



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:43 AM UTC

PDB ID : 3A74 / pdb_00003a74
Title : Lysyl-tRNA synthetase from *Bacillus stearothermophilus* complexed with Diadenosine Tetraphosphate (AP4A)
Authors : Sakurama, H.; Takita, T.; Mikami, B.; Itoh, T.; Yasukawa, K.; Inouye, K.
Deposited on : 2009-09-13
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

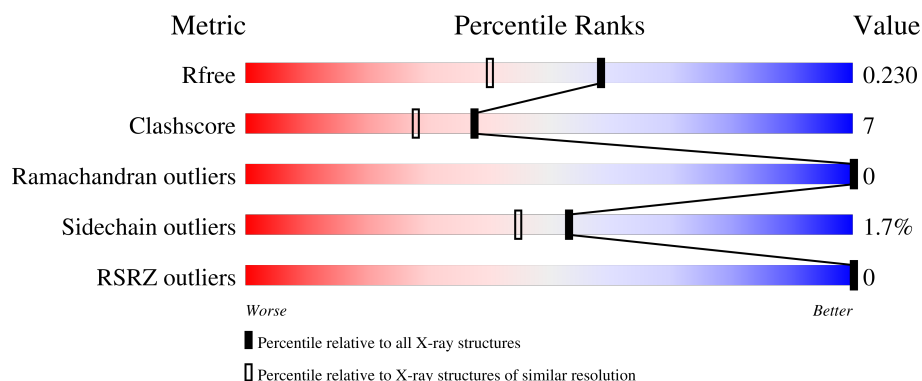
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	493	
1	B	493	
1	C	493	
1	D	493	

2 Entry composition [i](#)

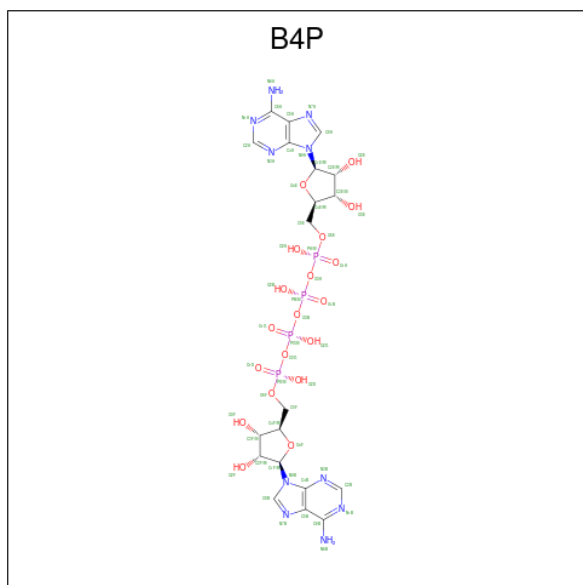
There are 5 unique types of molecules in this entry. The entry contains 16936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	1	0
			3965	2514	691	742	18			
1	B	484	Total	C	N	O	S	0	1	0
			3965	2514	691	742	18			
1	C	484	Total	C	N	O	S	0	1	0
			3965	2514	691	742	18			
1	D	484	Total	C	N	O	S	0	1	0
			3965	2514	691	742	18			

- Molecule 2 is BIS(ADENOSINE)-5'-TETRAPHOSPHATE (CCD ID: B4P) (formula: $C_{20}H_{28}N_{10}O_{19}P_4$).



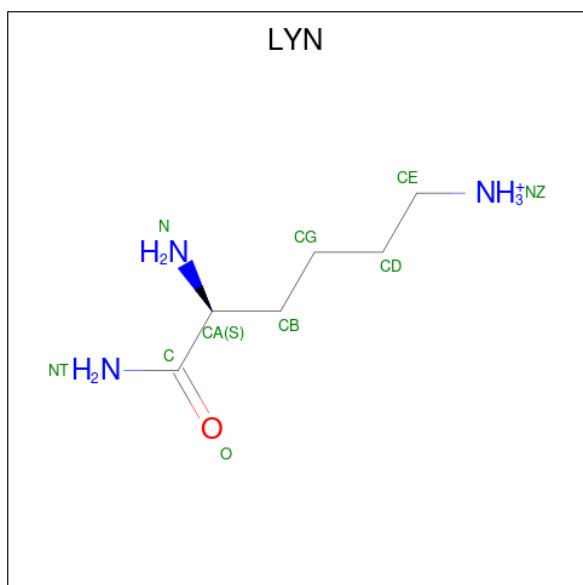
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
2	B	1	Total	C	N	O	P	0	0
			53	20	10	19	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
2	D	1	Total	C	N	O	P	0	0
			53	20	10	19	4		

- Molecule 3 is 2,6-DIAMINO-HEXANOIC ACID AMIDE (CCD ID: LYN) (formula: C₆H₁₆N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	3	1		
3	B	1	Total	C	N	O	0	0
			10	6	3	1		
3	C	1	Total	C	N	O	0	0
			10	6	3	1		
3	D	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Mg 3	0	0

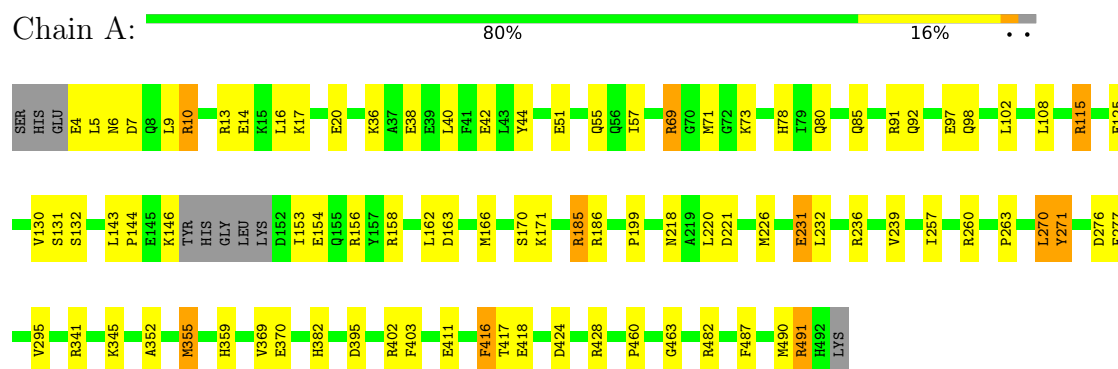
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total 216	O 216	0	0
5	B	195	Total 195	O 195	0	0
5	C	214	Total 214	O 214	0	0
5	D	187	Total 187	O 187	0	0

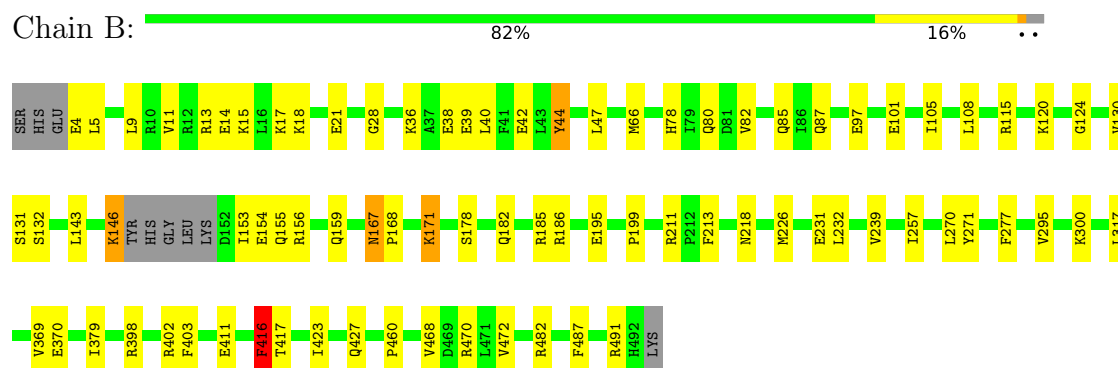
3 Residue-property plots [i](#)

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.

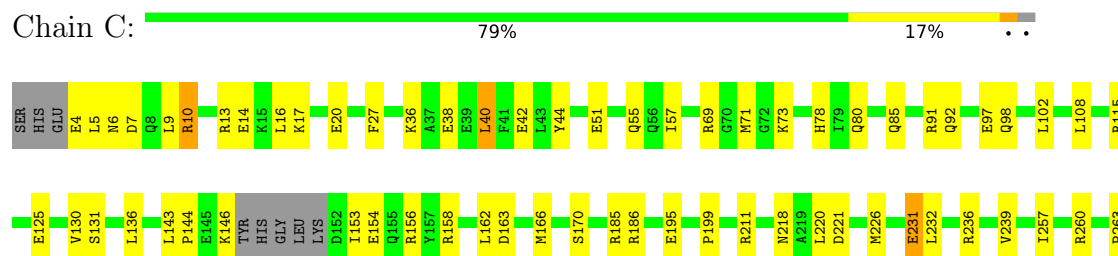
• Molecule 1: Lysyl-tRNA synthetase



• Molecule 1: Lysyl-tRNA synthetase

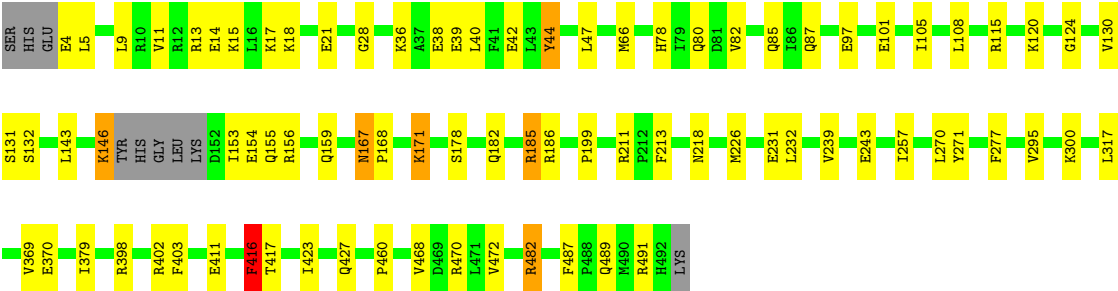
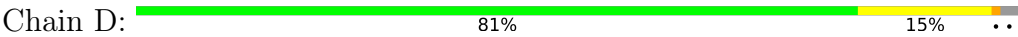


