



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:49 PM UTC

PDB ID : 1AN4 / pdb_00001an4
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)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

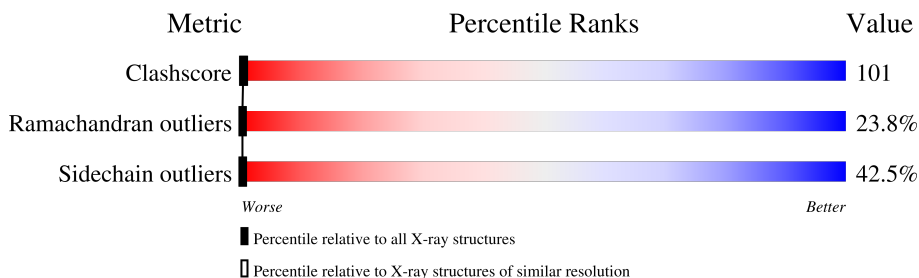
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	21	5% 57% 38%
2	D	21	5% 29% 43% 24%
3	A	65	9% 29% 48% 14%
3	B	65	6% 32% 40% 22%

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*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*GP*GP*TP*CP*AP*CP*GP*TP*GP*GP*CP*C P*TP*AP*CP*A)-3')

Chain C: 



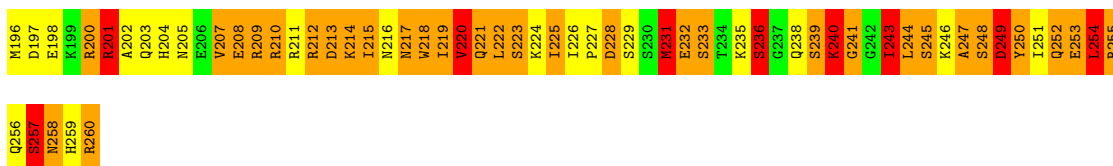
- Molecule 2: DNA (5'-D(*GP*TP*GP*TP*AP*GP*GP*CP*CP*AP*CP*GP*TP*GP*AP*CP*C P*GP*GP*GP*T)-3')

Chain D: 



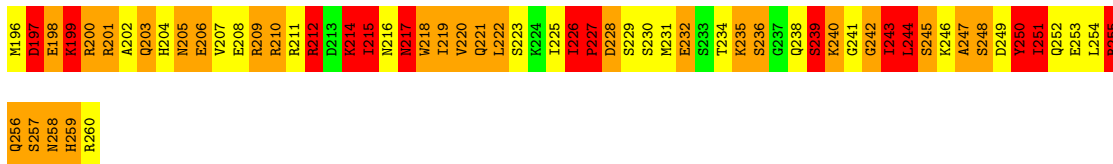
- Molecule 3: PROTEIN (UPSTREAM STIMULATORY FACTOR)

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	1.27	2/472 (0.4%)	2.53	51/725 (7.0%)
2	D	1.17	1/486 (0.2%)	2.33	42/750 (5.6%)
3	A	1.21	2/539 (0.4%)	1.74	15/716 (2.1%)
3	B	1.28	6/539 (1.1%)	2.20	27/716 (3.8%)
All	All	1.23	11/2036 (0.5%)	2.22	135/2907 (4.6%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	207	VAL	CA-CB	11.68	1.67	1.54
3	B	215	ILE	CA-C	8.55	1.61	1.52
3	B	216	ASN	N-CA	7.94	1.57	1.46
3	B	219	ILE	C-N	-6.96	1.24	1.33
3	B	231	MET	SD-CE	6.96	1.97	1.79
1	C	308	DT	O3'-P	6.70	1.71	1.61
3	A	243	ILE	CA-CB	6.16	1.60	1.55
1	C	304	DC	O3'-P	6.00	1.70	1.61
3	B	219	ILE	C-O	-5.56	1.18	1.24
2	D	323	DT	O3'-P	5.32	1.69	1.61
3	B	218	TRP	NE1-CE2	-5.08	1.31	1.37

