Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 01:03 AM EDT

PDB ID	:	1N6Q
Title	:	HIV-1 Reverse Transcriptase Crosslinked to pre-translocation AZTMP-terminated DNA (complex N)
Authors	:	Sarafianos, S.G.; Clark Jr., A.D.; Das, K.; Tuske, S.; Birktoft, J.J.; Ilankumaran, I.; Ramesha, A.R.; Sayer, J.M.; Jerina, D.M.; Boyer, P.L.; Hughes, S.H.; Arnold, E.
Deposited on	:	2002-11-11
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

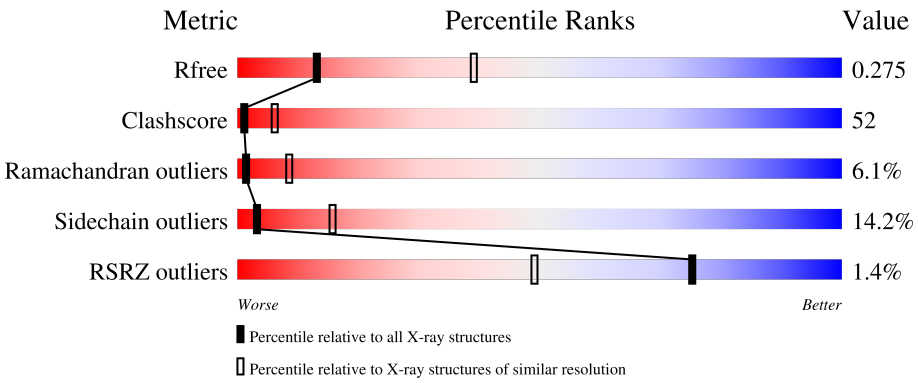
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

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

Mol	Chain	Length	Quality of chain
1	T	27	4%, 11%, 70%, •, 15%
2	P	22	14%, 64%, 18%, 5%
3	A	558	3%, 31%, 53%, 15%, •
4	B	430	%, 28%, 58%, 12%, •
5	L	211	28%, 59%, 12%

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Mol	Chain	Length	Quality of chain
6	H	225	40% 52% 7%

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
2	ATM	P	823	-	-	X	-
7	MG	A	1002	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12250 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(*AP*T*GP*CP*AP*TP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	23	473	223	95	133	22	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*AP*(ATM))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	P	21	429	205	77	126	20	1	0	0	0

- Molecule 3 is a protein called Reverse Transcriptase.

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

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 Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	429	3534	2304	586	637	7	12	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called Monoclonal Antibody (Light Chain).

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

- Molecule 6 is a protein called Monoclonal Antibody (Heavy Chain).

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

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

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

- Molecule 8 is water.

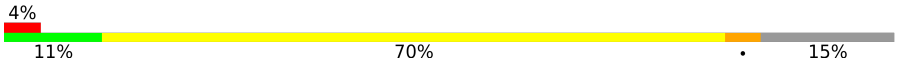
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	2	2	2	0	0

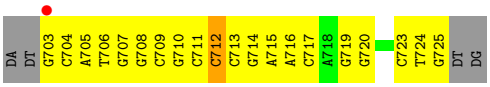
3 Residue-property plots (i)

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

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

Chain T:



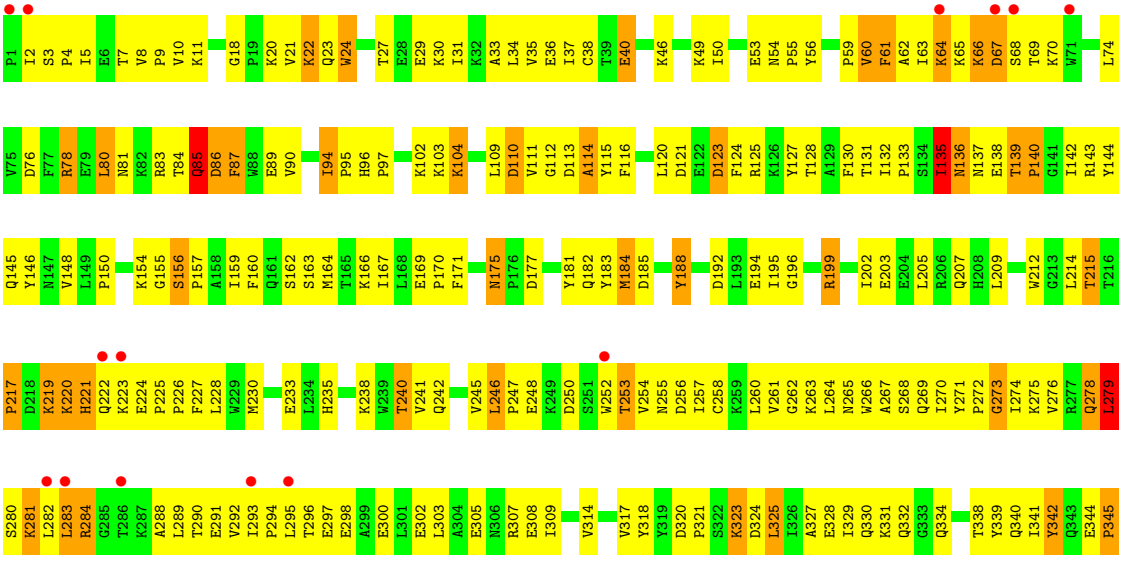


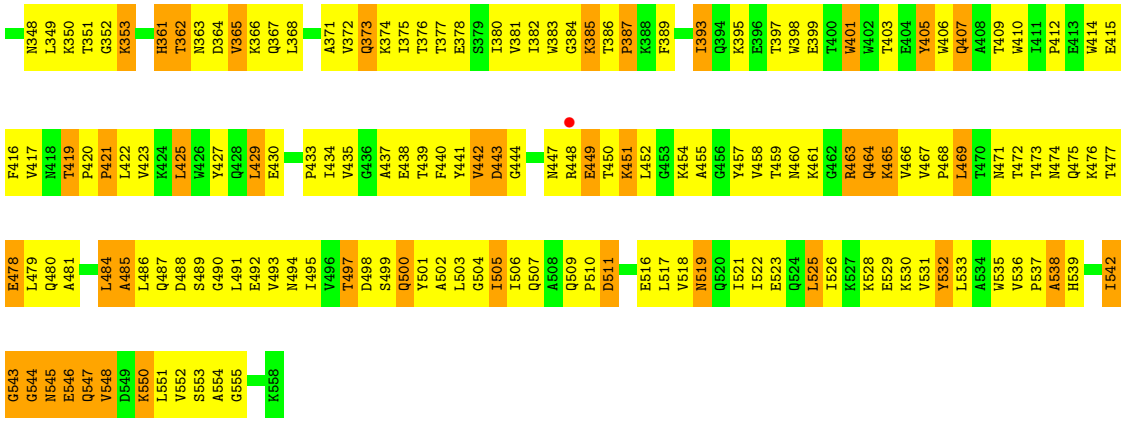
• Molecule 2: 5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*AP*(ATM))-3'

Chain P:

• Molecule 3: Reverse Transcriptase

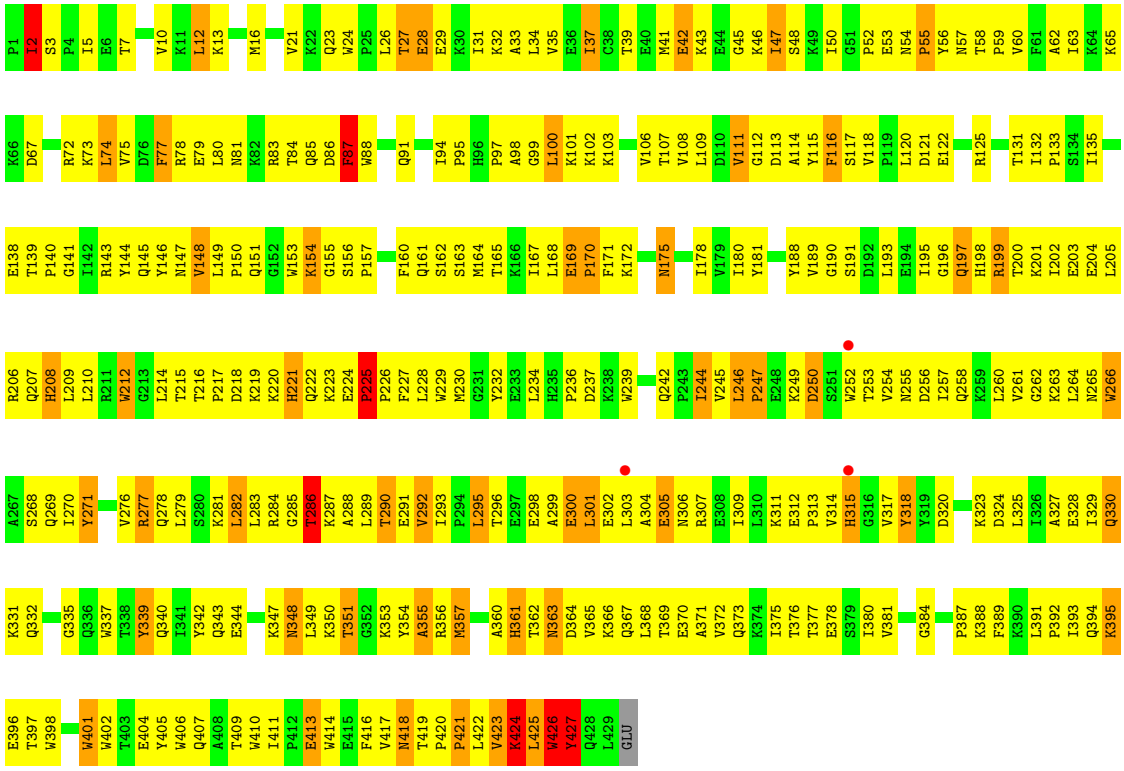
Chain A:





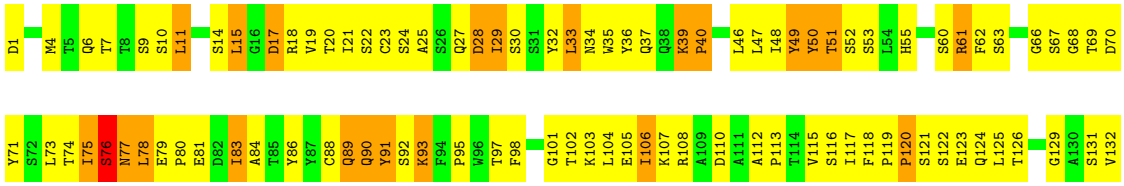
• Molecule 4: Reverse Transcriptase

Chain B:



