Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 06:32 AM EDT

PDB ID	:	3HTX
Title	:	Crystal structure of small RNA methyltransferase HEN1
Authors	:	Huang, Y.; Ji, L.-J.; Huang, Q.-C.; Vassylyev, D.G.; Chen, X.-M.; Ma, J.-B.
Deposited on	:	2009-06-12
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

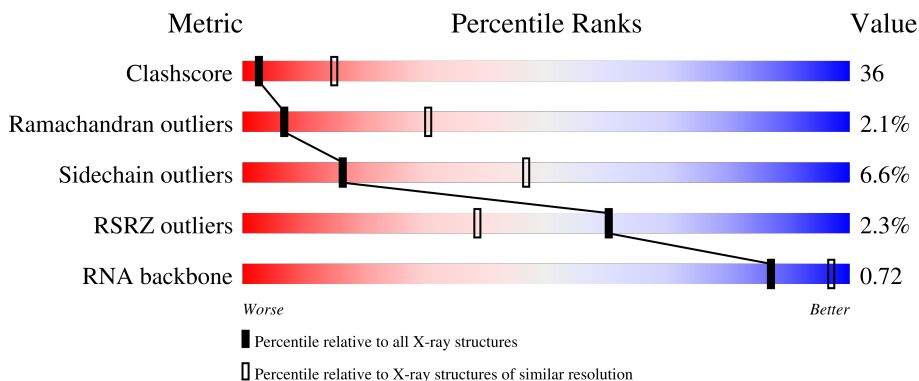|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.10 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	Percentile Ranks	Value
Clashscore		36
Ramachandran outliers		2.1%
Sidechain outliers		6.6%
RSRZ outliers		2.3%
RNA backbone		0.72

Worse *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	A	950	2% 37% 40% • 18%
1	D	950	2% 36% 44% • 16%
2	B	22	9% 77% 14%
2	E	22	32% 64% 5%
3	C	22	27% 59% 14%

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Mol	Chain	Length	Quality of chain
3	F	22	

50% 32% 14% 5%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 14269 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 protein called HEN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total 6093	C 3847	N 1046	O 1170	S 30	0	0	0
1	D	795	Total 6217	C 3928	N 1065	O 1194	S 30	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q945R3
A	-6	GLY	-	expression tag	UNP Q945R3
A	-5	HIS	-	expression tag	UNP Q945R3
A	-4	HIS	-	expression tag	UNP Q945R3
A	-3	HIS	-	expression tag	UNP Q945R3
A	-2	HIS	-	expression tag	UNP Q945R3
A	-1	HIS	-	expression tag	UNP Q945R3
A	0	HIS	-	expression tag	UNP Q945R3
A	604	PRO	LEU	engineered mutation	UNP Q945R3
A	640	LYS	ARG	engineered mutation	UNP Q945R3
D	-7	MET	-	expression tag	UNP Q945R3
D	-6	GLY	-	expression tag	UNP Q945R3
D	-5	HIS	-	expression tag	UNP Q945R3
D	-4	HIS	-	expression tag	UNP Q945R3
D	-3	HIS	-	expression tag	UNP Q945R3
D	-2	HIS	-	expression tag	UNP Q945R3
D	-1	HIS	-	expression tag	UNP Q945R3
D	0	HIS	-	expression tag	UNP Q945R3
D	604	PRO	LEU	engineered mutation	UNP Q945R3
D	640	LYS	ARG	engineered mutation	UNP Q945R3

- Molecule 2 is a RNA chain called 5'-R(*GP*AP*UP*UP*UP*CP*UP*CP*UP*CP*UP*G P*CP*AP*AP*GP*CP*GP*AP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	22	Total	C	N	O	P	0	0	0
			464	209	82	152	21			
2	E	22	Total	C	N	O	P	0	0	0
			464	209	82	152	21			

- Molecule 3 is a RNA chain called 5'-R(P*UP*UP*CP*GP*CP*UP*UP*GP*CP*AP*GP*AP*GP*AP*GP*AP*AP*AP*UP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	P	0	0	0
			470	210	85	153	22			
3	F	22	Total	C	N	O	P	0	0	0
			470	210	85	153	22			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).
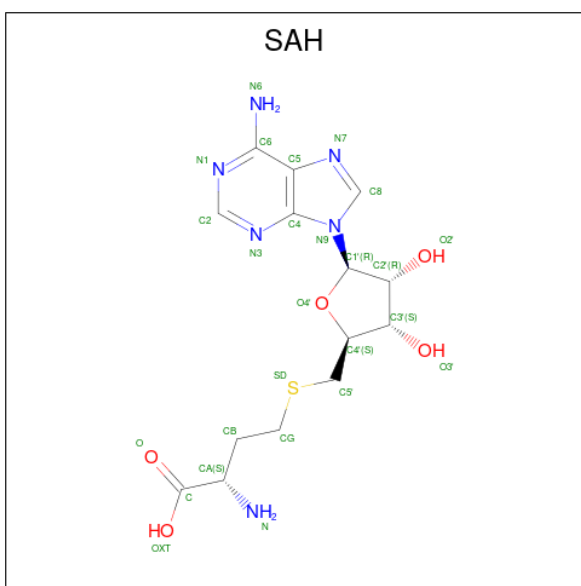
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	D	16	Total	O	0	0
			16	16		
6	E	1	Total	O	0	0
			1	1		
6	F	2	Total	O	0	0
			2	2		

3 Residue-property plots ⓘ

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: HEN1
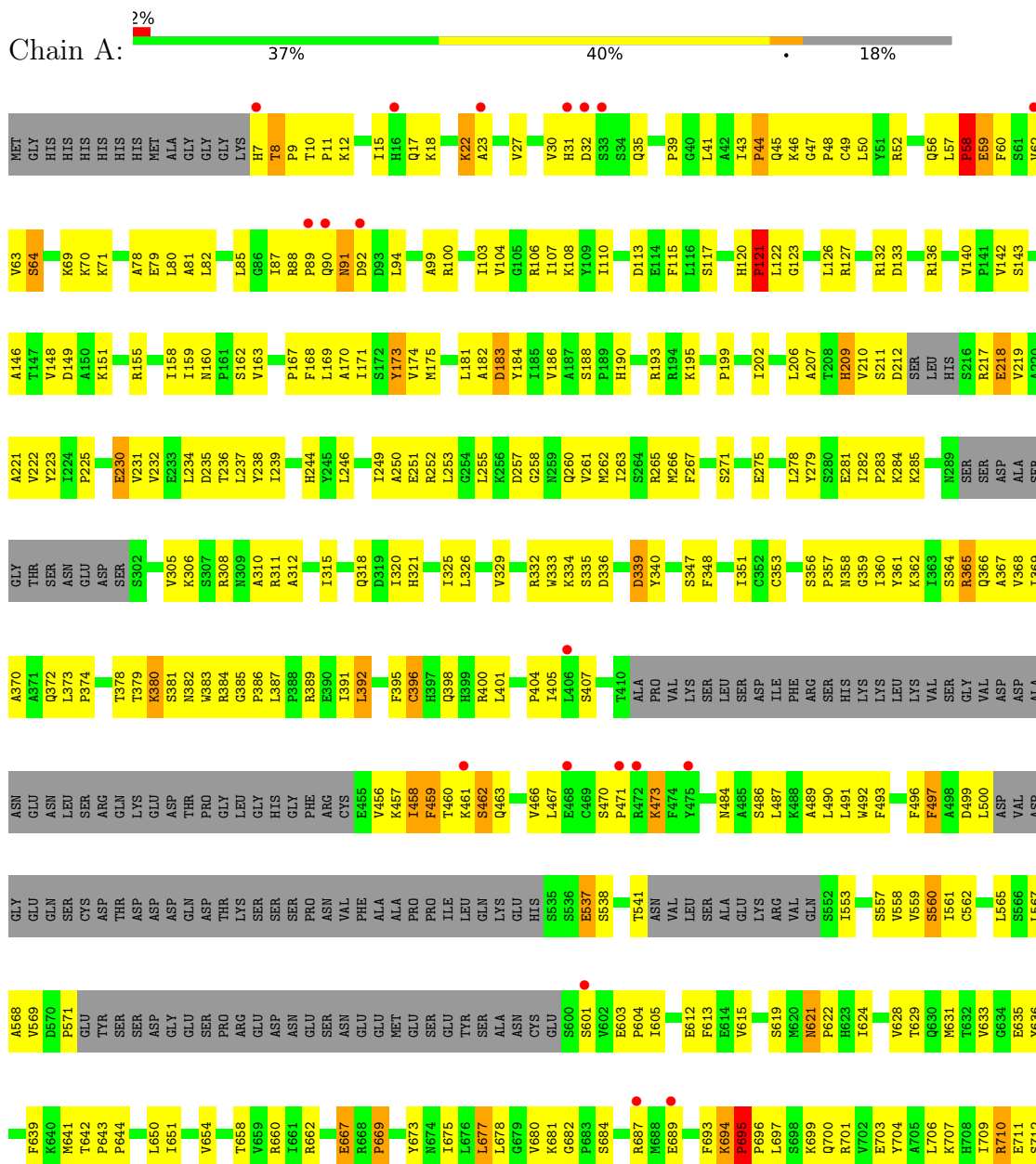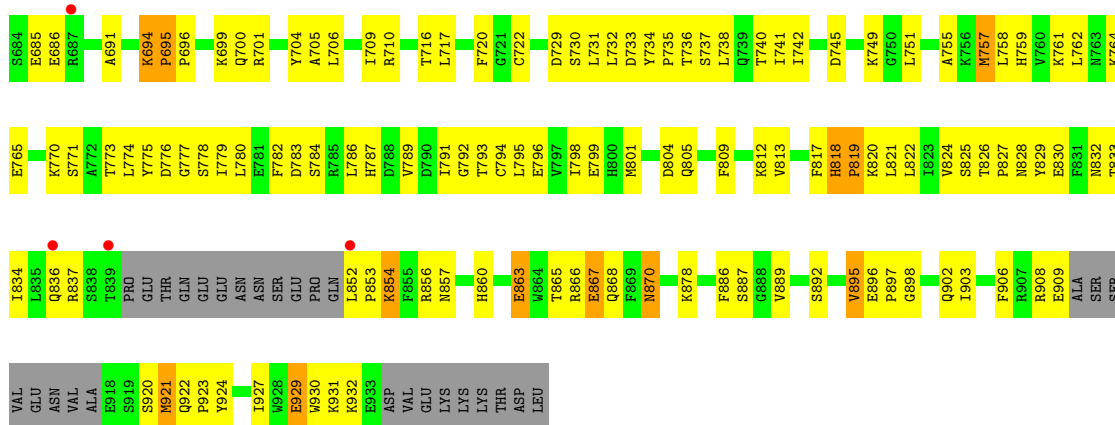
Chain A:

● Molecule 1: HEN1

Chain D:

• Molecule 2: 5'-R(*GP*AP*UP*UP*UP*CP*UP*CP*UP*CP*UP*GP*CP*AP*AP*GP*CP*G P*AP*AP*AP*G)-3'
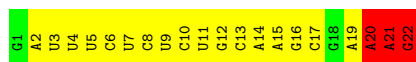
Chain B:

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

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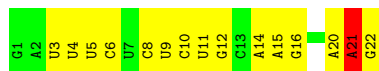
• Molecule 3: 5'-R(P*UP*UP*CP*GP*CP*UP*UP*GP*CP*AP*GP*AP*GP*AP*GP*AP*AP* AP*UP*CP*AP*C)-3'

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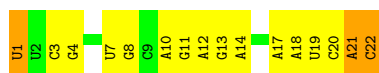
• Molecule 3: 5'-R(P*UP*UP*CP*GP*CP*UP*UP*GP*CP*AP*GP*AP*GP*AP*GP*AP*AP* AP*UP*CP*AP*C)-3'

Chain F:

4　Data and refinement statistics　ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.00Å　　124.35Å　　101.38Å 90.00°　　93.47°　　90.00°	Depositor
Resolution (Å)	20.00　–　3.10 19.99　–　3.10	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-3.10) 78.0 (19.99-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260　　,　　　0.288 0.246　　,　　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	72.0	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 11.0	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.054 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14269	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, SAH

