



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:16 pm BST

PDB ID : 3T79
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

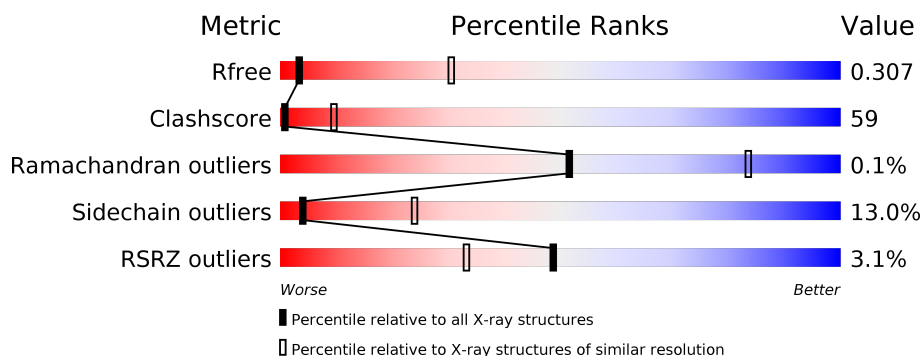
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 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	
2	C	15	
3	E	14	
4	F	15	
5	A	402	
5	D	402	

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


These plots are drawn for all protein, RNA and DNA 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*TP*T)-3')

Chain B: 



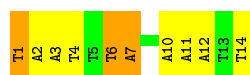
- Molecule 2: DNA (5'-D(P*AP*AP*AP*TP*TP*TP*TP*AP*TP*AP*AP*AP*TP*TP*A)-3')

Chain C: 



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

Chain E: 



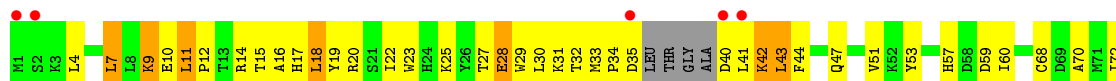
- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*AP*TP*TP*TP*TP*AP*TP*AP*AP*AP*T)-3')

Chain F: 

