



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:26 PM EDT

PDB ID : 2IS2  
Title : Crystal structure of UvrD-DNA binary complex  
Authors : Yang, W.; Lee, J.Y.  
Deposited on : 2006-10-16  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

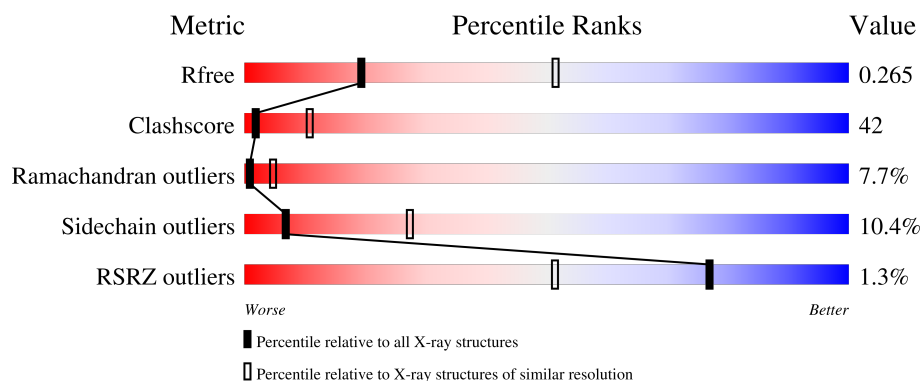
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	35	<div> <div>3%</div> <div>20%</div> <div>74%</div> <div>6%</div> </div>
1	D	35	<div> <div>14%</div> <div>80%</div> <div>6%</div> </div>
2	A	680	<div> <div>42%</div> <div>43%</div> <div>8%</div> <div>6%</div> </div>
2	B	680	<div> <div>2%</div> <div>31%</div> <div>52%</div> <div>11%</div> <div>6%</div> </div>

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
3	GOL	A	681	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11505 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 33-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	P	0	0	0
			673	321	120	200	32			
1	D	33	Total	C	N	O	P	0	0	0
			673	321	120	200	32			

- Molecule 2 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	642	Total	C	N	O	S	0	0	0
			5076	3180	924	946	26			
2	B	642	Total	C	N	O	S	0	0	0
			5060	3169	923	942	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	engineered mutation	UNP P03018
B	399	VAL	ALA	engineered mutation	UNP P03018

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		

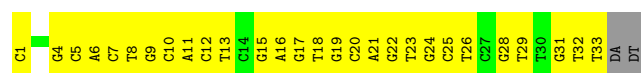
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

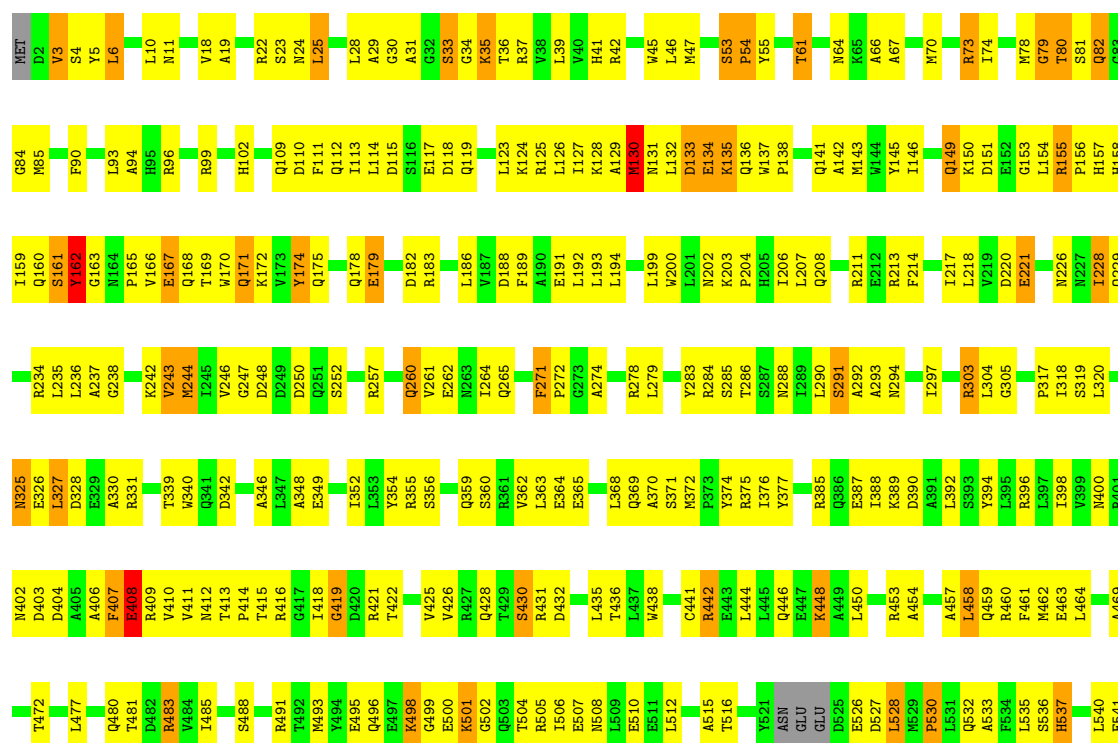
#### • Molecule 1: 33-MER

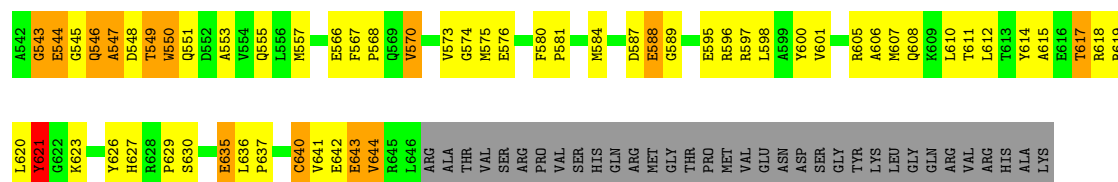


#### • Molecule 1: 33-MER

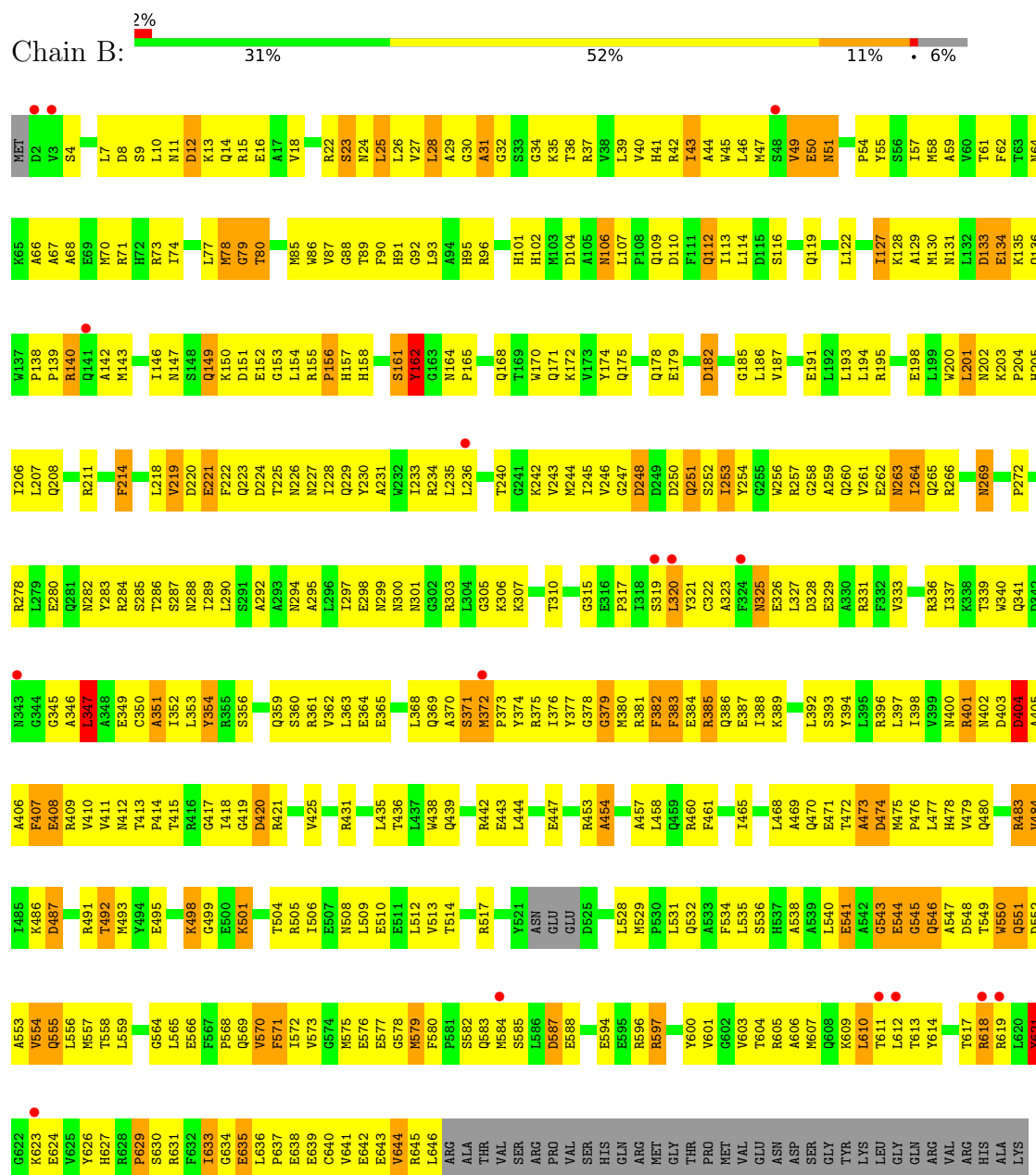


#### • Molecule 2: DNA helicase II





## • Molecule 2: DNA helicase II





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.60Å 105.97Å 295.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.00 49.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.7 (29.75-3.00) 83.6 (49.48-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.283 0.214 , 0.265	Depositor DCC
$R_{free}$ test set	3600 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C	0.51	0/753	0.80	0/1161
1	D	0.49	0/753	0.75	0/1161
2	A	0.49	1/5170 (0.0%)	0.73	0/6993
2	B	0.37	1/5154 (0.0%)	0.65	0/6972
All	All	0.44	2/11830 (0.0%)	0.70	0/16287

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	162	TYR	CB-CG	-6.50	1.41	1.51
2	B	162	TYR	CB-CG	-6.36	1.42	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	621	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	673	0	374	42	0
1	D	673	0	374	57	0
2	A	5076	0	4944	338	0
2	B	5060	0	4908	529	0
3	A	6	0	8	4	0
4	A	3	0	1	1	0
5	A	14	0	0	0	0
All	All	11505	0	10609	933	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 42.

