Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 03:10 pm BST

PDB ID	:	2XCT
Title	:	The twinned 3.35A structure of S. aureus Gyrase complex with Ciprofloxacin and DNA
Authors	:	Bax, B.D.; Chan, P.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.
Deposited on	:	2010-04-25
Resolution	:	3.35 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:

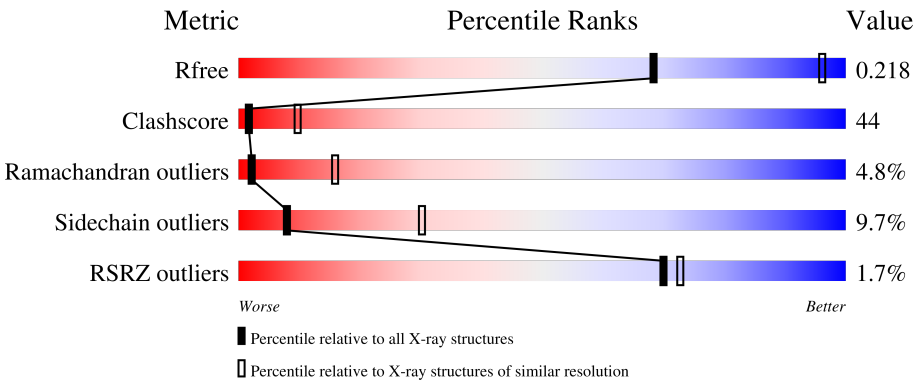
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	B	692	% 38% 52% 6% •
1	D	692	% 39% 50% 8% •
1	S	692	3% 33% 55% 9% •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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Mol	Chain	Length	Quality of chain
1	U	692	2% 37% 51% 9%
2	E	8	50% 38% 12%
2	V	8	12% 50% 25% 12%
3	F	8	12% 50% 25% 12%
3	W	8	12% 38% 25% 25%
4	G	12	58% 33% 8%
4	X	12	8% 25% 58% 8%
5	H	12	25% 75%
5	Y	12	25% 67% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CPF	H	1020	-	-	X	-
7	CPF	X	1020	-	-	X	-
7	CPF	Y	1020	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22370 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 DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	669	5262	3277	944	1015	26	0	2	0
1	D	669	5151	3212	913	1001	25	0	1	0
1	S	667	5199	3247	920	1007	25	0	0	1
1	U	665	5193	3239	926	1003	25	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	expression tag	UNP P66937
B	544	THR	-	insertion	UNP P66937
B	545	GLY	-	insertion	UNP P66937
B	1123	PHE	TYR	engineered mutation	UNP Q99XG5
D	409	MET	-	expression tag	UNP P66937
D	544	THR	-	insertion	UNP P66937
D	545	GLY	-	insertion	UNP P66937
D	1123	PHE	TYR	engineered mutation	UNP Q99XG5
S	409	MET	-	expression tag	UNP P66937
S	544	THR	-	insertion	UNP P66937
S	545	GLY	-	insertion	UNP P66937
S	1123	PHE	TYR	engineered mutation	UNP Q99XG5
U	409	MET	-	expression tag	UNP P66937
U	544	THR	-	insertion	UNP P66937
U	545	GLY	-	insertion	UNP P66937
U	1123	PHE	TYR	engineered mutation	UNP Q99XG5

- Molecule 2 is a DNA chain called 5'-D(TP*GP*TP*GP*CP*GP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	7	147	69	27	44	7	0	0	0
2	V	7	147	69	27	44	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	7	145	68	28	42	7	0	0	0
3	W	6	123	58	23	36	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	G	11	220	105	42	63	10	0	0	0
4	X	11	220	105	42	63	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	H	12	240	115	47	67	11	0	0	0
5	Y	11	219	105	42	62	10	0	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
6	B	1	1	1	0	0
6	D	1	1	1	0	0
6	F	1	1	1	0	0
6	G	1	1	1	0	0

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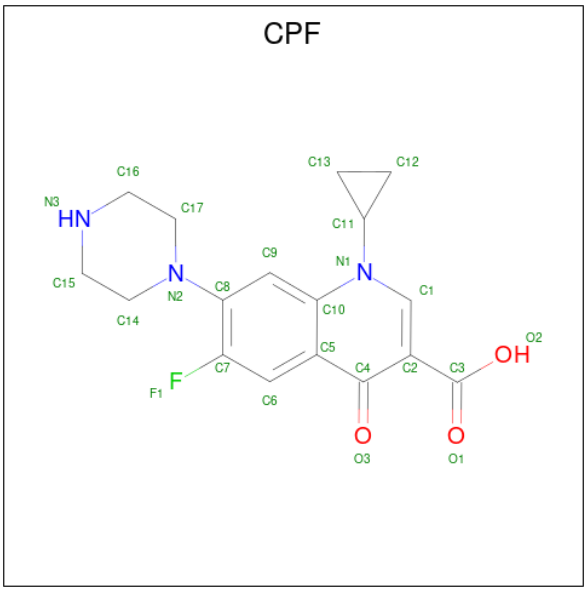
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
6	S	1	1	1	0	0
			Total	Mn		
6	U	1	1	1	0	0
			Total	Mn		
6	W	2	2	2	0	0

- Molecule 7 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula: $C_{17}H_{18}FN_3O_3$).



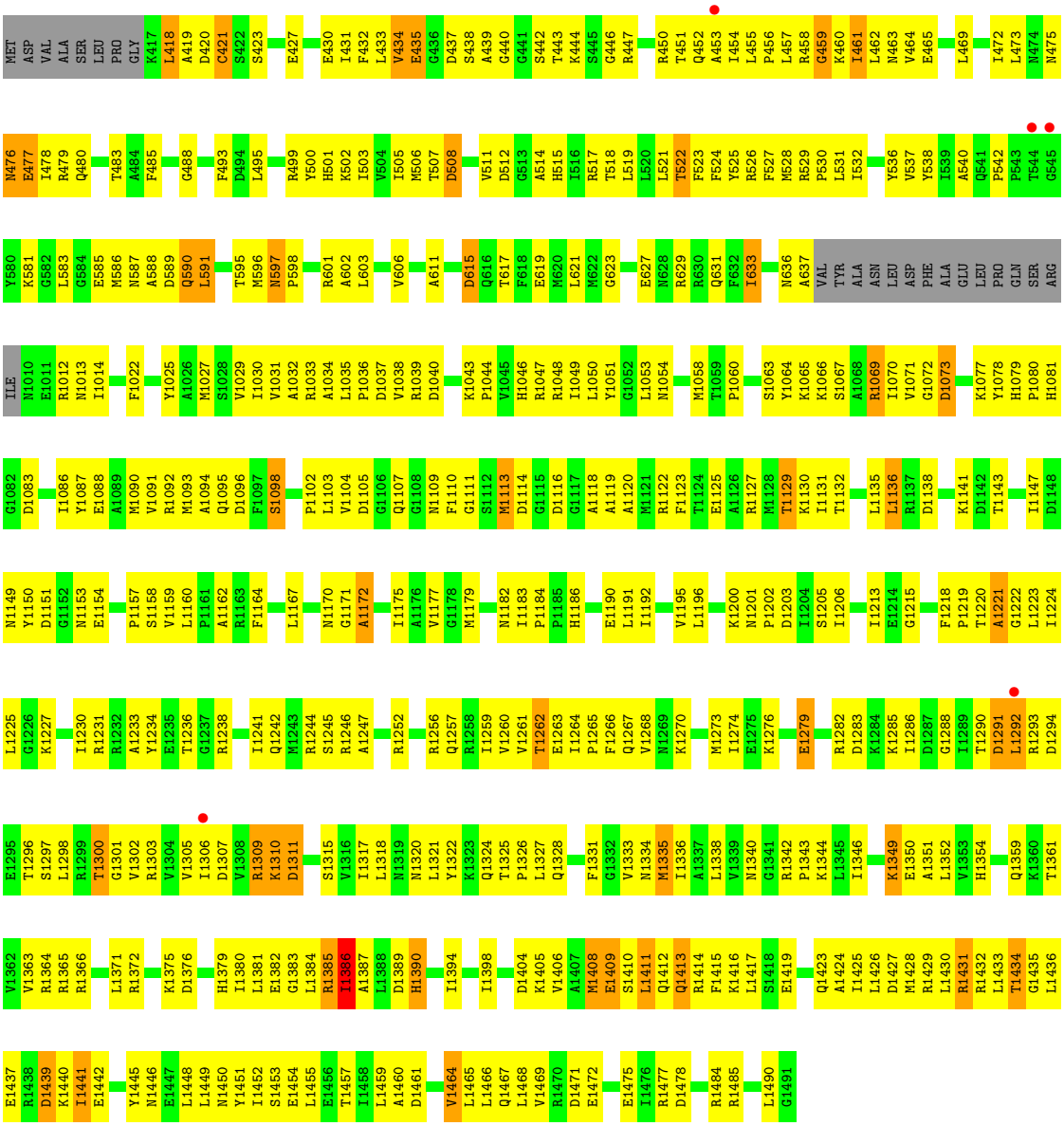
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
7	G	1	24	17	1	3	3	0	0
			Total	C	F	N	O		
7	H	1	24	17	1	3	3	0	0
			Total	C	F	N	O		
7	X	1	24	17	1	3	3	0	0
			Total	C	F	N	O		
7	Y	1	24	17	1	3	3	0	0

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.

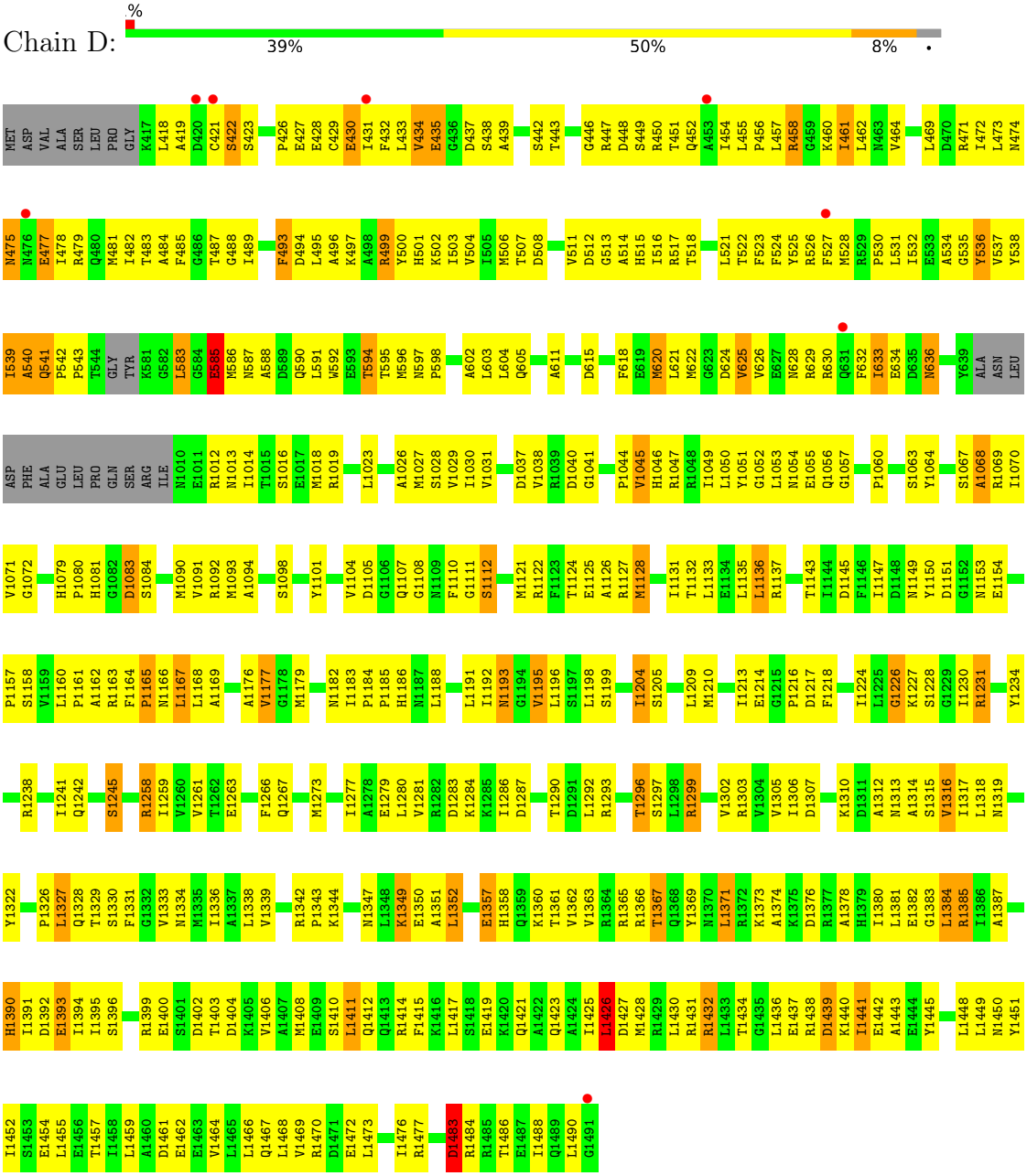
• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain B:



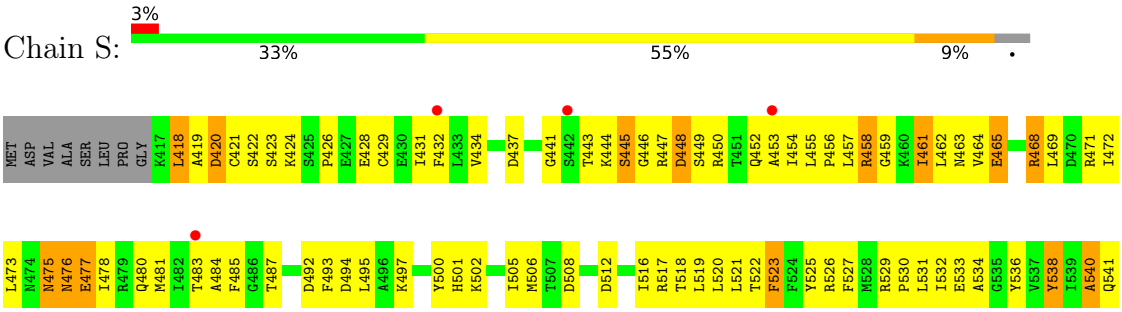
• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

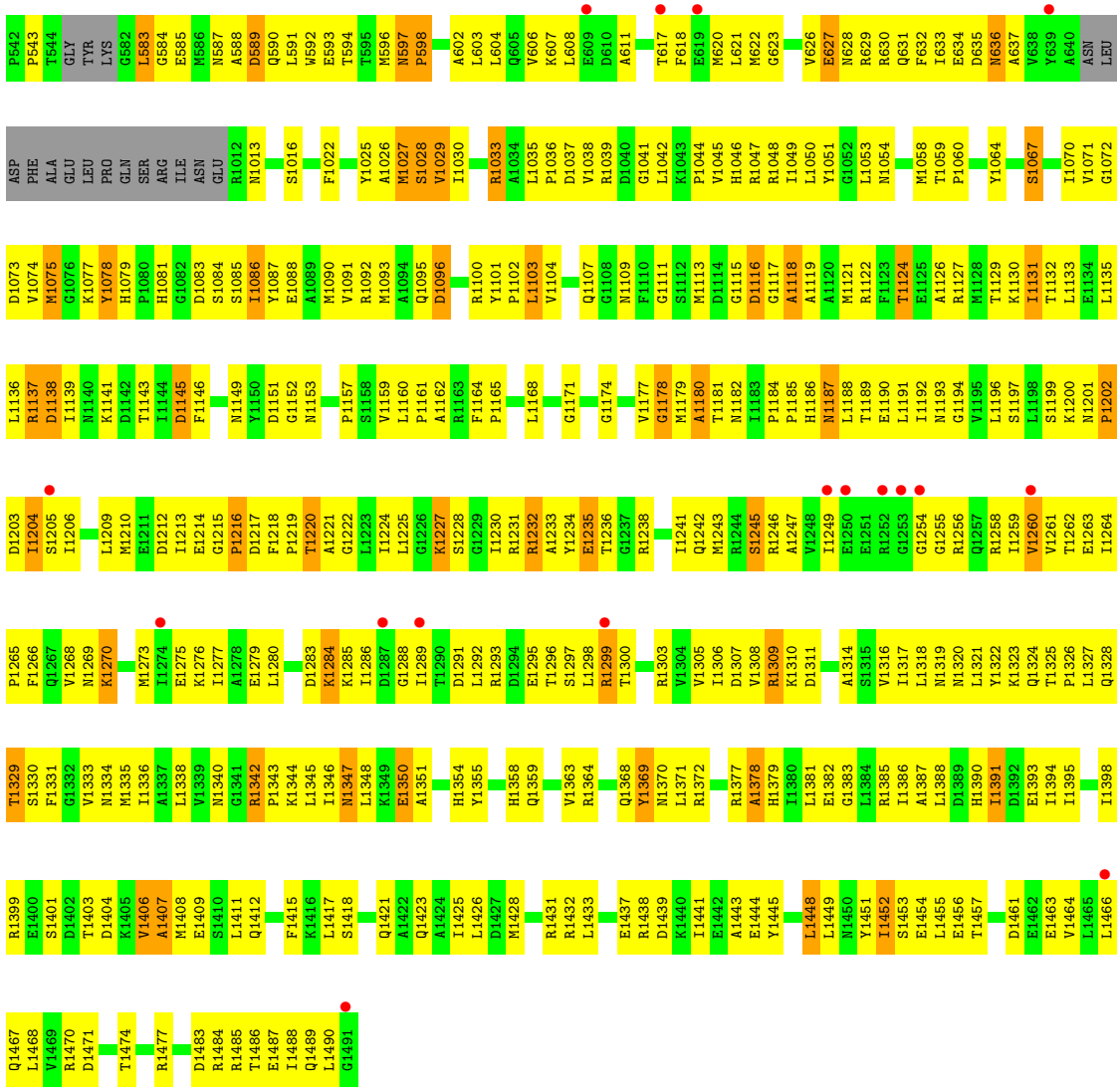
Chain D:



• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

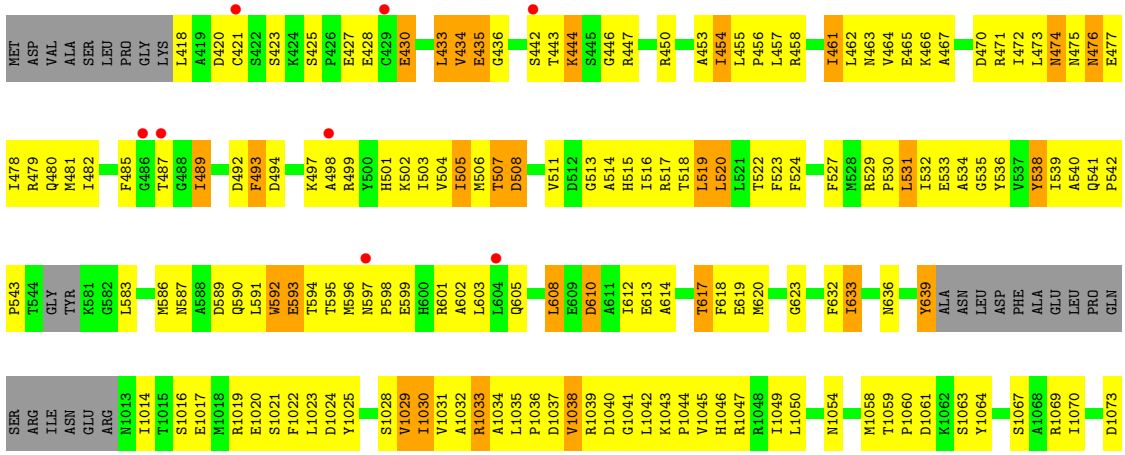
Chain S:

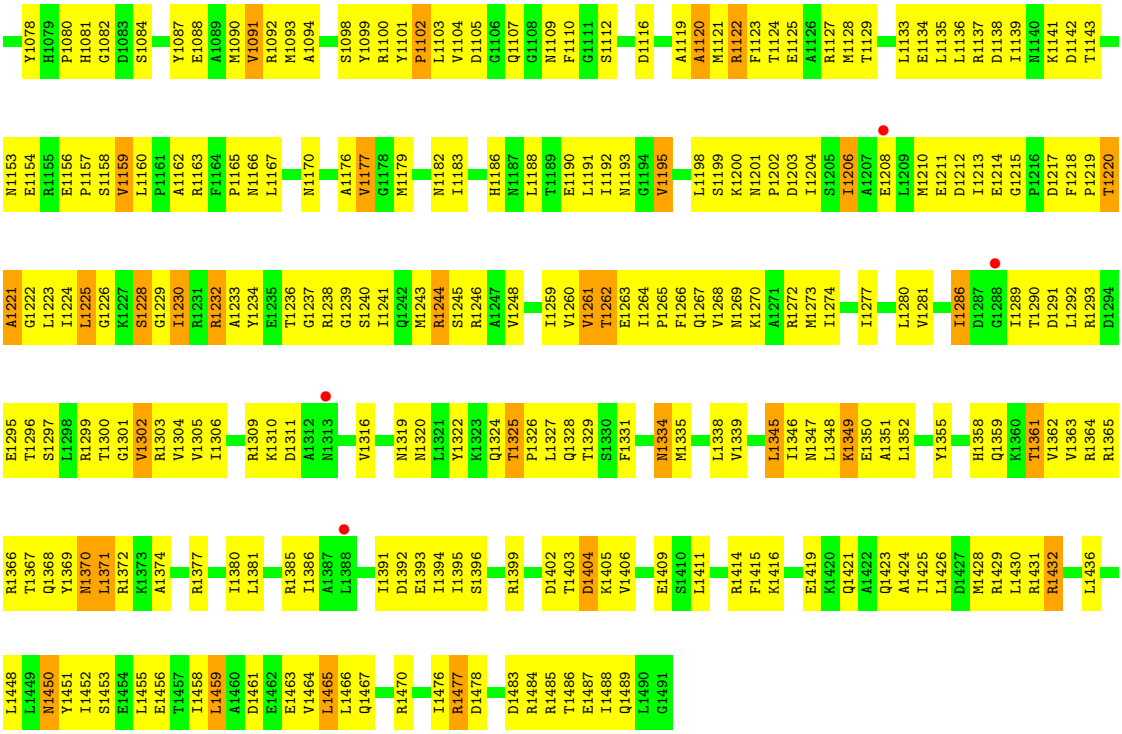




• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain U: 2% 37% 51% 9% •



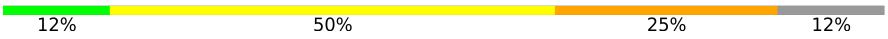


- Molecule 2: 5'-D(TP*GP*TP*GP*CP*GP*GP*T)-3'

Chain E:

- Molecule 2: 5'-D(TP*GP*TP*GP*CP*GP*GP*T)-3'

Chain V:



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

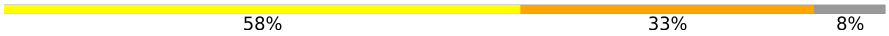
Chain F:

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

Chain W:

- Molecule 4: 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'

Chain G:



• Molecule 4: 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'

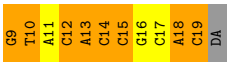
Chain X:

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

Chain H:

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

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.98Å 123.17Å 170.42Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	24.96 – 3.35 24.96 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (24.96-3.35) 97.3 (24.96-3.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.166 , 0.236 0.167 , 0.218	Depositor DCC
R_{free} test set	2115 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.277 for h,-k,-l	Xtriage
Reported twinning fraction	0.324 for h,-k,-l	Depositor
Outliers	0 of 52173 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22370	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CPF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	B	0.49	0/5332	0.70	0/7190
1	D	0.47	0/5220	0.69	1/7063 (0.0%)
1	S	0.45	0/5269	0.68	1/7112 (0.0%)
1	U	0.49	0/5263	0.71	1/7106 (0.0%)
2	E	1.02	0/164	2.13	7/252 (2.8%)
2	V	0.82	0/164	1.77	3/252 (1.2%)
3	F	0.94	1/162 (0.6%)	2.01	7/248 (2.8%)
3	W	0.80	0/137	1.81	6/209 (2.9%)
4	G	0.98	0/246	1.78	10/377 (2.7%)
4	X	1.00	0/246	2.04	17/377 (4.5%)
5	H	1.33	2/269 (0.7%)	2.72	31/412 (7.5%)
5	Y	1.00	0/245	2.42	18/375 (4.8%)
All	All	0.54	3/22717 (0.0%)	0.90	102/30973 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	17	DC	C3'-O3'	-5.51	1.36	1.44
5	H	16	DG	C3'-O3'	-5.48	1.36	1.44
3	F	6	DT	C1'-N1	5.42	1.56	1.49

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	9	DG	O4'-C1'-N9	17.19	120.03	108.00
5	H	17	DC	O4'-C1'-N1	-13.75	98.38	108.00
5	H	9	DG	O4'-C1'-N9	13.50	117.45	108.00
5	H	10	DT	O4'-C1'-N1	13.39	117.37	108.00
5	Y	9	DG	C1'-O4'-C4'	-11.73	98.36	110.10
2	E	6	DG	O4'-C1'-N9	11.35	115.94	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	6	DT	O4'-C1'-N1	10.85	115.60	108.00
4	X	19	DC	O4'-C1'-N1	10.82	115.57	108.00
5	Y	9	DG	O4'-C4'-C3'	-10.66	99.60	106.00
5	H	9	DG	N9-C4-C5	10.16	109.46	105.40
5	H	9	DG	N3-C4-N9	-9.94	120.04	126.00
5	H	9	DG	P-O3'-C3'	9.88	131.56	119.70
3	F	4	DC	O4'-C4'-C3'	-9.87	100.08	106.00
4	X	19	DC	O4'-C4'-C3'	-9.38	100.37	106.00
5	H	16	DG	O4'-C4'-C3'	-9.32	100.41	106.00
5	H	16	DG	C1'-O4'-C4'	-9.01	101.09	110.10
3	F	6	DT	N3-C4-O4	8.81	125.19	119.90
5	Y	16	DG	O4'-C4'-C3'	-8.68	100.79	106.00
5	Y	10	DT	O4'-C1'-N1	-8.63	101.96	108.00
5	H	14	DC	O4'-C4'-C3'	-8.46	100.92	106.00
4	G	9	DG	O4'-C1'-N9	8.22	113.75	108.00
5	H	9	DG	N3-C2-N2	-8.21	114.15	119.90
2	E	6	DG	C4'-C3'-C2'	-8.06	95.85	103.10
5	Y	9	DG	C4'-C3'-C2'	-8.03	95.87	103.10
5	Y	16	DG	C1'-O4'-C4'	-7.96	102.14	110.10
4	X	14	DC	O4'-C1'-N1	7.91	113.54	108.00
3	F	3	DC	O4'-C1'-N1	7.77	113.44	108.00
4	X	16	DC	O4'-C4'-C3'	-7.61	101.43	106.00
5	H	17	DC	C6-N1-C2	7.52	123.31	120.30
5	H	9	DG	C6-C5-N7	7.39	134.84	130.40
3	W	6	DT	N3-C2-O2	-7.37	117.88	122.30
4	X	16	DC	C1'-O4'-C4'	-7.36	102.74	110.10
5	Y	9	DG	C4-N9-C1'	-7.32	116.99	126.50
5	Y	13	DA	O4'-C1'-N9	7.04	112.92	108.00
5	H	10	DT	C5-C4-O4	-6.93	120.05	124.90
1	U	608	LEU	CA-CB-CG	6.83	131.01	115.30
4	G	16	DC	O4'-C4'-C3'	-6.78	101.79	104.50
5	Y	19	DC	O4'-C1'-N1	6.75	112.73	108.00
4	X	9	DG	O4'-C1'-N9	6.74	112.72	108.00
4	X	13	DC	N1-C2-O2	6.72	122.94	118.90
5	H	9	DG	C8-N9-C4	-6.71	103.72	106.40
4	X	18	DG	C1'-O4'-C4'	-6.63	103.47	110.10
5	H	16	DG	C8-N9-C4	6.55	109.02	106.40
4	X	19	DC	C4'-C3'-C2'	-6.54	97.21	103.10
5	H	19	DC	O4'-C1'-N1	6.53	112.57	108.00
5	H	9	DG	C4'-C3'-O3'	6.50	125.94	109.70
5	H	13	DA	C3'-C2'-C1'	-6.48	94.72	102.50
3	F	6	DT	O4'-C1'-C2'	-6.47	100.72	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	19	DC	C1'-O4'-C4'	-6.47	103.63	110.10
5	Y	9	DG	C8-N9-C1'	6.24	135.11	127.00
5	H	16	DG	O4'-C1'-N9	-6.22	103.65	108.00
4	X	16	DC	C6-N1-C2	6.22	122.79	120.30
5	H	18	DA	C3'-C2'-C1'	-6.19	95.07	102.50
4	G	10	DT	C1'-O4'-C4'	-6.18	103.92	110.10
4	G	13	DC	O4'-C1'-N1	6.15	112.31	108.00
5	Y	9	DG	C6-C5-N7	6.10	134.06	130.40
5	H	9	DG	C8-N9-C1'	6.07	134.88	127.00
5	H	9	DG	C4-C5-N7	-5.98	108.41	110.80
4	G	10	DT	O4'-C1'-N1	5.97	112.18	108.00
4	G	16	DC	C1'-O4'-C4'	-5.96	104.14	110.10
3	W	6	DT	N3-C4-O4	5.96	123.48	119.90
2	E	3	DT	C6-C5-C7	-5.96	119.32	122.90
1	D	418	LEU	CA-CB-CG	5.96	129.00	115.30
5	H	16	DG	N3-C4-C5	5.95	131.57	128.60
4	X	17	DG	C3'-C2'-C1'	-5.95	95.36	102.50
2	E	4	DG	P-O3'-C3'	5.90	126.78	119.70
4	X	16	DC	P-O3'-C3'	-5.89	112.63	119.70
2	V	5	DC	C3'-C2'-C1'	-5.84	95.49	102.50
1	S	1029	VAL	CB-CA-C	-5.84	100.31	111.40
5	H	17	DC	C1'-O4'-C4'	-5.83	104.27	110.10
2	E	3	DT	C4-C5-C7	5.77	122.46	119.00
5	H	10	DT	N3-C4-O4	5.77	123.36	119.90
5	Y	15	DC	N3-C4-C5	-5.75	119.60	121.90
2	V	5	DC	O4'-C4'-C3'	-5.69	102.22	104.50
4	G	17	DG	O4'-C1'-C2'	-5.63	101.40	105.90
5	Y	14	DC	O4'-C4'-C3'	-5.62	102.25	104.50
5	Y	18	DA	O4'-C1'-C2'	-5.57	101.44	105.90
4	X	14	DC	O4'-C4'-C3'	-5.56	102.28	104.50
5	H	12	DC	O4'-C4'-C3'	-5.52	102.29	104.50
5	Y	12	DC	C5-C6-N1	5.51	123.75	121.00
2	E	7	DG	C8-N9-C4	-5.50	104.20	106.40
4	X	12	DC	P-O3'-C3'	5.42	126.21	119.70
5	Y	10	DT	C5-C4-O4	-5.32	121.18	124.90
5	H	9	DG	N1-C2-N2	5.30	120.97	116.20
4	X	17	DG	O4'-C1'-C2'	-5.29	101.67	105.90
4	G	18	DG	C1'-O4'-C4'	-5.28	104.82	110.10
4	X	13	DC	N3-C2-O2	-5.28	118.21	121.90
5	H	18	DA	O4'-C1'-N9	-5.26	104.32	108.00
3	F	6	DT	C5-C4-O4	-5.25	121.22	124.90
4	G	18	DG	P-O5'-C5'	-5.24	112.52	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	18	DA	C1'-O4'-C4'	-5.24	104.86	110.10
3	W	8	DG	O4'-C1'-N9	-5.23	104.34	108.00
5	H	16	DG	N9-C4-C5	-5.23	103.31	105.40
4	G	17	DG	O4'-C1'-N9	-5.22	104.35	108.00
3	W	4	DC	C6-N1-C2	5.22	122.39	120.30
5	H	18	DA	O4'-C1'-C2'	-5.21	101.73	105.90
5	H	13	DA	O4'-C1'-N9	5.07	111.55	108.00
3	F	6	DT	C6-N1-C2	-5.06	118.77	121.30
2	V	8	DT	C5-C4-O4	-5.03	121.38	124.90
3	W	6	DT	N1-C2-O2	5.03	127.12	123.10
2	E	2	DG	O4'-C4'-C3'	-5.01	102.50	104.50
3	W	6	DT	O4'-C1'-C2'	-5.01	101.89	105.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5262	0	5259	446	0
1	D	5151	0	5043	443	0
1	S	5199	0	5178	502	0
1	U	5193	0	5163	464	0
2	E	147	0	80	8	0
2	V	147	0	80	8	0
3	F	145	0	79	14	0
3	W	123	0	68	8	0
4	G	220	0	124	27	0
4	X	220	0	124	35	0
5	H	240	0	135	38	0
5	Y	219	0	124	37	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	1	0	0	0	0
6	W	2	0	0	0	0
7	G	24	0	17	8	0
7	H	24	0	17	9	0
7	X	24	0	17	20	0
7	Y	24	0	17	10	0
All	All	22370	0	21525	1934	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 44.

