Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 11:18 AM EDT

PDB ID	:	1AN4
Title	:	STRUCTURE AND FUNCTION OF THE B/HLH/Z DOMAIN OF USF
Authors	:	Ferre-D'Amare, A.R.; Pognonec, P.; Roeder, R.G.; Burley, S.K.
Deposited on	:	1997-03-15
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

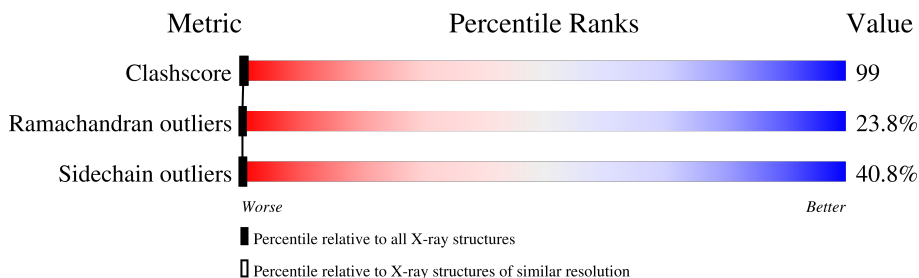|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Clashscore		99
Ramachandran outliers		23.8%
Sidechain outliers		40.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	21	62% 38%
2	D	21	19% 57% 24%
3	A	65	11% 43% 37% 9%
3	B	65	8% 37% 49% 6%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 1923 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 DNA chain called DNA (5'-D(*CP*AP*CP*CP*CP*GP*GP*TP*CP*AP* CP*GP*TP*GP*GP*CP*C P*TP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	21	Total	C	N	O	P	0	0	0
			422	201	78	123	20			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*GP*TP*AP*GP*GP*CP*CP*AP* CP*GP*TP*GP*AP*CP*C P*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	P	0	0	0
			433	205	83	125	20			

- Molecule 3 is a protein called PROTEIN (UPSTREAM STIMULATORY FACTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	65	Total	C	N	O	S	0	0	0
			534	320	109	103	2			
3	B	65	Total	C	N	O	S	0	0	0
			534	320	109	103	2			

There are 6 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	196	MET	ARG	cloning artifact	UNP P22415
A	229	SER	CYS	engineered mutation	UNP P22415
A	248	SER	CYS	engineered mutation	UNP P22415
B	196	MET	ARG	cloning artifact	UNP P22415
B	229	SER	CYS	engineered mutation	UNP P22415
B	248	SER	CYS	engineered mutation	UNP P22415

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.
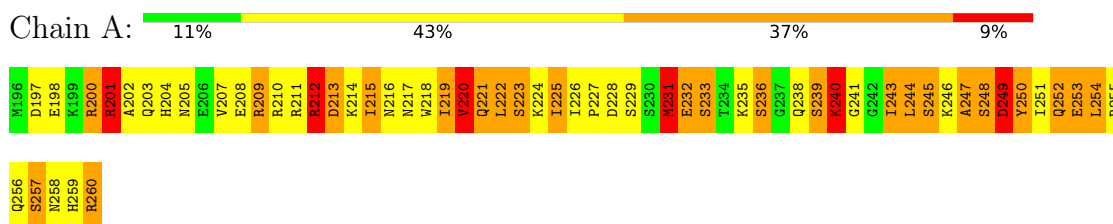
• Molecule 1: DNA (5'-D(*CP*AP*CP*CP*CP*GP*GP*TP*CP*AP*CP*GP*TP*GP*GP*CP *C P*TP*AP*CP*A)-3')

Chain C:

• Molecule 2: DNA (5'-D(*GP*TP*GP*TP*AP*GP*GP*CP*CP*AP*CP*GP*TP*GP*AP*CP *C P*GP*GP*GP*T)-3')
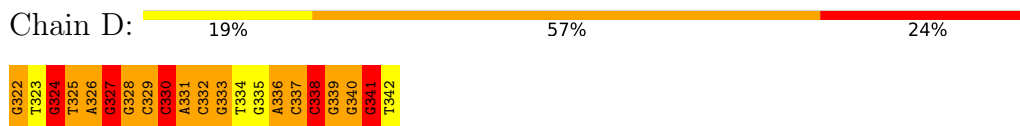
Chain D:

• Molecule 3: PROTEIN (UPSTREAM STIMULATORY FACTOR)

Chain A:

• Molecule 3: PROTEIN (UPSTREAM STIMULATORY FACTOR)

Chain B:
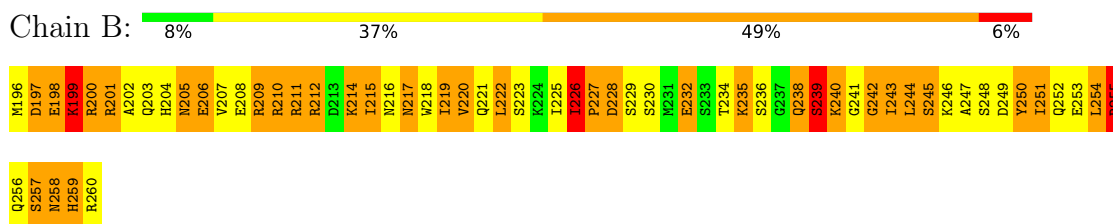
4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.60Å 54.70Å 44.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.236 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1923	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	C	2.46	32/472 (6.8%)	3.83	88/725 (12.1%)
2	D	2.42	25/486 (5.1%)	3.47	86/750 (11.5%)
3	A	0.89	1/539 (0.2%)	1.29	3/716 (0.4%)
3	B	0.95	1/539 (0.2%)	1.48	8/716 (1.1%)
All	All	1.80	59/2036 (2.9%)	2.78	185/2907 (6.4%)

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	C	0	9
2	D	0	6
3	B	0	1
All	All	0	16

