



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:43 AM UTC

PDB ID : 3T79 / pdb_00003t79
Title : Ndc10: a platform for inner kinetochore assembly in budding yeast
Authors : Cho, U.S.; Harrison, S.C.
Deposited on : 2011-07-29
Resolution : 3.61 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:

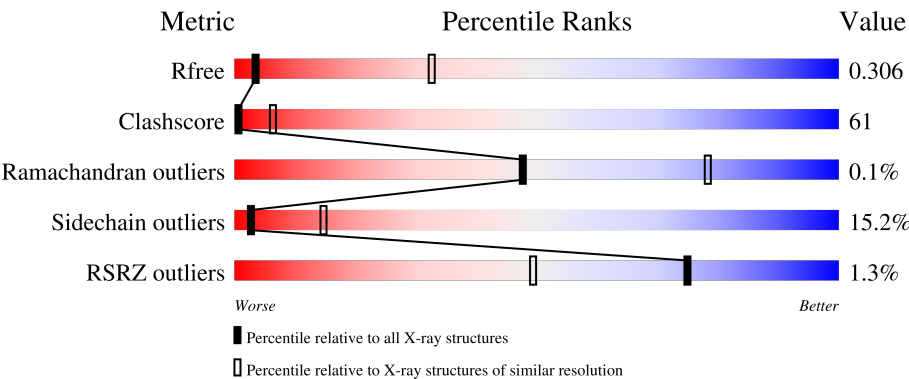
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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

Mol	Chain	Length	Quality of chain
1	B	15	7%93%
2	C	15	7%73%20%
3	E	14	29%71%
4	F	15	20%67%13%
5	A	402	%33%51%11%..

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Mol	Chain	Length	Quality of chain
5	D	402	% 35% 46% 14% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7603 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(P*TP*TP*AP*AP*TP*TP*TP*AP*TP*AP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	15	Total	C	N	O	P	0	0	0
			307	150	51	91	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			308	150	54	89	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	14	Total	C	N	O	P	0	0	0
			287	140	49	84	14			

- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*AP*TP*TP*TP*TP*AP*TP*AP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	15	Total	C	N	O	P	0	0	0
			309	150	57	87	15			

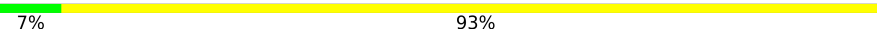
- Molecule 5 is a protein called KLLA0E03807p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	388	Total	C	N	O	S	0	0	0
			3196	2086	517	581	12			
5	D	388	Total	C	N	O	S	0	0	0
			3196	2086	517	581	12			

3 Residue-property plots [i](#)

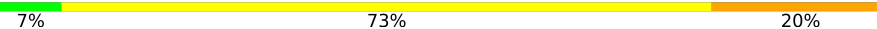
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

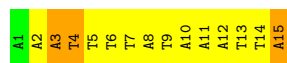
- Molecule 1: DNA (5'-D(P*TP*TP*AP*AP*TP*TP*TP*AP*TP*AP*AP*AP*AP*TP*T)-3')

Chain B: 

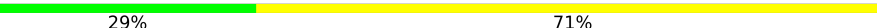


- Molecule 2: DNA (5'-D(P*AP*AP*AP*TP*TP*TP*TP*AP*TP*AP*AP*AP*TP*TP*A)-3')

Chain C: 



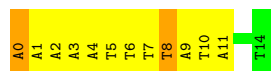
- Molecule 3: DNA (5'-D(P*TP*AP*AP*TP*TP*TP*AP*TP*AP*AP*AP*AP*TP*T)-3')

Chain E: 



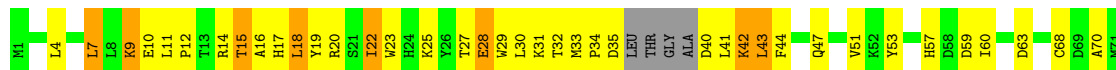
- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*AP*TP*TP*TP*TP*AP*TP*AP*AP*AP*T)-3')

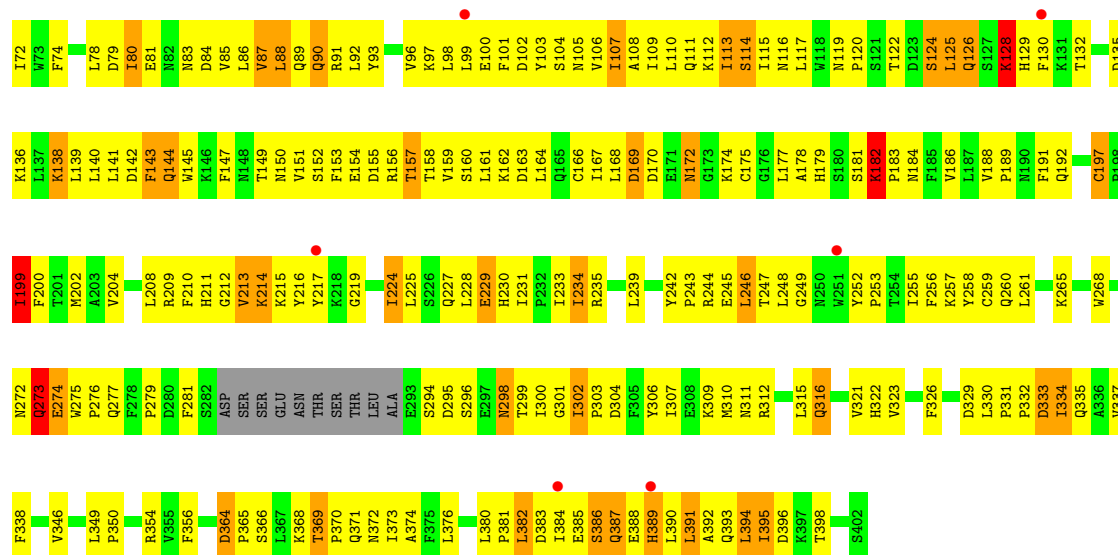
Chain F: 



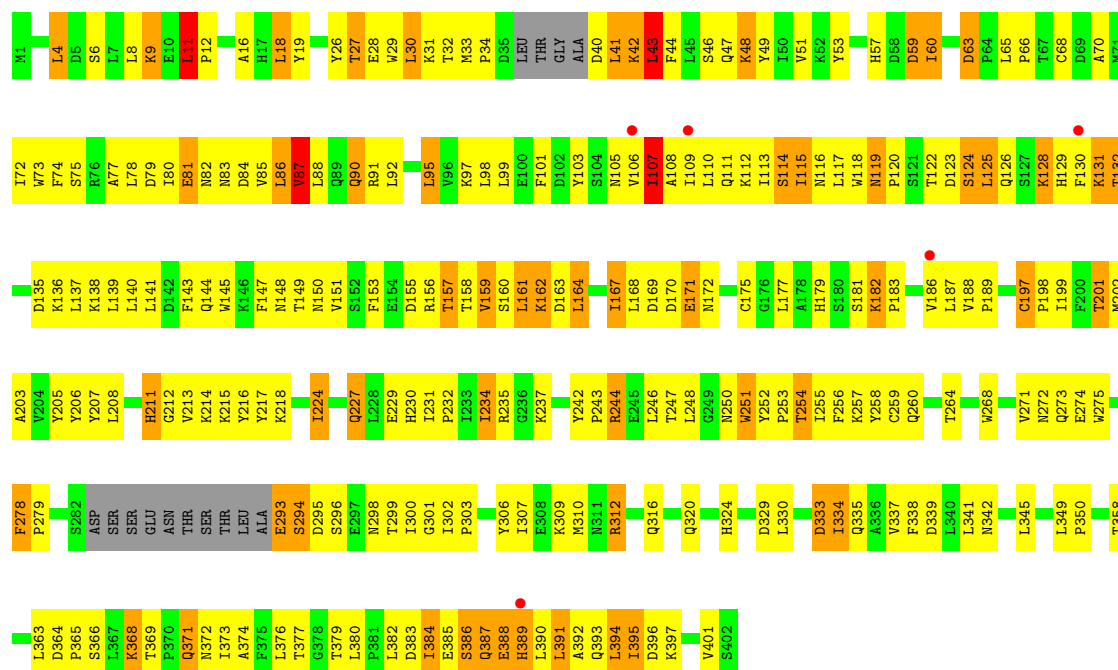
- Molecule 5: KLLA0E03807p

Chain A: 





• Molecule 5: KLLA0E03807p



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.06Å 99.65Å 125.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.65 – 3.61 43.65 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.65-3.61) 98.9 (43.65-3.61)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.286 , 0.331 0.272 , 0.306	Depositor DCC
R_{free} test set	688 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	92.2	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7603	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.23	0/343	0.90	0/527
2	C	0.43	0/345	1.38	7/530 (1.3%)
3	E	0.21	0/321	0.84	0/493
4	F	0.34	0/347	1.16	2/533 (0.4%)
5	A	0.53	0/3287	1.01	20/4473 (0.4%)
5	D	0.60	1/3287 (0.0%)	1.08	20/4473 (0.4%)
All	All	0.53	1/7930 (0.0%)	1.05	49/11029 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	43	LEU	CA-C	-5.14	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	DT	O5'-C5'-C4'	10.12	125.97	110.80
2	C	3	DA	C4'-C3'-O3'	-9.07	96.39	110.00
5	D	302	ILE	N-CA-C	8.75	117.43	107.89
5	A	182	LYS	CA-C-N	-7.71	112.05	119.76
5	A	182	LYS	C-N-CA	-7.71	112.05	119.76
2	C	4	DT	C5'-C4'-C3'	7.70	126.45	114.90
5	A	302	ILE	N-CA-C	7.34	115.89	107.89
2	C	3	DA	O5'-C5'-C4'	-7.25	99.93	110.80
2	C	4	DT	C2-N1-C1'	-7.06	108.76	119.35
5	D	11	LEU	CA-C-N	7.05	127.02	119.76
5	D	11	LEU	C-N-CA	7.05	127.02	119.76
5	D	87	VAL	N-CA-C	-6.69	103.81	110.30
5	D	278	PHE	CA-C-N	6.57	126.95	119.92
5	D	278	PHE	C-N-CA	6.57	126.95	119.92
5	D	43	LEU	N-CA-C	-6.48	103.33	111.11
5	D	107	ILE	N-CA-C	6.48	116.97	110.23
5	D	197	CYS	CA-C-N	6.38	125.95	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	197	CYS	C-N-CA	6.38	125.95	119.19
5	D	63	ASP	CA-C-N	6.32	125.89	119.19
5	D	63	ASP	C-N-CA	6.32	125.89	119.19
4	F	0	DA	C2'-C3'-O3'	6.25	120.88	111.50
2	C	3	DA	C5'-C4'-O4'	6.20	118.70	109.40
5	A	197	CYS	CA-C-N	5.87	125.41	119.19
5	A	197	CYS	C-N-CA	5.87	125.41	119.19
5	A	126	GLN	N-CA-C	-5.86	105.78	113.17
4	F	8	DT	C1'-O4'-C4'	-5.82	100.97	109.70
5	A	128	LYS	CB-CG-CD	-5.81	97.93	111.30
5	A	199	ILE	N-CA-CB	5.79	117.20	110.65
5	D	182	LYS	CA-C-N	-5.79	113.97	119.76
5	D	182	LYS	C-N-CA	-5.79	113.97	119.76
5	A	144	GLN	N-CA-C	-5.73	105.04	111.28
2	C	15	DA	O5'-C5'-C4'	-5.72	102.22	110.80
5	A	63	ASP	CA-C-N	5.70	125.23	119.19
5	A	63	ASP	C-N-CA	5.70	125.23	119.19
5	A	273	GLN	N-CA-C	5.67	119.37	112.23
5	D	119	ASN	CA-C-N	5.62	125.15	119.19
5	D	119	ASN	C-N-CA	5.62	125.15	119.19
5	D	27	THR	N-CA-C	5.48	117.25	111.28
5	A	128	LYS	CD-CE-NZ	-5.47	94.39	111.90
5	A	364	ASP	CA-C-N	-5.46	112.99	119.05
5	A	364	ASP	C-N-CA	-5.46	112.99	119.05
5	A	107	ILE	N-CA-C	5.41	116.04	110.36
5	A	114	SER	N-CA-C	-5.41	104.62	111.11
5	D	159	VAL	N-CA-C	5.37	115.93	108.84
5	A	274	GLU	N-CA-C	-5.36	105.38	112.34
5	D	60	ILE	CB-CA-C	-5.15	105.37	111.97
5	A	326	PHE	CA-C-N	5.13	125.14	119.90
5	A	326	PHE	C-N-CA	5.13	125.14	119.90
5	D	81	GLU	CB-CA-C	5.09	118.83	109.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	B	307	0	174	38	0
2	C	308	0	173	55	0
3	E	287	0	162	19	0
4	F	309	0	172	46	0
5	A	3196	0	3187	394	2
5	D	3196	0	3187	413	2
All	All	7603	0	7055	898	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 61.