All (1934) 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)
4:G:12:DC:N3	5:H:9:DG:N2	1.82	1.26
4:X:11:DA:N1	5:Y:10:DT:O4	1.78	1.15
5:H:11:DA:H2"	5:H:12:DC:C5'	1.86	1.06
1:U:1122:ARG:HH22	4:X:9:DG:H5"	1.18	1.06
1:D:1192:ILE:HD12	1:D:1477:ARG:HB2	1.39	1.05
1:U:1030:ILE:HG23	1:U:1035:LEU:HD12	1.39	1.04
4:X:9:DG:N2	5:Y:12:DC:O2	1.91	1.04
5:H:11:DA:C2'	5:H:12:DC:H5'	1.90	1.00
1:D:435:GLU:OE1	1:D:508:ASP:HB2	1.61	0.99
1:S:1277:ILE:HG12	1:S:1325:THR:HG21	1.45	0.99
1:S:1297:SER:HB2	1:S:1299:ARG:HH21	1.25	0.99
1:S:1309:ARG:HH11	1:S:1309:ARG:HG3	1.27	0.98
1:S:1256:ARG:HG2	1:S:1310:LYS:HB2	1.44	0.98
1:D:495:LEU:HD21	1:D:534:ALA:HB2	1.45	0.98
5:H:11:DA:H2"	5:H:12:DC:H5'	0.99	0.98
1:S:458:ARG:NH2	1:S:480:GLN:HE22	1.63	0.96
4:X:13:DC:H1'	7:X:1020:CPF:H161	1.44	0.96
1:S:1342:ARG:HG2	1:S:1342:ARG:HH21	1.30	0.96
1:S:1299:ARG:H	1:S:1299:ARG:HD2	1.31	0.95
1:U:1042:LEU:HD11	1:U:1160:LEU:HD12	1.47	0.94
1:B:458:ARG:HB2	7:G:1020:CPF:H162	1.50	0.94
1:U:434:VAL:HG22	1:U:456:PRO:HA	1.47	0.93
1:B:1296:THR:HG23	1:B:1301:GLY:O	1.69	0.93
1:U:1122:ARG:HH12	4:X:9:DG:H3'	1.32	0.92
1:B:1431:ARG:HG3	1:D:1426:LEU:O	1.69	0.92
1:S:620:MET:HE1	1:U:1019:ARG:HH12	1.34	0.91
1:B:1408:MET:HB3	1:B:1412:GLN:HE21	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1193:ASN:HA	1:S:1196:LEU:HD12	1.54	0.90
1:B:1256:ARG:HG2	1:B:1310:LYS:CB	2.02	0.90
1:S:1060:PRO:HG2	1:S:1133:LEU:HD11	1.55	0.89
1:U:1458:ILE:HA	1:U:1464:VAL:HG11	1.54	0.89
1:B:1371:LEU:HD11	1:B:1375:LYS:HE3	1.53	0.89
1:U:435:GLU:HG2	1:U:507:THR:HA	1.54	0.89
1:D:1027:MET:O	1:D:1031:VAL:HG22	1.71	0.89
1:B:585:GLU:O	1:D:1108:GLY:HA2	1.73	0.89
1:D:499:ARG:HH11	1:D:499:ARG:HG3	1.37	0.89
1:U:587:ASN:HB3	1:U:589:ASP:OD1	1.73	0.88
4:X:14:DC:H2"	4:X:15:DA:H5'	1.55	0.88
1:U:1122:ARG:NH2	4:X:9:DG:H5"	1.88	0.88
1:D:443:THR:HG22	1:D:454:ILE:HD11	1.56	0.88
3:F:8:DG:H5"	3:F:8:DG:H8	1.39	0.88
1:B:1095:GLN:HB2	1:B:1098:SER:HB2	1.54	0.87
1:D:636:ASN:HD22	1:D:636:ASN:N	1.72	0.87
1:S:1283:ASP:HB3	1:S:1285:LYS:HE3	1.56	0.87
1:D:454:ILE:HG22	1:D:456:PRO:HD3	1.57	0.87
1:D:437:ASP:CB	5:H:9:DG:H5"	2.05	0.87
1:S:1232:ARG:HG3	1:S:1232:ARG:HH11	1.38	0.87
1:D:1049:ILE:O	1:D:1053:LEU:HG	1.72	0.87
1:U:1361:THR:O	1:U:1365:ARG:HG3	1.75	0.87
1:B:1461:ASP:HB3	1:B:1464:VAL:HG23	1.57	0.87
5:H:19:DC:H2'	5:H:19:DC:OP2	1.75	0.87
1:U:475:ASN:O	1:U:479:ARG:HG3	1.75	0.87
3:W:7:DA:H2"	3:W:8:DG:H5"	1.55	0.86
1:D:434:VAL:HG12	1:D:506:MET:HE3	1.57	0.86
1:D:1030:ILE:CG2	1:D:1343:PRO:HG3	2.06	0.86
1:U:508:ASP:HB3	1:U:583:LEU:HD23	1.55	0.86
1:S:459:GLY:HA3	7:X:1020:CPF:H131	1.56	0.85
1:B:1153:ASN:O	1:B:1154:GLU:HG2	1.76	0.85
1:S:443:THR:HG22	1:S:454:ILE:HD11	1.57	0.85
1:U:1368:GLN:HG2	1:U:1459:LEU:HD11	1.58	0.85
1:S:1325:THR:HB	1:S:1326:PRO:HD2	1.59	0.85
1:U:493:PHE:HZ	1:U:531:LEU:HB2	1.39	0.85
1:U:435:GLU:CG	1:U:507:THR:HA	2.04	0.85
1:B:1049:ILE:HG21	1:B:1090:MET:HG3	1.56	0.85
4:G:12:DC:N4	5:H:9:DG:H22	1.74	0.85
1:S:1013:ASN:HB3	1:S:1016:SER:HB2	1.57	0.85
1:B:430:GLU:HB3	1:B:502:LYS:HB2	1.58	0.84
1:S:459:GLY:CA	7:X:1020:CPF:H131	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1363:VAL:HG13	1:B:1366:ARG:HH21	1.42	0.84
1:D:1049:ILE:HD13	1:D:1090:MET:HB2	1.58	0.83
1:B:1409:GLU:HA	1:B:1412:GLN:HG3	1.61	0.83
1:B:1222:GLY:O	1:B:1223:LEU:HD12	1.76	0.83
1:S:1232:ARG:HH11	1:S:1232:ARG:CG	1.92	0.83
1:B:435:GLU:HG3	1:B:508:ASP:OD1	1.77	0.83
1:S:1431:ARG:HG3	1:U:1426:LEU:HB3	1.60	0.83
4:X:13:DC:H1'	7:X:1020:CPF:C16	2.09	0.83
1:B:1230:ILE:HA	1:B:1241:ILE:HD11	1.58	0.82
4:X:9:DG:N1	5:Y:12:DC:N3	2.28	0.82
1:B:1066:LYS:HD3	1:B:1125:GLU:HG2	1.61	0.82
1:S:1309:ARG:HH11	1:S:1309:ARG:CG	1.92	0.82
1:U:1025:TYR:O	1:U:1029:VAL:HG23	1.78	0.82
1:S:1137:ARG:O	1:S:1138:ASP:HB2	1.76	0.82
1:S:1342:ARG:HH21	1:S:1342:ARG:CG	1.91	0.82
1:D:1064:TYR:HB3	1:D:1125:GLU:HB3	1.62	0.82
1:U:1192:ILE:HD12	1:U:1477:ARG:HB2	1.61	0.81
1:B:1071:VAL:HG13	1:B:1086:ILE:HG21	1.62	0.81
1:S:1295:GLU:HB2	1:S:1303:ARG:HG2	1.60	0.81
1:B:1425:ILE:O	1:D:1430:LEU:HD12	1.79	0.81
1:D:443:THR:HG23	1:D:596:MET:SD	2.20	0.81
1:U:461:ILE:HD11	1:U:477:GLU:HB3	1.61	0.81
1:U:522:THR:HA	1:U:618:PHE:CE2	2.15	0.81
1:B:1325:THR:HB	1:B:1326:PRO:HD2	1.60	0.81
1:D:493:PHE:CZ	1:D:495:LEU:HD13	2.16	0.81
1:D:458:ARG:HB2	7:H:1020:CPF:H172	1.59	0.81
1:D:1186:HIS:HB2	1:D:1191:LEU:HD11	1.60	0.81
3:F:8:DG:H5"	3:F:8:DG:C8	2.16	0.81
1:S:452:GLN:OE1	1:S:592:TRP:HZ3	1.63	0.81
1:S:1051:TYR:HH	1:S:1146:PHE:HE2	1.27	0.81
1:B:1138:ASP:HB3	1:B:1141:LYS:HD2	1.63	0.80
1:U:1054:ASN:HB2	1:U:1136:LEU:HD13	1.62	0.80
1:S:1342:ARG:HG2	1:S:1342:ARG:NH2	1.94	0.80
1:U:1450:ASN:HD22	1:U:1450:ASN:N	1.80	0.80
1:B:587:ASN:HB2	1:B:589:ASP:OD1	1.81	0.79
1:B:1245:SER:OG	1:B:1265:PRO:HD3	1.82	0.79
1:D:1030:ILE:HG21	1:D:1343:PRO:HG3	1.64	0.79
5:H:9:DG:H2'	5:H:10:DT:C5	2.17	0.79
1:U:458:ARG:HB3	7:Y:1020:CPF:H162	1.63	0.79
1:S:441:GLY:HA3	1:S:1109:ASN:HD21	1.48	0.79
4:X:12:DC:H42	5:Y:9:DG:H1	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1264:ILE:HG23	1:U:1302:VAL:HG11	1.64	0.79
1:B:606:VAL:HG11	1:B:1014:ILE:HD12	1.62	0.79
1:D:1319:ASN:HA	1:D:1322:TYR:HD2	1.47	0.79
1:S:1215:GLY:HA3	1:S:1488:ILE:HD11	1.63	0.79
1:S:1259:ILE:HD13	1:S:1318:LEU:HB2	1.64	0.79
4:X:9:DG:H5'	7:Y:1020:CPF:H1	1.65	0.79
1:D:1313:ASN:HD22	1:D:1316:VAL:HG23	1.46	0.79
4:G:10:DT:H2"	4:G:11:DA:C8	2.18	0.79
1:D:475:ASN:HD22	4:G:14:DC:H5'	1.46	0.79
1:U:1143:THR:HB	1:U:1362:VAL:HG13	1.64	0.79
1:D:1238:ARG:HG2	1:D:1334:ASN:HD22	1.48	0.78
1:B:1063:SER:O	1:B:1065:LYS:HE2	1.84	0.78
1:U:597:ASN:HD21	1:U:599:GLU:HG3	1.48	0.78
1:D:1231:ARG:HH11	1:D:1231:ARG:CG	1.95	0.78
1:S:1196:LEU:O	1:S:1200:LYS:HG3	1.83	0.78
4:G:9:DG:H5'	7:G:1020:CPF:H122	1.66	0.78
1:U:1105:ASP:HB3	1:U:1127:ARG:HG3	1.66	0.78
1:B:1244:ARG:HG2	1:B:1245:SER:H	1.49	0.78
1:D:1293:ARG:NH2	1:D:1305:VAL:HG11	1.99	0.78
1:S:1466:LEU:O	1:S:1466:LEU:HD12	1.84	0.78
1:D:508:ASP:HA	1:D:583:LEU:HD23	1.66	0.77
1:D:1414:ARG:HD2	1:D:1415:PHE:CE1	2.19	0.77
1:B:1064:TYR:HB3	1:B:1125:GLU:HB3	1.65	0.77
1:D:495:LEU:HD21	1:D:534:ALA:CB	2.13	0.77
1:D:1273:MET:O	1:D:1277:ILE:HG13	1.85	0.77
1:S:502:LYS:HA	1:S:538:TYR:HE1	1.50	0.77
1:D:1064:TYR:CE2	1:D:1107:GLN:HB2	2.19	0.77
1:D:1363:VAL:HG13	1:D:1366:ARG:NH2	1.99	0.77
1:S:1100:ARG:HD2	1:S:1485:ARG:NH1	1.99	0.77
1:D:1448:LEU:O	1:D:1452:ILE:HG13	1.85	0.77
5:Y:12:DC:H2'	7:Y:1020:CPF:H141	1.65	0.77
1:U:1064:TYR:HB3	1:U:1125:GLU:HB3	1.65	0.77
1:S:471:ARG:HG2	1:S:471:ARG:HH11	1.49	0.77
1:B:1039:ARG:HH21	1:B:1159:VAL:HB	1.49	0.76
1:D:485:PHE:HE1	1:D:503:ILE:HG12	1.50	0.76
1:D:1383:GLY:H	1:D:1421:GLN:HE21	1.32	0.76
1:U:461:ILE:HG21	1:U:520:LEU:HD23	1.67	0.76
1:B:1051:TYR:CE2	1:B:1157:PRO:HD3	2.20	0.76
1:U:529:ARG:HA	1:U:532:ILE:HD12	1.65	0.76
1:U:540:ALA:HA	1:U:603:LEU:HD23	1.67	0.76
1:B:434:VAL:HG21	1:B:440:GLY:CA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:VAL:HG13	1:B:1039:ARG:HG3	1.68	0.76
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.21	0.76
1:U:1191:LEU:O	1:U:1195:VAL:HG23	1.86	0.76
1:S:1241:ILE:HD12	1:S:1333:VAL:HG21	1.68	0.76
1:U:1165:PRO:HA	1:U:1355:TYR:CE2	2.20	0.76
1:D:587:ASN:HB2	1:D:590:GLN:HB3	1.67	0.75
1:D:1296:THR:OG1	1:D:1302:VAL:HA	1.86	0.75
1:S:629:ARG:O	1:S:633:ILE:HG13	1.86	0.75
1:B:1058:MET:HG2	1:B:1065:LYS:HE3	1.67	0.75
1:B:1225:LEU:HD11	1:B:1244:ARG:CZ	2.15	0.75
1:S:494:ASP:HB3	1:S:497:LYS:HB2	1.68	0.75
1:S:1448:LEU:O	1:S:1452:ILE:HG13	1.86	0.75
1:S:1468:LEU:O	1:S:1471:ASP:HB2	1.86	0.75
1:S:443:THR:HG22	1:S:454:ILE:CD1	2.15	0.75
1:S:1111:GLY:HA2	1:S:1116:ASP:HB2	1.67	0.75
1:B:1123:PHE:O	1:D:585:GLU:HB3	1.86	0.75
1:S:1042:LEU:HD22	1:S:1046:HIS:HB3	1.69	0.75
1:S:1192:ILE:O	1:S:1196:LEU:HG	1.86	0.74
1:U:1358:HIS:O	1:U:1362:VAL:HG23	1.87	0.74
1:S:1254:GLY:HA3	1:S:1256:ARG:HH12	1.50	0.74
1:U:427:GLU:HA	1:U:501:HIS:CD2	2.22	0.74
1:B:1288:GLY:HA2	1:B:1309:ARG:NH1	2.02	0.74
1:S:1025:TYR:HA	1:U:511:VAL:HB	1.69	0.74
1:U:1034:ALA:O	1:U:1043:LYS:HE2	1.87	0.74
1:U:1059:THR:HG22	1:U:1128:MET:HE3	1.70	0.74
1:S:1297:SER:HB2	1:S:1299:ARG:NH2	2.02	0.74
1:U:1218:PHE:HE2	1:U:1224:ILE:HD11	1.53	0.74
1:U:1377:ARG:HG2	1:U:1448:LEU:HD11	1.69	0.74
5:Y:18:DA:H2"	5:Y:19:DC:H5'	1.70	0.74
1:U:1182:ASN:O	1:U:1183:ILE:HG13	1.87	0.74
4:X:9:DG:N2	5:Y:12:DC:C2	2.51	0.74
1:B:1382:GLU:HG3	1:B:1445:TYR:HE2	1.52	0.74
1:B:469:LEU:HD12	1:B:472:ILE:HB	1.68	0.74
1:D:527:PHE:O	1:D:528:MET:HG2	1.88	0.74
1:B:433:LEU:HA	1:B:455:LEU:O	1.88	0.74
1:U:1265:PRO:HB2	1:U:1268:VAL:HG21	1.68	0.74
1:B:1031:VAL:HG23	1:B:1032:ALA:N	2.03	0.73
1:B:1219:PRO:HA	1:B:1485:ARG:HH11	1.52	0.73
1:B:1104:VAL:HG12	1:B:1105:ASP:H	1.53	0.73
5:H:10:DT:H2"	5:H:11:DA:N7	2.03	0.73
1:S:1306:ILE:O	1:S:1306:ILE:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1448:LEU:O	1:U:1452:ILE:HG13	1.89	0.73
1:B:1029:VAL:O	1:B:1033:ARG:HB3	1.89	0.73
1:U:461:ILE:HD11	1:U:477:GLU:CB	2.18	0.73
1:U:1138:ASP:HA	1:U:1141:LYS:HE3	1.71	0.73
1:D:540:ALA:HA	1:D:603:LEU:HD22	1.70	0.73
1:D:531:LEU:HD11	1:D:536:TYR:HB2	1.70	0.73
1:B:1030:ILE:HG23	1:B:1035:LEU:HD12	1.69	0.73
1:D:1279:GLU:O	1:D:1283:ASP:HB2	1.89	0.73
1:U:1245:SER:OG	1:U:1264:ILE:HA	1.89	0.73
1:S:1350:GLU:O	1:S:1354:HIS:HD2	1.72	0.73
1:S:1408:MET:O	1:S:1412:GLN:HG3	1.87	0.73
1:B:1192:ILE:HD13	1:B:1477:ARG:HB2	1.69	0.72
1:U:522:THR:HA	1:U:618:PHE:HE2	1.52	0.72
1:U:1299:ARG:H	1:U:1299:ARG:HD2	1.54	0.72
1:D:636:ASN:HD22	1:D:636:ASN:H	1.38	0.72
1:S:1204:ILE:HG13	1:S:1205:SER:H	1.53	0.72
1:S:1484:ARG:HG2	1:S:1486:THR:O	1.89	0.72
1:B:508:ASP:OD1	1:B:508:ASP:N	2.22	0.72
1:B:1046:HIS:HA	1:B:1049:ILE:HD12	1.71	0.72
1:B:1448:LEU:O	1:B:1452:ILE:HG13	1.90	0.72
1:D:430:GLU:HB2	1:D:502:LYS:O	1.90	0.72
1:S:1387:ALA:HA	1:S:1394:ILE:HG13	1.72	0.72
1:D:1259:ILE:HB	1:D:1306:ILE:HB	1.72	0.72
4:X:13:DC:N4	4:X:14:DC:C4	2.57	0.72
1:S:1079:HIS:NE2	1:S:1081:HIS:HD2	1.88	0.72
4:G:12:DC:N4	5:H:9:DG:N2	2.38	0.71
1:S:1184:PRO:HB2	1:S:1216:PRO:HB3	1.72	0.71
1:D:1184:PRO:HB2	1:D:1216:PRO:HB3	1.71	0.71
1:S:1071:VAL:HG12	1:S:1075:MET:HE2	1.71	0.71
1:S:1381:LEU:HD11	1:S:1444:GLU:OE2	1.90	0.71
1:U:1120:ALA:HB3	1:U:1123:PHE:CD1	2.24	0.71
1:U:1245:SER:OG	1:U:1265:PRO:HD3	1.90	0.71
1:U:1031:VAL:HA	1:U:1338:LEU:HD11	1.72	0.71
1:U:1206:ILE:O	1:U:1210:MET:HG3	1.89	0.71
1:D:543:PRO:HG3	1:D:594:THR:HB	1.72	0.71
1:D:1192:ILE:HD12	1:D:1477:ARG:CB	2.19	0.71
1:D:1468:LEU:O	1:D:1472:GLU:HG3	1.91	0.71
1:B:1381:LEU:HD13	1:B:1445:TYR:HA	1.71	0.71
1:S:1293:ARG:CZ	1:S:1293:ARG:HB2	2.21	0.71
1:U:1208:GLU:HA	1:U:1211:GLU:OE1	1.89	0.71
1:B:1071:VAL:HG13	1:B:1086:ILE:CG2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1408:MET:HB3	1:B:1412:GLN:NE2	2.04	0.71
1:B:1416:LYS:HA	1:B:1416:LYS:HE2	1.73	0.71
1:B:1431:ARG:HH11	1:D:1423:GLN:CD	1.94	0.71
1:B:586:MET:HB3	1:B:590:GLN:HB3	1.71	0.71
1:S:1221:ALA:HB1	1:S:1485:ARG:O	1.90	0.71
1:B:459:GLY:HA2	2:E:8:DT:H2"	1.73	0.70
1:S:1233:ALA:HB1	1:S:1333:VAL:HG11	1.72	0.70
1:S:1286:ILE:HD12	1:S:1324:GLN:NE2	2.06	0.70
1:U:1135:LEU:HA	1:U:1162:ALA:HA	1.73	0.70
1:D:1242:GLN:NE2	1:D:1330:SER:HB3	2.05	0.70
1:S:1036:PRO:HA	1:S:1042:LEU:O	1.91	0.70
1:S:1289:ILE:HG23	1:S:1306:ILE:HG23	1.74	0.70
1:B:1431:ARG:NH1	1:D:1423:GLN:HE22	1.90	0.70
1:U:1136:LEU:HD23	1:U:1160:LEU:HD22	1.72	0.70
1:U:1292:LEU:HD12	1:U:1293:ARG:H	1.54	0.70
1:B:447:ARG:HD3	1:B:454:ILE:HD12	1.73	0.70
4:G:12:DC:H42	5:H:9:DG:N2	1.90	0.70
1:S:432:PHE:O	1:S:434:VAL:HG13	1.92	0.70
1:S:540:ALA:O	1:S:541:GLN:HG3	1.92	0.70
1:U:1186:HIS:HE2	1:U:1234:TYR:HE1	1.37	0.70
1:B:1104:VAL:HG12	1:B:1105:ASP:N	2.06	0.70
1:U:531:LEU:CD1	1:U:536:TYR:HB2	2.21	0.70
1:B:1238:ARG:HH11	1:B:1334:ASN:ND2	1.90	0.70
1:D:461:ILE:HG22	1:D:462:LEU:H	1.54	0.70
1:S:1026:ALA:O	1:S:1030:ILE:HG13	1.92	0.70
1:D:508:ASP:CG	1:D:583:LEU:HB2	2.13	0.69
1:D:1204:ILE:H	1:D:1349:LYS:NZ	1.90	0.69
1:D:535:GLY:C	1:D:536:TYR:HD2	1.95	0.69
4:G:11:DA:H2"	4:G:12:DC:H5'	1.73	0.69
1:S:1185:PRO:HD2	1:S:1218:PHE:CE1	2.27	0.69
1:S:1249:ILE:HD11	1:S:1318:LEU:HD23	1.72	0.69
4:G:12:DC:C4	5:H:9:DG:N2	2.41	0.69
1:S:423:SER:HB3	1:S:450:ARG:O	1.93	0.69
1:U:1080:PRO:HD2	1:U:1081:HIS:CD2	2.28	0.69
1:B:1431:ARG:NH1	1:D:1423:GLN:NE2	2.40	0.69
1:D:512:ASP:O	1:D:516:ILE:HG13	1.93	0.69
1:S:1026:ALA:HB1	1:U:633:ILE:HD11	1.75	0.69
1:S:1039:ARG:HH21	1:S:1159:VAL:HB	1.58	0.68
1:D:1029:VAL:HG11	1:D:1177:VAL:HG23	1.75	0.68
1:S:1179:MET:O	5:Y:17:DC:H4'	1.93	0.68
1:U:494:ASP:OD1	1:U:497:LYS:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1408:MET:C	1:S:1412:GLN:HE21	1.96	0.68
1:B:469:LEU:HD13	1:B:472:ILE:HD12	1.75	0.68
1:D:587:ASN:HB2	1:D:590:GLN:CB	2.24	0.68
1:S:517:ARG:NH2	1:U:1021:SER:OG	2.26	0.68
1:S:1079:HIS:CE1	1:S:1081:HIS:HD2	2.11	0.68
1:U:464:VAL:O	1:U:472:ILE:HD11	1.93	0.68
1:U:487:THR:HG22	1:U:498:ALA:HB2	1.76	0.68
1:U:1093:MET:HG2	1:U:1099:TYR:CZ	2.29	0.68
1:S:1241:ILE:HD12	1:S:1333:VAL:CG2	2.24	0.68
1:B:1107:GLN:H	1:B:1110:PHE:HE1	1.41	0.68
1:S:1064:TYR:HE1	1:S:1127:ARG:CZ	2.07	0.68
1:S:1347:ASN:OD1	1:S:1347:ASN:N	2.24	0.67
1:B:1451:TYR:CE2	1:B:1455:LEU:HD11	2.28	0.67
1:U:1355:TYR:O	1:U:1359:GLN:HG2	1.94	0.67
1:D:1031:VAL:HA	1:D:1338:LEU:HD11	1.76	0.67
1:U:1222:GLY:N	1:U:1263:GLU:OE2	2.28	0.67
1:U:1458:ILE:HA	1:U:1464:VAL:CG1	2.24	0.67
1:B:1038:VAL:HG12	1:B:1338:LEU:O	1.95	0.67
1:D:1136:LEU:HD23	1:D:1160:LEU:HD22	1.77	0.67
1:U:1346:ILE:HD12	1:U:1351:ALA:HA	1.76	0.67
1:B:464:VAL:HG22	1:B:522:THR:CG2	2.25	0.67
1:D:626:VAL:HG11	4:G:17:DG:H3'	1.76	0.67
1:S:1100:ARG:HH11	1:S:1100:ARG:HG3	1.60	0.67
1:S:587:ASN:HB2	1:S:590:GLN:HB2	1.75	0.67
1:B:447:ARG:HA	1:B:596:MET:HE1	1.77	0.67
1:B:636:ASN:O	1:B:637:ALA:O	2.13	0.67
2:E:3:DT:H3	5:H:18:DA:H61	1.42	0.67
1:S:1185:PRO:HD2	1:S:1218:PHE:CD1	2.30	0.67
1:S:1383:GLY:HA3	1:S:1421:GLN:HG2	1.77	0.67
1:B:1109:ASN:HB3	1:B:1119:ALA:HB2	1.77	0.67
1:B:1390:HIS:ND1	1:B:1390:HIS:N	2.43	0.67
5:Y:13:DA:N3	7:Y:1020:CPF:H161	2.09	0.67
1:D:535:GLY:HA2	1:D:605:GLN:OE1	1.94	0.66
1:S:1299:ARG:H	1:S:1299:ARG:CD	2.02	0.66
1:U:421:CYS:H	1:U:453:ALA:HB2	1.60	0.66
1:D:586:MET:HE2	1:D:590:GLN:HG3	1.77	0.66
1:S:1254:GLY:HA3	1:S:1256:ARG:NH1	2.11	0.66
1:S:1320:ASN:O	1:S:1324:GLN:HG3	1.95	0.66
1:D:1110:PHE:HE1	1:D:1124:THR:HB	1.61	0.66
1:D:1313:ASN:ND2	1:D:1316:VAL:HG23	2.10	0.66
1:S:1259:ILE:CD1	1:S:1318:LEU:HB2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1188:LEU:O	1:S:1192:ILE:HG13	1.95	0.66
1:U:425:SER:OG	1:U:428:GLU:HG2	1.95	0.66
1:U:434:VAL:HG23	1:U:436:GLY:H	1.59	0.66
1:S:540:ALA:HA	1:S:603:LEU:HD22	1.77	0.66
1:U:586:MET:HB2	1:U:591:LEU:CD1	2.25	0.66
1:B:1104:VAL:O	1:B:1129:THR:HG23	1.95	0.66
1:S:1101:TYR:HB3	1:S:1131:ILE:HD13	1.77	0.66
1:S:1232:ARG:HG3	1:S:1232:ARG:NH1	2.04	0.66
1:B:1286:ILE:HD12	1:B:1324:GLN:NE2	2.11	0.66
1:B:1430:LEU:O	1:B:1433:LEU:HG	1.96	0.66
1:D:419:ALA:HB1	1:D:447:ARG:HH12	1.61	0.66
1:D:1277:ILE:O	1:D:1281:VAL:HG23	1.96	0.66
1:D:1415:PHE:HB2	1:D:1417:LEU:HG	1.77	0.66
1:S:1466:LEU:HD21	1:S:1470:ARG:HH21	1.61	0.66
1:B:461:ILE:HG22	1:B:462:LEU:H	1.59	0.65
1:D:1383:GLY:HA3	1:D:1421:GLN:HG2	1.78	0.65
1:S:1050:LEU:N	1:S:1050:LEU:HD23	2.10	0.65
1:D:586:MET:CE	1:D:590:GLN:HG3	2.26	0.65
1:D:1267:GLN:OE1	3:F:4:DC:H4'	1.96	0.65
1:S:1187:ASN:O	1:S:1191:LEU:HG	1.95	0.65
1:U:1100:ARG:HH12	1:U:1485:ARG:NE	1.95	0.65
1:D:508:ASP:OD1	1:D:583:LEU:HB2	1.97	0.65
1:S:461:ILE:HD11	1:S:477:GLU:HB2	1.78	0.65
1:S:583:LEU:O	1:S:585:GLU:N	2.29	0.65
1:U:1265:PRO:HB2	1:U:1268:VAL:CG2	2.26	0.65
4:X:18:DG:H2"	4:X:19:DC:C6	2.31	0.65
1:B:1325:THR:HB	1:B:1326:PRO:CD	2.25	0.65
1:U:1261:VAL:HG23	1:U:1304:VAL:O	1.95	0.65
1:S:1051:TYR:OH	1:S:1146:PHE:HE2	1.79	0.65
1:S:1256:ARG:CG	1:S:1310:LYS:HB2	2.23	0.65
1:D:1280:LEU:HB3	1:D:1286:ILE:HG22	1.77	0.65
1:D:1395:ILE:O	1:D:1399:ARG:HG3	1.96	0.65
1:B:1346:ILE:HD12	1:B:1351:ALA:HA	1.78	0.65
1:D:433:LEU:HD23	1:D:455:LEU:HB3	1.78	0.65
1:D:1313:ASN:HD22	1:D:1316:VAL:H	1.44	0.65
1:B:1273:MET:HG3	1:B:1326:PRO:HB2	1.78	0.65
1:D:430:GLU:CB	1:D:502:LYS:O	2.45	0.65
1:D:1132:THR:O	1:D:1135:LEU:HB2	1.97	0.65
1:U:461:ILE:HG21	1:U:520:LEU:CD2	2.26	0.65
1:U:1243:MET:SD	1:U:1266:PHE:HB3	2.37	0.65
1:U:1421:GLN:O	1:U:1425:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:13:DA:C2	7:Y:1020:CPF:H161	2.31	0.65
1:B:1411:LEU:O	1:B:1415:PHE:HB2	1.97	0.65
1:S:1426:LEU:HB3	1:U:1431:ARG:HB3	1.79	0.65
1:B:1218:PHE:HB3	1:B:1266:PHE:HB2	1.79	0.65
1:B:1361:THR:O	1:B:1365:ARG:HG3	1.97	0.65
1:B:1381:LEU:HD12	1:B:1448:LEU:HD12	1.77	0.65
1:D:1031:VAL:HG12	1:D:1338:LEU:HD21	1.79	0.65
5:Y:11:DA:H2"	5:Y:12:DC:OP2	1.96	0.65
1:B:597:ASN:HD22	1:B:598:PRO:HD2	1.61	0.64
1:S:531:LEU:O	1:S:536:TYR:HB2	1.96	0.64
1:S:1179:MET:O	1:S:1180:ALA:HB2	1.97	0.64
1:U:534:ALA:HB1	1:U:536:TYR:CE2	2.32	0.64
1:B:1183:ILE:HG12	1:B:1335:MET:HG2	1.79	0.64
1:B:1274:ILE:HD13	1:B:1294:ASP:HB2	1.79	0.64
1:B:1292:LEU:HG	1:B:1292:LEU:O	1.97	0.64
1:D:1050:LEU:N	1:D:1050:LEU:HD23	2.11	0.64
1:S:1067:SER:OG	1:S:1124:THR:O	2.13	0.64
1:U:1153:ASN:C	1:U:1154:GLU:HG2	2.18	0.64
1:D:541:GLN:HE21	1:D:541:GLN:HA	1.61	0.64
2:E:4:DG:N2	5:H:18:DA:C2	2.65	0.64
1:S:525:TYR:HE2	1:S:526:ARG:NH1	1.96	0.64
1:S:529:ARG:O	1:S:533:GLU:HG3	1.98	0.64
1:U:427:GLU:HA	1:U:501:HIS:CG	2.32	0.64
1:D:1329:THR:HG22	1:D:1330:SER:H	1.62	0.64
1:D:1400:GLU:HG3	1:D:1400:GLU:O	1.95	0.64
1:S:1218:PHE:CG	1:S:1266:PHE:HB2	2.32	0.64
1:B:1346:ILE:HD12	1:B:1351:ALA:CA	2.28	0.64
1:D:493:PHE:HZ	1:D:495:LEU:HD13	1.62	0.64
1:B:1386:ILE:HG22	1:B:1387:ALA:N	2.11	0.64
1:U:632:PHE:HD1	1:U:636:ASN:ND2	1.96	0.64
1:B:540:ALA:HA	1:B:603:LEU:HD22	1.79	0.64
1:B:1029:VAL:HA	1:B:1033:ARG:CB	2.28	0.64
1:U:632:PHE:O	1:U:636:ASN:HB2	1.98	0.64
1:D:633:ILE:HG22	1:D:634:GLU:N	2.13	0.64
1:S:1245:SER:OG	1:S:1327:LEU:HD12	1.98	0.64
1:U:597:ASN:ND2	1:U:599:GLU:HG3	2.12	0.64
1:D:604:LEU:HD22	1:D:1012:ARG:HB2	1.80	0.64
1:S:1309:ARG:HG3	1:S:1309:ARG:NH1	2.05	0.64
1:B:1247:ALA:HA	1:B:1260:VAL:O	1.97	0.63
1:U:531:LEU:HD12	1:U:531:LEU:O	1.98	0.63
1:B:629:ARG:O	1:B:633:ILE:HG13	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1030:ILE:HG22	1:D:1031:VAL:HG13	1.81	0.63
1:S:525:TYR:CE2	1:S:526:ARG:NH1	2.66	0.63
1:S:1452:ILE:O	1:S:1456:GLU:HG3	1.96	0.63
1:B:434:VAL:HG21	1:B:440:GLY:HA2	1.80	0.63
1:D:1231:ARG:HH11	1:D:1231:ARG:HG2	1.61	0.63
1:S:1025:TYR:CE2	1:U:515:HIS:CD2	2.86	0.63
1:S:1428:MET:HG3	1:S:1432:ARG:HG3	1.79	0.63
1:B:1215:GLY:HA2	1:B:1234:TYR:OH	1.99	0.63
1:D:1224:ILE:HD12	1:D:1486:THR:HG21	1.79	0.63
1:B:619:GLU:O	1:B:623:GLY:N	2.31	0.63
1:B:1247:ALA:HB2	1:B:1261:VAL:HG22	1.81	0.63
1:D:458:ARG:HD3	7:H:1020:CPF:H162	1.79	0.63
1:D:1440:LYS:O	1:D:1443:ALA:HB3	1.99	0.63
1:U:583:LEU:HD13	1:U:591:LEU:HD11	1.79	0.63
1:U:1335:MET:O	1:U:1345:LEU:HD12	1.98	0.63
1:B:430:GLU:CB	1:B:502:LYS:HB2	2.28	0.63
1:S:1130:LYS:HA	1:S:1133:LEU:HD12	1.81	0.63
1:S:1423:GLN:HA	1:S:1426:LEU:HD12	1.79	0.63
1:U:485:PHE:CE2	1:U:524:PHE:HE2	2.17	0.63
1:B:629:ARG:HB2	1:B:629:ARG:HH11	1.64	0.63
1:D:493:PHE:HE2	1:D:530:PRO:HB2	1.62	0.63
1:S:461:ILE:HD12	1:S:462:LEU:H	1.64	0.63
1:U:1042:LEU:CD1	1:U:1160:LEU:HD12	2.23	0.63
1:U:1059:THR:HA	1:U:1128:MET:HE3	1.80	0.63
1:B:1380:ILE:HD12	1:B:1424:ALA:HB2	1.80	0.63
1:D:636:ASN:N	1:D:636:ASN:ND2	2.42	0.63
1:S:1258:ARG:HB3	1:S:1307:ASP:HA	1.80	0.63
1:B:1413:GLN:HG2	1:B:1414:ARG:N	2.13	0.62
1:D:450:ARG:CZ	1:D:450:ARG:HB2	2.29	0.62
1:D:633:ILE:HD11	1:D:1026:ALA:HB1	1.80	0.62
1:D:1297:SER:C	1:D:1299:ARG:H	2.01	0.62
1:U:530:PRO:HA	1:U:533:GLU:HG3	1.81	0.62
1:B:478:ILE:HG23	1:B:523:PHE:CZ	2.34	0.62
1:B:1175:ILE:HD13	5:H:17:DC:N3	2.13	0.62
1:U:462:LEU:HG	1:U:463:ASN:N	2.12	0.62
1:U:485:PHE:HE2	1:U:524:PHE:HE2	1.46	0.62
1:B:1069:ARG:HG2	1:D:1072:GLY:O	2.00	0.62
1:D:541:GLN:HB2	1:D:602:ALA:HB3	1.79	0.62
1:D:1079:HIS:NE2	1:D:1081:HIS:HD2	1.96	0.62
1:U:586:MET:HB2	1:U:591:LEU:HD13	1.81	0.62
1:B:443:THR:HG22	1:B:454:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1466:LEU:HD12	1:B:1466:LEU:O	1.98	0.62
3:F:8:DG:H8	3:F:8:DG:C5'	2.10	0.62
1:U:531:LEU:HD11	1:U:536:TYR:HB2	1.81	0.62
1:B:606:VAL:HG13	1:B:1014:ILE:HB	1.82	0.62
1:B:1292:LEU:HD13	1:B:1306:ILE:HG12	1.80	0.62
1:S:1045:VAL:O	1:S:1049:ILE:HG13	1.99	0.62
1:D:434:VAL:CG1	1:D:506:MET:HE3	2.27	0.62
1:D:1231:ARG:HG2	1:D:1231:ARG:NH1	2.15	0.62
1:D:1391:ILE:HG23	1:D:1392:ASP:N	2.14	0.62
1:B:476:ASN:ND2	1:B:480:GLN:HG3	2.14	0.62
1:B:1066:LYS:HD3	1:B:1125:GLU:CG	2.30	0.62
1:S:621:LEU:O	1:S:629:ARG:HD3	2.00	0.62
1:U:435:GLU:HG3	1:U:507:THR:HA	1.80	0.62
1:U:1059:THR:HA	1:U:1128:MET:CE	2.29	0.62
1:S:1408:MET:SD	1:S:1426:LEU:HD11	2.39	0.62
1:U:508:ASP:CB	1:U:583:LEU:HD23	2.29	0.62
1:S:1314:ALA:HA	1:S:1317:ILE:HD12	1.80	0.62
1:U:522:THR:CA	1:U:618:PHE:HE2	2.13	0.62
1:U:535:GLY:O	1:U:605:GLN:OE1	2.17	0.62
1:B:514:ALA:O	1:B:518:THR:HG23	2.00	0.62
1:B:1225:LEU:HD11	1:B:1244:ARG:NE	2.14	0.62
1:B:1029:VAL:HG13	1:B:1033:ARG:HD2	1.82	0.61
1:S:418:LEU:HG	1:S:418:LEU:O	2.00	0.61
1:U:1367:THR:HG21	1:U:1459:LEU:HD23	1.82	0.61
1:B:1409:GLU:CA	1:B:1412:GLN:HG3	2.30	0.61
1:B:1415:PHE:HB3	1:B:1417:LEU:HG	1.80	0.61
1:D:499:ARG:HG3	1:D:499:ARG:NH1	2.13	0.61
1:S:1191:LEU:O	1:S:1194:GLY:N	2.33	0.61
1:U:592:TRP:CD1	1:U:593:GLU:N	2.68	0.61
1:B:528:MET:O	1:B:531:LEU:HB3	2.00	0.61
1:B:1244:ARG:HG2	1:B:1245:SER:N	2.15	0.61
1:S:1177:VAL:O	1:S:1179:MET:N	2.32	0.61
1:S:1215:GLY:O	1:S:1217:ASP:N	2.34	0.61
1:U:493:PHE:CZ	1:U:531:LEU:HB2	2.29	0.61
1:B:431:ILE:HG22	1:B:503:ILE:HA	1.83	0.61
1:B:1290:THR:O	1:B:1291:ASP:HB2	2.00	0.61
1:S:1382:GLU:CG	1:S:1445:TYR:HE1	2.13	0.61
1:U:443:THR:HG23	1:U:596:MET:SD	2.40	0.61
1:B:1384:LEU:HD22	1:B:1428:MET:SD	2.40	0.61
1:D:1414:ARG:HD2	1:D:1415:PHE:CZ	2.35	0.61
1:S:1461:ASP:HB3	1:S:1464:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1109:ASN:HB3	1:U:1119:ALA:HB2	1.81	0.61
1:S:1204:ILE:HG13	1:S:1205:SER:N	2.15	0.61
1:S:1329:THR:HG22	1:S:1330:SER:H	1.65	0.61
1:D:1381:LEU:O	1:D:1385:ARG:HG3	2.01	0.61
1:S:519:LEU:HD23	1:S:622:MET:CE	2.30	0.61
1:B:1408:MET:O	1:B:1412:GLN:HG2	2.01	0.61
1:U:1067:SER:HB2	1:U:1121:MET:O	2.00	0.61
1:B:1431:ARG:HH12	1:D:1423:GLN:HE22	1.46	0.61
1:S:1344:LYS:NZ	1:S:1350:GLU:OE1	2.33	0.61
1:D:539:ILE:O	1:D:539:ILE:HG22	2.01	0.61
1:S:458:ARG:HH22	1:S:480:GLN:HE22	1.46	0.61
4:X:11:DA:C6	5:Y:10:DT:O4	2.53	0.61
1:B:1031:VAL:HG23	1:B:1032:ALA:H	1.64	0.60
1:B:1223:LEU:HD11	1:B:1246:ARG:CZ	2.31	0.60
1:D:1357:GLU:OE1	1:D:1357:GLU:HA	2.00	0.60
1:S:1398:ILE:HD11	1:S:1411:LEU:HD11	1.83	0.60
1:B:511:VAL:HB	1:B:1025:TYR:HA	1.83	0.60
1:B:1245:SER:OG	1:B:1264:ILE:HA	2.01	0.60
1:D:1292:LEU:CD1	1:D:1306:ILE:HG12	2.31	0.60
1:S:620:MET:CE	1:U:1019:ARG:HH12	2.12	0.60
1:S:1071:VAL:HG13	1:S:1086:ILE:HD12	1.83	0.60
1:S:1255:GLY:HA3	1:S:1310:LYS:HE3	1.82	0.60
1:S:1399:ARG:CZ	1:U:1391:ILE:HG21	2.31	0.60
1:B:1387:ALA:HB2	1:B:1425:ILE:HD13	1.83	0.60
1:S:461:ILE:HD11	1:S:477:GLU:CB	2.32	0.60
1:S:1286:ILE:HD12	1:S:1324:GLN:HE22	1.66	0.60
1:U:420:ASP:HA	1:U:453:ALA:HB1	1.82	0.60
1:D:478:ILE:O	1:D:482:ILE:HG13	2.01	0.60
1:D:1196:LEU:O	1:D:1199:SER:OG	2.16	0.60
1:S:589:ASP:CG	1:S:590:GLN:N	2.54	0.60
1:U:632:PHE:CD1	1:U:636:ASN:ND2	2.70	0.60
1:B:1153:ASN:C	1:B:1154:GLU:HG2	2.21	0.60
1:D:522:THR:HA	1:D:618:PHE:CE2	2.36	0.60
4:G:13:DC:O2	7:H:1020:CPF:H161	2.02	0.60
1:B:1259:ILE:HD13	1:B:1318:LEU:HB2	1.84	0.60
1:S:458:ARG:HD2	7:X:1020:CPF:H162	1.83	0.60
1:U:435:GLU:HG3	1:U:508:ASP:H	1.67	0.60
1:B:1219:PRO:HA	1:B:1485:ARG:NH1	2.16	0.60
1:B:1454:GLU:O	1:B:1457:THR:HB	2.02	0.60
1:U:1059:THR:HG22	1:U:1128:MET:CE	2.32	0.60
1:U:1064:TYR:CB	1:U:1125:GLU:HB3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.32	0.60
1:S:1162:ALA:C	1:S:1164:PHE:H	2.03	0.60
1:S:1258:ARG:HD2	1:S:1305:VAL:CG1	2.32	0.60
1:U:1112:SER:OG	1:U:1116:ASP:OD1	2.19	0.60
1:B:1030:ILE:HG21	1:B:1343:PRO:HG3	1.84	0.59
1:B:1245:SER:HB3	1:B:1263:GLU:O	2.02	0.59
1:D:1049:ILE:HG22	1:D:1050:LEU:HD23	1.82	0.59
3:F:6:DT:C2	3:F:7:DA:C8	2.90	0.59
1:S:532:ILE:HD13	1:U:1014:ILE:HD12	1.83	0.59
1:S:1177:VAL:HG12	1:S:1178:GLY:N	2.17	0.59
1:B:514:ALA:HA	1:B:517:ARG:NH2	2.17	0.59
1:D:538:TYR:HA	1:D:604:LEU:O	2.03	0.59
1:D:1049:ILE:C	1:D:1050:LEU:HD23	2.22	0.59
1:U:511:VAL:O	1:U:514:ALA:HB3	2.02	0.59
1:D:435:GLU:HG3	1:D:516:ILE:HD12	1.83	0.59
1:D:1213:ILE:HG22	1:D:1213:ILE:O	2.02	0.59
1:S:1100:ARG:HA	1:S:1219:PRO:HB3	1.83	0.59
1:S:1029:VAL:O	1:S:1029:VAL:HG12	2.02	0.59
1:B:464:VAL:HG22	1:B:522:THR:HG23	1.84	0.59
1:B:1046:HIS:O	1:B:1047:ARG:C	2.40	0.59
1:S:1484:ARG:CG	1:S:1486:THR:O	2.49	0.59
4:X:11:DA:N1	5:Y:10:DT:C4	2.66	0.59
1:B:469:LEU:CD1	1:B:472:ILE:HD12	2.32	0.59
1:D:475:ASN:ND2	4:G:14:DC:H5'	2.18	0.59
1:D:1051:TYR:O	1:D:1054:ASN:HB3	2.03	0.59
1:D:1133:LEU:O	1:D:1137:ARG:N	2.35	0.59
1:S:1403:THR:HG22	1:U:1436:LEU:HD12	1.84	0.59
1:U:1218:PHE:HD1	1:U:1266:PHE:CD2	2.20	0.59
4:G:10:DT:H2"	4:G:11:DA:N7	2.17	0.59
1:S:1368:GLN:O	1:S:1372:ARG:NH1	2.36	0.59
1:S:1403:THR:HG22	1:U:1436:LEU:CD1	2.32	0.59
1:U:1364:ARG:O	1:U:1367:THR:HB	2.02	0.59
3:W:8:DG:H5'	3:W:8:DG:C8	2.38	0.59
4:X:12:DC:C2	7:X:1020:CPF:H141	2.37	0.59
1:D:1092:ARG:C	1:D:1094:ALA:H	2.04	0.59
1:U:462:LEU:HA	5:Y:14:DC:O3'	2.03	0.59
1:U:1182:ASN:C	1:U:1183:ILE:HG13	2.23	0.59
1:S:1177:VAL:C	1:S:1179:MET:H	2.05	0.58
1:U:1087:TYR:O	1:U:1091:VAL:HB	2.03	0.58
1:B:1224:ILE:HA	1:B:1242:GLN:O	2.02	0.58
1:S:1067:SER:HB2	1:S:1121:MET:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1183:ILE:HG12	1:U:1335:MET:HG2	1.83	0.58
3:W:8:DG:C4	7:X:1020:CPF:H132	2.38	0.58
1:D:1185:PRO:O	1:D:1217:ASP:N	2.34	0.58
1:U:458:ARG:HH11	7:Y:1020:CPF:H152	1.68	0.58
1:U:1064:TYR:CD1	1:U:1127:ARG:HG2	2.38	0.58
1:B:597:ASN:O	1:B:601:ARG:HB3	2.02	0.58
1:S:587:ASN:HB2	1:S:590:GLN:CB	2.34	0.58
1:D:432:PHE:CD2	1:D:504:VAL:HB	2.39	0.58
1:D:1064:TYR:CD1	1:D:1127:ARG:HG2	2.37	0.58
1:U:1157:PRO:C	1:U:1159:VAL:H	2.07	0.58
1:B:447:ARG:CD	1:B:454:ILE:HD12	2.33	0.58
1:S:1042:LEU:HD22	1:S:1046:HIS:CB	2.33	0.58
1:S:1064:TYR:HE1	1:S:1127:ARG:NE	2.00	0.58
1:S:1185:PRO:HD3	1:S:1266:PHE:CE2	2.38	0.58
1:U:444:LYS:NZ	1:U:454:ILE:HD12	2.19	0.58
1:U:1190:GLU:O	1:U:1213:ILE:HG13	2.04	0.58
1:U:1296:THR:HG23	1:U:1301:GLY:C	2.24	0.58
1:B:1051:TYR:CD2	1:B:1157:PRO:HD3	2.38	0.58
1:U:1049:ILE:HD13	1:U:1090:MET:HB2	1.86	0.58
1:B:463:ASN:OD1	1:B:465:GLU:HB3	2.04	0.58
1:B:525:TYR:O	1:B:529:ARG:HB2	2.04	0.58
1:B:1029:VAL:C	1:B:1033:ARG:HB3	2.24	0.58
1:B:1149:ASN:ND2	1:B:1154:GLU:HB2	2.19	0.58
1:D:443:THR:CG2	1:D:596:MET:SD	2.91	0.58
1:S:445:SER:O	1:S:588:ALA:HB1	2.04	0.58
1:B:1051:TYR:CZ	1:B:1157:PRO:HD3	2.39	0.58
1:B:1363:VAL:CG1	1:B:1468:LEU:HD23	2.34	0.58
1:D:1012:ARG:NH1	1:D:1016:SER:HB3	2.19	0.58
1:S:602:ALA:O	1:S:603:LEU:HD23	2.04	0.58
1:S:1060:PRO:O	1:S:1127:ARG:NH1	2.37	0.58
1:U:1380:ILE:HD12	1:U:1424:ALA:HB2	1.86	0.58
1:D:1132:THR:HG22	1:D:1136:LEU:HD11	1.86	0.57
1:S:1381:LEU:O	1:S:1385:ARG:HG3	2.04	0.57
1:U:1064:TYR:CE1	1:U:1127:ARG:HG2	2.39	0.57
1:U:1229:GLY:HA3	1:U:1240:SER:O	2.04	0.57
1:U:1347:ASN:ND2	1:U:1350:GLU:OE2	2.36	0.57
1:B:1096:ASP:HA	1:B:1102:PRO:HG3	1.86	0.57
1:U:1060:PRO:CD	1:U:1133:LEU:HD21	2.34	0.57
1:U:1377:ARG:CG	1:U:1448:LEU:HD11	2.32	0.57
5:Y:12:DC:H2'	7:Y:1020:CPF:C14	2.32	0.57
1:U:1289:ILE:HG22	1:U:1290:THR:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ASN:HD22	1:B:598:PRO:CD	2.17	0.57
1:D:1362:VAL:HG12	1:D:1363:VAL:N	2.18	0.57
1:S:1451:TYR:HE2	1:S:1455:LEU:HD21	1.70	0.57
1:U:489:ILE:HG22	1:U:527:PHE:HB3	1.85	0.57
1:U:1014:ILE:O	1:U:1014:ILE:HG12	2.04	0.57
1:B:1022:PHE:O	1:B:1025:TYR:HB3	2.04	0.57
1:B:1064:TYR:CE2	1:B:1127:ARG:NH2	2.73	0.57
1:B:1149:ASN:HD22	1:B:1154:GLU:HB2	1.68	0.57
1:D:1176:ALA:HB3	1:D:1179:MET:O	2.04	0.57
1:S:1090:MET:HA	1:S:1093:MET:HE2	1.85	0.57
1:S:1309:ARG:CG	1:S:1309:ARG:NH1	2.62	0.57
1:B:447:ARG:HA	1:B:596:MET:CE	2.33	0.57
1:B:454:ILE:HG22	1:B:456:PRO:HD3	1.86	0.57
1:S:632:PHE:CE1	1:S:636:ASN:ND2	2.72	0.57
1:S:1319:ASN:O	1:S:1323:LYS:HG3	2.04	0.57
1:S:1451:TYR:CE2	1:S:1455:LEU:HD21	2.39	0.57
1:U:598:PRO:HA	1:U:601:ARG:NE	2.19	0.57
1:B:1270:LYS:O	1:B:1274:ILE:HG13	2.04	0.57
1:D:1329:THR:HG22	1:D:1330:SER:N	2.18	0.57
5:H:10:DT:H2"	5:H:11:DA:C8	2.39	0.57
1:S:1072:GLY:O	1:U:1069:ARG:HG3	2.05	0.57
1:D:443:THR:HG22	1:D:454:ILE:CD1	2.32	0.57
1:U:1038:VAL:HG13	1:U:1039:ARG:HG3	1.86	0.57
1:U:1244:ARG:HH21	1:U:1322:TYR:HB3	1.70	0.57
1:B:506:MET:SD	1:B:595:THR:HG21	2.45	0.57
1:S:456:PRO:O	1:S:457:LEU:HG	2.04	0.57
1:U:477:GLU:N	1:U:477:GLU:OE1	2.38	0.57
1:U:610:ASP:C	1:U:610:ASP:OD1	2.43	0.57
1:U:1268:VAL:HG12	1:U:1269:ASN:N	2.20	0.57
1:U:1280:LEU:HD13	1:U:1286:ILE:HD12	1.87	0.57
1:B:457:LEU:HD12	1:B:477:GLU:HG3	1.87	0.57
1:D:1277:ILE:HB	1:D:1292:LEU:HD21	1.86	0.57
4:G:11:DA:N1	5:H:10:DT:O4	2.38	0.57
1:S:608:LEU:HD11	1:S:611:ALA:HA	1.87	0.57
1:B:501:HIS:HA	1:B:536:TYR:CD1	2.40	0.56
1:D:1449:LEU:HD23	1:D:1452:ILE:HD12	1.86	0.56
1:S:534:ALA:O	1:S:536:TYR:HD2	1.88	0.56
1:S:620:MET:HE1	1:U:1019:ARG:NH1	2.12	0.56
1:S:1217:ASP:HA	1:S:1486:THR:HB	1.87	0.56
1:S:1231:ARG:O	1:S:1235:GLU:HB2	2.05	0.56
1:U:1186:HIS:NE2	1:U:1234:TYR:HE1	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1215:GLY:HA3	1:U:1230:ILE:HD13	1.86	0.56
