



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:25 AM UTC

PDB ID : 3ANX / pdb_00003anx
Title : Crystal structure of triamine/agmatine aminopropyltransferase (SPEE) from thermus thermophilus, complexed with MTA
Authors : Ganbe, T.; Ohnuma, M.; Sato, T.; Tanaka, N.; Oshima, T.; Kumasaka, T.
Deposited on : 2010-09-14
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

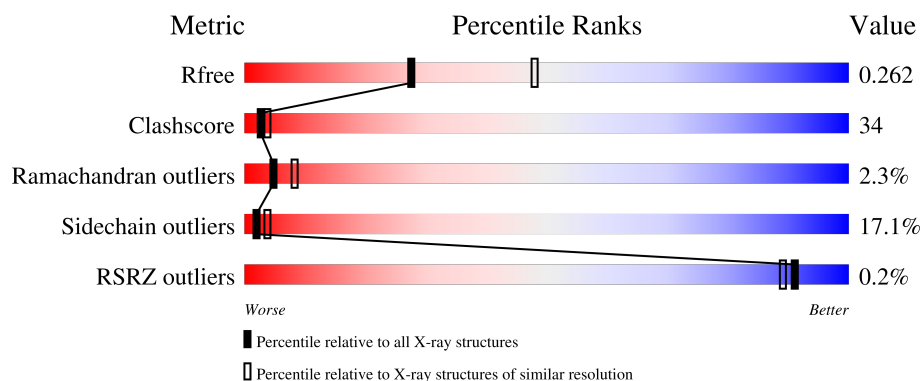
1 Overall quality at a glance

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))
R_{free}	180053	5829 (2.50-2.50)
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	314	 38% 42% 17% . .
1	B	314	 32% 45% 19% .

2 Entry composition [i](#)

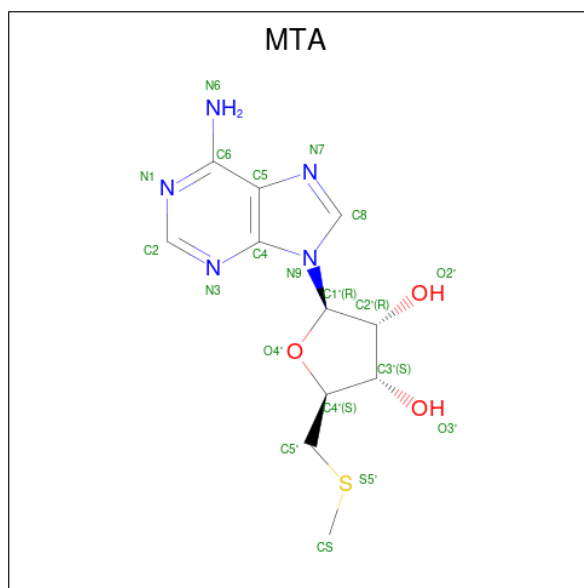
There are 3 unique types of molecules in this entry. The entry contains 5288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2528	1624	434	459	11			
1	B	313	Total	C	N	O	S	0	0	0
			2537	1630	436	460	11			

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	2	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	2	0
			20	11	5	3	1		

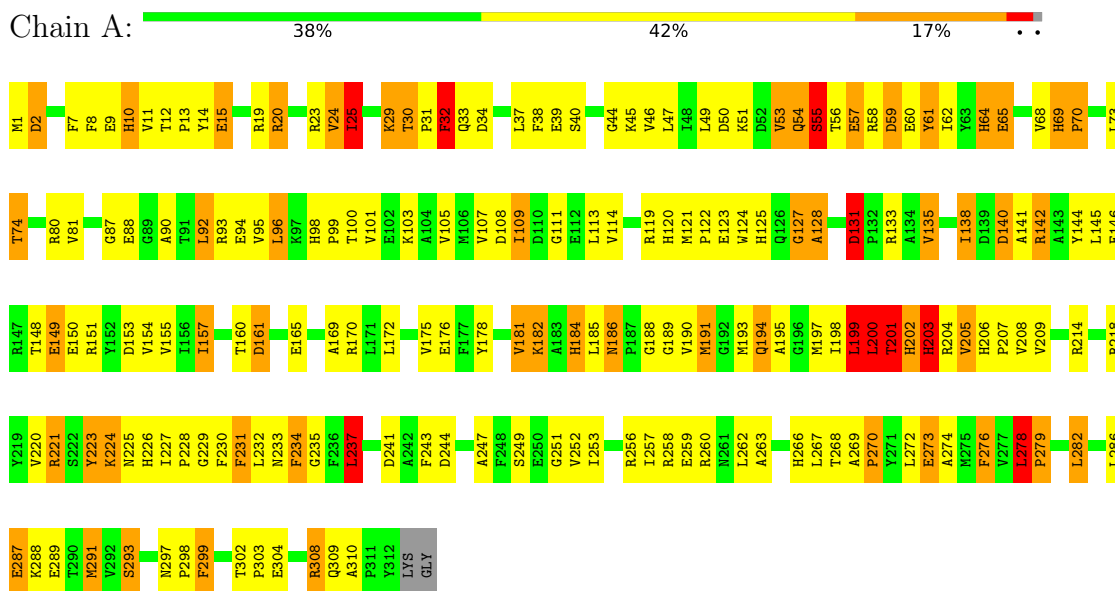
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	81	Total 81	O 81	0	0

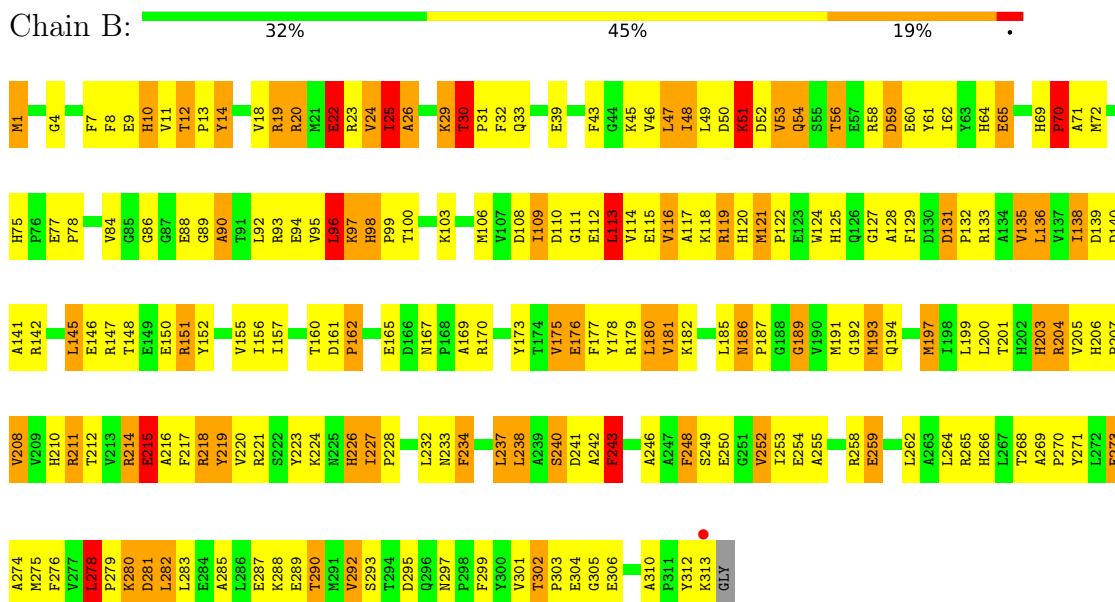
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: spermidine synthase



• Molecule 1: spermidine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.04Å 88.04Å 191.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.50) 91.5 (20.00-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.263 0.180 , 0.262	Depositor DCC
R_{free} test set	2419 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: MTA

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	1.82	35/2594 (1.3%)	1.79	58/3520 (1.6%)
1	B	1.60	28/2603 (1.1%)	1.69	60/3531 (1.7%)
All	All	1.72	63/5197 (1.2%)	1.74	118/7051 (1.7%)