All (898) 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)
5:D:30:LEU:HG	5:D:44:PHE:CZ	1.57	1.38
5:D:27:THR:HA	5:D:30:LEU:CD2	1.59	1.33
5:D:128:LYS:HD3	5:D:129:HIS:CE1	1.68	1.28
5:D:11:LEU:HD21	5:D:16:ALA:HB2	1.25	1.15
5:D:383:ASP:O	5:D:386:SER:OG	1.65	1.14
2:C:13:DT:H2'	2:C:14:DT:H5''	1.28	1.13
5:A:321:VAL:HG22	5:A:323:VAL:H	1.15	1.10
5:A:11:LEU:HD11	5:A:15:THR:HG22	1.32	1.09
5:A:321:VAL:HG21	5:A:346:VAL:HG11	1.28	1.09
5:D:312:ARG:HG2	5:D:312:ARG:HH11	1.01	1.08
1:B:3:DA:H2''	1:B:4:DA:H5'	1.31	1.07
5:D:179:HIS:CE1	5:D:181:SER:HB3	1.90	1.05
5:D:27:THR:CA	5:D:30:LEU:HD22	1.86	1.04
5:D:83:ASN:HA	5:D:86:LEU:HG	1.37	1.03
5:A:103:TYR:HB3	5:A:107:ILE:HD11	1.39	1.02
5:D:258:TYR:CE2	5:D:395:ILE:HD11	1.95	1.02
5:D:128:LYS:HD3	5:D:129:HIS:NE2	1.75	1.01
5:D:30:LEU:HG	5:D:44:PHE:CE1	1.97	1.00
1:B:3:DA:H2'	1:B:4:DA:C8	1.97	0.99
5:D:11:LEU:CD2	5:D:16:ALA:HB2	1.92	0.99
3:E:6:DT:H2''	3:E:7:DA:H8	1.27	0.99
5:A:260:GLN:HE22	5:D:260:GLN:HE22	1.06	0.99
5:D:124:SER:HB2	5:D:258:TYR:CE1	1.97	0.99
5:D:30:LEU:CG	5:D:44:PHE:CZ	2.45	0.98
5:D:27:THR:HA	5:D:30:LEU:HD22	1.00	0.98
4:F:8:DT:OP2	5:D:244:ARG:NE	1.96	0.97
5:D:30:LEU:HG	5:D:44:PHE:HZ	1.27	0.97
5:D:371:GLN:OE1	5:D:371:GLN:N	1.96	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:312:ARG:HH11	5:D:312:ARG:CG	1.77	0.96
4:F:2:DA:O5'	4:F:2:DA:H2'	1.65	0.95
5:D:130:PHE:HA	5:D:135:ASP:HB2	1.46	0.95
1:B:7:DT:H2''	1:B:8:DA:H8	1.30	0.92
3:E:6:DT:H2''	3:E:7:DA:C8	2.05	0.92
5:D:124:SER:HB2	5:D:258:TYR:HE1	1.32	0.92
5:D:252:TYR:HD1	5:D:256:PHE:HE2	1.11	0.92
5:D:388:GLU:O	5:D:391:LEU:HG	1.68	0.92
5:D:147:PHE:HD2	5:D:312:ARG:NH2	1.67	0.92
5:D:147:PHE:HD2	5:D:312:ARG:HH21	1.13	0.91
5:A:213:VAL:CG2	5:A:216:TYR:HB2	2.00	0.91
5:A:143:PHE:C	5:A:143:PHE:CD2	2.48	0.91
5:A:112:LYS:HA	5:A:393:GLN:HG2	1.54	0.90
5:D:131:LYS:HG2	5:D:132:THR:H	1.36	0.89
5:D:182:LYS:HB2	5:D:183:PRO:HD3	1.52	0.89
5:D:324:HIS:HA	5:D:342:ASN:HD21	1.35	0.89
5:A:86:LEU:O	5:A:90:GLN:NE2	2.06	0.89
5:D:244:ARG:HG2	5:D:244:ARG:HH11	1.37	0.89
5:D:162:LYS:HZ1	5:D:230:HIS:HA	1.38	0.88
5:A:260:GLN:NE2	5:D:260:GLN:HE22	1.71	0.88
5:A:113:ILE:HG22	5:A:259:CYS:SG	2.12	0.88
1:B:12:DA:H2''	1:B:13:DA:O5'	1.74	0.88
5:D:148:ASN:OD1	5:D:312:ARG:NH1	2.06	0.88
5:D:169:ASP:OD1	5:D:171:GLU:HG3	1.75	0.87
5:D:81:GLU:OE1	5:D:83:ASN:OD1	1.92	0.87
5:D:147:PHE:CD2	5:D:312:ARG:NH2	2.41	0.87
5:A:260:GLN:HE22	5:D:260:GLN:NE2	1.71	0.87
2:C:13:DT:C2'	2:C:14:DT:H5''	2.04	0.86
1:B:4:DA:OP2	1:B:4:DA:H2'	1.75	0.86
5:A:169:ASP:HB3	5:A:172:ASN:OD1	1.74	0.86
5:D:312:ARG:HG2	5:D:312:ARG:NH1	1.75	0.86
2:C:2:DA:H1'	2:C:3:DA:H5'	1.56	0.85
5:D:156:ARG:NH1	5:D:268:TRP:O	2.09	0.85
1:B:6:DT:H2''	1:B:7:DT:OP2	1.74	0.85
4:F:9:DA:H2''	4:F:10:DT:O5'	1.76	0.85
5:D:395:ILE:HD13	5:D:395:ILE:H	1.41	0.85
5:D:114:SER:OG	5:D:144:GLN:NE2	2.10	0.85
5:D:128:LYS:CD	5:D:129:HIS:CE1	2.59	0.85
5:A:9:LYS:NZ	5:A:10:GLU:HG2	1.91	0.85
5:A:9:LYS:HZ1	5:A:10:GLU:HG2	1.41	0.84
5:D:244:ARG:HH11	5:D:244:ARG:CG	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:103:TYR:HB3	5:A:107:ILE:CD1	2.06	0.84
5:A:115:ILE:HD12	5:A:390:LEU:O	1.76	0.84
5:D:86:LEU:O	5:D:90:GLN:NE2	2.10	0.84
5:D:271:VAL:HB	5:D:273:GLN:HE22	1.39	0.84
5:A:162:LYS:NZ	5:A:228:LEU:O	2.09	0.84
5:A:162:LYS:HG3	5:A:231:ILE:HD11	1.59	0.84
5:A:389:HIS:ND1	5:D:105:ASN:O	2.11	0.84
1:B:2:DT:H5'	1:B:2:DT:C6	2.12	0.83
5:A:140:LEU:HD11	5:A:144:GLN:HE21	1.42	0.83
5:D:11:LEU:HD21	5:D:16:ALA:CB	2.09	0.83
5:A:25:LYS:HG2	5:A:53:TYR:OH	1.79	0.83
5:D:95:LEU:C	5:D:95:LEU:HD12	2.03	0.83
5:D:253:PRO:O	5:D:257:LYS:HG2	1.78	0.83
5:A:11:LEU:HD11	5:A:15:THR:CG2	2.09	0.82
5:D:252:TYR:HD1	5:D:256:PHE:CE2	1.97	0.82
5:D:293:GLU:N	5:D:293:GLU:OE1	2.13	0.82
4:F:1:DA:OP2	4:F:1:DA:H2'	1.80	0.82
5:A:88:LEU:HD12	5:A:92:LEU:HG	1.62	0.82
5:A:244:ARG:O	5:A:247:THR:OG1	1.98	0.81
5:A:209:ARG:HE	5:A:235:ARG:HH12	1.28	0.81
5:D:234:ILE:HD11	5:D:243:PRO:HG2	1.61	0.81
5:D:162:LYS:NZ	5:D:229:GLU:O	2.12	0.81
5:A:153:PHE:HE1	5:A:248:LEU:HD12	1.44	0.81
5:D:115:ILE:HD11	5:D:391:LEU:HA	1.62	0.81
1:B:7:DT:H2''	1:B:8:DA:C8	2.14	0.81
5:D:115:ILE:HD12	5:D:390:LEU:O	1.80	0.81
5:A:164:LEU:HD21	5:A:177:LEU:HD22	1.63	0.81
5:D:84:ASP:O	5:D:87:VAL:HG22	1.81	0.80
5:A:143:PHE:HD2	5:A:144:GLN:N	1.78	0.80
5:D:95:LEU:CD1	5:D:99:LEU:HG	2.11	0.80
5:A:9:LYS:HG3	5:A:10:GLU:N	1.97	0.80
5:D:202:MET:HE3	5:D:341:LEU:HD21	1.63	0.80
4:F:2:DA:H2''	4:F:3:DA:OP2	1.82	0.80
2:C:4:DT:P	5:A:128:LYS:NZ	2.55	0.80
5:A:389:HIS:CD2	5:A:390:LEU:N	2.50	0.80
5:A:142:ASP:O	5:A:145:TRP:HB3	1.83	0.79
5:A:189:PRO:CA	5:A:199:ILE:HD11	2.13	0.79
5:A:143:PHE:C	5:A:143:PHE:HD2	1.90	0.79
4:F:7:DT:H5''	5:D:244:ARG:HD2	1.65	0.78
5:D:112:LYS:O	5:D:116:ASN:ND2	2.17	0.78
5:D:83:ASN:HA	5:D:86:LEU:CG	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:DA:H2''	2:C:9:DT:O5'	1.82	0.77
5:A:321:VAL:CG2	5:A:346:VAL:HG11	2.12	0.77
2:C:4:DT:OP2	5:A:128:LYS:NZ	2.16	0.77
5:D:128:LYS:HG2	5:D:129:HIS:N	1.99	0.77
5:D:234:ILE:HD11	5:D:243:PRO:CG	2.13	0.77
5:D:115:ILE:CD1	5:D:391:LEU:HA	2.15	0.77
5:A:209:ARG:NE	5:A:235:ARG:HH12	1.83	0.77
5:D:98:LEU:HD21	5:D:306:TYR:HA	1.66	0.77
5:A:300:ILE:HG23	5:A:301:GLY:H	1.48	0.77
5:D:40:ASP:HA	5:D:43:LEU:HD11	1.68	0.76
5:D:155:ASP:O	5:D:158:THR:HG22	1.84	0.76
5:D:294:SER:HB2	5:D:299:THR:HA	1.66	0.76
5:D:95:LEU:HD11	5:D:99:LEU:HG	1.68	0.76
5:A:112:LYS:NZ	5:A:259:CYS:O	2.18	0.76
5:A:97:LYS:O	5:A:101:PHE:HB2	1.86	0.76
5:A:235:ARG:NE	5:A:239:LEU:O	2.19	0.76
5:A:153:PHE:HE1	5:A:248:LEU:CD1	1.98	0.76
5:A:329:ASP:O	5:A:330:LEU:HG	1.86	0.75
5:D:83:ASN:CA	5:D:86:LEU:HG	2.16	0.75
5:A:150:ASN:OD1	5:A:277:GLN:HG2	1.86	0.75
5:A:235:ARG:HE	5:A:239:LEU:C	1.94	0.75
5:A:370:PRO:O	5:A:373:ILE:HG22	1.87	0.75
5:D:91:ARG:NH1	5:D:306:TYR:OH	2.20	0.75
5:A:388:GLU:N	5:A:388:GLU:OE1	2.19	0.75
5:D:30:LEU:CG	5:D:44:PHE:HZ	1.93	0.75
5:A:111:GLN:OE1	5:A:389:HIS:HE1	1.69	0.75
5:D:160:SER:OG	5:D:230:HIS:HD2	1.71	0.74
3:E:11:DA:H2''	3:E:12:DA:O5'	1.86	0.74
5:A:235:ARG:NE	5:A:239:LEU:HA	2.03	0.74
5:A:106:VAL:HG21	5:A:275:TRP:CZ2	2.23	0.74
5:A:161:LEU:HB3	5:A:231:ILE:HD12	1.70	0.74
5:A:164:LEU:HD11	5:A:177:LEU:HB3	1.69	0.74
5:D:235:ARG:NH2	5:D:237:LYS:O	2.21	0.73
5:A:235:ARG:HE	5:A:239:LEU:CA	2.02	0.73
5:D:333:ASP:OD2	5:D:333:ASP:N	2.20	0.73
5:A:388:GLU:O	5:A:391:LEU:HG	1.88	0.73
5:D:389:HIS:ND1	5:D:390:LEU:HD12	2.03	0.73
5:A:102:ASP:OD1	5:A:104:SER:N	2.21	0.73
5:D:380:LEU:HD12	5:D:380:LEU:O	1.88	0.73
5:A:156:ARG:NH1	5:A:268:TRP:O	2.21	0.72
5:A:235:ARG:CD	5:A:239:LEU:HA	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:321:VAL:HG22	5:A:323:VAL:N	1.98	0.72
2:C:2:DA:C1'	2:C:3:DA:H5'	2.20	0.72
5:A:88:LEU:CD1	5:A:92:LEU:HG	2.19	0.72
5:A:192:GLN:OE1	5:A:192:GLN:N	2.22	0.72
5:A:116:ASN:HD21	5:A:394:LEU:HA	1.55	0.72
5:A:211:HIS:HD2	5:A:212:GLY:O	1.72	0.72
5:A:235:ARG:HE	5:A:239:LEU:HA	1.53	0.72
5:D:145:TRP:O	5:D:149:THR:HG22	1.89	0.71
5:D:300:ILE:HG23	5:D:301:GLY:H	1.54	0.71
5:D:333:ASP:HB2	5:D:334:ILE:HD13	1.71	0.71
5:A:113:ILE:HD11	5:A:143:PHE:CE1	2.24	0.71
5:D:145:TRP:CZ3	5:D:156:ARG:HG2	2.25	0.71
4:F:0:DA:OP2	4:F:0:DA:H3'	1.90	0.71
5:A:11:LEU:HD12	5:A:16:ALA:N	2.05	0.71
5:D:388:GLU:OE1	5:D:388:GLU:N	2.23	0.71
5:A:155:ASP:O	5:A:158:THR:HG22	1.91	0.71
5:A:321:VAL:CG2	5:A:323:VAL:H	2.00	0.71
5:D:224:ILE:HA	5:D:227:GLN:CG	2.20	0.71
5:D:349:LEU:N	5:D:350:PRO:HD2	2.05	0.71
1:B:3:DA:H2''	1:B:4:DA:C5'	2.16	0.70
5:A:365:PRO:O	5:A:368:LYS:N	2.21	0.70
5:D:74:PHE:O	5:D:78:LEU:HD12	1.91	0.70
5:D:11:LEU:HB2	5:D:12:PRO:HD2	1.73	0.70
5:A:83:ASN:O	5:A:86:LEU:HG	1.92	0.70
5:D:177:LEU:HD13	5:D:202:MET:HE1	1.73	0.70
4:F:2:DA:O5'	4:F:2:DA:C2'	2.40	0.70