1:D:543:PRO:HG3	1:D:594:THR:CB	2.35	0.56
3:F:8:DG:C8	3:F:8:DG:C5'	2.86	0.56
1:B:1058:MET:SD	1:B:1065:LYS:HG3	2.46	0.56
1:B:1200:LYS:O	1:B:1202:PRO:HD3	2.06	0.56
1:D:431:ILE:HG22	1:D:503:ILE:HG13	1.86	0.56
1:D:458:ARG:HB2	7:H:1020:CPF:C17	2.32	0.56
1:D:1296:THR:HG1	1:D:1302:VAL:HA	1.69	0.56
1:S:476:ASN:CG	1:S:480:GLN:HE21	2.09	0.56
1:S:1042:LEU:HD13	1:S:1047:ARG:HA	1.87	0.56
1:S:1318:LEU:HD12	1:S:1318:LEU:O	2.05	0.56
1:U:1220:THR:O	1:U:1221:ALA:HB3	2.05	0.56
1:U:1289:ILE:HG22	1:U:1290:THR:H	1.70	0.56
1:U:1358:HIS:HD2	1:U:1359:GLN:HE21	1.52	0.56
1:U:1368:GLN:O	1:U:1372:ARG:HD3	2.04	0.56
5:Y:11:DA:H1'	5:Y:12:DC:H5"	1.87	0.56
1:U:1045:VAL:O	1:U:1049:ILE:HG13	2.06	0.56
1:U:1054:ASN:HB2	1:U:1136:LEU:CD1	2.34	0.56
1:U:1230:ILE:HA	1:U:1241:ILE:HD11	1.86	0.56
1:B:1270:LYS:NZ	1:B:1294:ASP:OD2	2.38	0.56
1:S:469:LEU:HG	1:S:473:LEU:HG	1.88	0.56
1:U:541:GLN:OE1	1:U:602:ALA:HB1	2.04	0.56
1:B:1029:VAL:HA	1:B:1033:ARG:HB2	1.88	0.56
1:B:1408:MET:O	1:B:1410:SER:N	2.39	0.56
1:U:1367:THR:CG2	1:U:1459:LEU:HD23	2.36	0.56
1:U:1464:VAL:HG12	1:U:1465:LEU:N	2.18	0.56
1:B:589:ASP:OD1	1:B:590:GLN:N	2.38	0.56
1:D:621:LEU:O	1:D:629:ARG:HD3	2.06	0.56
1:S:1187:ASN:OD1	1:S:1190:GLU:N	2.38	0.56
1:S:1247:ALA:HA	1:S:1260:VAL:O	2.05	0.56
1:S:1283:ASP:CB	1:S:1285:LYS:HE3	2.34	0.56
1:S:1454:GLU:O	1:S:1457:THR:HB	2.06	0.56
1:B:1441:ILE:HG22	1:B:1442:GLU:N	2.20	0.56
1:D:1164:PHE:O	1:D:1166:ASN:N	2.39	0.56
1:S:543:PRO:HD3	1:S:594:THR:HB	1.88	0.56
1:U:508:ASP:HB3	1:U:583:LEU:CD2	2.30	0.56
1:U:1135:LEU:HD23	1:U:1162:ALA:HA	1.88	0.56
1:U:1186:HIS:NE2	1:U:1234:TYR:CE1	2.70	0.56
1:B:1079:HIS:CE1	1:B:1081:HIS:HD2	2.24	0.56
1:B:1427:ASP:OD1	1:D:1431:ARG:NH2	2.39	0.56
1:D:472:ILE:O	1:D:478:ILE:HG21	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:461:ILE:O	1:S:519:LEU:HD13	2.04	0.56
1:U:1084:SER:O	1:U:1088:GLU:HB2	2.05	0.56
1:U:1153:ASN:O	1:U:1154:GLU:HG2	2.06	0.56
1:U:1273:MET:O	1:U:1277:ILE:HG13	2.06	0.56
1:D:501:HIS:O	1:D:536:TYR:HA	2.05	0.56
1:D:1110:PHE:CE1	1:D:1124:THR:HB	2.39	0.56
5:H:12:DC:H2"	5:H:13:DA:H5'	1.86	0.56
1:S:476:ASN:ND2	1:S:480:GLN:HE21	2.04	0.56
1:S:1288:GLY:O	1:S:1308:VAL:HG22	2.06	0.56
1:S:1382:GLU:HG2	1:S:1445:TYR:CE1	2.41	0.56
1:U:517:ARG:HD2	1:U:539:ILE:HG21	1.87	0.56
1:U:1192:ILE:HD12	1:U:1477:ARG:CB	2.33	0.56
1:B:1080:PRO:O	1:B:1081:HIS:CG	2.59	0.55
1:B:1196:LEU:O	1:B:1200:LYS:HG3	2.05	0.55
1:D:430:GLU:HA	1:D:500:TYR:HB3	1.89	0.55
1:D:1127:ARG:O	1:D:1128:MET:O	2.24	0.55
1:S:626:VAL:HG11	4:X:18:DG:OP2	2.06	0.55
1:S:1197:SER:OG	1:S:1212:ASP:OD2	2.23	0.55
1:S:1325:THR:HB	1:S:1326:PRO:CD	2.35	0.55
1:U:533:GLU:HA	1:U:608:LEU:HD22	1.87	0.55
1:U:598:PRO:HB3	1:U:601:ARG:NH2	2.21	0.55
1:U:1218:PHE:CD1	1:U:1266:PHE:CD2	2.94	0.55
1:U:1450:ASN:N	1:U:1450:ASN:ND2	2.50	0.55
1:D:474:ASN:O	1:D:479:ARG:HD2	2.07	0.55
1:S:1122:ARG:HH11	1:U:1082:GLY:HA2	1.71	0.55
1:S:1177:VAL:CG1	1:S:1178:GLY:N	2.70	0.55
1:S:1185:PRO:HG2	1:S:1219:PRO:HD2	1.87	0.55
1:U:1038:VAL:HG12	1:U:1338:LEU:O	2.07	0.55
1:B:1149:ASN:C	1:B:1149:ASN:OD1	2.44	0.55
1:D:514:ALA:O	1:D:518:THR:HG23	2.06	0.55
1:S:1215:GLY:HA2	1:S:1234:TYR:OH	2.06	0.55
1:D:539:ILE:HB	1:D:604:LEU:HB2	1.88	0.55
1:U:435:GLU:HG3	1:U:508:ASP:N	2.22	0.55
1:B:437:ASP:OD2	4:G:10:DT:H5'	2.06	0.55
1:B:1079:HIS:CE1	1:B:1081:HIS:CD2	2.95	0.55
1:S:418:LEU:HD13	1:S:454:ILE:O	2.07	0.55
1:S:1039:ARG:NH2	1:S:1159:VAL:HB	2.20	0.55
1:S:1073:ASP:O	1:S:1077:LYS:HB2	2.07	0.55
1:D:460:LYS:O	4:G:14:DC:H1'	2.06	0.55
1:S:1344:LYS:NZ	1:S:1346:ILE:HG22	2.22	0.55
1:U:1233:ALA:O	1:U:1237:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1083:ASP:HB3	1:D:1121:MET:HE3	1.89	0.55
3:F:8:DG:H2'	7:H:1020:CPF:H132	1.88	0.55
1:S:1467:GLN:OE1	1:S:1467:GLN:HA	2.07	0.55
1:U:1041:GLY:HA2	1:U:1167:LEU:HD13	1.89	0.55
1:D:454:ILE:CG2	1:D:456:PRO:HD3	2.35	0.55
5:H:9:DG:H2'	5:H:10:DT:C6	2.42	0.55
1:U:1243:MET:HE1	1:U:1331:PHE:HD1	1.72	0.55
1:U:1325:THR:C	1:U:1327:LEU:H	2.10	0.55
4:X:13:DC:N4	4:X:14:DC:N3	2.55	0.55
1:B:1136:LEU:HD21	1:B:1160:LEU:HD13	1.89	0.55
1:D:508:ASP:CA	1:D:583:LEU:HD23	2.37	0.55
1:D:1041:GLY:HA2	1:D:1167:LEU:HD13	1.88	0.55
1:S:420:ASP:HA	1:S:453:ALA:HB1	1.89	0.55
5:Y:13:DA:P	5:Y:13:DA:H2'	2.47	0.55
1:B:1220:THR:O	1:B:1221:ALA:HB3	2.06	0.54
1:D:596:MET:O	1:D:598:PRO:HD3	2.07	0.54
1:D:1184:PRO:O	1:D:1186:HIS:CE1	2.60	0.54
1:D:1451:TYR:CE1	1:D:1455:LEU:HD21	2.42	0.54
1:S:459:GLY:N	7:X:1020:CPF:H131	2.22	0.54
1:S:1265:PRO:HB2	1:S:1268:VAL:HG21	1.87	0.54
1:B:629:ARG:HB2	1:B:629:ARG:NH1	2.23	0.54
1:U:1246:ARG:HG2	1:U:1262:THR:OG1	2.07	0.54
1:B:606:VAL:CG1	1:B:1014:ILE:HD12	2.37	0.54
1:D:495:LEU:CD2	1:D:534:ALA:HB2	2.30	0.54
1:U:601:ARG:HD2	1:U:603:LEU:HG	1.90	0.54
1:U:1234:TYR:O	1:U:1347:ASN:HB2	2.06	0.54
1:D:1111:GLY:O	1:D:1112:SER:HB3	2.07	0.54
3:F:8:DG:H2'	7:H:1020:CPF:C13	2.38	0.54
1:S:1100:ARG:HG3	1:S:1100:ARG:NH1	2.22	0.54
1:B:434:VAL:HG21	1:B:440:GLY:N	2.22	0.54
1:B:1149:ASN:OD1	1:B:1149:ASN:O	2.26	0.54
1:B:1218:PHE:CB	1:B:1266:PHE:HB2	2.38	0.54
4:G:13:DC:H5"	4:G:13:DC:H6	1.73	0.54
1:S:1386:ILE:HG23	1:S:1390:HIS:HD2	1.73	0.54
1:S:1387:ALA:O	1:S:1391:ILE:HA	2.08	0.54
1:S:1411:LEU:O	1:S:1415:PHE:HB2	2.08	0.54
1:U:430:GLU:HB2	1:U:502:LYS:HB2	1.89	0.54
4:X:9:DG:C2	5:Y:12:DC:N3	2.75	0.54
1:B:619:GLU:O	1:B:623:GLY:CA	2.55	0.54
1:B:1113:MET:CE	1:B:1302:VAL:HG22	2.37	0.54
1:B:1230:ILE:H	1:B:1230:ILE:HD12	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1380:ILE:HD12	1:B:1424:ALA:CB	2.37	0.54
1:D:435:GLU:OE2	3:F:8:DG:O3'	2.26	0.54
1:D:1150:TYR:CE2	1:D:1151:ASP:HB3	2.42	0.54
1:D:1469:VAL:HG12	1:D:1473:LEU:CD1	2.37	0.54
1:U:463:ASN:ND2	1:U:466:LYS:HG3	2.22	0.54
4:X:13:DC:H1'	7:X:1020:CPF:N3	2.21	0.54
1:B:420:ASP:OD2	1:B:499:ARG:NH2	2.39	0.54
1:B:1037:ASP:HB3	1:B:1040:ASP:OD1	2.08	0.54
1:B:1129:THR:HB	1:B:1131:ILE:HG22	1.90	0.54
1:D:1191:LEU:HD23	1:D:1213:ILE:HD13	1.90	0.54
1:S:437:ASP:HB3	5:Y:9:DG:H5'	1.90	0.54
1:S:458:ARG:CD	1:S:477:GLU:OE2	2.56	0.54
1:S:1192:ILE:HD12	1:S:1477:ARG:HB2	1.89	0.54
1:D:1369:TYR:CZ	1:D:1373:LYS:HD2	2.42	0.54
1:S:1264:ILE:HB	1:S:1265:PRO:CD	2.38	0.54
1:U:1030:ILE:HG22	1:U:1031:VAL:N	2.23	0.54
1:D:1067:SER:HB2	1:D:1121:MET:O	2.07	0.54
1:D:1191:LEU:O	1:D:1195:VAL:HG23	2.08	0.54
1:D:1227:LYS:O	1:D:1231:ARG:HB2	2.08	0.54
1:S:538:TYR:HB3	1:S:604:LEU:O	2.07	0.54
1:S:1059:THR:HB	1:S:1060:PRO:CD	2.38	0.54
1:U:430:GLU:HB3	1:U:502:LYS:HE2	1.89	0.54
1:U:1100:ARG:HH12	1:U:1485:ARG:CZ	2.20	0.54
1:U:1461:ASP:OD2	1:U:1463:GLU:N	2.40	0.54
1:B:1336:ILE:HG23	1:B:1344:LYS:O	2.08	0.54
1:D:1055:GLU:C	1:D:1057:GLY:H	2.10	0.54
1:D:1266:PHE:O	1:D:1267:GLN:HB2	2.08	0.54
5:H:9:DG:C2'	5:H:10:DT:C6	2.91	0.54
1:S:1276:LYS:O	1:S:1280:LEU:HG	2.07	0.54
1:S:1406:VAL:O	1:S:1407:ALA:C	2.45	0.54
1:S:1474:THR:HG23	1:S:1477:ARG:NH2	2.23	0.54
1:B:1283:ASP:O	1:B:1285:LYS:HG3	2.08	0.53
1:U:1232:ARG:HG2	1:U:1239:GLY:HA2	1.90	0.53
1:U:1234:TYR:CD1	1:U:1348:LEU:HD13	2.42	0.53
1:U:1484:ARG:HD3	1:U:1486:THR:O	2.07	0.53
1:D:1326:PRO:C	1:D:1328:GLN:N	2.60	0.53
1:D:1384:LEU:O	1:D:1387:ALA:HB3	2.08	0.53
1:S:1177:VAL:CG1	1:S:1178:GLY:H	2.22	0.53
1:S:1190:GLU:HB3	1:S:1213:ILE:HA	1.91	0.53
1:U:470:ASP:O	1:U:474:ASN:ND2	2.41	0.53
1:U:1186:HIS:NE2	1:U:1234:TYR:OH	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1391:ILE:HG23	1:U:1392:ASP:N	2.23	0.53
1:B:522:THR:HG22	1:B:523:PHE:N	2.23	0.53
1:B:1382:GLU:HG3	1:B:1445:TYR:CE2	2.39	0.53
1:D:528:MET:O	1:D:531:LEU:HB3	2.08	0.53
1:D:1079:HIS:CE1	1:D:1081:HIS:HD2	2.26	0.53
1:U:1409:GLU:OE1	1:U:1409:GLU:HA	2.07	0.53
4:X:13:DC:C1'	7:X:1020:CPF:H161	2.28	0.53
1:B:472:ILE:HD13	1:B:527:PHE:CZ	2.44	0.53
1:B:501:HIS:CD2	1:B:536:TYR:CE1	2.97	0.53
1:B:536:TYR:O	1:B:538:TYR:HD1	1.91	0.53
1:B:1361:THR:O	1:B:1361:THR:HG22	2.08	0.53
1:S:1087:TYR:O	1:S:1091:VAL:HG23	2.09	0.53
1:S:1100:ARG:NH2	1:S:1217:ASP:OD2	2.41	0.53
4:X:14:DC:H2'	4:X:15:DA:H8	1.73	0.53
1:D:482:ILE:HG23	1:D:489:ILE:HG23	1.91	0.53
1:D:1292:LEU:HD13	1:D:1306:ILE:HG12	1.90	0.53
1:U:1054:ASN:CB	1:U:1136:LEU:HD13	2.37	0.53
3:W:8:DG:H5'	3:W:8:DG:H8	1.71	0.53
1:B:493:PHE:CZ	1:B:531:LEU:HB2	2.43	0.53
1:D:1266:PHE:CE2	1:D:1267:GLN:HG3	2.44	0.53
1:D:1290:THR:OG1	1:D:1307:ASP:HB3	2.07	0.53
1:D:1369:TYR:CE2	1:D:1373:LYS:HD2	2.44	0.53
1:S:602:ALA:C	1:S:603:LEU:HD23	2.28	0.53
1:S:1202:PRO:HB2	1:S:1203:ASP:OD1	2.09	0.53
1:B:442:SER:HB2	1:B:591:LEU:HD23	1.91	0.53
1:B:1191:LEU:HD23	1:B:1213:ILE:HD13	1.91	0.53
1:D:1363:VAL:HG13	1:D:1366:ARG:HH21	1.70	0.53
1:S:468:ARG:O	1:S:472:ILE:HG13	2.09	0.53
1:S:1182:ASN:OD1	1:S:1331:PHE:CZ	2.62	0.53
1:S:1350:GLU:O	1:S:1354:HIS:CD2	2.56	0.53
1:U:444:LYS:HA	1:U:447:ARG:HG2	1.89	0.53
4:X:12:DC:O2	7:X:1020:CPF:H141	2.08	0.53
1:B:447:ARG:HD2	1:B:452:GLN:O	2.09	0.53
1:B:1262:THR:O	1:B:1263:GLU:HG3	2.08	0.53
1:U:1100:ARG:NH1	1:U:1485:ARG:CZ	2.72	0.53
1:S:1321:LEU:C	1:S:1323:LYS:H	2.11	0.53
1:U:1091:VAL:O	1:U:1091:VAL:HG13	2.09	0.53
1:U:1190:GLU:HB3	1:U:1213:ILE:HA	1.91	0.53
1:B:1325:THR:CB	1:B:1326:PRO:HD2	2.35	0.53
1:D:1378:ALA:O	1:D:1382:GLU:HG3	2.08	0.53
4:G:11:DA:N1	5:H:10:DT:C4	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:18:DA:C5	5:H:19:DC:N4	2.76	0.53
1:S:1309:ARG:HD2	1:S:1309:ARG:O	2.09	0.53
1:U:493:PHE:HZ	1:U:531:LEU:CB	2.16	0.53
1:U:1037:ASP:O	1:U:1039:ARG:N	2.42	0.53
4:X:13:DC:C1'	7:X:1020:CPF:H142	2.39	0.53
1:D:1037:ASP:OD2	1:D:1038:VAL:N	2.42	0.52
1:D:1238:ARG:CG	1:D:1334:ASN:HD22	2.20	0.52
1:S:633:ILE:O	1:S:637:ALA:HB2	2.09	0.52
1:S:1026:ALA:CB	1:U:633:ILE:HD11	2.39	0.52
1:S:1289:ILE:HG12	1:S:1317:ILE:HG21	1.91	0.52
1:B:458:ARG:CB	7:G:1020:CPF:H162	2.30	0.52
1:B:1259:ILE:HG21	1:B:1318:LEU:HD13	1.91	0.52
1:B:1414:ARG:O	1:B:1415:PHE:CD1	2.63	0.52
1:D:1204:ILE:HG13	1:D:1205:SER:N	2.24	0.52
5:H:12:DC:H2"	5:H:13:DA:C5'	2.39	0.52
5:H:18:DA:H2"	5:H:19:DC:OP2	2.09	0.52
1:S:444:LYS:O	1:S:447:ARG:HG2	2.09	0.52
1:S:493:PHE:HE2	1:S:495:LEU:HB2	1.74	0.52
1:S:1077:LYS:O	1:S:1078:TYR:CG	2.62	0.52
1:S:1273:MET:HG3	1:S:1326:PRO:HB2	1.90	0.52
1:U:1136:LEU:O	1:U:1139:ILE:HB	2.08	0.52
1:B:1039:ARG:NH2	1:B:1159:VAL:HB	2.21	0.52
1:D:454:ILE:HG22	1:D:456:PRO:CD	2.34	0.52
1:D:1338:LEU:HD23	1:D:1342:ARG:C	2.30	0.52
4:G:9:DG:H5'	7:G:1020:CPF:C12	2.37	0.52
1:S:506:MET:HG2	1:S:583:LEU:HD11	1.91	0.52
1:S:1224:ILE:O	1:S:1489:GLN:HB2	2.10	0.52
1:U:583:LEU:CD1	1:U:591:LEU:HD11	2.39	0.52
1:B:446:GLY:N	1:B:588:ALA:HB1	2.24	0.52
1:B:1149:ASN:O	1:B:1151:ASP:N	2.42	0.52
1:S:607:LYS:O	1:U:1014:ILE:HG22	2.09	0.52
1:U:1087:TYR:HB2	1:U:1121:MET:HE2	1.92	0.52
1:B:636:ASN:O	1:B:637:ALA:C	2.48	0.52
1:B:1031:VAL:CG2	1:B:1032:ALA:N	2.70	0.52
1:B:1136:LEU:CD2	1:B:1160:LEU:HD13	2.40	0.52
1:D:1193:ASN:OD1	1:D:1193:ASN:N	2.41	0.52
1:D:1210:MET:SD	1:D:1234:TYR:HD2	2.31	0.52
1:S:1201:ASN:OD1	1:S:1202:PRO:HD2	2.09	0.52
1:S:1334:ASN:O	1:S:1336:ILE:N	2.42	0.52
1:U:1380:ILE:HD12	1:U:1424:ALA:CB	2.39	0.52
1:B:519:LEU:HD11	5:H:15:DC:H4'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1139:ILE:HD12	1:S:1161:PRO:HD3	1.91	0.52
1:U:1101:TYR:N	1:U:1170:ASN:OD1	2.42	0.52
5:Y:13:DA:H2"	5:Y:14:DC:OP2	2.10	0.52
1:B:1363:VAL:HG21	1:B:1469:VAL:HG22	1.90	0.52
1:D:1079:HIS:NE2	1:D:1081:HIS:CD2	2.77	0.52
1:D:1367:THR:HG22	1:D:1459:LEU:HD21	1.91	0.52
1:D:1410:SER:O	1:D:1412:GLN:N	2.42	0.52
1:S:1092:ARG:HB3	1:S:1092:ARG:CZ	2.38	0.52
1:S:1243:MET:O	1:S:1328:GLN:HG3	2.10	0.52
1:S:1369:TYR:CD2	1:S:1370:ASN:N	2.78	0.52
1:U:442:SER:HB3	1:U:591:LEU:HD22	1.92	0.52
1:U:1163:ARG:NH2	1:U:1363:VAL:HG23	2.24	0.52
1:U:1364:ARG:HB2	1:U:1465:LEU:HD11	1.90	0.52
1:U:1414:ARG:HB3	1:U:1415:PHE:CD1	2.44	0.52
1:B:602:ALA:O	1:B:603:LEU:HD23	2.09	0.52
1:B:1030:ILE:HG22	1:B:1031:VAL:N	2.23	0.52
1:D:422:SER:OG	1:D:450:ARG:HG2	2.10	0.52
1:S:521:LEU:HD21	1:S:606:VAL:HG11	1.91	0.52
1:S:1049:ILE:O	1:S:1053:LEU:HG	2.09	0.52
1:S:1258:ARG:HD2	1:S:1305:VAL:HG11	1.92	0.52
1:S:1344:LYS:HZ2	1:S:1346:ILE:HG22	1.75	0.52
1:S:1383:GLY:CA	1:S:1421:GLN:HG2	2.40	0.52
1:U:632:PHE:HD1	1:U:636:ASN:HD22	1.56	0.52
1:U:1091:VAL:O	1:U:1091:VAL:CG1	2.57	0.52
1:U:1290:THR:OG1	1:U:1291:ASP:N	2.43	0.52
1:B:433:LEU:HD12	1:B:505:ILE:HG12	1.91	0.52
1:B:1218:PHE:O	1:B:1221:ALA:N	2.37	0.52
1:D:419:ALA:HB1	1:D:447:ARG:NH1	2.24	0.52
1:S:1090:MET:HA	1:S:1093:MET:CE	2.40	0.52
1:S:1289:ILE:CG1	1:S:1317:ILE:HG21	2.40	0.52
1:S:1490:LEU:HD12	1:S:1490:LEU:O	2.09	0.52
1:U:461:ILE:HG22	1:U:519:LEU:HD13	1.91	0.52
1:U:473:LEU:C	1:U:474:ASN:HD22	2.14	0.52
1:U:540:ALA:HA	1:U:603:LEU:CD2	2.38	0.52
1:B:1363:VAL:HG13	1:B:1366:ARG:NH2	2.20	0.51
1:D:526:ARG:C	1:D:527:PHE:CD1	2.84	0.51
1:D:1030:ILE:HG21	1:D:1343:PRO:CG	2.38	0.51
1:S:1382:GLU:CG	1:S:1445:TYR:CE1	2.93	0.51
1:U:478:ILE:O	1:U:482:ILE:HG13	2.09	0.51
1:U:501:HIS:O	1:U:536:TYR:HB3	2.10	0.51
1:B:621:LEU:O	1:B:629:ARG:CD	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:VAL:HG11	1:D:540:ALA:HB2	1.92	0.51
1:S:1387:ALA:HA	1:S:1394:ILE:CG1	2.40	0.51
1:U:1381:LEU:O	1:U:1385:ARG:HG3	2.10	0.51
1:B:1431:ARG:CG	1:D:1426:LEU:O	2.51	0.51
1:D:625:VAL:HG21	1:D:628:ASN:ND2	2.26	0.51
1:D:1092:ARG:C	1:D:1094:ALA:N	2.64	0.51
1:D:1469:VAL:HG12	1:D:1473:LEU:HD12	1.93	0.51
1:S:441:GLY:HA3	1:S:1109:ASN:ND2	2.20	0.51
1:S:494:ASP:CB	1:S:497:LYS:HD2	2.40	0.51
1:S:630:ARG:HA	1:S:633:ILE:HD12	1.92	0.51
1:S:1463:GLU:OE2	1:S:1466:LEU:HD23	2.10	0.51
1:U:485:PHE:O	1:U:499:ARG:HG3	2.10	0.51
1:U:592:TRP:CG	1:U:593:GLU:N	2.79	0.51
1:U:1041:GLY:HA2	1:U:1167:LEU:CD1	2.40	0.51
1:B:418:LEU:HD12	1:B:419:ALA:N	2.25	0.51
1:B:1151:ASP:OD1	1:B:1153:ASN:HB2	2.10	0.51
1:S:1051:TYR:CZ	1:S:1157:PRO:HD3	2.45	0.51
1:S:1071:VAL:HG12	1:S:1075:MET:CE	2.39	0.51
1:S:1391:ILE:O	1:S:1395:ILE:HG12	2.10	0.51
1:U:1267:GLN:OE1	1:U:1331:PHE:HE1	1.93	0.51
1:B:1309:ARG:O	1:B:1310:LYS:O	2.29	0.51
1:D:500:TYR:O	1:D:536:TYR:CD1	2.63	0.51
1:D:1060:PRO:HD3	1:D:1128:MET:CB	2.41	0.51
2:E:8:DT:C2	7:G:1020:CPF:H132	2.45	0.51
1:S:1222:GLY:HA2	1:S:1263:GLU:HB3	1.92	0.51
1:S:1295:GLU:O	1:S:1300:THR:HG21	2.10	0.51
1:U:1362:VAL:O	1:U:1363:VAL:C	2.48	0.51
1:U:1452:ILE:O	1:U:1456:GLU:HG3	2.10	0.51
1:B:435:GLU:HG2	1:B:507:THR:HB	1.92	0.51
1:D:1071:VAL:HG11	1:D:1121:MET:HE1	1.92	0.51
1:D:1105:ASP:O	1:D:1126:ALA:HA	2.11	0.51
1:U:1030:ILE:HG12	1:U:1176:ALA:HB1	1.93	0.51
1:U:1087:TYR:HH	1:U:1124:THR:HG1	1.58	0.51
1:S:456:PRO:C	1:S:457:LEU:HG	2.31	0.51
1:S:1241:ILE:CD1	1:S:1333:VAL:HG21	2.38	0.51
1:S:1297:SER:HG	1:S:1300:THR:HG1	1.57	0.51
1:U:592:TRP:HA	1:U:596:MET:HE2	1.92	0.51
1:U:1295:GLU:OE1	1:U:1305:VAL:HG21	2.10	0.51
1:B:1416:LYS:HE2	1:B:1416:LYS:CA	2.37	0.51
1:D:517:ARG:NH1	1:D:517:ARG:HB2	2.25	0.51
1:S:1321:LEU:HB3	1:S:1327:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:586:MET:HB2	1:U:591:LEU:HD12	1.93	0.51
1:U:1087:TYR:CZ	1:U:1121:MET:HA	2.45	0.51
1:B:1103:LEU:HD21	1:B:1170:ASN:HD21	1.76	0.51
1:B:1153:ASN:O	1:B:1154:GLU:CG	2.56	0.51
1:D:1390:HIS:HB3	1:D:1393:GLU:OE2	2.11	0.51
1:S:1122:ARG:NH1	1:U:1082:GLY:HA2	2.26	0.51
1:U:1090:MET:HA	1:U:1093:MET:HE3	1.93	0.51
1:U:1320:ASN:HB3	1:U:1324:GLN:HE21	1.76	0.51
1:U:1335:MET:O	1:U:1345:LEU:CD1	2.59	0.51
1:B:1244:ARG:HA	1:B:1328:GLN:HG3	1.92	0.51
1:D:522:THR:HA	1:D:618:PHE:HE2	1.76	0.51
1:S:1151:ASP:O	1:S:1153:ASN:N	2.42	0.51
1:S:1355:TYR:O	1:S:1358:HIS:HB3	2.10	0.51
1:U:435:GLU:OE1	1:U:508:ASP:OD1	2.29	0.51
1:U:1093:MET:HB3	1:U:1104:VAL:HG23	1.92	0.51
1:U:1316:VAL:HA	1:U:1319:ASN:HB2	1.93	0.51
1:D:633:ILE:CD1	1:D:1026:ALA:HB1	2.41	0.50
1:S:458:ARG:HD2	1:S:477:GLU:OE2	2.11	0.50
1:B:1104:VAL:CG1	1:B:1105:ASP:N	2.74	0.50
1:D:1390:HIS:O	1:D:1394:ILE:HG12	2.11	0.50
1:S:421:CYS:N	1:S:453:ALA:HB2	2.26	0.50
1:S:422:SER:O	1:S:424:LYS:HD2	2.10	0.50
1:S:1067:SER:CB	1:S:1121:MET:HB2	2.41	0.50
1:S:1406:VAL:O	1:S:1408:MET:N	2.44	0.50
1:U:430:GLU:CB	1:U:502:LYS:HB2	2.41	0.50
1:U:589:ASP:CG	1:U:590:GLN:H	2.14	0.50
1:D:1293:ARG:HH22	1:D:1305:VAL:HG11	1.77	0.50
1:S:459:GLY:HA3	7:X:1020:CPF:C13	2.37	0.50
1:S:597:ASN:HD22	1:S:598:PRO:HD2	1.76	0.50
1:S:1100:ARG:NH1	1:S:1101:TYR:CZ	2.79	0.50
1:S:1433:LEU:HD23	1:S:1433:LEU:N	2.26	0.50
1:U:481:MET:HG2	1:U:485:PHE:CZ	2.46	0.50
1:B:1222:GLY:C	1:B:1223:LEU:HD12	2.30	0.50
1:D:514:ALA:O	1:D:517:ARG:HB3	2.12	0.50
1:D:1403:THR:OG1	1:D:1406:VAL:HG23	2.12	0.50
1:B:476:ASN:HD21	1:B:480:GLN:HG3	1.76	0.50
1:B:493:PHE:HZ	1:B:531:LEU:HB2	1.76	0.50
1:B:1040:ASP:OD2	1:B:1047:ARG:NH2	2.45	0.50
1:D:452:GLN:OE1	1:D:592:TRP:HZ3	1.95	0.50
1:D:540:ALA:HB1	1:D:595:THR:CG2	2.42	0.50
1:S:464:VAL:HG21	1:S:523:PHE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:471:ARG:HG2	1:S:471:ARG:NH1	2.20	0.50
1:S:1116:ASP:O	1:S:1118:ALA:N	2.44	0.50
1:S:1196:LEU:O	1:S:1200:LYS:HE3	2.11	0.50
1:S:1265:PRO:HB2	1:S:1268:VAL:CG2	2.42	0.50
1:B:1247:ALA:HA	1:B:1261:VAL:HA	1.93	0.50
1:B:1405:LYS:HE2	1:B:1409:GLU:OE1	2.12	0.50
1:D:1318:LEU:HG	1:D:1322:TYR:CE2	2.46	0.50
5:H:18:DA:C5	5:H:19:DC:C4	3.00	0.50
1:S:521:LEU:CD2	1:S:606:VAL:HG11	2.42	0.50
1:S:1246:ARG:NH2	1:S:1487:GLU:HB3	2.26	0.50
1:S:1321:LEU:C	1:S:1323:LYS:N	2.64	0.50
1:U:597:ASN:O	1:U:601:ARG:HB3	2.11	0.50
1:U:1270:LYS:O	1:U:1274:ILE:HG13	2.12	0.50
1:B:1186:HIS:NE2	1:B:1234:TYR:OH	2.30	0.50
1:D:1150:TYR:CD2	1:D:1151:ASP:N	2.80	0.50
1:S:1051:TYR:CZ	1:S:1146:PHE:HE2	2.29	0.50
1:S:1206:ILE:O	1:S:1210:MET:HG3	2.11	0.50
1:B:433:LEU:HB3	1:B:457:LEU:HD21	1.94	0.50
1:B:1292:LEU:HA	1:B:1305:VAL:O	2.12	0.50
1:D:1408:MET:O	1:D:1412:GLN:HG3	2.12	0.50
1:D:1472:GLU:O	1:D:1476:ILE:HG12	2.12	0.50
1:S:1096:ASP:HA	1:S:1102:PRO:HG3	1.93	0.50
1:S:1381:LEU:HD13	1:S:1445:TYR:N	2.27	0.50
1:U:444:LYS:HZ2	1:U:454:ILE:HD12	1.77	0.50
1:D:626:VAL:HA	1:D:629:ARG:NH2	2.27	0.50
1:D:1179:MET:O	4:G:17:DG:H4'	2.12	0.50
1:S:1037:ASP:O	1:S:1041:GLY:HA2	2.11	0.50
1:S:1193:ASN:CA	1:S:1196:LEU:HD12	2.36	0.50
1:S:1245:SER:CB	1:S:1261:VAL:HG11	2.41	0.50
1:U:433:LEU:HA	1:U:455:LEU:O	2.12	0.50
1:U:1157:PRO:O	1:U:1159:VAL:N	2.45	0.50
1:B:493:PHE:CE2	1:B:530:PRO:HB2	2.46	0.49
1:D:1313:ASN:HB3	1:D:1316:VAL:CG2	2.42	0.49
1:D:1329:THR:CG2	1:D:1330:SER:H	2.24	0.49
1:U:1195:VAL:O	1:U:1198:LEU:HB3	2.11	0.49
1:U:1281:VAL:HG22	1:U:1289:ILE:HD12	1.94	0.49
1:U:1451:TYR:CE1	1:U:1455:LEU:HD21	2.47	0.49
1:B:1071:VAL:C	1:B:1073:ASP:N	2.62	0.49
1:D:604:LEU:HD13	1:D:1012:ARG:CB	2.42	0.49
1:D:1466:LEU:HD23	1:D:1470:ARG:HH22	1.77	0.49
1:S:447:ARG:HG3	1:S:447:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1071:VAL:O	1:S:1074:VAL:N	2.46	0.49
1:U:1223:LEU:HD23	1:U:1487:GLU:OE2	2.12	0.49
1:B:1104:VAL:CG1	1:B:1105:ASP:H	2.22	0.49
1:D:587:ASN:O	1:D:591:LEU:HG	2.12	0.49
1:D:1060:PRO:HD3	1:D:1128:MET:HB2	1.94	0.49
1:S:455:LEU:HD12	1:S:456:PRO:HD2	1.93	0.49
1:U:506:MET:SD	1:U:595:THR:HG21	2.51	0.49
1:B:525:TYR:HE2	1:B:526:ARG:NH1	2.10	0.49
1:B:611:ALA:O	1:B:615:ASP:OD2	2.30	0.49
1:D:461:ILE:HG22	1:D:462:LEU:N	2.27	0.49
1:S:1030:ILE:HG23	1:S:1035:LEU:HD12	1.93	0.49
1:S:1401:SER:HB3	1:S:1406:VAL:HB	1.95	0.49
1:S:1432:ARG:O	1:S:1438:ARG:HG3	2.13	0.49
1:U:1292:LEU:HD12	1:U:1293:ARG:N	2.25	0.49
1:D:494:ASP:C	1:D:496:ALA:H	2.15	0.49
1:D:521:LEU:HD12	1:D:1018:MET:SD	2.53	0.49
1:S:418:LEU:O	1:S:420:ASP:N	2.43	0.49
1:S:1159:VAL:HG22	1:S:1160:LEU:N	2.27	0.49
1:U:476:ASN:O	1:U:480:GLN:N	2.40	0.49
1:U:1042:LEU:HD13	1:U:1047:ARG:HA	1.95	0.49
1:U:1090:MET:HG2	1:U:1090:MET:O	2.13	0.49
1:U:1193:ASN:HB3	1:U:1212:ASP:HB3	1.95	0.49
1:B:447:ARG:CA	1:B:596:MET:HE1	2.43	0.49
1:D:439:ALA:HB1	1:D:583:LEU:HD12	1.94	0.49
1:D:1068:ALA:HB2	1:D:1121:MET:HG3	1.94	0.49
1:D:1092:ARG:O	1:D:1094:ALA:N	2.46	0.49
1:D:1204:ILE:H	1:D:1349:LYS:HZ1	1.59	0.49
1:S:525:TYR:HE2	1:S:526:ARG:HH12	1.60	0.49
1:S:1199:SER:HB2	1:S:1466:LEU:HD11	1.94	0.49
1:U:619:GLU:O	1:U:623:GLY:HA3	2.12	0.49
1:U:1104:VAL:HG12	1:U:1105:ASP:N	2.27	0.49
1:B:432:PHE:HB2	1:B:454:ILE:HG12	1.94	0.49
1:B:1094:ALA:HB2	1:B:1104:VAL:HB	1.94	0.49
1:B:1291:ASP:HB3	1:B:1307:ASP:OD2	2.13	0.49
1:S:1233:ALA:HB1	1:S:1333:VAL:CG1	2.40	0.49
1:S:1291:ASP:OD2	1:S:1292:LEU:N	2.46	0.49
1:S:1385:ARG:O	1:S:1388:LEU:HB2	2.12	0.49
1:U:1192:ILE:CD1	1:U:1477:ARG:HB2	2.38	0.49
1:U:1296:THR:HG23	1:U:1302:VAL:N	2.27	0.49
1:B:1382:GLU:CG	1:B:1445:TYR:HE2	2.22	0.49
1:D:539:ILE:O	1:D:540:ALA:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:DG:N2	5:H:16:DG:N2	2.61	0.49
1:S:481:MET:O	1:S:485:PHE:CG	2.66	0.49
1:U:420:ASP:HA	1:U:453:ALA:CB	2.43	0.49
1:U:464:VAL:HG21	1:U:523:PHE:HA	1.95	0.49
1:U:1138:ASP:OD2	1:U:1366:ARG:HD3	2.12	0.49
1:B:431:ILE:HA	1:B:453:ALA:O	2.13	0.49
1:B:1064:TYR:O	1:B:1065:LYS:HD3	2.12	0.49
1:B:1349:LYS:O	1:B:1350:GLU:C	2.51	0.49
1:D:523:PHE:HD2	1:D:524:PHE:CD2	2.31	0.49
1:D:540:ALA:HB1	1:D:595:THR:HG23	1.95	0.49
1:D:1185:PRO:O	1:D:1217:ASP:O	2.31	0.49
1:S:437:ASP:N	5:Y:9:DG:H5'	2.28	0.49
1:S:518:THR:HG21	1:U:1022:PHE:HB2	1.94	0.49
1:S:620:MET:CE	1:U:1019:ARG:NH1	2.74	0.49
1:B:1147:ILE:HG23	1:B:1158:SER:HB3	1.95	0.49
1:S:1103:LEU:HD22	1:S:1135:LEU:HD11	1.94	0.49
1:S:1224:ILE:HD12	1:S:1488:ILE:HG12	1.95	0.49
1:U:508:ASP:O	1:U:513:GLY:HA3	2.12	0.49
1:U:1067:SER:CB	1:U:1121:MET:O	2.60	0.49
1:B:1030:ILE:O	1:B:1035:LEU:HB2	2.13	0.48
1:B:1225:LEU:HB2	1:B:1242:GLN:HB2	1.95	0.48
1:D:1030:ILE:HG23	1:D:1343:PRO:HG3	1.93	0.48
5:H:20:DA:OP1	5:H:20:DA:H4'	2.12	0.48
1:S:1203:ASP:OD1	1:S:1203:ASP:N	2.46	0.48
1:S:1381:LEU:CD2	1:S:1441:ILE:HG23	2.43	0.48
1:U:487:THR:HG22	1:U:498:ALA:CB	2.42	0.48
1:U:1032:ALA:O	1:U:1033:ARG:HB2	2.13	0.48
1:U:1461:ASP:HB3	1:U:1464:VAL:CG2	2.43	0.48
1:B:1230:ILE:HA	1:B:1241:ILE:CD1	2.38	0.48
1:B:1290:THR:O	1:B:1291:ASP:CB	2.60	0.48
1:D:511:VAL:C	1:D:513:GLY:H	2.16	0.48
1:D:1390:HIS:N	1:D:1390:HIS:ND1	2.60	0.48
1:S:437:ASP:H	5:Y:9:DG:H5'	1.78	0.48
1:S:1225:LEU:HD12	1:S:1242:GLN:HB3	1.95	0.48
1:U:1225:LEU:HD21	1:U:1244:ARG:HD2	1.95	0.48
1:B:1067:SER:O	1:B:1071:VAL:HG23	2.13	0.48
1:B:1389:ASP:HB2	1:B:1390:HIS:ND1	2.29	0.48
1:B:1434:THR:HG21	1:D:1404:ASP:OD1	2.13	0.48
1:B:1450:ASN:O	1:B:1453:SER:HB3	2.14	0.48
1:D:426:PRO:O	1:D:429:CYS:HB2	2.12	0.48
1:D:1238:ARG:HG2	1:D:1334:ASN:ND2	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1425:ILE:C	1:D:1427:ASP:H	2.17	0.48
5:H:15:DC:H2"	5:H:16:DG:O4'	2.12	0.48
1:S:461:ILE:HD12	1:S:462:LEU:N	2.27	0.48
1:S:1046:HIS:HE1	2:V:6:DG:OP1	1.97	0.48
1:S:1064:TYR:CE1	1:S:1127:ARG:NE	2.82	0.48
1:S:1288:GLY:O	1:S:1308:VAL:HG13	2.13	0.48
1:U:1230:ILE:HG23	1:U:1234:TYR:CE2	2.49	0.48
1:B:447:ARG:HB2	1:B:596:MET:HE1	1.96	0.48
1:B:511:VAL:O	1:B:514:ALA:HB3	2.13	0.48
1:B:619:GLU:O	1:B:623:GLY:HA3	2.13	0.48
1:B:1405:LYS:O	1:B:1409:GLU:HG3	2.13	0.48
1:B:1431:ARG:NH1	1:D:1423:GLN:CD	2.62	0.48
1:D:475:ASN:O	1:D:478:ILE:HB	2.14	0.48
1:D:494:ASP:HB3	1:D:497:LYS:HE3	1.95	0.48
1:U:1087:TYR:CB	1:U:1121:MET:HE2	2.43	0.48
1:U:1416:LYS:HB3	1:U:1416:LYS:HE2	1.54	0.48
4:X:11:DA:H2	5:Y:10:DT:H3	1.61	0.48
1:B:1025:TYR:O	1:B:1029:VAL:HG23	2.14	0.48
1:B:1113:MET:HE1	1:B:1302:VAL:HG22	1.96	0.48
1:S:1386:ILE:HG23	1:S:1390:HIS:CD2	2.48	0.48
1:S:1401:SER:HB3	1:S:1407:ALA:H	1.78	0.48
1:U:591:LEU:O	1:U:592:TRP:C	2.51	0.48
1:U:1110:PHE:HZ	1:U:1125:GLU:O	1.97	0.48
1:B:431:ILE:HG21	1:B:485:PHE:HE1	1.79	0.48
1:D:508:ASP:HA	1:D:583:LEU:CD2	2.41	0.48
1:S:1439:ASP:O	1:S:1443:ALA:CB	2.62	0.48
1:U:1040:ASP:O	1:U:1166:ASN:ND2	2.44	0.48
1:D:1195:VAL:HA	1:D:1198:LEU:HB3	1.95	0.48
1:D:1277:ILE:HB	1:D:1292:LEU:CD2	2.43	0.48
7:H:1020:CPF:H1	7:H:1020:CPF:H121	1.41	0.48
1:S:1084:SER:HB2	1:S:1088:GLU:OE1	2.14	0.48
1:U:1046:HIS:O	1:U:1047:ARG:C	2.52	0.48
2:V:4:DG:H2"	2:V:5:DC:H5'	1.96	0.48
1:B:1060:PRO:HG2	1:B:1130:LYS:HA	1.96	0.48
1:B:1265:PRO:O	1:B:1268:VAL:HB	2.14	0.48
1:B:1325:THR:CB	1:B:1326:PRO:CD	2.90	0.48
1:D:487:THR:HB	1:D:493:PHE:CE1	2.49	0.48
1:D:488:GLY:O	1:D:493:PHE:HD1	1.96	0.48
3:F:6:DT:N3	3:F:7:DA:N7	2.62	0.48
1:S:448:ASP:C	1:S:450:ARG:H	2.17	0.48
1:S:493:PHE:CE2	1:S:530:PRO:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:470:ASP:OD1	1:U:471:ARG:N	2.47	0.48
1:U:1134:GLU:O	1:U:1163:ARG:HG2	2.13	0.48
1:B:1029:VAL:HA	1:B:1033:ARG:HB3	1.95	0.47
1:B:1431:ARG:NH1	1:D:1423:GLN:OE1	2.34	0.47
1:B:1475:GLU:HA	1:B:1478:ASP:HB2	1.96	0.47
1:D:532:ILE:HA	1:D:537:VAL:CG2	2.42	0.47
1:D:1185:PRO:HG2	1:D:1218:PHE:HA	1.96	0.47
1:D:1287:ASP:OD1	1:D:1287:ASP:N	2.47	0.47
1:D:1383:GLY:H	1:D:1421:GLN:NE2	2.06	0.47
2:E:4:DG:H2"	2:E:5:DC:H5'	1.95	0.47
1:S:1404:ASP:OD2	1:U:1431:ARG:HB2	2.15	0.47
1:U:1093:MET:HG2	1:U:1099:TYR:CE2	2.49	0.47
1:U:1346:ILE:HA	1:U:1350:GLU:OE1	2.13	0.47
1:B:517:ARG:O	1:B:521:LEU:HG	2.14	0.47
1:B:525:TYR:CE2	1:B:526:ARG:NH1	2.82	0.47
1:B:1031:VAL:CG2	1:B:1032:ALA:H	2.25	0.47
1:B:1087:TYR:O	1:B:1090:MET:N	2.47	0.47
1:B:1190:GLU:CD	1:B:1484:ARG:HH21	2.16	0.47
1:D:429:CYS:O	1:D:430:GLU:HB3	2.14	0.47
1:D:458:ARG:CB	7:H:1020:CPF:H172	2.39	0.47
1:D:1038:VAL:HG11	1:D:1339:VAL:HG22	1.96	0.47
1:S:1051:TYR:CE2	1:S:1157:PRO:HD3	2.48	0.47
1:S:1113:MET:C	1:S:1115:GLY:H	2.17	0.47
1:S:1162:ALA:C	1:S:1164:PHE:N	2.68	0.47
1:S:1246:ARG:HH22	1:S:1487:GLU:HB3	1.79	0.47
1:D:485:PHE:CZ	1:D:524:PHE:CZ	3.03	0.47
1:S:1013:ASN:HB3	1:S:1016:SER:CB	2.36	0.47
1:S:1083:ASP:HA	1:S:1086:ILE:HG13	1.95	0.47
1:S:1151:ASP:C	1:S:1153:ASN:H	2.16	0.47
1:U:1225:LEU:N	1:U:1225:LEU:HD23	2.29	0.47
1:U:1406:VAL:O	1:U:1409:GLU:N	2.47	0.47
1:B:1120:ALA:HB3	1:B:1123:PHE:HD1	1.79	0.47
1:D:485:PHE:CE2	1:D:524:PHE:CE2	3.02	0.47
1:D:1079:HIS:CD2	1:D:1081:HIS:HD2	2.32	0.47
5:H:12:DC:C2'	5:H:13:DA:O5'	2.63	0.47
1:S:418:LEU:O	1:S:418:LEU:CG	2.62	0.47
1:S:1022:PHE:O	1:S:1025:TYR:HB3	2.14	0.47
3:W:7:DA:H2"	3:W:8:DG:C5'	2.35	0.47
4:X:14:DC:H2'	4:X:15:DA:C8	2.49	0.47
1:B:512:ASP:OD2	2:E:8:DT:H5'	2.14	0.47
1:B:1080:PRO:HD2	1:B:1081:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1406:VAL:O	1:B:1410:SER:N	2.47	0.47
1:D:536:TYR:CD2	1:D:536:TYR:N	2.83	0.47
1:D:1241:ILE:HD12	1:D:1333:VAL:CG2	2.44	0.47
1:D:1483:ASP:OD1	1:D:1483:ASP:N	2.44	0.47
1:S:1091:VAL:HG12	1:S:1095:GLN:NE2	2.28	0.47
1:S:1093:MET:HB3	1:S:1104:VAL:HG23	1.95	0.47
1:S:1215:GLY:HA3	1:S:1488:ILE:CD1	2.40	0.47
1:U:1230:ILE:HG23	1:U:1234:TYR:HE2	1.78	0.47
1:U:1476:ILE:C	1:U:1478:ASP:H	2.18	0.47
1:B:469:LEU:HG	1:B:473:LEU:HG	1.97	0.47
1:B:1467:GLN:NE2	1:B:1471:ASP:OD1	2.43	0.47
1:D:626:VAL:HG22	1:D:629:ARG:HH21	1.77	0.47
1:D:1445:TYR:CE1	1:D:1449:LEU:HD11	2.50	0.47
1:D:1461:ASP:OD1	1:D:1464:VAL:HG23	2.15	0.47
1:U:1022:PHE:CD2	1:U:1022:PHE:O	2.68	0.47
1:U:1031:VAL:HA	1:U:1338:LEU:CD1	2.42	0.47
1:U:1264:ILE:HB	1:U:1265:PRO:CD	2.43	0.47
1:U:1395:ILE:O	1:U:1399:ARG:HG3	2.15	0.47
1:B:452:GLN:HE22	1:B:596:MET:HB3	1.78	0.47
1:B:1201:ASN:C	1:B:1203:ASP:H	2.16	0.47
1:B:1245:SER:CB	1:B:1263:GLU:O	2.63	0.47
1:B:1349:LYS:O	1:B:1352:LEU:N	2.47	0.47
1:B:1431:ARG:HH12	1:D:1423:GLN:NE2	2.09	0.47
1:B:1468:LEU:O	1:B:1472:GLU:HG3	2.13	0.47
1:D:428:GLU:O	1:D:451:THR:HG22	2.15	0.47
1:D:1052:GLY:O	1:D:1056:GLN:HB2	2.15	0.47
1:D:1163:ARG:NH2	1:D:1363:VAL:HG22	2.28	0.47
1:D:1231:ARG:HH11	1:D:1231:ARG:HG3	1.75	0.47
1:D:1391:ILE:CG2	1:D:1392:ASP:N	2.78	0.47
1:S:418:LEU:C	1:S:418:LEU:HD12	2.35	0.47
1:S:437:ASP:OD2	5:Y:10:DT:OP1	2.33	0.47
1:S:437:ASP:OD2	5:Y:10:DT:H5"	2.15	0.47
1:S:1261:VAL:HG12	1:S:1263:GLU:O	2.15	0.47
1:U:1040:ASP:CG	1:U:1042:LEU:HD12	2.35	0.47
1:U:1122:ARG:NH1	4:X:9:DG:H3'	2.14	0.47
1:U:1137:ARG:O	1:U:1138:ASP:HB2	2.14	0.47
1:U:1291:ASP:OD2	1:U:1292:LEU:N	2.47	0.47
4:X:13:DC:C4	4:X:14:DC:C4	3.03	0.47
1:B:514:ALA:HA	1:B:517:ARG:CZ	2.45	0.47
1:D:446:GLY:O	1:D:592:TRP:HB2	2.14	0.47
1:D:1055:GLU:C	1:D:1057:GLY:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:424:LYS:O	1:S:426:PRO:HD3	2.14	0.47
1:S:495:LEU:HD11	1:S:534:ALA:CB	2.45	0.47
1:S:1466:LEU:HD11	1:S:1470:ARG:HE	1.79	0.47
1:U:493:PHE:HE2	1:U:530:PRO:HB2	1.79	0.47
5:Y:12:DC:C5'	5:Y:12:DC:H6	2.28	0.47
1:D:1104:VAL:CG1	1:D:1126:ALA:HB1	2.45	0.47
1:D:1224:ILE:HG21	1:D:1230:ILE:HD11	1.96	0.47
1:S:418:LEU:CD1	1:S:454:ILE:O	2.63	0.47
1:S:423:SER:O	1:S:429:CYS:SG	2.73	0.47
1:S:1070:ILE:HD12	1:S:1126:ALA:HB3	1.97	0.47
1:U:1157:PRO:C	1:U:1159:VAL:N	2.68	0.47
1:B:1069:ARG:HE	1:B:1069:ARG:HB3	1.25	0.47
1:D:504:VAL:HG13	1:D:540:ALA:H	1.80	0.47
1:S:1111:GLY:CA	1:S:1116:ASP:HB2	2.43	0.47
1:B:444:LYS:HA	1:B:447:ARG:HH11	1.80	0.46
1:B:1432:ARG:HG2	1:B:1437:GLU:HB3	1.97	0.46
1:D:1165:PRO:O	1:D:1169:ALA:HB2	2.15	0.46
1:S:1204:ILE:CG1	1:S:1205:SER:N	2.77	0.46
1:U:1037:ASP:C	1:U:1039:ARG:H	2.18	0.46
1:U:1301:GLY:O	1:U:1302:VAL:C	2.53	0.46
1:B:1135:LEU:HG	1:B:1164:PHE:HE2	1.81	0.46
1:D:1383:GLY:N	1:D:1421:GLN:HE21	2.08	0.46
1:S:1406:VAL:O	1:S:1409:GLU:N	2.48	0.46
1:U:1020:GLU:O	1:U:1024:ASP:HB2	2.16	0.46
1:U:1092:ARG:NH1	1:U:1098:SER:HB3	2.30	0.46
1:U:1201:ASN:O	1:U:1202:PRO:C	2.54	0.46
1:U:1371:LEU:HG	1:U:1372:ARG:N	2.30	0.46
1:B:1244:ARG:CG	1:B:1245:SER:H	2.23	0.46
1:D:472:ILE:C	1:D:474:ASN:H	2.19	0.46
1:D:1091:VAL:O	1:D:1094:ALA:HB3	2.15	0.46
1:D:1168:LEU:HD21	1:D:1351:ALA:HB1	1.97	0.46
1:S:1245:SER:HB2	1:S:1261:VAL:HG11	1.97	0.46
1:U:1467:GLN:OE1	1:U:1470:ARG:HD2	2.15	0.46
1:D:448:ASP:OD1	1:D:449:SER:N	2.48	0.46
