



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:44 am GMT

PDB ID : 1R0A
Title : Crystal structure of HIV-1 reverse transcriptase covalently tethered to DNA template-primer solved to 2.8 angstroms
Authors : Tuske, S.; Ding, J.; Arnold, E.
Deposited on : 2003-09-19
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

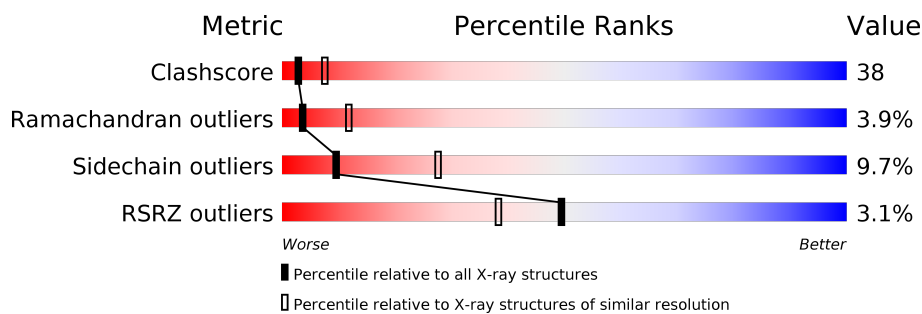
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>11%</div> <div>7%</div> <div>74%</div> <div>7%</div> <div>11%</div> </div>
2	P	21	<div> <div>5%</div> <div>14%</div> <div>67%</div> <div>14%</div> <div>5%</div> </div>
3	A	558	<div> <div>4%</div> <div>37%</div> <div>53%</div> <div>9%</div> <div>.</div> </div>
4	B	429	<div> <div>3%</div> <div>40%</div> <div>53%</div> <div>7%</div> </div>
5	L	211	<div> <div>36%</div> <div>55%</div> <div>9%</div> </div>
6	H	225	<div> <div>3%</div> <div>56%</div> <div>38%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	MG	A	559	-	-	-	X
9	GOL	B	3001	-	X	-	-
9	GOL	P	3002	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12292 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 5'-D(*A*TP*GP*CP*AP*TP*CP*GP*GP*CP*GP*CP*TP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*GP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	24	Total	C	N	O	P	0	0	0
			493	233	97	140	23			

- Molecule 2 is a DNA chain called 5'-D(*C*CP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*AP*GP*CP*GP*CP*CP*GP*(2DA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	20	Total	C	N	O	P	0	0	0
			402	192	72	119	19			

- Molecule 3 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	558	Total	C	N	O	S	15	0	0
			4482	2901	741	832	8			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	429	Total	C	N	O	S	4	0	0
			3534	2304	586	637	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

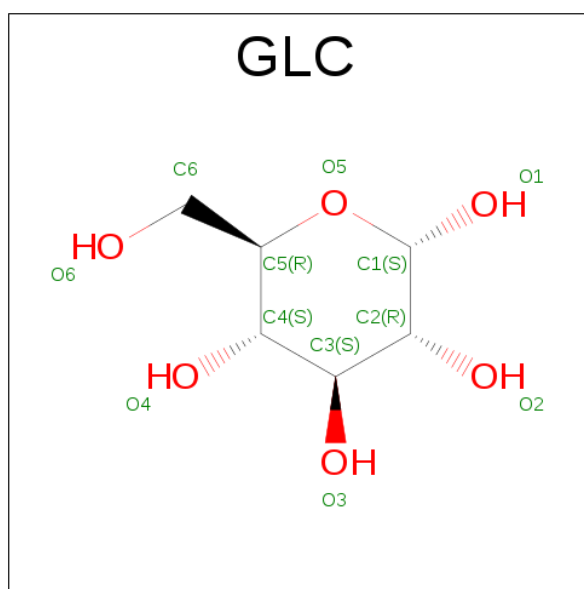
- Molecule 5 is a protein called monoclonal antibody (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	211	Total	C	N	O	S	0	0	0
			1643	1025	270	342	6			

- Molecule 6 is a protein called monoclonal antibody (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	225	Total	C	N	O	S	0	0	0
			1685	1060	276	340	9			

- Molecule 7 is SUGAR (GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	P	1	Total	C	O	0	0
			6	3	3		

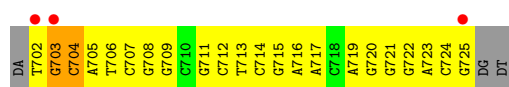
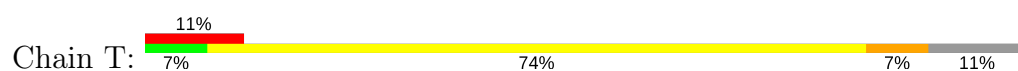
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	7	Total	O	0	0
			7	7		
10	B	15	Total	O	0	0
			15	15		
10	H	3	Total	O	0	0
			3	3		
10	L	2	Total	O	0	0
			2	2		
10	T	1	Total	O	0	0
			1	1		

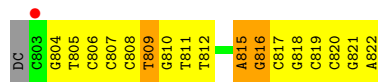
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

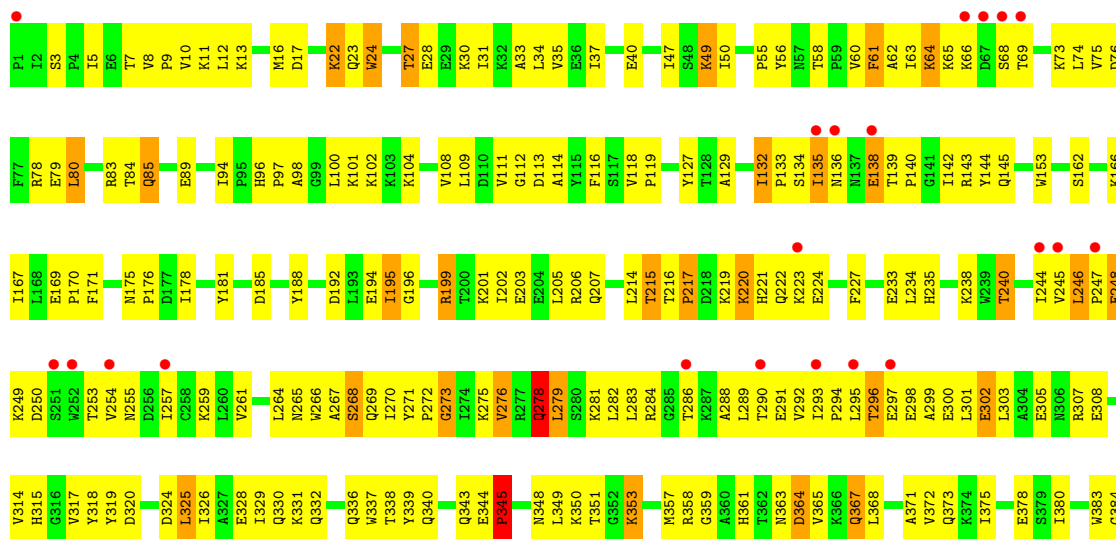
- Molecule 1: 5'-D(*A*TP*GP*CP*AP*TP*CP*GP*GP*CP*GP*CP*TP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*GP*GP*T)-3'



- Molecule 2: 5'-D(*C*CP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*AP*GP*CP*GP*CP*CP*GP*(2DA))-3'

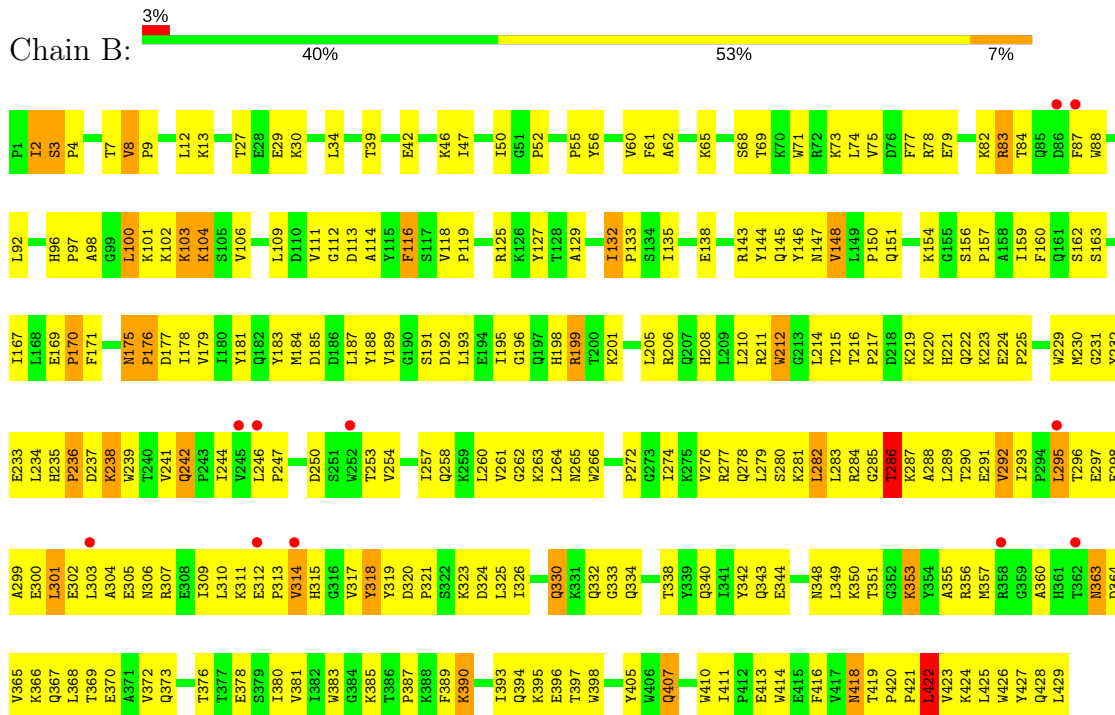


- Molecule 3: Reverse transcriptase





• Molecule 4: Reverse transcriptase

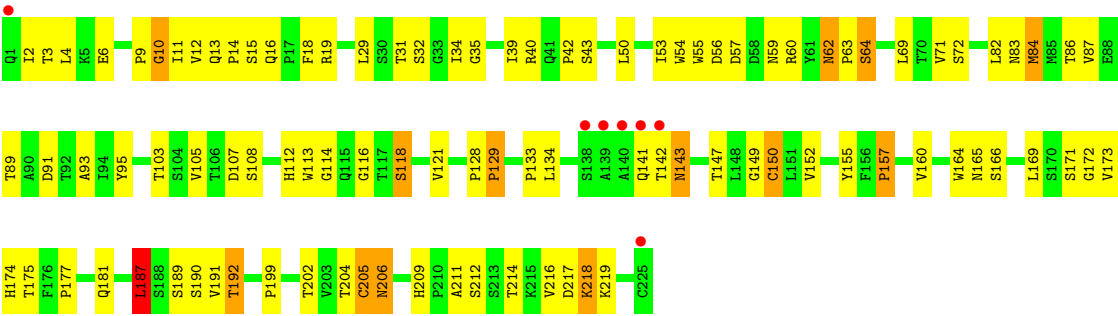


• Molecule 5: monoclonal antibody (light chain)



• Molecule 6: monoclonal antibody (heavy chain)





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	165.82Å 165.82Å 220.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.80 39.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.96-2.80) 94.6 (39.20-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.239 , 0.272 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, MG, GLC, 2DA

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	0.77	1/554 (0.2%)	1.12	3/854 (0.4%)
2	P	0.69	0/426	1.02	3/655 (0.5%)
3	A	0.51	1/4600 (0.0%)	0.76	1/6259 (0.0%)
4	B	0.59	0/3639	0.79	1/4949 (0.0%)
5	L	0.52	0/1681	0.78	1/2283 (0.0%)
6	H	0.53	0/1729	0.80	1/2372 (0.0%)
All	All	0.56	2/12629 (0.0%)	0.81	10/17372 (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
4	B	0	2
5	L	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	248	GLU	CD-OE2	6.89	1.33	1.25
1	T	703	DG	O3'-P	5.73	1.68	1.61

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	704	DC	O5'-P-OP1	-14.16	92.96	105.70
2	P	816	DG	N9-C1'-C2'	7.49	126.83	112.60
2	P	815	DA	N9-C1'-C2'	7.13	126.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	187	LEU	CA-CB-CG	6.72	130.75	115.30
3	A	289	LEU	N-CA-C	5.74	126.50	111.00
5	L	6	GLN	N-CA-C	-5.50	96.14	111.00
4	B	390	LYS	N-CA-C	-5.38	96.49	111.00
1	T	703	DG	O4'-C1'-N9	5.25	111.68	108.00
1	T	703	DG	C3'-C2'-C1'	-5.24	96.21	102.50
2	P	809	DT	C5'-C4'-C3'	-5.13	104.86	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	188	TYR	Sidechain
4	B	405	TYR	Sidechain
5	L	49	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	493	0	269	38	0
2	P	402	0	226	23	0
3	A	4482	0	4485	400	0
4	B	3534	0	3568	270	2
5	L	1643	0	1565	136	0
6	H	1685	0	1640	92	0
7	H	12	0	12	2	0
8	A	1	0	0	0	0
9	B	6	0	4	0	0
9	P	6	0	4	0	0
10	A	7	0	0	1	0
10	B	15	0	0	0	0
10	H	3	0	0	0	0
10	L	2	0	0	0	0
10	T	1	0	0	0	0
All	All	12292	0	11773	918	2

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 38.