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	318	DT	C5-C7	10.03	1.56	1.50
2	D	342	DT	C5-C7	9.54	1.55	1.50
2	D	331	DA	P-O5'	8.80	1.68	1.59
1	C	313	DT	C5-C7	8.66	1.55	1.50
1	C	308	DT	O3'-P	8.37	1.71	1.61
1	C	311	DC	P-O5'	8.35	1.68	1.59
2	D	331	DA	C5'-C4'	8.23	1.60	1.51
2	D	328	DG	P-O5'	7.64	1.67	1.59
2	D	338	DC	N3-C4	7.57	1.39	1.33
1	C	303	DC	P-O5'	7.56	1.67	1.59
1	C	311	DC	C4'-O4'	-7.50	1.37	1.45
1	C	304	DC	O3'-P	7.49	1.70	1.61
1	C	320	DC	P-O5'	7.33	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	333	DG	C2-N3	7.32	1.38	1.32
2	D	342	DT	C3'-C2'	7.12	1.60	1.52
2	D	339	DG	C6-N1	-6.84	1.34	1.39
2	D	323	DT	O3'-P	6.65	1.69	1.61
2	D	324	DG	C4'-C3'	6.63	1.59	1.53
1	C	318	DT	N1-C2	6.51	1.43	1.38
2	D	342	DT	P-O5'	6.50	1.66	1.59
2	D	337	DC	P-O5'	6.40	1.66	1.59
1	C	306	DG	P-O5'	6.37	1.66	1.59
1	C	311	DC	C5'-C4'	-6.36	1.44	1.51
1	C	310	DA	P-O5'	6.34	1.66	1.59
2	D	333	DG	N3-C4	6.25	1.39	1.35
1	C	319	DA	C5'-C4'	6.23	1.58	1.51
1	C	317	DC	C5'-C4'	6.11	1.58	1.51
2	D	336	DA	N9-C8	-6.03	1.32	1.37
3	A	207	VAL	CA-CB	5.98	1.67	1.54
2	D	322	DG	C4'-C3'	5.95	1.59	1.53
2	D	337	DC	C5'-C4'	5.94	1.57	1.51
1	C	306	DG	C5'-C4'	5.86	1.57	1.51
1	C	310	DA	C3'-C2'	5.85	1.59	1.52
2	D	330	DC	C5'-C4'	5.84	1.57	1.51
1	C	304	DC	P-O5'	5.82	1.65	1.59
2	D	324	DG	C5-C6	-5.78	1.36	1.42
2	D	323	DT	P-O5'	5.69	1.65	1.59
2	D	323	DT	N3-C4	-5.60	1.34	1.38
1	C	315	DG	C2'-C1'	-5.59	1.46	1.52
2	D	337	DC	N1-C6	5.59	1.40	1.37
1	C	310	DA	N7-C5	-5.49	1.35	1.39
2	D	324	DG	C5'-C4'	5.47	1.57	1.51
3	B	216	ASN	N-CA	5.46	1.57	1.46
1	C	311	DC	O3'-P	5.40	1.67	1.61
1	C	306	DG	C2-N3	5.39	1.37	1.32
1	C	308	DT	C3'-C2'	5.37	1.58	1.52
1	C	301	DC	C2'-C1'	5.35	1.57	1.52
1	C	303	DC	O3'-P	5.35	1.67	1.61
1	C	310	DA	N3-C4	-5.34	1.31	1.34
2	D	328	DG	C5'-C4'	5.30	1.57	1.51
1	C	319	DA	N9-C4	-5.28	1.34	1.37
1	C	314	DG	C2-N3	5.25	1.36	1.32
2	D	338	DC	C2-N3	5.14	1.39	1.35
1	C	304	DC	C5'-C4'	5.12	1.56	1.51
1	C	302	DA	C2'-C1'	-5.06	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	332	DC	O3'-P	5.06	1.67	1.61
1	C	314	DG	O4'-C1'	5.03	1.48	1.42
1	C	308	DT	C5'-C4'	5.02	1.56	1.51
1	C	308	DT	C5-C7	5.00	1.53	1.50