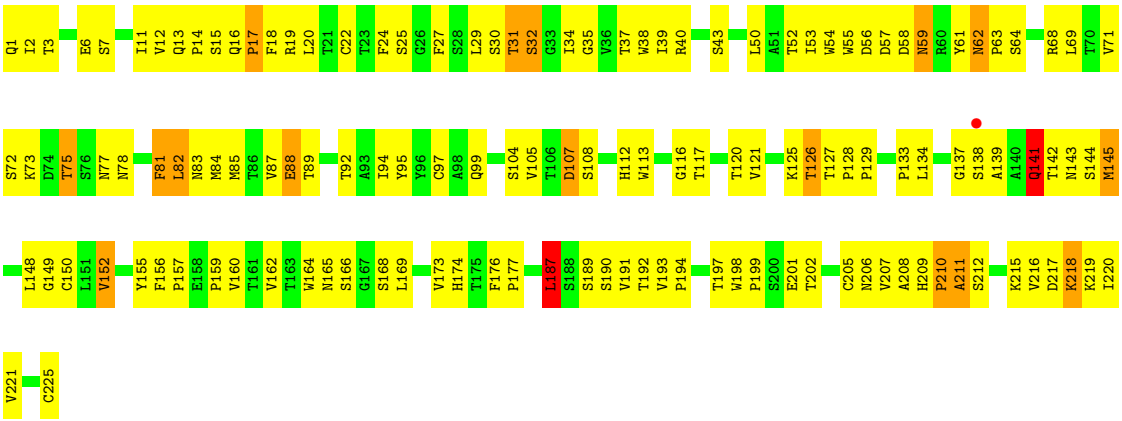
• Molecule 5: Monoclonal Antibody (Light Chain)

Chain L:



• Molecule 6: Monoclonal Antibody (Heavy Chain)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	166.35Å 166.35Å 220.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 39.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	85.0 (20.00-3.00) 85.0 (39.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.284 0.239 , 0.275	Depositor DCC
R_{free} test set	2631 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12250	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.76	0/532	1.04	1/820 (0.1%)
2	P	0.66	0/424	1.13	5/649 (0.8%)
3	A	0.48	2/4600 (0.0%)	0.72	0/6259
4	B	0.59	2/3639 (0.1%)	0.83	6/4949 (0.1%)
5	L	0.50	1/1681 (0.1%)	0.74	0/2283
6	H	0.49	0/1729	0.83	2/2372 (0.1%)
All	All	0.54	5/12605 (0.0%)	0.80	14/17332 (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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	425	LEU	C-N	-7.72	1.16	1.34
3	A	248	GLU	CD-OE2	7.38	1.33	1.25
4	B	426	TRP	N-CA	-6.47	1.33	1.46
5	L	50	TYR	C-N	-5.06	1.22	1.34
3	A	421	PRO	C-N	-5.06	1.22	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	815	DG	N9-C1'-C2'	9.97	131.55	112.60
2	P	816	DG	N9-C1'-C2'	7.73	127.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	427	TYR	N-CA-C	7.72	131.84	111.00
4	B	425	LEU	O-C-N	7.16	134.16	122.70
2	P	815	DG	O4'-C1'-C2'	6.40	111.02	105.90
4	B	425	LEU	CA-C-N	-6.31	103.31	117.20
2	P	816	DG	O4'-C1'-N9	6.24	112.37	108.00
4	B	426	TRP	N-CA-C	-6.06	94.65	111.00
1	T	712	DC	N1-C1'-C2'	6.01	124.02	112.60
2	P	815	DG	O4'-C1'-N9	5.91	112.14	108.00
6	H	141	GLN	N-CA-C	5.91	126.95	111.00
6	H	187	LEU	CA-CB-CG	5.77	128.57	115.30
4	B	225	PRO	N-CA-C	5.60	126.65	112.10
4	B	2	ILE	N-CA-C	5.25	125.17	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	427	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	473	0	257	34	0
2	P	429	0	242	28	0
3	A	4482	0	4484	506	0
4	B	3534	0	3567	407	0
5	L	1643	0	1564	208	0
6	H	1685	0	1640	137	0
7	A	2	0	0	0	0
8	A	2	0	0	0	0
All	All	12250	0	11754	1256	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 52.

