Full wwPDB X-ray Structure Validation Report (i)

Apr 18, 2026 – 01:03 PM UTC

PDB ID	:	2QKK / pdb_00002qkk
Title	:	Human RNase H catalytic domain mutant D210N in complex with 14-mer RNA/DNA hybrid
Authors	:	Nowotny, M.; Gaidamakov, S.A.; Ghirlando, R.; Cerritelli, S.M.; Crouch, R.J.; Yang, W.
Deposited on	:	2007-07-11
Resolution	:	3.20 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 (i)) were used in the production of this report:

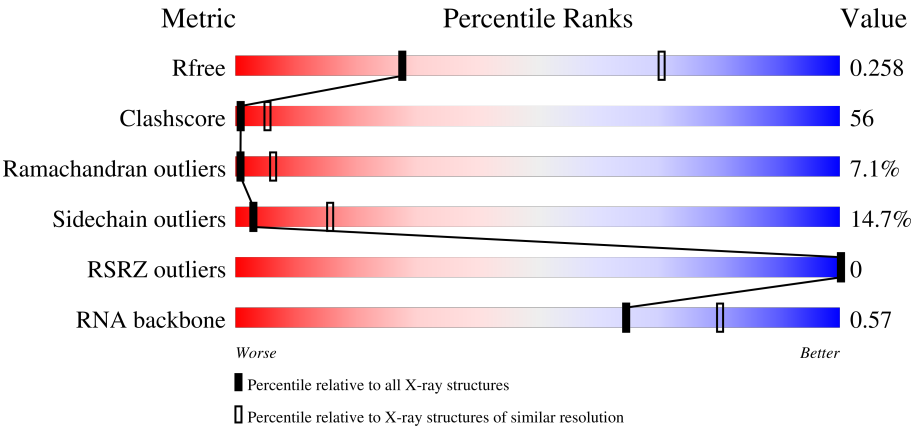
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	C	14	64% 36%
1	G	14	36% 57% 7%
1	K	14	93% 7%
1	O	14	7% 86% 7%

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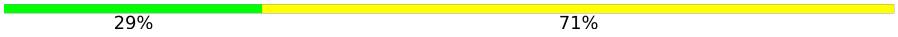
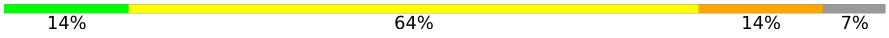
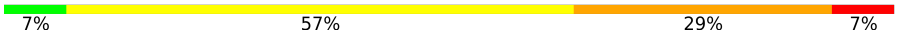
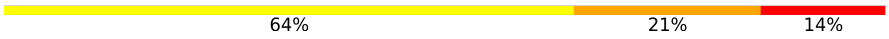
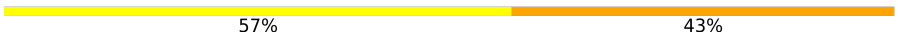
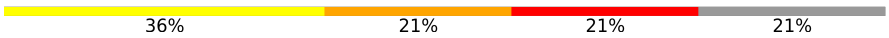
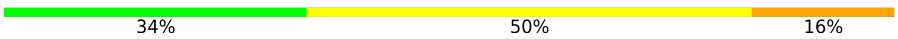
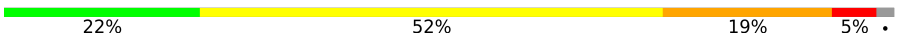
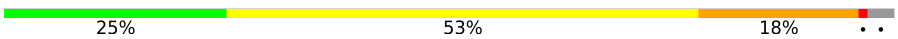
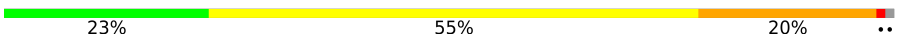
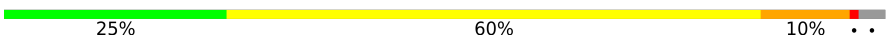
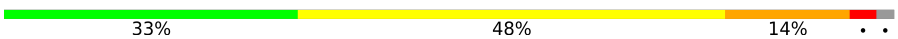
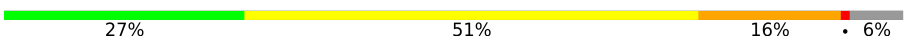
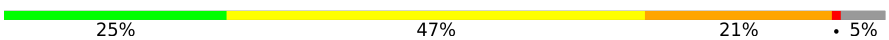
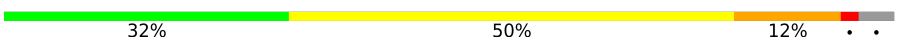
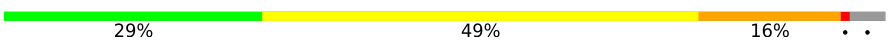
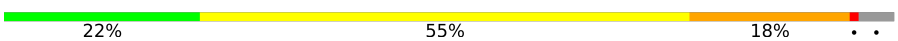
Mol	Chain	Length	Quality of chain
1	T	14	
1	X	14	
2	D	14	
2	H	14	
2	L	14	
2	P	14	
2	U	14	
2	Z	14	
3	A	154	
3	B	154	
3	E	154	
3	F	154	
3	I	154	
3	J	154	
3	M	154	
3	N	154	
3	R	154	
3	S	154	
3	W	154	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16231 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(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	G	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	K	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	O	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	T	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	X	13	Total	C	N	O	P	0	0	0
			269	122	46	89	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	H	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	L	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	P	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	U	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	Z	11	Total	C	N	O	P	0	0	0
			229	109	47	63	10			

- Molecule 3 is a protein called Ribonuclease H1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	154	Total	C	N	O	S	0	0	0
			1186	737	222	220	7			
3	B	151	Total	C	N	O	S	1	0	0
			1175	731	223	214	7			
3	E	149	Total	C	N	O	S	0	0	0
			1147	715	217	209	6			
3	F	152	Total	C	N	O	S	3	0	0
			1175	733	219	216	7			
3	I	149	Total	C	N	O	S	6	0	0
			1133	706	213	208	6			
3	J	151	Total	C	N	O	S	5	0	0
			1166	728	218	213	7			
3	M	145	Total	C	N	O	S	3	0	0
			1117	700	208	203	6			
3	N	146	Total	C	N	O	S	0	0	0
			1121	701	208	206	6			
3	R	148	Total	C	N	O	S	0	0	0
			1144	714	215	208	7			
3	S	148	Total	C	N	O	S	7	0	0
			1126	704	210	206	6			
3	W	148	Total	C	N	O	S	9	0	0
			1141	716	211	207	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	GLY	-	expression tag	UNP O60930
A	134	SER	-	expression tag	UNP O60930
A	135	HIS	-	expression tag	UNP O60930
A	210	ASN	ASP	engineered mutation	UNP O60930
B	133	GLY	-	expression tag	UNP O60930
B	134	SER	-	expression tag	UNP O60930
B	135	HIS	-	expression tag	UNP O60930
B	210	ASN	ASP	engineered mutation	UNP O60930
E	133	GLY	-	expression tag	UNP O60930
E	134	SER	-	expression tag	UNP O60930
E	135	HIS	-	expression tag	UNP O60930
E	210	ASN	ASP	engineered mutation	UNP O60930
F	133	GLY	-	expression tag	UNP O60930
F	134	SER	-	expression tag	UNP O60930
F	135	HIS	-	expression tag	UNP O60930
F	210	ASN	ASP	engineered mutation	UNP O60930
I	133	GLY	-	expression tag	UNP O60930
I	134	SER	-	expression tag	UNP O60930

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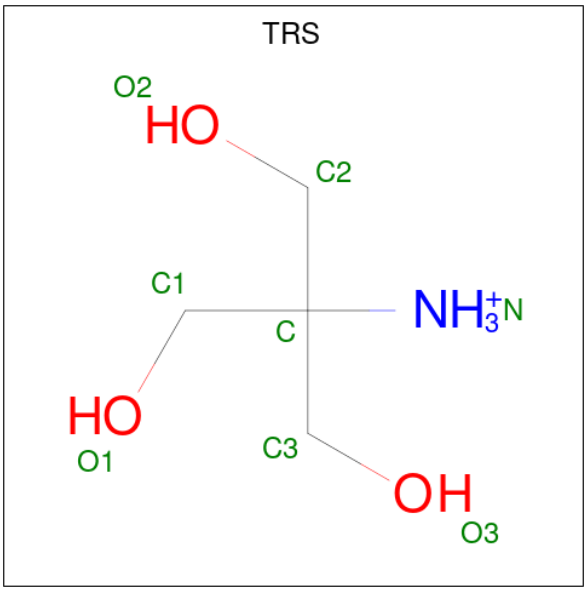
Chain	Residue	Modelled	Actual	Comment	Reference
I	135	HIS	-	expression tag	UNP O60930
I	210	ASN	ASP	engineered mutation	UNP O60930
J	133	GLY	-	expression tag	UNP O60930
J	134	SER	-	expression tag	UNP O60930
J	135	HIS	-	expression tag	UNP O60930
J	210	ASN	ASP	engineered mutation	UNP O60930
M	133	GLY	-	expression tag	UNP O60930
M	134	SER	-	expression tag	UNP O60930
M	135	HIS	-	expression tag	UNP O60930
M	210	ASN	ASP	engineered mutation	UNP O60930
N	133	GLY	-	expression tag	UNP O60930
N	134	SER	-	expression tag	UNP O60930
N	135	HIS	-	expression tag	UNP O60930
N	210	ASN	ASP	engineered mutation	UNP O60930
R	133	GLY	-	expression tag	UNP O60930
R	134	SER	-	expression tag	UNP O60930
R	135	HIS	-	expression tag	UNP O60930
R	210	ASN	ASP	engineered mutation	UNP O60930
S	133	GLY	-	expression tag	UNP O60930
S	134	SER	-	expression tag	UNP O60930
S	135	HIS	-	expression tag	UNP O60930
S	210	ASN	ASP	engineered mutation	UNP O60930
W	133	GLY	-	expression tag	UNP O60930
W	134	SER	-	expression tag	UNP O60930
W	135	HIS	-	expression tag	UNP O60930
W	210	ASN	ASP	engineered mutation	UNP O60930

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).

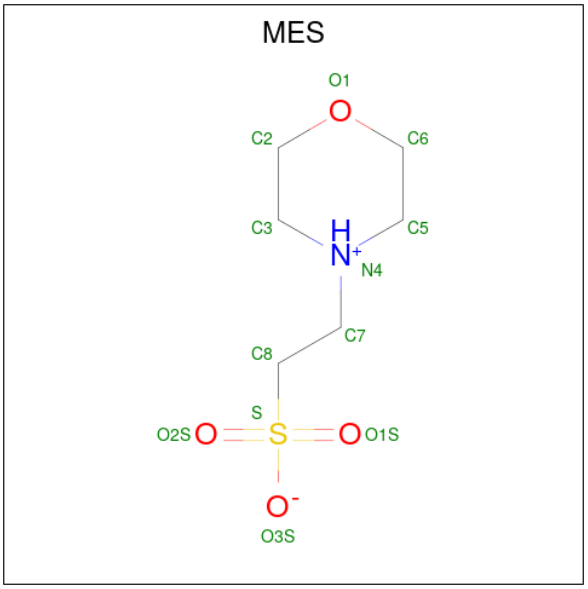


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	1	Total Ca 1 1	0	0
5	E	2	Total Ca 2 2	0	0
5	F	1	Total Ca 1 1	0	0
5	I	1	Total Ca 1 1	0	0
5	J	1	Total Ca 1 1	0	0
5	M	2	Total Ca 2 2	0	0
5	N	1	Total Ca 1 1	0	0
5	R	1	Total Ca 1 1	0	0
5	S	1	Total Ca 1 1	0	0
5	W	1	Total Ca 1 1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total	O	0	0
			2	2		
8	D	5	Total	O	0	0
			5	5		
8	G	8	Total	O	0	0
			8	8		
8	H	9	Total	O	0	0
			9	9		
8	K	4	Total	O	0	0
			4	4		
8	L	4	Total	O	0	0
			4	4		

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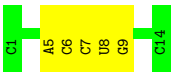
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	O	4	Total O 4 4	0	0
8	P	6	Total O 6 6	0	0
8	T	3	Total O 3 3	0	0
8	U	3	Total O 3 3	0	0
8	X	5	Total O 5 5	0	0
8	Z	3	Total O 3 3	0	0
8	A	16	Total O 16 16	0	0
8	B	15	Total O 15 15	0	0
8	E	16	Total O 16 16	0	0
8	F	13	Total O 13 13	0	0
8	I	3	Total O 3 3	0	0
8	J	12	Total O 12 12	0	0
8	M	6	Total O 6 6	0	0
8	N	7	Total O 7 7	0	0
8	R	7	Total O 7 7	0	0
8	S	11	Total O 11 11	0	0
8	W	10	Total O 10 10	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.

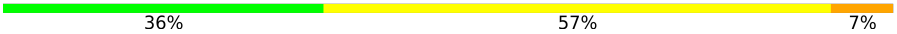
• Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

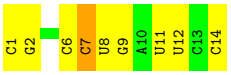
Chain C:



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

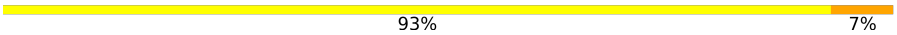
Chain G:

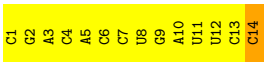




• Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

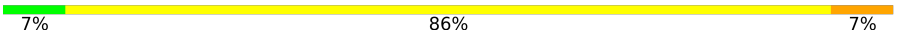
Chain K:





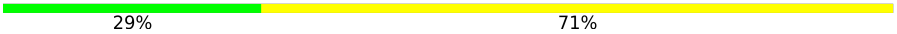
• Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain O:



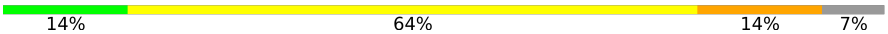
• Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain T:



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

Chain X:

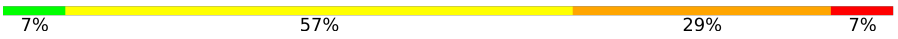


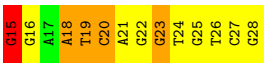
• Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'

Chain D:

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

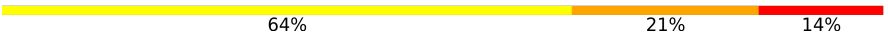
Chain H:





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

Chain L:

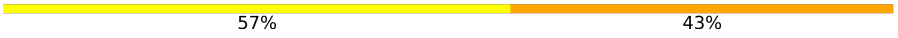


• Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'

Chain P:

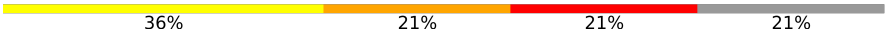
• Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'

Chain U:



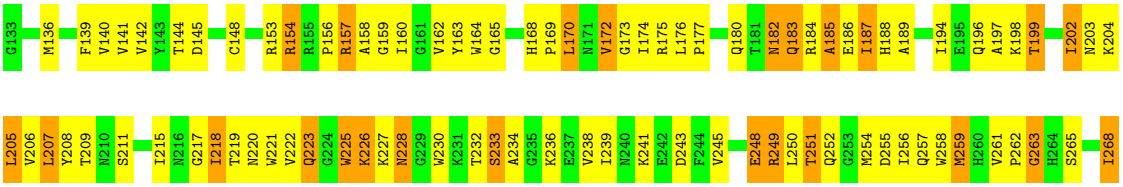
• Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'

Chain Z:



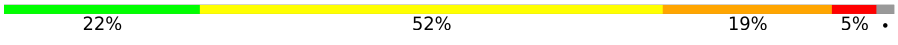
• Molecule 3: Ribonuclease H1

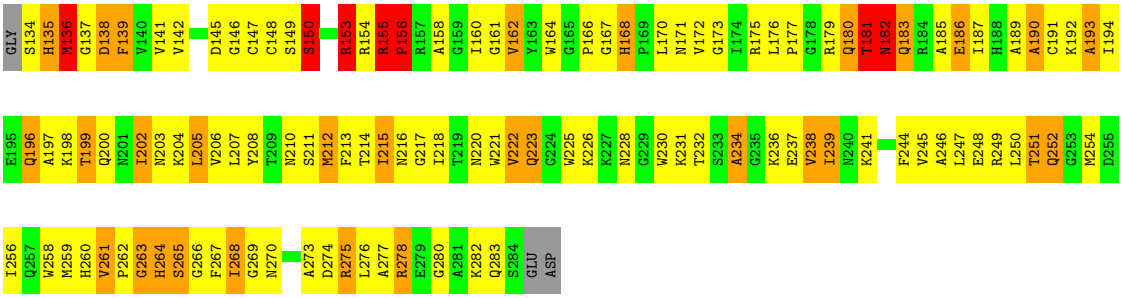
Chain A:



• Molecule 3: Ribonuclease H1

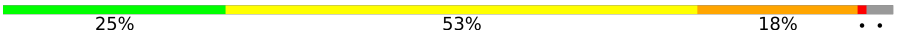
Chain B:

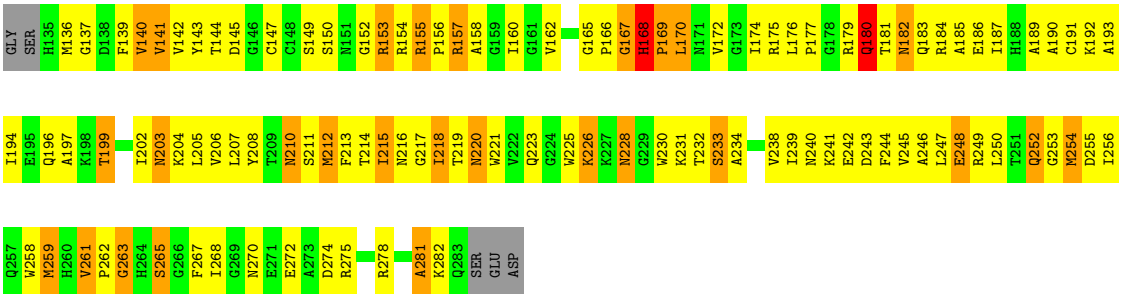




• Molecule 3: Ribonuclease H1

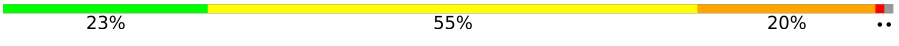
Chain E:

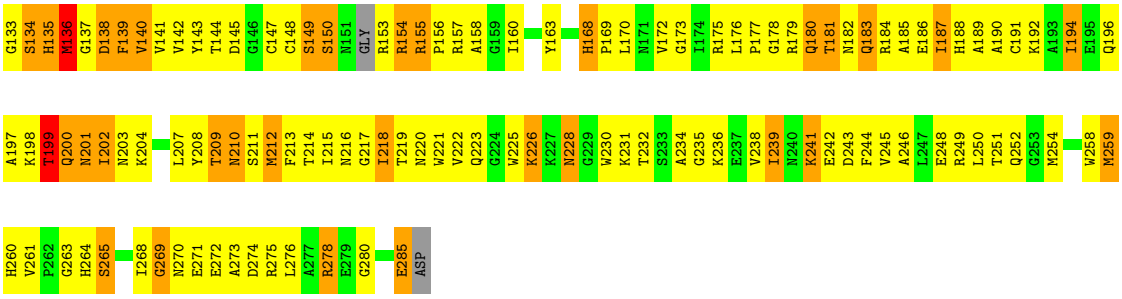




• Molecule 3: Ribonuclease H1

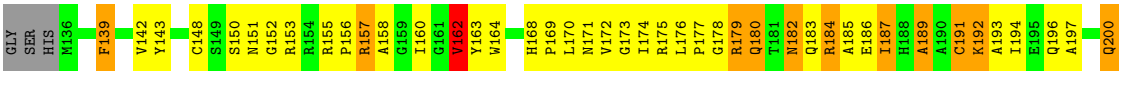
Chain F:

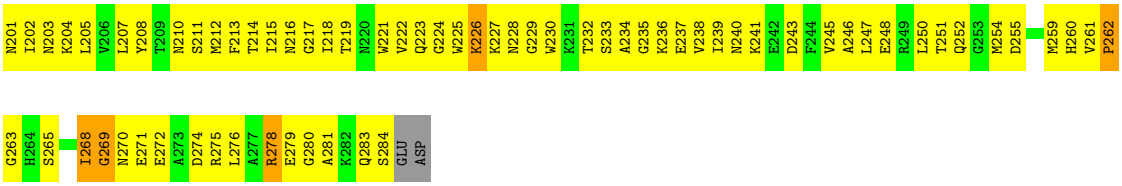




• Molecule 3: Ribonuclease H1

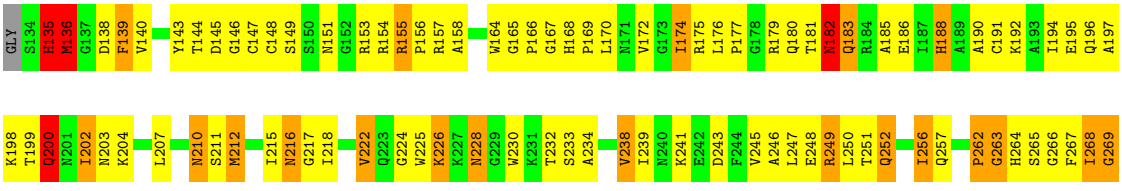
Chain I:





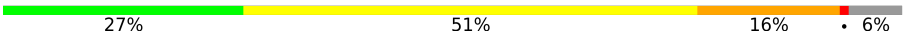
• Molecule 3: Ribonuclease H1

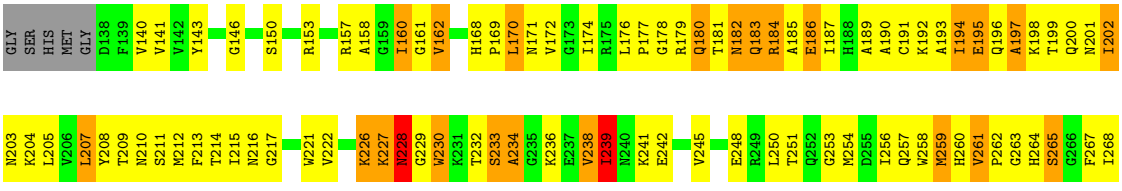
Chain J:



• Molecule 3: Ribonuclease H1

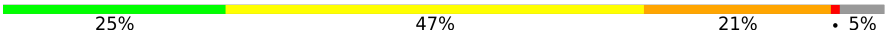
Chain M:

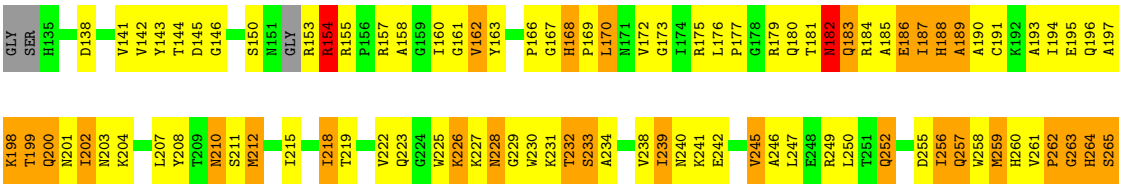




• Molecule 3: Ribonuclease H1

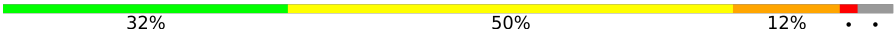
Chain N:

