



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:40 PM UTC

PDB ID : 1E19 / pdb_00001e19
Title : Structure of the carbamate kinase-like carbamoyl phosphate synthetase from the hyperthermophilic archaeon *Pyrococcus furiosus* bound to ADP
Authors : Ramon-Maiques, S.; Marina, A.; Uriarte, M.; Fita, I.; Rubio, V.
Deposited on : 2000-04-28
Resolution : 1.50 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

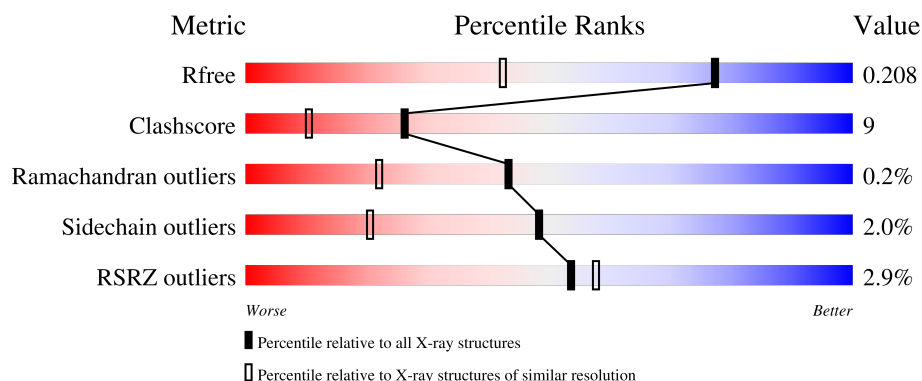
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

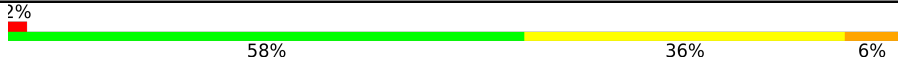
The reported resolution of this entry is 1.50 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	
1	B	314	

2 Entry composition [i](#)

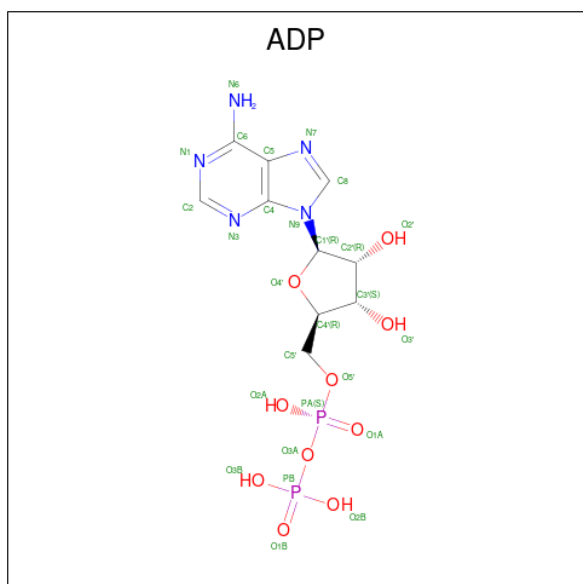
There are 4 unique types of molecules in this entry. The entry contains 5734 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CARBAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	15	0
			2479	1573	428	468	10			
1	B	313	Total	C	N	O	S	0	16	0
			2483	1575	431	467	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0

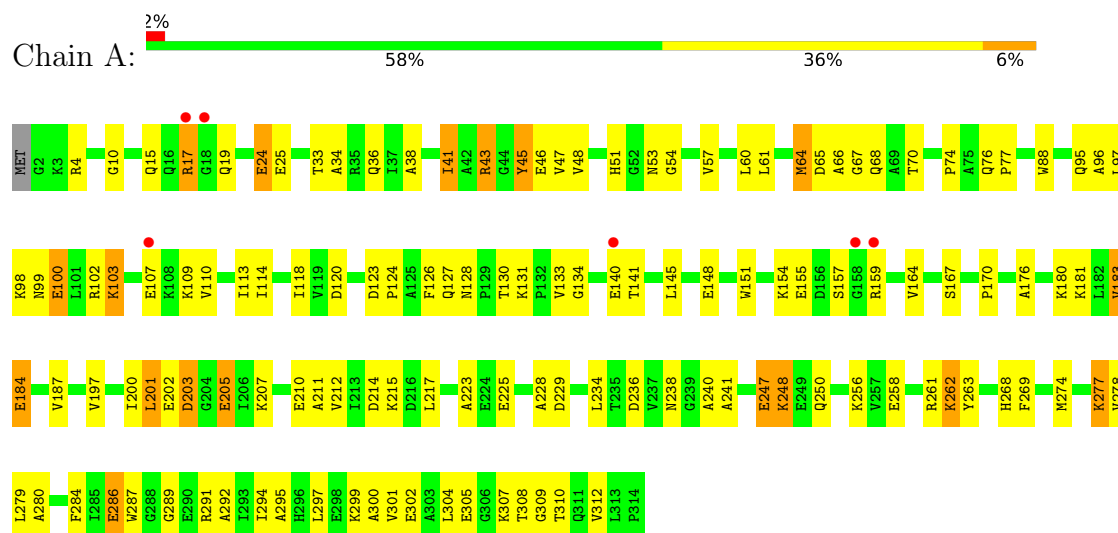
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	391	Total 391	O 391	0	0
4	B	325	Total 325	O 325	0	0

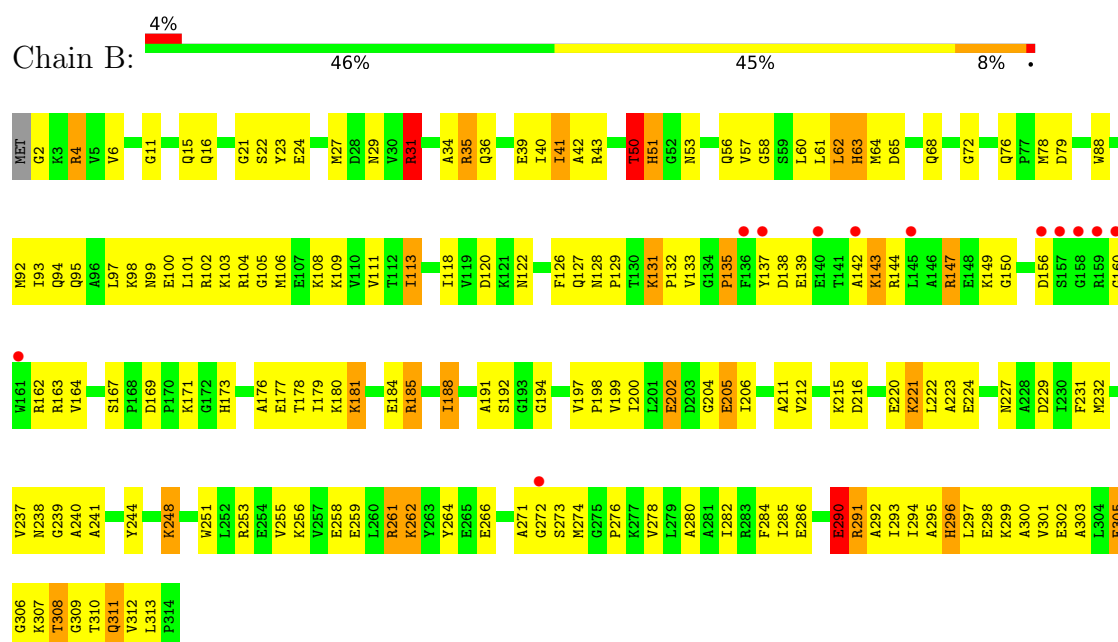
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CARBAMATE KINASE



• Molecule 1: CARBAMATE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.40Å 91.70Å 133.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.50 15.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-1.50) 98.2 (15.00-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.218 0.176 , 0.208	Depositor DCC
R_{free} test set	6517 reflections (6.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5734	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.70	23/2580 (0.9%)	2.28	144/3474 (4.1%)
1	B	1.81	46/2588 (1.8%)	2.62	226/3484 (6.5%)
All	All	1.76	69/5168 (1.3%)	2.46	370/6958 (5.3%)