All (1256) 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)
6:H:92:THR:HG23	6:H:120:THR:HA	1.34	1.07
3:A:22:LYS:H	3:A:22:LYS:HD3	1.13	1.06
3:A:441:TYR:CE2	3:A:544:GLY:HA3	1.91	1.05
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.37	1.04
3:A:501:TYR:CE1	3:A:505:ILE:HD11	1.93	1.04
3:A:61:PHE:H	3:A:61:PHE:HD2	1.06	1.03
4:B:247:PRO:HG3	4:B:427:TYR:OH	1.57	1.02
5:L:34:ASN:HB2	5:L:89:GLN:NE2	1.74	1.01
5:L:34:ASN:HD22	5:L:89:GLN:HE22	1.06	1.01
1:T:704:DC:H2"	1:T:705:DA:H5'	1.41	1.00
3:A:373:GLN:NE2	4:B:397:THR:HG23	1.78	0.98
6:H:53:ILE:HB	6:H:71:VAL:HG11	1.45	0.98
1:T:707:DG:H2"	1:T:708:DG:H5'	1.45	0.98
3:A:233:GLU:HB2	3:A:240:THR:HG23	1.43	0.96
3:A:138:GLU:HG2	3:A:139:THR:H	1.28	0.96
3:A:344:GLU:HB3	3:A:345:PRO:HD2	1.49	0.95
4:B:257:ILE:O	4:B:261:VAL:HG23	1.64	0.94
4:B:244:ILE:HD13	4:B:244:ILE:H	1.31	0.94
6:H:166:SER:N	6:H:206:ASN:HD21	1.64	0.94
3:A:500:GLN:H	3:A:500:GLN:NE2	1.66	0.94
5:L:11:LEU:HD21	5:L:19:VAL:HG11	1.49	0.93
3:A:34:LEU:HD21	3:A:62:ALA:HB2	1.50	0.93
3:A:64:LYS:HD2	3:A:66:LYS:NZ	1.83	0.93
6:H:142:THR:HG22	6:H:143:ASN:H	1.34	0.93
3:A:215:THR:O	3:A:217:PRO:HD3	1.69	0.92
3:A:3:SER:HB3	3:A:5:ILE:HG13	1.51	0.92
4:B:222:GLN:HG3	4:B:224:GLU:H	1.34	0.92
6:H:53:ILE:HB	6:H:71:VAL:CG1	1.99	0.92
3:A:331:LYS:HB3	3:A:421:PRO:HG2	1.50	0.91
3:A:293:ILE:HD12	3:A:294:PRO:HD2	1.52	0.91
3:A:136:ASN:HD22	3:A:136:ASN:N	1.69	0.91
5:L:15:LEU:HD12	5:L:15:LEU:H	1.36	0.90
3:A:340:GLN:HB3	3:A:348:ASN:OD1	1.71	0.90
6:H:166:SER:H	6:H:206:ASN:HD21	0.91	0.90
5:L:195:GLU:HG2	5:L:206:VAL:HG22	1.54	0.89
3:A:111:VAL:HG11	3:A:214:LEU:HD12	1.54	0.89
3:A:136:ASN:HD22	3:A:136:ASN:H	0.89	0.89
4:B:371:ALA:O	4:B:375:ILE:HG13	1.73	0.88
3:A:136:ASN:H	3:A:136:ASN:ND2	1.71	0.88
3:A:489:SER:HB3	3:A:528:LYS:NZ	1.89	0.88
3:A:501:TYR:O	3:A:505:ILE:HG13	1.74	0.87
1:T:705:DA:H2"	1:T:706:DT:H5'	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:459:THR:HG22	3:A:463:ARG:HB3	1.56	0.87
6:H:148:LEU:HD22	6:H:220:ILE:HG21	1.56	0.86
3:A:275:LYS:HE2	3:A:332:GLN:OE1	1.75	0.86
3:A:143:ARG:HG3	3:A:143:ARG:HH11	1.39	0.86
4:B:225:PRO:HB2	4:B:226:PRO:HD3	1.55	0.86
5:L:34:ASN:ND2	5:L:89:GLN:HE22	1.74	0.86
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.06	0.85
3:A:454:LYS:HE2	3:A:554:ALA:HB3	1.56	0.85
3:A:469:LEU:HD21	3:A:480:GLN:HG2	1.58	0.85
4:B:34:LEU:HD11	4:B:73:LYS:HG3	1.58	0.85
3:A:478:GLU:HG2	3:A:499:SER:HB3	1.59	0.85
4:B:162:SER:O	4:B:165:THR:HG22	1.77	0.85
4:B:340:GLN:HG3	4:B:351:THR:HG22	1.58	0.85
3:A:489:SER:HB3	3:A:528:LYS:HZ3	1.39	0.84
3:A:473:THR:HG22	3:A:474:ASN:H	1.41	0.84
5:L:147:LYS:HZ2	5:L:149:LYS:HG2	1.43	0.84
1:T:705:DA:C2'	1:T:706:DT:H5'	2.07	0.84
2:P:817:MRG:H2"	2:P:818:DC:O5'	1.77	0.84
4:B:361:HIS:CE1	4:B:366:LYS:HE3	2.13	0.83
6:H:166:SER:H	6:H:206:ASN:ND2	1.73	0.83
3:A:344:GLU:CB	3:A:345:PRO:HD2	2.09	0.83
4:B:393:ILE:HD13	4:B:398:TRP:HB2	1.60	0.83
3:A:64:LYS:HD2	3:A:66:LYS:HZ3	1.42	0.83
5:L:33:LEU:HD21	5:L:88:CYS:HB2	1.60	0.83
2:P:818:DC:H2'	2:P:819:DG:H8	1.44	0.82
5:L:34:ASN:HB2	5:L:89:GLN:HE21	1.44	0.82
3:A:439:THR:HG21	4:B:289:LEU:H	1.42	0.82
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.60	0.82
5:L:89:GLN:HB2	5:L:98:PHE:CD1	2.15	0.82
3:A:90:VAL:HG12	4:B:140:PRO:HB3	1.60	0.82
4:B:222:GLN:HE21	4:B:224:GLU:HG3	1.44	0.82
5:L:11:LEU:CD2	5:L:19:VAL:HG11	2.09	0.82
5:L:90:GLN:HE21	5:L:92:SER:H	1.26	0.81
3:A:22:LYS:HD3	3:A:22:LYS:N	1.93	0.81
4:B:80:LEU:O	4:B:84:THR:HG23	1.80	0.81
3:A:135:ILE:HG12	3:A:136:ASN:N	1.95	0.81
4:B:12:LEU:HD12	4:B:12:LEU:H	1.46	0.81
4:B:116:PHE:HA	4:B:148:VAL:HG21	1.61	0.81
4:B:225:PRO:CG	5:L:92:SER:HA	2.11	0.80
5:L:40:PRO:HD3	5:L:84:ALA:HB2	1.63	0.80
3:A:296:THR:HG22	3:A:298:GLU:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:GLN:H	3:A:500:GLN:HE21	1.27	0.80
4:B:135:ILE:HD12	4:B:135:ILE:O	1.82	0.80
4:B:377:THR:O	4:B:381:VAL:HG23	1.82	0.79
3:A:23:GLN:HE22	3:A:60:VAL:H	1.30	0.79
3:A:439:THR:HG21	4:B:289:LEU:N	1.97	0.79
3:A:441:TYR:CD2	3:A:544:GLY:HA3	2.17	0.79
5:L:147:LYS:HZ2	5:L:149:LYS:HE3	1.46	0.79
5:L:124:GLN:HG2	5:L:129:GLY:O	1.81	0.78
4:B:422:LEU:O	4:B:423:VAL:HG23	1.83	0.78
6:H:16:GLN:O	6:H:87:VAL:HG22	1.84	0.78
3:A:61:PHE:CD2	3:A:61:PHE:N	2.49	0.78
3:A:497:THR:HG22	3:A:498:ASP:H	1.48	0.77
5:L:86:TYR:O	5:L:101:GLY:HA2	1.84	0.77
3:A:5:ILE:CD1	3:A:167:ILE:HD11	2.14	0.77
3:A:22:LYS:H	3:A:22:LYS:CD	1.90	0.77
4:B:387:PRO:HG2	4:B:389:PHE:CE1	2.20	0.77
3:A:447:ASN:HD22	3:A:450:THR:HG23	1.49	0.77
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.14	0.77
4:B:223:LYS:HD2	4:B:223:LYS:N	2.00	0.77
4:B:296:THR:HG22	4:B:298:GLU:H	1.49	0.77
5:L:190:ASN:HD22	5:L:211:ARG:HG2	1.50	0.76
1:T:704:DC:H2"	1:T:705:DA:C5'	2.16	0.76
5:L:17:ASP:O	5:L:77:ASN:HA	1.86	0.76
3:A:63:ILE:HD12	3:A:64:LYS:H	1.51	0.75
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.66	0.75
5:L:150:ILE:HD11	5:L:155:ARG:HD3	1.68	0.75
4:B:97:PRO:HG2	4:B:181:TYR:HB2	1.68	0.75
4:B:225:PRO:HG3	5:L:92:SER:HA	1.67	0.75
5:L:106:ILE:HG13	5:L:166:GLN:OE1	1.85	0.75
3:A:175:ASN:N	3:A:175:ASN:HD22	1.84	0.75
4:B:366:LYS:HG2	4:B:370:GLU:OE2	1.86	0.75
3:A:60:VAL:HG11	3:A:130:PHE:HD1	1.52	0.75
3:A:430:GLU:HB2	3:A:532:TYR:HB2	1.69	0.75
3:A:288:ALA:HB3	3:A:291:GLU:HB2	1.69	0.74
4:B:304:ALA:O	4:B:307:ARG:HG2	1.86	0.74
2:P:818:DC:H2'	2:P:819:DG:C8	2.22	0.74
4:B:285:GLY:H	4:B:287:LYS:HZ1	1.36	0.74
3:A:457:TYR:HA	3:A:548:VAL:CG1	2.17	0.74
3:A:500:GLN:HE21	3:A:500:GLN:N	1.85	0.74
4:B:365:VAL:O	4:B:369:THR:HG23	1.88	0.74
3:A:371:ALA:O	3:A:375:ILE:HG12	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:104:LYS:HB2	3:A:192:ASP:HA	1.69	0.73
4:B:314:VAL:HG12	4:B:315:HIS:H	1.53	0.73
3:A:31:ILE:O	3:A:35:VAL:HG23	1.87	0.73
6:H:34:ILE:CG2	6:H:35:GLY:N	2.52	0.73
3:A:203:GLU:HG3	3:A:207:GLN:NE2	2.03	0.73
2:P:807:DC:H4'	3:A:448:ARG:HD2	1.70	0.73
3:A:479:LEU:HD21	3:A:518:VAL:CG2	2.19	0.73
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.24	0.73
4:B:254:VAL:HB	4:B:289:LEU:O	1.89	0.72