1:D:1179:MET:C	4:G:17:DG:H4'	2.36	0.46
1:D:1209:LEU:HD13	1:D:1352:LEU:CD1	2.46	0.46
1:U:504:VAL:HA	1:U:538:TYR:O	2.15	0.46
1:U:538:TYR:N	1:U:538:TYR:CD1	2.83	0.46
1:U:1268:VAL:CG1	1:U:1269:ASN:N	2.78	0.46
1:U:1402:ASP:OD2	1:U:1403:THR:HG23	2.15	0.46
1:B:1131:ILE:HG13	1:B:1131:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:GLU:HA	1:B:1282:ARG:NH2	2.30	0.46
1:D:464:VAL:HG23	1:D:522:THR:HG22	1.97	0.46
1:D:1258:ARG:HD2	1:D:1305:VAL:HG13	1.96	0.46
1:D:1182:ASN:ND2	1:D:1331:PHE:CZ	2.84	0.46
1:D:1242:GLN:HE21	1:D:1330:SER:HB3	1.79	0.46
1:D:1245:SER:HA	1:D:1263:GLU:O	2.16	0.46
5:H:9:DG:H2"	5:H:10:DT:C6	2.51	0.46
1:S:458:ARG:HB3	7:X:1020:CPF:H172	1.97	0.46
1:S:1079:HIS:NE2	1:S:1081:HIS:CD2	2.77	0.46
1:S:1221:ALA:HA	1:S:1485:ARG:C	2.36	0.46
1:S:1293:ARG:NH2	1:S:1295:GLU:OE2	2.40	0.46
1:B:585:GLU:O	1:D:1108:GLY:CA	2.55	0.46
1:B:1047:ARG:HE	1:B:1047:ARG:HB2	1.54	0.46
1:D:522:THR:OG1	1:D:622:MET:HG3	2.16	0.46
1:D:526:ARG:NH1	1:D:615:ASP:OD1	2.41	0.46
1:D:604:LEU:CD2	1:D:1012:ARG:HB2	2.44	0.46
1:S:1291:ASP:HB3	1:S:1307:ASP:HB2	1.97	0.46
1:B:459:GLY:HA3	2:E:8:DT:O2	2.16	0.46
1:B:1311:ASP:OD1	1:B:1311:ASP:N	2.49	0.46
1:D:532:ILE:HA	1:D:537:VAL:HG21	1.97	0.46
1:D:539:ILE:HB	1:D:604:LEU:CB	2.46	0.46
1:D:1261:VAL:O	1:D:1303:ARG:HA	2.15	0.46
1:D:1436:LEU:O	1:D:1440:LYS:N	2.33	0.46
1:S:1100:ARG:HD2	1:S:1485:ARG:HH11	1.80	0.46
1:S:1412:GLN:HB3	1:S:1417:LEU:O	2.15	0.46
1:B:1342:ARG:HB3	1:B:1343:PRO:HD2	1.96	0.46
1:D:481:MET:HE3	1:D:523:PHE:CE2	2.51	0.46
1:D:1198:LEU:CD2	1:D:1352:LEU:HB2	2.46	0.46
1:D:1218:PHE:HE2	1:D:1224:ILE:HD11	1.81	0.46
1:S:1070:ILE:CD1	1:S:1126:ALA:HB3	2.46	0.46
1:S:1387:ALA:CA	1:S:1394:ILE:HG13	2.45	0.46
1:U:1165:PRO:CA	1:U:1355:TYR:CZ	2.99	0.46
1:U:1190:GLU:HB3	1:U:1212:ASP:O	2.16	0.46
4:X:13:DC:C6	7:X:1020:CPF:H142	2.51	0.46
1:B:526:ARG:HB3	1:B:527:PHE:CE1	2.51	0.46
1:B:1429:ARG:NH1	1:D:1427:ASP:O	2.48	0.46
1:D:543:PRO:HG3	1:D:594:THR:CG2	2.46	0.46
1:D:1101:TYR:HB3	1:D:1131:ILE:HD13	1.97	0.46
1:S:484:ALA:O	1:S:500:TYR:HE1	1.99	0.46
1:S:538:TYR:N	1:S:538:TYR:CD1	2.83	0.46
1:S:1101:TYR:HB3	1:S:1131:ILE:CD1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1245:SER:OG	1:S:1327:LEU:CD1	2.63	0.46
1:S:1269:ASN:O	1:S:1270:LYS:C	2.54	0.46
1:U:1262:THR:HA	1:U:1302:VAL:O	2.15	0.46
1:B:423:SER:HB2	1:B:450:ARG:O	2.16	0.45
1:B:1039:ARG:HH21	1:B:1159:VAL:CB	2.24	0.45
1:D:526:ARG:HB2	1:D:527:PHE:CD1	2.51	0.45
1:D:1192:ILE:CD1	1:D:1477:ARG:HB2	2.28	0.45
1:D:1442:GLU:O	1:D:1442:GLU:HG3	2.15	0.45
1:S:1371:LEU:HD11	1:S:1452:ILE:HG22	1.97	0.45
1:S:1404:ASP:HA	1:S:1407:ALA:HB3	1.97	0.45
1:U:1040:ASP:OD2	1:U:1159:VAL:HG23	2.17	0.45
2:V:5:DC:H2'	2:V:5:DC:O5'	2.17	0.45
1:B:1088:GLU:HA	1:B:1091:VAL:HB	1.97	0.45
1:B:1111:GLY:N	1:B:1118:ALA:HA	2.31	0.45
1:B:1408:MET:HE1	1:B:1423:GLN:HE21	1.81	0.45
1:D:620:MET:HE3	1:D:621:LEU:HG	1.98	0.45
1:D:1080:PRO:HG3	1:D:1150:TYR:CD1	2.51	0.45
1:S:1033:ARG:CZ	2:V:7:DG:H4'	2.46	0.45
1:S:1079:HIS:CE1	1:S:1081:HIS:CD2	2.99	0.45
1:S:1213:ILE:HG22	1:S:1214:GLU:N	2.31	0.45
1:S:1346:ILE:HD12	1:S:1351:ALA:HB2	1.98	0.45
1:U:610:ASP:OD1	1:U:613:GLU:N	2.49	0.45
1:U:1038:VAL:HG22	1:U:1038:VAL:O	2.16	0.45
5:Y:14:DC:H2'	5:Y:15:DC:H6	1.82	0.45
1:B:526:ARG:CB	1:B:527:PHE:CD1	2.99	0.45
1:B:1201:ASN:C	1:B:1201:ASN:OD1	2.55	0.45
1:B:1225:LEU:HB2	1:B:1242:GLN:CB	2.47	0.45
1:B:1459:LEU:O	1:B:1461:ASP:N	2.44	0.45
1:D:528:MET:O	1:D:531:LEU:N	2.48	0.45
1:S:1149:ASN:ND2	1:S:1151:ASP:OD1	2.48	0.45
1:S:1201:ASN:HA	1:S:1202:PRO:HD3	1.80	0.45
1:S:1310:LYS:O	1:S:1311:ASP:HB2	2.16	0.45
1:U:1033:ARG:N	1:U:1044:PRO:HG2	2.31	0.45
1:U:1349:LYS:O	1:U:1350:GLU:C	2.54	0.45
2:V:8:DT:C2	7:Y:1020:CPF:H132	2.51	0.45
7:X:1020:CPF:H141	7:X:1020:CPF:F1	2.06	0.45
7:Y:1020:CPF:H9	7:Y:1020:CPF:H171	1.52	0.45
1:B:1080:PRO:C	1:B:1081:HIS:CG	2.89	0.45
1:B:1293:ARG:NH2	1:B:1305:VAL:HG11	2.31	0.45
1:B:1379:HIS:O	1:B:1382:GLU:HB2	2.16	0.45
1:D:527:PHE:O	1:D:528:MET:CG	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1179:MET:O	1:S:1180:ALA:CB	2.62	0.45
1:S:1227:LYS:O	1:S:1230:ILE:HB	2.16	0.45
1:U:1104:VAL:CG1	1:U:1105:ASP:N	2.80	0.45
1:B:1044:PRO:O	1:B:1048:ARG:HB2	2.16	0.45
1:B:1364:ARG:HB2	1:B:1465:LEU:HD21	1.99	0.45
1:B:1412:GLN:OE1	1:B:1419:GLU:HA	2.16	0.45
1:D:462:LEU:HA	4:G:14:DC:O3'	2.17	0.45
1:S:421:CYS:H	1:S:453:ALA:HB2	1.82	0.45
1:U:457:LEU:HD11	1:U:520:LEU:HD11	1.97	0.45
1:U:1218:PHE:CD1	1:U:1266:PHE:CG	3.05	0.45
1:U:1324:GLN:O	1:U:1325:THR:HG23	2.16	0.45
1:U:1368:GLN:O	1:U:1372:ARG:CD	2.64	0.45
1:B:432:PHE:HD2	1:B:506:MET:HE2	1.81	0.45
1:B:1038:VAL:HG21	1:B:1354:HIS:CB	2.47	0.45
1:B:1066:LYS:HE3	1:B:1125:GLU:OE2	2.17	0.45
1:D:1019:ARG:O	1:D:1023:LEU:HB2	2.17	0.45
1:S:446:GLY:O	1:S:592:TRP:HB2	2.17	0.45
1:S:527:PHE:N	1:S:527:PHE:CD1	2.84	0.45
1:S:1029:VAL:HG13	1:S:1033:ARG:HB3	1.98	0.45
1:S:1072:GLY:C	1:U:1069:ARG:HG3	2.37	0.45
1:U:1217:ASP:OD2	1:U:1484:ARG:HA	2.17	0.45
1:U:1266:PHE:O	1:U:1268:VAL:HG23	2.16	0.45
1:U:1290:THR:CG2	1:U:1309:ARG:N	2.80	0.45
1:U:1368:GLN:CG	1:U:1459:LEU:HD11	2.39	0.45
1:U:1393:GLU:O	1:U:1396:SER:N	2.50	0.45
1:B:438:SER:O	1:B:439:ALA:C	2.55	0.45
1:B:621:LEU:HD22	1:B:1022:PHE:CD2	2.52	0.45
1:B:1107:GLN:HG2	1:B:1125:GLU:OE1	2.17	0.45
1:B:1175:ILE:HD13	5:H:17:DC:C2	2.51	0.45
1:B:1363:VAL:HG11	1:B:1468:LEU:HD23	1.97	0.45
1:D:484:ALA:O	1:D:500:TYR:HE1	1.99	0.45
1:S:1322:TYR:O	1:S:1328:GLN:HB3	2.17	0.45
1:U:446:GLY:O	1:U:592:TRP:CE3	2.70	0.45
1:U:1204:ILE:HG23	1:U:1204:ILE:O	2.15	0.45
1:U:1310:LYS:HG2	1:U:1311:ASP:OD1	2.17	0.45
1:B:447:ARG:CB	1:B:596:MET:HE1	2.47	0.45
1:B:1012:ARG:HD2	1:B:1013:ASN:N	2.31	0.45
1:D:450:ARG:HB2	1:D:450:ARG:NH1	2.31	0.45
1:D:1310:LYS:O	1:D:1312:ALA:N	2.48	0.45
1:S:457:LEU:O	1:S:459:GLY:N	2.50	0.45
1:S:463:ASN:C	1:S:463:ASN:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1346:ILE:HG22	1:S:1350:GLU:OE1	2.16	0.45
1:U:536:TYR:O	1:U:538:TYR:CE1	2.70	0.45
1:U:541:GLN:HB2	1:U:602:ALA:HB3	1.99	0.45
1:U:1038:VAL:HG21	1:U:1339:VAL:HG22	1.98	0.45
1:B:527:PHE:CD1	1:B:527:PHE:N	2.85	0.45
1:B:587:ASN:CB	1:B:589:ASP:OD1	2.60	0.45
1:B:1446:ASN:HA	1:B:1449:LEU:HD12	1.99	0.45
1:D:475:ASN:C	1:D:475:ASN:OD1	2.54	0.45
1:D:586:MET:HE3	1:D:590:GLN:HG3	1.99	0.45
1:D:1150:TYR:CD2	1:D:1151:ASP:HB3	2.51	0.45
1:S:1177:VAL:O	1:S:1179:MET:HG2	2.17	0.45
1:U:461:ILE:HG12	1:U:520:LEU:HD21	1.99	0.45
1:B:529:ARG:N	1:B:530:PRO:CD	2.80	0.45
1:B:621:LEU:O	1:B:629:ARG:HD2	2.17	0.45
1:D:446:GLY:O	1:D:592:TRP:CE3	2.70	0.45
1:D:1044:PRO:O	1:D:1046:HIS:N	2.50	0.45
1:D:1153:ASN:C	1:D:1154:GLU:HG2	2.36	0.45
1:D:1185:PRO:HG2	1:D:1217:ASP:O	2.17	0.45
1:D:1455:LEU:O	1:D:1459:LEU:HG	2.16	0.45
3:F:2:DG:N2	4:G:19:DC:O2	2.43	0.45
1:S:461:ILE:CD1	1:S:477:GLU:CB	2.94	0.45
1:S:1035:LEU:HA	1:S:1036:PRO:HD3	1.58	0.45
1:D:602:ALA:C	1:D:603:LEU:HD23	2.38	0.44
1:D:1031:VAL:HG12	1:D:1338:LEU:CD2	2.45	0.44
1:D:1064:TYR:CE2	1:D:1107:GLN:OE1	2.70	0.44
7:H:1020:CPF:H142	7:H:1020:CPF:F1	2.07	0.44
1:S:459:GLY:HA3	3:W:8:DG:N3	2.32	0.44
1:S:597:ASN:HA	1:S:598:PRO:HD2	1.63	0.44
1:S:1388:LEU:CD2	1:S:1438:ARG:HG2	2.47	0.44
1:U:617:THR:HG22	1:U:618:PHE:N	2.32	0.44
1:U:1198:LEU:C	1:U:1200:LYS:H	2.20	0.44
1:U:1243:MET:O	1:U:1244:ARG:HB2	2.17	0.44
2:V:3:DT:H2"	2:V:4:DG:OP2	2.17	0.44
4:X:9:DG:N1	5:Y:11:DA:N6	2.66	0.44
1:S:1083:ASP:OD2	1:S:1084:SER:N	2.50	0.44
1:S:1132:THR:O	1:S:1135:LEU:HB2	2.17	0.44
1:U:1025:TYR:CZ	1:U:1029:VAL:HG21	2.52	0.44
1:B:1027[B]:MET:HA	1:B:1027[B]:MET:CE	2.47	0.44
1:D:626:VAL:HG22	4:G:17:DG:P	2.57	0.44
1:D:1184:PRO:HG3	1:D:1333:VAL:HG22	1.99	0.44
1:S:471:ARG:NH1	1:S:471:ARG:CG	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1071:VAL:O	1:B:1073:ASP:N	2.50	0.44
1:D:494:ASP:CB	1:D:497:LYS:HE3	2.47	0.44
7:G:1020:CPF:H171	7:G:1020:CPF:H9	1.54	0.44
1:S:1093:MET:HE2	1:S:1093:MET:HB2	1.50	0.44
1:S:1221:ALA:HA	1:S:1486:THR:N	2.32	0.44
1:S:1428:MET:HE2	1:S:1428:MET:HB3	1.70	0.44
1:U:493:PHE:CE2	1:U:530:PRO:HB2	2.53	0.44
1:B:444:LYS:HA	1:B:447:ARG:HD3	2.00	0.44
1:B:1063:SER:O	1:B:1065:LYS:CE	2.60	0.44
1:B:1092:ARG:C	1:B:1094:ALA:H	2.21	0.44
1:D:597:ASN:HD22	1:D:598:PRO:HD2	1.83	0.44
1:S:522:THR:HA	1:S:618:PHE:CE2	2.53	0.44
1:S:597:ASN:HD22	1:S:598:PRO:CD	2.31	0.44
1:S:1221:ALA:CB	1:S:1485:ARG:O	2.62	0.44
1:U:529:ARG:O	1:U:533:GLU:HG3	2.17	0.44
1:U:1218:PHE:HD1	1:U:1266:PHE:CG	2.35	0.44
1:B:1191:LEU:CD2	1:B:1213:ILE:HD13	2.48	0.44
1:B:1331:PHE:HD2	1:B:1333:VAL:HG23	1.83	0.44
1:B:1394:ILE:O	1:B:1398:ILE:HG13	2.18	0.44
1:B:1405:LYS:NZ	1:B:1409:GLU:OE1	2.47	0.44
1:D:1425:ILE:HG23	1:D:1428:MET:HE2	2.00	0.44
1:S:437:ASP:HB3	5:Y:9:DG:O3'	2.17	0.44
1:S:1129:THR:OG1	1:S:1131:ILE:HG23	2.17	0.44
1:U:462:LEU:HD11	1:U:467:ALA:HB2	1.99	0.44
1:U:520:LEU:HD22	1:U:520:LEU:HA	1.77	0.44
1:U:1025:TYR:CE2	1:U:1029:VAL:HG21	2.52	0.44
1:B:1054:ASN:HB2	1:B:1136:LEU:HD13	1.98	0.44
1:B:1058:MET:CE	1:B:1065:LYS:HG3	2.47	0.44
1:B:1071:VAL:O	1:B:1072:GLY:C	2.55	0.44
1:B:1430:LEU:O	1:B:1432:ARG:N	2.51	0.44
1:D:526:ARG:HB2	1:D:527:PHE:CE1	2.52	0.44
1:D:604:LEU:HD13	1:D:1012:ARG:HB2	2.00	0.44
1:S:458:ARG:NE	1:S:477:GLU:OE2	2.51	0.44
1:S:508:ASP:HB2	1:S:583:LEU:H	1.83	0.44
1:U:612:ILE:HD13	1:U:612:ILE:HA	1.83	0.44
1:B:1171:GLY:O	1:B:1172:ALA:HB2	2.18	0.44
1:B:1381:LEU:CD1	1:B:1448:LEU:HD12	2.46	0.44
1:D:536:TYR:HD2	1:D:536:TYR:N	2.16	0.44
1:D:1318:LEU:HG	1:D:1322:TYR:HE2	1.82	0.44
1:S:1177:VAL:C	1:S:1179:MET:N	2.70	0.44
1:U:1093:MET:HA	1:U:1099:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:1020:CPF:H9	7:X:1020:CPF:H11	1.65	0.44
1:B:597:ASN:ND2	1:B:598:PRO:HD2	2.30	0.44
1:B:1218:PHE:HA	1:B:1219:PRO:HD2	1.79	0.44
1:B:1300:THR:CG2	1:B:1303:ARG:HD3	2.47	0.44
1:B:1382:GLU:O	1:B:1383:GLY:C	2.56	0.44
1:B:1435:GLY:O	1:B:1439:ASP:OD2	2.34	0.44
1:D:632:PHE:CE1	1:D:1019:ARG:NH2	2.86	0.44
1:S:475:ASN:O	1:S:478:ILE:HB	2.17	0.44
1:S:1417:LEU:HD22	1:S:1421:GLN:HB3	2.00	0.44
1:U:597:ASN:HA	1:U:598:PRO:HD2	1.84	0.44
1:U:1381:LEU:HD12	1:U:1448:LEU:HD12	1.99	0.44
7:X:1020:CPF:F1	7:X:1020:CPF:C14	2.54	0.44
1:B:499:ARG:HB2	1:B:500:TYR:CD1	2.53	0.43
1:B:586:MET:H	1:B:586:MET:HG3	1.58	0.43
1:B:1317:ILE:O	1:B:1320:ASN:N	2.47	0.43
1:D:446:GLY:C	1:D:592:TRP:HB2	2.39	0.43
1:D:457:LEU:HD13	1:D:461:ILE:HD11	1.99	0.43
1:S:1145:ASP:OD1	1:S:1145:ASP:N	2.49	0.43
1:S:1382:GLU:HG3	1:S:1445:TYR:HE1	1.80	0.43
1:U:1226:GLY:C	1:U:1228:SER:H	2.20	0.43
1:B:444:LYS:O	1:B:447:ARG:NH1	2.51	0.43
1:B:1282:ARG:HG2	1:B:1283:ASP:OD1	2.17	0.43
1:B:1372:ARG:O	1:B:1376:ASP:HB2	2.18	0.43
1:D:1314:ALA:O	1:D:1318:LEU:N	2.51	0.43
1:D:1467:GLN:O	1:D:1468:LEU:C	2.56	0.43
5:H:12:DC:H2"	5:H:13:DA:O5'	2.18	0.43
1:S:1215:GLY:H	1:S:1484:ARG:NH2	2.16	0.43
1:S:1358:HIS:HD2	1:S:1359:GLN:NE2	2.16	0.43
1:U:464:VAL:HG23	1:U:465:GLU:N	2.32	0.43
1:U:1177:VAL:O	1:U:1177:VAL:HG12	2.17	0.43
1:U:1419:GLU:O	1:U:1423:GLN:HB2	2.17	0.43
2:V:6:DG:H1	5:Y:15:DC:N4	2.16	0.43
5:Y:13:DA:OP2	5:Y:13:DA:H8	2.01	0.43
1:B:444:LYS:CA	1:B:447:ARG:HH11	2.30	0.43
1:B:503:ILE:O	1:B:503:ILE:HG22	2.18	0.43
1:B:1107:GLN:HB3	1:B:1125:GLU:HB2	2.00	0.43
1:B:1230:ILE:O	1:B:1233:ALA:HB3	2.18	0.43
1:D:1051:TYR:CD2	1:D:1157:PRO:HD3	2.53	0.43
1:S:520:LEU:HD23	1:S:520:LEU:HA	1.76	0.43
1:S:1129:THR:OG1	1:S:1132:THR:OG1	2.29	0.43
1:S:1174:GLY:H	1:S:1181:THR:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1220:THR:O	1:S:1221:ALA:HB3	2.18	0.43
1:S:1394:ILE:HD13	1:S:1415:PHE:CE1	2.52	0.43
1:U:433:LEU:HD12	1:U:505:ILE:HG12	2.00	0.43
1:U:1188:LEU:HD12	1:U:1188:LEU:HA	1.71	0.43
1:B:420:ASP:OD1	1:B:421:CYS:N	2.51	0.43
1:B:1183:ILE:HA	1:B:1184:PRO:HD3	1.66	0.43
1:B:1415:PHE:CB	1:B:1417:LEU:HG	2.49	0.43
1:D:532:ILE:HD13	1:D:1014:ILE:HD12	2.01	0.43
1:D:1131:ILE:O	1:D:1131:ILE:CG1	2.66	0.43
1:D:1164:PHE:O	1:D:1164:PHE:CD1	2.71	0.43
1:S:501:HIS:CD2	1:S:536:TYR:HH	2.35	0.43
1:S:1224:ILE:HD12	1:S:1488:ILE:CG1	2.48	0.43
1:S:1318:LEU:HD12	1:S:1318:LEU:C	2.39	0.43
1:S:1398:ILE:CD1	1:S:1411:LEU:HD11	2.48	0.43
1:S:1428:MET:HA	1:S:1432:ARG:NH1	2.32	0.43
1:U:435:GLU:HG3	1:U:507:THR:CA	2.48	0.43
1:U:592:TRP:HE3	1:U:596:MET:HE3	1.81	0.43
4:X:13:DC:H1'	7:X:1020:CPF:H142	2.01	0.43
1:B:627:GLU:OE1	1:B:627:GLU:HA	2.18	0.43
1:B:1071:VAL:C	1:B:1073:ASP:H	2.21	0.43
1:B:1122:ARG:NH2	1:B:1123:PHE:CE1	2.86	0.43
1:B:1265:PRO:HB2	1:B:1268:VAL:CG2	2.48	0.43
1:B:1334:ASN:O	1:B:1336:ILE:HG13	2.18	0.43
1:B:1384:LEU:O	1:B:1385:ARG:C	2.56	0.43
1:D:525:TYR:HE2	1:D:526:ARG:NH1	2.16	0.43
1:D:1132:THR:O	1:D:1136:LEU:HD12	2.18	0.43
1:D:1462:GLU:O	1:D:1464:VAL:N	2.52	0.43
1:S:1185:PRO:O	1:S:1216:PRO:HA	2.19	0.43
1:S:1275:GLU:O	1:S:1279:GLU:HB2	2.19	0.43
1:S:1283:ASP:O	1:S:1284:LYS:HB2	2.17	0.43
1:U:418:LEU:HD13	1:U:455:LEU:HD13	2.00	0.43
1:U:1025:TYR:CZ	1:U:1029:VAL:CG2	3.01	0.43
1:U:1060:PRO:HD3	1:U:1133:LEU:HD21	2.00	0.43
1:B:1331:PHE:CD2	1:B:1333:VAL:HG23	2.53	0.43
1:D:1361:THR:O	1:D:1365:ARG:HG3	2.19	0.43
1:S:476:ASN:CG	1:S:480:GLN:NE2	2.71	0.43
1:S:521:LEU:HD22	1:U:1014:ILE:HG13	2.00	0.43
1:S:1432:ARG:H	1:S:1432:ARG:HG2	1.58	0.43
1:S:1439:ASP:O	1:S:1443:ALA:HB3	2.18	0.43
1:S:1449:LEU:HA	1:S:1452:ILE:HD12	2.00	0.43
1:B:540:ALA:O	1:B:542:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:PHE:CE1	1:D:596:MET:HE3	2.54	0.43
1:D:1410:SER:O	1:D:1411:LEU:C	2.57	0.43
1:S:1185:PRO:HG2	1:S:1218:PHE:HD1	1.84	0.43
1:U:1058:MET:SD	1:U:1070:ILE:HG12	2.59	0.43
1:U:1176:ALA:O	1:U:1177:VAL:HG23	2.19	0.43
1:U:1361:THR:O	1:U:1365:ARG:CG	2.57	0.43
1:B:1050:LEU:HD23	1:B:1053:LEU:HD12	2.01	0.43
1:B:1218:PHE:CG	1:B:1266:PHE:HB2	2.54	0.43
1:B:1411:LEU:HD23	1:B:1417:LEU:CD1	2.48	0.43
1:D:540:ALA:O	1:D:542:PRO:HD3	2.19	0.43
1:D:1425:ILE:HG23	1:D:1428:MET:CE	2.48	0.43
1:S:593:GLU:OE1	1:S:593:GLU:HA	2.18	0.43
1:S:1238:ARG:HA	1:S:1333:VAL:O	2.18	0.43
1:S:1245:SER:HB3	1:S:1261:VAL:HG11	2.01	0.43
1:U:1028:SER:C	1:U:1030:ILE:N	2.71	0.43
1:U:1100:ARG:HA	1:U:1219:PRO:HG3	2.00	0.43
1:U:1110:PHE:CZ	1:U:1124:THR:HB	2.54	0.43
1:U:1467:GLN:OE1	1:U:1467:GLN:HA	2.19	0.43
7:X:1020:CPF:H122	5:Y:9:DG:O5'	2.18	0.43
1:B:488:GLY:O	1:B:493:PHE:HD1	2.01	0.43
1:B:1079:HIS:HA	1:B:1080:PRO:HD3	1.89	0.43
1:B:1426:LEU:HD23	1:B:1426:LEU:HA	1.75	0.43
1:D:435:GLU:OE1	1:D:508:ASP:CB	2.49	0.43
1:D:592:TRP:O	1:D:597:ASN:N	2.51	0.43
1:D:1186:HIS:HB2	1:D:1191:LEU:CD1	2.42	0.43
1:D:1186:HIS:CD2	1:D:1216:PRO:HA	2.54	0.43
1:D:1421:GLN:O	1:D:1425:ILE:HG13	2.19	0.43
3:F:6:DT:C4	3:F:7:DA:N7	2.87	0.43
1:S:493:PHE:CG	1:S:494:ASP:N	2.86	0.43
1:U:542:PRO:HA	1:U:543:PRO:HD3	1.86	0.43
1:U:639:TYR:N	1:U:639:TYR:CD1	2.87	0.43
1:U:1101:TYR:O	1:U:1102:PRO:C	2.57	0.43
1:U:1156:GLU:HB2	1:U:1157:PRO:HD2	2.01	0.43
1:B:1029:VAL:O	1:B:1029:VAL:HG12	2.18	0.43
1:B:1034:ALA:HA	1:B:1043:LYS:HD3	2.01	0.43
1:D:448:ASP:H	1:D:592:TRP:HZ3	1.66	0.43
1:D:500:TYR:HB2	1:D:503:ILE:HD11	2.01	0.43
1:D:1127:ARG:O	1:D:1128:MET:C	2.57	0.43
1:D:1183:ILE:HA	1:D:1184:PRO:HD3	1.88	0.43
1:D:1366:ARG:O	1:D:1369:TYR:N	2.51	0.43
7:G:1020:CPF:H1	7:G:1020:CPF:H121	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:9:DG:C2'	5:H:10:DT:C5	2.94	0.43
1:S:1135:LEU:HD23	1:S:1162:ALA:HA	2.00	0.43
1:S:1224:ILE:HG23	1:S:1242:GLN:O	2.19	0.43
1:S:1348:LEU:O	1:S:1351:ALA:HB3	2.19	0.43
1:S:1377:ARG:O	1:S:1378:ALA:C	2.57	0.43
1:U:1035:LEU:HA	1:U:1036:PRO:HD3	1.75	0.43
1:U:1133:LEU:O	1:U:1137:ARG:N	2.52	0.43
1:B:495:LEU:HD12	1:B:495:LEU:O	2.19	0.42
1:B:1114:ASP:OD1	1:B:1270:LYS:NZ	2.48	0.42
1:B:1120:ALA:O	1:B:1122:ARG:N	2.52	0.42
1:D:458:ARG:HD2	1:D:477:GLU:HG3	2.01	0.42
1:D:1313:ASN:ND2	1:D:1316:VAL:H	2.12	0.42
1:D:1349:LYS:O	1:D:1350:GLU:C	2.57	0.42
1:S:1247:ALA:CB	1:S:1260:VAL:O	2.67	0.42
1:U:458:ARG:HB3	7:Y:1020:CPF:C16	2.43	0.42
1:U:592:TRP:O	1:U:593:GLU:C	2.56	0.42
1:U:592:TRP:O	1:U:596:MET:N	2.51	0.42
1:U:1030:ILE:C	1:U:1032:ALA:H	2.20	0.42
1:U:1165:PRO:CA	1:U:1355:TYR:CE2	2.97	0.42
1:U:1190:GLU:O	1:U:1213:ILE:CG1	2.66	0.42
1:U:1246:ARG:HB3	1:U:1263:GLU:HB2	2.01	0.42
1:U:1273:MET:SD	1:U:1327:LEU:HA	2.58	0.42
1:U:1450:ASN:HD22	1:U:1450:ASN:H	1.60	0.42
1:D:477:GLU:O	1:D:481:MET:HG3	2.18	0.42
1:D:1161:PRO:O	1:D:1162:ALA:C	2.56	0.42
1:D:1466:LEU:O	1:D:1470:ARG:HG3	2.20	0.42
1:U:430:GLU:O	1:U:430:GLU:HG2	2.19	0.42
1:U:587:ASN:HB2	1:U:590:GLN:HB2	2.00	0.42
1:U:1028:SER:O	1:U:1029:VAL:C	2.58	0.42
1:U:1119:ALA:O	1:U:1120:ALA:O	2.37	0.42
1:U:1165:PRO:HG3	1:U:1355:TYR:CE1	2.54	0.42
1:U:1238:ARG:CD	1:U:1345:LEU:HD21	2.48	0.42
1:U:1260:VAL:HG11	1:U:1303:ARG:NH1	2.34	0.42
1:B:473:LEU:O	1:B:479:ARG:HD2	2.19	0.42
1:B:1192:ILE:CD1	1:B:1477:ARG:HB2	2.42	0.42
1:D:1067:SER:C	1:D:1069:ARG:H	2.22	0.42
1:D:1143:THR:HG21	1:D:1362:VAL:HG13	2.01	0.42
1:D:1402:ASP:CG	1:D:1403:THR:H	2.23	0.42
3:F:6:DT:O4	3:F:7:DA:N6	2.52	0.42
5:H:12:DC:H3'	5:H:12:DC:OP2	2.19	0.42
1:S:431:ILE:HG13	1:S:453:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:522:THR:HG1	1:S:618:PHE:HE2	1.64	0.42
1:S:1038:VAL:HG21	1:S:1354:HIS:HB2	2.02	0.42
1:S:1293:ARG:HB2	1:S:1293:ARG:NH1	2.33	0.42
1:U:1070:ILE:O	1:U:1073:ASP:HB3	2.18	0.42
1:U:1281:VAL:CG2	1:U:1289:ILE:HD12	2.49	0.42
1:U:1450:ASN:ND2	1:U:1450:ASN:H	2.16	0.42
1:B:493:PHE:CD2	1:B:530:PRO:HB2	2.55	0.42
1:B:1405:LYS:CE	1:B:1409:GLU:OE1	2.67	0.42
1:D:512:ASP:HA	1:D:515:HIS:HB3	2.00	0.42
1:D:1145:ASP:O	1:D:1158:SER:HB3	2.20	0.42
1:D:1199:SER:CB	1:D:1470:ARG:HE	2.33	0.42
1:D:1461:ASP:O	1:D:1462:GLU:C	2.58	0.42
1:D:1467:GLN:O	1:D:1470:ARG:N	2.52	0.42
1:S:1027:MET:O	1:S:1030:ILE:N	2.47	0.42
1:S:1437:GLU:O	1:S:1441:ILE:HG13	2.20	0.42
1:U:1186:HIS:CD2	1:U:1234:TYR:OH	2.72	0.42
1:U:1346:ILE:HD12	1:U:1351:ALA:CA	2.47	0.42
1:U:1411:LEU:HA	1:U:1411:LEU:HD23	1.74	0.42
1:B:478:ILE:CG2	1:B:523:PHE:CZ	3.02	0.42
1:B:1365:ARG:HE	1:B:1365:ARG:HB3	1.51	0.42
1:D:586:MET:HB2	1:D:591:LEU:HD21	2.01	0.42
1:D:591:LEU:HD23	1:D:591:LEU:HA	1.80	0.42
1:D:1297:SER:C	1:D:1299:ARG:N	2.69	0.42
1:S:446:GLY:O	1:S:592:TRP:CE3	2.72	0.42
1:S:494:ASP:OD1	1:S:497:LYS:HE3	2.18	0.42
1:S:1317:ILE:H	1:S:1317:ILE:HG13	1.47	0.42
1:S:1457:THR:O	1:S:1464:VAL:HG11	2.20	0.42
1:U:1094:ALA:HB2	1:U:1104:VAL:HB	2.01	0.42
1:B:435:GLU:HB2	1:B:583:LEU:HD12	2.01	0.42
1:B:1036:PRO:HG3	1:B:1172:ALA:HB1	2.02	0.42
1:D:485:PHE:HZ	1:D:524:PHE:CZ	2.37	0.42
1:S:485:PHE:O	1:S:487:THR:HG23	2.19	0.42
1:S:1029:VAL:O	1:S:1029:VAL:CG1	2.65	0.42
1:S:1185:PRO:O	1:S:1186:HIS:ND1	2.53	0.42
1:S:1470:ARG:H	1:S:1470:ARG:HG3	1.62	0.42
1:U:1453:SER:O	1:U:1456:GLU:HB2	2.19	0.42
1:B:1201:ASN:O	1:B:1203:ASP:N	2.52	0.42
1:B:1408:MET:C	1:B:1410:SER:N	2.72	0.42
1:D:1394:ILE:CD1	1:D:1415:PHE:CZ	3.03	0.42
4:G:14:DC:H2"	4:G:15:DA:H5'	2.02	0.42
7:G:1020:CPF:F1	7:G:1020:CPF:C14	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:421:CYS:N	1:U:453:ALA:HB2	2.32	0.42
1:U:514:ALA:O	1:U:518:THR:HG23	2.20	0.42
1:U:598:PRO:HB3	1:U:601:ARG:CZ	2.48	0.42
1:U:1035:LEU:HA	1:U:1035:LEU:HD23	1.88	0.42
1:U:1134:GLU:OE2	1:U:1137:ARG:HD3	2.19	0.42
1:U:1238:ARG:HD2	1:U:1345:LEU:HD21	2.01	0.42
1:B:524:PHE:N	1:B:524:PHE:CD2	2.85	0.42
1:B:1195:VAL:HG12	1:B:1196:LEU:N	2.34	0.42
1:B:1286:ILE:O	1:B:1286:ILE:HG23	2.18	0.42
1:D:472:ILE:O	1:D:474:ASN:N	2.53	0.42
1:D:1467:GLN:OE1	1:D:1467:GLN:HA	2.20	0.42
1:S:1101:TYR:CB	1:S:1131:ILE:HD13	2.48	0.42
1:S:1138:ASP:OD1	1:S:1141:LYS:HD2	2.20	0.42
1:S:1217:ASP:HB2	1:S:1484:ARG:NH1	2.34	0.42
1:S:1219:PRO:HA	1:S:1485:ARG:HH11	1.84	0.42
1:U:492:ASP:O	1:U:494:ASP:N	2.53	0.42
1:U:1050:LEU:HD11	1:U:1103:LEU:HD13	2.01	0.42
1:U:1296:THR:HG22	1:U:1297:SER:N	2.35	0.42
1:U:1429:ARG:O	1:U:1432:ARG:HB2	2.19	0.42
4:X:17:DG:H2'	4:X:17:DG:O5'	2.20	0.42
1:B:519:LEU:O	1:B:522:THR:HB	2.19	0.42
1:D:611:ALA:O	1:D:615:ASP:HB2	2.19	0.42
1:D:1329:THR:CG2	1:D:1330:SER:N	2.81	0.42
1:D:1412:GLN:NE2	1:D:1419:GLU:HA	2.34	0.42
4:G:11:DA:H2"	4:G:12:DC:C5'	2.46	0.42
1:S:1259:ILE:HG22	1:S:1260:VAL:N	2.35	0.42
1:S:1296:THR:OG1	1:S:1303:ARG:N	2.47	0.42
1:S:1388:LEU:HD21	1:S:1438:ARG:HG2	2.02	0.42
1:S:1398:ILE:O	1:S:1399:ARG:C	2.58	0.42
1:S:1408:MET:HE1	1:S:1423:GLN:HG2	2.02	0.42
1:U:1264:ILE:CG2	1:U:1302:VAL:HG11	2.42	0.42
1:U:1295:GLU:HG3	1:U:1305:VAL:HG23	2.01	0.42
1:U:1425:ILE:O	1:U:1428:MET:HB3	2.20	0.42
1:B:500:TYR:O	1:B:501:HIS:HD2	2.03	0.42
1:B:1113:MET:HE2	1:B:1302:VAL:HG22	2.00	0.42
1:B:1224:ILE:HD13	1:B:1241:ILE:CG2	2.49	0.42
1:B:1266:PHE:O	1:B:1267:GLN:HB2	2.19	0.42
1:D:435:GLU:O	1:D:457:LEU:O	2.37	0.42
1:D:1013:ASN:HB3	1:D:1016:SER:HB2	2.01	0.42
1:D:1226:GLY:C	1:D:1228:SER:H	2.22	0.42
1:S:1071:VAL:O	1:S:1075:MET:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1193:ASN:O	1:S:1197:SER:OG	2.37	0.42
1:S:1245:SER:HB3	1:S:1263:GLU:O	2.20	0.42
1:U:485:PHE:HB3	1:U:487:THR:HG23	2.02	0.42
1:U:1043:LYS:HB3	1:U:1044:PRO:HD2	2.01	0.42
1:U:1046:HIS:CE1	3:W:6:DT:OP1	2.73	0.42
1:U:1238:ARG:HH11	1:U:1334:ASN:ND2	2.18	0.42
1:D:1037:ASP:HB3	1:D:1040:ASP:OD1	2.20	0.41
1:D:1049:ILE:HG21	1:D:1090:MET:HB2	2.02	0.41
1:D:1293:ARG:CZ	1:D:1305:VAL:HG11	2.50	0.41
1:D:1454:GLU:O	1:D:1457:THR:N	2.53	0.41
1:S:636:ASN:O	1:U:1023:LEU:HD21	2.19	0.41
1:S:1309:ARG:HD2	1:S:1309:ARG:C	2.40	0.41
1:S:1425:ILE:O	1:S:1426:LEU:C	2.57	0.41
1:U:1320:ASN:CB	1:U:1324:GLN:HE21	2.33	0.41
1:B:475:ASN:O	1:B:479:ARG:CD	2.68	0.41
1:B:1244:ARG:CG	1:B:1245:SER:N	2.81	0.41
1:B:1381:LEU:HB3	1:B:1445:TYR:HD2	1.85	0.41
1:D:493:PHE:CE2	1:D:495:LEU:HD13	2.55	0.41
1:D:494:ASP:C	1:D:496:ALA:N	2.73	0.41
1:S:1064:TYR:CE2	1:S:1107:GLN:CB	3.03	0.41
1:U:462:LEU:HD11	1:U:467:ALA:CB	2.50	0.41
1:U:1349:LYS:O	1:U:1352:LEU:N	2.53	0.41
1:U:1358:HIS:HD2	1:U:1359:GLN:NE2	2.17	0.41
1:B:515:HIS:HB2	1:B:1025:TYR:CG	2.54	0.41
1:B:532:ILE:HG12	1:B:537:VAL:HG21	2.02	0.41
1:B:536:TYR:N	1:B:536:TYR:CD2	2.88	0.41
1:B:1177:VAL:C	1:B:1179:MET:H	2.23	0.41
1:B:1201:ASN:OD1	1:B:1201:ASN:O	2.38	0.41
1:B:1322:TYR:CD1	1:B:1327:LEU:HD23	2.55	0.41
1:D:471:ARG:O	1:D:472:ILE:C	2.59	0.41
1:D:625:VAL:CB	1:D:628:ASN:ND2	2.84	0.41
1:D:1198:LEU:HG	1:D:1198:LEU:O	2.20	0.41
1:D:1336:ILE:HA	1:D:1344:LYS:O	2.19	0.41
1:D:1357:GLU:OE1	1:D:1357:GLU:CA	2.65	0.41
1:S:1030:ILE:CG2	1:S:1343:PRO:HG3	2.50	0.41
1:S:1067:SER:OG	1:S:1121:MET:O	2.38	0.41
1:S:1074:VAL:O	1:S:1074:VAL:HG12	2.21	0.41
1:S:1193:ASN:HA	1:S:1196:LEU:HB2	2.02	0.41
1:S:1363:VAL:CG1	1:S:1468:LEU:HD23	2.50	0.41
1:U:493:PHE:CE2	1:U:531:LEU:N	2.88	0.41
1:U:1243:MET:O	1:U:1328:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1391:ILE:O	1:U:1395:ILE:HG12	2.19	0.41
1:B:519:LEU:HA	1:B:519:LEU:HD23	1.73	0.41
1:B:1227:LYS:O	1:B:1231:ARG:HB2	2.20	0.41
1:B:1238:ARG:HG2	1:B:1334:ASN:HD22	1.85	0.41
1:B:1436:LEU:HD23	1:B:1440:LYS:HE3	2.01	0.41
1:S:437:ASP:H	5:Y:9:DG:C5'	2.32	0.41
1:S:627:GLU:O	1:S:629:ARG:N	2.53	0.41
1:U:1036:PRO:HA	1:U:1042:LEU:O	2.20	0.41
1:U:1038:VAL:HG11	1:U:1339:VAL:HA	2.01	0.41
1:U:1214:GLU:HB3	1:U:1488:ILE:HD12	2.02	0.41
1:B:457:LEU:CD1	1:B:477:GLU:HG3	2.50	0.41
1:B:1035:LEU:HA	1:B:1036:PRO:HD3	1.87	0.41
1:B:1049:ILE:O	1:B:1053:LEU:HG	2.21	0.41
1:B:1050:LEU:HD21	1:B:1093:MET:HE3	2.02	0.41
1:B:1058:MET:HG2	1:B:1065:LYS:HG3	2.01	0.41
1:B:1066:LYS:O	1:B:1070:ILE:HG13	2.20	0.41
1:D:1164:PHE:HA	1:D:1165:PRO:HD3	1.89	0.41
1:S:1185:PRO:HD2	1:S:1218:PHE:HE1	1.83	0.41
1:U:482:ILE:HG12	1:U:523:PHE:HZ	1.85	0.41
1:U:503:ILE:HD13	1:U:531:LEU:HD11	2.03	0.41
1:U:1299:ARG:H	1:U:1299:ARG:CD	2.29	0.41
1:B:526:ARG:C	1:B:527:PHE:CD1	2.94	0.41
1:B:1404:ASP:O	1:B:1408:MET:HG2	2.20	0.41
1:D:421:CYS:SG	1:D:429:CYS:SG	3.07	0.41
1:D:442:SER:CB	1:D:591:LEU:HD12	2.50	0.41
1:S:1027:MET:O	1:S:1028:SER:C	2.59	0.41
1:U:1107:GLN:C	1:U:1110:PHE:HE1	2.24	0.41
1:U:1259:ILE:H	1:U:1259:ILE:HG13	1.70	0.41
1:B:1171:GLY:HA2	1:B:1184:PRO:O	2.21	0.41
1:B:1274:ILE:HG23	1:B:1292:LEU:HD11	2.02	0.41
1:D:497:LYS:H	1:D:497:LYS:HG3	1.64	0.41
1:D:1376:ASP:O	1:D:1380:ILE:HG12	2.21	0.41
1:D:1400:GLU:O	1:D:1400:GLU:CG	2.61	0.41
1:D:1484:ARG:HD3	1:D:1486:THR:O	2.20	0.41
1:S:1037:ASP:HA	1:S:1338:LEU:HB2	2.01	0.41
1:S:1358:HIS:CD2	1:S:1359:GLN:HE21	2.39	0.41
1:U:1037:ASP:C	1:U:1039:ARG:N	2.73	0.41
1:U:1100:ARG:NH1	1:U:1485:ARG:NE	2.66	0.41
1:B:1077:LYS:HB3	1:B:1078:TYR:CE1	2.56	0.41
1:B:1221:ALA:HB2	1:B:1485:ARG:HB3	2.02	0.41
1:D:1402:ASP:OD2	1:D:1403:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:9:DG:H4'	5:H:10:DT:OP1	2.21	0.41
1:S:596:MET:HE3	1:S:596:MET:HB3	1.70	0.41
1:S:631:GLN:O	1:S:634:GLU:N	2.51	0.41
1:S:1038:VAL:HG12	1:S:1338:LEU:O	2.21	0.41
1:S:1074:VAL:O	1:S:1079:HIS:N	2.53	0.41
1:S:1075:MET:O	1:S:1075:MET:HG2	2.19	0.41
1:S:1452:ILE:HG13	1:S:1452:ILE:H	1.43	0.41
1:U:470:ASP:OD1	1:U:470:ASP:C	2.59	0.41
1:U:1238:ARG:CG	1:U:1345:LEU:HD21	2.51	0.41
1:U:1320:ASN:HB3	1:U:1324:GLN:NE2	2.36	0.41
1:U:1369:TYR:CD2	1:U:1370:ASN:N	2.89	0.41
2:V:6:DG:H1	5:Y:15:DC:H42	1.68	0.41
1:B:427:GLU:CD	1:B:427:GLU:H	2.24	0.41
1:B:1029:VAL:CA	1:B:1033:ARG:HB3	2.50	0.41
1:B:1064:TYR:CD1	1:B:1107:GLN:HB2	2.56	0.41
1:B:1252:ARG:HG2	1:B:1257:GLN:O	2.21	0.41
1:D:442:SER:HB2	1:D:591:LEU:HD12	2.02	0.41
1:D:469:LEU:HA	1:D:472:ILE:HD12	2.01	0.41
1:D:542:PRO:HA	1:D:543:PRO:HD3	1.79	0.41
1:D:587:ASN:HB2	1:D:590:GLN:HB2	2.02	0.41
1:D:630:ARG:O	1:D:633:ILE:HB	2.21	0.41
1:D:1013:ASN:HB3	1:D:1016:SER:CB	2.51	0.41
1:D:1266:PHE:CZ	1:D:1267:GLN:HG3	2.56	0.41
1:D:1439:ASP:O	1:D:1440:LYS:C	2.59	0.41
1:S:617:THR:O	1:S:621:LEU:HG	2.21	0.41
1:S:1113:MET:C	1:S:1115:GLY:N	2.74	0.41
1:S:1288:GLY:O	1:S:1317:ILE:HD13	2.21	0.41
1:S:1309:ARG:HH11	1:S:1309:ARG:CB	2.32	0.41
1:S:1325:THR:CB	1:S:1326:PRO:CD	2.98	0.41
1:S:1331:PHE:HD2	1:S:1333:VAL:HG22	1.86	0.41
1:S:1428:MET:HE2	1:U:1430:LEU:CD1	2.51	0.41
1:U:1041:GLY:HA3	1:U:1167:LEU:HA	2.03	0.41
1:U:1295:GLU:N	1:U:1303:ARG:O	2.41	0.41
1:U:1355:TYR:CZ	1:U:1359:GLN:HG3	2.56	0.41
1:U:1381:LEU:CD1	1:U:1448:LEU:HD12	2.51	0.41
1:U:1399:ARG:HG3	1:U:1399:ARG:H	1.59	0.41
1:U:1476:ILE:O	1:U:1478:ASP:N	2.54	0.41
3:W:3:DC:H6	3:W:3:DC:H2'	1.68	0.41
4:X:17:DG:C2	4:X:18:DG:C2	3.08	0.41
1:B:472:ILE:HD13	1:B:527:PHE:HZ	1.85	0.41
1:B:525:TYR:HE2	1:B:526:ARG:HH12	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1132:THR:O	1:B:1132:THR:HG22	2.20	0.41
1:D:429:CYS:O	1:D:430:GLU:CB	2.68	0.41
1:D:517:ARG:HB2	1:D:517:ARG:CZ	2.51	0.41
1:D:1313:ASN:O	1:D:1317:ILE:HG13	2.21	0.41
1:D:1358:HIS:O	1:D:1358:HIS:CG	2.73	0.41
3:F:8:DG:C2	4:G:14:DC:O2	2.74	0.41
5:H:19:DC:H1'	5:H:20:DA:O4'	2.21	0.41
1:U:464:VAL:HA	1:U:472:ILE:HG12	2.03	0.41
1:U:536:TYR:N	1:U:536:TYR:CD2	2.89	0.41
1:U:612:ILE:C	1:U:614:ALA:N	2.75	0.41
1:U:1269:ASN:CB	1:U:1272:ARG:NH1	2.84	0.41
5:Y:13:DA:OP2	5:Y:13:DA:C8	2.74	0.41
1:B:1162:ALA:O	1:B:1359:GLN:NE2	2.54	0.40
1:D:523:PHE:CD2	1:D:524:PHE:CE2	3.09	0.40
1:D:1160:LEU:HB3	1:D:1161:PRO:HD2	2.02	0.40
1:D:1437:GLU:O	1:D:1441:ILE:HG13	2.21	0.40
1:S:1100:ARG:NH1	1:S:1485:ARG:CZ	2.84	0.40
1:S:1185:PRO:HB2	1:S:1217:ASP:O	2.22	0.40
1:U:427:GLU:HA	1:U:501:HIS:CE1	2.56	0.40
1:U:1059:THR:CG2	1:U:1128:MET:CE	2.98	0.40
4:X:17:DG:C2	4:X:18:DG:N3	2.89	0.40
1:B:536:TYR:N	1:B:536:TYR:HD2	2.20	0.40
1:D:501:HIS:HA	1:D:536:TYR:CD1	2.56	0.40
1:S:437:ASP:CB	5:Y:9:DG:H5'	2.51	0.40
1:S:608:LEU:O	1:S:608:LEU:HG	2.20	0.40
1:S:1273:MET:HA	1:S:1326:PRO:HG2	2.03	0.40
1:S:1364:ARG:O	1:S:1368:GLN:HG3	2.21	0.40
1:S:1390:HIS:HB3	1:S:1393:GLU:CB	2.51	0.40
1:U:1195:VAL:O	1:U:1198:LEU:N	2.54	0.40
1:U:1374:ALA:HB1	1:U:1448:LEU:CD2	2.51	0.40
1:B:1225:LEU:HA	1:B:1225:LEU:HD23	1.79	0.40
1:B:1321:LEU:HD23	1:B:1321:LEU:HA	1.92	0.40
1:B:1445:TYR:CD1	1:B:1445:TYR:C	2.94	0.40
1:D:588:ALA:O	1:D:591:LEU:HB2	2.21	0.40
1:D:1012:ARG:NH2	1:D:1016:SER:O	2.54	0.40
1:S:517:ARG:NH2	1:U:1017:GLU:OE2	2.50	0.40
1:U:1165:PRO:HA	1:U:1355:TYR:CZ	2.55	0.40
5:Y:12:DC:H6	5:Y:12:DC:H5'	1.87	0.40
1:B:1080:PRO:O	1:B:1081:HIS:ND1	2.55	0.40
1:D:461:ILE:H	1:D:461:ILE:HG13	1.67	0.40
1:D:506:MET:HE2	1:D:506:MET:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1049:ILE:HD13	1:D:1090:MET:CB	2.42	0.40
1:D:1188:LEU:O	1:D:1192:ILE:HG13	2.21	0.40
1:D:1214:GLU:HB3	1:D:1488:ILE:HD12	2.04	0.40
1:D:1432:ARG:CG	1:D:1441:ILE:HD11	2.52	0.40
1:D:1438:ARG:O	1:D:1441:ILE:HB	2.22	0.40
1:S:465:GLU:OE1	1:S:465:GLU:O	2.38	0.40
1:B:443:THR:O	1:B:447:ARG:HB3	2.20	0.40
1:B:461:ILE:O	5:H:14:DC:H2"	2.21	0.40
1:B:598:PRO:HA	1:B:601:ARG:HD3	2.03	0.40
1:B:1103:LEU:HD21	1:B:1170:ASN:ND2	2.37	0.40
1:B:1182:ASN:ND2	1:B:1331:PHE:CE2	2.89	0.40
1:B:1411:LEU:HD23	1:B:1417:LEU:HD12	2.04	0.40
1:D:531:LEU:CD1	1:D:536:TYR:HB2	2.48	0.40
1:D:625:VAL:HB	1:D:628:ASN:ND2	2.37	0.40
1:D:1371:LEU:O	1:D:1374:ALA:N	2.50	0.40
1:S:1247:ALA:CA	1:S:1260:VAL:O	2.69	0.40
1:S:1369:TYR:CD2	1:S:1369:TYR:C	2.94	0.40
1:S:1448:LEU:O	1:S:1449:LEU:C	2.59	0.40
1:U:423:SER:HB3	1:U:450:ARG:O	2.21	0.40
1:U:1237:GLY:HA2	1:U:1335:MET:HE3	2.03	0.40
1:U:1404:ASP:O	1:U:1405:LYS:C	2.60	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	B	667/692 (96%)	545 (82%)	100 (15%)	22 (3%)	4 24
1	D	664/692 (96%)	526 (79%)	108 (16%)	30 (4%)	2 17
1	S	661/692 (96%)	493 (75%)	123 (19%)	45 (7%)	1 9
1	U	659/692 (95%)	532 (81%)	97 (15%)	30 (5%)	2 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2651/2768 (96%)	2096 (79%)	428 (16%)	127 (5%)	2 16