All (918) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:703:DG:H1'	1:T:704:DC:OP1	1.50	1.11
3:A:498:ASP:HB2	3:A:538:ALA:HB2	1.17	1.10
3:A:22:LYS:H	3:A:22:LYS:HD3	1.12	1.09
1:T:721:DG:H2''	1:T:722:DG:H5''	1.10	1.08
4:B:296:THR:HG22	4:B:298:GLU:H	1.09	1.07
3:A:246:LEU:H	3:A:246:LEU:HD23	1.17	1.07
4:B:261:VAL:HG13	4:B:276:VAL:HG11	1.37	1.06
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.36	1.05
3:A:104:LYS:HB2	3:A:192:ASP:HA	1.39	1.05
1:T:721:DG:C2'	1:T:722:DG:H5''	1.87	1.04
3:A:293:ILE:HD12	3:A:294:PRO:HD2	1.38	1.01
4:B:330:GLN:HE22	4:B:340:GLN:HE22	1.05	1.01
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.39	1.00
3:A:459:THR:HG23	3:A:463:ARG:HB3	1.44	1.00
1:T:703:DG:H1'	1:T:704:DC:P	2.01	0.99
3:A:5:ILE:HD11	3:A:167:ILE:HD11	1.45	0.98
1:T:721:DG:H2''	1:T:722:DG:C5'	1.95	0.95
3:A:440:PHE:HE2	3:A:489:SER:HG	0.94	0.94
5:L:15:LEU:HD12	5:L:15:LEU:H	1.30	0.94
3:A:13:LYS:HD2	3:A:16:MET:HE1	1.49	0.94
5:L:34:ASN:HD22	5:L:89:GLN:HE22	1.08	0.94
3:A:248:GLU:HB3	3:A:307:ARG:HH22	1.31	0.93
3:A:498:ASP:CB	3:A:538:ALA:HB2	1.99	0.92
6:H:165:ASN:HB2	6:H:169:LEU:HD13	1.51	0.92
4:B:260:LEU:HD21	4:B:303:LEU:HD13	1.52	0.92
5:L:90:GLN:HE21	5:L:92:SER:H	1.09	0.92
4:B:330:GLN:HE22	4:B:340:GLN:NE2	1.69	0.90
3:A:278:GLN:HG3	3:A:302:GLU:CB	2.02	0.90
3:A:111:VAL:HG11	3:A:214:LEU:HD12	1.54	0.90
3:A:406:TRP:HE1	4:B:418:ASN:ND2	1.69	0.89
4:B:135:ILE:HD12	4:B:135:ILE:O	1.73	0.89
2:P:807:DC:H4'	3:A:448:ARG:HD2	1.55	0.89
3:A:550:LYS:HA	3:A:550:LYS:HE2	1.55	0.88
3:A:73:LYS:HB3	3:A:73:LYS:HZ2	1.37	0.88
3:A:3:SER:OG	3:A:5:ILE:HG13	1.74	0.87
4:B:296:THR:HG22	4:B:298:GLU:N	1.90	0.87
5:L:61:ARG:HB2	5:L:76:SER:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.10	0.86
3:A:253:THR:HA	3:A:292:VAL:HA	1.58	0.86
3:A:435:VAL:HG22	4:B:290:THR:CG2	2.06	0.85
1:T:713:DT:H2''	1:T:714:DC:H5'	1.59	0.85
3:A:296:THR:HG22	3:A:298:GLU:H	1.41	0.84
4:B:222:GLN:HG3	4:B:224:GLU:H	1.40	0.84
3:A:420:PRO:HG3	3:A:422:LEU:HG	1.56	0.84
5:L:195:GLU:HG2	5:L:206:VAL:HG22	1.59	0.84
4:B:257:ILE:O	4:B:261:VAL:HG23	1.79	0.83
6:H:84:MET:HG2	6:H:87:VAL:HG12	1.59	0.83
3:A:233:GLU:HB2	3:A:240:THR:HG23	1.58	0.83
3:A:24:TRP:HZ3	3:A:61:PHE:HB3	1.44	0.83
3:A:246:LEU:H	3:A:246:LEU:CD2	1.91	0.83
2:P:809:DT:H2''	2:P:810:DG:C8	2.14	0.82
3:A:34:LEU:HD21	3:A:62:ALA:HB2	1.58	0.82
4:B:61:PHE:CZ	4:B:74:LEU:HD23	2.14	0.82
4:B:266:TRP:HH2	4:B:422:LEU:HD22	1.46	0.81
6:H:141:GLN:OE1	6:H:199:PRO:HD3	1.80	0.81
4:B:332:GLN:HG2	4:B:427:TYR:CD1	2.16	0.80
5:L:147:LYS:NZ	5:L:149:LYS:HD2	1.96	0.80
4:B:175:ASN:N	4:B:176:PRO:HD3	1.97	0.80
3:A:450:THR:O	3:A:451:LYS:HG2	1.80	0.80
3:A:406:TRP:HE1	4:B:418:ASN:HD21	1.27	0.80
3:A:303:LEU:O	3:A:307:ARG:HG3	1.82	0.79
4:B:106:VAL:HG13	4:B:234:LEU:HB2	1.65	0.79
5:L:155:ARG:HE	5:L:157:ASN:HB2	1.45	0.79
3:A:199:ARG:NH2	3:A:220:LYS:HE2	1.98	0.79
3:A:498:ASP:HB2	3:A:538:ALA:CB	2.09	0.79
5:L:90:GLN:HE21	5:L:92:SER:N	1.80	0.79
2:P:818:DG:H2'	2:P:819:DC:C6	2.19	0.78
3:A:466:VAL:HG21	3:A:551:LEU:HG	1.63	0.78
3:A:439:THR:HG21	4:B:289:LEU:H	1.49	0.77
3:A:317:VAL:HG22	3:A:318:TYR:N	2.00	0.76
3:A:466:VAL:O	3:A:466:VAL:HG12	1.84	0.76
4:B:261:VAL:HG13	4:B:276:VAL:CG1	2.13	0.76
3:A:443:ASP:O	3:A:481:ALA:HB2	1.85	0.76
4:B:356:ARG:HE	4:B:360:ALA:CB	1.97	0.76
3:A:23:GLN:HE22	3:A:60:VAL:H	1.31	0.76
4:B:8:VAL:HG11	4:B:159:ILE:HG12	1.68	0.76
3:A:465:LYS:O	3:A:466:VAL:HG23	1.86	0.76
1:T:703:DG:C1'	1:T:704:DC:OP1	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:10:GLY:HA2	6:H:118:SER:O	1.87	0.75
1:T:722:DG:H2''	1:T:723:DA:H5'	1.68	0.75
3:A:420:PRO:HA	3:A:422:LEU:N	2.01	0.75
3:A:430:GLU:HB2	3:A:532:TYR:HB2	1.67	0.75
4:B:238:LYS:HD3	4:B:238:LYS:O	1.85	0.75
4:B:34:LEU:HD11	4:B:73:LYS:HG3	1.69	0.75
3:A:517:LEU:O	3:A:521:ILE:HG13	1.87	0.75
3:A:400:THR:O	3:A:403:THR:HG22	1.87	0.75
4:B:387:PRO:HG2	4:B:389:PHE:CE1	2.21	0.75
6:H:103:THR:HG21	7:H:1725:GLC:H4	1.69	0.74
6:H:53:ILE:HB	6:H:71:VAL:CG1	2.16	0.74
6:H:62:ASN:HD22	6:H:62:ASN:C	1.89	0.74
4:B:253:THR:O	4:B:257:ILE:HG12	1.87	0.74
4:B:317:VAL:HG12	4:B:349:LEU:HD23	1.68	0.74
3:A:478:GLU:OE1	3:A:498:ASP:OD1	2.05	0.74
3:A:460:ASN:ND2	4:B:288:ALA:HB2	2.03	0.74
3:A:253:THR:HG22	3:A:292:VAL:HG22	1.69	0.73
3:A:297:GLU:HA	3:A:300:GLU:HB2	1.70	0.73
4:B:266:TRP:CH2	4:B:422:LEU:HD22	2.22	0.73
6:H:160:VAL:HG21	6:H:187:LEU:HD11	1.68	0.73
3:A:533:LEU:N	3:A:533:LEU:HD12	2.02	0.73
3:A:555:GLY:O	3:A:556:ILE:HG13	1.88	0.73
4:B:254:VAL:HB	4:B:289:LEU:O	1.88	0.73
3:A:317:VAL:HG22	3:A:318:TYR:H	1.53	0.73
3:A:473:THR:O	3:A:476:LYS:N	2.21	0.73
3:A:491:LEU:HD23	3:A:529:GLU:OE2	1.88	0.73
4:B:356:ARG:HE	4:B:360:ALA:HB3	1.54	0.73
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.70	0.73
3:A:463:ARG:C	3:A:464:GLN:HE21	1.91	0.73
3:A:61:PHE:H	3:A:61:PHE:HD2	1.37	0.72
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.17	0.72
4:B:112:GLY:HA3	4:B:151:GLN:HE21	1.52	0.72
6:H:19:ARG:NH1	6:H:83:ASN:HD21	1.86	0.72
3:A:494:ASN:HB3	4:B:289:LEU:HD12	1.71	0.72
4:B:237:ASP:C	4:B:239:TRP:H	1.93	0.72
6:H:62:ASN:HD22	6:H:63:PRO:N	1.88	0.72
5:L:151:ASP:HA	5:L:191:SER:HB3	1.71	0.72
4:B:46:LYS:HD2	4:B:148:VAL:HG21	1.72	0.72
3:A:266:TRP:O	3:A:269:GLN:HG2	1.90	0.71
4:B:79:GLU:OE1	4:B:83:ARG:NH1	2.22	0.71
1:T:702:DT:H4'	1:T:703:DG:OP2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:713:DT:H2'	1:T:714:DC:C6	2.24	0.71
3:A:419:THR:H	3:A:422:LEU:HD21	1.55	0.71
5:L:17:ASP:O	5:L:77:ASN:HA	1.91	0.71
1:T:713:DT:H2'	1:T:714:DC:H6	1.56	0.71
3:A:64:LYS:HE2	3:A:66:LYS:NZ	2.06	0.71
5:L:34:ASN:OD1	5:L:49:TYR:HA	1.91	0.71
3:A:22:LYS:N	3:A:22:LYS:HD3	1.97	0.71
3:A:73:LYS:HB3	3:A:73:LYS:NZ	2.05	0.71
3:A:447:ASN:ND2	3:A:450:THR:HG23	2.06	0.70
3:A:175:ASN:HB3	3:A:178:ILE:HD12	1.72	0.70
3:A:275:LYS:HE3	3:A:332:GLN:OE1	1.91	0.70
6:H:18:PHE:CD2	6:H:87:VAL:HG11	2.26	0.70
3:A:279:LEU:H	3:A:279:LEU:CD2	2.05	0.70
5:L:4:MET:HE1	5:L:90:GLN:HB2	1.74	0.70
3:A:320:ASP:H	3:A:343:GLN:HE22	1.38	0.70
4:B:260:LEU:HG	4:B:264:LEU:HD12	1.72	0.70
3:A:7:THR:HG22	3:A:119:PRO:HB2	1.72	0.70
4:B:103:LYS:HE3	4:B:103:LYS:HA	1.74	0.69
4:B:175:ASN:H	4:B:176:PRO:HD3	1.56	0.69
1:T:703:DG:C1'	1:T:704:DC:P	2.80	0.69
4:B:363:ASN:HD22	4:B:363:ASN:C	1.95	0.69
5:L:105:GLU:OE2	5:L:173:TYR:OH	2.10	0.69
3:A:444:GLY:HA2	3:A:552:VAL:HG11	1.73	0.69
4:B:365:VAL:O	4:B:369:THR:HG23	1.92	0.69
3:A:139:THR:HG22	3:A:140:PRO:O	1.92	0.69
3:A:522:ILE:O	3:A:526:ILE:HG22	1.91	0.69
3:A:217:PRO:HB2	3:A:219:LYS:HG2	1.75	0.69
5:L:146:VAL:HG21	5:L:175:MET:CE	2.22	0.69
3:A:350:LYS:NZ	3:A:378:GLU:OE1	2.27	0.68
3:A:454:LYS:NZ	3:A:554:ALA:HB3	2.08	0.68
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.74	0.68
4:B:292:VAL:O	4:B:292:VAL:HG12	1.93	0.68
3:A:456:GLY:O	3:A:548:VAL:HG12	1.94	0.68
3:A:547:GLN:HE21	3:A:547:GLN:N	1.92	0.68
1:T:704:DC:H4'	1:T:705:DA:H5'	1.76	0.68
3:A:96:HIS:HD1	3:A:98:ALA:H	1.40	0.67
5:L:31:SER:O	5:L:50:TYR:HD1	1.76	0.67
3:A:22:LYS:H	3:A:22:LYS:CD	1.96	0.67
5:L:146:VAL:HG21	5:L:175:MET:HE1	1.75	0.67
5:L:34:ASN:HB2	5:L:89:GLN:NE2	2.09	0.67
3:A:278:GLN:HE21	3:A:302:GLU:HA	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:368:LEU:O	3:A:372:VAL:HG23	1.94	0.67
3:A:261:VAL:HG23	3:A:276:VAL:HG11	1.76	0.67
4:B:229:TRP:HA	4:B:232:TYR:CE1	2.30	0.67
3:A:49:LYS:HB2	3:A:49:LYS:NZ	2.10	0.66
4:B:12:LEU:HD23	4:B:84:THR:HG22	1.76	0.66
3:A:246:LEU:N	3:A:246:LEU:HD23	2.00	0.66
3:A:440:PHE:CZ	3:A:488:ASP:O	2.48	0.66
4:B:195:ILE:HG12	4:B:199:ARG:NE	2.10	0.66
1:T:715:DG:H1'	1:T:716:DA:C8	2.29	0.66
3:A:35:VAL:CG2	3:A:132:ILE:HD11	2.24	0.66
4:B:242:GLN:OE1	4:B:353:LYS:HD2	1.95	0.66
3:A:438:GLU:OE2	3:A:463:ARG:NH2	2.28	0.66
3:A:11:LYS:O	3:A:85:GLN:HG2	1.95	0.66
3:A:397:THR:HG21	3:A:424:LYS:HA	1.78	0.66
3:A:139:THR:HG23	3:A:140:PRO:HD2	1.78	0.66
3:A:463:ARG:HG3	3:A:464:GLN:N	2.09	0.66
1:T:716:DA:H2''	1:T:717:DA:H5'	1.78	0.66
3:A:447:ASN:HD22	3:A:450:THR:HG23	1.58	0.66
4:B:220:LYS:NZ	4:B:222:GLN:HB2	2.11	0.66
1:T:704:DC:O2	1:T:704:DC:C2'	2.43	0.66
3:A:222:GLN:O	3:A:224:GLU:HG3	1.95	0.65
4:B:366:LYS:O	4:B:370:GLU:HG3	1.97	0.65
5:L:137:ASN:HB3	5:L:138:ASN:HD22	1.61	0.65
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.31	0.65
3:A:293:ILE:CD1	3:A:294:PRO:HD2	2.22	0.65
6:H:157:PRO:HD2	6:H:211:ALA:CB	2.27	0.65
5:L:18:ARG:HA	5:L:76:SER:O	1.97	0.65
3:A:104:LYS:HB2	3:A:192:ASP:CA	2.23	0.65
3:A:296:THR:HG22	3:A:298:GLU:N	2.09	0.65
3:A:219:LYS:O	3:A:219:LYS:HG3	1.97	0.65
4:B:98:ALA:O	4:B:101:LYS:HG2	1.96	0.65
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.32	0.64
2:P:812:DT:H6	3:A:358:ARG:HH12	1.45	0.64
3:A:34:LEU:CD2	3:A:62:ALA:HB2	2.28	0.64
5:L:23:CYS:SG	5:L:33:LEU:HD11	2.37	0.64
3:A:445:ALA:O	3:A:477:THR:HG21	1.97	0.64
3:A:485:ALA:O	3:A:489:SER:HB2	1.97	0.64
3:A:458:VAL:O	3:A:458:VAL:HG12	1.97	0.64
3:A:407:GLN:HG3	4:B:393:ILE:HA	1.80	0.64
4:B:427:TYR:CG	4:B:428:GLN:N	2.66	0.64
3:A:361:HIS:NE2	3:A:505:ILE:HD13	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:199:LYS:HG3	5:L:199:LYS:O	1.98	0.64
3:A:501:TYR:O	3:A:505:ILE:HG13	1.98	0.63
1:T:713:DT:H2''	1:T:714:DC:C5'	2.27	0.63
3:A:33:ALA:O	3:A:37:ILE:HG13	1.98	0.63
4:B:175:ASN:N	4:B:176:PRO:CD	2.61	0.63
4:B:220:LYS:HZ3	4:B:222:GLN:HB2	1.63	0.63
6:H:3:THR:C	6:H:4:LEU:HD12	2.19	0.63
6:H:53:ILE:HB	6:H:71:VAL:HG12	1.79	0.63
3:A:265:ASN:HA	3:A:268:SER:OG	1.99	0.63
3:A:403:THR:HG23	3:A:404:GLU:HG2	1.81	0.63
6:H:53:ILE:HB	6:H:71:VAL:HG11	1.79	0.63
3:A:24:TRP:CZ3	3:A:61:PHE:HB3	2.32	0.63
4:B:363:ASN:ND2	4:B:366:LYS:H	1.97	0.62
6:H:62:ASN:ND2	6:H:62:ASN:C	2.49	0.62
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.63	0.62
3:A:270:ILE:HD11	3:A:315:HIS:O	1.99	0.62
6:H:13:GLN:HB2	6:H:16:GLN:HG3	1.80	0.62
3:A:199:ARG:HH22	3:A:220:LYS:HE2	1.65	0.62
3:A:203:GLU:HG3	3:A:207:GLN:HE21	1.64	0.62
3:A:288:ALA:O	3:A:291:GLU:HB3	1.99	0.62
5:L:46:LEU:HD23	5:L:55:HIS:CG	2.35	0.62
2:P:805:DT:OP1	2:P:805:DT:H4'	1.99	0.62
4:B:104:LYS:NZ	4:B:104:LYS:HB3	2.14	0.62
2:P:809:DT:C2'	2:P:810:DG:C8	2.82	0.62
1:T:720:DG:OP1	1:T:720:DG:H4'	1.99	0.62
