



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:57 AM UTC

PDB ID : 2GLI / pdb_00002gli
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

<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

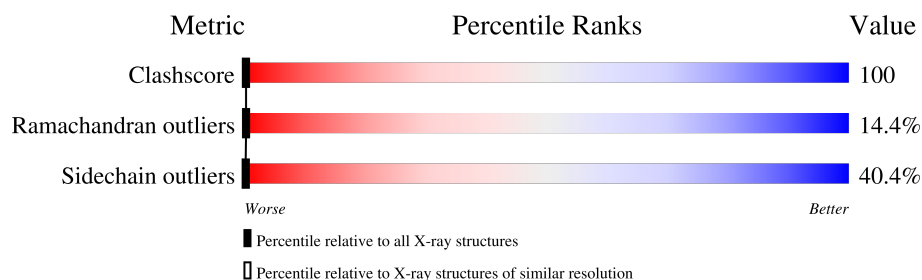
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 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	29% 57% 14%
2	D	21	14% 19% 57% 10%
3	A	155	9% 40% 37% 14%

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 (CCD ID: 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	C	18	Total	O	0	0
			18	18		
5	D	14	Total	O	0	0
			14	14		
5	A	12	Total	O	0	0
			12	12		

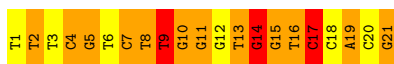
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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(*TP*TP*TP*CP*GP*TP*CP*TP*TP*GP*GP*GP*TP*GP*GP*TP*CP*CP*AP*CP*G)-3')

Chain C: 



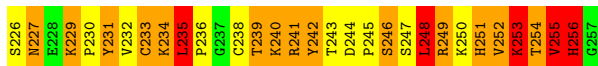
- Molecule 2: DNA (5'-D(*AP*CP*GP*TP*GP*GP*AP*CP*CP*AP*CP*CP*CP*AP*AP*GP*AP*CP*GP*AP*A)-3')

Chain D: 



- Molecule 3: PROTEIN (FIVE-FINGER GLI)