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	B	0	2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	ILE	C-O	9.05	1.33	1.24
1	B	51	HIS	ND1-CE1	8.89	1.41	1.32
1	B	300	ALA	C-N	8.09	1.44	1.33
1	B	98	LYS	C-O	8.09	1.33	1.24
1	B	272	GLY	N-CA	8.04	1.57	1.45
1	A	151	TRP	C-O	7.40	1.33	1.23
1	B	296	HIS	CG-ND1	7.14	1.46	1.38
1	B	299	LYS	C-N	7.07	1.43	1.33
1	B	103	LYS	C-O	7.00	1.32	1.24
1	A	184[A]	GLU	C-O	6.84	1.32	1.24
1	A	184[B]	GLU	C-O	6.84	1.32	1.24
1	B	100	GLU	C-O	6.74	1.32	1.24
1	B	100	GLU	N-CA	6.61	1.54	1.46
1	A	312	VAL	C-N	6.48	1.41	1.32
1	A	277	LYS	C-N	6.37	1.41	1.33
1	B	132	PRO	C-N	-6.32	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	MET	C-O	6.18	1.31	1.24
1	B	282	ILE	C-N	6.16	1.42	1.33
1	B	63	HIS	ND1-CE1	6.12	1.38	1.32
1	B	92	MET	C-O	6.11	1.31	1.24
1	B	109	LYS	N-CA	6.02	1.53	1.46
1	B	309	GLY	N-CA	5.97	1.53	1.45
1	B	200	ILE	N-CA	5.90	1.52	1.46
1	A	103	LYS	C-O	5.82	1.31	1.24
1	B	36	GLN	C-N	5.75	1.41	1.33
1	A	110	VAL	N-CA	5.74	1.53	1.46
1	B	93	ILE	C-O	5.73	1.30	1.24
1	B	51	HIS	CD2-NE2	5.63	1.44	1.37
1	B	40	ILE	CA-CB	5.63	1.61	1.54
1	B	284	PHE	CA-C	5.60	1.60	1.52
1	B	231	PHE	C-O	5.57	1.30	1.24
1	B	35	ARG	C-N	5.54	1.41	1.33
1	B	311	GLN	N-CA	-5.52	1.39	1.46
1	A	99	ASN	C-O	5.46	1.30	1.24
1	A	241	ALA	N-CA	5.46	1.52	1.46
1	A	114	ILE	C-O	5.42	1.29	1.24
1	B	266	GLU	C-N	5.42	1.40	1.33
1	A	170	PRO	C-O	5.41	1.29	1.23
1	B	101	LEU	C-O	5.41	1.30	1.24
1	B	220	GLU	C-N	5.39	1.41	1.34
1	B	142	ALA	N-CA	5.38	1.52	1.46
1	A	200	ILE	N-CA	5.38	1.52	1.46
1	A	123	ASP	CA-CB	5.36	1.61	1.53
1	A	268	HIS	CD2-NE2	5.35	1.43	1.37
1	B	206	ILE	N-CA	5.34	1.52	1.46
1	B	58	GLY	N-CA	5.29	1.52	1.45
1	B	42	ALA	N-CA	5.27	1.52	1.46
1	B	99	ASN	C-O	5.24	1.30	1.24
1	A	167	SER	C-N	-5.23	1.27	1.33
1	A	240	ALA	CA-C	5.21	1.58	1.52
1	B	61	LEU	C-N	-5.20	1.27	1.33
1	B	162	ARG	C-O	5.19	1.30	1.23
1	B	88	TRP	N-CA	5.19	1.52	1.46
1	B	253	ARG	C-O	5.18	1.30	1.24
1	A	309	GLY	C-O	5.16	1.30	1.23
1	B	232	MET	CA-CB	5.16	1.61	1.53
1	A	97	LEU	N-CA	5.15	1.52	1.46
1	A	234	LEU	C-O	5.14	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	VAL	N-CA	5.13	1.53	1.47
1	B	308	THR	CA-C	5.11	1.58	1.52
1	B	131	LYS	CA-C	-5.09	1.46	1.52
1	B	295	ALA	C-O	5.06	1.30	1.23
1	B	200	ILE	C-N	5.06	1.40	1.33
1	B	285	ILE	N-CA	5.06	1.52	1.46
1	B	120	ASP	N-CA	5.05	1.52	1.46
1	A	96	ALA	C-O	5.04	1.30	1.24
1	A	210	GLU	CD-OE1	5.03	1.34	1.25
1	A	36	GLN	C-N	5.03	1.40	1.33
1	B	221	LYS	C-O	-5.02	1.17	1.24

