



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:53 pm GMT

PDB ID : 1E19
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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

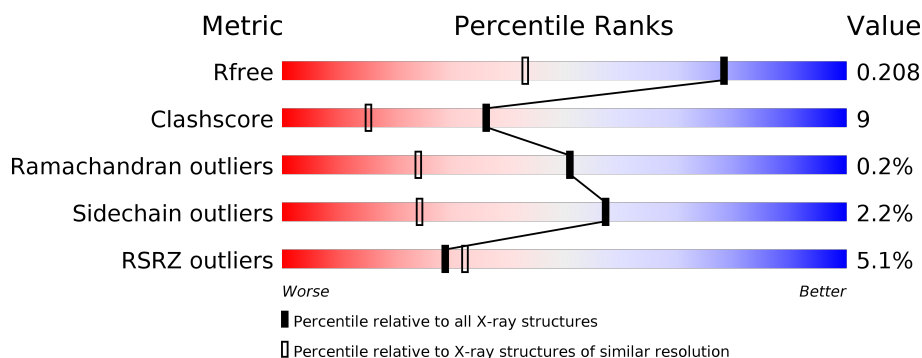
1 Overall quality at a glance

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}	100719	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>•</div> </div> </div>
1	B	314	<div> <div>8%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>5%</div> <div>•</div> </div> </div>

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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

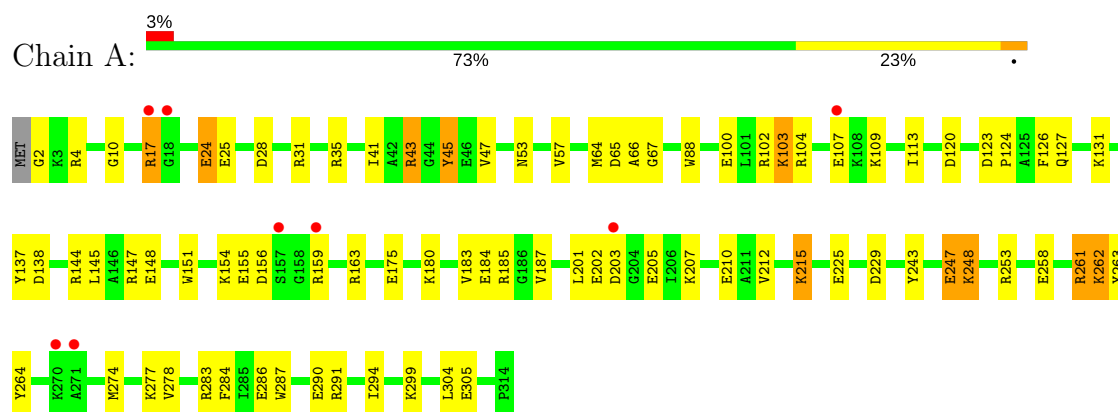
- Molecule 4 is water.

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

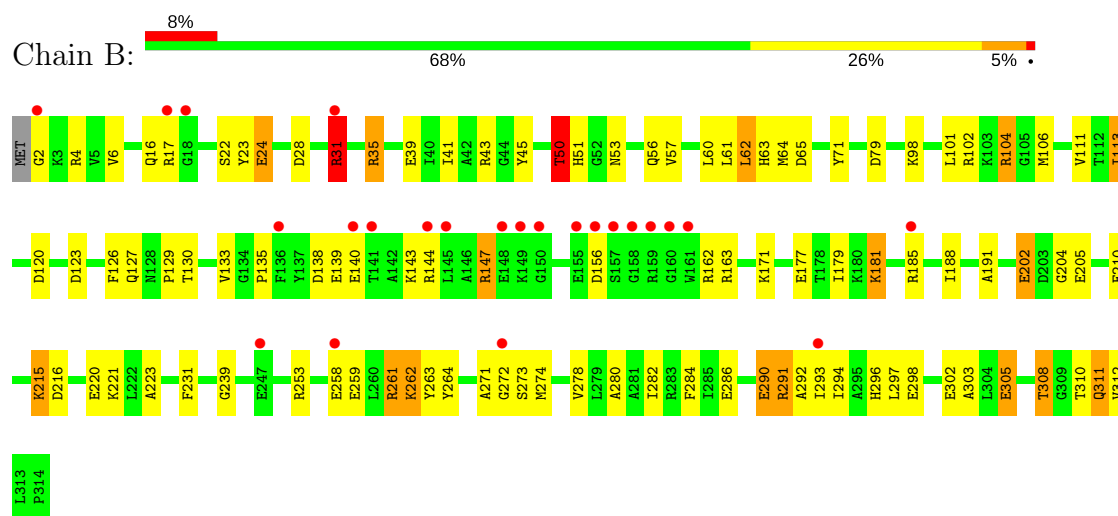
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 19.34 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-1.50) 98.3 (19.34-1.50)	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 (6.43%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.3	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