1:T:716:DA:H1'	1:T:717:DC:H5'	1.71	0.72
3:A:434:ILE:HG22	3:A:494:ASN:HD21	1.55	0.72
4:B:13:LYS:HE2	4:B:85:GLN:HB3	1.69	0.72
6:H:56:ASP:OD2	6:H:58:ASP:HB2	1.89	0.72
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.71	0.72
6:H:129:PRO:HB3	6:H:155:TYR:HB3	1.70	0.72
6:H:150:CYS:HB2	6:H:164:TRP:CH2	2.25	0.72
3:A:257:ILE:HB	3:A:283:LEU:HD21	1.71	0.72
3:A:454:LYS:CE	3:A:554:ALA:HB3	2.20	0.72
5:L:90:GLN:NE2	5:L:92:SER:H	1.85	0.72
5:L:34:ASN:OD1	5:L:49:TYR:HA	1.88	0.72
6:H:95:TYR:O	6:H:116:GLY:HA2	1.88	0.72
3:A:138:GLU:HG2	3:A:139:THR:N	2.05	0.72
3:A:429:LEU:HD22	3:A:533:LEU:HD13	1.72	0.72
5:L:15:LEU:HD12	5:L:15:LEU:N	2.05	0.72
4:B:34:LEU:HD13	4:B:62:ALA:HB2	1.70	0.71
3:A:279:LEU:O	3:A:282:LEU:HG	1.91	0.71
5:L:40:PRO:HD3	5:L:84:ALA:CB	2.20	0.71
3:A:247:PRO:HD2	3:A:260:LEU:HD12	1.71	0.71
4:B:12:LEU:HD12	4:B:12:LEU:N	2.05	0.71
4:B:363:ASN:O	4:B:367:GLN:HG3	1.90	0.71
6:H:38:TRP:CZ3	6:H:97:CYS:HB3	2.25	0.71
4:B:222:GLN:NE2	4:B:224:GLU:HG3	2.04	0.71
4:B:263:LYS:HA	4:B:423:VAL:HG11	1.71	0.71
4:B:171:PHE:HE1	4:B:205:LEU:HA	1.55	0.70
5:L:170:ASP:O	5:L:172:THR:HG23	1.91	0.70
4:B:106:VAL:HG13	4:B:234:LEU:HB2	1.72	0.70
4:B:85:GLN:HG3	4:B:88:TRP:CE2	2.26	0.70
4:B:237:ASP:C	4:B:239:TRP:H	1.92	0.70
4:B:263:LYS:HG2	4:B:423:VAL:HG12	1.74	0.70
3:A:222:GLN:O	3:A:224:GLU:HG3	1.92	0.70
3:A:473:THR:HG22	3:A:474:ASN:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:5:ILE:HD13	3:A:167:ILE:HD11	1.72	0.69
4:B:199:ARG:HH11	4:B:199:ARG:HG2	1.56	0.69
3:A:479:LEU:HD21	3:A:518:VAL:HG22	1.73	0.69
6:H:19:ARG:HD2	6:H:83:ASN:HD21	1.57	0.69
3:A:317:VAL:HG22	3:A:318:TYR:N	2.07	0.69
3:A:417:VAL:HG13	3:A:419:THR:HG22	1.75	0.69
3:A:235:HIS:HB2	3:A:238:LYS:O	1.93	0.69
4:B:332:GLN:NE2	4:B:426:TRP:O	2.25	0.69
5:L:1:ASP:N	5:L:95:PRO:HG2	2.07	0.69
5:L:150:ILE:CD1	5:L:155:ARG:HD3	2.22	0.69
5:L:206:VAL:O	5:L:207:LYS:HG2	1.93	0.69
6:H:89:THR:HA	6:H:121:VAL:HB	1.73	0.69
3:A:450:THR:O	3:A:451:LYS:HG2	1.93	0.68
3:A:543:GLY:O	3:A:545:ASN:N	2.26	0.68
6:H:142:THR:HG22	6:H:143:ASN:N	2.07	0.68
5:L:19:VAL:HG12	5:L:20:THR:N	2.08	0.68
6:H:133:PRO:O	6:H:134:LEU:HD23	1.94	0.68
3:A:406:TRP:CZ2	4:B:420:PRO:HG3	2.29	0.68
5:L:23:CYS:SG	5:L:33:LEU:HD11	2.34	0.68
6:H:38:TRP:O	6:H:50:LEU:HB2	1.94	0.68
3:A:34:LEU:CD2	3:A:62:ALA:HB2	2.22	0.68
3:A:209:LEU:HB3	3:A:214:LEU:HB2	1.76	0.68
3:A:523:GLU:HA	3:A:523:GLU:OE2	1.94	0.68
3:A:437:ALA:HB1	3:A:493:VAL:HA	1.76	0.67
5:L:83:ILE:HD12	5:L:106:ILE:HG23	1.76	0.67
6:H:69:LEU:HD22	6:H:82:LEU:HD11	1.75	0.67
6:H:145:MET:HE1	6:H:194:PRO:HG3	1.76	0.67
5:L:183:LYS:HE2	5:L:187:GLU:OE1	1.94	0.67
3:A:473:THR:O	3:A:477:THR:HG23	1.95	0.67
3:A:27:THR:OG1	3:A:30:LYS:HG3	1.94	0.67
3:A:138:GLU:OE1	3:A:139:THR:HG22	1.95	0.67
3:A:254:VAL:HG11	3:A:288:ALA:O	1.94	0.67
5:L:120:PRO:HG3	5:L:131:SER:O	1.95	0.67
3:A:278:GLN:HB2	3:A:302:GLU:CB	2.24	0.67
4:B:56:TYR:O	4:B:143:ARG:NH2	2.27	0.67
4:B:85:GLN:O	4:B:85:GLN:HG2	1.95	0.67
4:B:171:PHE:CE1	4:B:205:LEU:HA	2.28	0.67
4:B:285:GLY:O	4:B:287:LYS:HG2	1.94	0.67
4:B:395:LYS:HB2	4:B:416:PHE:CD2	2.28	0.67
4:B:34:LEU:CD1	4:B:73:LYS:HG3	2.24	0.67
3:A:463:ARG:HG3	3:A:464:GLN:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:363:ASN:C	4:B:363:ASN:HD22	1.97	0.67
2:P:805:DG:H1'	2:P:806:DT:H5"	1.75	0.67
3:A:425:LEU:HD13	3:A:509:GLN:OE1	1.94	0.67
4:B:250:ASP:OD2	4:B:250:ASP:N	2.22	0.67
3:A:362:THR:OG1	3:A:363:ASN:N	2.28	0.66
4:B:229:TRP:HA	4:B:232:TYR:CE1	2.30	0.66
5:L:147:LYS:NZ	5:L:149:LYS:HE3	2.08	0.66
5:L:48:ILE:HG23	5:L:53:SER:O	1.95	0.66
3:A:139:THR:OG1	3:A:140:PRO:HD2	1.94	0.66
4:B:97:PRO:HD3	4:B:181:TYR:CD1	2.31	0.66
4:B:234:LEU:HD21	4:B:377:THR:HG21	1.77	0.66
4:B:311:LYS:O	4:B:312:GLU:HG2	1.94	0.66
5:L:15:LEU:H	5:L:15:LEU:CD1	2.04	0.66
3:A:170:PRO:HG2	3:A:171:PHE:H	1.61	0.66
4:B:7:THR:OG1	4:B:121:ASP:HA	1.95	0.66
4:B:47:ILE:HG23	4:B:144:TYR:HD1	1.59	0.66
1:T:707:DG:C2'	1:T:708:DG:H5'	2.23	0.66
3:A:501:TYR:CZ	3:A:505:ILE:HD11	2.30	0.66
3:A:293:ILE:CD1	3:A:294:PRO:HD2	2.23	0.66
4:B:266:TRP:CZ2	4:B:422:LEU:HD13	2.31	0.66
3:A:469:LEU:CD2	3:A:480:GLN:HG2	2.24	0.66
3:A:548:VAL:O	3:A:552:VAL:HG23	1.96	0.66
5:L:48:ILE:HD12	5:L:73:LEU:HD13	1.78	0.66
3:A:331:LYS:HD3	3:A:332:GLN:N	2.12	0.65
4:B:426:TRP:HA	4:B:426:TRP:CE3	2.30	0.65
3:A:49:LYS:HB2	3:A:49:LYS:NZ	2.11	0.65
3:A:143:ARG:HG3	3:A:143:ARG:NH1	2.08	0.65
3:A:175:ASN:N	3:A:175:ASN:ND2	2.42	0.65
3:A:194:GLU:O	3:A:196:GLY:N	2.29	0.65
3:A:471:ASN:O	3:A:472:THR:HG23	1.96	0.65
3:A:30:LYS:O	3:A:33:ALA:HB3	1.96	0.65
4:B:360:ALA:HB1	4:B:367:GLN:HE21	1.60	0.65
4:B:263:LYS:HG2	4:B:423:VAL:CG1	2.25	0.65
4:B:33:ALA:O	4:B:37:ILE:HG22	1.96	0.65
3:A:255:ASN:HD22	3:A:289:LEU:HG	1.62	0.65
3:A:484:LEU:O	3:A:486:LEU:N	2.30	0.65
4:B:101:LYS:O	4:B:236:PRO:HB2	1.97	0.65
4:B:293:ILE:HD13	4:B:293:ILE:N	2.12	0.65
4:B:314:VAL:HG12	4:B:315:HIS:N	2.11	0.65
5:L:107:LYS:HA	5:L:140:TYR:OH	1.97	0.65
2:P:815:DG:H2'	2:P:816:DG:H8	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:486:LEU:HD21	3:A:495:ILE:HD11	1.79	0.65
4:B:43:LYS:C	4:B:45:GLY:H	2.00	0.65
1:T:706:DT:H2'	1:T:707:DG:C8	2.32	0.64
4:B:79:GLU:HB3	4:B:83:ARG:NH1	2.12	0.64
3:A:303:LEU:O	3:A:307:ARG:HG3	1.97	0.64
4:B:225:PRO:HB3	5:L:32:TYR:CE1	2.33	0.64
3:A:254:VAL:HG13	3:A:255:ASN:N	2.13	0.64
5:L:39:LYS:NZ	5:L:39:LYS:HB3	2.13	0.64
4:B:223:LYS:HE3	6:H:58:ASP:HB3	1.80	0.64
3:A:171:PHE:CE2	3:A:205:LEU:HD12	2.33	0.64
3:A:258:CYS:HA	3:A:261:VAL:CG1	2.28	0.64
3:A:499:SER:OG	3:A:502:ALA:HB3	1.98	0.64
3:A:458:VAL:HG11	4:B:286:THR:HG21	1.80	0.64
3:A:215:THR:C	3:A:217:PRO:HD3	2.18	0.64
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.33	0.64
5:L:34:ASN:HB2	5:L:89:GLN:HE22	1.60	0.63
4:B:266:TRP:CE3	4:B:423:VAL:HG21	2.32	0.63
3:A:267:ALA:HB1	3:A:271:TYR:HD2	1.63	0.63
3:A:473:THR:CG2	3:A:474:ASN:H	2.11	0.63
4:B:314:VAL:HB	4:B:317:VAL:CG2	2.28	0.63
6:H:162:VAL:HG22	6:H:207:VAL:HG22	1.79	0.63
2:P:808:DC:H5'	2:P:808:DC:H6	1.61	0.63
6:H:169:LEU:HD21	6:H:193:VAL:CG1	2.28	0.63
3:A:429:LEU:HD22	3:A:533:LEU:CD1	2.29	0.63
