



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 09:39 PM EDT

PDB ID : 1T05  
Title : HIV-1 reverse transcriptase crosslinked to template-primer with tenofovir-dip  
hosphate bound as the incoming nucleotide substrate  
Authors : Tuske, S.; Sarafianos, S.G.; Ding, J.; Arnold, E.  
Deposited on : 2004-04-07  
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  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

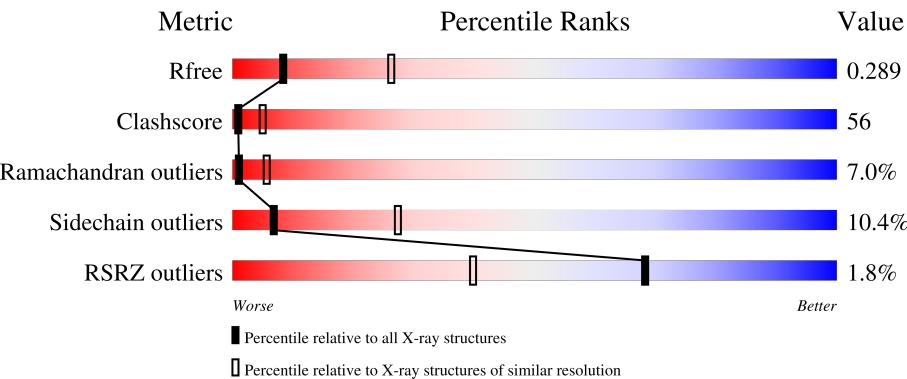
# 1 Overall quality at a glance i

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	T	27	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>11%78%11%</div></div>
2	P	21	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>10%57%29%5%</div></div>
3	A	558	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>%28%59%11%..</div></div>
4	B	437	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>3%24%57%13%• 5%</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
7	GOL	A	824	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8898 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 oligonucleotide template.

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

- Molecule 2 is a DNA chain called oligonucleotide primer.

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

- Molecule 3 is a protein called POL polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	554	Total	C	N	O	S	0	0	0
			4506	2917	749	832	8			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called POL polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	414	Total	C	N	O	S	0	0	0
			3415	2221	567	621	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P04585
B	430	GLY	-	cloning artifact	UNP P04585

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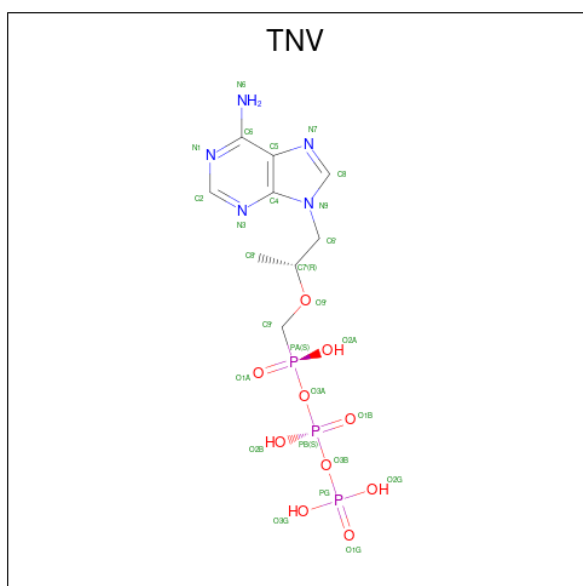
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Chain	Residue	Modelled	Actual	Comment	Reference
B	431	GLY	-	cloning artifact	UNP P04585
B	432	HIS	-	expression tag	UNP P04585
B	433	HIS	-	expression tag	UNP P04585
B	434	HIS	-	expression tag	UNP P04585
B	435	HIS	-	expression tag	UNP P04585
B	436	HIS	-	expression tag	UNP P04585
B	437	HIS	-	expression tag	UNP P04585

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is [2-(6-AMINO-9H-PURIN-9-YL)-1-METHYLETHOXY]METHYL-TRIPHOSPHATE (three-letter code: TNV) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>5</sub>O<sub>10</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 27 9 5 10 3	0	0

- Molecule 7 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
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

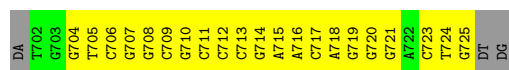
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	T	2	Total	O	0	0
			2	2		
8	P	3	Total	O	0	0
			3	3		
8	A	10	Total	O	0	0
			10	10		
8	B	6	Total	O	0	0
			6	6		

### 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: oligonucleotide template

Chain T: 



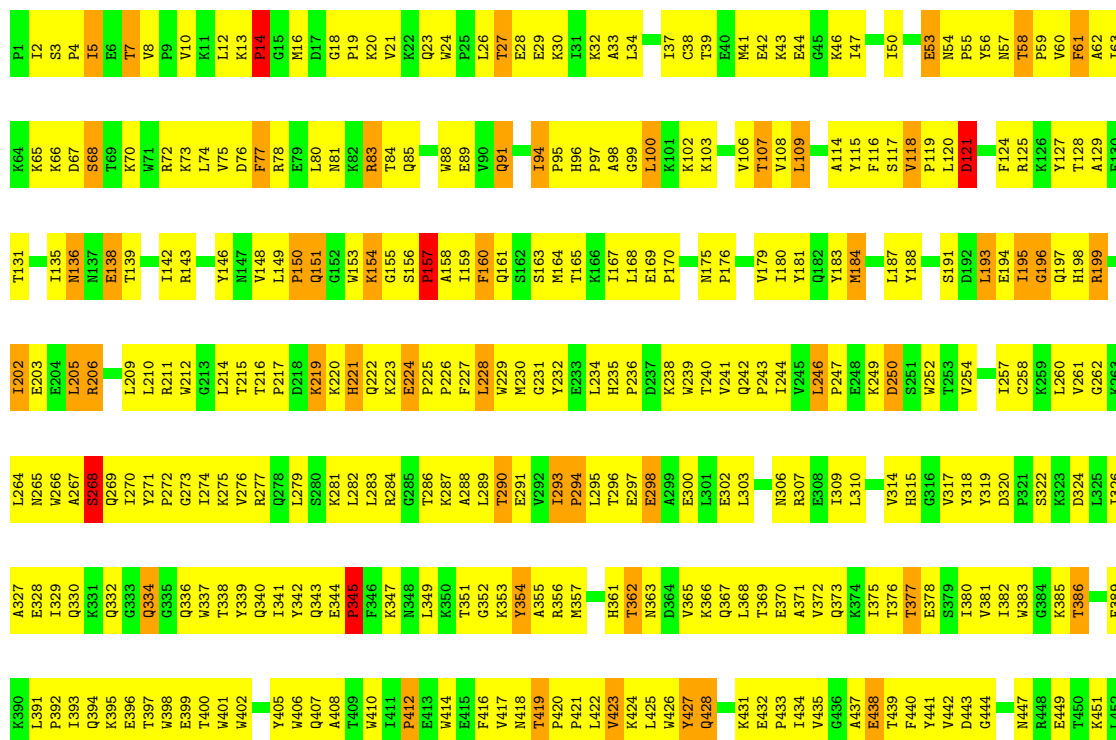
- Molecule 2: oligonucleotide primer

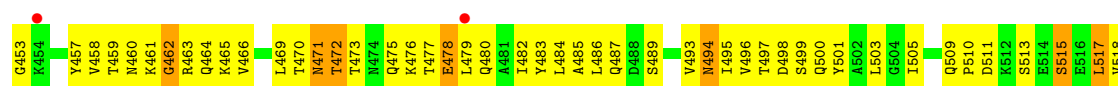
Chain P: 



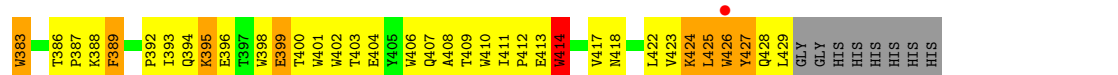
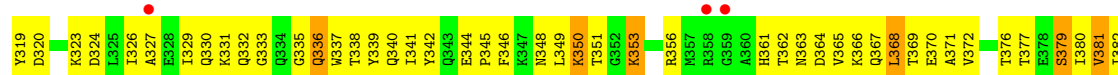
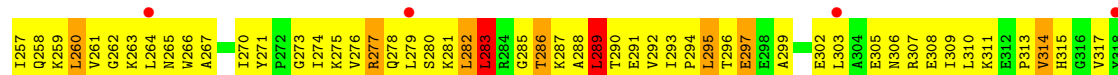
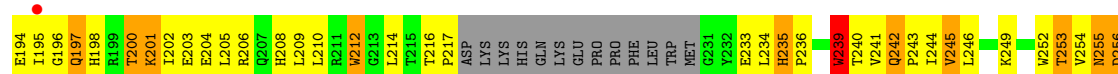
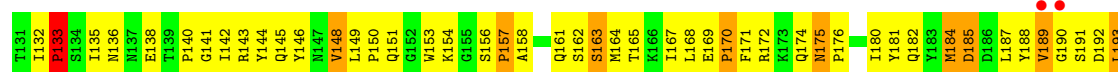
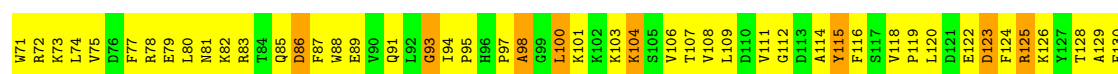
- Molecule 3: POL polypeptide

Chain A: 





### • Molecule 4: POL polypeptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.57Å 171.57Å 156.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 39.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-3.00) 91.3 (39.85-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.253 , 0.292 0.255 , 0.289	Depositor DCC
$R_{free}$ test set	1926 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 66.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: GOL, TNV, DDG, MRG, 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	T	0.59	0/555	1.13	2/856 (0.2%)
2	P	0.59	0/400	1.24	5/612 (0.8%)
3	A	0.55	1/4624 (0.0%)	0.80	3/6282 (0.0%)
4	B	0.48	0/3512	0.78	4/4774 (0.1%)
All	All	0.53	1/9091 (0.0%)	0.84	14/12524 (0.1%)

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
3	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	478	GLU	CD-OE2	7.31	1.33	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3	SER	C-N-CD	-20.07	76.44	120.60
4	B	295	LEU	N-CA-C	6.77	129.27	111.00
1	T	718	DA	N9-C1'-C2'	6.35	124.66	112.60
3	A	100	LEU	CA-CB-CG	6.22	129.60	115.30
2	P	815	DG	N9-C1'-C2'	6.15	124.28	112.60
4	B	4	PRO	N-CA-C	5.76	127.07	112.10
3	A	219	LYS	N-CA-C	-5.65	95.75	111.00
3	A	199	ARG	NE-CZ-NH2	5.65	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	719	DG	N9-C1'-C2'	5.57	123.18	112.60
2	P	809	DC	O4'-C1'-N1	5.57	111.89	108.00
2	P	813	DT	N1-C1'-C2'	5.25	122.57	112.60
2	P	814	DC	O4'-C1'-N1	5.24	111.67	108.00
4	B	3	SER	C-N-CA	5.18	143.77	122.00
2	P	814	DC	N1-C1'-C2'	5.14	122.37	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	160	PHE	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	T	494	0	269	24	0
2	P	403	0	224	30	0
3	A	4506	0	4567	517	0
4	B	3415	0	3448	443	0
5	A	2	0	0	0	0
6	A	27	0	12	7	0
7	A	18	0	21	5	0
7	B	12	0	14	1	0
8	A	10	0	0	1	0
8	B	6	0	0	1	0
8	P	3	0	0	0	0
8	T	2	0	0	0	0
All	All	8898	0	8555	981	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 56.

