



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

PDB ID : 2GLI
Title : FIVE-FINGER GLI/DNA COMPLEX
Authors : Pavletich, N.P.; Pabo, C.O.
Deposited on : 1993-11-09
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

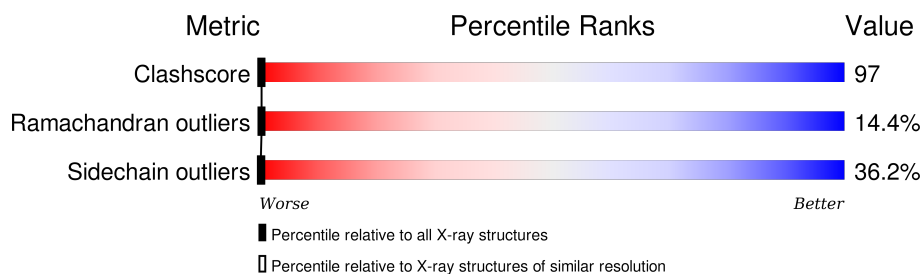
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	21	
2	D	21	
3	A	155	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2174 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(*TP*TP*TP*CP*GP*TP*CP*TP*TP*GP*GP*GP*TP*GP*GP*TP*CP*CP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	21	Total	C	N	O	P	0	0	0
			427	205	71	131	20			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*GP*TP*GP*GP*AP*CP*CP*AP*CP*CP*CP*AP*AP*GP*AP*CP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	P	0	0	0
			428	203	88	117	20			

- Molecule 3 is a protein called PROTEIN (FIVE-FINGER GLI).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	155	Total	C	N	O	S	0	0	0
			1270	776	250	231	13			

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Co	0	0
			5	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	C	18	Total	O	0	0
			18	18		
5	D	14	Total	O	0	0
			14	14		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

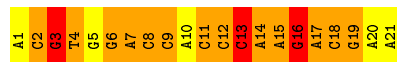
- Molecule 1: DNA (5'-D(*TP*TP*TP*CP*GP*TP*CP*TP*TP*GP*GP*GP*TP*GP*GP*TP*CP*CP*AP*CP*G)-3')

Chain C: 



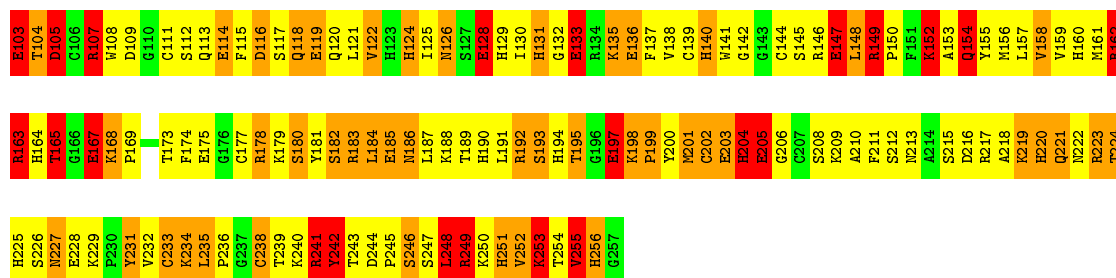
- Molecule 2: DNA (5'-D(*AP*CP*GP*TP*GP*GP*AP*CP*CP*AP*CP*CP*CP*AP*AP*GP*AP*CP*GP*AP*A)-3')

Chain D: 



- Molecule 3: PROTEIN (FIVE-FINGER GLI)

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.00 Å 50.20 Å 45.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.228 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2174	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.63	4/476 (0.8%)	2.83	49/734 (6.7%)
2	D	1.68	6/482 (1.2%)	2.80	49/741 (6.6%)
3	A	1.07	14/1304 (1.1%)	1.79	36/1746 (2.1%)
All	All	1.35	24/2262 (1.1%)	2.32	134/3221 (4.2%)

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	6
2	D	0	6
3	A	2	0
All	All	2	12

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	12	DC	N1-C6	-9.60	1.31	1.37
2	D	13	DC	C3'-O3'	-7.57	1.34	1.44
3	A	119	GLU	CD-OE2	7.53	1.33	1.25
2	D	11	DC	C1'-N1	-7.28	1.37	1.47
3	A	205	GLU	CD-OE2	7.20	1.33	1.25
3	A	203	GLU	CD-OE2	6.98	1.33	1.25
3	A	147	GLU	CD-OE2	6.83	1.33	1.25
1	C	11	DG	N9-C4	6.83	1.43	1.38
1	C	14	DG	C3'-O3'	-6.75	1.35	1.44
3	A	228	GLU	CD-OE2	6.69	1.33	1.25
3	A	133	GLU	CD-OE2	6.29	1.32	1.25
2	D	13	DC	C1'-N1	-6.26	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	136	GLU	CD-OE2	6.20	1.32	1.25
1	C	12	DG	C6-N1	-6.17	1.35	1.39
3	A	103	GLU	CD-OE2	6.15	1.32	1.25
3	A	167	GLU	CD-OE2	5.94	1.32	1.25
2	D	11	DC	N1-C6	-5.85	1.33	1.37
3	A	114	GLU	CD-OE2	5.81	1.32	1.25
3	A	175	GLU	CD-OE2	5.63	1.31	1.25
1	C	6	DT	C1'-N1	5.55	1.56	1.49
3	A	128	GLU	CD-OE2	5.46	1.31	1.25
3	A	197	GLU	CD-OE2	5.12	1.31	1.25
3	A	185	GLU	CD-OE2	5.04	1.31	1.25
2	D	12	DC	N3-C4	-5.01	1.30	1.33