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	A	0.51	0/6214	0.75	4/8395 (0.0%)
1	D	0.52	0/6343	0.76	5/8573 (0.1%)
2	B	0.46	0/518	0.92	3/805 (0.4%)
2	E	0.46	0/518	0.78	1/805 (0.1%)
3	C	0.55	1/525 (0.2%)	0.69	0/814
3	F	0.58	1/525 (0.2%)	0.84	1/814 (0.1%)
All	All	0.51	2/14643 (0.0%)	0.77	14/20206 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	U	OP3-P	-6.77	1.53	1.61
3	F	1	U	OP3-P	-6.57	1.53	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	20	A	C2'-C3'-O3'	9.92	131.33	109.50
3	F	19	U	C2'-C3'-O3'	8.29	127.75	109.50
1	A	789	VAL	CB-CA-C	-7.54	97.08	111.40
1	D	20	GLY	N-CA-C	-7.19	95.12	113.10
1	D	818	HIS	C-N-CD	-7.07	105.05	120.60
1	D	695	PRO	N-CA-C	-6.44	95.36	112.10
2	B	21	A	C5'-C4'-C3'	-6.41	105.74	116.00
2	B	22	G	C2'-C3'-O3'	5.88	123.10	113.70
1	D	499	ASP	N-CA-C	-5.69	95.64	111.00
2	E	21	A	N9-C1'-C2'	5.44	121.07	114.00
1	A	764	LYS	N-CA-C	-5.43	96.33	111.00
1	A	695	PRO	N-CA-C	-5.15	98.71	112.10
1	D	819	PRO	N-CA-C	-5.06	98.95	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	562	CYS	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6093	0	6031	434	0
1	D	6217	0	6139	493	0
2	B	464	0	236	35	0
2	E	464	0	236	21	0
3	C	470	0	238	20	0
3	F	470	0	238	17	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	26	0	19	2	0
5	D	26	0	19	1	0
6	A	14	0	0	5	0
6	B	2	0	0	2	0
6	C	2	0	0	0	0
6	D	16	0	0	2	0
6	E	1	0	0	0	0
6	F	2	0	0	1	0
All	All	14269	0	13156	987	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (987) 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)
1:A:802:GLU:HB2	1:A:805:GLN:HG3	1.21	1.20
3:F:21:A:H2'	6:F:226:HOH:O	1.45	1.12
1:A:262:MET:HE3	1:A:263:ILE:H	1.16	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:776:ASP:HB2	1:D:927:ILE:HD11	1.34	1.07
1:A:45:GLN:HE21	1:A:752:ALA:HB1	1.18	1.07
1:A:401:LEU:HD22	1:A:461:LYS:HB2	1.39	1.03
1:A:142:VAL:HG11	1:A:171:ILE:HG23	1.43	1.01
1:A:15:ILE:HG21	1:A:82:LEU:HD11	1.43	1.00
1:D:537:GLU:HA	1:D:641:MET:HE2	1.42	1.00
1:D:570:ASP:H	1:D:571:PRO:HD2	1.27	0.98
1:D:457:LYS:HE2	1:D:457:LYS:HA	1.46	0.97
1:A:183:ASP:HA	6:A:947:HOH:O	1.66	0.95
1:D:43:ILE:N	1:D:44:PRO:HD3	1.82	0.94
1:D:836:GLN:HE22	1:D:854:LYS:HB2	1.29	0.94
1:A:45:GLN:NE2	1:A:752:ALA:HB1	1.82	0.93
1:D:401:LEU:HD22	1:D:461:LYS:HD3	1.51	0.93
1:A:82:LEU:HD23	1:A:85:LEU:HD12	1.50	0.92
1:D:262:MET:HB2	1:D:282:ILE:HG12	1.52	0.92
1:A:405:ILE:HB	1:A:458:ILE:HG12	1.53	0.91
1:D:116:LEU:HG	1:D:206:LEU:HD11	1.53	0.89
1:D:757:MET:HG3	1:D:758:LEU:N	1.85	0.89
1:D:265:ARG:H	1:D:318:GLN:NE2	1.71	0.88
1:A:244:HIS:HD2	1:A:246:LEU:H	1.18	0.88
1:D:244:HIS:CD2	1:D:246:LEU:HB2	2.09	0.88
1:A:400:ARG:O	1:A:401:LEU:HD23	1.74	0.87
1:D:570:ASP:H	1:D:571:PRO:CD	1.88	0.87
1:D:716:THR:HG22	1:D:740:THR:HB	1.56	0.87
1:A:810:GLY:HA3	1:A:876:LEU:HD21	1.57	0.86
1:A:457:LYS:HZ3	1:A:486:SER:HA	1.41	0.86
1:A:401:LEU:HD22	1:A:461:LYS:CB	2.04	0.86
1:D:88:ARG:HG2	1:D:89:PRO:HD2	1.57	0.86
1:D:262:MET:HB2	1:D:282:ILE:CG1	2.06	0.86
1:D:817:PHE:O	1:D:819:PRO:HD2	1.77	0.85
1:D:43:ILE:N	1:D:44:PRO:CD	2.39	0.84
1:A:831:PHE:O	1:A:834:ILE:HG22	1.76	0.83
1:A:365:ARG:HG3	1:A:365:ARG:HH11	1.44	0.83
1:D:265:ARG:H	1:D:318:GLN:HE22	1.21	0.83
1:D:729:ASP:HB2	1:D:757:MET:SD	2.19	0.83
1:D:710:ARG:NH2	1:D:734:TYR:HB2	1.92	0.83
1:D:776:ASP:HB2	1:D:927:ILE:CD1	2.07	0.83
1:A:255:LEU:HD11	1:A:281:GLU:HB2	1.62	0.82
1:A:88:ARG:HG3	1:A:89:PRO:HD3	1.59	0.82
1:A:742:ILE:HD13	1:A:786:LEU:HD22	1.62	0.82
1:D:387:LEU:HB3	1:D:483:GLN:HE22	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ALA:CB	1:D:57:LEU:HD23	2.09	0.81
1:A:405:ILE:HD12	1:A:458:ILE:HD11	1.61	0.81
1:A:127:ARG:HG3	1:A:206:LEU:HD21	1.63	0.81
1:D:124:ALA:HA	1:D:127:ARG:NH1	1.96	0.81
1:D:621:ASN:HD22	1:D:624:ILE:HG13	1.45	0.81
1:D:548:LYS:O	1:D:552:SER:HB2	1.80	0.81
1:D:892:SER:HB2	1:D:895:VAL:HG23	1.62	0.80
1:A:126:LEU:HD23	1:A:140:VAL:HG21	1.63	0.80
1:D:43:ILE:HD11	1:D:927:ILE:HD13	1.64	0.80
1:A:569:VAL:HG23	1:A:601:SER:HB2	1.61	0.80
1:A:865:THR:H	1:A:868:GLN:NE2	1.80	0.80
1:D:817:PHE:C	1:D:819:PRO:HD2	2.02	0.80
1:A:624:ILE:HG23	1:A:675:ILE:HD11	1.65	0.79
1:D:57:LEU:HB3	1:D:58:PRO:HD2	1.62	0.79
1:D:105:GLY:O	1:D:108:LYS:HG2	1.82	0.79
1:D:570:ASP:N	1:D:571:PRO:HD2	1.96	0.79
1:A:895:VAL:HG12	1:A:897:PRO:HD2	1.64	0.79
1:D:387:LEU:HB3	1:D:483:GLN:NE2	1.98	0.79
1:A:537:GLU:HB3	1:A:641:MET:CE	2.12	0.79
1:D:559:VAL:HG12	1:D:561:ILE:HG23	1.63	0.79
1:D:799:GLU:HG3	1:D:860:HIS:CD2	2.18	0.79
1:A:537:GLU:HB3	1:A:641:MET:HE1	1.64	0.78
1:D:740:THR:HG23	1:D:771:SER:HB3	1.66	0.78
1:D:829:TYR:HD1	1:D:832:ASN:HD21	1.29	0.78
1:D:266:MET:HB3	1:D:277:ARG:HE	1.47	0.78
1:A:457:LYS:NZ	1:A:486:SER:HA	1.98	0.78
1:D:405:ILE:HB	1:D:458:ILE:HG13	1.66	0.78
2:E:8:C:H2'	2:E:9:U:C6	2.20	0.77
1:A:108:LYS:HD2	1:A:181:LEU:HD21	1.66	0.77
1:A:151:LYS:O	1:A:155:ARG:HG2	1.85	0.77
1:D:557:SER:O	1:D:615:VAL:HG23	1.84	0.77
1:D:461:LYS:HG3	1:D:466:VAL:HG21	1.65	0.77
1:A:123:GLY:O	1:A:127:ARG:HB2	1.86	0.76
1:D:552:SER:HA	1:D:629:THR:O	1.86	0.76
1:A:852:LEU:HB2	1:A:855:PHE:CE1	2.20	0.76
1:A:865:THR:H	1:A:868:GLN:HE21	1.30	0.76
3:F:19:U:O2'	3:F:20:C:H5'	1.86	0.76
1:D:164:GLU:HB3	1:D:400:ARG:HH12	1.48	0.75
1:A:318:GLN:HG3	1:A:400:ARG:HH22	1.50	0.75
1:D:895:VAL:HG12	1:D:897:PRO:HD2	1.67	0.75
1:A:827:PRO:HA	1:A:901:SER:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:18:A:H2'	3:F:19:U:C6	2.21	0.75
1:A:553:ILE:HD12	1:A:629:THR:HA	1.68	0.75
1:D:568:ALA:HB1	1:D:601:SER:O	1.85	0.75
1:D:830:GLU:HG3	1:D:865:THR:HG23	1.69	0.75
1:D:181:LEU:HG	1:D:184:TYR:HB2	1.68	0.74
1:A:704:TYR:HA	1:A:707:LYS:HE3	1.69	0.74
1:D:41:LEU:HD21	1:D:755:ALA:HB1	1.69	0.74
1:D:606:GLU:HB3	1:D:654:VAL:HG11	1.70	0.74
1:A:650:LEU:O	1:A:654:VAL:HG23	1.86	0.74
1:D:552:SER:HA	1:D:629:THR:HG22	1.68	0.74
1:D:12:LYS:HG3	1:D:79:GLU:HB2	1.69	0.74
1:A:368:VAL:HB	1:A:650:LEU:HD11	1.68	0.74
1:D:16:HIS:NE2	1:D:82:LEU:HG	2.03	0.74
3:F:19:U:H2'	3:F:20:C:H6	1.53	0.73
1:A:47:GLY:HA2	2:B:15:A:H4'	1.69	0.73
1:D:283:PRO:HG2	1:D:286:TYR:HD1	1.54	0.73
1:D:627:GLU:HB2	6:D:955:HOH:O	1.86	0.73
1:D:731:LEU:HD21	1:D:738:LEU:HD13	1.71	0.73
1:A:392:LEU:HD22	1:A:457:LYS:HZ2	1.54	0.73
1:A:864:TRP:HA	1:A:868:GLN:NE2	2.03	0.73
1:D:866:ARG:NH1	1:D:898:GLY:HA3	2.03	0.73
1:A:10:THR:HG21	1:A:90:GLN:HG2	1.69	0.72
1:D:836:GLN:NE2	1:D:854:LYS:HB2	2.04	0.72
1:A:94:LEU:HD23	1:A:99:ALA:HB2	1.72	0.72
1:A:569:VAL:O	1:A:571:PRO:HD3	1.88	0.72
1:D:710:ARG:CZ	1:D:734:TYR:HB2	2.19	0.72
1:D:88:ARG:CG	1:D:89:PRO:HD2	2.20	0.72
1:A:364:SER:HB3	1:A:386:PRO:HG2	1.70	0.72
1:D:784:SER:HB3	1:D:920:SER:HA	1.73	0.71
1:D:628:VAL:CG2	1:D:675:ILE:HD12	2.21	0.71
1:D:731:LEU:HD11	1:D:738:LEU:HD12	1.72	0.71
1:D:164:GLU:HB3	1:D:400:ARG:NH1	2.05	0.71
1:A:253:LEU:HD21	1:A:325:ILE:HG12	1.72	0.71
1:D:244:HIS:HD2	1:D:246:LEU:HB2	1.54	0.71
1:D:402:ALA:HB3	1:D:460:THR:O	1.91	0.71
1:A:364:SER:CB	1:A:386:PRO:HG2	2.21	0.71
1:D:283:PRO:HG2	1:D:286:TYR:CD1	2.26	0.71
1:D:553:ILE:H	1:D:629:THR:HG23	1.56	0.71
1:D:278:LEU:HD21	1:D:312:ALA:HB1	1.73	0.70
1:A:262:MET:HE3	1:A:263:ILE:N	2.00	0.70
1:D:742:ILE:HG21	1:D:786:LEU:HD21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:628:VAL:HG22	1:D:675:ILE:HD12	1.72	0.70
1:D:160:ASN:O	1:D:163:VAL:HG23	1.92	0.70
1:D:232:VAL:HG23	1:D:311:ARG:NH2	2.07	0.70
1:A:332:ARG:HG2	1:A:333:TRP:H	1.57	0.70
1:A:392:LEU:HD11	1:A:459:PHE:HE1	1.57	0.70
1:D:567:LEU:HB2	1:D:605:ILE:HD11	1.72	0.70
1:D:827:PRO:HB3	1:D:856:ARG:HD2	1.72	0.69
1:A:367:ALA:HB1	1:A:370:ALA:HB3	1.74	0.69
1:A:255:LEU:HB3	1:A:260:GLN:OE1	1.92	0.69
1:A:667:GLU:O	1:A:669:PRO:HD3	1.93	0.69
1:A:887:SER:O	1:A:903:ILE:HB	1.93	0.69
1:A:369:ILE:HG21	1:A:565:LEU:HD11	1.74	0.69
1:D:81:ALA:O	1:D:85:LEU:HG	1.93	0.69
1:A:809:PHE:O	1:A:813:VAL:HG23	1.93	0.69
1:A:108:LYS:HB2	1:A:181:LEU:HD21	1.74	0.69
3:C:7:U:H2'	3:C:8:G:C8	2.28	0.69
1:A:110:ILE:HG22	1:A:126:LEU:HD11	1.74	0.68
3:F:21:A:H1'	3:F:22:C:H5	1.57	0.68
1:D:731:LEU:HD21	1:D:738:LEU:CD1	2.23	0.68
1:D:219:VAL:HG21	1:D:239:ILE:HD11	1.74	0.68
1:A:244:HIS:CD2	1:A:246:LEU:H	2.06	0.68
1:D:257:ASP:H	1:D:260:GLN:HE21	1.42	0.68
1:D:809:PHE:O	1:D:813:VAL:HG23	1.93	0.68
1:A:721:GLY:HA3	1:A:797:VAL:HG21	1.75	0.68
1:D:559:VAL:CG1	1:D:561:ILE:HG23	2.23	0.68
1:D:406:LEU:HD13	1:D:457:LYS:HE3	1.74	0.68
1:A:362:LYS:HB3	1:A:368:VAL:HA	1.76	0.67
1:A:18:LYS:HE2	3:C:19:U:H4'	1.75	0.67
1:A:117:SER:HB3	1:A:206:LEU:HD13	1.77	0.67
1:D:43:ILE:O	1:D:43:ILE:HG22	1.91	0.67
1:D:152:ILE:O	1:D:156:CYS:HB2	1.94	0.67
1:D:265:ARG:HH12	1:D:400:ARG:HE	1.42	0.67
1:D:828:ASN:HA	1:D:902:GLN:NE2	2.10	0.67
1:D:30:VAL:HG12	1:D:32:ASP:H	1.58	0.67
1:D:124:ALA:HA	1:D:127:ARG:HH12	1.57	0.67
1:D:194:ARG:HH12	1:D:198:TYR:HA	1.60	0.67
1:D:344:THR:H	1:D:347:SER:HB2	1.60	0.67
1:A:108:LYS:HB2	1:A:181:LEU:CD2	2.24	0.67
1:D:43:ILE:HD11	1:D:927:ILE:CD1	2.23	0.67
1:A:742:ILE:HD13	1:A:786:LEU:CD2	2.24	0.67
1:D:459:PHE:HB2	1:D:466:VAL:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:691:ALA:HB2	2:E:20:A:H5"	1.75	0.67
1:D:347:SER:O	1:D:351:ILE:HG12	1.94	0.66
1:A:94:LEU:HB2	1:A:158:ILE:HD13	1.78	0.66
3:C:7:U:H2'	3:C:8:G:H8	1.59	0.66
3:C:21:A:H5'	3:C:22:C:OP1	1.96	0.66
1:A:753:ARG:O	1:A:756:LYS:HG2	1.94	0.66
1:D:23:ALA:HB1	1:D:56:GLN:O	1.95	0.66
1:D:458:ILE:HG22	1:D:468:GLU:HA	1.76	0.66
1:A:658:THR:O	1:A:662:ARG:CG	2.43	0.66
1:A:888:GLY:C	1:A:899:PHE:CD2	2.70	0.66
1:A:149:ASP:OD1	1:A:151:LYS:HB2	1.95	0.65
1:D:567:LEU:CB	1:D:605:ILE:HD11	2.26	0.65
1:A:561:ILE:HD11	1:A:613:PHE:HE1	1.62	0.65
1:A:829:TYR:HD1	1:A:863:GLU:HB3	1.61	0.65
1:A:888:GLY:O	1:A:899:PHE:CE2	2.50	0.65
1:A:113:ASP:HB3	1:A:202:ILE:HD13	1.78	0.65
1:D:257:ASP:H	1:D:260:GLN:NE2	1.94	0.65
1:D:467:LEU:HD13	1:D:492:TRP:CZ3	2.31	0.65
1:A:168:PHE:HE2	1:A:282:ILE:HA	1.62	0.65
1:A:57:LEU:HG	1:A:58:PRO:HD2	1.79	0.64
1:D:210:VAL:HG12	1:D:211:SER:N	2.12	0.64
1:D:655:GLY:HA3	1:D:661:ILE:HD11	1.78	0.64
1:A:639:PHE:HE1	1:A:641:MET:HE3	1.61	0.64
1:A:639:PHE:CE1	1:A:641:MET:HE3	2.33	0.64
1:D:362:LYS:HD3	1:D:368:VAL:O	1.97	0.64
1:A:85:LEU:HD22	1:A:88:ARG:NH2	2.12	0.64
1:D:798:ILE:HD11	1:D:826:THR:OG1	1.98	0.64
3:F:21:A:H1'	3:F:22:C:C5	2.33	0.64
1:A:239:ILE:N	1:A:239:ILE:HD12	2.13	0.64
1:D:168:PHE:CD2	1:D:282:ILE:HG23	2.32	0.64
1:D:265:ARG:HH12	1:D:400:ARG:NE	1.94	0.64
1:D:701:ARG:NH1	1:D:796:GLU:HG2	2.13	0.64
1:A:88:ARG:CG	1:A:89:PRO:HD3	2.28	0.63
1:A:392:LEU:HD13	1:A:457:LYS:HZ1	1.63	0.63
1:D:60:PHE:HE1	1:D:62:VAL:HG22	1.64	0.63
1:A:365:ARG:HH11	1:A:365:ARG:CG	2.12	0.63
1:A:624:ILE:HG23	1:A:675:ILE:CD1	2.28	0.63
1:A:12:LYS:HA	1:A:15:ILE:HD12	1.79	0.63
1:A:658:THR:O	1:A:662:ARG:HG2	1.98	0.63
1:A:883:SER:HB3	1:A:907:ARG:HB2	1.78	0.63
1:D:14:ILE:HD11	2:E:5:U:H1'	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:LEU:HD22	1:D:68:LYS:HA	1.79	0.63
1:D:401:LEU:HA	1:D:461:LYS:HG2	1.78	0.63
1:D:627:GLU:N	6:D:955:HOH:O	2.31	0.63
1:D:929:GLU:HG3	1:D:930:TRP:N	2.13	0.63
1:A:796:GLU:HA	1:A:825:SER:O	1.99	0.63
1:D:240:SER:HB2	1:D:242:ASN:OD1	1.98	0.63
1:A:795:LEU:O	1:A:796:GLU:HG3	1.99	0.63
1:D:243:ARG:HH11	1:D:248:SER:HB3	1.63	0.63
1:A:565:LEU:HD21	1:A:673:TYR:CE2	2.33	0.63