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	3
1	B	0	2
All	All	0	5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	VAL	CA-CB	-10.71	1.43	1.54
1	A	61	TYR	C-O	9.32	1.35	1.24
1	B	84	VAL	CA-CB	-8.65	1.44	1.54
1	B	14	TYR	CA-C	-8.43	1.41	1.52
1	B	243	PHE	CA-C	7.85	1.64	1.53
1	B	135	VAL	CA-CB	7.77	1.62	1.53
1	B	24	VAL	CA-CB	-7.76	1.45	1.54
1	A	181	VAL	CA-C	7.75	1.61	1.52
1	A	227	ILE	CA-C	7.59	1.60	1.52
1	B	18	VAL	C-O	-7.50	1.15	1.24
1	A	45	LYS	N-CA	-7.14	1.37	1.46
1	A	270	PRO	CA-C	7.04	1.61	1.52
1	A	157	ILE	C-O	6.91	1.31	1.24
1	B	282	LEU	N-CA	-6.78	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	LEU	C-O	-6.36	1.16	1.24
1	A	25	ILE	CA-CB	6.35	1.63	1.54
1	A	135	VAL	CA-CB	6.32	1.63	1.54
1	B	51	LYS	CA-C	-6.24	1.44	1.52
1	B	292	VAL	CA-CB	6.20	1.62	1.54
1	A	231	PHE	CA-C	-6.13	1.45	1.53
1	A	198	ILE	N-CA	-6.05	1.39	1.46
1	A	279	PRO	CA-C	-6.04	1.45	1.52
1	A	198	ILE	CA-C	-6.03	1.45	1.52
1	A	201	THR	CA-C	6.01	1.60	1.52
1	B	18	VAL	CA-CB	6.01	1.61	1.53
1	A	127	GLY	C-O	-5.94	1.17	1.23
1	A	200	LEU	CA-C	-5.86	1.44	1.52
1	A	181	VAL	CB-CG2	5.85	1.71	1.52
1	A	25	ILE	C-O	-5.78	1.17	1.24
1	B	45	LYS	CA-C	-5.78	1.45	1.52
1	B	180	LEU	CA-C	-5.75	1.45	1.52
1	A	24	VAL	CA-CB	5.74	1.61	1.53
1	B	19	ARG	CA-C	5.73	1.59	1.52
1	B	226	HIS	N-CA	5.71	1.53	1.46
1	A	243	PHE	N-CA	5.71	1.53	1.46
1	A	55	SER	CA-C	-5.68	1.45	1.52
1	A	157	ILE	CA-CB	-5.55	1.47	1.54
1	B	227	ILE	CG1-CD1	-5.49	1.30	1.51
1	B	152	TYR	N-CA	5.43	1.52	1.45
1	A	150	GLU	N-CA	5.41	1.52	1.46
1	A	149	GLU	CA-CB	5.40	1.60	1.53
1	B	197	MET	CA-C	-5.39	1.45	1.53
1	A	203	HIS	CA-C	5.37	1.59	1.53
1	B	290	THR	CA-CB	5.35	1.62	1.53
1	B	217	PHE	N-CA	5.33	1.52	1.45
1	B	97	LYS	CA-C	-5.28	1.45	1.52
1	B	50	ASP	C-O	-5.25	1.17	1.24
1	A	38	PHE	CA-C	-5.24	1.46	1.52
1	A	57	GLU	CA-C	-5.18	1.46	1.52
1	A	310	ALA	CA-C	5.18	1.58	1.52
1	B	281	ASP	CA-CB	5.14	1.61	1.53
1	B	199	LEU	C-O	5.12	1.28	1.23
1	B	208	VAL	CA-C	-5.12	1.46	1.52
1	B	210	HIS	N-CA	-5.10	1.40	1.46
1	A	195	ALA	N-CA	5.08	1.52	1.46
1	B	150	GLU	CA-C	5.07	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	LEU	C-N	5.06	1.39	1.33
1	B	285	ALA	CA-CB	-5.06	1.45	1.53
1	A	30	THR	N-CA	5.05	1.53	1.46
1	A	178	TYR	N-CA	-5.03	1.39	1.46
1	A	54	GLN	C-O	-5.03	1.18	1.23
1	A	237	LEU	N-CA	5.03	1.52	1.45
1	B	65	GLU	CA-C	-5.00	1.46	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	HIS	N-CA-C	12.54	124.80	108.24
1	A	186	ASN	CA-C-N	-11.93	107.50	120.14
1	A	186	ASN	C-N-CA	-11.93	107.50	120.14
1	B	25	ILE	N-CA-C	-11.55	102.21	113.53
1	A	200	LEU	N-CA-C	-11.10	99.74	113.28
1	B	227	ILE	N-CA-C	10.85	117.43	107.56
1	B	12	THR	CA-C-N	-10.84	108.42	120.45
1	B	12	THR	C-N-CA	-10.84	108.42	120.45
1	A	87	GLY	N-CA-C	10.49	126.04	114.40
1	B	65	GLU	N-CA-C	-9.44	101.07	111.36
1	A	161	ASP	CA-C-N	-8.84	108.79	119.84
1	A	161	ASP	C-N-CA	-8.84	108.79	119.84
1	A	105	VAL	N-CA-C	-8.49	96.26	108.48
1	B	248	PHE	N-CA-C	-8.35	98.10	110.46
1	A	25	ILE	CB-CA-C	-8.33	97.62	111.29
1	A	268	THR	N-CA-C	-8.19	96.94	109.14
1	B	98	HIS	CA-C-N	8.16	130.04	119.84
1	B	98	HIS	C-N-CA	8.16	130.04	119.84
1	A	142	ARG	N-CA-C	-8.00	101.64	111.40
1	B	131	ASP	N-CA-C	-7.71	100.08	109.72
1	B	22	GLU	N-CA-C	-7.41	102.58	111.69
1	A	178	TYR	N-CA-C	-7.35	103.94	113.12
1	A	69	HIS	CA-C-N	-7.33	111.42	119.19
1	A	69	HIS	C-N-CA	-7.33	111.42	119.19
1	B	203	HIS	N-CA-C	7.25	119.40	107.73
1	B	29	LYS	N-CA-C	7.21	120.38	110.06
1	A	165	GLU	N-CA-C	7.13	119.66	111.11
1	A	289	GLU	N-CA-C	7.10	120.67	110.24
1	B	252	VAL	CB-CA-C	-6.92	102.97	112.24
1	B	312	TYR	N-CA-C	6.88	120.06	108.23
1	A	278	LEU	CA-C-N	6.79	126.73	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	LEU	C-N-CA	6.79	126.73	120.21
1	B	121	MET	CA-C-N	6.79	126.30	119.24
1	B	121	MET	C-N-CA	6.79	126.30	119.24
1	B	112	GLU	N-CA-C	-6.78	103.36	111.69
1	A	140	ASP	N-CA-C	-6.74	98.71	109.76
1	A	198	ILE	N-CA-C	-6.73	98.43	108.12
1	A	94	GLU	CA-C-N	-6.72	111.96	120.56
1	A	94	GLU	C-N-CA	-6.72	111.96	120.56
1	B	161	ASP	N-CA-C	-6.71	101.88	109.60
1	B	243	PHE	N-CA-C	6.67	118.93	110.33
1	B	268	THR	N-CA-C	-6.59	99.32	109.14
1	A	247	ALA	N-CA-C	-6.50	98.59	108.67
1	B	97	LYS	N-CA-C	-6.48	105.30	113.72
1	A	131	ASP	CA-C-N	6.35	126.56	119.32
1	A	131	ASP	C-N-CA	6.35	126.56	119.32
1	A	30	THR	CA-C-N	-6.33	111.93	119.84
1	A	30	THR	C-N-CA	-6.33	111.93	119.84
1	A	310	ALA	N-CA-C	6.30	113.68	108.07
1	B	297	ASN	CA-C-N	-6.28	113.49	120.14
1	B	297	ASN	C-N-CA	-6.28	113.49	120.14
1	A	90	ALA	N-CA-C	6.26	118.19	111.36
1	A	24	VAL	N-CA-C	6.21	112.85	106.21
1	B	287	GLU	N-CA-C	-6.15	104.68	111.82
1	A	221	ARG	CG-CD-NE	-6.13	98.52	112.00
1	B	90	ALA	N-CA-C	-6.11	105.65	113.23
1	B	116	VAL	N-CA-CB	6.09	117.01	110.62
1	B	45	LYS	N-CA-C	-6.08	100.59	110.20
1	A	149	GLU	N-CA-C	6.00	120.33	111.87
1	A	223	TYR	N-CA-C	5.99	119.31	109.85
1	A	287	GLU	N-CA-C	5.94	117.56	111.14
1	A	207	PRO	N-CA-C	5.87	121.57	113.65
1	A	65	GLU	N-CA-C	-5.86	104.25	111.40
1	B	302	THR	CA-C-N	-5.83	113.65	120.12
1	B	302	THR	C-N-CA	-5.83	113.65	120.12
1	B	84	VAL	CB-CA-C	-5.79	102.97	110.84
1	A	251	GLY	N-CA-C	5.77	123.03	115.47
1	B	310	ALA	CA-C-N	5.72	126.04	119.92
1	B	310	ALA	C-N-CA	5.72	126.04	119.92
1	A	53	VAL	CB-CA-C	-5.72	102.00	111.32
1	A	184	HIS	N-CA-C	5.72	119.03	112.97
1	B	208	VAL	CB-CA-C	-5.72	104.33	112.22
1	A	20	ARG	N-CA-C	5.67	118.55	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	GLU	N-CA-C	5.65	118.20	111.71
1	A	15	GLU	N-CA-C	-5.64	98.43	108.13
1	A	235	GLY	O-C-N	-5.63	119.19	123.35
1	A	193	MET	N-CA-C	5.62	117.64	108.76
1	B	113	LEU	N-CA-C	-5.62	105.07	111.14
1	A	221	ARG	CA-C-N	-5.56	115.27	123.05
1	A	221	ARG	C-N-CA	-5.56	115.27	123.05
1	B	186	ASN	CA-C-N	-5.52	112.83	118.85
1	B	186	ASN	C-N-CA	-5.52	112.83	118.85
1	B	33	GLN	N-CA-C	5.51	116.64	108.60
1	B	136	LEU	CA-C-N	-5.49	115.95	123.14
1	B	136	LEU	C-N-CA	-5.49	115.95	123.14
1	A	25	ILE	N-CA-CB	5.48	120.28	111.23
1	A	24	VAL	CA-C-O	-5.43	117.90	122.63
1	B	273	GLU	N-CA-C	-5.41	104.94	112.45
1	B	227	ILE	CA-C-O	5.40	122.14	119.12
1	A	64	HIS	N-CA-C	5.40	118.97	112.38
1	A	169	ALA	N-CA-C	-5.38	106.67	113.18
1	B	24	VAL	CA-C-N	5.37	128.16	121.71
1	B	24	VAL	C-N-CA	5.37	128.16	121.71
1	B	19	ARG	N-CA-C	5.37	117.99	109.24
1	B	219	TYR	N-CA-C	5.35	117.03	108.41
1	A	199	LEU	N-CA-C	-5.35	99.41	110.80
1	A	276	PHE	N-CA-C	5.35	119.81	113.28
1	B	180	LEU	N-CA-C	-5.33	105.37	111.07
1	A	32	PHE	CB-CA-C	-5.29	99.89	110.42
1	B	133	ARG	N-CA-C	5.27	119.56	113.18
1	A	70	PRO	N-CA-C	-5.25	106.69	113.57
1	B	48	ILE	CB-CA-C	5.24	118.37	110.98
1	A	298	PRO	N-CA-C	5.24	119.10	111.03
1	B	197	MET	N-CA-CB	5.21	117.89	110.44
1	B	287	GLU	N-CA-CB	5.20	118.35	110.28
1	B	278	LEU	CA-C-N	-5.20	115.37	120.52
1	B	278	LEU	C-N-CA	-5.20	115.37	120.52
1	B	96	LEU	N-CA-C	-5.17	107.26	113.21
1	B	189	GLY	N-CA-C	5.16	125.41	113.18
1	A	237	LEU	N-CA-C	5.15	117.02	109.24
1	B	131	ASP	CA-C-N	5.12	126.24	119.84
1	B	131	ASP	C-N-CA	5.12	126.24	119.84
1	A	194	GLN	N-CA-C	-5.12	102.28	109.96
1	A	308	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	B	46	VAL	CA-C-N	-5.11	115.79	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	VAL	C-N-CA	-5.11	115.79	122.99
1	B	131	ASP	CB-CA-C	5.07	116.64	109.08
1	A	56	THR	N-CA-C	-5.04	101.53	109.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	LEU	Peptide
1	A	202	HIS	Peptide
1	A	203	HIS	Peptide
1	B	243	PHE	Peptide
1	B	70	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2491	150	0
1	B	2537	0	2504	200	0
2	A	20	0	13	1	0
2	B	20	0	13	3	0
3	A	102	0	0	19	2
3	B	81	0	0	8	0
All	All	5288	0	5021	339	2