5:L:137:ASN:HB3	5:L:138:ASN:ND2	2.14	0.63
4:B:111:VAL:HG23	4:B:111:VAL:O	1.97	0.63
3:A:40:GLU:HA	3:A:40:GLU:OE1	1.98	0.63
3:A:182:GLN:O	3:A:182:GLN:HG3	1.98	0.63
3:A:518:VAL:O	3:A:522:ILE:HG13	1.99	0.63
4:B:266:TRP:HE3	4:B:423:VAL:HG21	1.63	0.63
5:L:120:PRO:HB2	5:L:125:LEU:HD21	1.80	0.63
3:A:76:ASP:OD1	3:A:78:ARG:HB2	1.98	0.63
3:A:255:ASN:HB2	3:A:289:LEU:O	1.98	0.63
6:H:18:PHE:HD2	6:H:87:VAL:HG11	1.62	0.63
5:L:34:ASN:HD22	5:L:89:GLN:NE2	1.89	0.62
4:B:260:LEU:HD21	4:B:303:LEU:HD13	1.81	0.62
5:L:147:LYS:NZ	5:L:149:LYS:HG2	2.13	0.62
3:A:297:GLU:HA	3:A:300:GLU:CG	2.30	0.62
4:B:85:GLN:HG3	4:B:88:TRP:CZ2	2.34	0.62
4:B:325:LEU:HB3	4:B:387:PRO:HB3	1.79	0.62
4:B:329:ILE:O	4:B:392:PRO:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:261:VAL:HA	3:A:264:LEU:HD12	1.81	0.62
4:B:285:GLY:H	4:B:287:LYS:NZ	1.96	0.62
4:B:387:PRO:HG2	4:B:389:PHE:HE1	1.63	0.62
3:A:115:TYR:OH	3:A:157:PRO:HA	2.00	0.62
3:A:203:GLU:C	3:A:207:GLN:HE21	2.02	0.62
4:B:224:GLU:HB3	4:B:225:PRO:HD2	1.81	0.62
5:L:144:ILE:HG23	5:L:145:ASN:N	2.15	0.62
3:A:297:GLU:HA	3:A:300:GLU:HB2	1.82	0.62
4:B:305:GLU:OE1	4:B:309:ILE:HD11	2.00	0.62
3:A:317:VAL:HG22	3:A:318:TYR:H	1.63	0.62
5:L:118:PHE:CD2	6:H:134:LEU:HB3	2.35	0.62
6:H:62:ASN:HD21	6:H:64:SER:HB2	1.65	0.62
4:B:302:GLU:HA	4:B:305:GLU:HB2	1.82	0.61
5:L:124:GLN:HE22	5:L:131:SER:HB2	1.65	0.61
6:H:145:MET:CE	6:H:194:PRO:HG3	2.29	0.61
6:H:18:PHE:CD2	6:H:87:VAL:HG11	2.35	0.61
2:P:803:DC:H2"	2:P:804:DA:C8	2.35	0.61
3:A:87:PHE:N	3:A:87:PHE:CD2	2.67	0.61
3:A:405:TYR:HD1	3:A:406:TRP:H	1.48	0.61
4:B:75:VAL:HG11	4:B:77:PHE:CZ	2.33	0.61
4:B:247:PRO:CG	4:B:427:TYR:OH	2.43	0.61
4:B:360:ALA:CB	4:B:367:GLN:HE21	2.13	0.61
3:A:102:LYS:HG2	3:A:318:TYR:HD1	1.65	0.61
3:A:466:VAL:HG21	3:A:551:LEU:HG	1.82	0.61
3:A:473:THR:H	3:A:476:LYS:HG3	1.64	0.61
3:A:550:LYS:HE2	3:A:550:LYS:HA	1.82	0.61
4:B:244:ILE:HD13	4:B:244:ILE:N	2.09	0.61
6:H:169:LEU:HD21	6:H:193:VAL:HG11	1.82	0.61
3:A:90:VAL:CG1	4:B:140:PRO:HB3	2.30	0.61
6:H:19:ARG:NH2	6:H:81:PHE:CD2	2.69	0.61
1:T:709:DC:H2'	1:T:710:DG:H8	1.65	0.61
3:A:460:ASN:HA	4:B:286:THR:O	2.01	0.61
6:H:208:ALA:HB2	6:H:215:LYS:HD2	1.83	0.61
3:A:258:CYS:HA	3:A:261:VAL:HG12	1.82	0.61
6:H:142:THR:CG2	6:H:143:ASN:H	2.11	0.61
1:T:713:DC:H2'	1:T:714:DG:C8	2.36	0.61
4:B:106:VAL:HA	4:B:190:GLY:HA2	1.82	0.61
4:B:125:ARG:HD3	4:B:147:ASN:HA	1.81	0.61
5:L:60:SER:C	5:L:62:PHE:H	2.03	0.61
3:A:438:GLU:HB3	3:A:459:THR:OG1	2.01	0.61
3:A:438:GLU:OE2	3:A:463:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:491:LEU:HD23	3:A:529:GLU:OE1	2.01	0.61
4:B:262:GLY:O	4:B:265:ASN:HB3	2.01	0.61
3:A:511:ASP:OD2	3:A:511:ASP:C	2.40	0.60
2:P:815:DG:H2'	2:P:816:DG:C8	2.36	0.60
6:H:6:GLU:N	6:H:6:GLU:OE1	2.32	0.60
4:B:206:ARG:NH1	4:B:217:PRO:O	2.35	0.60
1:T:715:DA:H2"	1:T:716:DA:OP2	2.02	0.60
3:A:550:LYS:HA	3:A:550:LYS:CE	2.31	0.60
6:H:133:PRO:HD3	6:H:218:LYS:HD2	1.84	0.60
3:A:23:GLN:HE22	3:A:60:VAL:N	1.97	0.60
3:A:459:THR:HG22	3:A:463:ARG:CB	2.29	0.60
4:B:279:LEU:HD11	4:B:302:GLU:HB2	1.84	0.60
3:A:7:THR:OG1	3:A:121:ASP:HA	2.02	0.59
4:B:46:LYS:HD3	4:B:116:PHE:HB3	1.83	0.59
6:H:128:PRO:HA	6:H:209:HIS:HD2	1.67	0.59
4:B:43:LYS:C	4:B:45:GLY:N	2.54	0.59
4:B:108:VAL:HG12	4:B:188:TYR:CE1	2.37	0.59
5:L:89:GLN:HB2	5:L:98:PHE:CE1	2.37	0.59
4:B:131:THR:HG22	4:B:132:ILE:N	2.17	0.59
4:B:266:TRP:CE3	4:B:423:VAL:CG2	2.86	0.59
5:L:146:VAL:CG1	5:L:147:LYS:N	2.65	0.59
3:A:503:LEU:CD2	3:A:535:TRP:HB2	2.32	0.59
4:B:116:PHE:HA	4:B:148:VAL:CG2	2.31	0.59
5:L:181:LEU:N	5:L:181:LEU:HD12	2.18	0.59
1:T:711:DC:H2'	1:T:712:DC:C6	2.37	0.59
3:A:363:ASN:OD1	3:A:364:ASP:N	2.36	0.59
3:A:417:VAL:HG13	3:A:419:THR:CG2	2.33	0.59
5:L:137:ASN:HB3	5:L:138:ASN:HD22	1.67	0.59
3:A:305:GLU:O	3:A:308:GLU:HB2	2.02	0.59
3:A:221:HIS:N	3:A:221:HIS:CD2	2.70	0.59
3:A:440:PHE:HE2	3:A:489:SER:HG	1.50	0.59
3:A:542:ILE:HD12	3:A:542:ILE:H	1.68	0.59
5:L:61:ARG:HB2	5:L:76:SER:HB3	1.84	0.59
6:H:59:ASN:ND2	6:H:59:ASN:H	1.98	0.59
6:H:81:PHE:CD1	6:H:81:PHE:N	2.68	0.59
3:A:542:ILE:HD12	3:A:542:ILE:N	2.17	0.59
4:B:163:SER:O	4:B:167:ILE:HG13	2.03	0.59
4:B:199:ARG:HG2	4:B:199:ARG:NH1	2.17	0.59
3:A:33:ALA:O	3:A:36:GLU:HB2	2.02	0.59
3:A:257:ILE:HD11	3:A:293:ILE:HG21	1.85	0.59
4:B:342:TYR:HB3	4:B:348:ASN:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:200:THR:HG22	4:B:201:LYS:N	2.17	0.58
5:L:115:VAL:HG12	5:L:116:SER:N	2.18	0.58
3:A:368:LEU:O	3:A:372:VAL:HG23	2.03	0.58
3:A:420:PRO:HG3	3:A:422:LEU:HG	1.85	0.58
5:L:61:ARG:CZ	5:L:79:GLU:HG3	2.32	0.58
4:B:47:ILE:HD12	4:B:146:TYR:HA	1.85	0.58
5:L:161:ASN:HB3	5:L:163:TRP:CH2	2.37	0.58
3:A:457:TYR:HA	3:A:548:VAL:HG11	1.85	0.58
3:A:493:VAL:HG22	3:A:494:ASN:N	2.18	0.58
4:B:97:PRO:HB2	4:B:100:LEU:HB2	1.84	0.58
6:H:34:ILE:HG22	6:H:35:GLY:N	2.19	0.58
3:A:279:LEU:N	3:A:279:LEU:HD23	2.19	0.58
5:L:35:TRP:CZ3	5:L:88:CYS:HB3	2.38	0.58
2:P:820:DC:H2'	2:P:821:DC:H6	1.68	0.58
3:A:274:ILE:O	3:A:276:VAL:HG23	2.04	0.58
4:B:309:ILE:N	4:B:309:ILE:HD13	2.19	0.58
4:B:329:ILE:HD11	4:B:375:ILE:HD12	1.85	0.58
3:A:254:VAL:HG13	3:A:255:ASN:H	1.68	0.58
5:L:63:SER:O	5:L:73:LEU:HD12	2.04	0.58
3:A:50:ILE:HG23	3:A:145:GLN:HB3	1.86	0.58
3:A:329:ILE:HG21	3:A:368:LEU:CD1	2.34	0.58
3:A:542:ILE:H	3:A:542:ILE:CD1	2.17	0.58
5:L:173:TYR:N	5:L:173:TYR:CD1	2.71	0.58
3:A:533:LEU:HD12	3:A:533:LEU:N	2.18	0.57
4:B:295:LEU:HD13	4:B:300:GLU:OE1	2.03	0.57
4:B:314:VAL:CG1	4:B:315:HIS:H	2.17	0.57
4:B:332:GLN:HA	4:B:332:GLN:OE1	2.03	0.57
5:L:88:CYS:O	5:L:98:PHE:HA	2.03	0.57
6:H:53:ILE:HG23	6:H:53:ILE:O	2.04	0.57
4:B:226:PRO:O	4:B:228:LEU:HG	2.03	0.57
4:B:423:VAL:O	4:B:424:LYS:HB2	2.04	0.57
6:H:56:ASP:OD2	6:H:58:ASP:CB	2.51	0.57
6:H:174:HIS:O	6:H:189:SER:HA	2.04	0.57
3:A:406:TRP:HE1	4:B:418:ASN:ND2	2.02	0.57
3:A:458:VAL:HG21	3:A:547:GLN:HB3	1.85	0.57
4:B:225:PRO:CB	4:B:226:PRO:HD3	2.32	0.57
5:L:146:VAL:HG12	5:L:147:LYS:N	2.18	0.57
2:P:814:DC:H2"	2:P:815:DG:H8	1.68	0.57
5:L:6:GLN:HA	5:L:22:SER:O	2.05	0.57
3:A:502:ALA:O	3:A:506:ILE:HG12	2.05	0.57