4:B:175:ASN:HD21	4:B:201:LYS:NZ	1.97	0.62
3:A:28:GLU:HG3	3:A:135:ILE:HG13	1.82	0.62
3:A:338:THR:HG22	3:A:339:TYR:N	2.14	0.62
6:H:192:THR:HG22	6:H:192:THR:O	1.98	0.62
3:A:248:GLU:HB3	3:A:307:ARG:NH2	2.11	0.61
4:B:116:PHE:O	4:B:148:VAL:HG11	2.01	0.61
6:H:32:SER:HA	6:H:55:TRP:CD1	2.35	0.61
2:P:818:DG:H2'	2:P:819:DC:H6	1.63	0.61
3:A:460:ASN:HA	4:B:286:THR:O	1.99	0.61
3:A:13:LYS:CD	3:A:16:MET:HE1	2.28	0.61
4:B:246:LEU:HG	4:B:310:LEU:HD12	1.81	0.61
3:A:473:THR:O	3:A:475:GLN:N	2.34	0.61
2:P:808:DC:H2''	2:P:809:DT:O5'	1.99	0.61
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.23	0.61
3:A:202:ILE:O	3:A:206:ARG:HG3	2.00	0.61
3:A:325:LEU:HD21	3:A:383:TRP:CE3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:106:ILE:HG13	5:L:166:GLN:OE1	1.99	0.61
3:A:143:ARG:HH11	3:A:143:ARG:HG3	1.63	0.61
3:A:469:LEU:HD21	3:A:480:GLN:HG2	1.81	0.61
3:A:529:GLU:O	3:A:530:LYS:HG3	2.01	0.61
4:B:101:LYS:O	4:B:236:PRO:HB2	2.00	0.61
5:L:15:LEU:CD1	5:L:15:LEU:H	2.08	0.61
3:A:61:PHE:N	3:A:61:PHE:HD2	1.98	0.61
4:B:206:ARG:HD2	4:B:216:THR:OG1	2.00	0.61
5:L:34:ASN:ND2	5:L:89:GLN:HE22	1.90	0.61
5:L:193:THR:HG23	5:L:206:VAL:HG13	1.83	0.60
5:L:6:GLN:OE1	5:L:101:GLY:N	2.34	0.60
4:B:393:ILE:HD11	4:B:397:THR:HG22	1.82	0.60
4:B:97:PRO:HD3	4:B:181:TYR:CD1	2.36	0.60
5:L:31:SER:O	5:L:50:TYR:CD1	2.54	0.60
5:L:4:MET:CE	5:L:90:GLN:HB2	2.30	0.60
3:A:447:ASN:HD22	3:A:450:THR:CG2	2.14	0.60
4:B:326:ILE:HG21	4:B:390:LYS:HE2	1.82	0.60
6:H:202:THR:HB	6:H:219:LYS:HE3	1.83	0.60
6:H:166:SER:H	6:H:206:ASN:HD21	1.47	0.60
3:A:503:LEU:CD2	3:A:535:TRP:HB2	2.31	0.60
3:A:61:PHE:N	3:A:61:PHE:CD2	2.69	0.60
3:A:365:VAL:HG11	3:A:401:TRP:CD1	2.36	0.60
3:A:64:LYS:HE2	3:A:66:LYS:HZ1	1.65	0.60
4:B:50:ILE:HG21	4:B:145:GLN:HG2	1.84	0.60
4:B:279:LEU:HD12	4:B:279:LEU:N	2.17	0.60
3:A:246:LEU:N	3:A:246:LEU:CD2	2.61	0.60
2:P:811:DT:OP2	3:A:359:GLY:HA2	2.00	0.60
3:A:279:LEU:H	3:A:279:LEU:HD23	1.67	0.59
4:B:114:ALA:HB1	4:B:160:PHE:CZ	2.37	0.59
5:L:137:ASN:HB3	5:L:138:ASN:ND2	2.17	0.59
4:B:279:LEU:HD12	4:B:279:LEU:H	1.66	0.59
6:H:3:THR:O	6:H:4:LEU:HD12	2.01	0.59
3:A:35:VAL:HG22	3:A:132:ILE:HD11	1.82	0.59
1:T:721:DG:C3'	1:T:722:DG:H5''	2.31	0.59
3:A:365:VAL:HG11	3:A:401:TRP:CG	2.37	0.59
3:A:399:GLU:O	3:A:403:THR:HB	2.02	0.59
3:A:17:ASP:O	3:A:83:ARG:NH1	2.35	0.59
6:H:6:GLU:OE1	6:H:116:GLY:N	2.33	0.59
2:P:805:DT:H2'	2:P:806:DC:C6	2.38	0.59
3:A:194:GLU:O	3:A:196:GLY:N	2.36	0.59
3:A:443:ASP:OD1	3:A:478:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:175:ASN:O	4:B:177:ASP:N	2.35	0.59
6:H:18:PHE:HD2	6:H:87:VAL:HG11	1.67	0.59
5:L:144:ILE:HG23	5:L:145:ASN:N	2.18	0.59
3:A:272:PRO:O	3:A:273:GLY:O	2.21	0.59
3:A:279:LEU:N	3:A:279:LEU:HD23	2.18	0.59
4:B:320:ASP:OD2	4:B:323:LYS:HG3	2.01	0.59
3:A:463:ARG:HG3	3:A:464:GLN:H	1.68	0.59
3:A:498:ASP:HA	3:A:536:VAL:O	2.03	0.59
5:L:48:ILE:HD12	5:L:73:LEU:HD13	1.85	0.59
3:A:455:ALA:HB2	3:A:477:THR:HB	1.84	0.59
5:L:106:ILE:H	5:L:166:GLN:HE22	1.50	0.59
3:A:11:LYS:H	3:A:85:GLN:HE21	1.51	0.59
3:A:371:ALA:O	3:A:375:ILE:HG12	2.03	0.59
3:A:473:THR:O	3:A:474:ASN:C	2.41	0.59
3:A:361:HIS:CD2	3:A:505:ILE:HD13	2.38	0.59
6:H:19:ARG:HH12	6:H:83:ASN:HD21	1.51	0.59
4:B:262:GLY:O	4:B:265:ASN:HB3	2.02	0.58
4:B:2:ILE:H	4:B:2:ILE:HD12	1.67	0.58
4:B:8:VAL:CG1	4:B:159:ILE:HG12	2.33	0.58
6:H:204:THR:HG23	6:H:218:LYS:C	2.24	0.58
4:B:344:GLU:OE2	4:B:344:GLU:HA	2.02	0.58
1:T:723:DA:H2"	1:T:724:DC:OP2	2.02	0.58
3:A:451:LYS:O	3:A:471:ASN:N	2.36	0.58
3:A:463:ARG:O	3:A:464:GLN:NE2	2.36	0.58
3:A:50:ILE:CG2	3:A:145:GLN:HB3	2.34	0.58
6:H:128:PRO:HA	6:H:209:HIS:HD2	1.67	0.58
5:L:179:LEU:HG	5:L:181:LEU:HD21	1.84	0.58
3:A:452:LEU:HB3	3:A:470:THR:HA	1.84	0.58
4:B:106:VAL:HG13	4:B:234:LEU:CB	2.33	0.58
3:A:244:ILE:HD13	3:A:267:ALA:HB2	1.86	0.58
3:A:279:LEU:HD22	3:A:302:GLU:CB	2.33	0.58
3:A:458:VAL:HG11	3:A:547:GLN:HB3	1.85	0.58
4:B:239:TRP:CH2	4:B:378:GLU:HA	2.38	0.58
3:A:326:ILE:HG21	3:A:390:LYS:HE2	1.86	0.58
3:A:317:VAL:CG2	3:A:318:TYR:H	2.16	0.58
3:A:438:GLU:CD	3:A:463:ARG:HH21	2.07	0.58
3:A:441:TYR:CD2	3:A:544:GLY:CA	2.86	0.58
6:H:165:ASN:HD22	6:H:169:LEU:HD11	1.69	0.58
4:B:330:GLN:NE2	4:B:340:GLN:OE1	2.37	0.58
3:A:30:LYS:O	3:A:33:ALA:HB3	2.04	0.57
3:A:132:ILE:O	3:A:132:ILE:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:317:VAL:CG2	3:A:318:TYR:N	2.68	0.57
3:A:434:ILE:HG22	3:A:494:ASN:HD21	1.67	0.57
4:B:104:LYS:HG2	4:B:192:ASP:HA	1.85	0.57
5:L:138:ASN:ND2	6:H:174:HIS:HE1	2.02	0.57
3:A:254:VAL:HG13	3:A:255:ASN:N	2.18	0.57
3:A:79:GLU:O	3:A:83:ARG:HD2	2.05	0.57
4:B:342:TYR:HB3	4:B:348:ASN:HA	1.87	0.57
5:L:136:LEU:HD23	5:L:144:ILE:HD13	1.86	0.57
5:L:146:VAL:HG12	5:L:147:LYS:N	2.19	0.57
3:A:56:TYR:O	3:A:143:ARG:NH2	2.37	0.57
6:H:89:THR:HA	6:H:121:VAL:HB	1.86	0.57
4:B:285:GLY:H	4:B:287:LYS:NZ	2.02	0.57
5:L:162:SER:OG	6:H:177:PRO:HG2	2.05	0.57
4:B:169:GLU:HB3	4:B:170:PRO:HD3	1.84	0.57
4:B:210:LEU:C	4:B:212:TRP:H	2.07	0.57
4:B:360:ALA:HB1	4:B:367:GLN:NE2	2.20	0.57
6:H:133:PRO:O	6:H:134:LEU:HD23	2.05	0.57
3:A:434:ILE:CG2	3:A:494:ASN:HD21	2.18	0.57
3:A:220:LYS:O	3:A:220:LYS:HD3	2.05	0.56
3:A:494:ASN:HB3	4:B:289:LEU:CD1	2.35	0.56
4:B:393:ILE:HD13	4:B:398:TRP:HB2	1.87	0.56
6:H:6:GLU:HG2	6:H:95:TYR:O	2.04	0.56
5:L:89:GLN:HB2	5:L:98:PHE:CD1	2.40	0.56
1:T:724:DC:H2"	1:T:725:DG:H8	1.70	0.56
3:A:245:VAL:O	3:A:245:VAL:HG23	2.04	0.56
4:B:295:LEU:HD13	4:B:300:GLU:OE1	2.04	0.56
6:H:34:ILE:CG2	6:H:35:GLY:N	2.67	0.56
3:A:220:LYS:C	3:A:220:LYS:HD3	2.25	0.56
3:A:536:VAL:HG21	3:A:542:ILE:HG21	1.86	0.56
4:B:324:ASP:O	4:B:343:GLN:HG2	2.05	0.56
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.39	0.56
3:A:429:LEU:HD13	3:A:533:LEU:HD13	1.87	0.56
6:H:164:TRP:CH2	6:H:205:CYS:HB2	2.40	0.56
3:A:329:ILE:HG13	3:A:391:LEU:CD2	2.36	0.56
4:B:111:VAL:HG23	4:B:111:VAL:O	2.04	0.56
6:H:166:SER:N	6:H:206:ASN:HD21	2.01	0.56
4:B:219:LYS:HB3	4:B:232:TYR:CE2	2.40	0.56
3:A:466:VAL:HG21	3:A:551:LEU:CG	2.35	0.56
3:A:492:GLU:HG2	3:A:530:LYS:HB2	1.88	0.56
4:B:112:GLY:HA3	4:B:151:GLN:NE2	2.18	0.56
2:P:815:DA:C6	2:P:816:DG:C6	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:706:DT:H2'	1:T:707:DC:C6	2.41	0.56
3:A:63:ILE:HD12	3:A:64:LYS:H	1.71	0.56
3:A:494:ASN:CB	4:B:289:LEU:HD12	2.34	0.56
4:B:2:ILE:HG21	4:B:46:LYS:HE2	1.88	0.56
5:L:83:ILE:HG21	5:L:106:ILE:HG12	1.87	0.56
3:A:328:GLU:HG2	3:A:330:GLN:HE22	1.70	0.56
3:A:478:GLU:OE1	3:A:498:ASP:CG	2.43	0.56
4:B:291:GLU:O	4:B:293:ILE:N	2.39	0.56
3:A:102:LYS:HG2	3:A:318:TYR:HD1	1.70	0.55
3:A:441:TYR:O	3:A:548:VAL:HG21	2.06	0.55
3:A:466:VAL:CG2	3:A:551:LEU:HG	2.35	0.55
4:B:317:VAL:CG1	4:B:349:LEU:HD23	2.34	0.55
5:L:146:VAL:CG1	5:L:147:LYS:N	2.69	0.55
4:B:223:LYS:HB3	5:L:94:PHE:HE1	1.71	0.55
3:A:317:VAL:HG13	3:A:349:LEU:HD23	1.88	0.55
3:A:493:VAL:HG22	3:A:494:ASN:N	2.22	0.55
3:A:435:VAL:CG2	4:B:290:THR:HG21	2.24	0.55
5:L:150:ILE:N	5:L:153:SER:O	2.31	0.55
5:L:108:ARG:HH11	5:L:108:ARG:HG3	1.72	0.55
3:A:364:ASP:HB3	3:A:423:VAL:HG13	1.89	0.55
4:B:393:ILE:HG12	4:B:394:GLN:N	2.22	0.55
6:H:209:HIS:CD2	6:H:212:SER:OG	2.60	0.55
1:T:704:DC:O2	1:T:704:DC:H2'	2.05	0.55
3:A:268:SER:O	3:A:351:THR:O	2.25	0.55
4:B:106:VAL:HA	4:B:189:VAL:O	2.07	0.55
3:A:247:PRO:HB3	3:A:249:LYS:HE3	1.88	0.55
3:A:279:LEU:N	3:A:279:LEU:CD2	2.70	0.55
3:A:417:VAL:O	3:A:417:VAL:HG13	2.07	0.55
3:A:441:TYR:CE2	3:A:544:GLY:N	2.74	0.55
4:B:281:LYS:O	4:B:284:ARG:HB2	2.07	0.55
4:B:312:GLU:HB3	4:B:315:HIS:CE1	2.42	0.54
4:B:369:THR:O	4:B:373:GLN:HG3	2.07	0.54
6:H:165:ASN:CB	6:H:169:LEU:HD13	2.33	0.54
3:A:301:LEU:O	3:A:305:GLU:HG3	2.06	0.54
4:B:253:THR:HA	4:B:292:VAL:HA	1.90	0.54
6:H:164:TRP:CZ3	6:H:205:CYS:HB2	2.42	0.54
4:B:175:ASN:C	4:B:177:ASP:H	2.11	0.54
3:A:278:GLN:HE21	3:A:302:GLU:CA	2.21	0.54
4:B:277:ARG:HG3	4:B:278:GLN:H	1.71	0.54
3:A:338:THR:CG2	3:A:339:TYR:N	2.70	0.54
4:B:223:LYS:HZ1	6:H:56:ASP:CG	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:61:PHE:CZ	3:A:74:LEU:HD23	2.42	0.54
5:L:61:ARG:HB2	5:L:76:SER:CB	2.33	0.54
4:B:191:SER:HB2	4:B:193:LEU:HG	1.89	0.54
4:B:302:GLU:HA	4:B:302:GLU:OE1	2.08	0.54
3:A:61:PHE:CE2	3:A:74:LEU:HD23	2.43	0.54
4:B:2:ILE:HD12	4:B:3:SER:H	1.73	0.54
6:H:69:LEU:HD22	6:H:82:LEU:HD11	1.90	0.54
5:L:90:GLN:NE2	5:L:93:LYS:H	2.06	0.54
3:A:69:THR:HG22	3:A:69:THR:O	2.08	0.54
4:B:298:GLU:O	4:B:301:LEU:HB3	2.08	0.53
3:A:406:TRP:CZ2	4:B:420:PRO:HG3	2.43	0.53
5:L:149:LYS:HE3	5:L:152:GLY:O	2.08	0.53
3:A:456:GLY:O	3:A:548:VAL:CG1	2.56	0.53
4:B:237:ASP:C	4:B:239:TRP:N	2.59	0.53
5:L:48:ILE:HG21	5:L:52:SER:HA	1.90	0.53
3:A:233:GLU:HB2	3:A:240:THR:CG2	2.34	0.53
3:A:340:GLN:HB3	3:A:348:ASN:OD1	2.08	0.53
4:B:318:TYR:HD2	4:B:318:TYR:H	1.55	0.53
3:A:441:TYR:CD2	3:A:544:GLY:C	2.82	0.53
5:L:193:THR:HG23	5:L:206:VAL:CG1	2.39	0.53
4:B:195:ILE:HG12	4:B:199:ARG:CD	2.39	0.53
4:B:396:GLU:HG2	4:B:396:GLU:O	2.08	0.53
4:B:244:ILE:HD11	4:B:310:LEU:HD22	1.89	0.53
3:A:518:VAL:O	3:A:522:ILE:HG13	2.08	0.53
4:B:65:LYS:HA	4:B:407:GLN:OE1	2.08	0.53
5:L:205:ILE:N	5:L:205:ILE:HD12	2.23	0.53
3:A:437:ALA:HB1	3:A:492:GLU:O	2.09	0.53
4:B:214:LEU:HD12	4:B:214:LEU:N	2.24	0.53
5:L:62:PHE:CE1	5:L:75:ILE:HG12	2.44	0.53
5:L:138:ASN:HD21	6:H:174:HIS:HE1	1.55	0.52
5:L:35:TRP:CZ3	5:L:88:CYS:HB3	2.44	0.52
5:L:90:GLN:NE2	5:L:92:SER:N	2.55	0.52
2:P:820:DC:H2''	2:P:821:DG:H5'	1.90	0.52
3:A:478:GLU:OE1	3:A:498:ASP:OD2	2.26	0.52
3:A:477:THR:O	3:A:480:GLN:N	2.40	0.52
4:B:101:LYS:HG3	4:B:102:LYS:HG3	1.90	0.52
4:B:420:PRO:O	4:B:422:LEU:HG	2.08	0.52
4:B:356:ARG:NE	4:B:360:ALA:HB3	2.22	0.52
3:A:463:ARG:C	3:A:464:GLN:NE2	2.63	0.52
3:A:457:TYR:OH	3:A:488:ASP:OD2	2.15	0.52
6:H:175:THR:HA	6:H:189:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:712:DC:H2'	1:T:713:DT:C6	2.44	0.52
3:A:503:LEU:HD22	3:A:535:TRP:HB2	1.92	0.52
3:A:454:LYS:HZ2	3:A:554:ALA:HB3	1.74	0.52
4:B:12:LEU:HD11	4:B:127:TYR:CZ	2.44	0.52
4:B:307:ARG:O	4:B:311:LYS:HG3	2.10	0.52
4:B:330:GLN:NE2	4:B:340:GLN:NE2	2.50	0.52
3:A:254:VAL:HG13	3:A:255:ASN:H	1.75	0.52
1:T:722:DG:H2''	1:T:723:DA:H8	1.75	0.52
3:A:465:LYS:O	3:A:466:VAL:CG2	2.57	0.51