5.1 Standard geometry

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	1.27	3/2580 (0.1%)	1.97	65/3474 (1.9%)
1	B	1.31	5/2588 (0.2%)	2.25	104/3484 (3.0%)
All	All	1.29	8/5168 (0.2%)	2.12	169/6958 (2.4%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLU	CD-OE1	8.42	1.34	1.25
1	B	272	GLY	N-CA	7.49	1.57	1.46
1	A	210	GLU	CD-OE2	-6.88	1.18	1.25
1	B	210	GLU	CD-OE1	6.33	1.32	1.25
1	A	151	TRP	C-O	5.58	1.33	1.23
1	B	39	GLU	CD-OE1	-5.40	1.19	1.25
1	B	98	LYS	C-O	5.39	1.33	1.23
1	B	293	ILE	C-O	5.09	1.33	1.23

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ARG	NE-CZ-NH1	-25.08	107.76	120.30
1	A	102	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	B	31	ARG	NE-CZ-NH2	19.21	129.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	NE-CZ-NH1	17.16	128.88	120.30
1	B	4	ARG	NE-CZ-NH1	14.90	127.75	120.30
1	B	35	ARG	NE-CZ-NH1	14.48	127.54	120.30
1	A	43	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	B	291	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	B	39	GLU	OE1-CD-OE2	13.31	139.27	123.30
1	B	147	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	A	291	ARG	NE-CZ-NH2	-12.87	113.86	120.30
1	B	120	ASP	CB-CG-OD2	-12.83	106.75	118.30
1	B	35	ARG	CD-NE-CZ	12.60	141.24	123.60
1	B	35	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	A	123	ASP	CB-CG-OD1	11.99	129.09	118.30
1	B	163	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	B	23	TYR	CB-CG-CD1	11.88	128.13	121.00
1	A	147	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	B	23	TYR	CG-CD1-CE1	10.99	130.09	121.30
1	B	185	ARG	CD-NE-CZ	10.85	138.79	123.60
1	A	185	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	B	23	TYR	CD1-CE1-CZ	-10.47	110.37	119.80
1	B	104	ARG	NE-CZ-NH2	-10.33	115.14	120.30
1	B	147	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	A	65	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	A	156	ASP	CB-CG-OD1	10.04	127.34	118.30
1	A	4	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	104	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	B	202	GLU	OE1-CD-OE2	9.25	134.41	123.30
1	B	23	TYR	CB-CG-CD2	-9.19	115.49	121.00
1	B	43	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	B	50[A]	THR	N-CA-CB	9.12	127.62	110.30
1	B	50[B]	THR	N-CA-CB	9.12	127.62	110.30
1	B	185	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	A	159	ARG	CD-NE-CZ	9.06	136.29	123.60
1	A	43	ARG	NH1-CZ-NH2	9.04	129.34	119.40
1	B	65	ASP	CB-CG-OD2	-8.78	110.39	118.30
1	B	4	ARG	NH1-CZ-NH2	-8.55	110.00	119.40
1	A	147	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	163	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	4	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	B	271	ALA	C-N-CA	-8.21	105.07	122.30
1	B	120	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	65	ASP	OD1-CG-OD2	8.19	138.86	123.30
1	B	282	ILE	O-C-N	-8.05	109.82	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ALA	CA-C-O	7.98	136.85	120.10