5:D:83:ASN:O	5:D:87:VAL:HG13	1.91	0.70
5:D:126:GLN:H	5:D:126:GLN:CD	1.99	0.70
5:D:368:LYS:HA	5:D:373:ILE:HD11	1.72	0.69
5:A:81:GLU:HB3	5:A:83:ASN:OD1	1.92	0.69
5:A:211:HIS:NE2	5:A:364:ASP:OD2	2.23	0.69
5:A:369:THR:OG1	5:A:371:GLN:HG2	1.92	0.69
1:B:1:DT:H72	1:B:1:DT:OP2	1.92	0.69
5:A:153:PHE:CE1	5:A:248:LEU:HD12	2.26	0.69
5:A:189:PRO:HA	5:A:199:ILE:HD11	1.73	0.69
5:D:30:LEU:HD13	5:D:30:LEU:N	2.05	0.69
5:D:252:TYR:CD1	5:D:256:PHE:HE2	2.02	0.69
5:A:103:TYR:O	5:A:107:ILE:HD13	1.93	0.69
5:D:131:LYS:HG2	5:D:132:THR:N	2.07	0.69
5:A:197:CYS:SG	5:A:199:ILE:HG12	2.33	0.69
5:A:93:TYR:O	5:A:96:VAL:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:DT:H2'	2:C:14:DT:C5'	2.16	0.68
2:C:6:DT:H2''	2:C:7:DT:H5''	1.76	0.68
5:A:122:THR:OG1	5:A:125:LEU:HD11	1.93	0.68
5:A:209:ARG:HE	5:A:235:ARG:NH1	1.89	0.68
5:A:105:ASN:O	5:D:389:HIS:CG	2.47	0.68
5:A:105:ASN:ND2	5:D:386:SER:O	2.27	0.68
5:A:235:ARG:HD3	5:A:239:LEU:HA	1.74	0.68
5:A:214:LYS:H	5:A:214:LYS:HD2	1.59	0.68
5:A:389:HIS:CG	5:D:105:ASN:O	2.47	0.68
5:A:186:VAL:HG11	5:A:307:ILE:HD13	1.75	0.68
5:D:389:HIS:NE2	5:D:393:GLN:NE2	2.42	0.68
5:A:143:PHE:HB2	5:A:252:TYR:OH	1.95	0.67
5:D:126:GLN:N	5:D:126:GLN:OE1	2.26	0.67
5:A:115:ILE:HD11	5:A:391:LEU:HA	1.76	0.67
5:A:389:HIS:CG	5:D:105:ASN:C	2.73	0.67
5:A:389:HIS:CG	5:A:390:LEU:N	2.63	0.67
5:D:162:LYS:NZ	5:D:230:HIS:HA	2.08	0.67
5:D:211:HIS:NE2	5:D:364:ASP:OD2	2.28	0.67
5:A:145:TRP:O	5:A:149:THR:HG22	1.94	0.67
3:E:2:DA:H2'	3:E:3:DA:O4'	1.95	0.66
5:A:115:ILE:HG23	5:A:116:ASN:N	2.09	0.66
5:D:70:ALA:O	5:D:74:PHE:CD2	2.48	0.66
5:A:162:LYS:HG3	5:A:231:ILE:CD1	2.26	0.66
3:E:6:DT:C2'	3:E:7:DA:H8	2.05	0.66
5:A:333:ASP:OD2	5:A:333:ASP:N	2.14	0.66
5:D:150:ASN:HD21	5:D:275:TRP:HE3	1.44	0.66
5:D:397:LYS:HE2	5:D:401:VAL:CG1	2.26	0.66
4:F:2:DA:C6	4:F:3:DA:N6	2.64	0.66
5:D:8:LEU:HA	5:D:11:LEU:CD1	2.26	0.66
5:D:140:LEU:O	5:D:144:GLN:HG3	1.95	0.66
5:D:161:LEU:C	5:D:161:LEU:HD12	2.21	0.66
5:D:252:TYR:O	5:D:255:ILE:HG22	1.96	0.66
2:C:4:DT:H2''	2:C:5:DT:H72	1.77	0.66
5:D:26:TYR:CE2	5:D:44:PHE:CE2	2.84	0.66
5:D:387:GLN:HA	5:D:387:GLN:OE1	1.96	0.66
5:A:40:ASP:HA	5:A:44:PHE:CE2	2.31	0.65
5:D:244:ARG:HG2	5:D:244:ARG:NH1	2.11	0.65
2:C:4:DT:H2'	5:A:128:LYS:NZ	2.12	0.65
5:A:188:VAL:HG13	5:A:189:PRO:HD2	1.78	0.65
5:A:294:SER:HB2	5:A:299:THR:HA	1.78	0.65
5:A:83:ASN:OD1	5:A:84:ASP:N	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:333:ASP:HB2	5:A:334:ILE:HD13	1.78	0.65
5:D:59:ASP:OD1	5:D:59:ASP:N	2.28	0.65
5:D:365:PRO:HA	5:D:368:LYS:CG	2.26	0.65
5:D:129:HIS:O	5:D:130:PHE:HB2	1.96	0.65
5:A:115:ILE:HB	5:A:390:LEU:CD2	2.27	0.65
5:A:96:VAL:HG23	5:A:97:LYS:N	2.11	0.65
5:A:279:PRO:HD3	5:A:306:TYR:CE1	2.32	0.65
5:D:33:MET:HB3	5:D:34:PRO:HD2	1.79	0.65
5:D:128:LYS:HD3	5:D:129:HIS:CD2	2.31	0.65
5:A:300:ILE:CG2	5:A:301:GLY:H	2.09	0.65
2:C:12:DA:H1'	2:C:13:DT:C6	2.32	0.64
4:F:5:DT:H2''	4:F:6:DT:H72	1.79	0.64
5:A:105:ASN:HB3	5:D:389:HIS:HB3	1.78	0.64
4:F:1:DA:C2	4:F:2:DA:C2	2.85	0.64
5:A:299:THR:HG23	5:A:304:ASP:OD1	1.95	0.64
5:D:186:VAL:HG11	5:D:307:ILE:HD13	1.78	0.64
5:D:6:SER:O	5:D:9:LYS:HB2	1.97	0.64
5:D:8:LEU:HA	5:D:11:LEU:HD11	1.78	0.64
5:D:365:PRO:O	5:D:368:LYS:N	2.24	0.64
1:B:4:DA:C2	2:C:14:DT:O2	2.51	0.64
5:A:209:ARG:NE	5:A:235:ARG:NH1	2.44	0.64
5:D:118:TRP:CZ2	5:D:201:THR:HG23	2.33	0.64
5:D:211:HIS:C	5:D:211:HIS:CD2	2.75	0.64
1:B:2:DT:H2''	1:B:3:DA:H5''	1.78	0.64
5:A:179:HIS:CE1	5:A:181:SER:HB2	2.33	0.64
2:C:4:DT:H3'	5:A:128:LYS:HE3	1.78	0.63
2:C:8:DA:H2''	2:C:9:DT:C5'	2.27	0.63
3:E:2:DA:N6	3:E:3:DA:C6	2.65	0.63
3:E:14:DT:H5''	5:D:237:LYS:O	1.99	0.63
4:F:3:DA:H1'	4:F:4:DA:H5'	1.81	0.63
1:B:11:DA:H2''	1:B:12:DA:C8	2.33	0.63
4:F:0:DA:H3'	4:F:0:DA:P	2.39	0.63
5:A:300:ILE:HG23	5:A:301:GLY:N	2.13	0.63
5:A:40:ASP:N	5:A:44:PHE:CE2	2.67	0.63
5:A:167:ILE:O	5:A:175:CYS:HA	1.99	0.63
5:D:40:ASP:C	5:D:41:LEU:HD12	2.23	0.63
5:A:189:PRO:N	5:A:199:ILE:HD11	2.12	0.63
5:A:204:VAL:O	5:A:208:LEU:HD12	1.98	0.63
5:A:386:SER:OG	5:A:387:GLN:OE1	2.13	0.63
5:D:27:THR:HA	5:D:30:LEU:HD23	1.74	0.63
1:B:6:DT:H3'	5:A:265:LYS:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:101:PHE:CD2	5:A:276:PRO:HD3	2.33	0.63
5:D:148:ASN:OD1	5:D:312:ARG:NH2	2.32	0.63
2:C:4:DT:P	5:A:128:LYS:HZ1	2.18	0.62
3:E:6:DT:C2'	3:E:7:DA:C8	2.78	0.62
5:A:160:SER:HB2	5:A:230:HIS:HD2	1.63	0.62
5:D:256:PHE:O	5:D:260:GLN:N	2.32	0.62
5:A:33:MET:HB3	5:A:34:PRO:CD	2.28	0.62
5:A:214:LYS:HD2	5:A:214:LYS:N	2.12	0.62
5:D:148:ASN:OD1	5:D:312:ARG:CZ	2.47	0.62
5:D:251:TRP:CE3	5:D:251:TRP:N	2.67	0.62
5:D:389:HIS:HD1	5:D:390:LEU:HD12	1.63	0.62
5:A:103:TYR:C	5:A:107:ILE:HD13	2.25	0.62
5:A:272:ASN:O	5:A:275:TRP:HB2	1.98	0.62
5:D:224:ILE:HA	5:D:227:GLN:HG3	1.79	0.62
5:D:371:GLN:O	5:D:374:ALA:N	2.33	0.62
5:D:139:LEU:HD13	5:D:251:TRP:HB3	1.81	0.62
4:F:1:DA:C1'	4:F:2:DA:H5'	2.30	0.62
5:A:160:SER:CB	5:A:230:HIS:HD2	2.12	0.62
5:A:22:ILE:HG22	5:A:23:TRP:N	2.13	0.62
5:A:246:LEU:HD12	5:A:247:THR:N	2.15	0.62
5:D:95:LEU:HD12	5:D:95:LEU:O	1.97	0.62
5:D:11:LEU:HD22	5:D:11:LEU:H	1.65	0.62
4:F:0:DA:H2''	4:F:1:DA:C8	2.34	0.62
5:A:109:ILE:HD11	5:D:389:HIS:HD2	1.64	0.62
5:D:112:LYS:NZ	5:D:259:CYS:O	2.30	0.61
5:A:115:ILE:HG23	5:A:116:ASN:H	1.66	0.61
5:D:160:SER:O	5:D:163:ASP:HB2	2.00	0.61
5:D:115:ILE:HG23	5:D:116:ASN:H	1.65	0.61
5:A:153:PHE:CE2	5:A:157:THR:HG21	2.36	0.61
5:D:128:LYS:HD3	5:D:129:HIS:ND1	2.14	0.61
2:C:14:DT:H1'	2:C:15:DA:H5'	1.82	0.61
5:D:213:VAL:HG12	5:D:216:TYR:CD2	2.36	0.61
4:F:1:DA:H1'	4:F:2:DA:H5'	1.83	0.61
5:A:11:LEU:HD12	5:A:16:ALA:HB2	1.81	0.61
5:D:160:SER:CB	5:D:230:HIS:HD2	2.13	0.61
5:A:7:LEU:HD12	5:A:7:LEU:O	2.02	0.60
1:B:14:DT:H5'	1:B:14:DT:C6	2.36	0.60
5:A:389:HIS:CD2	5:D:105:ASN:HB3	2.36	0.60
5:D:30:LEU:CD2	5:D:44:PHE:CZ	2.83	0.60
4:F:1:DA:H2''	4:F:2:DA:OP2	2.00	0.60
5:A:79:ASP:OD1	5:A:79:ASP:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:110:LEU:HD12	5:A:143:PHE:HE2	1.64	0.60
5:A:113:ILE:CD1	5:A:143:PHE:CE1	2.84	0.60
5:A:145:TRP:CZ3	5:A:156:ARG:HG2	2.35	0.60
5:D:371:GLN:H	5:D:371:GLN:CD	2.01	0.60
5:A:153:PHE:CE2	5:A:245:GLU:HG3	2.36	0.60
5:D:107:ILE:HG22	5:D:108:ALA:N	2.17	0.60
5:D:182:LYS:HB2	5:D:183:PRO:CD	2.26	0.60
5:D:8:LEU:O	5:D:11:LEU:HD21	2.02	0.60
5:D:113:ILE:HD12	5:D:143:PHE:CE1	2.37	0.60
5:D:338:PHE:O	5:D:341:LEU:N	2.35	0.60
4:F:6:DT:H2''	4:F:7:DT:O5'	2.02	0.59
5:A:209:ARG:NH2	5:A:235:ARG:HH12	1.99	0.59
5:D:300:ILE:HG23	5:D:301:GLY:N	2.17	0.59
5:D:371:GLN:O	5:D:374:ALA:HB3	2.02	0.59
5:D:141:LEU:HD23	5:D:234:ILE:CG2	2.33	0.59
5:A:106:VAL:HG22	5:A:147:PHE:CZ	2.37	0.59
5:D:18:LEU:HD13	5:D:19:TYR:CD1	2.37	0.59
5:D:106:VAL:HG21	5:D:275:TRP:CZ2	2.38	0.59
5:D:167:ILE:O	5:D:175:CYS:HA	2.02	0.59
5:D:149:THR:HG23	5:D:151:VAL:HG23	1.84	0.59
5:A:130:PHE:HA	5:A:135:ASP:HB2	1.83	0.59
5:A:209:ARG:CZ	5:A:235:ARG:HH12	2.15	0.59
5:D:252:TYR:O	5:D:256:PHE:HD2	1.85	0.59
5:D:18:LEU:HD13	5:D:19:TYR:HD1	1.65	0.59
5:D:300:ILE:CG2	5:D:301:GLY:H	2.14	0.59
4:F:8:DT:P	5:D:244:ARG:HE	2.23	0.59
5:A:108:ALA:HB3	5:D:393:GLN:NE2	2.18	0.59
5:D:81:GLU:CD	5:D:83:ASN:OD1	2.45	0.59
5:D:335:GLN:O	5:D:339:ASP:OD2	2.20	0.59
5:A:389:HIS:CD2	5:D:105:ASN:HD22	2.21	0.59
5:D:380:LEU:HD12	5:D:380:LEU:C	2.28	0.59
5:A:103:TYR:O	5:A:105:ASN:N	2.36	0.58
5:A:191:PHE:CE2	5:A:316:GLN:HG3	2.38	0.58
5:D:70:ALA:O	5:D:74:PHE:HD2	1.86	0.58
4:F:1:DA:H1'	4:F:2:DA:C5'	2.34	0.58
5:A:371:GLN:O	5:A:374:ALA:N	2.37	0.58
5:D:389:HIS:O	5:D:392:ALA:N	2.36	0.58
3:E:7:DA:C2	4:F:11:DA:C2	2.91	0.58
5:A:140:LEU:O	5:A:144:GLN:HG3	2.03	0.58
4:F:0:DA:H2''	4:F:1:DA:H5'	1.85	0.58
5:A:108:ALA:HB3	5:D:393:GLN:HE21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:29:TRP:HE3	5:D:30:LEU:CD1	2.17	0.58