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	DT	P-O3'-C3'	17.31	140.47	119.70
2	D	12	DC	O4'-C4'-C3'	-15.47	96.72	106.00
2	D	11	DC	C1'-O4'-C4'	-13.88	96.22	110.10
2	D	16	DG	O4'-C4'-C3'	-13.48	97.91	106.00
2	D	15	DA	O4'-C4'-C3'	-12.84	98.29	106.00
1	C	8	DT	P-O5'-C5'	-12.30	101.22	120.90
1	C	12	DG	N1-C6-O6	-11.90	112.76	119.90
1	C	10	DG	O4'-C1'-N9	11.35	115.95	108.00
2	D	12	DC	C1'-O4'-C4'	-11.07	99.03	110.10
1	C	11	DG	N9-C4-C5	10.93	109.77	105.40
2	D	15	DA	P-O3'-C3'	10.74	132.59	119.70
3	A	192	ARG	NE-CZ-NH2	-10.71	114.94	120.30
2	D	21	DA	O4'-C1'-N9	10.66	115.46	108.00
1	C	11	DG	C4-C5-N7	-10.43	106.63	110.80
2	D	15	DA	O4'-C1'-N9	10.29	115.20	108.00
1	C	11	DG	O4'-C4'-C3'	-10.27	99.84	106.00
2	D	12	DC	O4'-C1'-C2'	-9.92	97.97	105.90
2	D	18	DC	P-O3'-C3'	9.86	131.54	119.70
2	D	7	DA	O4'-C1'-N9	9.81	114.87	108.00
2	D	17	DA	C4'-C3'-C2'	-9.76	94.31	103.10
2	D	16	DG	O4'-C1'-N9	-9.32	101.47	108.00
1	C	7	DC	P-O3'-C3'	9.25	130.80	119.70
1	C	11	DG	O4'-C1'-N9	9.22	114.46	108.00
1	C	19	DA	P-O3'-C3'	9.15	130.68	119.70
1	C	4	DC	O4'-C1'-N1	9.01	114.31	108.00
1	C	13	DT	P-O5'-C5'	-8.99	106.51	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	149	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	C	12	DG	P-O5'-C5'	-8.56	107.21	120.90
1	C	17	DC	O4'-C1'-N1	8.55	113.99	108.00
1	C	20	DC	O4'-C1'-N1	8.54	113.98	108.00
2	D	11	DC	C6-N1-C2	8.53	123.71	120.30
2	D	12	DC	O4'-C1'-N1	-8.47	102.07	108.00
1	C	1	DT	O4'-C4'-C3'	-8.38	100.97	106.00
1	C	14	DG	O4'-C1'-N9	-8.37	102.14	108.00
2	D	8	DC	P-O3'-C3'	8.36	129.73	119.70
1	C	12	DG	C5-C6-O6	8.30	133.58	128.60
1	C	11	DG	C8-N9-C4	-8.05	103.18	106.40
1	C	9	DT	O4'-C1'-N1	8.01	113.61	108.00
1	C	11	DG	C4'-C3'-C2'	-7.95	95.95	103.10
3	A	154	GLN	CB-CA-C	7.88	126.17	110.40
2	D	9	DC	O4'-C4'-C3'	-7.86	101.29	106.00
2	D	21	DA	O4'-C1'-C2'	-7.70	99.74	105.90
1	C	15	DG	O4'-C1'-N9	-7.66	102.64	108.00
1	C	6	DT	O4'-C1'-N1	7.65	113.36	108.00
2	D	16	DG	P-O3'-C3'	-7.49	110.72	119.70
3	A	107	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	C	11	DG	C8-N9-C1'	7.45	136.68	127.00
1	C	21	DG	N3-C2-N2	-7.44	114.69	119.90
3	A	223	ARG	CD-NE-CZ	7.30	133.82	123.60
1	C	14	DG	P-O3'-C3'	7.27	128.43	119.70
2	D	11	DC	O4'-C4'-C3'	-7.20	101.62	104.50
2	D	12	DC	N3-C4-N4	-6.93	113.15	118.00
3	A	241	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	10	DG	O4'-C1'-C2'	-6.91	100.37	105.90
3	A	249	ARG	NE-CZ-NH1	6.89	123.75	120.30
3	A	223	ARG	CG-CD-NE	6.88	126.24	111.80
1	C	19	DA	O4'-C1'-N9	6.81	112.77	108.00
3	A	216	ASP	CB-CG-OD2	-6.77	112.21	118.30
2	D	13	DC	C2-N1-C1'	-6.74	111.38	118.80
1	C	4	DC	O4'-C4'-C3'	-6.72	101.81	104.50
3	A	203	GLU	N-CA-CB	6.69	122.64	110.60
2	D	13	DC	N3-C2-O2	6.65	126.56	121.90
3	A	182	SER	N-CA-CB	-6.63	100.55	110.50
3	A	116	ASP	CB-CG-OD2	-6.59	112.37	118.30
3	A	165	THR	N-CA-CB	6.53	122.71	110.30
1	C	20	DC	C6-N1-C2	-6.52	117.69	120.30
2	D	18	DC	N1-C2-O2	-6.47	115.02	118.90
2	D	4	DT	O4'-C1'-C2'	-6.46	100.73	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	DA	C1'-O4'-C4'	-6.44	103.66	110.10
2	D	13	DC	O3'-P-O5'	-6.39	91.86	104.00
1	C	20	DC	N3-C4-C5	-6.39	119.34	121.90
1	C	19	DA	N1-C6-N6	6.34	122.40	118.60
1	C	18	DC	C6-N1-C2	6.33	122.83	120.30
1	C	15	DG	C5-C6-O6	-6.33	124.80	128.60
3	A	241	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	11	DG	C6-C5-N7	6.26	134.16	130.40
1	C	2	DT	N3-C4-O4	6.25	123.65	119.90
1	C	21	DG	C1'-O4'-C4'	-6.25	103.85	110.10
3	A	183	ARG	CB-CA-C	6.22	122.84	110.40
3	A	152	LYS	N-CA-CB	6.19	121.75	110.60
2	D	13	DC	N1-C2-O2	-6.17	115.20	118.90
2	D	2	DC	O4'-C1'-N1	6.15	112.31	108.00
3	A	242	TYR	CB-CG-CD1	6.09	124.65	121.00
2	D	12	DC	C2-N3-C4	-6.09	116.86	119.90
3	A	192	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	11	DG	C5-N7-C8	6.04	107.32	104.30
2	D	18	DC	C4'-C3'-C2'	-6.02	97.69	103.10
3	A	109	ASP	CB-CG-OD1	6.01	123.71	118.30
3	A	223	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	1	DT	C6-C5-C7	-5.99	119.31	122.90
1	C	19	DA	P-O5'-C5'	5.92	130.38	120.90
1	C	7	DC	C4'-C3'-C2'	-5.91	97.79	103.10
3	A	116	ASP	CB-CG-OD1	5.83	123.55	118.30
3	A	109	ASP	CB-CG-OD2	-5.78	113.10	118.30
3	A	107	ARG	NE-CZ-NH2	-5.72	117.44	120.30
3	A	124	HIS	CA-CB-CG	5.70	123.29	113.60
2	D	11	DC	C3'-C2'-C1'	-5.68	95.69	102.50
3	A	223	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	D	2	DC	O4'-C1'-C2'	-5.65	101.38	105.90
3	A	231	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	C	2	DT	C5-C4-O4	-5.63	120.96	124.90
1	C	21	DG	C4-N9-C1'	-5.60	119.22	126.50
3	A	204	HIS	CB-CA-C	5.59	121.59	110.40
3	A	178	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	D	5	DG	C4'-C3'-C2'	-5.59	98.07	103.10
2	D	7	DA	O4'-C4'-C3'	-5.58	102.27	104.50
2	D	9	DC	P-O5'-C5'	-5.56	112.01	120.90
2	D	9	DC	O4'-C1'-N1	5.52	111.86	108.00
2	D	13	DC	C1'-O4'-C4'	-5.52	104.58	110.10
3	A	242	TYR	CB-CG-CD2	-5.51	117.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	DG	O4'-C1'-N9	5.47	111.83	108.00
3	A	216	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	9	DT	C5-C4-O4	5.45	128.71	124.90
2	D	6	DG	C4'-C3'-C2'	-5.38	98.26	103.10
2	D	14	DA	O4'-C4'-C3'	-5.34	102.36	104.50
3	A	205	GLU	C-N-CA	-5.31	111.15	122.30
2	D	2	DC	N1-C2-O2	5.28	122.07	118.90
2	D	3	DG	O4'-C1'-N9	-5.27	104.31	108.00
3	A	255	VAL	N-CA-CB	5.26	123.07	111.50
1	C	12	DG	N3-C2-N2	5.25	123.58	119.90
3	A	202	CYS	N-CA-CB	5.20	119.95	110.60
3	A	227	ASN	CB-CA-C	5.17	120.73	110.40
3	A	131	HIS	N-CA-CB	5.17	119.90	110.60
3	A	154	GLN	CB-CG-CD	5.16	125.00	111.60
2	D	13	DC	O4'-C1'-N1	5.15	111.61	108.00
1	C	21	DG	N1-C2-N2	5.12	120.81	116.20
2	D	10	DA	O4'-C1'-N9	5.12	111.58	108.00
1	C	17	DC	N3-C4-N4	-5.11	114.43	118.00
2	D	18	DC	O4'-C1'-N1	5.10	111.57	108.00
1	C	17	DC	P-O5'-C5'	5.04	128.97	120.90
2	D	12	DC	C6-N1-C1'	-5.04	114.75	120.80
1	C	18	DC	N3-C4-C5	5.04	123.92	121.90
2	D	12	DC	N1-C2-O2	-5.03	115.88	118.90
2	D	9	DC	P-O3'-C3'	5.01	125.72	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	131	HIS	CA
3	A	152	LYS	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	10	DG	Sidechain
1	C	14	DG	Sidechain
1	C	15	DG	Sidechain
1	C	16	DT	Sidechain
1	C	17	DC	Sidechain
1	C	9	DT	Sidechain
2	D	13	DC	Sidechain
2	D	16	DG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	19	DG	Sidechain
2	D	3	DG	Sidechain
2	D	6	DG	Sidechain
2	D	7	DA	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	427	0	241	60	2
2	D	428	0	234	56	2
3	A	1270	0	1199	259	0
4	A	5	0	0	0	0
5	A	12	0	0	0	0
5	C	18	0	0	0	0
5	D	14	0	0	2	0
All	All	2174	0	1674	346	2