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	320	DC	O4'-C1'-N1	25.93	126.15	108.00
1	C	309	DC	O4'-C1'-N1	25.79	126.05	108.00
1	C	310	DA	O4'-C4'-C3'	-20.02	93.99	106.00
2	D	322	DG	O4'-C1'-N9	18.81	121.17	108.00
2	D	327	DG	C1'-O4'-C4'	-18.54	91.56	110.10
1	C	305	DC	C1'-O4'-C4'	-18.39	91.71	110.10
1	C	305	DC	O4'-C4'-C3'	-17.61	95.43	106.00
1	C	317	DC	O4'-C1'-N1	17.45	120.22	108.00
1	C	302	DA	O4'-C4'-C3'	-17.00	95.80	106.00
2	D	337	DC	O4'-C1'-N1	16.99	119.89	108.00
1	C	301	DC	O4'-C1'-N1	15.26	118.68	108.00
1	C	315	DG	O4'-C4'-C3'	-13.86	97.68	106.00
1	C	310	DA	O4'-C1'-C2'	-13.39	95.19	105.90
2	D	322	DG	C1'-O4'-C4'	-12.18	97.92	110.10
1	C	315	DG	C1'-O4'-C4'	-12.17	97.93	110.10
2	D	336	DA	O4'-C1'-C2'	-12.02	96.28	105.90
2	D	327	DG	O4'-C4'-C3'	-11.94	98.84	106.00
1	C	302	DA	P-O3'-C3'	-11.64	105.73	119.70
2	D	322	DG	C3'-C2'-C1'	-11.16	89.10	102.50
2	D	327	DG	O4'-C1'-N9	11.06	115.75	108.00
2	D	326	DA	C1'-O4'-C4'	-10.94	99.16	110.10
2	D	338	DC	N3-C4-N4	10.85	125.59	118.00
3	B	219	ILE	O-C-N	-10.64	105.67	122.70
1	C	304	DC	P-O3'-C3'	10.55	132.36	119.70
2	D	339	DG	O4'-C1'-N9	10.35	115.25	108.00
2	D	325	DT	P-O3'-C3'	10.25	132.00	119.70
1	C	317	DC	O4'-C4'-C3'	-9.86	100.08	106.00
2	D	328	DG	O4'-C4'-C3'	-9.85	100.09	106.00
2	D	338	DC	P-O3'-C3'	-9.79	107.95	119.70
1	C	309	DC	N1-C2-O2	9.79	124.77	118.90
2	D	325	DT	O4'-C1'-N1	9.74	114.82	108.00
1	C	317	DC	C4'-C3'-C2'	-9.71	94.36	103.10
1	C	311	DC	O4'-C1'-C2'	-9.67	98.16	105.90
2	D	341	DG	C1'-O4'-C4'	-9.62	100.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	326	DA	O4'-C4'-C3'	-9.54	100.28	106.00
2	D	338	DC	C5-C4-N4	-9.38	113.64	120.20
1	C	316	DC	P-O3'-C3'	9.33	130.89	119.70
2	D	342	DT	O4'-C1'-C2'	-9.25	98.50	105.90
2	D	342	DT	N3-C2-O2	-9.21	116.77	122.30
1	C	307	DG	O4'-C4'-C3'	-9.18	100.49	106.00
2	D	323	DT	C4'-C3'-C2'	-8.98	95.02	103.10
1	C	320	DC	P-O3'-C3'	8.93	130.41	119.70
1	C	308	DT	O4'-C1'-N1	8.89	114.22	108.00
2	D	323	DT	N3-C2-O2	-8.89	116.97	122.30
1	C	305	DC	N1-C2-O2	8.88	124.23	118.90
2	D	323	DT	O4'-C1'-N1	8.87	114.21	108.00
2	D	337	DC	P-O3'-C3'	-8.87	109.06	119.70
1	C	309	DC	N3-C2-O2	-8.81	115.73	121.90
3	B	219	ILE	C-N-CA	-8.81	99.68	121.70
1	C	315	DG	C3'-C2'-C1'	-8.67	92.09	102.50
1	C	319	DA	O4'-C4'-C3'	-8.66	100.80	106.00
2	D	326	DA	O4'-C1'-N9	8.52	113.96	108.00
2	D	323	DT	C6-C5-C7	-8.50	117.80	122.90
2	D	325	DT	C4'-C3'-C2'	-8.42	95.52	103.10
1	C	318	DT	O4'-C1'-N1	8.37	113.86	108.00
1	C	305	DC	C4'-C3'-C2'	-8.30	95.63	103.10
1	C	319	DA	C1'-O4'-C4'	-8.21	101.89	110.10
1	C	312	DG	O4'-C1'-N9	8.10	113.67	108.00
1	C	315	DG	P-O3'-C3'	8.08	129.40	119.70
1	C	303	DC	N3-C4-C5	-8.05	118.68	121.90
2	D	335	DG	P-O3'-C3'	8.05	129.36	119.70
1	C	303	DC	P-O3'-C3'	8.02	129.32	119.70
1	C	313	DT	P-O5'-C5'	-7.88	108.29	120.90
2	D	332	DC	C5-C4-N4	-7.80	114.74	120.20
2	D	331	DA	O4'-C1'-N9	7.72	113.41	108.00
1	C	313	DT	C1'-O4'-C4'	-7.68	102.42	110.10
1	C	306	DG	O4'-C1'-N9	7.58	113.31	108.00
2	D	336	DA	P-O3'-C3'	-7.58	110.61	119.70
1	C	313	DT	O4'-C1'-C2'	7.53	111.92	105.90
1	C	318	DT	C4'-C3'-C2'	-7.53	96.33	103.10
1	C	311	DC	C5'-C4'-O4'	-7.45	95.14	109.30
1	C	308	DT	C4-C5-C6	7.44	122.47	118.00
1	C	305	DC	O4'-C1'-C2'	-7.41	99.97	105.90
1	C	303	DC	O4'-C4'-C3'	-7.37	101.55	104.50
1	C	314	DG	O4'-C1'-N9	7.34	113.14	108.00
1	C	306	DG	C5'-C4'-O4'	7.34	123.24	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	328	DG	P-O3'-C3'	7.31	128.47	119.70
3	A	239	SER	N-CA-C	7.30	130.71	111.00
2	D	324	DG	O4'-C1'-N9	7.29	113.10	108.00
2	D	323	DT	O4'-C4'-C3'	7.29	110.37	106.00
2	D	327	DG	P-O3'-C3'	7.22	128.37	119.70
2	D	332	DC	P-O3'-C3'	7.11	128.23	119.70
1	C	319	DA	P-O3'-C3'	6.99	128.09	119.70
3	A	203	GLN	N-CA-C	-6.95	92.22	111.00
1	C	311	DC	O4'-C1'-N1	-6.90	103.17	108.00
1	C	306	DG	C5'-C4'-C3'	-6.88	101.72	114.10
1	C	308	DT	O4'-C1'-C2'	-6.75	100.50	105.90
1	C	320	DC	C5-C6-N1	6.71	124.36	121.00
2	D	342	DT	O4'-C1'-N1	-6.70	103.31	108.00
2	D	322	DG	P-O3'-C3'	6.64	127.67	119.70
2	D	328	DG	O4'-C1'-C2'	-6.60	100.62	105.90
2	D	324	DG	P-O5'-C5'	6.58	131.43	120.90
1	C	302	DA	O4'-C1'-N9	6.58	112.60	108.00
2	D	332	DC	N1-C2-O2	6.54	122.82	118.90
2	D	334	DT	O4'-C1'-C2'	-6.54	100.67	105.90
1	C	320	DC	C4'-C3'-C2'	-6.54	97.22	103.10
1	C	303	DC	N3-C4-N4	6.53	122.57	118.00
1	C	309	DC	N1-C1'-C2'	-6.47	100.31	112.60