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ALA	CA-C-O	15.50	136.85	120.42
1	B	31	ARG	NE-CZ-NH1	-13.74	107.76	121.50
1	B	282	ILE	O-C-N	-12.34	109.82	121.91
1	B	35	ARG	CD-NE-CZ	12.03	141.24	124.40
1	B	31	ARG	NE-CZ-NH2	11.89	129.90	119.20
1	B	127	GLN	OE1-CD-NE2	11.80	134.41	122.60
1	B	22	SER	CA-C-O	11.73	134.77	121.87
1	B	311	GLN	OE1-CD-NE2	11.64	134.24	122.60
1	B	61	LEU	CA-C-O	-11.57	108.15	120.42
1	B	282	ILE	CA-C-O	10.94	132.76	121.17
1	B	131	LYS	O-C-N	-10.49	111.69	121.35
1	A	66	ALA	O-C-N	-10.44	110.81	122.09
1	B	185	ARG	CD-NE-CZ	10.28	138.79	124.40
1	A	102	ARG	NE-CZ-NH2	-10.13	110.08	119.20
1	B	62	LEU	CA-C-O	9.83	131.15	120.82
1	B	180	LYS	CA-C-O	-9.55	110.43	120.55
1	B	312	VAL	CA-C-O	9.55	131.82	120.65
1	B	63	HIS	CE1-NE2-CD2	9.55	118.55	109.00
1	B	176	ALA	CA-C-O	-9.52	110.35	120.63
1	B	310	THR	O-C-N	-9.47	112.24	123.13
1	B	129	PRO	O-C-N	9.28	132.86	123.03
1	B	305	GLU	CB-CG-CD	9.19	128.22	112.60
1	B	308	THR	O-C-N	9.18	133.24	123.42
1	B	284	PHE	O-C-N	9.02	131.68	122.12
1	B	227	ASN	OD1-CG-ND2	8.97	131.57	122.60
1	B	308	THR	CA-CB-OG1	8.96	123.04	109.60
1	B	293	ILE	CA-C-O	-8.90	110.70	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ALA	CA-C-O	-8.86	111.81	121.28
1	B	64	MET	O-C-N	8.76	133.04	122.27
1	B	58	GLY	O-C-N	8.75	130.59	122.19
1	B	57[A]	VAL	O-C-N	8.74	130.83	121.83
1	B	57[B]	VAL	O-C-N	8.74	130.83	121.83
1	B	62	LEU	O-C-N	-8.71	113.10	122.07
1	B	61	LEU	O-C-N	8.62	131.97	122.15
1	B	264	TYR	O-C-N	8.57	130.90	122.07
1	B	22	SER	O-C-N	-8.55	112.75	122.75
1	A	159	ARG	CD-NE-CZ	8.49	136.29	124.40
1	B	60	LEU	O-C-N	8.49	131.12	122.12
1	A	100[A]	GLU	CA-C-O	-8.41	111.50	120.42
1	A	100[B]	GLU	CA-C-O	-8.41	111.50	120.42
1	B	39	GLU	CA-C-O	8.38	129.44	120.55
1	B	204	GLY	O-C-N	8.37	132.75	122.46
1	B	156	ASP	CA-CB-CG	8.37	120.97	112.60
1	B	253	ARG	O-C-N	-8.25	111.61	122.59
1	A	262	LYS	CA-CB-CG	8.19	130.48	114.10
1	B	280	ALA	O-C-N	8.09	131.37	122.15
1	B	303	ALA	O-C-N	-7.95	113.09	122.15
1	A	295	ALA	CA-C-O	-7.90	113.00	121.45
1	A	68	GLN	CA-C-O	-7.88	112.06	120.42
1	A	145	LEU	O-C-N	-7.86	113.79	122.12
1	B	181	LYS	CA-CB-CG	7.86	129.81	114.10
1	A	176	ALA	CA-C-O	-7.85	112.15	120.63
1	A	68	GLN	N-CA-C	-7.83	102.83	111.36
1	B	147	ARG	O-C-N	7.82	130.13	122.07
1	A	74	PRO	CA-C-O	-7.78	111.97	121.31
1	A	43	ARG	NH1-CZ-NH2	7.73	129.34	119.30
1	A	284	PHE	O-C-N	7.66	130.88	122.15
1	A	308	THR	O-C-N	7.63	131.59	123.42
1	B	238	ASN	OD1-CG-ND2	-7.58	115.02	122.60
1	B	311	GLN	CG-CD-NE2	-7.57	105.05	116.40
1	A	130	THR	CA-C-O	-7.57	110.55	118.65
1	B	98	LYS	CA-C-O	-7.56	112.53	120.55
1	B	147	ARG	CA-C-O	-7.56	112.89	120.82
1	B	57[A]	VAL	CA-C-N	-7.44	111.73	119.98
1	B	57[A]	VAL	C-N-CA	-7.44	111.73	119.98
1	B	57[B]	VAL	CA-C-N	-7.44	111.73	119.98
1	B	57[B]	VAL	C-N-CA	-7.44	111.73	119.98
1	A	102	ARG	NE-CZ-NH1	7.38	128.88	121.50
1	A	312	VAL	CA-C-O	7.38	129.05	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	GLN	CA-C-O	-7.33	113.15	120.70
1	A	211	ALA	O-C-N	7.32	130.61	123.29
1	B	100	GLU	N-CA-C	-7.28	103.42	111.36
1	A	65	ASP	N-CA-C	-7.26	103.45	111.36
1	B	160	GLY	CA-C-O	-7.25	116.21	122.16
1	B	262[A]	LYS	CA-C-O	7.25	128.10	120.42
1	B	262[B]	LYS	CA-C-O	7.25	128.10	120.42
1	B	313	LEU	O-C-N	-7.25	115.19	121.35
1	A	141	THR	CA-C-O	-7.24	112.75	120.42
1	B	126	PHE	O-C-N	7.24	132.12	122.43
1	B	31	ARG	CD-NE-CZ	-7.22	114.29	124.40
1	B	122	ASN	CA-CB-CG	-7.22	105.38	112.60
1	A	141	THR	O-C-N	7.21	130.36	122.15
1	B	4	ARG	NH1-CZ-NH2	-7.16	110.00	119.30
1	B	188	ILE	CA-C-N	-7.08	113.97	123.10
1	B	188	ILE	C-N-CA	-7.08	113.97	123.10
1	B	57[A]	VAL	CA-C-O	-7.04	113.39	120.85
1	B	57[B]	VAL	CA-C-O	-7.04	113.39	120.85
1	B	292	ALA	O-C-N	-7.03	114.05	123.19
1	B	58	GLY	CA-C-O	-6.99	113.55	120.75
1	B	36	GLN	CA-C-O	6.97	127.94	120.55
1	B	15	GLN	CB-CG-CD	6.95	124.42	112.60
1	A	15	GLN	CB-CG-CD	6.95	124.42	112.60
1	B	126	PHE	CA-C-O	-6.95	110.84	119.38
1	B	173	HIS	CG-CD2-NE2	6.92	114.12	107.20
1	B	29	ASN	CA-C-O	6.91	127.75	120.42
1	A	304	LEU	O-C-N	6.91	130.77	122.27
1	B	102	ARG	N-CA-C	-6.91	103.83	111.36
1	B	251	TRP	O-C-N	-6.89	114.97	123.04
1	A	51	HIS	ND1-CE1-NE2	6.84	115.24	108.40
1	B	255	VAL	O-C-N	-6.83	115.69	123.07
1	B	68	GLN	O-C-N	6.83	129.36	122.12
1	B	299	LYS	CA-C-O	6.83	129.05	120.65
1	A	65	ASP	CA-C-O	-6.83	113.19	120.42
1	A	262	LYS	O-C-N	-6.82	114.89	122.12
1	B	39	GLU	OE1-CD-OE2	6.82	139.27	122.90
1	B	105	GLY	CA-C-O	6.78	128.40	119.58
1	B	63	HIS	ND1-CE1-NE2	-6.77	101.63	108.40
1	B	147	ARG	CD-NE-CZ	6.75	133.86	124.40
1	A	236	ASP	O-C-N	6.75	130.29	122.25
1	B	51	HIS	ND1-CG-CD2	6.74	112.83	106.10
1	A	68	GLN	OE1-CD-NE2	6.69	129.29	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ARG	CA-C-O	6.68	127.51	120.36
1	B	64	MET	CA-C-O	-6.66	112.31	119.97
1	A	65	ASP	OD1-CG-OD2	6.65	138.86	122.90
1	A	124	PRO	O-C-N	-6.65	113.33	122.24
1	B	197	VAL	O-C-N	-6.65	113.92	121.57
1	B	60	LEU	CA-C-O	-6.63	113.52	120.55
1	B	99	ASN	CA-C-O	-6.58	113.44	120.42
1	B	180	LYS	O-C-N	6.58	129.10	122.12
1	B	63	HIS	CG-CD2-NE2	-6.58	100.62	107.20
1	A	99	ASN	CA-C-O	-6.56	113.94	120.70
1	A	127	GLN	O-C-N	-6.56	113.40	122.46
1	B	34	ALA	CA-C-N	-6.55	111.00	120.29
1	B	34	ALA	C-N-CA	-6.55	111.00	120.29