• Molecule 1: Lysyl-tRNA synthetase





● Molecule 1: Lysyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.18Å 85.08Å 151.76Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	14.96 – 1.80 14.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (14.96-1.80) 98.1 (14.96-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.228 0.208 , 0.230	Depositor DCC
R_{free} test set	21886 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 19.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16936	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: LYN, B4P, MG

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	0.36	0/4044	1.06	44/5445 (0.8%)
1	B	0.34	0/4044	1.00	35/5445 (0.6%)
1	C	0.36	0/4044	1.02	43/5445 (0.8%)
1	D	0.35	0/4044	0.99	35/5445 (0.6%)
All	All	0.36	0/16176	1.02	157/21780 (0.7%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH2	10.60	128.74	119.20
1	B	369	VAL	N-CA-C	10.42	119.85	111.62
1	A	185	ARG	NE-CZ-NH1	-10.13	111.37	121.50
1	C	417	THR	N-CA-C	-9.72	93.61	108.67
1	A	417	THR	N-CA-C	-9.71	93.62	108.67
1	D	482	ARG	NE-CZ-NH2	9.69	127.92	119.20
1	D	482	ARG	NE-CZ-NH1	-9.54	111.96	121.50
1	A	69	ARG	NE-CZ-NH2	9.22	127.50	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	GLU	N-CA-C	9.21	122.25	111.02
1	B	417	THR	N-CA-C	-9.20	95.17	109.25
1	D	417	THR	N-CA-C	-9.17	95.21	109.25
1	C	231	GLU	N-CA-C	9.06	122.07	111.02
1	B	211	ARG	NE-CZ-NH2	8.96	127.27	119.20
1	C	369	VAL	N-CA-C	8.91	118.66	111.62
1	B	186	ARG	NE-CZ-NH2	8.84	127.15	119.20
1	A	369	VAL	N-CA-C	8.81	118.58	111.62
1	B	231	GLU	N-CA-C	8.79	121.75	111.02
1	D	185	ARG	NE-CZ-NH2	-8.72	111.35	119.20
1	C	115	ARG	NE-CZ-NH2	8.62	126.96	119.20
1	A	69	ARG	NE-CZ-NH1	-8.52	112.98	121.50
1	A	10	ARG	NE-CZ-NH2	8.39	126.75	119.20
1	D	13	ARG	NE-CZ-NH2	8.37	126.73	119.20
1	A	186	ARG	NE-CZ-NH2	8.34	126.71	119.20
1	B	186	ARG	NE-CZ-NH1	-8.32	113.18	121.50
1	B	211	ARG	NE-CZ-NH1	-8.24	113.26	121.50
1	C	491	ARG	NE-CZ-NH2	8.22	126.59	119.20
1	C	115	ARG	NE-CZ-NH1	-8.12	113.38	121.50
1	A	91	ARG	NE-CZ-NH2	8.02	126.41	119.20
1	C	236	ARG	NE-CZ-NH2	8.00	126.40	119.20
1	C	491	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	A	10	ARG	NE-CZ-NH1	-7.87	113.63	121.50
1	A	186	ARG	NE-CZ-NH1	-7.82	113.68	121.50
1	A	236	ARG	NE-CZ-NH2	-7.81	112.17	119.20
1	D	13	ARG	NE-CZ-NH1	-7.76	113.74	121.50
1	D	185	ARG	CD-NE-CZ	7.75	135.26	124.40
1	B	185	ARG	NE-CZ-NH2	7.69	126.12	119.20
1	C	236	ARG	NE-CZ-NH1	-7.64	113.86	121.50
1	A	185	ARG	CD-NE-CZ	7.56	134.98	124.40
1	A	91	ARG	NE-CZ-NH1	-7.53	113.97	121.50
1	A	236	ARG	CD-NE-CZ	7.50	134.90	124.40
1	A	482	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	A	491	ARG	NE-CZ-NH2	-7.37	112.57	119.20
1	B	185	ARG	NE-CZ-NH1	-7.36	114.14	121.50
1	D	185	ARG	NE-CZ-NH1	7.29	128.79	121.50
1	D	482	ARG	CD-NE-CZ	7.20	134.48	124.40
1	D	186	ARG	NE-CZ-NH2	-7.11	112.80	119.20
1	B	239	VAL	N-CA-C	-7.08	103.57	110.72
1	D	239	VAL	N-CA-C	-7.04	103.61	110.72
1	A	491	ARG	CD-NE-CZ	6.89	134.04	124.40
1	A	69	ARG	CD-NE-CZ	6.83	133.96	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	B	370	GLU	N-CA-C	6.77	119.53	111.33
1	D	370	GLU	N-CA-C	6.77	119.52	111.33
1	A	236	ARG	NE-CZ-NH1	6.76	128.26	121.50
1	A	115	ARG	CD-NE-CZ	6.76	133.86	124.40
1	B	482	ARG	CD-NE-CZ	6.69	133.77	124.40
1	D	211	ARG	NE-CZ-NH2	-6.67	113.19	119.20
1	D	186	ARG	CD-NE-CZ	6.65	133.71	124.40
1	B	186	ARG	CD-NE-CZ	6.62	133.67	124.40
1	B	211	ARG	CD-NE-CZ	6.59	133.63	124.40
1	A	115	ARG	NE-CZ-NH2	-6.53	113.33	119.20
1	B	482	ARG	NE-CZ-NH2	-6.42	113.43	119.20
1	D	231	GLU	N-CA-C	6.41	121.88	111.37
1	C	186	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	B	13	ARG	CD-NE-CZ	6.29	133.21	124.40
1	A	491	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	C	130	VAL	N-CA-C	6.26	117.13	109.30
1	C	108	LEU	N-CA-C	-6.26	101.15	110.23
1	C	115	ARG	CD-NE-CZ	6.23	133.12	124.40
1	A	370	GLU	N-CA-C	6.22	119.71	111.75
1	B	13	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	C	370	GLU	N-CA-C	6.20	119.68	111.75
1	D	13	ARG	CD-NE-CZ	6.19	133.07	124.40
1	C	91	ARG	CD-NE-CZ	6.17	133.03	124.40
1	A	10	ARG	CD-NE-CZ	6.16	133.02	124.40
1	A	186	ARG	CD-NE-CZ	6.15	133.01	124.40
1	B	218	ASN	N-CA-C	6.15	117.78	111.14
1	C	69	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	D	211	ARG	CD-NE-CZ	6.15	133.01	124.40
1	C	91	ARG	NE-CZ-NH2	-6.14	113.68	119.20
1	C	69	ARG	CD-NE-CZ	6.13	132.98	124.40
1	D	218	ASN	N-CA-C	6.12	117.75	111.14
1	A	108	LEU	N-CA-C	-6.11	101.37	110.23
1	A	130	VAL	N-CA-C	6.07	116.89	109.30
1	B	108	LEU	N-CA-C	-6.05	101.46	110.23
1	C	185	ARG	NE-CZ-NH2	-6.04	113.76	119.20
1	C	491	ARG	CD-NE-CZ	6.04	132.86	124.40
1	D	108	LEU	N-CA-C	-6.04	101.47	110.23
1	B	167	ASN	CA-C-N	6.00	125.68	119.56
1	B	167	ASN	C-N-CA	6.00	125.68	119.56
1	C	186	ARG	CD-NE-CZ	6.00	132.79	124.40
1	C	10	ARG	NE-CZ-NH2	-5.99	113.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	ARG	CD-NE-CZ	5.97	132.76	124.40
1	C	482	ARG	NE-CZ-NH2	-5.96	113.83	119.20
1	D	186	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	D	130	VAL	N-CA-C	5.90	117.33	109.37
1	D	167	ASN	CA-C-N	5.89	125.57	119.56
1	D	167	ASN	C-N-CA	5.89	125.57	119.56
1	A	218	ASN	N-CA-C	5.84	117.33	110.97
1	C	10	ARG	CD-NE-CZ	5.83	132.56	124.40
1	C	218	ASN	N-CA-C	5.83	117.32	110.97
1	A	115	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	B	130	VAL	N-CA-C	5.80	117.21	109.37
1	A	232	LEU	N-CA-C	5.77	117.57	111.28
1	C	232	LEU	N-CA-C	5.74	117.54	111.28
1	A	91	ARG	CD-NE-CZ	5.70	132.38	124.40
1	C	185	ARG	CD-NE-CZ	5.64	132.29	124.40
1	C	352	ALA	CA-C-N	5.58	125.69	119.32
1	C	352	ALA	C-N-CA	5.58	125.69	119.32
1	D	211	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	A	352	ALA	CA-C-N	5.58	125.68	119.32
1	A	352	ALA	C-N-CA	5.58	125.68	119.32
1	B	398	ARG	N-CA-C	-5.58	105.74	112.54
1	B	369	VAL	CB-CA-C	-5.54	106.12	111.05
1	D	398	ARG	N-CA-C	-5.54	105.79	112.54
1	B	185	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	482	ARG	NE-CZ-NH1	5.45	126.95	121.50
1	C	482	ARG	CD-NE-CZ	5.43	132.01	124.40
1	A	355	MET	N-CA-C	5.42	118.31	110.28
1	B	13	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	C	355	MET	N-CA-C	5.42	118.30	110.28
1	C	482	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	B	213	PHE	N-CA-C	-5.36	100.95	109.96
1	C	295	VAL	N-CA-C	5.35	116.83	111.00
1	A	295	VAL	N-CA-C	5.34	116.82	111.00
1	C	186	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	B	131	SER	N-CA-C	-5.33	107.14	113.97
1	B	97	GLU	N-CA-C	5.33	116.78	111.07
1	C	36	LYS	N-CA-C	-5.32	101.49	109.95
1	A	170	SER	N-CA-C	5.32	117.76	111.33
1	D	213	PHE	N-CA-C	-5.32	101.03	109.96
1	A	239	VAL	N-CA-C	-5.31	105.20	110.62
1	C	170	SER	N-CA-C	5.29	117.73	111.33
1	C	460	PRO	N-CA-C	-5.29	102.89	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	PRO	N-CA-C	-5.27	102.92	111.14
1	A	36	LYS	N-CA-C	-5.26	101.59	109.95
1	D	131	SER	N-CA-C	-5.25	107.25	113.97
1	B	295	VAL	N-CA-C	5.24	116.71	111.00
1	D	295	VAL	N-CA-C	5.23	116.70	111.00
1	C	239	VAL	N-CA-C	-5.23	105.29	110.62
1	A	131	SER	N-CA-C	-5.22	107.57	114.31
1	D	28	GLY	N-CA-C	5.22	125.55	113.18
1	D	97	GLU	N-CA-C	5.22	116.65	111.07
1	B	28	GLY	N-CA-C	5.21	125.52	113.18
1	C	91	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	D	232	LEU	N-CA-C	5.15	116.89	111.28
1	B	416	PHE	N-CA-C	5.13	116.09	108.60
1	B	460	PRO	N-CA-C	-5.13	103.13	111.14
1	C	131	SER	N-CA-C	-5.11	107.71	114.31
1	D	460	PRO	N-CA-C	-5.09	103.20	111.14
1	D	416	PHE	N-CA-C	5.08	116.01	108.60
1	C	10	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	C	69	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	D	369	VAL	N-CA-C	5.02	119.79	109.34
1	D	243	GLU	N-CA-C	5.02	121.49	110.80
1	A	482	ARG	CD-NE-CZ	5.01	131.42	124.40
1	B	232	LEU	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	TYR	Sidechain
1	B	271	TYR	Sidechain
1	C	271	TYR	Sidechain
1	D	271	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3965	0	3926	59	0
1	B	3965	0	3926	54	0
1	C	3965	0	3926	63	0
1	D	3965	0	3926	53	0
2	A	53	0	24	1	0
2	B	53	0	24	2	0
2	C	53	0	24	2	0
2	D	53	0	24	1	0
3	A	10	0	16	0	0
3	B	10	0	16	0	0
3	C	10	0	16	0	0
3	D	10	0	16	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	216	0	0	3	0
5	B	195	0	0	1	0
5	C	214	0	0	5	0
5	D	187	0	0	0	0
All	All	16936	0	15864	225	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (225) 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:D:44:TYR:HB3	1:D:47:LEU:HD22	1.55	0.86
1:B:44:TYR:HB3	1:B:47:LEU:HD22	1.56	0.85
1:B:257:ILE:HD11	1:B:491:ARG:HH21	1.43	0.83
1:D:411[B]:GLU:CD	1:D:411[B]:GLU:H	1.86	0.83
1:A:143:LEU:HD12	1:A:143:LEU:H	1.43	0.83
1:D:257:ILE:HD11	1:D:491:ARG:HH21	1.44	0.83
1:C:143:LEU:HD12	1:C:143:LEU:H	1.44	0.83
1:A:6:ASN:H	1:A:9:LEU:HD12	1.51	0.76
1:C:6:ASN:H	1:C:9:LEU:HD12	1.52	0.75
1:B:155:GLN:NE2	1:B:159:GLN:HE21	1.86	0.72
1:D:155:GLN:NE2	1:D:159:GLN:HE21	1.87	0.72
1:A:153:ILE:HG23	1:A:156:ARG:HH22	1.55	0.70
1:C:153:ILE:HG23	1:C:156:ARG:HH22	1.55	0.70
1:D:482:ARG:NH1	1:D:489:GLN:O	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:C	1:A:7:ASP:H	1.99	0.70
1:C:5:LEU:C	1:C:7:ASP:H	1.99	0.70
1:D:155:GLN:HE21	1:D:159:GLN:HE21	1.38	0.70
1:B:155:GLN:HE21	1:B:159:GLN:HE21	1.38	0.69
1:A:10:ARG:O	1:A:14:GLU:HG3	1.93	0.69
1:C:10:ARG:O	1:C:14:GLU:HG3	1.93	0.69