1	C	302	DA	C1'-O4'-C4'	-6.45	103.65	110.10
2	D	336	DA	N1-C2-N3	6.42	132.51	129.30
2	D	334	DT	C4-C5-C6	6.39	121.83	118.00
1	C	305	DC	N3-C2-O2	-6.35	117.45	121.90
1	C	310	DA	C4-C5-C6	6.31	120.15	117.00
1	C	311	DC	P-O3'-C3'	6.29	127.25	119.70
2	D	336	DA	C6-N1-C2	-6.27	114.84	118.60
2	D	337	DC	C5'-C4'-C3'	-6.23	102.88	114.10
1	C	310	DA	C8-N9-C4	-6.21	103.32	105.80
2	D	342	DT	P-O5'-C5'	6.20	130.83	120.90
2	D	326	DA	O4'-C1'-C2'	-6.17	100.96	105.90
2	D	325	DT	C4-C5-C6	6.17	121.70	118.00
1	C	303	DC	C2-N3-C4	6.16	122.98	119.90
3	A	212	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	308	DT	P-O3'-C3'	6.13	127.05	119.70
2	D	326	DA	P-O3'-C3'	-6.12	112.35	119.70
2	D	339	DG	N3-C2-N2	6.09	124.17	119.90
2	D	339	DG	C5-C6-N1	6.08	114.54	111.50
1	C	315	DG	O4'-C1'-C2'	-6.07	101.04	105.90
1	C	314	DG	C5'-C4'-C3'	-6.05	103.21	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	335	DG	C4'-C3'-C2'	-6.01	97.69	103.10
1	C	311	DC	C6-N1-C2	6.00	122.70	120.30
2	D	327	DG	N9-C1'-C2'	5.98	123.95	112.60
2	D	328	DG	P-O5'-C5'	5.97	130.45	120.90
2	D	328	DG	N3-C4-C5	-5.95	125.62	128.60
1	C	314	DG	C8-N9-C4	-5.93	104.03	106.40
1	C	310	DA	O4'-C1'-N9	-5.92	103.85	108.00
1	C	301	DC	O4'-C1'-C2'	-5.92	101.16	105.90
2	D	333	DG	O4'-C1'-N9	-5.89	103.88	108.00
2	D	323	DT	P-O3'-C3'	5.88	126.76	119.70
1	C	312	DG	P-O3'-C3'	5.88	126.75	119.70
1	C	320	DC	C2-N3-C4	5.87	122.84	119.90
2	D	338	DC	C4'-C3'-C2'	5.81	108.33	103.10
2	D	325	DT	O4'-C1'-C2'	-5.79	101.27	105.90
3	B	219	ILE	CA-C-N	5.78	129.92	117.20
2	D	336	DA	C5'-C4'-C3'	-5.73	103.78	114.10
1	C	301	DC	N1-C2-O2	5.67	122.30	118.90
1	C	308	DT	C2-N3-C4	-5.67	123.80	127.20
2	D	336	DA	C4-C5-C6	5.66	119.83	117.00
2	D	323	DT	N1-C2-O2	5.65	127.62	123.10
1	C	315	DG	O4'-C1'-N9	5.64	111.95	108.00
3	B	255	ARG	N-CA-C	-5.62	95.83	111.00
1	C	320	DC	P-O5'-C5'	5.59	129.84	120.90
2	D	328	DG	C4'-C3'-C2'	-5.58	98.08	103.10
2	D	327	DG	C3'-C2'-C1'	-5.58	95.81	102.50
1	C	308	DT	N3-C4-O4	5.55	123.23	119.90
1	C	316	DC	O4'-C1'-N1	5.54	111.88	108.00
3	B	254	LEU	CA-CB-CG	5.54	128.03	115.30
3	B	220	VAL	O-C-N	5.46	131.44	122.70
1	C	315	DG	N9-C1'-C2'	5.46	122.97	112.60
2	D	330	DC	N3-C4-C5	-5.46	119.72	121.90
2	D	340	DG	C3'-C2'-C1'	-5.45	95.96	102.50
2	D	342	DT	C1'-O4'-C4'	5.45	115.55	110.10
2	D	338	DC	N3-C2-O2	5.45	125.71	121.90
2	D	338	DC	N1-C2-N3	-5.44	115.39	119.20
2	D	333	DG	N3-C4-N9	5.39	129.24	126.00
1	C	314	DG	N3-C4-C5	-5.38	125.91	128.60
2	D	329	DC	N1-C2-O2	5.38	122.13	118.90
2	D	332	DC	N3-C4-N4	5.37	121.76	118.00
1	C	321	DA	C5'-C4'-C3'	-5.35	104.47	114.10
1	C	306	DG	C4'-C3'-C2'	5.33	107.90	103.10
2	D	336	DA	C5'-C4'-O4'	5.33	119.43	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	314	DG	C5'-C4'-O4'	5.32	119.41	109.30
2	D	331	DA	N9-C1'-C2'	-5.30	102.52	112.60
1	C	309	DC	C5-C4-N4	-5.30	116.49	120.20
1	C	311	DC	C5-C4-N4	-5.29	116.50	120.20
2	D	339	DG	O4'-C1'-C2'	-5.26	101.69	105.90
2	D	331	DA	C2-N3-C4	-5.26	107.97	110.60
2	D	324	DG	C8-N9-C1'	5.21	133.78	127.00
2	D	338	DC	C5-C6-N1	5.18	123.59	121.00
2	D	323	DT	O3'-P-O5'	-5.17	94.17	104.00
2	D	323	DT	O4'-C1'-C2'	-5.17	101.76	105.90
1	C	310	DA	N1-C6-N6	5.16	121.69	118.60
2	D	322	DG	N9-C1'-C2'	5.16	122.39	112.60
3	B	199	LYS	N-CA-C	5.15	124.91	111.00
2	D	332	DC	P-O5'-C5'	5.13	129.11	120.90
1	C	316	DC	C4'-C3'-C2'	5.12	107.70	103.10
2	D	342	DT	C6-N1-C2	-5.12	118.74	121.30
1	C	311	DC	P-O5'-C5'	-5.10	112.74	120.90
1	C	307	DG	C8-N9-C4	-5.10	104.36	106.40
2	D	332	DC	C6-N1-C1'	-5.08	114.70	120.80
3	B	226	ILE	C-N-CD	-5.05	109.48	120.60
1	C	307	DG	C4'-C3'-C2'	-5.05	98.55	103.10
1	C	311	DC	O3'-P-O5'	5.04	113.58	104.00
1	C	317	DC	C1'-O4'-C4'	-5.03	105.07	110.10
1	C	317	DC	N3-C4-C5	-5.02	119.89	121.90
2	D	340	DG	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	250	TYR	Sidechain
1	C	301	DC	Sidechain
1	C	302	DA	Sidechain
1	C	306	DG	Sidechain
1	C	307	DG	Sidechain
1	C	309	DC	Sidechain
1	C	312	DG	Sidechain
1	C	313	DT	Sidechain
1	C	320	DC	Sidechain
1	C	321	DA	Sidechain
2	D	322	DG	Sidechain
2	D	324	DG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	327	DG	Sidechain
2	D	330	DC	Sidechain
2	D	338	DC	Sidechain
2	D	341	DG	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	C	422	0	236	62	0
2	D	433	0	237	50	0
3	A	534	0	537	106	0
3	B	534	0	537	166	0
All	All	1923	0	1547	335	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 99.