1:A:813:VAL:HA	1:A:817:PHE:HD1	1.64	0.63
1:A:852:LEU:HB2	1:A:855:PHE:HE1	1.62	0.63
1:D:278:LEU:HD23	1:D:320:ILE:HG13	1.81	0.63
1:A:69:LYS:HE3	3:C:8:G:OP1	1.98	0.62
1:D:455:GLU:HG2	1:D:482:ILE:HA	1.81	0.62
1:D:661:ILE:O	1:D:665:LEU:HG	1.99	0.62
1:A:329:VAL:HG12	1:A:340:TYR:HB3	1.82	0.62
1:D:102:GLU:HG3	1:D:155:ARG:HD2	1.81	0.62
1:D:710:ARG:HH22	1:D:734:TYR:HB2	1.65	0.62
1:A:717:LEU:HD12	1:A:718:VAL:N	2.14	0.62
2:B:2:A:H2'	2:B:3:U:O4'	1.99	0.62
1:D:373:LEU:HD12	1:D:374:PRO:HD2	1.81	0.62
1:D:751:LEU:HD13	1:D:927:ILE:HD13	1.81	0.62
1:A:238:TYR:HE1	1:A:252:ARG:HH22	1.46	0.62
1:A:255:LEU:HD22	1:A:260:GLN:NE2	2.15	0.62
1:D:23:ALA:HB2	1:D:57:LEU:HD23	1.81	0.62
1:D:256:LYS:H	1:D:260:GLN:HE22	1.46	0.62
1:D:169:LEU:HB3	1:D:173:TYR:CE1	2.34	0.62
1:D:729:ASP:HB2	1:D:757:MET:CE	2.30	0.62
1:A:182:ALA:O	6:A:947:HOH:O	2.16	0.62
1:D:283:PRO:C	1:D:285:LYS:H	2.02	0.62
1:D:467:LEU:HD22	1:D:492:TRP:CE3	2.34	0.62
1:A:368:VAL:CG2	1:A:654:VAL:HG22	2.30	0.62
1:D:45:GLN:HE22	1:D:749:LYS:HA	1.65	0.62
1:A:694:LYS:HB3	1:A:695:PRO:CD	2.29	0.61
1:D:43:ILE:H	1:D:44:PRO:HD3	1.63	0.61
1:D:41:LEU:HD21	1:D:755:ALA:CB	2.29	0.61
1:D:387:LEU:O	1:D:391:ILE:HG13	2.00	0.61
1:D:716:THR:HA	1:D:740:THR:O	2.00	0.61
1:A:60:PHE:HB2	6:A:948:HOH:O	2.01	0.61
1:A:710:ARG:HG2	1:A:711:GLU:N	2.11	0.61
3:C:19:U:O2'	3:C:20:C:H5'	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:THR:HG22	1:D:97:ASP:H	1.64	0.61
1:A:41:LEU:HG	1:A:43:ILE:H	1.66	0.61
1:D:636:TYR:HD1	1:D:676:LEU:HD13	1.65	0.61
1:A:17:GLN:NE2	2:B:4:U:O2'	2.28	0.61
1:A:757:MET:HE2	1:A:758:LEU:HD23	1.82	0.61
1:D:309:ASN:HB2	1:D:322:GLY:O	2.00	0.61
1:D:170:ALA:HA	1:D:173:TYR:HD1	1.66	0.61
1:A:856:ARG:HD3	2:B:21:A:O2'	2.01	0.60
2:B:22:G:H1'	3:C:1:U:O2	2.01	0.60
1:D:219:VAL:CG2	1:D:239:ILE:HD11	2.30	0.60
1:D:694:LYS:HB2	1:D:695:PRO:HD2	1.82	0.60
1:A:133:ASP:O	1:A:136:ARG:HB2	2.01	0.60
1:D:358:ASN:ND2	1:D:373:LEU:H	1.99	0.60
1:A:828:ASN:HA	1:A:902:GLN:NE2	2.16	0.60
1:D:120:HIS:ND1	1:D:121:PRO:HD2	2.16	0.60
1:D:732:LEU:HD23	1:D:761:LYS:HB3	1.84	0.60
1:A:308:ARG:HD3	1:A:321:HIS:CE1	2.36	0.60
1:D:642:THR:O	1:D:644:PRO:HD3	2.02	0.60
1:A:870:ASN:HA	1:A:886:PHE:CE2	2.36	0.60
1:D:183:ASP:OD2	1:D:183:ASP:N	2.32	0.60
1:A:103:ILE:O	1:A:107:ILE:HG13	2.00	0.60
1:D:11:PRO:HD2	1:D:14:ILE:HD12	1.83	0.60
1:D:113:ASP:HB3	1:D:202:ILE:HD13	1.83	0.60
1:D:141:PRO:HB2	1:D:144:VAL:HG23	1.84	0.60
3:F:19:U:H2'	3:F:20:C:C6	2.36	0.60
1:A:499:ASP:O	1:A:500:LEU:HB2	2.02	0.60
1:A:921:MET:C	1:A:923:PRO:HD3	2.22	0.60
1:D:368:VAL:HB	1:D:654:VAL:CG2	2.32	0.60
1:D:780:LEU:O	1:D:812:LYS:HD2	2.01	0.60
1:A:255:LEU:HD22	1:A:260:GLN:HE22	1.66	0.59
1:D:401:LEU:CD1	1:D:461:LYS:HE2	2.33	0.59
1:D:406:LEU:HD21	1:D:482:ILE:HD13	1.82	0.59
1:D:731:LEU:HD11	1:D:738:LEU:CD1	2.32	0.59
1:A:633:VAL:HG22	1:A:677:LEU:HD12	1.84	0.59
2:B:8:C:H2'	2:B:9:U:C6	2.38	0.59
1:A:266:MET:SD	1:A:275:GLU:HB3	2.43	0.59
1:D:559:VAL:HG23	1:D:615:VAL:CG2	2.33	0.59
1:D:716:THR:HG22	1:D:740:THR:CB	2.32	0.59
1:D:243:ARG:NH1	1:D:248:SER:HB3	2.18	0.59
1:A:697:LEU:HD23	2:B:22:G:OP2	2.03	0.59
1:D:404:PRO:HB3	1:D:459:PHE:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:LYS:HG3	1:D:765:GLU:HG3	1.83	0.59
1:D:386:PRO:HG2	1:D:391:ILE:HD11	1.85	0.59
3:C:18:A:H2'	3:C:19:U:C6	2.38	0.58
3:C:21:A:H5'	3:C:22:C:P	2.42	0.58
1:A:810:GLY:CA	1:A:876:LEU:HD21	2.32	0.58
1:D:265:ARG:NH1	1:D:400:ARG:HH21	2.01	0.58
1:D:362:LYS:HB3	1:D:368:VAL:HA	1.85	0.58
3:F:2:U:H2'	3:F:3:C:C6	2.38	0.58
1:A:392:LEU:HD22	1:A:457:LYS:NZ	2.18	0.58
1:A:818:HIS:O	1:A:908:ARG:NH1	2.36	0.58
1:A:473:LYS:HE3	1:A:484:ASN:ND2	2.18	0.58
1:A:560:SER:O	1:A:678:LEU:HB2	2.03	0.58
1:A:642:THR:HB	1:A:643:PRO:CD	2.33	0.58
1:D:559:VAL:O	1:D:612:GLU:HA	2.04	0.58
1:D:866:ARG:HD2	1:D:897:PRO:O	2.04	0.58
1:A:895:VAL:C	1:A:897:PRO:HD2	2.24	0.58
1:A:262:MET:CE	1:A:263:ILE:H	2.04	0.58
1:D:60:PHE:CE1	1:D:62:VAL:HG22	2.38	0.58
1:D:95:THR:HB	1:D:98:GLU:HG3	1.86	0.58
1:D:777:GLY:HA3	1:D:924:TYR:CD1	2.39	0.58
1:D:829:TYR:HA	1:D:832:ASN:ND2	2.18	0.58
1:A:567:LEU:HB2	1:A:605:ILE:HD11	1.85	0.58
1:A:642:THR:O	1:A:644:PRO:HD3	2.04	0.57
1:D:16:HIS:CD2	1:D:78:ALA:HB1	2.38	0.57
1:D:870:ASN:HA	1:D:886:PHE:CE2	2.39	0.57
1:A:835:LEU:HD13	2:B:21:A:H1'	1.87	0.57
1:D:210:VAL:HG12	1:D:211:SER:H	1.69	0.57
1:A:46:LYS:HE3	2:B:14:A:O3'	2.04	0.57
1:D:539:LYS:HG3	1:D:638:SER:O	2.04	0.57
1:A:207:ALA:HA	1:A:210:VAL:HG23	1.84	0.57
1:A:332:ARG:HB2	1:A:339:ASP:OD2	2.04	0.57
2:B:15:A:H2'	2:B:16:G:H8	1.69	0.57
1:D:315:ILE:HD11	1:D:352:CYS:SG	2.45	0.57
1:A:460:THR:HG23	6:A:944:HOH:O	2.04	0.57
1:D:813:VAL:O	1:D:817:PHE:O	2.21	0.57
1:D:829:TYR:HA	1:D:832:ASN:HD21	1.69	0.57
1:D:266:MET:HA	1:D:276:CYS:O	2.05	0.57
1:A:368:VAL:HG23	1:A:369:ILE:N	2.20	0.57
1:D:98:GLU:O	1:D:102:GLU:HG2	2.03	0.57
1:D:113:ASP:HB3	1:D:202:ILE:CD1	2.35	0.57
1:D:255:LEU:HD13	1:D:260:GLN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PRO:HG3	1:A:619:SER:HB3	1.87	0.57
1:D:368:VAL:HB	1:D:654:VAL:HG21	1.86	0.57
1:D:374:PRO:HG3	1:D:619:SER:HA	1.86	0.57
1:A:94:LEU:CB	1:A:158:ILE:HD13	2.34	0.57
1:A:142:VAL:CG1	1:A:171:ILE:HG23	2.26	0.57
1:D:94:LEU:HD12	1:D:158:ILE:HD13	1.87	0.57
3:F:21:A:C2	3:F:21:A:OP2	2.58	0.57
1:A:658:THR:O	1:A:662:ARG:HG3	2.04	0.57
1:A:81:ALA:O	1:A:85:LEU:HG	2.05	0.56
1:A:694:LYS:CB	1:A:695:PRO:CD	2.83	0.56
1:A:762:LEU:HD13	1:A:930:TRP:CE3	2.40	0.56
1:A:798:ILE:O	1:A:801:MET:HG2	2.06	0.56
2:B:20:A:O2'	2:B:21:A:H5"	2.05	0.56
1:D:720:PHE:HB3	1:D:779:ILE:HG21	1.86	0.56
1:A:360:ILE:HD11	1:A:398:GLN:NE2	2.20	0.56
1:D:142:VAL:HG23	1:D:259:ASN:OD1	2.05	0.56
1:D:390:GLU:OE1	1:D:390:GLU:HA	2.06	0.56
1:D:694:LYS:HB2	1:D:695:PRO:CD	2.36	0.56
3:F:18:A:H2'	3:F:19:U:H6	1.70	0.56
1:A:43:ILE:CD1	1:A:927:ILE:HD13	2.35	0.56
1:D:467:LEU:HG	1:D:468:GLU:N	2.20	0.56
1:A:603:GLU:HG3	1:A:604:PRO:HD2	1.88	0.56
2:B:4:U:H2'	2:B:5:U:C6	2.40	0.56
1:A:46:LYS:NZ	2:B:14:A:H5"	2.20	0.56
1:A:400:ARG:C	1:A:401:LEU:HD23	2.26	0.56
1:A:405:ILE:CD1	1:A:458:ILE:HD11	2.35	0.56
1:D:624:ILE:HG22	1:D:624:ILE:O	2.05	0.56
2:B:15:A:H2'	2:B:16:G:C8	2.40	0.56
1:D:567:LEU:HB2	1:D:605:ILE:CD1	2.35	0.56
1:A:365:ARG:CG	1:A:365:ARG:NH1	2.67	0.56
1:D:11:PRO:HD2	1:D:14:ILE:CD1	2.35	0.56
1:D:563:TYR:CE2	1:D:608:ASN:HB2	2.41	0.56
1:D:570:ASP:N	1:D:571:PRO:CD	2.51	0.56
1:D:570:ASP:HB3	1:D:640:LYS:NZ	2.21	0.56
1:D:865:THR:HG22	1:D:866:ARG:N	2.21	0.56
1:A:493:PHE:HA	1:A:496:PHE:CD1	2.41	0.56
1:D:122:LEU:O	1:D:125:HIS:HB2	2.06	0.56
1:D:551:GLN:O	1:D:629:THR:O	2.24	0.56
1:A:568:ALA:HA	1:A:601:SER:O	2.06	0.56
1:A:814:LEU:HD12	1:A:876:LEU:HG	1.86	0.56
1:A:719:ASP:HB3	1:A:722:CYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:ILE:HG21	1:D:565:LEU:CD2	2.36	0.55
1:D:568:ALA:HB2	1:D:602:VAL:HA	1.88	0.55
1:A:169:LEU:O	1:A:173:TYR:CD1	2.59	0.55
1:A:725:GLY:O	1:A:729:ASP:N	2.38	0.55
1:D:222:VAL:HB	1:D:326:LEU:HB3	1.87	0.55
1:D:401:LEU:HD13	1:D:461:LYS:HE2	1.88	0.55
1:A:369:ILE:CG2	1:A:565:LEU:HD11	2.35	0.55
1:A:387:LEU:O	1:A:391:ILE:HG22	2.06	0.55
1:A:405:ILE:HB	1:A:458:ILE:CG1	2.32	0.55
1:D:253:LEU:HD13	1:D:325:ILE:HG12	1.87	0.55
1:D:455:GLU:O	1:D:471:PRO:HD2	2.06	0.55
1:A:283:PRO:O	1:A:285:LYS:N	2.39	0.55
1:A:392:LEU:O	1:A:395:PHE:HB3	2.07	0.55
1:A:852:LEU:HB2	1:A:855:PHE:CD1	2.42	0.55
1:D:606:GLU:CB	1:D:654:VAL:HG11	2.35	0.55
1:A:146:ALA:HB2	1:A:174:VAL:HG21	1.88	0.55
1:A:160:ASN:HD21	1:A:169:LEU:HD13	1.71	0.55
1:A:908:ARG:HE	1:A:911:SER:HB3	1.71	0.55
1:D:345:VAL:CG1	1:D:658:THR:HG21	2.37	0.55
1:D:553:ILE:H	1:D:629:THR:CG2	2.20	0.55
1:D:821:LEU:HD12	1:D:906:PHE:O	2.06	0.55
1:A:27:VAL:HG11	1:A:70:LYS:HE2	1.89	0.55
1:A:132:ARG:NH2	1:A:257:ASP:OD1	2.39	0.55
1:A:360:ILE:HD11	1:A:398:GLN:HE22	1.72	0.55
1:A:864:TRP:HA	1:A:868:GLN:HE22	1.72	0.55
1:A:865:THR:N	1:A:868:GLN:HE21	2.04	0.55
1:A:365:ARG:HG3	1:A:365:ARG:NH1	2.18	0.55
1:D:103:ILE:HG23	1:D:152:ILE:HD12	1.87	0.55
1:D:496:PHE:N	1:D:496:PHE:CD2	2.74	0.55
1:D:570:ASP:O	1:D:572:GLU:HG3	2.07	0.55
1:D:829:TYR:OH	1:D:853:PRO:HG2	2.07	0.55
2:B:13:C:O2'	2:B:14:A:H5'	2.07	0.55
1:D:12:LYS:HD2	1:D:82:LEU:HD12	1.90	0.54
1:D:168:PHE:HD2	1:D:282:ILE:HG23	1.71	0.54
1:D:392:LEU:HD13	1:D:490:LEU:HG	1.89	0.54
1:D:568:ALA:CB	1:D:601:SER:O	2.53	0.54
1:A:358:ASN:HA	1:A:373:LEU:HB2	1.90	0.54
1:A:558:VAL:CG1	1:A:681:LYS:HD3	2.37	0.54
1:A:851:GLN:O	1:A:852:LEU:HG	2.08	0.54
1:D:569:VAL:HG22	1:D:668:ARG:O	2.08	0.54
1:D:710:ARG:NH1	1:D:734:TYR:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HD2	1:A:385:GLY:HA3	1.89	0.54
1:A:537:GLU:HB3	1:A:641:MET:HE2	1.90	0.54
1:A:855:PHE:HZ	1:A:862:PHE:HA	1.73	0.54
1:D:88:ARG:CB	1:D:89:PRO:HD2	2.37	0.54
1:A:374:PRO:HG3	1:A:619:SER:CB	2.38	0.54
1:D:11:PRO:HB2	1:D:75:GLN:HE22	1.72	0.54
1:D:17:GLN:O	1:D:17:GLN:HG3	2.07	0.54
1:D:736:THR:HG22	1:D:737:SER:N	2.23	0.54
1:D:829:TYR:HB2	1:D:863:GLU:O	2.07	0.54
1:A:171:ILE:HD13	1:A:282:ILE:HD13	1.89	0.54
1:A:255:LEU:HD13	1:A:260:GLN:HB3	1.90	0.54
1:A:62:VAL:HG11	1:A:80:LEU:HB2	1.90	0.54
1:A:168:PHE:CE2	1:A:282:ILE:HA	2.42	0.54
1:A:700:GLN:HB2	1:A:889:VAL:HG11	1.90	0.54
1:D:121:PRO:HD3	1:D:333:TRP:CD2	2.43	0.54
1:D:571:PRO:HD3	1:D:670:CYS:HB2	1.88	0.54
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.73	0.54
1:A:871:GLN:O	1:A:875:LYS:HG3	2.08	0.54
1:D:257:ASP:N	1:D:260:GLN:HE21	2.03	0.54
1:D:627:GLU:O	1:D:630:GLN:HG2	2.07	0.54
1:D:895:VAL:HG12	1:D:896:GLU:N	2.22	0.54
1:A:12:LYS:HB3	1:A:78:ALA:CB	2.39	0.53
2:B:10:C:H2'	2:B:11:U:C6	2.43	0.53
1:A:392:LEU:HD21	1:A:404:PRO:HG3	1.90	0.53
1:D:704:TYR:HH	1:D:887:SER:HG	1.55	0.53
1:A:12:LYS:HE3	1:A:79:GLU:CD	2.29	0.53
1:D:18:LYS:HD3	3:F:19:U:O2'	2.08	0.53
1:D:265:ARG:N	1:D:318:GLN:HE22	1.98	0.53
1:A:23:ALA:HB2	1:A:57:LEU:CD1	2.38	0.53
1:D:392:LEU:HD21	1:D:459:PHE:HZ	1.74	0.53
1:D:685:GLU:HG3	1:D:686:GLU:H	1.73	0.53
1:D:857:ASN:OD1	3:F:2:U:H4'	2.08	0.53
1:D:188:SER:O	1:D:190:HIS:N	2.41	0.53
1:D:257:ASP:OD1	1:D:258:GLY:N	2.42	0.53
1:A:278:LEU:HD23	1:A:320:ILE:HD12	1.90	0.53
1:A:677:LEU:HD13	1:A:678:LEU:N	2.23	0.53
1:D:194:ARG:HH12	1:D:198:TYR:CA	2.20	0.53
1:D:551:GLN:O	1:D:553:ILE:HG13	2.08	0.53
1:D:896:GLU:HB2	1:D:897:PRO:HD3	1.91	0.53
1:D:39:PRO:HD2	1:D:759:HIS:CD2	2.44	0.53
1:D:119:GLU:HA	1:D:119:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:GLU:HA	1:D:204:GLU:OE1	2.09	0.53
1:D:146:ALA:HB2	1:D:174:VAL:HG21	1.91	0.53
1:D:828:ASN:HA	1:D:902:GLN:HE21	1.74	0.53
1:A:246:LEU:HD22	1:A:261:VAL:HG11	1.90	0.53
3:F:19:U:H2'	3:F:20:C:O4'	2.09	0.53
1:A:160:ASN:ND2	1:A:169:LEU:HD13	2.24	0.53
1:A:392:LEU:HA	1:A:490:LEU:HD21	1.91	0.53
1:A:407:SER:HB2	1:A:456:VAL:HB	1.90	0.53
1:D:50:LEU:CD2	1:D:68:LYS:HG3	2.39	0.53
1:D:818:HIS:N	1:D:819:PRO:HD2	2.11	0.53
1:A:8:THR:O	1:A:10:THR:N	2.42	0.52
1:A:813:VAL:HG11	1:A:822:LEU:HD11	1.92	0.52
1:A:365:ARG:NH2	1:A:612:GLU:O	2.42	0.52
1:A:368:VAL:HG21	1:A:654:VAL:HG22	1.90	0.52
1:A:642:THR:HB	1:A:643:PRO:HD2	1.90	0.52
1:D:357:PRO:HB3	1:D:490:LEU:HD22	1.90	0.52
1:D:655:GLY:HA3	1:D:661:ILE:CD1	2.38	0.52
1:A:221:ALA:O	1:A:234:LEU:HD12	2.09	0.52
1:A:278:LEU:HD21	1:A:312:ALA:HB1	1.90	0.52
1:A:793:THR:CG2	1:A:795:LEU:HG	2.39	0.52