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.00Å 50.20Å 45.40Å 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	0.73	0/476	2.03	19/734 (2.6%)
2	D	0.77	0/482	1.83	16/741 (2.2%)
3	A	1.22	1/1304 (0.1%)	2.22	72/1746 (4.1%)
All	All	1.05	1/2262 (0.0%)	2.09	107/3221 (3.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	203	GLU	CA-C	-5.37	1.46	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	DT	P-O3'-C3'	13.51	140.47	120.20
1	C	8	DT	P-O5'-C5'	-12.52	101.22	120.00
3	A	115	PHE	N-CA-C	10.01	121.06	108.45
3	A	154	GLN	CB-CA-C	9.89	126.17	109.55
3	A	124	HIS	CA-CB-CG	9.49	123.29	113.80
1	C	13	DT	P-O5'-C5'	-8.99	106.51	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	11	DC	C1'-O4'-C4'	-8.99	96.22	109.70
1	C	14	DG	C4'-C3'-O3'	-8.53	97.20	110.00
1	C	12	DG	P-O5'-C5'	-8.53	107.21	120.00
3	A	165	THR	N-CA-CB	8.48	122.71	110.16
3	A	131	HIS	N-CA-C	8.27	123.92	107.62
2	D	15	DA	P-O3'-C3'	8.26	132.59	120.20
3	A	256	HIS	CA-CB-CG	-8.21	105.59	113.80
3	A	152	LYS	N-CA-CB	8.12	121.75	109.98
2	D	13	DC	O3'-P-O5'	-8.09	91.86	104.00
3	A	154	GLN	CA-C-O	7.95	127.79	119.05
1	C	6	DT	C2'-C3'-O3'	7.92	123.39	111.50
3	A	211	PHE	CA-CB-CG	-7.65	106.15	113.80
2	D	18	DC	P-O3'-C3'	7.56	131.54	120.20
3	A	203	GLU	N-CA-CB	7.44	122.64	110.37
3	A	210	ALA	N-CA-C	7.38	120.66	109.23
3	A	154	GLN	CB-CG-CD	7.29	125.00	112.60
3	A	199	PRO	CB-CA-C	-7.29	99.53	111.56
3	A	143	GLY	CA-C-N	-7.27	112.75	122.42
3	A	143	GLY	C-N-CA	-7.27	112.75	122.42
3	A	183	ARG	CB-CA-C	7.26	122.84	109.70
3	A	255	VAL	N-CA-CB	7.17	123.07	111.23
3	A	239	THR	CA-C-N	7.14	131.59	121.02
3	A	239	THR	C-N-CA	7.14	131.59	121.02
2	D	12	DC	C1'-O4'-C4'	-7.11	99.03	109.70
1	C	7	DC	P-O3'-C3'	7.07	130.80	120.20
3	A	126	ASN	CA-CB-CG	-7.06	105.54	112.60
1	C	19	DA	P-O3'-C3'	6.99	130.68	120.20
3	A	235	LEU	O-C-N	6.96	127.58	121.39
1	C	19	DA	P-O5'-C5'	6.92	130.38	120.00
3	A	214	ALA	O-C-N	6.86	129.50	122.09
1	C	19	DA	C4'-C3'-O3'	6.80	120.21	110.00
3	A	181	TYR	N-CA-C	-6.80	99.88	108.45
3	A	223	ARG	CD-NE-CZ	6.73	133.82	124.40
3	A	207	CYS	N-CA-C	6.68	119.55	111.40
3	A	223	ARG	CG-CD-NE	6.47	126.24	112.00
1	C	11	DG	C8-N9-C1'	6.46	136.68	127.00
3	A	151	PHE	CA-C-N	-6.43	111.89	120.63
3	A	151	PHE	C-N-CA	-6.43	111.89	120.63
2	D	14	DA	C4'-C3'-O3'	-6.41	100.39	110.00
3	A	203	GLU	O-C-N	6.41	130.68	123.05
3	A	230	PRO	N-CA-CB	6.39	108.34	101.88
3	A	202	CYS	N-CA-CB	6.38	119.95	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	165	THR	N-CA-C	6.37	118.31	111.36