1:A:411[B]:GLU:CD	1:A:411[B]:GLU:H	2.02	0.67
1:A:78:HIS:HE1	1:A:125:GLU:OE1	1.79	0.66
1:C:78:HIS:HE1	1:C:125:GLU:OE1	1.79	0.66
1:D:4:GLU:HG2	1:D:5:LEU:H	1.59	0.66
1:B:4:GLU:HG2	1:B:5:LEU:H	1.59	0.66
1:C:144:PRO:HG2	1:C:162:LEU:HD13	1.77	0.66
1:A:144:PRO:HG2	1:A:162:LEU:HD13	1.77	0.65
1:D:146:LYS:C	1:D:146:LYS:HE3	2.23	0.64
1:B:146:LYS:C	1:B:146:LYS:HE3	2.23	0.64
1:B:257:ILE:CD1	1:B:491:ARG:HE	2.11	0.63
1:D:257:ILE:CD1	1:D:491:ARG:HE	2.11	0.63
1:B:153:ILE:HD11	5:B:1108:HOH:O	1.99	0.63
1:D:78:HIS:CE1	1:D:87:GLN:HB2	2.34	0.63
1:A:153:ILE:HG23	1:A:156:ARG:NH2	2.14	0.63
1:C:153:ILE:HG23	1:C:156:ARG:NH2	2.13	0.63
1:D:11:VAL:O	1:D:14:GLU:HG2	1.99	0.62
1:B:78:HIS:CE1	1:B:87:GLN:HB2	2.34	0.62
1:B:11:VAL:O	1:B:14:GLU:HG2	2.00	0.62
1:D:36:LYS:HB2	1:D:39:GLU:HG3	1.82	0.62
1:A:16:LEU:O	1:A:20:GLU:HG3	1.99	0.61
1:A:143:LEU:HD12	1:A:143:LEU:N	2.14	0.61
1:C:482:ARG:HD3	5:C:785:HOH:O	2.01	0.61
1:D:38:GLU:O	1:D:42:GLU:HG3	2.00	0.61
1:B:36:LYS:HB2	1:B:39:GLU:HG3	1.83	0.61
1:C:16:LEU:O	1:C:20:GLU:HG3	2.00	0.61
1:B:423:ILE:O	1:B:427:GLN:HG3	2.01	0.61
1:C:143:LEU:HD12	1:C:143:LEU:N	2.15	0.61
1:B:38:GLU:O	1:B:42:GLU:HG3	2.01	0.61
1:D:82:VAL:O	1:D:171:LYS:HE2	2.02	0.60
1:B:257:ILE:HD11	1:B:491:ARG:NH2	2.14	0.60
1:D:257:ILE:HD11	1:D:491:ARG:NH2	2.15	0.60
1:A:226:MET:HE2	1:B:226:MET:HE2	1.82	0.60
1:D:423:ILE:O	1:D:427:GLN:HG3	2.01	0.60
1:B:82:VAL:O	1:B:171:LYS:HE2	2.02	0.59
1:C:226:MET:HE2	1:D:226:MET:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PRO:O	1:B:171:LYS:HG2	2.03	0.58
1:D:168:PRO:O	1:D:171:LYS:HG2	2.03	0.58
1:C:411[B]:GLU:H	1:C:411[B]:GLU:CD	2.08	0.58
1:B:120:LYS:HB3	1:B:124:GLY:HA2	1.85	0.58
1:D:120:LYS:HB3	1:D:124:GLY:HA2	1.85	0.57
1:D:257:ILE:HD11	1:D:491:ARG:HE	1.68	0.57
1:B:18:LYS:HE3	1:B:105:ILE:HD11	1.87	0.56
1:B:257:ILE:HD11	1:B:491:ARG:HE	1.68	0.56
1:D:18:LYS:HE3	1:D:105:ILE:HD11	1.88	0.56
1:A:38:GLU:O	1:A:42:GLU:HG3	2.06	0.56
1:C:5:LEU:HD13	1:C:6:ASN:OD1	2.06	0.56
1:C:98:GLN:O	1:C:102:LEU:HD13	2.05	0.56
1:A:5:LEU:HD13	1:A:6:ASN:OD1	2.06	0.56
1:A:98:GLN:O	1:A:102:LEU:HD13	2.05	0.56
1:C:156:ARG:HG3	1:C:163:ASP:CG	2.30	0.56
1:C:38:GLU:O	1:C:42:GLU:HG3	2.06	0.55
1:A:73:LYS:HG2	5:A:1297:HOH:O	2.05	0.55
1:A:156:ARG:HG3	1:A:163:ASP:CG	2.31	0.55
1:A:80:GLN:HB2	1:A:85:GLN:HG2	1.89	0.55
1:A:270:LEU:C	1:A:270:LEU:HD12	2.32	0.55
1:C:270:LEU:HD12	1:C:270:LEU:C	2.32	0.55
1:B:411[B]:GLU:CD	1:B:411[B]:GLU:H	2.15	0.54
1:C:80:GLN:HB2	1:C:85:GLN:HG2	1.90	0.54
1:C:17:LYS:NZ	1:C:17:LYS:HB3	2.23	0.53
1:A:17:LYS:NZ	1:A:17:LYS:HB3	2.23	0.53
1:A:143:LEU:H	1:A:143:LEU:CD1	2.17	0.53
1:B:5:LEU:C	1:B:5:LEU:HD13	2.33	0.53
1:C:143:LEU:H	1:C:143:LEU:CD1	2.17	0.53
2:B:494:B4P:O3A	2:B:494:B4P:H3E	2.09	0.53
1:D:5:LEU:C	1:D:5:LEU:HD13	2.33	0.53
1:B:171:LYS:HZ2	1:B:171:LYS:HB2	1.74	0.53
1:C:44:TYR:CE2	1:C:57:ILE:HD13	2.43	0.53
1:D:44:TYR:HA	1:D:47:LEU:HD13	1.90	0.53
1:B:17:LYS:O	1:B:21:GLU:HG3	2.09	0.52
1:D:17:LYS:O	1:D:21:GLU:HG3	2.09	0.52
1:D:178:SER:O	1:D:182:GLN:HG3	2.10	0.52
1:A:44:TYR:CE2	1:A:57:ILE:HD13	2.44	0.52
1:C:257:ILE:HG22	1:C:263:PRO:HD3	1.91	0.52
1:B:44:TYR:HA	1:B:47:LEU:HD13	1.91	0.52
1:B:178:SER:O	1:B:182:GLN:HG3	2.10	0.52
1:A:6:ASN:H	1:A:9:LEU:CD1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASN:HA	1:A:9:LEU:HB2	1.91	0.52
1:C:6:ASN:HA	1:C:9:LEU:HB2	1.91	0.52
1:A:257:ILE:HG22	1:A:263:PRO:HD3	1.92	0.51
1:C:6:ASN:H	1:C:9:LEU:CD1	2.23	0.51
1:A:6:ASN:N	1:A:9:LEU:HD12	2.22	0.51
1:C:158:ARG:HD2	1:C:490:MET:CE	2.40	0.51
1:D:146:LYS:HE3	1:D:146:LYS:CA	2.41	0.51
1:A:158:ARG:HD2	1:A:490:MET:HE2	1.92	0.51
1:A:158:ARG:HD2	1:A:490:MET:CE	2.40	0.51
1:B:146:LYS:HE3	1:B:146:LYS:CA	2.41	0.51
1:C:154:GLU:OE2	1:C:490:MET:HE1	2.11	0.51
1:A:6:ASN:CA	1:A:9:LEU:HB2	2.42	0.50
1:A:154:GLU:OE2	1:A:490:MET:HE1	2.12	0.50
1:B:15:LYS:HA	1:B:18:LYS:HE3	1.93	0.50
1:C:6:ASN:CA	1:C:9:LEU:HB2	2.42	0.50
1:C:158:ARG:HD2	1:C:490:MET:HE2	1.92	0.50
1:D:15:LYS:HA	1:D:18:LYS:HE3	1.94	0.50
1:C:263:PRO:HB2	5:C:847:HOH:O	2.12	0.50
1:C:6:ASN:N	1:C:9:LEU:HD12	2.23	0.50
1:C:6:ASN:O	1:C:10:ARG:HB2	2.12	0.50
1:A:263:PRO:HB2	5:A:882:HOH:O	2.12	0.50
1:C:402:ARG:HG3	1:C:416:PHE:HD1	1.78	0.49
1:D:171:LYS:HZ2	1:D:171:LYS:HB2	1.78	0.49
1:B:153:ILE:HG23	1:B:154:GLU:N	2.26	0.49
1:A:402:ARG:HG3	1:A:416:PHE:HD1	1.78	0.49
1:B:153:ILE:HG23	1:B:154:GLU:H	1.78	0.49
1:B:403:PHE:CD1	1:B:403:PHE:C	2.90	0.49
1:C:73:LYS:HD2	1:C:92:GLN:HE22	1.78	0.48
1:A:73:LYS:HD2	1:A:92:GLN:HE22	1.78	0.48
1:D:153:ILE:HG23	1:D:154:GLU:H	1.78	0.48
1:D:153:ILE:HG23	1:D:154:GLU:N	2.27	0.48
2:D:494:B4P:O3A	2:D:494:B4P:H3E	2.13	0.48
1:D:403:PHE:CD1	1:D:403:PHE:C	2.91	0.48
1:A:6:ASN:O	1:A:10:ARG:HB2	2.14	0.48
1:D:270:LEU:C	1:D:270:LEU:HD23	2.38	0.48
1:D:402:ARG:HG3	1:D:416:PHE:HD1	1.79	0.48
1:A:185:ARG:HH12	1:B:195:GLU:CD	2.21	0.48
1:C:418:GLU:OE1	1:C:463:GLY:HA3	2.14	0.48
2:C:494:B4P:H3F	2:C:494:B4P:O3G	2.15	0.47
1:A:5:LEU:O	1:A:6:ASN:HB2	2.14	0.47
1:C:231:GLU:HG3	1:C:271:TYR:OH	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLU:OE1	1:A:463:GLY:HA3	2.14	0.47
1:B:270:LEU:C	1:B:270:LEU:HD23	2.39	0.47
1:C:5:LEU:O	1:C:6:ASN:HB2	2.14	0.47
1:C:73:LYS:HD2	1:C:92:GLN:NE2	2.29	0.47
1:A:73:LYS:HD2	1:A:92:GLN:NE2	2.30	0.47
1:A:13:ARG:O	1:A:16:LEU:HB3	2.15	0.46
1:A:146:LYS:HB2	1:A:166:MET:HE2	1.97	0.46
1:A:231:GLU:HG3	1:A:271:TYR:OH	2.14	0.46
1:B:402:ARG:HG3	1:B:416:PHE:HD1	1.80	0.46
1:A:185:ARG:NH1	1:B:195:GLU:OE1	2.46	0.46
1:C:13:ARG:O	1:C:16:LEU:HB3	2.16	0.46
1:C:51:GLU:O	1:C:55:GLN:HG3	2.16	0.46
1:C:424:ASP:O	1:C:428:ARG:HG2	2.16	0.46
1:C:195:GLU:OE1	1:D:185:ARG:NH2	2.49	0.45
1:C:146:LYS:HB2	1:C:166:MET:HE2	1.98	0.45
1:C:260:ARG:HG2	1:C:260:ARG:HH11	1.80	0.45
1:A:171:LYS:NZ	5:A:1262:HOH:O	2.33	0.45
1:A:260:ARG:HH11	1:A:260:ARG:HG2	1.81	0.45
1:A:424:ASP:O	1:A:428:ARG:HG2	2.16	0.45
1:D:66:MET:HE1	1:D:143:LEU:HD21	1.98	0.45
1:A:491:ARG:NH2	1:C:55:GLN:O	2.45	0.45
1:B:66:MET:HE1	1:B:143:LEU:HD21	1.99	0.45
1:D:47:LEU:C	1:D:120:LYS:HZ2	2.25	0.45
1:A:51:GLU:O	1:A:55:GLN:HG3	2.17	0.45
1:B:171:LYS:HB2	1:B:171:LYS:NZ	2.31	0.45
1:C:403:PHE:CD1	1:C:403:PHE:C	2.94	0.45
1:C:38:GLU:HA	1:C:38:GLU:OE2	2.17	0.45
1:B:47:LEU:C	1:B:120:LYS:HZ2	2.25	0.45
1:C:487:PHE:HB2	1:D:199:PRO:CG	2.47	0.45
1:D:80:GLN:HB2	1:D:85:GLN:HG2	1.98	0.45
1:A:38:GLU:OE2	1:A:38:GLU:HA	2.17	0.45
1:D:171:LYS:HB2	1:D:171:LYS:NZ	2.32	0.45
1:A:403:PHE:CD1	1:A:403:PHE:C	2.94	0.44
1:A:487:PHE:HB2	1:B:199:PRO:CG	2.47	0.44
1:B:80:GLN:HB2	1:B:85:GLN:HG2	1.99	0.44
1:C:491:ARG:HG3	5:C:1227:HOH:O	2.18	0.44
1:A:382:HIS:HB2	1:A:402:ARG:HD3	1.99	0.44
1:B:411[B]:GLU:HG2	1:B:470:ARG:NH2	2.33	0.43
2:C:494:B4P:O5E	2:C:494:B4P:H2E	2.18	0.43
1:D:153:ILE:HA	1:D:156:ARG:HE	1.84	0.43
1:B:468:VAL:O	1:B:472:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LYS:HA	1:B:18:LYS:CE	2.49	0.43
1:B:153:ILE:HA	1:B:156:ARG:HE	1.84	0.43
1:C:211:ARG:NH1	5:C:685:HOH:O	2.51	0.43
1:C:382:HIS:HB2	1:C:402:ARG:HD3	2.00	0.43
1:D:468:VAL:O	1:D:472:VAL:HG23	2.19	0.43
1:D:15:LYS:HA	1:D:18:LYS:CE	2.49	0.43
1:D:146:LYS:HE3	1:D:146:LYS:HA	2.00	0.42
1:B:167:ASN:HA	1:B:168:PRO:HD2	1.89	0.42
1:C:276:ASP:OD1	1:C:276:ASP:C	2.62	0.42
1:C:154:GLU:OE2	1:C:482:ARG:NH2	2.52	0.42
1:D:167:ASN:HA	1:D:168:PRO:HD2	1.89	0.42
1:A:4:GLU:HG2	1:A:5:LEU:N	2.34	0.42
1:B:4:GLU:HG2	1:B:5:LEU:N	2.29	0.42
1:B:146:LYS:HE3	1:B:146:LYS:HA	2.01	0.42
2:B:494:B4P:H2F	2:B:494:B4P:O5F	2.19	0.42
1:C:4:GLU:HG2	1:C:5:LEU:N	2.34	0.42
1:D:257:ILE:HD11	1:D:491:ARG:NE	2.33	0.42
1:A:276:ASP:C	1:A:276:ASP:OD1	2.63	0.42
1:B:257:ILE:HD11	1:B:491:ARG:NE	2.33	0.42
1:C:199:PRO:CG	1:D:487:PHE:HB2	2.50	0.42
1:D:4:GLU:HG2	1:D:5:LEU:N	2.29	0.42
1:C:355:MET:HB3	1:C:359:HIS:HB2	2.01	0.42
1:A:199:PRO:CG	1:B:487:PHE:HB2	2.50	0.42
1:C:5:LEU:C	1:C:7:ASP:N	2.67	0.42
1:C:341:ARG:O	1:C:345:LYS:HG3	2.20	0.42
1:A:5:LEU:C	1:A:7:ASP:N	2.67	0.41
1:B:317:LEU:O	1:B:379:ILE:HA	2.19	0.41
1:D:101:GLU:OE2	1:D:101:GLU:HA	2.21	0.41
1:D:317:LEU:O	1:D:379:ILE:HA	2.20	0.41
1:A:341:ARG:O	1:A:345:LYS:HG3	2.21	0.41
1:B:257:ILE:HD13	1:B:491:ARG:HE	1.85	0.41
1:C:220:LEU:O	1:C:221:ASP:C	2.63	0.41
1:B:101:GLU:HA	1:B:101:GLU:OE2	2.21	0.41
1:D:257:ILE:HD13	1:D:491:ARG:HE	1.86	0.41
1:A:220:LEU:O	1:A:221:ASP:C	2.63	0.41
2:A:494:B4P:H3F	2:A:494:B4P:O3G	2.21	0.41
1:C:27:PHE:C	1:C:136:LEU:O	2.64	0.41
1:C:324:LYS:HE3	5:C:1045:HOH:O	2.20	0.41
1:C:415:ALA:HB1	1:C:463:GLY:O	2.21	0.41
1:B:5:LEU:O	1:B:9:LEU:HG	2.21	0.40
1:D:411[B]:GLU:HG2	1:D:470:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HB3	1:A:359:HIS:HB2	2.02	0.40
1:A:115:ARG:HB2	1:A:132:SER:HB3	2.03	0.40
1:C:40:LEU:HD12	1:C:40:LEU:HA	1.93	0.40
1:D:115:ARG:HB2	1:D:132:SER:HB3	2.02	0.40
1:D:5:LEU:O	1:D:9:LEU:HG	2.21	0.40
1:B:115:ARG:HB2	1:B:132:SER:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/493 (98%)	466 (97%)	15 (3%)	0	100	100
1	B	481/493 (98%)	468 (97%)	13 (3%)	0	100	100
1	C	481/493 (98%)	466 (97%)	15 (3%)	0	100	100
1	D	481/493 (98%)	468 (97%)	13 (3%)	0	100	100
All	All	1924/1972 (98%)	1868 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	426/433 (98%)	418 (98%)	8 (2%)	50	41
1	B	426/433 (98%)	419 (98%)	7 (2%)	55	47
1	C	426/433 (98%)	419 (98%)	7 (2%)	55	47
1	D	426/433 (98%)	419 (98%)	7 (2%)	55	47
All	All	1704/1732 (98%)	1675 (98%)	29 (2%)	53	45