5:D:41:LEU:H	5:D:43:LEU:HD21	1.69	0.58
5:D:251:TRP:N	5:D:251:TRP:HE3	2.02	0.58
3:E:3:DA:H2''	3:E:4:DT:C6	2.39	0.57
5:A:161:LEU:HB3	5:A:231:ILE:CD1	2.35	0.57
5:D:27:THR:CA	5:D:30:LEU:CD2	2.55	0.57
5:D:44:PHE:O	5:D:44:PHE:CG	2.56	0.57
2:C:4:DT:H2'	5:A:128:LYS:CE	2.33	0.57
5:A:112:LYS:HG2	5:A:261:LEU:HD11	1.86	0.57
2:C:6:DT:C2'	2:C:7:DT:H5''	2.35	0.57
5:A:209:ARG:HH21	5:A:235:ARG:HH12	1.52	0.57
5:A:213:VAL:HG23	5:A:216:TYR:HB2	1.82	0.57
5:A:279:PRO:HB2	5:A:281:PHE:CE2	2.40	0.57
5:D:26:TYR:CE2	5:D:44:PHE:HE2	2.22	0.57
5:A:9:LYS:CE	5:A:10:GLU:HG2	2.34	0.57
5:A:329:ASP:O	5:A:329:ASP:OD1	2.22	0.57
5:D:114:SER:OG	5:D:140:LEU:HD11	2.04	0.57
5:A:245:GLU:CD	5:A:245:GLU:H	2.12	0.57
5:D:87:VAL:CG2	5:D:88:LEU:N	2.67	0.57
5:D:113:ILE:HD12	5:D:143:PHE:CZ	2.39	0.57
1:B:3:DA:H2'	1:B:4:DA:H8	1.64	0.57
5:A:11:LEU:CD1	5:A:16:ALA:N	2.67	0.57
5:A:84:ASP:O	5:A:87:VAL:HG22	2.04	0.57
5:A:389:HIS:CD2	5:A:390:LEU:CA	2.87	0.57
1:B:12:DA:H2''	1:B:13:DA:C5'	2.35	0.56
4:F:2:DA:C2'	4:F:3:DA:OP2	2.53	0.56
5:D:365:PRO:HA	5:D:368:LYS:HG3	1.86	0.56
5:D:107:ILE:CG2	5:D:108:ALA:N	2.68	0.56
5:A:113:ILE:HD11	5:A:143:PHE:HE1	1.69	0.56
5:A:380:LEU:HG	5:A:381:PRO:HD2	1.87	0.56
5:A:384:ILE:O	5:A:386:SER:N	2.38	0.56
5:A:79:ASP:C	5:A:80:ILE:HD12	2.31	0.56
5:A:213:VAL:HG22	5:A:217:TYR:CD2	2.39	0.56
5:A:119:ASN:O	5:A:136:LYS:NZ	2.39	0.56
5:D:216:TYR:CD2	5:D:216:TYR:N	2.72	0.56
5:D:388:GLU:HA	5:D:391:LEU:HD21	1.86	0.56
5:A:199:ILE:HG22	5:A:202:MET:CE	2.35	0.56
5:D:42:LYS:H	5:D:42:LYS:HZ2	1.54	0.56
1:B:4:DA:H1'	1:B:5:DT:H5'	1.88	0.56
5:A:43:LEU:HD23	5:A:43:LEU:H	1.71	0.56
2:C:4:DT:P	5:A:128:LYS:HZ2	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:184:ASN:OD1	5:A:302:ILE:HD11	2.06	0.56
5:A:395:ILE:HD13	5:A:395:ILE:H	1.71	0.56
5:A:96:VAL:O	5:A:97:LYS:C	2.49	0.55
5:A:256:PHE:CZ	5:A:268:TRP:CH2	2.94	0.55
5:A:321:VAL:HG21	5:A:346:VAL:CG1	2.19	0.55
5:D:115:ILE:HG23	5:D:116:ASN:N	2.21	0.55
1:B:6:DT:H3'	5:A:265:LYS:CD	2.36	0.55
1:B:1:DT:OP2	1:B:1:DT:C7	2.54	0.55
3:E:10:DA:H2''	3:E:11:DA:OP2	2.05	0.55
5:D:129:HIS:O	5:D:130:PHE:CB	2.54	0.55
1:B:4:DA:H2	2:C:14:DT:O2	1.89	0.55
2:C:12:DA:H2''	2:C:13:DT:H72	1.88	0.55
5:D:365:PRO:HA	5:D:368:LYS:HG2	1.89	0.55
2:C:6:DT:OP2	5:A:247:THR:HG21	2.07	0.55
5:A:395:ILE:HD13	5:A:395:ILE:N	2.21	0.55
5:D:211:HIS:CD2	5:D:211:HIS:O	2.59	0.55
5:D:98:LEU:HD12	5:D:309:LYS:HG2	1.88	0.55
5:A:91:ARG:HG3	5:A:91:ARG:HH11	1.71	0.55
5:D:29:TRP:CE3	5:D:30:LEU:CD1	2.90	0.55
5:D:161:LEU:HG	5:D:231:ILE:CG2	2.36	0.55
5:D:179:HIS:HE1	5:D:181:SER:HB3	1.64	0.54
2:C:2:DA:C2'	2:C:3:DA:H5'	2.37	0.54
5:A:42:LYS:HE3	5:A:79:ASP:OD1	2.07	0.54
5:A:96:VAL:CG2	5:A:97:LYS:N	2.70	0.54
5:A:253:PRO:O	5:A:257:LYS:HG3	2.08	0.54
5:A:160:SER:HB2	5:A:230:HIS:CD2	2.41	0.54
5:A:372:ASN:O	5:A:376:LEU:HG	2.08	0.54
2:C:11:DA:C2	2:C:12:DA:C2	2.96	0.54
5:A:14:ARG:O	5:A:17:HIS:HB3	2.07	0.54
5:D:103:TYR:C	5:D:105:ASN:H	2.15	0.54
5:D:169:ASP:OD2	5:D:172:ASN:ND2	2.27	0.54
5:D:395:ILE:HD13	5:D:395:ILE:N	2.19	0.54
4:F:7:DT:C5'	5:D:244:ARG:HD2	2.36	0.54
5:A:83:ASN:CG	5:A:84:ASP:H	2.14	0.54
5:A:119:ASN:HA	5:A:356:PHE:CE1	2.42	0.54
5:D:211:HIS:CE1	5:D:364:ASP:OD2	2.60	0.54
5:A:149:THR:HG23	5:A:151:VAL:HG23	1.90	0.54
5:A:166:CYS:SG	5:A:168:LEU:HG	2.48	0.54
5:D:95:LEU:HD11	5:D:99:LEU:CG	2.36	0.54
4:F:0:DA:C2'	4:F:1:DA:H5'	2.38	0.54
5:A:40:ASP:CA	5:A:44:PHE:CE2	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:DA:O4'	4:F:2:DA:H5'	2.07	0.54
5:A:115:ILE:CD1	5:A:391:LEU:HA	2.38	0.54
5:D:68:CYS:O	5:D:72:ILE:HG13	2.07	0.54
5:D:73:TRP:O	5:D:74:PHE:C	2.50	0.54
5:D:111:GLN:OE1	5:D:389:HIS:HE1	1.90	0.54
5:A:111:GLN:OE1	5:A:389:HIS:CE1	2.56	0.54
5:D:18:LEU:HD22	5:D:18:LEU:O	2.07	0.54
5:D:214:LYS:O	5:D:216:TYR:CD2	2.61	0.54
5:A:11:LEU:HD12	5:A:16:ALA:CA	2.38	0.53
5:A:33:MET:HB3	5:A:34:PRO:HD2	1.89	0.53
5:A:105:ASN:O	5:D:389:HIS:ND1	2.41	0.53
5:D:8:LEU:O	5:D:11:LEU:CD2	2.55	0.53
5:D:29:TRP:O	5:D:32:THR:HB	2.07	0.53
5:A:177:LEU:HD13	5:A:202:MET:HE1	1.90	0.53
5:D:130:PHE:HZ	5:D:251:TRP:HB3	1.72	0.53
5:D:161:LEU:O	5:D:164:LEU:HB2	2.08	0.53
5:A:79:ASP:O	5:A:80:ILE:HD12	2.08	0.53
5:A:389:HIS:CD2	5:D:105:ASN:CB	2.91	0.53
2:C:14:DT:H5'	2:C:14:DT:C6	2.43	0.53
5:A:321:VAL:HG22	5:A:322:HIS:N	2.23	0.53
5:A:384:ILE:C	5:A:386:SER:N	2.65	0.53
2:C:4:DT:C2	2:C:5:DT:C4	2.97	0.53
5:A:138:LYS:HG2	5:A:234:ILE:HD12	1.89	0.53
5:A:274:GLU:OE1	5:A:275:TRP:HD1	1.91	0.53
5:D:26:TYR:O	5:D:30:LEU:HD22	2.08	0.53
5:A:140:LEU:HD11	5:A:144:GLN:NE2	2.20	0.53
5:D:161:LEU:HG	5:D:231:ILE:HG23	1.89	0.53
5:D:389:HIS:CE1	5:D:390:LEU:HD12	2.43	0.53
5:D:380:LEU:HD13	5:D:382:LEU:C	2.34	0.53
2:C:6:DT:H5''	5:A:244:ARG:HG2	1.91	0.52
2:C:14:DT:H4'	2:C:14:DT:OP1	2.09	0.52
5:A:274:GLU:OE1	5:A:275:TRP:CD1	2.62	0.52
5:D:60:ILE:O	5:D:63:ASP:N	2.41	0.52
5:D:203:ALA:HB1	5:D:345:LEU:HB2	1.91	0.52
1:B:3:DA:N1	2:C:15:DA:C6	2.77	0.52
5:A:109:ILE:CD1	5:D:389:HIS:HD2	2.22	0.52
5:A:384:ILE:O	5:A:387:GLN:N	2.39	0.52
5:D:106:VAL:HG22	5:D:147:PHE:CZ	2.44	0.52
5:D:214:LYS:O	5:D:215:LYS:HB2	2.08	0.52
5:A:199:ILE:O	5:A:202:MET:N	2.43	0.52
5:D:294:SER:HA	5:D:299:THR:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:113:ILE:O	5:A:114:SER:C	2.51	0.52
5:D:18:LEU:HD22	5:D:18:LEU:C	2.35	0.52
5:D:111:GLN:OE1	5:D:389:HIS:CE1	2.63	0.52
5:D:250:ASN:HB3	5:D:251:TRP:CE3	2.44	0.52
5:D:251:TRP:CE3	5:D:251:TRP:CA	2.93	0.52
5:D:345:LEU:O	5:D:349:LEU:HB2	2.10	0.52
5:A:151:VAL:HG12	5:A:152:SER:O	2.10	0.52
5:A:179:HIS:NE2	5:A:181:SER:HB2	2.25	0.52
1:B:3:DA:N6	2:C:14:DT:O4	2.43	0.52
5:A:18:LEU:HD22	5:A:18:LEU:O	2.10	0.52
5:A:224:ILE:HA	5:A:227:GLN:HG2	1.92	0.52
5:D:388:GLU:HG2	5:D:389:HIS:N	2.24	0.52
5:A:388:GLU:HG2	5:A:389:HIS:N	2.24	0.52
1:B:6:DT:C4	1:B:7:DT:C4	2.99	0.51
5:A:98:LEU:HD11	5:A:310:MET:HG3	1.92	0.51
5:A:109:ILE:CD1	5:D:389:HIS:CD2	2.94	0.51
5:A:153:PHE:CD2	5:A:153:PHE:C	2.88	0.51
5:D:122:THR:HG23	5:D:136:LYS:HZ1	1.75	0.51
2:C:5:DT:H2''	2:C:6:DT:O5'	2.11	0.51
5:A:32:THR:HG22	5:A:32:THR:O	2.10	0.51
5:D:138:LYS:NZ	5:D:205:TYR:OH	2.43	0.51
5:D:148:ASN:O	5:D:310:MET:HG2	2.09	0.51
5:A:88:LEU:HD12	5:A:88:LEU:C	2.36	0.51
5:A:233:ILE:N	5:A:233:ILE:HD12	2.25	0.51
5:D:95:LEU:HD12	5:D:99:LEU:HG	1.93	0.51
5:D:46:SER:HB3	5:D:49:TYR:CD2	2.45	0.51
5:A:210:PHE:O	5:A:219:GLY:HA3	2.10	0.51
5:D:122:THR:HG23	5:D:136:LYS:NZ	2.25	0.51
5:D:179:HIS:CE1	5:D:181:SER:CB	2.81	0.51
5:D:397:LYS:HE2	5:D:401:VAL:HG11	1.92	0.51
5:D:83:ASN:OD1	5:D:83:ASN:N	2.41	0.51
5:D:177:LEU:CD1	5:D:202:MET:HE1	2.40	0.51
5:D:211:HIS:HD2	5:D:212:GLY:O	1.93	0.51
5:D:254:THR:HA	5:D:257:LYS:HD2	1.93	0.51
4:F:6:DT:OP1	5:D:129:HIS:HD2	1.94	0.51
5:A:124:SER:HB2	5:A:258:TYR:CE1	2.46	0.51
5:A:384:ILE:C	5:A:386:SER:H	2.18	0.51
5:D:368:LYS:HA	5:D:373:ILE:CD1	2.40	0.51
5:D:57:HIS:HB3	5:D:59:ASP:OD1	2.11	0.50
2:C:11:DA:C6	2:C:12:DA:C6	3.00	0.50
5:D:42:LYS:HB2	5:D:42:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:117:LEU:HD11	5:D:139:LEU:HD23	1.92	0.50
5:D:130:PHE:HZ	5:D:251:TRP:CB	2.24	0.50
5:D:143:PHE:C	5:D:143:PHE:CD2	2.88	0.50
5:D:211:HIS:CD2	5:D:212:GLY:O	2.65	0.50
5:D:189:PRO:HA	5:D:197:CYS:SG	2.50	0.50
5:A:191:PHE:HE2	5:A:316:GLN:HG3	1.74	0.50
5:A:174:LYS:HE3	5:A:299:THR:HG22	1.94	0.50
5:D:11:LEU:HD23	5:D:12:PRO:O	2.11	0.50
5:D:397:LYS:HE2	5:D:401:VAL:HG13	1.92	0.50
5:A:90:GLN:HA	5:A:90:GLN:OE1	2.12	0.50
5:A:389:HIS:O	5:A:392:ALA:N	2.45	0.50
5:D:160:SER:OG	5:D:230:HIS:CD2	2.58	0.50
2:C:2:DA:C6	2:C:3:DA:C6	3.00	0.49
5:D:40:ASP:CA	5:D:43:LEU:HD11	2.40	0.49
5:D:246:LEU:O	5:D:246:LEU:HD23	2.12	0.49
5:D:294:SER:OG	5:D:295:ASP:N	2.40	0.49
2:C:13:DT:C3'	2:C:14:DT:H5''	2.41	0.49
5:A:115:ILE:CG2	5:A:116:ASN:N	2.75	0.49