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 34.

All (339) 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:58:ARG:HD2	3:A:390:HOH:O	1.41	1.14
1:B:141:ALA:O	1:B:145:LEU:HD11	1.51	1.11
1:B:141:ALA:O	1:B:145:LEU:CD1	2.04	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HG	1:B:96:LEU:HD22	1.38	1.05
1:A:202:HIS:HB2	1:A:203:HIS:CD2	1.98	0.99
1:A:272:LEU:HD23	1:A:272:LEU:C	1.87	0.98
1:B:176:GLU:HG3	1:B:295:ASP:OD1	1.68	0.93
1:B:145:LEU:HD12	1:B:145:LEU:H	1.30	0.93
1:A:201:THR:C	1:B:58:ARG:HH12	1.78	0.92
1:A:202:HIS:HB3	1:A:203:HIS:HD2	1.33	0.92
1:A:202:HIS:CB	1:A:203:HIS:CD2	2.52	0.92
1:A:202:HIS:CB	1:A:203:HIS:HD2	1.82	0.91
1:B:108:ASP:OD2	2:B:315:MTA:H1'	1.69	0.91
1:B:221:ARG:HG3	1:B:246:ALA:HB2	1.52	0.91
1:B:218:ARG:HB3	1:B:219:TYR:CE1	2.07	0.90
1:B:175:VAL:HG11	1:B:215:GLU:HB3	1.53	0.87
1:B:48:ILE:O	1:B:49:LEU:HD12	1.73	0.87
1:B:129:PHE:HB2	3:B:344:HOH:O	1.74	0.86
1:A:201:THR:O	1:B:58:ARG:NH1	2.09	0.85
1:A:182:LYS:NZ	1:A:241:ASP:OD1	2.08	0.85
1:B:92:LEU:HG	1:B:96:LEU:CD2	2.08	0.82
1:B:86:GLY:H	2:B:315:MTA:H4'	1.43	0.82
1:A:278:LEU:HG	1:A:282:LEU:HD13	1.63	0.79
1:B:145:LEU:HD12	1:B:145:LEU:N	1.98	0.79
1:B:214:ARG:HA	1:B:220:VAL:HG21	1.65	0.79
1:B:177:PHE:O	1:B:181:VAL:HG23	1.83	0.78
1:B:138:ILE:HG22	1:B:138:ILE:O	1.83	0.78
1:A:293:SER:HB2	1:A:299:PHE:HB3	1.65	0.77
1:A:197:MET:HE1	3:A:375:HOH:O	1.84	0.77
1:B:223:TYR:CD2	1:B:275:MET:HE3	2.21	0.76
1:A:103:LYS:HE2	1:A:135:VAL:HG21	1.68	0.76
1:B:141:ALA:O	1:B:145:LEU:HD12	1.86	0.76
1:B:221:ARG:HG3	1:B:246:ALA:CB	2.16	0.75
1:B:218:ARG:HB3	1:B:219:TYR:CD1	2.22	0.75
1:A:224:LYS:HE2	3:A:357:HOH:O	1.86	0.75
1:B:22:GLU:HB2	1:B:39:GLU:O	1.87	0.74
1:B:259:GLU:C	1:B:259:GLU:OE1	2.30	0.74
1:B:25:ILE:O	1:B:26:ALA:HB2	1.88	0.73
1:A:155:VAL:HG23	1:A:185:LEU:HD21	1.68	0.72
1:A:121:MET:HB3	1:A:124:TRP:CE3	2.25	0.72
1:B:249:SER:HB3	1:B:252:VAL:HG23	1.71	0.72
1:B:157:ILE:HD12	1:B:191:MET:SD	2.30	0.72
1:B:215:GLU:HG2	1:B:292:VAL:HG11	1.71	0.71
1:B:182:LYS:HE2	1:B:241:ASP:OD1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:OE2	3:A:396:HOH:O	2.08	0.71
1:B:193:MET:CG	1:B:237:LEU:HD22	2.21	0.71
1:A:272:LEU:C	1:A:272:LEU:CD2	2.64	0.71
1:B:243:PHE:CD1	1:B:243:PHE:N	2.60	0.69
1:B:43:PHE:HB3	1:B:56:THR:CG2	2.22	0.68
1:B:47:LEU:HD12	1:B:54:GLN:HB2	1.75	0.68
1:B:221:ARG:CG	1:B:246:ALA:HB2	2.22	0.68
1:A:12:THR:HB	1:A:13:PRO:HD2	1.75	0.68
1:B:175:VAL:CG1	1:B:215:GLU:HB3	2.22	0.68
1:A:142:ARG:HD3	3:A:396:HOH:O	1.94	0.68
1:A:225:ASN:OD1	3:A:317:HOH:O	2.12	0.67
1:A:293:SER:CB	1:A:299:PHE:HB3	2.24	0.67
1:B:243:PHE:N	1:B:243:PHE:HD1	1.91	0.67
1:A:11:VAL:HG12	1:A:12:THR:HG23	1.77	0.67
1:B:98:HIS:CE1	1:B:262:LEU:HD11	2.30	0.67
1:A:8:PHE:HE2	1:B:1:MET:HE2	1.60	0.66
1:A:111:GLY:HA2	1:A:138:ILE:CD1	2.25	0.66
1:B:106:MET:HE2	3:B:319:HOH:O	1.96	0.66
1:A:154:VAL:HG22	1:A:190:VAL:HG22	1.77	0.66
1:B:223:TYR:HD2	1:B:275:MET:HE3	1.61	0.66
1:A:131:ASP:OD1	1:A:133:ARG:N	2.29	0.66
1:A:120:HIS:C	1:A:122:PRO:HD2	2.21	0.65
1:A:202:HIS:HB3	1:A:203:HIS:CD2	2.22	0.65
1:B:94:GLU:O	1:B:97:LYS:HB2	1.96	0.65
1:B:43:PHE:HB3	1:B:56:THR:HG23	1.78	0.65
1:B:98:HIS:HE1	1:B:262:LEU:HD11	1.62	0.65
1:B:186:ASN:HB3	1:B:187:PRO:HD2	1.78	0.65
1:A:272:LEU:HD23	1:A:272:LEU:O	1.96	0.64
1:A:278:LEU:HG	1:A:282:LEU:CD1	2.27	0.64
1:B:61:TYR:CE2	1:B:62:ILE:HG12	2.33	0.64
1:B:211:ARG:HD3	1:B:289:GLU:O	1.98	0.64
1:B:47:LEU:HD11	1:B:49:LEU:CD1	2.28	0.64
1:A:9:GLU:CD	1:A:53:VAL:HG23	2.23	0.64
1:B:47:LEU:CD1	1:B:49:LEU:HD13	2.28	0.64
1:A:53:VAL:HG12	1:A:54:GLN:N	2.11	0.64
1:A:8:PHE:CE2	1:B:1:MET:HE2	2.31	0.63
1:A:64:HIS:O	1:A:68:VAL:HG23	1.96	0.63
1:B:255:ALA:O	1:B:259:GLU:HB2	1.99	0.63
1:B:176:GLU:HG3	1:B:295:ASP:CG	2.24	0.63
1:A:99:PRO:HD2	1:A:260:ARG:HG2	1.79	0.63
1:B:186:ASN:HB3	1:B:187:PRO:CD	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG23	1:A:266:HIS:CD2	2.34	0.62
1:B:120:HIS:C	1:B:122:PRO:HD2	2.25	0.62
1:A:249:SER:HB2	1:A:252:VAL:HG21	1.82	0.61
1:A:12:THR:HB	1:A:13:PRO:CD	2.30	0.61
1:B:86:GLY:N	2:B:315:MTA:H4'	2.16	0.60
1:B:193:MET:HG2	1:B:237:LEU:CD2	2.30	0.60
1:B:249:SER:HB3	1:B:252:VAL:CG2	2.32	0.60
1:B:182:LYS:CE	1:B:241:ASP:OD1	2.50	0.59
1:A:249:SER:O	1:A:252:VAL:HG23	2.02	0.59
1:A:25:ILE:HD13	1:A:25:ILE:H	1.67	0.59
1:B:155:VAL:HG21	1:B:181:VAL:HG12	1.84	0.59
1:B:95:VAL:C	1:B:97:LYS:H	2.11	0.59
1:A:293:SER:HB2	1:A:299:PHE:H	1.67	0.59
1:B:56:THR:CG2	1:B:59:ASP:OD2	2.51	0.59
1:B:48:ILE:O	1:B:49:LEU:CD1	2.50	0.59
1:B:252:VAL:O	1:B:255:ALA:HB3	2.03	0.58
1:A:151:ARG:HB3	1:A:186:ASN:ND2	2.18	0.58
1:B:194:GLN:OE1	1:B:234:PHE:HE1	1.86	0.58
1:A:127:GLY:O	1:A:128:ALA:C	2.46	0.58
1:B:219:TYR:CD1	1:B:219:TYR:N	2.70	0.58
1:A:65:GLU:HB3	1:A:267:LEU:HD12	1.86	0.57
1:B:10:HIS:HD2	1:B:52:ASP:OD1	1.87	0.57
1:B:139:ASP:OD2	1:B:140:ASP:N	2.37	0.57
1:A:201:THR:O	1:B:58:ARG:NH2	2.38	0.57
1:B:282:LEU:O	1:B:282:LEU:HD12	2.04	0.57
1:B:151:ARG:HB3	1:B:186:ASN:HD21	1.69	0.57
1:B:175:VAL:HG22	1:B:293:SER:O	2.04	0.56
1:A:233:ASN:HB2	1:B:226:HIS:CD2	2.41	0.56