1	B	204	GLY	CA-C-N	-6.51	113.81	122.99
1	B	204	GLY	C-N-CA	-6.51	113.81	122.99
1	A	66	ALA	CA-C-N	6.50	127.19	119.98
1	A	66	ALA	C-N-CA	6.50	127.19	119.98
1	B	31	ARG	CA-C-O	-6.48	113.55	120.42
1	A	43	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	B	129	PRO	CA-C-O	-6.45	113.37	120.92
1	A	197	VAL	N-CA-C	-6.44	102.64	108.95
1	A	118	ILE	CA-C-O	6.43	128.18	120.85
1	B	290	GLU	O-C-N	-6.42	113.73	122.33
1	B	297	LEU	O-C-N	6.41	131.12	122.59
1	A	38	ALA	CA-C-O	-6.41	112.86	120.10
1	A	201	LEU	CA-C-O	-6.40	113.28	120.32
1	A	269	PHE	CA-C-O	-6.40	113.89	120.54
1	A	126	PHE	O-C-N	6.39	130.13	122.27
1	B	296	HIS	CB-CG-CD2	6.38	139.50	131.20
1	A	134	GLY	O-C-N	6.37	128.14	121.77
1	A	217	LEU	CA-C-O	6.35	127.16	120.42
1	B	222	LEU	O-C-N	6.35	128.85	122.12
1	A	38	ALA	O-C-N	6.34	129.64	122.22
1	B	292	ALA	CA-C-O	6.33	128.27	121.11
1	A	183	VAL	O-C-N	6.32	128.00	121.87
1	B	167	SER	CA-C-N	6.32	126.28	120.03
1	B	167	SER	C-N-CA	6.32	126.28	120.03
1	A	280	ALA	O-C-N	6.31	129.35	122.15
1	A	223	ALA	CA-C-O	-6.31	113.73	120.42
1	B	241	ALA	CA-C-O	6.29	128.21	121.11
1	A	120	ASP	O-C-N	6.28	130.39	123.04
1	B	162	ARG	CD-NE-CZ	-6.28	115.60	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LYS	CB-CG-CD	-6.26	96.91	111.30
1	A	61	LEU	O-C-N	6.26	129.28	122.15
1	B	4	ARG	NE-CZ-NH1	6.25	127.75	121.50
1	B	301	VAL	N-CA-C	6.25	117.03	110.72
1	B	211	ALA	CA-C-N	-6.24	114.97	123.14
1	B	211	ALA	C-N-CA	-6.24	114.97	123.14
1	A	287	TRP	CD2-CE2-CZ2	-6.23	116.17	122.40
1	B	133	VAL	N-CA-C	6.22	118.08	108.44
1	A	95	GLN	CA-C-O	-6.21	114.30	120.82
1	A	256	LYS	O-C-N	6.18	129.98	123.06
1	B	300	ALA	CA-C-O	6.18	127.30	120.63
1	B	253	ARG	CA-C-N	6.17	130.12	121.24
1	B	253	ARG	C-N-CA	6.17	130.12	121.24
1	B	204	GLY	CA-C-O	-6.16	112.87	119.27
1	A	211	ALA	CA-C-N	-6.15	114.57	123.06
1	A	211	ALA	C-N-CA	-6.15	114.57	123.06
1	A	70	THR	CA-C-N	6.14	132.03	122.26
1	A	70	THR	C-N-CA	6.14	132.03	122.26
1	B	108	LYS	O-C-N	6.14	130.60	123.17
1	A	299	LYS	O-C-N	-6.12	113.99	122.20
1	B	138	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	79	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	39	GLU	CG-CD-OE2	-6.11	104.36	118.40
1	B	298	GLU	O-C-N	-6.09	114.06	122.46
1	A	155	GLU	CA-C-O	6.08	127.41	120.54
1	B	301	VAL	O-C-N	6.08	128.09	121.83
1	A	4	ARG	CD-NE-CZ	-6.06	115.92	124.40
1	A	60	LEU	O-C-N	6.05	129.30	122.22
1	A	167	SER	CA-C-N	6.04	126.01	120.03
1	A	167	SER	C-N-CA	6.04	126.01	120.03
1	B	35	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	A	304	LEU	CA-C-O	-6.03	113.04	119.97
1	B	211	ALA	O-C-N	6.01	129.57	123.26
1	B	101	LEU	CA-C-O	-6.01	114.05	120.42
1	B	271	ALA	CA-C-N	-6.00	105.07	122.46
1	B	271	ALA	C-N-CA	-6.00	105.07	122.46
1	B	205	GLU	CA-C-O	5.98	126.82	120.36
1	A	64	MET	CA-C-O	-5.97	113.10	119.97
1	B	129	PRO	CA-C-N	-5.97	112.67	121.99
1	B	129	PRO	C-N-CA	-5.97	112.67	121.99
1	B	72	GLY	CA-C-O	5.97	126.89	119.25
1	B	147	ARG	NE-CZ-NH2	-5.96	113.83	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	GLY	O-C-N	-5.94	115.37	122.68
1	A	302[A]	GLU	CA-C-O	5.93	126.84	120.55
1	A	302[B]	GLU	CA-C-O	5.93	126.84	120.55
1	B	194	GLY	O-C-N	5.93	130.24	122.35
1	A	291	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	B	23	TYR	CG-CD1-CE1	5.93	130.09	121.20
1	A	126	PHE	CA-C-O	-5.92	113.16	119.97
1	B	40	ILE	CA-C-O	5.92	127.12	120.85
1	A	300	ALA	N-CA-C	5.91	117.72	111.28
1	B	97	LEU	O-C-N	-5.91	115.42	122.15
1	A	248	LYS	CA-CB-CG	5.91	125.91	114.10
1	A	19	GLN	CG-CD-NE2	5.90	125.25	116.40
1	A	279	LEU	CA-C-O	5.89	126.79	120.55
1	B	150	GLY	O-C-N	5.89	129.39	122.38
1	B	163	ARG	CD-NE-CZ	-5.88	116.16	124.40
1	A	41[A]	ILE	CA-C-O	-5.88	114.28	120.57
1	A	41[B]	ILE	CA-C-O	-5.88	114.28	120.57
1	A	148	GLU	CA-CB-CG	-5.87	102.36	114.10
1	B	284	PHE	CA-C-O	-5.87	114.33	120.55
1	B	312	VAL	O-C-N	-5.86	115.79	122.94
1	B	202	GLU	CG-CD-OE2	-5.85	104.94	118.40
1	A	102	ARG	CA-C-O	-5.84	114.36	120.55
1	B	63	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	B	278	VAL	O-C-N	-5.82	115.83	121.83
1	A	64	MET	O-C-N	5.80	129.41	122.27
1	A	310	THR	CA-C-N	5.79	131.87	123.13
1	A	310	THR	C-N-CA	5.79	131.87	123.13
1	B	41[A]	ILE	CA-C-O	-5.78	114.73	120.85
1	B	41[B]	ILE	CA-C-O	-5.78	114.73	120.85
1	B	95	GLN	N-CA-C	-5.77	104.90	111.14
1	B	132	PRO	CA-C-O	-5.77	114.38	121.31
1	A	310	THR	O-C-N	-5.77	116.64	123.22
1	A	133	VAL	O-C-N	-5.77	116.50	123.02
1	B	164	VAL	N-CA-CB	5.76	121.42	111.39
1	B	43	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	B	244	TYR	O-C-N	-5.74	115.97	122.97
1	A	297	LEU	O-C-N	5.73	130.21	122.59
1	A	164	VAL	N-CA-CB	5.72	121.35	111.39
1	A	262	LYS	CA-C-O	5.72	126.62	120.55
1	A	34	ALA	CA-C-O	-5.71	113.41	119.97
1	B	27	MET	CA-C-O	-5.70	114.51	120.55
1	B	251	TRP	CA-C-O	5.70	127.19	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ILE	O-C-N	-5.70	115.96	121.83
1	B	198	PRO	CA-C-O	-5.70	114.54	121.03
1	B	35	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	B	173	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
1	B	200	ILE	CA-C-O	5.68	128.45	121.75
1	B	276	PRO	O-C-N	5.65	129.98	122.30
1	B	194	GLY	CA-C-O	-5.65	112.02	119.25
1	B	36	GLN	O-C-N	-5.63	116.15	122.12
1	B	310	THR	CA-C-N	5.63	131.63	123.13
