



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 AM GMT

PDB ID : 2TSC  
Title : STRUCTURE, MULTIPLE SITE BINDING, AND SEGMENTAL ACCOMMODATION IN THYMIDYLATE SYNTHASE ON BINDING D/UMP AND AN ANTI-FOLATE  
Authors : Montfort, W.R.; Stroud, R.M.  
Deposited on : 1991-07-03  
Resolution : 1.97 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.

---

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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

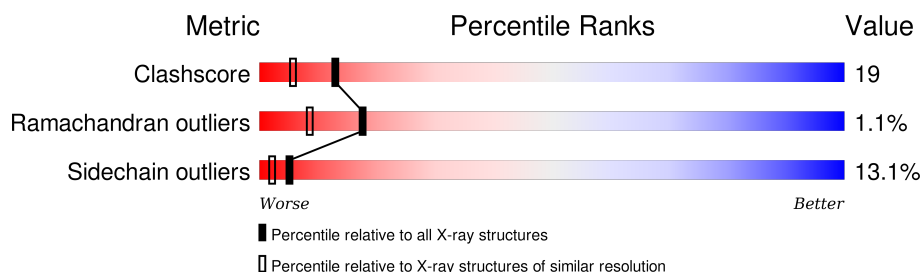
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

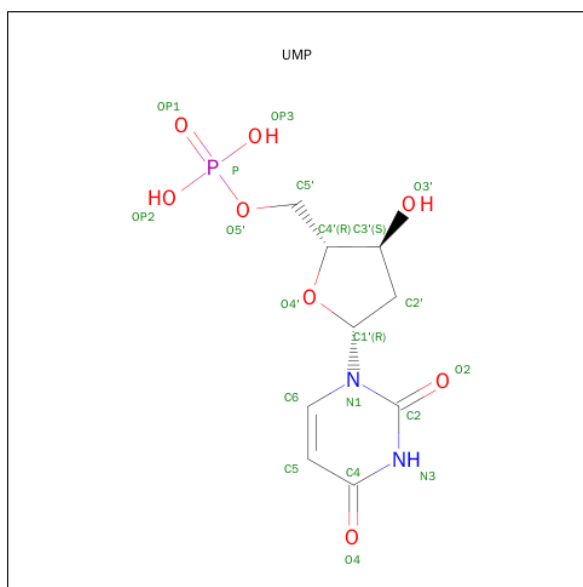
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2146	1371	370	393	12			
1	B	264	Total	C	N	O	S	0	0	0
			2146	1371	370	393	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	ALA	LYS	CONFLICT	UNP P0A884
B	235	ALA	LYS	CONFLICT	UNP P0A884

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula:  $C_9H_{13}N_2O_8P$ ).



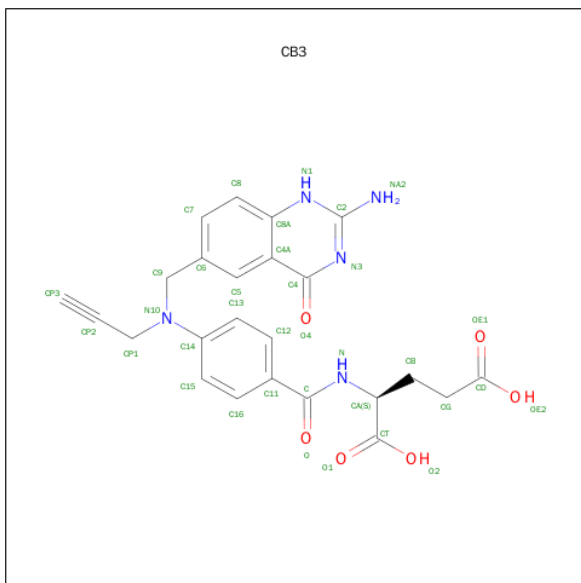
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula:  $C_{24}H_{23}N_5O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is water.

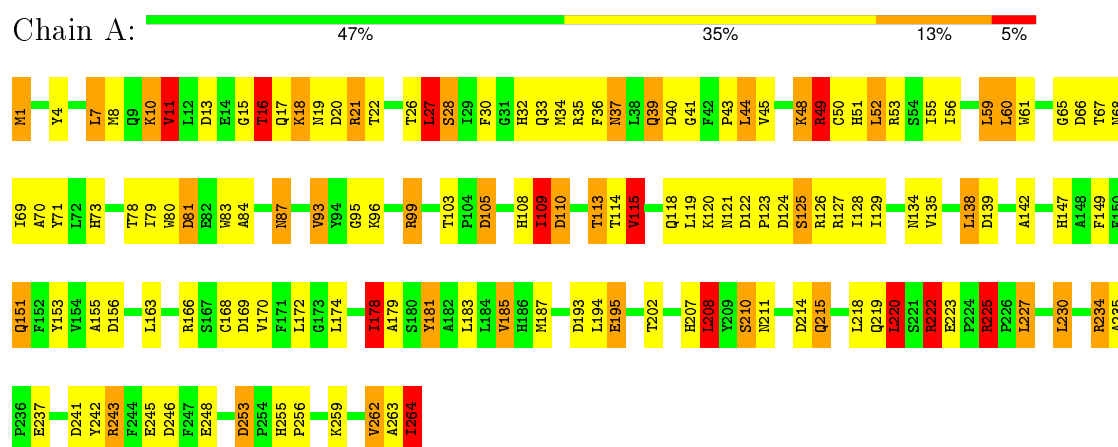
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	85	Total	O	0	0
			85	85		

