Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 07:46 AM EDT

PDB ID	:	1HYS
Title	:	CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH A POLYPURINE TRACT RNA:DNA
Authors	:	Sarafianos, S.G.; Das, K.; Tantillo, C.; Clark Jr., A.D.; Ding, J.; Whitcomb, J.; Boyer, P.L.; Hughes, S.H.; Arnold, E.
Deposited on	:	2001-01-22
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

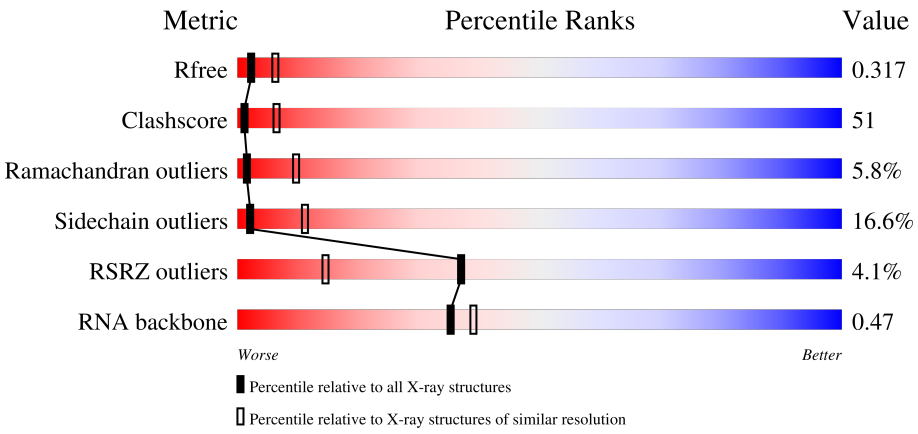
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 <=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	E	23	74% 22% •
2	F	22	86% 14%
3	A	553	7% 33% 52% 15% •
4	B	425	4% 30% 55% 14% •

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Mol	Chain	Length	Quality of chain
5	C	214	2%, 40%, 47%, 13%
6	D	220	33%, 54%, 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12139 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 RNA chain called 5'-R(*UP*CP*AP*GP*CP*CP*AP*CP*UP*UP*UP*UP *UP*AP*AP*AP*AP*GP*AP*AP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	23	486	220	89	155	22	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	22	447	217	74	135	21	0	0	0

- Molecule 3 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	553	4465	2894	739	825	7	249	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 4 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	425	3481	2265	578	632	6	77	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 5 is a protein called FAB-28 MONOCLONAL ANTIBODY FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	214	1612	1008	256	341	7	0	0	0

- Molecule 6 is a protein called FAB-28 MONOCLONAL ANTIBODY FRAGMENT HEAVY CHAIN.

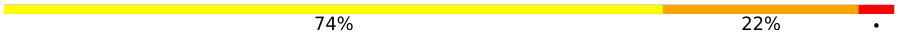
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	220	1648	1037	270	333	8	5	0	0

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.

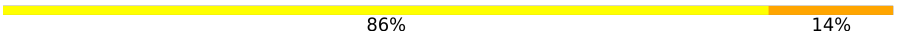
• Molecule 1: 5'-R(*UP*CP*AP*GP*CP*CP*AP*CP*UP*UP*UP*UP*UP*AP*AP*AP*AP*G P*AP*AP*AP*AP*G)-3'

Chain E:



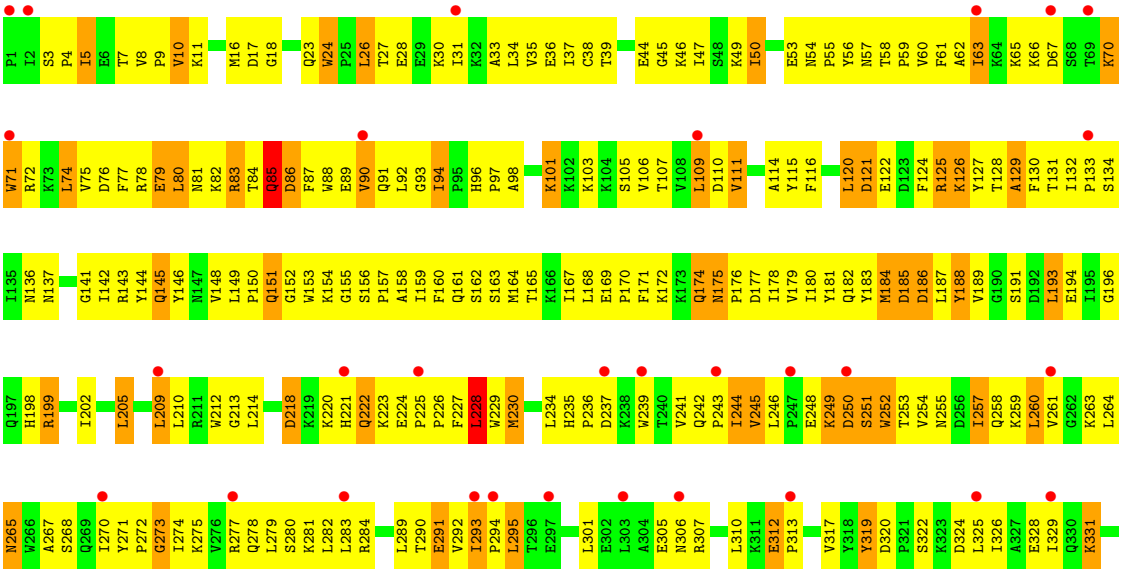
• Molecule 2: 5'-D(*CP*TP*TP*TP*TP*CP*TP*TP*TP*TP*AP*AP*AP*AP*AP*GP*TP*G P*GP*CP*TP*G)-3'

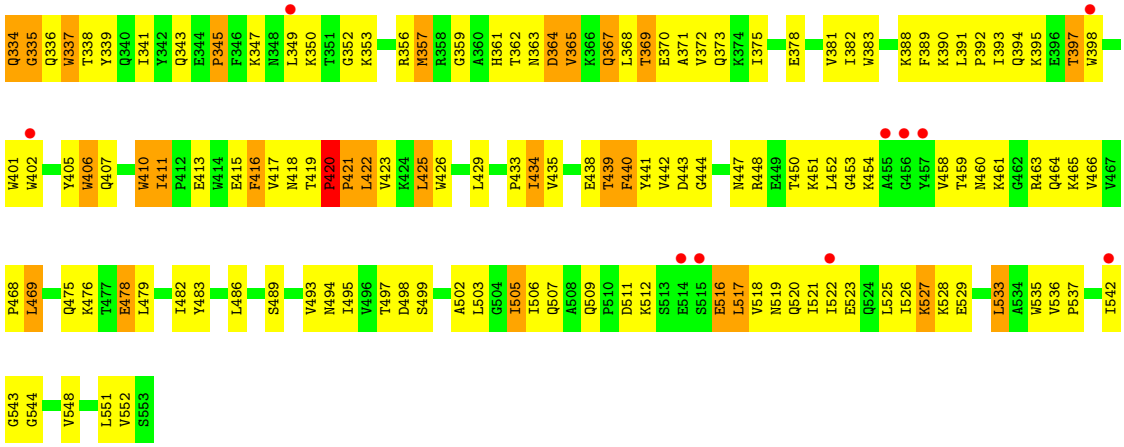
Chain F:



• Molecule 3: HIV-1 REVERSE TRANSCRIPTASE

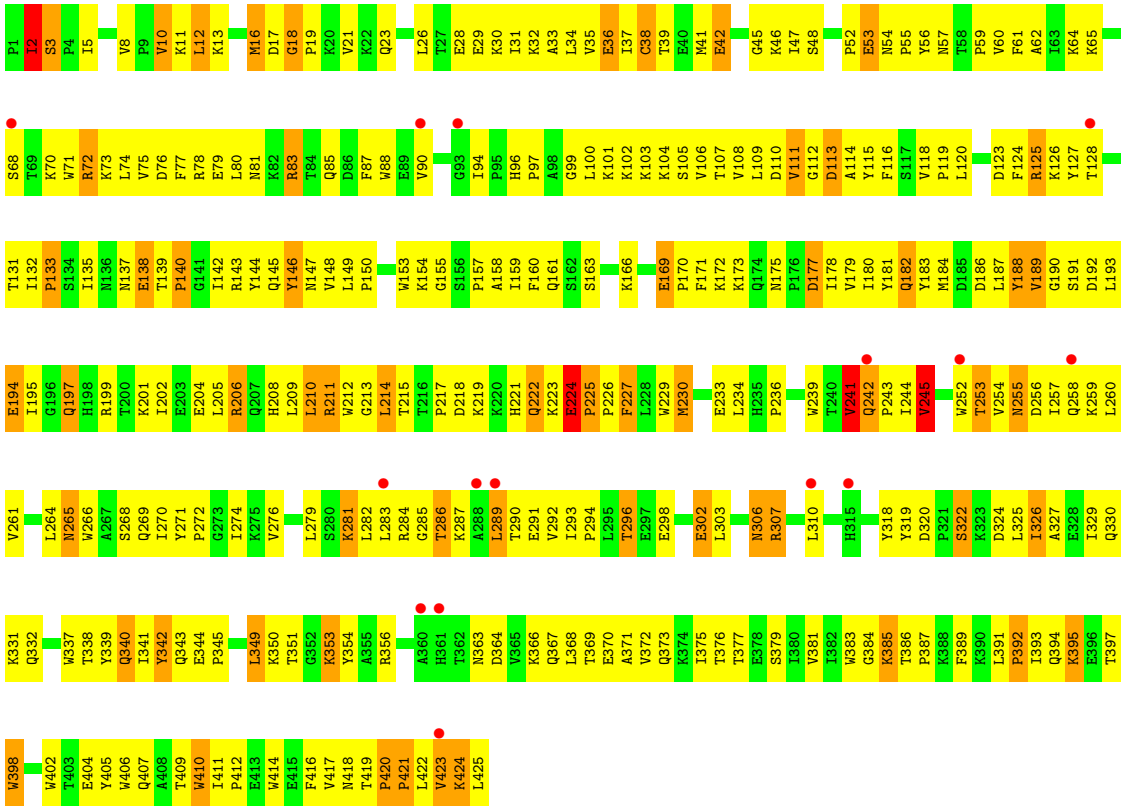
Chain A:





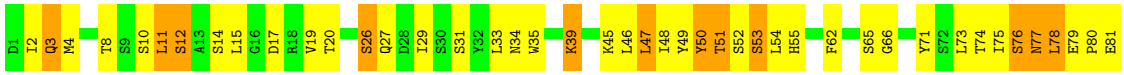
• Molecule 4: HIV-1 REVERSE TRANSCRIPTASE

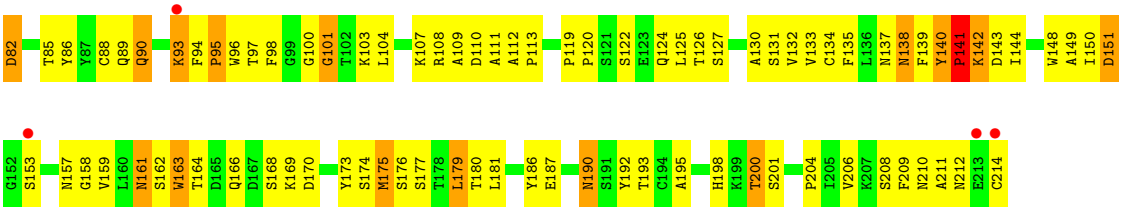
Chain B:



• Molecule 5: FAB-28 MONOCLONAL ANTIBODY FRAGMENT LIGHT CHAIN

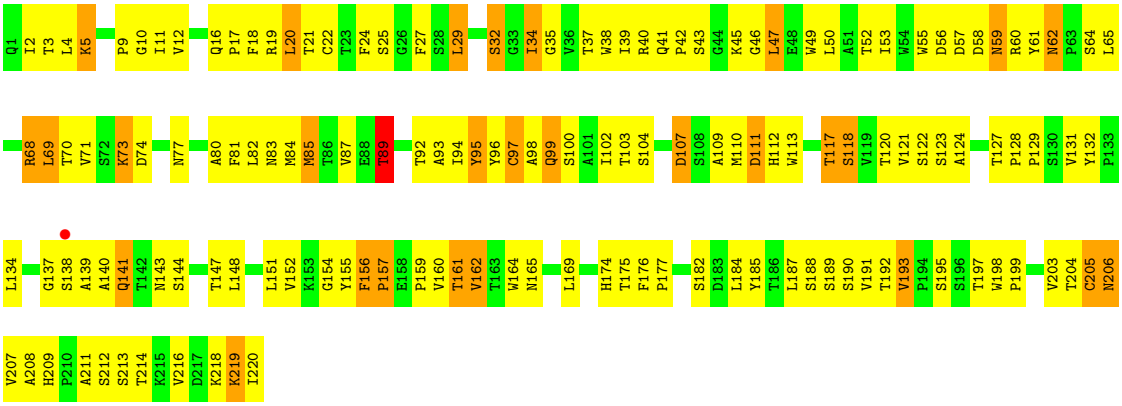
Chain C:





- Molecule 6: FAB-28 MONOCLONAL ANTIBODY FRAGMENT HEAVY CHAIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	166.16Å 166.16Å 218.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00 24.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	74.1 (8.00-3.00) 75.2 (24.98-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.274 , 0.316 0.274 , 0.317	Depositor DCC
R_{free} test set	1286 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 14.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	12139	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	E	0.76	1/544 (0.2%)	1.11	7/845 (0.8%)
2	F	0.66	0/499	1.05	5/769 (0.7%)
3	A	0.55	0/4583	0.80	6/6232 (0.1%)
4	B	0.79	2/3583 (0.1%)	1.10	8/4871 (0.2%)
5	C	0.55	0/1650	0.80	1/2251 (0.0%)
6	D	0.64	0/1691	0.88	0/2320
All	All	0.65	3/12550 (0.0%)	0.93	27/17288 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	B	0	5
6	D	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	211	ARG	CZ-NH1	22.86	1.62	1.33
1	E	854	U	C5-C6	7.03	1.40	1.34
4	B	211	ARG	CZ-NH2	-5.46	1.25	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	211	ARG	NE-CZ-NH2	34.23	137.41	120.30
4	B	211	ARG	NE-CZ-NH1	-28.40	106.10	120.30
4	B	211	ARG	NH1-CZ-NH2	-15.12	102.77	119.40
1	E	854	U	N1-C1'-C2'	8.67	125.28	114.00
2	F	892	DA	N9-C1'-C2'	8.29	128.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	72	ARG	NE-CZ-NH2	7.15	123.87	120.30
4	B	211	ARG	CD-NE-CZ	7.03	133.45	123.60
1	E	859	C	O3'-P-O5'	-6.42	91.79	104.00
1	E	863	U	O3'-P-O5'	6.30	115.97	104.00
2	F	887	DT	O3'-P-O5'	6.30	115.97	104.00
1	E	854	U	O4'-C4'-C3'	-6.16	97.84	104.00
3	A	421	PRO	N-CA-C	-6.15	96.11	112.10
4	B	230	MET	CG-SD-CE	6.02	109.83	100.20
3	A	357	MET	CG-SD-CE	5.84	109.55	100.20
2	F	886	DT	O3'-P-O5'	-5.72	93.13	104.00
4	B	16	MET	CG-SD-CE	5.71	109.34	100.20
3	A	230	MET	CG-SD-CE	5.65	109.25	100.20
4	B	184	MET	CG-SD-CE	5.57	109.11	100.20
3	A	517	LEU	CA-CB-CG	5.50	127.95	115.30
4	B	421	PRO	N-CA-C	5.43	126.21	112.10
1	E	860	A	O3'-P-O5'	5.30	114.08	104.00
3	A	24	TRP	CB-CA-C	-5.26	99.88	110.40
5	C	4	MET	CG-SD-CE	5.25	108.60	100.20
1	E	859	C	OP2-P-O3'	5.22	116.68	105.20
2	F	887	DT	OP1-P-O3'	-5.15	93.88	105.20
2	F	887	DT	P-O3'-C3'	-5.09	113.59	119.70
1	E	862	U	P-O3'-C3'	5.02	125.73	119.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	146	TYR	Sidechain
4	B	183	TYR	Sidechain
4	B	188	TYR	Sidechain
4	B	211	ARG	Sidechain
4	B	342	TYR	Sidechain
6	D	95	TYR	Sidechain