1	B	310	THR	C-N-CA	5.63	131.63	123.13
1	A	48	VAL	CA-C-O	-5.60	114.51	120.39
1	B	2	GLY	O-C-N	5.60	131.96	123.00
1	B	128	ASN	CA-C-O	5.60	127.71	121.22
1	B	64	MET	CA-C-N	-5.58	112.37	120.29
1	B	64	MET	C-N-CA	-5.58	112.37	120.29
1	A	289	GLY	CA-C-O	-5.57	114.84	122.31
1	A	123	ASP	CA-C-O	-5.57	115.03	119.71
1	B	94	GLN	CA-C-O	-5.56	114.52	120.42
1	B	291	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	A	51	HIS	CA-C-O	-5.51	115.53	121.38
1	A	64	MET	CA-C-N	-5.50	112.47	120.29
1	A	64	MET	C-N-CA	-5.50	112.47	120.29
1	B	39	GLU	O-C-N	-5.49	116.30	122.12
1	B	178	THR	O-C-N	-5.49	115.89	122.15
1	A	170	PRO	CA-C-O	-5.49	114.77	121.03
1	B	65	ASP	OD1-CG-OD2	5.48	136.04	122.90
1	B	50[A]	THR	O-C-N	-5.46	115.20	122.74
1	B	50[B]	THR	O-C-N	-5.46	115.20	122.74
1	B	160	GLY	O-C-N	5.46	128.25	123.06
1	A	51	HIS	CA-C-N	-5.42	116.72	122.30
1	A	51	HIS	C-N-CA	-5.42	116.72	122.30
1	A	250	GLN	CB-CG-CD	5.42	121.81	112.60
1	B	169	ASP	CA-C-O	5.41	124.58	119.76
1	B	280	ALA	CA-C-O	-5.41	114.68	120.42
1	B	176	ALA	O-C-N	5.41	127.85	122.12
1	B	137	TYR	CA-C-O	-5.41	114.86	121.78
1	B	132	PRO	CB-CA-C	-5.40	104.03	111.21
1	A	33	THR	CA-C-O	5.40	126.27	120.55
1	B	34	ALA	O-C-N	5.39	128.53	122.22
1	A	214	ASP	CA-CB-CG	-5.38	107.22	112.60
1	B	222	LEU	CA-C-O	-5.38	114.85	120.55
1	A	60	LEU	CA-C-O	-5.37	114.03	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	GLU	CB-CG-CD	-5.37	103.47	112.60
1	B	36	GLN	N-CA-C	5.35	117.11	111.28
1	B	296	HIS	CG-CD2-NE2	5.35	112.55	107.20
1	B	163	ARG	O-C-N	-5.35	116.23	122.81
1	B	11	GLY	O-C-N	5.34	127.42	122.13
1	B	212	VAL	CA-C-O	-5.34	114.79	120.39
1	A	128	ASN	OD1-CG-ND2	5.33	127.92	122.60
1	A	140	GLU	N-CA-CB	-5.32	102.30	110.12
1	B	31	ARG	O-C-N	5.32	128.21	122.15
1	B	122	ASN	CB-CA-C	-5.31	102.17	110.94
1	A	98	LYS	CA-C-O	-5.31	113.86	119.97
1	B	290	GLU	CA-C-O	5.30	126.05	119.79
1	A	292	ALA	O-C-N	-5.30	116.30	123.19
1	A	262	LYS	CB-CG-CD	5.30	123.48	111.30
1	A	46	GLU	CA-C-N	-5.29	116.28	123.10
1	A	46	GLU	C-N-CA	-5.29	116.28	123.10
1	B	224	GLU	O-C-N	-5.29	116.38	122.09
1	B	301	VAL	N-CA-CB	-5.28	102.66	110.58
1	B	248	LYS	O-C-N	5.28	128.67	122.34
1	A	301	VAL	N-CA-CB	-5.27	103.83	110.57
1	A	238	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	151	TRP	CA-C-N	5.26	129.56	122.93
1	A	151	TRP	C-N-CA	5.26	129.56	122.93
1	A	51	HIS	O-C-N	5.26	128.78	123.26
1	B	306	GLY	O-C-N	-5.26	116.30	122.45
1	B	118	ILE	O-C-N	5.25	128.64	122.81
1	A	312	VAL	O-C-N	-5.25	116.97	122.95
1	A	54	GLY	CA-C-N	5.24	124.75	119.19
1	A	54	GLY	C-N-CA	5.24	124.75	119.19
1	A	184[A]	GLU	CA-C-N	5.24	131.58	122.56
1	A	184[A]	GLU	C-N-CA	5.24	131.58	122.56
1	A	184[B]	GLU	CA-C-N	5.24	131.58	122.56
1	A	184[B]	GLU	C-N-CA	5.24	131.58	122.56
1	A	181	LYS	O-C-N	-5.24	116.56	122.12
1	B	135	PRO	CB-CA-C	-5.23	104.37	111.12
1	A	229	ASP	CA-C-O	5.23	126.04	120.24
1	B	133	VAL	CB-CA-C	-5.22	101.08	110.48
1	A	45	TYR	N-CA-C	5.22	118.21	110.48
1	B	229	ASP	CA-C-N	5.22	130.20	122.94
1	B	229	ASP	C-N-CA	5.22	130.20	122.94
1	B	253	ARG	CA-CB-CG	-5.20	103.69	114.10
1	A	159	ARG	N-CA-CB	-5.20	102.48	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	MET	CA-C-O	-5.19	114.24	120.10
1	B	199	VAL	O-C-N	5.18	128.91	123.00
1	B	307	LYS	N-CA-C	5.18	119.60	113.28
1	B	164	VAL	CA-C-O	5.18	126.73	120.67
1	B	293	ILE	CA-C-N	5.18	129.98	123.10
1	B	293	ILE	C-N-CA	5.18	129.98	123.10
1	A	19	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	B	76	GLN	CA-C-N	5.16	125.63	120.52
1	B	76	GLN	C-N-CA	5.16	125.63	120.52
1	A	307	LYS	O-C-N	-5.16	115.67	122.42
1	A	205	GLU	CB-CG-CD	5.15	121.36	112.60
1	A	43	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	B	143	LYS	O-C-N	-5.14	115.95	122.27
1	B	23	TYR	CD1-CE1-CZ	-5.12	110.37	119.60
1	B	132	PRO	CA-C-N	5.11	129.21	122.51
1	B	132	PRO	C-N-CA	5.11	129.21	122.51
1	A	25	GLU	CA-C-O	5.11	125.96	120.70
1	A	76	GLN	CA-C-O	5.11	126.82	120.54
1	A	269	PHE	N-CA-CB	-5.11	101.94	110.37
1	B	21	GLY	CA-C-O	5.10	125.48	119.46
1	B	41[A]	ILE	O-C-N	5.10	127.08	121.83
1	B	41[B]	ILE	O-C-N	5.10	127.08	121.83
1	A	88	TRP	N-CA-CB	-5.10	102.62	110.01
1	A	286	GLU	O-C-N	-5.09	116.26	122.22
1	A	24	GLU	CG-CD-OE1	5.09	130.12	118.40
1	B	42	ALA	CA-C-O	5.09	125.85	120.10
1	B	300	ALA	CA-C-N	-5.09	113.19	120.42
1	B	300	ALA	C-N-CA	-5.09	113.19	120.42
1	A	157	SER	CA-C-O	-5.09	114.72	121.08
1	A	263	TYR	O-C-N	5.08	127.51	122.12
1	B	231	PHE	O-C-N	-5.08	117.38	123.27
1	B	137	TYR	O-C-N	5.08	130.03	122.97
1	B	31	ARG	CG-CD-NE	5.07	123.16	112.00
1	A	228	ALA	O-C-N	5.07	128.84	122.86
1	A	17	ARG	CD-NE-CZ	5.07	131.49	124.40
1	A	295	ALA	N-CA-C	5.07	116.51	108.96
1	A	203	ASP	O-C-N	5.06	129.19	122.41
1	B	120	ASP	CB-CG-OD2	-5.06	106.75	118.40
1	B	261	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	B	192	SER	CB-CA-C	5.06	119.51	111.51
1	B	42	ALA	O-C-N	-5.06	116.30	122.22
1	B	149	LYS	O-C-N	5.05	128.56	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	LYS	CA-CB-CG	-5.05	104.00	114.10
1	A	256	LYS	CA-C-O	-5.02	115.33	121.36
1	A	308	THR	CA-C-O	-5.02	115.86	121.23
1	B	100	GLU	CA-C-O	-5.02	115.10	120.42
1	B	237	VAL	O-C-N	-5.02	117.47	123.04
1	B	51	HIS	CA-C-O	-5.01	116.07	121.38
1	A	77	PRO	O-C-N	5.01	129.07	122.86