1:D:123:GLY:HA2	1:D:126:LEU:HB2	1.91	0.52
1:D:375:PHE:HA	1:D:491:LEU:HD11	1.92	0.52
1:A:267:PHE:CE1	1:A:315:ILE:HG22	2.45	0.52
1:D:14:ILE:CD1	2:E:5:U:H1'	2.39	0.52
1:D:265:ARG:NH1	1:D:400:ARG:HE	2.07	0.52
1:D:359:GLY:O	1:D:363:ILE:HG13	2.09	0.52
1:D:829:TYR:HD1	1:D:832:ASN:ND2	2.04	0.52
1:D:621:ASN:HD21	1:D:623:HIS:HB2	1.73	0.52
1:D:679:GLY:O	1:D:680:VAL:HG23	2.10	0.52
1:A:155:ARG:O	1:A:159:ILE:HG13	2.10	0.52
1:A:318:GLN:HG3	1:A:400:ARG:NH2	2.24	0.52
1:A:391:ILE:HG23	1:A:490:LEU:HD11	1.90	0.52
1:D:132:ARG:O	1:D:137:CYS:HB2	2.10	0.52
1:D:789:VAL:O	1:D:819:PRO:HA	2.10	0.52
2:E:14:A:H2'	2:E:15:A:C8	2.44	0.52
1:D:358:ASN:HD21	1:D:373:LEU:H	1.58	0.52
1:D:570:ASP:O	1:D:572:GLU:N	2.39	0.52
1:D:778:SER:HA	5:D:951:SAH:N1	2.24	0.52
2:B:4:U:H5'	6:B:23:HOH:O	2.10	0.52
1:D:176:LYS:O	1:D:180:LYS:HG3	2.10	0.51
1:A:353:CYS:O	1:A:359:GLY:HA3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASN:HD22	1:A:622:PRO:N	2.08	0.51
1:D:121:PRO:HD3	1:D:333:TRP:CE2	2.45	0.51
1:A:23:ALA:HA	1:A:56:GLN:O	2.09	0.51
1:A:895:VAL:HG12	1:A:897:PRO:CD	2.37	0.51
1:D:18:LYS:HD3	3:F:20:C:H5'	1.92	0.51
1:D:459:PHE:CB	1:D:466:VAL:HB	2.41	0.51
1:D:867:GLU:HG3	1:D:868:GLN:N	2.25	0.51
1:A:35:GLN:NE2	1:A:47:GLY:HA3	2.25	0.51
1:A:828:ASN:CG	1:A:866:ARG:HG3	2.30	0.51
1:A:829:TYR:OH	1:A:853:PRO:O	2.26	0.51
1:D:921:MET:O	1:D:923:PRO:HD3	2.11	0.51
1:A:160:ASN:ND2	1:A:173:TYR:OH	2.42	0.51
1:A:378:THR:CG2	1:A:382:ASN:HD22	2.24	0.51
1:A:389:ARG:O	1:A:392:LEU:HB3	2.10	0.51
1:A:704:TYR:CD2	1:A:903:ILE:HD13	2.46	0.51
1:A:886:PHE:N	1:A:886:PHE:CD1	2.78	0.51
1:D:921:MET:O	1:D:921:MET:HG2	2.10	0.51
1:A:43:ILE:HG22	1:A:44:PRO:N	2.25	0.51
1:D:373:LEU:HD12	1:D:374:PRO:CD	2.41	0.51
1:D:406:LEU:HD11	1:D:482:ILE:HG23	1.91	0.51
1:A:57:LEU:O	1:A:58:PRO:C	2.49	0.51
1:D:224:ILE:HG22	1:D:309:ASN:HD21	1.76	0.51
1:D:701:ARG:NH1	1:D:796:GLU:CG	2.73	0.51
1:D:479:ASN:O	1:D:483:GLN:HG2	2.11	0.51
1:D:48:PRO:HD2	1:D:48:PRO:O	2.12	0.50
1:D:401:LEU:HD13	1:D:461:LYS:CG	2.41	0.50
1:D:496:PHE:HB3	1:D:524:PHE:CD1	2.46	0.50
1:A:558:VAL:HG12	1:A:681:LYS:HB2	1.92	0.50
1:D:780:LEU:CD1	1:D:805:GLN:HB3	2.41	0.50
1:A:258:GLY:HA2	1:A:261:VAL:HG23	1.94	0.50
1:D:605:ILE:HD13	1:D:651:ILE:HG23	1.94	0.50
1:D:818:HIS:N	1:D:819:PRO:CD	2.69	0.50
1:A:7:HIS:C	1:A:9:PRO:HD2	2.32	0.50
1:A:697:LEU:HD23	2:B:22:G:P	2.50	0.50
1:D:819:PRO:HB2	1:D:821:LEU:O	2.12	0.50
1:A:12:LYS:O	1:A:15:ILE:HB	2.11	0.50
1:A:22:LYS:O	1:A:22:LYS:HG3	2.10	0.50
1:A:865:THR:N	1:A:868:GLN:NE2	2.55	0.50
1:A:920:SER:O	1:A:921:MET:HG3	2.11	0.50
1:D:47:GLY:HA2	2:E:14:A:O2'	2.11	0.50
1:D:706:LEU:HD11	1:D:730:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:8:G:H2'	3:F:9:C:C6	2.46	0.50
1:A:369:ILE:HG21	1:A:565:LEU:CD1	2.41	0.50
1:A:769:VAL:HG12	1:A:770:LYS:N	2.27	0.50
1:D:643:PRO:O	1:D:644:PRO:C	2.48	0.50
1:A:567:LEU:HB2	1:A:605:ILE:CD1	2.42	0.50
1:A:706:LEU:HA	1:A:709:ILE:HD12	1.94	0.50
1:D:25:TYR:CD2	1:D:55:LEU:HD13	2.47	0.50
1:D:396:CYS:O	1:D:401:LEU:HB2	2.11	0.50
1:D:553:ILE:HG22	1:D:557:SER:HB2	1.94	0.50
1:D:103:ILE:O	1:D:107:ILE:HG13	2.12	0.50
1:D:262:MET:HE3	1:D:263:ILE:H	1.76	0.50
1:D:640:LYS:HD2	1:D:670:CYS:SG	2.51	0.50
1:D:621:ASN:ND2	1:D:624:ILE:HG13	2.23	0.49
1:A:7:HIS:NE2	3:C:17:A:H4'	2.27	0.49
1:D:770:LYS:O	1:D:931:LYS:HA	2.12	0.49
1:A:694:LYS:HB3	1:A:695:PRO:HD3	1.93	0.49
1:D:246:LEU:HD22	1:D:261:VAL:HB	1.92	0.49
1:D:403:GLU:HG3	1:D:404:PRO:HD2	1.93	0.49
1:A:188:SER:C	1:A:190:HIS:H	2.15	0.49
1:A:487:LEU:O	1:A:491:LEU:HG	2.12	0.49
1:A:18:LYS:CE	3:C:19:U:H4'	2.42	0.49
1:D:42:ALA:C	1:D:44:PRO:HD3	2.33	0.49
1:D:567:LEU:O	1:D:568:ALA:HB2	2.12	0.49
1:A:87:ILE:O	1:A:91:ASN:HB2	2.13	0.49
1:A:396:CYS:SG	1:A:459:PHE:CZ	3.02	0.49
1:D:16:HIS:HD2	1:D:78:ALA:HB1	1.78	0.49
1:D:262:MET:HA	1:D:282:ILE:HD11	1.94	0.49
1:A:315:ILE:HD11	1:A:348:PHE:HE1	1.77	0.49
1:A:329:VAL:HG12	1:A:340:TYR:CB	2.43	0.49
1:A:798:ILE:HG13	1:A:799:GLU:N	2.28	0.49
1:A:43:ILE:CG2	1:A:44:PRO:CD	2.91	0.49
1:A:265:ARG:HG2	1:A:266:MET:N	2.28	0.49
1:A:565:LEU:HD21	1:A:673:TYR:CZ	2.48	0.49
1:A:642:THR:CB	1:A:643:PRO:CD	2.91	0.49
1:A:803:GLU:HG2	1:A:862:PHE:CD2	2.48	0.49
1:D:704:TYR:CE2	1:D:903:ILE:HD11	2.47	0.49
1:A:358:ASN:ND2	1:A:373:LEU:H	2.11	0.49
1:D:43:ILE:HD11	1:D:927:ILE:CG1	2.43	0.49
1:A:106:ARG:HD3	1:A:151:LYS:HD2	1.95	0.48
1:A:265:ARG:HG2	1:A:266:MET:H	1.76	0.48
1:D:242:ASN:OD1	1:D:243:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:CD2	1:A:461:LYS:HB2	2.26	0.48
1:D:287:LEU:O	1:D:291:SER:HB3	2.13	0.48
1:D:462:SER:O	1:D:463:GLN:HB2	2.13	0.48
1:D:467:LEU:HD22	1:D:492:TRP:HE3	1.76	0.48
1:D:757:MET:HG3	1:D:758:LEU:H	1.73	0.48
1:D:887:SER:O	1:D:903:ILE:HG12	2.13	0.48
1:A:357:PRO:HB3	1:A:490:LEU:HD22	1.95	0.48
1:A:700:GLN:HB2	1:A:889:VAL:CG1	2.44	0.48
1:D:780:LEU:HD21	1:D:801:MET:SD	2.53	0.48
1:A:110:ILE:HG23	1:A:115:PHE:CE2	2.48	0.48
1:A:392:LEU:CD2	1:A:404:PRO:HG3	2.44	0.48
1:D:138:GLY:O	1:D:193:ARG:HG3	2.12	0.48
1:D:189:PRO:O	1:D:259:ASN:ND2	2.46	0.48
1:D:820:LYS:HG2	1:D:908:ARG:NH2	2.29	0.48
1:D:278:LEU:HD22	1:D:316:CYS:SG	2.54	0.48
1:D:357:PRO:CB	1:D:490:LEU:HD22	2.44	0.48
1:D:832:ASN:HB3	1:D:856:ARG:HE	1.79	0.48
2:E:15:A:H2'	2:E:16:G:C8	2.49	0.48
1:A:779:ILE:HD12	1:A:809:PHE:CE1	2.48	0.48
1:A:905:ILE:N	1:A:905:ILE:HD12	2.29	0.48
1:A:907:ARG:HG3	6:A:952:HOH:O	2.13	0.48
1:D:87:ILE:O	1:D:87:ILE:HG22	2.13	0.48
1:D:567:LEU:HD12	1:D:670:CYS:O	2.13	0.48
1:A:170:ALA:O	1:A:174:VAL:HG23	2.13	0.48
2:B:19:A:O2'	2:B:20:A:H5'	2.14	0.48
1:A:23:ALA:HB2	1:A:57:LEU:HD12	1.95	0.48
1:A:43:ILE:HD11	1:A:927:ILE:HD13	1.96	0.48
1:D:50:LEU:HB3	1:D:66:VAL:CG1	2.43	0.48
1:D:107:ILE:HG22	1:D:185:ILE:HD13	1.96	0.48
1:D:181:LEU:HD11	1:D:184:TYR:CD1	2.49	0.48
1:D:188:SER:O	1:D:189:PRO:C	2.52	0.48
2:E:11:U:H2'	2:E:12:G:H8	1.78	0.48
1:A:822:LEU:HD23	1:A:823:ILE:N	2.29	0.48
1:D:315:ILE:HG23	1:D:351:ILE:HG21	1.95	0.48
1:D:852:LEU:N	1:D:853:PRO:CD	2.77	0.48
1:A:35:GLN:HE22	1:A:47:GLY:HA3	1.79	0.47
1:A:380:LYS:O	1:A:380:LYS:HG2	2.14	0.47
1:A:462:SER:O	1:A:463:GLN:HB2	2.13	0.47
1:A:467:LEU:HD22	1:A:492:TRP:HE3	1.79	0.47
1:D:43:ILE:HG13	1:D:927:ILE:HG23	1.96	0.47
1:D:345:VAL:HG12	1:D:658:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:825:SER:HA	1:D:903:ILE:HG22	1.96	0.47
2:E:9:U:C2	3:F:13:G:N2	2.82	0.47
3:F:19:U:O2'	3:F:20:C:C5'	2.61	0.47
1:A:461:LYS:HE2	1:A:466:VAL:HG21	1.97	0.47
1:D:71:LYS:HD2	2:E:6:C:OP2	2.14	0.47
1:A:59:GLU:HB3	1:A:60:PHE:HD1	1.79	0.47
1:A:467:LEU:HD13	1:A:492:TRP:CE3	2.50	0.47
1:A:834:ILE:HG23	1:A:835:LEU:N	2.29	0.47
1:D:552:SER:CA	1:D:629:THR:O	2.61	0.47
1:A:680:VAL:C	1:A:681:LYS:HD2	2.35	0.47
3:C:10:A:O2'	3:C:11:G:H5'	2.14	0.47
1:D:642:THR:HB	1:D:643:PRO:HD3	1.97	0.47
1:A:365:ARG:NH2	1:A:384:ARG:HB3	2.29	0.47
1:A:538:SER:O	1:A:639:PHE:HB2	2.14	0.47
1:A:709:ILE:O	1:A:712:SER:O	2.33	0.47
1:D:272:CYS:HB2	1:D:351:ILE:HD11	1.97	0.47
1:A:160:ASN:O	1:A:163:VAL:HG23	2.15	0.47
1:A:382:ASN:HD21	1:A:684:SER:HB2	1.79	0.47
1:A:383:TRP:HH2	1:A:487:LEU:HD21	1.79	0.47
1:A:693:PHE:O	1:A:694:LYS:C	2.51	0.47
1:D:392:LEU:HD11	1:D:459:PHE:CZ	2.50	0.47
1:D:856:ARG:HB3	2:E:21:A:O2'	2.13	0.47
1:A:22:LYS:HE2	1:A:22:LYS:HA	1.97	0.47
1:A:739:GLN:HE22	1:A:770:LYS:NZ	2.12	0.47
1:A:821:LEU:HD11	1:A:905:ILE:CG2	2.45	0.47
1:D:210:VAL:CG1	1:D:211:SER:N	2.77	0.47
1:D:382:ASN:O	1:D:614:GLU:HG3	2.14	0.47
1:D:795:LEU:HA	1:D:825:SER:HB3	1.95	0.47
1:A:190:HIS:HA	1:A:257:ASP:OD2	2.15	0.47
1:A:383:TRP:CH2	1:A:487:LEU:HD21	2.50	0.47
1:A:745:ASP:HB3	1:A:751:LEU:HD21	1.96	0.47
2:E:10:C:O2'	2:E:11:U:H5'	2.15	0.47
1:A:43:ILE:HD12	1:A:927:ILE:HD13	1.97	0.47
1:D:210:VAL:CG1	1:D:211:SER:H	2.28	0.47
1:D:691:ALA:CB	2:E:20:A:H5"	2.45	0.47
1:D:764:LYS:HG3	1:D:765:GLU:N	2.30	0.47
1:A:160:ASN:ND2	1:A:162:SER:OG	2.47	0.46
1:A:392:LEU:HD11	1:A:459:PHE:CE1	2.45	0.46
2:B:8:C:H2'	2:B:9:U:H6	1.80	0.46
1:D:401:LEU:HD22	1:D:461:LYS:CD	2.33	0.46
1:A:22:LYS:HG2	1:A:58:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:LYS:C	1:D:932:LYS:HD3	2.35	0.46
1:A:199:PRO:HD2	1:A:202:ILE:HD12	1.96	0.46
1:A:365:ARG:O	1:A:366:GLN:HB2	2.15	0.46
1:A:59:GLU:HB3	1:A:60:PHE:CD1	2.51	0.46
1:A:223:TYR:HB2	1:A:235:ASP:HB2	1.97	0.46
1:A:557:SER:HB2	1:A:681:LYS:O	2.15	0.46
1:D:181:LEU:CG	1:D:184:TYR:HB2	2.42	0.46
1:D:190:HIS:O	1:D:259:ASN:HB2	2.15	0.46
1:D:599:GLU:HG2	1:D:600:SER:N	2.31	0.46
1:A:46:LYS:CE	2:B:14:A:H4'	2.45	0.46
1:A:110:ILE:CG2	1:A:126:LEU:HD11	2.44	0.46
1:A:372:GLN:O	1:A:374:PRO:HD3	2.15	0.46
1:A:486:SER:O	1:A:490:LEU:HG	2.16	0.46
1:A:797:VAL:O	1:A:800:HIS:HB2	2.16	0.46
1:D:54:HIS:ND1	1:D:63:VAL:HG22	2.30	0.46
1:D:642:THR:N	1:D:643:PRO:CD	2.78	0.46
1:D:199:PRO:HG2	1:D:202:ILE:HD12	1.98	0.46
1:A:106:ARG:O	1:A:110:ILE:HG13	2.16	0.46
1:A:305:VAL:HG12	1:A:306:LYS:N	2.31	0.46
1:A:931:LYS:HG3	1:A:931:LYS:O	2.16	0.46
1:D:741:ILE:C	1:D:742:ILE:HG13	2.35	0.46
1:A:689:GLU:OE2	3:C:3:C:H1'	2.16	0.46
1:A:870:ASN:HA	1:A:886:PHE:HE2	1.78	0.46
1:D:55:LEU:HD23	1:D:81:ALA:HB2	1.97	0.46
1:D:396:CYS:O	1:D:399:HIS:O	2.33	0.46
1:D:705:ALA:O	1:D:709:ILE:HG13	2.16	0.46
1:A:221:ALA:HB1	1:A:326:LEU:O	2.16	0.46
1:A:636:TYR:HA	1:A:675:ILE:O	2.16	0.46
1:D:12:LYS:HD2	1:D:79:GLU:HA	1.97	0.46
1:A:315:ILE:HD11	1:A:348:PHE:CE1	2.51	0.45
1:A:796:GLU:OE2	5:A:951:SAH:HB2	2.16	0.45
1:D:232:VAL:HG23	1:D:311:ARG:HH21	1.79	0.45
1:D:773:THR:C	1:D:774:LEU:HD23	2.36	0.45
2:B:14:A:O2'	2:B:15:A:H5'	2.17	0.45
1:D:282:ILE:HG23	1:D:283:PRO:HD2	1.98	0.45
1:A:17:GLN:NE2	2:B:4:U:H4'	2.31	0.45
1:A:237:LEU:CD2	1:A:249:ILE:HG12	2.46	0.45
1:A:368:VAL:CG2	1:A:654:VAL:CG2	2.94	0.45
1:A:565:LEU:HD21	1:A:673:TYR:CD2	2.52	0.45
1:D:107:ILE:HG22	1:D:185:ILE:CD1	2.46	0.45
1:D:265:ARG:HH12	1:D:400:ARG:CZ	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PRO:C	1:A:285:LYS:H	2.20	0.45
1:D:524:PHE:CD1	1:D:524:PHE:O	2.70	0.45
1:D:783:ASP:H	1:D:817:PHE:HZ	1.65	0.45
1:A:271:SER:HB3	1:A:351:ILE:HA	1.98	0.45
1:A:714:ALA:O	1:A:737:SER:O	2.34	0.45
1:D:100:ARG:O	1:D:104:VAL:HG23	2.16	0.45
1:D:104:VAL:HG22	1:D:177:ALA:HB1	1.99	0.45
1:A:46:LYS:HZ1	2:B:14:A:H5"	1.81	0.45
1:D:88:ARG:HG2	1:D:89:PRO:CD	2.38	0.45
1:D:700:GLN:HB3	1:D:889:VAL:HG11	1.97	0.45
1:D:826:THR:HG23	1:D:827:PRO:HD2	1.98	0.45
1:A:231:VAL:HG12	1:A:232:VAL:N	2.32	0.45
1:D:628:VAL:HG23	1:D:675:ILE:HD12	1.98	0.45
1:A:12:LYS:HB3	1:A:78:ALA:HB1	1.99	0.45
1:A:169:LEU:O	1:A:173:TYR:HD1	1.97	0.45
1:A:255:LEU:CD1	1:A:281:GLU:HB2	2.40	0.45
1:A:379:THR:C	1:A:381:SER:H	2.20	0.45
1:A:821:LEU:HD11	1:A:905:ILE:HG23	1.99	0.45
1:A:822:LEU:HB3	1:A:906:PHE:HB2	1.99	0.45
3:C:13:G:H2'	3:C:14:A:C8	2.52	0.45
1:D:116:LEU:HG	1:D:206:LEU:CD1	2.36	0.45
1:D:553:ILE:HG22	1:D:554:THR:N	2.32	0.45
1:D:717:LEU:HD12	1:D:791:ILE:O	2.16	0.45
1:D:792:GLY:O	1:D:822:LEU:HD12	2.16	0.45
1:A:719:ASP:OD2	1:A:727:LEU:HD23	2.17	0.45
1:A:727:LEU:CD2	1:A:793:THR:HG21	2.46	0.45
1:D:11:PRO:HG3	2:E:5:U:O2'	2.17	0.45
1:D:696:PRO:O	1:D:699:LYS:HB2	2.17	0.45
1:D:775:TYR:HB3	1:D:924:TYR:HB3	1.97	0.45
1:A:108:LYS:CD	1:A:181:LEU:HD21	2.43	0.45
1:A:235:ASP:OD1	1:A:252:ARG:HD2	2.18	0.45
1:A:896:GLU:N	1:A:897:PRO:HD2	2.31	0.44