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	69	ARG
1	A	71	MET
1	A	97	GLU
1	A	270	LEU
1	A	277	PHE
1	A	395	ASP
1	A	416	PHE
1	B	40	LEU
1	B	44	TYR
1	B	146	LYS
1	B	171	LYS
1	B	277	PHE
1	B	300	LYS
1	B	416	PHE
1	C	40	LEU
1	C	71	MET
1	C	97	GLU
1	C	270	LEU
1	C	277	PHE
1	C	395	ASP
1	C	416	PHE
1	D	40	LEU
1	D	44	TYR
1	D	146	LYS
1	D	171	LYS
1	D	277	PHE
1	D	300	LYS
1	D	416	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	78	HIS
1	A	80	GLN
1	A	85	GLN
1	A	92	GLN
1	A	167	ASN
1	A	216	HIS
1	A	218	ASN
1	A	362	ASN
1	A	412	HIS
1	B	78	HIS
1	B	80	GLN
1	B	85	GLN
1	B	155	GLN
1	B	167	ASN
1	B	216	HIS
1	B	233	HIS
1	B	302	GLN
1	B	489	GLN
1	C	55	GLN
1	C	78	HIS
1	C	80	GLN
1	C	85	GLN
1	C	92	GLN
1	C	167	ASN
1	C	182	GLN
1	C	218	ASN
1	C	362	ASN
1	C	412	HIS
1	D	78	HIS
1	D	80	GLN
1	D	85	GLN
1	D	155	GLN
1	D	167	ASN
1	D	216	HIS
1	D	233	HIS
1	D	302	GLN