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	255	ARG	N-CA-C	-14.68	95.83	113.88
3	A	239	SER	N-CA-C	13.88	130.71	110.59
3	B	219	ILE	CA-C-N	-13.04	99.68	120.55
3	B	219	ILE	C-N-CA	-13.04	99.68	120.55
3	B	219	ILE	O-C-N	-12.48	105.67	121.90
2	D	327	DG	C1'-O4'-C4'	-12.09	91.56	109.70
1	C	305	DC	C1'-O4'-C4'	-11.99	91.71	109.70
1	C	320	DC	O4'-C1'-N1	11.83	126.15	108.40
1	C	309	DC	O4'-C1'-N1	11.77	126.05	108.40
3	B	251	ILE	N-CA-C	-11.41	99.47	110.42
3	B	226	ILE	CA-C-N	11.28	133.94	119.84
3	B	226	ILE	C-N-CA	11.28	133.94	119.84
3	B	256	GLN	N-CA-C	-10.67	100.21	113.01
3	B	250	TYR	N-CA-C	-10.13	101.05	113.41
1	C	302	DA	P-O3'-C3'	-9.65	105.73	120.20
1	C	311	DC	C5'-C4'-O4'	-9.50	95.14	109.40
3	B	214	LYS	N-CA-C	-9.47	101.28	113.12
1	C	306	DG	C5'-C4'-O4'	9.23	123.24	109.40
1	C	309	DC	N1-C1'-C2'	-8.79	100.31	113.50
1	C	306	DG	C5'-C4'-C3'	-8.78	101.72	114.90
3	A	203	GLN	N-CA-C	-8.72	92.22	110.80
3	B	203	GLN	N-CA-C	-8.67	101.77	111.14
1	C	320	DC	C2'-C3'-O3'	-8.54	98.69	111.50
2	D	322	DG	O4'-C1'-N9	8.51	121.17	108.40
3	A	217	ASN	N-CA-C	8.35	123.08	113.15
2	D	322	DG	C3'-C2'-C1'	-8.33	89.10	101.60
3	B	197	ASP	N-CA-C	-8.22	99.54	111.30
2	D	338	DC	P-O3'-C3'	-8.16	107.95	120.20
3	A	208	GLU	N-CA-C	8.15	120.08	111.03
1	C	304	DC	P-O3'-C3'	8.11	132.36	120.20
2	D	337	DC	C5'-C4'-C3'	-8.01	102.88	114.90
1	C	317	DC	O4'-C1'-N1	7.88	120.22	108.40
2	D	325	DT	P-O3'-C3'	7.87	132.00	120.20
2	D	322	DG	C1'-O4'-C4'	-7.86	97.92	109.70
1	C	315	DG	C1'-O4'-C4'	-7.85	97.93	109.70
1	C	313	DT	P-O5'-C5'	-7.81	108.29	120.00
1	C	314	DG	C5'-C4'-C3'	-7.80	103.21	114.90
2	D	337	DC	O4'-C1'-N1	7.66	119.89	108.40
3	A	241	GLY	N-CA-C	-7.63	102.33	115.61
2	D	324	DG	P-O5'-C5'	7.62	131.43	120.00
1	C	310	DA	O4'-C4'-C3'	-7.61	93.99	105.40
2	D	330	DC	O5'-C5'-C4'	7.53	122.10	110.80
1	C	310	DA	O4'-C1'-C2'	-7.47	95.19	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	337	DC	P-O3'-C3'	-7.43	109.06	120.20