1:D:169:LEU:O	1:D:173:TYR:CD1	2.70	0.44
1:D:267:PHE:CE1	1:D:315:ILE:HG22	2.52	0.44
1:D:401:LEU:HD11	1:D:461:LYS:HE2	1.99	0.44
2:E:20:A:O2'	2:E:21:A:H5"	2.17	0.44
1:D:358:ASN:ND2	1:D:373:LEU:N	2.65	0.44
1:D:733:ASP:OD1	1:D:761:LYS:HE2	2.17	0.44
1:A:347:SER:O	1:A:351:ILE:HG13	2.18	0.44
1:D:59:GLU:HB3	1:D:60:PHE:HD2	1.82	0.44
1:D:278:LEU:CD2	1:D:320:ILE:HG13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG23	1:A:239:ILE:HD13	1.99	0.44
1:A:621:ASN:C	1:A:621:ASN:ND2	2.70	0.44
1:D:47:GLY:HA2	2:E:14:A:HO2'	1.80	0.44
1:D:127:ARG:NH1	1:D:336:ASP:OD1	2.50	0.44
1:D:283:PRO:C	1:D:285:LYS:N	2.68	0.44
1:D:396:CYS:HA	1:D:401:LEU:HG	1.99	0.44
1:D:570:ASP:HB3	1:D:640:LYS:HZ3	1.81	0.44
1:D:745:ASP:O	1:D:776:ASP:HA	2.18	0.44
1:A:113:ASP:HB3	1:A:202:ILE:CD1	2.46	0.44
1:A:759:HIS:O	1:A:763:ASN:ND2	2.51	0.44
1:A:837:ARG:O	1:A:838:SER:HB3	2.17	0.44
2:B:7:U:O2	2:B:7:U:H2'	2.18	0.44
1:D:487:LEU:HD23	1:D:491:LEU:HD12	2.00	0.44
1:D:556:GLY:HA3	1:D:683:PRO:HB3	1.99	0.44
1:D:648:GLU:OE1	1:D:665:LEU:HD13	2.18	0.44
1:A:48:PRO:HD3	2:B:15:A:O2'	2.18	0.44
1:A:222:VAL:CG1	1:A:223:TYR:N	2.81	0.44
2:B:11:U:O2'	2:B:12:G:H5'	2.17	0.44
1:D:778:SER:C	1:D:780:LEU:H	2.20	0.44
1:A:94:LEU:HB3	1:A:158:ILE:HG21	2.00	0.44
3:C:19:U:H2'	3:C:20:C:H6	1.83	0.44
1:D:172:SER:O	1:D:176:LYS:HG3	2.18	0.44
1:D:559:VAL:HG23	1:D:615:VAL:HG22	1.99	0.44
1:A:8:THR:N	1:A:9:PRO:CD	2.81	0.43
1:A:188:SER:C	1:A:190:HIS:N	2.70	0.43
1:A:696:PRO:HD2	1:A:699:LYS:HD2	2.00	0.43
3:C:11:G:H2'	3:C:12:A:H8	1.83	0.43
1:D:110:ILE:HD13	1:D:122:LEU:HD13	2.00	0.43
1:D:262:MET:CE	1:D:263:ILE:H	2.31	0.43
1:A:50:LEU:HD23	1:A:50:LEU:N	2.32	0.43
1:A:120:HIS:O	1:A:121:PRO:C	2.56	0.43
1:A:467:LEU:HD22	1:A:492:TRP:CE3	2.53	0.43
1:D:121:PRO:O	1:D:124:ALA:HB3	2.18	0.43
1:D:153:ASN:O	1:D:157:LYS:HG3	2.18	0.43
1:A:121:PRO:HB2	1:A:148:VAL:CG1	2.48	0.43
1:A:217:ARG:HD3	1:A:340:TYR:CE2	2.53	0.43
1:A:318:GLN:CG	1:A:400:ARG:HH22	2.24	0.43
1:A:356:SER:O	1:A:360:ILE:HG13	2.18	0.43
1:A:407:SER:HB2	1:A:456:VAL:O	2.18	0.43
2:B:16:G:O2'	2:B:17:C:H5'	2.19	0.43
1:D:164:GLU:CB	1:D:400:ARG:HH12	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ARG:HD2	1:D:389:ARG:O	2.18	0.43
1:D:461:LYS:HG3	1:D:466:VAL:CG2	2.41	0.43
1:D:496:PHE:N	1:D:496:PHE:HD2	2.14	0.43
1:D:652:LEU:HD23	1:D:661:ILE:HG21	1.99	0.43
1:D:695:PRO:HG2	1:D:700:GLN:NE2	2.33	0.43
2:E:4:U:H2'	2:E:5:U:C6	2.53	0.43
1:A:71:LYS:HE2	2:B:6:C:P	2.58	0.43
3:C:10:A:H2'	3:C:11:G:C8	2.53	0.43
1:D:126:LEU:O	1:D:129:ALA:HB3	2.18	0.43
1:D:257:ASP:N	1:D:260:GLN:NE2	2.65	0.43
1:D:391:ILE:HB	1:D:490:LEU:HD11	2.00	0.43
1:D:406:LEU:HD13	1:D:457:LYS:CE	2.44	0.43
1:D:824:VAL:HG12	1:D:825:SER:N	2.33	0.43
1:D:227:ILE:HB	1:D:230:GLU:OE2	2.18	0.43
1:D:234:LEU:HB2	1:D:345:VAL:HG23	1.99	0.43
1:D:667:GLU:O	1:D:669:PRO:HD3	2.19	0.43
1:D:832:ASN:O	1:D:836:GLN:HG3	2.18	0.43
1:A:57:LEU:CG	1:A:58:PRO:HD2	2.48	0.43
1:A:680:VAL:HG12	1:A:681:LYS:N	2.34	0.43
1:A:785:ARG:NH2	1:A:922:GLN:HB3	2.34	0.43
1:A:920:SER:C	1:A:921:MET:HG3	2.39	0.43
1:A:694:LYS:CB	1:A:695:PRO:HD2	2.48	0.43
1:D:158:ILE:H	1:D:158:ILE:HG13	1.66	0.43
1:D:265:ARG:HH12	1:D:400:ARG:NH2	2.17	0.43
1:D:537:GLU:HA	1:D:641:MET:CE	2.31	0.43
1:D:657:ASP:CG	1:D:660:ARG:HE	2.22	0.43
1:D:732:LEU:HD21	1:D:762:LEU:HD23	2.00	0.43
1:D:895:VAL:HG12	1:D:896:GLU:H	1.83	0.43
1:D:12:LYS:CD	1:D:82:LEU:HD12	2.48	0.43
1:D:69:LYS:HB2	1:D:72:ASP:HB2	2.00	0.43
1:D:314:TYR:CE2	1:D:355:MET:HG3	2.54	0.43
1:D:329:VAL:HG12	1:D:340:TYR:HB3	2.00	0.43
1:A:11:PRO:O	1:A:12:LYS:C	2.57	0.43
1:A:120:HIS:HD2	1:A:122:LEU:HB2	1.84	0.43
1:A:160:ASN:HB2	1:A:173:TYR:OH	2.19	0.43
1:A:624:ILE:O	1:A:628:VAL:HG23	2.18	0.43
1:D:92:ASP:O	1:D:94:LEU:HG	2.19	0.43
1:D:492:TRP:CD1	1:D:495:LYS:HD3	2.53	0.43
1:D:742:ILE:HD13	1:D:786:LEU:CD2	2.48	0.43
1:A:126:LEU:HD23	1:A:140:VAL:CG2	2.42	0.43
1:A:742:ILE:HG21	1:A:786:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ILE:CG2	1:A:835:LEU:N	2.82	0.43
1:D:326:LEU:HG	1:D:343:VAL:HG11	2.01	0.43
1:D:729:ASP:HB2	1:D:757:MET:HE3	1.98	0.43
1:D:762:LEU:HD13	1:D:930:TRP:CE3	2.54	0.43
1:A:120:HIS:O	1:A:122:LEU:N	2.52	0.42
1:A:741:ILE:HG13	1:A:772:ALA:HA	2.00	0.42
1:A:796:GLU:HB3	1:A:825:SER:OG	2.19	0.42
1:D:11:PRO:HB2	1:D:75:GLN:NE2	2.34	0.42
1:D:329:VAL:HG12	1:D:340:TYR:CB	2.49	0.42
1:A:10:THR:CG2	1:A:90:GLN:HG2	2.45	0.42
1:A:225:PRO:HG3	1:A:230:GLU:HG2	2.01	0.42
1:A:695:PRO:HA	1:A:696:PRO:HD3	1.88	0.42
1:D:255:LEU:HD13	1:D:260:GLN:CB	2.48	0.42
1:D:624:ILE:O	1:D:624:ILE:CG2	2.66	0.42
1:A:127:ARG:CG	1:A:206:LEU:HD21	2.42	0.42
1:A:250:ALA:HB2	1:A:261:VAL:CG2	2.49	0.42
1:A:864:TRP:CA	1:A:868:GLN:NE2	2.78	0.42
1:A:924:TYR:N	1:A:924:TYR:CD2	2.86	0.42
5:A:951:SAH:HG2	2:B:22:G:N2	2.34	0.42
2:B:20:A:O2'	2:B:21:A:C5'	2.68	0.42
1:A:796:GLU:O	1:A:796:GLU:CD	2.58	0.42
2:B:4:U:O2'	2:B:5:U:H5'	2.19	0.42
1:D:12:LYS:HE3	1:D:79:GLU:OE2	2.19	0.42
1:D:94:LEU:HD12	1:D:158:ILE:CD1	2.49	0.42
1:D:632:THR:C	1:D:677:LEU:HD23	2.39	0.42
1:D:818:HIS:HA	1:D:819:PRO:HD2	1.34	0.42
1:A:8:THR:O	1:A:8:THR:HG22	2.19	0.42
1:A:621:ASN:HD22	1:A:622:PRO:CD	2.33	0.42
1:A:795:LEU:C	1:A:796:GLU:HG3	2.40	0.42
3:C:11:G:H2'	3:C:12:A:C8	2.54	0.42
1:D:262:MET:CA	1:D:282:ILE:HD11	2.49	0.42
1:D:608:ASN:ND2	1:D:611:ILE:HD11	2.35	0.42
1:D:742:ILE:HD13	1:D:786:LEU:HD23	2.01	0.42
1:D:870:ASN:C	1:D:870:ASN:OD1	2.56	0.42
1:D:895:VAL:CG1	1:D:897:PRO:HD2	2.43	0.42
1:D:227:ILE:HG22	1:D:229:GLU:H	1.84	0.42
1:D:271:SER:O	1:D:350:ARG:NH1	2.52	0.42
1:D:694:LYS:CB	1:D:695:PRO:CD	2.97	0.42
2:E:3:U:H2'	2:E:4:U:O4'	2.20	0.42
1:A:218:GLU:OE1	1:A:236:THR:HG21	2.20	0.42
2:B:6:C:H2'	2:B:7:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HD2	1:A:759:HIS:NE2	2.34	0.42
1:A:857:ASN:HB3	1:A:859:ASP:H	1.84	0.42
1:D:14:ILE:O	1:D:17:GLN:HB3	2.20	0.42
1:D:126:LEU:HD23	1:D:140:VAL:HG21	2.02	0.42
1:D:151:LYS:O	1:D:155:ARG:HG2	2.19	0.42
1:D:377:PHE:C	1:D:377:PHE:CD2	2.93	0.42
1:D:833:THR:O	1:D:837:ARG:HG3	2.19	0.42
1:D:834:ILE:HD12	1:D:897:PRO:HB3	2.01	0.42
1:D:283:PRO:O	1:D:285:LYS:N	2.52	0.42
1:D:387:LEU:CB	1:D:483:GLN:HE22	2.24	0.42
1:D:908:ARG:HG2	1:D:909:GLU:H	1.84	0.42
1:A:391:ILE:HG12	1:A:391:ILE:O	2.20	0.42
1:A:693:PHE:CD1	1:A:693:PHE:N	2.88	0.42
1:A:822:LEU:CD2	1:A:824:VAL:HG23	2.50	0.42
3:C:13:G:H2'	3:C:14:A:H8	1.85	0.42
1:D:535:SER:N	1:D:643:PRO:HB2	2.35	0.42
1:D:559:VAL:HG13	1:D:677:LEU:HD11	2.01	0.42
1:D:836:GLN:HG2	2:E:21:A:N1	2.34	0.42
1:A:39:PRO:HD2	1:A:759:HIS:CD2	2.55	0.41
1:A:368:VAL:HG22	1:A:654:VAL:HG22	1.99	0.41
1:A:559:VAL:HG23	1:A:615:VAL:CG2	2.50	0.41
1:A:745:ASP:OD1	1:A:746:ILE:N	2.53	0.41
1:D:62:VAL:HG11	1:D:80:LEU:HB3	2.02	0.41
1:D:96:VAL:O	1:D:100:ARG:HD2	2.19	0.41
1:D:383:TRP:HZ2	1:D:386:PRO:O	2.03	0.41
1:D:387:LEU:HD13	1:D:483:GLN:NE2	2.35	0.41
1:D:817:PHE:C	1:D:819:PRO:CD	2.81	0.41
1:A:12:LYS:CB	1:A:78:ALA:HB3	2.51	0.41
1:A:30:VAL:HG12	1:A:31:HIS:N	2.34	0.41
1:A:209:HIS:O	1:A:209:HIS:CG	2.71	0.41
1:D:524:PHE:O	1:D:524:PHE:CG	2.74	0.41
1:D:658:THR:O	1:D:662:ARG:HG3	2.20	0.41
1:D:18:LYS:HG3	1:D:18:LYS:O	2.19	0.41
1:D:47:GLY:HA3	1:D:48:PRO:HD3	1.91	0.41
1:A:168:PHE:HD2	1:A:282:ILE:HG23	1.84	0.41
1:A:246:LEU:HD22	1:A:261:VAL:CG1	2.50	0.41
1:A:368:VAL:CG2	1:A:369:ILE:N	2.82	0.41
1:A:864:TRP:CA	1:A:868:GLN:HE21	2.32	0.41
2:B:13:C:H2'	2:B:14:A:H8	1.85	0.41
1:D:380:LYS:HD2	1:D:479:ASN:ND2	2.35	0.41
1:D:783:ASP:OD1	1:D:922:GLN:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:857:ASN:HB3	1:D:860:HIS:CE1	2.56	0.41
1:A:32:ASP:HB2	1:A:50:LEU:CD1	2.50	0.41
1:A:52:ARG:HB2	1:A:64:SER:O	2.21	0.41
1:A:356:SER:HA	1:A:497:PHE:CE1	2.55	0.41
1:D:38:CYS:HB3	1:D:41:LEU:CD1	2.50	0.41
1:D:231:VAL:HG12	1:D:232:VAL:O	2.21	0.41
1:D:272:CYS:HB2	1:D:351:ILE:CD1	2.51	0.41
1:D:482:ILE:O	1:D:485:ALA:HB3	2.20	0.41
1:D:599:GLU:C	1:D:601:SER:H	2.22	0.41
1:D:773:THR:O	1:D:774:LEU:HD23	2.20	0.41
1:A:631:MET:HA	1:A:635:GLU:OE1	2.20	0.41
1:D:527:PRO:N	1:D:528:PRO:CD	2.84	0.41
1:D:793:THR:HG22	1:D:795:LEU:HG	2.02	0.41
3:C:3:C:H2'	3:C:4:G:C8	2.55	0.41
1:D:358:ASN:HA	1:D:373:LEU:HB2	2.02	0.41
1:D:370:ALA:O	1:D:620:MET:HB2	2.20	0.41
1:D:561:ILE:HG22	1:D:677:LEU:HD12	2.02	0.41
2:E:11:U:O2'	2:E:12:G:H5'	2.21	0.41
1:A:244:HIS:HD2	1:A:246:LEU:N	2.01	0.41
1:A:667:GLU:O	1:A:669:PRO:CD	2.64	0.41
1:D:43:ILE:O	1:D:44:PRO:C	2.58	0.41
1:D:154:SER:O	1:D:158:ILE:HG13	2.20	0.41
1:D:168:PHE:HE2	1:D:282:ILE:HG12	1.86	0.41
1:D:262:MET:N	1:D:280:SER:O	2.46	0.41
1:A:186:VAL:CG2	1:A:195:LYS:HG3	2.50	0.41
1:A:237:LEU:HD22	1:A:249:ILE:HG12	2.03	0.41
1:A:263:ILE:HG12	1:A:279:TYR:CE2	2.56	0.41
1:A:392:LEU:HD21	1:A:404:PRO:CG	2.51	0.41
1:A:470:SER:HA	1:A:471:PRO:HD3	1.83	0.41
1:A:753:ARG:HA	1:A:756:LYS:HE2	2.03	0.41
1:D:18:LYS:O	1:D:18:LYS:CG	2.69	0.41
1:D:199:PRO:HB2	1:D:201:GLU:OE1	2.20	0.41
1:D:782:PHE:HD1	1:D:817:PHE:CE1	2.39	0.41
1:D:857:ASN:HB3	1:D:860:HIS:ND1	2.36	0.41
1:A:401:LEU:HD22	1:A:461:LYS:HB3	1.98	0.41
1:A:728:LEU:HD22	1:A:741:ILE:HD12	2.03	0.41
1:A:783:ASP:OD1	1:A:922:GLN:HA	2.21	0.41
1:A:821:LEU:HD12	1:A:906:PHE:O	2.21	0.41
1:A:827:PRO:HB2	1:A:856:ARG:CZ	2.50	0.41
1:A:887:SER:O	1:A:903:ILE:N	2.54	0.41
1:D:212:ASP:HB3	1:D:337:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:LEU:CD2	1:D:461:LYS:HD3	2.37	0.41
1:D:780:LEU:HD11	1:D:805:GLN:HB3	2.03	0.41
2:E:11:U:H2'	2:E:12:G:C8	2.55	0.41
1:A:160:ASN:CB	1:A:173:TYR:OH	2.69	0.40
1:A:211:SER:O	1:A:212:ASP:C	2.60	0.40
1:A:624:ILE:HD11	1:A:673:TYR:CE2	2.55	0.40
1:A:719:ASP:O	1:A:721:GLY:N	2.54	0.40
1:D:43:ILE:O	1:D:43:ILE:CG2	2.62	0.40
1:A:12:LYS:HE2	1:A:90:GLN:HE22	1.85	0.40
1:A:82:LEU:CD2	1:A:85:LEU:HD12	2.37	0.40
1:A:120:HIS:CD2	1:A:122:LEU:H	2.38	0.40
1:A:252:ARG:HH11	1:A:252:ARG:CG	2.33	0.40
1:A:361:TYR:HB2	1:A:391:ILE:CD1	2.52	0.40
1:A:457:LYS:NZ	1:A:489:ALA:HB3	2.36	0.40
1:A:493:PHE:HA	1:A:496:PHE:HD1	1.84	0.40
1:A:621:ASN:HD22	1:A:621:ASN:C	2.25	0.40
1:A:798:ILE:HA	1:A:801:MET:CE	2.51	0.40
2:B:20:A:C2'	2:B:21:A:H5"	2.51	0.40
1:D:73:SER:OG	1:D:74:GLU:N	2.53	0.40
1:D:483:GLN:HA	1:D:483:GLN:OE1	2.21	0.40
1:D:570:ASP:OD2	1:D:672:ASN:OD1	2.38	0.40
1:D:695:PRO:HG2	1:D:700:GLN:CG	2.50	0.40
1:A:493:PHE:HA	1:A:496:PHE:CE1	2.55	0.40
1:A:605:ILE:HD13	1:A:651:ILE:HG23	2.03	0.40
1:D:38:CYS:HA	1:D:39:PRO:HD3	1.86	0.40
1:D:62:VAL:HG21	1:D:81:ALA:HA	2.02	0.40
1:D:373:LEU:HA	1:D:374:PRO:HD3	1.80	0.40
1:D:824:VAL:O	1:D:903:ILE:HB	2.21	0.40
1:A:17:GLN:HG2	6:B:23:HOH:O	2.22	0.40
1:A:100:ARG:O	1:A:104:VAL:HG23	2.22	0.40
1:A:757:MET:HE2	1:A:758:LEU:CD2	2.48	0.40
1:D:149:ASP:OD2	1:D:152:ILE:HG12	2.21	0.40
1:D:392:LEU:HD11	1:D:459:PHE:HZ	1.87	0.40
1:D:648:GLU:OE1	1:D:665:LEU:HD22	2.22	0.40
1:D:736:THR:CG2	1:D:738:LEU:HG	2.52	0.40
1:A:12:LYS:HB3	1:A:78:ALA:HB3	2.04	0.40
1:A:217:ARG:HD3	1:A:340:TYR:HE2	1.85	0.40
1:A:333:TRP:C	1:A:335:SER:H	2.25	0.40
1:A:457:LYS:HZ3	1:A:489:ALA:HB3	1.87	0.40
1:A:813:VAL:HA	1:A:817:PHE:CD1	2.50	0.40
1:D:777:GLY:HA3	1:D:924:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	761/950 (80%)	671 (88%)	72 (10%)	18 (2%)	6	27
1	D	777/950 (82%)	692 (89%)	70 (9%)	15 (2%)	8	33
All	All	1538/1900 (81%)	1363 (89%)	142 (9%)	33 (2%)	7	30