All (933) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:DG:H2''	1:D:20:DC:H5''	1.32	1.09
2:B:155:ARG:HG3	2:B:156:PRO:HD2	1.14	1.08
2:B:261:VAL:HG21	2:B:597:ARG:HH21	1.24	1.01
2:B:7:LEU:HD11	2:B:45:TRP:HZ3	1.21	0.99
2:A:288:ASN:ND2	2:A:317:PRO:HA	1.78	0.98
2:B:112:GLN:HE21	2:B:113:ILE:H	1.04	0.98
2:B:400:ASN:HD21	2:B:402:ASN:HB2	1.24	0.96
2:A:161:SER:O	2:A:162:TYR:CG	2.18	0.96
2:A:203:LYS:O	2:A:206:ILE:HG12	1.67	0.94
2:A:73:ARG:HG2	2:A:73:ARG:HH11	1.32	0.93
2:A:325:ASN:HD22	2:A:325:ASN:C	1.72	0.93
2:A:284:ARG:HD3	2:A:566:GLU:HB3	1.51	0.93
2:A:161:SER:HB3	2:A:168:GLN:HE21	1.34	0.93
2:B:320:LEU:HD11	2:B:633:ILE:HG21	1.51	0.92
2:B:155:ARG:CG	2:B:156:PRO:HD2	2.01	0.91
2:B:285:SER:HB3	2:B:606:ALA:O	1.71	0.90
1:C:14:DC:H1'	2:B:453:ARG:HH21	1.37	0.88
2:A:284:ARG:HG3	2:A:566:GLU:OE1	1.73	0.88
2:B:475:MET:HE3	2:B:479:VAL:HG12	1.55	0.87
2:B:7:LEU:HD11	2:B:45:TRP:CZ3	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:TYR:C	2:B:164:ASN:H	1.77	0.87
2:B:79:GLY:O	2:B:80:THR:HG23	1.76	0.86
2:B:23:SER:HA	2:B:242:LYS:HG3	1.55	0.85
2:B:349:GLU:HB3	2:B:568:PRO:HG2	1.58	0.85
1:D:19:DG:C2'	1:D:20:DC:H5''	2.06	0.85
2:A:217:ILE:HB	2:A:243:VAL:HB	1.56	0.85
2:B:453:ARG:HB2	2:B:453:ARG:NH1	1.91	0.84
2:B:112:GLN:HG2	2:B:396:ARG:HH11	1.40	0.84
2:B:261:VAL:HG21	2:B:597:ARG:NH2	1.92	0.84
2:B:453:ARG:HB2	2:B:453:ARG:HH11	1.40	0.84
2:B:575:MET:HB2	2:B:613:THR:O	1.77	0.84
2:B:61:THR:HG22	2:B:62:PHE:H	1.41	0.83
2:B:154:LEU:HD22	2:B:158:HIS:HB3	1.61	0.83
2:B:112:GLN:HE21	2:B:113:ILE:N	1.76	0.83
2:A:643:GLU:HG3	2:A:644:VAL:H	1.42	0.83
2:B:43:ILE:HD12	2:B:74:ILE:HD12	1.60	0.82
1:D:22:DG:H2''	1:D:23:DT:OP2	1.77	0.82
2:B:246:VAL:HG12	2:B:247:GLY:H	1.45	0.82
2:B:360:SER:HA	2:B:363:LEU:HD12	1.63	0.81
2:B:300:ASN:HB2	2:B:303:ARG:HD3	1.62	0.81
2:B:472:THR:HA	2:B:475:MET:SD	2.21	0.81
2:B:252:SER:OG	2:B:261:VAL:HG22	1.81	0.81
2:A:42:ARG:HG2	2:A:244:MET:CE	2.11	0.81
2:B:401:ARG:HH22	2:B:469:ALA:HB2	1.46	0.80
2:B:300:ASN:OD1	2:B:596:ARG:HD2	1.81	0.80
2:B:322:CYS:HG	2:B:614:TYR:HE1	1.30	0.80
1:C:2:DG:H2''	1:C:3:DA:OP2	1.81	0.80
2:A:504:THR:HG22	2:A:508:ASN:HD21	1.46	0.80
2:A:78:MET:O	2:A:80:THR:N	2.15	0.79
2:B:112:GLN:OE1	2:B:396:ARG:HD3	1.82	0.79
2:A:414:PRO:HA	2:A:493:MET:CE	2.12	0.79
1:D:7:DC:H2'	1:D:8:DT:H72	1.63	0.79
2:B:44:ALA:HB2	2:B:77:LEU:HD23	1.63	0.79
2:A:285:SER:HB3	2:A:606:ALA:O	1.81	0.79
1:D:23:DT:H2''	1:D:24:DG:O4'	1.83	0.79
2:A:138:PRO:HG2	2:A:141:GLN:HB3	1.64	0.79
2:B:396:ARG:HD2	2:B:403:ASP:OD2	1.83	0.78
1:C:6:DA:H2''	1:C:7:DC:O5'	1.81	0.78
2:A:131:ASN:OD1	2:A:132:LEU:N	2.17	0.78
2:B:288:ASN:HD21	2:B:317:PRO:HA	1.48	0.78
2:A:42:ARG:HG2	2:A:244:MET:HE1	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:MET:CE	2:B:479:VAL:HG12	2.14	0.77
2:B:112:GLN:NE2	2:B:113:ILE:H	1.81	0.77
2:B:323:ALA:HB1	2:B:328:ASP:HB3	1.66	0.77
2:B:42:ARG:O	2:B:46:LEU:HG	1.84	0.77
1:C:14:DC:H1'	2:B:453:ARG:NH2	2.00	0.77
2:B:26:LEU:HD12	2:B:27:VAL:H	1.48	0.76
2:B:504:THR:HG22	2:B:508:ASN:ND2	2.00	0.76
2:B:436:THR:OG1	2:B:439:GLN:HG3	1.86	0.76
1:C:18:DT:H2''	1:C:19:DG:H5'	1.68	0.76
2:A:112:GLN:HE21	2:A:113:ILE:N	1.83	0.76
2:B:341:GLN:NE2	2:B:347:LEU:HD11	2.00	0.76
2:A:252:SER:OG	2:A:261:VAL:HG22	1.85	0.76
2:B:156:PRO:HD3	2:B:174:TYR:HE1	1.50	0.75
2:B:597:ARG:O	2:B:601:VAL:HG23	1.87	0.75
2:A:119:GLN:HE21	2:A:143:MET:CE	1.99	0.75
2:B:618:ARG:HH11	2:B:618:ARG:HB2	1.51	0.75
2:A:288:ASN:OD1	2:A:640:CYS:HB3	1.87	0.75
2:B:400:ASN:ND2	2:B:402:ASN:H	1.84	0.75
2:B:570:VAL:HG11	2:B:606:ALA:HA	1.69	0.75
2:A:30:GLY:O	2:A:31:ALA:HB3	1.86	0.74
2:A:73:ARG:HG2	2:A:73:ARG:NH1	2.00	0.74
2:A:200:TRP:HB3	2:A:207:LEU:HD13	1.69	0.74
2:B:346:ALA:HB3	2:B:349:GLU:CD	2.08	0.74
2:A:64:ASN:ND2	2:A:541:GLU:HB3	2.03	0.74
2:B:353:LEU:HB3	2:B:559:LEU:CD2	2.18	0.74
2:A:637:PRO:HB2	2:A:640:CYS:SG	2.28	0.73
2:B:113:ILE:H	2:B:113:ILE:HD12	1.53	0.73
2:B:129:ALA:HB1	2:B:431:ARG:HD2	1.69	0.73
2:B:381:ARG:HD3	2:B:543:GLY:H	1.53	0.73
2:A:644:VAL:HG12	2:A:644:VAL:O	1.86	0.73
2:B:26:LEU:HD12	2:B:27:VAL:N	2.04	0.73
2:B:263:ASN:HA	2:B:266:ARG:HB3	1.71	0.73
2:B:504:THR:HG22	2:B:508:ASN:HD21	1.54	0.73
2:A:288:ASN:HD21	2:A:317:PRO:HA	1.49	0.72
2:A:346:ALA:HB3	2:A:349:GLU:HG3	1.70	0.72
2:A:112:GLN:HG2	2:A:396:ARG:HH11	1.54	0.72
1:C:11:DA:H2''	1:C:12:DC:C5'	2.19	0.72
2:B:472:THR:O	2:B:475:MET:HB2	1.90	0.72
1:D:7:DC:H2''	1:D:8:DT:C6	2.25	0.72
2:A:188:ASP:OD2	2:A:191:GLU:HB2	1.90	0.72
2:B:321:TYR:HE2	2:B:323:ALA:HB2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:325:ASN:ND2	2:A:328:ASP:H	1.88	0.71
2:B:554:VAL:HG12	2:B:555:GLN:N	2.04	0.71
1:D:24:DG:H4'	1:D:24:DG:OP1	1.89	0.71
2:A:134:GLU:O	2:A:136:GLN:N	2.23	0.71
2:B:54:PRO:HA	2:B:57:ILE:HD13	1.71	0.71
2:B:501:LYS:HE3	2:B:505:ARG:HH12	1.55	0.71
2:B:569:GLN:HG3	2:B:571:PHE:CE2	2.25	0.71
2:B:43:ILE:CG2	2:B:57:ILE:HG21	2.20	0.71
2:B:468:LEU:HD21	2:B:487:ASP:HB3	1.73	0.70
2:B:509:LEU:O	2:B:512:LEU:HB3	1.91	0.70
2:B:23:SER:HA	2:B:242:LYS:CG	2.21	0.70
2:B:468:LEU:O	2:B:472:THR:HG22	1.91	0.70
2:A:549:THR:O	2:A:551:GLN:N	2.19	0.70
2:A:643:GLU:HG3	2:A:644:VAL:N	2.05	0.70
2:B:388:ILE:HG13	2:B:512:LEU:HD22	1.73	0.70
2:B:554:VAL:HG12	2:B:555:GLN:H	1.56	0.70
2:B:498:LYS:HB2	2:B:501:LYS:HB2	1.74	0.70
1:C:14:DC:C1'	2:B:453:ARG:HH21	2.04	0.69
2:A:28:LEU:HD22	2:A:304:LEU:HD12	1.72	0.69
2:A:161:SER:HB3	2:A:168:GLN:NE2	2.05	0.69
1:D:7:DC:H2'	1:D:8:DT:C7	2.21	0.69
2:B:106:ASN:O	2:B:107:LEU:HD23	1.93	0.69
2:B:234:ARG:HG3	2:B:235:LEU:N	2.08	0.69
2:B:550:TRP:O	2:B:551:GLN:C	2.31	0.69
2:A:325:ASN:HD21	2:A:327:LEU:HB2	1.56	0.69
2:B:380:MET:HG3	2:B:385:ARG:NH2	2.08	0.69
2:B:288:ASN:ND2	2:B:317:PRO:HA	2.08	0.68
2:B:298:GLU:HG3	2:B:303:ARG:HH21	1.56	0.68
1:D:10:DC:H2'	1:D:11:DA:C8	2.28	0.68
2:A:414:PRO:HA	2:A:493:MET:HE1	1.74	0.68
2:B:603:VAL:C	2:B:605:ARG:H	1.94	0.68
2:A:110:ASP:OD1	2:A:532:GLN:HG2	1.94	0.68
2:B:478:HIS:CD2	2:B:517:ARG:HE	2.12	0.68
2:B:162:TYR:C	2:B:164:ASN:N	2.48	0.68
2:B:383:PHE:CD1	2:B:538:ALA:HA	2.29	0.68
2:B:601:VAL:O	2:B:605:ARG:HG2	1.93	0.68
2:B:571:PHE:C	2:B:572:ILE:HD12	2.15	0.67
2:A:325:ASN:C	2:A:325:ASN:ND2	2.47	0.67
2:A:568:PRO:N	2:A:607:MET:HE3	2.10	0.67
2:B:58:MET:HB2	2:B:214:PHE:CD1	2.29	0.67
2:B:353:LEU:HB3	2:B:559:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:413:THR:HA	2:A:414:PRO:C	2.13	0.67
2:A:610:LEU:HD12	2:A:611:THR:N	2.09	0.67
2:A:472:THR:HG21	2:A:480:GLN:HG3	1.75	0.67
2:B:333:VAL:HG13	2:B:571:PHE:CE1	2.29	0.67
1:C:18:DT:OP1	2:A:422:THR:OG1	2.08	0.66
1:D:1:DC:HO5'	1:D:1:DC:H6	1.43	0.66
1:C:11:DA:H2''	1:C:12:DC:H5'	1.75	0.66
2:A:189:PHE:HA	2:A:192:LEU:HD12	1.76	0.66
2:B:638:GLU:O	2:B:638:GLU:HG2	1.95	0.66
2:B:326:GLU:OE2	2:B:327:LEU:HD22	1.95	0.66
2:B:382:PHE:HD2	2:B:383:PHE:CD2	2.13	0.66
2:B:569:GLN:HG3	2:B:571:PHE:HE2	1.60	0.66
2:B:10:LEU:CD1	2:B:18:VAL:HG21	2.25	0.66
2:A:138:PRO:HG2	2:A:141:GLN:CB	2.24	0.66
2:A:601:VAL:O	2:A:605:ARG:HG2	1.96	0.66
2:B:349:GLU:HB3	2:B:568:PRO:CG	2.25	0.66
2:A:165:PRO:HA	2:A:168:GLN:HB2	1.77	0.65
1:D:19:DG:H2''	1:D:20:DC:C5'	2.18	0.65
2:B:398:ILE:HA	2:B:401:ARG:HH21	1.61	0.65
2:B:457:ALA:HA	2:B:460:ARG:NH1	2.11	0.65
2:B:472:THR:HG23	2:B:480:GLN:HE21	1.61	0.65
2:B:475:MET:HE3	2:B:479:VAL:CG1	2.25	0.65
2:A:150:LYS:NZ	2:A:178:GLN:HE22	1.95	0.65
2:B:347:LEU:HD12	2:B:552:ASP:OD2	1.96	0.65
1:C:17:DG:H8	2:A:421:ARG:NH1	1.95	0.65
2:A:355:ARG:NH2	2:A:595:GLU:OE2	2.22	0.65
2:A:112:GLN:CG	2:A:396:ARG:HH11	2.10	0.65
2:B:220:ASP:OD1	2:B:221:GLU:N	2.30	0.65
2:B:549:THR:O	2:B:551:GLN:N	2.30	0.65
2:A:326:GLU:OE1	2:A:618:ARG:HA	1.97	0.64
2:B:380:MET:HG3	2:B:385:ARG:HH22	1.62	0.64
1:D:18:DT:H5'	2:B:419:GLY:HA3	1.79	0.64
2:B:341:GLN:HE21	2:B:347:LEU:HD11	1.59	0.64
1:D:17:DG:H3'	2:B:421:ARG:HD2	1.78	0.64
2:B:356:SER:OG	2:B:359:GLN:HG3	1.96	0.64
2:B:453:ARG:HH11	2:B:453:ARG:CB	2.09	0.64
2:A:142:ALA:O	2:A:146:ILE:HG13	1.97	0.64
2:B:570:VAL:CG1	2:B:606:ALA:HA	2.28	0.64
2:A:284:ARG:HD3	2:A:566:GLU:CB	2.26	0.64
2:B:39:LEU:CD2	2:B:218:LEU:HD23	2.28	0.64
2:B:403:ASP:HB3	2:B:406:ALA:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:290:LEU:O	2:A:293:ALA:HB3	1.98	0.63