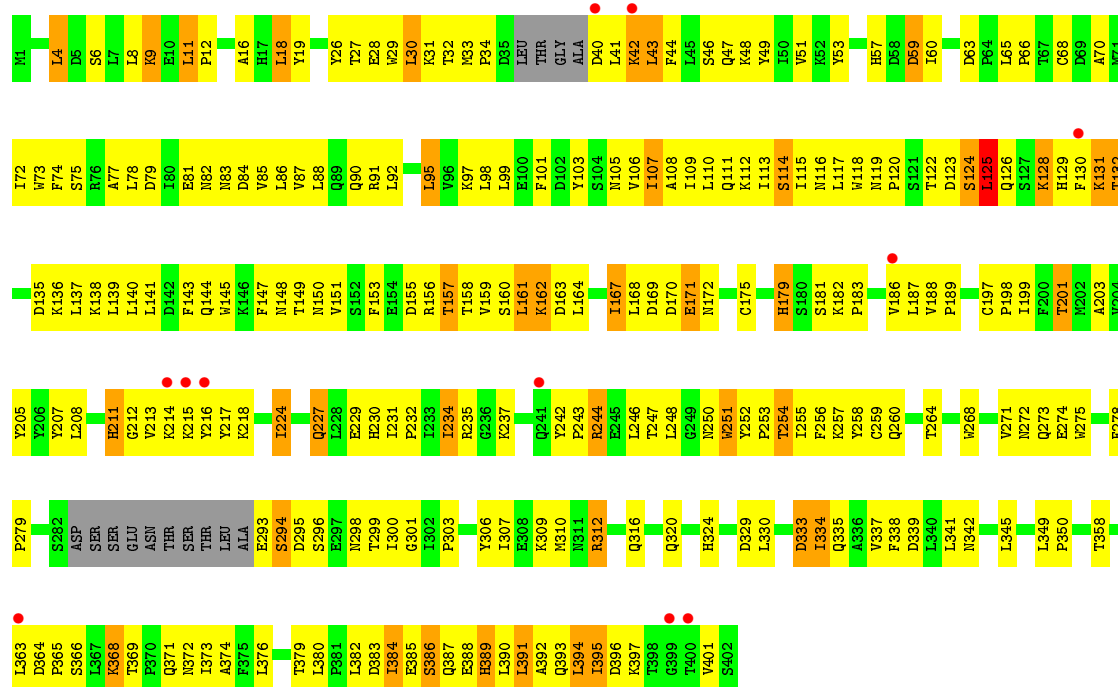


- Molecule 5: KLLA0E03807p

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	93.06 Å 99.65 Å 125.92 Å 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) 99.0 (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 3.57 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.286 , 0.331 0.270 , 0.307	Depositor DCC
R_{free} test set	688 reflections (4.98%)	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)	0.28 , 55.4	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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.60	0/343	1.57	5/527 (0.9%)
2	C	0.84	1/345 (0.3%)	1.86	15/530 (2.8%)
3	E	0.57	0/321	1.43	4/493 (0.8%)
4	F	0.78	0/347	1.77	8/533 (1.5%)
5	A	0.40	0/3287	0.66	3/4473 (0.1%)
5	D	0.47	0/3287	0.72	1/4473 (0.0%)
All	All	0.49	1/7930 (0.0%)	0.95	36/11029 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	DT	C5'-C4'	5.44	1.57	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	DA	O4'-C4'-C3'	-12.44	98.54	106.00
1	B	2	DT	O4'-C4'-C3'	-10.62	99.63	106.00
4	F	8	DT	C1'-O4'-C4'	-9.12	100.97	110.10
2	C	4	DT	O4'-C1'-N1	-8.53	102.03	108.00
4	F	2	DA	O4'-C4'-C3'	-8.38	100.97	106.00
1	B	1	DT	O4'-C4'-C3'	-7.85	101.29	106.00
2	C	8	DA	O4'-C4'-C3'	-7.53	101.48	106.00
5	A	128	LYS	CD-CE-NZ	-7.53	94.39	111.70
2	C	3	DA	O4'-C4'-C3'	-7.51	101.50	106.00
5	A	11	LEU	CA-CB-CG	7.33	132.15	115.30
4	F	7	DT	C1'-O4'-C4'	-7.05	103.05	110.10
1	B	1	DT	O4'-C1'-N1	-7.02	103.09	108.00
2	C	4	DT	C5-C6-N1	-6.98	119.51	123.70
2	C	9	DT	O4'-C1'-N1	6.97	112.88	108.00
2	C	4	DT	C5'-C4'-C3'	6.86	126.45	114.10
2	C	4	DT	C6-N1-C2	6.85	124.72	121.30
4	F	7	DT	O4'-C1'-N1	6.64	112.65	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7	DA	C1'-O4'-C4'	-6.58	103.52	110.10
3	E	6	DT	O4'-C1'-N1	6.55	112.58	108.00
4	F	8	DT	O4'-C1'-N1	6.29	112.40	108.00
3	E	7	DA	O4'-C4'-C3'	-6.21	102.02	104.50
1	B	2	DT	N3-C4-O4	6.17	123.60	119.90
2	C	4	DT	O5'-C5'-C4'	5.99	125.97	111.00
2	C	3	DA	C3'-C2'-C1'	-5.91	95.41	102.50
2	C	4	DT	C2-N1-C1'	-5.90	108.76	118.20
4	F	2	DA	C3'-C2'-C1'	-5.88	95.44	102.50
2	C	8	DA	O4'-C1'-N9	5.82	112.08	108.00
2	C	6	DT	C1'-O4'-C4'	-5.80	104.30	110.10
2	C	3	DA	C8-N9-C4	5.80	108.12	105.80
1	B	2	DT	C5-C4-O4	-5.41	121.12	124.90
2	C	3	DA	N9-C4-C5	-5.35	103.66	105.80
2	C	3	DA	C4'-C3'-O3'	-5.32	96.39	109.70
5	D	125	LEU	CA-CB-CG	5.31	127.51	115.30
5	A	128	LYS	CB-CG-CD	-5.26	97.93	111.60
4	F	2	DA	C4'-C3'-C2'	-5.21	98.41	103.10
3	E	1	DT	C5-C4-O4	-5.20	121.26	124.90

There are no chirality outliers.

There are no planarity outliers.

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	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	385	2
5	D	3196	0	3187	390	2
All	All	7603	0	7055	868	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 59.