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 97.

All (346) 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:A:126:ASN:H	3:A:126:ASN:ND2	1.24	1.14
3:A:103:GLU:N	3:A:107:ARG:HH22	1.47	1.12
3:A:126:ASN:HD22	3:A:126:ASN:N	1.49	1.08
3:A:231:TYR:HB3	3:A:248:LEU:HD12	1.37	1.04
3:A:189:THR:HG21	3:A:213:ASN:HB3	1.41	1.02
3:A:252:VAL:HA	3:A:256:HIS:HD2	1.29	0.98
3:A:130:ILE:HD13	3:A:158:VAL:HG22	1.46	0.97
3:A:201:MET:HA	3:A:210:ALA:HB2	1.44	0.95
3:A:130:ILE:HG21	3:A:158:VAL:CG2	1.96	0.94
3:A:192:ARG:HB3	3:A:197:GLU:HB3	1.48	0.94
1:C:21:DG:O6	2:D:2:DC:N3	2.01	0.94
1:C:19:DA:N1	2:D:4:DT:N3	2.17	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:DG:C2'	2:D:17:DA:H5'	1.99	0.92
3:A:126:ASN:ND2	3:A:126:ASN:N	2.03	0.92
3:A:235:LEU:HD13	3:A:256:HIS:CG	2.03	0.92
2:D:1:DA:H2''	2:D:2:DC:OP2	1.69	0.92
2:D:14:DA:H5'	3:A:163:ARG:HD2	1.52	0.92
3:A:135:LYS:HE3	3:A:135:LYS:HA	1.49	0.92
3:A:130:ILE:HG21	3:A:158:VAL:HG23	1.52	0.91
3:A:103:GLU:N	3:A:107:ARG:NH2	2.17	0.90
3:A:192:ARG:HB3	3:A:197:GLU:CB	2.00	0.90
3:A:137:PHE:H	3:A:154:GLN:NE2	1.70	0.90
1:C:5:DG:H1	2:D:18:DC:N4	1.71	0.89
1:C:16:DT:H2''	1:C:17:DC:H5'	1.56	0.88
3:A:199:PRO:HG2	3:A:200:TYR:CD1	2.08	0.87
1:C:4:DC:H2'	1:C:5:DG:C8	2.11	0.86
3:A:231:TYR:CB	3:A:248:LEU:HD12	2.04	0.86
3:A:152:LYS:HE3	3:A:152:LYS:H	1.40	0.86
3:A:202:CYS:N	3:A:209:LYS:O	2.08	0.84
1:C:19:DA:N6	2:D:4:DT:O4	2.10	0.84
1:C:5:DG:H1	2:D:18:DC:H42	1.24	0.84
3:A:201:MET:HA	3:A:210:ALA:CB	2.08	0.83
3:A:130:ILE:HD13	3:A:158:VAL:CG2	2.09	0.82
2:D:17:DA:OP2	2:D:17:DA:H2'	1.80	0.82
3:A:209:LYS:HG3	3:A:210:ALA:N	1.95	0.82
3:A:137:PHE:HB2	3:A:154:GLN:NE2	1.95	0.81
3:A:235:LEU:HD13	3:A:256:HIS:ND1	1.94	0.81
3:A:116:ASP:OD1	3:A:120:GLN:NE2	2.14	0.81
3:A:147:GLU:OE2	3:A:147:GLU:HA	1.81	0.81
3:A:137:PHE:H	3:A:154:GLN:HE22	1.30	0.80
3:A:144:CYS:SG	3:A:146:ARG:HG2	2.21	0.80
1:C:1:DT:C2'	1:C:2:DT:H5'	2.12	0.79
1:C:2:DT:H2'	1:C:3:DT:H6	1.47	0.79
3:A:232:VAL:HG12	3:A:241:ARG:HE	1.47	0.79
2:D:16:DG:H2'	2:D:17:DA:H5'	1.65	0.77
3:A:223:ARG:O	3:A:226:SER:HB3	1.84	0.77
3:A:137:PHE:HB2	3:A:154:GLN:HB3	1.66	0.77
1:C:20:DC:H42	2:D:3:DG:H1	1.31	0.77
1:C:3:DT:OP2	3:A:155:TYR:HB3	1.86	0.76
3:A:130:ILE:CD1	3:A:158:VAL:HG22	2.14	0.76
3:A:169:PRO:HD2	3:A:182:SER:HA	1.68	0.75
3:A:201:MET:HG2	3:A:210:ALA:HB2	1.69	0.75
1:C:2:DT:H2'	1:C:3:DT:C6	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:DC:H2''	1:C:5:DG:O5'	1.86	0.74
1:C:14:DG:O6	2:D:9:DC:N4	2.19	0.74
3:A:157:LEU:O	3:A:160:HIS:HB3	1.86	0.74
3:A:201:MET:SD	3:A:208:SER:HA	2.28	0.74
3:A:252:VAL:HA	3:A:256:HIS:CD2	2.20	0.74
3:A:167:GLU:HG3	3:A:167:GLU:O	1.88	0.73
3:A:211:PHE:CD1	3:A:217:ARG:HA	2.23	0.73
1:C:14:DG:H2''	1:C:15:DG:C5'	2.18	0.73
3:A:240:LYS:HG3	3:A:251:HIS:CE1	2.24	0.73
2:D:20:DA:N7	5:D:204:HOH:O	2.20	0.73
3:A:219:LYS:O	3:A:221:GLN:N	2.22	0.73
2:D:16:DG:H2''	2:D:17:DA:H5'	1.71	0.73
1:C:5:DG:N2	2:D:18:DC:N3	2.37	0.73
3:A:251:HIS:O	3:A:253:LYS:N	2.19	0.72