2	D	8	DC	P-O3'-C3'	6.36	129.73	120.20
2	D	16	DG	P-O3'-C3'	-6.32	110.72	120.20
3	A	147	GLU	CA-C-N	-6.28	112.56	122.79
3	A	147	GLU	C-N-CA	-6.28	112.56	122.79
1	C	4	DC	O5'-C5'-C4'	-6.25	101.43	110.80
3	A	214	ALA	CA-C-O	-6.24	114.28	120.70
3	A	254	THR	N-CA-C	-6.16	103.17	112.04
3	A	239	THR	N-CA-CB	-6.12	103.17	113.15
2	D	13	DC	C2'-C3'-O3'	-6.09	102.36	111.50
3	A	172	CYS	N-CA-C	-6.02	101.61	110.52
1	C	17	DC	P-O5'-C5'	5.98	128.97	120.00
3	A	124	HIS	CB-CG-ND1	-5.96	113.76	122.70
3	A	202	CYS	CA-C-N	-5.93	115.12	122.84
3	A	202	CYS	C-N-CA	-5.93	115.12	122.84
3	A	190	HIS	CA-CB-CG	-5.93	107.87	113.80
3	A	152	LYS	CB-CA-C	5.90	120.09	110.95
3	A	217	ARG	N-CA-C	-5.86	104.84	112.23
3	A	114	GLU	CB-CG-CD	5.85	122.55	112.60
3	A	151	PHE	O-C-N	-5.81	116.44	122.94
2	D	12	DC	O4'-C4'-C3'	-5.79	96.72	105.40
3	A	182	SER	N-CA-CB	-5.79	100.55	111.43
3	A	137	PHE	N-CA-C	5.76	118.12	108.73
1	C	2	DT	O3'-P-O5'	5.75	112.63	104.00
3	A	116	ASP	CA-CB-CG	5.75	118.35	112.60
2	D	1	DA	C5'-C4'-O4'	5.66	117.89	109.40
2	D	12	DC	O4'-C1'-C2'	-5.62	97.97	106.40
3	A	204	HIS	CB-CA-C	5.61	121.59	110.42
3	A	131	HIS	N-CA-CB	5.59	119.90	110.46
1	C	5	DG	O3'-P-O5'	-5.57	95.65	104.00
3	A	124	HIS	CB-CG-CD2	5.55	138.41	131.20
2	D	13	DC	C2-N1-C1'	-5.54	111.38	119.70
1	C	14	DG	P-O3'-C3'	5.48	128.43	120.20
3	A	229	LYS	O-C-N	5.47	125.98	121.44
1	C	9	DT	N1-C1'-C2'	5.43	121.64	113.50
3	A	152	LYS	N-CA-C	5.41	117.03	111.03
2	D	17	DA	C4'-C3'-C2'	-5.39	94.31	102.40
3	A	167	GLU	N-CA-C	5.34	116.95	108.67
2	D	9	DC	P-O5'-C5'	-5.33	112.01	120.00
3	A	256	HIS	ND1-CG-CD2	5.32	111.42	106.10
3	A	231	TYR	CA-CB-CG	-5.31	104.34	113.90
3	A	137	PHE	CA-C-N	5.26	130.29	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	137	PHE	C-N-CA	5.26	130.29	122.71
3	A	205	GLU	CA-C-N	-5.24	111.15	121.41
3	A	205	GLU	C-N-CA	-5.24	111.15	121.41
3	A	190	HIS	N-CA-CB	5.20	119.28	110.49
3	A	182	SER	CA-CB-OG	-5.20	100.71	111.10
1	C	21	DG	C4-N9-C1'	-5.19	119.22	127.00
3	A	227	ASN	CB-CA-C	5.18	120.73	110.42
3	A	203	GLU	CB-CG-CD	5.13	121.33	112.60
2	D	13	DC	N1-C1'-C2'	-5.12	105.81	113.50
3	A	172	CYS	CA-C-O	-5.08	115.72	121.72
3	A	225	HIS	CA-C-N	5.07	131.23	121.54
3	A	225	HIS	C-N-CA	5.07	131.23	121.54
3	A	214	ALA	CA-C-N	5.04	127.30	120.65
3	A	214	ALA	C-N-CA	5.04	127.30	120.65
3	A	159	VAL	CA-C-N	5.03	127.28	120.44
3	A	159	VAL	C-N-CA	5.03	127.28	120.44
1	C	10	DG	O4'-C1'-N9	5.03	115.95	108.40