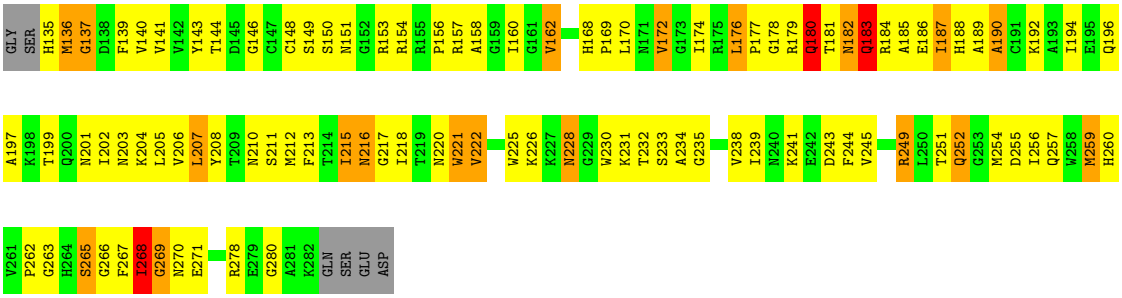




• Molecule 3: Ribonuclease H1

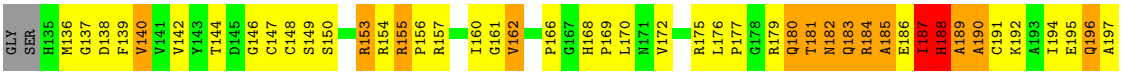
Chain R:

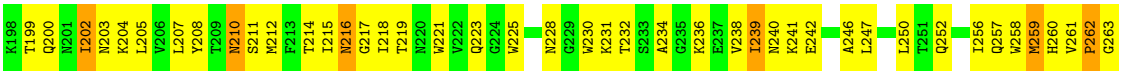




• Molecule 3: Ribonuclease H1

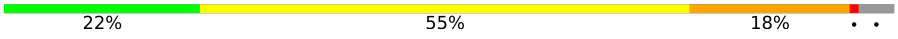
Chain S:

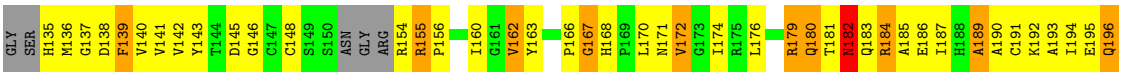




• Molecule 3: Ribonuclease H1

Chain W:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.06Å 176.20Å 125.84Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-3.20) 91.8 (30.00-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.269 0.212 , 0.258	Depositor DCC
R_{free} test set	1752 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.177 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16231	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA, MES, TRS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.46	0/321	0.84	0/497
1	G	0.45	0/321	0.88	0/497
1	K	0.35	0/321	0.69	0/497
1	O	0.33	0/321	0.66	0/497
1	T	0.36	0/321	0.68	0/497
1	X	0.32	0/299	0.64	0/463
2	D	0.40	0/326	1.20	4/503 (0.8%)
2	H	0.41	0/326	0.93	3/503 (0.6%)
2	L	0.32	0/326	1.15	3/503 (0.6%)
2	P	0.36	0/326	1.24	4/503 (0.8%)
2	U	0.31	0/326	1.22	2/503 (0.4%)
2	Z	0.29	0/258	1.25	4/398 (1.0%)
3	A	0.61	0/1212	1.12	3/1637 (0.2%)
3	B	0.56	1/1201 (0.1%)	1.45	17/1622 (1.0%)
3	E	0.56	0/1172	1.08	12/1586 (0.8%)
3	F	0.59	0/1200	1.09	6/1620 (0.4%)
3	I	0.43	0/1158	0.98	3/1571 (0.2%)
3	J	0.49	0/1192	1.08	10/1611 (0.6%)
3	M	0.48	0/1142	1.09	11/1546 (0.7%)
3	N	0.55	0/1145	1.16	16/1550 (1.0%)
3	R	0.50	0/1170	1.06	6/1583 (0.4%)
3	S	0.47	0/1151	1.04	11/1560 (0.7%)
3	W	0.42	0/1166	1.02	10/1576 (0.6%)
All	All	0.49	1/16701 (0.0%)	1.08	125/23323 (0.5%)

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
2	D	0	6
2	H	0	4
2	L	0	6
2	P	0	6
2	U	0	5
2	Z	0	6
All	All	0	33

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	212	MET	SD-CE	6.03	1.94	1.79

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	155	ARG	CA-C-N	23.37	149.06	119.84
3	B	155	ARG	C-N-CA	23.37	149.06	119.84
3	I	152	GLY	N-CA-C	-13.69	99.08	111.67
3	S	279	GLU	N-CA-C	-9.90	100.96	113.43
3	B	155	ARG	C-N-CD	-9.81	84.79	125.00
3	M	239	ILE	N-CA-C	9.64	119.67	110.42
3	S	184	ARG	N-CA-C	-9.18	101.36	114.12
3	B	213	PHE	N-CA-C	-9.02	99.05	112.04
3	W	264	HIS	N-CA-C	-8.71	101.96	112.58
3	W	184	ARG	N-CA-C	-8.61	102.22	112.89
3	N	233	SER	N-CA-C	-8.47	102.96	113.38
2	U	28	DG	C2'-C3'-O3'	8.30	123.96	111.50
2	U	28	DG	C4'-C3'-O3'	8.08	122.11	110.00
3	M	253	GLY	N-CA-C	-8.03	104.25	114.37
3	F	168	HIS	CA-C-N	8.02	127.95	119.05
3	F	168	HIS	C-N-CA	8.02	127.95	119.05
2	P	28	DG	C2'-C3'-O3'	8.01	123.51	111.50
3	N	218	ILE	N-CA-C	7.95	119.68	110.62
3	S	188	HIS	N-CA-C	-7.86	103.83	113.41
3	I	184	ARG	N-CA-C	-7.77	102.75	111.14
3	N	168	HIS	CA-C-N	7.66	127.30	119.56
3	N	168	HIS	C-N-CA	7.66	127.30	119.56
3	R	221	TRP	N-CA-C	7.56	119.21	110.97
3	A	189	ALA	N-CA-C	-7.44	103.11	111.07
3	B	273	ALA	N-CA-C	-7.42	103.13	111.07
3	S	271	GLU	N-CA-C	-7.27	104.39	113.18
3	M	195	GLU	N-CA-C	-7.26	103.37	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	262	PRO	N-CA-C	7.06	127.02	112.47
3	R	218	ILE	N-CA-C	7.00	118.60	110.62
3	B	168	HIS	CA-C-N	6.98	128.56	119.84
3	B	168	HIS	C-N-CA	6.98	128.56	119.84
3	S	273	ALA	N-CA-C	-6.95	103.39	110.97
3	M	189	ALA	N-CA-C	-6.94	103.64	111.07
3	N	229	GLY	N-CA-C	-6.92	105.27	115.72
3	B	156	PRO	CA-N-CD	-6.92	102.32	112.00
3	M	279	GLU	N-CA-C	-6.86	104.78	113.01
3	E	155	ARG	CA-C-N	6.78	126.77	119.78
3	E	155	ARG	C-N-CA	6.78	126.77	119.78
3	J	273	ALA	N-CA-C	-6.78	103.89	111.28
3	E	212	MET	N-CA-C	-6.64	103.96	111.07
2	Z	23	DG	N9-C1'-C2'	-6.63	103.56	113.50
3	A	274	ASP	N-CA-C	-6.59	104.02	111.14
3	R	176	LEU	N-CA-C	6.57	118.37	109.24
3	B	138	ASP	N-CA-C	6.51	124.66	110.80
3	F	135	HIS	N-CA-C	6.50	124.64	110.80
3	E	168	HIS	CA-C-N	6.39	127.83	119.84
3	E	168	HIS	C-N-CA	6.39	127.83	119.84
3	J	270	ASN	N-CA-C	-6.36	97.26	110.80
2	Z	16	DG	N9-C1'-C2'	-6.34	103.99	113.50
3	F	155	ARG	N-CA-C	-6.31	100.95	110.73
2	D	28	DG	C2'-C3'-O3'	6.26	120.89	111.50
2	L	28	DG	C2'-C3'-O3'	6.23	120.85	111.50
3	J	200	GLN	N-CA-C	-6.23	104.84	112.88
3	S	190	ALA	N-CA-C	-6.23	104.41	111.07
3	F	136	MET	N-CA-C	6.20	124.01	110.80
3	W	137	GLY	N-CA-C	6.15	120.41	112.54
3	N	265	SER	CA-C-N	6.06	133.30	121.41
3	N	265	SER	C-N-CA	6.06	133.30	121.41
3	W	189	ALA	N-CA-C	-6.01	104.30	111.69
2	P	17	DA	C5'-C4'-C3'	-6.00	105.89	114.90
3	J	271	GLU	N-CA-C	-5.99	105.27	113.30
3	E	218	ILE	N-CA-C	5.93	116.10	110.53
3	J	135	HIS	CA-C-O	5.89	121.36	117.94
3	J	135	HIS	CB-CA-C	-5.85	108.65	117.07
3	J	269	GLY	N-CA-C	-5.82	105.93	114.90
2	L	22	DG	N9-C1'-C2'	-5.73	104.91	113.50
2	H	15	DG	O5'-C5'-C4'	5.71	119.36	110.80
3	B	190	ALA	N-CA-C	-5.68	106.47	113.41
3	S	189	ALA	N-CA-C	-5.67	105.11	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	16	DG	C5'-C4'-C3'	-5.65	106.43	114.90
3	N	188	HIS	N-CA-C	-5.64	106.35	113.18
3	J	153	ARG	N-CA-C	-5.61	105.12	112.41
3	W	272	GLU	N-CA-C	-5.60	105.23	112.68
2	Z	22	DG	N9-C1'-C2'	-5.58	105.13	113.50
3	E	180	GLN	N-CA-C	5.57	118.59	107.62
3	A	185	ALA	N-CA-C	-5.57	104.43	111.11
3	S	185	ALA	N-CA-C	-5.55	104.73	112.45
3	M	160	ILE	N-CA-C	5.55	116.27	108.17
2	L	27	DC	N1-C1'-C2'	-5.54	105.19	113.50
2	Z	25	DG	C4'-C3'-O3'	5.51	118.26	110.00
3	M	271	GLU	N-CA-C	-5.48	105.39	111.36
3	W	221	TRP	N-CA-C	5.48	118.18	111.82
3	B	155	ARG	N-CA-C	5.47	121.91	109.81
3	N	264	HIS	N-CA-C	5.47	122.46	110.80
2	D	20	DC	N1-C1'-C2'	-5.46	105.31	113.50
3	J	151	ASN	N-CA-C	5.45	118.13	109.96
3	E	136	MET	N-CA-C	5.42	117.74	108.90
3	S	239	ILE	N-CA-C	5.41	116.04	110.36
3	F	149	SER	N-CA-C	5.41	115.50	107.88
3	E	141	VAL	N-CA-C	5.37	116.51	109.58
3	E	265	SER	N-CA-C	-5.36	105.45	112.41
3	B	214	THR	N-CA-C	-5.35	105.34	111.07
3	I	189	ALA	N-CA-C	-5.35	105.11	111.69
3	E	221	TRP	N-CA-C	5.35	118.59	111.75
3	N	198	LYS	N-CA-C	-5.34	105.63	111.82
3	M	265	SER	N-CA-C	-5.33	106.82	113.38
3	R	172	VAL	N-CA-C	5.31	116.23	108.53
3	N	183	GLN	N-CA-C	5.30	120.40	113.88
2	D	28	DG	C4'-C3'-O3'	5.30	117.94	110.00
3	B	149	SER	N-CA-C	5.29	122.06	110.80
3	B	139	PHE	N-CA-C	5.29	118.15	110.17
3	B	264	HIS	N-CA-C	-5.28	105.48	112.24
3	R	180	GLN	N-CA-C	5.27	117.07	108.63
2	H	15	DG	C2'-C3'-O3'	5.25	119.38	111.50
3	R	190	ALA	N-CA-C	-5.25	105.64	111.36
3	E	189	ALA	N-CA-C	-5.23	105.47	111.07
3	M	234	ALA	N-CA-C	-5.22	106.50	112.92
3	N	278	ARG	N-CA-C	-5.21	106.19	112.54
2	P	20	DC	N1-C1'-C2'	-5.19	105.71	113.50
3	W	273	ALA	N-CA-C	-5.19	104.88	111.11
3	W	245	VAL	N-CA-C	-5.17	105.29	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	196	GLN	N-CA-C	-5.15	105.66	111.28
2	D	15	DG	O5'-C5'-C4'	5.14	118.51	110.80
3	S	183	GLN	N-CA-C	5.14	119.24	112.25
3	N	264	HIS	CA-C-N	5.13	131.34	121.54
3	N	264	HIS	C-N-CA	5.13	131.34	121.54
3	N	189	ALA	N-CA-C	-5.12	105.78	112.23
3	W	233	SER	N-CA-C	-5.10	107.12	113.19
3	M	181	THR	N-CA-C	5.06	116.76	109.07
3	B	196	GLN	N-CA-C	-5.06	105.86	112.23
3	M	233	SER	N-CA-C	-5.04	106.96	113.01
3	J	256	ILE	N-CA-C	5.04	115.34	107.99
3	W	196	GLN	N-CA-C	-5.04	105.79	111.28
3	B	181	THR	N-CA-C	5.02	116.86	108.99
2	H	18	DA	C5'-C4'-C3'	-5.00	107.39	114.90

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	15	DG	Sidechain
2	D	18	DA	Sidechain
2	D	19	DT	Sidechain
2	D	20	DC	Sidechain
2	D	22	DG	Sidechain
2	D	23	DG	Sidechain
2	H	15	DG	Sidechain
2	H	19	DT	Sidechain
2	H	20	DC	Sidechain
2	H	23	DG	Sidechain
2	L	19	DT	Sidechain
2	L	20	DC	Sidechain
2	L	22	DG	Sidechain
2	L	23	DG	Sidechain
2	L	24	DT	Sidechain
2	L	27	DC	Sidechain
2	P	19	DT	Sidechain
2	P	20	DC	Sidechain
2	P	22	DG	Sidechain
2	P	23	DG	Sidechain
2	P	26	DT	Sidechain
2	P	27	DC	Sidechain
2	U	16	DG	Sidechain

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Mol	Chain	Res	Type	Group
2	U	19	DT	Sidechain
2	U	22	DG	Sidechain
2	U	23	DG	Sidechain
2	U	26	DT	Sidechain
2	Z	16	DG	Sidechain
2	Z	20	DC	Sidechain
2	Z	22	DG	Sidechain
2	Z	23	DG	Sidechain
2	Z	24	DT	Sidechain
2	Z	25	DG	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	C	289	0	153	3	0
1	G	289	0	153	13	0
1	K	289	0	153	17	0
1	O	289	0	153	14	0
1	T	289	0	153	13	0
1	X	269	0	142	9	0
2	D	290	0	159	27	0
2	H	290	0	159	33	1
2	L	290	0	159	47	0
2	P	290	0	159	35	0
2	U	290	0	159	41	0
2	Z	229	0	125	36	0
3	A	1186	0	1137	124	0
3	B	1175	0	1144	128	0
3	E	1147	0	1105	130	0
3	F	1175	0	1135	164	0
3	I	1133	0	1074	140	0
3	J	1166	0	1130	118	0
3	M	1117	0	1083	121	0
3	N	1121	0	1075	132	0
3	R	1144	0	1104	120	0
3	S	1126	0	1077	145	0
3	W	1141	0	1101	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	12	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	M	2	0	0	0	0
5	N	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	W	1	0	0	0	0
6	A	12	0	13	1	0
7	B	1	0	0	0	0
8	A	16	0	0	1	0
8	B	15	0	0	4	0
8	C	2	0	0	0	0
8	D	5	0	0	1	0
8	E	16	0	0	4	0
8	F	13	0	0	1	0
8	G	8	0	0	0	0
8	H	9	0	0	0	0
8	I	3	0	0	1	0
8	J	12	0	0	5	0
8	K	4	0	0	1	0
8	L	4	0	0	2	0
8	M	6	0	0	1	0
8	N	7	0	0	0	0
8	O	4	0	0	0	0
8	P	6	0	0	3	0
8	R	7	0	0	2	0
8	S	11	0	0	2	0
8	T	3	0	0	0	0
8	U	3	0	0	0	0
8	W	10	0	0	2	0
8	X	5	0	0	1	0
8	Z	3	0	0	0	0
All	All	16231	0	14017	1668	1

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 56.