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	E	486	0	249	75	0
2	F	447	0	254	98	0
3	A	4465	0	4497	436	0
4	B	3481	0	3505	336	0
5	C	1612	0	1516	144	0
6	D	1648	0	1602	176	0
All	All	12139	0	11623	1181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (1181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:439:THR:HG21	4:B:289:LEU:H	1.15	1.10
2:F:878:DC:H1'	2:F:879:DT:H5"	1.35	1.08
2:F:897:DC:H2"	2:F:898:DT:H5'	1.28	1.08
1:E:868:A:H2'	1:E:869:A:C8	1.89	1.08
2:F:884:DT:C2'	2:F:885:DT:H71	1.82	1.07
2:F:894:DT:H2"	3:A:258:GLN:HE22	1.19	1.06
1:E:854:U:C4'	1:E:855:C:H5'	1.86	1.06
2:F:893:DG:H2"	2:F:894:DT:H5'	1.32	1.05
6:D:165:ASN:HD21	6:D:203:VAL:HA	1.17	1.05
2:F:893:DG:H2"	2:F:894:DT:C5'	1.85	1.05
6:D:40:ARG:HB2	6:D:50:LEU:HD11	1.38	1.04
1:E:855:C:H2'	1:E:856:A:C8	1.93	1.03
1:E:861:C:H2'	1:E:862:U:C6	1.93	1.03
1:E:855:C:H2'	1:E:856:A:H8	1.24	1.03
2:F:884:DT:H2'	2:F:885:DT:C7	1.88	1.03
6:D:4:LEU:HD12	6:D:97:CYS:SG	2.00	1.02
4:B:282:LEU:HD21	4:B:294:PRO:HG2	1.41	1.02
1:E:865:U:H2'	1:E:866:U:H6	1.23	1.01
4:B:245:VAL:HG11	4:B:310:LEU:HD12	1.43	0.99
4:B:223:LYS:HG3	4:B:224:GLU:H	1.26	0.99
1:E:854:U:H4'	1:E:855:C:H5'	1.00	0.98
1:E:865:U:H2'	1:E:866:U:C6	1.99	0.98
3:A:120:LEU:HD12	3:A:121:ASP:H	1.29	0.97
1:E:854:U:H4'	1:E:855:C:C5'	1.93	0.97
3:A:440:PHE:HE2	3:A:489:SER:HB3	1.26	0.97
3:A:438:GLU:HA	3:A:460:ASN:ND2	1.81	0.96
5:C:149:ALA:HB1	5:C:153:SER:HA	1.47	0.95
3:A:503:LEU:HD11	3:A:507:GLN:HE21	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:895:DG:H5'	3:A:258:GLN:NE2	1.83	0.94
4:B:34:LEU:HD13	4:B:62:ALA:HB2	1.46	0.93
4:B:114:ALA:HB2	4:B:215:THR:HG23	1.51	0.93
4:B:223:LYS:HE3	6:D:60:ARG:HH22	1.31	0.93
1:E:867:A:H2'	1:E:868:A:O4'	1.69	0.92
6:D:34:ILE:HG22	6:D:35:GLY:H	1.34	0.92
1:E:864:U:H2'	1:E:865:U:H6	1.35	0.92
2:F:883:DC:C6	2:F:884:DT:H72	2.05	0.92
3:A:120:LEU:HD12	3:A:121:ASP:N	1.85	0.92
3:A:291:GLU:HG2	3:A:292:VAL:N	1.85	0.91
4:B:47:ILE:HG22	4:B:146:TYR:HA	1.53	0.91
5:C:161:ASN:HB2	5:C:163:TRP:CZ3	2.04	0.91
2:F:884:DT:H2'	2:F:885:DT:H71	0.93	0.90
3:A:225:PRO:HG2	3:A:226:PRO:HD3	1.53	0.90
3:A:151:GLN:H	3:A:151:GLN:NE2	1.71	0.89
2:F:894:DT:C2'	3:A:258:GLN:HE22	1.87	0.88
1:E:864:U:H2'	1:E:865:U:C6	2.09	0.88
2:F:894:DT:H2"	3:A:258:GLN:NE2	1.89	0.87
1:E:854:U:O2'	1:E:855:C:C6	2.27	0.87
2:F:897:DC:H2"	2:F:898:DT:C5'	2.03	0.87
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.56	0.87
3:A:329:ILE:HG23	3:A:392:PRO:HD3	1.57	0.86
5:C:113:PRO:HD3	5:C:200:THR:HG21	1.57	0.86
3:A:151:GLN:N	3:A:151:GLN:HE21	1.71	0.85
3:A:115:TYR:HD2	3:A:156:SER:OG	1.59	0.85
5:C:142:LYS:O	5:C:144:ILE:HG22	1.77	0.85
4:B:23:GLN:HE22	4:B:60:VAL:H	1.24	0.84
4:B:326:ILE:O	4:B:341:ILE:HA	1.78	0.84
5:C:137:ASN:HA	5:C:174:SER:HB2	1.60	0.84
4:B:12:LEU:HD11	4:B:127:TYR:CE1	2.13	0.84
6:D:89:THR:O	6:D:92:THR:HG22	1.78	0.83
5:C:2:ILE:HD11	5:C:93:LYS:HB2	1.59	0.83
2:F:895:DG:H2'	2:F:896:DG:H8	1.40	0.83
6:D:38:TRP:CD1	6:D:82:LEU:HD23	2.13	0.83
3:A:357:MET:HG3	3:A:362:THR:HG21	1.58	0.83
6:D:165:ASN:ND2	6:D:203:VAL:HA	1.94	0.83
3:A:84:THR:HB	3:A:154:LYS:HD3	1.60	0.83
3:A:440:PHE:CE2	3:A:489:SER:HB3	2.13	0.83
2:F:878:DC:H1'	2:F:879:DT:C5'	2.09	0.82
5:C:140:TYR:CG	5:C:141:PRO:HD3	2.14	0.82
2:F:887:DT:H2"	2:F:888:DA:OP2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:47:ILE:HG22	3:A:146:TYR:HA	1.60	0.82
3:A:415:GLU:HG2	3:A:416:PHE:H	1.43	0.82
3:A:106:VAL:HB	3:A:227:PHE:CE1	2.15	0.82
2:F:878:DC:H2"	2:F:879:DT:H5'	1.60	0.82
2:F:880:DT:H2"	2:F:881:DT:OP2	1.80	0.81
3:A:151:GLN:H	3:A:151:GLN:HE21	1.22	0.81
2:F:883:DC:H2"	2:F:884:DT:OP2	1.77	0.81
4:B:12:LEU:HD12	4:B:12:LEU:H	1.44	0.81
4:B:395:LYS:HA	4:B:416:PHE:CE2	2.14	0.81
5:C:140:TYR:CD1	5:C:141:PRO:HD3	2.15	0.81
6:D:42:PRO:HG2	6:D:45:LYS:HD2	1.59	0.81
4:B:21:VAL:HG21	4:B:79:GLU:HG3	1.63	0.81
5:C:48:ILE:HG22	5:C:54:LEU:HA	1.60	0.81
6:D:18:PHE:HD2	6:D:87:VAL:HG21	1.44	0.81
3:A:122:GLU:HA	3:A:125:ARG:HD2	1.61	0.81
1:E:875:A:H2'	1:E:876:G:C8	2.16	0.81
1:E:869:A:H2'	1:E:870:A:C8	2.17	0.80
3:A:31:ILE:O	3:A:35:VAL:HG23	1.81	0.80
4:B:222:GLN:HE21	4:B:222:GLN:N	1.80	0.80
3:A:181:TYR:CE2	4:B:138:GLU:HA	2.17	0.79
2:F:896:DG:C2'	2:F:897:DC:H5'	2.12	0.79
1:E:873:A:H2'	1:E:874:A:H8	1.48	0.79
3:A:438:GLU:HA	3:A:460:ASN:HD21	1.43	0.79
4:B:225:PRO:HB2	4:B:226:PRO:CD	2.12	0.79
3:A:459:THR:HG22	3:A:463:ARG:HB3	1.64	0.79
1:E:861:C:H2'	1:E:862:U:H6	1.45	0.78
3:A:115:TYR:HD2	3:A:156:SER:HG	0.79	0.78
4:B:206:ARG:HG2	4:B:217:PRO:HG3	1.66	0.78
4:B:225:PRO:HB2	4:B:226:PRO:HD2	1.66	0.78
6:D:65:LEU:HD22	6:D:68:ARG:NH1	1.99	0.78
1:E:875:A:H2'	1:E:876:G:H8	1.46	0.78
3:A:164:MET:HE1	3:A:187:LEU:HD21	1.65	0.78
3:A:439:THR:HG21	4:B:289:LEU:N	1.95	0.78
6:D:18:PHE:CD2	6:D:87:VAL:HG21	2.18	0.77
4:B:59:PRO:HG2	4:B:76:ASP:HB3	1.67	0.77
5:C:3:GLN:H	5:C:26:SER:HB2	1.49	0.77
2:F:895:DG:H2'	2:F:896:DG:C8	2.19	0.77
6:D:74:ASP:OD1	6:D:77:ASN:HB2	1.84	0.77
1:E:873:A:O2'	1:E:874:A:H5'	1.84	0.77
4:B:170:PRO:HG2	4:B:212:TRP:HZ3	1.49	0.77
6:D:122:SER:HB3	6:D:156:PHE:CZ	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:15:LEU:HD12	5:C:15:LEU:H	1.49	0.76
1:E:869:A:H2'	1:E:870:A:H8	1.51	0.76
4:B:33:ALA:O	4:B:37:ILE:HG22	1.86	0.76
1:E:858:C:H4'	3:A:93:GLY:HA2	1.65	0.76
4:B:209:LEU:HD22	4:B:215:THR:HG21	1.68	0.76
3:A:373:GLN:OE1	4:B:397:THR:HA	1.86	0.76
6:D:122:SER:HB3	6:D:156:PHE:HZ	1.50	0.76
3:A:418:ASN:ND2	3:A:422:LEU:HD11	1.99	0.76
4:B:420:PRO:HB3	4:B:421:PRO:HD2	1.65	0.75
3:A:87:PHE:CE1	3:A:155:GLY:HA3	2.20	0.75
3:A:291:GLU:HG2	3:A:292:VAL:H	1.48	0.75
5:C:133:VAL:HG11	6:D:134:LEU:HD13	1.69	0.75
3:A:319:TYR:HD1	3:A:343:GLN:NE2	1.83	0.75
3:A:502:ALA:O	3:A:506:ILE:HG12	1.86	0.74
4:B:90:VAL:HG23	4:B:158:ALA:HB2	1.68	0.74
4:B:387:PRO:HG2	4:B:389:PHE:CE1	2.22	0.74
3:A:459:THR:HG23	3:A:461:LYS:H	1.51	0.74
3:A:544:GLY:O	3:A:548:VAL:HG23	1.87	0.74
5:C:86:TYR:O	5:C:101:GLY:HA2	1.88	0.74
5:C:198:HIS:HB3	5:C:200:THR:HG23	1.69	0.74
3:A:419:THR:N	3:A:420:PRO:HD3	2.03	0.74
5:C:190:ASN:H	5:C:190:ASN:HD22	1.35	0.74
1:E:866:U:H2'	1:E:867:A:C8	2.23	0.73
2:F:892:DA:H2'	2:F:893:DG:H8	1.53	0.73
2:F:878:DC:H2"	2:F:879:DT:C5'	2.17	0.73
2:F:894:DT:H2"	2:F:895:DG:H5'	1.70	0.73
2:F:897:DC:C2'	2:F:898:DT:H5'	2.16	0.73
4:B:171:PHE:CZ	4:B:205:LEU:HB2	2.24	0.73
1:E:854:U:O2'	1:E:855:C:H6	1.69	0.73
2:F:896:DG:H2"	2:F:897:DC:H5'	1.69	0.73
3:A:244:ILE:HG13	3:A:271:TYR:HE2	1.53	0.72
3:A:209:LEU:HB3	3:A:214:LEU:HB2	1.69	0.72
3:A:465:LYS:O	3:A:466:VAL:HG23	1.88	0.72
4:B:41:MET:HG2	4:B:46:LYS:HD2	1.70	0.72
6:D:62:ASN:HD21	6:D:64:SER:HB3	1.54	0.72
3:A:261:VAL:HG21	3:A:283:LEU:HD11	1.71	0.72
3:A:368:LEU:HD21	3:A:391:LEU:HD13	1.71	0.72
4:B:19:PRO:HD3	4:B:80:LEU:HD13	1.71	0.72
6:D:17:PRO:HB3	6:D:85:MET:HG3	1.71	0.72
2:F:893:DG:H2"	2:F:894:DT:H5"	1.71	0.72
4:B:146:TYR:CE2	4:B:150:PRO:HA	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:878:DC:C1'	2:F:879:DT:H5"	2.17	0.72
5:C:79:GLU:HB3	5:C:81:GLU:OE1	1.90	0.72
6:D:156:PHE:HB3	6:D:157:PRO:HD3	1.71	0.72
4:B:100:LEU:HD23	4:B:381:VAL:HA	1.71	0.72
4:B:349:LEU:HD12	4:B:349:LEU:H	1.55	0.71
2:F:892:DA:H2'	2:F:893:DG:C8	2.24	0.71
6:D:155:TYR:OH	6:D:187:LEU:HB2	1.89	0.71
3:A:155:GLY:O	3:A:159:ILE:HG12	1.90	0.71
3:A:122:GLU:HA	3:A:125:ARG:CD	2.19	0.71
3:A:453:GLY:O	3:A:469:LEU:HD12	1.89	0.71
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.19	0.71
4:B:119:PRO:HA	4:B:148:VAL:HG12	1.72	0.71
4:B:395:LYS:HA	4:B:416:PHE:CD2	2.25	0.71
5:C:51:THR:HG21	5:C:71:TYR:CD2	2.26	0.71
6:D:61:TYR:HE2	6:D:70:THR:HA	1.55	0.71
6:D:103:THR:HB	6:D:107:ASP:HB2	1.73	0.71
4:B:281:LYS:HB2	4:B:281:LYS:NZ	2.04	0.71
6:D:56:ASP:OD2	6:D:58:ASP:HB3	1.90	0.71
1:E:865:U:C2	1:E:866:U:C5	2.78	0.71
4:B:163:SER:O	4:B:166:LYS:HG2	1.90	0.71
6:D:19:ARG:O	6:D:19:ARG:HG2	1.89	0.70
3:A:329:ILE:HD13	3:A:368:LEU:HD12	1.72	0.70
4:B:222:GLN:HE21	4:B:222:GLN:H	1.36	0.70
4:B:389:PHE:HB3	4:B:391:LEU:CD2	2.20	0.70
6:D:92:THR:OG1	6:D:120:THR:HA	1.90	0.70
5:C:79:GLU:HG2	5:C:80:PRO:HD2	1.73	0.70
6:D:47:LEU:HD23	6:D:47:LEU:H	1.56	0.70
6:D:164:TRP:CZ3	6:D:205:CYS:HB2	2.26	0.70
2:F:881:DT:H2"	2:F:882:DT:OP2	1.92	0.70
5:C:135:PHE:HB3	5:C:137:ASN:HD21	1.55	0.70
3:A:3:SER:OG	3:A:5:ILE:HG22	1.91	0.70
3:A:331:LYS:HE3	3:A:421:PRO:HB2	1.73	0.70
4:B:170:PRO:HG2	4:B:212:TRP:CZ3	2.25	0.70
4:B:241:VAL:HB	4:B:243:PRO:HD3	1.72	0.70
2:F:894:DT:C2'	2:F:895:DG:O5'	2.39	0.70
4:B:224:GLU:HG3	5:C:94:PHE:CD2	2.27	0.69
4:B:291:GLU:O	4:B:293:ILE:HG23	1.92	0.69
4:B:125:ARG:HD3	4:B:147:ASN:HA	1.73	0.69
3:A:250:ASP:C	3:A:252:TRP:H	1.93	0.69
4:B:264:LEU:HG	4:B:276:VAL:HG11	1.74	0.69
6:D:198:TRP:CZ2	6:D:220:ILE:HG23	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:881:DT:H2"	2:F:882:DT:H5'	1.75	0.69
2:F:895:DG:C2'	2:F:896:DG:H8	2.05	0.69
4:B:131:THR:HG23	4:B:143:ARG:HG2	1.75	0.69
4:B:325:LEU:HD21	4:B:383:TRP:CE3	2.28	0.69
5:C:107:LYS:HA	5:C:140:TYR:OH	1.93	0.69
3:A:225:PRO:CG	3:A:226:PRO:HD3	2.23	0.69
3:A:425:LEU:HD12	3:A:425:LEU:H	1.58	0.69
3:A:8:VAL:CG1	4:B:53:GLU:HB3	2.23	0.68
3:A:169:GLU:N	3:A:170:PRO:HD2	2.08	0.68
4:B:223:LYS:CE	6:D:60:ARG:HH22	2.06	0.68
4:B:260:LEU:HD21	4:B:303:LEU:HD11	1.75	0.68
6:D:53:ILE:HA	6:D:59:ASN:HB3	1.74	0.68
1:E:873:A:H2'	1:E:874:A:C8	2.27	0.68
6:D:206:ASN:N	6:D:206:ASN:HD22	1.91	0.68
3:A:273:GLY:HA2	3:A:338:THR:HG21	1.75	0.68
3:A:26:LEU:HD23	3:A:133:PRO:HG2	1.75	0.68
4:B:282:LEU:HD21	4:B:294:PRO:CG	2.20	0.68
3:A:279:LEU:HD23	3:A:282:LEU:HD12	1.76	0.68
5:C:11:LEU:HD21	5:C:19:VAL:HG13	1.76	0.68
5:C:162:SER:HB3	6:D:177:PRO:HG2	1.76	0.68
1:E:858:C:H1'	3:A:94:ILE:HD13	1.76	0.68
3:A:493:VAL:HG13	3:A:495:ILE:HD11	1.76	0.68
3:A:85:GLN:NE2	3:A:87:PHE:CE2	2.61	0.67
4:B:194:GLU:HG3	4:B:197:GLN:H	1.59	0.67
4:B:373:GLN:HE22	4:B:406:TRP:HA	1.60	0.67
6:D:65:LEU:HB3	6:D:69:LEU:HD23	1.75	0.67
6:D:99:GLN:C	6:D:99:GLN:HE21	1.97	0.67
3:A:88:TRP:CZ3	3:A:90:VAL:HA	2.29	0.67
1:E:868:A:C2'	1:E:869:A:C8	2.75	0.67
3:A:372:VAL:HG13	3:A:389:PHE:CE1	2.29	0.67
4:B:234:LEU:HD11	4:B:377:THR:HG21	1.76	0.67
3:A:372:VAL:HG11	3:A:411:ILE:HG22	1.78	0.66
3:A:30:LYS:O	3:A:34:LEU:HG	1.95	0.66
4:B:23:GLN:NE2	4:B:60:VAL:H	1.93	0.66
4:B:75:VAL:HG11	4:B:77:PHE:CZ	2.30	0.66
5:C:112:ALA:HA	5:C:200:THR:HG21	1.77	0.66
6:D:152:VAL:HG22	6:D:207:VAL:HG21	1.77	0.66
4:B:281:LYS:HE3	4:B:284:ARG:HH12	1.61	0.66
6:D:61:TYR:CE2	6:D:70:THR:HA	2.31	0.66
3:A:180:ILE:HG12	3:A:189:VAL:HG12	1.77	0.66
4:B:306:ASN:O	4:B:310:LEU:HD23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:LYS:HD3	3:A:144:TYR:CE2	2.29	0.66
3:A:375:ILE:HB	3:A:389:PHE:HZ	1.61	0.66
4:B:34:LEU:O	4:B:38:CYS:HB2	1.95	0.66
3:A:503:LEU:HD11	3:A:507:GLN:NE2	2.08	0.66
3:A:23:GLN:CG	3:A:133:PRO:HG3	2.26	0.66
3:A:253:THR:HG22	3:A:255:ASN:H	1.61	0.66
4:B:373:GLN:NE2	4:B:406:TRP:HA	2.11	0.66
5:C:45:LYS:HD2	5:C:46:LEU:H	1.61	0.65
3:A:447:ASN:HB3	3:A:450:THR:OG1	1.95	0.65
3:A:84:THR:HG21	3:A:153:TRP:NE1	2.11	0.65
3:A:54:ASN:ND2	3:A:56:TYR:HD1	1.94	0.65
3:A:265:ASN:O	3:A:268:SER:HB3	1.97	0.65
3:A:274:ILE:HG23	3:A:306:ASN:ND2	2.11	0.65
5:C:130:ALA:HB3	5:C:181:LEU:O	1.95	0.65
3:A:394:GLN:HA	3:A:416:PHE:CZ	2.31	0.65
4:B:2:ILE:HD13	4:B:119:PRO:HD3	1.77	0.65
4:B:224:GLU:HA	4:B:227:PHE:CE2	2.32	0.65
5:C:120:PRO:HG2	5:C:186:TYR:CE1	2.31	0.65
5:C:12:SER:HB3	5:C:107:LYS:HD3	1.79	0.65
4:B:242:GLN:H	4:B:243:PRO:HD3	1.62	0.65
4:B:252:TRP:CH2	4:B:260:LEU:HD22	2.32	0.65
6:D:4:LEU:HD11	6:D:98:ALA:HA	1.79	0.65
3:A:178:ILE:HA	3:A:191:SER:HB3	1.79	0.64
1:E:873:A:C2	1:E:874:A:C4	2.85	0.64
2:F:878:DC:C1'	2:F:879:DT:C5'	2.75	0.64
2:F:894:DT:H2"	2:F:895:DG:C5'	2.26	0.64
3:A:181:TYR:CD1	4:B:138:GLU:HG3	2.33	0.64
3:A:397:THR:HG22	3:A:425:LEU:HD12	1.80	0.64
4:B:23:GLN:HE22	4:B:60:VAL:N	1.94	0.64
6:D:21:THR:HG23	6:D:81:PHE:CE2	2.32	0.64
2:F:897:DC:C2'	2:F:898:DT:C5'	2.75	0.64
3:A:275:LYS:HD2	3:A:336:GLN:NE2	2.12	0.64
4:B:199:ARG:HH22	4:B:230:MET:HE3	1.63	0.64
6:D:204:THR:HG22	6:D:219:LYS:HA	1.79	0.64
3:A:77:PHE:CD1	3:A:80:LEU:HD12	2.32	0.64
3:A:239:TRP:CZ3	3:A:270:ILE:HG12	2.33	0.64
6:D:92:THR:HB	6:D:121:VAL:HG23	1.80	0.64
3:A:365:VAL:HG11	3:A:401:TRP:CE2	2.33	0.63
4:B:242:GLN:N	4:B:243:PRO:HD3	2.13	0.63
5:C:190:ASN:H	5:C:190:ASN:ND2	1.96	0.63
3:A:319:TYR:CD1	3:A:343:GLN:NE2	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:19:PRO:CD	4:B:80:LEU:HD13	2.28	0.63
5:C:11:LEU:HD21	5:C:19:VAL:CG1	2.28	0.63
4:B:193:LEU:HD13	4:B:197:GLN:NE2	2.13	0.63
6:D:53:ILE:HG12	6:D:71:VAL:CG2	2.29	0.63
1:E:857:G:O2'	1:E:858:C:H5'	1.98	0.63
4:B:230:MET:HE2	6:D:104:SER:HA	1.80	0.63
3:A:255:ASN:O	3:A:258:GLN:HB2	1.98	0.63
3:A:434:ILE:HG23	3:A:494:ASN:ND2	2.13	0.63
6:D:34:ILE:HG22	6:D:35:GLY:N	2.10	0.63
1:E:859:C:N4	1:E:860:A:N6	2.46	0.63
2:F:882:DT:H1'	2:F:883:DC:H5'	1.81	0.63
4:B:72:ARG:NH2	4:B:409:THR:HB	2.14	0.63
2:F:878:DC:C2'	2:F:879:DT:C5'	2.77	0.63
3:A:181:TYR:CE1	4:B:138:GLU:HG3	2.34	0.63
3:A:337:TRP:N	3:A:337:TRP:CD1	2.67	0.62
4:B:369:THR:HA	4:B:398:TRP:CH2	2.34	0.62