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1150	TYR
1	B	1291	ASP
1	B	1310	LYS
1	B	1409	GLU
1	B	1431	ARG
1	D	435	GLU
1	D	540	ALA
1	D	1128	MET
1	D	1434	THR
1	D	1483	ASP
1	S	583	LEU
1	S	627	GLU
1	S	1118	ALA
1	S	1138	ASP
1	S	1335	MET
1	S	1406	VAL
1	U	1038	VAL
1	U	1120	ALA
1	U	1142	ASP
1	U	1302	VAL
1	U	1477	ARG
1	B	1335	MET
1	B	1340	ASN
1	B	1408	MET
1	B	1460	ALA
1	D	427	GLU
1	D	493	PHE
1	D	585	GLU
1	D	633	ILE
1	D	1165	PRO
1	D	1167	LEU
1	D	1411	LEU
1	D	1426	LEU
1	S	419	ALA
1	S	420	ASP
1	S	458	ARG
1	S	516	ILE

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Mol	Chain	Res	Type
1	S	540	ALA
1	S	584	GLY
1	S	628	ASN
1	S	635	ASP
1	S	1027	MET
1	S	1054	ASN
1	S	1117	GLY
1	S	1119	ALA
1	S	1152	GLY
1	S	1178	GLY
1	S	1180	ALA
1	S	1284	LYS
1	S	1378	ALA
1	S	1379	HIS
1	S	1407	ALA
1	U	593	GLU
1	U	1030	ILE
1	U	1033	ARG
1	U	1158	SER
1	U	1159	VAL
1	U	1228	SER
1	B	1172	ALA
1	B	1221	ALA
1	B	1309	ARG
1	B	1434	THR
1	D	430	GLU
1	D	473	LEU
1	D	1045	VAL
1	D	1112	SER
1	D	1316	VAL
1	S	449	SER
1	S	468	ARG
1	S	1044	PRO
1	S	1165	PRO
1	S	1216	PRO
1	S	1227	LYS
1	U	519	LEU
1	U	592	TRP
1	U	1199	SER
1	U	1244	ARG
1	B	1167	LEU
1	B	1276	LYS