2:B:89:THR:O	2:B:93:LEU:HG	1.98	0.63
2:B:258:GLY:O	2:B:260:GLN:NE2	2.31	0.63
2:B:621:TYR:HD1	2:B:621:TYR:O	1.80	0.63
2:B:4:SER:HB3	2:B:7:LEU:HD12	1.81	0.63
2:B:129:ALA:HB1	2:B:431:ARG:CD	2.29	0.63
1:D:29:DT:O2	1:D:29:DT:H5'	1.99	0.63
2:A:119:GLN:HE21	2:A:143:MET:HE2	1.62	0.63
2:B:113:ILE:N	2:B:113:ILE:HD12	2.12	0.63
2:B:396:ARG:HG2	2:B:535:LEU:HD13	1.81	0.63
2:A:431:ARG:HG3	2:A:431:ARG:HH11	1.62	0.63
2:A:288:ASN:O	2:A:291:SER:HB3	1.99	0.63
2:A:288:ASN:HD22	2:A:317:PRO:HA	1.60	0.63
2:A:491:ARG:O	2:A:495:GLU:HG3	1.99	0.63
2:B:23:SER:CA	2:B:242:LYS:HG3	2.28	0.63
2:B:246:VAL:HG12	2:B:247:GLY:N	2.11	0.63
2:B:582:SER:OG	2:B:585:SER:HB3	1.98	0.63
2:B:222:PHE:O	2:B:225:THR:HG23	1.99	0.62
2:B:610:LEU:HD12	2:B:611:THR:N	2.15	0.62
2:B:325:ASN:HD22	2:B:325:ASN:H	1.45	0.62
2:A:457:ALA:HA	2:A:460:ARG:NH2	2.14	0.62
2:B:182:ASP:O	2:B:185:GLY:N	2.31	0.62
2:B:341:GLN:CD	2:B:347:LEU:HD21	2.20	0.62
1:C:17:DG:H1'	1:C:18:DT:H5''	1.81	0.62
1:D:6:DA:H2'	1:D:7:DC:C6	2.35	0.62
1:C:27:DC:H1'	1:C:28:DG:C8	2.35	0.62
2:B:483:ARG:HG2	2:B:483:ARG:HH11	1.64	0.62
2:B:10:LEU:HD11	2:B:18:VAL:HG21	1.82	0.62
2:B:36:THR:O	2:B:40:VAL:HG23	2.00	0.61
2:B:247:GLY:O	2:B:248:ASP:HB2	2.00	0.61
2:B:641:VAL:HG12	2:B:642:GLU:N	2.15	0.61
2:A:53:SER:O	2:A:55:TYR:N	2.33	0.61
2:A:412:ASN:O	2:A:415:THR:HA	2.00	0.61
2:B:262:GLU:O	2:B:264:ILE:N	2.34	0.61
1:D:17:DG:H2''	1:D:18:DT:O5'	1.99	0.61
2:A:156:PRO:HD3	2:A:174:TYR:HE1	1.64	0.61
2:B:340:TRP:CD1	2:B:345:GLY:HA3	2.36	0.61
2:B:320:LEU:HD11	2:B:633:ILE:CG2	2.30	0.61
2:A:133:ASP:O	2:A:135:LYS:N	2.34	0.61
2:B:39:LEU:HD22	2:B:218:LEU:HD23	1.82	0.61
2:B:146:ILE:HG23	2:B:174:TYR:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:MET:O	2:B:74:ILE:HG12	2.00	0.61
2:B:280:GLU:HB3	2:B:307:LYS:O	2.00	0.61
2:B:321:TYR:CE2	2:B:323:ALA:HB2	2.35	0.61
2:A:129:ALA:C	2:A:130:MET:HG3	2.21	0.61
2:B:546:GLN:O	2:B:548:ASP:N	2.34	0.60
1:D:16:DA:H2''	1:D:17:DG:C5'	2.31	0.60
2:B:161:SER:O	2:B:162:TYR:CG	2.54	0.60
2:B:383:PHE:CE1	2:B:538:ALA:HA	2.36	0.60
2:A:37:ARG:NH1	3:A:681:GOL:H2	2.15	0.60
2:B:401:ARG:HH22	2:B:469:ALA:CB	2.13	0.60
2:A:39:LEU:HD21	2:A:246:VAL:HG21	1.83	0.60
2:B:122:LEU:HD12	2:B:122:LEU:O	2.01	0.60
1:C:6:DA:C2'	1:C:7:DC:O5'	2.50	0.60
2:B:155:ARG:HG3	2:B:156:PRO:CD	2.09	0.60
2:B:412:ASN:HB2	2:B:418:ILE:HB	1.84	0.60
2:A:573:VAL:HG13	2:A:574:GLY:N	2.17	0.60
2:B:347:LEU:N	2:B:552:ASP:OD2	2.34	0.60
2:A:156:PRO:HD3	2:A:174:TYR:CE1	2.36	0.60
2:B:12:ASP:O	2:B:16:GLU:N	2.30	0.60
2:B:23:SER:O	2:B:25:LEU:HD23	2.01	0.60
2:B:501:LYS:CE	2:B:505:ARG:HH12	2.14	0.60
2:A:6:LEU:HD12	2:A:45:TRP:HE3	1.66	0.60
2:B:161:SER:O	2:B:162:TYR:CB	2.49	0.60
2:B:326:GLU:HB3	2:B:618:ARG:HH12	1.66	0.60
1:C:11:DA:H1'	1:C:12:DC:H5''	1.84	0.60
2:A:42:ARG:HG2	2:A:244:MET:HE3	1.84	0.60
2:A:236:LEU:HD12	2:A:236:LEU:O	2.01	0.60
2:B:152:GLU:OE2	2:B:227:ASN:ND2	2.34	0.60
2:B:112:GLN:HB3	2:B:186:LEU:CD2	2.32	0.60
2:B:107:LEU:HD21	2:B:195:ARG:HE	1.66	0.59
2:A:459:GLN:O	2:A:463:GLU:HG3	2.01	0.59
2:B:150:LYS:HE2	2:B:178:GLN:HE22	1.66	0.59
2:A:162:TYR:CG	2:A:162:TYR:O	2.56	0.59
2:B:253:ILE:CD1	2:B:253:ILE:H	2.15	0.59
2:B:226:ASN:OD1	2:B:229:GLN:HG3	2.01	0.59
2:A:70:MET:O	2:A:74:ILE:HG13	2.03	0.59
1:C:17:DG:H2'	2:A:421:ARG:HD2	1.84	0.59
2:A:28:LEU:HD12	2:A:247:GLY:O	2.03	0.59
2:B:398:ILE:HG23	2:B:469:ALA:HA	1.85	0.59
2:B:165:PRO:HA	2:B:168:GLN:HB2	1.84	0.59
2:B:253:ILE:H	2:B:253:ILE:HD13	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:ARG:O	2:B:495:GLU:HG3	2.03	0.59
2:A:319:SER:C	2:A:320:LEU:HD23	2.22	0.59
2:A:414:PRO:HA	2:A:493:MET:HE3	1.83	0.59
1:D:18:DT:H5'	2:B:419:GLY:CA	2.33	0.58
2:A:23:SER:HA	2:A:242:LYS:HG3	1.83	0.58
2:A:325:ASN:HA	2:A:617:THR:O	2.03	0.58
2:A:504:THR:HG22	2:A:508:ASN:ND2	2.18	0.58
2:B:226:ASN:OD1	2:B:228:ILE:HG22	2.04	0.58
2:B:400:ASN:HD21	2:B:402:ASN:CB	2.08	0.58
2:A:119:GLN:HE21	2:A:143:MET:HE3	1.66	0.58
2:A:290:LEU:O	2:A:294:ASN:ND2	2.36	0.58
2:B:351:ALA:HA	2:B:555:GLN:O	2.03	0.58
2:A:134:GLU:C	2:A:136:GLN:H	2.07	0.58
2:A:601:VAL:O	2:A:605:ARG:NH1	2.35	0.58
2:B:333:VAL:HG11	2:B:352:ILE:HD12	1.85	0.58
2:B:142:ALA:HB2	2:B:170:TRP:HZ3	1.67	0.58
2:B:571:PHE:N	2:B:571:PHE:CD2	2.72	0.58
1:D:17:DG:H5'	2:B:421:ARG:NH1	2.18	0.58
2:A:368:LEU:O	2:A:370:ALA:N	2.36	0.58
2:A:643:GLU:O	2:A:644:VAL:HG23	2.02	0.58
2:A:543:GLY:O	2:A:544:GLU:CB	2.52	0.58
2:B:329:GLU:CD	2:B:573:VAL:HG13	2.24	0.57
1:D:17:DG:H5'	2:B:421:ARG:HH11	1.69	0.57
2:A:112:GLN:HG2	2:A:396:ARG:NH1	2.18	0.57
2:B:557:MET:HG3	2:B:558:THR:O	2.04	0.57
2:A:10:LEU:HD11	2:A:18:VAL:HG21	1.85	0.57
1:C:7:DC:H2''	1:C:8:DT:OP2	2.05	0.57
2:B:230:TYR:HB2	2:B:263:ASN:ND2	2.19	0.57
2:B:603:VAL:HG23	2:B:610:LEU:HD21	1.86	0.57
1:C:12:DC:C6	1:C:13:DT:H72	2.40	0.57
1:C:18:DT:C2'	1:C:19:DG:H5'	2.35	0.57
2:B:461:PHE:CZ	2:B:465:ILE:HD11	2.40	0.57
2:A:53:SER:C	2:A:55:TYR:H	2.06	0.57
2:A:149:GLN:HG3	2:A:154:LEU:HB2	1.87	0.57
2:A:217:ILE:C	2:A:218:LEU:HD12	2.24	0.57
2:B:421:ARG:O	2:B:425:VAL:HG23	2.04	0.57
2:B:569:GLN:HE22	2:B:609:LYS:HB3	1.70	0.57
1:D:16:DA:H2''	1:D:17:DG:H5'	1.86	0.57
1:D:18:DT:H5'	2:B:419:GLY:N	2.20	0.57
2:A:506:ILE:O	2:A:510:GLU:HG3	2.05	0.57
2:A:568:PRO:HA	2:A:607:MET:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ASP:HB3	2:B:203:LYS:HG3	1.85	0.57
2:A:374:TYR:HA	2:A:553:ALA:HB1	1.85	0.57
2:B:140:ARG:HG3	2:B:140:ARG:HH11	1.69	0.57
2:B:483:ARG:HG2	2:B:483:ARG:NH1	2.20	0.57
2:A:30:GLY:O	2:A:31:ALA:CB	2.52	0.57
2:A:325:ASN:ND2	2:A:327:LEU:HB2	2.18	0.56
2:A:112:GLN:HE21	2:A:113:ILE:H	1.50	0.56
2:A:260:GLN:HA	2:A:260:GLN:HE21	1.70	0.56
2:B:298:GLU:HG3	2:B:303:ARG:NH2	2.20	0.56
2:B:543:GLY:O	2:B:544:GLU:CB	2.53	0.56
2:A:119:GLN:NE2	2:A:143:MET:HE2	2.20	0.56
2:A:262:GLU:OE1	2:A:262:GLU:N	2.21	0.56
2:B:154:LEU:HD23	2:B:158:HIS:HD2	1.70	0.56
2:B:550:TRP:O	2:B:552:ASP:N	2.38	0.56
2:A:325:ASN:ND2	2:A:327:LEU:N	2.53	0.56
2:B:292:ALA:HA	2:B:637:PRO:HD2	1.88	0.56
2:B:483:ARG:O	2:B:486:LYS:N	2.38	0.56
2:B:579:MET:HE2	2:B:618:ARG:NE	2.21	0.56
2:B:597:ARG:O	2:B:600:TYR:HB3	2.05	0.56
2:B:337:ILE:HD12	2:B:350:CYS:SG	2.45	0.56
2:A:154:LEU:O	2:A:155:ARG:CB	2.54	0.55
2:B:114:LEU:CD1	2:B:186:LEU:HD13	2.36	0.55
2:B:161:SER:O	2:B:162:TYR:HB3	2.06	0.55
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.71	0.55
2:B:329:GLU:OE2	2:B:573:VAL:HG13	2.06	0.55
2:B:412:ASN:O	2:B:413:THR:HG23	2.05	0.55
2:B:614:TYR:CE1	2:B:629:PRO:HG3	2.41	0.55
2:B:198:GLU:O	2:B:202:ASN:ND2	2.39	0.55
2:B:299:ASN:HD21	2:B:635:GLU:HB3	1.71	0.55
2:B:410:VAL:HA	2:B:413:THR:OG1	2.05	0.55
1:C:11:DA:C2'	1:C:12:DC:H5''	2.36	0.55
2:A:402:ASN:HB3	2:A:436:THR:HG21	1.88	0.55
1:D:18:DT:H2''	1:D:19:DG:O5'	2.06	0.55
2:A:349:GLU:HB3	2:A:568:PRO:HD2	1.89	0.55
2:B:7:LEU:O	2:B:9:SER:N	2.39	0.55
2:A:80:THR:HG22	2:A:81:SER:H	1.71	0.55
2:A:199:LEU:HG	2:A:206:ILE:CD1	2.37	0.55
2:A:573:VAL:CG1	2:A:574:GLY:N	2.69	0.55
1:D:11:DA:H2''	1:D:12:DC:H5'	1.89	0.55
1:D:28:DG:H4'	1:D:28:DG:OP1	2.06	0.55
2:A:154:LEU:O	2:A:155:ARG:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:202:ASN:O	2:A:204:PRO:HD3	2.07	0.55
2:A:292:ALA:HB1	2:A:636:LEU:HD22	1.88	0.55
2:A:349:GLU:HB3	2:A:568:PRO:HG2	1.89	0.55
1:C:33:DT:H3'	2:A:540:LEU:O	2.07	0.55
1:D:20:DC:H2''	1:D:21:DA:C8	2.42	0.55
2:A:394:TYR:CE2	2:A:488:SER:HB2	2.42	0.55
2:B:368:LEU:HD21	2:B:374:TYR:HE2	1.71	0.55
2:A:403:ASP:HB3	2:A:406:ALA:HB3	1.88	0.55
2:A:348:ALA:HA	2:A:553:ALA:O	2.07	0.55
2:A:394:TYR:O	2:A:398:ILE:HG13	2.07	0.54
2:B:341:GLN:NE2	2:B:347:LEU:HD21	2.21	0.54
2:A:125:ARG:NE	2:A:408:GLU:OE1	2.40	0.54
2:A:619:ARG:HG3	2:A:623:LYS:O	2.07	0.54
2:B:495:GLU:HA	2:B:506:ILE:HD11	1.90	0.54
2:A:360:SER:O	2:A:364:GLU:HG3	2.07	0.54
2:B:32:GLY:O	2:B:283:TYR:HD1	1.91	0.54
2:B:35:LYS:HE2	2:B:221:GLU:OE2	2.07	0.54
2:B:350:CYS:O	2:B:351:ALA:HB2	2.07	0.54
2:A:394:TYR:CE1	2:A:410:VAL:HB	2.43	0.54
2:B:325:ASN:HD22	2:B:325:ASN:N	2.05	0.54
2:B:603:VAL:C	2:B:605:ARG:N	2.61	0.54
1:C:2:DG:H4'	2:B:361:ARG:NH1	2.23	0.54
1:C:17:DG:H2''	1:C:18:DT:H5'	1.89	0.54
2:A:137:TRP:CZ3	2:A:169:THR:HB	2.43	0.54