All (981) 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)
3:A:498:ASP:HB2	3:A:538:ALA:HB2	1.31	1.08
3:A:103:LYS:H	7:A:824:GOL:H32	1.13	1.08
3:A:205:LEU:HD22	3:A:209:LEU:HD11	1.35	1.07
3:A:408:ALA:HB1	4:B:364:ASP:HB3	1.37	1.07
3:A:72:ARG:HH12	6:A:823:TNV:H8'3	1.12	1.07
4:B:140:PRO:HA	8:B:441:HOH:O	1.54	1.06
4:B:278:GLN:HB3	4:B:299:ALA:HA	1.40	1.03
3:A:517:LEU:HD22	3:A:521:ILE:HD11	1.43	1.00
4:B:194:GLU:H	4:B:197:GLN:HE22	1.07	0.98
4:B:44:GLU:O	4:B:46:LYS:HD2	1.65	0.94
4:B:332:GLN:HB2	4:B:336:GLN:HB3	1.48	0.94
4:B:122:GLU:HA	4:B:125:ARG:HD2	1.50	0.93
4:B:167:ILE:HG23	4:B:212:TRP:CE3	2.04	0.93
3:A:484:LEU:HA	3:A:487:GLN:HE21	1.30	0.93
3:A:324:ASP:O	3:A:343:GLN:HG2	1.69	0.93
4:B:104:LYS:HB2	4:B:192:ASP:HA	1.51	0.92
3:A:254:VAL:HG13	3:A:283:LEU:HD22	1.51	0.92
3:A:419:THR:H	3:A:422:LEU:HD21	1.33	0.92
3:A:493:VAL:HG12	3:A:494:ASN:H	1.34	0.92
3:A:222:GLN:N	3:A:224:GLU:HG3	1.84	0.91
3:A:317:VAL:HG22	3:A:318:TYR:H	1.32	0.91
3:A:221:HIS:HE1	3:A:228:LEU:HB2	1.36	0.91
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.05	0.91
3:A:484:LEU:HD23	3:A:487:GLN:NE2	1.86	0.90
3:A:439:THR:HG21	4:B:289:LEU:HD13	1.50	0.90
3:A:47:ILE:HG22	3:A:146:TYR:HA	1.54	0.90
3:A:293:ILE:HG13	3:A:294:PRO:HD2	1.53	0.88
4:B:326:ILE:HG22	4:B:327:ALA:H	1.36	0.88
4:B:326:ILE:HG22	4:B:327:ALA:N	1.88	0.88
1:T:705:DT:H3	6:A:823:TNV:HN61	1.22	0.87
3:A:135:ILE:H	3:A:135:ILE:HD12	1.39	0.87
3:A:199:ARG:HH21	3:A:223:LYS:HB2	1.40	0.87
4:B:246:LEU:HD22	4:B:260:LEU:HD11	1.58	0.85
3:A:72:ARG:HH12	6:A:823:TNV:C8'	1.87	0.85
3:A:156:SER:HB2	3:A:157:PRO:HD3	1.59	0.85
3:A:103:LYS:H	7:A:824:GOL:C3	1.89	0.85
3:A:222:GLN:H	3:A:224:GLU:HG3	1.38	0.83
4:B:194:GLU:HG3	4:B:196:GLY:H	1.43	0.83
3:A:72:ARG:NH1	6:A:823:TNV:H8'3	1.94	0.83
3:A:500:GLN:HG2	4:B:422:LEU:HD22	1.59	0.83
4:B:252:TRP:HB3	4:B:257:ILE:HD11	1.59	0.82
3:A:205:LEU:HD22	3:A:209:LEU:CD1	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:296:THR:HB	4:B:299:ALA:HB3	1.60	0.82
4:B:194:GLU:H	4:B:197:GLN:NE2	1.78	0.82
3:A:59:PRO:HG2	3:A:76:ASP:HB3	1.59	0.81
4:B:118:VAL:HB	4:B:149:LEU:HD12	1.62	0.81
4:B:175:ASN:HD21	4:B:201:LYS:HE2	1.47	0.80
4:B:389:PHE:HD1	4:B:389:PHE:H	1.30	0.80
3:A:95:PRO:HA	4:B:136:ASN:O	1.80	0.79
3:A:417:VAL:O	3:A:417:VAL:HG13	1.81	0.79
4:B:365:VAL:O	4:B:369:THR:HG23	1.81	0.79
3:A:72:ARG:HG2	3:A:74:LEU:HD21	1.65	0.79
4:B:326:ILE:CG2	4:B:327:ALA:H	1.96	0.79
3:A:397:THR:HG21	3:A:424:LYS:HA	1.63	0.79
3:A:498:ASP:CB	3:A:538:ALA:HB2	2.12	0.79
4:B:276:VAL:HG22	4:B:280:SER:HB3	1.63	0.79
3:A:362:THR:HG22	3:A:366:LYS:HD3	1.64	0.79
4:B:62:ALA:HB1	4:B:71:TRP:HE3	1.48	0.79
3:A:157:PRO:O	3:A:161:GLN:HG3	1.83	0.78
4:B:401:TRP:O	4:B:404:GLU:HB2	1.83	0.78
3:A:441:TYR:HB2	3:A:458:VAL:HG12	1.66	0.78
3:A:246:LEU:HD21	3:A:264:LEU:HD11	1.65	0.78
3:A:199:ARG:NH2	3:A:223:LYS:HB2	1.99	0.78
4:B:266:TRP:HB3	4:B:426:TRP:CZ2	2.19	0.77
4:B:79:GLU:O	4:B:83:ARG:HG3	1.84	0.77
4:B:335:GLY:HA3	4:B:356:ARG:HB2	1.66	0.77
1:T:714:DG:H4'	3:A:286:THR:HG21	1.66	0.76
3:A:67:ASP:O	3:A:68:SER:HB2	1.85	0.76
4:B:372:VAL:HG13	4:B:389:PHE:CE2	2.21	0.76
4:B:61:PHE:HE2	4:B:63:ILE:HD11	1.50	0.76
3:A:205:LEU:CD2	3:A:209:LEU:HD11	2.15	0.76
3:A:50:ILE:HD12	3:A:54:ASN:HB3	1.67	0.76
3:A:220:LYS:O	3:A:220:LYS:HG3	1.86	0.76
4:B:287:LYS:HE2	4:B:287:LYS:HA	1.68	0.76
4:B:314:VAL:HG22	4:B:315:HIS:H	1.50	0.76
4:B:114:ALA:CB	4:B:214:LEU:HD22	2.16	0.75
3:A:478:GLU:HG2	3:A:499:SER:HB3	1.68	0.75
4:B:120:LEU:HD12	4:B:149:LEU:HD23	1.67	0.75
4:B:278:GLN:HB3	4:B:299:ALA:CA	2.16	0.75
4:B:240:THR:HG22	4:B:241:VAL:H	1.51	0.75
3:A:408:ALA:HA	4:B:364:ASP:OD1	1.85	0.75
2:P:818:DC:H2''	2:P:819:DG:H5'	1.69	0.74
4:B:239:TRP:HA	4:B:239:TRP:CE3	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:149:LEU:CD2	3:A:156:SER:HA	2.17	0.74
4:B:115:TYR:CD1	4:B:156:SER:HB3	2.22	0.74
3:A:484:LEU:HA	3:A:487:GLN:NE2	2.01	0.74
4:B:171:PHE:HA	4:B:174:GLN:HG3	1.70	0.74
4:B:180:ILE:HD11	4:B:205:LEU:HD11	1.67	0.74
3:A:537:PRO:HG2	4:B:262:GLY:HA2	1.68	0.74
4:B:406:TRP:O	4:B:407:GLN:HG3	1.87	0.74
3:A:544:GLY:O	3:A:548:VAL:HG23	1.88	0.74
3:A:3:SER:OG	3:A:5:ILE:HG22	1.86	0.73
3:A:118:VAL:HB	3:A:149:LEU:CD1	2.18	0.73
4:B:262:GLY:O	4:B:265:ASN:HB3	1.88	0.73
3:A:221:HIS:CE1	3:A:228:LEU:HB2	2.23	0.73
4:B:406:TRP:CH2	4:B:412:PRO:HD2	2.23	0.73
4:B:266:TRP:HB3	4:B:426:TRP:HZ2	1.50	0.73
4:B:329:ILE:HG22	4:B:330:GLN:N	2.04	0.73
3:A:103:LYS:N	7:A:824:GOL:H32	1.97	0.73
4:B:115:TYR:HD1	4:B:156:SER:HB3	1.54	0.72
4:B:388:LYS:HD2	4:B:388:LYS:O	1.88	0.72
3:A:509:GLN:N	3:A:510:PRO:HD3	2.04	0.72
3:A:478:GLU:O	3:A:482:ILE:HG13	1.88	0.72
3:A:470:THR:HG22	3:A:471:ASN:OD1	1.89	0.72
3:A:76:ASP:O	3:A:78:ARG:N	2.21	0.72
3:A:221:HIS:HB3	3:A:224:GLU:HB2	1.72	0.72
3:A:337:TRP:CZ3	3:A:368:LEU:HD23	2.24	0.72
3:A:116:PHE:C	3:A:148:VAL:HG21	2.09	0.72
3:A:441:TYR:HB3	3:A:548:VAL:HG21	1.72	0.71
3:A:206:ARG:HG2	3:A:216:THR:OG1	1.89	0.71
3:A:317:VAL:HG22	3:A:318:TYR:N	2.04	0.71
3:A:529:GLU:O	3:A:530:LYS:HG3	1.91	0.71
3:A:89:GLU:OE1	3:A:89:GLU:HA	1.90	0.71
3:A:242:GLN:HB3	3:A:243:PRO:HD2	1.72	0.71
3:A:293:ILE:HG13	3:A:294:PRO:CD	2.21	0.70
4:B:120:LEU:HB2	4:B:148:VAL:O	1.91	0.70
4:B:255:ASN:ND2	4:B:259:LYS:HE2	2.06	0.70
4:B:65:LYS:HB2	4:B:68:SER:HB3	1.73	0.70
3:A:3:SER:HB2	3:A:212:TRP:O	1.91	0.70
3:A:257:ILE:O	3:A:261:VAL:HG23	1.92	0.70
4:B:115:TYR:OH	4:B:157:PRO:HB3	1.90	0.70
4:B:44:GLU:HB2	4:B:46:LYS:HE3	1.73	0.70
3:A:221:HIS:CE1	3:A:228:LEU:H	2.09	0.70
4:B:329:ILE:HG22	4:B:330:GLN:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.73	0.70
3:A:97:PRO:HA	3:A:100:LEU:CD2	2.21	0.70
4:B:98:ALA:HA	4:B:101:LYS:HD3	1.72	0.70
3:A:406:TRP:CD1	3:A:407:GLN:HG3	2.26	0.70
4:B:406:TRP:HH2	4:B:412:PRO:HD2	1.55	0.70
3:A:451:LYS:HB3	3:A:471:ASN:HA	1.74	0.69
4:B:326:ILE:CG2	4:B:327:ALA:N	2.54	0.69
3:A:482:ILE:O	3:A:486:LEU:HG	1.92	0.69
4:B:372:VAL:HA	4:B:389:PHE:HE2	1.56	0.69
3:A:135:ILE:HD12	3:A:135:ILE:N	2.06	0.69
4:B:175:ASN:N	4:B:176:PRO:HD3	2.08	0.69
3:A:84:THR:HG22	3:A:85:GLN:N	2.08	0.69
3:A:59:PRO:HG2	3:A:76:ASP:CB	2.23	0.69
3:A:391:LEU:HB2	3:A:414:TRP:CE3	2.28	0.69
3:A:498:ASP:HB2	3:A:538:ALA:CB	2.17	0.69
4:B:24:TRP:HH2	4:B:61:PHE:CD1	2.10	0.69
4:B:379:SER:OG	4:B:387:PRO:HD3	1.93	0.69
3:A:2:ILE:HD11	3:A:46:LYS:HD2	1.75	0.69
4:B:61:PHE:CE2	4:B:63:ILE:HD11	2.27	0.68
3:A:91:GLN:CG	3:A:161:GLN:HE22	2.07	0.68
4:B:168:LEU:HD12	4:B:172:ARG:NH2	2.08	0.68
4:B:242:GLN:HE21	4:B:353:LYS:HE3	1.58	0.68
3:A:410:TRP:CH2	3:A:412:PRO:HA	2.29	0.68
4:B:167:ILE:HA	4:B:212:TRP:CZ3	2.29	0.68
3:A:417:VAL:HG22	3:A:419:THR:CG2	2.24	0.68
3:A:518:VAL:HA	3:A:521:ILE:HD12	1.75	0.68
4:B:255:ASN:HB3	4:B:289:LEU:HG	1.76	0.68
3:A:402:TRP:HH2	4:B:362:THR:HB	1.59	0.67
4:B:25:PRO:O	4:B:26:LEU:HD23	1.95	0.67
4:B:260:LEU:O	4:B:264:LEU:HD12	1.95	0.67
4:B:170:PRO:HB2	4:B:208:HIS:CE1	2.29	0.67
3:A:518:VAL:O	3:A:522:ILE:HG13	1.95	0.67
4:B:314:VAL:HG22	4:B:315:HIS:N	2.08	0.67
4:B:368:LEU:HD23	4:B:368:LEU:O	1.94	0.67
4:B:233:GLU:CD	4:B:233:GLU:H	1.97	0.67
3:A:394:GLN:HB2	3:A:397:THR:OG1	1.95	0.67
4:B:103:LYS:HG3	4:B:191:SER:O	1.95	0.67
3:A:453:GLY:O	3:A:469:LEU:N	2.27	0.67
3:A:91:GLN:HG3	3:A:161:GLN:HE22	1.60	0.67
4:B:114:ALA:HB1	4:B:214:LEU:HD22	1.77	0.67
4:B:254:VAL:HB	4:B:289:LEU:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:58:THR:HG22	3:A:59:PRO:HD2	1.77	0.66
3:A:164:MET:HG3	3:A:168:LEU:HD12	1.76	0.66
3:A:109:LEU:HD23	3:A:109:LEU:N	2.09	0.66
3:A:242:GLN:HB3	3:A:243:PRO:CD	2.25	0.66
4:B:78:ARG:O	4:B:82:LYS:HG3	1.95	0.66
4:B:254:VAL:O	4:B:258:GLN:HG3	1.96	0.66
4:B:277:ARG:HA	4:B:280:SER:OG	1.95	0.66
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.30	0.66
4:B:239:TRP:HA	4:B:239:TRP:HE3	1.61	0.66
3:A:13:LYS:HG2	3:A:84:THR:O	1.96	0.66
4:B:100:LEU:HD23	4:B:101:LYS:N	2.10	0.66
4:B:194:GLU:N	4:B:197:GLN:HE22	1.88	0.66
3:A:392:PRO:O	3:A:423:VAL:HG23	1.96	0.65
3:A:439:THR:CG2	4:B:289:LEU:HD13	2.24	0.65
3:A:517:LEU:O	3:A:520:GLN:HG2	1.96	0.65
4:B:50:ILE:HG21	4:B:145:GLN:HB2	1.76	0.65
3:A:149:LEU:HD23	3:A:156:SER:HA	1.78	0.65
3:A:391:LEU:C	3:A:417:VAL:HG12	2.16	0.65
4:B:120:LEU:HD21	4:B:124:PHE:HD2	1.60	0.65
3:A:97:PRO:HA	3:A:100:LEU:HD22	1.77	0.65
3:A:369:THR:O	3:A:373:GLN:HG3	1.96	0.65
4:B:85:GLN:HA	4:B:88:TRP:CE2	2.32	0.65
3:A:402:TRP:CH2	4:B:362:THR:HB	2.32	0.65
3:A:457:TYR:CE2	3:A:465:LYS:HB3	2.31	0.65
3:A:221:HIS:H	3:A:221:HIS:CD2	2.14	0.64
3:A:376:THR:HG23	3:A:386:THR:HG22	1.79	0.64
3:A:339:TYR:CZ	3:A:352:GLY:HA3	2.31	0.64
4:B:151:GLN:HB3	4:B:185:ASP:OD2	1.97	0.64
3:A:273:GLY:H	3:A:338:THR:HG21	1.62	0.64
3:A:427:TYR:HE1	3:A:522:ILE:HG23	1.63	0.64
4:B:126:LYS:HA	4:B:145:GLN:OE1	1.96	0.64
4:B:308:GLU:HA	4:B:311:LYS:HE2	1.78	0.64
4:B:243:PRO:O	4:B:244:ILE:HD13	1.98	0.64
3:A:344:GLU:HB2	3:A:347:LYS:HB2	1.79	0.64
4:B:72:ARG:HG3	4:B:72:ARG:HH11	1.62	0.64
4:B:244:ILE:HG23	4:B:426:TRP:HB3	1.80	0.64
3:A:347:LYS:HE2	3:A:347:LYS:HA	1.80	0.64
3:A:547:GLN:O	3:A:551:LEU:HG	1.96	0.64
4:B:85:GLN:HG3	4:B:86:ASP:N	2.12	0.64
4:B:320:ASP:OD2	4:B:323:LYS:HE2	1.97	0.64
3:A:376:THR:HG23	3:A:386:THR:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:114:ALA:HB2	4:B:214:LEU:HD22	1.80	0.63
3:A:135:ILE:H	3:A:135:ILE:CD1	2.10	0.63
3:A:303:LEU:HD21	3:A:307:ARG:NH2	2.14	0.63
4:B:109:LEU:HD11	4:B:206:ARG:NH2	2.14	0.63
3:A:202:ILE:HG22	3:A:203:GLU:N	2.13	0.63
3:A:420:PRO:HA	3:A:421:PRO:C	2.18	0.63
3:A:434:ILE:H	3:A:494:ASN:HD21	1.47	0.63
3:A:497:THR:O	3:A:535:TRP:HA	1.97	0.63
4:B:170:PRO:HB2	4:B:208:HIS:HE1	1.63	0.63
4:B:341:ILE:HD12	4:B:350:LYS:HB3	1.80	0.63
3:A:238:LYS:HD2	3:A:315:HIS:CD2	2.34	0.62
3:A:337:TRP:CH2	3:A:368:LEU:HB2	2.34	0.62
4:B:59:PRO:O	4:B:75:VAL:HG13	1.98	0.62
4:B:369:THR:HG22	4:B:398:TRP:HH2	1.61	0.62
3:A:23:GLN:OE1	3:A:59:PRO:HA	2.00	0.62
3:A:417:VAL:HG22	3:A:419:THR:HG22	1.81	0.62
3:A:441:TYR:HB2	3:A:458:VAL:CG1	2.28	0.62
4:B:330:GLN:O	4:B:337:TRP:HA	1.99	0.62
3:A:370:GLU:HA	3:A:373:GLN:HG3	1.82	0.62
4:B:106:VAL:HG12	4:B:107:THR:N	2.15	0.62
4:B:241:VAL:HG12	4:B:242:GLN:H	1.64	0.62
3:A:247:PRO:HG2	3:A:260:LEU:CD1	2.30	0.62
4:B:54:ASN:O	4:B:143:ARG:NH2	2.32	0.62
4:B:249:LYS:HE2	4:B:256:ASP:OD1	2.00	0.62
3:A:540:LYS:O	3:A:542:ILE:HG13	1.99	0.62
4:B:62:ALA:HB1	4:B:71:TRP:CE3	2.31	0.62
4:B:100:LEU:HD23	4:B:101:LYS:H	1.64	0.62
4:B:291:GLU:O	4:B:293:ILE:HG23	1.99	0.62
3:A:222:GLN:O	3:A:227:PHE:CE2	2.53	0.62
3:A:458:VAL:HG22	3:A:459:THR:H	1.65	0.62
3:A:473:THR:O	3:A:477:THR:HG23	1.99	0.62
4:B:34:LEU:H	4:B:34:LEU:HD23	1.64	0.61
3:A:438:GLU:OE1	3:A:461:LYS:HD2	1.99	0.61
1:T:707:DG:H2''	1:T:708:DG:H5'	1.82	0.61
3:A:368:LEU:HD11	3:A:391:LEU:HD22	1.81	0.61
4:B:252:TRP:HB3	4:B:257:ILE:CD1	2.31	0.61
4:B:296:THR:HG22	4:B:297:GLU:N	2.15	0.61