1	A	144	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	262	LYS	CA-CB-CG	7.77	130.48	113.40
1	B	261	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	B	138	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	65	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	A	24	GLU	OE1-CD-OE2	-7.68	114.08	123.30
1	A	31	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	181	LYS	CA-CB-CG	7.46	129.81	113.40
1	B	220	GLU	OE1-CD-OE2	-7.41	114.41	123.30
1	B	23	TYR	CG-CD2-CE2	-7.36	115.41	121.30
1	B	147	ARG	CD-NE-CZ	7.33	133.86	123.60
1	A	66	ALA	O-C-N	-7.29	110.81	123.20
1	B	253	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	163	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	22	SER	CA-C-O	6.99	134.77	120.10
1	B	39	GLU	CG-CD-OE2	-6.97	104.36	118.30
1	B	253	ARG	O-C-N	-6.93	111.61	122.70
1	A	229	ASP	CB-CG-OD2	6.85	124.46	118.30
1	B	79	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	283	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	137	TYR	CB-CG-CD1	6.78	125.07	121.00
1	B	130	THR	CA-CB-CG2	-6.75	102.95	112.40
1	B	65	ASP	OD1-CG-OD2	6.71	136.04	123.30
1	A	25	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	B	308	THR	CA-CB-OG1	6.69	123.04	109.00
1	B	202	GLU	CG-CD-OE2	-6.68	104.94	118.30
1	B	31	ARG	CD-NE-CZ	-6.65	114.29	123.60
1	A	263	TYR	CB-CG-CD1	6.64	124.98	121.00
1	B	185	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	253	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	310	THR	O-C-N	-6.54	112.24	122.70
1	A	291	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	64	MET	O-C-N	6.46	133.04	122.70
1	A	159	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	50[A]	THR	CB-CA-C	-6.38	94.37	111.60
1	B	50[B]	THR	CB-CA-C	-6.38	94.37	111.60
1	A	243	TYR	CB-CG-CD2	6.38	124.83	121.00
1	B	129	PRO	O-C-N	6.35	132.86	122.70
1	B	204	GLY	O-C-N	6.28	132.75	122.70
1	B	22	SER	O-C-N	-6.22	112.75	122.70
1	B	17	ARG	NE-CZ-NH2	-6.18	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	43	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	B	282	ILE	CA-C-O	6.03	132.76	120.10
1	B	23	TYR	CZ-CE2-CD2	6.02	125.22	119.80
1	B	303	ALA	O-C-N	-6.01	113.09	122.70
1	B	62	LEU	O-C-N	-6.00	113.10	122.70
1	B	231	PHE	CB-CG-CD1	5.94	124.96	120.80
1	A	24	GLU	CG-CD-OE1	5.91	130.12	118.30
1	B	308	THR	O-C-N	5.91	133.24	123.20
1	B	140	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	B	126	PHE	O-C-N	5.89	132.12	122.70
1	A	126	PHE	CB-CG-CD1	-5.88	116.68	120.80
1	A	261	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	293	ILE	CA-C-N	5.87	130.11	117.20
1	A	124	PRO	O-C-N	-5.86	113.33	122.70
1	A	127	GLN	O-C-N	-5.81	113.40	122.70
1	A	156	ASP	OD1-CG-OD2	-5.81	112.26	123.30
1	B	61	LEU	O-C-N	5.79	131.97	122.70
1	B	2	GLY	O-C-N	5.79	131.96	122.70