All (1668) 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)
2:L:15:DG:H4'	2:L:16:DG:H5'	1.16	1.15
2:L:15:DG:H4'	2:L:16:DG:C5'	1.77	1.14
3:W:199:THR:HG23	3:W:200:GLN:HE21	1.12	1.14
3:A:183:GLN:HE21	3:A:183:GLN:HA	1.10	1.11
3:R:187:ILE:HD11	3:R:243:ASP:HB3	1.37	1.07
3:N:176:LEU:HD12	3:N:177:PRO:HD2	1.31	1.05
3:J:186:GLU:HG2	3:J:211:SER:HB2	1.35	1.05
2:P:15:DG:H2'	2:U:15:DG:H5"	1.35	1.04
3:E:186:GLU:HG2	3:E:211:SER:HB3	1.31	1.04
2:Z:19:DT:H3'	3:W:239:ILE:HD12	1.32	1.03
3:N:256:ILE:HG22	3:N:257:GLN:H	1.24	1.03
3:W:268:ILE:HD13	3:W:268:ILE:H	1.21	1.02
3:F:232:THR:HG23	3:F:234:ALA:H	1.22	1.00
3:N:226:LYS:HA	3:N:226:LYS:HZ3	1.28	0.99
3:R:268:ILE:HD13	3:R:268:ILE:H	1.25	0.97
3:M:196:GLN:O	3:M:199:THR:HG22	1.65	0.97
3:N:175:ARG:HH12	3:N:180:GLN:NE2	1.62	0.97
3:N:228:ASN:HD21	3:N:231:LYS:HB2	1.27	0.97
3:B:183:GLN:HA	3:B:183:GLN:HE21	1.29	0.95
3:F:183:GLN:HE21	3:F:183:GLN:HA	1.30	0.95
3:F:210:ASN:HD22	3:F:210:ASN:H	1.13	0.95
2:L:15:DG:H3'	2:Z:15:DG:H5'	1.45	0.95
3:M:183:GLN:HE21	3:M:183:GLN:HA	1.31	0.94
3:I:182:ASN:ND2	3:I:183:GLN:H	1.66	0.94
3:S:199:THR:HG23	3:S:200:GLN:HE21	1.29	0.94
3:N:228:ASN:HD22	3:N:228:ASN:C	1.76	0.93
3:J:262:PRO:HG2	3:J:265:SER:OG	1.69	0.93
3:B:160:ILE:HD11	3:B:176:LEU:HD13	1.52	0.92
3:N:190:ALA:O	3:N:194:ILE:HG22	1.69	0.91
3:N:186:GLU:HG2	3:N:211:SER:HB2	1.51	0.91
3:I:278:ARG:HH11	3:I:278:ARG:HB2	1.35	0.90
3:N:226:LYS:HA	3:N:226:LYS:NZ	1.86	0.90
3:J:269:GLY:HA2	3:J:272:GLU:HB2	1.52	0.90
3:W:283:GLN:HG3	3:W:284:SER:H	1.34	0.90
3:A:262:PRO:HB2	3:A:265:SER:OG	1.72	0.90
3:E:225:TRP:HA	3:E:228:ASN:ND2	1.87	0.89
3:R:232:THR:HG23	3:R:234:ALA:H	1.36	0.89
3:I:218:ILE:HD13	3:I:247:LEU:HD23	1.55	0.89
3:N:232:THR:HG22	3:N:233:SER:H	1.36	0.88
3:A:182:ASN:ND2	3:A:183:GLN:H	1.72	0.88
3:A:186:GLU:HG2	3:A:211:SER:HB2	1.54	0.88
3:R:212:MET:HE3	3:R:212:MET:HA	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:196:GLN:O	3:S:199:THR:HG22	1.72	0.88
3:E:154:ARG:O	3:E:156:PRO:HD3	1.74	0.88
3:I:204:LYS:HB3	3:I:255:ASP:HB3	1.55	0.86
2:P:15:DG:C2'	2:U:15:DG:H5"	2.06	0.86
3:S:139:PHE:O	3:S:140:VAL:HG12	1.75	0.86
3:E:144:THR:HG21	3:E:190:ALA:HA	1.57	0.86
2:Z:18:DA:H2"	2:Z:19:DT:H5"	1.56	0.86
3:I:187:ILE:HD11	3:I:243:ASP:HB3	1.56	0.85
3:M:186:GLU:HG2	3:M:211:SER:HB3	1.56	0.85
2:L:15:DG:C4'	2:L:16:DG:H5'	2.04	0.85
2:P:15:DG:H2'	2:U:15:DG:C5'	2.05	0.85
3:N:183:GLN:O	3:N:187:ILE:HG22	1.77	0.85
3:F:147:CYS:HB3	3:F:278:ARG:HH21	1.41	0.84
3:F:194:ILE:HD11	3:F:250:LEU:HB3	1.59	0.84
3:S:156:PRO:O	3:S:180:GLN:HG2	1.76	0.84
3:W:281:ALA:O	3:W:282:LYS:HG2	1.76	0.84
3:R:203:ASN:HA	3:R:254:MET:HE1	1.57	0.83
3:A:157:ARG:HH21	3:A:175:ARG:NH1	1.77	0.83
3:R:225:TRP:HA	3:R:228:ASN:ND2	1.92	0.83
2:L:25:DG:H5"	8:L:65:HOH:O	1.77	0.83
3:R:249:ARG:HB2	3:R:249:ARG:NH1	1.93	0.83
2:Z:15:DG:H2"	2:Z:16:DG:OP2	1.78	0.83
3:E:186:GLU:HG2	3:E:211:SER:CB	2.08	0.82
3:I:157:ARG:HB3	3:I:281:ALA:HB1	1.59	0.82
2:L:15:DG:H5"	2:Z:15:DG:H3'	1.61	0.82
2:Z:19:DT:C3'	3:W:239:ILE:HD12	2.08	0.82
3:F:180:GLN:HA	3:F:180:GLN:HE21	1.43	0.82
3:S:274:ASP:O	3:S:278:ARG:HG2	1.79	0.82
3:A:222:VAL:HG13	3:A:223:GLN:H	1.42	0.81
3:W:176:LEU:HD22	3:W:185:ALA:HB2	1.61	0.81
3:F:176:LEU:HD22	3:F:185:ALA:HA	1.62	0.81
3:J:186:GLU:HG2	3:J:211:SER:CB	2.09	0.81
3:N:199:THR:C	3:N:201:ASN:H	1.89	0.81
3:M:232:THR:HG22	3:M:236:LYS:N	1.96	0.80
3:F:210:ASN:HD22	3:F:210:ASN:N	1.77	0.80
3:F:160:ILE:HD11	3:F:176:LEU:HD13	1.63	0.80
2:D:26:DT:H3'	3:A:239:ILE:HD12	1.62	0.80
3:F:135:HIS:HB3	3:F:136:MET:SD	2.21	0.80
3:I:183:GLN:O	3:I:187:ILE:HG23	1.82	0.80
3:B:261:VAL:HG21	3:B:270:ASN:HD21	1.45	0.80
3:A:156:PRO:HB2	3:A:180:GLN:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:145:ASP:HA	3:J:186:GLU:OE2	1.82	0.80
3:F:264:HIS:O	3:F:265:SER:HB3	1.82	0.79
3:N:157:ARG:NH1	3:N:175:ARG:HE	1.80	0.79
3:S:199:THR:HG23	3:S:200:GLN:NE2	1.98	0.79
3:S:207:LEU:HD23	3:S:258:TRP:CZ3	2.17	0.79
3:E:246:ALA:O	3:E:249:ARG:HG2	1.82	0.79
3:R:186:GLU:CG	3:R:211:SER:HB2	2.12	0.79
3:R:187:ILE:CD1	3:R:243:ASP:HB3	2.11	0.79
3:R:225:TRP:HA	3:R:228:ASN:HD21	1.48	0.79
2:U:19:DT:H3'	3:S:239:ILE:HD12	1.62	0.79
2:H:18:DA:C3'	2:H:19:DT:H5"	2.12	0.78
2:H:27:DC:OP1	3:E:239:ILE:HD12	1.84	0.78
3:A:232:THR:CG2	3:A:236:LYS:HG2	2.13	0.78
3:M:228:ASN:C	3:M:228:ASN:HD22	1.92	0.78
3:R:179:ARG:HG2	3:R:179:ARG:HH21	1.49	0.78
2:Z:15:DG:H1'	2:Z:16:DG:C8	2.18	0.78
3:N:157:ARG:HH12	3:N:175:ARG:HE	1.30	0.78
2:L:18:DA:H2"	2:L:19:DT:H5"	1.66	0.78
3:M:217:GLY:O	3:M:222:VAL:HG13	1.83	0.78
3:N:186:GLU:CG	3:N:211:SER:HB2	2.13	0.78
3:A:183:GLN:HA	3:A:183:GLN:NE2	1.91	0.78
3:I:139:PHE:HB3	3:I:205:LEU:HA	1.65	0.78
2:P:15:DG:H4'	2:P:16:DG:O5'	1.84	0.77
3:W:202:ILE:O	3:W:254:MET:HE1	1.84	0.77
3:W:230:TRP:HE3	3:W:238:VAL:HG11	1.47	0.77
2:L:21:DA:H2'	2:L:22:DG:C8	2.19	0.77
3:N:197:ALA:O	3:N:202:ILE:HG22	1.84	0.77
3:W:268:ILE:H	3:W:268:ILE:CD1	1.94	0.77
3:W:268:ILE:HD13	3:W:268:ILE:N	1.99	0.77
1:G:2:G:O6	2:H:27:DC:N4	2.18	0.76
2:L:15:DG:H3'	2:Z:15:DG:C5'	2.14	0.76
3:F:210:ASN:N	3:F:210:ASN:ND2	2.33	0.76
3:F:183:GLN:HA	3:F:183:GLN:NE2	2.00	0.76
3:F:194:ILE:CD1	3:F:250:LEU:HB3	2.15	0.76
2:U:15:DG:H4'	2:U:16:DG:C5'	2.14	0.76
3:R:203:ASN:HA	3:R:254:MET:CE	2.15	0.76
3:S:162:VAL:HG13	3:S:172:VAL:HB	1.68	0.76
1:X:3:A:H2'	1:X:4:C:C6	2.21	0.76
3:E:182:ASN:N	3:E:182:ASN:HD22	1.84	0.76
3:I:186:GLU:HG2	3:I:211:SER:HB3	1.66	0.76
3:I:225:TRP:HA	3:I:228:ASN:HD21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:18:DA:H2"	2:Z:19:DT:C5'	2.15	0.75
3:E:176:LEU:HD12	3:E:177:PRO:HD2	1.67	0.75
3:J:283:GLN:HG2	8:J:1011:HOH:O	1.85	0.75
3:N:268:ILE:HG22	3:N:272:GLU:HG2	1.66	0.75
3:J:268:ILE:HD12	3:J:268:ILE:H	1.51	0.75
3:A:196:GLN:O	3:A:199:THR:HG22	1.86	0.75
3:A:257:GLN:HG3	3:R:220:ASN:HD22	1.50	0.75
3:M:176:LEU:HD12	3:M:177:PRO:HD2	1.68	0.75
3:F:230:TRP:CE3	3:F:241:LYS:HG2	2.22	0.75
3:F:145:ASP:HA	3:F:186:GLU:OE2	1.86	0.75
3:B:205:LEU:HD21	3:B:256:ILE:HD13	1.68	0.74
3:F:192:LYS:O	3:F:196:GLN:HG3	1.86	0.74
3:S:232:THR:HG23	3:S:234:ALA:H	1.52	0.74
3:F:168:HIS:HE1	3:F:170:LEU:HD23	1.52	0.74
3:B:250:LEU:HD12	3:B:250:LEU:H	1.52	0.74
3:S:162:VAL:CG1	3:S:172:VAL:HB	2.18	0.74
3:S:197:ALA:O	3:S:202:ILE:HG22	1.88	0.74
2:U:19:DT:OP1	3:S:181:THR:HG21	1.86	0.74
2:U:25:DG:H2"	2:U:26:DT:C5'	2.17	0.74
3:N:266:GLY:O	3:N:267:PHE:HB2	1.87	0.74
3:S:148:CYS:HB2	3:S:182:ASN:HA	1.68	0.74
2:U:15:DG:H4'	2:U:16:DG:O5'	1.88	0.73
3:F:140:VAL:HG11	3:F:202:ILE:HG13	1.69	0.73
3:S:194:ILE:O	3:S:197:ALA:HB3	1.88	0.73
3:E:160:ILE:HD11	3:E:174:ILE:HD11	1.70	0.73
3:M:203:ASN:HA	3:M:254:MET:SD	2.28	0.73
3:A:168:HIS:CE1	3:A:170:LEU:HB2	2.23	0.73
3:A:172:VAL:HG12	3:A:174:ILE:HG13	1.70	0.73
3:B:205:LEU:HD23	3:B:205:LEU:H	1.54	0.73
3:J:190:ALA:O	3:J:194:ILE:HG22	1.88	0.73
3:S:140:VAL:O	3:S:140:VAL:HG13	1.88	0.73
2:P:15:DG:H5'	2:P:16:DG:O4'	1.89	0.73
3:F:180:GLN:HE21	3:F:180:GLN:CA	2.00	0.73
2:H:18:DA:H3'	2:H:19:DT:H5"	1.71	0.73
3:B:176:LEU:HD22	3:B:185:ALA:HB2	1.69	0.73
3:J:232:THR:C	3:J:234:ALA:H	1.97	0.72
3:S:202:ILE:C	3:S:202:ILE:HD13	2.14	0.72
3:S:176:LEU:HD22	3:S:185:ALA:HB2	1.70	0.72
2:H:18:DA:C2'	2:H:19:DT:H5"	2.20	0.72
2:U:21:DA:H2'	2:U:22:DG:C8	2.23	0.72
3:E:254:MET:HB3	3:E:256:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:210:ASN:HB3	3:S:261:VAL:HG23	1.71	0.72
3:A:160:ILE:HD11	3:A:174:ILE:HD12	1.72	0.72
3:I:196:GLN:O	3:I:200:GLN:HG2	1.89	0.72
3:N:168:HIS:CE1	3:N:170:LEU:HB2	2.25	0.72
3:R:249:ARG:HB2	3:R:249:ARG:HH11	1.52	0.72
3:E:226:LYS:HA	3:E:226:LYS:NZ	2.04	0.71
3:E:249:ARG:HG2	3:E:250:LEU:HD12	1.72	0.71
3:I:157:ARG:HG2	3:I:281:ALA:O	1.89	0.71
3:I:278:ARG:HB2	3:I:278:ARG:NH1	2.05	0.71
3:N:175:ARG:NH1	3:N:180:GLN:NE2	2.37	0.71
3:R:186:GLU:HG2	3:R:211:SER:HB2	1.70	0.71
3:W:140:VAL:O	3:W:205:LEU:HB2	1.91	0.71
2:L:17:DA:H2"	2:L:18:DA:H5'	1.72	0.71
3:B:150:SER:O	3:B:156:PRO:HD3	1.89	0.71
3:B:261:VAL:HG21	3:B:270:ASN:ND2	2.05	0.71
3:N:228:ASN:ND2	3:N:231:LYS:H	1.88	0.71
3:F:175:ARG:HB2	3:F:280:GLY:O	1.91	0.71
3:W:160:ILE:HB	3:W:174:ILE:HG13	1.71	0.71
3:A:145:ASP:HA	8:A:2004:HOH:O	1.89	0.71
3:I:164:TRP:CD1	3:I:170:LEU:HB3	2.25	0.71
3:R:249:ARG:HD3	8:R:1016:HOH:O	1.89	0.71
3:F:211:SER:HB2	8:F:1014:HOH:O	1.90	0.71
3:I:232:THR:C	3:I:234:ALA:H	1.97	0.71
3:J:138:ASP:OD1	3:J:204:LYS:HD2	1.91	0.71
3:J:194:ILE:HD12	3:J:256:ILE:HD11	1.72	0.71
3:R:182:ASN:CG	3:R:183:GLN:H	1.97	0.71
3:R:231:LYS:HE3	3:R:235:GLY:O	1.89	0.71
3:A:139:PHE:CE1	3:A:204:LYS:HD3	2.25	0.71
3:I:200:GLN:HE21	3:I:200:GLN:HA	1.56	0.70
3:M:205:LEU:HD21	3:M:256:ILE:HG12	1.72	0.70
3:A:182:ASN:ND2	3:A:183:GLN:N	2.39	0.70
3:A:176:LEU:HD22	3:A:185:ALA:HA	1.72	0.70
3:J:192:LYS:O	3:J:196:GLN:HG3	1.91	0.70
3:W:199:THR:CG2	3:W:200:GLN:HE21	2.00	0.70
3:W:283:GLN:HG3	3:W:284:SER:N	2.07	0.70
2:D:16:DG:H4'	2:D:16:DG:OP1	1.91	0.70
2:H:19:DT:H3'	3:F:239:ILE:CD1	2.21	0.70
3:J:157:ARG:HG2	3:J:175:ARG:NH2	2.07	0.70
2:U:25:DG:H2"	2:U:26:DT:H5"	1.72	0.70
3:R:249:ARG:O	3:R:252:GLN:HB2	1.92	0.70
3:R:278:ARG:C	3:R:280:GLY:H	1.97	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:241:LYS:O	3:W:245:VAL:HG23	1.92	0.70
3:M:169:PRO:HA	3:R:174:ILE:HG22	1.72	0.69
3:I:187:ILE:CD1	3:I:243:ASP:HB3	2.23	0.69
3:W:230:TRP:HB3	3:W:238:VAL:HG12	1.74	0.69
3:S:261:VAL:HG21	3:S:270:ASN:ND2	2.06	0.69
3:W:196:GLN:O	3:W:199:THR:HG22	1.92	0.69
2:D:19:DT:H3'	3:B:239:ILE:HD11	1.73	0.69
3:B:154:ARG:HG3	3:B:155:ARG:HG2	1.73	0.69
3:E:225:TRP:HA	3:E:228:ASN:HD21	1.54	0.69
3:N:271:GLU:HA	3:N:274:ASP:HB2	1.74	0.69
2:U:23:DG:H2"	2:U:24:DT:OP2	1.93	0.69
3:E:183:GLN:NE2	3:E:213:PHE:CD2	2.61	0.69
3:I:224:GLY:O	3:I:228:ASN:ND2	2.25	0.69
3:N:256:ILE:HG22	3:N:257:GLN:N	2.05	0.69
2:H:15:DG:H4'	2:H:16:DG:H5'	1.75	0.69
3:N:228:ASN:C	3:N:228:ASN:ND2	2.50	0.69
3:N:276:LEU:O	3:N:279:GLU:HB2	1.93	0.69
3:W:160:ILE:HG23	3:W:189:ALA:HA	1.75	0.69
3:B:207:LEU:C	3:B:207:LEU:HD23	2.17	0.68
3:M:232:THR:HG22	3:M:236:LYS:H	1.57	0.68
3:E:205:LEU:HD21	3:E:256:ILE:HD12	1.75	0.68
3:I:184:ARG:HB3	3:I:184:ARG:NH1	2.07	0.68
2:L:25:DG:H1'	3:I:182:ASN:HD21	1.57	0.68
3:E:205:LEU:H	3:E:205:LEU:HD23	1.57	0.68
3:F:184:ARG:HA	3:F:187:ILE:HG23	1.76	0.68
3:W:231:LYS:HD2	3:W:235:GLY:O	1.93	0.68
3:N:204:LYS:HG3	3:N:204:LYS:O	1.94	0.68
3:A:205:LEU:HD23	3:A:205:LEU:N	2.08	0.68
3:B:205:LEU:HD21	3:B:256:ILE:CD1	2.23	0.68
3:F:232:THR:HG23	3:F:234:ALA:N	2.04	0.68
3:N:170:LEU:O	3:N:172:VAL:HG23	1.93	0.68
2:Z:18:DA:C2'	2:Z:19:DT:H5"	2.24	0.68
3:J:148:CYS:HA	3:J:157:ARG:O	1.94	0.68
3:M:184:ARG:HG2	3:M:184:ARG:HH11	1.59	0.67
2:H:21:DA:H2"	2:H:22:DG:H8	1.57	0.67
2:H:26:DT:H3'	3:E:239:ILE:HD13	1.76	0.67
3:F:194:ILE:HD12	3:F:194:ILE:C	2.20	0.67
3:R:158:ALA:H	3:R:180:GLN:HG3	1.59	0.67
3:S:232:THR:C	3:S:234:ALA:H	2.01	0.67
2:L:20:DC:P	3:J:239:ILE:HG12	2.34	0.67
3:R:172:VAL:CG1	3:R:174:ILE:HG23	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:222:VAL:O	3:M:226:LYS:HG3	1.95	0.67
3:R:232:THR:HG23	3:R:234:ALA:N	2.09	0.67
3:A:139:PHE:HB3	3:A:206:VAL:HG23	1.75	0.67
3:A:174:ILE:HG22	3:A:175:ARG:N	2.09	0.67
3:B:156:PRO:O	3:B:180:GLN:HG2	1.95	0.67
3:B:270:ASN:O	3:B:274:ASP:HB2	1.95	0.67
3:R:262:PRO:HB2	3:R:265:SER:HB3	1.76	0.67
3:A:186:GLU:CG	3:A:211:SER:HB2	2.25	0.67
1:K:12:U:H2'	1:K:13:C:H6	1.60	0.67
1:T:11:U:H4'	3:S:212:MET:HG3	1.77	0.67
3:S:142:VAL:HG13	3:S:207:LEU:HD12	1.76	0.66
3:E:182:ASN:HD22	3:E:182:ASN:H	1.43	0.66
3:I:176:LEU:HD12	3:I:177:PRO:HD2	1.77	0.66
3:N:202:ILE:HD13	3:N:203:ASN:N	2.10	0.66
3:S:211:SER:HB2	8:S:1011:HOH:O	1.94	0.66
3:W:197:ALA:O	3:W:202:ILE:HG22	1.94	0.66
3:B:166:PRO:HA	8:B:2015:HOH:O	1.93	0.66
3:E:154:ARG:C	3:E:156:PRO:HD3	2.21	0.66
3:E:249:ARG:CG	3:E:250:LEU:HD12	2.25	0.66
3:N:154:ARG:HD3	3:N:155:ARG:N	2.10	0.66
3:I:160:ILE:HG23	3:I:189:ALA:HA	1.76	0.66
3:J:172:VAL:HA	8:J:1016:HOH:O	1.95	0.66
3:S:179:ARG:HG3	3:S:180:GLN:N	2.10	0.66
3:A:157:ARG:NH2	3:A:175:ARG:NH1	2.43	0.66
3:J:147:CYS:HB3	3:J:278:ARG:NH1	2.09	0.66
3:W:230:TRP:CE3	3:W:241:LYS:HG3	2.30	0.66
3:I:150:SER:HB2	3:I:156:PRO:HA	1.76	0.66
3:S:181:THR:HG22	3:S:184:ARG:N	2.11	0.66
3:W:192:LYS:O	3:W:196:GLN:HG3	1.96	0.66
3:A:232:THR:HG22	3:A:236:LYS:HG2	1.77	0.66
3:A:241:LYS:O	3:A:245:VAL:HG23	1.96	0.66
3:E:253:GLY:O	3:E:254:MET:HG2	1.95	0.66
3:R:183:GLN:HA	3:R:183:GLN:HE21	1.60	0.66
3:S:261:VAL:HG23	3:S:261:VAL:O	1.96	0.66
3:E:278:ARG:HH11	3:E:278:ARG:HG2	1.60	0.66
3:M:208:TYR:HD2	3:M:261:VAL:HG12	1.61	0.66
3:N:225:TRP:HA	3:N:228:ASN:HB3	1.77	0.66
2:H:15:DG:H4'	2:H:16:DG:C5'	2.26	0.65
2:L:27:DC:C2'	2:L:28:DG:H8	2.09	0.65
3:J:232:THR:HG22	3:J:233:SER:N	2.11	0.65
3:N:175:ARG:HH12	3:N:180:GLN:CD	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:210:ASN:H	3:F:210:ASN:ND2	1.88	0.65
3:A:227:LYS:O	3:A:228:ASN:HB3	1.95	0.65
3:I:179:ARG:HH22	3:I:239:ILE:CG2	2.10	0.65
3:M:162:VAL:CG1	3:M:172:VAL:HG12	2.26	0.65
3:F:160:ILE:CG2	3:F:189:ALA:HA	2.27	0.65
3:B:202:ILE:CD1	3:B:204:LYS:H	2.09	0.65
3:F:212:MET:HE2	3:F:212:MET:HA	1.79	0.65
3:A:182:ASN:HD22	3:A:182:ASN:N	1.95	0.65
3:A:187:ILE:HG13	3:A:188:HIS:N	2.10	0.65
3:F:181:THR:OG1	3:F:184:ARG:HG2	1.97	0.65
3:F:199:THR:C	3:F:200:GLN:HG2	2.22	0.65
3:F:202:ILE:HD13	3:F:203:ASN:N	2.12	0.65
3:B:194:ILE:O	3:B:197:ALA:HB3	1.97	0.65
3:S:192:LYS:O	3:S:196:GLN:HG3	1.96	0.65
3:S:262:PRO:HG2	3:S:265:SER:OG	1.97	0.65
3:A:182:ASN:HD22	3:A:183:GLN:H	1.44	0.64
3:N:249:ARG:HA	3:N:252:GLN:NE2	2.12	0.64
3:R:141:VAL:HG22	3:R:206:VAL:HB	1.80	0.64
3:N:249:ARG:O	3:N:252:GLN:HB2	1.97	0.64
3:F:203:ASN:HA	3:F:254:MET:HE2	1.80	0.64
3:J:230:TRP:O	3:J:238:VAL:HG12	1.97	0.64
3:I:201:ASN:HD22	3:I:201:ASN:H	1.46	0.64
3:M:183:GLN:HE21	3:M:183:GLN:CA	2.03	0.64
3:R:263:GLY:C	3:R:265:SER:H	2.04	0.64
3:A:222:VAL:HG13	3:A:223:GLN:N	2.12	0.64
3:E:183:GLN:NE2	3:E:213:PHE:CG	2.66	0.64
3:E:217:GLY:HA3	3:E:244:PHE:CE1	2.31	0.64
3:I:168:HIS:ND1	3:I:170:LEU:HB2	2.11	0.64
2:L:25:DG:H2"	2:L:26:DT:O5'	1.97	0.64
3:R:180:GLN:HE21	3:R:180:GLN:N	1.95	0.64
3:S:202:ILE:HD13	3:S:203:ASN:N	2.13	0.64
3:F:182:ASN:CG	3:F:183:GLN:N	2.55	0.64
3:F:218:ILE:HA	3:F:222:VAL:HG11	1.79	0.64
3:M:176:LEU:HD21	3:M:184:ARG:HG2	1.78	0.64
3:W:251:THR:O	3:W:254:MET:HB2	1.97	0.64
3:J:199:THR:C	3:J:200:GLN:HE21	2.05	0.64
3:A:226:LYS:HE2	3:A:248:GLU:OE1	1.98	0.64
3:W:256:ILE:HG22	3:W:257:GLN:N	2.13	0.64
2:L:27:DC:H2'	2:L:28:DG:H8	1.62	0.64
3:F:179:ARG:O	3:F:184:ARG:HD3	1.98	0.64
3:M:168:HIS:ND1	3:M:169:PRO:HD2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:228:ASN:ND2	3:N:231:LYS:HB2	2.08	0.64
3:S:261:VAL:HG21	3:S:270:ASN:HD21	1.63	0.64
3:W:199:THR:HG23	3:W:200:GLN:NE2	1.98	0.64
3:W:227:LYS:C	3:W:229:GLY:H	2.06	0.64
3:W:274:ASP:O	3:W:278:ARG:HG2	1.98	0.64
2:H:26:DT:OP2	3:E:179:ARG:NH1	2.32	0.63
1:O:5:A:O2'	3:M:186:GLU:OE1	2.16	0.63
3:I:240:ASN:O	3:I:243:ASP:HB2	1.97	0.63
3:J:263:GLY:C	3:J:265:SER:H	2.06	0.63
3:M:194:ILE:HD11	3:M:250:LEU:C	2.23	0.63
2:U:15:DG:H4'	2:U:16:DG:H5'	1.81	0.63
3:F:186:GLU:HG2	3:F:211:SER:HB3	1.80	0.63
3:I:182:ASN:ND2	3:I:183:GLN:N	2.42	0.63
1:X:11:U:H2'	1:X:12:U:C6	2.33	0.63
3:J:176:LEU:HD22	3:J:185:ALA:HA	1.80	0.63
3:J:263:GLY:O	3:J:265:SER:N	2.31	0.63
3:R:179:ARG:HG2	3:R:179:ARG:NH2	2.13	0.63
3:B:183:GLN:HA	3:B:183:GLN:NE2	2.09	0.63
3:M:212:MET:HE3	3:M:216:ASN:OD1	1.98	0.63
3:R:183:GLN:O	3:R:187:ILE:HG23	1.98	0.63
3:W:212:MET:HE2	3:W:212:MET:HA	1.80	0.63
3:R:136:MET:HE1	3:R:208:TYR:OH	1.99	0.62
3:B:228:ASN:O	3:B:231:LYS:HG2	1.99	0.62
3:F:202:ILE:HD13	3:F:202:ILE:C	2.24	0.62
3:I:205:LEU:HD23	3:I:205:LEU:N	2.14	0.62
3:S:218:ILE:HG23	3:S:219:THR:HG23	1.80	0.62
3:I:203:ASN:ND2	3:I:204:LYS:HE2	2.14	0.62
3:F:194:ILE:CG1	3:F:250:LEU:HB3	2.28	0.62
1:O:12:U:OP1	3:N:263:GLY:N	2.32	0.62
3:B:186:GLU:HG2	3:B:211:SER:OG	1.99	0.62
3:E:153:ARG:HG2	3:E:153:ARG:HH11	1.65	0.62
3:S:232:THR:HG23	3:S:234:ALA:N	2.15	0.62
3:E:205:LEU:CD2	3:E:256:ILE:HD12	2.30	0.62
3:F:226:LYS:HB3	3:F:226:LYS:HZ2	1.65	0.62
3:I:150:SER:O	3:I:153:ARG:HB2	2.00	0.62
3:M:257:GLN:OE1	3:M:259:MET:SD	2.57	0.62
3:W:254:MET:HB3	3:W:256:ILE:HD11	1.80	0.62
3:A:172:VAL:CG1	3:A:174:ILE:HG13	2.30	0.62
3:S:148:CYS:CB	3:S:182:ASN:HA	2.29	0.62
1:X:8:U:O2'	1:X:9:G:H5'	2.00	0.61
3:F:141:VAL:HG12	3:F:142:VAL:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:176:LEU:HD12	3:N:177:PRO:CD	2.19	0.61
3:R:263:GLY:C	3:R:265:SER:N	2.54	0.61
3:B:176:LEU:HD12	3:B:177:PRO:HD2	1.81	0.61
3:I:184:ARG:HB3	3:I:184:ARG:HH11	1.63	0.61
3:I:225:TRP:HA	3:I:228:ASN:ND2	2.14	0.61
3:N:162:VAL:CG2	3:N:193:ALA:HB2	2.30	0.61
3:N:162:VAL:HG21	3:N:193:ALA:HB2	1.82	0.61
3:W:212:MET:HE3	3:W:260:HIS:HB2	1.81	0.61
3:M:169:PRO:HA	3:R:174:ILE:CG2	2.29	0.61
3:W:146:GLY:HA3	3:W:186:GLU:HA	1.82	0.61
3:E:262:PRO:O	3:E:263:GLY:O	2.19	0.61
3:S:140:VAL:HG21	3:S:202:ILE:HG13	1.83	0.61
3:R:186:GLU:HG2	3:R:211:SER:CB	2.31	0.61
3:S:142:VAL:HG13	3:S:207:LEU:CD1	2.31	0.61
3:E:228:ASN:HB3	8:E:1013:HOH:O	2.00	0.61
2:P:21:DA:H2"	2:P:22:DG:H8	1.65	0.61
3:A:186:GLU:HG2	3:A:211:SER:CB	2.27	0.61
3:E:170:LEU:O	3:E:172:VAL:HG13	2.00	0.61
3:J:186:GLU:CG	3:J:211:SER:HB2	2.21	0.61
3:A:183:GLN:HE21	3:A:183:GLN:CA	1.94	0.61
3:B:181:THR:HA	8:B:2016:HOH:O	2.00	0.61
3:J:266:GLY:O	3:W:275:ARG:NH2	2.34	0.61
3:M:210:ASN:HB3	3:M:261:VAL:HG22	1.82	0.61
3:N:256:ILE:O	3:N:257:GLN:HB2	1.99	0.61
2:L:15:DG:H4'	2:L:16:DG:O5'	2.01	0.61
2:Z:19:DT:H3'	3:W:239:ILE:CD1	2.20	0.61
3:J:267:PHE:O	3:J:270:ASN:HB3	2.00	0.61
3:S:202:ILE:HD13	3:S:204:LYS:H	1.65	0.61
3:B:176:LEU:HD22	3:B:185:ALA:CB	2.31	0.60
3:S:139:PHE:CD2	3:S:140:VAL:N	2.65	0.60
3:S:230:TRP:CE3	3:S:241:LYS:HG3	2.36	0.60
2:P:28:DG:H5"	3:M:233:SER:HB2	1.83	0.60
3:I:268:ILE:O	3:I:271:GLU:HB2	2.02	0.60
3:M:259:MET:HE3	3:M:259:MET:HA	1.83	0.60
3:B:208:TYR:CD2	3:B:259:MET:HB3	2.37	0.60
3:R:268:ILE:O	3:R:269:GLY:C	2.44	0.60
3:B:160:ILE:HG23	3:B:189:ALA:HA	1.83	0.60
3:B:183:GLN:O	3:B:187:ILE:HG13	2.01	0.60
3:F:210:ASN:HB3	3:F:261:VAL:O	2.01	0.60
2:P:27:DC:OP1	3:M:239:ILE:HG12	2.01	0.60