All (335) 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)
3:B:219:ILE:CD1	3:B:240:LYS:HE3	1.55	1.36
3:B:227:PRO:HG3	3:B:250:TYR:HE2	0.99	1.12
3:B:220:VAL:CG2	3:B:221:GLN:OE1	1.99	1.10
3:B:227:PRO:HG3	3:B:250:TYR:CE2	1.84	1.10
3:B:219:ILE:HG21	3:B:240:LYS:HG3	1.33	1.10
3:B:219:ILE:HD12	3:B:240:LYS:HE3	1.19	1.09
3:B:223:SER:HB3	3:B:243:ILE:HG21	1.14	1.08
3:A:226:ILE:HG21	3:A:247:ALA:HA	1.36	1.07
3:B:220:VAL:HG22	3:B:221:GLN:OE1	1.54	1.07
3:B:215:ILE:HA	3:B:218:TRP:NE1	1.70	1.06
3:B:219:ILE:HD12	3:B:240:LYS:CE	1.89	1.02
3:B:219:ILE:CD1	3:B:240:LYS:CE	2.39	1.00
1:C:316:DC:H1'	1:C:317:DC:H5"	1.41	1.00
3:B:209:ARG:HA	3:B:212:ARG:HB2	1.42	0.97
3:B:211:ARG:O	3:B:215:ILE:HG22	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:212:ARG:HH11	3:A:212:ARG:HG2	1.30	0.95
3:B:206:GLU:HA	3:B:209:ARG:CZ	1.96	0.94
1:C:305:DC:H2'	1:C:306:DG:C8	2.05	0.91
3:B:211:ARG:O	3:B:214:LYS:HB2	1.70	0.89
3:B:215:ILE:HA	3:B:218:TRP:HE1	1.30	0.89
3:B:223:SER:CB	3:B:243:ILE:HG21	2.01	0.88
3:B:220:VAL:HG23	3:B:221:GLN:OE1	1.74	0.88
2:D:328:DG:H2'	2:D:329:DC:C6	2.09	0.87
2:D:324:DG:H2"	2:D:325:DT:OP1	1.73	0.85
3:A:209:ARG:HA	3:A:212:ARG:HD2	1.59	0.84
3:B:212:ARG:O	3:B:215:ILE:HG23	1.78	0.84
1:C:302:DA:H2'	1:C:303:DC:C1'	2.11	0.81
3:B:209:ARG:CA	3:B:212:ARG:HB2	2.11	0.81
3:B:248:SER:O	3:B:251:ILE:HG22	1.80	0.81
3:B:215:ILE:O	3:B:219:ILE:HG12	1.82	0.80
1:C:303:DC:H2"	1:C:304:DC:OP1	1.82	0.80
3:B:219:ILE:CG1	3:B:240:LYS:HE3	2.12	0.79
1:C:318:DT:OP2	1:C:318:DT:H2'	1.83	0.79
1:C:310:DA:H2"	1:C:311:DC:H5'	1.66	0.78
3:B:215:ILE:O	3:B:219:ILE:CG1	2.32	0.78
3:B:219:ILE:HD11	3:B:240:LYS:HE3	1.63	0.78
3:B:249:ASP:O	3:B:253:GLU:HG2	1.85	0.76
3:B:207:VAL:O	3:B:210:ARG:HB3	1.86	0.76
3:A:218:TRP:CE2	3:A:219:ILE:HG12	2.21	0.75
1:C:303:DC:H2'	1:C:304:DC:C5	2.21	0.75
3:A:260:ARG:HH12	3:B:227:PRO:HA	1.52	0.75
3:B:218:TRP:HE3	3:B:222:LEU:HD22	1.51	0.74
3:B:215:ILE:HA	3:B:218:TRP:CD1	2.23	0.74
3:B:209:ARG:HA	3:B:212:ARG:CB	2.17	0.74
1:C:308:DT:OP2	1:C:308:DT:H6	1.69	0.73
1:C:305:DC:N3	2:D:339:DG:O6	2.23	0.71
3:A:222:LEU:H	3:A:222:LEU:HD22	1.55	0.71
3:B:211:ARG:HA	3:B:214:LYS:HB2	1.72	0.71
2:D:324:DG:H8	2:D:324:DG:O5'	1.72	0.71
2:D:326:DA:H8	3:B:200:ARG:NH2	1.90	0.70
2:D:325:DT:H2'	2:D:326:DA:O4'	1.90	0.70
3:B:238:GLN:O	3:B:239:SER:HB2	1.89	0.70
3:A:252:GLN:HG3	3:A:253:GLU:N	2.06	0.69
1:C:302:DA:H2'	1:C:303:DC:H1'	1.74	0.69
2:D:326:DA:OP2	3:B:200:ARG:HG3	1.93	0.69
3:A:252:GLN:HA	3:B:225:ILE:CD1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:208:GLU:HG2	3:A:212:ARG:CZ	2.23	0.69
3:B:210:ARG:CZ	3:B:211:ARG:HB3	2.21	0.69
2:D:326:DA:C8	3:B:200:ARG:NH2	2.61	0.68
3:B:211:ARG:CA	3:B:214:LYS:HB2	2.24	0.68
3:A:240:LYS:HA	3:A:243:ILE:HB	1.74	0.68
3:B:257:SER:O	3:B:259:HIS:ND1	2.27	0.67
1:C:302:DA:O4'	1:C:302:DA:OP2	2.12	0.67
1:C:315:DG:H2"	1:C:316:DC:OP2	1.95	0.67
3:B:221:GLN:OE1	3:B:221:GLN:N	2.28	0.67
3:B:227:PRO:CG	3:B:250:TYR:HE2	1.93	0.67
3:B:202:ALA:O	3:B:205:ASN:HB3	1.94	0.67
1:C:301:DC:H2"	1:C:302:DA:OP2	1.95	0.66
2:D:339:DG:H2"	2:D:340:DG:OP2	1.95	0.66
3:B:211:ARG:C	3:B:214:LYS:HB2	2.16	0.66
1:C:318:DT:H3	2:D:326:DA:N6	1.94	0.65
3:A:217:ASN:OD1	3:A:220:VAL:HG11	1.97	0.65
3:B:219:ILE:HD11	3:B:240:LYS:CE	2.22	0.65
3:B:199:LYS:HD3	3:B:202:ALA:HB3	1.77	0.65
3:B:203:GLN:HG3	3:B:204:HIS:H	1.60	0.65
3:B:219:ILE:CG2	3:B:240:LYS:HG3	2.20	0.65
3:A:211:ARG:O	3:A:214:LYS:HB2	1.97	0.65
1:C:318:DT:H3	2:D:326:DA:H61	1.42	0.64
2:D:329:DC:H6	2:D:329:DC:O5'	1.79	0.64
3:A:222:LEU:H	3:A:222:LEU:CD2	2.10	0.64
3:B:226:ILE:CB	3:B:227:PRO:HD2	2.28	0.64
3:A:244:LEU:HD22	3:A:244:LEU:O	1.98	0.64
3:A:243:ILE:O	3:A:246:LYS:N	2.30	0.64
3:A:260:ARG:NH1	3:B:227:PRO:HA	2.12	0.64
3:A:228:ASP:CG	3:A:243:ILE:HA	2.18	0.63
3:A:216:ASN:O	3:A:220:VAL:HG12	1.98	0.63
3:A:252:GLN:HG3	3:A:253:GLU:H	1.63	0.63
1:C:304:DC:H2"	1:C:305:DC:O5'	1.98	0.63
1:C:319:DA:N1	2:D:325:DT:O4	2.31	0.62
3:A:244:LEU:HD13	3:A:244:LEU:C	2.20	0.62
1:C:316:DC:H1'	1:C:317:DC:C5'	2.24	0.62
3:B:218:TRP:CZ2	3:B:219:ILE:CD1	2.82	0.62
3:B:203:GLN:HG3	3:B:204:HIS:N	2.15	0.62
3:B:210:ARG:HG2	3:B:211:ARG:N	2.15	0.62
3:A:238:GLN:HG3	3:A:239:SER:N	2.15	0.61
3:B:206:GLU:O	3:B:209:ARG:HG2	2.01	0.61
3:A:252:GLN:HA	3:B:225:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:DA:OP2	1:C:302:DA:H8	1.85	0.60
1:C:302:DA:N6	2:D:341:DG:C6	2.69	0.60
3:A:215:ILE:HA	3:A:218:TRP:CD1	2.37	0.60
1:C:320:DC:H2'	1:C:320:DC:O5'	2.01	0.60
2:D:329:DC:H2"	2:D:330:DC:H5'	1.84	0.60
3:A:215:ILE:HA	3:A:218:TRP:HD1	1.67	0.59
1:C:320:DC:H42	2:D:324:DG:H1	1.48	0.59
1:C:305:DC:N3	2:D:339:DG:C6	2.70	0.59
3:A:248:SER:HB3	3:B:222:LEU:HG	1.85	0.59
3:B:211:ARG:HA	3:B:214:LYS:HG3	1.85	0.59
3:A:212:ARG:HH11	3:A:212:ARG:CG	2.09	0.59
3:A:231:MET:SD	3:A:232:GLU:N	2.74	0.59