1	B	264	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	138	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	162	ARG	CD-NE-CZ	-5.71	115.60	123.60
1	B	61	LEU	CA-C-O	-5.69	108.15	120.10
1	A	248	LYS	CA-CB-CG	5.69	125.91	113.40
1	A	103	LYS	CB-CG-CD	-5.65	96.91	111.60
1	A	17	ARG	CD-NE-CZ	5.64	131.49	123.60
1	B	290	GLU	OE1-CD-OE2	5.62	130.04	123.30
1	B	284	PHE	O-C-N	5.61	131.68	122.70
1	B	290	GLU	O-C-N	-5.61	113.73	122.70
1	B	291	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	312	VAL	CA-C-O	5.58	131.82	120.10
1	A	145	LEU	O-C-N	-5.57	113.79	122.70
1	A	264	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	A	287	TRP	CH2-CZ2-CE2	5.54	122.94	117.40
1	B	253	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	162	ARG	CB-CA-C	-5.50	99.41	110.40
1	A	4	ARG	CD-NE-CZ	-5.49	115.92	123.60
1	A	263	TYR	CZ-CE2-CD2	-5.47	114.88	119.80
1	A	299	LYS	O-C-N	-5.44	113.99	122.70
1	B	127	GLN	OE1-CD-NE2	5.44	134.41	121.90
1	B	133	VAL	CB-CA-C	-5.43	101.08	111.40
1	B	138	ASP	OD1-CG-OD2	-5.43	112.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	CA-C-N	5.43	129.14	117.20
1	A	155	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	B	280	ALA	O-C-N	5.42	131.37	122.70
1	B	31	ARG	CG-CD-NE	5.41	123.16	111.80
1	B	292	ALA	O-C-N	-5.41	114.05	122.70
1	B	298	GLU	O-C-N	-5.40	114.06	122.70
1	B	123	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	311	GLN	OE1-CD-NE2	5.37	134.24	121.90
1	B	28	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	163	ARG	CD-NE-CZ	-5.31	116.16	123.60
1	B	24[A]	GLU	CG-CD-OE1	5.30	128.90	118.30
1	B	24[B]	GLU	CG-CD-OE1	5.30	128.90	118.30
1	A	175	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	290	GLU	OE1-CD-OE2	5.28	129.64	123.30
1	A	45	TYR	CG-CD1-CE1	-5.28	117.08	121.30
1	B	65	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	60	LEU	O-C-N	5.26	131.12	122.70
1	B	297	LEU	O-C-N	5.26	131.12	122.70
1	B	62	LEU	CA-C-O	5.26	131.15	120.10
1	A	120	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	25	GLU	CG-CD-OE1	5.22	128.74	118.30
1	B	305	GLU	CB-CG-CD	5.19	128.22	114.20
1	B	71	TYR	CB-CG-CD2	5.18	124.11	121.00
1	B	45	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	B	263	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	B	264	TYR	O-C-N	5.12	130.90	122.70
1	A	284	PHE	O-C-N	5.11	130.88	122.70
1	A	287	TRP	CD2-CE2-CZ2	-5.11	116.17	122.30
1	B	156	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	43	ARG	CG-CD-NE	-5.10	101.10	111.80
1	B	102	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	263	TYR	CG-CD1-CE1	-5.07	117.24	121.30
1	A	2	GLY	O-C-N	5.05	130.79	122.70
1	A	28	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	A	35	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	304	LEU	O-C-N	5.04	130.77	122.70
1	B	57[A]	VAL	C-N-CA	-5.04	111.73	122.30
1	B	57[B]	VAL	C-N-CA	-5.04	111.73	122.30
1	A	148	GLU	CA-CB-CG	-5.02	102.36	113.40
1	A	88	TRP	CD1-CG-CD2	5.01	110.31	106.30