1:T:706:DT:H2'	1:T:707:DG:H8	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:166:LYS:O	3:A:169:GLU:HB3	2.05	0.57
3:A:518:VAL:O	3:A:518:VAL:HG12	2.03	0.57
6:H:145:MET:HA	6:H:194:PRO:HA	1.87	0.57
1:T:704:DC:O2	1:T:704:DC:H2'	2.05	0.57
3:A:479:LEU:O	3:A:521:ILE:HD11	2.04	0.57
4:B:191:SER:OG	4:B:198:HIS:ND1	2.27	0.57
4:B:302:GLU:HA	4:B:305:GLU:CB	2.35	0.57
3:A:498:ASP:OD2	3:A:538:ALA:HB2	2.04	0.57
4:B:209:LEU:O	4:B:212:TRP:N	2.36	0.57
4:B:23:GLN:OE1	4:B:59:PRO:HA	2.05	0.56
4:B:237:ASP:C	4:B:239:TRP:N	2.58	0.56
5:L:33:LEU:HD23	5:L:89:GLN:O	2.04	0.56
5:L:136:LEU:HD23	5:L:144:ILE:HD13	1.87	0.56
6:H:166:SER:N	6:H:206:ASN:ND2	2.41	0.56
3:A:440:PHE:HD2	3:A:493:VAL:HG21	1.69	0.56
3:A:280:SER:O	3:A:282:LEU:N	2.38	0.56
3:A:323:LYS:HD3	3:A:344:GLU:OE1	2.05	0.56
4:B:263:LYS:HE2	4:B:424:LYS:HB3	1.87	0.56
4:B:291:GLU:HG2	4:B:293:ILE:HD13	1.86	0.56
4:B:393:ILE:HG12	4:B:394:GLN:N	2.19	0.56
5:L:179:LEU:CD2	5:L:181:LEU:HD11	2.35	0.56
3:A:135:ILE:CG1	3:A:136:ASN:N	2.66	0.56
3:A:442:VAL:O	3:A:443:ASP:HB2	2.05	0.56
3:A:458:VAL:CG1	4:B:286:THR:HG21	2.35	0.56
4:B:283:LEU:HD23	4:B:287:LYS:HE2	1.87	0.56
4:B:394:GLN:O	4:B:395:LYS:C	2.44	0.56
6:H:34:ILE:N	6:H:34:ILE:HD12	2.20	0.56
6:H:84:MET:HG2	6:H:87:VAL:HG12	1.85	0.56
6:H:134:LEU:HD12	6:H:149:GLY:HA3	1.88	0.56
4:B:171:PHE:CD1	4:B:205:LEU:HD13	2.40	0.56
4:B:254:VAL:O	4:B:257:ILE:HG12	2.06	0.56
5:L:146:VAL:CG2	5:L:175:MET:HE1	2.36	0.56
3:A:247:PRO:O	3:A:252:TRP:HH2	1.88	0.56
5:L:34:ASN:CB	5:L:89:GLN:NE2	2.62	0.56
6:H:22:CYS:HB2	6:H:38:TRP:CH2	2.40	0.56
2:P:808:DC:H5'	2:P:808:DC:C6	2.41	0.56
3:A:96:HIS:ND1	3:A:97:PRO:HD2	2.20	0.56
5:L:146:VAL:HG21	5:L:175:MET:CE	2.35	0.56
2:P:814:DC:H2"	2:P:815:DG:C8	2.40	0.56
2:P:823:ATM:H1'	3:A:115:TYR:HE2	1.70	0.56
3:A:109:LEU:O	3:A:110:ASP:OD2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:245:VAL:HG22	4:B:246:LEU:N	2.21	0.56
2:P:823:ATM:H1'	3:A:115:TYR:CE2	2.41	0.56
3:A:361:HIS:CD2	3:A:505:ILE:HG23	2.41	0.56
4:B:72:ARG:HG3	4:B:72:ARG:HH11	1.70	0.56
3:A:181:TYR:CE1	4:B:138:GLU:HA	2.40	0.55
3:A:536:VAL:HG13	3:A:537:PRO:HD2	1.87	0.55
4:B:57:ASN:ND2	4:B:58:THR:H	2.05	0.55
4:B:206:ARG:HD2	4:B:216:THR:OG1	2.06	0.55
3:A:63:ILE:CD1	3:A:64:LYS:H	2.18	0.55
4:B:63:ILE:HG13	4:B:63:ILE:O	2.05	0.55
4:B:314:VAL:HB	4:B:317:VAL:HG21	1.86	0.55
5:L:66:GLY:HA3	5:L:71:TYR:HA	1.88	0.55
3:A:86:ASP:HA	3:A:154:LYS:HZ2	1.71	0.55
3:A:484:LEU:O	3:A:487:GLN:N	2.40	0.55
3:A:486:LEU:CD2	3:A:495:ILE:HD11	2.36	0.55
3:A:439:THR:HG23	4:B:288:ALA:HA	1.88	0.55
4:B:116:PHE:CA	4:B:148:VAL:HG21	2.33	0.55
4:B:227:PHE:O	4:B:230:MET:HB2	2.07	0.55
4:B:420:PRO:HB3	4:B:421:PRO:HD2	1.88	0.55
5:L:20:THR:HA	5:L:73:LEU:O	2.07	0.55
3:A:420:PRO:HA	3:A:421:PRO:C	2.27	0.55
3:A:457:TYR:CZ	3:A:465:LYS:HB3	2.42	0.55
4:B:350:LYS:HE2	4:B:378:GLU:OE1	2.06	0.55
5:L:146:VAL:HG21	5:L:175:MET:HE1	1.88	0.55
6:H:55:TRP:HE3	6:H:55:TRP:H	1.53	0.55
6:H:59:ASN:ND2	6:H:59:ASN:N	2.54	0.55
2:P:820:DC:H2"	2:P:821:DC:H5'	1.88	0.55
3:A:338:THR:HG22	3:A:339:TYR:N	2.22	0.55
3:A:427:TYR:CZ	3:A:525:LEU:HD23	2.42	0.55
3:A:465:LYS:HD2	3:A:467:VAL:HG13	1.87	0.55
5:L:33:LEU:HD23	5:L:34:ASN:N	2.22	0.55
4:B:277:ARG:C	4:B:279:LEU:H	2.10	0.55
3:A:344:GLU:CB	3:A:345:PRO:CD	2.84	0.55
3:A:344:GLU:CG	3:A:345:PRO:HD2	2.37	0.55
4:B:198:HIS:O	4:B:199:ARG:C	2.45	0.55
5:L:78:LEU:HD21	5:L:104:LEU:HD21	1.89	0.55
4:B:33:ALA:O	4:B:37:ILE:CG2	2.55	0.55
5:L:21:ILE:HD13	5:L:102:THR:HB	1.89	0.55
5:L:50:TYR:O	5:L:52:SER:N	2.38	0.55
1:T:709:DC:H2'	1:T:710:DG:C8	2.41	0.54
1:T:711:DC:H2"	1:T:712:DC:H5'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:57:ASN:ND2	4:B:58:THR:N	2.55	0.54
4:B:320:ASP:OD2	4:B:323:LYS:HG3	2.07	0.54
3:A:5:ILE:HD11	3:A:167:ILE:HD11	1.89	0.54
3:A:328:GLU:O	3:A:339:TYR:HA	2.06	0.54
4:B:223:LYS:NZ	6:H:56:ASP:OD1	2.36	0.54
5:L:46:LEU:HD23	5:L:55:HIS:CG	2.42	0.54
5:L:91:TYR:CD1	6:H:108:SER:HB3	2.42	0.54
6:H:29:LEU:HD23	6:H:34:ILE:HG22	1.89	0.54
6:H:134:LEU:HB2	6:H:149:GLY:CA	2.38	0.54
4:B:264:LEU:HD22	4:B:306:ASN:ND2	2.22	0.54
5:L:61:ARG:CA	5:L:76:SER:HB3	2.37	0.54
6:H:56:ASP:O	6:H:57:ASP:HB2	2.08	0.54
6:H:148:LEU:HD13	6:H:220:ILE:HG21	1.90	0.54
3:A:439:THR:HG1	3:A:441:TYR:HE1	1.53	0.54
4:B:295:LEU:HD13	4:B:300:GLU:CD	2.28	0.54
3:A:162:SER:OG	4:B:52:PRO:HD3	2.08	0.54
3:A:463:ARG:HG3	3:A:464:GLN:N	2.22	0.54
3:A:506:ILE:O	3:A:510:PRO:HD2	2.08	0.54
6:H:148:LEU:HD22	6:H:220:ILE:CG2	2.32	0.54
3:A:434:ILE:HG22	3:A:494:ASN:ND2	2.22	0.54
3:A:492:GLU:HG2	3:A:530:LYS:HB2	1.90	0.54
3:A:3:SER:HB3	3:A:5:ILE:CG1	2.31	0.54
6:H:205:CYS:O	6:H:217:ASP:HA	2.07	0.54
4:B:78:ARG:CZ	4:B:411:ILE:HG21	2.37	0.54
4:B:266:TRP:CH2	4:B:422:LEU:HD13	2.43	0.53
2:P:822:DA:H2"	2:P:823:ATM:H5'	1.89	0.53
4:B:260:LEU:O	4:B:264:LEU:HD12	2.08	0.53
4:B:281:LYS:HA	4:B:284:ARG:HH11	1.72	0.53
5:L:136:LEU:N	5:L:136:LEU:HD12	2.23	0.53
3:A:279:LEU:HD23	3:A:279:LEU:H	1.73	0.53
4:B:50:ILE:HG21	4:B:145:GLN:HG2	1.90	0.53
4:B:79:GLU:HB3	4:B:83:ARG:HH12	1.72	0.53
3:A:439:THR:CG2	4:B:289:LEU:H	2.16	0.53
3:A:550:LYS:HA	3:A:550:LYS:HZ3	1.72	0.53
4:B:175:ASN:OD1	4:B:201:LYS:NZ	2.35	0.53
4:B:389:PHE:HB3	4:B:391:LEU:HD23	1.90	0.53
5:L:61:ARG:HA	5:L:76:SER:HB3	1.91	0.53
5:L:179:LEU:HD23	5:L:181:LEU:HD11	1.91	0.53
5:L:206:VAL:HG12	5:L:207:LYS:N	2.24	0.53
3:A:253:THR:HG23	3:A:256:ASP:OD2	2.08	0.53
3:A:261:VAL:HG23	3:A:276:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:86:ASP:HB3	4:B:91:GLN:HE21	1.73	0.53
4:B:295:LEU:HD22	4:B:300:GLU:N	2.24	0.53
4:B:361:HIS:ND1	4:B:366:LYS:HE3	2.23	0.53
5:L:190:ASN:O	5:L:210:ASN:HA	2.07	0.53
6:H:92:THR:HG23	6:H:120:THR:CA	2.24	0.53
6:H:209:HIS:CD2	6:H:212:SER:OG	2.61	0.53
3:A:260:LEU:O	3:A:264:LEU:HG	2.08	0.53
3:A:427:TYR:CE2	3:A:525:LEU:HD23	2.44	0.53
3:A:447:ASN:ND2	3:A:450:THR:HG23	2.23	0.53
3:A:465:LYS:NZ	3:A:488:ASP:OD2	2.41	0.53
4:B:291:GLU:HG2	4:B:293:ILE:CD1	2.39	0.53
3:A:128:THR:CB	3:A:146:TYR:HB2	2.38	0.53
4:B:54:ASN:HB3	4:B:143:ARG:HH12	1.74	0.53
4:B:360:ALA:HB1	4:B:367:GLN:HG2	1.91	0.53