4:B:13:LYS:HG2	4:B:83:ARG:O	2.10	0.51
3:A:166:LYS:O	3:A:169:GLU:HB3	2.09	0.51
3:A:227:PHE:HB2	3:A:234:LEU:HB2	1.91	0.51
3:A:493:VAL:CG2	3:A:494:ASN:N	2.74	0.51
3:A:257:ILE:O	3:A:261:VAL:HG12	2.10	0.51
3:A:509:GLN:N	3:A:510:PRO:CD	2.73	0.51
3:A:60:VAL:O	3:A:60:VAL:HG13	2.09	0.51
4:B:163:SER:O	4:B:167:ILE:HG13	2.11	0.51
4:B:2:ILE:CG2	4:B:46:LYS:HE2	2.41	0.51
4:B:56:TYR:O	4:B:143:ARG:NH2	2.37	0.51
5:L:86:TYR:O	5:L:101:GLY:HA2	2.10	0.51
5:L:108:ARG:HG2	5:L:109:ALA:N	2.26	0.51
1:T:704:DC:C4'	1:T:705:DA:H5'	2.41	0.51
3:A:464:GLN:HE21	3:A:464:GLN:N	2.08	0.51
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.93	0.51
5:L:146:VAL:CG2	5:L:175:MET:HE1	2.40	0.51
3:A:331:LYS:HD3	3:A:332:GLN:O	2.11	0.51
3:A:325:LEU:HD21	3:A:383:TRP:CD2	2.46	0.51
3:A:434:ILE:HG22	3:A:494:ASN:ND2	2.26	0.51
3:A:361:HIS:CD2	3:A:505:ILE:HG23	2.45	0.51
4:B:146:TYR:CG	4:B:150:PRO:HB3	2.46	0.51
4:B:321:PRO:O	4:B:385:LYS:NZ	2.43	0.51
5:L:46:LEU:HD23	5:L:55:HIS:ND1	2.26	0.51
1:T:705:DA:H2''	1:T:706:DT:C5'	2.41	0.51
4:B:313:PRO:O	4:B:314:VAL:C	2.48	0.51
5:L:117:ILE:HD12	5:L:194:CYS:HB2	1.93	0.51
4:B:296:THR:HG22	4:B:297:GLU:N	2.24	0.51
5:L:34:ASN:HB2	5:L:89:GLN:HE21	1.74	0.51
1:T:708:DG:OP1	3:A:89:GLU:HG3	2.09	0.51
3:A:64:LYS:HE2	3:A:66:LYS:HZ3	1.76	0.51
4:B:231:GLY:O	4:B:232:TYR:C	2.50	0.51
4:B:330:GLN:HG2	4:B:338:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:149:LYS:HA	5:L:154:GLU:HA	1.92	0.51
3:A:221:HIS:CD2	3:A:221:HIS:N	2.78	0.50
3:A:296:THR:O	3:A:299:ALA:HB3	2.11	0.50
4:B:246:LEU:HD12	4:B:307:ARG:HB3	1.93	0.50
6:H:133:PRO:HD3	6:H:218:LYS:HD2	1.93	0.50
5:L:138:ASN:N	5:L:138:ASN:ND2	2.59	0.50
3:A:332:GLN:HB2	3:A:336:GLN:HB2	1.92	0.50
3:A:380:ILE:O	3:A:384:GLY:HA2	2.10	0.50
4:B:65:LYS:HB3	4:B:65:LYS:NZ	2.26	0.50
6:H:62:ASN:ND2	6:H:64:SER:H	2.09	0.50
1:T:722:DG:H2''	1:T:723:DA:C8	2.46	0.50
4:B:285:GLY:H	4:B:287:LYS:HZ2	1.58	0.50
3:A:35:VAL:HG23	3:A:132:ILE:HD11	1.92	0.50
3:A:427:TYR:CE1	3:A:525:LEU:HD23	2.47	0.50
3:A:533:LEU:N	3:A:533:LEU:CD1	2.73	0.50
4:B:195:ILE:CG2	4:B:196:GLY:N	2.74	0.50
3:A:257:ILE:CG2	3:A:283:LEU:HD21	2.41	0.50
6:H:172:GLY:O	6:H:191:VAL:HA	2.11	0.50
6:H:212:SER:O	6:H:214:THR:HG23	2.12	0.50
5:L:34:ASN:HD22	5:L:89:GLN:NE2	1.92	0.50
1:T:704:DC:C5'	1:T:705:DA:H5'	2.42	0.50
3:A:457:TYR:CE2	3:A:465:LYS:HB3	2.47	0.50
6:H:155:TYR:CE1	6:H:160:VAL:HG13	2.46	0.50
6:H:6:GLU:OE2	6:H:114:GLY:HA3	2.11	0.50
5:L:120:PRO:O	5:L:121:SER:O	2.30	0.50
1:T:705:DA:H2''	1:T:706:DT:H5'	1.93	0.50
3:A:474:ASN:OD1	3:A:474:ASN:N	2.43	0.50
3:A:49:LYS:HB2	3:A:49:LYS:HZ3	1.76	0.50
4:B:353:LYS:O	4:B:353:LYS:HG3	2.11	0.50
5:L:165:ASP:O	5:L:166:GLN:C	2.50	0.50
5:L:90:GLN:NE2	5:L:92:SER:H	1.93	0.50
3:A:416:PHE:CZ	3:A:418:ASN:HA	2.46	0.50
4:B:100:LEU:HD13	4:B:381:VAL:HG13	1.94	0.50
5:L:135:PHE:HB3	5:L:137:ASN:HD21	1.77	0.50
3:A:466:VAL:O	3:A:466:VAL:CG1	2.55	0.49
3:A:472:THR:HB	3:A:476:LYS:HB2	1.93	0.49
4:B:87:PHE:HZ	4:B:159:ILE:HG13	1.77	0.49
3:A:247:PRO:HG2	3:A:259:LYS:HE2	1.93	0.49
5:L:31:SER:HA	5:L:51:THR:OG1	2.12	0.49
2:P:806:DC:C2	2:P:807:DC:C5	3.00	0.49
4:B:219:LYS:HB3	4:B:232:TYR:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:393:ILE:CG1	4:B:394:GLN:N	2.75	0.49
5:L:205:ILE:H	5:L:205:ILE:HD12	1.78	0.49
3:A:350:LYS:HE2	3:A:378:GLU:OE1	2.11	0.49
5:L:190:ASN:O	5:L:210:ASN:HA	2.13	0.49
3:A:420:PRO:HB3	3:A:421:PRO:HA	1.94	0.49
4:B:263:LYS:HA	4:B:423:VAL:HG11	1.94	0.49
3:A:350:LYS:CE	3:A:378:GLU:OE1	2.60	0.49
4:B:376:THR:O	4:B:380:ILE:HG13	2.12	0.49
5:L:58:VAL:HG13	5:L:59:PRO:HD2	1.94	0.49
3:A:136:ASN:HB2	3:A:138:GLU:HG3	1.94	0.49
6:H:152:VAL:HB	6:H:187:LEU:HD13	1.95	0.49
6:H:165:ASN:HD22	6:H:169:LEU:CD1	2.25	0.49
6:H:169:LEU:N	6:H:169:LEU:HD12	2.28	0.49
3:A:171:PHE:CE2	3:A:205:LEU:HD13	2.48	0.49
3:A:507:GLN:C	3:A:509:GLN:H	2.16	0.49
3:A:76:ASP:OD1	3:A:78:ARG:HG3	2.13	0.49
4:B:317:VAL:HG11	4:B:348:ASN:O	2.13	0.49
3:A:410:TRP:HB3	4:B:365:VAL:HG23	1.95	0.49
4:B:424:LYS:C	4:B:426:TRP:N	2.66	0.49
5:L:45:LYS:HG2	5:L:46:LEU:N	2.26	0.49
3:A:331:LYS:HB3	3:A:421:PRO:HG2	1.95	0.49
3:A:463:ARG:CG	3:A:464:GLN:N	2.76	0.49
6:H:34:ILE:HG22	6:H:35:GLY:N	2.27	0.49
6:H:53:ILE:HA	6:H:59:ASN:ND2	2.28	0.49
5:L:170:ASP:OD1	5:L:170:ASP:C	2.51	0.49
1:T:708:DG:H2'	1:T:709:DG:C8	2.48	0.49
3:A:447:ASN:HB3	3:A:450:THR:OG1	2.13	0.49
4:B:104:LYS:HZ3	4:B:104:LYS:HB3	1.77	0.49
6:H:107:ASP:HB3	7:H:1725:GLC:O3	2.13	0.49
3:A:24:TRP:HZ3	3:A:61:PHE:CB	2.22	0.48
4:B:304:ALA:HA	4:B:307:ARG:HE	1.78	0.48
4:B:223:LYS:NZ	6:H:56:ASP:OD2	2.46	0.48
5:L:175:MET:HE3	5:L:177:SER:HB2	1.94	0.48
3:A:441:TYR:CD2	3:A:544:GLY:HA3	2.47	0.48
6:H:12:VAL:HG21	6:H:18:PHE:HB3	1.95	0.48
3:A:27:THR:HG23	3:A:30:LYS:HD2	1.95	0.48
3:A:541:GLY:HA2	3:A:546:GLU:HG3	1.96	0.48
4:B:333:GLY:O	4:B:334:GLN:HB2	2.13	0.48
5:L:15:LEU:HD12	5:L:15:LEU:N	2.13	0.48
5:L:49:TYR:O	5:L:50:TYR:HB3	2.13	0.48
4:B:154:LYS:HA	4:B:184:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:357:MET:SD	4:B:370:GLU:OE1	2.71	0.48
3:A:339:TYR:CD2	3:A:375:ILE:HD11	2.49	0.48
4:B:278:GLN:HB3	4:B:279:LEU:HD12	1.95	0.48
5:L:45:LYS:HG2	5:L:46:LEU:H	1.78	0.48
3:A:222:GLN:O	3:A:223:LYS:C	2.51	0.48
5:L:151:ASP:CA	5:L:191:SER:HB3	2.43	0.48
3:A:181:TYR:CD1	4:B:138:GLU:HA	2.48	0.48
3:A:40:GLU:OE1	3:A:40:GLU:HA	2.14	0.48
3:A:454:LYS:C	3:A:552:VAL:HG13	2.34	0.48
3:A:96:HIS:CG	3:A:97:PRO:HD2	2.48	0.48
6:H:209:HIS:CE1	6:H:211:ALA:HB3	2.49	0.48
5:L:138:ASN:HD22	5:L:138:ASN:N	2.12	0.48
3:A:109:LEU:HD23	3:A:220:LYS:HB2	1.96	0.48
4:B:104:LYS:O	4:B:235:HIS:HD2	1.96	0.48
4:B:210:LEU:O	4:B:212:TRP:N	2.39	0.48
5:L:36:TYR:HE2	5:L:89:GLN:HB3	1.78	0.48
2:P:816:DG:H2'	2:P:817:DC:H6	1.77	0.48
3:A:97:PRO:HA	3:A:100:LEU:HD12	1.96	0.47
3:A:23:GLN:HE22	3:A:60:VAL:N	2.05	0.47
2:P:807:DC:C4'	3:A:448:ARG:HD2	2.36	0.47
3:A:7:THR:CG2	3:A:119:PRO:HB2	2.43	0.47
3:A:132:ILE:HG23	3:A:142:ILE:HB	1.95	0.47
3:A:215:THR:C	3:A:217:PRO:HD3	2.34	0.47
3:A:235:HIS:HB2	3:A:238:LYS:O	2.13	0.47
3:A:302:GLU:O	3:A:303:LEU:C	2.52	0.47
4:B:171:PHE:CE1	4:B:205:LEU:HA	2.49	0.47
4:B:195:ILE:HG23	4:B:196:GLY:N	2.29	0.47
4:B:420:PRO:HB3	4:B:421:PRO:HD2	1.95	0.47
5:L:61:ARG:HG2	5:L:61:ARG:HH11	1.79	0.47
3:A:343:GLN:HE21	3:A:349:LEU:HD21	1.80	0.47
3:A:429:LEU:HD11	3:A:506:ILE:HG22	1.94	0.47
3:A:516:GLU:O	3:A:519:ASN:N	2.47	0.47
4:B:363:ASN:HD21	4:B:365:VAL:HB	1.80	0.47
4:B:263:LYS:CA	4:B:423:VAL:HG11	2.45	0.47
6:H:40:ARG:HB2	6:H:50:LEU:HD11	1.95	0.47
3:A:357:MET:HG3	3:A:367:GLN:HE22	1.80	0.47
4:B:101:LYS:O	4:B:236:PRO:CB	2.61	0.47
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.49	0.47
1:T:719:DA:H2''	1:T:720:DG:O5'	2.14	0.47
3:A:497:THR:HG22	3:A:498:ASP:H	1.79	0.47
5:L:4:MET:HE1	5:L:29:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:187:LEU:HA	4:B:187:LEU:HD12	1.76	0.47
6:H:134:LEU:HD12	6:H:149:GLY:HA3	1.95	0.47
5:L:199:LYS:O	5:L:199:LYS:CG	2.61	0.47
4:B:151:GLN:HB3	4:B:185:ASP:OD2	2.15	0.47
4:B:326:ILE:HD12	4:B:326:ILE:N	2.30	0.47
5:L:175:MET:CE	5:L:177:SER:HB2	2.45	0.47
3:A:319:TYR:HA	3:A:343:GLN:HE22	1.80	0.47
3:A:486:LEU:CD1	3:A:521:ILE:HG23	2.45	0.47
4:B:206:ARG:NH1	4:B:216:THR:O	2.48	0.47
4:B:79:GLU:O	4:B:83:ARG:HG2	2.15	0.47
6:H:31:THR:HB	6:H:34:ILE:HD12	1.96	0.47
3:A:547:GLN:CA	3:A:547:GLN:HE21	2.28	0.47
3:A:5:ILE:HD11	3:A:167:ILE:CD1	2.32	0.47
4:B:330:GLN:CG	4:B:338:THR:OG1	2.63	0.47
2:P:815:DA:H2'	2:P:816:DG:C8	2.50	0.47
4:B:210:LEU:C	4:B:212:TRP:N	2.68	0.46
2:P:822:2DA:H3'1	3:A:185:ASP:OD1	2.14	0.46
3:A:328:GLU:HG3	3:A:390:LYS:HB2	1.96	0.46
4:B:225:PRO:HB2	5:L:32:TYR:CE1	2.51	0.46
4:B:363:ASN:ND2	4:B:363:ASN:C	2.67	0.46
3:A:129:ALA:HA	3:A:144:TYR:O	2.16	0.46
3:A:473:THR:OG1	3:A:476:LYS:HG2	2.14	0.46
4:B:175:ASN:HD21	4:B:201:LYS:HZ1	1.61	0.46
4:B:277:ARG:HG3	4:B:278:GLN:N	2.31	0.46
3:A:194:GLU:O	3:A:195:ILE:C	2.54	0.46
3:A:278:GLN:HG2	3:A:278:GLN:H	1.34	0.46
3:A:339:TYR:CD2	3:A:375:ILE:CD1	2.99	0.46
6:H:150:CYS:HB2	6:H:164:TRP:CZ2	2.50	0.46
5:L:11:LEU:HD21	5:L:19:VAL:CG1	2.45	0.46
3:A:31:ILE:O	3:A:35:VAL:HG23	2.16	0.46
3:A:473:THR:H	3:A:476:LYS:HB2	1.80	0.46
4:B:183:TYR:CD2	4:B:380:ILE:HD13	2.50	0.46
4:B:285:GLY:O	4:B:287:LYS:N	2.49	0.46
6:H:14:PRO:O	6:H:15:SER:HB2	2.15	0.46
6:H:40:ARG:HD3	6:H:50:LEU:HD11	1.97	0.46
5:L:2:ILE:HG23	5:L:27:GLN:HG3	1.98	0.46
1:T:705:DA:H2''	1:T:706:DT:O5'	2.15	0.46
3:A:461:LYS:O	3:A:463:ARG:N	2.48	0.46
4:B:260:LEU:O	4:B:260:LEU:HG	2.16	0.46
5:L:136:LEU:HD21	5:L:146:VAL:HG22	1.97	0.46
3:A:269:GLN:HA	3:A:351:THR:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:142:THR:HG22	6:H:143:ASN:N	2.31	0.46
6:H:62:ASN:HD22	6:H:63:PRO:CD	2.28	0.46
3:A:12:LEU:HD11	3:A:127:TYR:CZ	2.51	0.46
3:A:257:ILE:HG22	3:A:283:LEU:HD21	1.97	0.46
4:B:146:TYR:CD2	4:B:150:PRO:HB3	2.51	0.46
4:B:75:VAL:HG11	4:B:77:PHE:CE2	2.51	0.46
5:L:78:LEU:HD21	5:L:104:LEU:HD21	1.98	0.46
5:L:190:ASN:HD22	5:L:211:ARG:HG2	1.79	0.46
2:P:804:DG:H2'	2:P:805:DT:H71	1.96	0.46
3:A:442:VAL:HB	3:A:481:ALA:HB1	1.96	0.45
3:A:529:GLU:O	3:A:530:LYS:CG	2.64	0.45
4:B:118:VAL:O	4:B:148:VAL:HA	2.15	0.45
4:B:199:ARG:HH12	4:B:229:TRP:HZ3	1.63	0.45
6:H:42:PRO:HA	6:H:93:ALA:HB2	1.96	0.45
5:L:206:VAL:HG12	5:L:207:LYS:N	2.31	0.45
3:A:297:GLU:HA	3:A:300:GLU:CB	2.42	0.45
3:A:305:GLU:O	3:A:308:GLU:HB2	2.16	0.45
3:A:50:ILE:HG23	3:A:145:GLN:HB3	1.98	0.45
4:B:368:LEU:O	4:B:372:VAL:HG23	2.16	0.45
5:L:51:THR:HG23	5:L:71:TYR:HD2	1.80	0.45
3:A:112:GLY:O	3:A:113:ASP:HB2	2.15	0.45
3:A:139:THR:HG23	3:A:140:PRO:CD	2.46	0.45
3:A:257:ILE:HD13	3:A:282:LEU:HB2	1.97	0.45
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.52	0.45
4:B:214:LEU:CD1	4:B:214:LEU:N	2.78	0.45
4:B:276:VAL:HG12	4:B:276:VAL:O	2.16	0.45
6:H:54:TRP:H	6:H:59:ASN:HD22	1.64	0.45
5:L:125:LEU:HD23	5:L:129:GLY:O	2.16	0.45
3:A:536:VAL:HG11	3:A:542:ILE:HB	1.97	0.45
6:H:42:PRO:HA	6:H:93:ALA:CB	2.47	0.45
5:L:6:GLN:HA	5:L:22:SER:O	2.17	0.45
5:L:27:GLN:O	5:L:28:ASP:C	2.55	0.45
4:B:39:THR:O	4:B:42:GLU:HB3	2.16	0.45
5:L:115:VAL:HG12	5:L:207:LYS:HG3	1.99	0.45
4:B:135:ILE:CD1	4:B:135:ILE:O	2.57	0.45
4:B:160:PHE:CD2	4:B:160:PHE:O	2.70	0.45