5:D:95:LEU:C	5:D:95:LEU:CD1	2.77	0.49
5:A:40:ASP:O	5:A:41:LEU:HD12	2.12	0.49
5:A:89:GLN:HE21	5:A:93:TYR:HE2	1.60	0.49
5:D:254:THR:O	5:D:257:LYS:HG3	2.12	0.49
5:A:68:CYS:O	5:A:72:ILE:HG13	2.13	0.49
5:A:199:ILE:O	5:A:200:PHE:C	2.55	0.49
5:D:113:ILE:CD1	5:D:143:PHE:CE1	2.95	0.49
5:D:125:LEU:HD12	5:D:125:LEU:C	2.38	0.49
5:A:18:LEU:HD13	5:A:19:TYR:HD1	1.77	0.49
5:A:295:ASP:OD1	5:A:298:ASN:ND2	2.46	0.49
5:A:382:LEU:HD21	5:A:386:SER:OG	2.13	0.49
5:D:11:LEU:CD2	5:D:11:LEU:C	2.85	0.49
1:B:3:DA:C2	2:C:15:DA:C2	3.01	0.49
5:A:235:ARG:CD	5:A:239:LEU:HD23	2.43	0.49
5:D:47:GLN:O	5:D:51:VAL:HG23	2.13	0.49
5:A:47:GLN:O	5:A:51:VAL:HG23	2.12	0.49
5:A:102:ASP:OD1	5:A:104:SER:HB3	2.13	0.49
5:A:125:LEU:HG	5:A:258:TYR:CE1	2.47	0.49
5:A:162:LYS:N	5:A:231:ILE:HD11	2.28	0.49
5:D:349:LEU:N	5:D:350:PRO:CD	2.73	0.49
2:C:4:DT:C3'	5:A:128:LYS:HE3	2.43	0.49
2:C:12:DA:H2''	2:C:13:DT:C7	2.43	0.49
5:A:11:LEU:HD22	5:A:12:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:59:ASP:OD2	5:A:59:ASP:N	2.46	0.49
5:A:83:ASN:O	5:A:87:VAL:HG13	2.13	0.49
5:A:83:ASN:CG	5:A:84:ASP:N	2.71	0.49
5:A:300:ILE:CG2	5:A:301:GLY:N	2.73	0.49
5:A:371:GLN:O	5:A:374:ALA:HB3	2.12	0.49
5:D:124:SER:CB	5:D:258:TYR:HE1	2.15	0.49
5:A:27:THR:OG1	5:A:28:GLU:N	2.45	0.49
5:A:90:GLN:OE1	5:A:90:GLN:CA	2.60	0.49
1:B:1:DT:C6	1:B:1:DT:O5'	2.66	0.49
5:D:397:LYS:HG2	5:D:401:VAL:HG22	1.95	0.49
5:A:330:LEU:HB2	5:A:335:GLN:OE1	2.12	0.48
5:A:385:GLU:HB3	5:D:274:GLU:HG3	1.95	0.48
3:E:11:DA:H4'	3:E:12:DA:OP1	2.11	0.48
5:A:11:LEU:HD12	5:A:16:ALA:CB	2.42	0.48
5:D:11:LEU:HB2	5:D:12:PRO:CD	2.43	0.48
4:F:6:DT:OP1	5:D:129:HIS:CD2	2.67	0.48
5:A:29:TRP:O	5:A:32:THR:N	2.41	0.48
2:C:4:DT:O2	2:C:5:DT:C4	2.66	0.48
5:A:27:THR:O	5:A:30:LEU:N	2.46	0.48
5:A:70:ALA:HB1	5:A:74:PHE:HE2	1.79	0.48
5:A:160:SER:O	5:A:163:ASP:HB2	2.13	0.48
5:A:110:LEU:HD12	5:A:143:PHE:CE2	2.46	0.48
5:A:113:ILE:CD1	5:A:143:PHE:HE1	2.26	0.48
5:D:44:PHE:O	5:D:44:PHE:CD1	2.66	0.48
5:D:167:ILE:HD11	5:D:293:GLU:N	2.29	0.48
3:E:2:DA:C2'	3:E:3:DA:H5'	2.44	0.48
5:D:369:THR:HB	5:D:371:GLN:OE1	2.14	0.48
1:B:2:DT:H6	1:B:2:DT:H2'	1.48	0.48
5:A:40:ASP:HA	5:A:44:PHE:CZ	2.48	0.48
5:D:132:THR:HG23	5:D:135:ASP:OD2	2.14	0.48
4:F:2:DA:C2	4:F:3:DA:C6	3.02	0.48
5:A:153:PHE:O	5:A:156:ARG:HB2	2.14	0.48
5:D:87:VAL:O	5:D:90:GLN:HB2	2.14	0.48
5:D:149:THR:CG2	5:D:151:VAL:HG23	2.43	0.48
5:D:150:ASN:ND2	5:D:275:TRP:HE3	2.10	0.48
5:D:227:GLN:H	5:D:227:GLN:HG2	1.43	0.48
4:F:3:DA:C8	4:F:4:DA:N7	2.82	0.47
5:A:115:ILE:CG2	5:A:116:ASN:H	2.27	0.47
5:A:188:VAL:HG21	5:A:315:LEU:HD21	1.95	0.47
5:D:271:VAL:HB	5:D:273:GLN:NE2	2.17	0.47
4:F:8:DT:P	5:D:244:ARG:HH21	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:258:TYR:OH	5:A:396:ASP:OD2	2.31	0.47
5:A:299:THR:OG1	5:A:307:ILE:HD11	2.14	0.47
5:A:125:LEU:HD12	5:A:125:LEU:O	2.15	0.47
5:A:143:PHE:CD2	5:A:144:GLN:N	2.67	0.47
5:A:334:ILE:CG2	5:A:338:PHE:HE2	2.28	0.47
5:A:370:PRO:C	5:A:373:ILE:HG22	2.39	0.47
5:D:125:LEU:HB3	5:D:258:TYR:CD1	2.49	0.47
2:C:12:DA:O5'	2:C:12:DA:H2'	2.15	0.47
5:A:105:ASN:C	5:D:389:HIS:CG	2.92	0.47
5:A:105:ASN:CA	5:D:389:HIS:ND1	2.77	0.47
5:A:125:LEU:O	5:A:125:LEU:CD1	2.62	0.47
5:A:388:GLU:O	5:A:389:HIS:C	2.54	0.47
5:D:103:TYR:C	5:D:105:ASN:N	2.73	0.47
5:D:231:ILE:HG23	5:D:231:ILE:O	2.15	0.47
5:A:91:ARG:NH1	5:A:279:PRO:HG3	2.29	0.47
5:A:120:PRO:HD2	5:A:356:PHE:CD1	2.50	0.47
5:A:233:ILE:N	5:A:233:ILE:CD1	2.78	0.47
5:A:242:TYR:CD2	5:A:243:PRO:HD2	2.50	0.47
5:D:88:LEU:HD23	5:D:88:LEU:C	2.39	0.47
5:D:116:ASN:OD1	5:D:395:ILE:HD13	2.15	0.47
5:D:388:GLU:CG	5:D:389:HIS:N	2.78	0.47
4:F:3:DA:H1'	4:F:4:DA:C5'	2.44	0.47
5:A:130:PHE:CZ	5:A:139:LEU:HD22	2.49	0.47
5:A:209:ARG:NH2	5:A:235:ARG:NH1	2.62	0.47
3:E:11:DA:H2''	3:E:12:DA:C5'	2.45	0.46
5:A:11:LEU:HD12	5:A:16:ALA:H	1.75	0.46
5:A:86:LEU:HD12	5:A:87:VAL:N	2.30	0.46
5:D:83:ASN:HA	5:D:86:LEU:CD2	2.45	0.46
5:D:198:PRO:HA	5:D:201:THR:OG1	2.15	0.46
5:A:389:HIS:CD2	5:D:105:ASN:ND2	2.83	0.46
5:D:11:LEU:HD23	5:D:11:LEU:C	2.41	0.46
5:A:96:VAL:O	5:A:99:LEU:N	2.48	0.46
5:A:113:ILE:HD11	5:A:143:PHE:CZ	2.50	0.46
5:A:235:ARG:NH2	5:A:239:LEU:O	2.48	0.46
5:A:252:TYR:O	5:A:255:ILE:HG22	2.14	0.46
5:A:273:GLN:C	5:A:275:TRP:N	2.71	0.46
5:D:26:TYR:HE2	5:D:44:PHE:CE2	2.33	0.46
5:D:187:LEU:HD23	5:D:187:LEU:HA	1.71	0.46
5:D:214:LYS:O	5:D:216:TYR:HD2	1.97	0.46
5:D:334:ILE:O	5:D:337:VAL:HB	2.15	0.46
5:D:372:ASN:O	5:D:376:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:DA:H5''	1:B:3:DA:H8	1.81	0.46
5:A:153:PHE:CD2	5:A:154:GLU:N	2.84	0.46
5:D:4:LEU:HD21	5:D:8:LEU:HD11	1.97	0.46
5:D:140:LEU:HD23	5:D:201:THR:CG2	2.45	0.46
5:D:250:ASN:HB3	5:D:251:TRP:CZ3	2.50	0.46
5:D:316:GLN:N	5:D:316:GLN:CD	2.74	0.46
4:F:1:DA:H1'	4:F:2:DA:O5'	2.16	0.46
5:A:110:LEU:O	5:A:111:GLN:C	2.57	0.46
5:A:224:ILE:HA	5:A:227:GLN:CG	2.46	0.46
5:D:82:ASN:O	5:D:85:VAL:CG1	2.63	0.46
2:C:4:DT:O5'	5:A:128:LYS:NZ	2.35	0.46
5:A:209:ARG:HH21	5:A:235:ARG:NH1	2.13	0.46
5:D:128:LYS:O	5:D:131:LYS:HD3	2.16	0.46
5:D:379:THR:HG22	5:D:380:LEU:N	2.31	0.46
3:E:11:DA:C2	3:E:12:DA:C2	3.04	0.46
5:A:97:LYS:O	5:A:101:PHE:CB	2.61	0.46
5:A:102:ASP:OD1	5:A:102:ASP:C	2.58	0.46
5:D:98:LEU:CD1	5:D:309:LYS:HG2	2.46	0.46
5:D:388:GLU:CG	5:D:389:HIS:H	2.29	0.46
5:A:25:LYS:HG2	5:A:53:TYR:HH	1.78	0.46
5:A:97:LYS:HD2	5:A:274:GLU:O	2.15	0.46
5:D:130:PHE:HD2	5:D:135:ASP:HB3	1.80	0.46
5:D:161:LEU:C	5:D:161:LEU:CD1	2.88	0.46
2:C:4:DT:O2	2:C:5:DT:N3	2.49	0.46
3:E:1:DT:H1'	3:E:2:DA:C8	2.51	0.46
5:A:90:GLN:N	5:A:90:GLN:CD	2.73	0.46
5:D:189:PRO:N	5:D:199:ILE:HD12	2.31	0.46
5:D:217:TYR:CE1	5:D:218:LYS:HG2	2.51	0.46
2:C:4:DT:C2'	5:A:128:LYS:CE	2.94	0.45
5:A:98:LEU:O	5:A:309:LYS:HE2	2.16	0.45
5:D:82:ASN:O	5:D:85:VAL:HG12	2.15	0.45
5:D:119:ASN:OD1	5:D:120:PRO:HD2	2.16	0.45
5:A:215:LYS:O	5:A:215:LYS:HG2	2.17	0.45
5:D:303:PRO:O	5:D:306:TYR:HB2	2.16	0.45
5:A:35:ASP:OD2	5:A:35:ASP:N	2.49	0.45
5:A:115:ILE:HD12	5:A:390:LEU:C	2.40	0.45
5:A:388:GLU:HA	5:A:391:LEU:HD21	1.99	0.45
4:F:1:DA:C2	4:F:2:DA:N3	2.84	0.45
5:A:18:LEU:HD22	5:A:18:LEU:C	2.41	0.45
5:A:105:ASN:CA	5:D:389:HIS:HD1	2.29	0.45
5:A:354:ARG:HG3	5:A:380:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:384:ILE:C	5:D:386:SER:N	2.71	0.45
1:B:6:DT:C2'	1:B:7:DT:OP2	2.53	0.45
5:A:91:ARG:NH1	5:A:306:TYR:OH	2.49	0.45
5:A:153:PHE:CE2	5:A:157:THR:CG2	2.99	0.45
5:A:192:GLN:N	5:A:192:GLN:CD	2.73	0.45
5:D:364:ASP:O	5:D:368:LYS:HG2	2.16	0.45
5:A:88:LEU:CD1	5:A:88:LEU:C	2.89	0.45
5:A:105:ASN:HA	5:D:389:HIS:ND1	2.31	0.45
5:A:382:LEU:HD12	5:A:383:ASP:N	2.32	0.45
5:D:73:TRP:O	5:D:77:ALA:N	2.44	0.45
2:C:12:DA:C2'	2:C:13:DT:H72	2.47	0.45
5:A:109:ILE:HD11	5:D:389:HIS:CD2	2.46	0.45
5:A:177:LEU:CD1	5:A:202:MET:HE1	2.46	0.45
5:D:65:LEU:N	5:D:66:PRO:HD2	2.31	0.45
5:D:168:LEU:HD23	5:D:175:CYS:HB2	1.99	0.45
5:A:85:VAL:O	5:A:88:LEU:HB3	2.16	0.45
5:A:209:ARG:CZ	5:A:235:ARG:NH1	2.80	0.45
5:D:112:LYS:HA	5:D:393:GLN:OE1	2.17	0.45
5:A:32:THR:O	5:A:32:THR:CG2	2.65	0.45
5:A:258:TYR:CE2	5:A:395:ILE:CG1	3.00	0.45
5:D:300:ILE:CG2	5:D:301:GLY:N	2.77	0.45
5:D:349:LEU:HD12	5:D:349:LEU:HA	1.75	0.45
5:A:106:VAL:CG2	5:A:275:TRP:CZ2	2.97	0.45
5:A:140:LEU:HG	5:A:144:GLN:HG3	1.98	0.44
5:A:213:VAL:HG22	5:A:216:TYR:HB2	1.90	0.44
5:A:386:SER:C	5:A:388:GLU:OE1	2.60	0.44
5:D:6:SER:O	5:D:9:LYS:CB	2.64	0.44
5:D:40:ASP:OD1	5:D:40:ASP:O	2.35	0.44
5:D:95:LEU:O	5:D:98:LEU:HB3	2.18	0.44
5:A:98:LEU:HD21	5:A:306:TYR:HA	1.98	0.44
5:A:108:ALA:CB	5:D:393:GLN:NE2	2.79	0.44
5:A:164:LEU:HD12	5:A:178:ALA:O	2.17	0.44
5:A:213:VAL:HG22	5:A:217:TYR:HD2	1.81	0.44
5:D:109:ILE:N	5:D:109:ILE:HD12	2.33	0.44
5:A:19:TYR:CE2	5:A:70:ALA:HA	2.52	0.44
5:A:321:VAL:CG2	5:A:322:HIS:N	2.81	0.44