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Mainchain
1	B	296	HIS	Mainchain

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	2479	0	2517	44	2
1	B	2483	0	2526	56	2
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	391	0	0	14	2
4	B	325	0	0	8	2
All	All	5734	0	5067	95	4

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 9.

All (95) 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:225:GLU:OE2	4:A:2286:HOH:O	1.71	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:NZ	1:A:184[B]:GLU:OE2	1.91	1.01
1:B:302[B]:GLU:HG2	1:B:308:THR:HG22	1.52	0.89
1:A:43:ARG:NH1	1:A:305[B]:GLU:OE2	2.08	0.87
1:B:290:GLU:OE2	4:B:2297:HOH:O	1.93	0.86
1:B:104:ARG:CB	1:B:106:MET:HE2	2.07	0.83
1:B:274[B]:MET:HE1	1:B:294:ILE:HD13	1.61	0.81
1:A:274[B]:MET:HE1	1:A:294:ILE:HD13	1.61	0.81
1:A:274[B]:MET:HE3	1:A:277:LYS:HB2	1.63	0.80
1:B:240:ALA:HB2	1:B:274[B]:MET:HE2	1.65	0.79
1:A:67:GLY:HA3	1:B:63:HIS:HD2	1.48	0.79
1:A:274[B]:MET:HE2	1:A:278:VAL:HG23	1.64	0.78
1:A:274[B]:MET:CE	1:A:277:LYS:HB2	2.14	0.77
1:B:50[A]:THR:HG23	1:B:191:ALA:O	1.84	0.77
1:B:221:LYS:NZ	4:B:2240:HOH:O	2.16	0.77
1:A:100[B]:GLU:CD	4:A:2141:HOH:O	2.28	0.76
1:B:104:ARG:HB2	1:B:106:MET:CE	2.16	0.75
1:B:104:ARG:HB3	1:B:106:MET:HE2	1.69	0.75
1:B:274[B]:MET:CE	1:B:294:ILE:HD13	2.18	0.74
1:B:50[A]:THR:CG2	1:B:191:ALA:O	2.35	0.74
1:B:104:ARG:HB2	1:B:106:MET:HE2	1.68	0.74
1:A:262:LYS:HD2	4:A:2322:HOH:O	1.87	0.72
1:B:50[B]:THR:HG22	1:B:51:HIS:H	1.52	0.72
1:A:247[A]:GLU:HG2	4:A:2299:HOH:O	1.89	0.71
1:B:274[B]:MET:HE1	1:B:294:ILE:HG21	1.71	0.71
1:A:305[A]:GLU:OE2	4:A:2370:HOH:O	2.09	0.69
1:B:144:ARG:HG3	1:B:147:ARG:NH2	2.09	0.67
1:A:184[B]:GLU:OE1	4:A:2246:HOH:O	2.14	0.66
1:B:202:GLU:OE2	4:B:2219:HOH:O	2.14	0.66
1:B:261:ARG:NE	1:B:286:GLU:OE2	2.29	0.65
1:A:67:GLY:HA3	1:B:63:HIS:CD2	2.32	0.65
1:A:305[A]:GLU:CD	4:A:2370:HOH:O	2.38	0.65
1:B:302[B]:GLU:HG2	1:B:308:THR:CG2	2.28	0.63
1:A:100[B]:GLU:CG	4:A:2141:HOH:O	2.47	0.62
1:A:183:VAL:HG22	4:A:2077:HOH:O	2.00	0.59
1:A:43:ARG:NH1	1:A:305[B]:GLU:CD	2.60	0.58
1:B:31:ARG:NE	4:B:2048:HOH:O	2.35	0.58
1:A:100[B]:GLU:HG3	4:A:2141:HOH:O	2.02	0.58
1:B:50[B]:THR:HG22	1:B:51:HIS:N	2.13	0.58
1:A:53:ASN:O	1:A:57[B]:VAL:HG22	2.05	0.57
1:A:274[B]:MET:CE	1:A:294:ILE:HD13	2.33	0.57
1:B:215[B]:LYS:HE2	1:B:216:ASP:CG	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ARG:HD3	1:A:286:GLU:OE2	2.05	0.56
1:B:104:ARG:CB	1:B:106:MET:CE	2.78	0.55
1:B:31:ARG:HD2	1:B:35:ARG:HH12	1.72	0.54
1:B:50[A]:THR:HG22	1:B:191:ALA:O	2.08	0.54
1:B:62:LEU:HD23	1:B:135:PRO:HG3	1.91	0.52
1:B:31:ARG:HD2	1:B:35:ARG:HH22	1.73	0.52
1:B:139:GLU:O	1:B:143:LYS:HG3	2.09	0.52
1:A:64:MET:HA	1:B:63:HIS:CD2	2.45	0.52
1:A:43:ARG:HH12	1:A:305[B]:GLU:CD	2.18	0.51
1:A:274[B]:MET:CE	1:A:278:VAL:HG23	2.35	0.50
1:A:41[B]:ILE:HD11	1:A:47:VAL:HB	1.93	0.50
1:A:274[B]:MET:HE1	1:A:277:LYS:HB2	1.94	0.49
1:B:177:GLU:O	1:B:181:LYS:HG2	2.13	0.48
1:B:215[B]:LYS:HE2	1:B:216:ASP:OD2	2.13	0.48
1:A:205:GLU:CD	1:A:207:LYS:HE2	2.40	0.47
1:B:31:ARG:HD2	1:B:35:ARG:NH2	2.30	0.47
1:B:31:ARG:HD2	1:B:35:ARG:NH1	2.30	0.47
1:A:131:LYS:HG2	1:A:212:VAL:HG21	1.96	0.46
1:B:31:ARG:HG2	1:B:35:ARG:NH1	2.29	0.46
1:B:259:GLU:CD	1:B:262[B]:LYS:NZ	2.73	0.46
1:B:41[B]:ILE:HD13	1:B:188:ILE:CD1	2.45	0.46
1:A:45:TYR:OH	1:A:305[A]:GLU:OE2	2.27	0.45
1:B:4:ARG:HH22	1:B:184[B]:GLU:CD	2.24	0.45
1:A:24:GLU:H	1:A:24:GLU:CD	2.23	0.45
1:B:6:VAL:HG21	1:B:223:ALA:HA	1.98	0.45
1:B:50[B]:THR:CG2	1:B:51:HIS:H	2.25	0.45
1:A:107:GLU:OE1	4:A:2156:HOH:O	2.20	0.45
1:B:50[B]:THR:HG21	4:B:2215:HOH:O	2.17	0.44
1:B:259:GLU:OE1	1:B:262[B]:LYS:NZ	2.50	0.44
1:B:50[B]:THR:HG23	1:B:191:ALA:O	2.17	0.44
1:A:201:LEU:HD12	4:A:2058:HOH:O	2.16	0.44
1:B:258:GLU:O	1:B:262[B]:LYS:HG3	2.18	0.43
1:A:109:LYS:HE2	1:A:187:VAL:HG22	2.00	0.43
1:A:113[B]:ILE:HD11	1:B:111:VAL:HG11	2.01	0.43
1:B:291:ARG:HD2	1:B:311:GLN:OE1	2.19	0.43
1:B:53:ASN:HA	1:B:56:GLN:HE21	1.83	0.42
1:B:131:LYS:NZ	4:B:2165:HOH:O	2.52	0.42
1:B:113[A]:ILE:HG21	1:B:179:ILE:HG12	2.02	0.42
1:B:171:LYS:HE2	4:B:2149:HOH:O	2.19	0.41
1:A:10:GLY:HA2	1:A:215[B]:LYS:NZ	2.36	0.41
1:A:103:LYS:HE3	1:B:205:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:MET:HE3	1:B:106:MET:HB2	1.89	0.41
1:A:100[B]:GLU:HG2	4:A:2143:HOH:O	2.21	0.41
1:B:31:ARG:CG	1:B:31:ARG:HH11	2.23	0.41
1:B:248:LYS:NZ	4:B:2257:HOH:O	2.54	0.41
1:A:154:LYS:HG2	4:A:2210:HOH:O	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:OE2	1:B:147:ARG:NH2[3_545]	1.67	0.53
4:A:2209:HOH:O	4:B:2154:HOH:O[3_545]	1.69	0.51
4:A:2296:HOH:O	4:B:2280:HOH:O[2_565]	2.14	0.06
1:A:203:ASP:OD2	1:B:144:ARG:NH2[3_545]	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	326/314 (104%)	319 (98%)	7 (2%)	0	100	100
1	B	327/314 (104%)	320 (98%)	6 (2%)	1 (0%)	36	17
All	All	653/628 (104%)	639 (98%)	13 (2%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	SER

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	262/248 (106%)	257 (98%)	5 (2%)	50	22
1	B	263/248 (106%)	255 (97%)	8 (3%)	36	9
All	All	525/496 (106%)	512 (98%)	13 (2%)	48	14

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	247[A]	GLU
1	A	247[B]	GLU
1	A	248	LYS
1	A	258	GLU
1	B	31	ARG
1	B	50[A]	THR
1	B	50[B]	THR
1	B	113[A]	ILE
1	B	113[B]	ILE
1	B	185	ARG
1	B	290	GLU
1	B	305	GLU

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

Mol	Chain	Res	Type
1	A	95	GLN
1	A	116	GLN
1	A	127	GLN
1	B	15	GLN
1	B	56	GLN
1	B	63	HIS
1	B	95	GLN
1	B	116	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ADP	A	315	3	28,29,29	1.27	4 (14%)	43,45,45	1.32	5 (11%)
2	ADP	B	315	3	28,29,29	1.45	5 (17%)	43,45,45	1.23	4 (9%)