3:A:494:ASN:HB3	4:B:289:LEU:HD12	1.90	0.53
4:B:325:LEU:HD12	4:B:343:GLN:HG2	1.90	0.53
6:H:125:LYS:O	6:H:127:THR:HG23	2.08	0.53
5:L:66:GLY:HA3	5:L:71:TYR:CD2	2.44	0.53
5:L:120:PRO:CB	5:L:125:LEU:HD21	2.38	0.53
6:H:62:ASN:ND2	6:H:64:SER:H	2.06	0.53
3:A:466:VAL:HG12	3:A:466:VAL:O	2.08	0.52
4:B:344:GLU:HA	4:B:344:GLU:OE2	2.09	0.52
2:P:820:DC:OP1	3:A:263:LYS:HE3	2.09	0.52
2:P:823:ATM:N4'	3:A:114:ALA:HB3	2.24	0.52
3:A:276:VAL:HG12	3:A:276:VAL:O	2.09	0.52
3:A:441:TYR:CD2	3:A:544:GLY:CA	2.89	0.52
4:B:88:TRP:CD1	4:B:154:LYS:HB3	2.44	0.52
5:L:76:SER:OG	5:L:77:ASN:N	2.40	0.52
6:H:12:VAL:HG21	6:H:18:PHE:HB3	1.90	0.52
3:A:49:LYS:HE3	3:A:142:ILE:CG2	2.40	0.52
3:A:128:THR:OG1	3:A:146:TYR:HB2	2.09	0.52
5:L:33:LEU:HD23	5:L:34:ASN:H	1.75	0.52
3:A:350:LYS:NZ	3:A:378:GLU:OE1	2.37	0.52
3:A:442:VAL:CG2	3:A:495:ILE:HG22	2.40	0.52
4:B:244:ILE:HD11	4:B:271:TYR:CE2	2.44	0.52
3:A:8:VAL:HG21	3:A:159:ILE:HG23	1.90	0.52
3:A:440:PHE:CZ	3:A:488:ASP:O	2.63	0.52
4:B:245:VAL:HG13	4:B:427:TYR:CE2	2.44	0.52
5:L:32:TYR:HA	5:L:91:TYR:CE2	2.44	0.52
6:H:34:ILE:HG23	6:H:35:GLY:H	1.74	0.52
6:H:129:PRO:HB2	6:H:152:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:517:LEU:HD13	3:A:521:ILE:HG13	1.90	0.52
3:A:523:GLU:O	3:A:526:ILE:HG22	2.10	0.52
4:B:146:TYR:CD2	4:B:150:PRO:HB3	2.45	0.52
6:H:32:SER:O	6:H:55:TRP:CD2	2.63	0.52
6:H:40:ARG:HB2	6:H:50:LEU:HD11	1.90	0.52
6:H:62:ASN:ND2	6:H:64:SER:N	2.57	0.52
6:H:19:ARG:HD2	6:H:83:ASN:ND2	2.22	0.52
3:A:65:LYS:O	3:A:67:ASP:N	2.43	0.52
3:A:500:GLN:NE2	3:A:500:GLN:N	2.44	0.52
4:B:249:LYS:HE3	4:B:256:ASP:OD2	2.08	0.52
5:L:1:ASP:H1	5:L:95:PRO:CG	2.23	0.52
3:A:86:ASP:OD2	3:A:86:ASP:N	2.39	0.52
3:A:296:THR:HG22	3:A:298:GLU:N	2.22	0.52
4:B:47:ILE:HD11	4:B:146:TYR:CD1	2.44	0.52
3:A:361:HIS:HD2	3:A:505:ILE:HG23	1.74	0.52
3:A:376:THR:HG22	3:A:377:THR:N	2.25	0.52
4:B:94:ILE:HG12	4:B:161:GLN:NE2	2.25	0.52
4:B:281:LYS:O	4:B:283:LEU:N	2.43	0.52
4:B:122:GLU:HA	4:B:122:GLU:OE2	2.10	0.51
4:B:223:LYS:HD3	6:H:58:ASP:OD2	2.09	0.51
4:B:225:PRO:HG2	5:L:92:SER:HA	1.92	0.51
3:A:181:TYR:CD1	4:B:138:GLU:HA	2.45	0.51
3:A:214:LEU:N	3:A:214:LEU:HD22	2.25	0.51
4:B:46:LYS:CD	4:B:116:PHE:HB3	2.40	0.51
5:L:190:ASN:ND2	5:L:211:ARG:HG2	2.21	0.51
3:A:113:ASP:O	3:A:114:ALA:C	2.49	0.51
3:A:454:LYS:HG2	3:A:468:PRO:HB3	1.90	0.51
3:A:130:PHE:CE2	3:A:144:TYR:HB2	2.45	0.51
3:A:148:VAL:O	3:A:150:PRO:HD3	2.11	0.51
3:A:246:LEU:HB2	3:A:260:LEU:CD1	2.40	0.51
5:L:27:GLN:O	5:L:29:ILE:N	2.44	0.51
5:L:133:VAL:HG11	5:L:135:PHE:CZ	2.45	0.51
6:H:176:PHE:O	6:H:187:LEU:HD23	2.11	0.51
3:A:435:VAL:HG22	4:B:290:THR:CG2	2.39	0.51
4:B:43:LYS:O	4:B:45:GLY:N	2.44	0.51
5:L:61:ARG:HB2	5:L:76:SER:CB	2.40	0.51
5:L:199:LYS:HG3	5:L:199:LYS:O	2.09	0.51
3:A:111:VAL:HG21	3:A:164:MET:HE1	1.93	0.51
3:A:220:LYS:O	3:A:220:LYS:HD3	2.10	0.51
6:H:137:GLY:O	6:H:138:SER:HB2	2.10	0.51
1:T:723:DC:H5"	3:A:474:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:TYR:CB	3:A:274:ILE:HD11	2.41	0.51
3:A:547:GLN:HG2	4:B:286:THR:HG22	1.92	0.51
5:L:79:GLU:HB3	5:L:80:PRO:HD2	1.91	0.51
5:L:198:HIS:HD2	5:L:200:THR:HG23	1.76	0.51
3:A:246:LEU:HB2	3:A:260:LEU:HD12	1.93	0.51
3:A:317:VAL:CG2	3:A:318:TYR:H	2.24	0.51
3:A:521:ILE:O	3:A:525:LEU:HD13	2.11	0.51
4:B:348:ASN:H	4:B:348:ASN:ND2	2.07	0.51
5:L:1:ASP:H1	5:L:95:PRO:HG2	1.76	0.51
5:L:108:ARG:HB3	5:L:140:TYR:CE1	2.45	0.51
6:H:202:THR:HB	6:H:219:LYS:HE3	1.93	0.51
3:A:457:TYR:HA	3:A:548:VAL:HG13	1.91	0.51
4:B:195:ILE:CG2	4:B:196:GLY:N	2.74	0.51
5:L:83:ILE:HG22	5:L:104:LEU:O	2.11	0.51
3:A:459:THR:HG22	3:A:463:ARG:N	2.25	0.51
4:B:113:ASP:C	4:B:115:TYR:N	2.65	0.51
4:B:328:GLU:O	4:B:339:TYR:HA	2.10	0.51
5:L:19:VAL:CG1	5:L:20:THR:N	2.73	0.51
5:L:124:GLN:HE22	5:L:131:SER:CB	2.22	0.51
1:T:712:DC:H2'	1:T:713:DC:H6	1.77	0.50
3:A:183:TYR:CD2	3:A:230:MET:SD	3.04	0.50
3:A:511:ASP:OD2	3:A:511:ASP:O	2.29	0.50
4:B:160:PHE:CD2	4:B:164:MET:HB2	2.46	0.50
4:B:372:VAL:HG13	4:B:389:PHE:CE2	2.46	0.50
5:L:140:TYR:CD2	5:L:141:PRO:HG3	2.46	0.50
6:H:32:SER:O	6:H:55:TRP:CE2	2.65	0.50
3:A:63:ILE:HG13	3:A:64:LYS:N	2.26	0.50
3:A:271:TYR:HB3	3:A:274:ILE:HD11	1.93	0.50
4:B:31:ILE:O	4:B:35:VAL:HG23	2.12	0.50
4:B:57:ASN:HD22	4:B:58:THR:N	2.10	0.50
5:L:66:GLY:CA	5:L:71:TYR:HA	2.41	0.50
3:A:341:ILE:O	3:A:349:LEU:HB2	2.11	0.50
4:B:13:LYS:HG2	4:B:83:ARG:O	2.11	0.50
4:B:295:LEU:HD22	4:B:300:GLU:HB2	1.93	0.50
5:L:1:ASP:H2	5:L:95:PRO:HG2	1.74	0.50
3:A:188:TYR:CD1	3:A:188:TYR:C	2.84	0.50
3:A:450:THR:O	3:A:451:LYS:CG	2.59	0.50
4:B:156:SER:N	4:B:157:PRO:HD2	2.26	0.50
4:B:263:LYS:CG	4:B:423:VAL:CG1	2.90	0.50
4:B:284:ARG:H	4:B:287:LYS:HZ1	1.58	0.50
4:B:299:ALA:O	4:B:301:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:339:TYR:CD1	4:B:339:TYR:C	2.84	0.50
6:H:141:GLN:OE1	6:H:199:PRO:HD3	2.12	0.50
3:A:23:GLN:NE2	3:A:59:PRO:HA	2.27	0.50
3:A:228:LEU:HD23	3:A:233:GLU:HG2	1.93	0.50
3:A:262:GLY:O	3:A:265:ASN:HB2	2.11	0.50
3:A:297:GLU:HA	3:A:300:GLU:CB	2.41	0.50
3:A:475:GLN:HB3	3:A:501:TYR:CD2	2.47	0.50
4:B:363:ASN:ND2	4:B:365:VAL:H	2.08	0.50
5:L:6:GLN:OE1	5:L:101:GLY:N	2.41	0.50
3:A:273:GLY:H	3:A:338:THR:HG21	1.77	0.50
3:A:450:THR:HB	3:A:452:LEU:HG	1.92	0.50
4:B:366:LYS:O	4:B:370:GLU:HG3	2.12	0.50
3:A:90:VAL:HG12	4:B:140:PRO:CB	2.37	0.50
4:B:84:THR:O	4:B:84:THR:OG1	2.28	0.50
4:B:395:LYS:HG2	4:B:396:GLU:N	2.27	0.50
5:L:19:VAL:HG12	5:L:20:THR:H	1.76	0.50
5:L:60:SER:O	5:L:62:PHE:N	2.45	0.50
6:H:82:LEU:HD12	6:H:83:ASN:N	2.26	0.50
2:P:823:ATM:N5'	3:A:114:ALA:N	2.60	0.50
3:A:401:TRP:HE3	3:A:401:TRP:HA	1.77	0.50
4:B:169:GLU:OE2	4:B:169:GLU:HA	2.11	0.50
4:B:223:LYS:N	4:B:223:LYS:CD	2.73	0.50
4:B:254:VAL:HB	4:B:289:LEU:HA	1.93	0.50
4:B:254:VAL:HG13	4:B:283:LEU:HD21	1.93	0.50
6:H:104:SER:OG	6:H:105:VAL:N	2.41	0.50
3:A:21:VAL:HB	3:A:59:PRO:HD3	1.93	0.50
3:A:317:VAL:CG2	3:A:318:TYR:N	2.73	0.50
4:B:207:GLN:O	4:B:209:LEU:N	2.45	0.50
3:A:80:LEU:O	3:A:83:ARG:N	2.39	0.49
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.76	0.49
