



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 12:34 PM EDT

PDB ID : 3JYT  
Title : K65R mutant HIV-1 reverse transcriptase cross-linked to DS-DNA and complexed with DATP as the incoming nucleotide substrate  
Authors : Das, K.; Arnold, E.  
Deposited on : 2009-09-22  
Resolution : 3.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

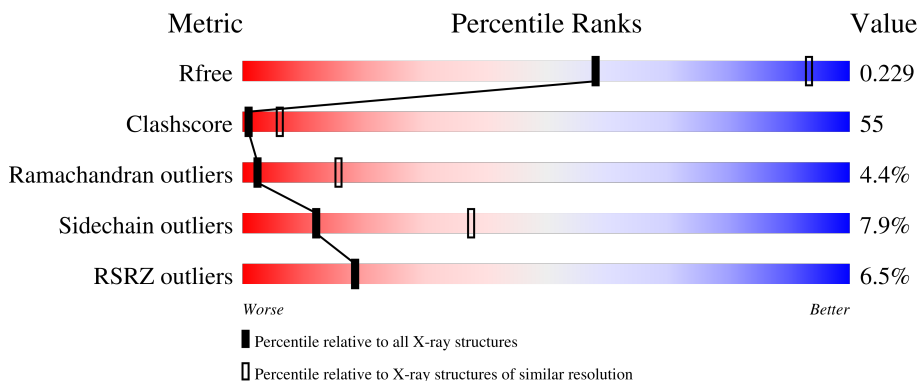
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	A	558	
2	B	437	
3	T	27	
4	P	21	

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
6	SO4	A	560	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8852 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	4508	2917	751	832	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ARG	LYS	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	413	3405	2215	564	620	6	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
B	430	GLY	-	expression tag	UNP P03366
B	431	GLY	-	expression tag	UNP P03366
B	432	HIS	-	expression tag	UNP P03366
B	433	HIS	-	expression tag	UNP P03366
B	434	HIS	-	expression tag	UNP P03366
B	435	HIS	-	expression tag	UNP P03366
B	436	HIS	-	expression tag	UNP P03366
B	437	HIS	-	expression tag	UNP P03366

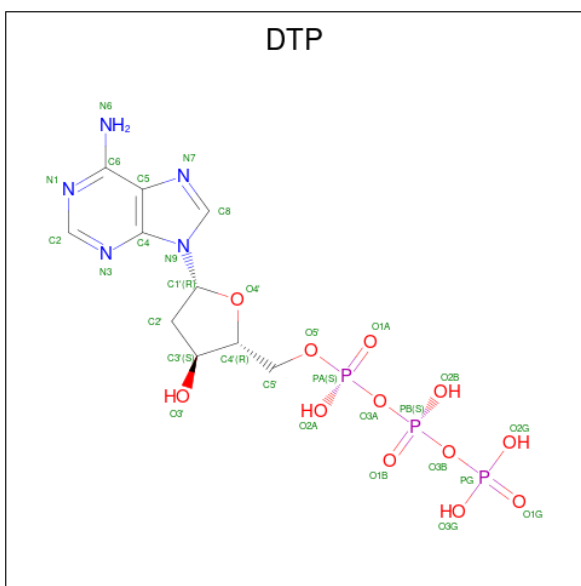
- Molecule 3 is a DNA chain called DNA (5'-D(\*A\*TP\*GP\*GP\*TP\*CP\*GP\*GP\*CP\*GP\*C  
P\*CP\*CP\*GP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	24	494	233	97	141	23	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(MRG)P\*CP\*GP\*CP\*CP\*(DDG))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	P	20	403	192	72	120	19	0	0	0

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	30	10	5	12	3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

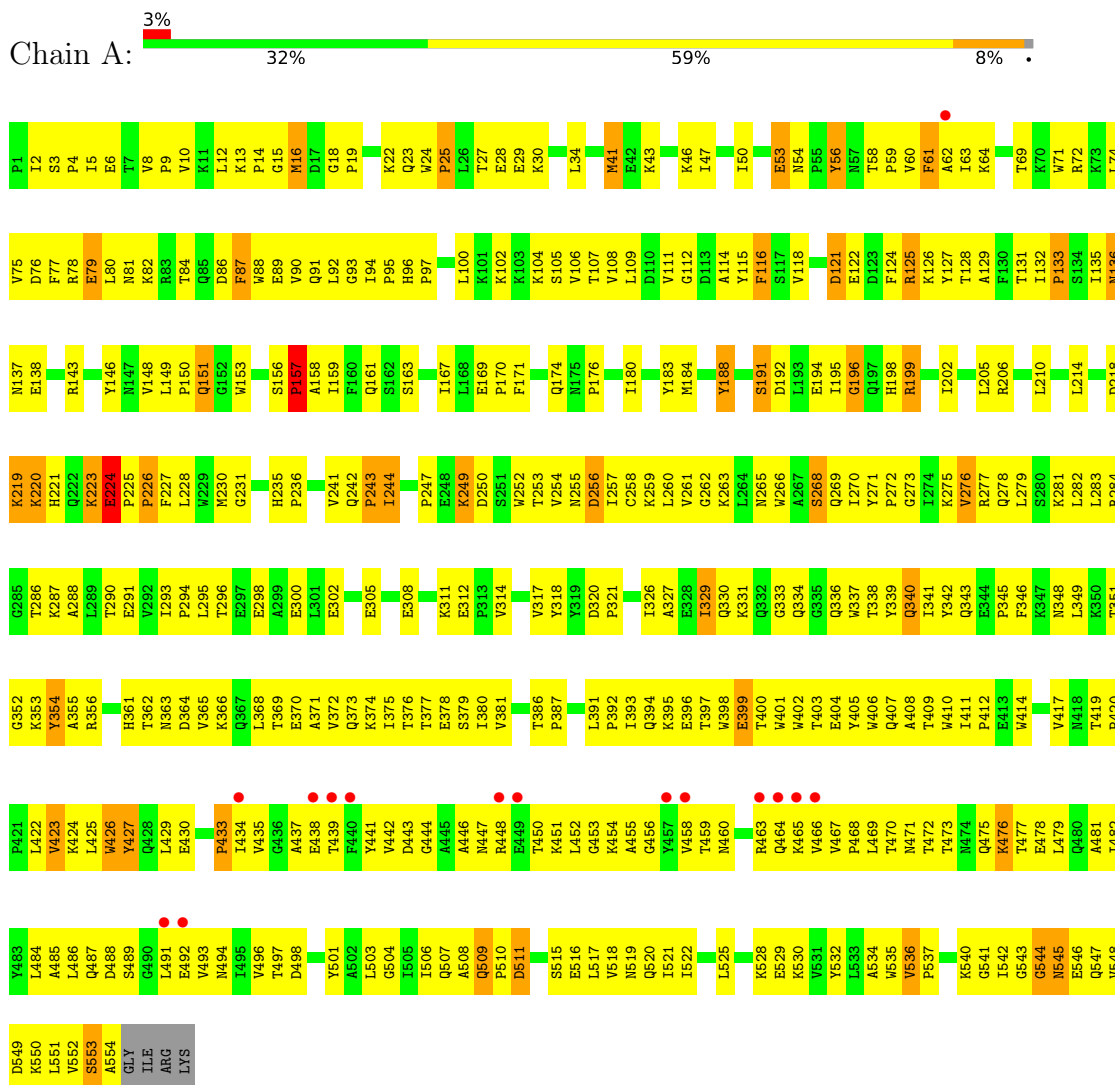
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		

### 3 Residue-property plots

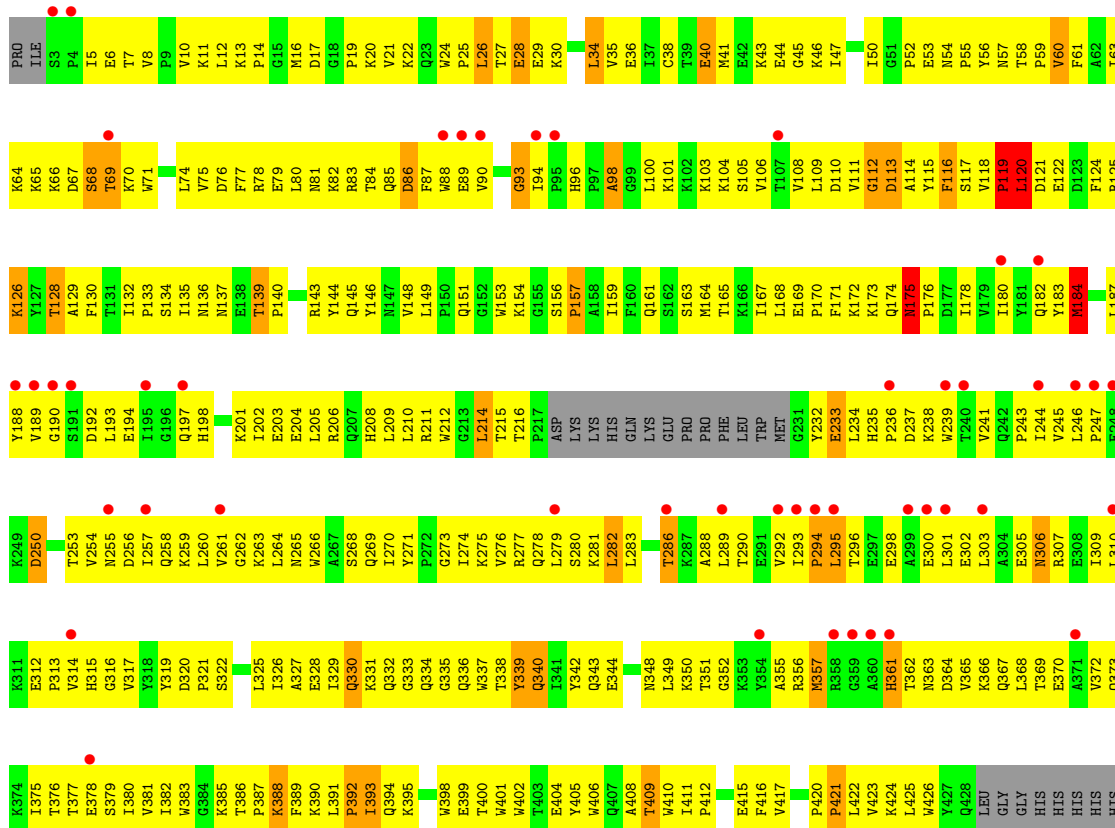
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Reverse transcriptase/ribonuclease H

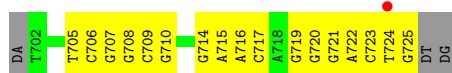


- Molecule 2: p51 RT

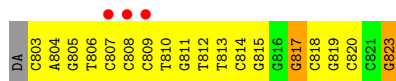




• Molecule 3: DNA (5'-D(\*A\*TP\*GP\*GP\*TP\*CP\*GP\*GP\*CP\*GP\*CP\*CP\*CP\*GP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3')



• Molecule 4: DNA (5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\*CP\*GP\*GP\*(MRG)P\*CP\*GP\*CP\*CP\*(DDG))-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.72Å 169.72Å 155.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.86 – 3.30 48.86 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.86-3.30) 98.6 (48.86-3.31)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.33Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.253 , 0.287 0.237 , 0.229	Depositor DCC
$R_{free}$ test set	1115 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.7	Xtrriage
Anisotropy	0.300	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 95.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, MRG, DDG, SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.46	0/4626	0.73	2/6285 (0.0%)
2	B	0.43	1/3502 (0.0%)	0.69	2/4760 (0.0%)
3	T	0.57	0/555	0.79	0/856
4	P	0.56	0/400	0.87	0/612
All	All	0.46	1/9083 (0.0%)	0.73	4/12513 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	339	TYR	CD2-CE2	-5.19	1.31	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	N-CA-C	-7.46	90.87	111.00
1	A	223	LYS	N-CA-C	-6.45	93.59	111.00
2	B	68	SER	N-CA-C	-5.49	96.17	111.00
2	B	120	LEU	CA-CB-CG	5.40	127.72	115.30

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	A	4508	0	4567	517	0
2	B	3405	0	3437	445	0
3	T	494	0	269	23	0
4	P	403	0	224	27	0
5	A	30	0	12	4	0
6	A	10	0	0	2	0
7	A	2	0	0	0	0
All	All	8852	0	8509	949	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 55.