5.3.3 RNA ⓘ

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 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	B4P	D	494	4	58,58,58	1.16	6 (10%)	84,91,91	1.75	16 (19%)
3	LYN	B	495	-	9,9,9	0.28	0	9,10,10	0.52	0
2	B4P	B	494	4	58,58,58	1.16	6 (10%)	84,91,91	1.74	16 (19%)
3	LYN	C	495	-	9,9,9	0.28	0	9,10,10	0.58	0
3	LYN	D	495	-	9,9,9	0.28	0	9,10,10	0.51	0
2	B4P	A	494	4	58,58,58	1.16	6 (10%)	84,91,91	1.75	17 (20%)
2	B4P	C	494	4	58,58,58	1.16	6 (10%)	84,91,91	1.75	18 (21%)
3	LYN	A	495	-	9,9,9	0.28	0	9,10,10	0.54	0

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	B4P	D	494	4	-	3/38/70/70	0/6/6/6
3	LYN	B	495	-	-	0/9/9/9	-
2	B4P	B	494	4	-	4/38/70/70	0/6/6/6
3	LYN	C	495	-	-	0/9/9/9	-
3	LYN	D	495	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B4P	A	494	4	-	3/38/70/70	0/6/6/6
2	B4P	C	494	4	-	3/38/70/70	0/6/6/6
3	LYN	A	495	-	-	0/9/9/9	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	494	B4P	C5B-N7B	-3.15	1.33	1.39
2	A	494	B4P	C5B-N7B	-3.15	1.33	1.39
2	C	494	B4P	C5A-N7A	-3.14	1.33	1.39
2	B	494	B4P	C5B-N7B	-3.13	1.33	1.39
2	A	494	B4P	C5A-N7A	-3.12	1.33	1.39
2	D	494	B4P	C5B-N7B	-3.11	1.33	1.39
2	B	494	B4P	C5A-N7A	-3.09	1.33	1.39
2	D	494	B4P	C5A-N7A	-3.07	1.33	1.39
2	B	494	B4P	C8B-N9B	-2.34	1.33	1.37
2	C	494	B4P	C8B-N9B	-2.34	1.33	1.37
2	C	494	B4P	C8A-N9A	-2.33	1.33	1.37
2	A	494	B4P	C8A-N9A	-2.31	1.33	1.37
2	D	494	B4P	C8B-N9B	-2.31	1.33	1.37
2	A	494	B4P	C8B-N9B	-2.31	1.33	1.37
2	D	494	B4P	C8A-N9A	-2.30	1.33	1.37
2	B	494	B4P	C8A-N9A	-2.27	1.33	1.37
2	D	494	B4P	C4A-N9A	-2.12	1.33	1.37
2	A	494	B4P	C4B-N9B	-2.09	1.33	1.37
2	D	494	B4P	C4B-N9B	-2.08	1.33	1.37
2	C	494	B4P	C4B-N9B	-2.08	1.33	1.37
2	A	494	B4P	C4A-N9A	-2.06	1.33	1.37
2	B	494	B4P	C4A-N9A	-2.06	1.33	1.37
2	C	494	B4P	C4A-N9A	-2.06	1.33	1.37
2	B	494	B4P	C4B-N9B	-2.01	1.33	1.37