5:A:380:LEU:CG	5:A:381:PRO:HD2	2.48	0.44
5:D:98:LEU:CD2	5:D:306:TYR:CD1	3.00	0.44
5:D:155:ASP:HB3	5:D:183:PRO:HG3	1.99	0.44
5:A:42:LYS:CE	5:A:79:ASP:OD1	2.66	0.44
5:A:177:LEU:CD1	5:A:199:ILE:CG2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:365:PRO:O	5:A:368:LYS:HB2	2.18	0.44
2:C:4:DT:H2'	5:A:128:LYS:HZ3	1.83	0.44
3:E:2:DA:H8	3:E:2:DA:H5''	1.82	0.44
5:D:81:GLU:O	5:D:84:ASP:HB3	2.18	0.44
5:A:162:LYS:HE3	5:A:229:GLU:O	2.17	0.44
5:A:235:ARG:CZ	5:A:239:LEU:O	2.65	0.44
4:F:1:DA:OP2	4:F:1:DA:H8	1.99	0.44
5:A:57:HIS:HB3	5:A:59:ASP:OD2	2.17	0.44
5:D:247:THR:HG23	5:D:251:TRP:CZ2	2.53	0.44
1:B:2:DT:C4	2:C:15:DA:N1	2.85	0.44
4:F:0:DA:H2''	4:F:1:DA:OP2	2.17	0.44
5:D:334:ILE:HD13	5:D:334:ILE:N	2.32	0.44
4:F:7:DT:H3'	5:D:244:ARG:HD2	2.00	0.44
5:A:105:ASN:C	5:D:389:HIS:ND1	2.75	0.44
5:D:338:PHE:O	5:D:339:ASP:C	2.59	0.44
1:B:4:DA:H1'	1:B:5:DT:C5'	2.48	0.43
4:F:2:DA:H2'	4:F:2:DA:P	2.58	0.43
5:A:100:GLU:O	5:A:101:PHE:C	2.60	0.43
5:A:116:ASN:ND2	5:A:394:LEU:HA	2.29	0.43
5:A:153:PHE:O	5:A:156:ARG:N	2.50	0.43
5:A:225:LEU:HD21	5:A:338:PHE:CZ	2.53	0.43
5:D:273:GLN:OE1	5:D:273:GLN:N	2.51	0.43
2:C:4:DT:H1'	2:C:5:DT:C5	2.53	0.43
2:C:12:DA:H2''	2:C:13:DT:OP2	2.18	0.43
5:A:126:GLN:H	5:A:126:GLN:HG2	1.44	0.43
5:A:312:ARG:O	5:A:312:ARG:HG2	2.17	0.43
5:A:350:PRO:HB2	5:A:381:PRO:HD3	2.00	0.43
5:D:115:ILE:HD12	5:D:391:LEU:HA	1.95	0.43
5:D:118:TRP:CZ3	5:D:137:LEU:HD21	2.53	0.43
5:D:371:GLN:C	5:D:374:ALA:H	2.26	0.43
1:B:10:DA:H2''	1:B:11:DA:C8	2.53	0.43
4:F:0:DA:C2'	4:F:1:DA:C8	3.01	0.43
5:A:349:LEU:N	5:A:350:PRO:CD	2.80	0.43
5:D:110:LEU:O	5:D:111:GLN:C	2.59	0.43
5:D:144:GLN:OE1	5:D:198:PRO:HA	2.18	0.43
5:D:211:HIS:C	5:D:211:HIS:HD2	2.23	0.43
4:F:8:DT:H2'	4:F:9:DA:C8	2.54	0.43
5:A:172:ASN:HB2	5:A:174:LYS:HD3	2.01	0.43
5:A:213:VAL:CG2	5:A:217:TYR:CD2	3.01	0.43
5:A:334:ILE:O	5:A:337:VAL:HB	2.18	0.43
5:D:163:ASP:HB3	5:D:179:HIS:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:9:DA:H4'	4:F:10:DT:OP1	2.18	0.43
5:A:182:LYS:HB2	5:A:183:PRO:HD3	1.99	0.43
5:A:189:PRO:O	5:A:316:GLN:NE2	2.51	0.43
5:D:388:GLU:O	5:D:389:HIS:C	2.59	0.43
4:F:1:DA:N1	4:F:2:DA:C2	2.86	0.43
5:A:256:PHE:HZ	5:A:268:TRP:CZ2	2.37	0.43
5:D:87:VAL:HG23	5:D:88:LEU:N	2.32	0.43
5:D:153:PHE:HE1	5:D:248:LEU:HD12	1.83	0.43
5:D:252:TYR:CD1	5:D:256:PHE:CE2	2.89	0.43
1:B:3:DA:N1	2:C:14:DT:N3	2.67	0.43
3:E:2:DA:C6	3:E:3:DA:C6	3.06	0.43
5:D:112:LYS:CA	5:D:393:GLN:OE1	2.67	0.43
5:D:131:LYS:CG	5:D:132:THR:N	2.78	0.43
1:B:2:DT:H5'	1:B:2:DT:H6	1.74	0.43
5:A:105:ASN:CG	5:D:390:LEU:HD13	2.43	0.43
5:A:349:LEU:N	5:A:350:PRO:HD2	2.34	0.43
5:A:349:LEU:HD12	5:A:349:LEU:HA	1.81	0.43
5:D:11:LEU:HD22	5:D:11:LEU:N	2.27	0.43
5:D:48:LYS:H	5:D:48:LYS:HG3	1.53	0.43
5:D:83:ASN:O	5:D:86:LEU:HG	2.19	0.43
5:D:181:SER:OG	5:D:182:LYS:N	2.49	0.43
5:D:213:VAL:CG1	5:D:216:TYR:CD2	3.02	0.43
5:D:216:TYR:CE1	5:D:363:LEU:HD23	2.54	0.43
5:D:242:TYR:CD2	5:D:243:PRO:HD2	2.54	0.43
5:D:388:GLU:HG2	5:D:389:HIS:H	1.83	0.43
5:D:394:LEU:HD22	5:D:396:ASP:O	2.19	0.43
5:A:334:ILE:O	5:A:338:PHE:HD2	2.02	0.43
5:A:302:ILE:HG22	5:A:303:PRO:O	2.19	0.42
5:A:366:SER:O	5:A:369:THR:CG2	2.67	0.42
5:D:106:VAL:CG2	5:D:275:TRP:CZ2	3.01	0.42
5:D:382:LEU:HD23	5:D:382:LEU:HA	1.90	0.42
5:D:389:HIS:O	5:D:390:LEU:C	2.60	0.42
5:A:235:ARG:HD3	5:A:239:LEU:HD23	2.01	0.42
5:D:110:LEU:HB2	5:D:147:PHE:CE1	2.53	0.42
5:D:188:VAL:HG13	5:D:189:PRO:HD2	2.00	0.42
5:D:271:VAL:CB	5:D:273:GLN:HE22	2.21	0.42
1:B:14:DT:H2''	1:B:15:DT:C6	2.55	0.42
5:A:9:LYS:HE3	5:A:10:GLU:HG2	1.99	0.42
5:A:229:GLU:OE1	5:A:229:GLU:HA	2.15	0.42
5:A:245:GLU:O	5:A:246:LEU:C	2.62	0.42
5:D:92:LEU:O	5:D:95:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:272:ASN:O	5:D:275:TRP:HB2	2.20	0.42
4:F:1:DA:C1'	4:F:2:DA:C5'	2.95	0.42
4:F:7:DT:H3'	5:D:244:ARG:CD	2.50	0.42
5:A:18:LEU:HD13	5:A:19:TYR:CD1	2.53	0.42
5:A:20:ARG:O	5:A:23:TRP:HB3	2.20	0.42
5:A:111:GLN:O	5:A:112:LYS:C	2.62	0.42
5:A:177:LEU:HD12	5:A:199:ILE:CG2	2.50	0.42
5:D:115:ILE:CG2	5:D:116:ASN:H	2.30	0.42
1:B:6:DT:N3	1:B:7:DT:C4	2.88	0.42
4:F:9:DA:H2''	4:F:10:DT:C5'	2.50	0.42
5:D:206:TYR:O	5:D:207:TYR:C	2.60	0.42
5:D:207:TYR:OH	5:D:211:HIS:CE1	2.72	0.42
5:A:113:ILE:O	5:A:117:LEU:N	2.51	0.42
5:A:174:LYS:HG2	5:A:315:LEU:HD13	2.01	0.42
5:A:258:TYR:CE2	5:A:395:ILE:HG12	2.55	0.42
5:A:307:ILE:O	5:A:311:ASN:OD1	2.37	0.42
5:D:97:LYS:O	5:D:101:PHE:HB2	2.20	0.42
5:D:115:ILE:O	5:D:118:TRP:HB2	2.20	0.42
5:D:139:LEU:CD1	5:D:251:TRP:HB3	2.47	0.42
5:D:273:GLN:C	5:D:275:TRP:N	2.75	0.42
5:A:331:PRO:HA	5:A:332:PRO:HD3	1.89	0.42
5:D:29:TRP:CZ3	5:D:53:TYR:HB2	2.55	0.42
5:D:130:PHE:HZ	5:D:251:TRP:CG	2.37	0.42
2:C:10:DA:C2	2:C:11:DA:C4	3.07	0.41
3:E:11:DA:C2	3:E:12:DA:N1	2.88	0.41
5:A:389:HIS:CD2	5:D:105:ASN:CA	3.03	0.41
5:D:30:LEU:HD13	5:D:30:LEU:H	1.82	0.41
5:D:365:PRO:O	5:D:366:SER:C	2.63	0.41
5:A:106:VAL:HG21	5:A:275:TRP:CH2	2.55	0.41
2:C:5:DT:C4	2:C:6:DT:C4	3.09	0.41
2:C:11:DA:N1	2:C:12:DA:C2	2.89	0.41
5:A:249:GLY:O	5:A:253:PRO:CD	2.68	0.41
5:D:117:LEU:HD23	5:D:117:LEU:HA	1.54	0.41
5:D:125:LEU:N	5:D:258:TYR:CE1	2.88	0.41
5:D:380:LEU:C	5:D:380:LEU:CD1	2.92	0.41
5:A:369:THR:HG1	5:A:371:GLN:HG2	1.85	0.41
5:A:384:ILE:HG23	5:A:385:GLU:N	2.33	0.41
5:D:88:LEU:HD21	5:D:92:LEU:HD11	2.01	0.41
5:D:217:TYR:CG	5:D:218:LYS:N	2.89	0.41
5:D:278:PHE:HA	5:D:279:PRO:HD3	1.84	0.41
5:D:371:GLN:O	5:D:374:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:DT:H2''	2:C:15:DA:OP2	2.21	0.41
4:F:8:DT:OP2	5:D:244:ARG:CZ	2.65	0.41
5:A:70:ALA:O	5:A:74:PHE:CD2	2.73	0.41
5:A:114:SER:HA	5:A:140:LEU:HD13	2.00	0.41
5:A:388:GLU:CG	5:A:389:HIS:N	2.83	0.41
5:A:160:SER:HA	5:A:230:HIS:CD2	2.56	0.41
5:D:141:LEU:HD23	5:D:234:ILE:HG22	2.02	0.41
5:D:251:TRP:O	5:D:254:THR:OG1	2.34	0.41
1:B:4:DA:C2	2:C:14:DT:C2	3.08	0.41
2:C:8:DA:C2'	2:C:9:DT:O5'	2.60	0.41
5:A:101:PHE:C	5:A:101:PHE:CD1	2.99	0.41
5:A:105:ASN:HA	5:D:389:HIS:HD1	1.85	0.41
5:D:43:LEU:HG	5:D:44:PHE:H	1.85	0.41
5:D:387:GLN:O	5:D:391:LEU:HD23	2.20	0.41
1:B:7:DT:C2'	1:B:8:DA:C8	2.96	0.41
5:A:86:LEU:HD12	5:A:86:LEU:C	2.46	0.41
5:A:274:GLU:HG3	5:D:385:GLU:HB3	2.02	0.41
5:D:83:ASN:O	5:D:84:ASP:C	2.64	0.41
5:D:83:ASN:C	5:D:86:LEU:HG	2.45	0.41
5:D:128:LYS:HD3	5:D:129:HIS:CG	2.56	0.41
5:D:153:PHE:O	5:D:157:THR:HG23	2.21	0.41
5:D:202:MET:HE2	5:D:202:MET:HB3	1.88	0.41
5:D:329:ASP:O	5:D:330:LEU:HG	2.21	0.41
5:D:368:LYS:C	5:D:373:ILE:HD12	2.46	0.41
5:A:105:ASN:O	5:D:389:HIS:CE1	2.74	0.41
5:A:199:ILE:HD12	5:A:199:ILE:HG21	1.84	0.41
5:A:329:ASP:O	5:A:330:LEU:CG	2.63	0.41
5:D:140:LEU:HA	5:D:140:LEU:HD12	1.85	0.41
5:D:366:SER:O	5:D:369:THR:HG23	2.22	0.41
5:A:141:LEU:O	5:A:142:ASP:C	2.62	0.40
5:D:81:GLU:CD	5:D:81:GLU:C	2.89	0.40
5:D:113:ILE:O	5:D:114:SER:C	2.65	0.40
5:D:231:ILE:HA	5:D:232:PRO:HD2	1.91	0.40
5:D:312:ARG:CG	5:D:312:ARG:NH1	2.48	0.40
5:A:29:TRP:C	5:A:31:LYS:N	2.80	0.40
5:A:60:ILE:N	5:A:60:ILE:HD13	2.35	0.40
5:A:279:PRO:HD3	5:A:306:TYR:CD1	2.56	0.40
5:A:382:LEU:HD12	5:A:383:ASP:H	1.87	0.40
5:D:153:PHE:O	5:D:156:ARG:HB2	2.20	0.40
5:A:227:GLN:HG2	5:A:227:GLN:H	1.73	0.40
5:A:388:GLU:O	5:A:391:LEU:CG	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:8:LEU:HA	5:D:11:LEU:HD13	2.00	0.40
5:D:26:TYR:O	5:D:30:LEU:HD13	2.20	0.40
5:D:120:PRO:HG3	5:D:358:THR:OG1	2.21	0.40
5:A:174:LYS:CE	5:A:299:THR:HG22	2.50	0.40
5:A:81:GLU:O	5:A:84:ASP:HB3	2.21	0.40
5:A:299:THR:OG1	5:A:307:ILE:CD1	2.69	0.40
5:D:246:LEU:HD23	5:D:246:LEU:C	2.47	0.40
5:D:252:TYR:O	5:D:256:PHE:CD2	2.72	0.40
5:D:369:THR:HB	5:D:371:GLN:CD	2.46	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)
5:A:170:ASP:OD2	5:D:320:GLN:NE2[3_454]	1.87	0.33
5:A:321:VAL:O	5:D:170:ASP:OD2[3_454]	2.03	0.17