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
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	57	2
3	A	1270	0	1199	271	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	358	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 100.

All (358) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:LYS:HE3	3:A:152:LYS:H	1.40	0.86
3:A:231:TYR:CB	3:A:248:LEU:HD12	2.04	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:H2'	2:D:17:DA:OP2	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
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:O	3:A:167:GLU:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:DA:N7	5:D:204:HOH:O	2.20	0.73
3:A:240:LYS:HG3	3:A:251:HIS:CE1	2.24	0.73
1:C:5:DG:N2	2:D:18:DC:N3	2.37	0.73
2:D:16:DG:H2''	2:D:17:DA:H5'	1.71	0.73
3:A:219:LYS:O	3:A:221:GLN:N	2.22	0.73
3:A:137:PHE:HB2	3:A:154:GLN:CD	2.13	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
1:C:3:DT:H2''	1:C:4:DC:H6	1.54	0.71
1:C:20:DC:N3	2:D:3:DG:N2	2.35	0.71
3:A:107:ARG:NH1	3:A:141:TRP:HZ2	1.88	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
2:D:16:DG:H2''	2:D:17:DA:C5'	2.21	0.71
3:A:107:ARG:HD2	3:A:141:TRP:CE2	2.26	0.71
3:A:250:LYS:O	3:A:254:THR:HG22	1.90	0.70
1:C:13:DT:H2''	1:C:14:DG:O5'	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
3:A:113:GLN:HB3	3:A:115:PHE:CZ	2.26	0.70
3:A:182:SER:O	3:A:183:ARG:HG3	1.91	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:219:LYS:O	3:A:220:HIS:C	2.34	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
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:128:GLU:N	3:A:128:GLU:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:138:VAL:HG22	3:A:150:PRO:HA	1.77	0.67
3:A:188:LYS:O	3:A:191:LEU:HB2	1.94	0.67
2:D:2:DC:H4'	2:D:3:DG:OP1	1.94	0.66
3:A:107:ARG:NH1	3:A:141:TRP:CZ2	2.63	0.66
1:C:16:DT:C2'	1:C:17:DC:H5'	2.25	0.66
3:A:163:ARG:HG2	3:A:163:ARG:HH21	1.59	0.66
1:C:15:DG:H2'	1:C:16:DT:H71	1.79	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:147:GLU:C	3:A:148:LEU:HD23	2.23	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
2:D:15:DA:C2'	2:D:16:DG:H8	2.12	0.63
3:A:126:ASN:H	3:A:126:ASN:HD22	0.66	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
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:107:ARG:HD2	3:A:141:TRP:NE1	2.15	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
3:A:168:LYS:HB3	3:A:181:TYR:C	2.26	0.60
1:C:4:DC:H4'	1:C:5:DG:OP1	2.01	0.60
3:A:232:VAL:CG1	3:A:241:ARG:HH21	2.14	0.60
3:A:117:SER:HB3	3:A:120:GLN:OE1	2.02	0.60
3:A:255:VAL:HG23	3:A:256:HIS:H	1.65	0.60
3:A:144:CYS:C	3:A:146:ARG:H	2.08	0.60
3:A:116:ASP:CG	3:A:120:GLN:NE2	2.60	0.59
3:A:135:LYS:HA	3:A:135:LYS:CE	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:ILE:HG21	3:A:158:VAL:HG22	1.85	0.59
3:A:192:ARG:O	3:A:195:THR:N	2.30	0.59
3:A:240:LYS:HG3	3:A:251:HIS:HE1	1.67	0.59
3:A:130:ILE:HG22	3:A:131:HIS:HD2	1.68	0.58
3:A:220:HIS:C	3:A:220:HIS:CD2	2.80	0.58
1:C:14:DG:C2'	1:C:15:DG:C5'	2.82	0.58
2:D:15:DA:C2'	2:D:16:DG:C8	2.87	0.58
3:A:242:TYR:N	3:A:242:TYR:CD1	2.72	0.58
3:A:168:LYS:HB2	3:A:180:SER:HB2	1.86	0.58
3:A:231:TYR:HB3	3:A:248:LEU:CD1	2.22	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:248:LEU:C	3:A:248:LEU:HD23	2.30	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:235:LEU:O	3:A:238:CYS:HB2	2.05	0.57