3:A:164:MET:HA	3:A:167:ILE:HD12	1.83	0.61
4:B:148:VAL:HG23	4:B:149:LEU:N	2.15	0.61
3:A:183:TYR:O	3:A:184:MET:HB3	2.01	0.60
3:A:336:GLN:C	3:A:337:TRP:CD1	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:372:VAL:HA	4:B:389:PHE:CE2	2.36	0.60
2:P:822:DDG:H2''	6:A:823:TNV:H6'1	1.82	0.60
3:A:221:HIS:HA	3:A:224:GLU:OE1	2.00	0.60
4:B:193:LEU:HD12	4:B:198:HIS:N	2.16	0.60
4:B:376:THR:HG1	4:B:389:PHE:HZ	1.49	0.60
3:A:75:VAL:HB	3:A:77:PHE:CE2	2.37	0.60
4:B:27:THR:HB	4:B:29:GLU:HG2	1.82	0.60
3:A:270:ILE:O	3:A:272:PRO:HD3	2.01	0.60
4:B:208:HIS:O	4:B:212:TRP:HB2	2.01	0.60
2:P:815:DG:H2'	2:P:816:DG:H8	1.67	0.60
4:B:233:GLU:C	4:B:234:LEU:HD12	2.20	0.60
4:B:30:LYS:O	4:B:33:ALA:HB3	2.01	0.60
3:A:223:LYS:C	3:A:225:PRO:HD2	2.22	0.60
3:A:521:ILE:O	3:A:525:LEU:HG	2.02	0.60
4:B:368:LEU:HD23	4:B:368:LEU:C	2.21	0.60
3:A:102:LYS:HE3	8:A:827:HOH:O	2.00	0.60
4:B:241:VAL:HA	4:B:351:THR:O	2.02	0.60
3:A:63:ILE:CD1	3:A:74:LEU:HD11	2.31	0.60
4:B:241:VAL:HG12	4:B:242:GLN:N	2.17	0.59
3:A:427:TYR:CE1	3:A:522:ILE:HG23	2.36	0.59
3:A:53:GLU:H	3:A:53:GLU:CD	2.06	0.59
3:A:478:GLU:HG2	3:A:499:SER:CB	2.31	0.59
3:A:547:GLN:H	3:A:547:GLN:NE2	2.00	0.59
4:B:406:TRP:CD1	4:B:407:GLN:N	2.70	0.59
1:T:706:DC:H2'	1:T:707:DG:C8	2.37	0.59
3:A:416:PHE:HZ	3:A:422:LEU:CD1	2.15	0.59
3:A:546:GLU:HB3	3:A:547:GLN:NE2	2.18	0.59
4:B:93:GLY:C	4:B:94:ILE:HD12	2.22	0.59
4:B:278:GLN:HB2	4:B:302:GLU:CD	2.23	0.59
3:A:332:GLN:HG3	3:A:338:THR:OG1	2.02	0.59
4:B:428:GLN:HG2	4:B:429:LEU:HD13	1.84	0.59
3:A:63:ILE:HD13	3:A:74:LEU:HD11	1.83	0.59
3:A:109:LEU:N	3:A:109:LEU:CD2	2.65	0.59
3:A:377:THR:HG22	3:A:378:GLU:N	2.17	0.59
4:B:111:VAL:HG12	4:B:216:THR:OG1	2.03	0.59
3:A:39:THR:HG22	3:A:43:LYS:HE3	1.85	0.59
3:A:118:VAL:HB	3:A:149:LEU:HD12	1.84	0.59
3:A:391:LEU:HB2	3:A:414:TRP:HE3	1.68	0.59
4:B:255:ASN:OD1	4:B:256:ASP:N	2.36	0.59
3:A:232:TYR:HB3	3:A:240:THR:O	2.03	0.59
3:A:484:LEU:HD23	3:A:487:GLN:HE22	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:278:GLN:CB	4:B:299:ALA:HA	2.26	0.59
3:A:72:ARG:CG	3:A:74:LEU:HD21	2.32	0.58
4:B:296:THR:HB	4:B:299:ALA:CB	2.31	0.58
4:B:47:ILE:HG22	4:B:145:GLN:O	2.03	0.58
4:B:241:VAL:HG22	4:B:350:LYS:HD2	1.84	0.58
4:B:356:ARG:HG3	4:B:367:GLN:NE2	2.17	0.58
3:A:75:VAL:HB	3:A:77:PHE:CD2	2.39	0.58
3:A:417:VAL:O	3:A:417:VAL:CG1	2.50	0.58
4:B:193:LEU:HB2	4:B:197:GLN:HE21	1.68	0.58
1:T:720:DG:H2'	1:T:721:DG:C8	2.39	0.58
3:A:10:VAL:HG23	3:A:124:PHE:CD1	2.38	0.58
3:A:405:TYR:CE2	3:A:407:GLN:HB2	2.39	0.58
4:B:306:ASN:HA	4:B:309:ILE:HD12	1.85	0.58
3:A:181:TYR:HB2	3:A:188:TYR:HB3	1.85	0.58
3:A:479:LEU:O	3:A:482:ILE:N	2.37	0.58
4:B:115:TYR:H	4:B:115:TYR:HD2	1.52	0.58
4:B:389:PHE:CD1	4:B:389:PHE:N	2.72	0.58
3:A:24:TRP:CD1	3:A:26:LEU:HD23	2.39	0.57
3:A:222:GLN:C	3:A:224:GLU:H	2.07	0.57
3:A:274:ILE:HG22	3:A:275:LYS:N	2.19	0.57
4:B:85:GLN:HA	4:B:88:TRP:CZ2	2.39	0.57
4:B:194:GLU:N	4:B:197:GLN:NE2	2.50	0.57
3:A:30:LYS:O	3:A:33:ALA:N	2.35	0.57
4:B:271:TYR:CD2	4:B:309:ILE:HG22	2.39	0.57
4:B:19:PRO:HG3	4:B:80:LEU:HD13	1.87	0.57
4:B:417:VAL:HG22	4:B:418:ASN:N	2.19	0.57
3:A:221:HIS:CD2	3:A:221:HIS:N	2.73	0.57
4:B:23:GLN:NE2	4:B:26:LEU:HD21	2.19	0.57
4:B:288:ALA:O	4:B:291:GLU:HG3	2.04	0.57
3:A:72:ARG:HG2	3:A:74:LEU:CD2	2.34	0.57
3:A:77:PHE:O	3:A:81:ASN:ND2	2.37	0.57
3:A:127:TYR:C	3:A:129:ALA:H	2.08	0.57
3:A:281:LYS:O	3:A:284:ARG:HG3	2.04	0.57
3:A:540:LYS:HD3	3:A:540:LYS:C	2.24	0.57
4:B:108:VAL:HG13	4:B:188:TYR:CE2	2.40	0.57
4:B:380:ILE:C	4:B:382:ILE:H	2.08	0.57
1:T:720:DG:O6	2:P:807:DC:N4	2.37	0.57
2:P:816:DG:H2'	2:P:817:MRG:H8	1.86	0.57
3:A:281:LYS:HG3	3:A:284:ARG:CZ	2.35	0.57
3:A:432:GLU:OE2	3:A:433:PRO:HD2	2.04	0.57
3:A:84:THR:CG2	3:A:85:GLN:N	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:PHE:CZ	3:A:422:LEU:HD13	2.40	0.56
3:A:548:VAL:O	3:A:552:VAL:HG22	2.05	0.56
4:B:205:LEU:HD23	4:B:205:LEU:O	2.05	0.56
3:A:96:HIS:O	3:A:99:GLY:N	2.35	0.56
4:B:161:GLN:O	4:B:165:THR:HG23	2.04	0.56
4:B:181:TYR:HD2	4:B:188:TYR:HD1	1.53	0.56
4:B:273:GLY:O	4:B:309:ILE:HD13	2.05	0.56
2:P:820:DC:H2''	2:P:821:DC:H5'	1.87	0.56
3:A:180:ILE:CG2	3:A:187:LEU:HD22	2.36	0.56
3:A:275:LYS:HD3	3:A:332:GLN:CD	2.25	0.56
4:B:13:LYS:HD3	4:B:86:ASP:H	1.70	0.56
4:B:33:ALA:O	4:B:34:LEU:C	2.42	0.56
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.87	0.56
4:B:80:LEU:O	4:B:83:ARG:N	2.35	0.56
4:B:274:ILE:HG23	4:B:306:ASN:CG	2.25	0.56
4:B:330:GLN:HB2	4:B:338:THR:OG1	2.05	0.56
4:B:271:TYR:HD2	4:B:309:ILE:HG22	1.70	0.56
4:B:274:ILE:HG12	4:B:309:ILE:HD12	1.86	0.56
4:B:143:ARG:O	4:B:144:TYR:CG	2.59	0.56
3:A:193:LEU:HD13	3:A:198:HIS:HA	1.86	0.56
3:A:275:LYS:CG	3:A:332:GLN:NE2	2.69	0.56
4:B:20:LYS:HG2	4:B:55:PRO:O	2.06	0.56
4:B:288:ALA:HB3	4:B:291:GLU:HG3	1.88	0.56
4:B:395:LYS:CG	4:B:399:GLU:OE2	2.54	0.56
3:A:493:VAL:HG12	3:A:494:ASN:N	2.15	0.56
4:B:78:ARG:HD3	4:B:411:ILE:O	2.06	0.56
4:B:100:LEU:HA	4:B:103:LYS:HB2	1.87	0.56
4:B:206:ARG:HH12	4:B:216:THR:HB	1.71	0.56
4:B:376:THR:HG23	4:B:386:THR:HG22	1.88	0.56
3:A:267:ALA:O	3:A:269:GLN:N	2.38	0.56
3:A:441:TYR:HA	3:A:496:VAL:HG12	1.87	0.56
3:A:28:GLU:O	3:A:32:LYS:HB2	2.06	0.55
3:A:220:LYS:O	3:A:220:LYS:CG	2.53	0.55
3:A:362:THR:HG22	3:A:366:LYS:CD	2.34	0.55
4:B:194:GLU:HB3	4:B:197:GLN:OE1	2.05	0.55
3:A:19:PRO:O	3:A:20:LYS:HG3	2.07	0.55
3:A:372:VAL:HG13	3:A:389:PHE:CE1	2.42	0.55
4:B:274:ILE:HD11	4:B:310:LEU:HD21	1.87	0.55
2:P:815:DG:H2'	2:P:816:DG:C8	2.41	0.55
3:A:97:PRO:HD3	3:A:232:TYR:CE2	2.41	0.55
3:A:121:ASP:O	3:A:125:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:366:LYS:O	4:B:370:GLU:HG3	2.05	0.55
1:T:714:DG:H4'	3:A:286:THR:CG2	2.37	0.55
3:A:529:GLU:O	3:A:529:GLU:HG2	2.06	0.55
4:B:278:GLN:HB2	4:B:302:GLU:OE2	2.06	0.55
3:A:81:ASN:HB3	3:A:154:LYS:HB2	1.87	0.55
3:A:136:ASN:HB2	3:A:138:GLU:HG3	1.88	0.55
3:A:23:GLN:HE21	3:A:26:LEU:HD21	1.71	0.55
3:A:76:ASP:C	3:A:78:ARG:H	2.10	0.55
3:A:306:ASN:HA	3:A:309:ILE:HG13	1.88	0.55
4:B:206:ARG:HH22	4:B:216:THR:HG22	1.72	0.55
4:B:275:LYS:O	4:B:306:ASN:ND2	2.39	0.55
3:A:188:TYR:HE2	3:A:234:LEU:CD1	2.19	0.55
3:A:354:TYR:CD2	3:A:371:ALA:HA	2.42	0.55
3:A:406:TRP:NE1	3:A:407:GLN:HG3	2.22	0.55
4:B:62:ALA:O	4:B:63:ILE:HD13	2.07	0.55
3:A:464:GLN:HG2	3:A:465:LYS:N	2.22	0.55
3:A:509:GLN:N	3:A:510:PRO:CD	2.70	0.55
4:B:395:LYS:HG3	4:B:399:GLU:OE2	2.07	0.55
3:A:63:ILE:HD11	3:A:72:ARG:HD2	1.89	0.54
3:A:274:ILE:HA	3:A:306:ASN:OD1	2.07	0.54
3:A:529:GLU:O	3:A:530:LYS:CG	2.55	0.54
3:A:68:SER:C	3:A:70:LYS:H	2.09	0.54
4:B:292:VAL:HG12	4:B:294:PRO:HD3	1.90	0.54
3:A:138:GLU:OE1	3:A:139:THR:HG23	2.07	0.54
3:A:265:ASN:OD1	3:A:353:LYS:NZ	2.40	0.54
3:A:401:TRP:O	3:A:405:TYR:HB2	2.06	0.54
3:A:416:PHE:HZ	3:A:422:LEU:HD13	1.71	0.54
4:B:54:ASN:HB3	4:B:143:ARG:HH21	1.71	0.54
4:B:180:ILE:CD1	4:B:205:LEU:HD11	2.37	0.54
3:A:249:LYS:HG3	3:A:252:TRP:CE2	2.43	0.54
3:A:472:THR:OG1	3:A:476:LYS:HB2	2.08	0.54
3:A:493:VAL:O	3:A:494:ASN:ND2	2.41	0.54
3:A:522:ILE:HA	3:A:525:LEU:HD12	1.90	0.54
4:B:181:TYR:HB3	4:B:188:TYR:HB2	1.90	0.54
4:B:394:GLN:O	4:B:395:LYS:C	2.45	0.54
3:A:254:VAL:HG13	3:A:283:LEU:CD2	2.32	0.54
3:A:275:LYS:HD3	3:A:332:GLN:OE1	2.08	0.54
3:A:484:LEU:CA	3:A:487:GLN:HE21	2.10	0.54
4:B:122:GLU:HA	4:B:125:ARG:CD	2.30	0.54
4:B:270:ILE:HG22	4:B:271:TYR:CD1	2.42	0.54
2:P:819:DG:H2'	2:P:820:DC:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4:PRO:O	3:A:5:ILE:C	2.44	0.54
3:A:109:LEU:HD23	3:A:187:LEU:O	2.08	0.54
4:B:109:LEU:HG	4:B:216:THR:HG21	1.90	0.54
4:B:193:LEU:HB2	4:B:197:GLN:NE2	2.23	0.54
1:T:711:DC:H2'	1:T:712:DC:C6	2.43	0.53
3:A:395:LYS:O	3:A:395:LYS:HD3	2.07	0.53
3:A:457:TYR:CZ	3:A:465:LYS:HB3	2.43	0.53
4:B:169:GLU:C	4:B:171:PHE:H	2.10	0.53
4:B:382:ILE:O	4:B:383:TRP:CG	2.61	0.53
2:P:819:DG:H2''	2:P:820:DC:H5'	1.90	0.53
4:B:303:LEU:HD11	4:B:307:ARG:NH2	2.23	0.53
3:A:34:LEU:HD11	3:A:62:ALA:HB2	1.91	0.53
4:B:382:ILE:HG22	4:B:383:TRP:CD2	2.43	0.53
4:B:60:VAL:O	4:B:61:PHE:HB3	2.09	0.53
4:B:282:LEU:O	4:B:283:LEU:HB3	2.08	0.53
4:B:329:ILE:CG2	4:B:330:GLN:H	2.21	0.53
3:A:470:THR:O	3:A:472:THR:N	2.41	0.53
4:B:255:ASN:C	4:B:257:ILE:N	2.62	0.53
3:A:288:ALA:C	3:A:290:THR:H	2.12	0.53
3:A:498:ASP:HA	3:A:536:VAL:O	2.09	0.53
4:B:81:ASN:HB3	4:B:154:LYS:HD2	1.90	0.53
4:B:382:ILE:O	4:B:382:ILE:CG2	2.57	0.53
4:B:395:LYS:CE	4:B:399:GLU:OE2	2.57	0.53
4:B:100:LEU:HG	4:B:381:VAL:HG12	1.90	0.53
3:A:5:ILE:HG23	3:A:5:ILE:O	2.09	0.53
3:A:74:LEU:CD2	3:A:151:GLN:HG2	2.39	0.52
4:B:369:THR:OG1	4:B:370:GLU:N	2.41	0.52
4:B:413:GLU:O	4:B:414:TRP:HB3	2.10	0.52
1:T:709:DC:H2'	1:T:710:DG:C8	2.44	0.52
3:A:229:TRP:CD2	3:A:230:MET:HG2	2.44	0.52
4:B:330:GLN:OE1	4:B:340:GLN:NE2	2.37	0.52
1:T:709:DC:H2'	1:T:710:DG:H8	1.74	0.52
3:A:39:THR:CG2	3:A:43:LYS:HE3	2.39	0.52
4:B:244:ILE:CG2	4:B:426:TRP:HB3	2.39	0.52
4:B:255:ASN:O	4:B:257:ILE:N	2.43	0.52
4:B:376:THR:OG1	4:B:389:PHE:CZ	2.62	0.52
3:A:239:TRP:CE3	3:A:240:THR:N	2.77	0.52
4:B:77:PHE:O	4:B:80:LEU:N	2.39	0.52
3:A:121:ASP:OD2	3:A:124:PHE:HB2	2.09	0.52
3:A:244:ILE:CD1	3:A:267:ALA:HB2	2.39	0.52
3:A:420:PRO:HA	3:A:422:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:546:GLU:HG3	3:A:547:GLN:N	2.24	0.52
3:A:72:ARG:NH1	6:A:823:TNV:C8'	2.62	0.52
3:A:500:GLN:HG2	4:B:422:LEU:CD2	2.36	0.52
1:T:704:DG:H5''	1:T:704:DG:N3	2.24	0.52
4:B:382:ILE:O	4:B:382:ILE:HG22	2.09	0.52
3:A:153:TRP:O	3:A:155:GLY:N	2.43	0.52
4:B:64:LYS:NZ	4:B:71:TRP:HE1	2.08	0.52
4:B:163:SER:O	4:B:167:ILE:HG13	2.09	0.52
4:B:332:GLN:HE22	4:B:425:LEU:CD1	2.23	0.52
4:B:376:THR:OG1	4:B:389:PHE:HZ	1.93	0.52
2:P:819:DG:H2'	2:P:820:DC:H6	1.75	0.52
3:A:334:GLN:OE1	3:A:334:GLN:HA	2.10	0.52
3:A:354:TYR:HE1	3:A:356:ARG:CB	2.22	0.52
3:A:442:VAL:O	3:A:443:ASP:HB2	2.09	0.52
4:B:255:ASN:C	4:B:257:ILE:H	2.14	0.52
3:A:156:SER:HB2	3:A:157:PRO:CD	2.38	0.51
4:B:153:TRP:HB3	4:B:156:SER:OG	2.10	0.51
3:A:53:GLU:CD	3:A:53:GLU:N	2.64	0.51
3:A:88:TRP:O	3:A:89:GLU:C	2.49	0.51
3:A:441:TYR:CD2	3:A:544:GLY:HA3	2.45	0.51
3:A:470:THR:C	3:A:472:THR:H	2.13	0.51
3:A:191:SER:OG	3:A:193:LEU:HD12	2.11	0.51
4:B:120:LEU:HD13	4:B:150:PRO:HD3	1.91	0.51
3:A:247:PRO:HD2	3:A:260:LEU:HD12	1.93	0.51
3:A:426:TRP:O	3:A:427:TYR:HB3	2.10	0.51
4:B:78:ARG:CD	4:B:411:ILE:HG22	2.41	0.51
2:P:818:DC:H2'	2:P:819:DG:H8	1.75	0.51
4:B:104:LYS:HD2	4:B:192:ASP:C	2.31	0.51
4:B:235:HIS:N	4:B:236:PRO:HD3	2.24	0.51
3:A:254:VAL:HB	3:A:289:LEU:HA	1.92	0.51
4:B:106:VAL:CG1	4:B:107:THR:N	2.73	0.51
4:B:189:VAL:HG21	4:B:202:ILE:HD12	1.91	0.51
3:A:440:PHE:O	3:A:496:VAL:HG12	2.11	0.51
4:B:365:VAL:HG23	4:B:366:LYS:H	1.75	0.51
3:A:2:ILE:CD1	3:A:46:LYS:HD2	2.40	0.51
3:A:55:PRO:HG2	3:A:56:TYR:CE2	2.46	0.51
3:A:94:ILE:HG23	3:A:95:PRO:CD	2.40	0.51
4:B:157:PRO:HG2	4:B:158:ALA:H	1.75	0.51