1:T:712:DC:OP1	3:A:353:LYS:NZ	2.49	0.45
3:A:134:SER:O	3:A:136:ASN:N	2.50	0.45
4:B:264:LEU:O	4:B:274:ILE:HG21	2.17	0.45
4:B:46:LYS:HD2	4:B:148:VAL:CG2	2.44	0.45
3:A:264:LEU:O	3:A:267:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:420:PRO:HA	3:A:421:PRO:C	2.36	0.45
3:A:478:GLU:HG2	3:A:499:SER:HB3	1.98	0.45
3:A:96:HIS:ND1	3:A:97:PRO:HD2	2.31	0.45
3:A:66:LYS:HA	3:A:66:LYS:HD3	1.77	0.45
4:B:113:ASP:O	4:B:114:ALA:C	2.54	0.45
3:A:435:VAL:HG22	4:B:290:THR:CB	2.46	0.45
6:H:129:PRO:HB2	6:H:152:VAL:CG1	2.47	0.45
5:L:11:LEU:HD23	5:L:104:LEU:HD13	1.99	0.45
3:A:517:LEU:HD13	3:A:517:LEU:C	2.37	0.44
3:A:547:GLN:HE21	3:A:547:GLN:H	1.59	0.44
4:B:170:PRO:HB2	4:B:208:HIS:CE1	2.52	0.44
4:B:258:GLN:HG2	4:B:283:LEU:CD1	2.48	0.44
4:B:282:LEU:HD23	4:B:282:LEU:N	2.33	0.44
6:H:174:HIS:O	6:H:189:SER:HA	2.17	0.44
5:L:63:SER:O	5:L:73:LEU:HD12	2.16	0.44
3:A:482:ILE:O	3:A:486:LEU:HG	2.17	0.44
4:B:193:LEU:HD12	4:B:198:HIS:HA	1.99	0.44
4:B:27:THR:OG1	4:B:30:LYS:HG3	2.16	0.44
3:A:108:VAL:O	3:A:109:LEU:HD23	2.18	0.44
3:A:23:GLN:HG2	3:A:133:PRO:HD3	1.99	0.44
3:A:552:VAL:C	3:A:554:ALA:H	2.20	0.44
6:H:129:PRO:HB2	6:H:152:VAL:HG13	1.97	0.44
3:A:408:ALA:HB1	4:B:364:ASP:HB3	1.98	0.44
3:A:452:LEU:HD23	3:A:470:THR:HG22	1.99	0.44
4:B:132:ILE:HA	4:B:133:PRO:HD3	1.79	0.44
4:B:212:TRP:O	4:B:212:TRP:HD1	1.99	0.44
5:L:190:ASN:CG	5:L:210:ASN:HD22	2.20	0.44
3:A:419:THR:HG22	3:A:419:THR:O	2.18	0.44
4:B:87:PHE:CE1	4:B:92:LEU:HD12	2.53	0.44
3:A:389:PHE:O	3:A:414:TRP:HA	2.17	0.44
6:H:128:PRO:HA	6:H:209:HIS:CD2	2.50	0.44
5:L:151:ASP:OD2	5:L:189:HIS:ND1	2.51	0.44
3:A:254:VAL:O	3:A:257:ILE:HB	2.18	0.44
3:A:337:TRP:CZ2	3:A:367:GLN:HB2	2.53	0.44
3:A:393:ILE:HG23	3:A:393:ILE:O	2.17	0.44
3:A:411:ILE:HG22	3:A:412:PRO:O	2.16	0.44
4:B:221:HIS:HA	4:B:229:TRP:CD1	2.52	0.44
4:B:325:LEU:HD12	4:B:343:GLN:HG2	2.00	0.44
4:B:3:SER:HA	4:B:4:PRO:HD3	1.88	0.44
6:H:173:VAL:HA	6:H:190:SER:O	2.18	0.44
3:A:261:VAL:HG23	3:A:276:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:454:LYS:O	3:A:552:VAL:CG1	2.66	0.44
3:A:541:GLY:HA2	3:A:546:GLU:CG	2.48	0.44
4:B:100:LEU:HD22	4:B:100:LEU:O	2.18	0.44
4:B:395:LYS:HA	4:B:416:PHE:CE1	2.53	0.44
5:L:14:SER:O	5:L:15:LEU:C	2.56	0.44
2:P:816:DG:H2'	2:P:817:DC:C6	2.52	0.44
3:A:167:ILE:O	3:A:170:PRO:HD2	2.18	0.43
4:B:29:GLU:HG2	4:B:71:TRP:CH2	2.53	0.43
3:A:452:LEU:HB3	3:A:470:THR:HG22	2.00	0.43
4:B:175:ASN:OD1	4:B:201:LYS:HE3	2.18	0.43
4:B:68:SER:O	4:B:69:THR:HB	2.18	0.43
4:B:96:HIS:HA	4:B:97:PRO:HD3	1.86	0.43
1:T:711:DG:H2'	1:T:712:DC:H6	1.83	0.43
3:A:281:LYS:NZ	3:A:284:ARG:CB	2.81	0.43
3:A:555:GLY:O	3:A:556:ILE:CG1	2.61	0.43
4:B:103:LYS:CE	4:B:103:LYS:HA	2.46	0.43
4:B:97:PRO:HG2	4:B:181:TYR:HB2	1.99	0.43
6:H:9:PRO:O	6:H:11:ILE:N	2.47	0.43
5:L:198:HIS:O	5:L:200:THR:N	2.47	0.43
5:L:198:HIS:C	5:L:200:THR:H	2.22	0.43
5:L:21:ILE:HD13	5:L:102:THR:HB	2.00	0.43
5:L:20:THR:OG1	5:L:74:THR:OG1	2.36	0.43
3:A:118:VAL:HA	3:A:119:PRO:HD3	1.79	0.43
4:B:350:LYS:HE2	4:B:378:GLU:OE1	2.18	0.43
5:L:147:LYS:HZ2	5:L:149:LYS:HD2	1.77	0.43
3:A:206:ARG:NH2	3:A:216:THR:O	2.52	0.43
3:A:278:GLN:HE21	3:A:302:GLU:CB	2.32	0.43
3:A:49:LYS:HB2	3:A:49:LYS:HZ2	1.83	0.43
3:A:458:VAL:HG11	3:A:547:GLN:HG2	2.00	0.43
4:B:154:LYS:HG2	4:B:184:MET:CE	2.48	0.43
4:B:278:GLN:HG3	4:B:299:ALA:HA	1.99	0.43
3:A:162:SER:OG	4:B:52:PRO:HD3	2.18	0.43
3:A:199:ARG:NH2	3:A:220:LYS:CE	2.76	0.43
3:A:338:THR:HG22	3:A:340:GLN:NE2	2.34	0.43
6:H:39:ILE:HG22	6:H:40:ARG:N	2.33	0.43
6:H:84:MET:HG2	6:H:87:VAL:CG1	2.40	0.43
3:A:363:ASN:OD1	3:A:363:ASN:C	2.57	0.43
3:A:455:ALA:HB3	3:A:469:LEU:HD11	2.01	0.43
3:A:506:ILE:O	3:A:510:PRO:HD2	2.19	0.43
6:H:60:ARG:HA	6:H:60:ARG:HD3	1.73	0.43
5:L:144:ILE:HG13	5:L:198:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.83	0.43
5:L:89:GLN:HB2	5:L:98:PHE:CE1	2.54	0.43
3:A:5:ILE:CD1	3:A:167:ILE:HD11	2.32	0.43
3:A:459:THR:HG23	3:A:463:ARG:CB	2.30	0.43
3:A:465:LYS:HD2	3:A:467:VAL:HG13	2.00	0.43
4:B:306:ASN:O	4:B:309:ILE:N	2.45	0.43
4:B:418:ASN:HD22	4:B:418:ASN:C	2.20	0.43
1:T:711:DG:H2'	1:T:712:DC:C6	2.54	0.43
3:A:257:ILE:HD13	3:A:282:LEU:CB	2.49	0.42
3:A:427:TYR:CZ	3:A:525:LEU:HD23	2.54	0.42
3:A:47:ILE:HD12	3:A:144:TYR:CD1	2.54	0.42
3:A:543:GLY:C	3:A:545:ASN:H	2.23	0.42
4:B:199:ARG:HH22	4:B:230:MET:CE	2.32	0.42
4:B:2:ILE:HD12	4:B:2:ILE:N	2.32	0.42
3:A:11:LYS:H	3:A:85:GLN:HG2	1.83	0.42
4:B:239:TRP:CZ2	4:B:378:GLU:HG2	2.54	0.42
4:B:279:LEU:CD1	4:B:279:LEU:H	2.32	0.42
5:L:146:VAL:HG21	5:L:175:MET:HE2	2.00	0.42
5:L:150:ILE:HA	5:L:191:SER:O	2.18	0.42
5:L:1:ASP:N	5:L:95:PRO:HG2	2.34	0.42
5:L:61:ARG:CZ	5:L:79:GLU:HG3	2.49	0.42
1:T:712:DC:H42	2:P:815:DA:N6	2.17	0.42
3:A:181:TYR:HB2	3:A:188:TYR:HB3	2.00	0.42
3:A:109:LEU:CD2	3:A:220:LYS:HB2	2.48	0.42
3:A:245:VAL:O	3:A:245:VAL:CG2	2.67	0.42
3:A:438:GLU:HG2	3:A:461:LYS:CD	2.49	0.42
4:B:210:LEU:HD12	4:B:210:LEU:HA	1.62	0.42
5:L:135:PHE:HB3	5:L:137:ASN:ND2	2.34	0.42
3:A:460:ASN:HA	4:B:286:THR:OG1	2.19	0.42
6:H:2:ILE:HG21	6:H:112:HIS:HD2	1.83	0.42
5:L:128:GLY:C	5:L:183:LYS:HB2	2.40	0.42
5:L:182:THR:HG22	5:L:183:LYS:N	2.33	0.42
4:B:260:LEU:CD2	4:B:303:LEU:HD13	2.35	0.42
6:H:39:ILE:HG13	6:H:113:TRP:CH2	2.55	0.42
5:L:149:LYS:HD3	5:L:195:GLU:OE2	2.19	0.42
5:L:54:LEU:HA	5:L:54:LEU:HD22	1.80	0.42
3:A:201:LYS:HA	3:A:201:LYS:HD2	1.84	0.42
3:A:409:THR:HG23	10:A:563:HOH:O	2.19	0.42
4:B:206:ARG:NH1	4:B:217:PRO:O	2.53	0.42
4:B:330:GLN:HE22	4:B:340:GLN:CD	2.21	0.42
4:B:319:TYR:CZ	4:B:383:TRP:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:124:GLN:HE22	5:L:131:SER:CB	2.32	0.42
3:A:10:VAL:HG11	3:A:153:TRP:HZ2	1.85	0.42
3:A:418:ASN:O	3:A:419:THR:OG1	2.31	0.42
3:A:547:GLN:H	3:A:547:GLN:NE2	2.18	0.42
4:B:50:ILE:CG2	4:B:145:GLN:HG2	2.47	0.42
4:B:199:ARG:NH2	4:B:230:MET:HE3	2.34	0.42
3:A:13:LYS:HB2	3:A:16:MET:CE	2.50	0.42
2:P:808:DC:H4'	3:A:475:GLN:OE1	2.18	0.42
3:A:523:GLU:HA	3:A:523:GLU:OE1	2.20	0.42
4:B:156:SER:N	4:B:157:PRO:HD2	2.34	0.42
5:L:118:PHE:HZ	6:H:147:THR:O	2.03	0.42
3:A:457:TYR:HA	3:A:548:VAL:HG11	2.02	0.42
3:A:458:VAL:HG11	3:A:547:GLN:CG	2.50	0.42
3:A:542:ILE:HD12	3:A:542:ILE:H	1.85	0.42
4:B:167:ILE:O	4:B:208:HIS:NE2	2.45	0.42
4:B:266:TRP:HH2	4:B:422:LEU:CD2	2.26	0.42
3:A:344:GLU:HA	3:A:345:PRO:HD2	1.79	0.41
4:B:212:TRP:O	4:B:212:TRP:CD1	2.72	0.41
3:A:494:ASN:OD1	4:B:289:LEU:HD12	2.20	0.41
4:B:7:THR:HG22	4:B:119:PRO:HG2	2.02	0.41
6:H:174:HIS:O	6:H:190:SER:N	2.50	0.41
5:L:201:SER:C	5:L:203:SER:N	2.74	0.41
5:L:90:GLN:HE22	5:L:93:LYS:H	1.66	0.41
3:A:279:LEU:HD22	3:A:279:LEU:H	1.84	0.41
4:B:394:GLN:O	4:B:395:LYS:C	2.58	0.41
4:B:263:LYS:HB2	4:B:423:VAL:CG1	2.50	0.41
2:P:810:DG:OP1	3:A:361:HIS:NE2	2.48	0.41
3:A:111:VAL:CG1	3:A:214:LEU:HD12	2.38	0.41
3:A:317:VAL:HG12	3:A:348:ASN:O	2.20	0.41
3:A:325:LEU:HB3	3:A:387:PRO:HB3	2.01	0.41
3:A:441:TYR:O	3:A:548:VAL:HG11	2.20	0.41
4:B:195:ILE:HG12	4:B:199:ARG:HE	1.83	0.41
5:L:201:SER:C	5:L:203:SER:H	2.23	0.41
3:A:526:ILE:HG12	3:A:526:ILE:O	2.19	0.41
4:B:299:ALA:O	4:B:300:GLU:C	2.59	0.41
6:H:86:THR:HG22	6:H:86:THR:O	2.20	0.41
5:L:146:VAL:CG1	5:L:147:LYS:H	2.34	0.41
3:A:490:GLY:C	3:A:492:GLU:H	2.24	0.41
4:B:47:ILE:HA	4:B:145:GLN:O	2.21	0.41
4:B:330:GLN:NE2	4:B:340:GLN:CD	2.74	0.41
6:H:54:TRP:H	6:H:59:ASN:ND2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:491:LEU:O	3:A:529:GLU:HB2	2.19	0.41
3:A:507:GLN:C	3:A:509:GLN:N	2.74	0.41
4:B:199:ARG:HH22	4:B:230:MET:HE3	1.85	0.41
4:B:424:LYS:O	4:B:425:LEU:C	2.58	0.41
5:L:138:ASN:HA	5:L:173:TYR:O	2.20	0.41
3:A:416:PHE:HZ	3:A:422:LEU:HD11	1.85	0.41
3:A:511:ASP:OD2	3:A:512:LYS:HE3	2.20	0.41
3:A:542:ILE:HD12	3:A:542:ILE:N	2.36	0.41
3:A:548:VAL:O	3:A:552:VAL:HG23	2.21	0.41
5:L:120:PRO:O	5:L:121:SER:C	2.59	0.41
5:L:61:ARG:HH21	5:L:82:ASP:CG	2.24	0.41
3:A:412:PRO:O	3:A:413:GLU:C	2.59	0.41
3:A:472:THR:O	3:A:473:THR:HG23	2.20	0.41
3:A:495:ILE:O	3:A:496:VAL:HG23	2.21	0.41
6:H:169:LEU:CD1	6:H:169:LEU:N	2.83	0.41
5:L:188:ARG:O	5:L:189:HIS:CG	2.74	0.41
3:A:458:VAL:HG23	3:A:548:VAL:HG13	2.03	0.41
4:B:175:ASN:C	4:B:177:ASP:N	2.73	0.41
4:B:241:VAL:HA	4:B:351:THR:O	2.20	0.41
6:H:105:VAL:HG12	6:H:105:VAL:O	2.20	0.41
6:H:40:ARG:HD2	6:H:95:TYR:CZ	2.56	0.41
5:L:48:ILE:HG23	5:L:53:SER:O	2.20	0.41
3:A:134:SER:C	3:A:136:ASN:N	2.74	0.41
4:B:104:LYS:O	4:B:235:HIS:CD2	2.74	0.41
6:H:204:THR:HG23	6:H:218:LYS:O	2.21	0.41
5:L:31:SER:CA	5:L:51:THR:OG1	2.69	0.41
3:A:10:VAL:HG11	3:A:153:TRP:CZ2	2.56	0.41
3:A:516:GLU:O	3:A:517:LEU:C	2.59	0.41
3:A:545:ASN:O	3:A:546:GLU:C	2.58	0.41
3:A:8:VAL:HA	3:A:9:PRO:HD3	1.89	0.41
4:B:125:ARG:HD3	4:B:146:TYR:O	2.21	0.41
4:B:146:TYR:CE2	4:B:150:PRO:HA	2.56	0.41
4:B:178:ILE:CD1	4:B:201:LYS:HG2	2.45	0.41
4:B:282:LEU:HD21	4:B:299:ALA:HB2	2.02	0.41
4:B:34:LEU:HD13	4:B:62:ALA:HB2	2.02	0.41
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.69	0.41
5:L:91:TYR:CE1	6:H:108:SER:HB3	2.56	0.41
4:B:129:ALA:HA	4:B:144:TYR:O	2.21	0.40
4:B:88:TRP:CD1	4:B:154:LYS:HB2	2.56	0.40
4:B:175:ASN:HD21	4:B:201:LYS:HZ2	1.64	0.40
4:B:34:LEU:HD12	4:B:34:LEU:HA	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:414:TRP:CD1	4:B:414:TRP:O	2.74	0.40
5:L:170:ASP:O	5:L:172:THR:HG23	2.21	0.40
2:P:804:DG:H2''	2:P:805:DT:O5'	2.21	0.40
3:A:434:ILE:CG2	3:A:494:ASN:ND2	2.82	0.40
6:H:216:VAL:HG12	6:H:217:ASP:N	2.36	0.40
3:A:470:THR:O	3:A:471:ASN:HB2	2.21	0.40
3:A:484:LEU:O	3:A:486:LEU:N	2.55	0.40
3:A:68:SER:O	3:A:69:THR:HB	2.21	0.40
4:B:169:GLU:N	4:B:170:PRO:CD	2.84	0.40
5:L:55:HIS:CD2	5:L:56:SER:H	2.39	0.40
4:B:125:ARG:NH1	4:B:147:ASN:OD1	2.54	0.40
4:B:46:LYS:HD3	4:B:46:LYS:HA	1.63	0.40
6:H:91:ASP:HB2	6:H:121:VAL:HG21	2.02	0.40
3:A:281:LYS:HD3	3:A:284:ARG:CB	2.52	0.40
3:A:297:GLU:CA	3:A:300:GLU:HB2	2.47	0.40
3:A:80:LEU:O	3:A:84:THR:N	2.47	0.40
4:B:199:ARG:NH2	4:B:230:MET:CE	2.84	0.40
4:B:257:ILE:H	4:B:257:ILE:HG12	1.69	0.40
4:B:301:LEU:HG	4:B:302:GLU:OE1	2.21	0.40
5:L:160:LEU:HD11	6:H:181:GLN:CD	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2:ILE:O	4:B:2:ILE:O[6_565]	1.96	0.24
4:B:3:SER:OG	4:B:3:SER:OG[6_565]	2.02	0.18