1:B:203:HIS:ND1	1:B:205:VAL:HG23	2.20	0.56
1:B:269:ALA:HB3	1:B:270:PRO:HD3	1.87	0.56
1:A:141:ALA:O	1:A:145:LEU:HD12	2.06	0.56
1:A:279:PRO:HG2	1:A:282:LEU:HB2	1.87	0.56
1:B:211:ARG:O	1:B:211:ARG:NH2	2.38	0.56
1:A:302:THR:HB	1:A:303:PRO:HD2	1.88	0.56
1:B:203:HIS:HB3	1:B:305:GLY:O	2.05	0.56
1:A:121:MET:N	1:A:122:PRO:CD	2.69	0.56
1:A:10:HIS:CG	1:A:11:VAL:N	2.74	0.56
1:B:61:TYR:HB3	3:B:322:HOH:O	2.05	0.55
1:A:99:PRO:CD	1:A:260:ARG:HG2	2.36	0.55
1:B:223:TYR:HE1	1:B:238:LEU:HD13	1.71	0.55
1:A:111:GLY:HA2	1:A:138:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HA	3:A:339:HOH:O	2.07	0.55
1:B:29:LYS:CG	1:B:29:LYS:O	2.54	0.55
1:A:214:ARG:HA	1:A:220:VAL:HG21	1.90	0.54
1:B:10:HIS:HB3	1:B:51:LYS:HB2	1.88	0.54
1:B:138:ILE:O	1:B:138:ILE:CG2	2.53	0.54
1:B:25:ILE:O	1:B:26:ALA:CB	2.53	0.54
1:A:61:TYR:HB3	3:A:320:HOH:O	2.08	0.54
1:A:146:GLU:HG3	3:A:396:HOH:O	2.08	0.54
1:B:193:MET:CG	1:B:237:LEU:CD2	2.85	0.54
1:B:31:PRO:HG2	1:B:32:PHE:CD2	2.43	0.54
1:B:56:THR:HG22	1:B:59:ASP:OD2	2.08	0.54
1:B:254:GLU:OE2	1:B:258:ARG:CZ	2.56	0.54
1:A:204:ARG:NH2	1:A:291:MET:HE3	2.22	0.54
1:A:172:LEU:HD11	2:A:315:MTA:N6	2.24	0.53
1:A:37:LEU:HD12	1:A:46:VAL:O	2.07	0.53
1:A:60:GLU:HG3	3:A:320:HOH:O	2.08	0.53
1:A:59:ASP:OD1	1:A:228:PRO:HD2	2.08	0.53
1:B:64:HIS:CE1	1:B:90:ALA:HB3	2.43	0.53
1:B:89:GLY:HA2	3:B:319:HOH:O	2.08	0.53
1:B:119:ARG:O	1:B:119:ARG:HG3	2.09	0.53
1:B:13:PRO:HG2	1:B:14:TYR:CE1	2.44	0.53
1:B:167:ASN:HD22	1:B:169:ALA:H	1.55	0.52
1:B:167:ASN:ND2	1:B:169:ALA:HB3	2.25	0.52
1:A:230:PHE:O	1:A:232:LEU:HB2	2.09	0.52
1:B:56:THR:HG22	1:B:59:ASP:H	1.74	0.52
1:A:81:VAL:HG11	1:A:95:VAL:HG11	1.90	0.52
1:B:204:ARG:C	1:B:207:PRO:HD2	2.33	0.52
1:B:274:ALA:O	1:B:275:MET:C	2.50	0.52
1:B:113:LEU:O	1:B:114:VAL:C	2.51	0.52
1:A:160:THR:O	1:A:161:ASP:C	2.50	0.52
1:A:263:ALA:N	3:A:339:HOH:O	1.86	0.52
1:A:121:MET:N	1:A:122:PRO:HD2	2.22	0.52
1:A:40:SER:HB3	1:A:44:GLY:O	2.10	0.52
1:B:20:ARG:HH11	1:B:20:ARG:CG	2.23	0.52
1:A:201:THR:C	1:B:58:ARG:NH1	2.59	0.51
1:B:178:TYR:HE2	3:B:318:HOH:O	1.92	0.51
1:A:170:ARG:C	1:A:172:LEU:H	2.17	0.51
1:B:9:GLU:CD	1:B:53:VAL:HG12	2.35	0.51
1:B:269:ALA:N	1:B:270:PRO:CD	2.73	0.51
1:A:200:LEU:HD11	3:A:365:HOH:O	2.11	0.51
1:B:151:ARG:HB3	1:B:186:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:NE2	1:A:49:LEU:HD13	2.26	0.51
1:B:117:ALA:HA	1:B:121:MET:HB2	1.93	0.51
1:A:123:GLU:HB3	3:A:331:HOH:O	2.10	0.50
1:A:51:LYS:O	1:A:51:LYS:HG3	2.10	0.50
1:B:69:HIS:NE2	1:B:94:GLU:OE1	2.39	0.50
1:A:201:THR:O	1:B:58:ARG:CZ	2.58	0.50
1:B:120:HIS:O	1:B:122:PRO:HD2	2.11	0.50
1:B:47:LEU:HD11	1:B:49:LEU:HD11	1.93	0.50
1:B:109:ILE:HG13	1:B:140:ASP:HA	1.93	0.50
1:B:4:GLY:HA3	1:B:20:ARG:HH12	1.76	0.49
1:B:278:LEU:N	1:B:278:LEU:HD22	2.26	0.49
1:A:145:LEU:O	1:A:184:HIS:NE2	2.46	0.49
1:B:47:LEU:HD11	1:B:49:LEU:HD13	1.91	0.49
1:A:146:GLU:CG	3:A:396:HOH:O	2.60	0.49
1:A:218:ARG:HD2	1:A:218:ARG:O	2.12	0.49
1:B:191:MET:CG	1:B:192:GLY:N	2.75	0.49
1:A:107:VAL:O	1:A:108:ASP:HB2	2.13	0.49
1:B:75:HIS:HB3	1:B:78:PRO:HG3	1.94	0.49
1:B:10:HIS:CD2	1:B:52:ASP:OD1	2.65	0.49
1:B:47:LEU:CD1	1:B:49:LEU:CD1	2.91	0.49
1:B:7:PHE:CZ	1:B:48:ILE:HG21	2.48	0.48
1:B:47:LEU:HD12	1:B:54:GLN:CB	2.42	0.48
1:B:49:LEU:HD22	1:B:54:GLN:HG2	1.94	0.48
1:A:32:PHE:CZ	1:A:109:ILE:HG12	2.48	0.48
1:A:194:GLN:HG3	3:A:364:HOH:O	2.12	0.48
1:A:151:ARG:CB	1:A:186:ASN:HD21	2.26	0.48
1:A:98:HIS:O	1:A:101:VAL:HG23	2.13	0.48
1:B:61:TYR:CE2	1:B:266:HIS:HB2	2.49	0.48
1:B:204:ARG:O	1:B:207:PRO:HD2	2.14	0.48
1:B:173:TYR:O	1:B:293:SER:OG	2.31	0.48
1:A:53:VAL:CG1	1:A:54:GLN:N	2.77	0.48
1:B:194:GLN:OE1	1:B:234:PHE:CE1	2.66	0.48
1:B:127:GLY:O	1:B:128:ALA:C	2.57	0.47
1:B:142:ARG:O	1:B:146:GLU:HB2	2.14	0.47
1:B:191:MET:HG2	1:B:192:GLY:N	2.30	0.47
1:B:303:PRO:HD3	3:B:356:HOH:O	2.14	0.47
1:A:25:ILE:HD13	1:A:25:ILE:N	2.30	0.47
1:A:69:HIS:O	1:A:73:LEU:HB2	2.14	0.47
1:A:2:ASP:HB2	1:A:20:ARG:NH1	2.29	0.47
1:A:244:ASP:OD1	1:A:244:ASP:C	2.58	0.47
1:B:48:ILE:HG23	1:B:52:ASP:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:O	1:B:115:GLU:HG2	2.15	0.47
1:B:145:LEU:CD1	1:B:145:LEU:N	2.72	0.47
1:B:156:ILE:HA	1:B:192:GLY:O	2.15	0.47
1:B:62:ILE:HG23	1:B:266:HIS:CD2	2.50	0.47
1:B:280:LYS:HB2	1:B:280:LYS:HE3	1.70	0.47
1:A:144:TYR:O	1:A:148:THR:HG22	2.15	0.47
1:B:47:LEU:O	1:B:54:GLN:N	2.46	0.47
1:B:227:ILE:O	1:B:228:PRO:C	2.57	0.47
1:B:274:ALA:C	1:B:276:PHE:N	2.68	0.47
1:A:92:LEU:O	1:A:93:ARG:C	2.55	0.47
1:A:214:ARG:HA	1:A:220:VAL:CG2	2.46	0.46
1:B:121:MET:HE2	1:B:124:TRP:CD2	2.51	0.46
1:B:165:GLU:O	1:B:170:ARG:HD2	2.15	0.46
1:B:264:LEU:HA	1:B:264:LEU:HD23	1.53	0.46
1:B:157:ILE:CD1	1:B:191:MET:SD	3.03	0.46
1:B:47:LEU:HD13	1:B:47:LEU:C	2.41	0.46
1:A:32:PHE:O	1:A:33:GLN:HB3	2.15	0.46
1:A:269:ALA:HB3	1:A:270:PRO:CD	2.45	0.46
1:A:269:ALA:HB3	1:A:270:PRO:HD3	1.96	0.46
1:B:98:HIS:HA	1:B:99:PRO:HD2	1.76	0.46
1:B:162:PRO:HD2	1:B:301:VAL:HG23	1.98	0.46
1:B:29:LYS:O	1:B:30:THR:O	2.33	0.46
1:B:131:ASP:HA	1:B:132:PRO:HD2	1.73	0.46
1:B:223:TYR:CD2	1:B:275:MET:CE	2.96	0.46
1:B:182:LYS:O	1:B:185:LEU:HB2	2.16	0.46