3:A:162:ARG:HD2	3:A:167:GLU:HG2	1.71	0.72
1:C:14:DG:N1	2:D:9:DC:N3	2.30	0.72
3:A:107:ARG:CZ	3:A:141:TRP:HZ2	2.03	0.72
3:A:229:LYS:HB2	3:A:241:ARG:HG3	1.72	0.71
3:A:107:ARG:NH1	3:A:141:TRP:HZ2	1.88	0.71
1:C:20:DC:N3	2:D:3:DG:N2	2.35	0.71
1:C:3:DT:H2''	1:C:4:DC:H6	1.54	0.71
3:A:137:PHE:CB	3:A:154:GLN:HB3	2.19	0.71
3:A:199:PRO:HG2	3:A:200:TYR:HD1	1.54	0.71
3:A:162:ARG:HD2	3:A:167:GLU:CG	2.20	0.71
3:A:152:LYS:HE3	3:A:152:LYS:N	2.06	0.71
3:A:107:ARG:HD2	3:A:141:TRP:CE2	2.26	0.71
2:D:16:DG:H2''	2:D:17:DA:C5'	2.21	0.71
3:A:250:LYS:O	3:A:254:THR:HG22	1.90	0.70
3:A:107:ARG:HD2	3:A:141:TRP:CZ2	2.26	0.70
3:A:252:VAL:HG12	3:A:252:VAL:O	1.91	0.70
1:C:13:DT:H2''	1:C:14:DG:O5'	1.90	0.70
3:A:182:SER:O	3:A:183:ARG:HG3	1.91	0.70
3:A:113:GLN:HB3	3:A:115:PHE:CZ	2.26	0.70
2:D:1:DA:H1'	2:D:2:DC:O5'	1.91	0.69
3:A:121:LEU:HD11	3:A:125:ILE:HD11	1.72	0.69
1:C:20:DC:N4	2:D:3:DG:H1	1.89	0.69
3:A:160:HIS:O	3:A:163:ARG:HB2	1.92	0.69
3:A:209:LYS:HE3	3:A:211:PHE:CE2	2.27	0.69
1:C:16:DT:H2''	1:C:17:DC:C5'	2.23	0.69
3:A:118:GLN:O	3:A:122:VAL:HG13	1.93	0.69
3:A:137:PHE:HB2	3:A:154:GLN:CD	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:DT:H2''	1:C:3:DT:O5'	1.92	0.68
1:C:9:DT:H73	3:A:215:SER:HB2	1.75	0.68
3:A:226:SER:OG	3:A:227:ASN:N	2.27	0.68
2:D:16:DG:H2'	2:D:17:DA:C8	2.29	0.67
3:A:232:VAL:HG11	3:A:241:ARG:HH21	1.58	0.67
3:A:144:CYS:O	3:A:146:ARG:N	2.27	0.67
3:A:138:VAL:HG22	3:A:150:PRO:HA	1.77	0.67
3:A:128:GLU:OE1	3:A:128:GLU:N	2.27	0.67
3:A:188:LYS:O	3:A:191:LEU:HB2	1.94	0.67
3:A:107:ARG:NH1	3:A:141:TRP:CZ2	2.63	0.66
2:D:2:DC:H4'	2:D:3:DG:OP1	1.94	0.66
1:C:16:DT:C2'	1:C:17:DC:H5'	2.25	0.66
3:A:163:ARG:HH21	3:A:163:ARG:HG2	1.59	0.66
1:C:15:DG:H2'	1:C:16:DT:H71	1.79	0.65
3:A:219:LYS:O	3:A:220:HIS:C	2.34	0.65
1:C:15:DG:H2'	1:C:16:DT:C6	2.32	0.65
1:C:14:DG:H2''	1:C:15:DG:O5'	1.97	0.64
3:A:104:THR:O	3:A:105:ASP:HB3	1.95	0.64
3:A:248:LEU:O	3:A:251:HIS:N	2.27	0.64
3:A:137:PHE:N	3:A:154:GLN:NE2	2.43	0.64
3:A:246:SER:OG	3:A:249:ARG:NH2	2.31	0.64
3:A:251:HIS:HA	3:A:254:THR:HG22	1.79	0.64
2:D:16:DG:C2'	2:D:17:DA:C5'	2.75	0.63
3:A:135:LYS:HE3	3:A:135:LYS:CA	2.26	0.63
3:A:126:ASN:H	3:A:126:ASN:HD22	0.66	0.63
2:D:15:DA:C2'	2:D:16:DG:H8	2.12	0.63
3:A:217:ARG:O	3:A:221:GLN:HB3	1.98	0.63
3:A:231:TYR:CA	3:A:248:LEU:HD12	2.28	0.62
3:A:232:VAL:HG12	3:A:241:ARG:HB3	1.80	0.62
3:A:146:ARG:NE	3:A:149:ARG:O	2.29	0.62
3:A:255:VAL:O	3:A:256:HIS:O	2.18	0.61
1:C:3:DT:H2''	1:C:4:DC:C6	2.35	0.61
3:A:130:ILE:O	3:A:137:PHE:CZ	2.53	0.61
1:C:1:DT:H2'	1:C:2:DT:H5'	1.82	0.61
3:A:107:ARG:HD2	3:A:141:TRP:NE1	2.15	0.61
2:D:14:DA:OP2	3:A:183:ARG:NH1	2.33	0.61
2:D:15:DA:H2''	2:D:16:DG:H8	1.65	0.61
3:A:255:VAL:HG23	3:A:256:HIS:N	2.15	0.61
3:A:203:GLU:O	3:A:204:HIS:HB2	2.01	0.61
3:A:122:VAL:O	3:A:122:VAL:HG23	2.00	0.60
1:C:4:DC:H4'	1:C:5:DG:OP1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:232:VAL:CG1	3:A:241:ARG:HH21	2.14	0.60
3:A:255:VAL:HG23	3:A:256:HIS:H	1.65	0.60