### 3 Residue-property plots

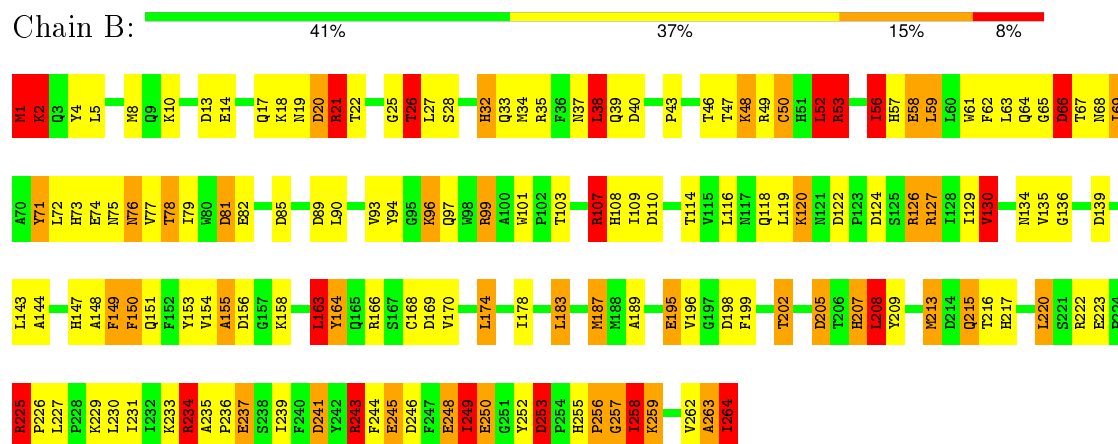
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: THYMIDYLATE SYNTHASE



#### • Molecule 1: THYMIDYLATE SYNTHASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.10 Å 127.10 Å 67.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.50 – 1.97	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-1.97)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CB3, UMP

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	1.15	2/2206 (0.1%)	2.50	129/2996 (4.3%)
1	B	1.15	5/2206 (0.2%)	2.76	148/2996 (4.9%)
All	All	1.15	7/4412 (0.2%)	2.63	277/5992 (4.6%)

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	5
1	B	0	3
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	GLY	N-CA	-7.22	1.35	1.46
1	B	257	GLY	CA-C	-6.38	1.41	1.51
1	B	264	ILE	N-CA	5.71	1.57	1.46
1	A	181	TYR	CG-CD2	5.52	1.46	1.39
1	B	127	ARG	CZ-NH2	5.36	1.40	1.33
1	A	234	ARG	CG-CD	5.27	1.65	1.51
1	B	264	ILE	CA-CB	5.20	1.66	1.54