2:A:567:PHE:O	2:A:607:MET:HG3	2.08	0.54
2:B:61:THR:HB	2:B:67:ALA:HB2	1.89	0.54
2:B:150:LYS:HE2	2:B:178:GLN:NE2	2.22	0.54
1:D:32:DT:H2''	1:D:33:DT:C6	2.42	0.54
2:A:576:GLU:OE2	2:A:627:HIS:HD2	1.90	0.54
2:B:44:ALA:CB	2:B:77:LEU:HD23	2.37	0.54
2:B:49:VAL:C	2:B:51:ASN:H	2.11	0.54
2:B:172:LYS:O	2:B:175:GLN:HB3	2.07	0.54
2:B:61:THR:HG22	2:B:62:PHE:N	2.15	0.54
2:B:618:ARG:HH11	2:B:618:ARG:CB	2.19	0.54
2:B:27:VAL:O	2:B:29:ALA:N	2.41	0.54
2:A:81:SER:O	2:A:82:GLN:HB2	2.08	0.53
2:B:112:GLN:HB3	2:B:186:LEU:HD23	1.88	0.53
2:B:398:ILE:HA	2:B:401:ARG:NH2	2.22	0.53
2:B:326:GLU:HA	2:B:329:GLU:HB3	1.89	0.53
1:D:25:DC:H2''	1:D:26:DT:OP2	2.08	0.53
2:B:203:LYS:N	2:B:204:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:ARG:HB3	2:B:543:GLY:N	2.23	0.53
2:B:570:VAL:C	2:B:571:PHE:CD2	2.82	0.53
2:A:153:GLY:HA2	2:A:194:LEU:HD13	1.90	0.53
2:B:606:ALA:HB2	2:B:610:LEU:HD22	1.91	0.53
2:A:442:ARG:NH1	2:A:442:ARG:HG2	2.22	0.53
2:B:642:GLU:HG2	2:B:643:GLU:O	2.09	0.53
2:A:202:ASN:C	2:A:204:PRO:HD3	2.29	0.53
2:A:30:GLY:N	2:A:33:SER:OG	2.41	0.53
2:A:400:ASN:HD21	2:A:402:ASN:HB2	1.74	0.53
2:A:53:SER:C	2:A:55:TYR:N	2.62	0.53
2:B:149:GLN:HG3	2:B:154:LEU:HB2	1.89	0.53
2:B:298:GLU:CG	2:B:303:ARG:HH21	2.21	0.53
1:D:32:DT:H3'	2:B:381:ARG:HH22	1.74	0.53
2:B:109:GLN:NE2	2:B:528:LEU:HD23	2.23	0.53
2:B:376:ILE:HG22	2:B:377:TYR:N	2.24	0.53
2:B:436:THR:HG1	2:B:439:GLN:HG3	1.74	0.53
2:B:458:LEU:O	2:B:461:PHE:HB3	2.09	0.53
2:B:556:LEU:HD12	2:B:556:LEU:N	2.24	0.53
2:A:54:PRO:O	2:A:85:MET:HA	2.10	0.52
2:B:385:ARG:HH21	2:B:385:ARG:HG2	1.74	0.52
2:A:158:HIS:O	2:A:160:GLN:N	2.43	0.52
2:B:396:ARG:HB3	2:B:403:ASP:OD2	2.10	0.52
2:A:264:ILE:CG2	2:A:265:GLN:N	2.71	0.52
2:B:407:PHE:O	2:B:409:ARG:N	2.41	0.52
2:B:554:VAL:CG1	2:B:555:GLN:H	2.23	0.52
2:B:443:GLU:O	2:B:447:GLU:HG3	2.10	0.52
2:B:244:MET:HG2	2:B:245:ILE:N	2.25	0.52
2:B:352:ILE:C	2:B:353:LEU:HD23	2.30	0.52
1:C:5:DC:H2''	1:C:6:DA:C8	2.45	0.52
2:A:156:PRO:HG2	2:A:157:HIS:H	1.75	0.52
2:B:253:ILE:HD13	2:B:253:ILE:N	2.25	0.52
2:B:340:TRP:O	2:B:345:GLY:HA3	2.09	0.52
2:B:435:LEU:HB3	2:B:439:GLN:HB2	1.91	0.52
1:D:32:DT:C4	2:B:257:ARG:HD2	2.45	0.52
2:A:80:THR:HG22	2:A:81:SER:N	2.24	0.52
2:B:265:GLN:NE2	2:B:269:ASN:OD1	2.43	0.52
2:B:470:GLN:O	2:B:472:THR:N	2.43	0.52
2:B:643:GLU:HG3	2:B:644:VAL:H	1.74	0.52
2:A:126:LEU:O	2:A:127:ILE:C	2.48	0.52
2:A:339:THR:O	2:A:342:ASP:N	2.43	0.52
2:B:107:LEU:HD21	2:B:195:ARG:NE	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASN:HA	2:B:297:ILE:HG22	1.92	0.52
2:B:438:TRP:HZ3	2:B:465:ILE:HD12	1.75	0.52
2:B:601:VAL:HG12	2:B:605:ARG:NH1	2.25	0.52
2:B:621:TYR:O	2:B:621:TYR:CD1	2.63	0.52
2:A:5:TYR:CZ	2:A:6:LEU:HD21	2.45	0.52
2:A:446:GLN:C	2:A:448:LYS:H	2.12	0.52
2:A:642:GLU:HG2	2:A:643:GLU:O	2.09	0.52
2:B:61:THR:HG21	2:B:66:ALA:HB3	1.92	0.52
2:B:472:THR:CG2	2:B:480:GLN:HE21	2.23	0.52
2:B:128:LYS:C	2:B:130:MET:H	2.13	0.51
2:B:306:LYS:HE3	2:B:600:TYR:OH	2.10	0.51
2:A:264:ILE:HG23	2:A:265:GLN:N	2.25	0.51
2:A:385:ARG:HH21	2:A:385:ARG:HG2	1.74	0.51
2:B:34:GLY:O	2:B:37:ARG:HB3	2.10	0.51
2:B:156:PRO:HG2	2:B:157:HIS:H	1.74	0.51
2:B:571:PHE:N	2:B:571:PHE:HD2	2.07	0.51
2:A:193:LEU:CD1	2:A:229:GLN:HE21	2.24	0.51
2:A:318:ILE:HD12	2:A:318:ILE:N	2.25	0.51
2:B:207:LEU:O	2:B:211:ARG:HG3	2.10	0.51
2:B:618:ARG:HG3	2:B:618:ARG:O	2.11	0.51
1:D:7:DC:C2'	1:D:8:DT:C6	2.93	0.51
2:A:320:LEU:O	2:A:644:VAL:HB	2.10	0.51
1:C:11:DA:H2''	1:C:12:DC:H5''	1.88	0.51
1:C:30:DT:H2''	1:C:31:DG:H5'	1.92	0.51
2:A:442:ARG:HG2	2:A:442:ARG:HH11	1.75	0.51
2:B:112:GLN:HG2	2:B:396:ARG:NH1	2.18	0.51
2:B:420:ASP:OD2	2:B:420:ASP:N	2.35	0.51
2:B:577:GLU:O	2:B:627:HIS:HB3	2.11	0.51
2:A:161:SER:OG	2:A:162:TYR:N	2.42	0.51
2:B:224:ASP:HA	2:B:259:ALA:HB1	1.91	0.51
2:A:252:SER:H	2:A:597:ARG:HD2	1.76	0.51
2:B:554:VAL:CG1	2:B:555:GLN:N	2.73	0.51
2:B:292:ALA:HB1	2:B:636:LEU:HD22	1.92	0.51
2:B:492:THR:HG22	2:B:493:MET:N	2.26	0.51
2:B:156:PRO:HD3	2:B:174:TYR:CE1	2.39	0.50
2:B:634:GLY:C	2:B:636:LEU:H	2.14	0.50
1:C:8:DT:H2''	1:C:9:DG:C8	2.46	0.50
2:A:119:GLN:NE2	2:A:143:MET:CE	2.74	0.50
2:B:411:VAL:HG13	2:B:412:ASN:N	2.26	0.50
2:B:414:PRO:HA	2:B:493:MET:CE	2.41	0.50
2:A:99:ARG:HD3	2:A:111:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:ARG:NH2	2:B:385:ARG:HG2	2.25	0.50
2:B:531:LEU:O	2:B:534:PHE:N	2.44	0.50
1:C:32:DT:C4	2:A:257:ARG:HD2	2.46	0.50
2:A:411:VAL:HG13	2:A:412:ASN:N	2.26	0.50
2:B:30:GLY:O	2:B:31:ALA:HB2	2.10	0.50
2:B:150:LYS:CE	2:B:178:GLN:HE22	2.24	0.50
2:B:49:VAL:O	2:B:51:ASN:N	2.44	0.50
2:B:382:PHE:HA	2:B:385:ARG:HD2	1.92	0.50
2:B:389:LYS:HB2	2:B:409:ARG:NH2	2.26	0.50
2:A:220:ASP:O	2:A:221:GLU:C	2.50	0.50
2:A:642:GLU:O	2:A:643:GLU:O	2.30	0.50
2:B:12:ASP:HA	2:B:15:ARG:HD3	1.93	0.50
2:B:401:ARG:HG2	2:B:438:TRP:CH2	2.47	0.50
2:B:603:VAL:O	2:B:605:ARG:N	2.44	0.50
2:B:39:LEU:O	2:B:43:ILE:HG13	2.12	0.50
2:B:114:LEU:HD13	2:B:186:LEU:HB3	1.92	0.50
1:D:1:DC:C2	2:A:621:TYR:HB2	2.47	0.50
2:A:596:ARG:NH1	2:A:635:GLU:OE1	2.45	0.50
2:B:360:SER:O	2:B:364:GLU:HG3	2.12	0.50
2:B:368:LEU:C	2:B:370:ALA:H	2.15	0.50
2:B:610:LEU:HD12	2:B:610:LEU:C	2.32	0.50
1:D:6:DA:H2'	1:D:7:DC:H6	1.76	0.50
2:A:36:THR:HG22	2:A:73:ARG:HH21	1.75	0.50
2:A:102:HIS:CD2	2:A:109:GLN:HB2	2.47	0.50
2:B:10:LEU:HD13	2:B:18:VAL:HG21	1.93	0.50
2:B:579:MET:HE2	2:B:618:ARG:HE	1.77	0.50
2:B:631:ARG:O	2:B:635:GLU:HG3	2.12	0.50
2:B:401:ARG:NH2	2:B:469:ALA:HB2	2.21	0.49
1:C:18:DT:O5'	2:A:419:GLY:HA3	2.12	0.49
1:D:16:DA:H2''	2:B:421:ARG:NH1	2.27	0.49
2:B:264:ILE:CG2	2:B:265:GLN:N	2.75	0.49
2:B:501:LYS:HE3	2:B:505:ARG:NH1	2.25	0.49
2:A:416:ARG:HB2	2:A:418:ILE:CD1	2.41	0.49
2:B:382:PHE:HD2	2:B:383:PHE:HD2	1.60	0.49
2:A:425:VAL:HG11	2:A:450:LEU:HD21	1.95	0.49
2:A:352:ILE:HG21	2:A:363:LEU:HD13	1.95	0.49
2:A:149:GLN:CA	2:A:149:GLN:HE21	2.26	0.49
2:B:39:LEU:HD11	2:B:246:VAL:HG21	1.93	0.49
2:B:290:LEU:CD1	2:B:310:THR:HB	2.43	0.49
2:B:644:VAL:HG12	2:B:644:VAL:O	2.13	0.49
1:D:9:DG:H2''	1:D:10:DC:O5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:568:PRO:CD	2:A:607:MET:HE3	2.42	0.49
2:B:119:GLN:HE22	2:B:147:ASN:HD21	1.60	0.49
2:B:370:ALA:O	2:B:371:SER:C	2.51	0.49
2:B:401:ARG:HG2	2:B:438:TRP:CE2	2.48	0.49
2:B:472:THR:OG1	2:B:480:GLN:HG3	2.13	0.49
2:B:154:LEU:HD23	2:B:158:HIS:CD2	2.47	0.48
2:B:472:THR:CA	2:B:475:MET:SD	2.99	0.48
2:B:596:ARG:HH11	2:B:596:ARG:HG3	1.78	0.48
2:A:374:TYR:HE1	2:A:376:ILE:HD11	1.77	0.48
2:A:614:TYR:CE1	2:A:629:PRO:HG3	2.48	0.48
2:B:223:GLN:OE1	2:B:223:GLN:N	2.40	0.48
2:A:115:ASP:OD1	2:A:389:LYS:NZ	2.37	0.48
2:B:401:ARG:HG2	2:B:438:TRP:CZ3	2.48	0.48
1:C:5:DC:H2''	1:C:6:DA:N7	2.29	0.48
2:A:461:PHE:O	2:A:464:LEU:HB3	2.13	0.48
2:B:68:ALA:HA	2:B:71:ARG:HH12	1.77	0.48
2:B:609:LYS:HG3	2:B:610:LEU:N	2.28	0.48
2:A:5:TYR:CE1	2:A:6:LEU:CD2	2.97	0.48
2:A:19:ALA:HA	2:A:45:TRP:CE2	2.49	0.48
2:A:172:LYS:O	2:A:175:GLN:HB3	2.14	0.48
2:A:398:ILE:HG23	2:A:469:ALA:HA	1.94	0.48
2:A:481:THR:O	2:A:485:ILE:HG13	2.13	0.48
2:B:333:VAL:HG13	2:B:571:PHE:CD1	2.48	0.48
2:B:545:GLY:O	2:B:546:GLN:CB	2.62	0.48
2:A:37:ARG:CZ	3:A:681:GOL:H2	2.44	0.48
2:B:41:HIS:HD1	2:B:77:LEU:HD21	1.78	0.48
2:A:392:LEU:O	2:A:396:ARG:HG3	2.14	0.48
2:B:219:VAL:HG21	2:B:233:ILE:HD13	1.96	0.48
2:B:394:TYR:O	2:B:398:ILE:HG12	2.13	0.48
2:B:407:PHE:C	2:B:409:ARG:H	2.17	0.48
2:A:112:GLN:CG	2:A:396:ARG:NH1	2.75	0.48
2:A:614:TYR:CD1	2:A:614:TYR:O	2.66	0.48
2:B:339:THR:HG23	2:B:340:TRP:N	2.29	0.48
1:C:21:DA:H2''	1:C:22:DG:H5'	1.95	0.48
2:A:349:GLU:HB3	2:A:568:PRO:CD	2.44	0.48
2:B:112:GLN:HE21	2:B:113:ILE:HD12	1.77	0.48
2:A:82:GLN:HB3	2:A:85:MET:HE3	1.96	0.48
2:A:235:LEU:C	2:A:237:ALA:H	2.16	0.48
2:A:483:ARG:HG3	2:A:483:ARG:NH1	2.28	0.48
2:B:505:ARG:HG2	2:B:505:ARG:HH11	1.79	0.48
1:D:18:DT:C5'	2:B:419:GLY:HA3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:LYS:HE2	2:A:220:ASP:OD1	2.14	0.47
2:A:150:LYS:HZ1	2:A:178:GLN:HE22	1.60	0.47
2:A:431:ARG:HG3	2:A:431:ARG:NH1	2.29	0.47
2:B:11:ASN:ND2	2:B:283:TYR:OH	2.47	0.47
2:B:68:ALA:HA	2:B:71:ARG:NH1	2.29	0.47
2:B:134:GLU:C	2:B:136:GLN:H	2.17	0.47
2:B:252:SER:CB	2:B:261:VAL:HG22	2.44	0.47
2:B:376:ILE:HD13	2:B:556:LEU:HB2	1.96	0.47