3:A:117:SER:HB3	3:A:120:GLN:OE1	2.02	0.60
3:A:135:LYS:CE	3:A:135:LYS:HA	2.27	0.59
3:A:252:VAL:O	3:A:253:LYS:HB3	2.01	0.59
3:A:192:ARG:HB3	3:A:197:GLU:HB2	1.79	0.59
3:A:147:GLU:C	3:A:148:LEU:HD23	2.23	0.59
3:A:130:ILE:HG21	3:A:158:VAL:HG22	1.85	0.59
3:A:240:LYS:HG3	3:A:251:HIS:HE1	1.67	0.59
3:A:192:ARG:O	3:A:195:THR:N	2.30	0.59
3:A:130:ILE:HG22	3:A:131:HIS:HD2	1.68	0.58
2:D:15:DA:C2'	2:D:16:DG:C8	2.87	0.58
1:C:14:DG:C2'	1:C:15:DG:C5'	2.82	0.58
3:A:242:TYR:N	3:A:242:TYR:CD1	2.72	0.58
3:A:231:TYR:HB3	3:A:248:LEU:CD1	2.22	0.58
3:A:168:LYS:HB2	3:A:180:SER:HB2	1.86	0.58
3:A:169:PRO:CD	3:A:182:SER:HA	2.33	0.58
3:A:248:LEU:O	3:A:250:LYS:N	2.37	0.57
3:A:235:LEU:HD13	3:A:256:HIS:CB	2.34	0.57
3:A:126:ASN:O	3:A:131:HIS:HB2	2.04	0.57
3:A:146:ARG:O	3:A:148:LEU:N	2.37	0.57
3:A:137:PHE:CD1	3:A:154:GLN:CB	2.87	0.57
3:A:168:LYS:O	3:A:180:SER:HB3	2.05	0.57
3:A:235:LEU:O	3:A:238:CYS:HB2	2.05	0.57
3:A:181:TYR:CE1	3:A:190:HIS:CB	2.88	0.57
3:A:192:ARG:NH2	3:A:199:PRO:HG3	2.20	0.57
3:A:184:LEU:HD13	3:A:188:LYS:HE3	1.87	0.57
3:A:157:LEU:O	3:A:160:HIS:N	2.36	0.57
3:A:235:LEU:CD1	3:A:256:HIS:CG	2.85	0.57
3:A:181:TYR:CZ	3:A:190:HIS:HB2	2.39	0.57
2:D:3:DG:H2''	2:D:4:DT:O5'	2.05	0.56
3:A:130:ILE:HA	3:A:137:PHE:CE2	2.40	0.56
1:C:1:DT:C3'	1:C:2:DT:H5'	2.34	0.56
1:C:14:DG:C2'	1:C:15:DG:H5''	2.36	0.56
3:A:174:PHE:CE2	3:A:194:HIS:HB3	2.41	0.56
3:A:168:LYS:HB3	3:A:181:TYR:C	2.26	0.56
3:A:152:LYS:NZ	3:A:156:MET:SD	2.73	0.56
1:C:9:DT:C7	3:A:215:SER:HB2	2.35	0.55
1:C:2:DT:C2'	1:C:3:DT:H6	2.19	0.55
3:A:144:CYS:C	3:A:146:ARG:H	2.08	0.55
3:A:116:ASP:CG	3:A:120:GLN:NE2	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:113:GLN:NE2	3:A:115:PHE:CE2	2.75	0.55
3:A:152:LYS:CE	3:A:152:LYS:H	2.15	0.55
3:A:231:TYR:CE1	3:A:243:THR:O	2.60	0.54
3:A:108:TRP:CG	3:A:129:HIS:CD2	2.95	0.54
3:A:137:PHE:HB2	3:A:154:GLN:CB	2.36	0.54
3:A:215:SER:O	3:A:218:ALA:N	2.37	0.54
3:A:147:GLU:HB3	3:A:148:LEU:HG	1.90	0.54
3:A:121:LEU:CD1	3:A:125:ILE:CD1	2.85	0.54
3:A:137:PHE:CG	3:A:154:GLN:HB3	2.43	0.54
3:A:139:CYS:HB2	3:A:157:LEU:HD11	1.90	0.54
3:A:232:VAL:HA	3:A:241:ARG:HA	1.90	0.54
3:A:220:HIS:C	3:A:220:HIS:CD2	2.80	0.54
2:D:17:DA:H2'	2:D:17:DA:P	2.48	0.54
3:A:238:CYS:O	3:A:239:THR:HB	2.08	0.53
3:A:181:TYR:CE1	3:A:190:HIS:HB2	2.43	0.53
3:A:118:GLN:HE22	3:A:167:GLU:CB	2.21	0.53
3:A:138:VAL:CG2	3:A:150:PRO:HA	2.38	0.53
3:A:148:LEU:O	3:A:150:PRO:HD3	2.08	0.53
3:A:114:GLU:O	3:A:115:PHE:CD2	2.61	0.53
3:A:137:PHE:CB	3:A:154:GLN:NE2	2.70	0.53
3:A:200:TYR:O	3:A:211:PHE:N	2.31	0.53
3:A:174:PHE:CD2	3:A:194:HIS:HB3	2.43	0.53
3:A:161:MET:O	3:A:165:THR:N	2.38	0.53
3:A:132:GLY:O	3:A:133:GLU:O	2.26	0.53
2:D:15:DA:C2	2:D:16:DG:C5	2.97	0.53
3:A:130:ILE:HG22	3:A:130:ILE:O	2.09	0.53
3:A:255:VAL:CG2	3:A:256:HIS:H	2.22	0.52
1:C:20:DC:N4	2:D:2:DC:C4	2.77	0.52
3:A:248:LEU:C	3:A:248:LEU:HD23	2.30	0.52
2:D:14:DA:H2''	2:D:15:DA:O5'	2.10	0.52
3:A:247:SER:O	3:A:248:LEU:O	2.28	0.51
3:A:211:PHE:HD1	3:A:217:ARG:CB	2.24	0.51