3:F:197:ALA:O	3:F:202:ILE:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:203:ASN:OD1	3:J:204:LYS:HG2	2.01	0.60
3:M:170:LEU:HG	3:M:196:GLN:NE2	2.15	0.60
3:R:278:ARG:C	3:R:280:GLY:N	2.58	0.60
2:D:18:DA:C2'	2:D:19:DT:H5"	2.31	0.60
3:F:144:THR:HG23	3:F:207:LEU:HD21	1.84	0.60
3:F:230:TRP:CZ3	3:F:241:LYS:HA	2.36	0.60
3:W:179:ARG:HB3	3:W:184:ARG:CZ	2.30	0.60
3:W:259:MET:HE3	3:W:259:MET:HA	1.82	0.60
1:K:11:U:H2'	1:K:12:U:C6	2.36	0.60
3:F:177:PRO:HA	3:F:285:GLU:OE2	2.02	0.60
2:P:25:DG:H2"	2:P:26:DT:H5"	1.82	0.60
3:M:232:THR:HG23	3:M:234:ALA:H	1.67	0.60
3:R:154:ARG:HD3	3:R:154:ARG:N	2.17	0.60
3:W:261:VAL:HG23	3:W:261:VAL:O	2.01	0.60
3:R:140:VAL:O	3:R:205:LEU:HB2	2.02	0.60
3:N:249:ARG:HD3	3:N:249:ARG:C	2.27	0.60
3:A:220:ASN:O	3:A:223:GLN:HG3	2.01	0.59
3:F:209:THR:O	3:F:261:VAL:HG22	2.02	0.59
3:I:182:ASN:CG	3:I:183:GLN:N	2.60	0.59
3:W:143:TYR:CD1	3:W:270:ASN:ND2	2.70	0.59
2:L:20:DC:OP1	3:J:239:ILE:HG12	2.02	0.59
2:Z:20:DC:H2"	2:Z:21:DA:C8	2.37	0.59
3:B:205:LEU:H	3:B:205:LEU:CD2	2.16	0.59
3:F:194:ILE:HD11	3:F:250:LEU:CB	2.32	0.59
3:F:176:LEU:HD22	3:F:185:ALA:CA	2.32	0.59
3:M:160:ILE:O	3:M:160:ILE:HG13	2.00	0.59
3:W:203:ASN:HA	3:W:254:MET:CE	2.31	0.59
1:O:13:C:H2'	1:O:14:C:C6	2.37	0.59
3:A:197:ALA:HB1	3:A:202:ILE:HG23	1.84	0.59
3:B:217:GLY:HA3	3:B:244:PHE:CE1	2.37	0.59
3:E:226:LYS:HA	3:E:226:LYS:HZ3	1.67	0.59
1:O:8:U:H2'	1:O:9:G:O4'	2.00	0.59
3:A:262:PRO:HD3	3:R:257:GLN:OE1	2.03	0.59
3:I:172:VAL:HG12	3:I:174:ILE:H	1.67	0.59
3:J:166:PRO:O	3:J:168:HIS:N	2.35	0.59
3:N:263:GLY:O	3:N:264:HIS:HB3	2.02	0.59
3:W:204:LYS:HB3	3:W:255:ASP:HB3	1.84	0.59
3:W:241:LYS:O	3:W:242:GLU:C	2.45	0.59
2:L:25:DG:C5'	8:L:65:HOH:O	2.43	0.59
3:E:182:ASN:N	3:E:182:ASN:ND2	2.50	0.59
3:F:222:VAL:HG23	3:F:223:GLN:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:261:VAL:O	3:F:261:VAL:HG23	2.01	0.59
3:M:262:PRO:HB2	3:M:265:SER:HB3	1.84	0.59
2:L:20:DC:H2"	2:L:21:DA:C8	2.37	0.59
3:B:199:THR:HG22	3:B:199:THR:O	2.03	0.59
3:B:202:ILE:HD13	3:B:203:ASN:N	2.17	0.59
3:F:241:LYS:O	3:F:245:VAL:HG23	2.02	0.59
3:I:232:THR:C	3:I:234:ALA:N	2.60	0.59
3:J:241:LYS:O	3:J:245:VAL:HG23	2.03	0.59
3:M:275:ARG:HH21	3:M:276:LEU:HD21	1.67	0.59
3:N:228:ASN:HD21	3:N:231:LYS:CB	2.10	0.59
2:U:26:DT:H3'	3:R:239:ILE:HD12	1.84	0.59
3:S:191:CYS:O	3:S:195:GLU:HB2	2.02	0.59
3:S:246:ALA:O	3:S:250:LEU:HD13	2.03	0.59
2:L:27:DC:H2'	2:L:28:DG:C8	2.37	0.59
3:N:157:ARG:HD3	3:N:281:ALA:HB1	1.84	0.59
3:R:160:ILE:HG23	3:R:189:ALA:HA	1.85	0.59
3:W:217:GLY:O	3:W:222:VAL:HG13	2.03	0.59
3:A:168:HIS:HE1	3:A:170:LEU:HB2	1.66	0.59
3:A:183:GLN:O	3:A:187:ILE:HG23	2.03	0.59
3:S:231:LYS:HA	3:S:236:LYS:O	2.03	0.59
3:A:164:TRP:CD1	3:A:170:LEU:HB3	2.38	0.58
3:F:153:ARG:O	3:F:155:ARG:N	2.36	0.58
3:N:262:PRO:O	3:N:263:GLY:C	2.45	0.58
3:S:175:ARG:O	3:S:177:PRO:HD3	2.03	0.58
3:S:182:ASN:C	3:S:182:ASN:ND2	2.61	0.58
1:G:7:C:H2'	1:G:8:U:C6	2.38	0.58
1:K:12:U:H2'	1:K:13:C:C6	2.36	0.58
2:U:18:DA:H2"	2:U:19:DT:O5'	2.03	0.58
3:N:188:HIS:HA	3:N:191:CYS:HB2	1.86	0.58
3:I:278:ARG:HH11	3:I:278:ARG:CB	2.12	0.58
1:G:6:C:H2'	1:G:7:C:H5"	1.86	0.58
1:K:1:C:O2'	1:K:2:G:H5'	2.02	0.58
3:E:196:GLN:O	3:E:199:THR:HG22	2.03	0.58
3:F:194:ILE:HD12	3:F:194:ILE:O	2.03	0.58
3:A:232:THR:HG23	3:A:234:ALA:H	1.67	0.58
3:E:190:ALA:O	3:E:194:ILE:HG22	2.03	0.58
3:W:232:THR:C	3:W:234:ALA:H	2.12	0.58
2:D:28:DG:H5"	3:A:233:SER:HB2	1.86	0.58
3:F:168:HIS:CE1	3:F:170:LEU:HD23	2.38	0.58
3:J:140:VAL:HG22	3:J:202:ILE:HG13	1.84	0.58
3:I:208:TYR:HD2	3:I:261:VAL:HG12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:200:GLN:HE21	3:J:200:GLN:CA	2.16	0.58
3:M:205:LEU:CD2	3:M:256:ILE:HG12	2.32	0.58
2:L:18:DA:C2'	2:L:19:DT:H5"	2.34	0.58
3:J:225:TRP:HB3	3:J:230:TRP:HA	1.85	0.58
3:M:217:GLY:HA2	3:M:221:TRP:CE3	2.38	0.58
2:L:20:DC:H2"	2:L:21:DA:H8	1.67	0.58
3:I:217:GLY:O	3:I:222:VAL:HG13	2.03	0.58
2:P:27:DC:H2"	2:P:28:DG:OP2	2.03	0.58
3:E:208:TYR:HD2	3:E:261:VAL:CG1	2.16	0.58
3:J:136:MET:HG3	3:J:136:MET:O	2.03	0.58
3:J:165:GLY:O	3:J:168:HIS:HB2	2.03	0.58
3:J:179:ARG:NH1	3:J:181:THR:HG21	2.18	0.58
3:M:150:SER:HB3	3:M:153:ARG:HB2	1.85	0.58
3:S:168:HIS:HE1	3:S:170:LEU:HD13	1.69	0.58
3:S:176:LEU:HD22	3:S:185:ALA:CB	2.33	0.58
3:S:179:ARG:HG3	3:S:180:GLN:H	1.68	0.58
3:I:230:TRP:O	3:I:238:VAL:HG13	2.03	0.57
3:W:176:LEU:HD22	3:W:185:ALA:CB	2.32	0.57
2:L:26:DT:O4'	3:I:183:GLN:OE1	2.22	0.57
3:I:201:ASN:HD22	3:I:201:ASN:N	2.00	0.57
3:N:261:VAL:O	3:N:261:VAL:HG13	2.04	0.57
3:B:198:LYS:C	3:B:200:GLN:H	2.12	0.57
3:W:256:ILE:HG22	3:W:257:GLN:H	1.68	0.57
3:E:205:LEU:HD23	3:E:205:LEU:N	2.18	0.57
3:N:163:TYR:CD2	3:N:272:GLU:HB3	2.39	0.57
3:N:203:ASN:O	3:N:255:ASP:N	2.29	0.57
2:U:21:DA:C2'	2:U:22:DG:C8	2.86	0.57
3:A:163:TYR:CD2	3:A:272:GLU:HB3	2.38	0.57
3:E:239:ILE:HD12	3:E:239:ILE:H	1.69	0.57
3:F:134:SER:O	3:F:135:HIS:HB2	2.04	0.57
3:J:166:PRO:C	3:J:168:HIS:H	2.12	0.57
3:M:272:GLU:OE2	3:M:272:GLU:HA	2.03	0.57
3:M:281:ALA:O	3:M:282:LYS:HB2	2.04	0.57
3:W:182:ASN:CG	3:W:183:GLN:N	2.61	0.57
3:S:160:ILE:HG23	3:S:189:ALA:CB	2.35	0.57
3:S:160:ILE:HG23	3:S:189:ALA:HA	1.87	0.57
3:W:140:VAL:HG12	3:W:202:ILE:HG13	1.85	0.57
1:G:7:C:H2'	1:G:8:U:H6	1.70	0.57
2:L:15:DG:O5'	2:Z:15:DG:H5"	2.05	0.57
3:E:192:LYS:O	3:E:196:GLN:HG3	2.05	0.57
3:E:272:GLU:O	3:E:275:ARG:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:158:ALA:N	3:R:180:GLN:HG3	2.19	0.57
3:B:173:GLY:HA3	3:B:276:LEU:HB3	1.87	0.57
3:F:147:CYS:HB3	3:F:278:ARG:NH2	2.16	0.57
3:I:175:ARG:HD2	3:I:176:LEU:N	2.20	0.57
3:I:251:THR:O	3:I:254:MET:HB2	2.03	0.57
3:S:190:ALA:O	3:S:194:ILE:HG22	2.04	0.57
3:E:208:TYR:HD2	3:E:261:VAL:HG13	1.70	0.57
3:R:170:LEU:O	3:R:172:VAL:HG23	2.05	0.57
1:T:11:U:H2'	1:T:12:U:C6	2.40	0.56
3:J:168:HIS:ND1	3:J:169:PRO:HD2	2.20	0.56
3:M:158:ALA:H	3:M:180:GLN:CG	2.17	0.56
2:H:27:DC:H2"	2:H:28:DG:C8	2.40	0.56
3:E:186:GLU:CG	3:E:211:SER:HB3	2.21	0.56
3:E:241:LYS:O	3:E:242:GLU:C	2.47	0.56
3:F:222:VAL:HG23	3:F:223:GLN:N	2.19	0.56
3:J:200:GLN:HA	3:J:200:GLN:NE2	2.20	0.56
3:S:170:LEU:O	3:S:172:VAL:HG23	2.05	0.56
1:G:11:U:H4'	3:F:212:MET:HG3	1.87	0.56
3:A:218:ILE:HG23	3:A:219:THR:HG23	1.86	0.56
3:B:249:ARG:O	3:B:252:GLN:HB2	2.03	0.56
3:M:143:TYR:CE2	3:M:269:GLY:HA3	2.40	0.56
3:N:186:GLU:HG2	3:N:211:SER:CB	2.31	0.56
3:W:212:MET:O	3:W:216:ASN:HB2	2.05	0.56
2:H:21:DA:H2"	2:H:22:DG:C8	2.39	0.56
3:R:186:GLU:HG3	3:R:211:SER:HB2	1.87	0.56
3:J:146:GLY:HA3	3:J:186:GLU:N	2.20	0.56
1:O:1:C:O2'	1:O:2:G:H5'	2.04	0.56
3:E:220:ASN:OD1	3:E:220:ASN:C	2.47	0.56
3:I:191:CYS:O	3:I:192:LYS:C	2.48	0.56
3:N:166:PRO:C	3:N:168:HIS:H	2.13	0.56
2:Z:21:DA:C2'	2:Z:22:DG:C8	2.89	0.56
3:E:182:ASN:CG	3:E:183:GLN:H	2.13	0.56
3:J:172:VAL:HG11	3:J:174:ILE:HD13	1.88	0.56
3:M:227:LYS:C	3:M:229:GLY:H	2.13	0.56
3:W:211:SER:C	3:W:213:PHE:H	2.13	0.56
3:B:218:ILE:HD13	3:B:247:LEU:HD23	1.88	0.56
3:F:194:ILE:HG12	3:F:250:LEU:HB3	1.88	0.56
3:M:183:GLN:O	3:M:184:ARG:C	2.49	0.56
3:M:186:GLU:HG2	3:M:211:SER:CB	2.33	0.56
3:M:251:THR:O	3:M:254:MET:HB2	2.05	0.56
3:B:208:TYR:CE2	3:B:259:MET:HG2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:240:ASN:O	3:E:244:PHE:HD2	1.88	0.56
3:I:232:THR:HG22	3:I:236:LYS:N	2.21	0.56
3:F:160:ILE:HG23	3:F:189:ALA:HA	1.88	0.56
3:M:208:TYR:CD2	3:M:261:VAL:HG12	2.40	0.56
3:R:228:ASN:H	3:R:228:ASN:HD22	1.53	0.56
3:W:278:ARG:HG3	3:W:278:ARG:HH11	1.71	0.56
3:A:232:THR:HG21	3:A:236:LYS:HG2	1.84	0.55
3:E:265:SER:HB2	3:E:267:PHE:CE2	2.41	0.55
3:F:199:THR:CG2	3:F:199:THR:O	2.53	0.55
3:N:256:ILE:HG21	3:N:258:TRP:CE2	2.41	0.55
2:L:15:DG:C3'	2:Z:15:DG:C5'	2.84	0.55
1:K:11:U:H2'	1:K:12:U:H6	1.69	0.55
3:B:153:ARG:C	3:B:155:ARG:N	2.62	0.55
3:B:197:ALA:O	3:B:202:ILE:HG22	2.05	0.55
3:E:176:LEU:HD22	3:E:185:ALA:HA	1.88	0.55
3:R:251:THR:O	3:R:254:MET:HB2	2.06	0.55
3:N:212:MET:HE2	3:N:212:MET:HA	1.88	0.55
3:R:197:ALA:O	3:R:202:ILE:HG22	2.07	0.55
3:S:139:PHE:HD2	3:S:140:VAL:H	1.51	0.55
3:A:154:ARG:O	3:A:156:PRO:HD3	2.07	0.55
3:B:252:GLN:OE1	3:B:252:GLN:HA	2.06	0.55
3:F:149:SER:O	3:F:150:SER:HB2	2.05	0.55
3:W:254:MET:HB3	3:W:256:ILE:CD1	2.36	0.55
3:B:205:LEU:CD2	3:B:205:LEU:N	2.70	0.55
3:R:204:LYS:HB3	3:R:255:ASP:HB3	1.89	0.55
3:A:160:ILE:HD11	3:A:174:ILE:HB	1.89	0.55
3:E:160:ILE:HD11	3:E:174:ILE:CD1	2.37	0.55
3:F:157:ARG:HA	3:F:180:GLN:HG2	1.88	0.55
3:J:156:PRO:HB2	3:J:180:GLN:HB2	1.87	0.55
3:R:150:SER:O	3:R:156:PRO:HA	2.07	0.55
3:R:178:GLY:O	3:R:180:GLN:NE2	2.38	0.55
3:S:202:ILE:C	3:S:202:ILE:CD1	2.80	0.55
3:S:273:ALA:O	3:S:274:ASP:C	2.49	0.55
3:W:135:HIS:O	3:W:136:MET:HB2	2.07	0.55
3:W:141:VAL:HG12	3:W:142:VAL:N	2.21	0.55
3:B:278:ARG:O	3:B:282:LYS:HG3	2.07	0.55
3:F:133:GLY:O	3:F:134:SER:C	2.50	0.55
3:M:174:ILE:HG22	3:R:169:PRO:HA	1.88	0.55
3:M:211:SER:O	3:M:212:MET:C	2.47	0.55
3:R:212:MET:HA	3:R:212:MET:CE	2.26	0.55
2:P:15:DG:H5"	2:U:15:DG:H3'	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:136:MET:SD	3:F:136:MET:N	2.80	0.55
3:N:160:ILE:HG23	3:N:189:ALA:HA	1.88	0.55
3:N:168:HIS:HE1	3:N:170:LEU:HB2	1.67	0.55
3:W:230:TRP:CE3	3:W:238:VAL:HG11	2.35	0.55
1:X:14:C:OP1	3:W:278:ARG:NH2	2.40	0.55
3:A:268:ILE:HA	3:A:271:GLU:HG2	1.89	0.55
3:E:139:PHE:HA	3:E:204:LYS:O	2.07	0.55
3:E:217:GLY:HA3	3:E:244:PHE:HE1	1.71	0.55
3:W:207:LEU:C	3:W:207:LEU:HD23	2.31	0.55
1:T:8:U:O2'	1:T:9:G:H5'	2.06	0.54
3:A:257:GLN:NE2	3:A:259:MET:SD	2.80	0.54
3:F:158:ALA:N	3:F:180:GLN:HG3	2.21	0.54
3:I:197:ALA:HB1	3:I:202:ILE:CG2	2.37	0.54
3:M:205:LEU:HD23	3:M:205:LEU:H	1.72	0.54
3:M:207:LEU:HD23	3:M:258:TRP:CZ3	2.42	0.54
3:W:143:TYR:HD1	3:W:270:ASN:ND2	2.04	0.54
3:I:239:ILE:HG22	3:I:239:ILE:O	2.07	0.54
3:J:138:ASP:O	3:J:139:PHE:HB3	2.07	0.54
3:N:202:ILE:HD13	3:N:202:ILE:C	2.32	0.54
2:P:15:DG:H3'	2:U:15:DG:H3'	1.88	0.54
3:A:257:GLN:HG3	3:R:220:ASN:ND2	2.21	0.54
3:B:225:TRP:HB3	3:B:230:TRP:CD2	2.42	0.54
2:D:18:DA:H1'	3:B:182:ASN:OD1	2.07	0.54
3:M:162:VAL:O	3:M:162:VAL:HG13	2.07	0.54
3:R:268:ILE:H	3:R:268:ILE:CD1	1.97	0.54
3:A:202:ILE:O	3:A:254:MET:HE1	2.07	0.54
3:A:205:LEU:HD23	3:A:205:LEU:H	1.71	0.54
3:A:232:THR:C	3:A:234:ALA:H	2.15	0.54
3:B:160:ILE:HG23	3:B:189:ALA:CB	2.37	0.54
3:F:217:GLY:HA3	3:F:244:PHE:CZ	2.42	0.54
3:I:178:GLY:O	3:I:180:GLN:NE2	2.41	0.54
2:D:18:DA:H2"	3:B:183:GLN:CG	2.36	0.54
3:E:212:MET:O	3:E:213:PHE:C	2.49	0.54
3:M:158:ALA:H	3:M:180:GLN:HG3	1.72	0.54
3:W:231:LYS:HA	3:W:236:LYS:O	2.07	0.54
2:U:18:DA:H4'	3:S:182:ASN:HB3	1.88	0.54
3:E:249:ARG:O	3:E:252:GLN:HB2	2.08	0.54
3:F:198:LYS:C	3:F:200:GLN:H	2.16	0.54
3:I:160:ILE:HD11	3:I:185:ALA:HA	1.90	0.54
3:N:238:VAL:HG22	3:N:238:VAL:O	2.08	0.54
1:G:8:U:H2'	1:G:9:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:230:TRP:HE3	3:W:238:VAL:CG1	2.18	0.54
2:H:15:DG:H5"	2:H:15:DG:N3	2.23	0.54
3:N:161:GLY:HA3	3:N:277:ALA:HB2	1.89	0.54
3:W:280:GLY:O	3:W:281:ALA:C	2.50	0.54
2:P:21:DA:H2"	2:P:22:DG:C8	2.42	0.53
2:U:16:DG:H2"	2:U:17:DA:OP2	2.08	0.53
3:M:195:GLU:HG3	3:M:196:GLN:N	2.23	0.53
3:N:228:ASN:ND2	3:N:228:ASN:O	2.34	0.53
3:S:228:ASN:HD21	3:S:231:LYS:H	1.57	0.53
2:L:18:DA:H2"	2:L:19:DT:C5'	2.37	0.53
3:F:182:ASN:CG	3:F:183:GLN:H	2.17	0.53
3:W:167:GLY:O	3:W:168:HIS:C	2.51	0.53
3:W:212:MET:HG2	3:W:260:HIS:CE1	2.43	0.53
2:L:15:DG:H1'	2:L:16:DG:C8	2.44	0.53
2:Z:15:DG:H4'	2:Z:16:DG:H5'	1.90	0.53
3:F:186:GLU:HG2	3:F:211:SER:CB	2.38	0.53
3:F:200:GLN:O	3:F:201:ASN:C	2.51	0.53
3:W:145:ASP:HA	3:W:186:GLU:OE2	2.09	0.53
3:W:227:LYS:C	3:W:229:GLY:N	2.66	0.53
3:B:197:ALA:HB1	3:B:202:ILE:CG2	2.39	0.53
3:I:175:ARG:HB2	3:I:280:GLY:O	2.08	0.53
3:I:227:LYS:C	3:I:229:GLY:H	2.14	0.53
2:D:18:DA:H2"	3:B:183:GLN:HG2	1.89	0.53
2:Z:21:DA:C2'	2:Z:22:DG:H8	2.22	0.53
3:B:179:ARG:O	3:B:181:THR:HG23	2.07	0.53
3:F:200:GLN:O	3:F:202:ILE:N	2.42	0.53
3:F:272:GLU:O	3:F:276:LEU:HD12	2.08	0.53
3:R:182:ASN:O	3:R:183:GLN:C	2.51	0.53
3:R:208:TYR:HA	3:R:259:MET:O	2.08	0.53
3:W:187:ILE:HD12	3:W:243:ASP:HB3	1.91	0.53
3:W:271:GLU:O	3:W:275:ARG:HG2	2.09	0.53
3:F:248:GLU:HA	3:F:251:THR:OG1	2.09	0.53
3:S:182:ASN:CG	3:S:183:GLN:N	2.66	0.53
3:W:179:ARG:HG3	3:W:180:GLN:N	2.23	0.53
3:I:197:ALA:O	3:I:202:ILE:HG22	2.09	0.53
3:N:154:ARG:HE	3:N:154:ARG:HA	1.74	0.53
2:D:16:DG:H8	2:D:16:DG:H5"	1.74	0.53
1:G:14:C:OP1	3:F:278:ARG:NH1	2.42	0.53
3:B:164:TRP:N	3:B:171:ASN:OD1	2.41	0.53
3:E:168:HIS:ND1	3:E:168:HIS:C	2.65	0.53
3:N:146:GLY:HA3	3:N:186:GLU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:232:THR:HG22	3:N:233:SER:N	2.15	0.53
3:E:184:ARG:HG2	3:E:184:ARG:HH11	1.74	0.53
3:S:256:ILE:HG22	3:S:257:GLN:N	2.24	0.53
2:D:18:DA:C3'	2:D:19:DT:H5"	2.39	0.53
3:E:140:VAL:HG11	3:E:202:ILE:HD12	1.89	0.53
3:R:148:CYS:HA	3:R:157:ARG:O	2.09	0.53
3:S:176:LEU:HD21	3:S:184:ARG:HG3	1.91	0.53
2:L:27:DC:C2'	2:L:28:DG:C8	2.91	0.52
3:F:225:TRP:HA	3:F:228:ASN:OD1	2.09	0.52
3:J:230:TRP:HB3	3:J:238:VAL:CG1	2.38	0.52
3:N:196:GLN:O	3:N:199:THR:HB	2.08	0.52
3:F:232:THR:HG22	3:F:236:LYS:H	1.72	0.52
3:I:279:GLU:OE2	3:I:279:GLU:HA	2.10	0.52
3:J:230:TRP:CG	3:J:241:LYS:HZ2	2.27	0.52
3:J:262:PRO:O	3:J:263:GLY:O	2.27	0.52
1:T:6:C:H2'	1:T:7:C:O4'	2.09	0.52
2:Z:17:DA:H2"	2:Z:18:DA:H5'	1.90	0.52
3:A:208:TYR:CD2	3:A:259:MET:HB3	2.45	0.52
3:E:223:GLN:O	3:E:226:LYS:HB2	2.10	0.52
3:A:148:CYS:SG	3:A:158:ALA:HB2	2.50	0.52
3:E:230:TRP:CD1	3:E:241:LYS:HE3	2.45	0.52
3:F:220:ASN:O	3:F:223:GLN:HG2	2.09	0.52
3:F:258:TRP:H	3:F:258:TRP:CD1	2.28	0.52
3:I:268:ILE:O	3:I:271:GLU:N	2.42	0.52
3:N:145:ASP:OD2	3:N:210:ASN:OD1	2.28	0.52
3:N:194:ILE:HG12	3:N:194:ILE:O	2.09	0.52
3:N:226:LYS:NZ	3:N:230:TRP:HE1	2.07	0.52
3:R:135:HIS:N	3:R:140:VAL:HA	2.25	0.52
3:R:210:ASN:CG	3:R:270:ASN:HD21	2.18	0.52
2:H:24:DT:H2"	2:H:25:DG:H5'	1.91	0.52
3:A:217:GLY:O	3:A:222:VAL:HG12	2.10	0.52
3:I:203:ASN:HD21	3:I:204:LYS:HE2	1.74	0.52
3:J:181:THR:HA	8:J:1012:HOH:O	2.09	0.52
3:S:140:VAL:HG11	3:S:202:ILE:HD11	1.90	0.52
2:H:19:DT:H3'	3:F:239:ILE:HD12	1.90	0.52
2:Z:21:DA:H2"	2:Z:22:DG:H8	1.74	0.52
3:A:157:ARG:HG2	3:A:157:ARG:HH11	1.74	0.52
3:F:160:ILE:HD11	3:F:176:LEU:HB2	1.91	0.52
3:M:176:LEU:HD12	3:M:177:PRO:CD	2.37	0.52
3:N:199:THR:HG22	3:N:200:GLN:N	2.24	0.52
3:S:208:TYR:HD2	3:S:261:VAL:CG1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:154:ARG:HA	3:N:154:ARG:NE	2.24	0.52
3:N:202:ILE:HD13	3:N:204:LYS:H	1.75	0.52
2:L:15:DG:H5"	2:Z:15:DG:C3'	2.37	0.52
3:A:174:ILE:CG2	3:A:175:ARG:N	2.73	0.52
3:I:139:PHE:CD2	3:I:204:LYS:HB2	2.45	0.52
3:N:143:TYR:O	3:N:162:VAL:HA	2.10	0.52
3:N:230:TRP:HE3	3:N:238:VAL:HG11	1.74	0.52
3:W:197:ALA:C	3:W:202:ILE:HG22	2.35	0.52
3:W:203:ASN:HA	3:W:254:MET:HE1	1.91	0.52
2:L:21:DA:H2'	2:L:22:DG:H8	1.70	0.51
3:I:200:GLN:HE21	3:I:200:GLN:CA	2.17	0.51
3:I:241:LYS:O	3:I:245:VAL:HG23	2.09	0.51
3:J:194:ILE:HG12	3:J:194:ILE:O	2.09	0.51
3:M:211:SER:HB2	8:M:100:HOH:O	2.10	0.51
3:W:202:ILE:HD11	3:W:204:LYS:O	2.11	0.51
2:P:19:DT:H3'	3:N:239:ILE:HD12	1.91	0.51
2:U:25:DG:H2"	2:U:26:DT:O5'	2.10	0.51
3:E:206:VAL:HG12	3:E:208:TYR:CE1	2.45	0.51
3:F:143:TYR:HB2	3:F:163:TYR:HB3	1.91	0.51
3:F:203:ASN:HA	3:F:254:MET:CE	2.40	0.51
3:I:208:TYR:HD2	3:I:261:VAL:CG1	2.23	0.51
3:J:175:ARG:H	3:J:283:GLN:NE2	2.09	0.51
2:P:19:DT:H2"	2:P:20:DC:C6	2.45	0.51
3:B:202:ILE:HD13	3:B:204:LYS:H	1.75	0.51
3:F:187:ILE:HG12	3:F:188:HIS:N	2.24	0.51
3:F:212:MET:HG2	3:F:260:HIS:CE1	2.46	0.51
3:I:157:ARG:HG2	3:I:157:ARG:HH11	1.76	0.51
3:N:274:ASP:O	3:N:278:ARG:HG2	2.10	0.51
3:R:268:ILE:O	3:R:271:GLU:N	2.43	0.51
3:S:179:ARG:HG2	3:S:179:ARG:NH2	2.25	0.51
2:H:19:DT:P	3:F:179:ARG:HH22	2.34	0.51
3:A:263:GLY:C	3:A:265:SER:H	2.18	0.51
3:E:258:TRP:C	3:E:259:MET:HG2	2.36	0.51
3:F:154:ARG:HG2	3:F:156:PRO:HD3	1.92	0.51
3:F:217:GLY:O	3:F:222:VAL:HG13	2.10	0.51
3:M:157:ARG:HG2	3:M:281:ALA:HB1	1.93	0.51
3:M:209:THR:OG1	3:M:210:ASN:N	2.42	0.51
3:N:266:GLY:O	3:N:267:PHE:CB	2.58	0.51
2:U:23:DG:C2'	2:U:24:DT:OP2	2.58	0.51
3:B:220:ASN:O	3:B:223:GLN:NE2	2.43	0.51
3:I:171:ASN:HD22	3:I:276:LEU:HD11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:202:ILE:HG23	3:I:202:ILE:O	2.11	0.51
3:J:200:GLN:CA	3:J:200:GLN:NE2	2.72	0.51
3:S:179:ARG:HB3	3:S:184:ARG:HD3	1.93	0.51
3:W:263:GLY:O	3:W:264:HIS:HB2	2.10	0.51
3:M:261:VAL:HG23	3:M:262:PRO:O	2.11	0.51
3:S:212:MET:HG2	3:S:260:HIS:CE1	2.46	0.51
3:W:154:ARG:O	3:W:155:ARG:C	2.53	0.51
1:T:12:U:H2'	1:T:13:C:H6	1.75	0.51
3:F:203:ASN:OD1	3:F:204:LYS:N	2.44	0.51
3:S:265:SER:O	3:S:266:GLY:O	2.28	0.51
3:W:232:THR:OG1	3:W:233:SER:N	2.42	0.51
3:B:160:ILE:CG2	3:B:189:ALA:HA	2.41	0.51
3:I:225:TRP:C	3:I:227:LYS:H	2.19	0.51
3:J:149:SER:N	3:J:157:ARG:O	2.43	0.51
3:R:232:THR:OG1	3:R:233:SER:N	2.41	0.51
3:B:150:SER:HB3	3:B:155:ARG:HB2	1.93	0.51
3:E:249:ARG:CG	3:E:250:LEU:N	2.73	0.51
3:M:279:GLU:OE2	3:M:279:GLU:HA	2.10	0.51
3:R:176:LEU:HD12	3:R:177:PRO:HD2	1.93	0.51
3:B:206:VAL:HG13	3:B:259:MET:HE3	1.93	0.51
3:F:218:ILE:HG23	3:F:219:THR:HG23	1.91	0.51
3:M:192:LYS:O	3:M:196:GLN:HG3	2.11	0.51
3:S:208:TYR:CE2	3:S:259:MET:HG2	2.46	0.51
3:W:194:ILE:O	3:W:197:ALA:HB3	2.11	0.51
3:W:210:ASN:HB3	3:W:261:VAL:O	2.11	0.51
3:A:194:ILE:HG21	3:A:250:LEU:HB3	1.91	0.50
3:J:269:GLY:HA2	3:J:272:GLU:CB	2.35	0.50
3:S:261:VAL:O	3:S:262:PRO:O	2.29	0.50
2:D:16:DG:H2'	2:D:17:DA:C8	2.47	0.50
2:L:15:DG:C5'	2:Z:15:DG:H5"	2.41	0.50
2:P:28:DG:OP2	2:P:28:DG:H8	1.95	0.50
2:Z:20:DC:OP1	3:W:239:ILE:HG13	2.11	0.50
3:E:210:ASN:OD1	3:E:210:ASN:N	2.44	0.50
3:F:133:GLY:O	3:F:135:HIS:ND1	2.43	0.50
3:F:215:ILE:HG12	3:F:258:TRP:HB3	1.93	0.50
3:M:195:GLU:HB3	3:M:250:LEU:HD21	1.91	0.50
2:Z:21:DA:H2'	2:Z:22:DG:C8	2.47	0.50
3:A:251:THR:O	3:A:254:MET:HB2	2.11	0.50
3:B:258:TRP:C	3:B:259:MET:HE2	2.37	0.50
3:J:212:MET:HA	3:J:212:MET:HE2	1.93	0.50
3:N:153:ARG:HE	3:N:153:ARG:HA	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:218:ILE:HD13	3:N:247:LEU:HD23	1.94	0.50
3:R:263:GLY:O	3:R:265:SER:N	2.45	0.50
3:B:262:PRO:O	3:B:263:GLY:C	2.53	0.50
3:M:230:TRP:HB3	3:M:238:VAL:CG1	2.42	0.50
3:S:196:GLN:O	3:S:199:THR:N	2.44	0.50
3:W:143:TYR:HB2	3:W:163:TYR:HB3	1.92	0.50