2:F:892:DA:C2'	2:F:893:DG:C8	2.81	0.62
3:A:53:GLU:O	3:A:55:PRO:HD3	1.99	0.62
3:A:92:LEU:HB3	4:B:137:ASN:OD1	1.99	0.62
2:F:892:DA:C2'	2:F:893:DG:H8	2.11	0.62
3:A:483:TYR:HA	3:A:486:LEU:HD12	1.81	0.62
6:D:39:ILE:HD11	6:D:110:MET:HE1	1.82	0.62
3:A:458:VAL:HG22	3:A:464:GLN:HG2	1.80	0.62
5:C:186:TYR:HA	5:C:192:TYR:OH	2.00	0.62
6:D:29:LEU:HD12	6:D:73:LYS:HG3	1.82	0.62
6:D:42:PRO:HA	6:D:93:ALA:HB1	1.80	0.62
5:C:66:GLY:HA3	5:C:71:TYR:HA	1.81	0.62
4:B:199:ARG:HH22	4:B:230:MET:CE	2.13	0.62
2:F:883:DC:C2	2:F:884:DT:C6	2.88	0.61
3:A:90:VAL:O	3:A:91:GLN:HG3	1.99	0.61
6:D:71:VAL:HG12	6:D:82:LEU:CD2	2.30	0.61
3:A:54:ASN:HD21	3:A:56:TYR:HB2	1.65	0.61
2:F:894:DT:H2'	2:F:895:DG:O5'	2.00	0.61
3:A:66:LYS:HG2	3:A:67:ASP:H	1.65	0.61
6:D:47:LEU:HD23	6:D:47:LEU:N	2.15	0.61
6:D:206:ASN:N	6:D:206:ASN:ND2	2.48	0.61
3:A:46:LYS:HZ3	3:A:116:PHE:HD2	1.48	0.61
4:B:201:LYS:O	4:B:201:LYS:HG3	2.00	0.61
1:E:862:U:H2'	1:E:863:U:C6	2.35	0.61
4:B:389:PHE:HB3	4:B:391:LEU:HD21	1.81	0.61
1:E:859:C:H2'	1:E:860:A:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:74:LEU:HG	3:A:75:VAL:N	2.14	0.61
3:A:443:ASP:HB3	3:A:552:VAL:HG21	1.83	0.61
4:B:223:LYS:HG3	4:B:224:GLU:N	2.08	0.61
3:A:482:ILE:HG22	3:A:486:LEU:HD11	1.83	0.61
4:B:11:LYS:O	4:B:85:GLN:HB3	2.00	0.61
5:C:33:LEU:HB3	5:C:51:THR:OG1	2.00	0.61
3:A:27:THR:O	3:A:31:ILE:HG12	1.99	0.61
3:A:273:GLY:CA	3:A:338:THR:HG21	2.31	0.61
3:A:465:LYS:O	3:A:551:LEU:HD21	2.01	0.60
4:B:172:LYS:CG	4:B:180:ILE:HD12	2.31	0.60
4:B:189:VAL:HG21	4:B:202:ILE:HD12	1.81	0.60
4:B:245:VAL:HG11	4:B:310:LEU:CD1	2.27	0.60
1:E:863:U:H6	1:E:863:U:O5'	1.84	0.60
4:B:65:LYS:HA	4:B:407:GLN:NE2	2.16	0.60
3:A:174:GLN:HE21	3:A:174:GLN:HA	1.66	0.60
3:A:441:TYR:CB	3:A:548:VAL:HG21	2.32	0.60
2:F:890:DA:H2"	2:F:891:DA:OP2	2.01	0.60
5:C:12:SER:CB	5:C:107:LYS:HD3	2.31	0.60
2:F:895:DG:C4	2:F:896:DG:N7	2.70	0.60
3:A:213:GLY:C	3:A:214:LEU:HD22	2.21	0.60
5:C:15:LEU:H	5:C:15:LEU:CD1	2.14	0.60
4:B:23:GLN:NE2	4:B:60:VAL:O	2.35	0.60
4:B:112:GLY:O	4:B:114:ALA:N	2.35	0.60
5:C:62:PHE:CE1	5:C:75:ILE:HG12	2.36	0.60
3:A:395:LYS:HG2	3:A:416:PHE:CD2	2.37	0.60
3:A:397:THR:HG22	3:A:425:LEU:CD1	2.32	0.60
3:A:516:GLU:O	3:A:520:GLN:HG3	2.02	0.60
4:B:55:PRO:HG2	4:B:56:TYR:N	2.17	0.60
5:C:35:TRP:HB2	5:C:48:ILE:CG1	2.32	0.60
5:C:66:GLY:HA3	5:C:71:TYR:CD2	2.36	0.60
5:C:78:LEU:HD21	5:C:104:LEU:HD21	1.82	0.60
6:D:5:LYS:HB2	6:D:5:LYS:NZ	2.16	0.60
3:A:441:TYR:HB3	3:A:548:VAL:HG21	1.83	0.59
6:D:53:ILE:HD11	6:D:71:VAL:HB	1.83	0.59
3:A:390:LYS:HB3	3:A:417:VAL:HG21	1.84	0.59
4:B:55:PRO:HG2	4:B:56:TYR:H	1.68	0.59
5:C:107:LYS:HD2	5:C:140:TYR:OH	2.02	0.59
1:E:857:G:H5'	3:A:89:GLU:HG3	1.83	0.59
1:E:859:C:N4	1:E:860:A:H62	1.99	0.59
3:A:364:ASP:HB3	3:A:423:VAL:HG13	1.84	0.59
4:B:12:LEU:HD11	4:B:127:TYR:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:258:GLN:O	4:B:261:VAL:HG12	2.02	0.59
3:A:365:VAL:HG11	3:A:401:TRP:CD2	2.38	0.59
5:C:138:ASN:OD1	6:D:174:HIS:CE1	2.56	0.59
1:E:864:U:O2'	1:E:865:U:H5'	2.03	0.59
2:F:880:DT:H1'	2:F:881:DT:C6	2.38	0.59
2:F:894:DT:C1'	3:A:258:GLN:HE22	2.15	0.59
4:B:420:PRO:CB	4:B:421:PRO:HD2	2.32	0.59
5:C:29:ILE:HG21	5:C:90:GLN:HG3	1.85	0.59
1:E:866:U:H2'	1:E:867:A:O4'	2.02	0.59
5:C:35:TRP:HB2	5:C:48:ILE:HG12	1.85	0.59
5:C:159:VAL:HG22	5:C:179:LEU:HD12	1.85	0.59
2:F:880:DT:C2'	2:F:881:DT:OP2	2.50	0.59
2:F:882:DT:C2'	2:F:883:DC:H5'	2.32	0.59
3:A:181:TYR:CD2	4:B:138:GLU:HA	2.37	0.59
3:A:429:LEU:HD11	3:A:533:LEU:HD23	1.85	0.59
1:E:871:G:N2	2:F:885:DT:C2	2.70	0.59
4:B:64:LYS:HB2	4:B:71:TRP:CH2	2.38	0.59
1:E:865:U:O2'	1:E:866:U:H5'	2.03	0.58
2:F:878:DC:C2'	2:F:879:DT:H5'	2.29	0.58
3:A:223:LYS:CB	3:A:226:PRO:HD2	2.33	0.58
3:A:267:ALA:HB1	3:A:271:TYR:CD2	2.38	0.58
4:B:108:VAL:HG22	4:B:188:TYR:CE1	2.38	0.58
6:D:151:LEU:HD12	6:D:188:SER:HB3	1.84	0.58
3:A:94:ILE:HG12	3:A:94:ILE:O	2.01	0.58
3:A:223:LYS:HB2	3:A:226:PRO:HD2	1.85	0.58
3:A:458:VAL:HB	3:A:548:VAL:HG22	1.84	0.58
5:C:94:PHE:O	5:C:96:TRP:N	2.35	0.58
5:C:190:ASN:ND2	5:C:190:ASN:N	2.50	0.58
3:A:44:GLU:O	3:A:46:LYS:N	2.37	0.58
4:B:75:VAL:HG11	4:B:77:PHE:CE2	2.38	0.58
4:B:236:PRO:HA	4:B:239:TRP:CE2	2.39	0.58
3:A:227:PHE:HB2	3:A:234:LEU:HB2	1.85	0.58
5:C:135:PHE:CE1	6:D:190:SER:HB3	2.38	0.58
3:A:96:HIS:CE1	3:A:97:PRO:HG2	2.38	0.58
3:A:328:GLU:O	3:A:339:TYR:HA	2.03	0.58
3:A:54:ASN:HD22	3:A:56:TYR:HD1	1.50	0.58
4:B:94:ILE:HG13	4:B:161:GLN:NE2	2.18	0.58
5:C:76:SER:OG	5:C:77:ASN:N	2.37	0.58
5:C:96:TRP:CE3	6:D:110:MET:HE3	2.38	0.58
5:C:112:ALA:HA	5:C:200:THR:CG2	2.33	0.58
1:E:865:U:C2	1:E:866:U:C6	2.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:146:TYR:CG	3:A:150:PRO:HG3	2.38	0.58
3:A:393:ILE:HG12	3:A:394:GLN:N	2.19	0.58
3:A:134:SER:HB3	3:A:141:GLY:HA2	1.86	0.58
3:A:38:CYS:HB3	3:A:144:TYR:CE1	2.38	0.58
3:A:58:THR:HG21	3:A:77:PHE:CE1	2.39	0.58
1:E:860:A:C4'	3:A:265:ASN:HD21	2.17	0.57
3:A:357:MET:HG3	3:A:362:THR:CG2	2.30	0.57
6:D:198:TRP:HB3	6:D:199:PRO:HD3	1.86	0.57
3:A:120:LEU:HB2	3:A:149:LEU:HD23	1.86	0.57
3:A:324:ASP:OD2	3:A:388:LYS:HE3	2.05	0.57
5:C:195:ALA:CB	5:C:206:VAL:HG12	2.34	0.57
3:A:90:VAL:HG23	4:B:143:ARG:HD2	1.86	0.57
5:C:186:TYR:O	5:C:212:ASN:ND2	2.37	0.57
2:F:883:DC:C2	2:F:884:DT:C5	2.93	0.57
3:A:23:GLN:HG3	3:A:133:PRO:HG3	1.86	0.57
3:A:349:LEU:HG	3:A:383:TRP:HZ2	1.68	0.57
5:C:124:GLN:HE22	5:C:131:SER:HB2	1.70	0.57
5:C:140:TYR:CB	5:C:141:PRO:HD3	2.34	0.57
3:A:31:ILE:HG23	3:A:133:PRO:O	2.03	0.57
3:A:46:LYS:HD3	3:A:116:PHE:CD2	2.40	0.57
3:A:167:ILE:HG23	3:A:212:TRP:CD1	2.40	0.57
2:F:896:DG:H2'	2:F:897:DC:H5'	1.84	0.57
3:A:132:ILE:HG23	3:A:142:ILE:HB	1.87	0.57
5:C:19:VAL:HG23	5:C:78:LEU:HG	1.86	0.57
5:C:45:LYS:HE3	5:C:55:HIS:CE1	2.40	0.57
2:F:897:DC:C2'	2:F:898:DT:O5'	2.53	0.57
3:A:370:GLU:OE1	3:A:370:GLU:HA	2.04	0.57
6:D:134:LEU:HD21	6:D:151:LEU:HB2	1.86	0.57
3:A:55:PRO:HD2	3:A:56:TYR:CD1	2.40	0.57
4:B:393:ILE:HD13	4:B:398:TRP:HB2	1.86	0.57
4:B:46:LYS:HD3	4:B:116:PHE:CE1	2.40	0.57
3:A:244:ILE:HG13	3:A:271:TYR:CE2	2.38	0.56
4:B:146:TYR:CD2	4:B:150:PRO:HB3	2.40	0.56
4:B:282:LEU:C	4:B:282:LEU:HD23	2.25	0.56
1:E:866:U:C2'	1:E:867:A:O4'	2.53	0.56
5:C:204:PRO:O	5:C:206:VAL:HG13	2.05	0.56
5:C:3:GLN:N	5:C:26:SER:HB2	2.18	0.56
5:C:149:ALA:CB	5:C:153:SER:HA	2.30	0.56
6:D:38:TRP:CE2	6:D:82:LEU:HB2	2.40	0.56
6:D:62:ASN:HD22	6:D:65:LEU:H	1.52	0.56
3:A:149:LEU:HD13	3:A:156:SER:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:416:PHE:N	4:B:416:PHE:CD1	2.73	0.56
5:C:161:ASN:N	5:C:161:ASN:OD1	2.38	0.56
6:D:128:PRO:HG3	6:D:212:SER:HB2	1.86	0.56
6:D:198:TRP:HZ2	6:D:220:ILE:HG12	1.71	0.56
2:F:882:DT:H2"	2:F:883:DC:H5'	1.87	0.56
3:A:420:PRO:HD2	3:A:422:LEU:HG	1.86	0.56
4:B:170:PRO:HB2	4:B:208:HIS:HE1	1.70	0.56
3:A:482:ILE:O	3:A:486:LEU:HG	2.06	0.56
4:B:153:TRP:O	4:B:155:GLY:N	2.38	0.56
4:B:261:VAL:O	4:B:265:ASN:HB3	2.06	0.56
4:B:230:MET:HE2	6:D:103:THR:O	2.05	0.56
3:A:274:ILE:HG23	3:A:306:ASN:HD21	1.69	0.56
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.87	0.56
4:B:282:LEU:HD23	4:B:282:LEU:O	2.06	0.56
5:C:144:ILE:HB	5:C:198:HIS:CD2	2.41	0.56
3:A:90:VAL:O	3:A:90:VAL:HG13	2.05	0.56
3:A:542:ILE:HG21	4:B:261:VAL:HG11	1.88	0.56
4:B:46:LYS:O	4:B:148:VAL:HG22	2.05	0.56
5:C:34:ASN:ND2	6:D:109:ALA:HB2	2.21	0.56
5:C:86:TYR:O	5:C:101:GLY:CA	2.53	0.56
2:F:895:DG:H2"	2:F:896:DG:O5'	2.04	0.56
3:A:88:TRP:HZ3	3:A:90:VAL:HA	1.71	0.56
3:A:319:TYR:HD1	3:A:343:GLN:HE21	1.53	0.56
4:B:175:ASN:HB3	4:B:178:ILE:HD12	1.87	0.56
4:B:224:GLU:HG3	5:C:94:PHE:CE2	2.41	0.56
4:B:276:VAL:O	4:B:276:VAL:HG23	2.06	0.56
6:D:53:ILE:CG1	6:D:71:VAL:HB	2.36	0.56
6:D:143:ASN:O	6:D:195:SER:HB3	2.05	0.56
1:E:860:A:O2'	1:E:861:C:H5'	2.06	0.55
3:A:329:ILE:HD13	3:A:368:LEU:CD1	2.35	0.55
3:A:434:ILE:HD12	3:A:435:VAL:N	2.21	0.55
2:F:892:DA:C2	2:F:893:DG:C6	2.94	0.55
4:B:10:VAL:HA	4:B:85:GLN:OE1	2.06	0.55
4:B:325:LEU:HB3	4:B:387:PRO:HA	1.88	0.55
5:C:193:THR:HG23	5:C:208:SER:OG	2.06	0.55
6:D:107:ASP:OD1	6:D:107:ASP:N	2.40	0.55
4:B:54:ASN:HD21	4:B:126:LYS:CB	2.18	0.55
4:B:170:PRO:HB2	4:B:208:HIS:CE1	2.41	0.55
5:C:31:SER:OG	5:C:50:TYR:CE1	2.57	0.55
6:D:65:LEU:CB	6:D:69:LEU:HD23	2.35	0.55
5:C:119:PRO:HB3	5:C:209:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:TYR:CD2	3:A:310:LEU:HD23	2.42	0.55
4:B:19:PRO:HB2	4:B:57:ASN:O	2.07	0.55
6:D:27:PHE:CE1	6:D:99:GLN:HG3	2.42	0.55
4:B:56:TYR:CZ	4:B:127:TYR:HE2	2.24	0.55
4:B:195:ILE:HD11	4:B:199:ARG:HE	1.72	0.55
4:B:341:ILE:O	4:B:349:LEU:HD12	2.06	0.55
5:C:85:THR:HG22	5:C:103:LYS:HG3	1.88	0.55
3:A:10:VAL:HG21	3:A:153:TRP:HZ2	1.71	0.55
6:D:157:PRO:C	6:D:159:PRO:HD2	2.27	0.55
2:F:881:DT:H1'	2:F:882:DT:H5"	1.89	0.55
3:A:38:CYS:SG	3:A:130:PHE:HE1	2.30	0.55
6:D:40:ARG:CB	6:D:50:LEU:HD11	2.26	0.55
6:D:10:GLY:HA2	6:D:118:SER:O	2.07	0.55
1:E:867:A:C2	2:F:888:DA:C2	2.95	0.55
4:B:2:ILE:HD11	4:B:119:PRO:HB3	1.89	0.55
1:E:862:U:H4'	3:A:284:ARG:HA	1.89	0.54
4:B:271:TYR:HB2	4:B:274:ILE:HD11	1.89	0.54
6:D:71:VAL:HG12	6:D:82:LEU:HD22	1.89	0.54
3:A:260:LEU:O	3:A:264:LEU:HG	2.06	0.54
2:F:894:DT:H1'	3:A:258:GLN:NE2	2.23	0.54
3:A:86:ASP:HA	3:A:154:LYS:HZ1	1.72	0.54
3:A:378:GLU:O	3:A:382:ILE:HG12	2.07	0.54
3:A:410:TRP:CG	3:A:411:ILE:N	2.75	0.54
6:D:42:PRO:CG	6:D:45:LYS:HD2	2.34	0.54
3:A:535:TRP:CH2	3:A:537:PRO:HG3	2.43	0.54
4:B:320:ASP:OD2	4:B:322:SER:HB3	2.07	0.54
6:D:176:PHE:HB3	6:D:177:PRO:HD2	1.89	0.54
3:A:519:ASN:O	3:A:522:ILE:HB	2.08	0.54
4:B:264:LEU:HG	4:B:276:VAL:CG1	2.37	0.54
3:A:393:ILE:HD11	3:A:397:THR:HB	1.88	0.54
6:D:2:ILE:HD13	6:D:112:HIS:CE1	2.43	0.54
1:E:871:G:O2'	1:E:872:A:H5'	2.08	0.54
2:F:895:DG:C2	2:F:896:DG:C5	2.96	0.54
3:A:479:LEU:O	3:A:482:ILE:HB	2.08	0.54
4:B:46:LYS:HD3	4:B:116:PHE:CD1	2.43	0.54
4:B:209:LEU:HD22	4:B:215:THR:CG2	2.36	0.54
4:B:281:LYS:HE3	4:B:284:ARG:NH1	2.23	0.54
4:B:372:VAL:HG13	4:B:389:PHE:CE2	2.42	0.54
6:D:62:ASN:HD21	6:D:64:SER:CB	2.21	0.54
6:D:94:ILE:HA	6:D:117:THR:O	2.07	0.54
3:A:38:CYS:HG	3:A:130:PHE:HE1	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:390:LYS:HB3	3:A:417:VAL:CG2	2.37	0.54
4:B:23:GLN:OE1	4:B:59:PRO:HA	2.08	0.54
4:B:349:LEU:O	4:B:350:LYS:HB2	2.08	0.54
5:C:2:ILE:HG13	5:C:90:GLN:CD	2.28	0.54
5:C:148:TRP:HE1	5:C:177:SER:HG	1.56	0.54
1:E:868:A:H2'	1:E:869:A:N9	2.21	0.53
3:A:242:GLN:N	3:A:243:PRO:HD2	2.24	0.53
2:F:887:DT:C2'	2:F:888:DA:OP2	2.54	0.53
3:A:522:ILE:HG22	3:A:526:ILE:HD11	1.90	0.53
3:A:85:GLN:HG2	3:A:86:ASP:N	2.24	0.53
3:A:107:THR:HB	3:A:189:VAL:HG23	1.91	0.53
3:A:479:LEU:HD21	3:A:518:VAL:HG22	1.91	0.53
4:B:389:PHE:HB3	4:B:391:LEU:HD23	1.89	0.53
3:A:105:SER:HB2	3:A:198:HIS:CD2	2.43	0.53
3:A:398:TRP:NE1	3:A:402:TRP:HD1	2.07	0.53
4:B:94:ILE:HG22	4:B:94:ILE:O	2.07	0.53
6:D:140:ALA:HB1	6:D:141:GLN:NE2	2.24	0.53
1:E:867:A:C2'	1:E:868:A:O4'	2.49	0.53
4:B:224:GLU:O	4:B:227:PHE:CE2	2.60	0.53
3:A:156:SER:N	3:A:157:PRO:HD2	2.23	0.53
3:A:405:TYR:CE2	3:A:407:GLN:HB3	2.43	0.53
5:C:81:GLU:CD	5:C:81:GLU:H	2.10	0.53
3:A:11:LYS:O	3:A:85:GLN:HB3	2.09	0.53
3:A:221:HIS:NE2	3:A:228:LEU:HG	2.23	0.53
3:A:250:ASP:C	3:A:252:TRP:N	2.62	0.53
4:B:296:THR:HG22	4:B:298:GLU:HB2	1.91	0.53
3:A:239:TRP:CH2	3:A:270:ILE:HG12	2.44	0.53
4:B:172:LYS:HG3	4:B:180:ILE:HD12	1.91	0.53
4:B:72:ARG:HH22	4:B:409:THR:HB	1.73	0.53
5:C:159:VAL:CG2	5:C:179:LEU:HD12	2.39	0.53
1:E:860:A:H4'	3:A:265:ASN:HD21	1.73	0.52
5:C:144:ILE:HB	5:C:198:HIS:HD2	1.74	0.52
6:D:62:ASN:ND2	6:D:64:SER:N	2.56	0.52
3:A:289:LEU:HD12	3:A:290:THR:N	2.24	0.52
3:A:179:VAL:O	3:A:189:VAL:HA	2.09	0.52
5:C:35:TRP:O	5:C:47:LEU:HB2	2.09	0.52
5:C:95:PRO:O	5:C:97:THR:HG23	2.09	0.52
5:C:140:TYR:CB	5:C:141:PRO:CD	2.87	0.52
3:A:44:GLU:C	3:A:46:LYS:H	2.13	0.52
3:A:86:ASP:HA	3:A:154:LYS:NZ	2.23	0.52
3:A:319:TYR:CD2	3:A:383:TRP:HD1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:407:GLN:OE1	4:B:418:ASN:HB3	2.09	0.52
3:A:418:ASN:HD21	3:A:422:LEU:HD11	1.71	0.52
4:B:55:PRO:HG2	4:B:56:TYR:CD2	2.45	0.52
6:D:206:ASN:ND2	6:D:206:ASN:H	2.08	0.52
6:D:219:LYS:HD2	6:D:219:LYS:O	2.09	0.52
3:A:50:ILE:HD11	3:A:144:TYR:O	2.09	0.52
3:A:415:GLU:HG2	3:A:416:PHE:N	2.18	0.52
3:A:442:VAL:HG12	3:A:443:ASP:N	2.24	0.52
4:B:12:LEU:HD12	4:B:12:LEU:N	2.19	0.52
4:B:389:PHE:CB	4:B:391:LEU:HD21	2.39	0.52
3:A:188:TYR:HE1	3:A:234:LEU:HD13	1.74	0.52
3:A:194:GLU:HG2	3:A:196:GLY:H	1.75	0.52
3:A:478:GLU:O	3:A:482:ILE:HG12	2.09	0.52
4:B:210:LEU:C	4:B:212:TRP:H	2.12	0.52
5:C:79:GLU:CG	5:C:80:PRO:HD2	2.40	0.52
3:A:114:ALA:HB1	3:A:160:PHE:CE1	2.45	0.52
3:A:253:THR:HG22	3:A:255:ASN:N	2.23	0.52
3:A:529:GLU:OE1	3:A:529:GLU:HA	2.10	0.52
1:E:874:A:O2'	1:E:875:A:H5'	2.09	0.52
4:B:172:LYS:HG2	4:B:180:ILE:HD12	1.90	0.52
1:E:874:A:H2'	1:E:875:A:O4'	2.09	0.52
3:A:454:LYS:HA	3:A:468:PRO:HA	1.91	0.52
6:D:42:PRO:HA	6:D:93:ALA:CB	2.40	0.52
6:D:61:TYR:CZ	6:D:71:VAL:HG22	2.45	0.52
6:D:169:LEU:HD22	6:D:191:VAL:HG21	1.90	0.52
2:F:882:DT:C1'	2:F:883:DC:H5'	2.40	0.52
3:A:10:VAL:HG21	3:A:153:TRP:CZ2	2.44	0.51
3:A:38:CYS:SG	3:A:130:PHE:CE1	3.01	0.51