2	D	336	DA	C5'-C4'-C3'	-7.41	103.78	114.90
3	B	248	SER	N-CA-C	-7.36	104.55	113.97
2	D	331	DA	N9-C1'-C2'	-7.32	102.52	113.50
3	B	220	VAL	O-C-N	7.27	131.44	121.84
2	D	342	DT	P-O5'-C5'	7.22	130.83	120.00
1	C	316	DC	P-O3'-C3'	7.13	130.89	120.20
2	D	326	DA	C1'-O4'-C4'	-7.03	99.16	109.70
2	D	327	DG	N9-C1'-C2'	6.97	123.95	113.50
2	D	328	DG	P-O5'-C5'	6.97	130.45	120.00
1	C	321	DA	C5'-C4'-C3'	-6.95	104.47	114.90
3	B	231	MET	N-CA-C	-6.91	104.17	112.59
1	C	320	DC	C4'-C3'-O3'	6.86	120.29	110.00
1	C	301	DC	O4'-C1'-N1	6.86	118.68	108.40
1	C	320	DC	P-O3'-C3'	6.81	130.41	120.20
2	D	323	DT	C4'-C3'-O3'	6.80	120.20	110.00
2	D	336	DA	O4'-C1'-C2'	-6.75	96.28	106.40
2	D	336	DA	C5'-C4'-O4'	6.69	119.43	109.40
1	C	314	DG	C5'-C4'-O4'	6.68	119.41	109.40
3	B	218	TRP	CA-C-N	-6.66	111.21	120.74
3	B	218	TRP	C-N-CA	-6.66	111.21	120.74
1	C	305	DC	O4'-C4'-C3'	-6.64	95.43	105.40
3	A	207	VAL	N-CA-C	6.62	116.73	110.30
3	B	199	LYS	N-CA-C	6.62	124.91	110.80
1	C	306	DG	O5'-C5'-C4'	6.62	120.72	110.80
1	C	320	DC	P-O5'-C5'	6.56	129.84	120.00
2	D	323	DT	O3'-P-O5'	-6.55	94.17	104.00
3	A	218	TRP	N-CA-C	-6.46	105.05	113.12
1	C	302	DA	O4'-C4'-C3'	-6.40	95.80	105.40
2	D	336	DA	P-O3'-C3'	-6.40	110.61	120.20
1	C	311	DC	O3'-P-O5'	6.38	113.58	104.00
1	C	315	DG	C3'-C2'-C1'	-6.34	92.09	101.60
3	A	228	ASP	N-CA-C	6.32	118.79	109.69
1	C	315	DG	N9-C1'-C2'	6.31	122.97	113.50
3	B	212	ARG	N-CA-C	-6.28	103.36	111.02
3	A	255	ARG	N-CA-C	-6.26	104.08	111.03
1	C	301	DC	N1-C1'-C2'	-6.25	104.13	113.50
1	C	312	DG	C4'-C3'-O3'	-6.22	100.67	110.00
2	D	341	DG	C1'-O4'-C4'	-6.15	100.48	109.70
1	C	315	DG	P-O3'-C3'	6.13	129.40	120.20
2	D	335	DG	P-O3'-C3'	6.11	129.36	120.20
1	C	303	DC	P-O3'-C3'	6.08	129.32	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	332	DC	P-O5'-C5'	6.07	129.11	120.00
3	B	215	ILE	O-C-N	-6.00	114.79	122.17
3	A	210	ARG	N-CA-C	-5.95	104.92	111.82
3	B	239	SER	N-CA-C	5.94	123.46	110.80
2	D	322	DG	N9-C1'-C2'	5.93	122.39	113.50