2:A:349:GLU:O	2:A:568:PRO:HD2	2.13	0.47
2:B:220:ASP:O	2:B:221:GLU:C	2.52	0.47
2:B:250:ASP:HB3	2:B:600:TYR:CE2	2.48	0.47
2:B:336:ARG:O	2:B:339:THR:HG22	2.13	0.47
2:A:235:LEU:N	2:A:235:LEU:HD23	2.28	0.47
2:B:400:ASN:ND2	2:B:402:ASN:N	2.58	0.47
2:B:564:GLY:C	2:B:565:LEU:HD23	2.33	0.47
2:B:570:VAL:C	2:B:571:PHE:HD2	2.18	0.47
2:B:579:MET:HE1	2:B:618:ARG:HD2	1.95	0.47
2:A:407:PHE:O	2:A:409:ARG:N	2.47	0.47
2:A:438:TRP:CE2	2:A:462:MET:HE3	2.50	0.47
2:A:271:PHE:CD1	2:A:271:PHE:N	2.83	0.47
2:A:375:ARG:NH1	2:A:548:ASP:CB	2.77	0.47
2:A:385:ARG:HG2	2:A:385:ARG:NH2	2.29	0.47
2:A:272:PRO:C	2:A:274:ALA:N	2.67	0.47
2:A:413:THR:CA	2:A:414:PRO:C	2.81	0.47
2:A:459:GLN:HE21	2:A:463:GLU:HG2	1.78	0.47
2:A:530:PRO:O	2:A:533:ALA:HB3	2.14	0.47
2:B:231:ALA:O	2:B:234:ARG:HG2	2.15	0.47
2:B:401:ARG:HG2	2:B:438:TRP:CZ2	2.49	0.47
2:B:565:LEU:HD23	2:B:565:LEU:N	2.30	0.47
2:B:506:ILE:O	2:B:510:GLU:HG2	2.15	0.47
2:A:325:ASN:ND2	2:A:327:LEU:H	2.13	0.47
2:B:321:TYR:HE2	2:B:323:ALA:CB	2.27	0.47
2:B:407:PHE:C	2:B:409:ARG:N	2.68	0.47
2:A:214:PHE:HB2	2:A:236:LEU:HD11	1.97	0.47
2:A:283:TYR:CZ	3:A:681:GOL:H12	2.50	0.47
2:A:498:LYS:H	2:A:498:LYS:HD3	1.80	0.47
2:B:454:ALA:O	2:B:457:ALA:N	2.47	0.47
2:A:472:THR:O	2:A:472:THR:HG22	2.15	0.46
2:B:256:TRP:C	2:B:258:GLY:H	2.18	0.46
2:B:354:TYR:CE2	2:B:360:SER:HB3	2.50	0.46
2:B:583:GLN:C	2:B:585:SER:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:DG:H2''	1:C:25:DC:OP2	2.15	0.46
1:D:17:DG:C3'	2:B:421:ARG:HD2	2.46	0.46
2:A:134:GLU:C	2:A:136:GLN:N	2.68	0.46
2:A:206:ILE:HG13	2:A:207:LEU:N	2.30	0.46
2:A:272:PRO:C	2:A:274:ALA:H	2.19	0.46
2:B:104:ASP:HA	2:B:203:LYS:NZ	2.30	0.46
2:B:119:GLN:HG2	2:B:143:MET:HE3	1.96	0.46
2:B:164:ASN:O	2:B:164:ASN:CG	2.52	0.46
2:B:205:HIS:CE1	2:B:206:ILE:HG13	2.50	0.46
2:B:337:ILE:HD11	2:B:571:PHE:CE2	2.50	0.46
1:C:17:DG:C8	2:A:421:ARG:NH1	2.80	0.46
2:A:80:THR:CG2	2:A:81:SER:H	2.25	0.46
2:A:199:LEU:HG	2:A:206:ILE:HD11	1.97	0.46
2:A:286:THR:HG23	2:A:607:MET:O	2.15	0.46
2:B:245:ILE:HG13	2:B:245:ILE:O	2.15	0.46
2:B:331:ARG:HG3	2:B:331:ARG:HH11	1.80	0.46
2:B:407:PHE:C	2:B:407:PHE:CD2	2.88	0.46
2:B:483:ARG:O	2:B:484:VAL:C	2.54	0.46
2:B:601:VAL:HG12	2:B:605:ARG:HH11	1.79	0.46
2:A:34:GLY:HA2	4:A:682:FMT:H	1.97	0.46
2:A:37:ARG:HG2	2:A:41:HIS:HD2	1.81	0.46
2:A:368:LEU:O	2:A:371:SER:N	2.47	0.46
2:A:546:GLN:O	2:A:547:ALA:C	2.53	0.46
2:B:157:HIS:CG	2:B:157:HIS:O	2.68	0.46
2:B:401:ARG:HG2	2:B:438:TRP:CD2	2.51	0.46
1:D:4:DG:H2''	1:D:5:DC:OP2	2.15	0.46
2:A:29:ALA:O	2:A:248:ASP:HB2	2.15	0.46
2:A:207:LEU:HD21	2:A:211:ARG:NH2	2.30	0.46
2:A:483:ARG:CG	2:A:483:ARG:HH11	2.28	0.46
2:B:47:MET:CE	2:B:78:MET:HG2	2.46	0.46
2:B:62:PHE:CE1	2:B:90:PHE:HE1	2.34	0.46
2:B:299:ASN:ND2	2:B:635:GLU:HB3	2.31	0.46
2:B:548:ASP:O	2:B:549:THR:C	2.53	0.46
2:B:278:ARG:HH11	2:B:278:ARG:HG3	1.81	0.46
2:B:420:ASP:O	2:B:421:ARG:C	2.54	0.46
2:B:644:VAL:O	2:B:646:LEU:N	2.41	0.46
2:A:441:CYS:O	2:A:442:ARG:C	2.53	0.46
2:A:504:THR:O	2:A:507:GLU:HB2	2.16	0.46
2:B:286:THR:OG1	2:B:289:ILE:HD13	2.16	0.46
2:B:373:PRO:HB2	2:B:553:ALA:HB2	1.96	0.46
1:D:16:DA:HI'	1:D:17:DG:H5''	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:154:LEU:O	2:A:155:ARG:HG2	2.16	0.46
2:A:425:VAL:HG12	2:A:444:LEU:CD1	2.46	0.46
2:A:584:MET:O	2:A:588:GLU:CB	2.64	0.46
2:B:260:GLN:C	2:B:262:GLU:N	2.69	0.46
2:B:290:LEU:HD12	2:B:310:THR:HB	1.98	0.46
2:B:329:GLU:O	2:B:333:VAL:HG23	2.16	0.46
2:B:346:ALA:HB3	2:B:349:GLU:OE1	2.16	0.46
2:A:151:ASP:O	2:A:228:ILE:HB	2.16	0.46
2:A:193:LEU:HD13	2:A:229:GLN:HE21	1.81	0.46
2:B:11:ASN:OD1	2:B:11:ASN:O	2.34	0.46
2:B:401:ARG:HG2	2:B:438:TRP:CE3	2.51	0.46
2:B:569:GLN:NE2	2:B:609:LYS:HB3	2.31	0.46
2:B:22:ARG:O	2:B:23:SER:CB	2.64	0.45
2:B:133:ASP:O	2:B:135:LYS:N	2.49	0.45
2:B:146:ILE:HG23	2:B:174:TYR:CD2	2.51	0.45
2:B:299:ASN:HB2	2:B:596:ARG:HD3	1.98	0.45
2:A:533:ALA:O	2:A:536:SER:HB3	2.16	0.45
2:A:535:LEU:HD23	2:A:535:LEU:HA	1.76	0.45
2:B:135:LYS:O	2:B:138:PRO:HD3	2.17	0.45
2:B:284:ARG:O	2:B:607:MET:HA	2.15	0.45
2:B:353:LEU:HD22	2:B:557:MET:HG2	1.99	0.45
1:C:16:DA:H2''	1:C:17:DG:H5'	1.98	0.45
2:A:114:LEU:CD1	2:A:186:LEU:HD13	2.47	0.45
2:A:325:ASN:HD22	2:A:328:ASP:H	1.64	0.45
2:A:570:VAL:HG22	2:A:610:LEU:HD13	1.97	0.45
1:C:6:DA:H2'	1:C:7:DC:C6	2.51	0.45
1:D:4:DG:H1'	1:D:5:DC:H5'	1.98	0.45
2:A:428:GLN:O	2:A:431:ARG:N	2.49	0.45
2:A:446:GLN:C	2:A:448:LYS:N	2.70	0.45
2:B:92:GLY:O	2:B:95:HIS:HB3	2.17	0.45
2:B:156:PRO:CD	2:B:174:TYR:HE1	2.26	0.45
2:B:264:ILE:HG23	2:B:265:GLN:N	2.32	0.45
2:B:609:LYS:HG3	2:B:610:LEU:H	1.82	0.45
1:D:15:DG:H5'	2:A:453:ARG:HG2	1.98	0.45
1:D:33:DT:H4'	2:B:91:HIS:HD2	1.81	0.45
2:B:618:ARG:CB	2:B:618:ARG:NH1	2.79	0.45
2:A:349:GLU:HB3	2:A:568:PRO:CG	2.46	0.45
2:A:457:ALA:CA	2:A:460:ARG:NH2	2.78	0.45
2:B:370:ALA:O	2:B:372:MET:N	2.49	0.45
2:A:29:ALA:HA	2:A:279:LEU:HB2	1.99	0.45
2:A:174:TYR:CD1	2:A:174:TYR:C	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:175:GLN:NE2	2:A:175:GLN:HA	2.31	0.45
2:B:43:ILE:HG23	2:B:57:ILE:HG21	1.95	0.45
2:B:57:ILE:HG21	2:B:85:MET:HE2	1.99	0.45
2:B:624:GLU:OE2	2:B:624:GLU:HA	2.17	0.45
1:D:16:DA:H2''	2:B:421:ARG:HH12	1.81	0.45
2:A:3:VAL:HG23	2:A:4:SER:N	2.31	0.45
2:A:47:MET:HE1	2:A:78:MET:HG3	1.98	0.45
2:A:457:ALA:HA	2:A:460:ARG:CZ	2.47	0.45
2:A:149:GLN:CD	2:A:154:LEU:HD12	2.38	0.45
2:B:11:ASN:O	2:B:13:LYS:N	2.49	0.45
2:B:24:ASN:O	2:B:25:LEU:HB3	2.17	0.45
2:B:40:VAL:HG21	2:B:73:ARG:HD3	1.97	0.45
2:B:295:ALA:HB3	2:B:637:PRO:HD3	1.98	0.45
2:B:392:LEU:O	2:B:396:ARG:HG3	2.16	0.45
2:B:397:LEU:HD13	2:B:465:ILE:CD1	2.47	0.45
2:A:235:LEU:C	2:A:237:ALA:N	2.69	0.45
2:A:339:THR:O	2:A:340:TRP:C	2.54	0.45
2:B:127:ILE:HG22	2:B:128:LYS:N	2.31	0.45
2:B:378:GLY:O	2:B:379:GLY:O	2.35	0.44
2:A:61:THR:HG21	2:A:66:ALA:HB1	1.98	0.44
2:A:368:LEU:HD23	2:A:368:LEU:HA	1.73	0.44
2:B:613:THR:O	2:B:614:TYR:HB3	2.17	0.44
2:A:118:ASP:OD2	2:A:396:ARG:NH2	2.50	0.44
2:A:326:GLU:OE2	2:A:327:LEU:HD22	2.17	0.44
2:B:134:GLU:O	2:B:136:GLN:N	2.48	0.44
2:A:250:ASP:CG	2:A:303:ARG:HE	2.20	0.44
2:B:101:HIS:HB3	2:B:104:ASP:OD2	2.18	0.44
2:B:576:GLU:N	2:B:630:SER:OG	2.51	0.44
1:D:25:DC:H2''	1:D:26:DT:H72	1.99	0.44
2:B:368:LEU:CD2	2:B:374:TYR:HE2	2.30	0.44
1:D:1:DC:H6	1:D:1:DC:O5'	2.01	0.44
2:A:134:GLU:O	2:A:136:GLN:HG3	2.18	0.44
2:A:472:THR:HG21	2:A:480:GLN:CG	2.43	0.44
2:A:483:ARG:NH1	2:A:483:ARG:CG	2.80	0.44
2:B:162:TYR:N	2:B:168:GLN:HE21	2.16	0.44
2:B:282:ASN:HB3	2:B:290:LEU:HD11	1.98	0.44
2:A:114:LEU:HD23	2:A:119:GLN:HB2	1.99	0.44
2:B:91:HIS:CE1	2:B:193:LEU:HD11	2.53	0.44
2:B:403:ASP:O	2:B:405:ALA:N	2.50	0.44
2:A:11:ASN:C	2:A:11:ASN:OD1	2.56	0.44
2:A:428:GLN:HG2	2:A:432:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:LEU:HD12	2:B:236:LEU:HA	1.80	0.44
2:A:167:GLU:O	2:A:171:GLN:HB2	2.18	0.44
2:A:472:THR:HG23	2:A:480:GLN:HB2	1.98	0.44
2:A:546:GLN:O	2:A:548:ASP:N	2.51	0.44
2:B:339:THR:CG2	2:B:340:TRP:N	2.81	0.44
1:C:11:DA:C1'	1:C:12:DC:H5''	2.47	0.43
2:B:605:ARG:HA	2:B:605:ARG:NE	2.33	0.43
2:A:5:TYR:CZ	2:A:6:LEU:CD2	3.01	0.43
2:A:217:ILE:HD11	2:A:236:LEU:HG	2.00	0.43
2:A:394:TYR:CZ	2:A:410:VAL:HB	2.53	0.43
2:B:39:LEU:HD21	2:B:246:VAL:CG2	2.47	0.43
2:B:369:GLN:O	2:B:369:GLN:HG3	2.17	0.43
2:A:133:ASP:O	2:A:134:GLU:C	2.56	0.43
2:B:59:ALA:HB3	2:B:87:VAL:HG22	2.00	0.43
2:B:113:ILE:H	2:B:113:ILE:CD1	2.26	0.43
2:B:155:ARG:HA	2:B:155:ARG:HD3	1.73	0.43
2:B:517:ARG:O	2:B:517:ARG:HG2	2.19	0.43
2:B:641:VAL:CG1	2:B:642:GLU:N	2.81	0.43
2:A:149:GLN:NE2	2:A:149:GLN:HA	2.33	0.43
2:A:179:GLU:HB2	2:A:183:ARG:HH12	1.83	0.43
2:B:42:ARG:NE	2:B:46:LEU:HD21	2.34	0.43
2:B:386:GLN:NE2	2:B:505:ARG:HH21	2.16	0.43
2:B:610:LEU:HD11	2:B:612:LEU:HD21	2.01	0.43
2:A:24:ASN:O	2:A:274:ALA:HA	2.18	0.43
2:A:644:VAL:O	2:A:644:VAL:CG1	2.58	0.43
2:B:39:LEU:HD23	2:B:218:LEU:HD23	1.99	0.43
2:B:127:ILE:HG21	2:B:133:ASP:HB3	2.01	0.43
2:B:350:CYS:HA	2:B:569:GLN:O	2.18	0.43
2:B:512:LEU:HD12	2:B:512:LEU:O	2.19	0.43
2:B:579:MET:CE	2:B:618:ARG:HE	2.32	0.43
1:C:1:DC:H4'	2:B:619:ARG:NH1	2.34	0.43
1:D:31:DG:N3	1:D:32:DT:H72	2.33	0.43
2:A:550:TRP:O	2:A:550:TRP:CD1	2.72	0.43