3:A:76:ASP:OD1	3:A:78:ARG:HB2	2.10	0.51
3:A:88:TRP:HD1	4:B:55:PRO:O	1.93	0.51
3:A:109:LEU:HD21	3:A:202:ILE:CG2	2.40	0.51
3:A:443:ASP:OD1	3:A:444:GLY:N	2.41	0.51
4:B:223:LYS:CG	4:B:224:GLU:H	2.07	0.51
6:D:209:HIS:NE2	6:D:211:ALA:HB3	2.24	0.51
3:A:66:LYS:HG2	3:A:67:ASP:N	2.25	0.51
3:A:167:ILE:HG23	3:A:212:TRP:CG	2.45	0.51
4:B:12:LEU:HB3	4:B:83:ARG:O	2.10	0.51
6:D:141:GLN:HE21	6:D:141:GLN:N	2.09	0.51
2:F:895:DG:C2'	2:F:896:DG:O5'	2.58	0.51
3:A:178:ILE:HD12	3:A:178:ILE:H	1.75	0.51
3:A:337:TRP:CZ2	3:A:367:GLN:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:453:GLY:O	3:A:469:LEU:N	2.42	0.51
3:A:548:VAL:O	3:A:552:VAL:HG23	2.10	0.51
3:A:188:TYR:CD2	3:A:188:TYR:C	2.84	0.51
3:A:363:ASN:HB3	3:A:511:ASP:H	1.76	0.51
4:B:125:ARG:O	4:B:145:GLN:HG2	2.11	0.51
2:F:888:DA:C2	2:F:889:DA:C4	2.97	0.51
2:F:894:DT:C2'	2:F:895:DG:C5'	2.89	0.51
3:A:11:LYS:HB2	3:A:11:LYS:NZ	2.25	0.51
5:C:12:SER:OG	5:C:107:LYS:HD3	2.10	0.51
6:D:45:LYS:HG2	6:D:46:GLY:H	1.76	0.51
1:E:854:U:O2'	1:E:855:C:OP2	2.29	0.51
3:A:246:LEU:HD23	3:A:263:LYS:HG2	1.93	0.51
3:A:439:THR:HB	4:B:289:LEU:HB2	1.92	0.51
4:B:163:SER:HA	4:B:166:LYS:HD3	1.92	0.51
5:C:66:GLY:CA	5:C:71:TYR:HA	2.40	0.51
6:D:61:TYR:OH	6:D:71:VAL:HG22	2.10	0.51
3:A:493:VAL:CG1	3:A:495:ILE:HD11	2.41	0.50
4:B:386:THR:HG23	4:B:387:PRO:HD2	1.92	0.50
1:E:870:A:H2'	1:E:871:G:O4'	2.11	0.50
4:B:28:GLU:O	4:B:31:ILE:N	2.45	0.50
4:B:286:THR:HG22	4:B:286:THR:O	2.12	0.50
2:F:891:DA:H2"	2:F:892:DA:O5'	2.11	0.50
3:A:406:TRP:O	4:B:331:LYS:HB3	2.12	0.50
4:B:227:PHE:CE2	6:D:102:ILE:HG12	2.46	0.50
6:D:161:THR:OG1	6:D:208:ALA:HB3	2.12	0.50
6:D:164:TRP:O	6:D:165:ASN:HB2	2.11	0.50
3:A:125:ARG:C	3:A:127:TYR:H	2.13	0.50
3:A:199:ARG:HA	3:A:202:ILE:HG12	1.93	0.50
4:B:253:THR:HG23	4:B:256:ASP:OD2	2.12	0.50
4:B:369:THR:HA	4:B:398:TRP:HH2	1.74	0.50
5:C:33:LEU:HD11	5:C:88:CYS:SG	2.51	0.50
6:D:162:VAL:HG21	6:D:189:SER:CB	2.41	0.50
6:D:164:TRP:CH2	6:D:205:CYS:HB2	2.47	0.50
4:B:421:PRO:O	4:B:424:LYS:HG3	2.11	0.50
5:C:139:PHE:CZ	5:C:144:ILE:HG21	2.47	0.50
6:D:37:THR:HG22	6:D:38:TRP:N	2.27	0.50
6:D:147:THR:HA	6:D:192:THR:HA	1.93	0.50
2:F:880:DT:C2	2:F:881:DT:C4	3.00	0.50
3:A:66:LYS:CG	3:A:67:ASP:H	2.24	0.50
3:A:96:HIS:CG	3:A:97:PRO:HD2	2.47	0.50
4:B:54:ASN:HD21	4:B:126:LYS:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:39:ILE:HG22	6:D:40:ARG:N	2.27	0.50
6:D:53:ILE:CD1	6:D:71:VAL:HB	2.42	0.50
1:E:859:C:H2'	1:E:860:A:H8	1.75	0.50
1:E:873:A:C4	1:E:874:A:C8	2.99	0.50
3:A:149:LEU:HD11	3:A:159:ILE:HB	1.93	0.50
3:A:381:VAL:HG12	3:A:382:ILE:HD13	1.94	0.50
4:B:266:TRP:CD1	4:B:422:LEU:HD21	2.46	0.50
2:F:894:DT:C2	2:F:895:DG:C8	2.99	0.50
3:A:434:ILE:HG23	3:A:494:ASN:HD22	1.77	0.50
3:A:277:ARG:HB2	3:A:336:GLN:HE21	1.77	0.49
3:A:493:VAL:HG13	3:A:495:ILE:CD1	2.41	0.49
5:C:124:GLN:HE21	6:D:132:TYR:HD2	1.59	0.49
3:A:271:TYR:CE2	3:A:310:LEU:HD23	2.47	0.49
3:A:334:GLN:O	3:A:334:GLN:NE2	2.45	0.49
3:A:494:ASN:HB3	4:B:289:LEU:HD23	1.94	0.49
4:B:135:ILE:HG13	4:B:135:ILE:O	2.11	0.49
4:B:325:LEU:HD12	4:B:343:GLN:HG2	1.94	0.49
6:D:40:ARG:HD2	6:D:95:TYR:OH	2.12	0.49
1:E:872:A:H2'	1:E:873:A:C8	2.48	0.49
3:A:63:ILE:HG23	3:A:63:ILE:O	2.12	0.49
3:A:254:VAL:O	3:A:257:ILE:HB	2.13	0.49
3:A:365:VAL:HG21	3:A:425:LEU:HG	1.94	0.49
4:B:194:GLU:HG3	4:B:197:GLN:HB2	1.95	0.49
4:B:339:TYR:CG	4:B:375:ILE:HG12	2.47	0.49
3:A:57:ASN:HA	3:A:129:ALA:O	2.12	0.49
5:C:134:CYS:HB3	5:C:148:TRP:CZ2	2.47	0.49
5:C:148:TRP:CE3	5:C:179:LEU:HD13	2.47	0.49
6:D:5:LYS:HB2	6:D:5:LYS:HZ3	1.77	0.49
3:A:229:TRP:CE3	3:A:234:LEU:HD11	2.47	0.49
4:B:42:GLU:C	4:B:45:GLY:H	2.16	0.49
4:B:64:LYS:HB2	4:B:71:TRP:CZ3	2.48	0.49
5:C:138:ASN:OD1	6:D:174:HIS:HE1	1.94	0.49
4:B:212:TRP:HD1	4:B:213:GLY:N	2.11	0.49
3:A:442:VAL:HG12	3:A:443:ASP:H	1.77	0.49
5:C:47:LEU:O	5:C:48:ILE:HG23	2.12	0.49
3:A:402:TRP:HE3	4:B:331:LYS:HZ1	1.60	0.49
2:F:881:DT:C5	2:F:882:DT:H73	2.48	0.49
2:F:882:DT:H2"	2:F:883:DC:OP2	2.12	0.49
2:F:883:DC:C5	2:F:884:DT:H72	2.44	0.49
2:F:892:DA:H2"	2:F:893:DG:O5'	2.13	0.49
3:A:274:ILE:HG23	3:A:306:ASN:CG	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:279:LEU:O	3:A:283:LEU:HD12	2.12	0.49
4:B:113:ASP:C	4:B:115:TYR:H	2.15	0.49
6:D:2:ILE:O	6:D:3:THR:HG23	2.13	0.49
6:D:129:PRO:HB3	6:D:155:TYR:HB3	1.94	0.49
3:A:218:ASP:C	3:A:220:LYS:H	2.16	0.49
3:A:273:GLY:HA2	3:A:338:THR:CG2	2.42	0.49
3:A:329:ILE:HD11	3:A:337:TRP:CE3	2.48	0.49
3:A:329:ILE:CG2	3:A:392:PRO:HD3	2.37	0.49
4:B:169:GLU:HG3	4:B:170:PRO:HD3	1.95	0.49
6:D:21:THR:HG23	6:D:81:PHE:HE2	1.75	0.49
2:F:894:DT:H1'	3:A:258:GLN:HE22	1.77	0.48
4:B:114:ALA:HB2	4:B:215:THR:CG2	2.34	0.48
4:B:271:TYR:CB	4:B:274:ILE:HD11	2.42	0.48
5:C:81:GLU:OE1	5:C:81:GLU:N	2.46	0.48
6:D:204:THR:HB	6:D:218:LYS:O	2.12	0.48
3:A:84:THR:CG2	3:A:153:TRP:HE1	2.26	0.48
3:A:106:VAL:O	3:A:227:PHE:CZ	2.66	0.48
3:A:419:THR:N	3:A:420:PRO:CD	2.75	0.48
4:B:96:HIS:HD2	4:B:181:TYR:CE1	2.32	0.48
3:A:244:ILE:HD11	3:A:310:LEU:HB3	1.94	0.48
3:A:319:TYR:HB2	3:A:349:LEU:HD21	1.95	0.48
3:A:325:LEU:HD22	3:A:349:LEU:HD23	1.95	0.48
4:B:26:LEU:HD11	4:B:60:VAL:O	2.13	0.48
4:B:402:TRP:HH2	4:B:411:ILE:HD13	1.78	0.48
6:D:2:ILE:HA	6:D:25:SER:O	2.12	0.48
6:D:22:CYS:O	6:D:80:ALA:N	2.41	0.48
3:A:128:THR:HB	3:A:146:TYR:HD1	1.78	0.48
3:A:158:ALA:O	3:A:161:GLN:N	2.46	0.48
4:B:307:ARG:HG3	4:B:307:ARG:HH11	1.77	0.48
6:D:27:PHE:HD2	6:D:34:ILE:HG21	1.79	0.48
6:D:65:LEU:HD22	6:D:68:ARG:HH12	1.78	0.48
3:A:126:LYS:HA	3:A:145:GLN:NE2	2.28	0.48
3:A:329:ILE:CD1	3:A:368:LEU:HD12	2.40	0.48
4:B:169:GLU:O	4:B:173:LYS:HB2	2.13	0.48
5:C:195:ALA:HB1	5:C:206:VAL:HG12	1.93	0.48
3:A:116:PHE:HA	3:A:148:VAL:HG21	1.95	0.48
4:B:387:PRO:HG2	4:B:389:PHE:HE1	1.78	0.48
5:C:140:TYR:CG	5:C:141:PRO:CD	2.90	0.48
3:A:171:PHE:CZ	3:A:205:LEU:HB2	2.49	0.48
3:A:417:VAL:HG12	3:A:418:ASN:N	2.29	0.48
4:B:366:LYS:HG2	4:B:370:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:865:U:N3	1:E:866:U:C4	2.82	0.48
3:A:361:HIS:CD2	3:A:505:ILE:HD13	2.48	0.48
2:F:894:DT:H2"	2:F:895:DG:O5'	2.14	0.48
3:A:459:THR:O	4:B:286:THR:HG21	2.14	0.48
4:B:17:ASP:O	4:B:18:GLY:O	2.31	0.48
4:B:376:THR:HB	4:B:410:TRP:CH2	2.48	0.48
4:B:414:TRP:O	4:B:414:TRP:CD1	2.67	0.48
3:A:224:GLU:O	3:A:227:PHE:CE1	2.67	0.47
3:A:267:ALA:HB1	3:A:271:TYR:HD2	1.78	0.47
4:B:146:TYR:CE2	4:B:150:PRO:HB3	2.49	0.47
4:B:417:VAL:HG12	4:B:418:ASN:N	2.28	0.47
5:C:46:LEU:HD22	6:D:111:ASP:HA	1.96	0.47
6:D:29:LEU:CD1	6:D:73:LYS:HG3	2.43	0.47
6:D:45:LYS:HD3	6:D:46:GLY:O	2.14	0.47
2:F:881:DT:C4	2:F:882:DT:H73	2.49	0.47
2:F:884:DT:C2	2:F:885:DT:C7	2.97	0.47
3:A:407:GLN:NE2	4:B:394:GLN:HG2	2.29	0.47
5:C:2:ILE:HG13	5:C:90:GLN:OE1	2.14	0.47
3:A:475:GLN:OE1	3:A:475:GLN:N	2.46	0.47
6:D:58:ASP:CG	6:D:58:ASP:O	2.50	0.47
3:A:519:ASN:HA	3:A:522:ILE:HD12	1.96	0.47
4:B:368:LEU:O	4:B:371:ALA:HB3	2.14	0.47
4:B:419:THR:HG21	4:B:423:VAL:HG11	1.95	0.47
5:C:111:ALA:O	5:C:139:PHE:HA	2.14	0.47
3:A:46:LYS:HE2	3:A:116:PHE:HB3	1.97	0.47
3:A:114:ALA:HB1	3:A:160:PHE:CZ	2.49	0.47
4:B:279:LEU:HD21	4:B:303:LEU:HD13	1.95	0.47
5:C:150:ILE:O	5:C:151:ASP:C	2.53	0.47
5:C:161:ASN:HB2	5:C:163:TRP:HZ3	1.74	0.47
6:D:140:ALA:C	6:D:141:GLN:HE21	2.18	0.47
4:B:12:LEU:HD11	4:B:127:TYR:CZ	2.48	0.47
4:B:236:PRO:HA	4:B:239:TRP:CD2	2.49	0.47
6:D:32:SER:O	6:D:55:TRP:CE2	2.67	0.47
1:E:857:G:C5'	3:A:89:GLU:HG3	2.45	0.47
3:A:46:LYS:NZ	3:A:116:PHE:HD2	2.10	0.47
3:A:54:ASN:ND2	3:A:56:TYR:CD1	2.79	0.47
3:A:86:ASP:C	3:A:87:PHE:HD2	2.18	0.47
3:A:183:TYR:CD1	3:A:230:MET:SD	3.08	0.47
3:A:277:ARG:HG3	3:A:336:GLN:NE2	2.30	0.47
3:A:368:LEU:O	3:A:371:ALA:HB3	2.14	0.47
4:B:119:PRO:HA	4:B:148:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:131:THR:CG2	4:B:143:ARG:HG2	2.44	0.47
4:B:260:LEU:O	4:B:264:LEU:HB2	2.13	0.47
6:D:27:PHE:CD2	6:D:34:ILE:HG21	2.49	0.47
6:D:41:GLN:NE2	6:D:96:TYR:OH	2.47	0.47
1:E:858:C:C4'	3:A:93:GLY:HA2	2.39	0.47
2:F:897:DC:H2'	2:F:898:DT:O5'	2.13	0.47
3:A:132:ILE:CG2	3:A:142:ILE:HB	2.45	0.47
3:A:253:THR:CG2	3:A:255:ASN:H	2.28	0.47
3:A:279:LEU:HD23	3:A:282:LEU:CD1	2.43	0.47
3:A:63:ILE:HG13	3:A:65:LYS:HD3	1.97	0.47
3:A:85:GLN:O	3:A:154:LYS:NZ	2.48	0.47
3:A:325:LEU:HD11	3:A:383:TRP:CG	2.50	0.47
3:A:395:LYS:HG2	3:A:416:PHE:HD2	1.80	0.47
3:A:527:LYS:CG	3:A:528:LYS:N	2.78	0.47
6:D:156:PHE:O	6:D:185:TYR:CE2	2.68	0.47
1:E:873:A:C2	1:E:874:A:N9	2.83	0.46
3:A:81:ASN:HA	3:A:84:THR:OG1	2.14	0.46
6:D:55:TRP:CG	6:D:56:ASP:N	2.83	0.46
4:B:199:ARG:NH1	4:B:230:MET:SD	2.85	0.46
5:C:134:CYS:HB3	5:C:148:TRP:HZ2	1.79	0.46
6:D:39:ILE:CG2	6:D:40:ARG:N	2.79	0.46
3:A:246:LEU:HD11	3:A:310:LEU:HD13	1.97	0.46
1:E:858:C:H4'	3:A:93:GLY:CA	2.40	0.46
2:F:895:DG:C2'	2:F:896:DG:C8	2.90	0.46
3:A:10:VAL:HG11	3:A:153:TRP:HH2	1.81	0.46
3:A:210:LEU:HA	3:A:214:LEU:H	1.81	0.46
4:B:210:LEU:C	4:B:212:TRP:N	2.69	0.46
6:D:18:PHE:CE1	6:D:20:LEU:HD21	2.50	0.46
6:D:53:ILE:HG12	6:D:71:VAL:HB	1.97	0.46
3:A:164:MET:HE1	3:A:168:LEU:HD11	1.97	0.46
3:A:339:TYR:CZ	3:A:352:GLY:HA3	2.50	0.46
4:B:111:VAL:HG21	4:B:187:LEU:HD13	1.96	0.46
4:B:186:ASP:OD1	4:B:409:THR:HG21	2.15	0.46
3:A:44:GLU:O	3:A:46:LYS:HG3	2.15	0.46
3:A:526:ILE:HG22	3:A:526:ILE:O	2.16	0.46
4:B:8:VAL:HG11	4:B:159:ILE:HG23	1.98	0.46
4:B:96:HIS:HD2	4:B:181:TYR:CZ	2.33	0.46
6:D:62:ASN:HD22	6:D:65:LEU:N	2.13	0.46
6:D:65:LEU:HD22	6:D:68:ARG:HH11	1.78	0.46
3:A:61:PHE:CD1	3:A:61:PHE:N	2.83	0.46
3:A:178:ILE:HD12	3:A:178:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:378:GLU:O	3:A:378:GLU:HG2	2.16	0.46
4:B:30:LYS:O	4:B:34:LEU:HB2	2.16	0.46
4:B:103:LYS:HA	4:B:192:ASP:OD1	2.16	0.46
4:B:223:LYS:HE3	6:D:60:ARG:NH2	2.15	0.46
3:A:4:PRO:HD2	3:A:212:TRP:O	2.15	0.46
3:A:50:ILE:HD11	3:A:144:TYR:C	2.35	0.46
3:A:111:VAL:HG11	3:A:214:LEU:HB3	1.98	0.46
3:A:149:LEU:HD22	3:A:153:TRP:CZ3	2.51	0.46
3:A:479:LEU:CD2	3:A:518:VAL:HG22	2.46	0.46
4:B:169:GLU:HG3	4:B:170:PRO:CD	2.46	0.46
4:B:404:GLU:O	4:B:405:TYR:CD1	2.69	0.46
5:C:125:LEU:C	5:C:127:SER:H	2.19	0.46
1:E:854:U:H5'	3:A:152:GLY:HA3	1.97	0.46
2:F:881:DT:C2'	2:F:882:DT:OP2	2.61	0.46
2:F:887:DT:C2	2:F:888:DA:C8	3.03	0.46
3:A:249:LYS:C	3:A:251:SER:H	2.19	0.46
4:B:422:LEU:C	4:B:424:LYS:H	2.19	0.46
3:A:495:ILE:HD12	3:A:495:ILE:N	2.31	0.46
4:B:337:TRP:HB2	4:B:354:TYR:HB3	1.97	0.46
4:B:384:GLY:O	4:B:385:LYS:HD3	2.15	0.46
5:C:200:THR:OG1	5:C:201:SER:N	2.48	0.45
2:F:895:DG:N3	2:F:896:DG:C8	2.84	0.45
3:A:98:ALA:O	3:A:383:TRP:NE1	2.48	0.45
3:A:103:LYS:NZ	3:A:179:VAL:HG21	2.31	0.45
4:B:340:GLN:HG3	4:B:351:THR:HG22	1.98	0.45
4:B:424:LYS:HD3	4:B:424:LYS:C	2.36	0.45
3:A:222:GLN:HG2	3:A:223:LYS:N	2.31	0.45
4:B:97:PRO:HD2	4:B:181:TYR:CD1	2.52	0.45
4:B:319:TYR:HE1	4:B:325:LEU:CD1	2.29	0.45
5:C:20:THR:HA	5:C:73:LEU:O	2.16	0.45
6:D:53:ILE:HG12	6:D:71:VAL:HG21	1.98	0.45
4:B:103:LYS:NZ	4:B:177:ASP:O	2.50	0.45
4:B:205:LEU:O	4:B:205:LEU:HD12	2.17	0.45
5:C:108:ARG:HG2	5:C:109:ALA:N	2.31	0.45
5:C:140:TYR:HB3	5:C:141:PRO:HD3	1.98	0.45
6:D:39:ILE:HD11	6:D:110:MET:CE	2.45	0.45
3:A:60:VAL:HG23	3:A:74:LEU:O	2.16	0.45
3:A:498:ASP:HA	3:A:536:VAL:O	2.17	0.45
4:B:2:ILE:HD12	4:B:2:ILE:N	2.32	0.45
4:B:125:ARG:HD3	4:B:146:TYR:O	2.17	0.45
4:B:224:GLU:HB2	4:B:225:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:242:GLN:CG	4:B:242:GLN:O	2.65	0.45
4:B:338:THR:HA	4:B:353:LYS:HA	1.97	0.45
5:C:96:TRP:O	6:D:49:TRP:HB3	2.16	0.45
5:C:174:SER:O	6:D:176:PHE:CE2	2.70	0.45
3:A:34:LEU:HB2	3:A:132:ILE:CD1	2.46	0.45
3:A:429:LEU:HD12	3:A:533:LEU:HB2	1.99	0.45
4:B:10:VAL:HG23	4:B:124:PHE:CD2	2.51	0.45
4:B:128:THR:OG1	4:B:146:TYR:HB2	2.15	0.45
4:B:254:VAL:HG23	4:B:292:VAL:HB	1.98	0.45
5:C:15:LEU:HD12	5:C:15:LEU:N	2.24	0.45
5:C:122:SER:HA	5:C:125:LEU:HB2	1.98	0.45
5:C:124:GLN:NE2	5:C:131:SER:HB2	2.32	0.45
1:E:854:U:C4'	3:A:152:GLY:HA2	2.47	0.45
3:A:420:PRO:HG2	3:A:422:LEU:HA	1.99	0.45
3:A:439:THR:CG2	4:B:289:LEU:H	2.06	0.45
4:B:229:TRP:CZ3	4:B:230:MET:SD	3.10	0.45
5:C:66:GLY:HA3	5:C:71:TYR:HD2	1.79	0.45
6:D:175:THR:HG22	6:D:189:SER:OG	2.16	0.45
2:F:894:DT:C2'	2:F:895:DG:H5'	2.44	0.45
4:B:100:LEU:HG	4:B:381:VAL:HG13	1.99	0.45
4:B:166:LYS:O	4:B:170:PRO:HD3	2.17	0.45
4:B:222:GLN:HG3	4:B:229:TRP:CG	2.52	0.45
4:B:402:TRP:CH2	4:B:411:ILE:HD13	2.52	0.45
6:D:148:LEU:HD11	6:D:198:TRP:CD1	2.52	0.45
2:F:878:DC:C1'	2:F:879:DT:H5'	2.46	0.45
4:B:259:LYS:HD3	4:B:259:LYS:HA	1.82	0.45
4:B:281:LYS:HB2	4:B:281:LYS:HZ2	1.81	0.45
5:C:132:VAL:HG12	5:C:148:TRP:CH2	2.51	0.45
6:D:4:LEU:N	6:D:4:LEU:HD23	2.32	0.45
3:A:169:GLU:N	3:A:170:PRO:CD	2.80	0.45
4:B:224:GLU:HA	4:B:227:PHE:HE2	1.77	0.45
4:B:281:LYS:HB2	4:B:281:LYS:HZ3	1.80	0.45
4:B:379:SER:OG	4:B:383:TRP:HZ3	2.00	0.45
5:C:108:ARG:HG2	5:C:109:ALA:H	1.81	0.45
6:D:12:VAL:HG21	6:D:18:PHE:HB3	1.98	0.45
3:A:23:GLN:CD	3:A:133:PRO:HG3	2.37	0.44
3:A:55:PRO:HD2	3:A:56:TYR:CE1	2.53	0.44
3:A:131:THR:O	3:A:133:PRO:HD3	2.17	0.44
3:A:191:SER:OG	3:A:193:LEU:HD23	2.17	0.44
3:A:454:LYS:HG3	3:A:468:PRO:HA	1.99	0.44
5:C:195:ALA:HB2	5:C:206:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:34:ILE:CG2	6:D:35:GLY:H	2.13	0.44