3:A:157:LEU:O	3:A:160:HIS:N	2.36	0.57
3:A:184:LEU:HD13	3:A:188:LYS:HE3	1.87	0.57
3:A:181:TYR:CZ	3:A:190:HIS:HB2	2.39	0.57
3:A:235:LEU:CD1	3:A:256:HIS:CG	2.85	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:152:LYS:NZ	3:A:156:MET:SD	2.73	0.56
1:C:2:DT:C2'	1:C:3:DT:H6	2.19	0.55
1:C:9:DT:C7	3:A:215:SER:HB2	2.35	0.55
3:A:253:LYS:CD	3:A:253:LYS:C	2.78	0.55
3:A:198:LYS:HB2	3:A:198:LYS:HZ2	1.72	0.55
3:A:113:GLN:NE2	3:A:115:PHE:CE2	2.75	0.55
3:A:152:LYS:H	3:A:152:LYS:CE	2.15	0.55
3:A:137:PHE:H	3:A:154:GLN:CD	2.14	0.55
3:A:108:TRP:CG	3:A:129:HIS:CD2	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:231:TYR:CE1	3:A:243:THR:O	2.60	0.54
3:A:121:LEU:CD1	3:A:125:ILE:CD1	2.85	0.54
3:A:133:GLU:CD	3:A:133:GLU:H	2.16	0.54
3:A:137:PHE:HB2	3:A:154:GLN:CB	2.36	0.54
3:A:147:GLU:HB3	3:A:148:LEU:HG	1.90	0.54
3:A:215:SER:O	3:A:218:ALA:N	2.37	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
2:D:17:DA:H2'	2:D:17:DA:P	2.48	0.54
3:A:189:THR:O	3:A:190:HIS:C	2.49	0.54
3:A:118:GLN:HE22	3:A:167:GLU:CB	2.21	0.53
3:A:181:TYR:CE1	3:A:190:HIS:HB2	2.43	0.53
3:A:229:LYS:HB3	3:A:242:TYR:C	2.34	0.53
3:A:238:CYS:O	3:A:239:THR:HB	2.08	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:253:LYS:C	3:A:253:LYS:HD3	2.34	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:132:GLY:O	3:A:133:GLU:O	2.26	0.53
3:A:161:MET:O	3:A:165:THR:N	2.38	0.53
3:A:174:PHE:CD2	3:A:194:HIS:HB3	2.43	0.53
2:D:15:DA:C2	2:D:16:DG:C5	2.97	0.53
3:A:130:ILE:O	3:A:130:ILE:HG22	2.09	0.53
1:C:20:DC:N4	2:D:2:DC:C4	2.77	0.52
3:A:255:VAL:CG2	3:A:256:HIS:H	2.22	0.52
3:A:186:ASN:O	3:A:187:LEU:C	2.50	0.52
3:A:117:SER:HB3	3:A:120:GLN:CD	2.35	0.52
2:D:14:DA:H2''	2:D:15:DA:O5'	2.10	0.52
3:A:173:THR:O	3:A:174:PHE:C	2.53	0.51
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
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:231:TYR:CZ	3:A:245:PRO:HD3	2.46	0.51
3:A:163:ARG:HG2	3:A:163:ARG:NH2	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
2:D:15:DA:H2'''	2:D:16:DG:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:133:GLU:CD	3:A:133:GLU:N	2.69	0.50
1:C:2:DT:C2'	1:C:3:DT:C6	2.91	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
2:D:6:DG:N7	3:A:250:LYS:NZ	2.55	0.50
3:A:121:LEU:HD11	3:A:125:ILE:CD1	2.41	0.50
3:A:187:LEU:O	3:A:187:LEU:HG	1.98	0.50
3:A:256:HIS:CD2	3:A:256:HIS:H	2.23	0.50
2:D:11:DC:H2''	2:D:12:DC:O5'	2.12	0.49
3:A:198:LYS:HB2	3:A:198:LYS:NZ	2.26	0.49
1:C:15:DG:H1	2:D:8:DC:N4	2.10	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
3:A:218:ALA:O	3:A:219:LYS:O	2.30	0.49
3:A:205:GLU:OE1	3:A:225:HIS:ND1	2.45	0.49
3:A:235:LEU:HD13	3:A:256:HIS:HB3	1.95	0.49
3:A:255:VAL:CG2	3:A:256:HIS:N	2.75	0.49
3:A:161:MET:O	3:A:164:HIS:N	2.46	0.49
2:D:17:DA:OP2	2:D:17:DA:H8	1.95	0.49
3:A:219:LYS:O	3:A:222:ASN:N	2.46	0.49
3:A:248:LEU:O	3:A:249:ARG:C	2.54	0.49
3:A:251:HIS:C	3:A:251:HIS:CD2	2.90	0.49
3:A:211:PHE:HD1	3:A:217:ARG:HG3	1.78	0.48
3:A:182:SER:C	3:A:183:ARG:HG3	2.38	0.48
3:A:108:TRP:HA	3:A:140:HIS:O	2.13	0.48
3:A:138:VAL:HG22	3:A:150:PRO:CA	2.43	0.48
3:A:217:ARG:O	3:A:221:GLN:CB	2.61	0.48
3:A:231:TYR:C	3:A:248:LEU:HD12	2.38	0.48
3:A:211:PHE:CD1	3:A:217:ARG:CB	2.96	0.48
3:A:121:LEU:CD1	3:A:125:ILE:HD11	2.42	0.48
3:A:162:ARG:HD2	3:A:167:GLU:HG3	1.94	0.48
1:C:5:DG:C6	2:D:18:DC:N4	2.74	0.48