All (868) 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
5:D:124:SER:HB2	5:D:258:TYR:CE1	1.97	0.99
5:A:260:GLN:HE22	5:D:260:GLN:HE22	1.06	0.99
3:E:6:DT:H2''	3:E:7:DA:H8	1.27	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:N	5:D:371:GLN:OE1	1.96	0.97
5:D:312:ARG:CG	5:D:312:ARG:HH11	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
5:D:124:SER:HB2	5:D:258:TYR:HE1	1.32	0.92
3:E:6:DT:H2''	3:E:7:DA:C8	2.05	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:112:LYS:HA	5:A:393:GLN:HG2	1.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
5:A:143:PHE:C	5:A:143:PHE:CD2	2.48	0.86
1:B:4:DA:H2'	1:B:4:DA:OP2	1.75	0.86
5:D:162:LYS:HZ1	5:D:230:HIS:HA	1.41	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
5:D:395:ILE:H	5:D:395:ILE:HD13	1.41	0.85
4:F:9:DA:H2''	4:F:10:DT:O5'	1.76	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:D:244:ARG:CG	5:D:244:ARG:HH11	1.90	0.84
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:271:VAL:HB	5:D:273:GLN:HE22	1.39	0.84
5:D:86:LEU:O	5:D:90:GLN:NE2	2.10	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:252:TYR:HD1	5:D:256:PHE:CE2	1.97	0.82
5:D:293:GLU:OE1	5:D:293:GLU:N	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
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
4:F:7:DT:H5''	5:D:244:ARG:HD2	1.65	0.78
5:D:95:LEU:HD12	5:D:95:LEU:C	2.03	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:143:PHE:C	5:A:143:PHE:HD2	1.90	0.74
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
5:A:321:VAL:HG22	5:A:323:VAL:N	1.98	0.72
5:A:192:GLN:N	5:A:192:GLN:OE1	2.22	0.72
5:A:88:LEU:CD1	5:A:92:LEU:HG	2.19	0.72
2:C:2:DA:C1'	2:C:3:DA:H5'	2.20	0.72
5:A:211:HIS:HD2	5:A:212:GLY:O	1.72	0.72
5:A:116:ASN:HD21	5:A:394:LEU:HA	1.55	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:H3'	4:F:0:DA:OP2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:235:ARG:HE	5:A:239:LEU:C	1.94	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:83:ASN:O	5:D:87:VAL:HG13	1.91	0.70
4:F:2:DA:O5'	4:F:2:DA:C2'	2.40	0.70
5:D:368:LYS:HA	5:D:373:ILE:HD11	1.72	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
5:A:81:GLU:HB3	5:A:83:ASN:OD1	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
1:B:1:DT:H72	1:B:1:DT:OP2	1.92	0.69
5:D:252:TYR:CD1	5:D:256:PHE:HE2	2.02	0.69
5:D:30:LEU:HD13	5:D:30:LEU:N	2.05	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
2:C:13:DT:H2'	2:C:14:DT:C5'	2.16	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
2:C:6:DT:H2''	2:C:7:DT:H5''	1.76	0.68
2:C:4:DT:P	5:A:128:LYS:HZ1	2.13	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:HD2	5:A:214:LYS:H	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:A:390:LEU:N	2.63	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:E:2:DA:H2'	3:E:3:DA:O4'	1.95	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
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
4:F:2:DA:C6	4:F:3:DA:N6	2.64	0.66
5:D:252:TYR:O	5:D:255:ILE:HG22	1.96	0.66
5:D:387:GLN:HA	5:D:387:GLN:OE1	1.96	0.66
5:D:26:TYR:CE2	5:D:44:PHE:CE2	2.84	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
5:A:188:VAL:HG13	5:A:189:PRO:HD2	1.78	0.65
2:C:4:DT:H2'	5:A:128:LYS:NZ	2.12	0.65
5:A:294:SER:HB2	5:A:299:THR:HA	1.78	0.65
5:A:333:ASP:HB2	5:A:334:ILE:HD13	1.78	0.65
5:A:83:ASN:OD1	5:A:84:ASP:N	2.23	0.65
5:D:365:PRO:HA	5:D:368:LYS:CG	2.26	0.65
5:D:59:ASP:N	5:D:59:ASP:OD1	2.28	0.65
5:D:129:HIS:O	5:D:130:PHE:HB2	1.96	0.65
5:D:126:GLN:H	5:D:126:GLN:CD	1.99	0.65
5:A:115:ILE:HB	5:A:390:LEU:CD2	2.27	0.65
5:A:279:PRO:HD3	5:A:306:TYR:CE1	2.32	0.65
5:A:96:VAL:HG23	5:A:97:LYS:N	2.11	0.65
5:D:128:LYS:HD3	5:D:129:HIS:CD2	2.31	0.65
5:D:33:MET:HB3	5:D:34:PRO:HD2	1.79	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
5:A:105:ASN:HB3	5:D:389:HIS:HB3	1.78	0.64
4:F:5:DT:H2''	4:F:6:DT:H72	1.79	0.64
5:A:299:THR:HG23	5:A:304:ASP:OD1	1.95	0.64
4:F:1:DA:C2	4:F:2:DA:C2	2.85	0.64
5:D:186:VAL:HG11	5:D:307:ILE:HD13	1.78	0.64
5:D:8:LEU:HA	5:D:11:LEU:HD11	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:6:SER:O	5:D:9:LYS:HB2	1.97	0.64
5:D:365:PRO:O	5:D:368:LYS:N	2.24	0.64
5:A:209:ARG:NE	5:A:235:ARG:NH1	2.44	0.64
1:B:4:DA:C2	2:C:14:DT:O2	2.51	0.64
5:D:118:TRP:CZ2	5:D:201:THR:HG23	2.33	0.64
5:A:179:HIS:CE1	5:A:181:SER:HB2	2.33	0.64
1:B:2:DT:H2''	1:B:3:DA:H5''	1.78	0.64
5:D:95:LEU:HD12	5:D:95:LEU:O	1.97	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:14:DT:H5''	5:D:237:LYS:O	1.99	0.63
3:E:2:DA:N6	3:E:3:DA:C6	2.65	0.63
4:F:3:DA:H1'	4:F:4:DA:H5'	1.81	0.63
5:A:300:ILE:HG23	5:A:301:GLY:N	2.13	0.63
1:B:11:DA:H2''	1:B:12:DA:C8	2.33	0.63
4:F:0:DA:P	4:F:0:DA:H3'	2.39	0.63
5:A:167:ILE:O	5:A:175:CYS:HA	1.99	0.63
5:A:40:ASP:N	5:A:44:PHE:CE2	2.67	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