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	ADP	A	315	3	-	5/16/32/32	0/3/3/3
2	ADP	B	315	3	-	5/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	ADP	C2-N1	3.69	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	ADP	PA-O3A	3.09	1.62	1.59
2	A	315	ADP	C2-N1	2.77	1.38	1.33
2	B	315	ADP	PA-O2A	-2.44	1.44	1.55
2	A	315	ADP	O2'-C2'	2.34	1.48	1.43
2	A	315	ADP	C6-N6	2.34	1.40	1.34
2	B	315	ADP	C5-N7	-2.31	1.34	1.39
2	A	315	ADP	C5-N7	-2.23	1.35	1.39
2	B	315	ADP	C8-N9	2.12	1.41	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	315	ADP	C4'-O4'-C1'	-4.25	100.08	109.47
2	A	315	ADP	C4'-O4'-C1'	-4.16	100.28	109.47
2	A	315	ADP	C5-C6-N6	3.12	131.00	123.29
2	A	315	ADP	N6-C6-N1	-2.99	111.72	118.38
2	A	315	ADP	O3A-PA-O1A	-2.64	102.75	110.70
2	B	315	ADP	C4-N9-C8	-2.36	103.26	105.74
2	B	315	ADP	O4'-C4'-C3'	-2.21	100.76	105.15
2	A	315	ADP	O3B-PB-O2B	2.15	115.86	107.80
2	B	315	ADP	O3B-PB-O2B	2.09	115.64	107.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

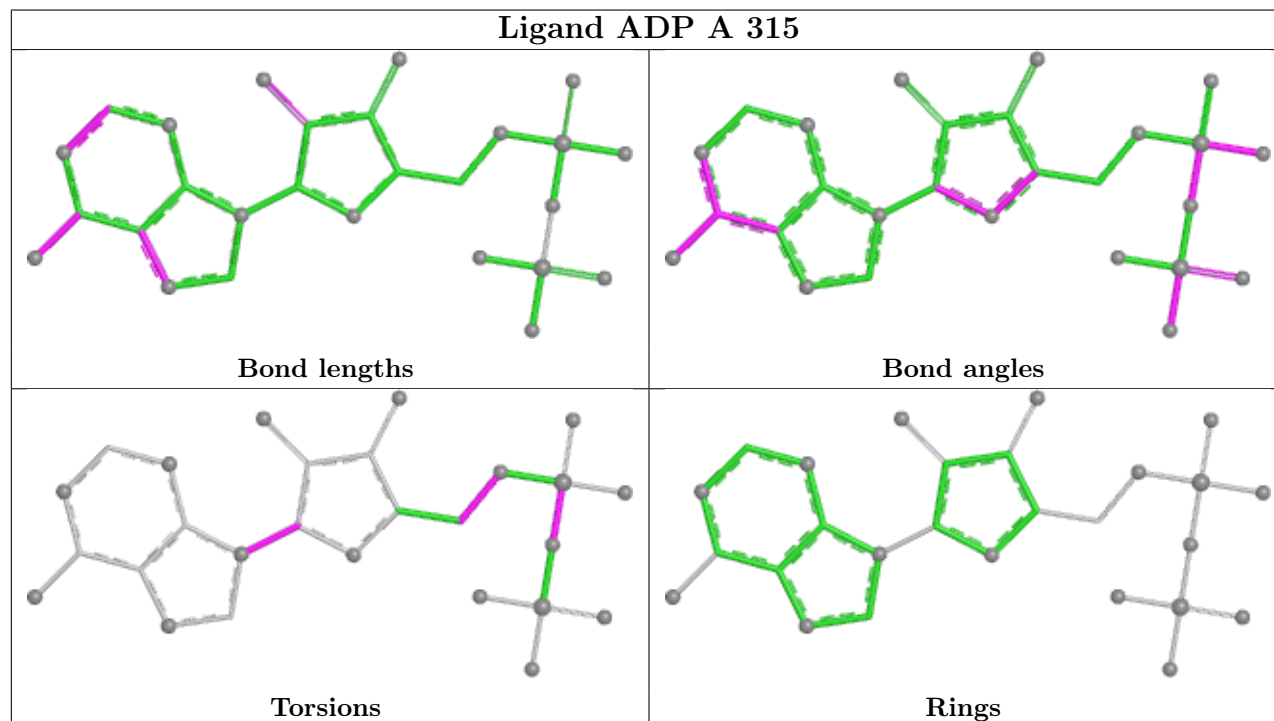
Mol	Chain	Res	Type	Atoms
2	B	315	ADP	C4'-C5'-O5'-PA
2	B	315	ADP	PA-O3A-PB-O3B
2	A	315	ADP	C4'-C5'-O5'-PA
2	A	315	ADP	PB-O3A-PA-O1A
2	A	315	ADP	PB-O3A-PA-O2A
2	A	315	ADP	O4'-C1'-N9-C8
2	B	315	ADP	PA-O3A-PB-O2B
2	A	315	ADP	C2'-C1'-N9-C8
2	B	315	ADP	O4'-C1'-N9-C8
2	B	315	ADP	PB-O3A-PA-O2A

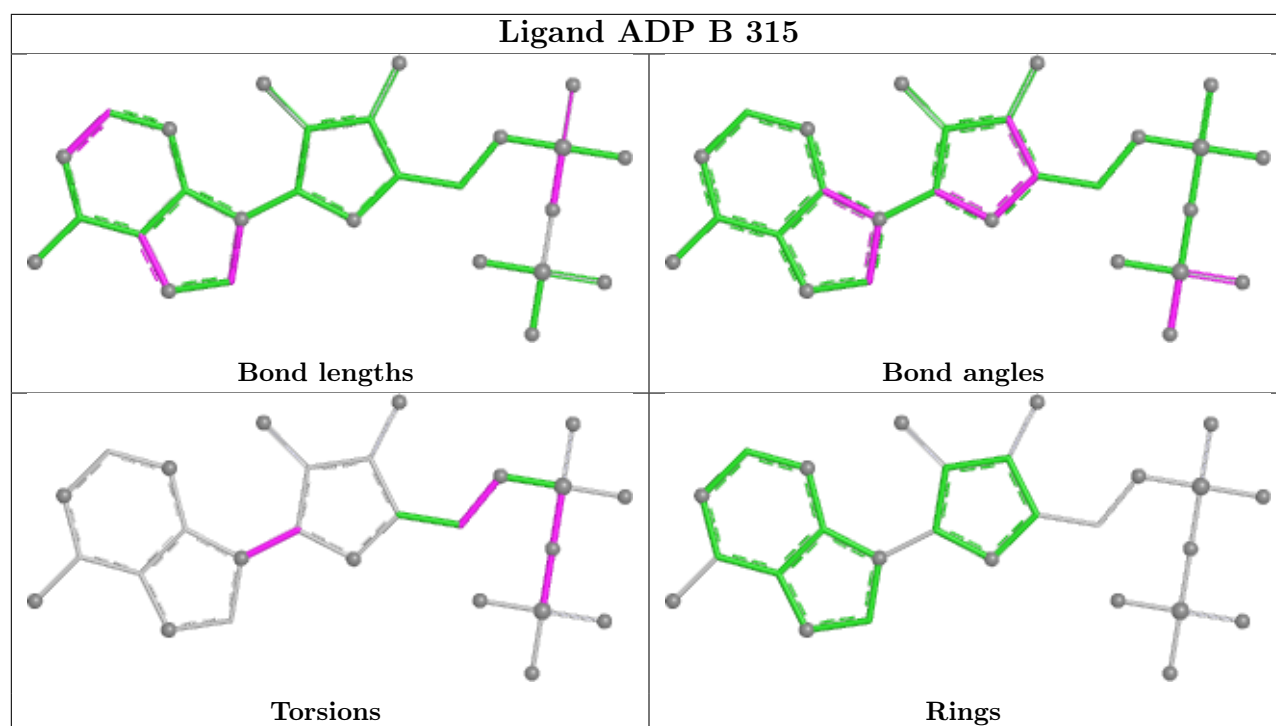
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	313/314 (99%)	-0.16	6 (1%) 66 70	11, 22, 38, 48	15 (4%)
1	B	313/314 (99%)	0.04	12 (3%) 44 48	11, 23, 37, 54	16 (5%)
All	All	626/628 (99%)	-0.06	18 (2%) 53 58	11, 22, 38, 54	31 (4%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	TRP	4.3
1	B	157	SER	3.3
1	A	159	ARG	3.0
1	B	160	GLY	2.8
1	A	17	ARG	2.7
1	B	140	GLU	2.4
1	A	107	GLU	2.4
1	B	156	ASP	2.3
1	B	145	LEU	2.2
1	B	142	ALA	2.2
1	A	140	GLU	2.2
1	B	137	TYR	2.2
1	A	18	GLY	2.2
1	A	158	GLY	2.2
1	B	136	PHE	2.2
1	B	158	GLY	2.1
1	B	159	ARG	2.1
1	B	272	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