1:B:212:THR:HA	1:B:292:VAL:HG13	1.97	0.46
1:B:186:ASN:N	1:B:186:ASN:HD22	2.13	0.46
1:B:206:HIS:HB3	1:B:207:PRO:HD3	1.97	0.46
1:A:13:PRO:HG2	1:A:14:TYR:CE1	2.51	0.45
1:B:167:ASN:ND2	1:B:169:ALA:H	2.14	0.45
1:B:95:VAL:C	1:B:97:LYS:N	2.75	0.45
1:A:237:LEU:C	1:A:237:LEU:HD12	2.41	0.45
1:A:258:ARG:O	1:A:259:GLU:C	2.59	0.45
1:A:25:ILE:HD11	1:A:39:GLU:HG2	1.97	0.45
1:A:205:VAL:O	1:A:206:HIS:C	2.57	0.45
1:B:211:ARG:NH2	1:B:211:ARG:HG3	2.30	0.45
1:A:9:GLU:OE1	1:A:19:ARG:NH1	2.49	0.45
1:A:181:VAL:HG11	1:A:191:MET:HG3	1.98	0.45
1:A:297:ASN:O	1:A:309:GLN:HG3	2.17	0.45
1:B:72:MET:HE3	1:B:98:HIS:CD2	2.51	0.45
1:B:60:GLU:O	1:B:61:TYR:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ARG:HG3	1:B:216:ALA:HB1	1.98	0.45
1:B:302:THR:HG23	1:B:306:GLU:O	2.16	0.45
1:A:30:THR:HB	1:A:31:PRO:HD2	1.98	0.45
1:A:24:VAL:HG12	1:A:24:VAL:O	2.16	0.44
1:A:220:VAL:CG1	1:A:237:LEU:HD22	2.47	0.44
1:B:61:TYR:HE2	1:B:266:HIS:HB2	1.82	0.44
1:B:279:PRO:HD2	1:B:282:LEU:HD23	1.99	0.44
1:A:151:ARG:CB	1:A:186:ASN:ND2	2.81	0.44
1:A:49:LEU:HD21	1:A:113:LEU:HD11	2.00	0.44
1:A:55:SER:HA	3:A:319:HOH:O	2.18	0.44
1:A:188:GLY:CA	3:A:414:HOH:O	2.65	0.44
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.65	0.44
1:B:155:VAL:HG21	1:B:181:VAL:CG1	2.47	0.44
1:A:194:GLN:OE1	1:A:234:PHE:CE1	2.71	0.44
1:A:197:MET:CE	3:A:375:HOH:O	2.53	0.44
1:B:178:TYR:HA	1:B:181:VAL:HG23	1.98	0.44
1:A:29:LYS:HG2	1:A:34:ASP:OD1	2.18	0.44
1:A:37:LEU:HA	1:A:46:VAL:O	2.17	0.44
1:B:65:GLU:OE2	1:B:265:ARG:N	2.47	0.44
1:B:193:MET:SD	1:B:237:LEU:HD22	2.57	0.44
1:A:194:GLN:OE1	1:A:234:PHE:HE1	2.00	0.44
1:A:231:PHE:CD1	1:A:231:PHE:N	2.85	0.44
1:B:69:HIS:N	1:B:70:PRO:CD	2.81	0.44
1:B:93:ARG:O	1:B:97:LYS:HG3	2.17	0.44
1:A:10:HIS:ND1	1:A:10:HIS:C	2.72	0.44
1:A:80:ARG:HD3	1:A:151:ARG:O	2.18	0.44
1:B:167:ASN:HD21	1:B:169:ALA:HB3	1.83	0.44
1:A:282:LEU:HD22	1:A:286:LEU:HG	2.00	0.43
1:A:274:ALA:C	1:A:276:PHE:N	2.75	0.43
1:A:1:MET:HE1	1:B:8:PHE:HE2	1.83	0.43
1:B:193:MET:HG3	1:B:237:LEU:HD22	1.98	0.43
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.80	0.43
1:A:96:LEU:HB3	1:A:133:ARG:NH2	2.34	0.43
1:A:70:PRO:O	1:A:74:THR:HB	2.19	0.43
1:B:77:GLU:HG3	1:B:100:THR:HG21	2.01	0.43
1:A:12:THR:OG1	1:A:15:GLU:HB2	2.18	0.43
1:A:170:ARG:C	1:A:172:LEU:N	2.76	0.43
1:B:208:VAL:O	1:B:208:VAL:HG12	2.18	0.43
1:A:175:VAL:O	1:A:176:GLU:C	2.62	0.43
1:A:221:ARG:HD3	1:A:244:ASP:OD1	2.19	0.43
1:B:108:ASP:OD1	1:B:109:ILE:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:VAL:C	1:B:12:THR:CG2	2.91	0.43
1:A:204:ARG:O	1:A:205:VAL:C	2.60	0.43
1:B:185:LEU:HA	1:B:185:LEU:HD23	1.61	0.43
1:A:125:HIS:O	1:A:128:ALA:HB2	2.18	0.42
1:B:136:LEU:N	3:B:370:HOH:O	2.40	0.42
1:A:223:TYR:HB3	1:A:276:PHE:CD1	2.54	0.42
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.82	0.42
1:B:9:GLU:OE2	1:B:53:VAL:HG12	2.18	0.42
1:A:24:VAL:O	1:A:25:ILE:C	2.63	0.42
1:A:88:GLU:OE1	1:A:88:GLU:N	2.50	0.42
1:A:131:ASP:HB2	3:A:370:HOH:O	2.19	0.42
1:B:118:LYS:HG2	3:B:383:HOH:O	2.19	0.42
1:B:250:GLU:O	1:B:250:GLU:HG2	2.19	0.42
1:B:147:ARG:O	1:B:147:ARG:HG2	2.20	0.42
1:A:160:THR:O	1:A:161:ASP:O	2.39	0.41
1:B:23:ARG:HG2	1:B:24:VAL:O	2.19	0.41
1:B:49:LEU:HB2	1:B:54:GLN:NE2	2.35	0.41
1:A:153:ASP:O	1:A:189:GLY:HA2	2.20	0.41
1:A:272:LEU:HD23	1:A:273:GLU:N	2.33	0.41
1:A:279:PRO:HD3	1:B:271:TYR:CE2	2.55	0.41
1:B:140:ASP:C	1:B:142:ARG:N	2.77	0.41
1:A:208:VAL:O	1:A:209:VAL:C	2.63	0.41
1:A:226:HIS:ND1	1:B:226:HIS:ND1	2.68	0.41
1:A:7:PHE:CD1	1:A:7:PHE:C	2.98	0.41
1:B:278:LEU:HD22	1:B:278:LEU:H	1.86	0.41
1:A:253:ILE:O	1:A:257:ILE:HG13	2.20	0.41
1:B:278:LEU:HD23	1:B:283:LEU:HD21	2.03	0.41
1:A:65:GLU:HA	1:A:69:HIS:HD2	1.84	0.41
1:A:267:LEU:HD22	1:A:272:LEU:HB2	2.03	0.41
1:B:145:LEU:HA	1:B:148:THR:HG22	2.03	0.41
1:A:1:MET:O	1:A:2:ASP:C	2.62	0.41
1:B:19:ARG:NH2	1:B:53:VAL:HG11	2.36	0.41
1:B:72:MET:CE	1:B:98:HIS:CD2	3.03	0.41
1:A:49:LEU:HD21	1:A:113:LEU:CD1	2.51	0.41
1:A:131:ASP:OD1	1:A:131:ASP:C	2.64	0.41
1:B:111:GLY:CA	1:B:138:ILE:HD13	2.51	0.41
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.89	0.41
1:B:121:MET:N	1:B:122:PRO:CD	2.84	0.40
1:B:167:ASN:HD22	1:B:167:ASN:C	2.29	0.40
1:B:227:ILE:HD12	1:B:227:ILE:N	2.35	0.40
1:B:122:PRO:HA	1:B:125:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HB	1:B:193:MET:CB	2.51	0.40
1:B:233:ASN:C	1:B:233:ASN:HD22	2.29	0.40
1:B:259:GLU:OE1	1:B:259:GLU:CA	2.64	0.40
1:A:113:LEU:O	1:A:114:VAL:C	2.62	0.40
1:A:256:ARG:O	1:A:257:ILE:C	2.59	0.40
1:B:219:TYR:HD1	1:B:240:SER:O	2.04	0.40
1:B:29:LYS:O	1:B:30:THR:C	2.64	0.40
1:B:56:THR:O	1:B:60:GLU:HB3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:406:HOH:O	3:A:406:HOH:O[7_556]	1.54	0.66
3:A:405:HOH:O	3:A:405:HOH:O[7_556]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	310/314 (99%)	268 (86%)	36 (12%)	6 (2%)	6	11
1	B	311/314 (99%)	261 (84%)	42 (14%)	8 (3%)	4	7
All	All	621/628 (99%)	529 (85%)	78 (13%)	14 (2%)	5	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ALA
1	B	26	ALA
1	B	30	THR
1	A	229	GLY