5:A:101:PHE:CD2	5:A:276:PRO:HD3	2.33	0.63
1:B:6:DT:H3'	5:A:265:LYS:HD3	1.79	0.63
5:D:148:ASN:OD1	5:D:312:ARG:NH2	2.32	0.63
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
3:E:6:DT:C2'	3:E:7:DA:C8	2.78	0.62
5:A:214:LYS:HD2	5:A:214:LYS:N	2.12	0.62
5:A:33:MET:HB3	5:A:34:PRO:CD	2.28	0.62
5:A:389:HIS:CG	5:D:105:ASN:C	2.73	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: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
5:A:160:SER:CB	5:A:230:HIS:HD2	2.12	0.62
4:F:1:DA:C1'	4:F:2:DA:H5'	2.30	0.62
5:A:22:ILE:HG22	5:A:23:TRP:N	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:246:LEU:HD12	5:A:247:THR:N	2.15	0.62
5:D:11:LEU:H	5:D:11:LEU:HD22	1.65	0.62
5:A:109:ILE:HD11	5:D:389:HIS:HD2	1.64	0.62
4:F:0:DA:H2''	4:F:1:DA:C8	2.34	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
2:C:4:DT:H2''	2:C:5:DT:H71	1.82	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
5:D:161:LEU:C	5:D:161:LEU:HD12	2.21	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
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
4:F:1:DA:H1'	4:F:2:DA:H5'	1.83	0.61
5:A:7:LEU:O	5:A:7:LEU:HD12	2.02	0.60
5:A:389:HIS:CD2	5:D:105:ASN:HB3	2.36	0.60
1:B:14:DT:C6	1:B:14:DT:H5'	2.36	0.60
5:D:30:LEU:CD2	5:D:44:PHE:CZ	2.83	0.60
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:A:79:ASP:OD1	5:A:79:ASP:O	2.19	0.60
4:F:1:DA:H2''	4:F:2:DA:OP2	2.00	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:113:ILE:HD12	5:D:143:PHE:CE1	2.37	0.60
5:D:8:LEU:O	5:D:11:LEU:HD21	2.02	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:211:HIS:CD2	5:D:211:HIS:C	2.75	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:167:ILE:O	5:D:175:CYS:HA	2.02	0.59
5:D:18:LEU:HD13	5:D:19:TYR:CD1	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:106:VAL:HG21	5:D:275:TRP:CZ2	2.38	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:D:335:GLN:O	5:D:339:ASP:OD2	2.20	0.59
5:A:108:ALA:HB3	5:D:393:GLN:NE2	2.18	0.59
5:A:389:HIS:CD2	5:D:105:ASN:HD22	2.21	0.59
5:D:122:THR:HG23	5:D:136:LYS:HZ1	1.68	0.58
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
5:A:9:LYS:HZ1	5:A:10:GLU:HG2	1.65	0.58
5:D:42:LYS:H	5:D:42:LYS:HZ2	1.51	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
4:F:1:DA:H1'	4:F:2:DA:C5'	2.34	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
5:D:40:ASP:C	5:D:41:LEU:HD12	2.23	0.58
5:A:172:ASN:OD1	5:A:172:ASN:N	2.36	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
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:HE3	5:D:251:TRP:N	2.02	0.58
5:A:103:TYR:C	5:A:107:ILE:HD13	2.25	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
3:E:3:DA:H2''	3:E:4:DT:C6	2.39	0.57
5:A:112:LYS:HG2	5:A:261:LEU:HD11	1.86	0.57
2:C:4:DT:H2'	5:A:128:LYS:CE	2.33	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
2:C:6:DT:C2'	2:C:7:DT:H5''	2.35	0.57
5:D:26:TYR:CE2	5:D:44:PHE:HE2	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:113:ILE:HD12	5:D:143:PHE:CZ	2.39	0.57
5:D:87:VAL:CG2	5:D:88:LEU:N	2.67	0.57
5:A:11:LEU:CD1	5:A:16:ALA:N	2.67	0.57
1:B:3:DA:H2'	1:B:4:DA:H8	1.64	0.57
5:A:389:HIS:CD2	5:A:390:LEU:CA	2.87	0.57
5:A:84:ASP:O	5:A:87:VAL:HG22	2.04	0.57
1:B:12:DA:H2''	1:B:13:DA:C5'	2.35	0.56
5:D:365:PRO:HA	5:D:368:LYS:HG3	1.86	0.56
4:F:2:DA:C2'	4:F:3:DA:OP2	2.53	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: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:A:43:LEU:H	5:A:43:LEU:HD23	1.71	0.56
1:B:4:DA:H1'	1:B:5:DT:H5'	1.88	0.56
5:A:184:ASN:OD1	5:A:302:ILE:HD11	2.06	0.56
5:A:395:ILE:H	5:A:395:ILE:HD13	1.71	0.56
5:D:371:GLN:CD	5:D:371:GLN:H	2.01	0.56
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:C7	1:B:1:DT:OP2	2.54	0.55
5:D:129:HIS:O	5:D:130:PHE:CB	2.54	0.55
3:E:10:DA:H2''	3:E:11:DA:OP2	2.05	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
5:A:395:ILE:N	5:A:395:ILE:HD13	2.21	0.55
2:C:6:DT:OP2	5:A:247:THR:HG21	2.07	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:HH11	5:A:91:ARG:HG3	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:161:LEU:HG	5:D:231:ILE:CG2	2.36	0.55
5:D:29:TRP:CE3	5:D:30:LEU:CD1	2.90	0.55
5:D:179:HIS:HE1	5:D:181:SER:HB3	1.64	0.54
5:A:253:PRO:O	5:A:257:LYS:HG3	2.08	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
2:C:2:DA:C2'	2:C:3:DA:H5'	2.37	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
5:A:14:ARG:O	5:A:17:HIS:HB3	2.07	0.54
2:C:11:DA:C2	2:C:12:DA:C2	2.96	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
5:A:119:ASN:HA	5:A:356:PHE:CE1	2.42	0.54
4:F:7:DT:C5'	5:D:244:ARG:HD2	2.36	0.54
5:D:211:HIS:CE1	5:D:364:ASP:OD2	2.60	0.54
5:D:81:GLU:CD	5:D:83:ASN:OD1	2.45	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:380:LEU:HD12	5:D:380:LEU:C	2.28	0.54
5:D:95:LEU:HD11	5:D:99:LEU:CG	2.36	0.54