All (277) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH1	41.98	141.29	120.30
1	B	127	ARG	NE-CZ-NH2	-31.80	104.40	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ARG	NE-CZ-NH1	-25.88	107.36	120.30
1	A	222	ARG	NE-CZ-NH1	22.60	131.60	120.30
1	B	35	ARG	NE-CZ-NH1	21.37	130.98	120.30
1	B	257	GLY	N-CA-C	20.43	164.17	113.10
1	A	53	ARG	NE-CZ-NH1	17.38	128.99	120.30
1	A	234	ARG	NE-CZ-NH1	-16.00	112.30	120.30
1	B	85	ASP	CB-CG-OD1	-16.00	103.90	118.30
1	B	253	ASP	N-CA-CB	14.93	137.48	110.60
1	B	94	TYR	CB-CG-CD2	-14.74	112.16	121.00
1	A	35	ARG	NE-CZ-NH2	14.19	127.39	120.30
1	A	166	ARG	NE-CZ-NH1	14.11	127.35	120.30
1	B	222	ARG	NE-CZ-NH2	-13.91	113.34	120.30
1	A	35	ARG	CD-NE-CZ	13.62	142.67	123.60
1	B	94	TYR	CB-CG-CD1	13.46	129.08	121.00
1	B	66	ASP	CB-CG-OD1	-12.94	106.65	118.30
1	B	205	ASP	CB-CG-OD1	12.88	129.89	118.30
1	A	4	TYR	CB-CG-CD1	12.61	128.56	121.00
1	B	122	ASP	CB-CG-OD1	12.57	129.61	118.30
1	A	222	ARG	NE-CZ-NH2	-12.53	114.03	120.30
1	A	166	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	A	40	ASP	CB-CG-OD2	-11.73	107.74	118.30
1	A	234	ARG	NE-CZ-NH2	11.51	126.05	120.30
1	B	48	LYS	N-CA-CB	11.43	131.17	110.60
1	A	243	ARG	NE-CZ-NH2	-11.39	114.60	120.30
1	A	4	TYR	CB-CG-CD2	-11.27	114.24	121.00
1	B	107	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	A	13	ASP	CB-CG-OD1	11.12	128.30	118.30
1	B	130	VAL	CA-CB-CG1	11.04	127.46	110.90
1	B	127	ARG	CD-NE-CZ	11.03	139.04	123.60
1	A	139	ASP	CB-CG-OD1	10.83	128.05	118.30
1	A	195	GLU	OE1-CD-OE2	10.69	136.13	123.30
1	B	126	ARG	NE-CZ-NH1	-10.59	115.00	120.30
1	B	20	ASP	N-CA-CB	-10.47	91.75	110.60
1	B	48	LYS	CA-CB-CG	10.04	135.48	113.40
1	A	49	ARG	NE-CZ-NH1	-9.97	115.32	120.30
1	B	164	TYR	CB-CG-CD2	9.97	126.98	121.00
1	A	49	ARG	CD-NE-CZ	-9.89	109.75	123.60
1	A	11	VAL	CA-CB-CG1	9.85	125.67	110.90
1	A	241	ASP	CB-CG-OD2	9.78	127.10	118.30
1	B	35	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	66	ASP	CB-CG-OD2	9.75	127.08	118.30
1	A	181	TYR	CB-CG-CD1	-9.65	115.21	121.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ARG	NH1-CZ-NH2	-9.54	108.90	119.40
1	B	225	ARG	NE-CZ-NH2	9.51	125.06	120.30
1	B	99	ARG	NH1-CZ-NH2	9.46	129.81	119.40
1	B	208	LEU	CB-CG-CD1	9.43	127.02	111.00
1	B	243	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	B	246	ASP	CB-CG-OD1	9.36	126.72	118.30
1	A	181	TYR	CB-CG-CD2	9.25	126.55	121.00
1	A	169	ASP	CB-CG-OD2	9.25	126.62	118.30
1	A	99	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	A	253	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	B	56	ILE	CA-CB-CG2	9.16	129.22	110.90
1	A	262	VAL	CB-CA-C	-9.11	94.09	111.40
1	B	37	ASN	CB-CA-C	8.95	128.31	110.40
1	B	223	GLU	N-CA-CB	8.85	126.53	110.60
1	A	125	SER	N-CA-CB	8.85	123.78	110.50
1	A	225	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	A	67	THR	CA-CB-CG2	8.74	124.63	112.40
1	B	26	THR	N-CA-CB	-8.66	93.84	110.30
1	B	126	ARG	NE-CZ-NH2	8.55	124.58	120.30
1	A	71	TYR	CB-CG-CD1	-8.49	115.91	121.00
1	B	34	MET	CB-CA-C	8.49	127.37	110.40
1	A	20	ASP	CB-CG-OD1	-8.45	110.69	118.30
1	A	71	TYR	CB-CG-CD2	8.40	126.04	121.00
1	A	234	ARG	CA-CB-CG	8.39	131.86	113.40
1	A	225	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	B	53	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	28	SER	N-CA-CB	-8.12	98.32	110.50
1	A	263	ALA	C-N-CA	8.11	141.98	121.70
1	B	253	ASP	CB-CG-OD1	8.07	125.56	118.30
1	B	243	ARG	CD-NE-CZ	8.05	134.88	123.60
1	A	7	LEU	CB-CG-CD1	7.95	124.52	111.00
1	B	124	ASP	CB-CG-OD1	-7.93	111.16	118.30
1	B	243	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	225	ARG	NH1-CZ-NH2	-7.84	110.77	119.40
1	A	124	ASP	CA-C-O	-7.77	103.79	120.10
1	A	138	LEU	CB-CA-C	7.76	124.95	110.20
1	A	48	LYS	N-CA-CB	7.74	124.53	110.60
1	B	189	ALA	CB-CA-C	7.74	121.71	110.10
1	B	169	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	126	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	222	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	234	ARG	N-CA-CB	7.57	124.22	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	VAL	N-CA-CB	7.49	127.98	111.50
1	B	148	ALA	N-CA-CB	-7.49	99.61	110.10
1	B	156	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	B	85	ASP	OD1-CG-OD2	7.47	137.50	123.30
1	A	61	TRP	CA-CB-CG	7.44	127.84	113.70
1	B	64	GLN	CB-CG-CD	7.44	130.95	111.60
1	A	122	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	B	64	GLN	N-CA-CB	7.42	123.95	110.60
1	A	19	ASN	OD1-CG-ND2	7.40	138.92	121.90
1	A	138	LEU	CA-CB-CG	7.39	132.30	115.30
1	A	40	ASP	N-CA-CB	7.38	123.89	110.60
1	A	243	ARG	NH1-CZ-NH2	7.36	127.50	119.40
1	B	2	LYS	N-CA-CB	7.36	123.86	110.60
1	A	227	LEU	CB-CA-C	7.32	124.11	110.20
1	A	126	ARG	CD-NE-CZ	7.31	133.84	123.60
1	A	81	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	149	PHE	N-CA-CB	-7.29	97.48	110.60
1	B	174	LEU	CB-CA-C	7.24	123.95	110.20
1	B	220	LEU	N-CA-CB	-7.23	95.93	110.40
1	A	142	ALA	N-CA-CB	-7.21	100.00	110.10
1	B	155	ALA	N-CA-CB	7.19	120.16	110.10
1	A	105	ASP	CB-CG-OD1	7.18	124.77	118.30
1	B	225	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	52	LEU	CB-CA-C	7.13	123.75	110.20
1	B	122	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	199	PHE	CB-CG-CD1	7.04	125.73	120.80
1	B	223	GLU	CA-CB-CG	7.02	128.85	113.40
1	A	230	LEU	O-C-N	7.00	133.90	122.70
1	B	21	ARG	CD-NE-CZ	6.96	133.35	123.60
1	A	27	LEU	CA-CB-CG	6.93	131.24	115.30
1	B	257	GLY	C-N-CA	6.86	138.85	121.70
1	B	155	ALA	CA-C-O	-6.85	105.71	120.10
1	B	156	ASP	CB-CG-OD1	6.82	124.44	118.30
1	B	252	TYR	CB-CG-CD2	6.78	125.07	121.00
1	A	35	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	195	GLU	N-CA-CB	-6.75	98.45	110.60
1	A	125	SER	CA-CB-OG	-6.72	93.05	111.20
1	A	178	ILE	CA-CB-CG2	6.68	124.27	110.90
1	B	52	LEU	N-CA-CB	-6.67	97.05	110.40
1	A	149	PHE	N-CA-CB	-6.66	98.62	110.60
1	B	195	GLU	CA-CB-CG	6.65	128.04	113.40
1	A	13	ASP	CB-CG-OD2	-6.64	112.33	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASN	CB-CA-C	6.61	123.61	110.40
1	A	99	ARG	NH1-CZ-NH2	-6.60	112.14	119.40
1	B	4	TYR	CB-CG-CD2	6.57	124.94	121.00
1	B	1	MET	O-C-N	-6.55	112.22	122.70
1	B	256	PRO	C-N-CA	6.54	136.04	122.30
1	A	70	ALA	CB-CA-C	6.51	119.86	110.10
1	B	150	PHE	CA-CB-CG	6.50	129.50	113.90
1	A	105	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	202	THR	CA-CB-CG2	6.50	121.50	112.40
1	B	263	ALA	CB-CA-C	-6.50	100.36	110.10
1	B	50	CYS	CB-CA-C	6.48	123.37	110.40
1	B	143	LEU	CA-CB-CG	6.45	130.14	115.30
1	A	108	HIS	O-C-N	6.45	133.01	122.70