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	45	2
1	B	2483	0	2526	52	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	6	2
All	All	5734	0	5067	92	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 (92) 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
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:HB2	1:B:106: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: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:B:104:ARG:HB2	1:B:106:MET:CE	2.16	0.75
1:B:274[B]:MET:CE	1:B:294:ILE:HD13	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50[A]:THR:CG2	1:B:191:ALA:O	2.35	0.74
1:A:274[B]:MET:HE1	1:A:277:LYS:HB2	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:A:100[B]:GLU:CD	4:A:2141:HOH:O	2.28	0.71
1:B:274[B]:MET:HE3	1:B:294:ILE:HD13	1.75	0.69
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:B:104:ARG:CB	1:B:106:MET:HE2	2.26	0.65
1:B:274[B]:MET:HE2	1:B:278:VAL:HG23	1.78	0.64
1:B:302[B]:GLU:HG2	1:B:308:THR:CG2	2.28	0.63
1:B:50[B]:THR:HG22	1:B:51:HIS:N	2.13	0.62
1:A:100[B]:GLU:CG	4:A:2141:HOH:O	2.47	0.62
1:B:104:ARG:CB	1:B:106:MET:CE	2.78	0.62
1:A:274[B]:MET:HE2	1:A:278:VAL:HG23	1.80	0.61
1:A:305[A]:GLU:CD	4:A:2370:HOH:O	2.38	0.60
1:A:274[B]:MET:HE1	1:A:277:LYS:CB	2.32	0.59
1:A:183:VAL:HG22	4:A:2077:HOH:O	2.00	0.59
1:B:31:ARG:NE	4:B:2048:HOH:O	2.35	0.58
1:A:274[B]:MET:HE1	1:A:294:ILE:HD13	1.84	0.58
1:A:100[B]:GLU:HG3	4:A:2141:HOH:O	2.02	0.58
1:A:274[B]:MET:CE	1:A:294:ILE:HD13	2.33	0.57
1:A:53:ASN:O	1:A:57[B]:VAL:HG22	2.05	0.57
1:A:274[B]:MET:CE	1:A:278:VAL:HG23	2.35	0.57
1:A:261:ARG:HD3	1:A:286:GLU:OE2	2.05	0.56
1:A:274[B]:MET:HE3	1:A:277:LYS:HB2	1.89	0.54
1:A:43:ARG:NH1	1:A:305[B]:GLU:CD	2.60	0.54
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:215[B]:LYS:HE2	1:B:216:ASP:CG	2.30	0.52
1:B:139:GLU:O	1:B:143:LYS:HG3	2.09	0.52
1:B:31:ARG:HD2	1:B:35:ARG:HH22	1.73	0.52
1:A:64:MET:HA	1:B:63:HIS:CD2	2.45	0.52
1:A:41[B]:ILE:HD11	1:A:47:VAL:HB	1.93	0.50
1:B:101:LEU:HD23	1:B:106:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:TYR:OH	1:A:305[A]:GLU:OE2	2.27	0.48
1:B:31:ARG:HD2	1:B:35:ARG:NH2	2.30	0.47
1:A:43:ARG:HH12	1:A:305[B]:GLU:CD	2.18	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:41[B]:ILE:HD13	1:B:188:ILE:CD1	2.45	0.46
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:259:GLU:OE1	1:B:262[B]:LYS:NZ	2.50	0.44
1:B:50[B]:THR:HG21	4:B:2215:HOH:O	2.17	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:274[B]:MET:HE1	1:B:294:ILE:HD13	1.99	0.42
1:A:205:GLU:CD	1:A:207:LYS:HE2	2.40	0.42
1:B:113[A]:ILE:HG21	1:B:179:ILE:HG12	2.02	0.42
1:B:259:GLU:CD	1:B:262[B]:LYS:NZ	2.73	0.41
1:B:171:LYS:HE2	4:B:2149:HOH:O	2.19	0.41
1:A:103:LYS:HE3	1:B:205:GLU:HG2	2.01	0.41
1:A:10:GLY:HA2	1:A:215[B]:LYS:NZ	2.36	0.41
1:B:31:ARG:HH11	1:B:31:ARG:CG	2.23	0.41
1:A:100[B]:GLU:HG2	4:A:2143:HOH:O	2.21	0.41
1:A:24:GLU:H	1:A:24:GLU:CD	2.23	0.40
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 [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	326/314 (104%)	319 (98%)	7 (2%)	0	100	100
1	B	327/314 (104%)	320 (98%)	6 (2%)	1 (0%)	44	19
All	All	653/628 (104%)	639 (98%)	13 (2%)	1 (0%)	51	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	SER