2:D:12:DC:C4	2:D:13:DC:C4	3.01	0.48
3:A:241:ARG:O	3:A:241:ARG:HG2	2.13	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:HG12	3:A:159:VAL:O	2.13	0.47
3:A:189:THR:C	3:A:191:LEU:N	2.66	0.47
1:C:21:DG:C6	2:D:2:DC:N3	2.81	0.47
3:A:130:ILE:O	3:A:130:ILE:CG2	2.62	0.47
3:A:201:MET:CA	3:A:210:ALA:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:DA:H2'	2:D:16:DG:C8	2.49	0.47
3:A:138:VAL:CG1	3:A:140:HIS:CE1	2.98	0.47
3:A:202:CYS:SG	3:A:221:GLN:NE2	2.88	0.47
2:D:11:DC:C2	2:D:12:DC:C6	3.02	0.47
3:A:234:LYS:HB2	3:A:234:LYS:HE3	1.53	0.47
3:A:159:VAL:O	3:A:162:ARG:HG3	2.15	0.46
3:A:107:ARG:CD	3:A:141:TRP:CZ2	2.98	0.46
3:A:137:PHE:HD1	3:A:154:GLN:CG	2.29	0.46
3:A:144:CYS:O	3:A:147:GLU:N	2.35	0.46
2:D:3:DG:H2'	2:D:4:DT:H71	1.97	0.46
3:A:251:HIS:CD2	3:A:252:VAL:N	2.83	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:253:LYS:HD3	3:A:253:LYS:O	2.17	0.45
3:A:146:ARG:O	3:A:149:ARG:N	2.37	0.45
3:A:218:ALA:HA	3:A:221:GLN:HB3	1.98	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
3:A:192:ARG:O	3:A:193:SER:C	2.57	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
1:C:18:DC:H4'	1:C:19:DA:OP1	2.14	0.44
3:A:135:LYS:CA	3:A:135:LYS:CE	2.92	0.44
3:A:137:PHE:CA	3:A:154:GLN:NE2	2.80	0.44
3:A:153:ALA:CB	3:A:155:TYR:CD1	3.00	0.44
3:A:248:LEU:C	3:A:248:LEU:CD2	2.89	0.44
3:A:130:ILE:HD13	3:A:130:ILE:HG21	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
2:D:20:DA:C8	5:D:204:HOH:O	2.66	0.44
3:A:121:LEU:HD12	3:A:125:ILE:HD12	2.00	0.44
3:A:138:VAL:HG23	3:A:150:PRO:HB3	2.00	0.44
3:A:161:MET:C	3:A:163:ARG:N	2.75	0.44
1:C:7:DC:H2'	1:C:7:DC:O5'	2.18	0.44
1:C:15:DG:H1	2:D:8:DC:H42	1.66	0.44
3:A:235:LEU:HA	3:A:236:PRO:HD3	1.74	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:118:GLN:O	3:A:119:GLU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:3:DT:C2'	1:C:4:DC:C6	3.02	0.43
3:A:199:PRO:HD2	3:A:212:SER:HA	2.00	0.43
3:A:147:GLU:O	3:A:148:LEU:HD23	2.18	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:N	3:A:154:GLN:CD	2.77	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:138:VAL:HG11	3:A:140:HIS:CE1	2.55	0.42
3:A:235:LEU:CD1	3:A:256:HIS:HB3	2.49	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:211:PHE:CD1	3:A:217:ARG:CA	2.99	0.42
3:A:251:HIS:CE1	3:A:255:VAL:CG2	3.03	0.42
3:A:121:LEU:C	3:A:123:HIS:N	2.78	0.42
3:A:121:LEU:O	3:A:125:ILE:HD12	2.20	0.42
3:A:144:CYS:C	3:A:146:ARG:N	2.72	0.42
3:A:174:PHE:CE1	3:A:191:LEU:HD22	2.54	0.42
3:A:200:TYR:C	3:A:210:ALA:HB1	2.45	0.42
3:A:105:ASP:O	3:A:106:CYS:C	2.59	0.41
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
2:D:8:DC:H6	2:D:8:DC:H2'	1.67	0.41
3:A:163:ARG:HH21	3:A:163:ARG:CG	2.31	0.41
3:A:197:GLU:O	3:A:199:PRO:HD3	2.20	0.41
3:A:255:VAL:C	3:A:256:HIS:O	2.64	0.41
3:A:198:LYS:C	3:A:200:TYR:H	2.28	0.41
1:C:5:DG:C2	2:D:18:DC:N3	2.88	0.41
3:A:191:LEU:O	3:A:194:HIS:N	2.52	0.41
2:D:11:DC:N3	2:D:12:DC:C5	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:DC:N3	2:D:16:DG:O6	2.54	0.41
1:C:11:DG:O6	3:A:219:LYS:NZ	2.46	0.41
3:A:146:ARG:O	3:A:147:GLU:C	2.64	0.41
3:A:251:HIS:CE1	3:A:255:VAL:HG21	2.56	0.41
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:HB3	3:A:155:TYR:CE1	2.56	0.40
3:A:153:ALA:HB1	3:A:155:TYR:HD1	1.85	0.40
3:A:122:VAL:O	3:A:122:VAL:CG2	2.59	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