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	
5	A	382/402 (95%)	345 (90%)	37 (10%)	0	100	100
5	D	382/402 (95%)	344 (90%)	37 (10%)	1 (0%)	36	64
All	All	764/804 (95%)	689 (90%)	74 (10%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	75	SER

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	
5	A	366/377 (97%)	317 (87%)	49 (13%)	4	18
5	D	366/377 (97%)	304 (83%)	62 (17%)	2	12
All	All	732/754 (97%)	621 (85%)	111 (15%)	3	15

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	4	LEU
5	A	7	LEU
5	A	9	LYS
5	A	15	THR
5	A	18	LEU
5	A	22	ILE
5	A	28	GLU
5	A	42	LYS
5	A	43	LEU
5	A	78	LEU
5	A	80	ILE
5	A	87	VAL
5	A	88	LEU
5	A	90	GLN
5	A	113	ILE
5	A	124	SER
5	A	125	LEU
5	A	128	LYS
5	A	129	HIS
5	A	132	THR
5	A	138	LYS
5	A	143	PHE
5	A	157	THR
5	A	159	VAL
5	A	169	ASP
5	A	172	ASN
5	A	182	LYS

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Mol	Chain	Res	Type
5	A	199	ILE
5	A	213	VAL
5	A	214	LYS
5	A	224	ILE
5	A	229	GLU
5	A	234	ILE
5	A	246	LEU
5	A	273	GLN
5	A	296	SER
5	A	298	ASN
5	A	316	GLN
5	A	333	ASP
5	A	334	ILE
5	A	369	THR
5	A	382	LEU
5	A	386	SER
5	A	387	GLN
5	A	389	HIS
5	A	391	LEU
5	A	394	LEU
5	A	395	ILE
5	A	398	THR
5	D	4	LEU
5	D	9	LYS
5	D	11	LEU
5	D	18	LEU
5	D	28	GLU
5	D	30	LEU
5	D	31	LYS
5	D	41	LEU
5	D	42	LYS
5	D	43	LEU
5	D	48	LYS
5	D	59	ASP
5	D	79	ASP
5	D	80	ILE
5	D	86	LEU
5	D	87	VAL
5	D	90	GLN
5	D	95	LEU
5	D	107	ILE
5	D	114	SER