5:A:40:ASP:CA	5:A:44:PHE:CE2	2.91	0.54
4:F:0:DA:C2'	4:F:1:DA:H5'	2.38	0.54
5:A:115:ILE:CD1	5:A:391:LEU:HA	2.38	0.54
2:C:4:DT:H2'	5:A:128:LYS:HZ3	1.73	0.54
5:D:68:CYS:O	5:D:72:ILE:HG13	2.07	0.54
4:F:1:DA:O4'	4:F:2:DA:H5'	2.07	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:O	5:D:18:LEU:HD22	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: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:105:ASN:O	5:D:389:HIS:ND1	2.41	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
5:A:321:VAL:HG22	5:A:322:HIS:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:DT:H5'	2:C:14:DT:C6	2.43	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
2:C:4:DT:C2	2:C:5:DT:C4	2.97	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
2:C:14:DT:OP1	2:C:14:DT:H4'	2.09	0.52
2:C:6:DT:H5"	5:A:244:ARG:HG2	1.91	0.52
5:A:274:GLU:OE1	5:A:275:TRP:CD1	2.62	0.52
5:A:245:GLU:CD	5:A:245:GLU:H	2.12	0.52
5:D:203:ALA:HB1	5:D:345:LEU:HB2	1.91	0.52
5:D:60:ILE:O	5:D:63:ASP:N	2.41	0.52
5:A:384:ILE:O	5:A:387:GLN:N	2.39	0.52
1:B:3:DA:N1	2:C:15:DA:C6	2.77	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:109:ILE:CD1	5:D:389:HIS:HD2	2.22	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
5:A:199:ILE:HG22	5:A:202:MET:HE2	1.92	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
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
1:B:3:DA:N6	2:C:14:DT:O4	2.43	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
5:A:79:ASP:C	5:A:80:ILE:HD12	2.31	0.51
5:A:98:LEU:HD11	5:A:310:MET:HG3	1.92	0.51
1:B:6:DT:C4	1:B:7:DT:C4	2.99	0.51
5:A:109:ILE:CD1	5:D:389:HIS:CD2	2.94	0.51
5:A:32:THR:O	5:A:32:THR:HG22	2.10	0.51
2:C:5:DT:H2"	2:C:6:DT:O5'	2.11	0.51
5:D:148:ASN:O	5:D:310:MET:HG2	2.09	0.51
5:D:138:LYS:NZ	5:D:205:TYR:OH	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:369:THR:HG1	5:A:371:GLN:HG2	1.75	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:A:96:VAL:O	5:A:97:LYS:C	2.49	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
5:D:83:ASN:N	5:D:83:ASN:OD1	2.41	0.51
5:A:124:SER:HB2	5:A:258:TYR:CE1	2.46	0.51
4:F:6:DT:OP1	5:D:129:HIS:HD2	1.94	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:130:PHE:HZ	5:D:251:TRP:CB	2.24	0.50
5:D:117:LEU:HD11	5:D:139:LEU:HD23	1.92	0.50
5:D:211:HIS:CD2	5:D:212:GLY:O	2.65	0.50
5:D:42:LYS:NZ	5:D:42:LYS:HB2	2.26	0.50
5:A:90:GLN:OE1	5:A:90:GLN:HA	2.12	0.50
5:D:189:PRO:HA	5:D:197:CYS:SG	2.50	0.50
2:C:4:DT:P	5:A:128:LYS:HZ2	2.34	0.50
5:A:191:PHE:HE2	5:A:316:GLN:HG3	1.74	0.50
5:D:122:THR:HG23	5:D:136:LYS:NZ	2.25	0.50
5:A:174:LYS:HE3	5:A:299:THR:HG22	1.94	0.50
5:A:384:ILE:C	5:A:386:SER:N	2.65	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: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:103:TYR:C	5:D:105:ASN:H	2.15	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
5:D:40:ASP:CA	5:D:43:LEU:HD11	2.40	0.49
5:A:115:ILE:CG2	5:A:116:ASN:N	2.75	0.49
2:C:13:DT:C3'	2:C:14:DT:H5''	2.41	0.49
5:A:40:ASP:O	5:A:41:LEU:HD12	2.12	0.49
5:A:83:ASN:CG	5:A:84:ASP:H	2.14	0.49
5:A:89:GLN:HE21	5:A:93:TYR:HE2	1.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:113:ILE:CD1	5:D:143:PHE:CE1	2.95	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:A:235:ARG:CD	5:A:239:LEU:HD23	2.43	0.49
1:B:3:DA:C2	2:C:15:DA:C2	3.01	0.49
5:D:47:GLN:O	5:D:51:VAL:HG23	2.13	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:A:47:GLN:O	5:A:51:VAL:HG23	2.12	0.49
5:D:349:LEU:N	5:D:350:PRO:CD	2.73	0.49
5:D:73:TRP:O	5:D:74:PHE:C	2.50	0.49
5:A:11:LEU:HD22	5:A:12:PRO:HD2	1.95	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: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
2:C:12:DA:H2''	2:C:13:DT:C7	2.43	0.49
2:C:4:DT:C3'	5:A:128:LYS:HE3	2.43	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
5:A:11:LEU:HD12	5:A:16:ALA:CB	2.42	0.48
3:E:11:DA:H4'	3:E:12:DA:OP1	2.11	0.48
5:D:11:LEU:HB2	5:D:12:PRO:CD	2.43	0.48
5:A:29:TRP:O	5:A:32:THR:N	2.41	0.48
4:F:6:DT:OP1	5:D:129:HIS:CD2	2.67	0.48
5:A:160:SER:O	5:A:163:ASP:HB2	2.13	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
2:C:4:DT:O2	2:C:5:DT:C4	2.66	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:167:ILE:HD11	5:D:293:GLU:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:44:PHE:CD1	5:D:44:PHE:O	2.66	0.48
5:D:369:THR:HB	5:D:371:GLN:OE1	2.14	0.48
5:D:380:LEU:HD13	5:D:382:LEU:C	2.34	0.48
3:E:2:DA:C2'	3:E:3:DA:H5'	2.44	0.48
5:A:40:ASP:HA	5:A:44:PHE:CZ	2.48	0.48
1:B:2:DT:H6	1:B:2:DT:H2'	1.48	0.48
5:D:132:THR:HG23	5:D:135:ASP:OD2	2.14	0.48
5:A:153:PHE:O	5:A:156:ARG:HB2	2.14	0.48
5:A:162:LYS:HZ1	5:A:229:GLU:HA	1.79	0.48
5:D:149:THR:CG2	5:D:151:VAL:HG23	2.43	0.48
5:D:227:GLN:H	5:D:227:GLN:HG2	1.43	0.48
5:D:150:ASN:ND2	5:D:275:TRP:HE3	2.10	0.48
5:D:87:VAL:O	5:D:90:GLN:HB2	2.14	0.48