All (949) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.25	1.18
2:B:357:MET:HE2	2:B:357:MET:H	1.04	1.16
2:B:169:GLU:HG3	2:B:170:PRO:HD3	1.18	1.12
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.20	1.10
2:B:422:LEU:HA	2:B:425:LEU:HD13	1.36	1.07
2:B:64:LYS:HD3	2:B:69:THR:HA	1.34	1.06
2:B:365:VAL:HG12	2:B:393:ILE:HD11	1.41	1.02
2:B:356:ARG:HD2	2:B:361:HIS:HA	1.41	1.00
2:B:13:LYS:HG3	2:B:85:GLN:HA	1.45	0.98
2:B:295:LEU:H	2:B:295:LEU:HD12	1.29	0.96
2:B:357:MET:HE2	2:B:357:MET:N	1.80	0.96
2:B:339:TYR:HB2	2:B:352:GLY:H	1.34	0.93
2:B:21:VAL:CG1	2:B:59:PRO:HD3	1.99	0.93
2:B:356:ARG:HB2	2:B:367:GLN:HE22	1.32	0.93
1:A:454:LYS:HE3	1:A:552:VAL:O	1.70	0.92
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.05	0.92
2:B:74:LEU:HD12	2:B:75:VAL:H	1.35	0.91
1:A:317:VAL:HG12	1:A:318:TYR:H	1.34	0.91
1:A:198:HIS:HE2	1:A:202:ILE:HD13	1.37	0.90
2:B:21:VAL:HG13	2:B:59:PRO:HD3	1.50	0.90
2:B:50:ILE:HD13	2:B:145:GLN:HG3	1.54	0.90
2:B:246:LEU:HD22	2:B:260:LEU:HD11	1.52	0.89
1:A:454:LYS:HA	1:A:469:LEU:HG	1.54	0.89
3:T:720:DG:H2'	3:T:721:DG:C8	2.07	0.89
1:A:393:ILE:HB	1:A:423:VAL:HG12	1.53	0.89
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.56	0.88
2:B:339:TYR:HB2	2:B:352:GLY:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:H	1:A:136:ASN:HD22	1.22	0.87
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.74	0.87
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.57	0.86
1:A:547:GLN:O	1:A:551:LEU:HG	1.75	0.86
2:B:100:LEU:HD23	2:B:103:LYS:HG3	1.56	0.86
1:A:408:ALA:CB	2:B:364:ASP:HB3	2.06	0.86
2:B:275:LYS:HB2	2:B:306:ASN:HD21	1.42	0.85
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.43	0.84
1:A:279:LEU:HB2	1:A:302:GLU:OE2	1.77	0.84
1:A:221:HIS:CE1	1:A:228:LEU:H	1.95	0.83
2:B:356:ARG:HB2	2:B:367:GLN:NE2	1.93	0.83
2:B:260:LEU:O	2:B:264:LEU:HD12	1.78	0.83
2:B:109:LEU:HG	2:B:216:THR:HG21	1.60	0.83
2:B:367:GLN:HA	2:B:370:GLU:OE1	1.79	0.83
1:A:157:PRO:O	1:A:161:GLN:HG3	1.79	0.82
1:A:254:VAL:HG13	1:A:283:LEU:HD22	1.62	0.82
1:A:92:LEU:HD12	2:B:133:PRO:HB3	1.61	0.81
2:B:365:VAL:HG12	2:B:393:ILE:CD1	2.10	0.81
2:B:167:ILE:HA	2:B:212:TRP:CZ3	2.15	0.81
2:B:357:MET:H	2:B:357:MET:CE	1.91	0.81
1:A:337:TRP:CZ3	1:A:368:LEU:HD13	2.16	0.81
2:B:335:GLY:O	2:B:355:ALA:HA	1.80	0.81
1:A:460:ASN:ND2	2:B:288:ALA:HB2	1.96	0.81
1:A:475:GLN:HE22	4:P:808:DC:H2"	1.47	0.80
1:A:247:PRO:HG2	1:A:260:LEU:HD11	1.64	0.80
2:B:296:THR:O	2:B:300:GLU:HB2	1.82	0.80
1:A:23:GLN:HE22	1:A:60:VAL:H	1.30	0.80
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.62	0.79
2:B:395:LYS:HG2	2:B:399:GLU:OE1	1.82	0.79
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.98	0.79
2:B:247:PRO:CG	2:B:260:LEU:HD22	2.11	0.79
1:A:354:TYR:HD2	1:A:371:ALA:HB2	1.48	0.78
2:B:390:LYS:HD2	2:B:415:GLU:OE2	1.84	0.78
2:B:178:ILE:HD11	2:B:201:LYS:NZ	1.98	0.78
2:B:13:LYS:N	2:B:85:GLN:HB2	1.98	0.78
2:B:333:GLY:O	2:B:336:GLN:HB2	1.84	0.78
2:B:169:GLU:HG3	2:B:170:PRO:CD	2.08	0.77
1:A:542:ILE:O	1:A:545:ASN:HB3	1.84	0.77
1:A:198:HIS:NE2	1:A:202:ILE:HD13	1.99	0.77
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.65	0.77
2:B:254:VAL:HB	2:B:289:LEU:HA	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.66	0.77
1:A:509:GLN:N	1:A:510:PRO:HD3	1.99	0.77
4:P:812:DT:H2'	4:P:813:DT:C6	2.20	0.77
2:B:246:LEU:HD21	2:B:264:LEU:HD21	1.65	0.76
2:B:206:ARG:HB3	2:B:206:ARG:HH11	1.49	0.76
1:A:376:THR:O	1:A:380:ILE:HG13	1.83	0.76
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.67	0.76
1:A:475:GLN:HE22	4:P:808:DC:C2'	1.98	0.76
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.68	0.76
1:A:247:PRO:CG	1:A:260:LEU:HD11	2.15	0.76
2:B:175:ASN:N	2:B:176:PRO:HD3	2.01	0.76
1:A:397:THR:HG21	1:A:424:LYS:HA	1.67	0.76
1:A:484:LEU:HD23	1:A:487:GLN:NE2	2.01	0.76
1:A:511:ASP:HA	1:A:522:ILE:HG21	1.67	0.76
2:B:128:THR:CB	2:B:146:TYR:HB2	2.15	0.76
1:A:89:GLU:HG2	3:T:708:DG:H5'	1.68	0.75
1:A:475:GLN:NE2	4:P:808:DC:H2''	2.01	0.75
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.85	0.75
1:A:425:LEU:HD13	1:A:509:GLN:HE22	1.49	0.75
2:B:74:LEU:HD12	2:B:75:VAL:N	2.02	0.75
1:A:136:ASN:OD1	1:A:138:GLU:HB3	1.87	0.74
1:A:536:VAL:HG11	2:B:258:GLN:HB3	1.68	0.74
2:B:319:TYR:O	2:B:321:PRO:HD3	1.87	0.74
1:A:276:VAL:HG21	1:A:353:LYS:NZ	2.03	0.74
1:A:184:MET:HG2	4:P:823:DDG:H2'	1.69	0.74
1:A:108:VAL:HB	1:A:221:HIS:HB2	1.70	0.73
1:A:354:TYR:HD2	1:A:371:ALA:CB	2.00	0.73
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.24	0.73
2:B:246:LEU:CD2	2:B:260:LEU:HD11	2.19	0.73
2:B:343:GLN:HG3	2:B:349:LEU:HD11	1.71	0.72
1:A:446:ALA:CB	1:A:453:GLY:HA3	2.19	0.72
2:B:66:LYS:O	2:B:66:LYS:HG2	1.87	0.72
1:A:244:ILE:HG12	1:A:244:ILE:O	1.88	0.72
2:B:193:LEU:HD22	2:B:197:GLN:HB2	1.71	0.72
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.72	0.72
2:B:13:LYS:HE3	2:B:16:MET:SD	2.30	0.72
2:B:244:ILE:HG13	2:B:426:TRP:O	1.88	0.72
1:A:118:VAL:HB	1:A:149:LEU:HD12	1.72	0.72
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.04	0.72
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.25	0.72
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:HG23	2:B:212:TRP:HE3	1.53	0.71
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.55	0.71
1:A:455:ALA:HB1	1:A:481:ALA:HB2	1.72	0.71
2:B:103:LYS:HE2	2:B:103:LYS:HA	1.72	0.71
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.25	0.71
1:A:426:TRP:CE3	1:A:426:TRP:HA	2.24	0.71
2:B:406:TRP:NE1	2:B:408:ALA:HB3	2.05	0.71
2:B:161:GLN:O	2:B:164:MET:HB3	1.91	0.71
1:A:337:TRP:HZ3	1:A:368:LEU:HD13	1.54	0.71
1:A:441:TYR:HB2	1:A:458:VAL:CG2	2.21	0.71
2:B:85:GLN:O	2:B:87:PHE:N	2.23	0.71
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.73	0.70
2:B:103:LYS:HD3	2:B:190:GLY:C	2.11	0.70
1:A:452:LEU:HG	1:A:470:THR:HA	1.73	0.70
2:B:330:GLN:O	2:B:337:TRP:HA	1.91	0.70
1:A:508:ALA:C	1:A:510:PRO:HD3	2.11	0.70
1:A:417:VAL:O	1:A:417:VAL:HG13	1.90	0.70
1:A:87:PHE:HB3	2:B:52:PRO:O	1.92	0.70
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.73	0.70
2:B:333:GLY:H	2:B:336:GLN:CB	2.04	0.70
2:B:279:LEU:HD21	2:B:295:LEU:HD23	1.71	0.70
1:A:94:ILE:HG23	1:A:95:PRO:HD2	1.74	0.69
1:A:220:LYS:O	1:A:220:LYS:HG3	1.90	0.69
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.55	0.69
2:B:93:GLY:O	2:B:94:ILE:HD12	1.92	0.69
1:A:395:LYS:HE3	1:A:414:TRP:NE1	2.08	0.69
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.74	0.69
2:B:13:LYS:HG2	2:B:85:GLN:HG3	1.74	0.69
2:B:85:GLN:HG2	2:B:86:ASP:N	2.08	0.69
1:A:92:LEU:CD1	2:B:133:PRO:HB3	2.22	0.68
2:B:274:ILE:HG13	2:B:309:ILE:HD12	1.74	0.68
1:A:34:LEU:HB3	1:A:132:ILE:HD13	1.74	0.68
1:A:105:SER:CB	1:A:198:HIS:ND1	2.57	0.68
2:B:35:VAL:HG13	2:B:36:GLU:N	2.08	0.68
2:B:270:ILE:HG23	2:B:271:TYR:CD1	2.28	0.68
1:A:331:LYS:HG2	1:A:333:GLY:H	1.57	0.68
2:B:266:TRP:C	2:B:268:SER:H	1.96	0.68
1:A:105:SER:HB3	1:A:198:HIS:ND1	2.08	0.68
2:B:85:GLN:C	2:B:87:PHE:H	1.96	0.68
2:B:305:GLU:C	2:B:307:ARG:H	1.95	0.68
4:P:809:DC:H2'	4:P:810:DT:C6	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:O	1:A:284:ARG:HG3	1.94	0.68
2:B:332:GLN:HB2	2:B:336:GLN:CB	2.16	0.68
2:B:5:ILE:HG22	2:B:6:GLU:H	1.57	0.68
1:A:23:GLN:OE1	1:A:59:PRO:HA	1.94	0.67
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.75	0.67
2:B:295:LEU:HD12	2:B:295:LEU:N	2.07	0.67
1:A:224:GLU:O	1:A:225:PRO:C	2.29	0.67
2:B:388:LYS:O	2:B:388:LYS:HD3	1.95	0.67
2:B:327:ALA:HA	2:B:340:GLN:O	1.95	0.67
1:A:91:GLN:HB2	1:A:161:GLN:HE22	1.59	0.67
2:B:293:ILE:HG13	2:B:293:ILE:O	1.94	0.67
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.77	0.67
1:A:106:VAL:HG21	6:A:560:SO4:O1	1.95	0.67
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.29	0.67
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.77	0.67
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.77	0.67
2:B:64:LYS:CD	2:B:69:THR:HA	2.18	0.67
2:B:169:GLU:CG	2:B:170:PRO:HD3	2.11	0.66
1:A:89:GLU:HG2	3:T:708:DG:C5'	2.25	0.66
1:A:95:PRO:HA	2:B:136:ASN:O	1.94	0.66
1:A:225:PRO:HG3	1:A:227:PHE:HE1	1.60	0.66
2:B:24:TRP:O	2:B:26:LEU:HD23	1.94	0.66
2:B:65:LYS:HG2	2:B:66:LYS:N	2.10	0.66
4:P:814:DC:H2'	4:P:815:DG:C8	2.31	0.66
2:B:356:ARG:CD	2:B:361:HIS:HA	2.24	0.66
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.78	0.66
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.31	0.66
1:A:452:LEU:HB3	1:A:469:LEU:O	1.96	0.66
2:B:24:TRP:HH2	2:B:61:PHE:CD1	2.14	0.66
4:P:807:DC:H2'	4:P:808:DC:C6	2.31	0.66
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.76	0.65
1:A:465:LYS:HE2	1:A:484:LEU:HD13	1.78	0.65
2:B:103:LYS:HD3	2:B:190:GLY:O	1.96	0.65
2:B:13:LYS:HG3	2:B:85:GLN:CA	2.24	0.65
1:A:88:TRP:HB3	2:B:143:ARG:NH1	2.11	0.65
1:A:484:LEU:HA	1:A:487:GLN:NE2	2.11	0.65
2:B:333:GLY:H	2:B:336:GLN:HB2	1.60	0.65
1:A:537:PRO:HB3	2:B:265:ASN:ND2	2.10	0.65
1:A:115:TYR:CE2	5:A:700:DTP:H2'1	2.32	0.65
1:A:149:LEU:HD22	1:A:156:SER:HA	1.77	0.65
1:A:19:PRO:O	1:A:56:TYR:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LYS:HE2	2:B:265:ASN:OD1	1.96	0.65
2:B:66:LYS:O	2:B:67:ASP:HB3	1.97	0.65
2:B:399:GLU:HA	2:B:402:TRP:CD1	2.31	0.65
1:A:94:ILE:HD11	3:T:708:DG:H21	1.61	0.64
2:B:122:GLU:HA	2:B:125:ARG:CD	2.26	0.64
1:A:279:LEU:O	1:A:282:LEU:HB3	1.96	0.64
1:A:286:THR:HG23	3:T:714:DG:H5'	1.79	0.64
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.79	0.64
1:A:136:ASN:H	1:A:136:ASN:ND2	1.91	0.64
1:A:206:ARG:NH1	1:A:220:LYS:HD3	2.12	0.64
3:T:705:DT:H2'	3:T:706:DC:H6	1.63	0.64
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.11	0.64
1:A:478:GLU:O	1:A:482:ILE:HG13	1.97	0.64
3:T:719:DG:H2''	3:T:720:DG:O5'	1.97	0.64
1:A:27:THR:OG1	1:A:29:GLU:HB3	1.97	0.64
4:P:817:MRG:H2'	4:P:818:DC:C6	2.32	0.64
1:A:464:GLN:HE21	1:A:551:LEU:HD13	1.62	0.64
2:B:154:LYS:O	2:B:157:PRO:HD2	1.97	0.64
3:T:720:DG:H2'	3:T:721:DG:H8	1.62	0.64
1:A:92:LEU:HD12	2:B:133:PRO:CB	2.28	0.64
2:B:393:ILE:CG2	2:B:398:TRP:HB2	2.27	0.64
1:A:369:THR:HG22	1:A:411:ILE:HD11	1.79	0.64
1:A:393:ILE:CB	1:A:423:VAL:HG12	2.26	0.64
2:B:114:ALA:CB	2:B:214:LEU:HD22	2.27	0.64
2:B:241:VAL:HG11	2:B:350:LYS:HG3	1.81	0.63
2:B:278:GLN:HB2	2:B:302:GLU:OE2	1.98	0.63
1:A:379:SER:OG	1:A:387:PRO:HD3	1.99	0.63
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.79	0.63
2:B:241:VAL:HB	2:B:351:THR:O	1.97	0.63
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.34	0.63
1:A:521:ILE:HG22	1:A:525:LEU:HD11	1.81	0.63
2:B:78:ARG:HE	2:B:411:ILE:CG2	2.12	0.63
1:A:535:TRP:HB3	2:B:422:LEU:CD2	2.29	0.62
2:B:120:LEU:HD12	2:B:121:ASP:N	2.15	0.62
1:A:317:VAL:HG12	1:A:318:TYR:N	2.08	0.62
2:B:8:VAL:CG2	2:B:159:ILE:HD13	2.29	0.62
4:P:812:DT:H2'	4:P:813:DT:H6	1.63	0.62
2:B:14:PRO:HD3	2:B:85:GLN:NE2	2.15	0.62
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.82	0.62
2:B:53:GLU:N	2:B:53:GLU:OE2	2.33	0.62
1:A:86:ASP:O	2:B:55:PRO:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD23	1:A:220:LYS:HB2	1.81	0.62
2:B:27:THR:HG22	2:B:28:GLU:N	2.13	0.62
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.65	0.61
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.80	0.61
1:A:254:VAL:HG13	1:A:283:LEU:CD2	2.30	0.61
1:A:454:LYS:HG3	1:A:552:VAL:HG13	1.82	0.61
1:A:467:VAL:HG13	1:A:468:PRO:HD2	1.82	0.61
2:B:78:ARG:HE	2:B:411:ILE:HG22	1.65	0.61
2:B:178:ILE:HD11	2:B:201:LYS:HZ2	1.65	0.61
2:B:81:ASN:HA	2:B:84:THR:HG22	1.83	0.61
1:A:354:TYR:HE1	1:A:356:ARG:HB3	1.64	0.61
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.65	0.61
4:P:811:DG:H2'	4:P:812:DT:C6	2.35	0.61
1:A:326:ILE:HG22	1:A:327:ALA:N	2.15	0.61
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.47	0.61
2:B:21:VAL:HG11	2:B:59:PRO:HD3	1.83	0.61
1:A:446:ALA:HB2	1:A:453:GLY:HA3	1.82	0.61
2:B:210:LEU:HA	2:B:214:LEU:O	2.00	0.61
1:A:509:GLN:N	1:A:510:PRO:CD	2.64	0.61
1:A:91:GLN:O	3:T:708:DG:H4'	2.01	0.60
1:A:446:ALA:HA	1:A:453:GLY:HA3	1.82	0.60
1:A:465:LYS:O	1:A:466:VAL:HG13	2.00	0.60
2:B:86:ASP:HB3	2:B:89:GLU:HB3	1.83	0.60
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.83	0.60
2:B:317:VAL:HG23	2:B:317:VAL:O	2.01	0.60
1:A:276:VAL:HG21	1:A:353:LYS:HZ3	1.65	0.60
2:B:203:GLU:O	2:B:203:GLU:HG2	2.00	0.60
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.14	0.60
2:B:422:LEU:CA	2:B:425:LEU:HD13	2.22	0.60
2:B:194:GLU:HB3	2:B:197:GLN:OE1	2.01	0.60
2:B:426:TRP:N	2:B:426:TRP:CD1	2.69	0.60
2:B:111:VAL:HG12	2:B:216:THR:OG1	2.01	0.60
1:A:53:GLU:H	1:A:53:GLU:CD	2.05	0.60
1:A:90:VAL:HG22	2:B:140:PRO:HB2	1.83	0.60
2:B:421:PRO:C	2:B:423:VAL:H	2.04	0.60
2:B:85:GLN:CG	2:B:86:ASP:N	2.64	0.60
2:B:178:ILE:HD11	2:B:201:LYS:HZ3	1.63	0.60
1:A:402:TRP:CG	1:A:403:THR:N	2.69	0.60
2:B:87:PHE:HZ	2:B:159:ILE:HG12	1.66	0.60
2:B:206:ARG:NH2	2:B:216:THR:O	2.35	0.60
2:B:379:SER:O	2:B:383:TRP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:813:DT:H2'	4:P:814:DC:C6	2.37	0.60
2:B:175:ASN:H	2:B:176:PRO:HD3	1.66	0.59
2:B:377:THR:O	2:B:381:VAL:HG23	2.01	0.59
1:A:493:VAL:HG12	1:A:494:ASN:H	1.66	0.59
1:A:518:VAL:O	1:A:522:ILE:HG13	2.02	0.59
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.37	0.59
1:A:498:ASP:HA	1:A:536:VAL:O	2.02	0.59
2:B:326:ILE:HG22	2:B:327:ALA:N	2.18	0.59
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.83	0.59
1:A:451:LYS:HB3	1:A:452:LEU:HD12	1.83	0.59
2:B:11:LYS:HG2	2:B:12:LEU:O	2.02	0.59
2:B:254:VAL:HG12	2:B:258:GLN:OE1	2.02	0.59
2:B:389:PHE:HD1	2:B:389:PHE:H	1.51	0.59
2:B:163:SER:O	2:B:167:ILE:HG13	2.03	0.59
2:B:421:PRO:HA	2:B:424:LYS:HG3	1.85	0.59
1:A:308:GLU:OE2	1:A:311:LYS:HD2	2.03	0.59
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.38	0.59
1:A:454:LYS:HZ2	1:A:554:ALA:HB3	1.66	0.59
1:A:127:TYR:C	1:A:129:ALA:H	2.06	0.58
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.85	0.58
2:B:24:TRP:CH2	2:B:61:PHE:CD1	2.91	0.58
2:B:325:LEU:O	2:B:387:PRO:HA	2.03	0.58
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.38	0.58
1:A:210:LEU:O	1:A:210:LEU:HD12	2.03	0.58
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.38	0.58
1:A:277:ARG:NH2	1:A:355:ALA:O	2.36	0.58
1:A:536:VAL:CG1	2:B:258:GLN:HB3	2.34	0.58
1:A:77:PHE:O	1:A:81:ASN:ND2	2.36	0.58
1:A:434:ILE:HB	1:A:494:ASN:ND2	2.17	0.58
2:B:128:THR:HB	2:B:146:TYR:HB2	1.85	0.58
1:A:92:LEU:HD23	1:A:92:LEU:N	2.18	0.58
1:A:430:GLU:OE2	1:A:530:LYS:HG2	2.03	0.58
1:A:550:LYS:HA	1:A:553:SER:OG	2.03	0.58
2:B:60:VAL:HG23	2:B:61:PHE:N	2.18	0.58
2:B:277:ARG:HA	2:B:280:SER:HB3	1.85	0.58
1:A:63:ILE:HG22	1:A:64:LYS:O	2.04	0.58
2:B:112:GLY:C	2:B:114:ALA:H	2.05	0.58