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	494	B4P	C5B-C4B-N3B	-5.40	119.28	126.72
2	B	494	B4P	C5B-C4B-N3B	-5.35	119.35	126.72
2	A	494	B4P	C5A-C4A-N3A	-5.33	119.38	126.72
2	C	494	B4P	C5A-C4A-N3A	-5.30	119.42	126.72
2	C	494	B4P	C5B-C4B-N3B	-5.29	119.44	126.72
2	A	494	B4P	C5B-C4B-N3B	-5.22	119.52	126.72
2	D	494	B4P	C5A-C4A-N3A	-5.22	119.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	494	B4P	C5A-C4A-N3A	-5.21	119.55	126.72
2	A	494	B4P	N3B-C2B-N1B	-4.59	121.63	128.58
2	B	494	B4P	N3A-C2A-N1A	-4.59	121.64	128.58
2	D	494	B4P	N3A-C2A-N1A	-4.58	121.64	128.58
2	C	494	B4P	N3B-C2B-N1B	-4.57	121.67	128.58
2	C	494	B4P	N3A-C2A-N1A	-4.56	121.69	128.58
2	A	494	B4P	N3A-C2A-N1A	-4.54	121.71	128.58
2	B	494	B4P	N3B-C2B-N1B	-4.54	121.72	128.58
2	D	494	B4P	N3B-C2B-N1B	-4.48	121.80	128.58
2	B	494	B4P	N3B-C4B-N9B	3.76	133.55	127.17
2	A	494	B4P	N3A-C4A-N9A	3.73	133.50	127.17
2	D	494	B4P	N3B-C4B-N9B	3.72	133.50	127.17
2	C	494	B4P	N3A-C4A-N9A	3.71	133.48	127.17
2	A	494	B4P	N3B-C4B-N9B	3.62	133.33	127.17
2	C	494	B4P	N3B-C4B-N9B	3.61	133.31	127.17
2	D	494	B4P	N3A-C4A-N9A	3.61	133.31	127.17
2	B	494	B4P	C2B-N3B-C4B	3.59	120.59	111.83
2	B	494	B4P	N3A-C4A-N9A	3.58	133.26	127.17
2	C	494	B4P	C2A-N3A-C4A	3.58	120.57	111.83
2	A	494	B4P	C2A-N3A-C4A	3.58	120.57	111.83
2	C	494	B4P	C2B-N3B-C4B	3.57	120.56	111.83
2	D	494	B4P	C2B-N3B-C4B	3.57	120.54	111.83
2	A	494	B4P	C2B-N3B-C4B	3.57	120.54	111.83
2	D	494	B4P	C2A-N3A-C4A	3.56	120.53	111.83
2	B	494	B4P	C2A-N3A-C4A	3.55	120.51	111.83
2	A	494	B4P	N9B-C8B-N7B	-3.10	109.54	113.94
2	D	494	B4P	N9A-C8A-N7A	-3.10	109.54	113.94
2	C	494	B4P	N9A-C8A-N7A	-3.05	109.60	113.94
2	C	494	B4P	N9B-C8B-N7B	-3.04	109.62	113.94
2	A	494	B4P	N9A-C8A-N7A	-3.03	109.64	113.94
2	B	494	B4P	N9A-C8A-N7A	-3.01	109.67	113.94
2	B	494	B4P	N9B-C8B-N7B	-2.98	109.71	113.94
2	D	494	B4P	N9B-C8B-N7B	-2.96	109.74	113.94
2	C	494	B4P	C4B-C5B-N7B	-2.91	107.26	110.58
2	A	494	B4P	C4B-C5B-N7B	-2.90	107.26	110.58
2	A	494	B4P	C5B-N7B-C8B	2.90	108.00	103.45
2	C	494	B4P	C5B-N7B-C8B	2.86	107.94	103.45
2	D	494	B4P	C4B-C5B-N7B	-2.85	107.32	110.58
2	B	494	B4P	C4A-C5A-N7A	-2.84	107.34	110.58
2	D	494	B4P	C4A-C5A-N7A	-2.83	107.34	110.58
2	C	494	B4P	C5A-N7A-C8A	2.82	107.88	103.45
2	D	494	B4P	C5A-N7A-C8A	2.82	107.88	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	494	B4P	C5A-N7A-C8A	2.82	107.88	103.45
2	A	494	B4P	C5A-N7A-C8A	2.81	107.86	103.45
2	B	494	B4P	C4B-C5B-N7B	-2.80	107.38	110.58
2	A	494	B4P	C4A-C5A-N7A	-2.80	107.38	110.58
2	B	494	B4P	C5B-N7B-C8B	2.80	107.85	103.45
2	D	494	B4P	C5B-N7B-C8B	2.80	107.85	103.45
2	C	494	B4P	C4A-C5A-N7A	-2.80	107.38	110.58
2	C	494	B4P	O4E-C1E-N9A	2.60	113.08	108.09
2	A	494	B4P	O4E-C1E-N9A	2.46	112.82	108.09
2	D	494	B4P	C4A-N9A-C8A	2.23	108.08	105.74
2	A	494	B4P	C4B-N9B-C8B	2.20	108.05	105.74
2	C	494	B4P	C4A-N9A-C8A	2.18	108.03	105.74
2	A	494	B4P	C4A-N9A-C8A	2.16	108.01	105.74
2	B	494	B4P	C4B-N9B-C8B	2.13	107.97	105.74
2	C	494	B4P	C4B-N9B-C8B	2.10	107.94	105.74
2	B	494	B4P	C4A-N9A-C8A	2.09	107.93	105.74
2	C	494	B4P	C2F-C3F-C4F	-2.04	98.68	102.61
2	D	494	B4P	C4B-N9B-C8B	2.03	107.87	105.74

There are no chirality outliers.

All (13) torsion outliers are listed below:

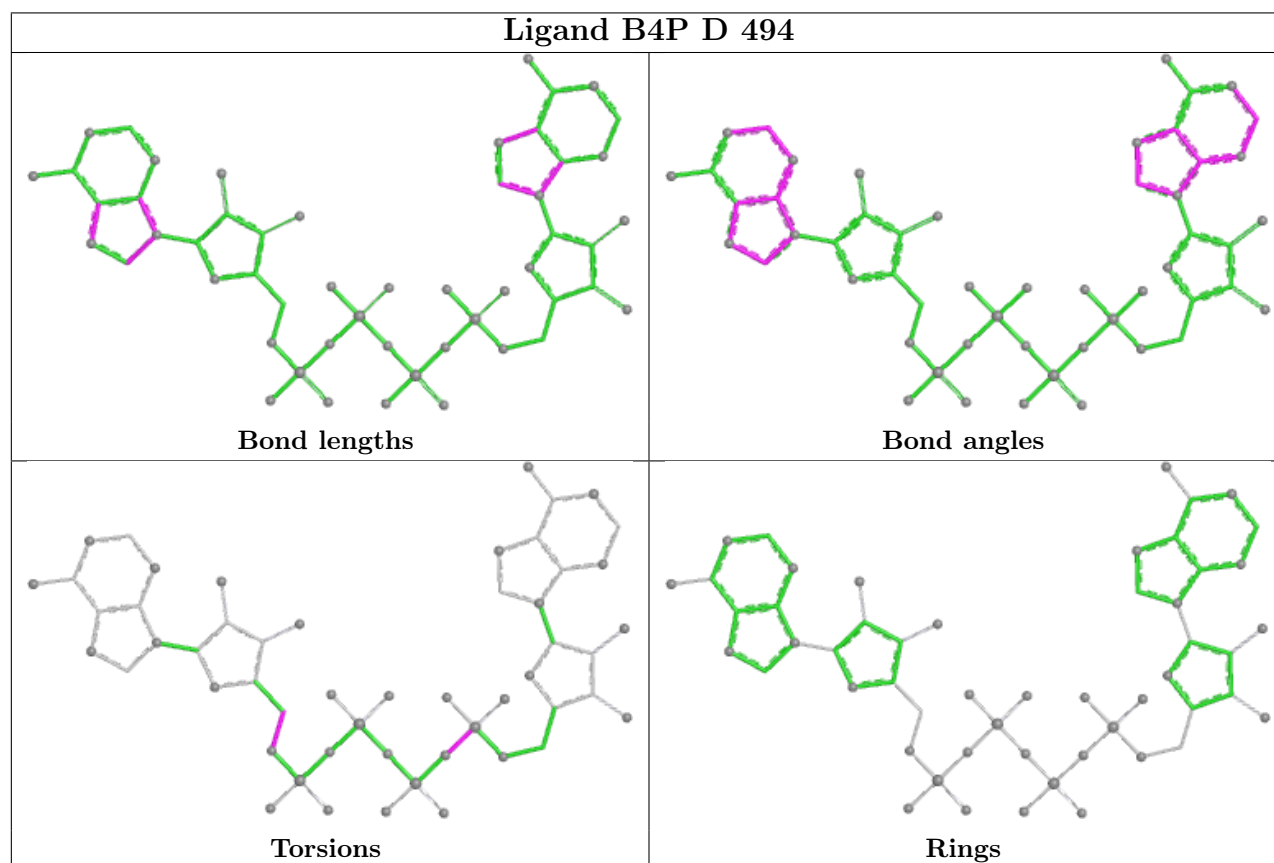
Mol	Chain	Res	Type	Atoms
2	B	494	B4P	C4E-C5E-O5E-PA
2	D	494	B4P	C4E-C5E-O5E-PA
2	A	494	B4P	PG-O3G-PD-O1D
2	D	494	B4P	PG-O3G-PD-O2D
2	B	494	B4P	PG-O3G-PD-O2D
2	A	494	B4P	C4F-C5F-O5F-PD
2	C	494	B4P	C4F-C5F-O5F-PD
2	C	494	B4P	PG-O3G-PD-O1D
2	D	494	B4P	PG-O3G-PD-O1D
2	A	494	B4P	PA-O3A-PB-O2B
2	B	494	B4P	PD-O3G-PG-O2G
2	B	494	B4P	PG-O3G-PD-O1D
2	C	494	B4P	PG-O3G-PD-O2D

There are no ring outliers.

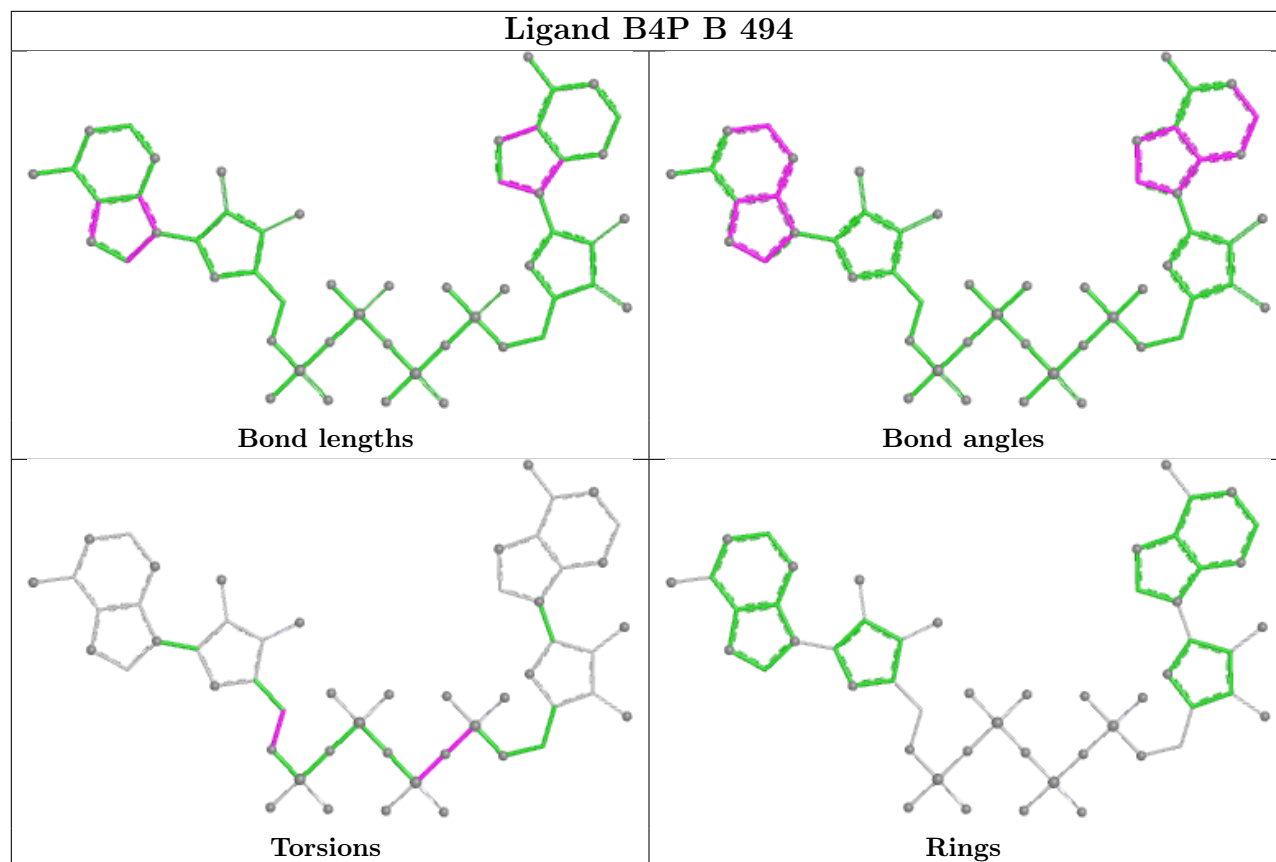
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	494	B4P	1	0
2	B	494	B4P	2	0
2	A	494	B4P	1	0
2	C	494	B4P	2	0