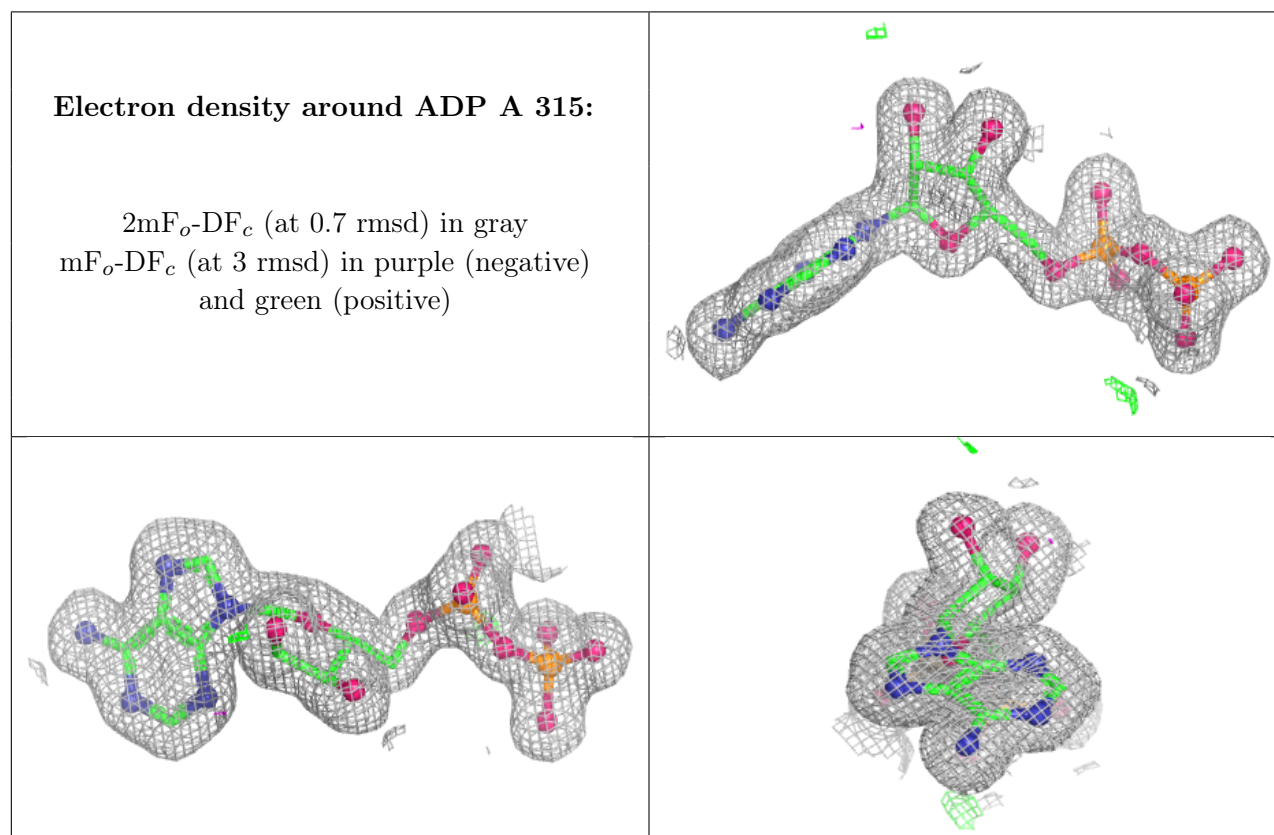
There are no oligosaccharides in this entry.

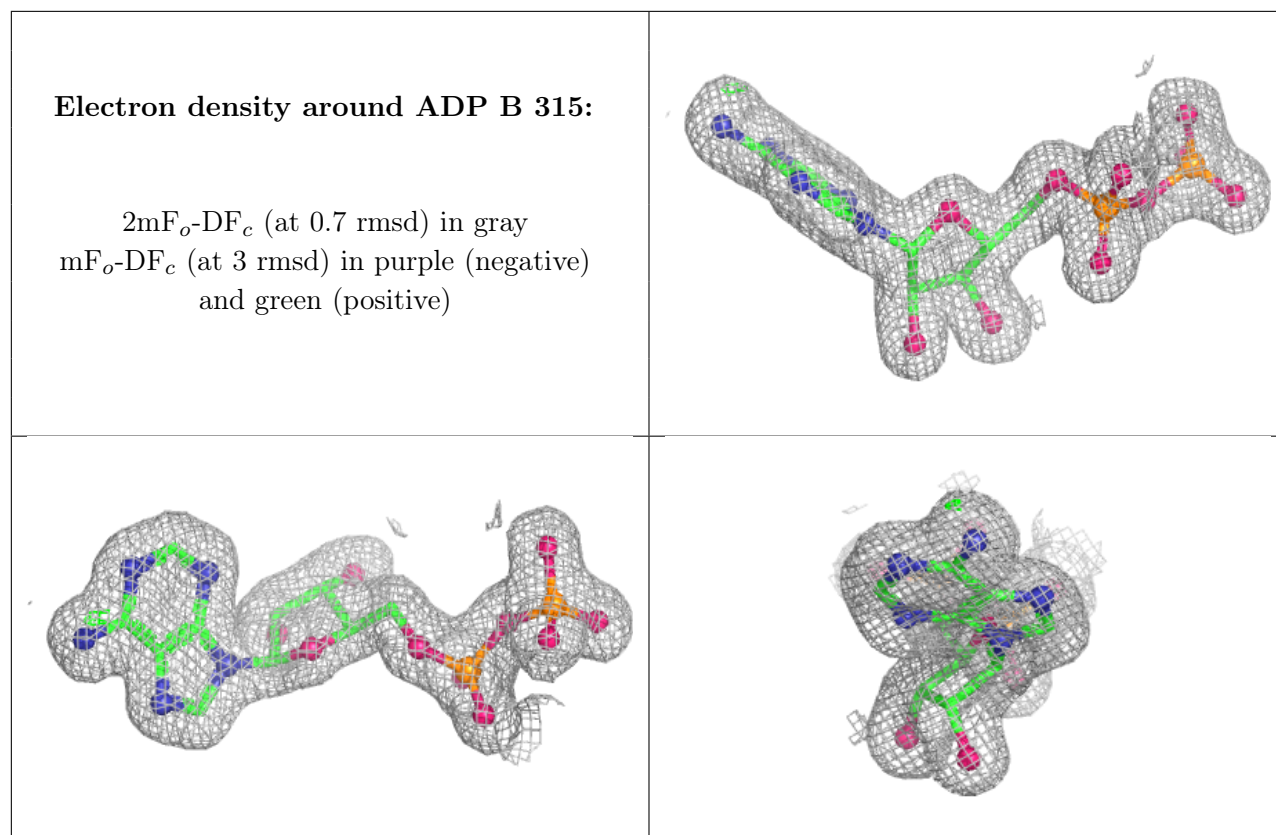
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	315	27/27	0.98	0.05	20,22,24,30	0
2	ADP	B	315	27/27	0.98	0.05	22,23,26,27	0
3	MG	A	316	1/1	0.99	0.08	25,25,25,25	0
3	MG	B	316	1/1	0.99	0.07	27,27,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.