1	A	124	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	234	ARG	CB-CG-CD	-6.43	94.88	111.60
1	B	108	HIS	N-CA-CB	6.42	122.16	110.60
1	A	1	MET	CG-SD-CE	-6.41	89.94	100.20
1	B	63	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	A	248	GLU	OE1-CD-OE2	-6.32	115.71	123.30
1	A	237	GLU	CG-CD-OE1	6.32	130.94	118.30
1	B	198	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	52	LEU	CB-CG-CD2	-6.32	100.26	111.00
1	A	19	ASN	CB-CG-OD1	-6.31	108.98	121.60
1	B	78	THR	N-CA-CB	-6.31	98.31	110.30
1	B	74	GLU	CB-CA-C	-6.30	97.80	110.40
1	A	7	LEU	CA-CB-CG	6.30	129.79	115.30
1	A	10	LYS	CD-CE-NZ	-6.29	97.22	111.70
1	A	28	SER	N-CA-CB	-6.29	101.07	110.50
1	B	208	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	41	GLY	O-C-N	6.27	132.73	122.70
1	B	78	THR	CA-CB-CG2	6.24	121.13	112.40
1	B	207	HIS	O-C-N	6.22	132.65	122.70
1	B	40	ASP	CB-CG-OD2	6.22	123.89	118.30
1	B	199	PHE	CB-CG-CD2	-6.21	116.45	120.80
1	A	235	ALA	N-CA-CB	6.20	118.78	110.10
1	B	20	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	110	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	127	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	222	ARG	CD-NE-CZ	-6.11	115.05	123.60
1	A	39	GLN	CB-CA-C	6.10	122.60	110.40
1	A	193	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	28	SER	CB-CA-C	-5.99	98.72	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	HIS	CA-CB-CG	-5.97	103.45	113.60
1	A	30	PHE	CB-CG-CD1	-5.96	116.63	120.80
1	B	239	ILE	CA-CB-CG1	5.96	122.32	111.00
1	A	128	ILE	O-C-N	5.95	132.22	122.70
1	B	119	LEU	CB-CG-CD1	5.93	121.08	111.00
1	A	70	ALA	N-CA-CB	-5.92	101.81	110.10
1	A	124	ASP	CA-C-N	5.92	130.22	117.20
1	B	250	GLU	N-CA-CB	5.91	121.23	110.60
1	A	115	VAL	CB-CA-C	5.89	122.59	111.40
1	B	250	GLU	CB-CA-C	-5.88	98.64	110.40
1	A	27	LEU	N-CA-C	-5.88	95.12	111.00
1	B	223	GLU	CB-CA-C	-5.87	98.65	110.40
1	A	195	GLU	CB-CA-C	-5.85	98.70	110.40
1	B	85	ASP	CB-CA-C	5.84	122.09	110.40
1	A	19	ASN	CA-CB-CG	-5.83	100.57	113.40
1	A	66	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	87	ASN	CB-CG-OD1	-5.80	109.99	121.60
1	A	169	ASP	CB-CA-C	5.77	121.95	110.40
1	B	168	CYS	N-CA-CB	-5.77	100.22	110.60
1	B	163	LEU	CB-CG-CD2	5.76	120.80	111.00
1	B	58	GLU	CG-CD-OE1	5.76	129.82	118.30
1	A	60	LEU	CB-CA-C	5.76	121.15	110.20
1	B	213	MET	CG-SD-CE	-5.76	90.98	100.20
1	A	21	ARG	CG-CD-NE	-5.73	99.76	111.80
1	A	264	ILE	N-CA-C	5.71	126.43	111.00
1	A	156	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	71	TYR	CB-CG-CD1	5.69	124.41	121.00
1	B	97	GLN	CA-CB-CG	5.68	125.91	113.40
1	B	127	ARG	NH1-CZ-NH2	-5.68	113.15	119.40
1	A	18	LYS	CA-CB-CG	5.68	125.90	113.40
1	B	187	MET	CG-SD-CE	-5.66	91.14	100.20
1	A	33	GLN	CG-CD-OE1	-5.64	110.31	121.60
1	B	148	ALA	N-CA-C	5.64	126.24	111.00
1	B	237	GLU	CA-CB-CG	5.64	125.80	113.40
1	B	19	ASN	C-N-CA	5.63	135.77	121.70
1	B	38	LEU	CA-CB-CG	5.63	128.25	115.30
1	B	81	ASP	O-C-N	5.63	131.70	122.70
1	A	53	ARG	NH1-CZ-NH2	-5.62	113.22	119.40
1	B	253	ASP	O-C-N	5.62	131.78	121.10
1	A	210	SER	N-CA-CB	-5.59	102.12	110.50
1	A	44	LEU	CB-CA-C	5.58	120.81	110.20
1	B	53	ARG	NH1-CZ-NH2	5.58	125.54	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	GLN	OE1-CD-NE2	-5.57	109.10	121.90
1	A	17	GLN	CB-CG-CD	-5.55	97.16	111.60
1	B	241	ASP	CA-CB-CG	5.55	125.60	113.40
1	A	195	GLU	CG-CD-OE2	-5.54	107.22	118.30
1	A	210	SER	CA-CB-OG	-5.49	96.37	111.20
1	B	249	ILE	CA-CB-CG2	5.49	121.88	110.90
1	A	218	LEU	CB-CA-C	5.49	120.62	110.20
1	B	27	LEU	N-CA-CB	5.48	121.36	110.40
1	B	153	TYR	CB-CG-CD1	5.46	124.28	121.00
1	B	38	LEU	CB-CA-C	5.43	120.52	110.20
1	A	138	LEU	N-CA-CB	-5.41	99.58	110.40
1	B	57	HIS	CA-CB-CG	-5.41	104.41	113.60
1	B	78	THR	OG1-CB-CG2	5.39	122.40	110.00
1	B	99	ARG	CD-NE-CZ	-5.38	116.07	123.60
1	B	248	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	A	34	MET	CB-CG-SD	-5.37	96.28	112.40
1	A	78	THR	CA-C-N	5.37	129.01	117.20
1	B	139	ASP	C-N-CA	5.35	135.07	121.70
1	B	49	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	208	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	B	164	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	249	ILE	N-CA-CB	5.32	123.03	110.80
1	A	96	LYS	CB-CG-CD	5.32	125.42	111.60
1	A	126	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	109	ILE	CB-CG1-CD1	5.31	128.77	113.90
1	B	35	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	B	246	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	185	VAL	CA-CB-CG2	5.30	118.84	110.90
1	B	250	GLU	CA-CB-CG	5.24	124.94	113.40
1	A	151	GLN	C-N-CA	5.24	134.80	121.70
1	A	53	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	144	ALA	N-CA-CB	-5.23	102.78	110.10
1	A	34	MET	N-CA-CB	5.22	120.00	110.60
1	A	223	GLU	CG-CD-OE2	-5.22	107.85	118.30
1	B	155	ALA	CA-C-N	5.22	128.68	117.20
1	B	120	LYS	CB-CA-C	-5.22	99.97	110.40
1	A	99	ARG	CB-CG-CD	5.20	125.12	111.60
1	B	13	ASP	N-CA-CB	5.20	119.96	110.60
1	B	76	ASN	OD1-CG-ND2	5.19	133.85	121.90
1	B	166	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	114	THR	CA-CB-CG2	5.17	119.64	112.40
1	A	214	ASP	CB-CG-OD1	5.17	122.95	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ASP	N-CA-CB	-5.16	101.31	110.60
1	A	168	CYS	N-CA-C	5.16	124.94	111.00
1	A	93	VAL	CB-CA-C	5.16	121.19	111.40
1	A	68	ASN	CB-CG-ND2	5.15	129.06	116.70
1	B	56	ILE	CB-CG1-CD1	5.15	128.32	113.90
1	B	234	ARG	CA-CB-CG	5.13	124.69	113.40
1	B	59	LEU	O-C-N	5.12	130.90	122.70
1	A	129	ILE	C-N-CA	5.12	134.51	121.70
1	B	62	PHE	CA-CB-CG	5.08	126.08	113.90
1	B	59	LEU	CA-C-O	-5.05	109.49	120.10
1	A	194	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	220	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	B	153	TYR	N-CA-CB	-5.05	101.51	110.60
1	B	264	ILE	N-CA-CB	5.04	122.40	110.80
1	A	16	THR	CA-CB-CG2	5.04	119.46	112.40
1	B	151	GLN	C-N-CA	5.04	134.29	121.70
1	B	163	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	B	209	TYR	CB-CG-CD2	5.03	124.02	121.00
1	A	11	VAL	N-CA-CB	5.03	122.56	111.50
1	B	33	GLN	CG-CD-OE1	5.02	131.65	121.60
1	B	19	ASN	N-CA-C	-5.01	97.47	111.00
1	A	59	LEU	CB-CG-CD2	5.01	119.51	111.00
1	B	135	VAL	C-N-CA	5.00	132.81	122.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	127	ARG	Sidechain
1	B	21	ARG	Sidechain
1	B	243	ARG	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	2146	0	2071	84	0
1	B	2146	0	2072	87	0
2	A	20	0	8	0	0
2	B	20	0	9	0	0
3	A	35	0	21	3	0
3	B	35	0	21	1	0
4	A	113	0	0	8	0
4	B	85	0	0	9	0
All	All	4600	0	4202	164	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 19.