2:A:575:MET:C	2:A:630:SER:OG	2.57	0.43
2:A:626:TYR:CD1	2:A:626:TYR:N	2.87	0.43
2:B:27:VAL:O	2:B:27:VAL:HG12	2.18	0.43
2:B:102:HIS:HB2	2:B:107:LEU:O	2.19	0.43
2:A:84:GLY:O	2:A:213:ARG:NH2	2.51	0.43
2:A:387:GLU:HG2	2:A:388:ILE:HD13	2.00	0.43
2:A:459:GLN:HE21	2:A:463:GLU:CG	2.32	0.43
2:B:579:MET:O	2:B:582:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:637:PRO:HB2	2:B:640:CYS:SG	2.59	0.43
2:A:39:LEU:HD21	2:A:246:VAL:CG2	2.49	0.43
2:A:42:ARG:O	2:A:45:TRP:HB3	2.19	0.43
2:A:54:PRO:O	2:A:85:MET:CA	2.67	0.43
2:A:109:GLN:NE2	2:A:528:LEU:HD23	2.33	0.43
2:A:320:LEU:HA	2:A:612:LEU:O	2.18	0.43
2:A:422:THR:O	2:A:426:VAL:HG23	2.19	0.43
2:B:31:ALA:O	2:B:282:ASN:ND2	2.52	0.43
2:B:301:ASN:OD1	2:B:301:ASN:N	2.52	0.43
1:D:18:DT:O3'	2:B:417:GLY:HA2	2.19	0.42
2:A:23:SER:CA	2:A:242:LYS:HG3	2.49	0.42
2:A:568:PRO:HB3	2:A:608:GLN:NE2	2.33	0.42
2:B:150:LYS:CE	2:B:178:GLN:NE2	2.81	0.42
2:B:250:ASP:O	2:B:597:ARG:HB3	2.19	0.42
2:B:403:ASP:O	2:B:406:ALA:N	2.52	0.42
2:B:643:GLU:HG3	2:B:644:VAL:N	2.34	0.42
1:D:24:DG:H2''	1:D:25:DC:C6	2.54	0.42
2:A:356:SER:OG	2:A:359:GLN:HG3	2.19	0.42
2:A:567:PHE:C	2:A:607:MET:HG3	2.39	0.42
2:B:156:PRO:O	2:B:171:GLN:NE2	2.52	0.42
2:B:325:ASN:N	2:B:325:ASN:ND2	2.67	0.42
2:B:325:ASN:HA	2:B:617:THR:O	2.18	0.42
2:B:513:VAL:O	2:B:514:THR:C	2.58	0.42
2:B:579:MET:CE	2:B:618:ARG:NE	2.82	0.42
1:D:10:DC:C2'	1:D:11:DA:C8	2.98	0.42
1:D:17:DG:H2'	2:B:421:ARG:HD2	2.01	0.42
2:B:57:ILE:HD12	2:B:57:ILE:N	2.34	0.42
2:B:139:PRO:O	2:B:142:ALA:HB3	2.20	0.42
2:B:641:VAL:HG12	2:B:642:GLU:H	1.83	0.42
1:D:17:DG:H8	2:B:421:ARG:NH1	2.17	0.42
2:A:93:LEU:O	2:A:94:ALA:C	2.56	0.42
2:A:252:SER:CB	2:A:261:VAL:HG22	2.49	0.42
2:A:411:VAL:HG13	2:A:412:ASN:H	1.85	0.42
2:B:225:THR:HA	2:B:229:GLN:OE1	2.19	0.42
2:B:234:ARG:HG3	2:B:235:LEU:H	1.83	0.42
2:B:386:GLN:HG3	2:B:387:GLU:N	2.34	0.42
2:B:476:PRO:HG2	2:B:479:VAL:HB	2.01	0.42
1:C:6:DA:C2'	1:C:7:DC:C6	3.03	0.42
2:A:123:LEU:O	2:A:124:LYS:C	2.58	0.42
2:A:125:ARG:HE	2:A:408:GLU:CD	2.23	0.42
2:A:129:ALA:O	2:A:130:MET:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:226:ASN:OD1	2:A:229:GLN:HB2	2.20	0.42
2:B:114:LEU:HD11	2:B:186:LEU:HD13	2.00	0.42
2:B:202:ASN:C	2:B:204:PRO:HD3	2.39	0.42
2:B:328:ASP:O	2:B:329:GLU:C	2.57	0.42
2:B:400:ASN:ND2	2:B:402:ASN:HB2	2.09	0.42
2:B:506:ILE:O	2:B:509:LEU:HB2	2.20	0.42
1:C:6:DA:H2'	1:C:7:DC:H6	1.84	0.42
1:C:14:DC:O2	2:B:453:ARG:NH2	2.52	0.42
1:D:6:DA:OP1	2:A:124:LYS:CE	2.67	0.42
1:D:12:DC:C6	1:D:13:DT:H72	2.55	0.42
2:B:265:GLN:HG3	2:B:269:ASN:HD21	1.85	0.42
2:B:290:LEU:O	2:B:294:ASN:ND2	2.52	0.42
2:A:128:LYS:C	2:A:130:MET:H	2.23	0.42
2:B:113:ILE:N	2:B:113:ILE:CD1	2.82	0.42
2:B:413:THR:HA	2:B:414:PRO:C	2.40	0.42
2:B:578:GLY:O	2:B:583:GLN:N	2.53	0.42
2:A:25:LEU:HD23	2:A:25:LEU:N	2.34	0.42
2:A:297:ILE:HB	2:A:600:TYR:CD1	2.54	0.42
2:A:642:GLU:C	2:A:643:GLU:O	2.57	0.42
2:B:57:ILE:HD12	2:B:57:ILE:H	1.85	0.42
2:B:146:ILE:HG12	2:B:174:TYR:HD2	1.84	0.42
2:B:473:ALA:C	2:B:475:MET:H	2.22	0.42
2:B:619:ARG:HG3	2:B:623:LYS:O	2.20	0.42
2:B:635:GLU:HG3	2:B:635:GLU:H	1.66	0.42
2:A:115:ASP:OD2	2:A:115:ASP:C	2.57	0.42
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.85	0.42
2:A:377:TYR:HB2	2:A:557:MET:HB3	2.02	0.42
2:A:390:ASP:OD1	2:A:409:ARG:NE	2.48	0.42
2:B:11:ASN:OD1	2:B:14:GLN:HG3	2.18	0.42
2:B:110:ASP:OD1	2:B:532:GLN:HG2	2.20	0.42
2:B:382:PHE:O	2:B:384:GLU:N	2.53	0.42
2:B:403:ASP:O	2:B:404:ASP:C	2.58	0.42
2:B:128:LYS:C	2:B:130:MET:N	2.73	0.42
2:B:370:ALA:O	2:B:372:MET:HB2	2.20	0.42
1:D:16:DA:H2''	1:D:17:DG:H5''	2.01	0.41
2:A:325:ASN:HD21	2:A:328:ASP:H	1.66	0.41
2:A:418:ILE:HG22	2:A:418:ILE:O	2.19	0.41
2:B:47:MET:HE1	2:B:78:MET:HG2	2.02	0.41
2:B:79:GLY:O	2:B:80:THR:CG2	2.57	0.41
2:B:153:GLY:CA	2:B:228:ILE:HD12	2.49	0.41
2:B:353:LEU:HA	2:B:557:MET:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:ARG:HA	2:B:483:ARG:HD3	1.81	0.41
2:A:319:SER:HB2	2:A:644:VAL:HG21	2.02	0.41
2:A:327:LEU:HD13	2:A:327:LEU:HA	1.91	0.41
2:A:330:ALA:O	2:A:331:ARG:C	2.58	0.41
2:B:11:ASN:O	2:B:12:ASP:C	2.59	0.41
2:B:389:LYS:HE2	2:B:389:LYS:HB3	1.85	0.41
2:B:540:LEU:O	2:B:541:GLU:HB3	2.20	0.41
2:B:576:GLU:HA	2:B:630:SER:N	2.34	0.41
1:C:6:DA:C2'	1:C:7:DC:H6	2.32	0.41
2:A:78:MET:O	2:A:79:GLY:C	2.57	0.41
2:A:537:HIS:O	2:A:537:HIS:CG	2.74	0.41
2:B:112:GLN:NE2	2:B:113:ILE:HD12	2.35	0.41
2:B:142:ALA:HB2	2:B:170:TRP:CZ3	2.51	0.41
2:B:247:GLY:O	2:B:248:ASP:CB	2.66	0.41
2:B:325:ASN:H	2:B:325:ASN:ND2	2.17	0.41
1:D:10:DC:H4'	1:D:10:DC:OP1	2.20	0.41
2:A:66:ALA:O	2:A:67:ALA:C	2.58	0.41
2:A:418:ILE:HD12	2:A:418:ILE:H	1.84	0.41
2:A:548:ASP:O	2:A:549:THR:C	2.59	0.41
2:A:598:LEU:HA	2:A:598:LEU:HD12	1.82	0.41
2:B:61:THR:CB	2:B:67:ALA:HB2	2.50	0.41
2:B:114:LEU:HD21	2:B:122:LEU:HD23	2.03	0.41
2:B:550:TRP:O	2:B:550:TRP:CD1	2.73	0.41
1:C:3:DA:OP2	1:C:3:DA:H2'	2.21	0.41
2:A:206:ILE:O	2:A:207:LEU:C	2.57	0.41
2:A:283:TYR:CE2	3:A:681:GOL:H12	2.55	0.41
2:A:320:LEU:HD23	2:A:320:LEU:N	2.35	0.41
2:A:505:ARG:HA	2:A:508:ASN:HD22	1.86	0.41
2:B:227:ASN:OD1	2:B:260:GLN:HG3	2.21	0.41
2:B:231:ALA:C	2:B:234:ARG:HG2	2.41	0.41
2:B:284:ARG:HD3	2:B:566:GLU:CB	2.50	0.41
2:B:397:LEU:HA	2:B:400:ASN:O	2.20	0.41
2:B:529:MET:HB2	2:B:532:GLN:OE1	2.19	0.41
2:A:430:SER:OG	2:A:435:LEU:O	2.31	0.41
2:B:10:LEU:HD21	2:B:41:HIS:CD2	2.55	0.41
2:B:306:LYS:CE	2:B:600:TYR:OH	2.69	0.41
2:B:382:PHE:O	2:B:385:ARG:HG3	2.20	0.41
2:A:22:ARG:HE	2:A:22:ARG:HB3	1.36	0.41
2:B:194:LEU:HD13	2:B:228:ILE:HD11	2.02	0.41
2:B:200:TRP:CH2	2:B:236:LEU:HD13	2.56	0.41
2:B:498:LYS:HB3	2:B:499:GLY:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:587:ASP:CG	2:B:588:GLU:N	2.73	0.41
1:C:17:DG:H5'	2:A:421:ARG:HH11	1.85	0.41
1:D:16:DA:C2'	1:D:17:DG:H5''	2.50	0.41
2:A:325:ASN:HA	2:A:615:ALA:HB1	2.02	0.41
2:A:477:LEU:HG	2:A:516:THR:HB	2.01	0.41
2:B:64:ASN:ND2	2:B:541:GLU:HB3	2.36	0.41
2:B:203:LYS:N	2:B:204:PRO:CD	2.84	0.41
2:B:352:ILE:O	2:B:353:LEU:HD23	2.21	0.41
2:B:406:ALA:O	2:B:410:VAL:HG22	2.20	0.41
2:A:149:GLN:CA	2:A:149:GLN:NE2	2.83	0.41
2:A:228:ILE:CG2	2:A:229:GLN:N	2.84	0.41
2:A:284:ARG:HH11	2:A:566:GLU:HB3	1.86	0.41
2:B:13:LYS:O	2:B:16:GLU:HB3	2.20	0.41
2:B:22:ARG:O	2:B:23:SER:HB3	2.20	0.41
2:B:49:VAL:HG12	2:B:50:GLU:N	2.36	0.41
2:B:88:GLY:HA3	2:B:93:LEU:HD21	2.03	0.41
2:B:187:VAL:CG1	2:B:191:GLU:HG2	2.51	0.41
2:B:223:GLN:HB2	2:B:252:SER:HB2	2.02	0.41
2:A:126:LEU:HD23	2:A:126:LEU:HA	1.81	0.41
2:B:55:TYR:N	2:B:55:TYR:CD1	2.89	0.41
2:B:385:ARG:HH21	2:B:385:ARG:CG	2.34	0.41
2:B:412:ASN:OD1	2:B:415:THR:HA	2.21	0.41
2:A:82:GLN:HB3	2:A:85:MET:CE	2.51	0.40
2:A:165:PRO:O	2:A:169:THR:N	2.41	0.40
2:B:175:GLN:O	2:B:179:GLU:HG3	2.20	0.40
2:B:253:ILE:CD1	2:B:253:ILE:N	2.81	0.40
2:B:472:THR:OG1	2:B:480:GLN:HA	2.21	0.40
2:B:61:THR:CG2	2:B:62:PHE:H	2.22	0.40
2:B:85:MET:O	2:B:86:TRP:HD1	2.04	0.40
2:B:211:ARG:HG2	2:B:236:LEU:O	2.20	0.40
2:B:251:GLN:HE21	2:B:251:GLN:HB2	1.66	0.40
2:B:556:LEU:O	2:B:557:MET:HB3	2.20	0.40
1:D:32:DT:OP2	1:D:32:DT:H6	2.05	0.40
2:A:188:ASP:OD2	2:A:191:GLU:CB	2.66	0.40
2:A:320:LEU:HG	2:A:641:VAL:CG1	2.51	0.40
2:B:200:TRP:HB3	2:B:207:LEU:HD22	2.04	0.40
2:B:442:ARG:HD3	2:B:442:ARG:HA	1.82	0.40
2:A:28:LEU:CD2	2:A:304:LEU:HD12	2.47	0.40
2:A:512:LEU:O	2:A:515:ALA:HB3	2.20	0.40
2:A:540:LEU:HA	2:A:540:LEU:HD23	1.79	0.40
2:A:580:PHE:HA	2:A:581:PRO:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:VAL:C	2:B:51:ASN:N	2.75	0.40
2:B:161:SER:OG	2:B:162:TYR:N	2.52	0.40
2:B:254:TYR:O	2:B:259:ALA:HB3	2.21	0.40
2:B:319:SER:HA	2:B:642:GLU:O	2.20	0.40
2:B:375:ARG:HG3	2:B:375:ARG:O	2.22	0.40
2:A:117:GLU:O	2:A:118:ASP:C	2.59	0.40
2:A:145:TYR:CD2	2:A:170:TRP:HB3	2.57	0.40
2:A:387:GLU:HG2	2:A:388:ILE:CD1	2.51	0.40
2:A:454:ALA:O	2:A:458:LEU:HB2	2.22	0.40
2:B:226:ASN:CG	2:B:229:GLN:HG3	2.42	0.40
2:B:472:THR:CG2	2:B:480:GLN:HG3	2.51	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	
2	A	638/680 (94%)	516 (81%)	82 (13%)	40 (6%)	<b>1</b>	<b>7</b>
2	B	638/680 (94%)	435 (68%)	145 (23%)	58 (9%)	<b>1</b>	<b>3</b>
All	All	1276/1360 (94%)	951 (74%)	227 (18%)	98 (8%)	<b>1</b>	<b>5</b>