1	C	317	DC	O5'-C5'-C4'	5.93	119.69	110.80
3	A	258	ASN	N-CA-C	5.90	123.37	110.80
3	B	236	SER	N-CA-C	-5.89	99.57	107.88
1	C	320	DC	N1-C1'-C2'	-5.89	104.66	113.50
3	A	254	LEU	N-CA-C	-5.87	106.77	114.04
2	D	324	DG	N9-C1'-C2'	-5.71	104.94	113.50
1	C	305	DC	N1-C1'-C2'	5.70	122.06	113.50
2	D	337	DC	C5'-C4'-O4'	5.68	117.93	109.40
1	C	313	DT	C4'-C3'-O3'	5.66	118.49	110.00
3	B	244	LEU	N-CA-C	-5.63	102.31	111.04
1	C	314	DG	O5'-C5'-C4'	5.61	119.22	110.80
1	C	303	DC	P-O5'-C5'	5.59	128.38	120.00
2	D	331	DA	C5'-C4'-O4'	5.54	117.72	109.40
1	C	302	DA	P-O5'-C5'	5.54	128.31	120.00
2	D	328	DG	P-O3'-C3'	5.51	128.47	120.20
1	C	307	DG	O3'-P-O5'	-5.50	95.74	104.00
1	C	311	DC	O4'-C1'-C2'	-5.49	98.16	106.40
1	C	307	DG	C5'-C4'-C3'	-5.48	106.68	114.90
2	D	342	DT	C2'-C3'-O3'	5.48	119.72	111.50
3	A	236	SER	N-CA-C	5.46	122.42	110.80
2	D	327	DG	P-O3'-C3'	5.45	128.37	120.20
2	D	323	DT	O5'-C5'-C4'	5.42	118.93	110.80
2	D	326	DA	P-O5'-C5'	5.41	128.12	120.00
2	D	324	DG	C4'-C3'-O3'	5.40	118.10	110.00
1	C	320	DC	C5'-C4'-C3'	-5.37	106.84	114.90
1	C	317	DC	C4'-C3'-C2'	-5.36	94.36	102.40
2	D	332	DC	P-O3'-C3'	5.36	128.23	120.20
2	D	331	DA	O5'-C5'-C4'	5.35	118.82	110.80
3	B	217	ASN	CA-C-N	-5.35	110.59	121.18
3	B	217	ASN	C-N-CA	-5.35	110.59	121.18
3	B	247	ALA	N-CA-C	-5.35	106.94	112.93
2	D	342	DT	O4'-C1'-C2'	-5.27	98.50	106.40
1	C	319	DA	P-O3'-C3'	5.26	128.09	120.20
2	D	325	DT	C4'-C3'-O3'	5.25	117.87	110.00
2	D	326	DA	P-O3'-C3'	-5.23	112.35	120.20
1	C	319	DA	C1'-O4'-C4'	-5.21	101.89	109.70
2	D	339	DG	C5'-C4'-C3'	-5.21	107.09	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	257	SER	N-CA-C	5.20	119.11	112.87
1	C	307	DG	C5'-C4'-O4'	5.18	117.17	109.40
1	C	310	DA	P-O5'-C5'	5.16	127.74	120.00
1	C	315	DG	O4'-C4'-C3'	-5.14	97.68	105.40
2	D	338	DC	N3-C4-N4	5.13	125.59	117.90
3	B	227	PRO	N-CA-C	5.06	122.89	112.47
1	C	306	DG	P-O5'-C5'	5.05	127.57	120.00
3	A	240	LYS	N-CA-C	5.01	121.48	110.80