1:A:446:ALA:HA	1:A:453:GLY:CA	2.33	0.58
2:B:41:MET:HB3	2:B:47:ILE:HG12	1.85	0.58
1:A:87:PHE:N	1:A:87:PHE:CD1	2.72	0.57
1:A:3:SER:OG	1:A:4:PRO:HD2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:VAL:C	2:B:113:ASP:N	2.57	0.57
1:A:441:TYR:HB2	1:A:458:VAL:HG22	1.86	0.57
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.39	0.57
1:A:454:LYS:HG3	1:A:552:VAL:CG1	2.33	0.57
2:B:161:GLN:HA	2:B:164:MET:HB3	1.86	0.57
2:B:368:LEU:HD13	2:B:393:ILE:HD12	1.87	0.57
1:A:96:HIS:O	1:A:97:PRO:C	2.41	0.57
2:B:11:LYS:HG2	2:B:12:LEU:N	2.18	0.57
2:B:64:LYS:HE3	2:B:71:TRP:NE1	2.19	0.57
1:A:491:LEU:HD22	1:A:529:GLU:HG2	1.86	0.57
1:A:521:ILE:O	1:A:525:LEU:HG	2.05	0.57
1:A:475:GLN:NE2	4:P:808:DC:C2'	2.66	0.57
2:B:85:GLN:CG	2:B:86:ASP:H	2.17	0.57
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.04	0.57
2:B:368:LEU:HD23	2:B:368:LEU:O	2.04	0.57
1:A:22:LYS:CD	1:A:23:GLN:H	2.18	0.57
1:A:41:MET:HG2	1:A:46:LYS:HB2	1.86	0.57
1:A:406:TRP:HZ3	1:A:507:GLN:HG3	1.70	0.57
1:A:93:GLY:HA3	2:B:137:ASN:OD1	2.04	0.56
1:A:354:TYR:CD2	1:A:371:ALA:HA	2.40	0.56
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.87	0.56
2:B:302:GLU:HG2	2:B:306:ASN:ND2	2.20	0.56
1:A:22:LYS:CG	1:A:23:GLN:H	2.18	0.56
2:B:106:VAL:HG22	2:B:190:GLY:HA3	1.85	0.56
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.40	0.56
1:A:188:TYR:CD1	1:A:188:TYR:C	2.79	0.56
1:A:417:VAL:O	1:A:419:THR:HG22	2.05	0.56
2:B:109:LEU:CG	2:B:216:THR:HG21	2.33	0.56
2:B:253:THR:OG1	2:B:256:ASP:HB2	2.05	0.56
2:B:234:LEU:HB3	2:B:236:PRO:HD3	1.87	0.56
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.40	0.56
1:A:188:TYR:HD1	1:A:188:TYR:O	1.88	0.56
1:A:406:TRP:CD1	1:A:407:GLN:HG3	2.41	0.56
1:A:479:LEU:HD11	1:A:501:TYR:HE2	1.70	0.56
2:B:90:VAL:HG12	2:B:90:VAL:O	2.06	0.56
2:B:295:LEU:HD13	2:B:300:GLU:CD	2.26	0.56
1:A:74:LEU:CD2	1:A:151:GLN:HG2	2.36	0.56
1:A:420:PRO:HA	1:A:422:LEU:N	2.20	0.56
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.33	0.56
1:A:105:SER:HB2	1:A:198:HIS:ND1	2.20	0.55
1:A:220:LYS:O	1:A:220:LYS:CG	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:O	1:A:71:TRP:HA	2.06	0.55
2:B:60:VAL:CG2	2:B:61:PHE:N	2.69	0.55
2:B:111:VAL:O	2:B:113:ASP:N	2.39	0.55
2:B:334:GLN:O	2:B:334:GLN:HG2	2.07	0.55
1:A:263:LYS:O	1:A:266:TRP:HB3	2.07	0.55
1:A:195:ILE:HG23	1:A:199:ARG:HD3	1.87	0.55
1:A:446:ALA:CA	1:A:453:GLY:HA3	2.36	0.55
2:B:393:ILE:HG23	2:B:394:GLN:N	2.21	0.55
3:T:708:DG:H2'	3:T:709:DC:C6	2.40	0.55
4:P:811:DG:H2'	4:P:812:DT:H6	1.70	0.55
1:A:376:THR:HG23	1:A:386:THR:OG1	2.07	0.55
2:B:247:PRO:CD	2:B:260:LEU:HD22	2.36	0.55
2:B:68:SER:OG	2:B:70:LYS:HB2	2.06	0.55
2:B:244:ILE:HG23	2:B:310:LEU:HD22	1.89	0.55
2:B:302:GLU:HG2	2:B:306:ASN:HD22	1.72	0.55
1:A:298:GLU:H	1:A:298:GLU:CD	2.10	0.55
1:A:342:TYR:HB3	1:A:348:ASN:HB3	1.89	0.55
1:A:22:LYS:HG3	1:A:23:GLN:N	2.22	0.55
1:A:30:LYS:O	1:A:34:LEU:HD12	2.07	0.55
1:A:225:PRO:HG3	1:A:227:PHE:CE1	2.41	0.55
1:A:282:LEU:O	1:A:293:ILE:HD11	2.07	0.55
1:A:484:LEU:HA	1:A:487:GLN:HE21	1.71	0.55
1:A:198:HIS:C	1:A:198:HIS:CD2	2.80	0.55
2:B:279:LEU:HA	2:B:282:LEU:HD13	1.89	0.55
2:B:362:THR:HB	2:B:366:LYS:HD3	1.88	0.55
2:B:406:TRP:CH2	2:B:412:PRO:HD2	2.42	0.55
1:A:195:ILE:HG23	1:A:199:ARG:CD	2.37	0.54
1:A:396:GLU:C	1:A:398:TRP:N	2.60	0.54
1:A:506:ILE:HG22	1:A:506:ILE:O	2.07	0.54
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.90	0.54
2:B:175:ASN:N	2:B:176:PRO:CD	2.70	0.54
2:B:235:HIS:N	2:B:236:PRO:HD3	2.22	0.54
2:B:391:LEU:O	2:B:417:VAL:N	2.35	0.54
1:A:362:THR:HB	1:A:366:LYS:HD3	1.90	0.54
2:B:40:GLU:OE1	2:B:40:GLU:HA	2.06	0.54
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.37	0.54
2:B:365:VAL:CG1	2:B:393:ILE:HD11	2.27	0.54
3:T:721:DG:H2'	3:T:722:DA:C8	2.42	0.54
1:A:369:THR:CG2	1:A:411:ILE:HD11	2.38	0.54
2:B:104:LYS:HG2	2:B:192:ASP:OD1	2.07	0.54
2:B:194:GLU:O	2:B:198:HIS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:H	2:B:295:LEU:CD1	2.11	0.54
2:B:134:SER:OG	2:B:139:THR:HG23	2.07	0.54
1:A:106:VAL:HG12	1:A:107:THR:N	2.22	0.54
1:A:354:TYR:C	1:A:354:TYR:CD1	2.80	0.54
1:A:459:THR:CG2	1:A:463:ARG:HB3	2.38	0.54
2:B:111:VAL:C	2:B:113:ASP:H	2.11	0.54
2:B:276:VAL:HG13	2:B:277:ARG:H	1.73	0.54
2:B:356:ARG:CB	2:B:367:GLN:HE22	2.15	0.54
2:B:388:LYS:O	2:B:388:LYS:CD	2.56	0.54
1:A:43:LYS:HD3	1:A:43:LYS:O	2.08	0.53
1:A:446:ALA:HB2	1:A:472:THR:HG23	1.91	0.53
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.89	0.53
1:A:398:TRP:C	1:A:400:THR:H	2.09	0.53
2:B:81:ASN:HA	2:B:84:THR:CG2	2.38	0.53
2:B:178:ILE:HG23	2:B:190:GLY:O	2.08	0.53
1:A:5:ILE:HG12	1:A:6:GLU:N	2.24	0.53
1:A:146:TYR:CE2	1:A:150:PRO:HA	2.43	0.53
2:B:21:VAL:CG1	2:B:58:THR:HA	2.38	0.53
1:A:23:GLN:NE2	1:A:60:VAL:H	2.01	0.53
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.44	0.53
2:B:7:THR:HG22	2:B:119:PRO:O	2.07	0.53
2:B:21:VAL:HG13	2:B:58:THR:HA	1.90	0.53
2:B:81:ASN:O	2:B:84:THR:HG22	2.08	0.53
1:A:406:TRP:CZ3	1:A:507:GLN:HG3	2.44	0.53
1:A:469:LEU:HD12	1:A:472:THR:HG21	1.91	0.53
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.90	0.53
2:B:241:VAL:CB	2:B:351:THR:O	2.56	0.53
1:A:223:LYS:C	1:A:225:PRO:CD	2.77	0.53
2:B:100:LEU:HA	2:B:103:LYS:HG2	1.91	0.53
1:A:115:TYR:CD2	5:A:700:DTP:H2'1	2.44	0.53
1:A:447:ASN:ND2	1:A:450:THR:HG23	2.24	0.53
3:T:716:DA:H2'	3:T:717:DC:O4'	2.09	0.53
1:A:23:GLN:HE22	1:A:60:VAL:N	2.03	0.53
1:A:60:VAL:HG12	1:A:75:VAL:HG13	1.91	0.53
1:A:259:LYS:HE2	4:P:819:DG:OP1	2.09	0.53
1:A:354:TYR:HE2	1:A:370:GLU:C	2.12	0.53
1:A:405:TYR:O	2:B:331:LYS:HE3	2.09	0.53
2:B:406:TRP:CZ2	2:B:412:PRO:HD2	2.44	0.53
1:A:395:LYS:HE3	1:A:414:TRP:CE2	2.45	0.52
2:B:35:VAL:CG1	2:B:36:GLU:N	2.72	0.52
1:A:78:ARG:HA	1:A:81:ASN:HD22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:O	1:A:312:GLU:HG3	2.09	0.52
1:A:529:GLU:O	1:A:530:LYS:HG3	2.10	0.52
1:A:61:PHE:CD1	1:A:61:PHE:N	2.77	0.52
1:A:391:LEU:C	1:A:417:VAL:HG12	2.29	0.52
1:A:537:PRO:HD3	2:B:262:GLY:CA	2.39	0.52
1:A:22:LYS:CG	1:A:23:GLN:N	2.72	0.52
1:A:89:GLU:CG	3:T:708:DG:H5'	2.39	0.52
1:A:398:TRP:O	1:A:402:TRP:HD1	1.92	0.52
1:A:447:ASN:HD22	1:A:450:THR:HG23	1.74	0.52
1:A:135:ILE:C	1:A:137:ASN:H	2.11	0.52
1:A:261:VAL:HG12	1:A:265:ASN:ND2	2.25	0.52
2:B:34:LEU:HD13	2:B:34:LEU:O	2.10	0.52
2:B:254:VAL:HG21	2:B:288:ALA:O	2.10	0.52
2:B:282:LEU:HD21	2:B:295:LEU:HB3	1.92	0.52
1:A:437:ALA:HB3	1:A:494:ASN:HD22	1.75	0.52
2:B:333:GLY:H	2:B:336:GLN:HB3	1.72	0.52
1:A:473:THR:H	1:A:476:LYS:HB2	1.74	0.52
2:B:104:LYS:CB	2:B:192:ASP:HA	2.38	0.52
1:A:198:HIS:CD2	1:A:202:ILE:HD13	2.45	0.52
1:A:435:VAL:HG22	2:B:290:THR:HG23	1.92	0.52
3:T:706:DC:H2'	3:T:707:DG:C8	2.45	0.52
1:A:64:LYS:HD3	1:A:71:TRP:CE2	2.45	0.51
1:A:231:GLY:HA2	1:A:242:GLN:NE2	2.24	0.51
1:A:470:THR:HG22	1:A:471:ASN:ND2	2.25	0.51
1:A:537:PRO:HD3	2:B:262:GLY:HA3	1.92	0.51
2:B:8:VAL:HG23	2:B:8:VAL:O	2.08	0.51
2:B:60:VAL:HG11	2:B:130:PHE:HB2	1.92	0.51
2:B:170:PRO:O	2:B:174:GLN:HG2	2.10	0.51
2:B:305:GLU:C	2:B:307:ARG:N	2.61	0.51
1:A:22:LYS:HD2	1:A:23:GLN:H	1.76	0.51
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.26	0.51
1:A:266:TRP:CZ3	1:A:269:GLN:NE2	2.78	0.51
1:A:467:VAL:CG1	1:A:468:PRO:HD2	2.40	0.51
2:B:13:LYS:CG	2:B:85:GLN:HG3	2.40	0.51
1:A:255:ASN:HA	1:A:258:CYS:HB2	1.90	0.51
1:A:430:GLU:O	1:A:532:TYR:HD1	1.94	0.51
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.92	0.51
1:A:536:VAL:HG12	2:B:258:GLN:O	2.10	0.51
2:B:376:THR:OG1	2:B:389:PHE:CZ	2.64	0.51
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.40	0.51
1:A:247:PRO:CG	1:A:260:LEU:CD1	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:C	1:A:337:TRP:CD1	2.84	0.51
1:A:338:THR:HG22	1:A:339:TYR:N	2.25	0.51
2:B:241:VAL:HG23	2:B:241:VAL:O	2.10	0.51
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.45	0.51
2:B:13:LYS:CA	2:B:85:GLN:HB2	2.39	0.51
2:B:174:GLN:HE21	2:B:175:ASN:HB2	1.75	0.51
2:B:193:LEU:HB3	2:B:198:HIS:HB2	1.93	0.51
2:B:279:LEU:CD2	2:B:295:LEU:HD23	2.40	0.51
1:A:276:VAL:CG2	1:A:353:LYS:HZ3	2.23	0.51
1:A:364:ASP:HB3	1:A:423:VAL:CG2	2.40	0.51
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.93	0.51
1:A:486:LEU:O	1:A:528:LYS:HE2	2.11	0.51
2:B:208:HIS:O	2:B:212:TRP:HB2	2.11	0.51
2:B:247:PRO:HG3	2:B:260:LEU:HD22	1.91	0.51
1:A:265:ASN:O	1:A:268:SER:OG	2.28	0.51
1:A:354:TYR:CD2	1:A:371:ALA:CA	2.94	0.51
2:B:64:LYS:HA	2:B:71:TRP:HA	1.92	0.51
4:P:805:DG:C2'	4:P:806:DT:O5'	2.59	0.51
1:A:266:TRP:CE2	4:P:820:DC:H4'	2.45	0.51
1:A:407:GLN:HG2	2:B:392:PRO:O	2.11	0.51
2:B:266:TRP:C	2:B:268:SER:N	2.65	0.51
2:B:273:GLY:O	2:B:309:ILE:HD13	2.11	0.51
1:A:441:TYR:HB2	1:A:458:VAL:HG23	1.92	0.51
2:B:368:LEU:O	2:B:372:VAL:HG23	2.10	0.51
1:A:231:GLY:CA	1:A:242:GLN:HE21	2.24	0.51
1:A:271:TYR:CE1	1:A:314:VAL:HG22	2.46	0.51
1:A:317:VAL:CG1	1:A:318:TYR:H	2.17	0.51
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.31	0.51
1:A:456:GLY:HA3	1:A:466:VAL:HG12	1.93	0.51
1:A:473:THR:O	1:A:477:THR:HG23	2.11	0.51
2:B:128:THR:HB	2:B:146:TYR:HD1	1.75	0.51
2:B:244:ILE:O	2:B:310:LEU:HD13	2.11	0.51
1:A:484:LEU:C	1:A:486:LEU:H	2.15	0.50
2:B:105:SER:HA	2:B:235:HIS:HD1	1.76	0.50
2:B:210:LEU:CD1	2:B:211:ARG:HG2	2.42	0.50
2:B:339:TYR:HE2	2:B:378:GLU:OE1	1.95	0.50
2:B:342:TYR:CD1	2:B:342:TYR:C	2.84	0.50
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.11	0.50
4:P:806:DT:H2'	4:P:807:DC:C6	2.46	0.50
1:A:78:ARG:HA	1:A:81:ASN:ND2	2.27	0.50
2:B:241:VAL:CG1	2:B:350:LYS:HG3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:O	1:A:291:GLU:HB3	2.11	0.50
2:B:118:VAL:O	2:B:149:LEU:HG	2.11	0.50
1:A:345:PRO:O	1:A:346:PHE:HB2	2.11	0.50
1:A:396:GLU:O	1:A:398:TRP:N	2.44	0.50
1:A:107:THR:HG21	1:A:202:ILE:HG12	1.93	0.50
1:A:333:GLY:C	1:A:334:GLN:HG2	2.32	0.50
1:A:377:THR:O	1:A:381:VAL:HG23	2.12	0.50
1:A:470:THR:O	1:A:471:ASN:HB2	2.11	0.50
1:A:489:SER:OG	1:A:493:VAL:HG21	2.12	0.50
1:A:493:VAL:HG12	1:A:494:ASN:N	2.27	0.50
2:B:8:VAL:HG21	2:B:159:ILE:HD13	1.92	0.50
2:B:203:GLU:HA	2:B:206:ARG:HG3	1.93	0.50
1:A:10:VAL:HG11	1:A:153:TRP:HH2	1.77	0.50
1:A:183:TYR:O	1:A:184:MET:HB3	2.12	0.50
1:A:340:GLN:CD	1:A:340:GLN:N	2.64	0.50
1:A:362:THR:HB	1:A:366:LYS:CD	2.41	0.50
2:B:85:GLN:C	2:B:87:PHE:N	2.64	0.50
1:A:221:HIS:CE1	1:A:228:LEU:HB2	2.46	0.50
1:A:361:HIS:NE2	4:P:810:DT:OP1	2.45	0.50
1:A:366:LYS:HE2	1:A:401:TRP:HH2	1.76	0.50
1:A:521:ILE:HG22	1:A:525:LEU:CD1	2.42	0.50
1:A:194:GLU:O	1:A:195:ILE:C	2.48	0.50
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.46	0.50
2:B:30:LYS:O	2:B:34:LEU:HB2	2.12	0.50
2:B:408:ALA:C	2:B:410:TRP:H	2.15	0.50
1:A:276:VAL:CG2	1:A:353:LYS:NZ	2.75	0.49
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.42	0.49
2:B:106:VAL:HG22	2:B:190:GLY:CA	2.42	0.49
1:A:91:GLN:HB2	1:A:161:GLN:NE2	2.26	0.49
1:A:419:THR:HG23	1:A:419:THR:O	2.11	0.49
1:A:72:ARG:HG2	1:A:74:LEU:HD21	1.94	0.49
2:B:362:THR:CG2	2:B:366:LYS:HD3	2.43	0.49
1:A:198:HIS:HE2	1:A:202:ILE:CD1	2.17	0.49
1:A:79:GLU:O	1:A:82:LYS:HB2	2.12	0.49
1:A:444:GLY:CA	1:A:552:VAL:HG11	2.38	0.49
1:A:454:LYS:HZ1	1:A:554:ALA:HB3	1.74	0.49
1:A:94:ILE:CD1	3:T:708:DG:H21	2.25	0.49
1:A:131:THR:O	1:A:133:PRO:HD3	2.12	0.49
1:A:354:TYR:HD2	1:A:371:ALA:CA	2.25	0.49
1:A:398:TRP:C	1:A:400:THR:N	2.65	0.49
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TYR:HE1	1:A:522:ILE:CG2	2.25	0.49
2:B:235:HIS:HB2	2:B:238:LYS:HB3	1.93	0.49
1:A:158:ALA:HB1	2:B:52:PRO:HB3	1.94	0.49
1:A:393:ILE:HG23	1:A:393:ILE:O	2.12	0.49
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.77	0.49
2:B:85:GLN:HG2	2:B:86:ASP:H	1.74	0.49
1:A:93:GLY:CA	2:B:137:ASN:OD1	2.61	0.49
1:A:109:LEU:CD2	1:A:220:LYS:HB2	2.42	0.49
1:A:195:ILE:CG2	1:A:199:ARG:HD3	2.43	0.49
1:A:221:HIS:HB3	1:A:227:PHE:CD2	2.48	0.49
2:B:21:VAL:HG12	2:B:57:ASN:O	2.12	0.49
2:B:279:LEU:HD12	2:B:302:GLU:OE1	2.13	0.49
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.48	0.49
1:A:75:VAL:HB	1:A:77:PHE:CE1	2.47	0.49
2:B:279:LEU:HD21	2:B:295:LEU:CD2	2.42	0.49
2:B:421:PRO:HB3	2:B:424:LYS:HD2	1.95	0.49
1:A:252:TRP:CH2	1:A:260:LEU:HD21	2.47	0.49
2:B:120:LEU:HD11	2:B:124:PHE:HD2	1.78	0.48
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.13	0.48
2:B:210:LEU:HD12	2:B:211:ARG:HG2	1.94	0.48
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.95	0.48
2:B:263:LYS:HG3	2:B:426:TRP:CD1	2.48	0.48
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.78	0.48
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.77	0.48
2:B:85:GLN:O	2:B:88:TRP:CD1	2.66	0.48
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.12	0.48
4:P:804:DA:H3'	4:P:805:DG:C8	2.48	0.48
1:A:331:LYS:HG2	1:A:333:GLY:N	2.27	0.48
1:A:377:THR:HG22	1:A:378:GLU:N	2.28	0.48
1:A:484:LEU:HD23	1:A:487:GLN:HE22	1.75	0.48
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.44	0.48
2:B:422:LEU:HD12	2:B:425:LEU:CD2	2.44	0.48
1:A:221:HIS:CE1	1:A:228:LEU:N	2.75	0.48
2:B:164:MET:HG2	2:B:182:GLN:OE1	2.14	0.48
1:A:281:LYS:HA	1:A:284:ARG:HE	1.78	0.48
1:A:329:ILE:HG13	1:A:338:THR:O	2.13	0.48
1:A:475:GLN:C	1:A:477:THR:H	2.16	0.48
1:A:53:GLU:CD	1:A:53:GLU:N	2.67	0.48
1:A:407:GLN:HE22	2:B:394:GLN:HE21	1.60	0.48
2:B:122:GLU:HG3	2:B:125:ARG:HH11	1.79	0.48
2:B:237:ASP:C	2:B:239:TRP:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:HE2	2:B:415:GLU:OE1	2.12	0.48
1:A:121:ASP:OD1	1:A:124:PHE:HB2	2.14	0.48
1:A:326:ILE:CG2	1:A:327:ALA:N	2.76	0.48
1:A:391:LEU:HB2	1:A:414:TRP:CZ3	2.49	0.48
2:B:78:ARG:O	2:B:82:LYS:HG3	2.13	0.48
1:A:169:GLU:N	1:A:170:PRO:HD2	2.28	0.48
1:A:535:TRP:HB3	2:B:422:LEU:HD21	1.96	0.48
2:B:245:VAL:O	2:B:263:LYS:NZ	2.46	0.48
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.49	0.48
1:A:41:MET:CG	1:A:46:LYS:HB2	2.44	0.48
1:A:112:GLY:HA2	5:A:700:DTP:O1G	2.14	0.48
1:A:259:LYS:O	1:A:263:LYS:HG3	2.14	0.48
2:B:171:PHE:HA	2:B:174:GLN:HG3	1.96	0.48
2:B:250:ASP:OD2	2:B:250:ASP:N	2.45	0.48
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.96	0.47
1:A:257:ILE:O	1:A:261:VAL:HG23	2.13	0.47
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.95	0.47
2:B:19:PRO:O	2:B:57:ASN:N	2.43	0.47
2:B:80:LEU:O	2:B:83:ARG:N	2.45	0.47
2:B:87:PHE:HZ	2:B:159:ILE:CG1	2.27	0.47
2:B:112:GLY:C	2:B:114:ALA:N	2.68	0.47
2:B:366:LYS:HA	2:B:405:TYR:CD2	2.49	0.47
1:A:231:GLY:HA2	1:A:242:GLN:HE21	1.78	0.47
1:A:366:LYS:O	1:A:370:GLU:HG3	2.13	0.47
2:B:57:ASN:HA	2:B:129:ALA:O	2.14	0.47
2:B:398:TRP:O	2:B:402:TRP:HB3	2.15	0.47
1:A:136:ASN:ND2	1:A:136:ASN:N	2.61	0.47
1:A:516:GLU:O	1:A:520:GLN:HG3	2.15	0.47