All (164) 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:B:243:ARG:HD3	1:B:244:PHE:H	1.18	1.09
1:B:243:ARG:CD	1:B:244:PHE:H	1.68	1.07
1:A:215:GLN:HE21	1:A:215:GLN:H	1.16	0.94
1:B:183:LEU:HD22	1:B:187:MET:HE2	1.53	0.91
1:A:172:LEU:HD12	3:A:266:CB3:OE2	1.74	0.87
1:A:234:ARG:NH2	1:A:246:ASP:OD2	2.11	0.83
1:B:245:GLU:OE2	4:B:677:HOH:O	1.96	0.83
1:B:107:ARG:HG3	4:B:704:HOH:O	1.75	0.83
1:B:103:THR:HG22	1:B:109:ILE:HD11	1.61	0.82
1:A:44:LEU:CD2	1:A:52:LEU:HD21	2.09	0.81
1:A:22:THR:O	1:A:264:ILE:HD11	1.79	0.81
1:B:243:ARG:CD	1:B:244:PHE:N	2.43	0.80
1:A:202:THR:HG21	1:B:202:THR:HG21	1.65	0.79
1:A:22:THR:O	1:A:264:ILE:CD1	2.31	0.78
1:B:22:THR:HG21	1:B:263:ALA:HB1	1.66	0.78
1:A:195:GLU:HA	4:A:570:HOH:O	1.85	0.77
1:A:37:ASN:HD22	1:A:39:GLN:H	1.31	0.75
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.17	0.75
1:B:66:ASP:OD2	4:B:689:HOH:O	2.05	0.73
1:A:8:MET:CE	1:A:220:LEU:HD13	2.19	0.72
1:A:56:ILE:HG12	1:A:183:LEU:HD21	1.72	0.72
1:A:172:LEU:HD12	3:A:266:CB3:HOE2	1.52	0.72
1:B:243:ARG:HD2	1:B:244:PHE:H	1.55	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:HD3	1:B:244:PHE:N	1.98	0.71
1:B:77:VAL:HG23	1:B:79:ILE:HG12	1.71	0.71
1:A:37:ASN:ND2	1:A:39:GLN:H	1.90	0.70
1:B:99:ARG:NH1	1:B:110:ASP:OD1	2.25	0.70
1:A:44:LEU:HD22	1:A:52:LEU:HD21	1.72	0.69
1:B:39:GLN:HE21	1:B:158:LYS:HE3	1.56	0.69
1:B:20:ASP:OD1	1:B:22:THR:HB	1.92	0.69
1:A:15:GLY:HA3	1:A:27:LEU:HD22	1.76	0.68
1:A:105:ASP:O	4:A:602:HOH:O	2.11	0.68
1:A:172:LEU:CD1	3:A:266:CB3:OE2	2.41	0.67
1:A:37:ASN:HD21	1:A:39:GLN:HB2	1.60	0.67
1:A:87:ASN:ND2	4:A:575:HOH:O	2.28	0.67
1:A:170:VAL:HB	1:A:208:LEU:HD13	1.78	0.66
1:A:45:VAL:HG22	1:A:50:CYS:SG	2.35	0.66
1:A:22:THR:HB	1:A:264:ILE:HG12	1.78	0.64
1:A:110:ASP:OD2	1:A:113:THR:HG23	1.98	0.64
1:A:52:LEU:HD23	4:A:619:HOH:O	1.98	0.63
1:B:215:GLN:HE21	1:B:215:GLN:H	1.45	0.63
1:B:59:LEU:HD23	1:B:187:MET:HE1	1.81	0.62
1:B:2:LYS:HE2	4:B:716:HOH:O	1.99	0.62
1:A:8:MET:HE1	1:A:220:LEU:HD13	1.81	0.61
1:A:215:GLN:NE2	1:A:215:GLN:H	1.93	0.61
1:B:99:ARG:HH12	1:B:110:ASP:CG	2.03	0.61
1:A:44:LEU:HD21	1:A:52:LEU:HD21	1.83	0.61
1:B:38:LEU:HB3	1:B:196:VAL:CG2	2.31	0.60
1:B:243:ARG:HD2	1:B:244:PHE:N	2.13	0.60
1:A:120:LYS:HG3	1:A:121:ASN:OD1	2.02	0.60
1:B:263:ALA:HB3	3:B:266:CB3:NA2	2.17	0.60
1:A:103:THR:CG2	1:A:109:ILE:HD13	2.32	0.60
1:B:75:ASN:O	1:B:76:ASN:HB2	2.00	0.60
1:B:38:LEU:HB3	1:B:196:VAL:HG21	1.84	0.60
1:B:234:ARG:O	1:B:236:PRO:HD3	2.02	0.59
1:B:114:THR:O	1:B:118:GLN:HG3	2.02	0.59
1:A:255:HIS:HB3	1:A:256:PRO:HD2	1.84	0.59
1:A:10:LYS:HE2	1:A:32:HIS:HD2	1.66	0.59
1:A:8:MET:HE2	1:A:220:LEU:HD13	1.85	0.58
1:B:158:LYS:HA	1:B:195:GLU:HB3	1.86	0.58
1:B:216:THR:O	1:B:220:LEU:HB2	2.03	0.58
1:B:21:ARG:HG3	1:B:22:THR:N	2.18	0.57
1:A:151:GLN:NE2	1:B:164:TYR:OH	2.37	0.57
1:A:234:ARG:HH21	1:A:246:ASP:CG	2.08	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE1	1:B:43:PRO:HA	1.86	0.56
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.71	0.55
1:A:264:ILE:O	1:A:264:ILE:CG1	2.54	0.55
1:A:79:ILE:O	1:A:83:TRP:HZ3	1.90	0.55
1:B:233:LYS:HE3	1:B:248:GLU:HB2	1.88	0.55
1:A:243:ARG:CB	1:A:243:ARG:HH11	2.20	0.55
1:B:20:ASP:HB3	1:B:25:GLY:H	1.71	0.54
1:B:237:GLU:HB2	4:B:721:HOH:O	2.07	0.54
1:A:73:HIS:HE1	1:A:81:ASP:OD1	1.91	0.54
1:A:44:LEU:HD11	1:A:50:CYS:HB2	1.90	0.54
1:A:16:THR:HG22	4:A:597:HOH:O	2.07	0.54
1:A:73:HIS:CE1	1:A:81:ASP:OD1	2.62	0.53
1:A:51:HIS:HB3	4:A:620:HOH:O	2.09	0.53
1:A:22:THR:O	1:A:264:ILE:HD13	2.08	0.53
1:A:36:PHE:CE1	1:A:178:ILE:HD13	2.43	0.53
1:B:65:GLY:CA	1:B:99:ARG:HG3	2.39	0.53
1:A:243:ARG:NH1	1:A:243:ARG:HB2	2.24	0.53
1:B:235:ALA:HB1	4:B:555:HOH:O	2.08	0.52
1:A:215:GLN:N	1:A:215:GLN:HE21	1.97	0.52
1:A:43:PRO:HB2	1:A:178:ILE:HD11	1.90	0.52
1:B:18:LYS:HB2	1:B:26:THR:HG22	1.91	0.52
1:A:245:GLU:H	1:A:245:GLU:CD	2.14	0.52
1:B:174:LEU:O	1:B:178:ILE:HG13	2.09	0.51
1:B:130:VAL:HG13	1:B:150:PHE:CE1	2.45	0.51
1:B:225:ARG:HB3	1:B:226:PRO:CD	2.41	0.51
1:B:262:VAL:HG13	1:B:264:ILE:CD1	2.40	0.51
1:B:170:VAL:HB	1:B:208:LEU:HD13	1.92	0.51
1:A:37:ASN:ND2	1:A:39:GLN:HB2	2.25	0.51
1:B:255:HIS:HB3	1:B:256:PRO:HD2	1.92	0.50
1:B:226:PRO:HD2	4:B:660:HOH:O	2.10	0.50
1:B:71:TYR:OH	1:B:243:ARG:NH1	2.44	0.50
1:B:53:ARG:HA	1:B:244:PHE:CE1	2.46	0.50
1:A:135:VAL:HA	1:A:138:LEU:HD22	1.93	0.50
1:B:39:GLN:NE2	1:B:158:LYS:HE3	2.24	0.49
1:A:110:ASP:CG	1:A:113:THR:HG23	2.33	0.49
1:A:16:THR:HG21	1:B:155:ALA:HB1	1.94	0.49
1:A:18:LYS:HE3	1:B:154:VAL:O	2.11	0.49
1:A:11:VAL:HG22	1:A:208:LEU:HD22	1.93	0.49
1:B:46:THR:O	1:B:255:HIS:HD2	1.94	0.49
1:A:222:ARG:NH1	1:A:256:PRO:O	2.44	0.49
1:A:195:GLU:HG3	4:A:565:HOH:O	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:HA	1:B:72:LEU:HD12	1.94	0.48
1:A:225:ARG:HD3	1:A:253:ASP:O	2.13	0.48
1:B:158:LYS:HG2	1:B:195:GLU:CG	2.44	0.48
1:B:10:LYS:HG3	1:B:14:GLU:OE2	2.13	0.48
1:A:65:GLY:HA2	1:A:95:GLY:O	2.12	0.48
1:B:58:GLU:O	1:B:61:TRP:HB3	2.14	0.48
1:B:56:ILE:HD11	1:B:244:PHE:HA	1.96	0.47
1:B:10:LYS:NZ	1:B:32:HIS:HD2	2.12	0.47
1:B:53:ARG:NH1	1:B:53:ARG:HB2	2.29	0.47
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.78	0.47
1:B:233:LYS:HE3	1:B:248:GLU:CB	2.45	0.46
1:B:73:HIS:HE2	1:B:81:ASP:CG	2.19	0.46
1:A:202:THR:HG21	1:B:202:THR:CG2	2.41	0.46
1:B:68:ASN:ND2	1:B:89:ASP:OD2	2.46	0.46
1:A:135:VAL:HB	1:B:101:TRP:CE2	2.51	0.45
1:A:259:LYS:HA	1:A:259:LYS:HD3	1.68	0.45
1:B:61:TRP:CD1	1:B:66:ASP:HB3	2.51	0.45
1:A:103:THR:HG22	1:B:136:GLY:HA2	1.99	0.45
1:A:174:LEU:O	1:A:178:ILE:HG23	2.16	0.45
1:A:69:ILE:HD13	1:A:84:ALA:CB	2.46	0.45
1:B:243:ARG:O	1:B:244:PHE:C	2.55	0.44
1:B:53:ARG:HA	1:B:244:PHE:HE1	1.81	0.44
1:B:61:TRP:HH2	1:B:90:LEU:CD1	2.30	0.44
1:A:243:ARG:NH1	1:A:243:ARG:CB	2.80	0.44
1:B:158:LYS:HG2	1:B:195:GLU:HB3	2.00	0.44
1:B:215:GLN:NE2	1:B:215:GLN:H	2.14	0.44
1:B:147:HIS:HB2	1:B:163:LEU:HD21	1.99	0.44
1:A:26:THR:HB	1:A:207:HIS:HB2	2.00	0.44
1:A:153:TYR:CE2	1:A:155:ALA:HB2	2.53	0.43
1:A:187:MET:HE2	1:A:242:TYR:CD2	2.53	0.43
1:A:22:THR:CB	1:A:264:ILE:HG12	2.45	0.43
1:A:234:ARG:HD3	1:A:246:ASP:OD1	2.19	0.43
1:B:225:ARG:HD2	1:B:253:ASP:O	2.19	0.43
1:B:170:VAL:HG23	1:B:207:HIS:O	2.19	0.42
1:A:79:ILE:HG13	1:A:80:TRP:CD1	2.54	0.42
1:B:67:THR:HG21	1:B:96:LYS:HB2	2.01	0.42
1:B:71:TYR:HB3	4:B:689:HOH:O	2.20	0.42
1:A:27:LEU:HD11	4:A:603:HOH:O	2.19	0.42
1:B:73:HIS:NE2	1:B:81:ASP:OD1	2.43	0.42
1:B:129:ILE:HG21	1:B:149:PHE:CZ	2.54	0.42
1:B:52:LEU:HD13	1:B:249:ILE:HG12	2.01	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:CB	1:B:226:PRO:CD	2.97	0.42
1:A:55:ILE:HD13	1:A:179:ALA:HB3	2.02	0.41
1:A:147:HIS:HB2	1:A:163:LEU:HD11	2.02	0.41
1:B:18:LYS:O	1:B:25:GLY:HA2	2.21	0.41
1:A:49:ARG:HH11	1:A:49:ARG:HD2	1.41	0.41
1:B:262:VAL:HG13	1:B:264:ILE:HD11	2.03	0.41
1:A:119:LEU:O	1:A:123:PRO:HB3	2.20	0.41
1:B:215:GLN:HG2	1:B:258:ILE:HG22	2.02	0.41
1:B:230:LEU:HD23	1:B:249:ILE:HG23	2.03	0.40
1:A:181:TYR:O	1:A:185:VAL:HG23	2.20	0.40
1:A:48:LYS:HG2	1:A:219:GLN:NE2	2.36	0.40
1:B:259:LYS:HE2	1:B:259:LYS:HB3	1.83	0.40
1:B:17:GLN:HG2	4:B:713:HOH:O	2.20	0.40
1:A:1:MET:CE	1:A:227:LEU:HD21	2.51	0.40
1:B:126:ARG:HD3	1:B:126:ARG:HH21	1.78	0.40
1:A:110:ASP:OD2	1:A:113:THR:CG2	2.66	0.40
1:A:1:MET:HE1	1:A:227:LEU:HD21	2.03	0.40
1:B:213:MET:O	1:B:217:HIS:CD2	2.74	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	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	39	31
1	B	262/264 (99%)	239 (91%)	18 (7%)	5 (2%)	10	3
All	All	524/528 (99%)	488 (93%)	30 (6%)	6 (1%)	17	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	ILE
1	B	257	GLY
1	B	107	ARG
1	B	205	ASP
1	B	93	VAL
1	A	93	VAL