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	79	GLY
2	A	134	GLU
2	A	135	LYS
2	A	155	ARG
2	A	369	GLN
2	A	498	LYS
2	A	543	GLY

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Mol	Chain	Res	Type
2	A	544	GLU
2	A	546	GLN
2	A	547	ALA
2	A	550	TRP
2	A	588	GLU
2	A	643	GLU
2	B	12	ASP
2	B	28	LEU
2	B	31	ALA
2	B	49	VAL
2	B	80	THR
2	B	134	GLU
2	B	162	TYR
2	B	201	LEU
2	B	248	ASP
2	B	263	ASN
2	B	351	ALA
2	B	371	SER
2	B	379	GLY
2	B	383	PHE
2	B	454	ALA
2	B	471	GLU
2	B	498	LYS
2	B	501	LYS
2	B	543	GLY
2	B	544	GLU
2	B	546	GLN
2	B	547	ALA
2	B	550	TRP
2	B	621	TYR
2	A	130	MET
2	A	159	ILE
2	A	238	GLY
2	A	408	GLU
2	A	419	GLY
2	A	502	GLY
2	A	589	GLY
2	A	621	TYR
2	A	635	GLU
2	A	644	VAL
2	B	8	ASP
2	B	50	GLU

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Mol	Chain	Res	Type
2	B	51	ASN
2	B	79	GLY
2	B	131	ASN
2	B	161	SER
2	B	214	PHE
2	B	305	GLY
2	B	347	LEU
2	B	551	GLN
2	B	604	THR
2	A	82	GLN
2	A	162	TYR
2	A	407	PHE
2	A	527	ASP
2	B	23	SER
2	B	272	PRO
2	B	382	PHE
2	B	404	ASP
2	B	408	GLU
2	B	474	ASP
2	B	487	ASP
2	B	541	GLU
2	B	645	ARG
2	A	54	PRO
2	A	80	THR
2	A	163	GLY
2	B	221	GLU
2	B	315	GLY
2	B	473	ALA
2	B	554	VAL
2	B	584	MET
2	B	635	GLU
2	A	90	PHE
2	A	500	GLU
2	A	526	GLU
2	A	530	PRO
2	B	477	LEU
2	B	545	GLY
2	B	629	PRO
2	A	161	SER
2	A	221	GLU
2	A	501	LYS
2	B	407	PHE