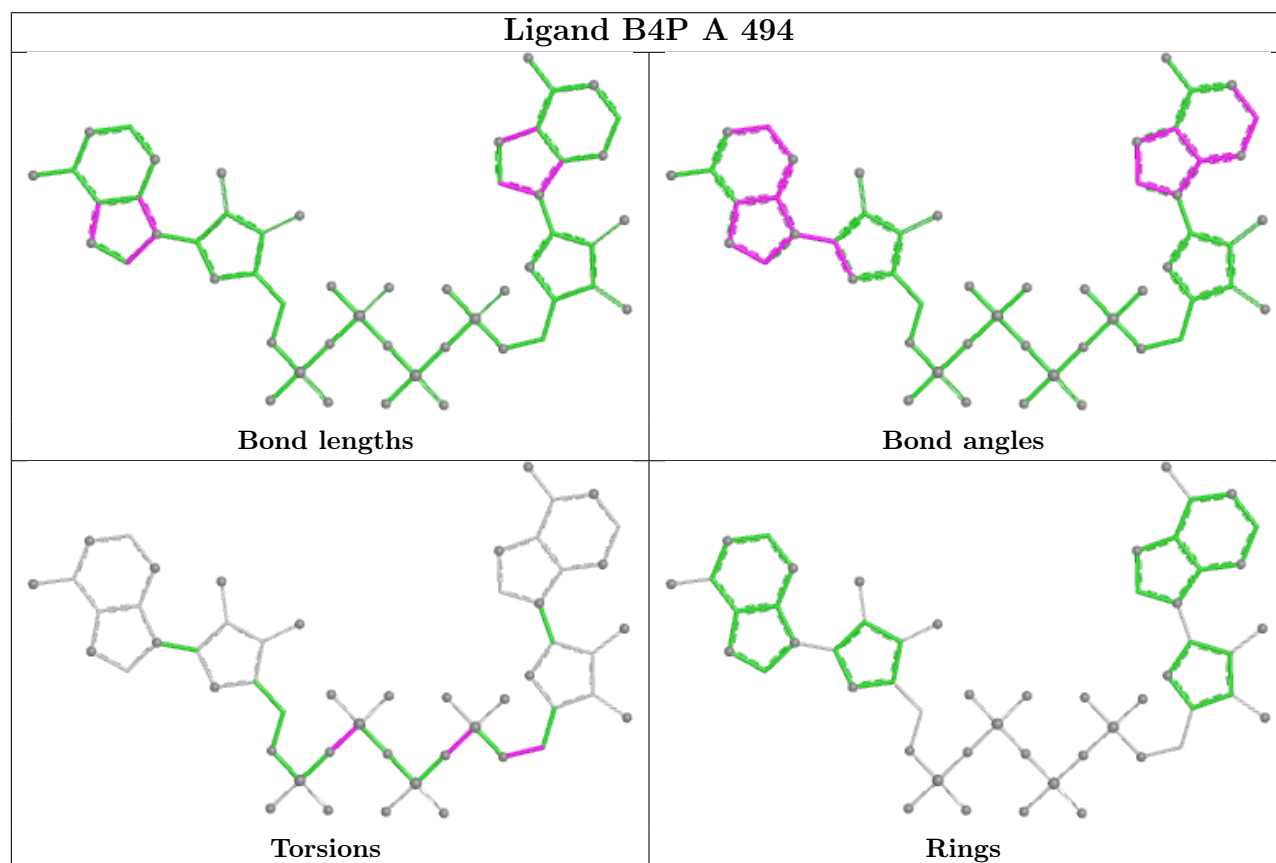
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

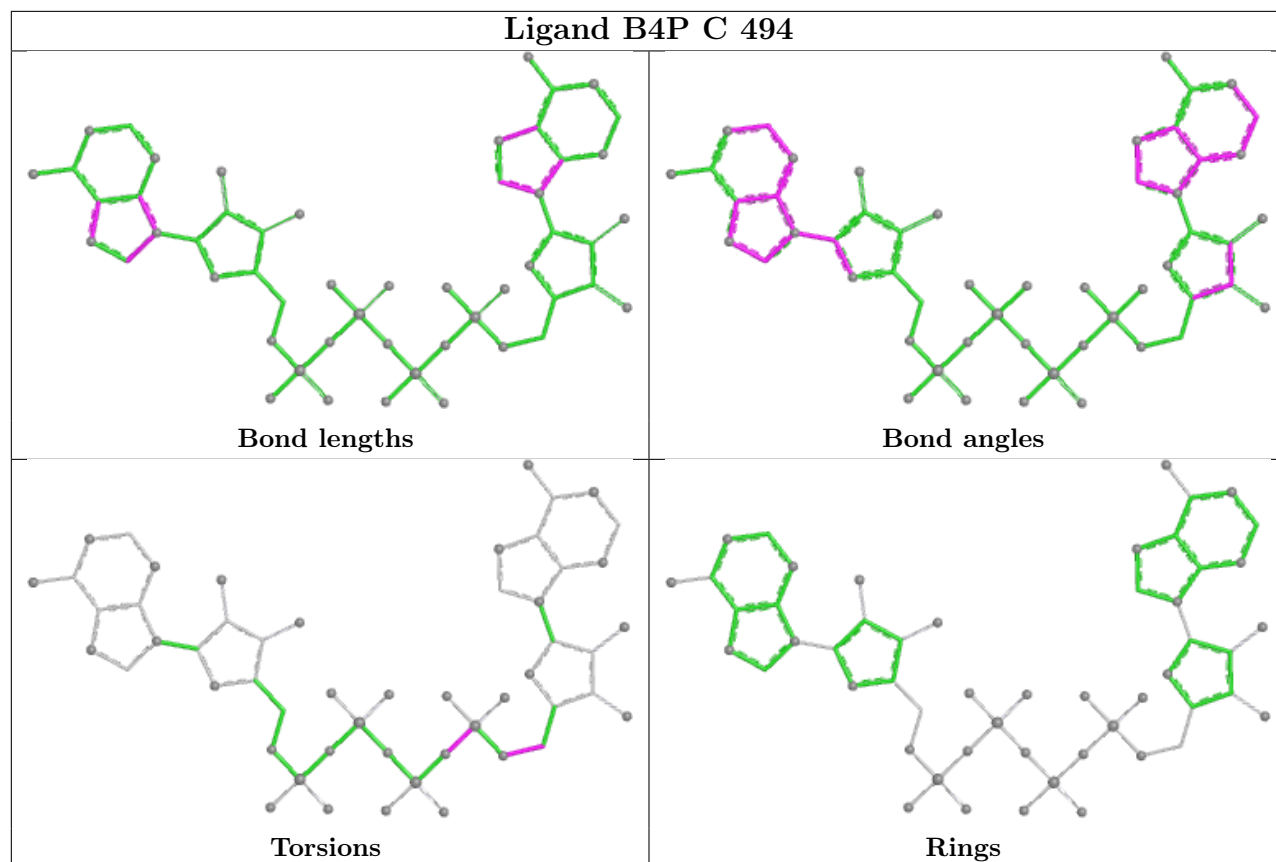


Ligand B4P B 494



Ligand B4P A 494





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	484/493 (98%)	-1.29	0 100 100	7, 15, 34, 50	1 (0%)
1	B	484/493 (98%)	-1.23	0 100 100	8, 16, 40, 44	1 (0%)
1	C	484/493 (98%)	-1.28	0 100 100	8, 16, 33, 50	1 (0%)
1	D	484/493 (98%)	-1.24	0 100 100	8, 16, 40, 44	1 (0%)
All	All	1936/1972 (98%)	-1.26	0 100 100	7, 16, 37, 50	4 (0%)

There are no RSRZ outliers to report.