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	262/248 (106%)	255 (97%)	7 (3%)	50	17
1	B	263/248 (106%)	253 (96%)	10 (4%)	38	9
All	All	525/496 (106%)	508 (97%)	17 (3%)	57	12

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	215[A]	LYS
1	A	215[B]	LYS
1	A	247[A]	GLU
1	A	247[B]	GLU

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Mol	Chain	Res	Type
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	215[A]	LYS
1	B	215[B]	LYS
1	B	262[A]	LYS
1	B	262[B]	LYS
1	B	305	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	B	56	GLN
1	B	63	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	25,29,29	1.29	3 (12%)	24,45,45	2.41	5 (20%)
2	ADP	B	315	3	25,29,29	1.29	2 (8%)	24,45,45	2.32	4 (16%)

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	-	0/12/32/32	0/3/3/3
2	ADP	B	315	3	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	ADP	PA-O2A	-2.21	1.44	1.55
2	A	315	ADP	C2'-C1'	-2.09	1.50	1.53
2	A	315	ADP	O2'-C2'	2.52	1.48	1.43
2	A	315	ADP	C2-N1	2.64	1.38	1.33
2	B	315	ADP	C2-N1	3.50	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	315	ADP	C4'-O4'-C1'	-9.10	100.08	109.77
2	A	315	ADP	C4'-O4'-C1'	-8.92	100.28	109.77
2	A	315	ADP	N6-C6-N1	-3.55	111.72	118.77
2	B	315	ADP	O4'-C4'-C3'	-2.21	100.76	105.17
2	A	315	ADP	O3B-PB-O2B	2.04	115.86	107.61
2	A	315	ADP	C1'-N9-C4	2.32	130.65	126.64
2	B	315	ADP	C5-C6-N6	2.71	125.99	120.47
2	B	315	ADP	C4-C5-N7	3.21	112.51	109.41
2	A	315	ADP	C5-C6-N6	5.17	131.00	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.18	8 (2%) 56 62	15, 22, 38, 48	0
1	B	313/314 (99%)	0.35	24 (7%) 14 16	16, 24, 39, 54	0
All	All	626/628 (99%)	0.27	32 (5%) 29 32	15, 23, 38, 54	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	GLY	6.9
1	B	157	SER	6.6
1	B	159	ARG	5.2
1	B	161	TRP	5.0
1	B	160	GLY	4.9
1	B	17	ARG	4.8
1	A	17	ARG	4.5
1	A	18	GLY	4.2
1	B	136	PHE	3.8
1	A	203	ASP	3.6
1	B	247[A]	GLU	3.5
1	A	159	ARG	3.4
1	B	156	ASP	3.4
1	B	155	GLU	3.2
1	A	107	GLU	3.0
1	B	148	GLU	3.0
1	B	18	GLY	3.0
1	B	145	LEU	2.9
1	B	140	GLU	2.8
1	A	157	SER	2.8
1	B	293	ILE	2.7
1	B	272	GLY	2.7
1	B	149	LYS	2.7
1	A	271	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	150	GLY	2.5
1	B	144	ARG	2.4
1	B	185	ARG	2.4
1	B	141	THR	2.3
1	A	270	LYS	2.3
1	B	258	GLU	2.1
1	B	2	GLY	2.0
1	B	31	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	A	315	27/27	0.96	0.07	-0.77	20,22,24,30	0
2	ADP	B	315	27/27	0.96	0.07	-0.86	22,23,26,27	0
3	MG	B	316	1/1	0.98	0.10	-	27,27,27,27	0
3	MG	A	316	1/1	0.99	0.12	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.