3:W:262:PRO:O	3:W:263:GLY:C	2.55	0.50
2:P:17:DA:N6	2:P:18:DA:C6	2.79	0.50
2:U:17:DA:H2"	2:U:18:DA:H5'	1.94	0.50
2:U:18:DA:H2"	2:U:19:DT:C5'	2.41	0.50
3:W:156:PRO:O	3:W:180:GLN:HG2	2.12	0.50
3:A:226:LYS:NZ	3:A:226:LYS:HB3	2.27	0.50
3:B:139:PHE:CD1	3:B:139:PHE:N	2.78	0.50
3:F:144:THR:CG2	3:F:207:LEU:HD21	2.42	0.50
3:F:271:GLU:O	3:F:274:ASP:HB2	2.11	0.50
3:I:187:ILE:HB	3:I:214:THR:HG23	1.93	0.50
3:J:182:ASN:C	3:J:182:ASN:ND2	2.66	0.50
3:M:140:VAL:HG21	3:M:202:ILE:HD12	1.92	0.50
3:W:203:ASN:HA	3:W:254:MET:HE2	1.94	0.50
2:P:23:DG:H2"	2:P:24:DT:OP2	2.12	0.50
3:B:192:LYS:O	3:B:196:GLN:HG3	2.11	0.50
3:B:248:GLU:HA	3:B:251:THR:OG1	2.12	0.50
3:E:202:ILE:HG22	3:E:203:ASN:N	2.27	0.50
3:I:208:TYR:CD2	3:I:261:VAL:HG12	2.46	0.50
3:J:192:LYS:O	3:J:195:GLU:HB3	2.12	0.50
3:F:252:GLN:OE1	3:F:252:GLN:HA	2.12	0.50
3:N:138:ASP:O	3:N:204:LYS:HD2	2.12	0.50
3:R:197:ALA:HB1	3:R:202:ILE:CG2	2.42	0.50
3:S:140:VAL:O	3:S:140:VAL:CG1	2.58	0.50
3:S:196:GLN:O	3:S:197:ALA:C	2.54	0.50
3:A:160:ILE:CD1	3:A:174:ILE:HB	2.41	0.50
3:B:221:TRP:O	3:B:225:TRP:CD2	2.65	0.50
3:J:144:THR:OG1	3:J:207:LEU:HD21	2.10	0.50
3:J:218:ILE:HD13	3:J:247:LEU:HD23	1.93	0.50
3:S:147:CYS:HB3	8:S:1008:HOH:O	2.11	0.49
3:R:154:ARG:O	3:R:156:PRO:HD3	2.12	0.49
3:S:202:ILE:HD13	3:S:204:LYS:N	2.26	0.49
3:W:222:VAL:HG23	3:W:223:GLN:N	2.27	0.49
3:A:222:VAL:HG13	3:A:223:GLN:HG2	1.94	0.49
3:F:208:TYR:CE2	3:F:259:MET:HG2	2.47	0.49
3:I:229:GLY:O	3:I:230:TRP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:143:TYR:CE2	3:N:269:GLY:HA3	2.47	0.49
2:P:17:DA:C2'	2:P:18:DA:O5'	2.60	0.49
3:A:283:GLN:O	3:A:284:SER:HB2	2.11	0.49
3:E:145:ASP:OD1	3:E:274:ASP:HA	2.13	0.49
3:E:168:HIS:HE1	3:E:170:LEU:HD13	1.77	0.49
3:E:192:LYS:O	3:E:193:ALA:C	2.55	0.49
3:E:241:LYS:O	3:E:245:VAL:HG23	2.11	0.49
3:I:270:ASN:O	3:I:274:ASP:HB2	2.13	0.49
3:M:257:GLN:HE22	3:M:259:MET:HE1	1.78	0.49
3:W:196:GLN:O	3:W:197:ALA:C	2.56	0.49
1:K:5:A:H5"	8:K:88:HOH:O	2.11	0.49
3:E:166:PRO:O	3:E:167:GLY:C	2.55	0.49
3:E:204:LYS:HA	3:E:255:ASP:O	2.12	0.49
3:F:268:ILE:O	3:F:271:GLU:N	2.45	0.49
3:J:274:ASP:O	3:J:278:ARG:HG2	2.13	0.49
3:N:166:PRO:O	3:N:168:HIS:N	2.46	0.49
3:W:202:ILE:O	3:W:202:ILE:HG23	2.12	0.49
3:A:230:TRP:CE3	3:A:241:LYS:HG3	2.48	0.49
3:F:180:GLN:HA	3:F:180:GLN:NE2	2.20	0.49
3:N:168:HIS:CG	3:N:169:PRO:HD2	2.47	0.49
3:N:170:LEU:HG	3:N:196:GLN:NE2	2.27	0.49
3:E:197:ALA:O	3:E:202:ILE:HB	2.11	0.49
3:M:184:ARG:HH11	3:M:184:ARG:CG	2.23	0.49
3:S:276:LEU:O	3:S:279:GLU:HB3	2.13	0.49
2:D:21:DA:H2'	2:D:22:DG:H8	1.78	0.49
2:P:27:DC:C2'	2:P:28:DG:OP2	2.61	0.49
3:E:140:VAL:O	3:E:205:LEU:HB2	2.12	0.49
3:I:217:GLY:HA2	3:I:221:TRP:HB2	1.94	0.49
3:M:278:ARG:C	3:M:280:GLY:N	2.70	0.49
3:N:160:ILE:HD11	3:N:176:LEU:HD13	1.95	0.49
3:S:181:THR:CG2	3:S:184:ARG:HB3	2.42	0.49
1:C:8:U:O2'	1:C:9:G:H5'	2.12	0.49
2:H:20:DC:H2"	2:H:21:DA:OP2	2.12	0.49
2:U:25:DG:C2'	2:U:26:DT:H5"	2.42	0.49
3:B:186:GLU:HG2	3:B:211:SER:CB	2.42	0.49
3:E:232:THR:O	3:E:233:SER:C	2.56	0.49
3:I:200:GLN:CA	3:I:200:GLN:NE2	2.72	0.49
3:J:230:TRP:HB3	3:J:238:VAL:HG11	1.94	0.49
2:L:15:DG:H2"	2:L:16:DG:OP2	2.12	0.49
1:X:6:C:H3'	8:X:16:HOH:O	2.12	0.49
3:E:158:ALA:CB	3:E:180:GLN:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:182:ASN:CG	3:E:183:GLN:N	2.70	0.49
3:J:175:ARG:HB2	3:J:283:GLN:HB2	1.95	0.49
3:J:198:LYS:HE3	3:J:250:LEU:O	2.13	0.49
3:J:271:GLU:HG3	3:W:275:ARG:HH12	1.78	0.49
3:S:160:ILE:HD12	3:S:189:ALA:CA	2.42	0.49
3:W:186:GLU:HG2	3:W:211:SER:HB3	1.94	0.49
2:D:15:DG:H4'	2:D:16:DG:OP1	2.12	0.48
3:A:141:VAL:HG12	3:A:142:VAL:N	2.27	0.48
3:F:156:PRO:O	3:F:180:GLN:HG2	2.13	0.48
3:F:187:ILE:CD1	3:F:243:ASP:HB3	2.43	0.48
3:I:160:ILE:CG2	3:I:189:ALA:HA	2.43	0.48
3:M:194:ILE:HD11	3:M:250:LEU:O	2.13	0.48
3:N:183:GLN:O	3:N:184:ARG:C	2.54	0.48
3:N:272:GLU:O	3:N:276:LEU:HB2	2.13	0.48
3:S:168:HIS:ND1	3:S:169:PRO:HD2	2.28	0.48
2:P:21:DA:C2'	2:P:22:DG:C8	2.97	0.48
3:A:265:SER:O	3:R:136:MET:HG2	2.13	0.48
3:B:232:THR:HG22	3:B:236:LYS:N	2.28	0.48
3:I:203:ASN:ND2	8:I:71:HOH:O	2.46	0.48
3:R:160:ILE:HD11	3:R:176:LEU:HD13	1.94	0.48
1:K:8:U:O2'	3:I:153:ARG:NH2	2.46	0.48
2:P:15:DG:C4'	2:P:16:DG:O5'	2.58	0.48
2:P:19:DT:H2"	2:P:20:DC:H6	1.78	0.48
3:E:168:HIS:HE1	3:E:170:LEU:HD22	1.78	0.48
3:E:207:LEU:HD22	3:E:258:TRP:CE3	2.48	0.48
3:E:228:ASN:OD1	3:E:231:LYS:HB2	2.12	0.48
3:I:179:ARG:HH22	3:I:239:ILE:HG22	1.78	0.48
3:J:140:VAL:CG2	3:J:202:ILE:HG13	2.43	0.48
3:M:239:ILE:N	3:M:239:ILE:HD13	2.28	0.48
3:R:259:MET:HE3	3:R:259:MET:HA	1.93	0.48
2:D:25:DG:H2"	2:D:26:DT:C5'	2.43	0.48
1:T:11:U:C4'	3:S:212:MET:HG3	2.42	0.48
3:A:176:LEU:HD22	3:A:185:ALA:CA	2.42	0.48
3:E:203:ASN:HA	3:E:254:MET:SD	2.54	0.48
3:I:163:TYR:HD2	3:I:171:ASN:HD21	1.59	0.48
3:I:268:ILE:O	3:I:269:GLY:C	2.55	0.48
3:M:232:THR:HG23	3:M:234:ALA:N	2.27	0.48
3:M:263:GLY:O	3:M:264:HIS:C	2.56	0.48
3:N:230:TRP:CE3	3:N:241:LYS:HG2	2.48	0.48
3:S:232:THR:C	3:S:234:ALA:N	2.69	0.48
1:O:12:U:H2'	1:O:13:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:168:HIS:CG	3:A:169:PRO:HD2	2.48	0.48
3:A:204:LYS:HB3	3:A:255:ASP:HB3	1.95	0.48
3:E:270:ASN:ND2	8:E:1012:HOH:O	2.46	0.48
3:I:248:GLU:O	3:I:251:THR:HB	2.14	0.48
3:N:245:VAL:CG1	3:N:246:ALA:N	2.76	0.48
3:A:141:VAL:CG1	3:A:142:VAL:N	2.76	0.48
3:A:257:GLN:HA	6:A:2002:MES:O1S	2.12	0.48
3:A:279:GLU:OE2	3:A:282:LYS:HE3	2.13	0.48
3:F:136:MET:HB2	3:F:137:GLY:H	1.46	0.48
3:R:230:TRP:HB2	8:R:1014:HOH:O	2.12	0.48
3:S:225:TRP:HA	3:S:228:ASN:OD1	2.14	0.48
3:S:256:ILE:HG22	3:S:257:GLN:H	1.79	0.48
3:W:231:LYS:NZ	3:W:237:GLU:HG2	2.29	0.48
2:D:17:DA:H2"	2:D:18:DA:H5"	1.96	0.48
2:H:15:DG:N3	2:H:15:DG:C5'	2.76	0.48
3:B:153:ARG:C	3:B:153:ARG:HD2	2.38	0.48
3:E:206:VAL:CG1	3:E:208:TYR:CE1	2.96	0.48
3:E:168:HIS:CE1	3:E:170:LEU:HD22	2.49	0.48
3:E:267:PHE:O	3:E:268:ILE:C	2.57	0.48
3:J:146:GLY:H	3:J:186:GLU:CD	2.21	0.48
3:J:197:ALA:HB1	3:J:202:ILE:HG22	1.96	0.48
3:J:230:TRP:CH2	3:J:245:VAL:HG22	2.49	0.48
3:N:160:ILE:CG2	3:N:189:ALA:HA	2.44	0.48
2:D:21:DA:H2'	2:D:22:DG:C8	2.48	0.48
2:P:25:DG:H2"	2:P:26:DT:C5'	2.44	0.48
3:J:168:HIS:CE1	3:J:170:LEU:HD13	2.49	0.48
3:M:211:SER:C	3:M:213:PHE:N	2.65	0.48
3:M:227:LYS:O	3:M:229:GLY:N	2.44	0.48
3:R:146:GLY:HA3	3:R:186:GLU:HA	1.96	0.48
3:R:182:ASN:CG	3:R:183:GLN:N	2.65	0.48
3:W:196:GLN:O	3:W:199:THR:N	2.47	0.48
2:D:16:DG:H5"	2:D:16:DG:C8	2.48	0.48
3:J:232:THR:C	3:J:234:ALA:N	2.64	0.48
2:H:20:DC:H2"	2:H:21:DA:C8	2.48	0.47
3:E:158:ALA:HB2	3:E:180:GLN:HG3	1.95	0.47
3:E:230:TRP:HE3	3:E:238:VAL:HG21	1.79	0.47
3:M:281:ALA:O	3:M:282:LYS:CB	2.60	0.47
3:N:168:HIS:ND1	3:N:169:PRO:HD2	2.28	0.47
3:R:137:GLY:C	3:R:139:PHE:H	2.22	0.47
3:R:143:TYR:O	3:R:162:VAL:HA	2.13	0.47
3:R:148:CYS:HA	3:R:158:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:158:ALA:H	3:R:180:GLN:CG	2.26	0.47
3:R:160:ILE:CG2	3:R:189:ALA:HA	2.43	0.47
3:S:157:ARG:HG2	3:S:175:ARG:CZ	2.43	0.47
3:S:176:LEU:HD13	3:S:185:ALA:HA	1.95	0.47
3:S:276:LEU:O	3:S:279:GLU:N	2.45	0.47
1:T:11:U:H4'	3:S:212:MET:CG	2.43	0.47
3:B:158:ALA:N	3:B:180:GLN:HG3	2.29	0.47
3:B:264:HIS:CD2	3:B:264:HIS:N	2.82	0.47
3:F:186:GLU:O	3:F:189:ALA:HB3	2.14	0.47
3:F:202:ILE:C	3:F:202:ILE:CD1	2.87	0.47
3:I:222:VAL:HG23	3:I:223:GLN:N	2.29	0.47
3:J:166:PRO:C	3:J:168:HIS:N	2.71	0.47
3:J:283:GLN:CG	8:J:1011:HOH:O	2.54	0.47
3:N:250:LEU:C	3:N:252:GLN:N	2.71	0.47
3:R:187:ILE:HD11	3:R:243:ASP:CB	2.27	0.47
3:S:179:ARG:HG2	3:S:179:ARG:HH21	1.79	0.47
1:C:5:A:C2	1:C:6:C:C2	3.01	0.47
1:T:4:C:H2'	1:T:5:A:O4'	2.15	0.47
2:U:25:DG:H4'	3:R:181:THR:HB	1.95	0.47
3:B:175:ARG:HD2	3:B:283:GLN:O	2.14	0.47
3:B:225:TRP:HA	3:B:228:ASN:OD1	2.15	0.47
3:E:191:CYS:SG	3:E:247:LEU:HD13	2.55	0.47
3:I:240:ASN:HB3	3:I:243:ASP:HB2	1.97	0.47
3:J:232:THR:CG2	3:J:233:SER:N	2.76	0.47
3:J:246:ALA:O	3:J:247:LEU:C	2.58	0.47
3:S:208:TYR:CZ	3:S:259:MET:HG2	2.50	0.47
3:S:241:LYS:O	3:S:242:GLU:C	2.56	0.47
2:Z:21:DA:H2"	2:Z:22:DG:C8	2.49	0.47
3:A:254:MET:HB3	3:A:256:ILE:HD11	1.96	0.47
3:A:283:GLN:O	3:A:284:SER:CB	2.63	0.47
3:B:266:GLY:O	3:B:267:PHE:HB2	2.15	0.47
3:F:212:MET:HA	3:F:212:MET:CE	2.43	0.47
3:I:218:ILE:CG2	3:I:219:THR:HG23	2.45	0.47
3:J:176:LEU:HD12	3:J:177:PRO:HD2	1.96	0.47
3:N:222:VAL:HG23	3:N:223:GLN:N	2.30	0.47
3:W:232:THR:C	3:W:234:ALA:N	2.72	0.47
2:P:18:DA:C2'	2:P:19:DT:H5"	2.44	0.47
3:B:141:VAL:HG12	3:B:142:VAL:N	2.29	0.47
3:B:232:THR:O	3:B:234:ALA:N	2.39	0.47
3:E:160:ILE:O	3:E:160:ILE:HG13	2.13	0.47
3:F:199:THR:O	3:F:200:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:197:ALA:HB1	3:I:202:ILE:HG23	1.96	0.47
3:I:227:LYS:C	3:I:229:GLY:N	2.72	0.47
3:J:135:HIS:O	3:J:136:MET:HB3	2.14	0.47
3:J:200:GLN:HE21	3:J:200:GLN:HA	1.75	0.47
3:J:278:ARG:O	3:J:281:ALA:HB3	2.14	0.47
3:R:176:LEU:HD22	3:R:185:ALA:HB2	1.97	0.47
2:L:27:DC:O3'	3:I:225:TRP:HZ2	1.96	0.47
3:B:230:TRP:CE3	3:B:241:LYS:HG3	2.50	0.47
3:B:238:VAL:HG22	3:B:238:VAL:O	2.13	0.47
3:B:252:GLN:C	3:B:254:MET:H	2.22	0.47
3:E:278:ARG:HG2	3:E:278:ARG:NH1	2.27	0.47
3:J:268:ILE:H	3:J:268:ILE:CD1	2.18	0.47
3:R:230:TRP:CD1	3:R:230:TRP:N	2.83	0.47
2:H:21:DA:H5"	3:F:221:TRP:CD1	2.48	0.47
2:U:19:DT:C4	2:U:20:DC:N4	2.83	0.47
1:X:5:A:H61	2:Z:24:DT:H3	1.62	0.47
3:B:134:SER:O	3:B:135:HIS:O	2.31	0.47
3:F:208:TYR:CD2	3:F:259:MET:HB3	2.50	0.47
3:F:275:ARG:NH1	3:F:275:ARG:HG2	2.29	0.47
3:I:191:CYS:O	3:I:194:ILE:HG12	2.15	0.47
3:I:262:PRO:HB2	3:I:265:SER:HB3	1.97	0.47
3:J:146:GLY:HA3	3:J:186:GLU:HA	1.97	0.47
3:J:182:ASN:CG	3:J:183:GLN:N	2.72	0.47
3:J:197:ALA:HB1	3:J:202:ILE:CG2	2.44	0.47
3:M:183:GLN:CA	3:M:183:GLN:NE2	2.76	0.47
3:N:154:ARG:NE	3:N:154:ARG:CA	2.78	0.47
3:R:156:PRO:HB2	3:R:180:GLN:HB3	1.96	0.47
3:S:138:ASP:OD1	3:S:139:PHE:N	2.48	0.47
3:S:181:THR:HG23	3:S:182:ASN:N	2.30	0.47
3:W:176:LEU:HD21	3:W:184:ARG:HG2	1.97	0.47
2:U:15:DG:N3	2:U:15:DG:O5'	2.48	0.47
3:B:268:ILE:O	3:B:269:GLY:C	2.58	0.47
3:F:187:ILE:HD11	3:F:243:ASP:C	2.40	0.47
3:F:202:ILE:HG23	3:F:202:ILE:O	2.15	0.47
3:F:207:LEU:HD13	3:F:258:TRP:CZ3	2.50	0.47
3:N:222:VAL:O	3:N:226:LYS:HG2	2.14	0.47
3:S:202:ILE:HG23	3:S:202:ILE:O	2.15	0.47
3:F:199:THR:HG22	3:F:200:GLN:HG2	1.97	0.47
3:I:272:GLU:HA	3:I:275:ARG:HH11	1.80	0.47
3:W:139:PHE:O	3:W:139:PHE:CD1	2.68	0.47
3:A:205:LEU:N	3:A:205:LEU:CD2	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:168:HIS:CE1	3:E:170:LEU:HB2	2.49	0.47
3:E:230:TRP:CE3	3:E:238:VAL:HG21	2.50	0.47
3:I:192:LYS:O	3:I:196:GLN:HG3	2.15	0.47
3:I:261:VAL:HG21	3:I:270:ASN:HD22	1.79	0.47
3:M:239:ILE:CD1	3:M:239:ILE:H	2.26	0.47
3:W:172:VAL:HG12	3:W:174:ILE:HG23	1.96	0.47
3:W:202:ILE:HD13	3:W:203:ASN:N	2.30	0.47
2:H:24:DT:H4'	3:E:152:GLY:O	2.15	0.46
3:B:205:LEU:CD2	3:B:256:ILE:HD13	2.42	0.46
3:S:202:ILE:CD1	3:S:204:LYS:H	2.26	0.46
3:W:199:THR:HG22	3:W:200:GLN:HG2	1.97	0.46
3:B:162:VAL:HG13	3:B:172:VAL:HG12	1.97	0.46
3:E:281:ALA:O	3:E:282:LYS:CB	2.63	0.46
3:M:174:ILE:CG2	3:R:169:PRO:HA	2.45	0.46
3:M:190:ALA:O	3:M:191:CYS:C	2.57	0.46
2:D:22:DG:H2'	8:D:2005:HOH:O	2.14	0.46
3:B:276:LEU:O	3:B:277:ALA:C	2.59	0.46
3:I:139:PHE:N	3:I:139:PHE:CD1	2.83	0.46
3:R:268:ILE:O	3:R:271:GLU:HB2	2.16	0.46
3:W:230:TRP:HB3	3:W:238:VAL:CG1	2.42	0.46
2:L:18:DA:H4'	3:J:182:ASN:HB3	1.98	0.46
3:F:209:THR:C	3:F:261:VAL:HG22	2.40	0.46
3:I:226:LYS:C	3:I:227:LYS:HG3	2.40	0.46
3:N:141:VAL:HG12	3:N:142:VAL:N	2.31	0.46
3:N:207:LEU:HD23	3:N:208:TYR:N	2.31	0.46
1:O:7:C:H2'	1:O:8:U:C6	2.49	0.46
3:A:232:THR:C	3:A:234:ALA:N	2.74	0.46
3:F:222:VAL:HA	3:F:225:TRP:CE3	2.50	0.46
3:F:274:ASP:O	3:F:278:ARG:HG2	2.15	0.46
3:F:275:ARG:HG2	3:F:275:ARG:HH11	1.81	0.46
3:R:182:ASN:O	3:R:185:ALA:N	2.48	0.46
3:A:140:VAL:O	3:A:140:VAL:HG13	2.14	0.46
3:A:257:GLN:HE21	3:A:259:MET:HE1	1.80	0.46
3:E:187:ILE:HG12	3:E:214:THR:HG23	1.98	0.46
3:I:186:GLU:HG2	3:I:211:SER:CB	2.40	0.46
3:N:183:GLN:C	3:N:185:ALA:N	2.72	0.46
3:N:232:THR:HB	3:N:234:ALA:H	1.80	0.46
3:S:230:TRP:CZ3	3:S:241:LYS:HG3	2.51	0.46
3:W:240:ASN:HB3	3:W:243:ASP:OD2	2.15	0.46
3:F:140:VAL:CG1	3:F:202:ILE:HG13	2.44	0.46
3:F:221:TRP:O	3:F:225:TRP:CD2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:158:ALA:HB2	3:I:180:GLN:HG3	1.97	0.46
3:I:201:ASN:N	3:I:201:ASN:ND2	2.64	0.46
3:W:207:LEU:HD13	3:W:258:TRP:CZ3	2.51	0.46
2:Z:20:DC:H2"	2:Z:21:DA:H8	1.81	0.46
3:A:262:PRO:HB2	3:A:265:SER:CB	2.45	0.46
3:I:168:HIS:C	3:I:170:LEU:H	2.24	0.46
3:N:158:ALA:H	3:N:180:GLN:HG3	1.80	0.46
3:W:198:LYS:HG2	3:W:254:MET:HE3	1.98	0.46
2:L:25:DG:H1'	3:I:182:ASN:ND2	2.29	0.46
2:Z:18:DA:H2"	2:Z:19:DT:O5'	2.16	0.46
3:A:136:MET:O	3:A:139:PHE:HB2	2.15	0.46
3:E:165:GLY:O	3:E:166:PRO:C	2.58	0.46
3:F:221:TRP:HB3	3:F:225:TRP:CZ2	2.50	0.46
3:F:246:ALA:O	3:F:250:LEU:HD13	2.16	0.46
3:J:146:GLY:HA3	3:J:186:GLU:CA	2.45	0.46
3:M:198:LYS:O	3:M:201:ASN:N	2.49	0.46
3:N:226:LYS:HZ1	3:N:230:TRP:HE1	1.63	0.46
3:R:135:HIS:N	3:R:135:HIS:CD2	2.84	0.46
3:R:168:HIS:HE1	3:R:170:LEU:HD13	1.81	0.46
3:S:273:ALA:O	3:S:276:LEU:N	2.48	0.46
3:W:227:LYS:O	3:W:229:GLY:N	2.48	0.46
3:W:250:LEU:H	3:W:250:LEU:CD1	2.28	0.46
3:A:217:GLY:HA2	3:A:221:TRP:HB2	1.98	0.46
3:M:146:GLY:HA3	3:M:186:GLU:HA	1.97	0.46
3:N:215:ILE:HG12	3:N:258:TRP:HB3	1.98	0.46
3:N:218:ILE:HG23	3:N:219:THR:HG23	1.98	0.46
3:N:261:VAL:HG21	3:N:270:ASN:ND2	2.31	0.46
3:S:157:ARG:NH1	3:S:175:ARG:NH1	2.64	0.46
3:W:143:TYR:O	3:W:163:TYR:N	2.46	0.46
3:W:160:ILE:CG2	3:W:189:ALA:HA	2.44	0.46
3:W:271:GLU:HG2	8:W:1022:HOH:O	2.16	0.46
2:D:18:DA:H2'	2:D:19:DT:H5"	1.98	0.45
2:D:25:DG:H2"	2:D:26:DT:H5"	1.99	0.45
1:K:5:A:H4'	3:I:210:ASN:O	2.16	0.45
2:L:16:DG:H2"	2:L:17:DA:OP2	2.16	0.45
2:U:21:DA:C2'	2:U:22:DG:H8	2.28	0.45
3:B:160:ILE:HG23	3:B:189:ALA:CA	2.45	0.45
3:B:176:LEU:HD22	3:B:185:ALA:CA	2.45	0.45
3:M:191:CYS:O	3:M:192:LYS:C	2.60	0.45
3:N:199:THR:C	3:N:201:ASN:N	2.58	0.45
3:W:138:ASP:O	3:W:139:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:168:HIS:C	3:W:170:LEU:H	2.23	0.45
3:W:282:LYS:O	3:W:283:GLN:HB3	2.16	0.45
3:B:139:PHE:CD2	3:B:206:VAL:HG23	2.52	0.45
3:B:199:THR:O	3:B:200:GLN:HG2	2.16	0.45
3:E:150:SER:HB3	3:E:153:ARG:HB3	1.99	0.45
3:I:178:GLY:O	3:I:179:ARG:C	2.59	0.45
3:I:248:GLU:HA	3:I:251:THR:OG1	2.17	0.45
3:M:193:ALA:O	3:M:196:GLN:HB2	2.16	0.45
3:N:175:ARG:HG2	3:N:175:ARG:HH11	1.82	0.45
3:N:225:TRP:CA	3:N:228:ASN:HB3	2.46	0.45
3:W:202:ILE:O	3:W:202:ILE:CG2	2.65	0.45
3:B:145:ASP:HB2	8:B:2004:HOH:O	2.14	0.45
3:B:232:THR:C	3:B:234:ALA:N	2.75	0.45
3:F:143:TYR:HD1	3:F:270:ASN:OD1	1.99	0.45
3:F:241:LYS:O	3:F:242:GLU:C	2.59	0.45
3:I:182:ASN:CG	3:I:183:GLN:H	2.14	0.45
3:S:277:ALA:C	3:S:279:GLU:H	2.23	0.45
2:D:23:DG:C8	2:D:24:DT:H72	2.52	0.45
2:L:19:DT:H2"	2:L:20:DC:H6	1.81	0.45
3:E:175:ARG:HD2	8:E:1010:HOH:O	2.16	0.45
3:E:181:THR:O	3:E:182:ASN:C	2.59	0.45
3:J:149:SER:O	3:J:156:PRO:HA	2.17	0.45
3:J:175:ARG:HB2	3:J:280:GLY:O	2.15	0.45
3:W:241:LYS:C	3:W:245:VAL:HG23	2.40	0.45
3:A:232:THR:O	3:A:234:ALA:N	2.50	0.45
3:E:250:LEU:HD12	3:E:250:LEU:H	1.81	0.45
3:F:217:GLY:C	3:F:222:VAL:HG13	2.41	0.45
3:M:182:ASN:O	3:M:185:ALA:HB3	2.16	0.45
3:N:199:THR:O	3:N:201:ASN:N	2.49	0.45
3:S:181:THR:HG22	3:S:184:ARG:H	1.80	0.45
3:W:262:PRO:O	3:W:265:SER:HB3	2.16	0.45
2:H:28:DG:H8	2:H:28:DG:OP2	2.00	0.45
2:L:17:DA:C6	2:L:18:DA:C6	3.04	0.45
2:Z:15:DG:H1'	2:Z:16:DG:N7	2.31	0.45
3:E:275:ARG:HH11	3:E:275:ARG:HG3	1.81	0.45
3:N:173:GLY:HA3	3:N:276:LEU:HD22	1.99	0.45
3:R:241:LYS:O	3:R:245:VAL:HG23	2.16	0.45
3:S:166:PRO:C	3:S:168:HIS:H	2.25	0.45
2:P:15:DG:N2	8:P:99:HOH:O	2.50	0.45
3:A:163:TYR:CE1	3:A:165:GLY:HA2	2.52	0.45
3:A:170:LEU:HD12	3:A:170:LEU:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:225:TRP:CE3	3:A:238:VAL:HG11	2.51	0.45
3:E:141:VAL:HG22	3:E:206:VAL:HB	1.98	0.45
2:H:20:DC:H2"	2:H:21:DA:H8	1.82	0.45
2:Z:19:DT:H2"	2:Z:20:DC:H6	1.81	0.45
3:A:153:ARG:O	3:A:154:ARG:C	2.60	0.45
3:A:172:VAL:HG12	3:A:173:GLY:N	2.31	0.45
3:A:174:ILE:HG22	3:A:175:ARG:O	2.17	0.45
3:B:191:CYS:O	3:B:192:LYS:C	2.59	0.45
3:B:198:LYS:O	3:B:200:GLN:N	2.44	0.45
3:E:168:HIS:CG	3:E:169:PRO:HD2	2.52	0.45
3:J:164:TRP:HB2	3:J:168:HIS:CG	2.51	0.45
3:N:181:THR:O	3:N:182:ASN:C	2.60	0.45
3:N:202:ILE:HD13	3:N:204:LYS:N	2.31	0.45
3:S:279:GLU:C	3:S:281:ALA:N	2.74	0.45
3:W:163:TYR:HA	3:W:171:ASN:OD1	2.16	0.45
2:D:18:DA:H3'	2:D:19:DT:H5"	1.98	0.45
1:G:8:U:H2'	1:G:9:G:H8	1.81	0.45
1:O:4:C:H2'	1:O:5:A:O4'	2.17	0.45
2:U:28:DG:H5"	3:R:233:SER:OG	2.16	0.45
3:A:172:VAL:HG11	3:A:174:ILE:HD11	1.99	0.45
3:I:168:HIS:O	3:I:170:LEU:N	2.49	0.45
3:I:172:VAL:CG1	3:I:174:ILE:HG23	2.47	0.45
3:M:278:ARG:C	3:M:280:GLY:H	2.24	0.45
3:N:256:ILE:CG2	3:N:257:GLN:H	2.05	0.45
3:S:149:SER:O	3:S:150:SER:HB3	2.16	0.45
3:S:179:ARG:HG2	3:S:184:ARG:HD2	1.99	0.45
3:S:188:HIS:O	3:S:191:CYS:HB2	2.17	0.45
3:W:179:ARG:HB3	3:W:184:ARG:NH1	2.32	0.45
3:W:211:SER:C	3:W:213:PHE:N	2.73	0.45
3:W:253:GLY:O	3:W:254:MET:HG2	2.16	0.45
2:L:25:DG:H2"	2:L:26:DT:C5'	2.46	0.45
2:P:18:DA:H2'	2:P:19:DT:H5"	1.99	0.45
3:E:225:TRP:HA	3:E:228:ASN:HD22	1.75	0.45
3:F:207:LEU:O	3:F:259:MET:N	2.47	0.45
3:I:211:SER:C	3:I:213:PHE:H	2.25	0.45
3:J:249:ARG:HH11	3:J:249:ARG:HB3	1.81	0.45
3:N:240:ASN:O	3:N:241:LYS:C	2.60	0.45
3:R:260:HIS:CD2	3:R:260:HIS:C	2.93	0.45
3:W:232:THR:HG22	3:W:236:LYS:O	2.17	0.45
3:A:170:LEU:O	3:A:172:VAL:HG23	2.17	0.44
3:B:250:LEU:HD12	3:B:250:LEU:N	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:191:CYS:O	3:J:192:LYS:C	2.58	0.44
1:K:14:C:H5'	3:W:264:HIS:CE1	2.52	0.44
2:P:23:DG:C2'	2:P:24:DT:H71	2.47	0.44
1:X:9:G:H2'	1:X:10:A:O4'	2.18	0.44
3:A:218:ILE:CG2	3:A:219:THR:HG23	2.47	0.44
3:A:268:ILE:O	3:A:269:GLY:C	2.59	0.44
3:B:210:ASN:ND2	3:B:261:VAL:O	2.46	0.44
3:M:261:VAL:HG21	3:M:270:ASN:CB	2.47	0.44
3:S:168:HIS:CG	3:S:169:PRO:HD2	2.52	0.44
3:S:281:ALA:O	3:S:282:LYS:O	2.35	0.44
3:A:274:ASP:O	3:A:275:ARG:C	2.58	0.44
3:E:255:ASP:C	3:E:256:ILE:HD13	2.41	0.44
3:F:218:ILE:HA	3:F:222:VAL:CG1	2.47	0.44
3:J:200:GLN:HE21	3:J:200:GLN:N	2.14	0.44
3:N:145:ASP:HA	3:N:186:GLU:OE2	2.18	0.44
3:R:183:GLN:HE21	3:R:183:GLN:CA	2.30	0.44