1:A:10:VAL:HG23	1:A:10:VAL:O	2.15	0.47
1:A:22:LYS:HG3	1:A:23:GLN:H	1.77	0.47
1:A:64:LYS:HD3	1:A:71:TRP:CZ2	2.48	0.47
1:A:174:GLN:O	1:A:174:GLN:HG2	2.15	0.47
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.95	0.47
1:A:224:GLU:N	1:A:225:PRO:CD	2.78	0.47
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.50	0.47
2:B:193:LEU:HD22	2:B:197:GLN:CB	2.42	0.47
2:B:328:GLU:HB2	2:B:340:GLN:CB	2.45	0.47
1:A:249:LYS:HG3	1:A:252:TRP:CE2	2.50	0.47
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.96	0.47
2:B:125:ARG:HG2	2:B:146:TYR:O	2.15	0.47
2:B:368:LEU:HD11	2:B:392:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:TRP:O	2:B:404:GLU:HB2	2.14	0.47
4:P:804:DA:C3'	4:P:805:DG:C8	2.97	0.47
1:A:13:LYS:HE2	1:A:84:THR:O	2.15	0.47
1:A:90:VAL:HG22	1:A:90:VAL:O	2.15	0.47
1:A:427:TYR:CE1	1:A:522:ILE:HG23	2.50	0.47
1:A:544:GLY:O	1:A:548:VAL:HG23	2.15	0.47
1:A:434:ILE:O	1:A:437:ALA:HB3	2.15	0.47
2:B:165:THR:HA	2:B:168:LEU:HD12	1.96	0.47
2:B:96:HIS:ND1	2:B:96:HIS:N	2.62	0.46
1:A:54:ASN:HB3	1:A:143:ARG:HH12	1.79	0.46
1:A:116:PHE:N	1:A:116:PHE:CD2	2.82	0.46
1:A:548:VAL:O	1:A:552:VAL:HG23	2.14	0.46
2:B:382:ILE:HG22	2:B:382:ILE:O	2.15	0.46
1:A:61:PHE:N	1:A:61:PHE:HD1	2.14	0.46
1:A:118:VAL:HB	1:A:149:LEU:CD1	2.42	0.46
2:B:47:ILE:HA	2:B:145:GLN:O	2.16	0.46
2:B:59:PRO:O	2:B:75:VAL:HG13	2.15	0.46
4:P:813:DT:H2'	4:P:814:DC:H6	1.79	0.46
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.60	0.46
1:A:455:ALA:CB	1:A:481:ALA:HB2	2.44	0.46
2:B:20:LYS:HG2	2:B:55:PRO:O	2.15	0.46
2:B:301:LEU:O	2:B:305:GLU:HB2	2.15	0.46
2:B:303:LEU:O	2:B:307:ARG:HB2	2.15	0.46
1:A:396:GLU:C	1:A:398:TRP:H	2.19	0.46
1:A:427:TYR:C	1:A:427:TYR:CD2	2.88	0.46
2:B:84:THR:HG23	2:B:88:TRP:CD1	2.50	0.46
2:B:275:LYS:HB2	2:B:306:ASN:ND2	2.21	0.46
2:B:314:VAL:O	2:B:315:HIS:HD2	1.97	0.46
1:A:124:PHE:O	1:A:126:LYS:N	2.48	0.46
1:A:191:SER:HB3	1:A:198:HIS:ND1	2.31	0.46
1:A:255:ASN:O	1:A:258:CYS:HB2	2.15	0.46
2:B:326:ILE:HG22	2:B:327:ALA:H	1.81	0.46
1:A:106:VAL:CG1	1:A:107:THR:N	2.79	0.46
2:B:340:GLN:HG3	2:B:348:ASN:HD21	1.80	0.46
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.98	0.46
1:A:441:TYR:HB3	1:A:548:VAL:HG21	1.98	0.46
1:A:484:LEU:O	1:A:488:ASP:HB2	2.16	0.46
2:B:84:THR:HG23	2:B:84:THR:O	2.16	0.46
2:B:307:ARG:HG2	2:B:307:ARG:HH11	1.81	0.46
1:A:102:LYS:HD2	6:A:560:SO4:O2	2.15	0.46
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:PRO:HB3	2:B:184:MET:O	2.16	0.46
2:B:211:ARG:HD3	2:B:211:ARG:HA	1.61	0.46
1:A:88:TRP:HB3	2:B:143:ARG:HH12	1.78	0.46
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.98	0.46
1:A:503:LEU:O	1:A:507:GLN:HB2	2.16	0.46
1:A:199:ARG:NH1	1:A:199:ARG:CG	2.77	0.45
1:A:272:PRO:HB3	1:A:351:THR:HG21	1.98	0.45
1:A:454:LYS:CA	1:A:469:LEU:HG	2.36	0.45
1:A:517:LEU:O	1:A:520:GLN:HB2	2.16	0.45
1:A:537:PRO:HG2	1:A:542:ILE:HD11	1.98	0.45
2:B:369:THR:HG21	2:B:405:TYR:O	2.16	0.45
1:A:156:SER:CB	1:A:157:PRO:HD3	2.43	0.45
1:A:329:ILE:HG12	1:A:330:GLN:N	2.30	0.45
1:A:423:VAL:CG1	1:A:423:VAL:O	2.64	0.45
1:A:519:ASN:HA	1:A:522:ILE:HD12	1.98	0.45
1:A:543:GLY:C	1:A:545:ASN:H	2.20	0.45
2:B:367:GLN:O	2:B:370:GLU:N	2.49	0.45
1:A:451:LYS:CB	1:A:452:LEU:HD12	2.45	0.45
1:A:401:TRP:O	1:A:405:TYR:HB2	2.16	0.45
2:B:75:VAL:HB	2:B:77:PHE:CE2	2.51	0.45
1:A:124:PHE:O	1:A:125:ARG:C	2.54	0.45
1:A:219:LYS:O	1:A:219:LYS:HG2	2.15	0.45
1:A:522:ILE:CA	1:A:525:LEU:HD12	2.43	0.45
2:B:50:ILE:O	2:B:143:ARG:HB2	2.16	0.45
2:B:328:GLU:O	2:B:340:GLN:HB2	2.17	0.45
1:A:13:LYS:O	1:A:14:PRO:C	2.54	0.45
1:A:406:TRP:C	2:B:331:LYS:HD3	2.37	0.45
1:A:363:ASN:OD1	1:A:365:VAL:N	2.50	0.45
1:A:391:LEU:HA	1:A:392:PRO:HD3	1.64	0.45
2:B:27:THR:CG2	2:B:28:GLU:N	2.79	0.45
2:B:66:LYS:HE2	2:B:68:SER:HB3	1.98	0.45
2:B:255:ASN:HD22	2:B:259:LYS:HE2	1.81	0.45
1:A:443:ASP:CG	1:A:444:GLY:N	2.70	0.45
1:A:497:THR:O	1:A:535:TRP:HA	2.16	0.45
2:B:86:ASP:C	2:B:88:TRP:N	2.70	0.45
4:P:804:DA:O3'	4:P:805:DG:O4'	2.34	0.45
1:A:2:ILE:HD11	1:A:148:VAL:HG12	1.98	0.45
1:A:75:VAL:HB	1:A:77:PHE:CD1	2.52	0.45
1:A:338:THR:HG22	1:A:339:TYR:H	1.82	0.45
1:A:447:ASN:HD22	1:A:450:THR:CG2	2.29	0.45
1:A:549:ASP:O	1:A:553:SER:N	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:N	1:A:338:THR:HG21	2.32	0.45
1:A:364:ASP:HB3	1:A:423:VAL:HG21	1.98	0.45
1:A:406:TRP:O	2:B:331:LYS:HB3	2.17	0.45
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.17	0.45
2:B:153:TRP:CE3	2:B:156:SER:N	2.84	0.45
2:B:202:ILE:O	2:B:206:ARG:HG3	2.17	0.45
1:A:50:ILE:HG13	1:A:143:ARG:HB2	1.98	0.44
1:A:287:LYS:HB3	1:A:288:ALA:H	1.63	0.44
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.17	0.44
2:B:66:LYS:O	2:B:66:LYS:CG	2.62	0.44
1:A:104:LYS:HE2	1:A:194:GLU:OE2	2.17	0.44
1:A:354:TYR:C	1:A:354:TYR:HD1	2.20	0.44
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.47	0.44
2:B:43:LYS:HB2	2:B:43:LYS:HE3	1.67	0.44
2:B:128:THR:HB	2:B:146:TYR:CD1	2.52	0.44
2:B:241:VAL:O	2:B:243:PRO:HD3	2.16	0.44
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.17	0.44
1:A:434:ILE:CB	1:A:494:ASN:HD21	2.26	0.44
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.98	0.44
2:B:156:SER:N	2:B:157:PRO:HD2	2.33	0.44
2:B:279:LEU:HG	2:B:302:GLU:OE1	2.17	0.44
1:A:115:TYR:CZ	5:A:700:DTP:H2'1	2.52	0.44
1:A:475:GLN:CD	4:P:808:DC:H2''	2.36	0.44
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.53	0.44
2:B:241:VAL:HG12	2:B:350:LYS:NZ	2.32	0.44
2:B:271:TYR:CD2	2:B:309:ILE:HG22	2.52	0.44
2:B:278:GLN:OE1	2:B:298:GLU:HB2	2.18	0.44
2:B:387:PRO:HB2	2:B:389:PHE:CE1	2.52	0.44
1:A:282:LEU:O	1:A:293:ILE:CD1	2.66	0.44
2:B:81:ASN:OD1	2:B:153:TRP:CD1	2.71	0.44
2:B:193:LEU:CB	2:B:198:HIS:HB2	2.47	0.44
1:A:163:SER:O	1:A:167:ILE:HG13	2.17	0.44
1:A:475:GLN:O	1:A:477:THR:N	2.51	0.44
2:B:232:TYR:HB2	2:B:233:GLU:OE2	2.17	0.44
1:A:230:MET:CE	4:P:823:DDG:H5'	2.48	0.44
1:A:339:TYR:CE1	1:A:352:GLY:C	2.91	0.44
1:A:380:ILE:HG22	2:B:26:LEU:O	2.17	0.44
1:A:399:GLU:O	1:A:403:THR:HG22	2.17	0.44
2:B:115:TYR:C	2:B:117:SER:H	2.21	0.44
2:B:295:LEU:HD13	2:B:300:GLU:OE1	2.17	0.44
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLY:O	1:A:334:GLN:HG2	2.17	0.44
1:A:362:THR:CB	1:A:366:LYS:HD3	2.48	0.44
2:B:178:ILE:HG21	2:B:189:VAL:HG13	2.00	0.44
2:B:369:THR:O	2:B:373:GLN:HG3	2.17	0.44
1:A:206:ARG:NH1	1:A:220:LYS:CD	2.78	0.43
1:A:127:TYR:C	1:A:129:ALA:N	2.71	0.43
1:A:504:GLY:HA3	2:B:420:PRO:CG	2.48	0.43
1:A:522:ILE:O	1:A:525:LEU:HB2	2.18	0.43
1:A:535:TRP:CE3	2:B:422:LEU:HD23	2.53	0.43
2:B:154:LYS:C	2:B:157:PRO:HD2	2.38	0.43
2:B:376:THR:CG2	2:B:386:THR:HG22	2.48	0.43
1:A:252:TRP:HZ3	1:A:260:LEU:CD1	2.31	0.43
1:A:363:ASN:H	1:A:366:LYS:HD2	1.83	0.43
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.86	0.43
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.53	0.43
2:B:50:ILE:HG21	2:B:145:GLN:CG	2.49	0.43
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.01	0.43
2:B:153:TRP:HB3	2:B:156:SER:HB2	2.00	0.43
2:B:161:GLN:HA	2:B:164:MET:CB	2.49	0.43
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.18	0.43
1:A:395:LYS:HD2	1:A:395:LYS:HA	1.77	0.43
2:B:247:PRO:HD2	2:B:260:LEU:HD22	2.00	0.43
2:B:257:ILE:O	2:B:261:VAL:HG23	2.18	0.43
2:B:295:LEU:HD13	2:B:300:GLU:OE2	2.18	0.43
2:B:380:ILE:HD11	2:B:386:THR:CG2	2.48	0.43
1:A:452:LEU:CB	1:A:469:LEU:O	2.63	0.43
2:B:367:GLN:O	2:B:368:LEU:C	2.57	0.43
2:B:400:THR:HB	2:B:401:TRP:CE3	2.54	0.43
1:A:74:LEU:HD13	3:T:705:DT:C2	2.53	0.43
1:A:366:LYS:HE2	1:A:401:TRP:CH2	2.54	0.43
1:A:547:GLN:NE2	2:B:286:THR:HG23	2.33	0.43
2:B:11:LYS:CG	2:B:12:LEU:N	2.80	0.43
2:B:44:GLU:O	2:B:46:LYS:HG3	2.18	0.43
2:B:110:ASP:OD2	2:B:409:THR:HG21	2.18	0.43
1:A:63:ILE:HD11	1:A:74:LEU:HD12	2.01	0.43
1:A:231:GLY:C	1:A:242:GLN:HE21	2.22	0.43
1:A:443:ASP:CG	1:A:444:GLY:H	2.21	0.43
2:B:112:GLY:O	2:B:114:ALA:N	2.52	0.43
1:A:89:GLU:OE2	1:A:158:ALA:HB2	2.19	0.43
2:B:421:PRO:C	2:B:423:VAL:N	2.68	0.43
1:A:438:GLU:CD	1:A:459:THR:HG21	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:O	1:A:443:ASP:HB2	2.19	0.42
1:A:452:LEU:HD12	1:A:452:LEU:N	2.33	0.42
1:A:517:LEU:HA	1:A:520:GLN:OE1	2.19	0.42
2:B:292:VAL:HG12	2:B:294:PRO:HD3	2.01	0.42
1:A:270:ILE:CG2	1:A:271:TYR:N	2.82	0.42
1:A:354:TYR:OH	1:A:370:GLU:HB3	2.20	0.42
2:B:78:ARG:NE	2:B:411:ILE:HG22	2.32	0.42
2:B:356:ARG:CB	2:B:367:GLN:NE2	2.76	0.42
3:T:709:DC:H2'	3:T:710:DG:C8	2.54	0.42
1:A:146:TYR:CD2	1:A:150:PRO:HA	2.55	0.42
1:A:149:LEU:HD21	1:A:159:ILE:CG2	2.47	0.42
1:A:373:GLN:O	1:A:374:LYS:C	2.58	0.42
2:B:279:LEU:CG	2:B:302:GLU:OE1	2.67	0.42
2:B:423:VAL:HA	2:B:426:TRP:CE2	2.55	0.42
1:A:288:ALA:C	1:A:290:THR:H	2.23	0.42
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.92	0.42
1:A:410:TRP:CD1	2:B:363:ASN:HB2	2.54	0.42
1:A:435:VAL:HA	2:B:290:THR:OG1	2.18	0.42
1:A:475:GLN:C	1:A:477:THR:N	2.72	0.42
1:A:375:ILE:O	1:A:379:SER:HB3	2.19	0.42
2:B:319:TYR:CE1	2:B:383:TRP:HD1	2.37	0.42
4:P:803:DC:H2'	4:P:804:DA:C8	2.55	0.42
1:A:487:GLN:H	1:A:487:GLN:HG2	1.64	0.42
1:A:517:LEU:C	1:A:517:LEU:HD23	2.39	0.42
2:B:122:GLU:HA	2:B:125:ARG:CG	2.50	0.42
2:B:270:ILE:O	2:B:314:VAL:HG23	2.20	0.42
2:B:367:GLN:O	2:B:369:THR:N	2.53	0.42
1:A:15:GLY:O	1:A:16:MET:HG2	2.20	0.42
1:A:28:GLU:HG3	1:A:135:ILE:CD1	2.50	0.42
1:A:80:LEU:O	1:A:84:THR:N	2.53	0.42
1:A:107:THR:HG22	1:A:108:VAL:N	2.34	0.42
1:A:368:LEU:O	1:A:372:VAL:HG23	2.19	0.42
2:B:5:ILE:HG22	2:B:6:GLU:N	2.30	0.42
2:B:81:ASN:HB3	2:B:154:LYS:HG2	2.01	0.42
2:B:86:ASP:CB	2:B:89:GLU:HB3	2.49	0.42
1:A:433:PRO:HG2	2:B:255:ASN:CG	2.41	0.42
2:B:79:GLU:OE1	2:B:79:GLU:HA	2.20	0.42
2:B:175:ASN:ND2	2:B:201:LYS:HZ3	2.18	0.42
2:B:254:VAL:CG2	2:B:288:ALA:O	2.68	0.42
2:B:367:GLN:C	2:B:369:THR:N	2.71	0.42
1:A:545:ASN:OD1	1:A:546:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ALA:HA	2:B:101:LYS:HE3	2.02	0.41
2:B:391:LEU:HA	2:B:392:PRO:HD3	1.96	0.41
1:A:27:THR:HG1	1:A:29:GLU:HB3	1.85	0.41
1:A:224:GLU:N	1:A:225:PRO:HD3	2.35	0.41
1:A:252:TRP:CZ3	1:A:260:LEU:CD2	3.03	0.41
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	0.41
1:A:508:ALA:C	1:A:510:PRO:CD	2.85	0.41
2:B:50:ILE:HG21	2:B:145:GLN:HG3	2.01	0.41
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.56	0.41
2:B:64:LYS:CE	2:B:71:TRP:NE1	2.82	0.41
2:B:149:LEU:HD23	2:B:149:LEU:HA	1.82	0.41
2:B:171:PHE:HA	2:B:174:GLN:CG	2.49	0.41
2:B:342:TYR:HA	2:B:349:LEU:HG	2.01	0.41
1:A:180:ILE:O	1:A:180:ILE:HG22	2.19	0.41
1:A:273:GLY:H	1:A:338:THR:HG21	1.85	0.41
1:A:276:VAL:HG21	1:A:353:LYS:HZ2	1.83	0.41
1:A:282:LEU:HD11	1:A:294:PRO:O	2.20	0.41
2:B:29:GLU:HG3	2:B:30:LYS:N	2.36	0.41
2:B:44:GLU:O	2:B:46:LYS:N	2.53	0.41
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.50	0.41
1:A:62:ALA:HB1	1:A:71:TRP:CE3	2.55	0.41
1:A:149:LEU:HD11	1:A:159:ILE:HG22	2.02	0.41
1:A:515:SER:CB	1:A:518:VAL:HG23	2.51	0.41
1:A:550:LYS:C	1:A:552:VAL:N	2.73	0.41
2:B:84:THR:CG2	2:B:84:THR:O	2.68	0.41
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.21	0.41
2:B:330:GLN:HB2	2:B:330:GLN:HE21	1.72	0.41
1:A:496:VAL:HG22	1:A:497:THR:N	2.35	0.41
2:B:54:ASN:ND2	2:B:145:GLN:OE1	2.54	0.41
2:B:235:HIS:HB2	2:B:238:LYS:CB	2.51	0.41
2:B:241:VAL:HG12	2:B:351:THR:O	2.20	0.41
2:B:270:ILE:HG23	2:B:271:TYR:HD1	1.84	0.41
3:T:716:DA:C2'	3:T:717:DC:O4'	2.68	0.41
1:A:188:TYR:CD1	1:A:188:TYR:O	2.71	0.41
1:A:486:LEU:HA	1:A:489:SER:OG	2.21	0.41
1:A:515:SER:HB3	1:A:518:VAL:HG23	2.01	0.41
2:B:201:LYS:HA	2:B:204:GLU:HG3	2.03	0.41
2:B:279:LEU:HA	2:B:282:LEU:CD1	2.49	0.41
1:A:43:LYS:HD3	1:A:43:LYS:C	2.41	0.41
1:A:183:TYR:O	1:A:184:MET:CB	2.69	0.41
1:A:439:THR:CG2	2:B:289:LEU:HG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG22	1:A:443:ASP:N	2.36	0.41
1:A:484:LEU:HA	1:A:487:GLN:CG	2.51	0.41
1:A:522:ILE:HG13	1:A:522:ILE:H	1.65	0.41
2:B:34:LEU:HD12	2:B:132:ILE:CD1	2.51	0.41
2:B:38:CYS:HA	2:B:41:MET:HB2	2.01	0.41
2:B:109:LEU:CD1	2:B:216:THR:HG21	2.51	0.41
2:B:365:VAL:HG23	2:B:366:LYS:N	2.36	0.41
1:A:195:ILE:O	1:A:196:GLY:C	2.58	0.41
1:A:226:PRO:HG2	1:A:226:PRO:O	2.21	0.41
1:A:398:TRP:HH2	1:A:409:THR:CG2	2.34	0.41
1:A:400:THR:HG22	1:A:401:TRP:N	2.35	0.41
1:A:452:LEU:HB3	1:A:453:GLY:H	1.70	0.41
2:B:10:VAL:HG12	2:B:11:LYS:N	2.36	0.41
2:B:98:ALA:CA	2:B:101:LYS:HE3	2.51	0.41
2:B:135:ILE:HG13	2:B:135:ILE:O	2.21	0.41
2:B:165:THR:O	2:B:168:LEU:HB2	2.21	0.41
2:B:204:GLU:C	2:B:206:ARG:N	2.74	0.41
2:B:241:VAL:CG1	2:B:351:THR:O	2.69	0.41
2:B:408:ALA:O	2:B:410:TRP:N	2.54	0.41
3:T:707:DG:H2'	3:T:708:DG:C8	2.56	0.41
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.51	0.41
1:A:399:GLU:HA	1:A:402:TRP:HE1	1.86	0.41
1:A:402:TRP:C	1:A:404:GLU:N	2.75	0.41
1:A:427:TYR:HE1	1:A:522:ILE:HG23	1.86	0.41
2:B:76:ASP:HA	2:B:411:ILE:HD12	2.01	0.41
2:B:314:VAL:HG22	2:B:315:HIS:N	2.35	0.41
2:B:406:TRP:CE2	2:B:408:ALA:HB3	2.56	0.41
3:T:723:DC:H2'	3:T:724:DT:C6	2.56	0.41
1:A:63:ILE:HG22	1:A:64:LYS:N	2.36	0.40
1:A:74:LEU:HD13	3:T:705:DT:N3	2.36	0.40
1:A:97:PRO:HA	1:A:100:LEU:HD12	2.03	0.40
1:A:484:LEU:HA	1:A:487:GLN:HG2	2.03	0.40
1:A:188:TYR:C	1:A:188:TYR:HD1	2.20	0.40
1:A:326:ILE:O	1:A:341:ILE:HG23	2.21	0.40
2:B:205:LEU:O	2:B:209:LEU:HG	2.21	0.40
2:B:312:GLU:HA	2:B:313:PRO:HD2	1.90	0.40
1:A:87:PHE:H	1:A:87:PHE:HD1	1.69	0.40
1:A:88:TRP:CZ2	2:B:57:ASN:ND2	2.90	0.40
1:A:111:VAL:HG11	1:A:214:LEU:HD22	2.01	0.40
1:A:135:ILE:HG23	1:A:136:ASN:N	2.36	0.40
1:A:262:GLY:O	1:A:265:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TRP:CH2	1:A:368:LEU:HB2	2.56	0.40
2:B:172:LYS:O	2:B:172:LYS:HG2	2.21	0.40
2:B:389:PHE:CD1	2:B:389:PHE:N	2.88	0.40
1:A:46:LYS:HD2	1:A:116:PHE:HB3	2.04	0.40
1:A:127:TYR:O	1:A:129:ALA:N	2.53	0.40
1:A:151:GLN:HE21	1:A:151:GLN:HB2	1.52	0.40
1:A:275:LYS:HE3	1:A:305:GLU:OE1	2.21	0.40
1:A:426:TRP:O	1:A:427:TYR:HB3	2.20	0.40
2:B:122:GLU:HA	2:B:125:ARG:HG3	2.02	0.40
2:B:215:THR:HG22	2:B:216:THR:N	2.37	0.40
2:B:305:GLU:O	2:B:307:ARG:N	2.55	0.40
2:B:362:THR:CB	2:B:366:LYS:HD3	2.49	0.40
3:T:715:DA:C6	3:T:716:DA:C6	3.09	0.40
3:T:724:DT:C2'	3:T:725:DG:O5'	2.70	0.40
1:A:56:TYR:O	1:A:143:ARG:NH2	2.55	0.40
1:A:88:TRP:HH2	2:B:22:LYS:HA	1.85	0.40
1:A:479:LEU:C	1:A:481:ALA:N	2.74	0.40
2:B:173:LYS:C	2:B:176:PRO:HD3	2.42	0.40
2:B:281:LYS:O	2:B:283:LEU:N	2.54	0.40
4:P:818:DC:H2''	4:P:819:DG:H5'	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	552/558 (99%)	438 (79%)	93 (17%)	21 (4%)	<b>3</b>   <b>19</b>
2	B	409/437 (94%)	312 (76%)	76 (19%)	21 (5%)	<b>2</b>   <b>13</b>
All	All	961/995 (97%)	750 (78%)	169 (18%)	42 (4%)	<b>2</b>   <b>16</b>