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	A	59	GLU
1	A	284	LYS
1	D	48	PRO
1	D	854	LYS
1	A	682	GLY
1	A	687	ARG
1	A	720	PHE
1	A	924	TYR
1	D	644	PRO
1	A	58	PRO
1	A	694	LYS
1	A	722	CYS
1	A	723	GLY
1	D	44	PRO
1	D	284	LYS
1	A	310	ALA
1	A	380	LYS
1	D	197	ALA
1	D	207	ALA
1	D	895	VAL
1	A	121	PRO

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Mol	Chain	Res	Type
1	A	334	LYS
1	A	669	PRO
1	D	189	PRO
1	A	8	THR
1	D	570	ASP
1	D	643	PRO
1	D	694	LYS
1	A	735	PRO
1	D	43	ILE
1	D	471	PRO
1	D	735	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	676/828 (82%)	621 (92%)	55 (8%)	11	39
1	D	689/828 (83%)	654 (95%)	35 (5%)	24	56
All	All	1365/1656 (82%)	1275 (93%)	90 (7%)	16	47

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	49	CYS
1	A	58	PRO
1	A	63	VAL
1	A	64	SER
1	A	91	ASN
1	A	92	ASP
1	A	121	PRO
1	A	143	SER
1	A	167	PRO
1	A	173	TYR
1	A	175	MET