3:A:10:VAL:HG23	3:A:10:VAL:O	2.11	0.50
3:A:28:GLU:HG2	3:A:32:LYS:HD3	1.92	0.50
3:A:235:HIS:HB2	3:A:238:LYS:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:723:DC:H2'	1:T:724:DT:C6	2.47	0.50
3:A:77:PHE:HE2	3:A:150:PRO:HB2	1.75	0.50
1:T:704:DG:N3	1:T:704:DG:H2'	2.26	0.50
3:A:486:LEU:HD13	3:A:524:GLN:HB3	1.94	0.50
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.47	0.50
4:B:233:GLU:O	4:B:234:LEU:HD12	2.12	0.50
2:P:814:DC:H2'	2:P:815:DG:C8	2.46	0.50
3:A:513:SER:OG	3:A:515:SER:HB3	2.11	0.50
3:A:293:ILE:CG1	3:A:294:PRO:HD2	2.34	0.50
4:B:290:THR:HG22	4:B:290:THR:O	2.12	0.50
4:B:329:ILE:CG2	4:B:330:GLN:N	2.71	0.50
3:A:91:GLN:HG2	3:A:161:GLN:NE2	2.26	0.50
3:A:136:ASN:HB2	3:A:138:GLU:OE2	2.12	0.50
4:B:365:VAL:HG23	4:B:366:LYS:N	2.27	0.50
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.93	0.50
4:B:24:TRP:CH2	4:B:61:PHE:CD1	2.96	0.50
3:A:317:VAL:CG2	3:A:318:TYR:H	2.15	0.50
3:A:319:TYR:CD1	3:A:383:TRP:CD1	3.00	0.50
4:B:154:LYS:O	4:B:157:PRO:HD2	2.11	0.50
3:A:33:ALA:O	3:A:37:ILE:HG12	2.10	0.49
3:A:163:SER:O	3:A:167:ILE:HG13	2.11	0.49
3:A:406:TRP:O	4:B:331:LYS:HD3	2.12	0.49
4:B:242:GLN:HB2	4:B:353:LYS:NZ	2.27	0.49
3:A:8:VAL:O	3:A:10:VAL:HG13	2.12	0.49
3:A:41:MET:O	3:A:44:GLU:N	2.46	0.49
3:A:154:LYS:O	3:A:154:LYS:HG2	2.12	0.49
3:A:131:THR:OG1	3:A:143:ARG:HG2	2.12	0.49
3:A:297:GLU:HA	3:A:300:GLU:HB2	1.95	0.49
3:A:501:TYR:O	3:A:505:ILE:HG13	2.12	0.49
3:A:246:LEU:HD22	3:A:310:LEU:HD12	1.93	0.49
3:A:447:ASN:ND2	3:A:449:GLU:H	2.10	0.49
3:A:434:ILE:HB	3:A:494:ASN:ND2	2.26	0.49
3:A:460:ASN:HA	4:B:286:THR:O	2.12	0.49
3:A:484:LEU:O	3:A:486:LEU:N	2.46	0.49
2:P:811:DG:H2'	2:P:812:DT:C6	2.47	0.49
3:A:396:GLU:O	3:A:397:THR:C	2.51	0.49
3:A:437:ALA:O	3:A:439:THR:N	2.45	0.49
1:T:724:DT:H2'	1:T:725:DG:C8	2.48	0.49
3:A:265:ASN:O	3:A:268:SER:OG	2.27	0.49
3:A:239:TRP:HE3	3:A:240:THR:N	2.11	0.49
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:78:ARG:NE	4:B:411:ILE:HG22	2.27	0.49
4:B:406:TRP:CD1	4:B:408:ALA:N	2.79	0.49
4:B:249:LYS:HB2	4:B:252:TRP:CE2	2.48	0.49
4:B:372:VAL:O	4:B:389:PHE:CZ	2.66	0.49
2:P:807:DC:H2'	2:P:808:DC:C6	2.48	0.49
2:P:818:DC:H2''	2:P:819:DG:C5'	2.40	0.49
3:A:46:LYS:O	3:A:47:ILE:HG23	2.12	0.49
3:A:106:VAL:HG12	3:A:107:THR:N	2.27	0.49
3:A:149:LEU:HD22	3:A:156:SER:HA	1.93	0.49
3:A:329:ILE:HG22	3:A:330:GLN:N	2.28	0.49
3:A:371:ALA:O	3:A:372:VAL:C	2.51	0.49
4:B:43:LYS:HG2	4:B:43:LYS:O	2.13	0.49
4:B:314:VAL:CG2	4:B:315:HIS:H	2.21	0.49
1:T:706:DC:H2'	1:T:707:DG:H8	1.77	0.48
3:A:269:GLN:HA	3:A:351:THR:O	2.13	0.48
3:A:277:ARG:NH1	3:A:355:ALA:O	2.46	0.48
3:A:537:PRO:CG	4:B:262:GLY:HA2	2.42	0.48
4:B:242:GLN:CB	4:B:353:LYS:NZ	2.76	0.48
3:A:37:ILE:HD13	3:A:37:ILE:N	2.28	0.48
3:A:222:GLN:H	3:A:224:GLU:CG	2.18	0.48
3:A:420:PRO:HB3	3:A:421:PRO:HA	1.95	0.48
3:A:458:VAL:HG22	3:A:459:THR:N	2.28	0.48
3:A:18:GLY:H	3:A:56:TYR:HE1	1.62	0.48
4:B:273:GLY:O	4:B:309:ILE:CD1	2.61	0.48
4:B:408:ALA:C	4:B:410:TRP:H	2.17	0.48
3:A:222:GLN:C	3:A:224:GLU:N	2.67	0.48
3:A:354:TYR:HE1	3:A:356:ARG:HB2	1.79	0.48
3:A:391:LEU:HD12	3:A:414:TRP:CB	2.43	0.48
3:A:451:LYS:O	3:A:471:ASN:N	2.46	0.48
4:B:112:GLY:HA2	4:B:115:TYR:CD2	2.48	0.48
4:B:175:ASN:N	4:B:176:PRO:CD	2.76	0.48
4:B:181:TYR:O	4:B:187:LEU:HD12	2.13	0.48
4:B:396:GLU:CD	4:B:396:GLU:H	2.17	0.48
2:P:810:DT:OP1	3:A:361:HIS:NE2	2.42	0.48
3:A:91:GLN:CG	3:A:161:GLN:NE2	2.75	0.48
3:A:115:TYR:OH	3:A:157:PRO:HG3	2.13	0.48
4:B:13:LYS:HD2	4:B:86:ASP:HB2	1.96	0.48
4:B:197:GLN:O	4:B:200:THR:N	2.45	0.48
4:B:285:GLY:O	4:B:287:LYS:N	2.42	0.48
3:A:247:PRO:HG2	3:A:260:LEU:HD13	1.95	0.48
4:B:77:PHE:O	4:B:78:ARG:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:164:MET:HG3	3:A:168:LEU:CD1	2.41	0.48
3:A:276:VAL:HA	3:A:302:GLU:CD	2.33	0.48
3:A:391:LEU:HD12	3:A:414:TRP:CE3	2.48	0.48
4:B:241:VAL:HG13	4:B:351:THR:OG1	2.13	0.48
4:B:245:VAL:O	4:B:263:LYS:NZ	2.47	0.48
4:B:253:THR:HG23	4:B:256:ASP:HB2	1.96	0.48
4:B:249:LYS:HD2	4:B:256:ASP:OD2	2.14	0.48
3:A:320:ASP:OD1	3:A:322:SER:HB3	2.13	0.48
3:A:339:TYR:CE1	3:A:352:GLY:C	2.87	0.48
3:A:376:THR:O	3:A:380:ILE:HG13	2.14	0.48
4:B:175:ASN:H	4:B:176:PRO:HD3	1.77	0.48
4:B:425:LEU:C	4:B:427:TYR:N	2.65	0.48
3:A:78:ARG:HA	3:A:81:ASN:ND2	2.28	0.47
3:A:95:PRO:HD2	3:A:230:MET:HE2	1.96	0.47
3:A:225:PRO:HB3	3:A:227:PHE:CE1	2.49	0.47
3:A:326:ILE:HD12	3:A:342:TYR:CE2	2.49	0.47
3:A:391:LEU:HD12	3:A:414:TRP:HB2	1.96	0.47
4:B:260:LEU:HG	4:B:264:LEU:HD12	1.95	0.47
3:A:94:ILE:HG23	3:A:95:PRO:HD2	1.96	0.47
3:A:545:ASN:O	3:A:546:GLU:C	2.52	0.47
4:B:401:TRP:O	4:B:404:GLU:N	2.45	0.47
3:A:23:GLN:NE2	3:A:26:LEU:HD21	2.28	0.47
3:A:146:TYR:CE2	3:A:150:PRO:HA	2.49	0.47
3:A:155:GLY:O	3:A:156:SER:C	2.53	0.47
4:B:169:GLU:OE1	4:B:169:GLU:HA	2.14	0.47
4:B:333:GLY:O	4:B:336:GLN:HB2	2.14	0.47
3:A:406:TRP:O	4:B:331:LYS:HB3	2.14	0.47
4:B:79:GLU:OE2	4:B:83:ARG:NH1	2.47	0.47
4:B:368:LEU:HD23	4:B:372:VAL:HG23	1.94	0.47
3:A:209:LEU:HB3	3:A:214:LEU:HB2	1.96	0.47
4:B:235:HIS:N	4:B:235:HIS:ND1	2.63	0.47
4:B:287:LYS:HD3	4:B:291:GLU:OE1	2.14	0.47
4:B:414:TRP:HD1	4:B:414:TRP:O	1.98	0.47
3:A:115:TYR:O	3:A:148:VAL:HG22	2.14	0.47
3:A:484:LEU:HA	3:A:487:GLN:HG2	1.96	0.47
3:A:461:LYS:C	3:A:463:ARG:H	2.17	0.47
3:A:489:SER:HB2	3:A:493:VAL:HG22	1.95	0.47
3:A:493:VAL:CG1	3:A:494:ASN:H	2.14	0.47
3:A:546:GLU:HB3	3:A:547:GLN:HE21	1.80	0.47
4:B:103:LYS:HG3	4:B:191:SER:C	2.35	0.47
4:B:124:PHE:O	4:B:126:LYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:175:ASN:ND2	4:B:201:LYS:HE2	2.23	0.47
4:B:242:GLN:HB2	4:B:243:PRO:HD2	1.97	0.47
4:B:257:ILE:O	4:B:261:VAL:HG23	2.15	0.47
3:A:13:LYS:O	3:A:14:PRO:C	2.53	0.47
3:A:158:ALA:HB1	4:B:52:PRO:HB2	1.97	0.47
3:A:247:PRO:CG	3:A:260:LEU:CD1	2.93	0.47
4:B:202:ILE:O	4:B:206:ARG:HG3	2.14	0.47
4:B:372:VAL:HG13	4:B:389:PHE:CZ	2.49	0.47
4:B:402:TRP:CG	4:B:403:THR:N	2.83	0.47
4:B:428:GLN:CG	4:B:429:LEU:HD13	2.44	0.47
2:P:820:DC:H4'	3:A:266:TRP:CE2	2.50	0.47
3:A:96:HIS:ND1	3:A:98:ALA:HB3	2.29	0.47
4:B:276:VAL:HG13	4:B:277:ARG:N	2.30	0.47
4:B:299:ALA:O	4:B:302:GLU:HB3	2.15	0.47
3:A:41:MET:O	3:A:42:GLU:C	2.54	0.47
3:A:498:ASP:O	3:A:535:TRP:NE1	2.48	0.47
4:B:97:PRO:O	4:B:100:LEU:HD22	2.14	0.47
4:B:234:LEU:HB3	4:B:236:PRO:HD3	1.97	0.47
4:B:281:LYS:C	4:B:283:LEU:H	2.19	0.47
3:A:354:TYR:C	3:A:354:TYR:CD1	2.86	0.46
3:A:363:ASN:HA	3:A:511:ASP:OD1	2.15	0.46
4:B:305:GLU:O	4:B:308:GLU:N	2.40	0.46
3:A:279:LEU:N	3:A:302:GLU:OE2	2.34	0.46
3:A:427:TYR:HD1	3:A:526:ILE:HG12	1.80	0.46
1:T:715:DA:C6	1:T:716:DA:C6	3.04	0.46
3:A:434:ILE:CB	3:A:494:ASN:HD21	2.28	0.46
4:B:194:GLU:HB3	4:B:197:GLN:CD	2.35	0.46
2:P:812:DT:H2''	2:P:813:DT:H5'	1.97	0.46
2:P:817:MRG:H4'	3:A:289:LEU:HD21	1.97	0.46
3:A:3:SER:CB	3:A:212:TRP:O	2.62	0.46
4:B:135:ILE:HD12	4:B:135:ILE:O	2.15	0.46
4:B:276:VAL:HG13	4:B:277:ARG:H	1.79	0.46
4:B:314:VAL:CG2	4:B:315:HIS:N	2.77	0.46
4:B:393:ILE:HG12	4:B:394:GLN:N	2.30	0.46
3:A:438:GLU:O	3:A:440:PHE:CD1	2.69	0.46
3:A:503:LEU:HD23	4:B:422:LEU:HD23	1.98	0.46
4:B:106:VAL:HA	4:B:190:GLY:HA2	1.97	0.46
4:B:296:THR:CG2	4:B:297:GLU:N	2.79	0.46
4:B:345:PRO:O	4:B:346:PHE:HB2	2.16	0.46
2:P:812:DT:H2'	2:P:813:DT:H6	1.81	0.46
3:A:61:PHE:CD1	3:A:61:PHE:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:LYS:O	7:A:824:GOL:H31	2.15	0.46
3:A:195:ILE:HG22	3:A:199:ARG:HD2	1.96	0.46
3:A:339:TYR:CD1	3:A:352:GLY:O	2.69	0.46
3:A:405:TYR:HE2	3:A:407:GLN:HB2	1.81	0.46
3:A:442:VAL:HG13	3:A:495:ILE:HG23	1.97	0.46
4:B:142:ILE:HD13	4:B:142:ILE:N	2.31	0.46
4:B:281:LYS:O	4:B:283:LEU:N	2.49	0.46
4:B:400:THR:HG22	4:B:401:TRP:CD2	2.51	0.46
2:P:822:DDG:H2'	3:A:184:MET:HG2	1.97	0.46
3:A:47:ILE:HG13	3:A:47:ILE:O	2.16	0.46
3:A:78:ARG:HA	3:A:81:ASN:HD22	1.80	0.46
4:B:276:VAL:CG2	4:B:280:SER:HB3	2.40	0.46
3:A:244:ILE:HD13	3:A:267:ALA:HB2	1.98	0.46
3:A:547:GLN:H	3:A:547:GLN:HE21	1.62	0.46
4:B:27:THR:HG22	4:B:28:GLU:N	2.31	0.46
4:B:162:SER:O	4:B:164:MET:N	2.49	0.46
4:B:164:MET:HG2	4:B:182:GLN:OE1	2.16	0.46
4:B:408:ALA:O	4:B:410:TRP:N	2.48	0.46
3:A:16:MET:CE	3:A:83:ARG:HD2	2.47	0.46
3:A:303:LEU:HD21	3:A:307:ARG:CZ	2.46	0.46
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.80	0.46
3:A:473:THR:H	3:A:476:LYS:HB2	1.81	0.46
3:A:484:LEU:O	3:A:487:GLN:HG2	2.15	0.46
4:B:200:THR:O	4:B:204:GLU:HG3	2.16	0.46
2:P:812:DT:H2'	2:P:813:DT:C6	2.51	0.45
3:A:127:TYR:C	3:A:129:ALA:N	2.70	0.45
3:A:377:THR:O	3:A:381:VAL:HG23	2.16	0.45
4:B:27:THR:HG22	4:B:28:GLU:H	1.82	0.45
4:B:44:GLU:HB2	4:B:46:LYS:CE	2.45	0.45
1:T:707:DG:O3'	3:A:89:GLU:HG3	2.17	0.45
3:A:270:ILE:HD12	3:A:270:ILE:HA	1.68	0.45
4:B:41:MET:HB3	4:B:47:ILE:HG12	1.98	0.45
3:A:77:PHE:O	3:A:81:ASN:CG	2.55	0.45
3:A:240:THR:OG1	3:A:241:VAL:N	2.50	0.45
3:A:517:LEU:HD22	3:A:521:ILE:CD1	2.30	0.45
4:B:361:HIS:CD2	4:B:363:ASN:HB2	2.51	0.45
2:P:809:DC:H2''	2:P:810:DT:C5'	2.47	0.45
3:A:458:VAL:HG12	3:A:548:VAL:HG22	1.98	0.45
4:B:114:ALA:O	4:B:116:PHE:N	2.50	0.45
3:A:341:ILE:HG22	3:A:342:TYR:N	2.32	0.45
3:A:427:TYR:CD2	3:A:427:TYR:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:252:TRP:CB	4:B:257:ILE:HD11	2.39	0.45
4:B:305:GLU:C	4:B:307:ARG:N	2.68	0.45
4:B:317:VAL:HG23	4:B:317:VAL:O	2.16	0.45
4:B:367:GLN:O	4:B:368:LEU:C	2.55	0.45
3:A:73:LYS:O	3:A:74:LEU:HD23	2.16	0.45
3:A:483:TYR:CE1	3:A:520:GLN:HG3	2.51	0.45
4:B:87:PHE:HA	4:B:91:GLN:NE2	2.31	0.45
4:B:128:THR:CB	4:B:146:TYR:HB2	2.47	0.45
3:A:7:THR:HG22	3:A:119:PRO:HB2	1.99	0.45
4:B:47:ILE:HA	4:B:145:GLN:O	2.17	0.45
4:B:62:ALA:CB	4:B:71:TRP:CE3	2.98	0.45
4:B:78:ARG:NE	4:B:411:ILE:CG2	2.80	0.45
4:B:395:LYS:HE3	4:B:399:GLU:OE2	2.16	0.45
2:P:809:DC:H2''	2:P:810:DT:H5'	1.98	0.45
3:A:158:ALA:HB1	4:B:52:PRO:CB	2.46	0.45
3:A:367:GLN:HA	3:A:370:GLU:CG	2.47	0.45
3:A:461:LYS:O	3:A:463:ARG:N	2.49	0.45
3:A:498:ASP:OD2	3:A:538:ALA:HB2	2.16	0.45
4:B:51:GLY:C	4:B:53:GLU:OE2	2.55	0.45
4:B:426:TRP:H	4:B:426:TRP:HE3	1.63	0.45
3:A:296:THR:O	3:A:300:GLU:N	2.33	0.45
3:A:326:ILE:HG22	3:A:327:ALA:N	2.31	0.45
3:A:328:GLU:HG2	3:A:330:GLN:NE2	2.31	0.45
4:B:42:GLU:C	4:B:44:GLU:H	2.20	0.45
4:B:81:ASN:O	4:B:88:TRP:HZ2	1.99	0.45
4:B:293:ILE:HB	4:B:295:LEU:HD13	1.99	0.45
4:B:302:GLU:O	4:B:305:GLU:HB3	2.17	0.45
4:B:332:GLN:HE22	4:B:425:LEU:HD12	1.80	0.45
4:B:380:ILE:C	4:B:382:ILE:N	2.70	0.45
3:A:252:TRP:CZ3	3:A:260:LEU:HD22	2.52	0.45
3:A:264:LEU:HD23	3:A:274:ILE:CG2	2.46	0.45
3:A:264:LEU:HD23	3:A:274:ILE:HG23	1.99	0.45
4:B:154:LYS:C	4:B:157:PRO:HD2	2.37	0.45
4:B:242:GLN:HG2	4:B:353:LYS:HG2	1.99	0.45
4:B:342:TYR:CD1	4:B:342:TYR:C	2.89	0.45
3:A:12:LEU:HD23	3:A:84:THR:HA	1.97	0.44
3:A:114:ALA:HB1	3:A:160:PHE:CE1	2.52	0.44
3:A:118:VAL:O	3:A:148:VAL:HG23	2.16	0.44
3:A:276:VAL:O	3:A:277:ARG:C	2.53	0.44
4:B:109:LEU:CD1	4:B:216:THR:HG21	2.47	0.44