3:A:60:VAL:C	3:A:61:PHE:HD1	2.21	0.44
3:A:259:LYS:O	3:A:263:LYS:HB2	2.17	0.44
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.99	0.44
5:C:34:ASN:ND2	6:D:109:ALA:CB	2.80	0.44
6:D:154:GLY:HA2	6:D:184:LEU:HB3	2.00	0.44
4:B:3:SER:C	4:B:5:ILE:H	2.20	0.44
4:B:99:GLY:HA2	4:B:102:LYS:HB2	1.99	0.44
3:A:33:ALA:O	3:A:37:ILE:HG13	2.17	0.44
3:A:128:THR:CB	3:A:146:TYR:HB2	2.47	0.44
3:A:444:GLY:HA2	3:A:552:VAL:HG11	1.99	0.44
5:C:110:ASP:HA	5:C:140:TYR:HB3	1.99	0.44
6:D:32:SER:O	6:D:55:TRP:CD2	2.71	0.44
6:D:37:THR:HG21	6:D:110:MET:CE	2.47	0.44
6:D:209:HIS:CE1	6:D:212:SER:HB3	2.53	0.44
3:A:8:VAL:CG2	3:A:159:ILE:HG23	2.48	0.44
3:A:325:LEU:HD23	3:A:343:GLN:HG3	2.00	0.44
3:A:357:MET:C	3:A:359:GLY:H	2.20	0.44
3:A:363:ASN:HA	3:A:511:ASP:HB3	1.98	0.44
3:A:398:TRP:CD2	3:A:411:ILE:HD11	2.53	0.44
4:B:28:GLU:O	4:B:29:GLU:C	2.56	0.44
4:B:229:TRP:CH2	4:B:230:MET:SD	3.10	0.44
5:C:34:ASN:OD1	5:C:49:TYR:HA	2.18	0.44
6:D:62:ASN:ND2	6:D:64:SER:H	2.14	0.44
3:A:172:LYS:HG3	3:A:180:ILE:HD12	2.00	0.44
4:B:195:ILE:CD1	4:B:233:GLU:HG2	2.48	0.44
5:C:192:TYR:O	5:C:208:SER:HB3	2.18	0.44
6:D:212:SER:O	6:D:213:SER:HB2	2.18	0.44
1:E:872:A:C2	1:E:873:A:C5	3.05	0.44
3:A:8:VAL:HG21	3:A:159:ILE:HG23	2.00	0.44
3:A:18:GLY:HA3	3:A:56:TYR:CD2	2.52	0.44
3:A:182:GLN:NE2	4:B:139:THR:OG1	2.51	0.44
3:A:228:LEU:HG	3:A:228:LEU:O	2.17	0.44
3:A:325:LEU:CD1	3:A:383:TRP:CD2	3.01	0.44
3:A:365:VAL:CG1	3:A:401:TRP:CE2	3.00	0.44
3:A:523:GLU:HA	3:A:526:ILE:HD12	2.00	0.44
4:B:319:TYR:HE1	4:B:325:LEU:HD13	1.83	0.44
5:C:144:ILE:HG23	5:C:175:MET:CE	2.48	0.44
6:D:21:THR:HG23	6:D:81:PHE:CD2	2.53	0.44
6:D:137:GLY:C	6:D:139:ALA:H	2.20	0.44
2:F:881:DT:H1'	2:F:882:DT:C5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:892:DA:C4	2:F:893:DG:N7	2.86	0.44
3:A:67:ASP:O	3:A:71:TRP:HB3	2.18	0.44
3:A:84:THR:CG2	3:A:153:TRP:NE1	2.78	0.44
3:A:101:LYS:H	3:A:101:LYS:HG2	1.64	0.44
4:B:54:ASN:HD21	4:B:126:LYS:CA	2.30	0.44
3:A:245:VAL:O	3:A:263:LYS:HE2	2.17	0.44
3:A:527:LYS:HB2	3:A:527:LYS:HE3	1.73	0.44
4:B:107:THR:HB	4:B:189:VAL:HG23	1.99	0.44
4:B:181:TYR:HB3	4:B:188:TYR:HB2	2.00	0.44
4:B:224:GLU:O	4:B:225:PRO:C	2.56	0.44
4:B:363:ASN:HB3	4:B:366:LYS:HB3	2.00	0.44
4:B:372:VAL:HG13	4:B:389:PHE:CD2	2.53	0.44
6:D:34:ILE:H	6:D:34:ILE:HG12	1.66	0.44
4:B:195:ILE:HD11	4:B:233:GLU:HG2	2.00	0.43
4:B:379:SER:HA	4:B:383:TRP:CZ3	2.53	0.43
5:C:164:THR:HG23	6:D:176:PHE:CD2	2.53	0.43
4:B:41:MET:O	4:B:46:LYS:N	2.33	0.43
4:B:77:PHE:O	4:B:81:ASN:ND2	2.51	0.43
4:B:253:THR:O	4:B:257:ILE:HG12	2.17	0.43
5:C:166:GLN:HB2	5:C:173:TYR:CZ	2.53	0.43
6:D:4:LEU:CD1	6:D:97:CYS:SG	2.90	0.43
6:D:62:ASN:ND2	6:D:65:LEU:H	2.17	0.43
6:D:92:THR:CB	6:D:121:VAL:HG23	2.47	0.43
3:A:148:VAL:O	3:A:150:PRO:HD3	2.18	0.43
3:A:185:ASP:OD2	3:A:185:ASP:N	2.50	0.43
3:A:293:ILE:HD12	3:A:294:PRO:HD2	2.01	0.43
4:B:395:LYS:CA	4:B:416:PHE:CD2	2.98	0.43
5:C:89:GLN:HG2	5:C:90:GLN:N	2.34	0.43
5:C:122:SER:HA	5:C:125:LEU:HD12	1.99	0.43
6:D:37:THR:CG2	6:D:38:TRP:N	2.81	0.43
3:A:151:GLN:NE2	3:A:151:GLN:N	2.41	0.43
4:B:10:VAL:HG12	4:B:87:PHE:HZ	1.83	0.43
4:B:146:TYR:CE2	4:B:150:PRO:CA	2.98	0.43
5:C:19:VAL:O	5:C:74:THR:HA	2.18	0.43
5:C:108:ARG:O	5:C:140:TYR:CE1	2.71	0.43
2:F:893:DG:C2	2:F:894:DT:C6	3.06	0.43
3:A:337:TRP:HZ2	3:A:367:GLN:HB2	1.82	0.43
3:A:522:ILE:O	3:A:526:ILE:HG13	2.18	0.43
4:B:10:VAL:CG1	4:B:87:PHE:HZ	2.32	0.43
4:B:268:SER:HA	4:B:274:ILE:HG13	1.99	0.43
6:D:160:VAL:CG1	6:D:187:LEU:HD12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:855:C:H5"	3:A:152:GLY:O	2.19	0.43
3:A:16:MET:HB3	3:A:17:ASP:H	1.63	0.43
3:A:81:ASN:O	3:A:84:THR:N	2.52	0.43
3:A:96:HIS:ND1	3:A:97:PRO:CD	2.82	0.43
3:A:115:TYR:H	3:A:115:TYR:HD1	1.66	0.43
3:A:188:TYR:HE1	3:A:234:LEU:CD1	2.32	0.43
3:A:312:GLU:HA	3:A:313:PRO:HD3	1.80	0.43
4:B:17:ASP:O	4:B:17:ASP:CG	2.57	0.43
4:B:160:PHE:CE1	4:B:163:SER:CB	3.01	0.43
4:B:254:VAL:CG2	4:B:292:VAL:HB	2.48	0.43
5:C:78:LEU:HD23	5:C:78:LEU:HA	1.84	0.43
6:D:27:PHE:HB2	6:D:34:ILE:HD12	1.99	0.43
3:A:87:PHE:HE1	3:A:155:GLY:HA3	1.75	0.43
3:A:96:HIS:HE1	3:A:239:TRP:CZ2	2.37	0.43
3:A:121:ASP:O	3:A:124:PHE:N	2.49	0.43
3:A:228:LEU:O	3:A:228:LEU:CG	2.67	0.43
3:A:274:ILE:HG23	3:A:306:ASN:OD1	2.18	0.43
4:B:34:LEU:CD1	4:B:73:LYS:HB3	2.48	0.43
4:B:391:LEU:O	4:B:393:ILE:N	2.51	0.43
5:C:135:PHE:CB	5:C:137:ASN:HD21	2.27	0.43
6:D:113:TRP:N	6:D:113:TRP:CD1	2.86	0.43
2:F:899:DG:H5"	3:A:186:ASP:OD1	2.19	0.43
3:A:249:LYS:O	3:A:251:SER:N	2.52	0.43
4:B:48:SER:N	4:B:147:ASN:ND2	2.67	0.43
4:B:379:SER:CB	4:B:387:PRO:HD3	2.49	0.43
3:A:70:LYS:HA	3:A:70:LYS:HD2	1.49	0.43
4:B:105:SER:O	4:B:190:GLY:HA2	2.18	0.43
4:B:125:ARG:NH1	4:B:147:ASN:OD1	2.52	0.43
4:B:253:THR:HA	4:B:293:ILE:HA	2.00	0.43
6:D:83:ASN:HB3	6:D:85:MET:HE3	2.01	0.43
4:B:178:ILE:CG2	4:B:179:VAL:N	2.82	0.43
4:B:302:GLU:OE1	4:B:302:GLU:HA	2.19	0.43
6:D:193:VAL:HB	6:D:197:THR:OG1	2.19	0.43
2:F:894:DT:C2'	3:A:258:GLN:NE2	2.64	0.42
3:A:81:ASN:O	3:A:83:ARG:N	2.52	0.42
3:A:317:VAL:HG21	3:A:347:LYS:HD3	2.01	0.42
3:A:392:PRO:HB3	3:A:420:PRO:HG3	2.00	0.42
3:A:425:LEU:HD23	3:A:509:GLN:OE1	2.19	0.42
4:B:52:PRO:O	4:B:54:ASN:N	2.51	0.42
4:B:100:LEU:HG	4:B:100:LEU:O	2.19	0.42
4:B:195:ILE:HD11	4:B:199:ARG:NE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:395:LYS:HB2	4:B:416:PHE:CG	2.54	0.42
6:D:38:TRP:HA	6:D:96:TYR:O	2.18	0.42
6:D:40:ARG:HD2	6:D:95:TYR:CZ	2.53	0.42
1:E:855:C:C5'	3:A:152:GLY:O	2.67	0.42
2:F:896:DG:C2'	2:F:897:DC:C5'	2.90	0.42
3:A:96:HIS:ND1	3:A:97:PRO:HD2	2.33	0.42
3:A:349:LEU:HG	3:A:383:TRP:CZ2	2.52	0.42
1:E:866:U:O2'	1:E:867:A:O4'	2.29	0.42
3:A:96:HIS:NE2	3:A:350:LYS:HG3	2.34	0.42
3:A:267:ALA:O	3:A:271:TYR:HB2	2.19	0.42
3:A:280:SER:HA	3:A:283:LEU:HD13	2.01	0.42
4:B:55:PRO:CG	4:B:56:TYR:N	2.81	0.42
4:B:109:LEU:HD11	4:B:206:ARG:HG3	2.01	0.42
4:B:341:ILE:HG22	4:B:349:LEU:CD1	2.50	0.42
6:D:68:ARG:NH2	6:D:84:MET:CG	2.83	0.42
3:A:175:ASN:O	3:A:177:ASP:N	2.52	0.42
3:A:275:LYS:HD2	3:A:336:GLN:CD	2.39	0.42
4:B:32:LYS:O	4:B:35:VAL:N	2.52	0.42
4:B:100:LEU:HD11	4:B:106:VAL:HG21	2.02	0.42
4:B:212:TRP:CD1	4:B:213:GLY:N	2.86	0.42
4:B:368:LEU:O	4:B:372:VAL:HG23	2.19	0.42
2:F:883:DC:C2'	2:F:884:DT:OP2	2.57	0.42
3:A:454:LYS:O	3:A:552:VAL:HG12	2.19	0.42
3:A:536:VAL:CG1	3:A:542:ILE:HB	2.49	0.42
5:C:82:ASP:O	5:C:104:LEU:HD23	2.19	0.42
2:F:890:DA:C2	2:F:891:DA:C5	3.07	0.42
2:F:898:DT:O3'	3:A:230:MET:HA	2.19	0.42
3:A:30:LYS:HB3	3:A:62:ALA:HB2	1.99	0.42
3:A:271:TYR:HA	3:A:272:PRO:HD2	1.89	0.42
3:A:373:GLN:NE2	4:B:397:THR:HG23	2.35	0.42
3:A:402:TRP:HE3	4:B:331:LYS:NZ	2.18	0.42
3:A:543:GLY:HA2	4:B:283:LEU:O	2.20	0.42
4:B:132:ILE:HG22	4:B:133:PRO:O	2.20	0.42
4:B:191:SER:OG	4:B:193:LEU:HG	2.20	0.42
4:B:202:ILE:HD13	4:B:202:ILE:HA	1.91	0.42
4:B:213:GLY:O	4:B:214:LEU:C	2.57	0.42
5:C:29:ILE:CG2	5:C:90:GLN:HG3	2.49	0.42
6:D:9:PRO:O	6:D:11:ILE:N	2.51	0.42
3:A:325:LEU:HD21	3:A:343:GLN:HE21	1.85	0.42
3:A:393:ILE:CG1	3:A:394:GLN:N	2.82	0.42
4:B:48:SER:N	4:B:147:ASN:HD21	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:206:ARG:NH1	4:B:218:ASP:O	2.50	0.42
4:B:363:ASN:H	4:B:367:GLN:NE2	2.18	0.42
1:E:861:C:C2'	1:E:862:U:C6	2.85	0.42
3:A:87:PHE:CE1	3:A:159:ILE:HD11	2.55	0.42
3:A:319:TYR:CG	3:A:383:TRP:CD1	3.08	0.42
5:C:89:GLN:HB2	5:C:98:PHE:CD1	2.55	0.42
1:E:862:U:O3'	3:A:284:ARG:HA	2.20	0.42
2:F:884:DT:C2	2:F:885:DT:H73	2.54	0.42
4:B:34:LEU:HD11	4:B:73:LYS:CB	2.50	0.42
4:B:370:GLU:HA	4:B:373:GLN:HG3	2.02	0.42
3:A:85:GLN:NE2	3:A:87:PHE:HE2	2.13	0.42
3:A:235:HIS:HB3	3:A:236:PRO:HD2	2.02	0.42
3:A:326:ILE:O	3:A:341:ILE:HA	2.20	0.42
4:B:157:PRO:O	4:B:161:GLN:HB2	2.19	0.42
5:C:96:TRP:HE3	6:D:110:MET:HE3	1.83	0.42
5:C:180:THR:O	5:C:181:LEU:HD23	2.20	0.42
3:A:79:GLU:O	3:A:83:ARG:HG3	2.20	0.41
3:A:165:THR:HG22	3:A:182:GLN:OE1	2.20	0.41
3:A:199:ARG:HA	3:A:202:ILE:CG1	2.50	0.41
3:A:407:GLN:HG2	4:B:393:ILE:HA	2.02	0.41
3:A:434:ILE:H	3:A:494:ASN:HD21	1.67	0.41
4:B:201:LYS:HA	4:B:204:GLU:HB2	2.01	0.41
4:B:234:LEU:HD11	4:B:377:THR:CG2	2.48	0.41
4:B:342:TYR:CD2	4:B:342:TYR:N	2.88	0.41
4:B:391:LEU:HA	4:B:392:PRO:HD2	1.89	0.41
5:C:113:PRO:HD3	5:C:200:THR:CG2	2.39	0.41
5:C:176:SER:HB3	6:D:176:PHE:CZ	2.55	0.41
6:D:134:LEU:HD21	6:D:151:LEU:CB	2.50	0.41
3:A:58:THR:HA	3:A:59:PRO:HD3	1.80	0.41
3:A:307:ARG:HH11	3:A:307:ARG:HG3	1.86	0.41
3:A:369:THR:O	3:A:372:VAL:N	2.53	0.41
3:A:478:GLU:HG2	3:A:499:SER:HB2	2.02	0.41
4:B:34:LEU:HD12	4:B:34:LEU:HA	1.64	0.41
4:B:97:PRO:HG3	4:B:181:TYR:HB2	2.02	0.41
4:B:331:LYS:NZ	4:B:364:ASP:OD2	2.52	0.41
5:C:124:GLN:HG3	6:D:132:TYR:CE2	2.55	0.41
5:C:142:LYS:HE3	5:C:163:TRP:HB3	2.02	0.41
2:F:894:DT:N3	2:F:895:DG:N7	2.69	0.41
3:A:98:ALA:O	3:A:319:TYR:HB3	2.20	0.41
3:A:161:GLN:O	3:A:163:SER:N	2.54	0.41
3:A:478:GLU:CG	3:A:499:SER:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:49:TYR:O	5:C:53:SER:HB2	2.20	0.41
5:C:85:THR:HG21	5:C:103:LYS:CE	2.50	0.41
5:C:120:PRO:HD2	5:C:186:TYR:OH	2.20	0.41
6:D:198:TRP:CD1	6:D:198:TRP:O	2.73	0.41
1:E:857:G:H5'	3:A:89:GLU:CG	2.50	0.41
1:E:860:A:N1	2:F:895:DG:C6	2.89	0.41
3:A:164:MET:CE	3:A:168:LEU:HD11	2.51	0.41
3:A:459:THR:HG21	3:A:463:ARG:HB3	2.00	0.41
4:B:118:VAL:HA	4:B:119:PRO:HD2	1.85	0.41
5:C:2:ILE:CD1	5:C:93:LYS:HB2	2.42	0.41
5:C:11:LEU:CD2	5:C:104:LEU:HD13	2.50	0.41
1:E:874:A:C2'	1:E:875:A:H5'	2.51	0.41
3:A:494:ASN:OD1	4:B:289:LEU:HD23	2.20	0.41
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.51	0.41
4:B:327:ALA:HA	4:B:340:GLN:O	2.20	0.41
6:D:187:LEU:HD23	6:D:188:SER:N	2.36	0.41
2:F:885:DT:H1'	2:F:886:DT:H5'	2.03	0.41
5:C:174:SER:O	6:D:176:PHE:HE2	2.02	0.41
6:D:131:VAL:HG11	6:D:216:VAL:HG13	2.03	0.41
3:A:120:LEU:HB2	3:A:148:VAL:O	2.21	0.41
3:A:441:TYR:HB2	3:A:548:VAL:HG21	2.00	0.41
3:A:542:ILE:HG22	4:B:258:GLN:HG3	2.03	0.41
4:B:54:ASN:HD21	4:B:126:LYS:HA	1.84	0.41
4:B:104:LYS:HD2	4:B:192:ASP:O	2.20	0.41
4:B:329:ILE:HD11	4:B:375:ILE:HD13	2.03	0.41
5:C:45:LYS:HE3	5:C:55:HIS:HE1	1.85	0.41
6:D:156:PHE:HB3	6:D:157:PRO:CD	2.48	0.41
2:F:881:DT:C6	2:F:882:DT:H71	2.56	0.41
3:A:261:VAL:HG21	3:A:283:LEU:CD1	2.46	0.41
3:A:433:PRO:HG3	4:B:255:ASN:OD1	2.21	0.41
4:B:47:ILE:HD12	4:B:144:TYR:CD1	2.56	0.41
4:B:160:PHE:O	4:B:160:PHE:CG	2.73	0.41
5:C:186:TYR:CE1	5:C:192:TYR:HE1	2.39	0.41
3:A:8:VAL:HA	3:A:9:PRO:HD3	1.84	0.41
3:A:120:LEU:HD11	3:A:124:PHE:CD2	2.56	0.41
3:A:131:THR:HG23	3:A:143:ARG:HD3	2.03	0.41
3:A:161:GLN:O	3:A:162:SER:C	2.59	0.41
3:A:193:LEU:N	3:A:193:LEU:CD2	2.84	0.41
3:A:362:THR:OG1	3:A:363:ASN:N	2.54	0.41
3:A:450:THR:O	3:A:451:LYS:HB2	2.21	0.41
4:B:119:PRO:CA	4:B:148:VAL:HG12	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:120:LEU:N	4:B:148:VAL:HA	2.36	0.41
4:B:149:LEU:HA	4:B:150:PRO:HD3	1.85	0.41
4:B:169:GLU:N	4:B:170:PRO:CD	2.84	0.41
4:B:171:PHE:CE1	4:B:205:LEU:HB2	2.54	0.41
4:B:209:LEU:O	4:B:215:THR:HB	2.20	0.41
4:B:376:THR:HG23	4:B:386:THR:HG23	2.02	0.41
4:B:393:ILE:HG12	4:B:394:GLN:N	2.36	0.41
5:C:79:GLU:HB2	5:C:82:ASP:OD2	2.21	0.41
6:D:24:PHE:HB2	6:D:27:PHE:CE1	2.55	0.41
6:D:41:GLN:O	6:D:94:ILE:HG12	2.20	0.41
6:D:53:ILE:HG12	6:D:71:VAL:CB	2.51	0.41
6:D:127:THR:HA	6:D:128:PRO:HD3	1.96	0.41
3:A:130:PHE:CZ	3:A:144:TYR:HB2	2.56	0.41
4:B:182:GLN:HG2	4:B:187:LEU:CD1	2.51	0.41
5:C:47:LEU:HD23	5:C:47:LEU:HA	1.76	0.41
5:C:107:LYS:HA	5:C:107:LYS:HD2	1.77	0.41
3:A:250:ASP:O	3:A:252:TRP:N	2.54	0.40
4:B:394:GLN:HB2	4:B:397:THR:OG1	2.21	0.40
6:D:62:ASN:ND2	6:D:65:LEU:N	2.69	0.40
6:D:164:TRP:CZ2	6:D:191:VAL:HG12	2.56	0.40
1:E:860:A:C6	2:F:895:DG:C6	3.10	0.40
3:A:182:GLN:HG3	4:B:140:PRO:HD3	2.03	0.40
3:A:325:LEU:HD11	3:A:383:TRP:CD2	2.56	0.40
4:B:213:GLY:O	4:B:215:THR:N	2.54	0.40
4:B:386:THR:HG21	4:B:412:PRO:HB3	2.03	0.40
1:E:857:G:HO2'	1:E:858:C:H5'	1.86	0.40
1:E:873:A:N3	3:A:448:ARG:NH2	2.67	0.40
3:A:11:LYS:NZ	3:A:11:LYS:CB	2.84	0.40
3:A:356:ARG:O	3:A:367:GLN:NE2	2.54	0.40
3:A:479:LEU:O	3:A:521:ILE:HD11	2.22	0.40
4:B:281:LYS:NZ	4:B:281:LYS:CB	2.78	0.40
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.36	0.40
5:C:39:LYS:HE3	5:C:39:LYS:HB2	1.82	0.40
6:D:49:TRP:HZ2	6:D:52:THR:HG1	1.64	0.40
3:A:184:MET:N	3:A:184:MET:SD	2.94	0.40
4:B:59:PRO:CG	4:B:76:ASP:HB3	2.44	0.40
4:B:187:LEU:HA	4:B:187:LEU:HD12	1.68	0.40
4:B:285:GLY:C	4:B:287:LYS:H	2.24	0.40
4:B:332:GLN:HE21	4:B:332:GLN:HB2	1.64	0.40
6:D:61:TYR:N	6:D:61:TYR:CD1	2.88	0.40
3:A:85:GLN:NE2	3:A:87:PHE:CD2	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:335:GLY:N	3:A:336:GLN:OE1	2.54	0.40
4:B:61:PHE:CZ	4:B:411:ILE:HD11	2.57	0.40
4:B:64:LYS:N	4:B:71:TRP:CZ3	2.90	0.40
5:C:31:SER:OG	5:C:50:TYR:HE1	2.01	0.40
6:D:17:PRO:HB3	6:D:85:MET:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	551/553 (100%)	431 (78%)	94 (17%)	26 (5%)	2 14
4	B	423/425 (100%)	319 (75%)	73 (17%)	31 (7%)	1 5
5	C	212/214 (99%)	171 (81%)	25 (12%)	16 (8%)	1 5
6	D	218/220 (99%)	181 (83%)	29 (13%)	8 (4%)	3 19
All	All	1404/1412 (99%)	1102 (78%)	221 (16%)	81 (6%)	1 10