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	45	GLY
2	B	86	ASP
1	A	268	SER
1	A	412	PRO
2	B	113	ASP
2	B	282	LEU
2	B	409	THR
1	A	25	PRO
1	A	116	PHE
1	A	128	THR
1	A	476	LYS
1	A	541	GLY
1	A	553	SER
1	A	114	ALA
1	A	125	ARG
1	A	448	ARG
2	B	25	PRO
2	B	98	ALA
2	B	116	PHE
2	B	126	LYS
2	B	157	PRO
2	B	184	MET
2	B	286	THR
2	B	306	ASN
2	B	421	PRO
1	A	157	PRO
1	A	224	GLU
1	A	485	ALA
2	B	119	PRO
2	B	294	PRO
1	A	196	GLY
1	A	243	PRO
1	A	509	GLN
2	B	93	GLY
2	B	112	GLY
1	A	133	PRO
2	B	175	ASN
1	A	176	PRO
1	A	544	GLY
2	B	316	GLY
1	A	433	PRO
2	B	148	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/498 (99%)	454 (92%)	41 (8%)	11	36
2	B	375/397 (94%)	347 (92%)	28 (8%)	13	39
All	All	870/895 (97%)	801 (92%)	69 (8%)	12	37

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	24	TRP
1	A	25	PRO
1	A	41	MET
1	A	53	GLU
1	A	56	TYR
1	A	58	THR
1	A	61	PHE
1	A	69	THR
1	A	79	GLU
1	A	87	PHE
1	A	121	ASP
1	A	136	ASN
1	A	151	GLN
1	A	157	PRO
1	A	188	TYR
1	A	191	SER
1	A	192	ASP
1	A	199	ARG
1	A	218	ASP
1	A	220	LYS
1	A	224	GLU
1	A	226	PRO
1	A	236	PRO
1	A	241	VAL
1	A	244	ILE
1	A	249	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	250	ASP
1	A	256	ASP
1	A	276	VAL
1	A	296	THR
1	A	329	ILE
1	A	340	GLN
1	A	354	TYR
1	A	399	GLU
1	A	423	VAL
1	A	426	TRP
1	A	427	TYR
1	A	511	ASP
1	A	536	VAL
1	A	545	ASN
2	B	17	ASP
2	B	26	LEU
2	B	28	GLU
2	B	34	LEU
2	B	40	GLU
2	B	60	VAL
2	B	63	ILE
2	B	69	THR
2	B	119	PRO
2	B	120	LEU
2	B	128	THR
2	B	139	THR
2	B	175	ASN
2	B	184	MET
2	B	214	LEU
2	B	233	GLU
2	B	250	ASP
2	B	269	GLN
2	B	295	LEU
2	B	329	ILE
2	B	330	GLN
2	B	340	GLN
2	B	357	MET
2	B	361	HIS
2	B	375	ILE
2	B	388	LYS
2	B	392	PRO
2	B	393	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	136	ASN
1	A	221	HIS
1	A	242	GLN
1	A	340	GLN
1	A	367	GLN
1	A	407	GLN
1	A	447	ASN
1	A	464	GLN
1	A	471	ASN
1	A	487	GLN
1	A	494	ASN
1	A	509	GLN
2	B	85	GLN
2	B	91	GLN
2	B	147	ASN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	208	HIS
2	B	269	GLN
2	B	315	HIS
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	348	ASN
2	B	361	HIS
2	B	367	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	DDG	P	823	-	17,23,24	1.28	2 (11%)	15,33,36	0.69	0
4	MRG	P	817	4,3	18,24,29	1.24	3 (16%)	19,35,42	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DDG	P	823	-	-	0/3/18/19	0/3/3/3
4	MRG	P	817	4,3	-	0/3/21/27	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	823	DDG	C5-C6	-3.48	1.40	1.47
4	P	817	MRG	C5-C6	-3.22	1.40	1.47
4	P	817	MRG	C8-N7	-2.49	1.30	1.35
4	P	823	DDG	C8-N7	-2.41	1.30	1.35
4	P	817	MRG	C5-C4	-2.09	1.37	1.43