3:S:269:GLY:O	3:S:272:GLU:HB2	2.17	0.44
3:W:166:PRO:C	3:W:168:HIS:H	2.26	0.44
3:W:256:ILE:CG2	3:W:257:GLN:N	2.81	0.44
2:P:27:DC:H5	8:P:171:HOH:O	1.99	0.44
3:B:204:LYS:HB3	3:B:204:LYS:HE2	1.79	0.44
3:F:178:GLY:O	3:F:180:GLN:NE2	2.50	0.44
3:I:158:ALA:CB	3:I:176:LEU:HB3	2.47	0.44
3:J:280:GLY:O	3:J:283:GLN:HG3	2.17	0.44
3:M:217:GLY:O	3:M:221:TRP:HB2	2.17	0.44
3:M:239:ILE:HD13	3:M:239:ILE:H	1.79	0.44
3:N:176:LEU:O	3:N:180:GLN:NE2	2.51	0.44
3:R:148:CYS:O	3:R:151:ASN:HB2	2.17	0.44
3:W:145:ASP:CG	3:W:274:ASP:OD1	2.61	0.44
3:W:222:VAL:HG23	3:W:223:GLN:H	1.83	0.44
2:H:23:DG:H2"	2:H:24:DT:OP2	2.17	0.44
3:A:221:TRP:HB3	3:A:225:TRP:CZ2	2.53	0.44
3:B:278:ARG:H	3:B:278:ARG:HG2	1.51	0.44
3:I:143:TYR:O	3:I:162:VAL:HA	2.17	0.44
3:M:143:TYR:CZ	3:M:269:GLY:HA3	2.53	0.44
3:M:168:HIS:H	3:M:171:ASN:ND2	2.15	0.44
3:M:170:LEU:HD12	3:M:170:LEU:HA	1.85	0.44
3:W:250:LEU:HD12	3:W:250:LEU:N	2.33	0.44
2:L:27:DC:C2'	2:L:28:DG:OP2	2.66	0.44
1:X:6:C:H2'	1:X:7:C:O5'	2.17	0.44
3:F:230:TRP:CD2	3:F:241:LYS:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:215:ILE:C	3:I:217:GLY:H	2.24	0.44
3:I:232:THR:O	3:I:234:ALA:N	2.51	0.44
3:J:224:GLY:O	3:J:228:ASN:HB3	2.18	0.44
3:M:196:GLN:O	3:M:197:ALA:C	2.60	0.44
3:M:275:ARG:HH21	3:M:276:LEU:CD2	2.31	0.44
3:S:139:PHE:HD2	3:S:140:VAL:N	2.12	0.44
3:W:168:HIS:CE1	3:W:170:LEU:HB2	2.53	0.44
3:W:194:ILE:HG13	3:W:250:LEU:HD23	1.99	0.44
3:W:283:GLN:CG	3:W:284:SER:H	2.08	0.44
1:T:12:U:H2'	1:T:13:C:C6	2.53	0.44
3:B:250:LEU:H	3:B:250:LEU:CD1	2.25	0.44
3:J:283:GLN:CD	8:J:1011:HOH:O	2.61	0.44
3:M:178:GLY:O	3:M:179:ARG:C	2.61	0.44
3:M:268:ILE:O	3:M:269:GLY:C	2.60	0.44
3:W:203:ASN:HD21	3:W:204:LYS:HE3	1.82	0.44
3:W:260:HIS:O	3:W:262:PRO:HD3	2.18	0.44
1:G:11:U:H2'	1:G:12:U:O4'	2.17	0.44
2:H:21:DA:OP2	2:H:21:DA:H8	2.01	0.44
2:L:15:DG:C3'	2:Z:15:DG:H5"	2.48	0.44
2:P:18:DA:H5"	8:P:133:HOH:O	2.17	0.44
3:B:155:ARG:CB	3:B:156:PRO:CD	2.94	0.44
3:E:149:SER:OG	3:E:157:ARG:HB2	2.18	0.44
3:E:168:HIS:CE1	3:E:170:LEU:HD13	2.53	0.44
3:F:168:HIS:HA	3:F:169:PRO:HD3	1.76	0.44
3:J:182:ASN:C	3:J:182:ASN:HD22	2.24	0.44
3:M:194:ILE:O	3:M:197:ALA:HB3	2.18	0.44
3:N:242:GLU:O	3:N:245:VAL:HG12	2.17	0.44
3:W:225:TRP:O	3:W:230:TRP:N	2.47	0.44
3:A:218:ILE:HG21	3:A:258:TRP:CE2	2.53	0.44
3:E:137:GLY:C	3:E:139:PHE:H	2.26	0.44
3:E:192:LYS:HD2	3:E:192:LYS:HA	1.80	0.44
3:F:232:THR:O	3:F:235:GLY:N	2.43	0.44
3:I:153:ARG:HA	3:I:153:ARG:HD3	1.83	0.44
3:N:230:TRP:HE3	3:N:238:VAL:CG1	2.31	0.44
3:R:186:GLU:CG	3:R:211:SER:CB	2.91	0.44
3:S:276:LEU:O	3:S:277:ALA:C	2.60	0.44
1:K:3:A:H2'	1:K:4:C:C6	2.52	0.43
3:A:159:GLY:N	3:A:281:ALA:HB2	2.33	0.43
3:B:160:ILE:HG22	3:B:161:GLY:N	2.32	0.43
3:F:138:ASP:O	3:F:139:PHE:HB3	2.18	0.43
3:I:215:ILE:C	3:I:217:GLY:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:168:HIS:H	3:M:171:ASN:HD21	1.66	0.43
3:M:228:ASN:C	3:M:228:ASN:ND2	2.64	0.43
3:R:137:GLY:O	3:R:139:PHE:HD1	2.01	0.43
3:R:217:GLY:HA3	3:R:244:PHE:CE1	2.53	0.43
3:A:136:MET:HE2	3:R:215:ILE:HG21	1.99	0.43
3:A:222:VAL:O	3:A:223:GLN:C	2.60	0.43
3:A:232:THR:HG22	3:A:236:LYS:H	1.83	0.43
3:B:215:ILE:HD12	3:B:260:HIS:HB2	2.00	0.43
3:I:207:LEU:HD23	3:I:207:LEU:C	2.43	0.43
3:J:251:THR:O	3:J:252:GLN:C	2.59	0.43
3:M:217:GLY:HA2	3:M:221:TRP:HE3	1.80	0.43
3:N:261:VAL:HG21	3:N:270:ASN:HD21	1.82	0.43
3:R:199:THR:C	3:R:201:ASN:H	2.26	0.43
3:S:184:ARG:HA	3:S:187:ILE:CG2	2.47	0.43
3:S:205:LEU:N	3:S:205:LEU:HD23	2.33	0.43
3:A:202:ILE:HD12	3:A:203:ASN:N	2.32	0.43
3:A:226:LYS:HB3	3:A:226:LYS:HZ2	1.82	0.43
3:B:146:GLY:HA3	3:B:186:GLU:HA	2.00	0.43
3:B:187:ILE:O	3:B:190:ALA:N	2.39	0.43
3:J:222:VAL:O	3:J:226:LYS:HG3	2.19	0.43
3:R:154:ARG:HD3	3:R:154:ARG:H	1.82	0.43
3:S:205:LEU:HD23	3:S:205:LEU:H	1.82	0.43
3:S:215:ILE:HA	3:S:218:ILE:HG22	2.00	0.43
2:D:19:DT:H5'	3:B:239:ILE:HD12	1.99	0.43
3:F:138:ASP:O	3:F:139:PHE:HD1	2.02	0.43
3:F:158:ALA:H	3:F:180:GLN:HG3	1.81	0.43
3:J:247:LEU:O	3:J:248:GLU:C	2.61	0.43
3:M:198:LYS:C	3:M:200:GLN:N	2.77	0.43
3:M:210:ASN:HA	3:M:260:HIS:CD2	2.53	0.43
3:M:274:ASP:O	3:M:275:ARG:C	2.61	0.43
3:R:217:GLY:O	3:R:222:VAL:HG22	2.18	0.43
3:S:204:LYS:HG3	3:S:204:LYS:O	2.18	0.43
3:W:143:TYR:HD1	3:W:270:ASN:HD22	1.65	0.43
3:W:228:ASN:ND2	3:W:231:LYS:H	2.16	0.43
1:K:12:U:C2	1:K:13:C:C6	3.07	0.43
2:U:26:DT:H2"	2:U:27:DC:C6	2.53	0.43
3:A:278:ARG:C	3:A:280:GLY:N	2.73	0.43
3:E:155:ARG:HG3	8:E:1005:HOH:O	2.17	0.43
3:E:203:ASN:N	3:E:203:ASN:OD1	2.52	0.43
3:E:218:ILE:HG23	3:E:219:THR:N	2.32	0.43
3:I:143:TYR:CD1	3:I:269:GLY:HA3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:170:LEU:O	3:J:172:VAL:HG23	2.18	0.43
3:J:188:HIS:O	3:J:191:CYS:HB2	2.19	0.43
3:M:232:THR:HG22	3:M:236:LYS:CA	2.47	0.43
3:R:151:ASN:OD1	3:R:181:THR:HA	2.17	0.43
3:R:210:ASN:OD1	3:R:210:ASN:N	2.45	0.43
3:S:154:ARG:O	3:S:155:ARG:HB2	2.19	0.43
3:W:160:ILE:HD12	3:W:189:ALA:CA	2.48	0.43
2:D:25:DG:H2"	2:D:26:DT:O5'	2.17	0.43
2:H:15:DG:N3	2:H:15:DG:O4'	2.51	0.43
3:B:258:TRP:CD1	3:B:258:TRP:H	2.36	0.43
3:E:142:VAL:HG22	3:E:143:TYR:N	2.33	0.43
3:E:249:ARG:CZ	3:E:250:LEU:HD11	2.49	0.43
3:E:261:VAL:O	3:E:262:PRO:C	2.61	0.43
3:F:184:ARG:HG3	3:F:185:ALA:N	2.34	0.43
3:M:184:ARG:CG	3:M:184:ARG:NH1	2.79	0.43
3:M:198:LYS:C	3:M:200:GLN:H	2.27	0.43
3:M:208:TYR:CE2	3:M:259:MET:HG2	2.54	0.43
1:G:11:U:H2'	1:G:12:U:C6	2.54	0.43
2:P:18:DA:H1'	3:N:182:ASN:OD1	2.18	0.43
2:Z:19:DT:OP1	3:W:240:ASN:ND2	2.41	0.43
3:A:163:TYR:CE1	3:A:165:GLY:CA	3.02	0.43
3:F:135:HIS:CB	3:F:136:MET:SD	3.00	0.43
3:I:218:ILE:CG2	3:I:219:THR:N	2.82	0.43
3:I:237:GLU:H	3:I:237:GLU:HG2	1.64	0.43
3:M:161:GLY:N	3:M:277:ALA:HB2	2.34	0.43
3:N:161:GLY:CA	3:N:277:ALA:HB2	2.49	0.43
3:S:146:GLY:O	3:S:186:GLU:HB2	2.18	0.43
3:S:160:ILE:HD11	3:S:176:LEU:HD13	2.01	0.43
3:W:179:ARG:HB3	3:W:184:ARG:HD3	2.00	0.43
2:H:15:DG:O4'	2:H:16:DG:C8	2.72	0.43
1:O:12:U:H2'	1:O:13:C:C6	2.53	0.43
3:B:153:ARG:O	3:B:154:ARG:C	2.60	0.43
3:B:262:PRO:O	3:B:265:SER:HB3	2.19	0.43
3:I:187:ILE:C	3:I:189:ALA:H	2.25	0.43
3:R:225:TRP:CA	3:R:228:ASN:ND2	2.74	0.43
3:R:254:MET:HB3	3:R:256:ILE:HD11	2.00	0.43
3:S:160:ILE:CG2	3:S:189:ALA:HA	2.48	0.43
3:S:205:LEU:HD21	3:S:256:ILE:CD1	2.49	0.43
3:W:204:LYS:CB	3:W:255:ASP:HB3	2.48	0.43
3:W:249:ARG:O	3:W:252:GLN:HB2	2.18	0.43
3:W:278:ARG:HG3	3:W:278:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:147:CYS:O	3:B:158:ALA:HA	2.19	0.43
3:B:183:GLN:HE21	3:B:183:GLN:CA	2.03	0.43
3:E:219:THR:O	3:E:220:ASN:HB2	2.19	0.43
3:M:194:ILE:HD11	3:M:250:LEU:HB3	2.01	0.43
3:S:221:TRP:C	3:S:223:GLN:N	2.75	0.43
2:L:27:DC:H2"	2:L:28:DG:H8	1.80	0.43
1:O:11:U:H2'	1:O:12:U:C6	2.54	0.43
2:U:19:DT:P	3:S:181:THR:OG1	2.77	0.43
3:B:180:GLN:HE21	3:B:180:GLN:N	2.17	0.43
3:F:211:SER:O	3:F:212:MET:C	2.61	0.43
3:I:180:GLN:HE21	3:I:180:GLN:CA	2.32	0.43
3:I:212:MET:O	3:I:216:ASN:HB2	2.18	0.43
3:J:135:HIS:HB3	3:J:136:MET:H	1.37	0.43
3:J:243:ASP:O	3:J:246:ALA:N	2.52	0.43
3:S:217:GLY:HA2	3:S:221:TRP:CE3	2.54	0.43
1:C:6:C:H2'	1:C:7:C:O4'	2.19	0.42
1:G:7:C:OP1	3:E:147:CYS:HB2	2.18	0.42
2:P:17:DA:H2"	2:P:18:DA:O5'	2.19	0.42
3:A:275:ARG:NH2	3:A:276:LEU:HD23	2.33	0.42
3:B:245:VAL:O	3:B:246:ALA:C	2.62	0.42
3:F:172:VAL:HG12	3:F:173:GLY:N	2.33	0.42
3:I:218:ILE:CD1	3:I:247:LEU:HD23	2.37	0.42
3:J:194:ILE:HD12	3:J:256:ILE:CD1	2.45	0.42
3:J:241:LYS:C	3:J:243:ASP:N	2.76	0.42
3:N:210:ASN:HA	3:N:261:VAL:O	2.18	0.42
3:S:214:THR:O	3:S:218:ILE:HG22	2.18	0.42
3:S:232:THR:CG2	3:S:234:ALA:HB3	2.49	0.42
3:W:181:THR:OG1	3:W:184:ARG:HB3	2.19	0.42
3:F:230:TRP:CG	3:F:241:LYS:HE3	2.54	0.42
3:I:200:GLN:HA	3:I:200:GLN:NE2	2.26	0.42
3:N:230:TRP:CE3	3:N:238:VAL:HG11	2.53	0.42
1:G:1:C:H2'	1:G:2:G:C8	2.54	0.42
1:K:8:U:O2'	1:K:9:G:H5'	2.18	0.42
2:Z:17:DA:H2'	2:Z:18:DA:C8	2.54	0.42
3:B:148:CYS:SG	3:B:181:THR:HA	2.59	0.42
3:B:198:LYS:C	3:B:200:GLN:N	2.77	0.42
3:F:187:ILE:HD11	3:F:243:ASP:HB3	2.01	0.42
3:J:216:ASN:HD22	3:J:216:ASN:HA	1.59	0.42
3:M:241:LYS:O	3:M:245:VAL:HG23	2.19	0.42
3:M:273:ALA:O	3:M:274:ASP:C	2.61	0.42
3:R:190:ALA:O	3:R:194:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:231:LYS:O	3:R:238:VAL:HG23	2.19	0.42
3:S:144:THR:HG21	3:S:190:ALA:HA	2.01	0.42
2:D:19:DT:H2"	2:D:20:DC:C6	2.53	0.42
2:Z:20:DC:C2'	2:Z:21:DA:C8	3.02	0.42
3:A:215:ILE:HG12	3:A:258:TRP:HB3	2.01	0.42
3:B:275:ARG:NH1	8:B:2011:HOH:O	2.51	0.42
3:E:247:LEU:HD21	3:E:258:TRP:CH2	2.54	0.42
3:F:228:ASN:O	3:F:231:LYS:HE3	2.19	0.42
3:I:168:HIS:C	3:I:170:LEU:N	2.77	0.42
3:I:208:TYR:CE2	3:I:259:MET:HG2	2.54	0.42
3:I:260:HIS:ND1	3:I:260:HIS:C	2.78	0.42
3:M:248:GLU:C	3:M:251:THR:HG1	2.26	0.42
3:N:183:GLN:H	3:N:183:GLN:HG2	1.59	0.42
3:R:149:SER:O	3:R:150:SER:C	2.61	0.42
3:R:192:LYS:O	3:R:196:GLN:HB2	2.20	0.42
3:S:232:THR:HG22	3:S:236:LYS:H	1.83	0.42
3:W:193:ALA:C	3:W:195:GLU:N	2.76	0.42
3:B:202:ILE:HD13	3:B:203:ASN:H	1.82	0.42
3:F:144:THR:HG21	3:F:190:ALA:HA	2.01	0.42
3:N:162:VAL:HG23	3:N:193:ALA:HB2	2.01	0.42
3:R:230:TRP:CE3	3:R:241:LYS:HG3	2.54	0.42
3:S:176:LEU:HD22	3:S:185:ALA:CA	2.50	0.42
3:S:250:LEU:C	3:S:252:GLN:N	2.76	0.42
3:W:182:ASN:OD1	3:W:183:GLN:HG2	2.19	0.42
3:W:209:THR:C	3:W:261:VAL:HG22	2.44	0.42
3:W:278:ARG:NH2	8:W:1018:HOH:O	2.49	0.42
2:H:21:DA:H2"	2:H:22:DG:OP2	2.19	0.42
2:L:28:DG:OP1	3:I:232:THR:HA	2.20	0.42
2:U:20:DC:H2"	2:U:21:DA:H8	1.85	0.42
2:Z:24:DT:H2"	2:Z:25:DG:H8	1.85	0.42
3:A:257:GLN:HE21	3:A:259:MET:CE	2.32	0.42
3:F:194:ILE:HG13	3:F:250:LEU:HD23	2.02	0.42
3:F:225:TRP:HB3	3:F:230:TRP:HA	2.02	0.42
3:I:270:ASN:O	3:I:274:ASP:CB	2.68	0.42
3:J:230:TRP:CZ3	3:J:241:LYS:HG3	2.55	0.42
3:M:178:GLY:O	3:M:180:GLN:NE2	2.53	0.42
3:M:211:SER:O	3:M:213:PHE:N	2.52	0.42
3:M:211:SER:OG	3:M:214:THR:HB	2.20	0.42
3:R:187:ILE:CG1	3:R:188:HIS:N	2.82	0.42
3:R:217:GLY:HA2	3:R:221:TRP:CE3	2.55	0.42
3:S:161:GLY:HA3	3:S:277:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:212:MET:HE3	3:W:260:HIS:CB	2.49	0.42
1:G:8:U:O2'	1:G:9:G:H5'	2.19	0.42
1:T:8:U:H2'	1:T:9:G:O4'	2.19	0.42
3:A:249:ARG:HG2	3:A:250:LEU:HD12	2.01	0.42
3:A:278:ARG:C	3:A:280:GLY:H	2.27	0.42
3:F:213:PHE:O	3:F:214:THR:C	2.62	0.42
3:I:156:PRO:O	3:I:157:ARG:HD2	2.19	0.42
3:I:275:ARG:HB3	3:I:275:ARG:NH1	2.35	0.42
3:M:168:HIS:C	3:M:170:LEU:H	2.27	0.42
3:N:144:THR:HG21	3:N:207:LEU:HD11	2.01	0.42
3:N:195:GLU:O	3:N:198:LYS:N	2.52	0.42
3:S:218:ILE:O	3:S:218:ILE:HG13	2.18	0.42
3:S:232:THR:HG23	3:S:234:ALA:HB3	2.01	0.42
3:W:148:CYS:CB	3:W:182:ASN:HA	2.50	0.42
1:K:12:U:H4'	3:J:210:ASN:O	2.20	0.42
2:L:21:DA:C2'	2:L:22:DG:C8	2.98	0.42
2:L:26:DT:H6	2:L:26:DT:H2'	1.69	0.42
2:U:18:DA:H4'	3:S:182:ASN:H	1.85	0.42
3:B:182:ASN:CG	3:B:183:GLN:N	2.76	0.42
3:F:141:VAL:CG1	3:F:142:VAL:N	2.83	0.42
3:J:218:ILE:HG13	3:J:218:ILE:O	2.20	0.42
3:S:207:LEU:HD23	3:S:258:TRP:CH2	2.54	0.42
3:W:183:GLN:CD	3:W:213:PHE:CD2	2.98	0.42
1:O:2:G:H2'	1:O:3:A:C8	2.55	0.42
3:B:166:PRO:O	3:B:168:HIS:N	2.52	0.42
3:B:166:PRO:C	3:B:168:HIS:H	2.27	0.42
3:E:207:LEU:HD22	3:E:258:TRP:CZ3	2.55	0.42
3:I:172:VAL:HG12	3:I:173:GLY:N	2.34	0.42
3:I:241:LYS:C	3:I:243:ASP:N	2.77	0.42
3:R:184:ARG:HG3	3:R:243:ASP:OD1	2.19	0.42
3:R:215:ILE:O	3:R:216:ASN:C	2.61	0.42
3:W:142:VAL:CG2	3:W:162:VAL:HG23	2.50	0.42
3:W:210:ASN:HB3	3:W:261:VAL:HG23	2.01	0.42
3:W:250:LEU:H	3:W:250:LEU:HD12	1.85	0.42
1:T:14:C:OP1	3:N:264:HIS:NE2	2.38	0.42
3:E:158:ALA:N	3:E:180:GLN:HG3	2.35	0.42
3:F:180:GLN:CA	3:F:180:GLN:NE2	2.72	0.42
2:P:23:DG:H2'	2:P:24:DT:H71	2.01	0.41
2:P:26:DT:H2"	2:P:27:DC:C6	2.55	0.41
3:A:208:TYR:HD2	3:A:261:VAL:HG13	1.85	0.41
3:A:232:THR:HG22	3:A:236:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:212:MET:O	3:E:216:ASN:N	2.52	0.41
3:I:142:VAL:HG11	3:I:205:LEU:HD12	2.02	0.41
3:J:263:GLY:C	3:J:265:SER:N	2.72	0.41
3:M:197:ALA:O	3:M:202:ILE:HG22	2.19	0.41
3:M:230:TRP:HB3	3:M:238:VAL:HG11	2.01	0.41
3:W:160:ILE:HG23	3:W:189:ALA:CA	2.48	0.41
1:K:4:C:H2'	1:K:5:A:O4'	2.20	0.41
1:K:10:A:H61	2:L:18:DA:N6	2.18	0.41
2:L:17:DA:N6	2:L:18:DA:C6	2.88	0.41
3:B:153:ARG:O	3:B:155:ARG:N	2.53	0.41
3:B:212:MET:O	3:B:216:ASN:HB2	2.21	0.41
3:I:151:ASN:CG	3:I:182:ASN:HB3	2.46	0.41
3:I:239:ILE:CG2	3:I:239:ILE:O	2.67	0.41
3:J:267:PHE:O	3:J:270:ASN:CB	2.66	0.41
3:R:245:VAL:O	3:R:249:ARG:HG2	2.18	0.41
3:S:153:ARG:O	3:S:154:ARG:C	2.63	0.41
2:Z:15:DG:H4'	2:Z:16:DG:C5'	2.49	0.41
3:A:163:TYR:CD1	3:A:163:TYR:C	2.99	0.41
3:A:184:ARG:O	3:A:185:ALA:C	2.63	0.41
3:A:197:ALA:O	3:A:198:LYS:C	2.63	0.41
3:A:222:VAL:CG1	3:A:223:GLN:H	2.23	0.41
3:E:262:PRO:O	3:E:263:GLY:C	2.63	0.41
3:F:272:GLU:O	3:F:273:ALA:C	2.62	0.41
3:J:241:LYS:O	3:J:243:ASP:N	2.54	0.41
3:M:279:GLU:OE2	3:M:282:LYS:HD3	2.20	0.41
1:K:6:C:O2'	3:I:148:CYS:O	2.34	0.41
1:K:14:C:P	3:W:264:HIS:HE2	2.43	0.41
1:T:14:C:H42	2:U:15:DG:H1	1.68	0.41
2:U:18:DA:C4'	3:S:182:ASN:HB3	2.50	0.41
3:A:257:GLN:CG	3:R:220:ASN:HD22	2.27	0.41
3:B:217:GLY:HA3	3:B:244:PHE:CZ	2.55	0.41
3:B:225:TRP:HB3	3:B:230:TRP:CE3	2.56	0.41
3:E:243:ASP:O	3:E:246:ALA:HB3	2.21	0.41
3:F:141:VAL:HG12	3:F:142:VAL:H	1.83	0.41
3:F:177:PRO:HG2	3:I:155:ARG:NH2	2.35	0.41
3:F:194:ILE:CD1	3:F:194:ILE:C	2.85	0.41
3:N:195:GLU:C	3:N:197:ALA:N	2.77	0.41
3:R:181:THR:O	3:R:182:ASN:C	2.63	0.41
2:D:18:DA:H2"	3:B:183:GLN:HG3	2.02	0.41
2:H:25:DG:N3	3:E:183:GLN:OE1	2.53	0.41
1:O:5:A:C2	2:P:25:DG:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:15:DG:C2'	2:Z:16:DG:OP2	2.61	0.41
3:A:176:LEU:HA	3:A:177:PRO:HD2	1.92	0.41
3:B:136:MET:HB3	3:B:137:GLY:H	1.54	0.41
3:E:247:LEU:O	3:E:248:GLU:C	2.62	0.41
3:F:179:ARG:CZ	3:F:181:THR:HG21	2.51	0.41
3:F:198:LYS:C	3:F:200:GLN:N	2.77	0.41
3:F:202:ILE:HD11	3:F:204:LYS:O	2.21	0.41
3:F:207:LEU:HD23	3:F:208:TYR:N	2.35	0.41
3:F:218:ILE:O	3:F:218:ILE:HG13	2.21	0.41
3:F:248:GLU:O	3:F:249:ARG:C	2.64	0.41
3:I:158:ALA:HB3	3:I:176:LEU:HB3	2.01	0.41
3:I:211:SER:C	3:I:213:PHE:N	2.77	0.41
3:J:143:TYR:CG	3:J:269:GLY:O	2.74	0.41
3:J:246:ALA:O	3:J:250:LEU:HD13	2.21	0.41
3:J:262:PRO:HG2	3:J:265:SER:HG	1.78	0.41
3:N:245:VAL:HG12	3:N:246:ALA:N	2.35	0.41
3:R:212:MET:O	3:R:213:PHE:C	2.63	0.41
3:S:261:VAL:HA	3:S:262:PRO:HD2	1.92	0.41
1:O:6:C:H2'	1:O:7:C:O4'	2.21	0.41
1:O:11:U:H4'	3:N:212:MET:HG3	2.02	0.41
1:T:7:C:H42	2:U:22:DG:H1	1.67	0.41
2:U:17:DA:H2'	2:U:18:DA:C8	2.56	0.41
3:E:153:ARG:HH11	3:E:153:ARG:CG	2.30	0.41
3:I:176:LEU:HD22	3:I:185:ALA:HA	2.02	0.41
3:I:179:ARG:HD3	3:I:184:ARG:HD2	2.03	0.41
3:I:252:GLN:OE1	3:I:252:GLN:HA	2.20	0.41
3:J:241:LYS:C	3:J:243:ASP:H	2.28	0.41
3:M:215:ILE:O	3:M:216:ASN:C	2.63	0.41
3:S:274:ASP:OD2	3:S:278:ARG:NH1	2.53	0.41
2:H:15:DG:H4'	2:H:16:DG:O5'	2.21	0.41
3:A:187:ILE:HD11	3:A:243:ASP:HB3	2.01	0.41
3:E:162:VAL:HG21	3:E:192:LYS:HB3	2.03	0.41
3:I:246:ALA:O	3:I:250:LEU:HD13	2.21	0.41
3:R:249:ARG:HH11	3:R:249:ARG:CB	2.27	0.41
3:S:215:ILE:O	3:S:216:ASN:C	2.63	0.41
3:A:182:ASN:ND2	3:A:182:ASN:N	2.65	0.41
3:A:230:TRP:CD2	3:A:241:LYS:HG3	2.56	0.41
3:B:205:LEU:HD23	3:B:205:LEU:N	2.22	0.41
3:B:215:ILE:CD1	3:B:260:HIS:HB2	2.50	0.41
3:E:215:ILE:O	3:E:216:ASN:C	2.63	0.41
3:E:225:TRP:CA	3:E:228:ASN:ND2	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:241:LYS:O	3:M:242:GLU:C	2.64	0.41
3:N:179:ARG:HG2	3:N:181:THR:CG2	2.51	0.41
3:S:261:VAL:O	3:S:261:VAL:CG2	2.65	0.41
2:D:15:DG:H1'	2:D:16:DG:C8	2.55	0.41
2:H:27:DC:H2"	2:H:28:DG:H8	1.84	0.41
2:U:18:DA:H2"	2:U:19:DT:H5"	2.02	0.41
3:B:192:LYS:O	3:B:193:ALA:C	2.63	0.41
3:B:245:VAL:HG12	3:B:246:ALA:N	2.35	0.41
3:B:280:GLY:C	3:B:282:LYS:N	2.79	0.41
3:E:230:TRP:CG	3:E:241:LYS:HE3	2.56	0.41
3:F:230:TRP:CD2	3:F:241:LYS:HE3	2.56	0.41
3:J:154:ARG:O	3:J:155:ARG:CB	2.68	0.41
3:M:160:ILE:O	3:M:160:ILE:CG1	2.67	0.41
3:M:190:ALA:O	3:M:193:ALA:HB3	2.21	0.41
3:M:203:ASN:OD1	3:M:204:LYS:HE3	2.20	0.41
3:N:146:GLY:HA3	3:N:186:GLU:N	2.36	0.41
3:R:208:TYR:CD2	3:R:259:MET:HB3	2.56	0.41
3:S:212:MET:O	3:S:216:ASN:HB2	2.21	0.41
3:S:250:LEU:HD12	3:S:250:LEU:N	2.36	0.41
3:W:141:VAL:CG1	3:W:142:VAL:N	2.84	0.41
3:W:190:ALA:O	3:W:194:ILE:HG12	2.21	0.41
2:U:19:DT:C3'	3:S:239:ILE:HD12	2.43	0.41
1:X:8:U:C2'	1:X:9:G:H5'	2.51	0.41
3:B:168:HIS:CE1	3:B:170:LEU:HB2	2.56	0.41
3:F:268:ILE:O	3:F:269:GLY:C	2.64	0.41
3:J:207:LEU:C	3:J:207:LEU:HD23	2.46	0.41
3:S:168:HIS:CE1	3:S:170:LEU:HD13	2.52	0.41
3:A:207:LEU:HD23	3:A:207:LEU:C	2.46	0.40
3:B:222:VAL:O	3:B:223:GLN:C	2.63	0.40
3:F:268:ILE:O	3:F:270:ASN:N	2.54	0.40
2:U:20:DC:H2"	2:U:21:DA:C8	2.57	0.40
2:U:21:DA:H2'	2:U:22:DG:H8	1.75	0.40
3:B:180:GLN:HE21	3:B:180:GLN:CA	2.34	0.40
3:B:262:PRO:O	3:B:265:SER:CA	2.69	0.40
3:E:232:THR:O	3:E:234:ALA:N	2.55	0.40
3:N:146:GLY:HA3	3:N:186:GLU:CA	2.51	0.40
3:S:160:ILE:HG23	3:S:189:ALA:CA	2.49	0.40
3:S:160:ILE:HD12	3:S:189:ALA:HA	2.03	0.40
3:W:187:ILE:CD1	3:W:243:ASP:HB3	2.52	0.40
3:W:230:TRP:CD2	3:W:241:LYS:HG3	2.56	0.40
3:E:153:ARG:CG	3:E:153:ARG:NH1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:278:ARG:HH11	3:E:278:ARG:CG	2.31	0.40
3:J:147:CYS:O	3:J:158:ALA:HA	2.21	0.40
3:J:169:PRO:HG2	3:J:170:LEU:HD12	2.03	0.40
3:J:257:GLN:HE21	3:J:257:GLN:HB3	1.63	0.40
3:N:158:ALA:HB3	3:N:180:GLN:HG3	2.03	0.40
3:S:216:ASN:HD22	3:S:216:ASN:HA	1.58	0.40
3:S:250:LEU:N	3:S:250:LEU:CD1	2.84	0.40
2:H:20:DC:H5'	3:F:213:PHE:CE1	2.57	0.40
3:A:153:ARG:NH1	3:A:153:ARG:HG2	2.37	0.40
3:F:188:HIS:O	3:F:191:CYS:HB2	2.20	0.40
3:F:226:LYS:CB	3:F:226:LYS:NZ	2.84	0.40
3:M:168:HIS:ND1	3:M:169:PRO:CD	2.81	0.40
3:M:258:TRP:O	3:M:259:MET:HE3	2.22	0.40
3:N:208:TYR:CD2	3:N:259:MET:HB3	2.57	0.40
3:R:144:THR:HG21	3:R:207:LEU:HD21	2.04	0.40
3:W:191:CYS:O	3:W:195:GLU:HB2	2.21	0.40
3:B:155:ARG:N	3:B:156:PRO:HD2	2.33	0.40
3:B:212:MET:HA	3:B:215:ILE:HB	2.04	0.40
3:F:160:ILE:HG23	3:F:189:ALA:CA	2.52	0.40
3:F:221:TRP:CD1	3:F:221:TRP:N	2.90	0.40
3:I:160:ILE:HG12	3:I:176:LEU:HB2	2.03	0.40
3:I:187:ILE:C	3:I:189:ALA:N	2.79	0.40
3:J:215:ILE:C	3:J:217:GLY:N	2.78	0.40
3:N:215:ILE:HD12	3:N:260:HIS:HB2	2.02	0.40
3:R:202:ILE:O	3:R:254:MET:HE1	2.21	0.40
3:S:218:ILE:HD13	3:S:247:LEU:HD23	2.02	0.40
3:W:283:GLN:O	3:W:284:SER:CB	2.69	0.40