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	63	ILE
3	A	245	VAL
3	A	248	GLU
3	A	273	GLY
3	A	345	PRO
3	A	420	PRO
3	A	440	PHE
4	B	18	GLY
4	B	138	GLU
4	B	224	GLU

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Mol	Chain	Res	Type
4	B	225	PRO
4	B	227	PHE
4	B	245	VAL
4	B	272	PRO
4	B	289	LEU
5	C	138	ASN
5	C	141	PRO
5	C	151	ASP
5	C	169	LYS
6	D	32	SER
6	D	43	SER
3	A	45	GLY
3	A	85	GLN
3	A	125	ARG
3	A	126	LYS
3	A	176	PRO
3	A	250	ASP
3	A	426	TRP
4	B	53	GLU
4	B	68	SER
4	B	113	ASP
4	B	154	LYS
4	B	214	LEU
4	B	290	THR
4	B	296	THR
4	B	398	TRP
4	B	423	VAL
5	C	76	SER
5	C	101	GLY
5	C	140	TYR
5	C	143	ASP
5	C	211	ALA
6	D	124	ALA
6	D	138	SER
3	A	90	VAL
3	A	228	LEU
3	A	241	VAL
3	A	295	LEU
3	A	413	GLU
3	A	422	LEU
4	B	2	ILE
4	B	125	ARG