### 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	232/232 (100%)	210 (90%)	22 (10%)	11	5
1	B	232/232 (100%)	193 (83%)	39 (17%)	2	1
All	All	464/464 (100%)	403 (87%)	61 (13%)	5	2

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	VAL
1	A	16	THR
1	A	27	LEU
1	A	28	SER
1	A	37	ASN
1	A	59	LEU
1	A	60	LEU
1	A	109	ILE
1	A	113	THR
1	A	115	VAL
1	A	125	SER
1	A	134	ASN
1	A	178	ILE
1	A	208	LEU
1	A	210	SER
1	A	215	GLN
1	A	220	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	225	ARG
1	A	230	LEU
1	A	262	VAL
1	A	264	ILE
1	B	1	MET
1	B	2	LYS
1	B	5	LEU
1	B	8	MET
1	B	26	THR
1	B	38	LEU
1	B	47	THR
1	B	48	LYS
1	B	50	CYS
1	B	52	LEU
1	B	53	ARG
1	B	56	ILE
1	B	66	ASP
1	B	69	ILE
1	B	78	THR
1	B	82	GLU
1	B	96	LYS
1	B	116	LEU
1	B	120	LYS
1	B	130	VAL
1	B	134	ASN
1	B	163	LEU
1	B	183	LEU
1	B	208	LEU
1	B	215	GLN
1	B	225	ARG
1	B	227	LEU
1	B	229	LYS
1	B	231	ILE
1	B	234	ARG
1	B	241	ASP
1	B	243	ARG
1	B	245	GLU
1	B	249	ILE
1	B	250	GLU
1	B	253	ASP
1	B	258	ILE
1	B	259	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	264	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	ASN
1	A	73	HIS
1	A	87	ASN
1	A	97	GLN
1	A	117	ASN
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	186	HIS
1	A	215	GLN
1	A	217	HIS
1	B	32	HIS
1	B	75	ASN
1	B	76	ASN
1	B	117	ASN
1	B	118	GLN
1	B	121	ASN
1	B	134	ASN
1	B	151	GLN
1	B	215	GLN
1	B	217	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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	UMP	A	265	1	16,21,21	2.34	7 (43%)	23,31,31	3.26	7 (30%)
3	CB3	A	266	-	31,37,37	2.55	9 (29%)	35,51,51	2.66	15 (42%)
2	UMP	B	265	1	16,21,21	1.89	5 (31%)	23,31,31	3.12	9 (39%)
3	CB3	B	266	-	31,37,37	2.71	12 (38%)	35,51,51	2.86	19 (54%)