3:A:215:ILE:HG23	3:A:218:TRP:HE1	1.68	0.59
3:A:212:ARG:HG2	3:A:212:ARG:NH1	2.10	0.59
3:B:234:THR:C	3:B:236:SER:H	2.05	0.59
3:B:218:TRP:CZ2	3:B:219:ILE:HD11	2.38	0.59
3:B:218:TRP:CH2	3:B:219:ILE:HD13	2.37	0.59
1:C:316:DC:OP2	1:C:316:DC:H2'	2.03	0.58
2:D:339:DG:O5'	2:D:339:DG:H2'	2.04	0.58
3:B:210:ARG:NH2	3:B:211:ARG:HB3	2.19	0.58
3:B:253:GLU:O	3:B:256:GLN:HB3	2.03	0.58
1:C:318:DT:OP2	1:C:318:DT:H6	1.87	0.58
3:A:254:LEU:HD12	3:B:254:LEU:HG	1.85	0.57
3:B:219:ILE:HG21	3:B:240:LYS:CG	2.21	0.57
1:C:305:DC:C4	2:D:339:DG:O6	2.57	0.57
1:C:320:DC:O3'	1:C:321:DA:C8	2.58	0.57
3:B:218:TRP:CE3	3:B:218:TRP:O	2.58	0.57
3:A:250:TYR:O	3:A:254:LEU:HD23	2.05	0.57
3:A:223:SER:HA	3:A:243:ILE:HG13	1.87	0.56
3:B:254:LEU:O	3:B:257:SER:OG	2.21	0.56
1:C:310:DA:H2"	1:C:311:DC:C5'	2.34	0.56
2:D:326:DA:H2"	2:D:327:DG:O5'	2.06	0.56
3:A:228:ASP:CG	3:A:229:SER:N	2.58	0.56
3:A:251:ILE:HD12	3:A:251:ILE:H	1.71	0.56
3:A:260:ARG:HH22	3:B:228:ASP:H	1.54	0.56
3:A:209:ARG:O	3:A:213:ASP:HB2	2.06	0.56
3:B:219:ILE:O	3:B:220:VAL:C	2.25	0.56
3:A:218:TRP:CD2	3:B:244:LEU:HB3	2.41	0.55
2:D:331:DA:H2"	2:D:332:DC:O5'	2.07	0.55
3:B:211:ARG:HA	3:B:214:LYS:CG	2.37	0.55
1:C:302:DA:H2'	1:C:303:DC:N1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:209:ARG:O	3:A:213:ASP:CB	2.56	0.54
3:B:196:MET:SD	3:B:198:GLU:HG3	2.47	0.54
1:C:305:DC:H5'	1:C:306:DG:OP2	2.08	0.54
3:A:215:ILE:O	3:A:218:TRP:CD1	2.60	0.54
1:C:302:DA:H2'	1:C:303:DC:C6	2.43	0.54
3:A:200:ARG:HG2	3:A:200:ARG:O	2.07	0.54
3:B:242:GLY:O	3:B:245:SER:N	2.41	0.54
3:B:211:ARG:HA	3:B:214:LYS:CB	2.38	0.54
1:C:302:DA:OP2	1:C:302:DA:C8	2.61	0.54
3:A:243:ILE:CG2	3:A:244:LEU:N	2.71	0.54
3:B:219:ILE:O	3:B:223:SER:HB2	2.07	0.54
3:B:218:TRP:CZ2	3:B:219:ILE:HD13	2.43	0.54
3:B:206:GLU:HA	3:B:209:ARG:NH1	2.23	0.53
3:B:215:ILE:O	3:B:219:ILE:HG13	2.07	0.53
3:B:251:ILE:O	3:B:255:ARG:CB	2.56	0.53
1:C:313:DT:C4	1:C:314:DG:C6	2.96	0.53
2:D:337:DC:H1'	2:D:338:DC:C6	2.43	0.53
3:A:212:ARG:O	3:A:215:ILE:N	2.42	0.53
3:A:218:TRP:O	3:A:221:GLN:HB2	2.09	0.53
3:A:254:LEU:CD1	3:B:254:LEU:HG	2.38	0.53
3:B:242:GLY:HA2	3:B:245:SER:OG	2.09	0.53
2:D:333:DG:N7	3:A:212:ARG:NH2	2.57	0.53
1:C:310:DA:H2'	1:C:311:DC:C6	2.43	0.52
3:B:219:ILE:HG13	3:B:240:LYS:HE3	1.90	0.52
3:A:254:LEU:O	3:B:254:LEU:HD21	2.10	0.52
3:A:255:ARG:HB3	3:B:225:ILE:HD12	1.91	0.52
3:A:260:ARG:NH2	3:B:228:ASP:H	2.08	0.52
2:D:330:DC:H2''	2:D:331:DA:C8	2.44	0.52
3:B:210:ARG:NE	3:B:211:ARG:H	2.07	0.52
3:B:210:ARG:HE	3:B:211:ARG:H	1.57	0.52
3:B:212:ARG:O	3:B:215:ILE:CG2	2.54	0.52
3:B:206:GLU:HG3	3:B:207:VAL:N	2.24	0.52
2:D:324:DG:O5'	2:D:324:DG:C8	2.59	0.52
3:A:222:LEU:HB3	3:A:226:ILE:HD12	1.90	0.52
3:A:228:ASP:OD2	3:A:243:ILE:HA	2.10	0.52
3:A:248:SER:OG	3:B:222:LEU:CD2	2.58	0.52
3:B:206:GLU:HG3	3:B:207:VAL:H	1.75	0.52
3:B:257:SER:O	3:B:259:HIS:N	2.43	0.52
2:D:330:DC:C5'	3:A:239:SER:HB2	2.40	0.51
3:A:225:ILE:O	3:A:225:ILE:HG23	2.09	0.51
3:A:218:TRP:CZ2	3:A:219:ILE:HG12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:DC:H2'	1:C:304:DC:C6	2.46	0.51
3:B:199:LYS:HD3	3:B:202:ALA:CB	2.41	0.51
3:B:243:ILE:HG22	3:B:244:LEU:HD12	1.93	0.51
1:C:308:DT:OP2	1:C:308:DT:C6	2.58	0.51
3:B:206:GLU:O	3:B:209:ARG:CG	2.58	0.50
3:B:215:ILE:CA	3:B:218:TRP:CD1	2.92	0.50
3:B:255:ARG:C	3:B:257:SER:N	2.63	0.50
1:C:320:DC:O3'	1:C:321:DA:H8	1.93	0.50
3:B:204:HIS:O	3:B:208:GLU:N	2.45	0.50
3:A:243:ILE:O	3:A:245:SER:N	2.45	0.50
3:A:215:ILE:O	3:A:219:ILE:HG13	2.12	0.50
2:D:326:DA:H8	3:B:200:ARG:HH21	1.56	0.50
3:A:240:LYS:O	3:A:243:ILE:HG22	2.12	0.50
3:A:248:SER:OG	3:B:222:LEU:HD21	2.11	0.50
3:A:255:ARG:CZ	3:B:225:ILE:HB	2.41	0.50
3:B:258:ASN:ND2	3:B:258:ASN:H	2.10	0.50
1:C:312:DG:OP2	3:B:209:ARG:NH1	2.45	0.49
3:A:200:ARG:O	3:A:202:ALA:N	2.45	0.49
3:A:212:ARG:O	3:A:213:ASP:C	2.50	0.49
3:B:217:ASN:O	3:B:221:GLN:HB2	2.12	0.49
2:D:332:DC:H2'	2:D:333:DG:C8	2.48	0.49
3:B:210:ARG:CG	3:B:211:ARG:N	2.74	0.49
3:B:244:LEU:N	3:B:244:LEU:CD1	2.75	0.49
3:B:255:ARG:C	3:B:257:SER:H	2.15	0.49
3:A:222:LEU:O	3:A:226:ILE:N	2.45	0.49
3:B:220:VAL:HG23	3:B:221:GLN:N	2.26	0.49
3:B:241:GLY:O	3:B:244:LEU:HD13	2.12	0.49
3:B:211:ARG:O	3:B:214:LYS:CB	2.53	0.49
3:A:218:TRP:CE3	3:B:244:LEU:HB3	2.47	0.49
3:B:217:ASN:HD22	3:B:217:ASN:HA	1.53	0.49
3:A:212:ARG:O	3:A:214:LYS:N	2.46	0.49
3:A:217:ASN:HA	3:A:220:VAL:CG1	2.43	0.49
3:A:228:ASP:CG	3:A:229:SER:H	2.16	0.49
3:B:198:GLU:OE2	3:B:199:LYS:HG2	2.13	0.49
3:B:251:ILE:O	3:B:255:ARG:HB3	2.13	0.48
3:B:206:GLU:HA	3:B:209:ARG:NH2	2.26	0.48
2:D:330:DC:H5"	3:A:239:SER:CB	2.43	0.48
3:A:244:LEU:O	3:A:244:LEU:HD13	2.14	0.48
3:B:251:ILE:CG2	3:B:252:GLN:N	2.76	0.48
2:D:338:DC:H5'	2:D:339:DG:OP2	2.13	0.48
2:D:326:DA:C2	2:D:327:DG:H1'	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:219:ILE:O	3:B:223:SER:CB	2.62	0.48