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Mol	Chain	Res	Type
1	B	1349	LYS
1	B	1386	ILE
1	D	423	SER
1	D	1149	ASN
1	S	448	ASP
1	S	475	ASN
1	S	1078	TYR
1	S	1171	GLY
1	S	1340	ASN
1	U	493	PHE
1	U	1063	SER
1	U	1489	GLN
1	B	581	LYS
1	B	1279	GLU
1	D	1068	ALA
1	D	1327	LEU
1	D	1367	THR
1	D	1371	LEU
1	S	1028	SER
1	S	1033	ARG
1	S	1137	ARG
1	S	1189	THR
1	S	1270	LYS
1	U	1326	PRO
1	U	1349	LYS
1	U	1370	ASN
1	B	633	ILE
1	D	1093	MET
1	D	1349	LYS
1	S	598	PRO
1	U	1203	ASP
1	U	1221	ALA
1	S	623	GLY
1	U	1102	PRO
1	D	1226	GLY
1	S	1202	PRO
1	S	1316	VAL
1	U	1195	VAL
1	U	1206	ILE
1	B	461	ILE
1	D	1177	VAL
1	D	1441	ILE

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Mol	Chain	Res	Type
1	U	1029	VAL
1	U	1177	VAL
1	U	1386	ILE
1	B	459	GLY
1	D	539	ILE
1	U	1394	ILE