4:F:2:DA:C2	4:F:3:DA:C6	3.02	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
5:D:42:LYS:HB2	5:D:42:LYS:HZ3	1.79	0.47
5:A:299:THR:OG1	5:A:307:ILE:HD11	2.14	0.47
5:A:258:TYR:OH	5:A:396:ASP:OD2	2.31	0.47
4:F:8:DT:P	5:D:244:ARG:HH21	2.38	0.47
5:A:113:ILE:O	5:A:114:SER:C	2.51	0.47
5:A:125:LEU:O	5:A:125:LEU:HD12	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:D:125:LEU:HB3	5:D:258:TYR:CD1	2.49	0.47
5:D:18:LEU:C	5:D:18:LEU:HD22	2.35	0.47
5:D:231:ILE:O	5:D:231:ILE:HG23	2.15	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
2:C:12:DA:H2'	2:C:12:DA:O5'	2.15	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: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: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
5:A:130:PHE:CZ	5:A:139:LEU:HD22	2.49	0.47
5:A:153:PHE:CD2	5:A:153:PHE:C	2.88	0.47
5:A:209:ARG:NH2	5:A:235:ARG:NH1	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:DA:H1'	4:F:4:DA:C5'	2.44	0.47
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:198:PRO:HA	5:D:201:THR:OG1	2.15	0.46
5:D:83:ASN:HA	5:D:86:LEU:CD2	2.45	0.46
3:E:11:DA:H2''	3:E:12:DA:C5'	2.45	0.46
5:A:88:LEU:C	5:A:88:LEU:HD12	2.36	0.46
5:A:389:HIS:CD2	5:D:105:ASN:ND2	2.83	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:96:VAL:O	5:A:99:LEU:N	2.48	0.46
5:A:384:ILE:C	5:A:386:SER:H	2.18	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
5:D:26:TYR:HE2	5:D:44:PHE:CE2	2.33	0.46
5:A:153:PHE:CD2	5:A:154:GLU:N	2.84	0.46
1:B:3:DA:H5''	1:B:3:DA:H8	1.81	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:4:LEU:HD21	5:D:8:LEU:HD11	1.97	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
4:F:1:DA:H1'	4:F:2:DA:O5'	2.16	0.46
5:A:209:ARG:HH21	5:A:235:ARG:NH1	2.13	0.46
2:C:4:DT:O5'	5:A:128:LYS:NZ	2.35	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
5:A:97:LYS:O	5:A:101:PHE:CB	2.61	0.46
5:D:388:GLU:CG	5:D:389:HIS:H	2.29	0.46
5:D:98:LEU:CD1	5:D:309:LYS:HG2	2.46	0.46
3:E:11:DA:C2	3:E:12:DA:C2	3.04	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:143:PHE:C	5:D:143:PHE:CD2	2.88	0.46
2:C:4:DT:O2	2:C:5:DT:N3	2.49	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
3:E:1:DT:H1'	3:E:2:DA:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:98:LEU:O	5:A:309:LYS:HE2	2.16	0.45
2:C:4:DT:C2'	5:A:128:LYS:CE	2.94	0.45
5:D:119:ASN:OD1	5:D:120:PRO:HD2	2.16	0.45
5:D:82:ASN:O	5:D:85:VAL:HG12	2.15	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:N	5:A:35:ASP:OD2	2.49	0.45
5:A:388:GLU:HA	5:A:391:LEU:HD21	1.99	0.45
5:D:95:LEU:C	5:D:95:LEU:CD1	2.77	0.45
5:A:354:ARG:HG3	5:A:380:LEU:HD11	1.99	0.45
5:A:105:ASN:CA	5:D:389:HIS:HD1	2.29	0.45
4:F:1:DA:C2	4:F:2:DA:N3	2.84	0.45
5:A:153:PHE:CE2	5:A:157:THR:CG2	2.99	0.45
5:A:91:ARG:NH1	5:A:306:TYR:OH	2.49	0.45
1:B:6:DT:C2'	1:B:7:DT:OP2	2.53	0.45
5:D:364:ASP:O	5:D:368:LYS:HG2	2.16	0.45
5:A:382:LEU:HD12	5:A:383:ASP:N	2.32	0.45
5:A:105:ASN:HA	5:D:389:HIS:ND1	2.31	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:D:168:LEU:HD23	5:D:175:CYS:HB2	1.99	0.45
5:A:109:ILE:HD11	5:D:389:HIS:CD2	2.46	0.45
5:D:65:LEU:N	5:D:66:PRO:HD2	2.31	0.45
5:A:209:ARG:CZ	5:A:235:ARG:NH1	2.80	0.45
5:A:85:VAL:O	5:A:88:LEU:HB3	2.16	0.45
5:D:112:LYS:HA	5:D:393:GLN:OE1	2.17	0.45
5:A:258:TYR:CE2	5:A:395:ILE:CG1	3.00	0.45
5:A:32:THR:O	5:A:32:THR:CG2	2.65	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:199:ILE:O	5:A:200:PHE:C	2.55	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:D:11:LEU:CD2	5:D:11:LEU:C	2.85	0.44
5:D:125:LEU:HD12	5:D:125:LEU:C	2.38	0.44
5:D:40:ASP:OD1	5:D:40:ASP:O	2.35	0.44
5:D:6:SER:O	5:D:9:LYS:CB	2.64	0.44
5:D:95:LEU:O	5:D:98:LEU:HB3	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:213:VAL:HG22	5:A:217:TYR:HD2	1.81	0.44
5:A:98:LEU:HD21	5:A:306:TYR:HA	1.98	0.44
5:D:109:ILE:HD12	5:D:109:ILE:N	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:155:ASP:HB3	5:D:183:PRO:HG3	1.99	0.44
5:D:98:LEU:CD2	5:D:306:TYR:CD1	3.00	0.44
5:A:177:LEU:CD1	5:A:199:ILE:CG2	2.95	0.44
5:A:365:PRO:O	5:A:368:LYS:HB2	2.18	0.44
5:A:42:LYS:CE	5:A:79:ASP:OD1	2.66	0.44
5:A:83:ASN:CG	5:A:84:ASP:N	2.71	0.44
5:D:81:GLU:O	5:D:84:ASP:HB3	2.18	0.44
3:E:2:DA:H5''	3:E:2:DA:H8	1.82	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
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
4:F:1:DA:OP2	4:F:1:DA:H8	1.99	0.44
1:B:2:DT:C4	2:C:15:DA:N1	2.85	0.44
5:D:334:ILE:HD13	5:D:334:ILE:N	2.32	0.44
4:F:0:DA:H2''	4:F:1:DA:OP2	2.17	0.44
4:F:7:DT:H3'	5:D:244:ARG:HD2	2.00	0.44
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:A:116:ASN:ND2	5:A:394:LEU:HA	2.29	0.43
1:B:4:DA:H1'	1:B:5:DT:C5'	2.48	0.43
5:D:273:GLN:OE1	5:D:273:GLN:N	2.51	0.43
4:F:2:DA:H2'	4:F:2:DA:P	2.58	0.43
5:A:126:GLN:H	5:A:126:GLN:HG2	1.44	0.43
5:A:312:ARG:HG2	5:A:312:ARG:O	2.17	0.43