3:B:219:ILE:HD12	3:B:240:LYS:HE2	1.89	0.48
3:A:215:ILE:O	3:A:218:TRP:NE1	2.47	0.48
3:B:242:GLY:O	3:B:244:LEU:N	2.47	0.48
2:D:333:DG:OP2	3:A:205:ASN:ND2	2.46	0.47
3:B:209:ARG:HG2	3:B:209:ARG:NH1	2.29	0.47
3:B:250:TYR:N	3:B:250:TYR:CD1	2.80	0.47
1:C:309:DC:H5	3:A:211:ARG:NE	2.12	0.47
3:B:223:SER:O	3:B:243:ILE:HD13	2.14	0.47
1:C:314:DG:H1	2:D:330:DC:H42	1.62	0.47
1:C:317:DC:H2"	1:C:318:DT:OP2	2.13	0.47
3:B:234:THR:C	3:B:236:SER:N	2.67	0.47
1:C:310:DA:N6	2:D:333:DG:O6	2.48	0.47
1:C:317:DC:H2'	1:C:317:DC:H5'	1.46	0.47
1:C:319:DA:N1	2:D:325:DT:C4	2.82	0.47
3:A:243:ILE:C	3:A:245:SER:N	2.67	0.47
3:B:207:VAL:O	3:B:210:ARG:NE	2.48	0.47
3:A:218:TRP:NE1	3:A:219:ILE:HG12	2.29	0.47
1:C:305:DC:H2'	1:C:306:DG:N7	2.28	0.47
3:A:208:GLU:O	3:A:211:ARG:N	2.42	0.47
3:A:222:LEU:HD22	3:A:222:LEU:N	2.28	0.46
3:B:219:ILE:HD11	3:B:240:LYS:NZ	2.30	0.46
3:A:260:ARG:HH22	3:B:228:ASP:N	2.13	0.46
3:B:226:ILE:HB	3:B:227:PRO:HD2	1.96	0.46
2:D:330:DC:H5"	3:A:239:SER:HB2	1.98	0.46
3:B:241:GLY:HA2	3:B:244:LEU:HD22	1.97	0.46
3:A:210:ARG:O	3:A:214:LYS:HG2	2.14	0.46
3:B:234:THR:O	3:B:236:SER:N	2.49	0.46
3:A:246:LYS:O	3:A:247:ALA:C	2.54	0.46
2:D:330:DC:H2"	2:D:331:DA:H5'	1.98	0.46
3:B:215:ILE:C	3:B:219:ILE:HG12	2.36	0.46
3:B:218:TRP:CE3	3:B:218:TRP:C	2.89	0.46
3:A:208:GLU:HG2	3:A:212:ARG:NH2	2.30	0.45
3:B:207:VAL:O	3:B:207:VAL:CG1	2.64	0.45
3:B:251:ILE:HG22	3:B:252:GLN:N	2.31	0.45
3:B:209:ARG:C	3:B:212:ARG:HB2	2.36	0.45
3:A:211:ARG:HA	3:A:214:LYS:HG3	1.98	0.45
3:A:225:ILE:HA	3:A:225:ILE:HD12	1.57	0.45
3:A:208:GLU:C	3:A:210:ARG:N	2.69	0.45
3:B:220:VAL:CG2	3:B:221:GLN:N	2.80	0.45
3:B:226:ILE:H	3:B:226:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:DC:H6	1:C:309:DC:C5'	2.29	0.45
1:C:316:DC:P	1:C:316:DC:H3'	2.57	0.45
2:D:338:DC:H5"	2:D:338:DC:H6	1.81	0.45
3:B:218:TRP:CH2	3:B:219:ILE:CD1	2.99	0.45
1:C:320:DC:N4	2:D:324:DG:H1	2.13	0.45
3:B:217:ASN:C	3:B:219:ILE:N	2.69	0.45
3:B:218:TRP:HE3	3:B:218:TRP:O	1.99	0.45
1:C:320:DC:H2'	1:C:320:DC:P	2.57	0.45
3:A:249:ASP:OD1	3:A:250:TYR:N	2.50	0.44
3:B:248:SER:C	3:B:251:ILE:HG22	2.38	0.44
3:A:226:ILE:CD1	3:A:251:ILE:HD11	2.47	0.44
3:A:226:ILE:HD11	3:A:251:ILE:HD11	2.00	0.44
1:C:309:DC:N4	3:A:208:GLU:OE1	2.51	0.44
3:A:214:LYS:HE2	3:A:214:LYS:HB3	1.69	0.44
3:B:209:ARG:HG2	3:B:209:ARG:HH11	1.82	0.44
3:B:227:PRO:CG	3:B:250:TYR:CE2	2.78	0.44
3:B:218:TRP:CE3	3:B:222:LEU:HD22	2.41	0.44
2:D:336:DA:H2"	2:D:337:DC:H5'	1.99	0.44
3:A:243:ILE:HG22	3:A:244:LEU:N	2.32	0.44
3:A:204:HIS:HB3	3:A:205:ASN:H	1.59	0.44
3:B:220:VAL:O	3:B:221:GLN:C	2.56	0.43
3:A:257:SER:O	3:A:258:ASN:ND2	2.51	0.43
3:B:242:GLY:C	3:B:244:LEU:N	2.71	0.43
1:C:320:DC:H1'	1:C:321:DA:O4'	2.17	0.43
3:B:241:GLY:CA	3:B:244:LEU:HD22	2.49	0.43
3:A:253:GLU:HG3	3:A:254:LEU:HD23	2.00	0.43
3:B:247:ALA:O	3:B:251:ILE:HB	2.19	0.43
3:B:256:GLN:HG3	3:B:260:ARG:HB3	2.00	0.43
1:C:308:DT:OP2	1:C:308:DT:O4'	2.36	0.43
3:B:197:ASP:O	3:B:197:ASP:CG	2.56	0.43
3:B:203:GLN:O	3:B:205:ASN:N	2.51	0.43
3:B:218:TRP:CZ3	3:B:219:ILE:HD13	2.54	0.43
3:B:257:SER:O	3:B:259:HIS:CE1	2.72	0.43
3:A:252:GLN:CG	3:A:253:GLU:N	2.80	0.42
3:A:255:ARG:HD2	3:A:255:ARG:C	2.39	0.42
3:B:206:GLU:CG	3:B:207:VAL:N	2.82	0.42
3:A:260:ARG:HH22	3:B:227:PRO:HA	1.84	0.42
3:B:204:HIS:HA	3:B:207:VAL:HB	2.02	0.42
3:A:218:TRP:CG	3:A:219:ILE:N	2.87	0.42
1:C:304:DC:H2"	1:C:305:DC:C5'	2.50	0.42
3:A:232:GLU:CD	3:A:233:SER:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:ARG:HE	3:A:201:ARG:HA	1.85	0.42
1:C:318:DT:H2'	1:C:318:DT:P	2.59	0.42
3:B:254:LEU:HD12	3:B:257:SER:OG	2.20	0.42
3:A:208:GLU:O	3:A:210:ARG:N	2.52	0.41
3:B:218:TRP:O	3:B:222:LEU:HD22	2.20	0.41
2:D:330:DC:H5''	3:A:239:SER:OG	2.19	0.41
3:A:219:ILE:HG13	3:A:219:ILE:H	1.63	0.41
2:D:330:DC:OP1	3:A:241:GLY:N	2.53	0.41
1:C:305:DC:O2	2:D:339:DG:N1	2.48	0.41
2:D:329:DC:OP2	3:B:210:ARG:NH1	2.52	0.41
1:C:319:DA:H2	2:D:325:DT:H3	1.64	0.41
3:A:215:ILE:O	3:A:215:ILE:CG2	2.68	0.41
3:A:259:HIS:CD2	3:A:260:ARG:N	2.88	0.41
3:B:198:GLU:O	3:B:200:ARG:N	2.53	0.41
3:B:211:ARG:O	3:B:211:ARG:HG2	2.20	0.41
1:C:304:DC:N3	2:D:340:DG:O6	2.54	0.41
1:C:309:DC:H5'	1:C:309:DC:C6	2.55	0.41
2:D:325:DT:C2'	2:D:326:DA:O4'	2.63	0.41
1:C:314:DG:H2''	1:C:315:DG:C5'	2.50	0.41
2:D:332:DC:H2''	2:D:333:DG:OP1	2.20	0.41
2:D:339:DG:O5'	2:D:339:DG:C2'	2.64	0.41
3:B:222:LEU:N	3:B:222:LEU:CD1	2.83	0.41
3:B:226:ILE:HG22	3:B:227:PRO:HD2	2.03	0.41
3:B:256:GLN:CG	3:B:260:ARG:HB3	2.50	0.41
2:D:328:DG:H2'	2:D:329:DC:O4'	2.21	0.40
1:C:304:DC:C2	1:C:305:DC:C6	3.10	0.40
1:C:314:DG:C2	1:C:315:DG:C5	3.09	0.40
3:A:259:HIS:HD2	3:A:260:ARG:N	2.20	0.40
3:B:201:ARG:NH1	3:B:201:ARG:HB3	2.36	0.40
1:C:320:DC:H2'	1:C:320:DC:OP2	2.21	0.40
3:A:260:ARG:NH2	3:B:227:PRO:HA	2.36	0.40
3:B:241:GLY:O	3:B:244:LEU:HB2	2.22	0.40
3:B:256:GLN:O	3:B:257:SER:C	2.60	0.40