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	B	563/591 (95%)	518 (92%)	45 (8%)	12	39
1	D	539/591 (91%)	483 (90%)	56 (10%)	7	27
1	S	555/591 (94%)	497 (90%)	58 (10%)	7	26
1	U	553/591 (94%)	499 (90%)	54 (10%)	8	30
All	All	2210/2364 (94%)	1997 (90%)	213 (10%)	8	30

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	LEU
1	B	421	CYS
1	B	434	VAL
1	B	435	GLU
1	B	451	THR
1	B	460	LYS
1	B	476	ASN
1	B	477	GLU
1	B	483	THR
1	B	508	ASP
1	B	522	THR
1	B	590	GLN
1	B	591	LEU
1	B	597	ASN
1	B	615	ASP

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Mol	Chain	Res	Type
1	B	617	THR
1	B	631	GLN
1	B	1069	ARG
1	B	1073	ASP
1	B	1083	ASP
1	B	1098	SER
1	B	1113	MET
1	B	1116	ASP
1	B	1129	THR
1	B	1136	LEU
1	B	1143	THR
1	B	1205	SER
1	B	1206	ILE
1	B	1236	THR
1	B	1262	THR
1	B	1292	LEU
1	B	1297	SER
1	B	1298	LEU
1	B	1300	THR
1	B	1311	ASP
1	B	1315	SER
1	B	1385	ARG
1	B	1386	ILE
1	B	1390	HIS
1	B	1411	LEU
1	B	1413	GLN
1	B	1439	ASP
1	B	1441	ILE
1	B	1464	VAL
1	B	1490	LEU
1	D	422	SER
1	D	434	VAL
1	D	438	SER
1	D	458	ARG
1	D	461	ILE
1	D	475	ASN
1	D	477	GLU
1	D	483	THR
1	D	499	ARG
1	D	507	THR
1	D	536	TYR
1	D	541	GLN

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Mol	Chain	Res	Type
1	D	583	LEU
1	D	585	GLU
1	D	594	THR
1	D	620	MET
1	D	624	ASP
1	D	625	VAL
1	D	636	ASN
1	D	1028	SER
1	D	1045	VAL
1	D	1047	ARG
1	D	1063	SER
1	D	1070	ILE
1	D	1083	ASP
1	D	1084	SER
1	D	1098	SER
1	D	1122	ARG
1	D	1136	LEU
1	D	1147	ILE
1	D	1193	ASN
1	D	1195	VAL
1	D	1204	ILE
1	D	1231	ARG
1	D	1245	SER
1	D	1258	ARG
1	D	1284	LYS
1	D	1296	THR
1	D	1299	ARG
1	D	1315	SER
1	D	1327	LEU
1	D	1347	ASN
1	D	1352	LEU
1	D	1357	GLU
1	D	1360	LYS
1	D	1384	LEU
1	D	1385	ARG
1	D	1390	HIS
1	D	1393	GLU
1	D	1396	SER
1	D	1426	LEU
1	D	1432	ARG
1	D	1439	ASP
1	D	1450	ASN

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Mol	Chain	Res	Type
1	D	1483	ASP
1	D	1490	LEU
1	S	418	LEU
1	S	428	GLU
1	S	445	SER
1	S	461	ILE
1	S	465	GLU
1	S	476	ASN
1	S	477	GLU
1	S	483	THR
1	S	492	ASP
1	S	505	ILE
1	S	512	ASP
1	S	523	PHE
1	S	538	TYR
1	S	589	ASP
1	S	591	LEU
1	S	597	ASN
1	S	636	ASN
1	S	1048	ARG
1	S	1058	MET
1	S	1067	SER
1	S	1075	MET
1	S	1085	SER
1	S	1086	ILE
1	S	1096	ASP
1	S	1103	LEU
1	S	1116	ASP
1	S	1124	THR
1	S	1131	ILE
1	S	1136	LEU
1	S	1143	THR
1	S	1145	ASP
1	S	1168	LEU
1	S	1187	ASN
1	S	1204	ILE
1	S	1209	LEU
1	S	1220	THR
1	S	1228	SER
1	S	1232	ARG
1	S	1235	GLU
1	S	1236	THR

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Mol	Chain	Res	Type
1	S	1245	SER
1	S	1260	VAL
1	S	1262	THR
1	S	1298	LEU
1	S	1299	ARG
1	S	1309	ARG
1	S	1329	THR
1	S	1342	ARG
1	S	1345	LEU
1	S	1347	ASN
1	S	1350	GLU
1	S	1369	TYR
1	S	1391	ILE
1	S	1418	SER
1	S	1448	LEU
1	S	1452	ILE
1	S	1453	SER
1	S	1483	ASP
1	U	430	GLU
1	U	433	LEU
1	U	434	VAL
1	U	435	GLU
1	U	444	LYS
1	U	454	ILE
1	U	461	ILE
1	U	474	ASN
1	U	476	ASN
1	U	489	ILE
1	U	505	ILE
1	U	507	THR
1	U	508	ASP
1	U	516	ILE
1	U	520	LEU
1	U	531	LEU
1	U	538	TYR
1	U	594	THR
1	U	610	ASP
1	U	617	THR
1	U	620	MET
1	U	633	ILE
1	U	639	TYR
1	U	1016	SER

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Mol	Chain	Res	Type
1	U	1061	ASP
1	U	1078	TYR
1	U	1091	VAL
1	U	1122	ARG
1	U	1129	THR
1	U	1179	MET
1	U	1220	THR
1	U	1225	LEU
1	U	1230	ILE
1	U	1232	ARG
1	U	1236	THR
1	U	1248	VAL
1	U	1261	VAL
1	U	1262	THR
1	U	1286	ILE
1	U	1300	THR
1	U	1306	ILE
1	U	1325	THR
1	U	1329	THR
1	U	1334	ASN
1	U	1345	LEU
1	U	1361	THR
1	U	1371	LEU
1	U	1404	ASP
1	U	1432	ARG
1	U	1450	ASN
1	U	1459	LEU
1	U	1465	LEU
1	U	1466	LEU
1	U	1483	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	476	ASN
1	B	501	HIS
1	B	597	ASN
1	B	605	GLN
1	B	628	ASN
1	B	1081	HIS
1	B	1170	ASN
1	B	1334	ASN

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Mol	Chain	Res	Type
1	B	1358	HIS
1	B	1359	GLN
1	B	1446	ASN
1	D	474	ASN
1	D	501	HIS
1	D	541	GLN
1	D	597	ASN
1	D	628	ASN
1	D	636	ASN
1	D	1081	HIS
1	D	1313	ASN
1	D	1334	ASN
1	D	1421	GLN
1	D	1450	ASN
1	S	480	GLN
1	S	597	ASN
1	S	1046	HIS
1	S	1054	ASN
1	S	1081	HIS
1	S	1324	GLN
1	S	1390	HIS
1	S	1412	GLN
1	U	474	ASN
1	U	501	HIS
1	U	515	HIS
1	U	597	ASN
1	U	605	GLN
1	U	636	ASN
1	U	1046	HIS
1	U	1107	GLN
1	U	1242	GLN
1	U	1324	GLN
1	U	1334	ASN
1	U	1358	HIS
1	U	1450	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
7	CPF	H	1020	6	27,27,27	2.34	7 (25%)	40,40,40	2.89	17 (42%)
7	CPF	X	1020	6	27,27,27	2.29	7 (25%)	40,40,40	2.36	14 (35%)
7	CPF	G	1020	6	27,27,27	2.27	5 (18%)	40,40,40	2.50	17 (42%)
7	CPF	Y	1020	6	27,27,27	2.32	7 (25%)	40,40,40	2.74	20 (50%)

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
7	CPF	H	1020	6	-	6/12/22/22	0/4/4/4
7	CPF	X	1020	6	-	4/12/22/22	0/4/4/4
7	CPF	G	1020	6	-	6/12/22/22	0/4/4/4
7	CPF	Y	1020	6	-	2/12/22/22	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1020	CPF	O3-C4	7.17	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	1020	CPF	O3-C4	6.49	1.36	1.23
7	H	1020	CPF	O3-C4	6.07	1.36	1.23
7	H	1020	CPF	C5-C4	-5.96	1.36	1.48
7	Y	1020	CPF	C5-C4	-5.75	1.37	1.48
7	Y	1020	CPF	O3-C4	5.71	1.35	1.23
7	Y	1020	CPF	O2-C3	5.63	1.47	1.30
7	H	1020	CPF	O2-C3	5.55	1.46	1.30
7	X	1020	CPF	O2-C3	5.49	1.46	1.30
7	G	1020	CPF	O2-C3	5.23	1.45	1.30
7	X	1020	CPF	C5-C4	-5.10	1.38	1.48
7	G	1020	CPF	C10-N1	-4.77	1.34	1.40
7	Y	1020	CPF	C10-N1	-4.62	1.34	1.40
7	G	1020	CPF	C5-C4	-4.39	1.39	1.48
7	H	1020	CPF	C10-N1	-4.06	1.35	1.40
7	X	1020	CPF	C10-N1	-3.87	1.35	1.40
7	X	1020	CPF	C2-C4	-2.54	1.38	1.44
7	H	1020	CPF	C2-C3	2.51	1.52	1.48
7	H	1020	CPF	C2-C4	-2.43	1.38	1.44
7	Y	1020	CPF	C2-C4	-2.33	1.39	1.44
7	G	1020	CPF	C2-C4	-2.24	1.39	1.44
7	X	1020	CPF	C2-C3	2.17	1.52	1.48
7	X	1020	CPF	C12-C11	2.16	1.53	1.48
7	H	1020	CPF	C12-C11	2.15	1.53	1.48
7	Y	1020	CPF	C13-C11	2.10	1.53	1.48
7	Y	1020	CPF	C2-C3	2.09	1.52	1.48