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Mol	Chain	Res	Type
1	B	71	ALA
1	B	242	ALA
1	B	70	PRO
1	A	50	ASP
1	A	109	ILE
1	B	110	ASP
1	A	32	PHE
1	B	162	PRO
1	A	25	ILE
1	B	189	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/270 (100%)	232 (86%)	37 (14%)	3	7
1	B	270/270 (100%)	215 (80%)	55 (20%)	1	2
All	All	539/540 (100%)	447 (83%)	92 (17%)	2	4

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	10	HIS
1	A	23	ARG
1	A	25	ILE
1	A	29	LYS
1	A	47	LEU
1	A	55	SER
1	A	57	GLU
1	A	59	ASP
1	A	74	THR
1	A	92	LEU
1	A	100	THR
1	A	119	ARG

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Mol	Chain	Res	Type
1	A	131	ASP
1	A	138	ILE
1	A	140	ASP
1	A	149	GLU
1	A	157	ILE
1	A	182	LYS
1	A	191	MET
1	A	199	LEU
1	A	200	LEU
1	A	201	THR
1	A	205	VAL
1	A	224	LYS
1	A	234	PHE
1	A	237	LEU
1	A	273	GLU
1	A	278	LEU
1	A	282	LEU
1	A	287	GLU
1	A	288	LYS
1	A	291	MET
1	A	293	SER
1	A	299	PHE
1	A	304	GLU
1	A	308	ARG
1	B	1	MET
1	B	10	HIS
1	B	20	ARG
1	B	22	GLU
1	B	25	ILE
1	B	30	THR
1	B	47	LEU
1	B	51	LYS
1	B	53	VAL
1	B	54	GLN
1	B	56	THR
1	B	59	ASP
1	B	88	GLU
1	B	96	LEU
1	B	103	LYS
1	B	109	ILE
1	B	113	LEU
1	B	116	VAL

