89	LYS
1	A	90	TRP

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Mol	Chain	Res	Type
1	A	94	ASP
1	A	97	HIS
1	A	106	HIS
1	A	109	GLN
1	A	113	GLU
1	A	114	PHE
1	A	121	GLU
1	A	127	ASP
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	210	LYS
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	262	VAL
1	A	270	GLU
1	A	274	ARG
1	A	278	PRO
1	A	286	PRO
1	A	297	LYS
1	A	300	LYS
1	A	302	LEU
1	A	308	PRO



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

Mol	Chain	Res	Type
1	A	35	GLN
1	A	76	GLN
1	A	80	HIS
1	A	207	ASN

### 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 carbohydrates 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	$\# Z  > 2$
2	UFP	A	317	-	18,22,22	2.56	5 (27%)	19,33,33	2.01	4 (21%)
3	CB3	A	318	-	31,37,37	2.60	11 (35%)	35,51,51	2.08	10 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UFP	A	317	-	-	0/6/22/22	0/2/2/2
3	CB3	A	318	-	-	0/21/28/28	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	UFP	P-O3P	-2.29	1.46	1.54
2	A	317	UFP	C6-C5	2.10	1.41	1.38
3	A	318	CB3	C4-N3	2.30	1.37	1.33
2	A	317	UFP	C4-N3	2.42	1.40	1.36
2	A	317	UFP	O4'-C1'	2.62	1.48	1.42
3	A	318	CB3	C5-C6	2.69	1.43	1.37
3	A	318	CB3	C16-C11	2.81	1.44	1.39
3	A	318	CB3	CA-N	2.88	1.50	1.46
3	A	318	CB3	C13-C12	3.10	1.44	1.38
3	A	318	CB3	C8-C7	3.23	1.43	1.36
3	A	318	CB3	C13-C14	3.71	1.46	1.39
3	A	318	CB3	C12-C11	4.49	1.47	1.39
3	A	318	CB3	C9-N10	5.70	1.54	1.46
3	A	318	CB3	CP1-N10	5.99	1.51	1.46
3	A	318	CB3	O4-C4	6.16	1.39	1.24
2	A	317	UFP	C4-C5	8.93	1.49	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	318	CB3	C9-N10-C14	-4.61	112.64	120.93
3	A	318	CB3	N1-C2-N3	-4.51	120.58	127.44
3	A	318	CB3	C15-C14-N10	-4.40	115.46	121.38
2	A	317	UFP	O2P-P-O5'	-2.46	99.49	106.56
2	A	317	UFP	C2'-C3'-C4'	-2.11	98.40	102.77
3	A	318	CB3	C12-C11-C	2.10	127.25	120.60
3	A	318	CB3	C8-C8A-N1	2.18	122.19	118.73
3	A	318	CB3	C6-C9-N10	2.57	118.78	114.51
3	A	318	CB3	C13-C14-N10	2.72	125.04	121.38
3	A	318	CB3	CG-CB-CA	2.75	118.58	112.99
3	A	318	CB3	C4-N3-C2	3.35	120.59	115.94
2	A	317	UFP	C2'-C1'-N1	3.45	122.56	114.16
3	A	318	CB3	CP1-N10-C14	5.51	129.08	119.05
2	A	317	UFP	O4'-C1'-N1	6.34	118.70	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	316/316 (100%)	1.30	79 (25%) <b>1</b> <b>1</b>	3, 10, 18, 23	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	SER	23.9
1	A	252	ILE	12.4
1	A	237	THR	11.7
1	A	235	LEU	11.4
1	A	234	ALA	11.2
1	A	232	SER	10.7
1	A	293	ASP	10.0
1	A	61	LEU	9.9
1	A	205	TYR	9.8
1	A	233	TYR	9.5
1	A	231	ALA	9.2
1	A	238	HIS	9.0
1	A	236	LEU	8.3
1	A	58	LYS	8.3
1	A	62	LEU	8.2
1	A	272	LEU	8.2
1	A	204	PHE	8.2
1	A	55	GLY	8.1
1	A	270	GLU	7.5
1	A	213	LEU	7.2
1	A	292	PHE	6.7
1	A	296	MET	6.1
1	A	37	ARG	5.9
1	A	32	PHE	5.8
1	A	181	ILE	5.8
1	A	23	ARG	5.4
1	A	212	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	HIS	5.0
1	A	59	SER	4.8
1	A	73	PHE	4.8
1	A	203	GLN	4.8
1	A	66	HIS	4.5
1	A	65	LEU	4.4
1	A	5	PRO	4.3
1	A	290	ASP	4.3
1	A	274	ARG	4.1
1	A	99	PRO	4.1
1	A	291	ILE	4.1
1	A	266	ASP	4.1
1	A	177	SER	4.0
1	A	98	GLY	3.9
1	A	35	GLN	3.8
1	A	120	GLU	3.6
1	A	156	SER	3.6
1	A	214	GLN	3.6
1	A	34	HIS	3.6
1	A	64	PHE	3.5
1	A	57	ILE	3.5
1	A	155	THR	3.4
1	A	227	PRO	3.3
1	A	63	TRP	3.3
1	A	68	ASP	3.1
1	A	10	ALA	3.0
1	A	4	GLN	3.0
1	A	215	LEU	3.0
1	A	239	LEU	3.0
1	A	54	PHE	2.9
1	A	250	GLU	2.8
1	A	13	VAL	2.8
1	A	251	PHE	2.7
1	A	310	ILE	2.7
1	A	124	LYS	2.7
1	A	249	GLY	2.6
1	A	33	GLY	2.5
1	A	309	ALA	2.5
1	A	116	ALA	2.4
1	A	202	TYR	2.4
1	A	77	HIS	2.4
1	A	180	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	241	ALA	2.3
1	A	248	VAL	2.3
1	A	24	THR	2.3
1	A	27	GLY	2.3
1	A	269	LYS	2.2
1	A	121	GLU	2.2
1	A	96	TYR	2.2
1	A	60	GLN	2.1
1	A	295	ASP	2.1
1	A	28	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CB3	A	318	35/35	0.83	0.19	-0.10	12,20,22,24	0
2	UFP	A	317	21/21	0.93	0.09	-0.94	12,15,18,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.