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	556/558 (100%)	456 (82%)	69 (12%)	31 (6%)	2	6
4	B	427/429 (100%)	361 (84%)	52 (12%)	14 (3%)	4	15
5	L	209/211 (99%)	184 (88%)	18 (9%)	7 (3%)	4	15
6	H	223/225 (99%)	198 (89%)	22 (10%)	3 (1%)	14	41
All	All	1415/1423 (99%)	1199 (85%)	161 (11%)	55 (4%)	3	12

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	273	GLY
3	A	278	GLN
3	A	286	THR
3	A	345	PRO
3	A	466	VAL
3	A	474	ASN
4	B	247	PRO
4	B	286	THR
4	B	292	VAL
4	B	355	ALA
5	L	76	SER
5	L	121	SER
3	A	195	ILE
3	A	462	GLY
3	A	543	GLY
3	A	547	GLN
3	A	556	ILE
4	B	176	PRO
4	B	236	PRO
4	B	272	PRO
4	B	314	VAL
5	L	143	ASP
6	H	57	ASP
3	A	114	ALA
3	A	295	LEU
3	A	324	ASP
3	A	538	ALA
4	B	170	PRO
4	B	211	ARG
4	B	212	TRP
4	B	422	LEU
5	L	28	ASP
5	L	60	SER