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
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	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	534	0	537	172	0
All	All	1923	0	1547	343	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 101.

All (343) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:ARG:C	3:B:214:LYS:HB2	2.16	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
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:A:228:ASP:CG	3:A:243:ILE:HA	2.18	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:A:244:LEU:HD13	3:A:244:LEU:C	2.20	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
1:C:318:DT:H3	2:D:326:DA:N6	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:THR:C	3:B:236:SER:H	2.05	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: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
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
3:B:219:ILE:O	3:B:220:VAL:C	2.25	0.61
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
3:A:228:ASP:CG	3:A:229:SER:N	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
3:B:255:ARG:C	3:B:257:SER:N	2.63	0.55
1:C:302:DA:H2'	1:C:303:DC:N1	2.21	0.55
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:255:ARG:C	3:B:257:SER:H	2.15	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:A:212:ARG:O	3:A:213:ASP:C	2.50	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:ASP:CG	3:A:229:SER:H	2.16	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
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:234:THR:C	3:B:236:SER:N	2.67	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:A:246:LYS:O	3:A:247:ALA:C	2.54	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:B:215:ILE:C	3:B:219:ILE:HG12	2.36	0.50
3:B:218:TRP:CE3	3:B:218:TRP:C	2.89	0.50
3:A:243:ILE:O	3:A:245:SER:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:215:ILE:O	3:A:219:ILE:HG13	2.12	0.50
3:B:209:ARG:C	3:B:212:ARG:HB2	2.36	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:208:GLU:C	3:A:210:ARG:N	2.69	0.50
3:A:255:ARG:CZ	3:B:225:ILE:HB	2.41	0.50
1:C:312:DG:OP2	3:B:209:ARG:NH1	2.45	0.49
3:B:258:ASN:ND2	3:B:258:ASN:H	2.10	0.49
3:A:200:ARG:O	3:A:202:ALA:N	2.45	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:A:243:ILE:C	3:A:245:SER:N	2.67	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:A:222:LEU:O	3:A:226:ILE:N	2.45	0.49
3:B:217:ASN:C	3:B:219:ILE:N	2.69	0.49
3:B:241:GLY:O	3:B:244:LEU:HD13	2.12	0.49
3:B:248:SER:C	3:B:251:ILE:HG22	2.38	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:B:198:GLU:OE2	3:B:199:LYS:HG2	2.13	0.49
3:B:220:VAL:HG23	3:B:221:GLN:N	2.26	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
3:B:220:VAL:O	3:B:221:GLN:C	2.56	0.48
2:D:330:DC:H5''	3:A:239:SER:CB	2.43	0.48
3:A:244:LEU:HD13	3:A:244:LEU:O	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
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:197:ASP:O	3:B:197:ASP:CG	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:255:ARG:HD2	3:A:255:ARG:C	2.39	0.47
1:C:310:DA:N6	2:D:333:DG:O6	2.48	0.47
3:B:242:GLY:C	3:B:244:LEU:N	2.71	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: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
3:A:232:GLU:CD	3:A:233:SER:H	2.23	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
2:D:330:DC:H2''	2:D:331:DA:H5'	1.98	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: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:B:226:ILE:H	3:B:226:ILE:HD12	1.82	0.45
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:218:TRP:HE3	3:B:218:TRP:O	1.99	0.45
3:B:256:GLN:O	3:B:257:SER:C	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:DC:N4	3:A:208:GLU:OE1	2.51	0.44
3:B:212:ARG:C	3:B:214:LYS:H	2.23	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
3:A:222:LEU:O	3:A:223:SER:C	2.60	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:B:205:ASN:OD1	3:B:205:ASN:C	2.60	0.44
3:A:204:HIS:HB3	3:A:205:ASN:H	1.59	0.44
3:B:220:VAL:CG2	3:B:221:GLN:N	2.80	0.44
3:A:257:SER:O	3:A:258:ASN:ND2	2.51	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:218:TRP:C	3:B:218:TRP:CD2	2.95	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: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:B:206:GLU:CG	3:B:207:VAL:N	2.82	0.42
3:B:257:SER:C	3:B:259:HIS:N	2.77	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:201:ARG:HE	3:A:201:ARG:HA	1.85	0.42
3:B:207:VAL:C	3:B:210:ARG:HB3	2.44	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:C	3:A:210:ARG:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:GLY:C	3:B:244:LEU:H	2.29	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

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
3	A	63/65 (97%)	23 (36%)	25 (40%)	15 (24%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	32 (53%)	28 (47%)	0	0
3	B	60/60 (100%)	37 (62%)	23 (38%)	0	0
All	All	120/120 (100%)	69 (58%)	51 (42%)	0	0

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	196	MET
3	A	198	GLU
3	A	200	ARG
3	A	201	ARG
3	A	207	VAL
3	A	209	ARG
3	A	212	ARG
3	A	214	LYS
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	243	ILE
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

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Mol	Chain	Res	Type
3	B	205	ASN
3	B	206	GLU
3	B	209	ARG
3	B	210	ARG
3	B	212	ARG
3	B	214	LYS
3	B	215	ILE
3	B	217	ASN
3	B	221	GLN
3	B	222	LEU
3	B	226	ILE
3	B	232	GLU
3	B	235	LYS
3	B	239	SER
3	B	243	ILE
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	203	GLN
3	A	204	HIS
3	A	258	ASN
3	A	259	HIS
3	B	203	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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.