4:B:120:LEU:CD1	4:B:150:PRO:HD3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:122:GLU:C	4:B:124:PHE:H	2.20	0.44
1:T:714:DG:H5'	3:A:286:THR:HG23	2.00	0.44
3:A:21:VAL:HG13	3:A:59:PRO:HD3	1.98	0.44
3:A:375:ILE:O	3:A:376:THR:C	2.55	0.44
4:B:348:ASN:C	4:B:350:LYS:H	2.21	0.44
2:P:816:DG:H2'	2:P:817:MRG:C8	2.46	0.44
3:A:117:SER:N	3:A:148:VAL:HG21	2.33	0.44
3:A:194:GLU:O	3:A:196:GLY:N	2.50	0.44
3:A:252:TRP:CE3	3:A:257:ILE:HD13	2.51	0.44
3:A:420:PRO:CB	3:A:421:PRO:HA	2.47	0.44
4:B:23:GLN:HE22	4:B:26:LEU:HD21	1.83	0.44
4:B:149:LEU:HA	4:B:150:PRO:HD3	1.82	0.44
4:B:209:LEU:HD22	4:B:214:LEU:HD12	2.00	0.44
3:A:169:GLU:HB3	3:A:170:PRO:HD3	1.98	0.44
3:A:477:THR:O	3:A:478:GLU:C	2.56	0.44
3:A:543:GLY:C	3:A:545:ASN:H	2.21	0.44
4:B:180:ILE:HA	4:B:188:TYR:O	2.17	0.44
4:B:210:LEU:C	4:B:212:TRP:H	2.21	0.44
3:A:57:ASN:HB2	3:A:143:ARG:NH2	2.32	0.44
3:A:88:TRP:CD1	4:B:143:ARG:HD3	2.53	0.44
3:A:349:LEU:HA	3:A:349:LEU:HD23	1.75	0.44
3:A:365:VAL:HG22	3:A:393:ILE:CD1	2.48	0.44
4:B:94:ILE:HD12	4:B:94:ILE:N	2.32	0.44
4:B:393:ILE:HG12	4:B:394:GLN:H	1.82	0.44
3:A:13:LYS:O	3:A:16:MET:HG3	2.16	0.44
3:A:149:LEU:HD21	3:A:159:ILE:HB	1.98	0.44
3:A:221:HIS:HE1	3:A:228:LEU:CB	2.20	0.44
4:B:184:MET:HB3	4:B:185:ASP:H	1.55	0.44
4:B:206:ARG:NH1	4:B:216:THR:HB	2.32	0.44
2:P:813:DT:H2'	2:P:814:DC:C6	2.53	0.44
3:A:96:HIS:N	4:B:136:ASN:OD1	2.44	0.44
4:B:424:LYS:O	4:B:425:LEU:O	2.36	0.44
3:A:224:GLU:N	3:A:225:PRO:CD	2.81	0.44
3:A:416:PHE:CZ	3:A:418:ASN:HA	2.53	0.44
3:A:480:GLN:HG2	3:A:517:LEU:HD11	2.00	0.44
3:A:408:ALA:O	4:B:393:ILE:HG13	2.18	0.43
4:B:65:LYS:HE3	4:B:72:ARG:HB2	2.00	0.43
4:B:255:ASN:HA	4:B:258:GLN:HB2	2.00	0.43
2:P:818:DC:H2'	2:P:819:DG:C8	2.51	0.43
3:A:118:VAL:HA	3:A:119:PRO:HD3	1.69	0.43
3:A:136:ASN:HB2	3:A:138:GLU:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:287:LYS:HD2	3:A:291:GLU:OE2	2.18	0.43
3:A:462:GLY:O	3:A:463:ARG:C	2.56	0.43
3:A:484:LEU:C	3:A:486:LEU:N	2.72	0.43
4:B:174:GLN:NE2	4:B:175:ASN:OD1	2.52	0.43
1:T:724:DT:H2'	1:T:725:DG:H8	1.82	0.43
3:A:423:VAL:O	3:A:424:LYS:HB3	2.19	0.43
4:B:195:ILE:C	4:B:197:GLN:N	2.71	0.43
3:A:24:TRP:CD1	3:A:24:TRP:O	2.72	0.43
3:A:286:THR:O	3:A:287:LYS:HG2	2.18	0.43
3:A:391:LEU:HA	3:A:392:PRO:HD3	1.58	0.43
4:B:85:GLN:O	4:B:89:GLU:N	2.51	0.43
3:A:367:GLN:HA	3:A:370:GLU:HG2	1.99	0.43
3:A:465:LYS:O	3:A:466:VAL:HG13	2.17	0.43
4:B:21:VAL:HB	4:B:59:PRO:HD3	1.99	0.43
4:B:254:VAL:HG12	4:B:258:GLN:OE1	2.18	0.43
4:B:260:LEU:HG	4:B:264:LEU:CD1	2.49	0.43
4:B:369:THR:O	4:B:370:GLU:C	2.56	0.43
3:A:96:HIS:O	3:A:97:PRO:C	2.55	0.43
3:A:279:LEU:HB2	3:A:302:GLU:OE1	2.17	0.43
3:A:365:VAL:HG22	3:A:393:ILE:HD12	2.01	0.43
3:A:427:TYR:HE1	3:A:522:ILE:CG2	2.30	0.43
4:B:253:THR:O	4:B:257:ILE:HG12	2.19	0.43
1:T:716:DA:H2'	1:T:717:DC:O4'	2.18	0.43
3:A:54:ASN:O	3:A:143:ARG:NH1	2.51	0.43
3:A:60:VAL:HG12	3:A:75:VAL:HG22	2.00	0.43
3:A:88:TRP:HD1	4:B:143:ARG:HD3	1.83	0.43
3:A:288:ALA:HB3	3:A:291:GLU:HB2	2.01	0.43
3:A:345:PRO:O	7:A:825:GOL:H31	2.19	0.43
3:A:511:ASP:HA	3:A:522:ILE:HG21	1.99	0.43
3:A:27:THR:OG1	3:A:29:GLU:HB3	2.19	0.43
3:A:275:LYS:HG3	3:A:332:GLN:NE2	2.34	0.43
3:A:297:GLU:O	3:A:300:GLU:N	2.52	0.43
4:B:259:LYS:O	4:B:261:VAL:N	2.52	0.43
4:B:376:THR:O	4:B:377:THR:C	2.56	0.43
3:A:38:CYS:O	3:A:39:THR:C	2.54	0.43
3:A:318:TYR:O	3:A:349:LEU:HD21	2.19	0.43
3:A:354:TYR:CE2	3:A:371:ALA:HA	2.54	0.43
4:B:100:LEU:HG	4:B:381:VAL:CG1	2.48	0.43
4:B:253:THR:HG23	4:B:256:ASP:CB	2.49	0.43
3:A:150:PRO:HG2	3:A:153:TRP:HB2	2.01	0.43
3:A:244:ILE:HG12	3:A:244:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:398:TRP:O	3:A:399:GLU:C	2.57	0.43
3:A:484:LEU:C	3:A:486:LEU:H	2.23	0.43
3:A:540:LYS:HD2	3:A:542:ILE:HD11	2.01	0.43
4:B:296:THR:HG22	4:B:297:GLU:H	1.83	0.43
4:B:363:ASN:O	4:B:367:GLN:HG3	2.19	0.43
4:B:402:TRP:CD2	4:B:403:THR:N	2.87	0.43
4:B:65:LYS:CB	4:B:68:SER:HB3	2.47	0.42
4:B:93:GLY:O	4:B:94:ILE:HG13	2.18	0.42
4:B:118:VAL:HB	4:B:149:LEU:CD1	2.40	0.42
4:B:167:ILE:HG23	4:B:212:TRP:CD2	2.51	0.42
4:B:180:ILE:HD11	4:B:205:LEU:CD1	2.45	0.42
4:B:382:ILE:HG22	4:B:383:TRP:CE3	2.52	0.42
7:B:438:GOL:H32	7:B:439:GOL:O1	2.18	0.42
3:A:270:ILE:HG23	3:A:271:TYR:CD2	2.54	0.42
3:A:500:GLN:CG	4:B:422:LEU:HD22	2.41	0.42
4:B:34:LEU:N	4:B:34:LEU:CD2	2.82	0.42
4:B:115:TYR:CE1	4:B:156:SER:C	2.92	0.42
4:B:168:LEU:HD12	4:B:172:ARG:CZ	2.49	0.42
3:A:221:HIS:HA	3:A:224:GLU:CD	2.39	0.42
3:A:288:ALA:C	3:A:290:THR:N	2.72	0.42
3:A:441:TYR:HB3	3:A:548:VAL:CG2	2.47	0.42
4:B:38:CYS:SG	4:B:130:PHE:HE2	2.42	0.42
4:B:339:TYR:HE2	4:B:341:ILE:HD11	1.83	0.42
4:B:380:ILE:O	4:B:382:ILE:N	2.52	0.42
3:A:50:ILE:HD12	3:A:54:ASN:CB	2.43	0.42
3:A:293:ILE:HG13	3:A:294:PRO:N	2.34	0.42
3:A:427:TYR:C	3:A:428:GLN:OE1	2.57	0.42
4:B:242:GLN:HB2	4:B:353:LYS:HZ1	1.83	0.42
3:A:221:HIS:H	3:A:221:HIS:HD2	1.61	0.42
3:A:367:GLN:C	3:A:369:THR:N	2.73	0.42
4:B:77:PHE:O	4:B:79:GLU:N	2.52	0.42
4:B:198:HIS:O	4:B:202:ILE:HG12	2.20	0.42
3:A:77:PHE:CE2	3:A:150:PRO:HB2	2.54	0.42
3:A:215:THR:O	3:A:217:PRO:HD3	2.19	0.42
3:A:239:TRP:CE3	3:A:240:THR:CA	3.02	0.42
3:A:392:PRO:N	3:A:417:VAL:HG12	2.34	0.42
3:A:434:ILE:HB	3:A:494:ASN:HD21	1.85	0.42
4:B:24:TRP:HH2	4:B:61:PHE:CE1	2.37	0.42
4:B:38:CYS:O	4:B:47:ILE:HD11	2.20	0.42
4:B:72:ARG:HH11	4:B:72:ARG:CG	2.27	0.42
4:B:174:GLN:O	4:B:175:ASN:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:342:TYR:CB	4:B:348:ASN:HA	2.49	0.42
3:A:80:LEU:HD12	3:A:80:LEU:O	2.20	0.42
3:A:294:PRO:O	3:A:294:PRO:HG2	2.20	0.42
4:B:140:PRO:O	4:B:142:ILE:HD13	2.19	0.42
4:B:203:GLU:OE2	4:B:206:ARG:HD2	2.20	0.42
1:T:713:DC:H2'	1:T:714:DG:C8	2.55	0.42
3:A:432:GLU:CD	3:A:433:PRO:HD2	2.40	0.42
4:B:115:TYR:CE1	4:B:156:SER:HB3	2.55	0.42
4:B:143:ARG:O	4:B:144:TYR:CD2	2.73	0.42
1:T:705:DT:H2''	1:T:706:DC:C5'	2.50	0.42
3:A:382:ILE:HG22	3:A:383:TRP:CE2	2.55	0.42
4:B:263:LYS:C	4:B:265:ASN:H	2.23	0.42
4:B:332:GLN:NE2	4:B:425:LEU:CD1	2.83	0.42
4:B:13:LYS:HE3	4:B:85:GLN:HG2	2.02	0.42
4:B:73:LYS:O	4:B:74:LEU:HB2	2.20	0.42
4:B:164:MET:O	4:B:165:THR:C	2.58	0.42
4:B:279:LEU:HD11	4:B:303:LEU:HA	2.02	0.42
3:A:228:LEU:HD22	3:A:228:LEU:HA	1.83	0.41
3:A:274:ILE:C	3:A:275:LYS:HG3	2.39	0.41
3:A:391:LEU:HD12	3:A:414:TRP:CD2	2.55	0.41
3:A:417:VAL:HG22	3:A:419:THR:HG21	2.00	0.41
4:B:16:MET:HB3	4:B:17:ASP:H	1.63	0.41
4:B:356:ARG:HG3	4:B:367:GLN:HE21	1.85	0.41
3:A:287:LYS:HG3	3:A:291:GLU:OE1	2.19	0.41
4:B:141:GLY:C	4:B:142:ILE:HD13	2.41	0.41
4:B:242:GLN:HB3	4:B:353:LYS:HZ2	1.86	0.41
4:B:368:LEU:O	4:B:371:ALA:HB3	2.20	0.41
4:B:401:TRP:O	4:B:402:TRP:C	2.59	0.41
3:A:194:GLU:C	3:A:196:GLY:N	2.74	0.41
3:A:231:GLY:O	3:A:242:GLN:HG3	2.19	0.41
3:A:249:LYS:HG3	3:A:252:TRP:NE1	2.35	0.41
3:A:279:LEU:O	3:A:282:LEU:CB	2.69	0.41
3:A:363:ASN:O	3:A:367:GLN:HG3	2.20	0.41
3:A:398:TRP:C	3:A:400:THR:N	2.73	0.41
4:B:243:PRO:C	4:B:244:ILE:HD13	2.39	0.41
4:B:344:GLU:OE1	4:B:344:GLU:HA	2.20	0.41
2:P:805:DG:H2'	2:P:806:DT:O5'	2.21	0.41
3:A:72:ARG:CD	3:A:74:LEU:HD21	2.51	0.41
3:A:441:TYR:O	3:A:457:TYR:HA	2.19	0.41
4:B:54:ASN:HB3	4:B:143:ARG:NH2	2.35	0.41
4:B:341:ILE:H	4:B:341:ILE:HG13	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:LEU:HD11	3:A:264:LEU:HD12	2.03	0.41
3:A:279:LEU:O	3:A:282:LEU:HB2	2.20	0.41
3:A:398:TRP:O	3:A:400:THR:N	2.54	0.41
3:A:522:ILE:O	3:A:525:LEU:N	2.54	0.41
3:A:546:GLU:OE2	3:A:550:LYS:HB2	2.20	0.41
4:B:21:VAL:HG12	4:B:59:PRO:CG	2.51	0.41
4:B:66:LYS:HB2	4:B:407:GLN:HE21	1.84	0.41
4:B:128:THR:OG1	4:B:146:TYR:HB2	2.19	0.41
3:A:106:VAL:CG1	3:A:107:THR:N	2.84	0.41
4:B:63:ILE:HG21	4:B:407:GLN:HA	2.02	0.41
4:B:194:GLU:HB3	4:B:197:GLN:NE2	2.35	0.41
4:B:195:ILE:C	4:B:197:GLN:H	2.23	0.41
4:B:313:PRO:O	4:B:314:VAL:O	2.39	0.41
4:B:417:VAL:CG2	4:B:418:ASN:N	2.83	0.41
3:A:224:GLU:O	3:A:225:PRO:C	2.57	0.41
3:A:336:GLN:O	3:A:337:TRP:CD1	2.74	0.41
3:A:391:LEU:HD12	3:A:414:TRP:CG	2.56	0.41
4:B:115:TYR:HE1	4:B:157:PRO:N	2.19	0.41
4:B:189:VAL:HB	4:B:202:ILE:HD11	2.01	0.41
4:B:241:VAL:CG1	4:B:242:GLN:H	2.33	0.41
3:A:210:LEU:HA	3:A:214:LEU:O	2.21	0.41
3:A:339:TYR:CG	3:A:375:ILE:HD11	2.55	0.41
3:A:341:ILE:CG2	3:A:342:TYR:N	2.83	0.41
4:B:132:ILE:HG22	4:B:133:PRO:N	2.34	0.41
4:B:267:ALA:N	4:B:426:TRP:HE1	2.18	0.41
4:B:425:LEU:C	4:B:427:TYR:H	2.22	0.41
3:A:65:LYS:HE2	3:A:72:ARG:HB2	2.03	0.41
3:A:107:THR:HA	3:A:227:PHE:CE2	2.55	0.41
3:A:175:ASN:N	3:A:176:PRO:HD3	2.35	0.41
3:A:194:GLU:O	3:A:195:ILE:C	2.58	0.41
3:A:249:LYS:HB2	3:A:250:ASP:H	1.74	0.41
3:A:306:ASN:HA	3:A:309:ILE:CD1	2.51	0.41
3:A:473:THR:C	3:A:475:GLN:N	2.75	0.41
4:B:50:ILE:CG2	4:B:145:GLN:HB2	2.49	0.41
4:B:189:VAL:HG11	4:B:202:ILE:HD13	2.03	0.41
4:B:194:GLU:O	4:B:198:HIS:N	2.49	0.41
4:B:216:THR:HA	4:B:217:PRO:HD3	1.96	0.41
3:A:281:LYS:C	3:A:283:LEU:H	2.23	0.41
3:A:459:THR:C	3:A:461:LYS:H	2.24	0.41
3:A:94:ILE:HG22	3:A:95:PRO:O	2.20	0.40
3:A:95:PRO:HB2	3:A:229:TRP:HH2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:341:ILE:O	3:A:342:TYR:HB3	2.21	0.40
6:A:823:TNV:H6'1	6:A:823:TNV:H9'1	1.51	0.40
4:B:169:GLU:C	4:B:171:PHE:N	2.75	0.40
4:B:279:LEU:HD11	4:B:303:LEU:CA	2.52	0.40
4:B:368:LEU:HD11	4:B:392:PRO:HD2	2.02	0.40
2:P:805:DG:H2'	2:P:806:DT:O4'	2.20	0.40
3:A:181:TYR:CD2	4:B:138:GLU:HA	2.56	0.40
3:A:226:PRO:HG2	3:A:226:PRO:O	2.21	0.40
3:A:262:GLY:O	3:A:265:ASN:HB2	2.22	0.40
3:A:367:GLN:O	3:A:369:THR:N	2.55	0.40
3:A:416:PHE:HZ	3:A:422:LEU:HD11	1.86	0.40
4:B:7:THR:HG22	4:B:119:PRO:HG2	2.03	0.40
4:B:8:VAL:O	4:B:8:VAL:HG23	2.22	0.40
4:B:57:ASN:HA	4:B:129:ALA:O	2.22	0.40
4:B:112:GLY:HA2	4:B:115:TYR:CE2	2.57	0.40
4:B:410:TRP:O	4:B:411:ILE:HG13	2.21	0.40
4:B:423:VAL:HG21	4:B:426:TRP:CH2	2.56	0.40
1:T:705:DT:H2''	1:T:706:DC:H5'	2.04	0.40
1:T:714:DG:C5'	3:A:286:THR:HG23	2.51	0.40
2:P:805:DG:C2'	2:P:806:DT:O5'	2.69	0.40
3:A:27:THR:HG1	3:A:29:GLU:HB3	1.85	0.40
3:A:65:LYS:O	3:A:68:SER:N	2.55	0.40
3:A:272:PRO:HG3	3:A:351:THR:HG21	2.02	0.40
4:B:162:SER:C	4:B:164:MET:N	2.74	0.40
4:B:206:ARG:HH22	4:B:216:THR:CG2	2.34	0.40
4:B:408:ALA:C	4:B:410:TRP:N	2.74	0.40
3:A:443:ASP:OD1	3:A:444:GLY:N	2.55	0.40
4:B:13:LYS:CD	4:B:86:ASP:H	2.35	0.40
4:B:255:ASN:HD21	4:B:259:LYS:HE2	1.83	0.40
4:B:278:GLN:O	4:B:299:ALA:HB2	2.22	0.40
3:A:34:LEU:CD1	3:A:62:ALA:HB2	2.51	0.40
3:A:198:HIS:CD2	3:A:198:HIS:C	2.95	0.40
3:A:385:LYS:HE3	3:A:385:LYS:HB2	1.66	0.40
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.57	0.40
3:A:495:ILE:O	3:A:533:LEU:HD12	2.22	0.40
4:B:319:TYR:CE2	4:B:383:TRP:HD1	2.40	0.40
4:B:365:VAL:HG12	4:B:393:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	552/558 (99%)	410 (74%)	112 (20%)	30 (5%)	2	11
4	B	410/437 (94%)	278 (68%)	95 (23%)	37 (9%)	1	3
All	All	962/995 (97%)	688 (72%)	207 (22%)	67 (7%)	1	6