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Mol	Chain	Res	Type
1	A	183	ASP
1	A	184	TYR
1	A	193	ARG
1	A	209	HIS
1	A	218	GLU
1	A	230	GLU
1	A	251	GLU
1	A	311	ARG
1	A	336	ASP
1	A	339	ASP
1	A	365	ARG
1	A	392	LEU
1	A	396	CYS
1	A	458	ILE
1	A	459	PHE
1	A	462	SER
1	A	473	LYS
1	A	497	PHE
1	A	537	GLU
1	A	541	THR
1	A	560	SER
1	A	621	ASN
1	A	660	ARG
1	A	667	GLU
1	A	677	LEU
1	A	695	PRO
1	A	701	ARG
1	A	703	GLU
1	A	710	ARG
1	A	715	SER
1	A	717	LEU
1	A	738	LEU
1	A	757	MET
1	A	776	ASP
1	A	784	SER
1	A	796	GLU
1	A	799	GLU
1	A	804	ASP
1	A	825	SER
1	A	855	PHE
1	A	857	ASN
1	A	865	THR

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Mol	Chain	Res	Type
1	A	886	PHE
1	D	51	TYR
1	D	72	ASP
1	D	88	ARG
1	D	156	CYS
1	D	183	ASP
1	D	194	ARG
1	D	200	SER
1	D	235	ASP
1	D	239	ILE
1	D	265	ARG
1	D	332	ARG
1	D	342	ASP
1	D	346	ASN
1	D	350	ARG
1	D	401	LEU
1	D	469	CYS
1	D	480	ASP
1	D	491	LEU
1	D	497	PHE
1	D	500	LEU
1	D	562	CYS
1	D	599	GLU
1	D	606	GLU
1	D	608	ASN
1	D	722	CYS
1	D	757	MET
1	D	787	HIS
1	D	794	CYS
1	D	804	ASP
1	D	863	GLU
1	D	867	GLU
1	D	870	ASN
1	D	878	LYS
1	D	921	MET
1	D	929	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	45	GLN
1	A	90	GLN
1	A	120	HIS
1	A	244	HIS
1	A	321	HIS
1	A	358	ASN
1	A	382	ASN
1	A	398	GLN
1	A	484	ASN
1	A	621	ASN
1	A	739	GLN
1	A	857	ASN
1	A	868	GLN
1	A	870	ASN
1	D	45	GLN
1	D	244	HIS
1	D	260	GLN
1	D	318	GLN
1	D	346	ASN
1	D	358	ASN
1	D	479	ASN
1	D	484	ASN
1	D	608	ASN
1	D	621	ASN
1	D	672	ASN
1	D	832	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	21/22 (95%)	3 (14%)	2 (9%)
2	E	21/22 (95%)	2 (9%)	0
3	C	21/22 (95%)	2 (9%)	0
3	F	21/22 (95%)	4 (19%)	1 (4%)
All	All	84/88 (95%)	11 (13%)	3 (3%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	A
2	B	21	A

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Mol	Chain	Res	Type
2	B	22	G
3	C	21	A
3	C	22	C
2	E	21	A
2	E	22	G
3	F	19	U
3	F	20	C
3	F	21	A
3	F	22	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	20	A
2	B	21	A
3	F	19	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	$\#|Z| > 2$
5	SAH	D	951	-	21,28,28	0.90	1 (4%)	20,40,40	1.05	2 (10%)
5	SAH	A	951	-	21,28,28	1.01	1 (4%)	20,40,40	1.17	1 (5%)

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
5	SAH	D	951	-	-	2/7/31/31	0/3/3/3
5	SAH	A	951	-	-	3/7/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	951	SAH	C2-N3	2.43	1.36	1.32
5	D	951	SAH	C2-N3	2.11	1.35	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	951	SAH	O4'-C1'-C2'	-3.90	101.23	106.93
5	D	951	SAH	O4'-C1'-C2'	-2.26	103.63	106.93
5	D	951	SAH	C5-C6-N6	2.04	123.45	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	951	SAH	N-CA-CB-CG
5	A	951	SAH	C-CA-CB-CG
5	D	951	SAH	N-CA-CB-CG
5	D	951	SAH	C-CA-CB-CG
5	A	951	SAH	CB-CG-SD-C5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	951	SAH	1	0
5	A	951	SAH	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAH D 951