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Mol	Chain	Res	Type
1	B	119	ARG
1	B	135	VAL
1	B	138	ILE
1	B	145	LEU
1	B	151	ARG
1	B	160	THR
1	B	175	VAL
1	B	176	GLU
1	B	180	LEU
1	B	181	VAL
1	B	193	MET
1	B	197	MET
1	B	201	THR
1	B	204	ARG
1	B	211	ARG
1	B	214	ARG
1	B	215	GLU
1	B	218	ARG
1	B	224	LYS
1	B	232	LEU
1	B	234	PHE
1	B	237	LEU
1	B	238	LEU
1	B	240	SER
1	B	243	PHE
1	B	248	PHE
1	B	253	ILE
1	B	259	GLU
1	B	273	GLU
1	B	278	LEU
1	B	280	LYS
1	B	281	ASP
1	B	288	LYS
1	B	290	THR
1	B	299	PHE
1	B	304	GLU
1	B	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

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Mol	Chain	Res	Type
1	A	54	GLN
1	A	186	ASN
1	A	203	HIS
1	A	309	GLN
1	B	10	HIS
1	B	54	GLN
1	B	126	GLN
1	B	167	ASN
1	B	186	ASN
1	B	233	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$
2	MTA	B	315	-	22,22,22	5.49	6 (27%)	32,32,32	3.74	16 (50%)
2	MTA	A	315	-	22,22,22	4.34	6 (27%)	32,32,32	3.78	15 (46%)

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	MTA	B	315	-	-	2/7/23/23	0/3/3/3
2	MTA	A	315	-	-	5/7/23/23	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	MTA	C5'-S5'	-24.21	1.23	1.81
2	A	315	MTA	C5'-S5'	-18.69	1.36	1.81
2	B	315	MTA	C5-C4	5.15	1.48	1.39
2	A	315	MTA	C5-C4	4.09	1.46	1.39
2	B	315	MTA	C5-C6	4.05	1.52	1.41
2	A	315	MTA	C1'-N9	3.39	1.55	1.46
2	A	315	MTA	C8-N7	3.28	1.38	1.31
2	A	315	MTA	C5-C6	3.23	1.50	1.41
2	B	315	MTA	O4'-C1'	3.05	1.49	1.42
2	A	315	MTA	C5-N7	-3.03	1.33	1.39
2	B	315	MTA	C8-N7	2.62	1.36	1.31
2	B	315	MTA	C1'-N9	2.38	1.52	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	315	MTA	C4'-C5'-S5'	14.08	160.76	113.89
2	A	315	MTA	C4'-C5'-S5'	13.34	158.27	113.89
2	A	315	MTA	C5-C4-N3	-8.41	115.14	126.72
2	B	315	MTA	C5-C4-N3	-6.30	118.05	126.72
2	B	315	MTA	O4'-C1'-N9	6.07	119.75	108.09
2	A	315	MTA	O4'-C1'-N9	5.99	119.60	108.09
2	A	315	MTA	C4-C5-N7	-5.42	104.38	110.58
2	A	315	MTA	C2-N3-C4	5.17	124.45	111.83
2	B	315	MTA	N3-C4-N9	4.98	135.63	127.17
2	B	315	MTA	O4'-C4'-C5'	4.87	121.36	108.83
2	A	315	MTA	N3-C4-N9	4.66	135.10	127.17
2	A	315	MTA	C5-N7-C8	4.19	110.03	103.45
2	B	315	MTA	C2-N3-C4	4.14	121.95	111.83
2	B	315	MTA	C4-C5-N7	-3.92	106.10	110.58
2	A	315	MTA	C5-C4-N9	3.62	109.76	105.81
2	B	315	MTA	C5-N7-C8	3.45	108.87	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	315	MTA	O4'-C4'-C5'	3.28	117.29	108.83
2	B	315	MTA	N3-C2-N1	-3.11	123.87	128.58
2	B	315	MTA	C2'-C3'-C4'	3.09	108.58	102.61
2	A	315	MTA	N3-C2-N1	-3.03	123.99	128.58
2	B	315	MTA	O3'-C3'-C2'	-2.93	102.43	111.82
2	B	315	MTA	C4-N9-C8	2.88	108.77	105.74
2	A	315	MTA	C6-C5-N7	2.83	137.55	132.09
2	B	315	MTA	N9-C8-N7	-2.78	109.99	113.94
2	B	315	MTA	C6-C5-N7	2.67	137.24	132.09
2	B	315	MTA	CS-S5'-C5'	-2.57	87.89	101.71
2	B	315	MTA	C3'-C2'-C1'	-2.39	96.94	101.46
2	A	315	MTA	O3'-C3'-C4'	-2.34	104.36	111.08
2	A	315	MTA	C2'-C3'-C4'	2.18	106.82	102.61
2	A	315	MTA	C3'-C2'-C1'	2.05	105.34	101.46
2	A	315	MTA	C4'-O4'-C1'	2.02	113.92	109.47

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	315	MTA	O4'-C4'-C5'-S5'
2	A	315	MTA	C3'-C4'-C5'-S5'
2	B	315	MTA	O4'-C4'-C5'-S5'
2	B	315	MTA	C3'-C4'-C5'-S5'
2	A	315	MTA	C4'-C5'-S5'-CS
2	A	315	MTA	C2'-C1'-N9-C8
2	A	315	MTA	O4'-C1'-N9-C8