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	UMP	A	265	1	-	0/6/22/22	0/2/2/2
3	CB3	A	266	-	-	0/21/28/28	0/3/3/3
2	UMP	B	265	1	-	0/6/22/22	0/2/2/2
3	CB3	B	266	-	-	0/21/28/28	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	266	CB3	C4-C4A	-4.78	1.33	1.41
3	B	266	CB3	C4-C4A	-4.78	1.33	1.41
2	A	265	UMP	O5'-C5'	-3.30	1.31	1.44
2	A	265	UMP	C5'-C4'	-3.24	1.41	1.51
2	B	265	UMP	O5'-C5'	-2.65	1.33	1.44
3	A	266	CB3	CA-N	-2.35	1.43	1.46
3	B	266	CB3	C8-C8A	-2.25	1.37	1.41
3	B	266	CB3	C5-C4A	-2.06	1.37	1.41
3	B	266	CB3	C14-N10	2.03	1.44	1.38
2	B	265	UMP	O4'-C1'	2.20	1.47	1.42
2	B	265	UMP	C6-C5	2.38	1.43	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	266	CB3	C16-C15	2.47	1.43	1.38
2	A	265	UMP	C4-N3	2.48	1.37	1.33
3	B	266	CB3	C7-C6	2.51	1.44	1.38
3	B	266	CB3	C11-C	2.79	1.56	1.50
3	A	266	CB3	C11-C	2.82	1.56	1.50
2	A	265	UMP	O4'-C1'	3.07	1.49	1.42
3	A	266	CB3	C14-N10	3.11	1.47	1.38
2	A	265	UMP	C6-C5	3.27	1.45	1.38
3	A	266	CB3	CB-CA	3.28	1.57	1.53
2	B	265	UMP	C4-N3	3.68	1.39	1.33
3	B	266	CB3	CB-CA	3.69	1.58	1.53
2	B	265	UMP	C2'-C1'	3.77	1.62	1.52
2	A	265	UMP	C6-N1	3.81	1.41	1.35
3	A	266	CB3	C7-C6	3.84	1.47	1.38
2	A	265	UMP	C2'-C1'	4.04	1.63	1.52
3	A	266	CB3	C9-N10	4.26	1.52	1.46
3	B	266	CB3	C9-N10	4.72	1.52	1.46
3	B	266	CB3	CP1-N10	5.65	1.51	1.46
3	B	266	CB3	CP1-CP2	6.28	1.55	1.47
3	A	266	CB3	CP1-CP2	6.29	1.55	1.47
3	B	266	CB3	C2-NA2	6.34	1.47	1.34
3	A	266	CB3	C2-NA2	6.88	1.48	1.34