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Mol	Chain	Res	Type
5	L	199	LYS
6	H	143	ASN
3	A	135	ILE
3	A	138	GLU
3	A	217	PRO
3	A	302	GLU
3	A	364	ASP
3	A	465	LYS
3	A	485	ALA
3	A	508	ALA
3	A	528	LYS
5	L	78	LEU
3	A	116	PHE
3	A	176	PRO
3	A	458	VAL
4	B	116	PHE
3	A	296	THR
4	B	175	ASN
6	H	10	GLY
3	A	537	PRO
3	A	276	VAL
3	A	421	PRO

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	485/498 (97%)	437 (90%)	48 (10%)	9	26
4	B	388/391 (99%)	351 (90%)	37 (10%)	10	28
5	L	190/190 (100%)	169 (89%)	21 (11%)	7	21
6	H	196/196 (100%)	180 (92%)	16 (8%)	13	37
All	All	1259/1275 (99%)	1137 (90%)	122 (10%)	9	27

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	22	LYS
3	A	24	TRP
3	A	27	THR
3	A	49	LYS
3	A	55	PRO
3	A	58	THR
3	A	61	PHE
3	A	64	LYS
3	A	65	LYS
3	A	75	VAL
3	A	80	LEU
3	A	85	GLN
3	A	94	ILE
3	A	101	LYS
3	A	132	ILE
3	A	199	ARG
3	A	215	THR
3	A	220	LYS
3	A	240	THR
3	A	246	LEU
3	A	250	ASP
3	A	268	SER
3	A	278	GLN
3	A	279	LEU
3	A	290	THR
3	A	325	LEU
3	A	345	PRO
3	A	353	LYS
3	A	367	GLN
3	A	373	GLN
3	A	385	LYS
3	A	397	THR
3	A	409	THR
3	A	452	LEU
3	A	459	THR
3	A	464	GLN
3	A	468	PRO
3	A	469	LEU
3	A	474	ASN
3	A	478	GLU
3	A	497	THR
3	A	499	SER
3	A	526	ILE