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	1020	CPF	C12-C11-N1	-7.64	107.38	118.84
7	H	1020	CPF	C13-C11-N1	-7.26	107.95	118.84
7	Y	1020	CPF	C12-C11-N1	-6.86	108.55	118.84
7	G	1020	CPF	C13-C11-N1	-6.81	108.63	118.84
7	H	1020	CPF	F1-C7-C8	6.15	124.02	118.42
7	X	1020	CPF	C13-C11-N1	-5.75	110.21	118.84
7	G	1020	CPF	C12-C11-N1	-5.73	110.24	118.84
7	Y	1020	CPF	C6-C7-C8	-5.44	118.85	123.34
7	X	1020	CPF	C6-C7-C8	-4.88	119.31	123.34
7	Y	1020	CPF	C9-C8-N2	-4.70	115.56	122.52
7	Y	1020	CPF	C5-C4-C2	4.69	121.54	115.59
7	H	1020	CPF	C14-N2-C17	4.58	121.64	111.52
7	Y	1020	CPF	C13-C11-N1	-4.57	111.98	118.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	1020	CPF	F1-C7-C8	4.57	122.58	118.42
7	X	1020	CPF	C14-N2-C17	4.56	121.59	111.52
7	X	1020	CPF	C12-C11-N1	-4.38	112.27	118.84
7	H	1020	CPF	O3-C4-C5	-4.26	114.67	121.56
7	Y	1020	CPF	C14-N2-C17	4.24	120.87	111.52
7	G	1020	CPF	C14-N2-C17	4.15	120.69	111.52
7	H	1020	CPF	C6-C7-C8	-4.14	119.92	123.34
7	G	1020	CPF	C9-C8-C7	4.09	120.46	116.48
7	H	1020	CPF	C5-C4-C2	4.08	120.78	115.59
7	H	1020	CPF	C9-C8-C7	4.04	120.41	116.48
7	G	1020	CPF	C6-C7-C8	-3.99	120.04	123.34
7	H	1020	CPF	C1-C2-C4	-3.95	116.95	119.88
7	X	1020	CPF	F1-C7-C8	3.85	121.93	118.42
7	Y	1020	CPF	C2-C1-N1	-3.82	120.21	124.49
7	G	1020	CPF	C5-C10-N1	3.77	121.59	118.81
7	G	1020	CPF	C9-C8-N2	-3.77	116.94	122.52
7	X	1020	CPF	C5-C4-C2	3.72	120.31	115.59
7	Y	1020	CPF	C7-C8-N2	3.63	124.78	120.47
7	G	1020	CPF	C2-C1-N1	-3.58	120.47	124.49
7	X	1020	CPF	C9-C8-C7	3.52	119.91	116.48
7	X	1020	CPF	C1-C2-C3	3.36	123.93	118.35
7	H	1020	CPF	C6-C5-C10	3.32	122.61	118.73
7	Y	1020	CPF	C9-C8-C7	3.26	119.66	116.48
7	Y	1020	CPF	O3-C4-C5	-3.26	116.29	121.56
7	H	1020	CPF	C9-C10-N1	3.16	122.82	120.53
7	X	1020	CPF	C2-C1-N1	-3.11	121.01	124.49
7	G	1020	CPF	C16-C17-N2	-3.09	103.80	110.48
7	Y	1020	CPF	C10-C5-C4	-3.00	118.42	121.44
7	X	1020	CPF	C15-N3-C16	2.98	118.91	110.34
7	Y	1020	CPF	C1-C2-C4	-2.95	117.69	119.88
7	Y	1020	CPF	C5-C10-N1	2.93	120.97	118.81
7	H	1020	CPF	C17-N2-C8	2.78	122.86	116.27
7	G	1020	CPF	C10-C5-C4	-2.74	118.69	121.44
7	G	1020	CPF	C5-C4-C2	2.69	119.00	115.59
7	H	1020	CPF	C10-N1-C1	2.68	121.47	119.59
7	G	1020	CPF	C9-C10-N1	-2.68	118.59	120.53
7	G	1020	CPF	C14-N2-C8	2.57	122.35	116.27
7	Y	1020	CPF	C1-C2-C3	2.55	122.58	118.35
7	H	1020	CPF	C15-N3-C16	2.54	117.64	110.34
7	H	1020	CPF	C2-C1-N1	-2.53	121.66	124.49
7	X	1020	CPF	C1-C2-C4	-2.51	118.02	119.88
7	Y	1020	CPF	C14-N2-C8	2.50	122.20	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	1020	CPF	C1-C2-C3	2.43	122.39	118.35
7	G	1020	CPF	C15-N3-C16	2.38	117.19	110.34
7	G	1020	CPF	F1-C7-C8	2.32	120.53	118.42
7	Y	1020	CPF	C15-N3-C16	2.30	116.96	110.34
7	X	1020	CPF	C3-C2-C4	-2.30	118.05	121.56
7	X	1020	CPF	O2-C3-O1	-2.24	118.47	123.61
7	X	1020	CPF	C6-C5-C10	2.24	121.34	118.73
7	Y	1020	CPF	C10-N1-C1	2.23	121.16	119.59
7	Y	1020	CPF	C6-C5-C10	2.22	121.33	118.73
7	G	1020	CPF	O3-C4-C2	-2.08	119.74	123.22
7	H	1020	CPF	C6-C5-C4	-2.03	116.48	119.95
7	G	1020	CPF	C15-C14-N2	-2.00	106.15	110.48
7	Y	1020	CPF	C15-C14-N2	-2.00	106.15	110.48

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	1020	CPF	C12-C11-N1-C1
7	G	1020	CPF	C9-C8-N2-C14
7	Y	1020	CPF	C9-C8-N2-C14
7	H	1020	CPF	C12-C11-N1-C10
7	G	1020	CPF	C7-C8-N2-C14
7	Y	1020	CPF	C7-C8-N2-C14
7	X	1020	CPF	C9-C8-N2-C14
7	G	1020	CPF	C13-C11-N1-C1
7	H	1020	CPF	C7-C8-N2-C17
7	X	1020	CPF	C7-C8-N2-C14
7	X	1020	CPF	C12-C11-N1-C1
7	G	1020	CPF	C13-C11-N1-C10
7	X	1020	CPF	C12-C11-N1-C10
7	G	1020	CPF	C12-C11-N1-C1
7	H	1020	CPF	C13-C11-N1-C1
7	G	1020	CPF	C12-C11-N1-C10
7	H	1020	CPF	C9-C8-N2-C17
7	H	1020	CPF	C13-C11-N1-C10

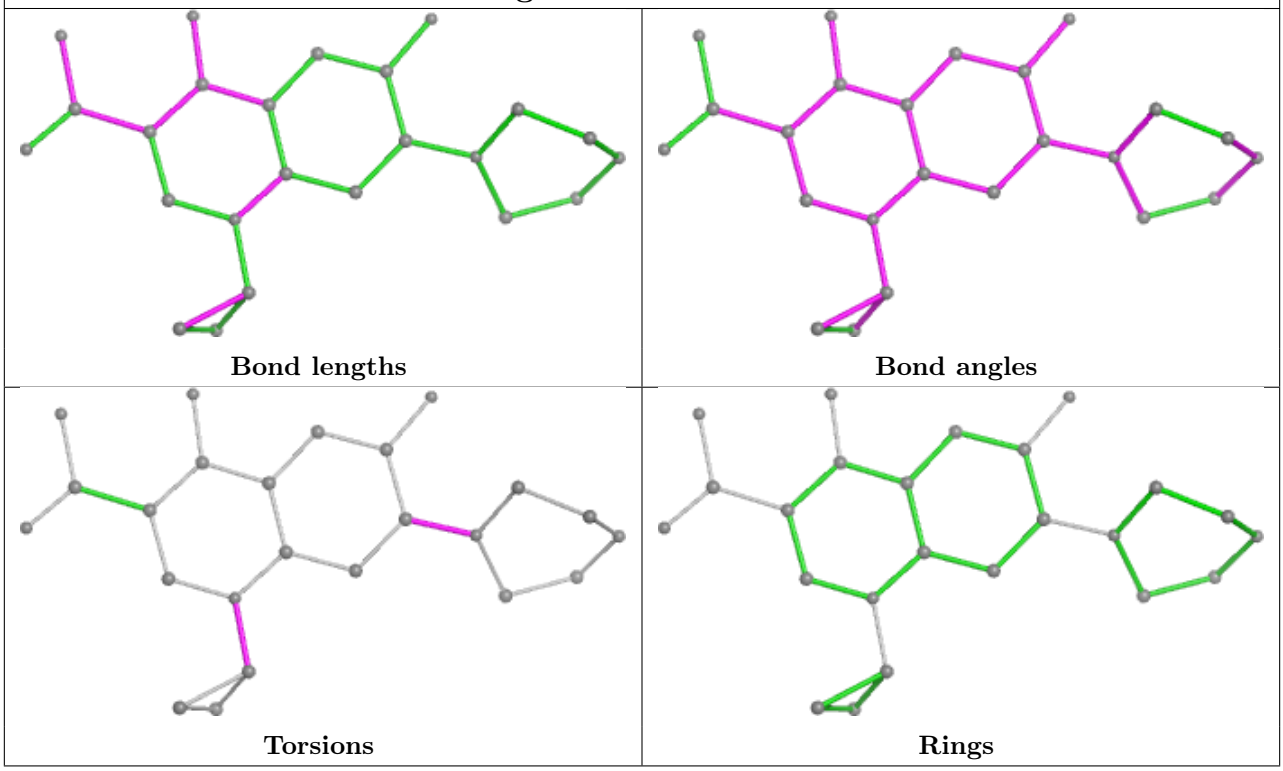
There are no ring outliers.

4 monomers are involved in 47 short contacts:

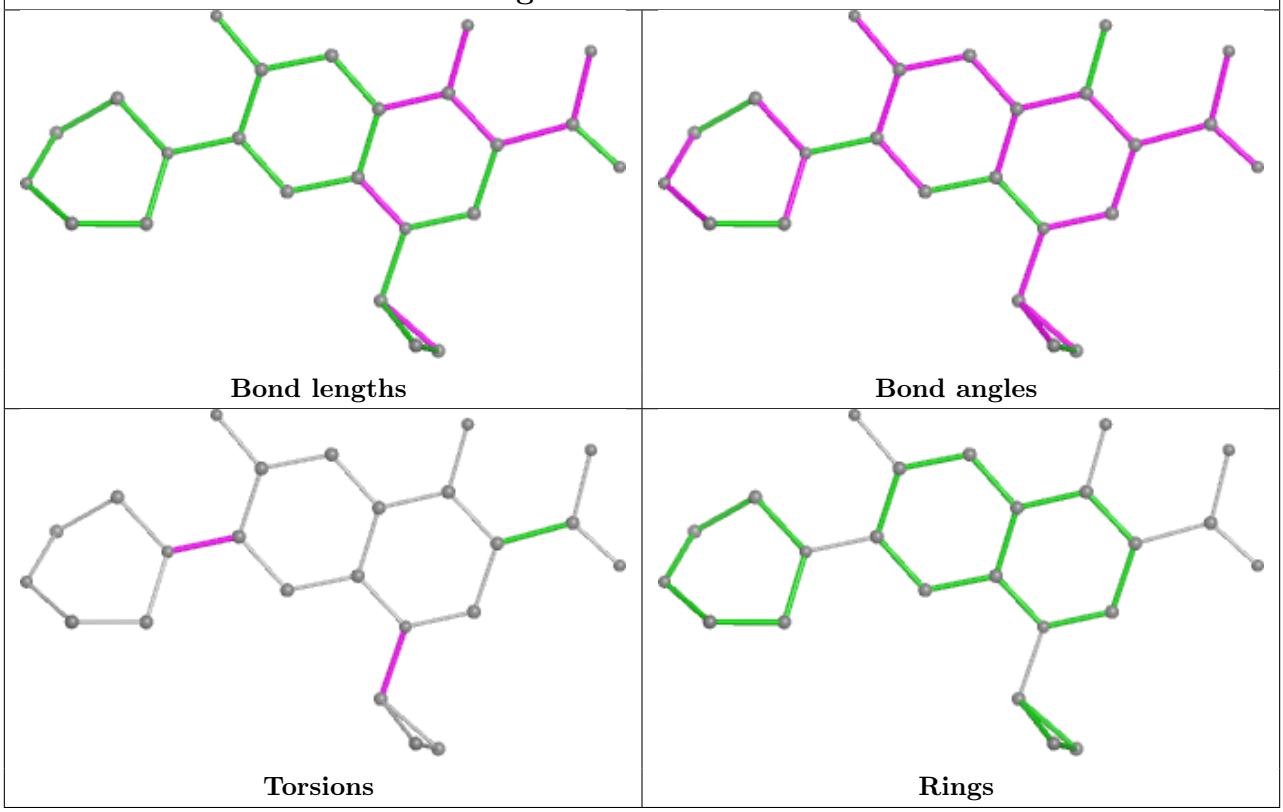
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	1020	CPF	9	0
7	X	1020	CPF	20	0
7	G	1020	CPF	8	0
7	Y	1020	CPF	10	0

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.

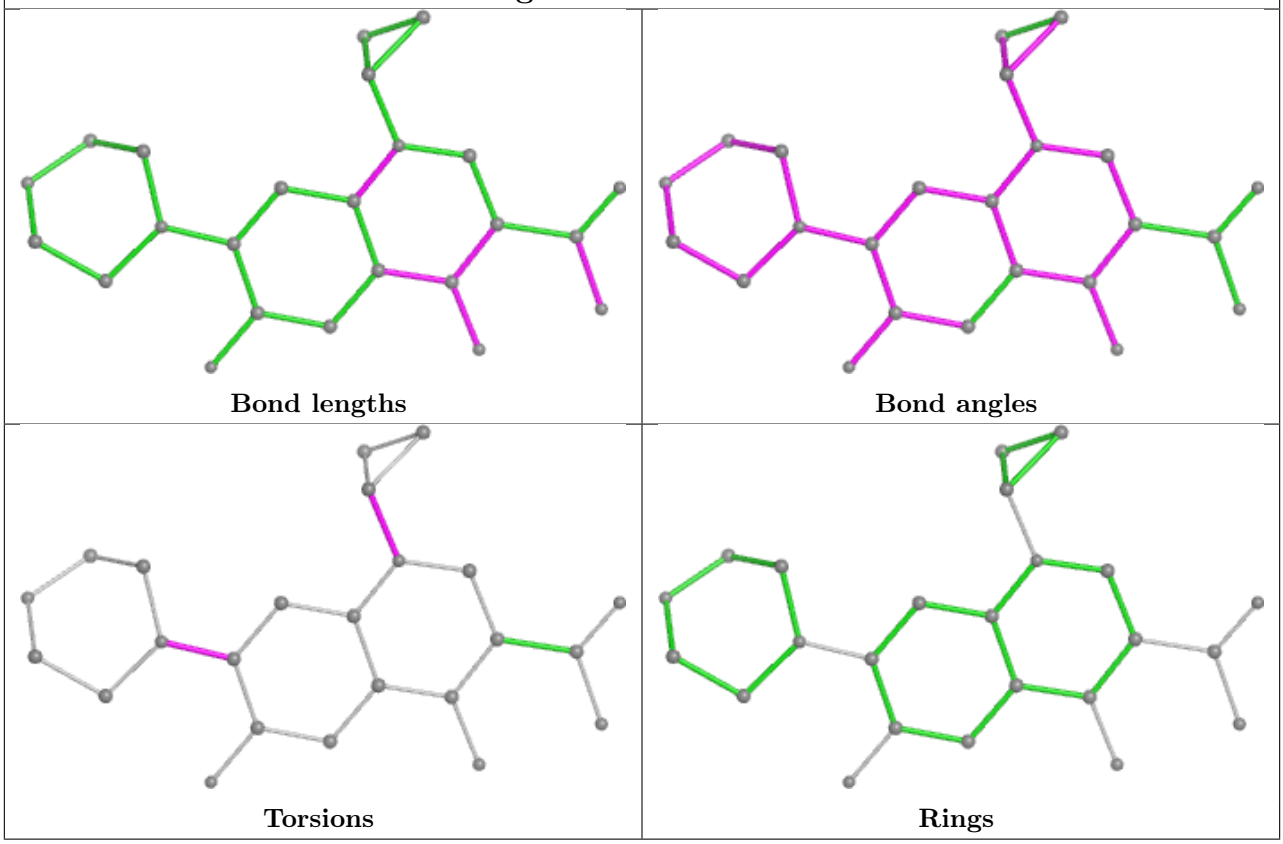
Ligand CPF H 1020



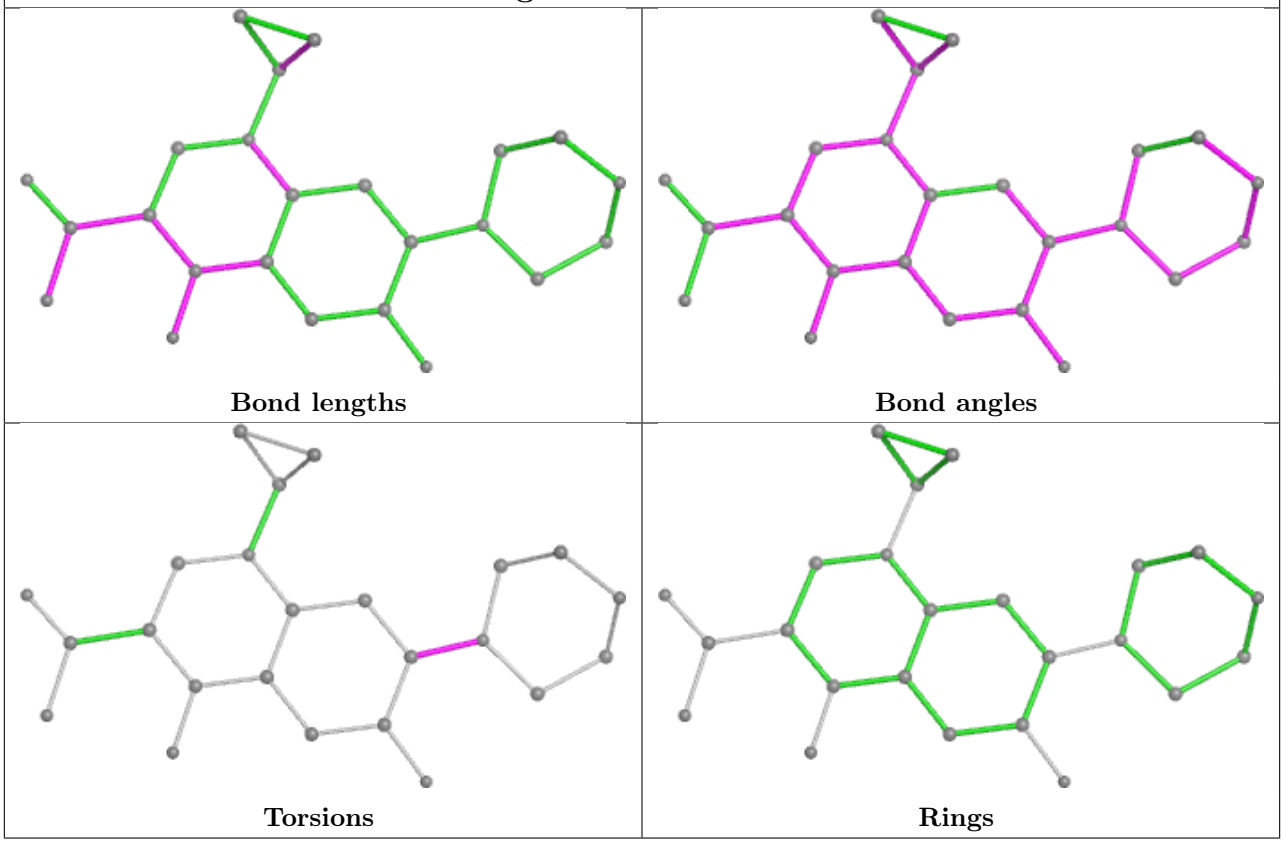
Ligand CPF X 1020



Ligand CPF G 1020



Ligand CPF Y 1020



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	669/692 (96%)	-0.03	5 (0%)	87	91	29, 64, 101, 143	0
1	D	669/692 (96%)	-0.02	8 (1%)	79	82	35, 69, 108, 143	0
1	S	667/692 (96%)	0.12	21 (3%)	49	52	43, 78, 119, 218	0
1	U	665/692 (96%)	0.07	12 (1%)	68	71	39, 72, 110, 158	0
2	E	7/8 (87%)	-0.02	0	100	100	48, 52, 83, 89	0
2	V	7/8 (87%)	-0.23	0	100	100	51, 62, 76, 86	0
3	F	7/8 (87%)	-0.20	0	100	100	51, 57, 77, 80	0
3	W	6/8 (75%)	-0.25	0	100	100	62, 75, 86, 86	0
4	G	11/12 (91%)	-0.11	0	100	100	60, 67, 90, 120	0
4	X	11/12 (91%)	0.34	0	100	100	68, 88, 102, 125	0
5	H	12/12 (100%)	0.01	0	100	100	48, 77, 111, 123	0
5	Y	11/12 (91%)	-0.04	0	100	100	67, 75, 106, 117	0
All	All	2742/2848 (96%)	0.03	46 (1%)	70	73	29, 71, 112, 218	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1491	GLY	4.7
1	S	619	GLU	4.6
1	U	486	GLY	3.8
1	U	604	LEU	3.8
1	B	545	GLY	3.7
1	S	432	PHE	3.4
1	D	431	ILE	3.1
1	S	453	ALA	3.1
1	U	498	ALA	3.0
1	S	1249	ILE	2.8
1	U	1313	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	631	GLN	2.7
1	S	1253	GLY	2.7
1	U	487	THR	2.7
1	D	421	CYS	2.7
1	S	609	GLU	2.6
1	S	1289	ILE	2.6
1	S	617	THR	2.6
1	S	442	SER	2.5
1	S	483	THR	2.5
1	S	1254	GLY	2.5
1	D	420	ASP	2.5
1	U	1288	GLY	2.5
1	D	476	ASN	2.5
1	S	1252	ARG	2.5
1	S	639	TYR	2.5
1	S	1274	ILE	2.4
1	U	1388	LEU	2.4
1	S	1491	GLY	2.4
1	S	1287	ASP	2.4
1	B	453	ALA	2.3
1	U	597	ASN	2.3
1	B	1292	LEU	2.2
1	S	1205	SER	2.2
1	U	1208	GLU	2.2
1	U	442	SER	2.2
1	S	1260	VAL	2.2
1	S	1466	LEU	2.1
1	U	421	CYS	2.1
1	S	1250	GLU	2.1
1	U	429	CYS	2.1
1	B	1306	ILE	2.1
1	B	544	THR	2.1
1	S	1299	ARG	2.1
1	D	453	ALA	2.0
1	D	527	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

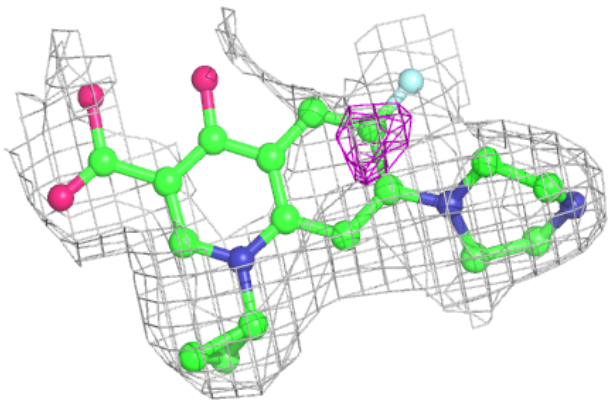
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

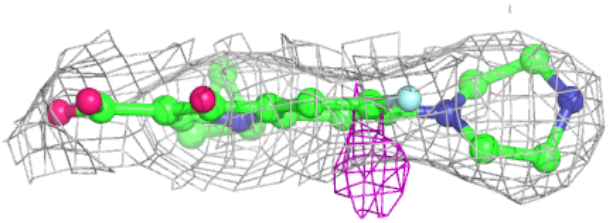
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MN	F	2000	1/1	0.86	0.10	86,86,86,86	0
7	CPF	H	1020	24/24	0.90	0.24	86,86,86,86	0
7	CPF	X	1020	24/24	0.92	0.20	86,86,86,86	0
7	CPF	Y	1020	24/24	0.93	0.18	76,76,76,76	0
7	CPF	G	1020	24/24	0.94	0.19	70,70,70,70	0
6	MN	W	2000	1/1	0.94	0.12	86,86,86,86	0
6	MN	D	2492	1/1	0.95	0.22	85,85,85,85	0
6	MN	W	2001	1/1	0.95	0.07	76,76,76,76	0
6	MN	B	2492	1/1	0.96	0.25	76,76,76,76	0
6	MN	S	2492	1/1	0.98	0.16	70,70,70,70	0
6	MN	U	2492	1/1	0.98	0.22	64,64,64,64	0
6	MN	G	2000	1/1	0.99	0.07	70,70,70,70	0

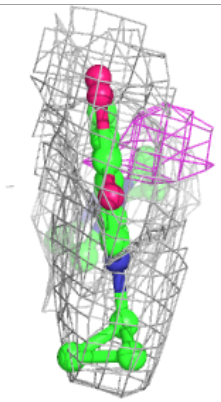
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPF H 1020:

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

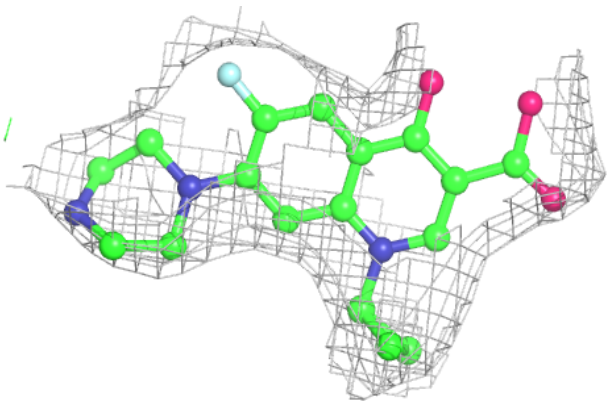


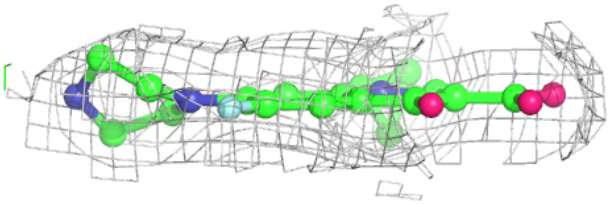


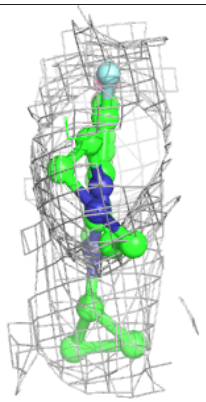


Electron density around CPF X 1020:

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

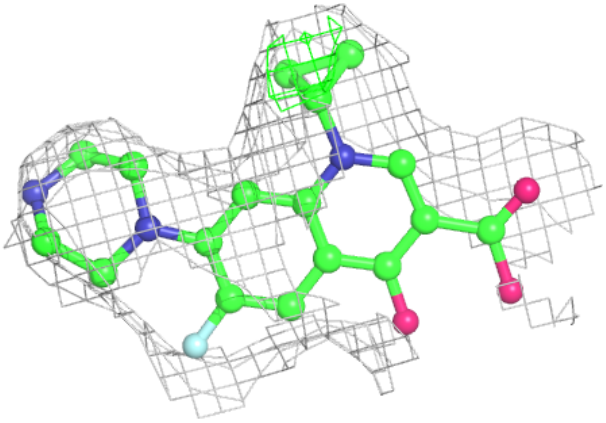


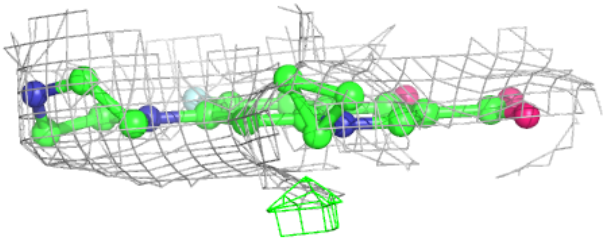


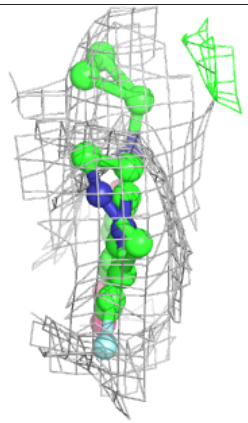


Electron density around CPF Y 1020:

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

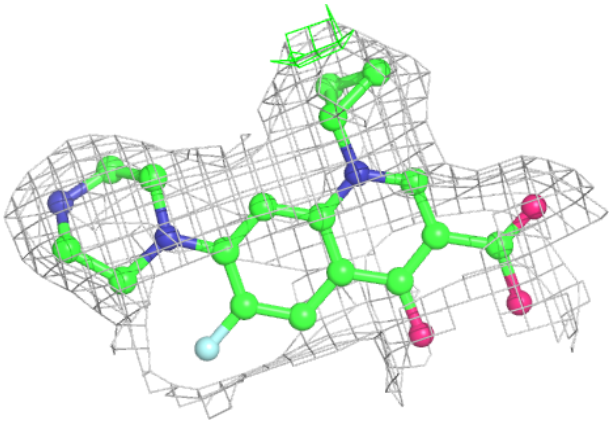


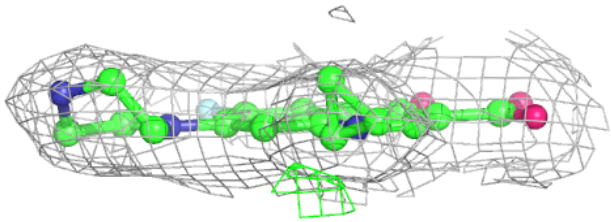


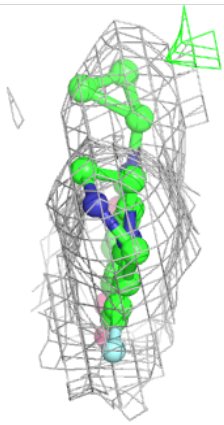


Electron density around CPF G 1020:

$2mF_o$-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 (i)

There are no such residues in this entry.