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	823	DDG	2	0
4	P	817	MRG	1	0

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
6	SO4	A	560	-	4,4,4	0.38	0	6,6,6	0.29	0
5	DTP	A	700	7	26,32,32	2.74	10 (38%)	30,50,50	2.04	5 (16%)
6	SO4	A	559	-	4,4,4	0.37	0	6,6,6	0.08	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
5	DTP	A	700	7	-	4/18/34/34	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	DTP	C2-N3	5.83	1.41	1.32
5	A	700	DTP	PA-O1A	4.81	1.68	1.50
5	A	700	DTP	PG-O1G	4.78	1.66	1.50
5	A	700	DTP	PB-O1B	4.67	1.67	1.50
5	A	700	DTP	C4-N3	-4.41	1.29	1.35
5	A	700	DTP	PG-O2G	3.88	1.69	1.54
5	A	700	DTP	PG-O3G	3.48	1.68	1.54
5	A	700	DTP	PB-O2B	2.74	1.68	1.55
5	A	700	DTP	O4'-C4'	-2.73	1.38	1.45
5	A	700	DTP	PA-O2A	2.65	1.67	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	DTP	PB-O3B-PG	-6.44	110.74	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	DTP	PA-O3A-PB	-5.71	113.23	132.83
5	A	700	DTP	N3-C2-N1	-3.48	123.24	128.68
5	A	700	DTP	C2'-C1'-N9	-3.28	106.69	114.27
5	A	700	DTP	O3G-PG-O3B	2.64	113.49	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