All (1) 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)
2:H:15:DG:C5'	2:H:15:DG:C5'[2_455]	1.91	0.29

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	152/154 (99%)	112 (74%)	34 (22%)	6 (4%)	2 18
3	B	149/154 (97%)	106 (71%)	28 (19%)	15 (10%)	0 2
3	E	147/154 (96%)	111 (76%)	29 (20%)	7 (5%)	2 14
3	F	148/154 (96%)	112 (76%)	23 (16%)	13 (9%)	0 3
3	I	147/154 (96%)	104 (71%)	30 (20%)	13 (9%)	0 3
3	J	149/154 (97%)	111 (74%)	29 (20%)	9 (6%)	1 10
3	M	143/154 (93%)	103 (72%)	34 (24%)	6 (4%)	2 16
3	N	142/154 (92%)	98 (69%)	31 (22%)	13 (9%)	0 3
3	R	146/154 (95%)	107 (73%)	30 (20%)	9 (6%)	1 9
3	S	146/154 (95%)	98 (67%)	38 (26%)	10 (7%)	1 7
3	W	144/154 (94%)	101 (70%)	29 (20%)	14 (10%)	0 3
All	All	1613/1694 (95%)	1163 (72%)	335 (21%)	115 (7%)	1 6

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	228	ASN
3	B	135	HIS
3	B	150	SER
3	B	155	ARG
3	B	156	PRO
3	B	234	ALA
3	B	265	SER
3	F	134	SER
3	F	136	MET
3	F	150	SER
3	F	154	ARG
3	F	201	ASN
3	J	136	MET
3	J	139	PHE
3	J	182	ASN
3	J	263	GLY
3	J	264	HIS
3	M	162	VAL
3	M	182	ASN