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Mol	Chain	Res	Type
3	A	533	LEU
3	A	545	ASN
3	A	547	GLN
3	A	548	VAL
3	A	550	LYS
4	B	2	ILE
4	B	3	SER
4	B	8	VAL
4	B	55	PRO
4	B	82	LYS
4	B	83	ARG
4	B	100	LEU
4	B	103	LYS
4	B	104	LYS
4	B	109	LEU
4	B	132	ILE
4	B	148	VAL
4	B	162	SER
4	B	179	VAL
4	B	199	ARG
4	B	215	THR
4	B	233	GLU
4	B	238	LYS
4	B	242	GLN
4	B	250	ASP
4	B	280	SER
4	B	282	LEU
4	B	286	THR
4	B	295	LEU
4	B	301	LEU
4	B	305	GLU
4	B	318	TYR
4	B	330	GLN
4	B	353	LYS
4	B	363	ASN
4	B	407	GLN
4	B	410	TRP
4	B	413	GLU
4	B	418	ASN
4	B	419	THR
4	B	422	LEU
4	B	429	LEU

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Mol	Chain	Res	Type
5	L	1	ASP
5	L	7	THR
5	L	15	LEU
5	L	27	GLN
5	L	39	LYS
5	L	41	GLU
5	L	43	THR
5	L	53	SER
5	L	54	LEU
5	L	65	SER
5	L	77	ASN
5	L	89	GLN
5	L	90	GLN
5	L	106	ILE
5	L	116	SER
5	L	126	THR
5	L	138	ASN
5	L	144	ILE
5	L	180	THR
5	L	190	ASN
5	L	203	SER
6	H	29	LEU
6	H	43	SER
6	H	62	ASN
6	H	64	SER
6	H	72	SER
6	H	84	MET
6	H	118	SER
6	H	129	PRO
6	H	150	CYS
6	H	157	PRO
6	H	171	SER
6	H	187	LEU
6	H	192	THR
6	H	205	CYS
6	H	206	ASN
6	H	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	GLN

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Mol	Chain	Res	Type
3	A	85	GLN
3	A	147	ASN
3	A	174	GLN
3	A	207	GLN
3	A	221	HIS
3	A	269	GLN
3	A	278	GLN
3	A	306	ASN
3	A	330	GLN
3	A	340	GLN
3	A	343	GLN
3	A	367	GLN
3	A	373	GLN
3	A	447	ASN
3	A	464	GLN
3	A	494	ASN
3	A	500	GLN
3	A	520	GLN
4	B	151	GLN
4	B	161	GLN
4	B	175	ASN
4	B	235	HIS
4	B	330	GLN
4	B	363	ASN
4	B	418	ASN
5	L	77	ASN
5	L	89	GLN
5	L	90	GLN
5	L	137	ASN
5	L	138	ASN
5	L	190	ASN
5	L	210	ASN
6	H	1	GLN
6	H	59	ASN
6	H	62	ASN
6	H	83	ASN
6	H	112	HIS
6	H	174	HIS
6	H	181	GLN
6	H	206	ASN
6	H	209	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	2DA	P	822	1,2	16,22,23	0.72	0	13,31,34	0.83	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
2	2DA	P	822	1,2	-	0/3/18/19	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	822	2DA	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is 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$
9	GOL	B	3001	-	5,5,5	4.79	5 (100%)	5,5,5	5.48	3 (60%)
7	GLC	H	1725	-	12,12,12	0.65	0	17,17,17	0.67	0
9	GOL	P	3002	-	5,5,5	4.88	5 (100%)	5,5,5	5.50	3 (60%)

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
9	GOL	B	3001	-	-	0/4/4/4	0/0/0/0
7	GLC	H	1725	-	-	0/2/22/22	0/1/1/1
9	GOL	P	3002	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	3002	GOL	C3-C2	-8.41	1.21	1.52
9	B	3001	GOL	C3-C2	-8.13	1.22	1.52
9	B	3001	GOL	C1-C2	-3.01	1.41	1.52
9	P	3002	GOL	C1-C2	-2.87	1.41	1.52
9	P	3002	GOL	O2-C2	-2.61	1.35	1.43
9	B	3001	GOL	O2-C2	-2.28	1.36	1.43
9	P	3002	GOL	O3-C3	3.27	1.56	1.42
9	B	3001	GOL	O3-C3	3.42	1.56	1.42
9	P	3002	GOL	O1-C1	4.77	1.62	1.42
9	B	3001	GOL	O1-C1	4.78	1.62	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	B	3001	GOL	O1-C1-C2	3.02	125.30	110.07
9	P	3002	GOL	O1-C1-C2	3.10	125.71	110.07
9	P	3002	GOL	O2-C2-C3	6.27	138.45	108.84
9	B	3001	GOL	O2-C2-C3	6.37	138.92	108.84
9	B	3001	GOL	O3-C3-C2	10.01	160.49	110.07
9	P	3002	GOL	O3-C3-C2	10.07	160.82	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	1725	GLC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	24/27 (88%)	0.30	3 (12%) 4 2	43, 87, 120, 126	0
2	P	19/21 (90%)	-0.12	1 (5%) 27 18	60, 75, 109, 117	0
3	A	556/558 (99%)	0.17	23 (4%) 38 27	31, 73, 101, 109	1 (0%)
4	B	429/429 (100%)	-0.05	11 (2%) 56 45	26, 54, 101, 112	1 (0%)
5	L	211/211 (100%)	-0.07	1 (0%) 90 88	39, 64, 98, 104	0
6	H	225/225 (100%)	-0.18	7 (3%) 49 38	35, 55, 87, 109	0
All	All	1464/1471 (99%)	0.01	46 (3%) 49 38	26, 64, 101, 126	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	141	GLN	5.8
6	H	138	SER	5.3
3	A	297	GLU	5.2
3	A	252	TRP	4.8
1	T	702	DT	3.7
3	A	448	ARG	3.5
3	A	293	ILE	3.4
4	B	312	GLU	3.4
6	H	139	ALA	3.3
4	B	303	LEU	3.3
6	H	140	ALA	3.1
3	A	135	ILE	3.0
3	A	138	GLU	3.0
4	B	252	TRP	2.9
3	A	68	SER	2.7
3	A	295	LEU	2.7
3	A	136	ASN	2.7
3	A	244	ILE	2.7
5	L	209	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	T	703	DG	2.6
6	H	225	CYS	2.6
3	A	1	PRO	2.6
4	B	358	ARG	2.6
4	B	295	LEU	2.5
3	A	254	VAL	2.5
3	A	245	VAL	2.5
3	A	223	LYS	2.5
3	A	67	ASP	2.4
1	T	725	DG	2.4
3	A	251	SER	2.3
3	A	257	ILE	2.2
3	A	66	LYS	2.2
3	A	286	THR	2.2
4	B	246	LEU	2.1
6	H	1	GLN	2.1
3	A	290	THR	2.1
3	A	491	LEU	2.1
4	B	314	VAL	2.1
4	B	86	ASP	2.1
2	P	803	DC	2.1
3	A	247	PRO	2.1
4	B	245	VAL	2.1
4	B	362	THR	2.0
4	B	87	PHE	2.0
3	A	69	THR	2.0
6	H	142	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	2DA	P	822	20/21	0.97	0.20	-	51,54,57,58	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MG	A	559	1/1	0.97	0.27	2.04	37,37,37,37	0
9	GOL	B	3001	6/6	0.87	0.18	0.15	67,70,71,72	0
7	GLC	H	1725	12/12	0.90	0.16	-0.11	61,63,65,67	0
9	GOL	P	3002	6/6	0.92	0.13	-0.26	62,65,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.