5:A:350:PRO:HB2	5:A:381:PRO:HD3	2.00	0.43
2:C:12:DA:H2''	2:C:13:DT:OP2	2.18	0.43
2:C:4:DT:H1'	2:C:5:DT:C5	2.53	0.43
5:D:118:TRP:CZ3	5:D:137:LEU:HD21	2.53	0.43
5:D:115:ILE:HD12	5:D:391:LEU:HA	1.95	0.43
5:A:9:LYS:HZ2	5:A:10:GLU:HG2	1.79	0.43
5:A:349:LEU:N	5:A:350:PRO:CD	2.80	0.43
1:B:10:DA:H2''	1:B:11:DA:C8	2.53	0.43
5:D:144:GLN:OE1	5:D:198:PRO:HA	2.18	0.43
4:F:0:DA:C2'	4:F:1:DA:C8	3.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:F:8:DT:H2'	4:F:9:DA:C8	2.54	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
4:F:9:DA:H4'	4:F:10:DT:OP1	2.18	0.43
5:A:256:PHE:HZ	5:A:268:TRP:CZ2	2.37	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
5:D:384:ILE:C	5:D:386:SER:N	2.71	0.43
5:D:87:VAL:HG23	5:D:88:LEU:N	2.32	0.43
4:F:1:DA:N1	4:F:2:DA:C2	2.86	0.43
5:A:202:MET:HE3	5:A:202:MET:HB3	1.87	0.43
1:B:3:DA:N1	2:C:14:DT:N3	2.67	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
3:E:2:DA:C6	3:E:3:DA:C6	3.06	0.43
5:A:349:LEU:HD12	5:A:349:LEU:HA	1.81	0.43
5:A:349:LEU:N	5:A:350:PRO:HD2	2.34	0.43
1:B:2:DT:H5'	1:B:2:DT:H6	1.74	0.43
5:D:11:LEU:HD22	5:D:11:LEU:N	2.27	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:242:TYR:CD2	5:D:243:PRO:HD2	2.54	0.43
5:D:216:TYR:CE1	5:D:363:LEU:HD23	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:D:48:LYS:HG3	5:D:48:LYS:H	1.53	0.43
5:D:83:ASN:O	5:D:86:LEU:HG	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:HA	5:D:382:LEU:HD23	1.90	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
5:A:9:LYS:HE3	5:A:10:GLU:HG2	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:229:GLU:HA	5:A:229:GLU:OE1	2.15	0.42
1:B:14:DT:H2"	1:B:15:DT:C6	2.55	0.42
5:D:272:ASN:O	5:D:275:TRP:HB2	2.20	0.42
5:D:92:LEU:O	5:D:95:LEU:HB3	2.19	0.42
5:A:105:ASN:C	5:D:389:HIS:CG	2.92	0.42
5:A:18:LEU:HD13	5:A:19:TYR:CD1	2.53	0.42
5:A:388:GLU:O	5:A:389:HIS:C	2.54	0.42
4:F:7:DT:H3'	5:D:244:ARG:CD	2.50	0.42
4:F:1:DA:C1'	4:F:2:DA:C5'	2.95	0.42
5:D:103:TYR:C	5:D:105:ASN:N	2.73	0.42
5:A:177:LEU:HD12	5:A:199:ILE:CG2	2.50	0.42
5:A:20:ARG:O	5:A:23:TRP:HB3	2.20	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
5:D:88:LEU:C	5:D:88:LEU:HD23	2.39	0.42
4:F:9:DA:H2"	4:F:10:DT:C5'	2.50	0.42
5:D:207:TYR:OH	5:D:211:HIS:CE1	2.72	0.42
5:A:102:ASP:OD1	5:A:102:ASP:C	2.58	0.42
5:A:113:ILE:O	5:A:117:LEU:N	2.51	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:A:174:LYS:HG2	5:A:315:LEU:HD13	2.01	0.42
5:A:384:ILE:HG23	5:A:385:GLU:N	2.33	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:A:273:GLN:C	5:A:275:TRP:N	2.71	0.42
5:A:331:PRO:HA	5:A:332:PRO:HD3	1.89	0.42
5:D:11:LEU:HD23	5:D:11:LEU:C	2.41	0.42
5:D:130:PHE:HZ	5:D:251:TRP:CG	2.37	0.42
5:D:29:TRP:CZ3	5:D:53:TYR:HB2	2.55	0.42
5:A:389:HIS:CD2	5:D:105:ASN:CA	3.03	0.41
2:C:10:DA:C2	2:C:11:DA:C4	3.07	0.41
5:D:30:LEU:HD13	5:D:30:LEU:H	1.82	0.41
3:E:11:DA:C2	3:E:12:DA:N1	2.88	0.41
5:A:106:VAL:HG21	5:A:275:TRP:CH2	2.55	0.41
5:A:110:LEU:O	5:A:111:GLN:C	2.57	0.41
5:A:249:GLY:O	5:A:253:PRO:CD	2.68	0.41
2:C:11:DA:N1	2:C:12:DA:C2	2.89	0.41
2:C:5:DT:C4	2:C:6:DT:C4	3.09	0.41
5:D:117:LEU:HA	5:D:117:LEU:HD23	1.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:125:LEU:N	5:D:258:TYR:CE1	2.88	0.41
5:D:316:GLN:CD	5:D:316:GLN:N	2.74	0.41
5:D:217:TYR:HE1	5:D:218:LYS:HZ3	1.65	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
5:D:88:LEU:HD21	5:D:92:LEU:HD11	2.01	0.41
5:A:114:SER:HA	5:A:140:LEU:HD13	2.00	0.41
5:A:70:ALA:O	5:A:74:PHE:CD2	2.73	0.41
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: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:A:90:GLN:CD	5:A:90:GLN:N	2.73	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:105:ASN:HA	5:D:389:HIS:HD1	1.85	0.41
5:D:387:GLN:O	5:D:391:LEU:HD23	2.20	0.41
5:D:43:LEU:HG	5:D:44:PHE:H	1.85	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:329:ASP:O	5:D:330:LEU:HG	2.21	0.41
5:A:18:LEU:HD22	5:A:18:LEU:C	2.41	0.41
1:B:7:DT:C2'	1:B:8:DA:C8	2.96	0.41
5:A:274:GLU:HG3	5:D:385:GLU:HB3	2.02	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:115:ILE:HD12	5:A:390:LEU:C	2.40	0.40
5:D:231:ILE:HA	5:D:232:PRO:HD2	1.91	0.40
5:D:312:ARG:NH1	5:D:312:ARG:CG	2.48	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:A:60:ILE:N	5:A:60:ILE:HD13	2.35	0.40
5:A:87:VAL:CG2	5:A:88:LEU:N	2.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:88:LEU:CD1	5:A:88:LEU:C	2.89	0.40
5:D:120:PRO:HG3	5:D:358:THR:OG1	2.21	0.40
5:D:26:TYR:O	5:D:30:LEU:HD13	2.20	0.40
5:D:8:LEU:HA	5:D:11:LEU:HD13	2.00	0.40
5:A:174:LYS:CE	5:A:299:THR:HG22	2.50	0.40
5:A:299:THR:OG1	5:A:307:ILE:CD1	2.69	0.40
5:A:81:GLU:O	5:A:84:ASP:HB3	2.21	0.40
5:D:252:TYR:O	5:D:256:PHE:CD2	2.72	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%)	41	74
All	All	764/804 (95%)	689 (90%)	74 (10%)	1 (0%)	51	83