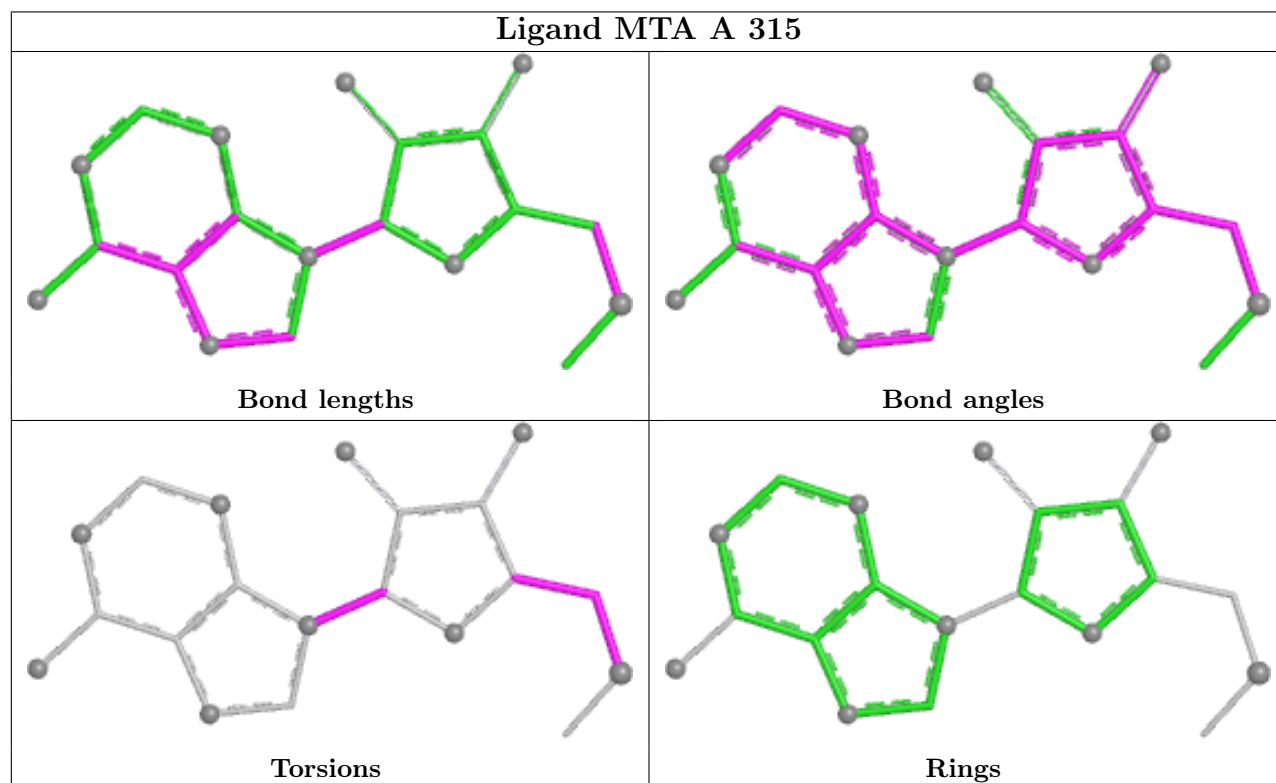
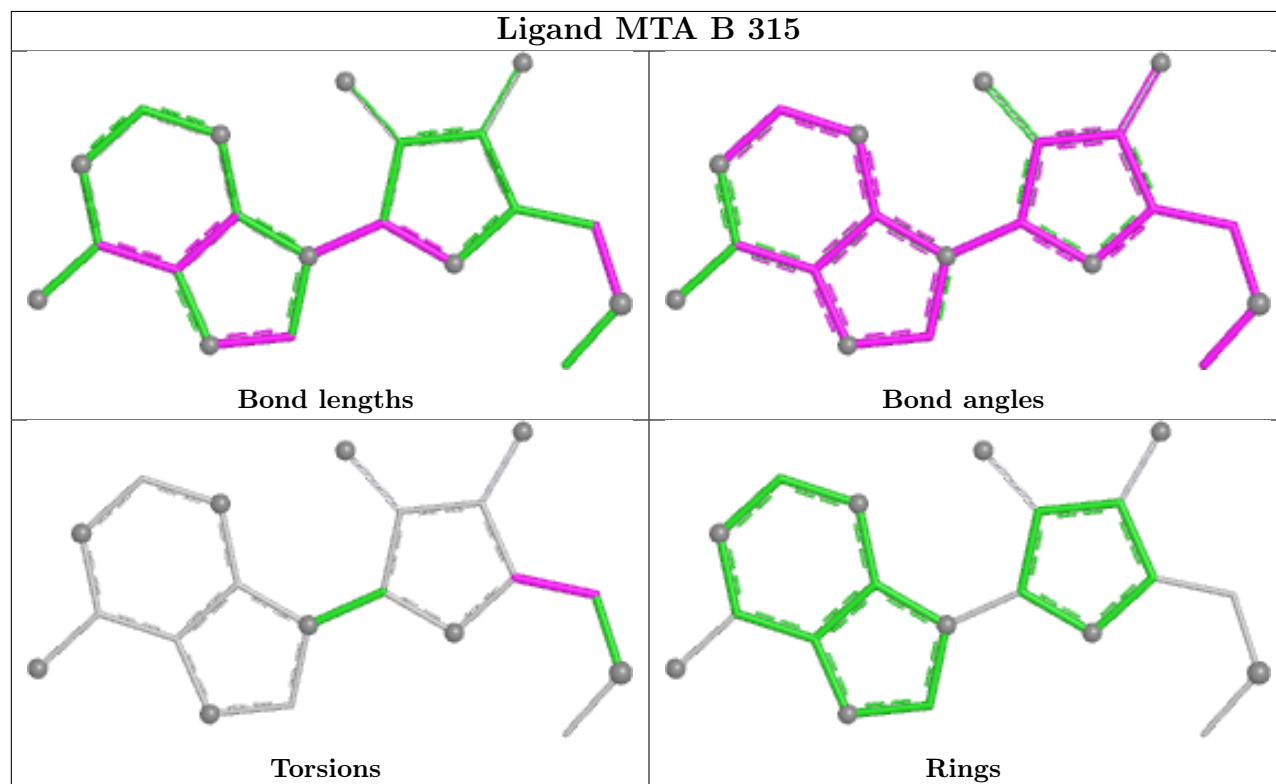
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	315	MTA	3	0
2	A	315	MTA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	312/314 (99%)	-0.75	0	100 100	15, 35, 55, 67	0
1	B	313/314 (99%)	-0.45	1 (0%)	90 87	16, 45, 75, 91	0
All	All	625/628 (99%)	-0.60	1 (0%)	91 89	15, 39, 67, 91	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	LYS	2.2

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.

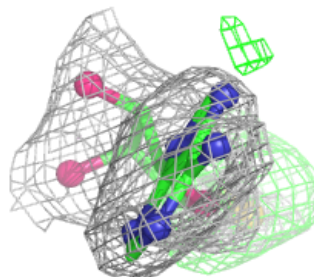
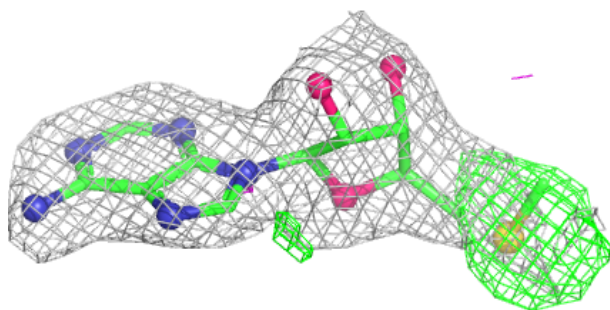
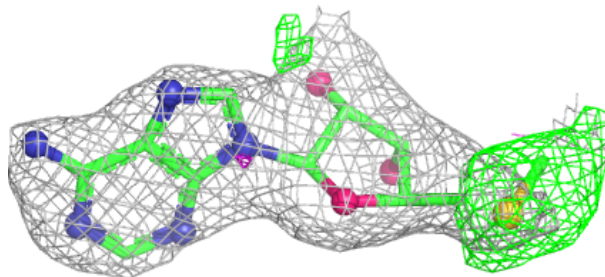
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	MTA	B	315	20/20	0.85	0.11	60,67,87,89	2
2	MTA	A	315	20/20	0.90	0.08	45,50,88,89	2

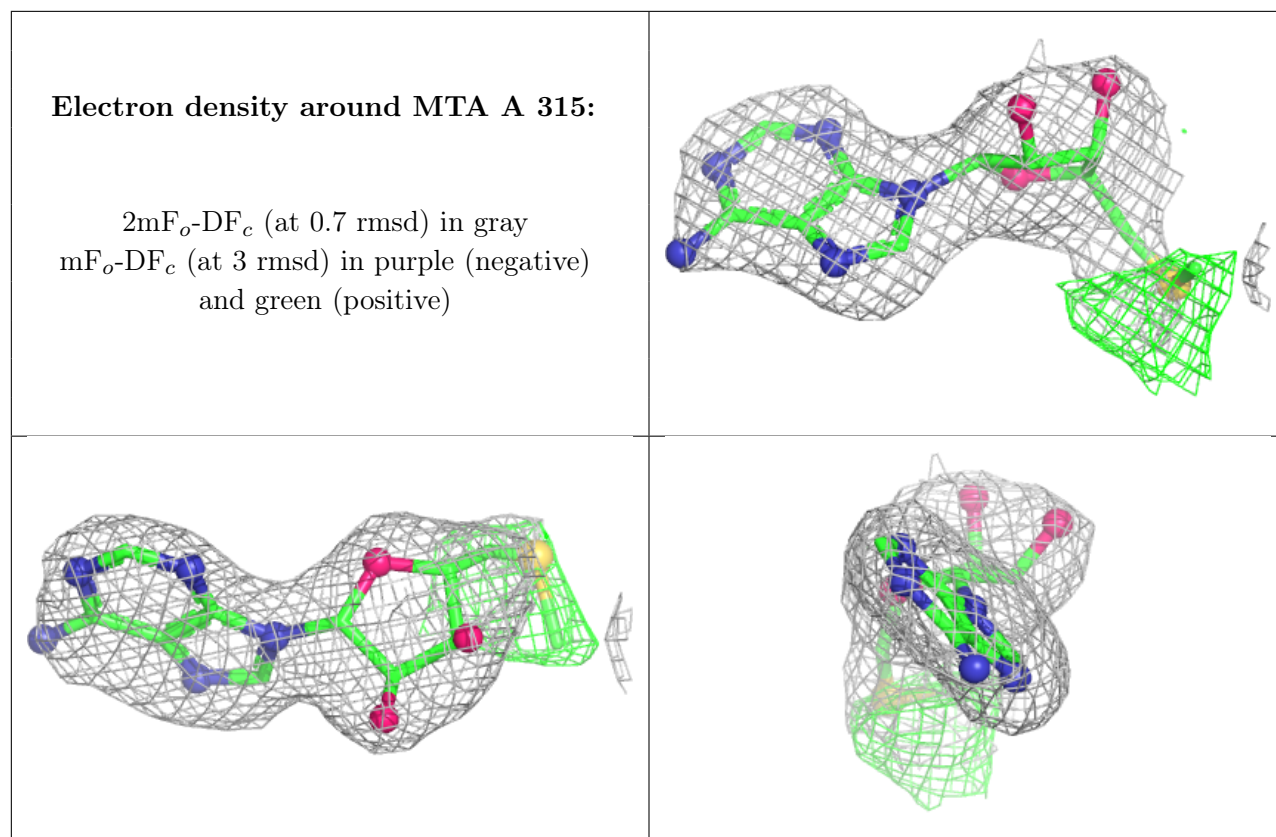
The following is a graphical depiction of the model fit to experimental electron density of all

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 MTA B 315:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.