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Mol	Chain	Res	Type
3	N	239	ILE
3	N	257	GLN
3	N	263	GLY
3	R	136	MET
3	R	182	ASN
3	R	265	SER
3	S	155	ARG
3	S	262	PRO
3	S	266	GLY
3	W	281	ALA
3	A	225	TRP
3	A	233	SER
3	A	263	GLY
3	B	153	ARG
3	B	167	GLY
3	B	263	GLY
3	E	167	GLY
3	E	220	ASN
3	E	233	SER
3	E	263	GLY
3	F	139	PHE
3	F	199	THR
3	F	263	GLY
3	I	191	CYS
3	I	235	GLY
3	I	263	GLY
3	I	269	GLY
3	I	283	GLN
3	J	167	GLY
3	J	183	GLN
3	M	228	ASN
3	M	281	ALA
3	N	162	VAL
3	N	256	ILE
3	R	137	GLY
3	R	268	ILE
3	R	269	GLY
3	S	136	MET
3	S	187	ILE
3	S	263	GLY
3	S	276	LEU
3	W	179	ARG

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Mol	Chain	Res	Type
3	W	266	GLY
3	W	283	GLN
3	W	284	SER
3	A	154	ARG
3	B	136	MET
3	B	182	ASN
3	B	199	THR
3	E	281	ALA
3	F	218	ILE
3	F	265	SER
3	I	193	ALA
3	M	230	TRP
3	N	150	SER
3	N	154	ARG
3	N	182	ASN
3	N	186	GLU
3	N	200	GLN
3	R	183	GLN
3	W	139	PHE
3	W	182	ASN
3	W	228	ASN
3	W	263	GLY
3	W	280	GLY
3	F	269	GLY
3	I	179	ARG
3	J	262	PRO
3	N	232	THR
3	N	267	PHE
3	W	155	ARG
3	W	167	GLY
3	B	193	ALA
3	E	169	PRO
3	F	148	CYS
3	I	169	PRO
3	I	233	SER
3	I	262	PRO
3	S	278	ARG
3	W	239	ILE
3	B	186	GLU
3	F	138	ASP
3	I	162	VAL
3	I	192	LYS

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Mol	Chain	Res	Type
3	M	197	ALA
3	N	167	GLY
3	S	137	GLY
3	S	140	VAL
3	I	268	ILE
3	R	215	ILE
3	R	266	GLY
3	W	215	ILE
3	A	268	ILE
3	B	215	ILE
3	E	215	ILE
3	J	155	ARG

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	120/124 (97%)	99 (82%)	21 (18%)	2 10
3	B	121/124 (98%)	97 (80%)	24 (20%)	1 8
3	E	115/124 (93%)	98 (85%)	17 (15%)	3 15
3	F	120/124 (97%)	98 (82%)	22 (18%)	2 9
3	I	112/124 (90%)	102 (91%)	10 (9%)	9 34
3	J	119/124 (96%)	102 (86%)	17 (14%)	3 16
3	M	113/124 (91%)	95 (84%)	18 (16%)	2 13
3	N	113/124 (91%)	97 (86%)	16 (14%)	3 17
3	R	116/124 (94%)	101 (87%)	15 (13%)	4 20
3	S	112/124 (90%)	98 (88%)	14 (12%)	4 21
3	W	115/124 (93%)	102 (89%)	13 (11%)	5 24
All	All	1276/1364 (94%)	1089 (85%)	187 (15%)	3 16

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	144	THR
3	A	157	ARG
3	A	162	VAL
3	A	170	LEU
3	A	172	VAL
3	A	182	ASN
3	A	183	GLN
3	A	187	ILE
3	A	199	THR
3	A	202	ILE
3	A	205	LEU
3	A	207	LEU
3	A	209	THR
3	A	218	ILE
3	A	223	GLN
3	A	226	LYS
3	A	248	GLU
3	A	249	ARG
3	A	251	THR
3	A	252	GLN
3	A	259	MET
3	B	136	MET
3	B	138	ASP
3	B	150	SER
3	B	153	ARG
3	B	156	PRO
3	B	162	VAL
3	B	180	GLN
3	B	181	THR
3	B	182	ASN
3	B	183	GLN
3	B	202	ILE
3	B	205	LEU
3	B	222	VAL
3	B	223	GLN
3	B	226	LYS
3	B	237	GLU
3	B	238	VAL
3	B	239	ILE
3	B	251	THR
3	B	252	GLN
3	B	261	VAL
3	B	268	ILE

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Mol	Chain	Res	Type
3	B	275	ARG
3	B	278	ARG
3	E	140	VAL
3	E	153	ARG
3	E	157	ARG
3	E	168	HIS
3	E	170	LEU
3	E	180	GLN
3	E	182	ASN
3	E	199	THR
3	E	203	ASN
3	E	210	ASN
3	E	226	LYS
3	E	228	ASN
3	E	248	GLU
3	E	252	GLN
3	E	254	MET
3	E	259	MET
3	E	261	VAL
3	F	136	MET
3	F	140	VAL
3	F	180	GLN
3	F	181	THR
3	F	183	GLN
3	F	187	ILE
3	F	194	ILE
3	F	199	THR
3	F	200	GLN
3	F	202	ILE
3	F	209	THR
3	F	210	ASN
3	F	212	MET
3	F	216	ASN
3	F	226	LYS
3	F	228	ASN
3	F	238	VAL
3	F	239	ILE
3	F	241	LYS
3	F	259	MET
3	F	278	ARG
3	F	285	GLU
3	I	139	PHE

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Mol	Chain	Res	Type
3	I	157	ARG
3	I	162	VAL
3	I	180	GLN
3	I	182	ASN
3	I	187	ILE
3	I	200	GLN
3	I	226	LYS
3	I	278	ARG
3	I	284	SER
3	J	135	HIS
3	J	136	MET
3	J	174	ILE
3	J	182	ASN
3	J	188	HIS
3	J	200	GLN
3	J	202	ILE
3	J	210	ASN
3	J	212	MET
3	J	216	ASN
3	J	222	VAL
3	J	226	LYS
3	J	228	ASN
3	J	238	VAL
3	J	249	ARG
3	J	252	GLN
3	J	268	ILE
3	M	141	VAL
3	M	170	LEU
3	M	180	GLN
3	M	183	GLN
3	M	184	ARG
3	M	186	GLU
3	M	187	ILE
3	M	194	ILE
3	M	202	ILE
3	M	207	LEU
3	M	226	LYS
3	M	227	LYS
3	M	228	ASN
3	M	238	VAL
3	M	239	ILE
3	M	259	MET

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Mol	Chain	Res	Type
3	M	261	VAL
3	M	267	PHE
3	N	154	ARG
3	N	170	LEU
3	N	182	ASN
3	N	187	ILE
3	N	199	THR
3	N	202	ILE
3	N	210	ASN
3	N	212	MET
3	N	226	LYS
3	N	227	LYS
3	N	228	ASN
3	N	245	VAL
3	N	252	GLN
3	N	259	MET
3	N	265	SER
3	N	276	LEU
3	R	153	ARG
3	R	162	VAL
3	R	180	GLN
3	R	183	GLN
3	R	187	ILE
3	R	207	LEU
3	R	216	ASN
3	R	222	VAL
3	R	226	LYS
3	R	228	ASN
3	R	249	ARG
3	R	252	GLN
3	R	259	MET
3	R	267	PHE
3	R	268	ILE
3	S	153	ARG
3	S	162	VAL
3	S	180	GLN
3	S	181	THR
3	S	182	ASN
3	S	187	ILE
3	S	188	HIS
3	S	202	ILE
3	S	210	ASN

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Mol	Chain	Res	Type
3	S	216	ASN
3	S	238	VAL
3	S	240	ASN
3	S	259	MET
3	S	274	ASP
3	W	162	VAL
3	W	172	VAL
3	W	180	GLN
3	W	182	ASN
3	W	199	THR
3	W	202	ILE
3	W	210	ASN
3	W	212	MET
3	W	248	GLU
3	W	252	GLN
3	W	259	MET
3	W	268	ILE
3	W	274	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	182	ASN
3	A	183	GLN
3	A	216	ASN
3	A	220	ASN
3	A	228	ASN
3	A	240	ASN
3	A	257	GLN
3	B	151	ASN
3	B	183	GLN
3	B	216	ASN
3	B	257	GLN
3	B	264	HIS
3	B	270	ASN
3	B	283	GLN
3	E	182	ASN
3	E	223	GLN
3	E	240	ASN
3	E	264	HIS
3	E	270	ASN
3	F	183	GLN

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Mol	Chain	Res	Type
3	F	200	GLN
3	F	210	ASN
3	F	216	ASN
3	F	283	GLN
3	I	171	ASN
3	I	182	ASN
3	I	196	GLN
3	I	200	GLN
3	I	201	ASN
3	I	216	ASN
3	I	283	GLN
3	J	151	ASN
3	J	182	ASN
3	J	200	GLN
3	J	201	ASN
3	J	216	ASN
3	J	257	GLN
3	J	283	GLN
3	M	180	GLN
3	M	183	GLN
3	M	228	ASN
3	M	257	GLN
3	M	264	HIS
3	N	180	GLN
3	N	200	GLN
3	N	216	ASN
3	N	228	ASN
3	N	240	ASN
3	N	260	HIS
3	N	270	ASN
3	R	135	HIS
3	R	180	GLN
3	R	183	GLN
3	R	216	ASN
3	R	220	ASN
3	R	223	GLN
3	R	228	ASN
3	R	257	GLN
3	R	260	HIS
3	R	270	ASN
3	S	183	GLN
3	S	200	GLN

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Mol	Chain	Res	Type
3	S	216	ASN
3	S	220	ASN
3	S	223	GLN
3	S	228	ASN
3	S	252	GLN
3	S	260	HIS
3	W	135	HIS
3	W	183	GLN
3	W	200	GLN
3	W	216	ASN
3	W	257	GLN
3	W	260	HIS
3	W	270	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	13/14 (92%)	0	0
1	G	13/14 (92%)	1 (7%)	0
1	K	13/14 (92%)	2 (15%)	0
1	O	13/14 (92%)	1 (7%)	0
1	T	13/14 (92%)	0	0
1	X	12/14 (85%)	2 (16%)	0
All	All	77/84 (91%)	6 (7%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	7	C
1	K	7	C
1	K	14	C
1	O	7	C
1	X	7	C
1	X	14	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 15 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TRS	D	2003	-	7,7,7	0.88	0	9,9,9	0.45	0
6	MES	A	2002	-	12,12,12	1.08	1 (8%)	15,16,16	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	D	2003	-	-	0/9/9/9	-
6	MES	A	2002	-	-	0/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2002	MES	C8-S	2.57	1.81	1.77

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2002	MES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	C	14/14 (100%)	-1.64	0	100	100	17, 24, 34, 40	0
1	G	14/14 (100%)	-1.65	0	100	100	24, 31, 38, 41	0
1	K	14/14 (100%)	-1.63	0	100	100	56, 62, 72, 75	0
1	O	14/14 (100%)	-1.76	0	100	100	44, 52, 74, 76	0
1	T	14/14 (100%)	-1.61	0	100	100	44, 57, 76, 85	0
1	X	13/14 (92%)	-1.07	0	100	100	68, 89, 144, 152	0
2	D	14/14 (100%)	-1.30	0	100	100	22, 32, 43, 50	0
2	H	14/14 (100%)	-1.22	0	100	100	28, 36, 43, 48	0
2	L	14/14 (100%)	-1.15	0	100	100	55, 74, 92, 123	0
2	P	14/14 (100%)	-1.27	0	100	100	42, 56, 81, 103	0
2	U	14/14 (100%)	-1.16	0	100	100	54, 69, 83, 91	0
2	Z	11/14 (78%)	-0.84	0	100	100	82, 88, 117, 131	0
3	A	154/154 (100%)	-1.20	0	100	100	18, 36, 73, 96	0
3	B	151/154 (98%)	-1.17	0	100	100	30, 51, 82, 108	1 (0%)
3	E	149/154 (96%)	-1.07	0	100	100	32, 51, 77, 93	0
3	F	152/154 (98%)	-1.16	0	100	100	30, 50, 83, 101	1 (0%)
3	I	149/154 (96%)	-0.94	0	100	100	44, 92, 117, 129	1 (0%)
3	J	151/154 (98%)	-1.05	0	100	100	35, 64, 87, 96	2 (1%)
3	M	145/154 (94%)	-1.19	0	100	100	35, 59, 80, 102	1 (0%)
3	N	146/154 (94%)	-1.07	0	100	100	46, 68, 87, 96	1 (0%)
3	R	148/154 (96%)	-1.22	0	100	100	34, 56, 80, 87	1 (0%)
3	S	148/154 (96%)	-1.07	0	100	100	29, 70, 98, 109	3 (2%)
3	W	148/154 (96%)	-1.06	0	100	100	45, 75, 96, 102	3 (2%)
All	All	1805/1862 (96%)	-1.13	0	100	100	17, 63, 98, 152	14 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRS	D	2003	8/8	0.92	0.10	94,96,97,97	0
5	CA	E	1004	1/1	0.96	0.04	68,68,68,68	0
7	CL	B	2001	1/1	0.97	0.09	49,49,49,49	0
6	MES	A	2002	12/12	0.98	0.08	136,136,138,138	0
5	CA	A	1001	1/1	0.99	0.03	44,44,44,44	0
5	CA	I	1006	1/1	0.99	0.04	78,78,78,78	0
5	CA	M	1014	1/1	0.99	0.03	106,106,106,106	0
5	CA	R	1011	1/1	0.99	0.03	64,64,64,64	0
5	CA	A	1002	1/1	0.99	0.02	23,23,23,23	0
5	CA	E	1003	1/1	0.99	0.03	44,44,44,44	0
5	CA	F	1013	1/1	1.00	0.03	32,32,32,32	0
5	CA	N	1005	1/1	1.00	0.02	56,56,56,56	0
5	CA	B	1009	1/1	1.00	0.02	38,38,38,38	0
5	CA	S	1007	1/1	1.00	0.02	77,77,77,77	0
5	CA	W	1012	1/1	1.00	0.03	81,81,81,81	0
5	CA	J	1008	1/1	1.00	0.03	53,53,53,53	0
5	CA	M	1010	1/1	1.00	0.01	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.