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%)	321 (88%)	45 (12%)	4	26
5	D	366/377 (97%)	316 (86%)	50 (14%)	3	22
All	All	732/754 (97%)	637 (87%)	95 (13%)	4	24

All (95) 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	18	LEU
5	A	28	GLU
5	A	31	LYS
5	A	42	LYS
5	A	43	LEU
5	A	78	LEU
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	169	ASP
5	A	172	ASN
5	A	182	LYS
5	A	199	ILE
5	A	213	VAL
5	A	214	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	224	ILE
5	A	229	GLU
5	A	234	ILE
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	375	PHE
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	42	LYS
5	D	43	LEU
5	D	59	ASP
5	D	79	ASP
5	D	95	LEU
5	D	107	ILE
5	D	114	SER
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	167	ILE
5	D	171	GLU
5	D	179	HIS
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	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	384	ILE
5	D	386	SER
5	D	389	HIS
5	D	391	LEU
5	D	394	LEU
5	D	395	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	134	GLN
5	A	230	HIS
5	A	298	ASN
5	A	311	ASN
5	A	389	HIS
5	D	90	GLN
5	D	105	ASN
5	D	129	HIS
5	D	144	GLN
5	D	179	HIS
5	D	211	HIS
5	D	230	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	260	GLN
5	D	273	GLN
5	D	316	GLN
5	D	342	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å ²)	Q<0.9
1	B	15/15 (100%)	-0.03	0 100 100	120, 140, 161, 168	0
2	C	15/15 (100%)	0.05	1 (6%) 17 10	114, 144, 169, 180	0
3	E	14/14 (100%)	-0.34	0 100 100	108, 138, 172, 187	0
4	F	15/15 (100%)	-0.24	0 100 100	103, 132, 161, 168	0
5	A	388/402 (96%)	-0.05	14 (3%) 42 29	65, 116, 176, 215	0
5	D	388/402 (96%)	0.04	11 (2%) 53 37	67, 119, 181, 231	0
All	All	835/863 (96%)	-0.01	26 (3%) 49 33	65, 120, 179, 231	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	399	GLY	5.6
5	A	41	LEU	4.5
2	C	1	DA	3.9
5	A	2	SER	3.9
5	D	214	LYS	3.4
5	D	40	ASP	3.4
5	D	215	LYS	3.3
5	D	399	GLY	3.1
5	A	131	LYS	3.1
5	A	400	THR	3.0
5	A	1	MET	2.9
5	A	402	SER	2.8
5	A	215	LYS	2.8
5	D	130	PHE	2.8
5	A	40	ASP	2.6
5	D	216	TYR	2.6
5	D	186	VAL	2.3
5	D	42	LYS	2.2
5	A	401	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	A	217	TYR	2.1
5	A	35	ASP	2.1
5	D	400	THR	2.1
5	A	282	SER	2.0
5	D	363	LEU	2.0
5	A	379	THR	2.0
5	D	241	GLN	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 carbohydrates 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.