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Mol	Chain	Res	Type
2	A	305	GLY
2	A	545	GLY
2	B	644	VAL
2	B	219	VAL
2	A	499	GLY
2	B	156	PRO
2	B	484	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	519/574 (90%)	467 (90%)	52 (10%)	7	29
2	B	513/574 (89%)	458 (89%)	55 (11%)	6	26
All	All	1032/1148 (90%)	925 (90%)	107 (10%)	7	27

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	VAL
2	A	6	LEU
2	A	25	LEU
2	A	33	SER
2	A	35	LYS
2	A	46	LEU
2	A	53	SER
2	A	61	THR
2	A	73	ARG
2	A	96	ARG
2	A	130	MET
2	A	133	ASP
2	A	149	GLN
2	A	166	VAL
2	A	167	GLU
2	A	171	GLN

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Mol	Chain	Res	Type
2	A	174	TYR
2	A	179	GLU
2	A	182	ASP
2	A	208	GLN
2	A	228	ILE
2	A	234	ARG
2	A	243	VAL
2	A	244	MET
2	A	260	GLN
2	A	271	PHE
2	A	291	SER
2	A	303	ARG
2	A	325	ASN
2	A	327	LEU
2	A	354	TYR
2	A	362	VAL
2	A	365	GLU
2	A	372	MET
2	A	404	ASP
2	A	408	GLU
2	A	430	SER
2	A	442	ARG
2	A	448	LYS
2	A	458	LEU
2	A	483	ARG
2	A	496	GLN
2	A	501	LYS
2	A	528	LEU
2	A	537	HIS
2	A	549	THR
2	A	555	GLN
2	A	570	VAL
2	A	587	ASP
2	A	617	THR
2	A	620	LEU
2	A	640	CYS
2	B	25	LEU
2	B	28	LEU
2	B	43	ILE
2	B	78	MET
2	B	96	ARG
2	B	106	ASN

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Mol	Chain	Res	Type
2	B	112	GLN
2	B	116	SER
2	B	127	ILE
2	B	133	ASP
2	B	140	ARG
2	B	149	GLN
2	B	151	ASP
2	B	182	ASP
2	B	201	LEU
2	B	208	GLN
2	B	240	THR
2	B	243	VAL
2	B	251	GLN
2	B	253	ILE
2	B	264	ILE
2	B	269	ASN
2	B	287	SER
2	B	320	LEU
2	B	325	ASN
2	B	347	LEU
2	B	354	TYR
2	B	362	VAL
2	B	365	GLU
2	B	372	MET
2	B	385	ARG
2	B	393	SER
2	B	401	ARG
2	B	404	ASP
2	B	408	GLU
2	B	420	ASP
2	B	444	LEU
2	B	474	ASP
2	B	483	ARG
2	B	492	THR
2	B	536	SER
2	B	555	GLN
2	B	570	VAL
2	B	571	PHE
2	B	579	MET
2	B	580	PHE
2	B	587	ASP
2	B	594	GLU

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Mol	Chain	Res	Type
2	B	597	ARG
2	B	610	LEU
2	B	618	ARG
2	B	621	TYR
2	B	626	TYR
2	B	633	ILE
2	B	639	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	41	HIS
2	A	64	ASN
2	A	109	GLN
2	A	112	GLN
2	A	119	GLN
2	A	149	GLN
2	A	168	GLN
2	A	175	GLN
2	A	178	GLN
2	A	208	GLN
2	A	227	ASN
2	A	229	GLN
2	A	260	GLN
2	A	281	GLN
2	A	325	ASN
2	A	446	GLN
2	A	459	GLN
2	A	480	GLN
2	A	508	ASN
2	A	569	GLN
2	A	583	GLN
2	A	608	GLN
2	A	627	HIS
2	B	11	ASN
2	B	64	ASN
2	B	82	GLN
2	B	91	HIS
2	B	112	GLN
2	B	119	GLN
2	B	141	GLN
2	B	147	ASN

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Mol	Chain	Res	Type
2	B	149	GLN
2	B	168	GLN
2	B	171	GLN
2	B	175	GLN
2	B	178	GLN
2	B	202	ASN
2	B	208	GLN
2	B	251	GLN
2	B	260	GLN
2	B	265	GLN
2	B	269	ASN
2	B	299	ASN
2	B	325	ASN
2	B	341	GLN
2	B	386	GLN
2	B	400	ASN
2	B	478	HIS
2	B	480	GLN
2	B	508	ASN
2	B	569	GLN
2	B	627	HIS

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	FMT	A	682	-	0,2,2	-	-	0,1,1	-	-
3	GOL	A	681	-	5,5,5	0.50	0	5,5,5	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	681	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	682	FMT	1	0
3	A	681	GOL	4	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	33/35 (94%)	-0.21	1 (3%)	50	22	43, 71, 131, 136	0
1	D	33/35 (94%)	-0.20	0	100	100	48, 84, 132, 137	0
2	A	642/680 (94%)	-0.28	0	100	100	26, 51, 91, 109	0
2	B	642/680 (94%)	0.17	16 (2%)	57	29	59, 101, 127, 149	0
All	All	1350/1430 (94%)	-0.06	17 (1%)	77	51	26, 79, 120, 149	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ASP	4.5
2	B	320	LEU	4.3
2	B	612	LEU	3.3
2	B	611	THR	3.2
2	B	319	SER	2.9
2	B	372	MET	2.6
2	B	236	LEU	2.6
2	B	141	GLN	2.5
2	B	3	VAL	2.5
2	B	618	ARG	2.4
2	B	324	PHE	2.3
2	B	48	SER	2.2
1	C	1	DC	2.1
2	B	584	MET	2.1
2	B	619	ARG	2.1
2	B	623	LYS	2.0
2	B	343	ASN	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	681	6/6	0.92	0.21	53,53,54,55	0
4	FMT	A	682	3/3	0.96	0.23	49,49,51,51	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.