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Mol	Chain	Res	Type
3	A	219	LYS
3	A	220	HIS
3	A	249	ARG
3	A	252	VAL
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	141/141 (100%)	84 (60%)	57 (40%)	0 0

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	103	GLU
3	A	104	THR
3	A	107	ARG
3	A	111	CYS
3	A	112	SER
3	A	113	GLN
3	A	118	GLN
3	A	119	GLU
3	A	122	VAL

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Mol	Chain	Res	Type
3	A	124	HIS
3	A	126	ASN
3	A	128	GLU
3	A	129	HIS
3	A	133	GLU
3	A	135	LYS
3	A	138	VAL
3	A	147	GLU
3	A	148	LEU
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	183	ARG
3	A	184	LEU
3	A	185	GLU
3	A	187	LEU
3	A	193	SER
3	A	195	THR
3	A	197	GLU
3	A	198	LYS
3	A	201	MET
3	A	203	GLU
3	A	205	GLU
3	A	209	LYS
3	A	219	LYS
3	A	221	GLN
3	A	223	ARG
3	A	224	THR
3	A	233	CYS
3	A	234	LYS
3	A	235	LEU
3	A	240	LYS
3	A	241	ARG
3	A	242	TYR

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Mol	Chain	Res	Type
3	A	244	ASP
3	A	246	SER
3	A	248	LEU
3	A	251	HIS
3	A	253	LYS
3	A	255	VAL

Sometimes 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 oligosaccharides 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 [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.