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
4	MG	C	1202	1/1	0.96	0.10	51,51,51,51	0
4	MG	D	1300	1/1	0.97	0.19	66,66,66,66	0
4	MG	A	1002	1/1	0.98	0.05	39,39,39,39	0
2	B4P	D	494	53/53	0.99	0.03	10,16,26,29	0

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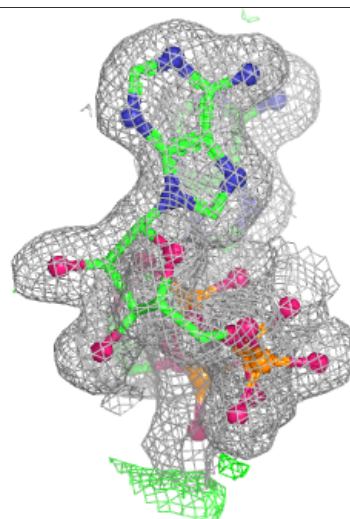
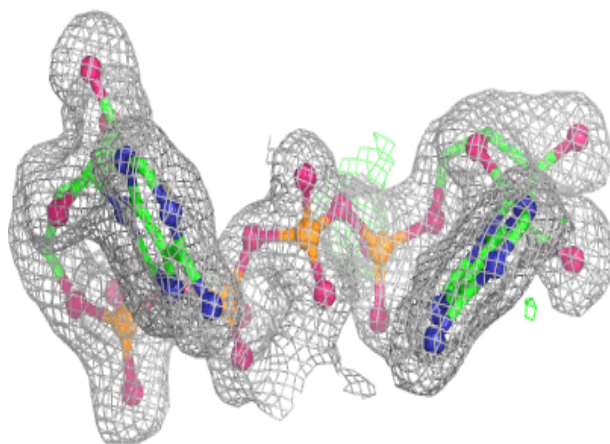
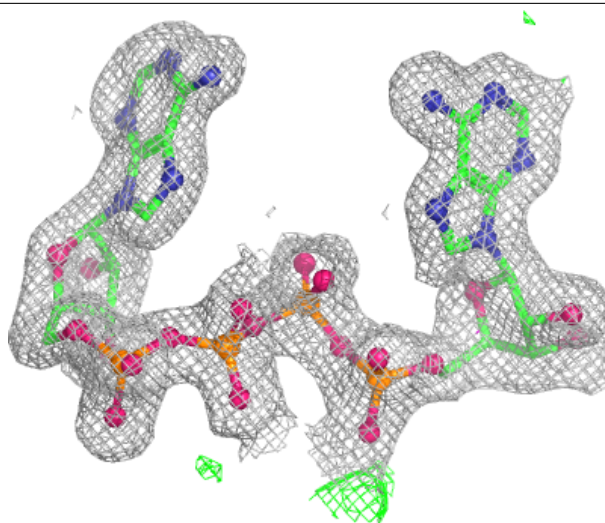
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LYN	A	495	10/10	0.99	0.03	7,10,11,14	0
3	LYN	B	495	10/10	0.99	0.04	10,11,12,14	0
3	LYN	C	495	10/10	0.99	0.02	7,10,11,14	0
3	LYN	D	495	10/10	0.99	0.03	8,10,12,13	0
4	MG	A	1001	1/1	0.99	0.03	16,16,16,16	0
2	B4P	A	494	53/53	0.99	0.03	11,17,26,27	0
4	MG	B	1102	1/1	0.99	0.03	31,31,31,31	0
4	MG	C	1200	1/1	0.99	0.04	23,23,23,23	0
2	B4P	B	494	53/53	0.99	0.03	10,16,26,28	0
2	B4P	C	494	53/53	0.99	0.03	11,17,26,26	0
4	MG	D	1302	1/1	0.99	0.03	33,33,33,33	0
4	MG	C	1201	1/1	1.00	0.05	14,14,14,14	0
4	MG	B	1101	1/1	1.00	0.06	12,12,12,12	0
4	MG	A	1000	1/1	1.00	0.04	21,21,21,21	0
4	MG	D	1301	1/1	1.00	0.03	12,12,12,12	0
4	MG	B	1100	1/1	1.00	0.01	22,22,22,22	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.

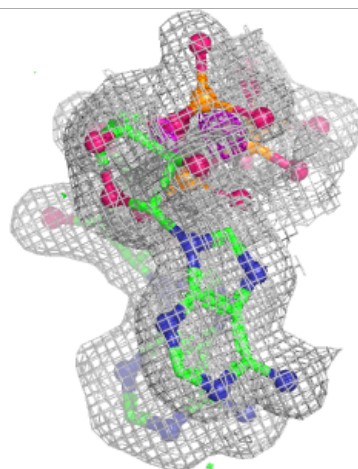
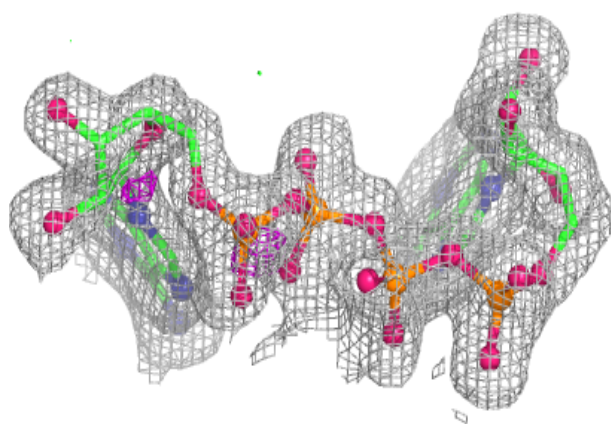
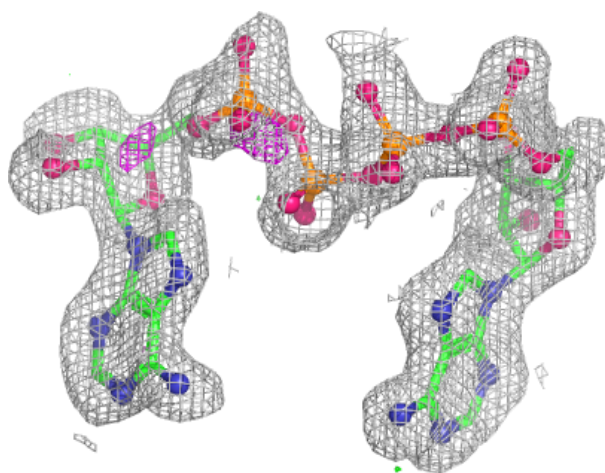
Electron density around B4P D 494:

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



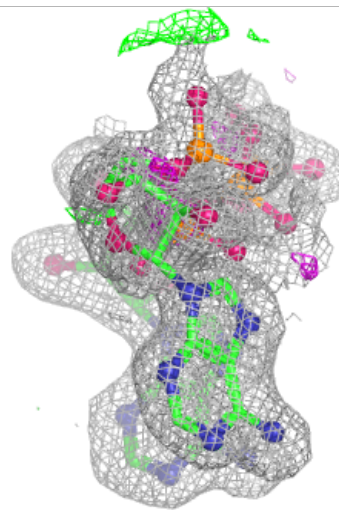
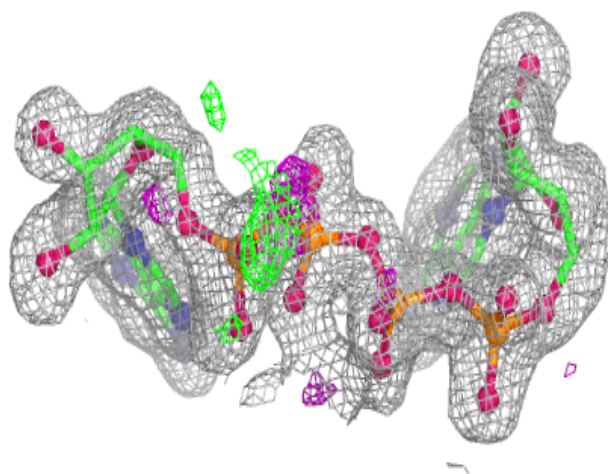
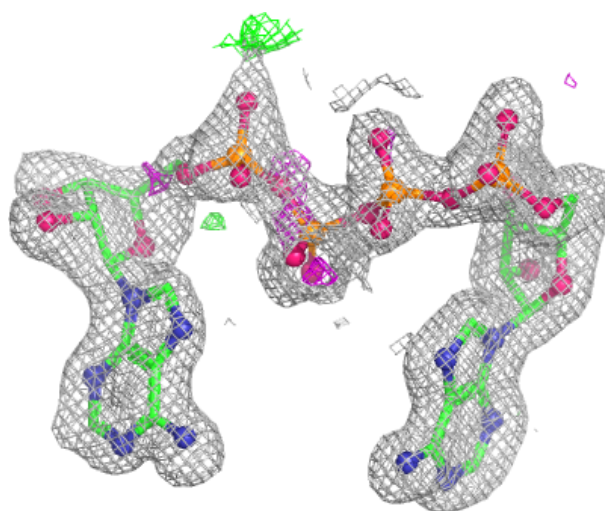
Electron density around B4P A 494:

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



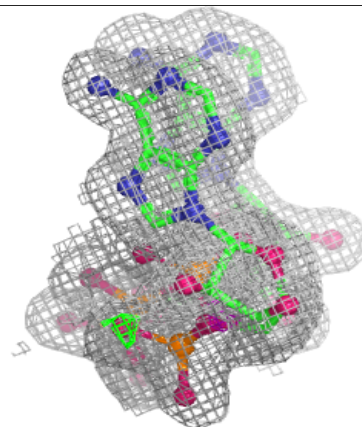
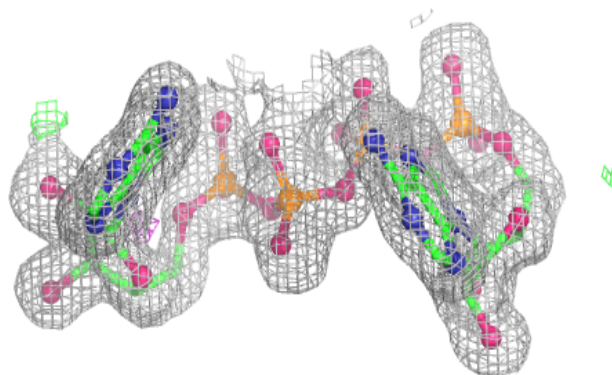
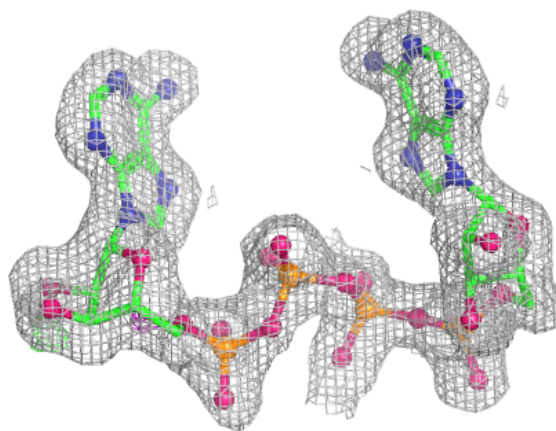
Electron density around B4P B 494:

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



Electron density around B4P C 494:

$2mF_o-DF_c$ (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.