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	77	PHE
3	A	154	LYS
3	A	268	SER
3	A	345	PRO
3	A	438	GLU
3	A	471	ASN
4	B	4	PRO
4	B	115	TYR
4	B	125	ARG
4	B	245	VAL
4	B	314	VAL
4	B	425	LEU
3	A	5	ILE
3	A	14	PRO
3	A	334	GLN
3	A	541	GLY
3	A	546	GLU
4	B	45	GLY
4	B	95	PRO
4	B	104	LYS
4	B	282	LEU
4	B	409	THR
3	A	68	SER
3	A	427	TYR
3	A	485	ALA

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Mol	Chain	Res	Type
4	B	93	GLY
4	B	163	SER
4	B	239	TRP
4	B	289	LEU
4	B	383	TRP
4	B	395	LYS
4	B	399	GLU
3	A	121	ASP
3	A	128	THR
3	A	157	PRO
3	A	184	MET
3	A	219	LYS
3	A	298	GLU
3	A	377	THR
3	A	412	PRO
3	A	472	THR
3	A	494	ASN
4	B	98	ALA
4	B	256	ASP
4	B	277	ARG
4	B	286	THR
3	A	66	LYS
3	A	196	GLY
3	A	537	PRO
4	B	61	PHE
4	B	260	LEU
4	B	283	LEU
4	B	368	LEU
4	B	379	SER
4	B	381	VAL
4	B	414	TRP
4	B	424	LYS
3	A	195	ILE
3	A	224	GLU
4	B	123	ASP
4	B	133	PRO
3	A	462	GLY
4	B	148	VAL
4	B	157	PRO
4	B	25	PRO
4	B	170	PRO
4	B	175	ASN