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Mol	Chain	Res	Type
4	B	420	PRO
5	C	17	ASP
5	C	82	ASP
5	C	100	GLY
3	A	82	LYS
3	A	129	ALA
3	A	251	SER
3	A	322	SER
3	A	335	GLY
4	B	36	GLU
4	B	111	VAL
4	B	286	THR
4	B	345	PRO
5	C	52	SER
5	C	126	THR
6	D	89	THR
3	A	121	ASP
4	B	324	ASP
5	C	95	PRO
6	D	34	ILE
6	D	157	PRO
4	B	110	ASP
4	B	322	SER
5	C	158	GLY
4	B	241	VAL
4	B	242	GLN
6	D	156	PHE
4	B	392	PRO
4	B	133	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	486/495 (98%)	399 (82%)	87 (18%)	2 9
4	B	381/387 (98%)	325 (85%)	56 (15%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	C	181/181 (100%)	149 (82%)	32 (18%)	2 9
6	D	191/191 (100%)	160 (84%)	31 (16%)	2 12
All	All	1239/1254 (99%)	1033 (83%)	206 (17%)	2 11

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	5	ILE
3	A	7	THR
3	A	10	VAL
3	A	24	TRP
3	A	26	LEU
3	A	28	GLU
3	A	36	GLU
3	A	39	THR
3	A	50	ILE
3	A	70	LYS
3	A	71	TRP
3	A	74	LEU
3	A	79	GLU
3	A	80	LEU
3	A	83	ARG
3	A	85	GLN
3	A	86	ASP
3	A	94	ILE
3	A	101	LYS
3	A	109	LEU
3	A	110	ASP
3	A	111	VAL
3	A	120	LEU
3	A	136	ASN
3	A	137	ASN
3	A	145	GLN
3	A	151	GLN
3	A	174	GLN
3	A	175	ASN
3	A	184	MET
3	A	185	ASP
3	A	186	ASP
3	A	188	TYR
3	A	193	LEU