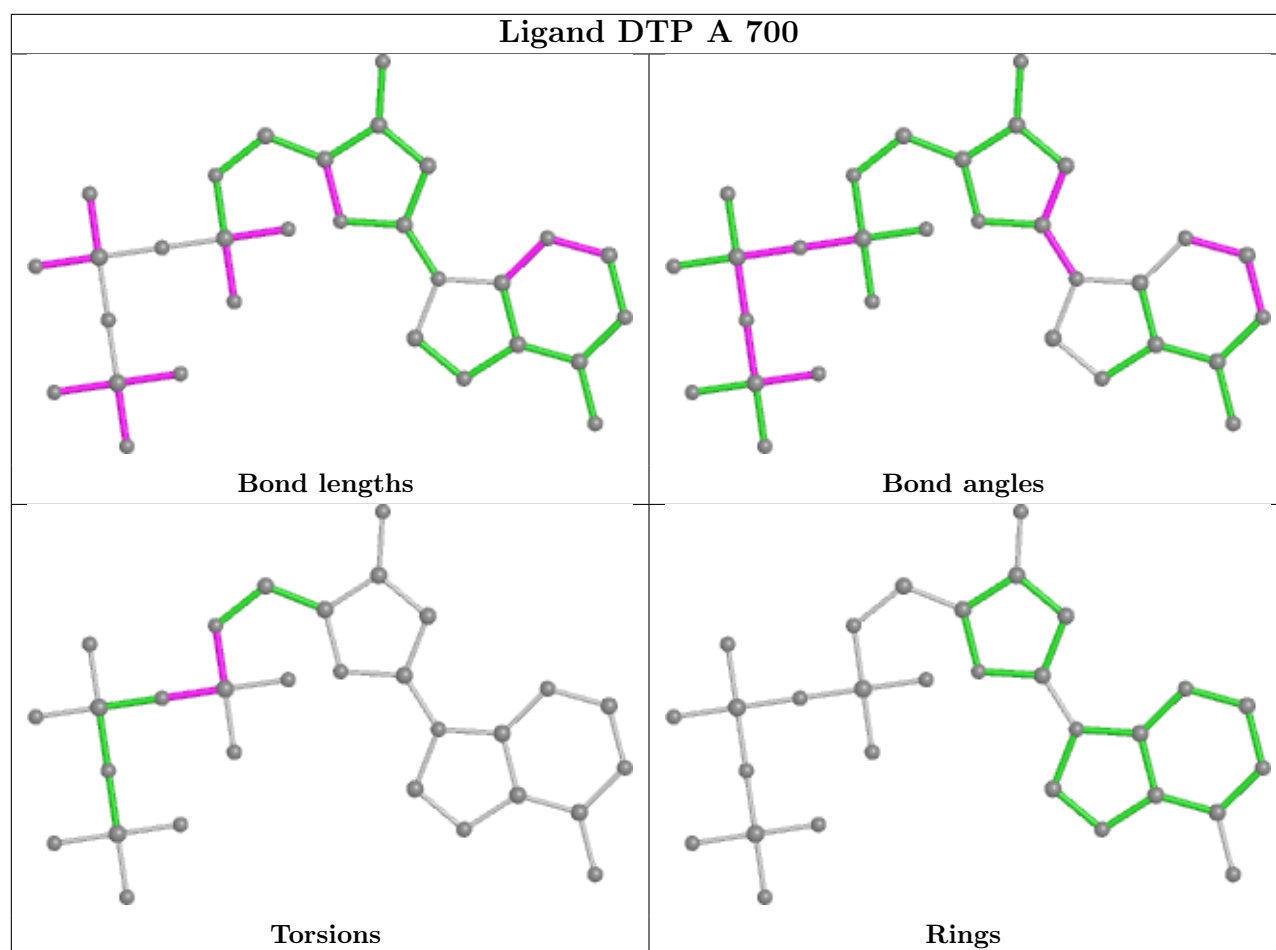
Mol	Chain	Res	Type	Atoms
5	A	700	DTP	C5'-O5'-PA-O1A
5	A	700	DTP	PB-O3A-PA-O5'
5	A	700	DTP	C5'-O5'-PA-O3A
5	A	700	DTP	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	560	SO4	2	0
5	A	700	DTP	4	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 than 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.