### 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	
3	A	495/498 (99%)	437 (88%)	58 (12%)	5	22
4	B	376/397 (95%)	343 (91%)	33 (9%)	10	36
All	All	871/895 (97%)	780 (90%)	91 (10%)	7	27

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	7	THR
3	A	14	PRO
3	A	27	THR
3	A	53	GLU
3	A	58	THR
3	A	61	PHE
3	A	83	ARG
3	A	91	GLN
3	A	94	ILE
3	A	107	THR
3	A	108	VAL
3	A	109	LEU
3	A	118	VAL
3	A	120	LEU
3	A	121	ASP
3	A	136	ASN
3	A	138	GLU
3	A	142	ILE
3	A	150	PRO
3	A	151	GLN
3	A	157	PRO
3	A	165	THR
3	A	179	VAL
3	A	193	LEU
3	A	197	GLN
3	A	202	ILE
3	A	205	LEU

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Mol	Chain	Res	Type
3	A	206	ARG
3	A	211	ARG
3	A	221	HIS
3	A	228	LEU
3	A	236	PRO
3	A	246	LEU
3	A	250	ASP
3	A	258	CYS
3	A	268	SER
3	A	290	THR
3	A	293	ILE
3	A	294	PRO
3	A	295	LEU
3	A	298	GLU
3	A	314	VAL
3	A	340	GLN
3	A	345	PRO
3	A	354	TYR
3	A	357	MET
3	A	362	THR
3	A	386	THR
3	A	419	THR
3	A	423	VAL
3	A	425	LEU
3	A	428	GLN
3	A	431	LYS
3	A	515	SER
3	A	517	LEU
3	A	520	GLN
3	A	524	GLN
3	A	547	GLN
4	B	24	TRP
4	B	34	LEU
4	B	46	LYS
4	B	53	GLU
4	B	86	ASP
4	B	100	LEU
4	B	123	ASP
4	B	133	PRO
4	B	184	MET
4	B	185	ASP
4	B	189	VAL