3:A:198:LYS:HB2	3:A:198:LYS:HZ2	1.76	0.51
3:A:231:TYR:CZ	3:A:245:PRO:HD3	2.46	0.51
1:C:16:DT:C2'	1:C:17:DC:C5'	2.87	0.51
3:A:138:VAL:HG12	3:A:140:HIS:ND1	2.25	0.51
3:A:253:LYS:CD	3:A:253:LYS:C	2.78	0.51
3:A:122:VAL:O	3:A:122:VAL:CG2	2.59	0.51
3:A:163:ARG:NH2	3:A:163:ARG:HG2	2.26	0.50
1:C:7:DC:N3	2:D:16:DG:C6	2.78	0.50
1:C:19:DA:H4'	1:C:20:DC:OP1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:DA:H2''	2:D:16:DG:C8	2.46	0.50
3:A:184:LEU:HD22	3:A:188:LYS:HG3	1.94	0.50
3:A:200:TYR:HB2	3:A:211:PHE:O	2.10	0.50
1:C:2:DT:C2'	1:C:3:DT:C6	2.91	0.50
3:A:198:LYS:HB2	3:A:198:LYS:NZ	2.26	0.50
3:A:137:PHE:H	3:A:154:GLN:CD	2.14	0.50
3:A:187:LEU:HG	3:A:187:LEU:O	1.98	0.50
3:A:121:LEU:HD11	3:A:125:ILE:CD1	2.41	0.50
3:A:256:HIS:H	3:A:256:HIS:CD2	2.23	0.50
2:D:11:DC:H2''	2:D:12:DC:O5'	2.12	0.49
3:A:130:ILE:HG22	3:A:131:HIS:CD2	2.46	0.49
3:A:137:PHE:CD1	3:A:154:GLN:HB3	2.47	0.49
1:C:15:DG:H1	2:D:8:DC:N4	2.10	0.49
3:A:133:GLU:CD	3:A:133:GLU:H	2.16	0.49
3:A:218:ALA:O	3:A:219:LYS:O	2.30	0.49
3:A:255:VAL:CG2	3:A:256:HIS:N	2.75	0.49
3:A:235:LEU:HD13	3:A:256:HIS:HB3	1.95	0.49
3:A:205:GLU:OE1	3:A:225:HIS:ND1	2.45	0.49
3:A:161:MET:O	3:A:164:HIS:N	2.46	0.49
3:A:189:THR:O	3:A:190:HIS:C	2.49	0.49
2:D:17:DA:OP2	2:D:17:DA:H8	1.95	0.49
3:A:229:LYS:HB3	3:A:242:TYR:C	2.34	0.49
3:A:219:LYS:O	3:A:222:ASN:N	2.46	0.49
3:A:211:PHE:HD1	3:A:217:ARG:HG3	1.78	0.48
3:A:253:LYS:HD3	3:A:253:LYS:C	2.34	0.48
3:A:217:ARG:O	3:A:221:GLN:CB	2.61	0.48
3:A:138:VAL:HG22	3:A:150:PRO:CA	2.43	0.48
3:A:108:TRP:HA	3:A:140:HIS:O	2.13	0.48
3:A:211:PHE:CD1	3:A:217:ARG:CB	2.96	0.48
3:A:162:ARG:HD2	3:A:167:GLU:HG3	1.94	0.48
3:A:121:LEU:CD1	3:A:125:ILE:HD11	2.42	0.48
1:C:5:DG:C6	2:D:18:DC:N4	2.74	0.48
3:A:241:ARG:O	3:A:241:ARG:HG2	2.13	0.48
2:D:12:DC:C4	2:D:13:DC:C4	3.01	0.48
3:A:198:LYS:HG2	3:A:210:ALA:O	2.14	0.48
2:D:11:DC:C4	2:D:12:DC:C5	3.02	0.47
3:A:159:VAL:O	3:A:159:VAL:HG12	2.13	0.47
3:A:130:ILE:CG2	3:A:130:ILE:O	2.62	0.47
3:A:186:ASN:O	3:A:187:LEU:C	2.50	0.47
1:C:21:DG:C6	2:D:2:DC:N3	2.81	0.47
3:A:117:SER:HB3	3:A:120:GLN:CD	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:MET:CA	3:A:210:ALA:HB2	2.30	0.47
3:A:202:CYS:SG	3:A:221:GLN:NE2	2.88	0.47
2:D:15:DA:H2'	2:D:16:DG:C8	2.49	0.47
3:A:138:VAL:CG1	3:A:140:HIS:CE1	2.98	0.47
3:A:189:THR:C	3:A:191:LEU:N	2.66	0.47
2:D:11:DC:C2	2:D:12:DC:C6	3.02	0.47
3:A:173:THR:O	3:A:174:PHE:C	2.53	0.47
3:A:234:LYS:HE3	3:A:234:LYS:HB2	1.53	0.47
3:A:159:VAL:O	3:A:162:ARG:HG3	2.15	0.46
3:A:137:PHE:HD1	3:A:154:GLN:CG	2.29	0.46
3:A:107:ARG:CD	3:A:141:TRP:CZ2	2.98	0.46
3:A:144:CYS:O	3:A:147:GLU:N	2.35	0.46
3:A:251:HIS:CD2	3:A:252:VAL:N	2.83	0.46
2:D:3:DG:H2'	2:D:4:DT:H71	1.97	0.46
3:A:248:LEU:O	3:A:249:ARG:C	2.54	0.46
1:C:5:DG:N1	2:D:18:DC:N4	2.40	0.46
1:C:2:DT:H2''	1:C:3:DT:O4'	2.16	0.46
3:A:133:GLU:N	3:A:133:GLU:CD	2.69	0.45
3:A:253:LYS:O	3:A:253:LYS:HD3	2.17	0.45
3:A:218:ALA:HA	3:A:221:GLN:HB3	1.98	0.45
3:A:146:ARG:O	3:A:149:ARG:N	2.37	0.45