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Mol	Chain	Res	Type
3	A	199	ARG
3	A	205	LEU
3	A	209	LEU
3	A	218	ASP
3	A	222	GLN
3	A	228	LEU
3	A	237	ASP
3	A	244	ILE
3	A	249	LYS
3	A	252	TRP
3	A	257	ILE
3	A	260	LEU
3	A	265	ASN
3	A	278	GLN
3	A	281	LYS
3	A	291	GLU
3	A	293	ILE
3	A	295	LEU
3	A	301	LEU
3	A	305	GLU
3	A	312	GLU
3	A	319	TYR
3	A	320	ASP
3	A	331	LYS
3	A	334	GLN
3	A	337	TRP
3	A	345	PRO
3	A	353	LYS
3	A	364	ASP
3	A	365	VAL
3	A	367	GLN
3	A	369	THR
3	A	397	THR
3	A	406	TRP
3	A	410	TRP
3	A	411	ILE
3	A	416	PHE
3	A	420	PRO
3	A	425	LEU
3	A	434	ILE
3	A	439	THR
3	A	452	LEU

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Mol	Chain	Res	Type
3	A	469	LEU
3	A	476	LYS
3	A	478	GLU
3	A	497	THR
3	A	505	ILE
3	A	512	LYS
3	A	516	GLU
3	A	517	LEU
3	A	525	LEU
3	A	527	LYS
3	A	533	LEU
4	B	2	ILE
4	B	3	SER
4	B	10	VAL
4	B	12	LEU
4	B	13	LYS
4	B	16	MET
4	B	36	GLU
4	B	38	CYS
4	B	39	THR
4	B	42	GLU
4	B	70	LYS
4	B	72	ARG
4	B	74	LEU
4	B	83	ARG
4	B	88	TRP
4	B	101	LYS
4	B	123	ASP
4	B	140	PRO
4	B	142	ILE
4	B	169	GLU
4	B	177	ASP
4	B	182	GLN
4	B	189	VAL
4	B	194	GLU
4	B	197	GLN
4	B	206	ARG
4	B	210	LEU
4	B	219	LYS
4	B	221	HIS
4	B	222	GLN
4	B	224	GLU

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Mol	Chain	Res	Type
4	B	241	VAL
4	B	244	ILE
4	B	245	VAL
4	B	253	THR
4	B	255	ASN
4	B	265	ASN
4	B	269	GLN
4	B	270	ILE
4	B	281	LYS
4	B	302	GLU
4	B	306	ASN
4	B	307	ARG
4	B	318	TYR
4	B	326	ILE
4	B	330	GLN
4	B	340	GLN
4	B	344	GLU
4	B	349	LEU
4	B	353	LYS
4	B	356	ARG
4	B	385	LYS
4	B	395	LYS
4	B	410	TRP
4	B	424	LYS
4	B	425	LEU
5	C	3	GLN
5	C	8	THR
5	C	10	SER
5	C	11	LEU
5	C	12	SER
5	C	14	SER
5	C	26	SER
5	C	27	GLN
5	C	39	LYS
5	C	47	LEU
5	C	50	TYR
5	C	51	THR
5	C	53	SER
5	C	65	SER
5	C	77	ASN
5	C	78	LEU
5	C	90	GLN

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Mol	Chain	Res	Type
5	C	93	LYS
5	C	141	PRO
5	C	142	LYS
5	C	157	ASN
5	C	161	ASN
5	C	163	TRP
5	C	168	SER
5	C	170	ASP
5	C	175	MET
5	C	179	LEU
5	C	187	GLU
5	C	190	ASN
5	C	200	THR
5	C	210	ASN
5	C	214	CYS
6	D	5	LYS
6	D	16	GLN
6	D	20	LEU
6	D	29	LEU
6	D	47	LEU
6	D	57	ASP
6	D	59	ASN
6	D	62	ASN
6	D	68	ARG
6	D	69	LEU
6	D	73	LYS
6	D	85	MET
6	D	89	THR
6	D	97	CYS
6	D	99	GLN
6	D	100	SER
6	D	107	ASP
6	D	111	ASP
6	D	117	THR
6	D	118	SER
6	D	123	SER
6	D	141	GLN
6	D	144	SER
6	D	161	THR
6	D	162	VAL
6	D	182	SER
6	D	193	VAL

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Mol	Chain	Res	Type
6	D	205	CYS
6	D	206	ASN
6	D	214	THR
6	D	219	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	145	GLN
3	A	151	GLN
3	A	174	GLN
3	A	175	ASN
3	A	182	GLN
3	A	208	HIS
3	A	258	GLN
3	A	265	ASN
3	A	343	GLN
3	A	418	ASN
3	A	507	GLN
3	A	520	GLN
4	B	23	GLN
4	B	54	ASN
4	B	57	ASN
4	B	81	ASN
4	B	96	HIS
4	B	151	GLN
4	B	175	ASN
4	B	222	GLN
4	B	255	ASN
4	B	269	GLN
4	B	278	GLN
4	B	306	ASN
4	B	330	GLN
4	B	332	GLN
4	B	340	GLN
4	B	407	GLN
4	B	418	ASN
5	C	38	GLN
5	C	137	ASN
5	C	157	ASN
5	C	190	ASN
5	C	212	ASN

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Mol	Chain	Res	Type
6	D	1	GLN
6	D	41	GLN
6	D	62	ASN
6	D	99	GLN
6	D	141	GLN
6	D	174	HIS
6	D	181	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	23/23 (100%)	1 (4%)	1 (4%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	855	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	854	U

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 monosaccharides 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 (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(Å^2)	Q<0.9
1	E	23/23 (100%)	-0.36	0	100	100	62, 66, 76, 78	0
2	F	22/22 (100%)	-0.18	0	100	100	52, 70, 80, 86	0
3	A	553/553 (100%)	0.48	40 (7%)	15	4	10, 51, 75, 87	61 (11%)
4	B	425/425 (100%)	0.34	15 (3%)	44	18	8, 25, 69, 83	20 (4%)
5	C	214/214 (100%)	0.27	4 (1%)	66	37	9, 37, 66, 75	0
6	D	220/220 (100%)	0.23	1 (0%)	91	75	8, 27, 49, 70	2 (0%)
All	All	1457/1457 (100%)	0.35	60 (4%)	37	14	8, 39, 71, 87	83 (5%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	2	ILE	5.8
3	A	456	GLY	5.7
4	B	315	HIS	5.5
5	C	213	GLU	4.7
3	A	542	ILE	4.1
3	A	69	THR	3.9
3	A	455	ALA	3.8
3	A	71	TRP	3.5
3	A	293	ILE	3.4
3	A	243	PRO	3.4
6	D	138	SER	3.3
4	B	242	GLN	3.3
4	B	361	HIS	3.2
3	A	514	GLU	3.2
3	A	67	ASP	3.2
3	A	277	ARG	3.2
4	B	252	TRP	3.1
3	A	294	PRO	3.1
3	A	297	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	63	ILE	3.0
3	A	515	SER	3.0
4	B	90	VAL	3.0
4	B	93	GLY	3.0
3	A	1	PRO	3.0
5	C	214	CYS	2.8
3	A	522	ILE	2.8
3	A	221	HIS	2.8
4	B	283	LEU	2.8
3	A	247	PRO	2.7
3	A	239	TRP	2.7
4	B	128	THR	2.6
3	A	109	LEU	2.6
4	B	258	GLN	2.5
3	A	261	VAL	2.5
3	A	90	VAL	2.5
3	A	225	PRO	2.5
3	A	283	LEU	2.5
3	A	457	TYR	2.5
3	A	329	ILE	2.5
4	B	310	LEU	2.4
3	A	306	ASN	2.4
4	B	289	LEU	2.3
3	A	402	TRP	2.3
3	A	31	ILE	2.3
3	A	209	LEU	2.3
3	A	250	ASP	2.3
3	A	237	ASP	2.3
4	B	288	ALA	2.2
3	A	325	LEU	2.2
3	A	303	LEU	2.2
4	B	360	ALA	2.2
3	A	133	PRO	2.2
5	C	93	LYS	2.2
3	A	270	ILE	2.1
3	A	349	LEU	2.1
5	C	153	SER	2.1
3	A	398	TRP	2.1
4	B	423	VAL	2.1
3	A	313	PRO	2.1
4	B	68	SER	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 monosaccharides 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.