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Mol	Chain	Res	Type
5	D	115	ILE
5	D	123	ASP
5	D	124	SER
5	D	125	LEU
5	D	128	LYS
5	D	131	LYS
5	D	132	THR
5	D	157	THR
5	D	159	VAL
5	D	161	LEU
5	D	162	LYS
5	D	164	LEU
5	D	167	ILE
5	D	171	GLU
5	D	201	THR
5	D	208	LEU
5	D	211	HIS
5	D	224	ILE
5	D	227	GLN
5	D	234	ILE
5	D	244	ARG
5	D	251	TRP
5	D	254	THR
5	D	264	THR
5	D	293	GLU
5	D	294	SER
5	D	296	SER
5	D	298	ASN
5	D	312	ARG
5	D	333	ASP
5	D	334	ILE
5	D	368	LYS
5	D	371	GLN
5	D	377	THR
5	D	384	ILE
5	D	386	SER
5	D	387	GLN
5	D	388	GLU
5	D	389	HIS
5	D	391	LEU
5	D	394	LEU
5	D	395	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	230	HIS
5	A	260	GLN
5	A	298	ASN
5	A	311	ASN
5	A	389	HIS
5	D	105	ASN
5	D	129	HIS
5	D	179	HIS
5	D	211	HIS
5	D	230	HIS
5	D	273	GLN
5	D	298	ASN
5	D	316	GLN
5	D	393	GLN

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](#)

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	B	15/15 (100%)	0.15	0	100	100	120, 140, 161, 168	0
2	C	15/15 (100%)	0.22	0	100	100	114, 144, 169, 180	0
3	E	14/14 (100%)	0.03	0	100	100	108, 138, 172, 187	0
4	F	15/15 (100%)	0.14	0	100	100	103, 132, 161, 168	0
5	A	388/402 (96%)	0.02	6 (1%)	72	46	65, 116, 176, 215	0
5	D	388/402 (96%)	0.08	5 (1%)	75	49	67, 119, 181, 231	0
All	All	835/863 (96%)	0.06	11 (1%)	75	49	65, 120, 179, 231	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	130	PHE	3.6
5	D	389	HIS	3.5
5	A	130	PHE	3.3
5	A	251	TRP	2.8
5	A	99	LEU	2.7
5	D	186	VAL	2.5
5	D	109	ILE	2.4
5	D	106	VAL	2.1
5	A	384	ILE	2.1
5	A	217	TYR	2.1
5	A	389	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.