2:D:16:DG:H2''	2:D:17:DA:H5''	1.95	0.45
1:C:18:DC:H1'	1:C:19:DA:N7	2.32	0.45
1:C:14:DG:H2''	1:C:15:DG:C4'	2.46	0.45
3:A:138:VAL:HG12	3:A:140:HIS:HD1	1.81	0.45
3:A:211:PHE:HD1	3:A:217:ARG:HB2	1.82	0.45
3:A:137:PHE:CA	3:A:154:GLN:NE2	2.80	0.44
1:C:18:DC:H4'	1:C:19:DA:OP1	2.14	0.44
3:A:135:LYS:CE	3:A:135:LYS:CA	2.92	0.44
3:A:153:ALA:CB	3:A:155:TYR:CD1	3.00	0.44
3:A:130:ILE:HG21	3:A:130:ILE:HD13	1.78	0.44
3:A:189:THR:O	3:A:191:LEU:N	2.50	0.44
3:A:232:VAL:HA	3:A:241:ARG:CB	2.46	0.44
3:A:251:HIS:C	3:A:251:HIS:CD2	2.90	0.44
2:D:20:DA:C8	5:D:204:HOH:O	2.66	0.44
3:A:138:VAL:HG23	3:A:150:PRO:HB3	2.00	0.44
3:A:121:LEU:HD12	3:A:125:ILE:HD12	2.00	0.44
1:C:7:DC:H2'	1:C:7:DC:O5'	2.18	0.44
3:A:147:GLU:O	3:A:148:LEU:HD23	2.18	0.44
3:A:231:TYR:C	3:A:248:LEU:HD12	2.38	0.44
3:A:182:SER:C	3:A:183:ARG:HG3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:235:LEU:HA	3:A:236:PRO:HD3	1.74	0.44
1:C:15:DG:H1	2:D:8:DC:H42	1.66	0.44
2:D:18:DC:H1'	2:D:19:DG:C8	2.53	0.43
1:C:19:DA:N1	2:D:4:DT:C2	2.85	0.43
2:D:8:DC:H3'	3:A:224:THR:OG1	2.18	0.43
3:A:226:SER:O	3:A:227:ASN:ND2	2.51	0.43
1:C:18:DC:H1'	1:C:19:DA:C8	2.54	0.43
3:A:138:VAL:HG12	3:A:140:HIS:CE1	2.54	0.43
3:A:199:PRO:HD2	3:A:212:SER:HA	2.00	0.43
1:C:3:DT:C2'	1:C:4:DC:C6	3.02	0.43
3:A:211:PHE:CD1	3:A:211:PHE:N	2.85	0.43
3:A:148:LEU:O	3:A:150:PRO:CD	2.67	0.42
1:C:15:DG:N2	2:D:8:DC:N3	2.64	0.42
3:A:152:LYS:N	3:A:152:LYS:CE	2.78	0.42
3:A:203:GLU:O	3:A:204:HIS:CB	2.67	0.42
3:A:152:LYS:HE3	3:A:152:LYS:CA	2.48	0.42
3:A:233:CYS:SG	3:A:234:LYS:N	2.92	0.42
3:A:137:PHE:HB2	3:A:154:GLN:HE21	1.82	0.42
3:A:181:TYR:CD1	3:A:187:LEU:HA	2.54	0.42
3:A:198:LYS:O	3:A:200:TYR:N	2.52	0.42
3:A:211:PHE:HD1	3:A:217:ARG:CG	2.32	0.42
3:A:235:LEU:CD1	3:A:256:HIS:HB3	2.49	0.42
3:A:138:VAL:HG11	3:A:140:HIS:CE1	2.55	0.42
3:A:211:PHE:CD1	3:A:217:ARG:CA	2.99	0.42
3:A:108:TRP:CD1	3:A:129:HIS:HD2	2.38	0.42
3:A:138:VAL:HG12	3:A:138:VAL:O	2.18	0.42
3:A:251:HIS:CE1	3:A:255:VAL:CG2	3.03	0.42
3:A:174:PHE:CE1	3:A:191:LEU:HD22	2.54	0.42
3:A:121:LEU:O	3:A:125:ILE:HD12	2.20	0.42
3:A:137:PHE:HD1	3:A:154:GLN:CB	2.33	0.41
3:A:137:PHE:HB2	3:A:154:GLN:CG	2.49	0.41
3:A:153:ALA:HB3	3:A:155:TYR:CD1	2.56	0.41
3:A:163:ARG:CG	3:A:163:ARG:HH21	2.31	0.41
3:A:197:GLU:O	3:A:199:PRO:HD3	2.20	0.41
2:D:8:DC:H6	2:D:8:DC:H2'	1.67	0.41
3:A:191:LEU:O	3:A:194:HIS:N	2.52	0.41
1:C:5:DG:C2	2:D:18:DC:N3	2.88	0.41
2:D:11:DC:N3	2:D:12:DC:C5	2.89	0.41
3:A:251:HIS:CE1	3:A:255:VAL:HG21	2.56	0.41
1:C:11:DG:O6	3:A:219:LYS:NZ	2.46	0.41
1:C:7:DC:N3	2:D:16:DG:O6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:DC:C6	1:C:8:DT:H72	2.56	0.40
1:C:13:DT:C2'	1:C:14:DG:O5'	2.63	0.40
3:A:121:LEU:HD12	3:A:125:ILE:CD1	2.51	0.40
3:A:153:ALA:HB1	3:A:155:TYR:HD1	1.85	0.40
3:A:153:ALA:HB3	3:A:155:TYR:CE1	2.56	0.40
3:A:192:ARG:O	3:A:193:SER:C	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:DT:N3	2:D:1:DA:N1[1_544]	2.03	0.17
1:C:1:DT:O4	2:D:1:DA:N6[1_544]	2.19	0.01