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	266	CB3	C9-C6-C7	-6.29	108.91	120.78
3	B	266	CB3	O-C-N	-6.15	111.32	122.44
2	A	265	UMP	C6-N1-C2	-6.02	111.52	121.28
2	B	265	UMP	C6-N1-C2	-5.55	112.30	121.28
3	A	266	CB3	N1-C2-N3	-5.29	119.38	127.44
3	B	266	CB3	CG-CB-CA	-5.07	102.69	112.99
3	A	266	CB3	O-C-N	-4.90	113.58	122.44
2	B	265	UMP	C5-C6-N1	-4.58	109.37	120.58
2	A	265	UMP	C5-C6-N1	-4.54	109.45	120.58
2	A	265	UMP	C5-C4-N3	-4.40	111.83	123.12
2	B	265	UMP	C5-C4-N3	-4.34	112.00	123.12
3	B	266	CB3	N1-C2-N3	-3.97	121.40	127.44
3	A	266	CB3	CG-CB-CA	-3.92	105.03	112.99
3	B	266	CB3	CP1-N10-C14	-3.57	112.55	119.05
3	A	266	CB3	CB-CG-CD	-3.54	98.59	113.02
3	B	266	CB3	CB-CG-CD	-3.33	99.45	113.02

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	CB3	C15-C16-C11	-3.25	116.99	120.76
3	B	266	CB3	C6-C5-C4A	-3.12	117.03	122.65
3	B	266	CB3	C15-C14-N10	-3.03	117.31	121.38
3	B	266	CB3	C13-C12-C11	-2.99	117.30	120.76
3	A	266	CB3	C5-C4A-C4	-2.97	118.56	122.22
3	A	266	CB3	C6-C5-C4A	-2.87	117.49	122.65
3	A	266	CB3	C9-N10-C14	-2.50	116.43	120.93
2	B	265	UMP	O4'-C1'-C2'	-2.47	101.35	106.27
3	B	266	CB3	C5-C4A-C4	-2.47	119.18	122.22
3	B	266	CB3	CP1-N10-C9	-2.25	111.75	117.28
3	A	266	CB3	C9-C6-C7	-2.19	116.65	120.78
2	B	265	UMP	O5'-P-OP1	-2.17	101.62	107.14
3	B	266	CB3	C12-C13-C14	2.11	123.08	120.36
2	A	265	UMP	O5'-C5'-C4'	2.22	117.30	109.12
2	B	265	UMP	OP3-P-OP1	2.33	118.09	110.58
3	B	266	CB3	C6-C9-N10	2.35	118.43	114.51
3	B	266	CB3	NA2-C2-N3	2.70	121.66	117.20
3	B	266	CB3	C9-C6-C5	2.95	129.57	121.32
3	A	266	CB3	NA2-C2-N3	3.01	122.18	117.20
3	A	266	CB3	C5-C4A-C8A	3.11	121.85	118.14
3	A	266	CB3	C16-C11-C12	3.16	123.30	118.60
3	B	266	CB3	C5-C4A-C8A	3.27	122.04	118.14
3	B	266	CB3	C9-N10-C14	3.45	127.14	120.93
2	A	265	UMP	C2'-C1'-N1	3.95	123.76	114.16
2	B	265	UMP	C4-N3-C2	4.07	118.17	114.14
3	A	266	CB3	C6-C9-N10	4.25	121.59	114.51
3	B	266	CB3	C4-N3-C2	4.34	121.96	115.94
3	A	266	CB3	O-C-C11	4.56	128.78	120.97
2	A	265	UMP	O4'-C1'-N1	4.59	115.66	107.72
3	B	266	CB3	C11-C-N	4.62	125.16	116.93
2	B	265	UMP	C2'-C1'-N1	5.61	127.79	114.16
3	A	266	CB3	C4-N3-C2	6.57	125.06	115.94
2	B	265	UMP	O4'-C1'-N1	8.65	122.69	107.72
2	A	265	UMP	C4-N3-C2	10.88	124.92	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	266	CB3	3	0
3	B	266	CB3	1	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.