There are no symmetry-related clashes.

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	
3	A	63/65 (97%)	23 (36%)	25 (40%)	15 (24%)	0	0
3	B	63/65 (97%)	35 (56%)	13 (21%)	15 (24%)	0	0
All	All	126/130 (97%)	58 (46%)	38 (30%)	30 (24%)	0	0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	201	ARG
3	A	231	MET
3	A	236	SER
3	A	240	LYS
3	A	247	ALA
3	A	256	GLN
3	B	199	LYS
3	B	201	ARG
3	B	227	PRO
3	B	232	GLU
3	B	239	SER
3	B	257	SER
3	B	259	HIS
3	A	233	SER
3	A	235	LYS
3	A	249	ASP
3	B	229	SER
3	B	240	LYS
3	B	258	ASN
3	A	197	ASP
3	A	213	ASP
3	A	248	SER
3	B	228	ASP
3	B	230	SER
3	B	235	LYS

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Mol	Chain	Res	Type
3	B	243	ILE
3	A	253	GLU
3	A	227	PRO
3	A	220	VAL
3	B	242	GLY

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	
3	A	60/60 (100%)	34 (57%)	26 (43%)	0	0
3	B	60/60 (100%)	37 (62%)	23 (38%)	0	0
All	All	120/120 (100%)	71 (59%)	49 (41%)	0	0

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	198	GLU
3	A	200	ARG
3	A	201	ARG
3	A	209	ARG
3	A	212	ARG
3	A	215	ILE
3	A	219	ILE
3	A	220	VAL
3	A	221	GLN
3	A	222	LEU
3	A	223	SER
3	A	224	LYS
3	A	225	ILE
3	A	231	MET
3	A	232	GLU
3	A	236	SER
3	A	240	LYS
3	A	243	ILE

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Mol	Chain	Res	Type
3	A	244	LEU
3	A	245	SER
3	A	249	ASP
3	A	250	TYR
3	A	252	GLN
3	A	254	LEU
3	A	257	SER
3	A	260	ARG
3	B	197	ASP
3	B	198	GLU
3	B	200	ARG
3	B	205	ASN
3	B	206	GLU
3	B	209	ARG
3	B	210	ARG
3	B	211	ARG
3	B	212	ARG
3	B	214	LYS
3	B	215	ILE
3	B	217	ASN
3	B	222	LEU
3	B	226	ILE
3	B	232	GLU
3	B	235	LYS
3	B	238	GLN
3	B	239	SER
3	B	244	LEU
3	B	245	SER
3	B	246	LYS
3	B	251	ILE
3	B	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	203	GLN
3	A	258	ASN
3	A	259	HIS
3	B	216	ASN
3	B	217	ASN
3	B	258	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.