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	153/155 (99%)	105 (69%)	26 (17%)	22 (14%)	0 0

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	105	ASP
3	A	133	GLU
3	A	145	SER
3	A	149	ARG
3	A	204	HIS
3	A	219	LYS
3	A	220	HIS
3	A	249	ARG
3	A	252	VAL

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Mol	Chain	Res	Type
3	A	253	LYS
3	A	255	VAL
3	A	256	HIS
3	A	142	GLY
3	A	147	GLU
3	A	248	LEU
3	A	136	GLU
3	A	162	ARG
3	A	163	ARG
3	A	186	ASN
3	A	206	GLY
3	A	158	VAL
3	A	199	PRO

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	141/141 (100%)	90 (64%)	51 (36%)	0 0

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

Mol	Chain	Res	Type
3	A	103	GLU
3	A	104	THR
3	A	105	ASP
3	A	107	ARG
3	A	111	CYS
3	A	112	SER
3	A	118	GLN
3	A	119	GLU
3	A	122	VAL
3	A	124	HIS
3	A	126	ASN
3	A	128	GLU
3	A	133	GLU

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Mol	Chain	Res	Type
3	A	135	LYS
3	A	140	HIS
3	A	147	GLU
3	A	148	LEU
3	A	149	ARG
3	A	152	LYS
3	A	154	GLN
3	A	162	ARG
3	A	163	ARG
3	A	165	THR
3	A	167	GLU
3	A	168	LYS
3	A	177	CYS
3	A	178	ARG
3	A	179	LYS
3	A	180	SER
3	A	184	LEU
3	A	185	GLU
3	A	193	SER
3	A	195	THR
3	A	197	GLU
3	A	198	LYS
3	A	201	MET
3	A	205	GLU
3	A	221	GLN
3	A	224	THR
3	A	233	CYS
3	A	234	LYS
3	A	235	LEU
3	A	238	CYS
3	A	241	ARG
3	A	242	TYR
3	A	244	ASP
3	A	246	SER
3	A	248	LEU
3	A	251	HIS
3	A	253	LYS
3	A	255	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	113	GLN
3	A	118	GLN
3	A	126	ASN
3	A	131	HIS
3	A	154	GLN
3	A	170	HIS
3	A	186	ASN
3	A	204	HIS
3	A	213	ASN
3	A	221	GLN
3	A	227	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.