## 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	A	554/558 (99%)	0.10	15 (2%) 54 52	33, 97, 157, 160	0
2	B	413/437 (94%)	0.53	47 (11%) 5 4	62, 141, 160, 160	0
3	T	24/27 (88%)	0.41	1 (4%) 36 34	71, 142, 160, 160	0
4	P	18/21 (85%)	0.66	3 (16%) 1 1	66, 140, 160, 160	0
All	All	1009/1043 (96%)	0.29	66 (6%) 18 18	33, 117, 160, 160	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	295	LEU	5.9
2	B	189	VAL	5.2
2	B	359	GLY	4.6
2	B	303	LEU	4.3
1	A	464	GLN	4.2
2	B	286	THR	4.2
2	B	358	ARG	4.0
2	B	239	TRP	3.9
2	B	300	GLU	3.8
1	A	457	TYR	3.7
2	B	94	ILE	3.7
1	A	434	ILE	3.7
2	B	195	ILE	3.6
2	B	3	SER	3.6
2	B	240	THR	3.4
1	A	440	PHE	3.4
2	B	292	VAL	3.3
2	B	107	THR	3.3
2	B	299	ALA	3.3
2	B	314	VAL	3.2
2	B	361	HIS	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	246	LEU	3.2
1	A	465	LYS	3.1
2	B	4	PRO	3.0
2	B	354	TYR	3.0
2	B	90	VAL	3.0
1	A	463	ARG	2.8
2	B	191	SER	2.8
4	P	809	DC	2.8
2	B	95	PRO	2.8
2	B	360	ALA	2.8
2	B	261	VAL	2.8
1	A	448	ARG	2.7
4	P	808	DC	2.7
2	B	89	GLU	2.7
4	P	807	DC	2.7
1	A	62	ALA	2.6
2	B	180	ILE	2.6
2	B	88	TRP	2.6
2	B	371	ALA	2.5
2	B	69	THR	2.5
2	B	293	ILE	2.5
2	B	190	GLY	2.5
2	B	294	PRO	2.5
2	B	182	GLN	2.4
2	B	279	LEU	2.4
2	B	188	TYR	2.4
2	B	257	ILE	2.4
2	B	255	ASN	2.3
2	B	289	LEU	2.3
2	B	301	LEU	2.3
1	A	439	THR	2.3
1	A	449	GLU	2.3
2	B	378	GLU	2.2
2	B	247	PRO	2.2
1	A	438	GLU	2.2
1	A	466	VAL	2.2
3	T	724	DT	2.2
2	B	197	GLN	2.2
1	A	491	LEU	2.1
1	A	492	GLU	2.1
1	A	458	VAL	2.1
2	B	310	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	236	PRO	2.1
2	B	248	GLU	2.1
2	B	244	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
4	MRG	P	817	22/27	0.96	0.14	83,94,104,106	0
4	DDG	P	823	21/22	0.96	0.22	58,68,81,88	0

## 6.3 Carbohydrates [i](#)

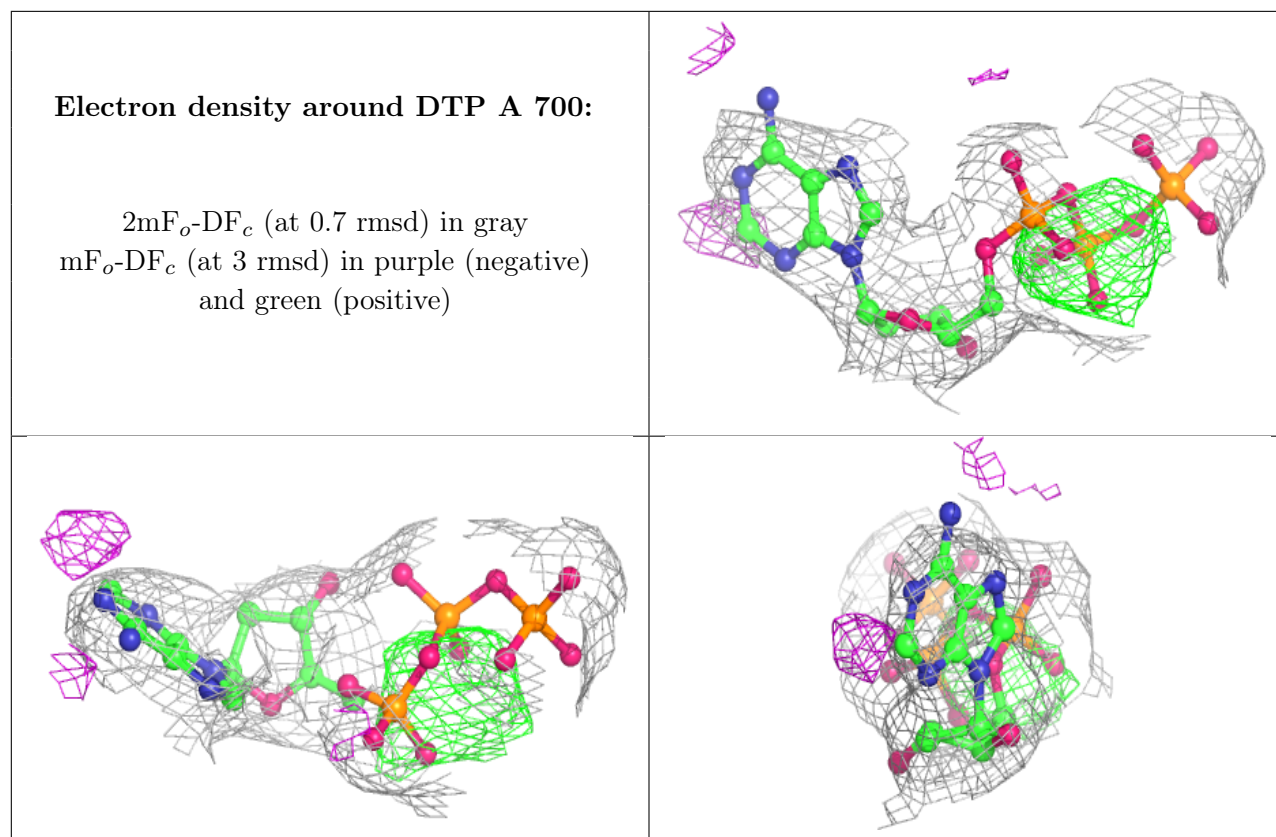
There are no monosaccharides in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
6	SO4	A	560	5/5	0.85	0.57	114,116,120,120	0
7	MG	A	601	1/1	0.87	0.12	104,104,104,104	0
6	SO4	A	559	5/5	0.94	0.24	132,133,137,138	0
5	DTP	A	700	30/30	0.97	0.24	58,71,82,85	0
7	MG	A	600	1/1	0.99	0.26	19,19,19,19	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.