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Mol	Chain	Res	Type
4	B	193	LEU
4	B	197	GLN
4	B	200	THR
4	B	201	LYS
4	B	212	TRP
4	B	235	HIS
4	B	239	TRP
4	B	242	GLN
4	B	253	THR
4	B	255	ASN
4	B	283	LEU
4	B	289	LEU
4	B	297	GLU
4	B	324	ASP
4	B	336	GLN
4	B	349	LEU
4	B	350	LYS
4	B	353	LYS
4	B	389	PHE
4	B	414	TRP
4	B	426	TRP
4	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	91	GLN
3	A	161	GLN
3	A	221	HIS
3	A	242	GLN
3	A	255	ASN
3	A	269	GLN
3	A	315	HIS
3	A	330	GLN
3	A	332	GLN
3	A	340	GLN
3	A	373	GLN
3	A	447	ASN
3	A	480	GLN
3	A	487	GLN
3	A	494	ASN
3	A	500	GLN

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Mol	Chain	Res	Type
3	A	509	GLN
3	A	519	ASN
3	A	547	GLN
4	B	91	GLN
4	B	147	ASN
4	B	174	GLN
4	B	175	ASN
4	B	197	GLN
4	B	242	GLN
4	B	278	GLN
4	B	330	GLN
4	B	340	GLN
4	B	361	HIS
4	B	407	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
2	MRG	P	817	1,2	18,24,29	1.45	3 (16%)	19,35,42	2.71	5 (26%)
2	DDG	P	822	1,2	17,23,24	1.19	2 (11%)	15,33,36	3.01	5 (33%)

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
2	MRG	P	817	1,2	-	0/3/21/27	0/3/3/3
2	DDG	P	822	1,2	-	0/3/18/19	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	817	MRG	C6-N1	4.56	1.41	1.33
2	P	822	DDG	C6-N1	3.68	1.39	1.33
2	P	817	MRG	C2-N1	2.38	1.39	1.35
2	P	817	MRG	C8-N7	-2.18	1.30	1.34
2	P	822	DDG	C8-N7	-2.12	1.30	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	822	DDG	C5-C6-N1	-8.63	111.62	123.43
2	P	817	MRG	C5-C6-N1	-8.60	111.66	123.43
2	P	822	DDG	C6-N1-C2	5.87	125.25	115.93
2	P	817	MRG	C6-N1-C2	5.67	124.94	115.93
2	P	822	DDG	C2-N3-C4	-3.01	111.92	115.36
2	P	817	MRG	O3'-C3'-C2'	-2.97	100.28	110.90
2	P	817	MRG	N3-C2-N1	-2.95	123.29	127.22
2	P	817	MRG	C2-N3-C4	-2.89	112.05	115.36
2	P	822	DDG	N3-C2-N1	-2.59	123.76	127.22
2	P	822	DDG	C6-C5-C4	-2.50	118.41	120.80

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
2	P	817	MRG	3	0
2	P	822	DDG	2	0

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	B	438	-	5,5,5	0.79	0	5,5,5	1.99	2 (40%)
7	GOL	A	824	-	5,5,5	1.22	0	5,5,5	2.00	2 (40%)
7	GOL	B	439	-	5,5,5	0.97	0	5,5,5	1.95	2 (40%)
7	GOL	A	826	-	5,5,5	1.02	0	5,5,5	1.96	2 (40%)
7	GOL	A	825	-	5,5,5	1.16	0	5,5,5	1.97	2 (40%)
6	TNV	A	823	5	22,28,28	1.61	5 (22%)	20,43,43	1.56	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	438	-	-	2/4/4/4	-
7	GOL	A	824	-	-	3/4/4/4	-
7	GOL	B	439	-	-	2/4/4/4	-
7	GOL	A	826	-	-	3/4/4/4	-
7	GOL	A	825	-	-	2/4/4/4	-
6	TNV	A	823	5	-	8/17/22/22	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	823	TNV	O9'-C9'	-3.64	1.37	1.42
6	A	823	TNV	PA-O3A	-3.02	1.55	1.58
6	A	823	TNV	C6'-N9	-2.96	1.45	1.48
6	A	823	TNV	C2-N3	2.52	1.36	1.32
6	A	823	TNV	C2-N1	2.03	1.37	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	823	TNV	PB-O3A-PA	-3.91	120.17	132.56
6	A	823	TNV	PB-O3B-PG	-3.05	122.35	132.83
6	A	823	TNV	C5-C6-N6	3.04	124.97	120.35
7	B	438	GOL	C3-C2-C1	2.95	123.18	111.70
7	A	825	GOL	O2-C2-C1	2.95	122.10	109.12
7	B	439	GOL	O2-C2-C1	2.89	121.84	109.12
7	A	826	GOL	O2-C2-C1	2.88	121.82	109.12
7	A	824	GOL	C3-C2-C1	2.86	122.84	111.70
7	A	824	GOL	O2-C2-C1	2.85	121.68	109.12
7	A	826	GOL	C3-C2-C1	2.78	122.50	111.70
7	A	825	GOL	C3-C2-C1	2.77	122.47	111.70
7	B	438	GOL	O2-C2-C1	2.71	121.07	109.12
7	B	439	GOL	C3-C2-C1	2.71	122.25	111.70

There are no chirality outliers.

All (20) torsion outliers are listed below:

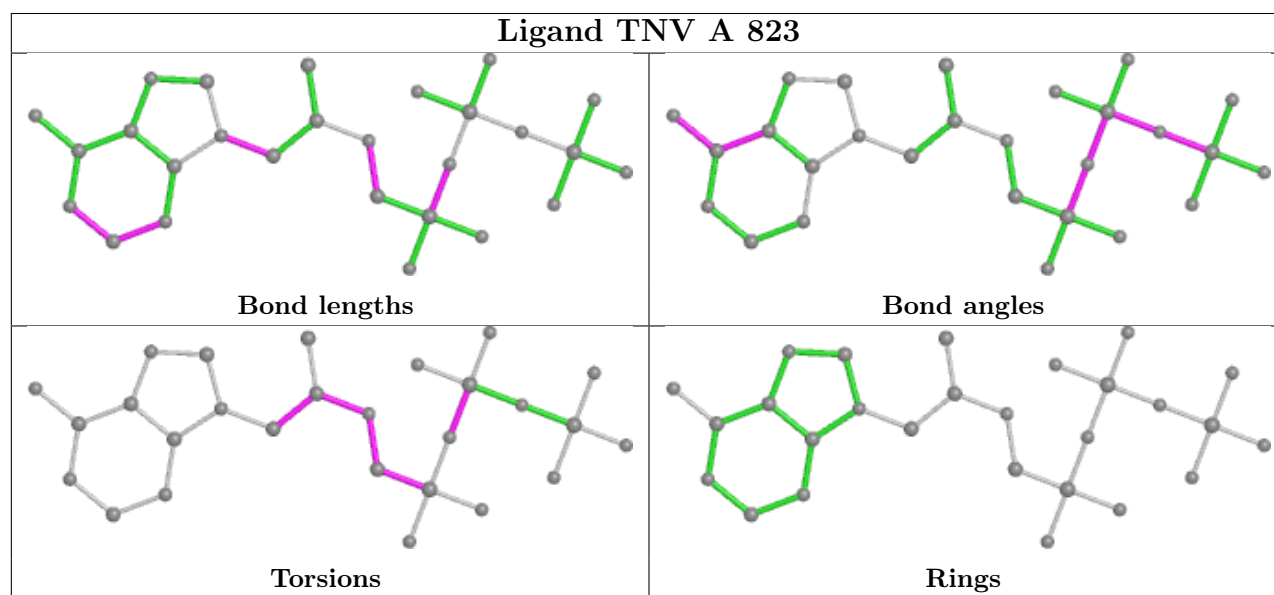
Mol	Chain	Res	Type	Atoms
6	A	823	TNV	O9'-C9'-PA-O2A
6	A	823	TNV	O9'-C9'-PA-O3A
6	A	823	TNV	C6'-C7'-O9'-C9'
6	A	823	TNV	N9-C6'-C7'-O9'
6	A	823	TNV	N9-C6'-C7'-C8'
7	A	824	GOL	C1-C2-C3-O3
7	A	825	GOL	O1-C1-C2-C3
7	A	825	GOL	C1-C2-C3-O3
7	A	826	GOL	C1-C2-C3-O3
7	B	438	GOL	C1-C2-C3-O3
7	B	439	GOL	O1-C1-C2-C3
7	B	439	GOL	C1-C2-C3-O3
7	B	438	GOL	O1-C1-C2-O2
7	A	826	GOL	O1-C1-C2-C3
7	A	824	GOL	O1-C1-C2-O2
7	A	826	GOL	O1-C1-C2-O2
6	A	823	TNV	O9'-C9'-PA-O1A
6	A	823	TNV	PA-O3A-PB-O2B
6	A	823	TNV	PA-C9'-O9'-C7'
7	A	824	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	438	GOL	1	0
7	A	824	GOL	4	0
7	B	439	GOL	1	0
7	A	825	GOL	1	0
6	A	823	TNV	7	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	T	24/27 (88%)	-0.26	0	100	100	42, 100, 120, 120	0
2	P	18/21 (85%)	-0.29	0	100	100	42, 104, 120, 120	0
3	A	554/558 (99%)	-0.27	3 (0%)	91	75	13, 71, 119, 120	0
4	B	414/437 (94%)	-0.02	15 (3%)	42	17	30, 100, 120, 120	0
All	All	1010/1043 (96%)	-0.17	18 (1%)	68	40	13, 86, 120, 120	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	3	SER	9.3
4	B	4	PRO	5.9
4	B	5	ILE	4.5
4	B	279	LEU	3.5
4	B	358	ARG	3.4
4	B	195	ILE	2.8
3	A	479	LEU	2.7
4	B	190	GLY	2.5
4	B	327	ALA	2.5
4	B	426	TRP	2.4
4	B	264	LEU	2.4
4	B	6	GLU	2.4
4	B	189	VAL	2.3
4	B	303	LEU	2.3
3	A	454	LYS	2.2
3	A	542	ILE	2.0
4	B	318	TYR	2.0
4	B	359	GLY	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
2	MRG	P	817	22/27	0.94	0.12	37,60,89,98	0
2	DDG	P	822	21/22	0.96	0.19	39,53,60,74	0

## 6.3 Carbohydrates [i](#)

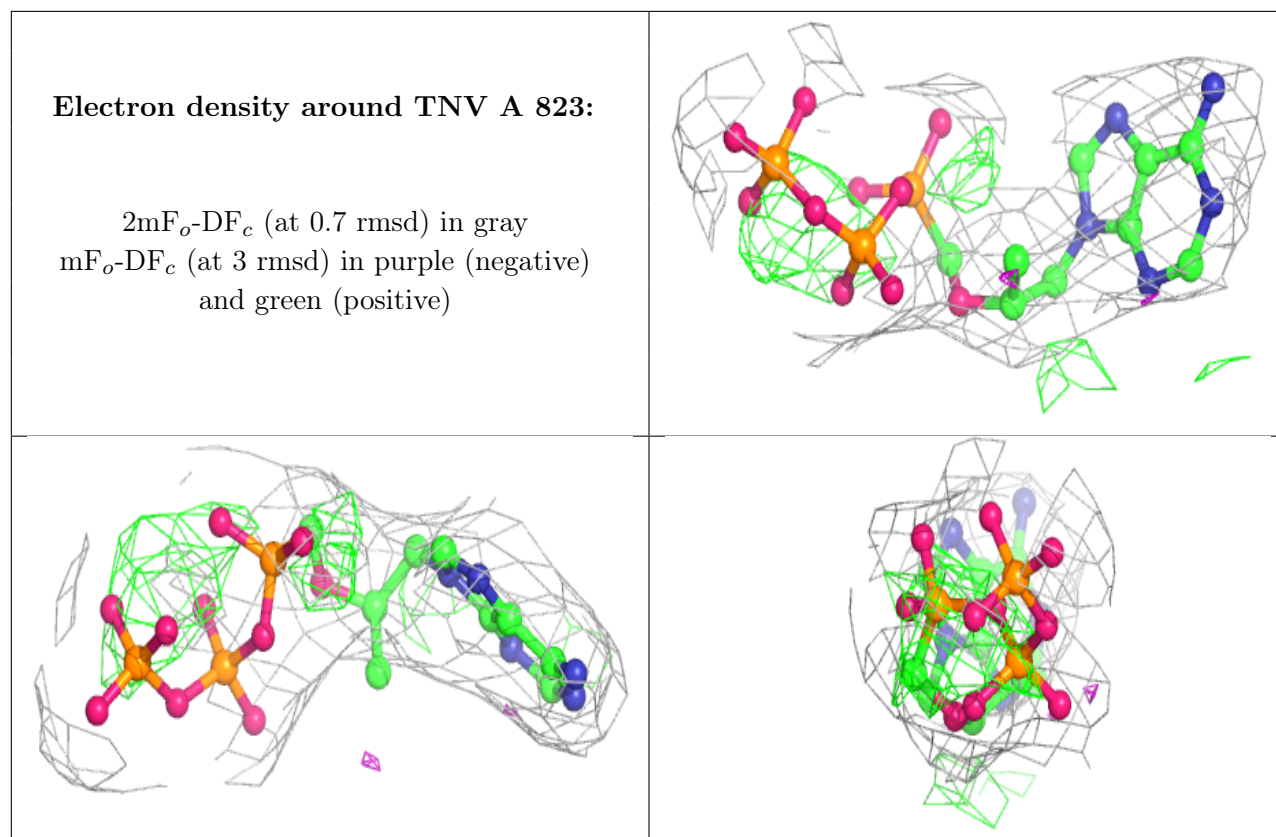
There are no monosaccharides in this entry.

## 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
7	GOL	A	824	6/6	0.83	0.25	54,58,60,63	6
7	GOL	A	826	6/6	0.85	0.28	36,42,49,50	6
7	GOL	A	825	6/6	0.87	0.18	45,59,68,81	6
7	GOL	B	439	6/6	0.89	0.48	63,70,74,75	6
7	GOL	B	438	6/6	0.90	0.47	56,70,72,74	6
5	MG	A	600	1/1	0.90	0.21	16,16,16,16	0
5	MG	A	601	1/1	0.94	0.24	73,73,73,73	0
6	TNV	A	823	27/27	0.96	0.21	34,54,64,71	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.