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH A 951

Bond lengths

Bond angles

Torsions

Rings
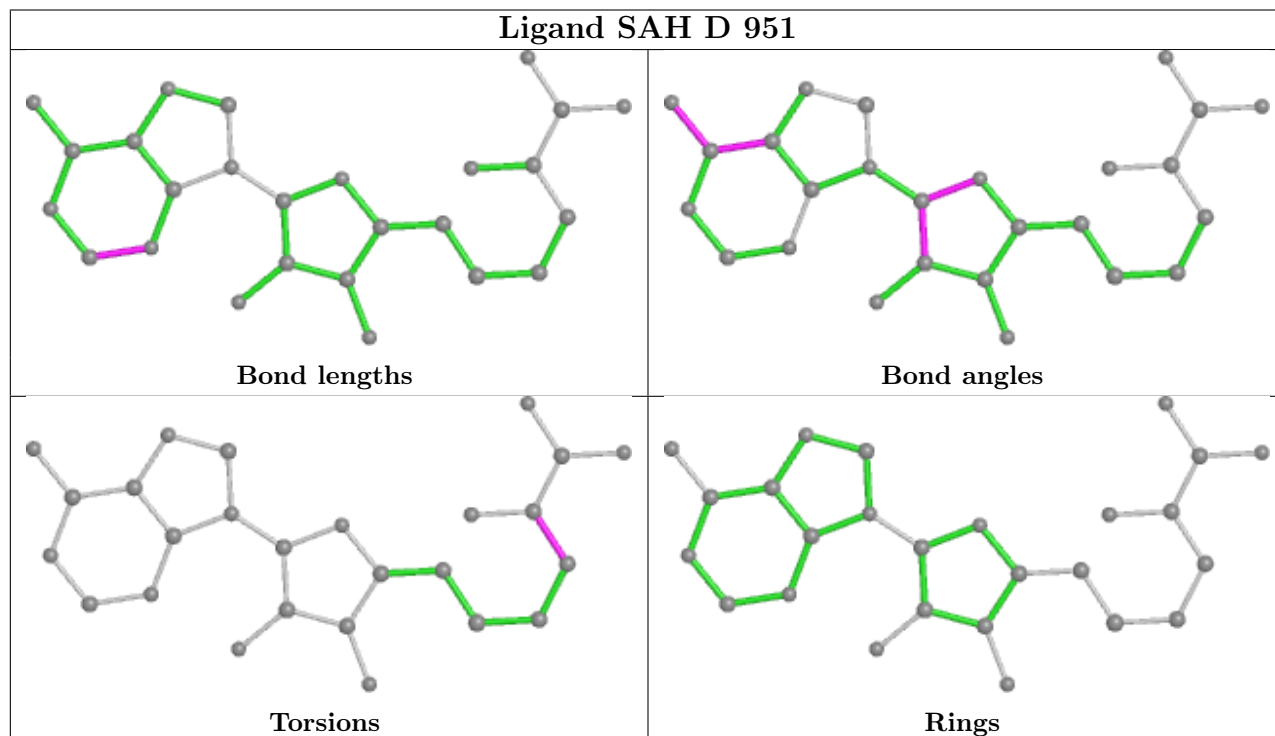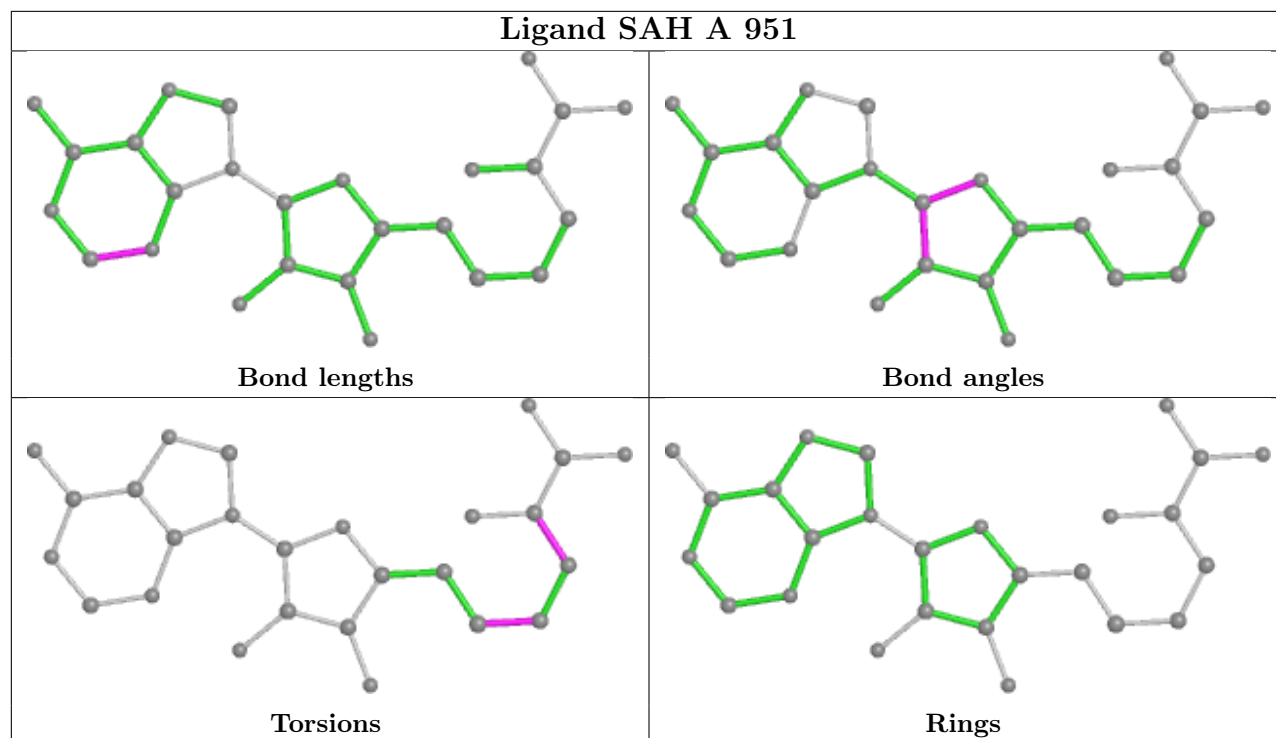
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	779/950 (82%)	-0.11	23 (2%)	50	27	60, 96, 160, 193	0
1	D	795/950 (83%)	-0.16	15 (1%)	66	46	55, 98, 154, 188	0
2	B	22/22 (100%)	-0.72	0	100	100	91, 120, 146, 151	0
2	E	22/22 (100%)	-0.71	0	100	100	99, 114, 123, 130	0
3	C	22/22 (100%)	-0.66	0	100	100	89, 137, 168, 199	0
3	F	22/22 (100%)	-0.64	0	100	100	91, 125, 144, 186	0
All	All	1662/1988 (83%)	-0.16	38 (2%)	60	39	55, 98, 159, 199	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	573	TYR	6.8
1	A	32	ASP	5.5
1	A	7	HIS	5.3
1	A	851	GLN	5.2
1	A	89	PRO	5.1
1	A	92	ASP	4.5
1	D	524	PHE	4.4
1	A	33	SER	4.4
1	A	406	LEU	4.1
1	D	91	ASN	3.9
1	A	90	GLN	3.8
1	A	475	TYR	3.5
1	A	23	ALA	3.4
1	A	919	SER	3.4
1	D	290	SER	3.4
1	D	93	ASP	3.3
1	D	687	ARG	3.2
1	D	839	THR	3.1
1	A	16	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	852	LEU	2.7
1	A	468	GLU	2.7
1	A	687	ARG	2.6
1	A	62	VAL	2.6
1	A	472	ARG	2.5
1	D	291	SER	2.5
1	A	461	LYS	2.4
1	A	853	PRO	2.4
1	D	852	LEU	2.4
1	D	409	SER	2.4
1	D	522	ASN	2.4
1	D	209	HIS	2.4
1	D	88	ARG	2.3
1	D	836	GLN	2.2
1	D	7	HIS	2.2
1	A	31	HIS	2.1
1	A	471	PRO	2.1
1	A	601	SER	2.1
1	A	689	GLU	2.0

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

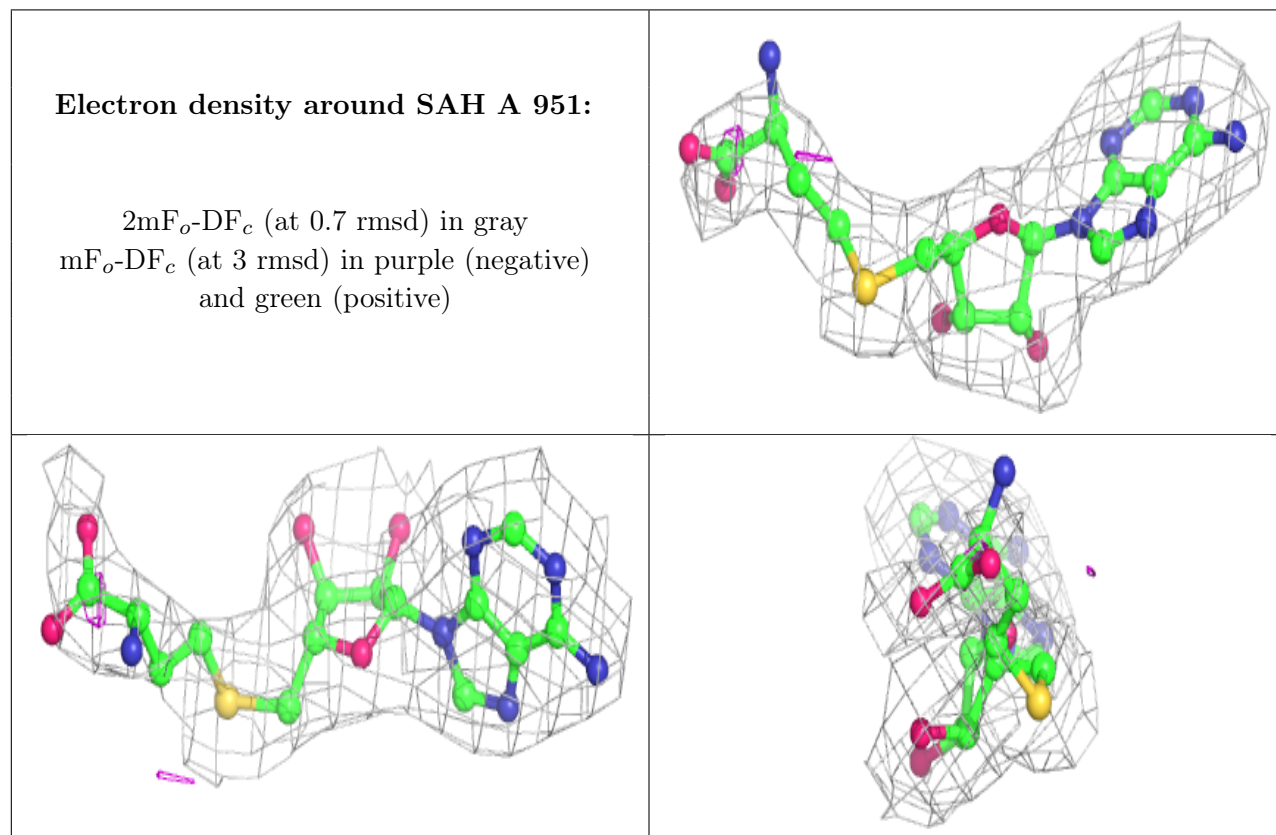There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

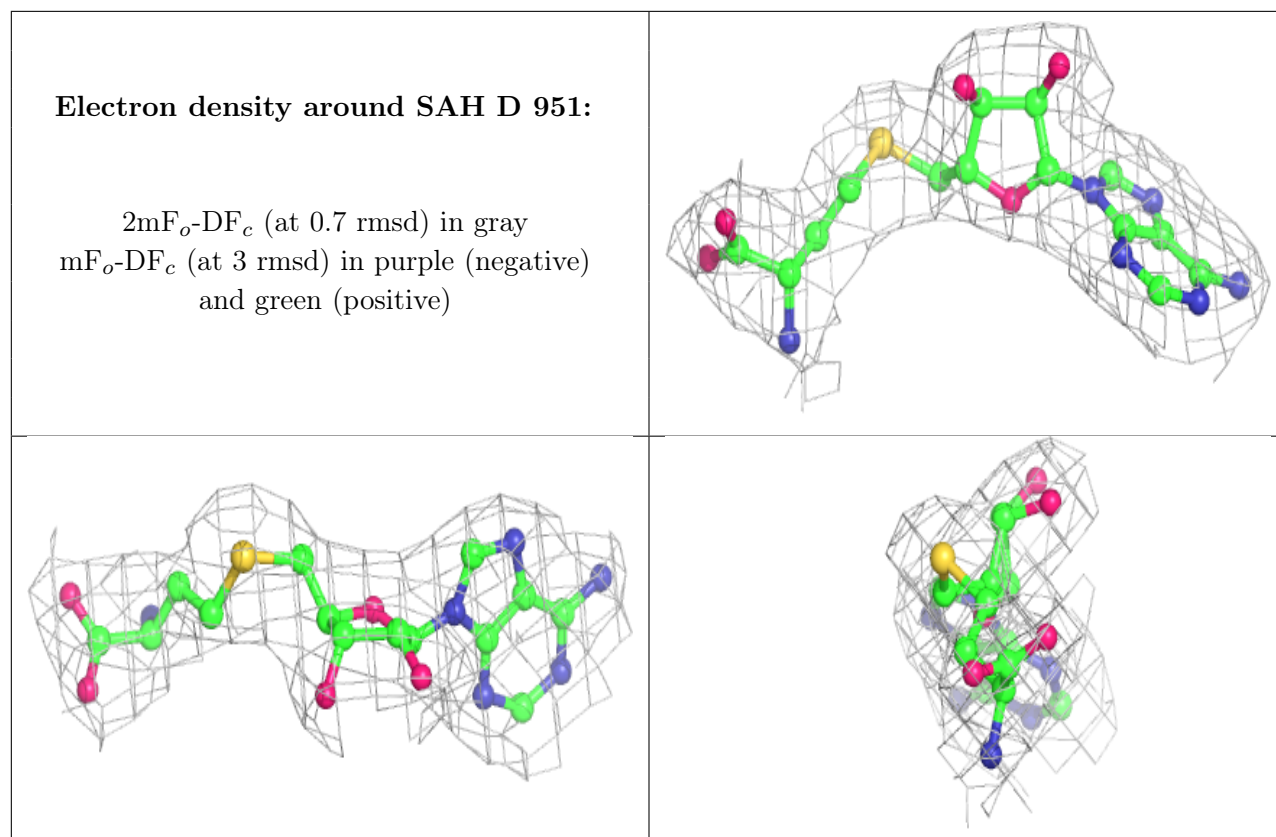There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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	MG	A	950	1/1	0.94	0.04	60,60,60,60	0
5	SAH	A	951	26/26	0.94	0.21	62,68,85,86	0
5	SAH	D	951	26/26	0.96	0.14	70,74,86,87	0
4	MG	D	950	1/1	0.98	0.10	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH A 951:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around SAH D 951:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.