3:A:545:ASN:O	3:A:546:GLU:C	2.50	0.49
4:B:204:GLU:O	4:B:207:GLN:HB2	2.11	0.49
5:L:74:THR:O	5:L:74:THR:HG22	2.12	0.49
5:L:201:SER:C	5:L:203:SER:H	2.16	0.49
2:P:820:DC:H2'	2:P:821:DC:C6	2.47	0.49
3:A:64:LYS:HD2	3:A:66:LYS:HZ1	1.70	0.49
3:A:224:GLU:O	3:A:225:PRO:C	2.50	0.49
3:A:262:GLY:O	3:A:265:ASN:N	2.45	0.49
3:A:433:PRO:HD3	4:B:255:ASN:ND2	2.27	0.49
3:A:439:THR:CG2	4:B:288:ALA:HA	2.42	0.49
4:B:47:ILE:HG23	4:B:144:TYR:CD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:55:PRO:HG2	4:B:56:TYR:CD1	2.47	0.49
4:B:113:ASP:O	4:B:115:TYR:N	2.45	0.49
5:L:105:GLU:OE2	5:L:173:TYR:OH	2.25	0.49
5:L:144:ILE:HG13	5:L:198:HIS:ND1	2.27	0.49
1:T:706:DT:H5"	3:A:81:ASN:ND2	2.27	0.49
4:B:422:LEU:O	4:B:423:VAL:CG2	2.58	0.49
5:L:205:ILE:N	5:L:205:ILE:HD12	2.27	0.49
6:H:39:ILE:HG13	6:H:113:TRP:CZ3	2.48	0.49
4:B:172:LYS:HE2	4:B:180:ILE:HB	1.94	0.49
5:L:147:LYS:HZ2	5:L:149:LYS:CG	2.20	0.49
5:L:176:SER:HB2	6:H:176:PHE:CD1	2.48	0.49
3:A:18:GLY:HA3	3:A:56:TYR:CD2	2.47	0.49
3:A:401:TRP:HA	3:A:401:TRP:CE3	2.48	0.49
3:A:507:GLN:O	3:A:509:GLN:HG3	2.12	0.49
4:B:138:GLU:HG2	4:B:139:THR:HG23	1.94	0.49
3:A:269:GLN:HA	3:A:351:THR:O	2.11	0.49
3:A:344:GLU:HG3	3:A:345:PRO:CD	2.43	0.49
4:B:363:ASN:HD22	4:B:365:VAL:H	1.61	0.49
5:L:81:GLU:OE1	5:L:81:GLU:N	2.42	0.49
3:A:278:GLN:O	3:A:280:SER:N	2.46	0.49
3:A:399:GLU:O	3:A:403:THR:HG22	2.12	0.49
3:A:447:ASN:HB3	3:A:450:THR:OG1	2.12	0.49
4:B:318:TYR:O	4:B:349:LEU:HD21	2.12	0.49
4:B:13:LYS:O	4:B:16:MET:HB2	2.13	0.49
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.95	0.49
4:B:244:ILE:HD11	4:B:271:TYR:HE2	1.76	0.49
2:P:807:DC:C2	2:P:808:DC:C5	3.01	0.49
3:A:504:GLY:O	3:A:505:ILE:C	2.50	0.49
4:B:153:TRP:CH2	4:B:155:GLY:HA3	2.48	0.49
3:A:87:PHE:HD2	3:A:87:PHE:H	1.60	0.49
3:A:493:VAL:CG2	3:A:494:ASN:N	2.75	0.49
4:B:168:LEU:HD13	4:B:180:ILE:HG21	1.95	0.49
5:L:156:GLN:HA	5:L:156:GLN:OE1	2.13	0.49
6:H:39:ILE:HG13	6:H:113:TRP:CH2	2.48	0.49
6:H:157:PRO:O	6:H:209:HIS:HE1	1.96	0.49
6:H:198:TRP:CD1	6:H:199:PRO:HA	2.48	0.49
3:A:50:ILE:HD12	3:A:54:ASN:HB3	1.94	0.48
3:A:56:TYR:O	3:A:143:ARG:NH2	2.46	0.48
3:A:63:ILE:CG1	3:A:64:LYS:N	2.76	0.48
3:A:382:ILE:HG22	3:A:382:ILE:O	2.13	0.48
4:B:108:VAL:HG12	4:B:188:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:150:PRO:HG2	4:B:153:TRP:HB3	1.94	0.48
4:B:246:LEU:HD12	4:B:307:ARG:HB3	1.95	0.48
4:B:277:ARG:O	4:B:279:LEU:N	2.46	0.48
5:L:34:ASN:CB	5:L:89:GLN:HE22	2.25	0.48
3:A:410:TRP:CZ3	4:B:363:ASN:HB2	2.48	0.48
3:A:412:PRO:O	3:A:414:TRP:HD1	1.95	0.48
4:B:112:GLY:HA3	4:B:151:GLN:NE2	2.27	0.48
4:B:247:PRO:HG3	4:B:427:TYR:HH	1.70	0.48
4:B:304:ALA:C	4:B:307:ARG:HG2	2.33	0.48
4:B:335:GLY:O	4:B:337:TRP:CD1	2.66	0.48
5:L:32:TYR:CA	5:L:91:TYR:CE2	2.96	0.48
3:A:221:HIS:HB2	3:A:227:PHE:CE2	2.49	0.48
4:B:281:LYS:C	4:B:283:LEU:H	2.16	0.48
6:H:62:ASN:HD21	6:H:64:SER:CB	2.27	0.48
3:A:539:HIS:N	3:A:539:HIS:CD2	2.81	0.48
4:B:227:PHE:HB2	6:H:105:VAL:HA	1.94	0.48
5:L:132:VAL:O	5:L:148:TRP:CH2	2.67	0.48
3:A:279:LEU:H	3:A:279:LEU:CD2	2.26	0.48
4:B:120:LEU:HD12	4:B:121:ASP:H	1.79	0.48
4:B:265:ASN:O	4:B:268:SER:OG	2.24	0.48
5:L:28:ASP:HA	5:L:68:GLY:O	2.13	0.48
5:L:62:PHE:CE1	5:L:75:ILE:HG23	2.49	0.48
5:L:123:GLU:HA	5:L:126:THR:HB	1.95	0.48
5:L:189:HIS:O	5:L:211:ARG:HD3	2.13	0.48
3:A:125:ARG:HB3	3:A:145:GLN:HG3	1.96	0.48
5:L:83:ILE:HG21	5:L:106:ILE:HG12	1.96	0.48
3:A:94:ILE:HG13	3:A:95:PRO:O	2.14	0.48
3:A:132:ILE:HG23	3:A:132:ILE:O	2.13	0.48
3:A:138:GLU:CG	3:A:139:THR:H	2.13	0.48
3:A:459:THR:HG21	3:A:463:ARG:HB3	1.90	0.48
4:B:116:PHE:C	4:B:148:VAL:HG21	2.33	0.48
4:B:226:PRO:O	4:B:228:LEU:N	2.36	0.48
5:L:206:VAL:C	5:L:207:LYS:HG2	2.34	0.48
1:T:713:DC:H2"	1:T:714:DG:H5'	1.96	0.48
3:A:3:SER:CB	3:A:5:ILE:HG13	2.35	0.48
3:A:114:ALA:HB1	3:A:160:PHE:CE1	2.48	0.48
3:A:516:GLU:HA	3:A:519:ASN:HB2	1.96	0.48
4:B:10:VAL:HG22	4:B:87:PHE:CE1	2.48	0.48
4:B:97:PRO:O	4:B:98:ALA:C	2.52	0.48
5:L:91:TYR:CE1	6:H:108:SER:HB3	2.48	0.48
5:L:198:HIS:CD2	5:L:200:THR:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:150:CYS:HB2	6:H:164:TRP:HH2	1.74	0.48
3:A:300:GLU:OE1	3:A:300:GLU:HA	2.14	0.47
4:B:266:TRP:O	4:B:269:GLN:HG3	2.14	0.47
4:B:389:PHE:HB3	4:B:391:LEU:CD2	2.44	0.47
5:L:24:SER:HA	5:L:69:THR:O	2.14	0.47
3:A:268:SER:O	3:A:352:GLY:HA2	2.14	0.47
4:B:323:LYS:HB2	4:B:343:GLN:NE2	2.28	0.47
5:L:66:GLY:HA2	5:L:70:ASP:O	2.14	0.47
3:A:112:GLY:O	3:A:113:ASP:HB2	2.15	0.47
3:A:120:LEU:O	3:A:121:ASP:C	2.53	0.47
3:A:385:LYS:HG2	3:A:386:THR:N	2.29	0.47
3:A:460:ASN:HA	4:B:286:THR:OG1	2.14	0.47
1:T:712:DC:H2'	1:T:713:DC:C6	2.49	0.47
3:A:136:ASN:N	3:A:136:ASN:ND2	2.42	0.47
3:A:444:GLY:HA2	3:A:552:VAL:HG11	1.97	0.47
4:B:420:PRO:CB	4:B:421:PRO:HD2	2.44	0.47
5:L:61:ARG:NH1	5:L:61:ARG:HG2	2.30	0.47
6:H:27:PHE:CE1	6:H:99:GLN:HG3	2.50	0.47
3:A:125:ARG:HG2	3:A:146:TYR:O	2.15	0.47
3:A:281:LYS:O	3:A:284:ARG:CB	2.62	0.47
5:L:103:LYS:HE2	5:L:105:GLU:OE1	2.14	0.47
4:B:221:HIS:HA	4:B:229:TRP:CD1	2.49	0.47
3:A:9:PRO:HA	3:A:121:ASP:OD2	2.14	0.47
3:A:11:LYS:O	3:A:85:GLN:HG2	2.15	0.47
3:A:74:LEU:HD12	3:A:74:LEU:HA	1.81	0.47
3:A:246:LEU:H	3:A:246:LEU:CD2	2.27	0.47
3:A:430:GLU:HG2	3:A:531:VAL:O	2.14	0.47
3:A:439:THR:OG1	3:A:441:TYR:HE1	1.98	0.47
3:A:498:ASP:N	3:A:498:ASP:OD1	2.48	0.47
4:B:205:LEU:C	4:B:207:GLN:H	2.18	0.47
4:B:298:GLU:O	4:B:301:LEU:HB3	2.15	0.47
4:B:311:LYS:O	4:B:312:GLU:CG	2.62	0.47
5:L:151:ASP:OD1	5:L:191:SER:HB3	2.14	0.47
5:L:201:SER:C	5:L:203:SER:N	2.67	0.47
6:H:128:PRO:HA	6:H:209:HIS:CD2	2.47	0.47
3:A:437:ALA:CB	3:A:493:VAL:HA	2.43	0.47
4:B:50:ILE:O	4:B:143:ARG:HB2	2.15	0.47
4:B:115:TYR:C	4:B:117:SER:H	2.18	0.47
4:B:325:LEU:HB3	4:B:387:PRO:CB	2.45	0.47
6:H:29:LEU:HD13	6:H:73:LYS:HD3	1.96	0.47
3:A:136:ASN:C	3:A:138:GLU:H	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:327:ALA:HB3	3:A:389:PHE:CE1	2.50	0.47
4:B:74:LEU:HD21	4:B:409:THR:O	2.15	0.47
4:B:239:TRP:CH2	4:B:378:GLU:HG2	2.49	0.47
4:B:27:THR:O	4:B:28:GLU:C	2.53	0.47
1:T:716:DA:C2	1:T:717:DC:C2	3.03	0.46
3:A:209:LEU:O	3:A:212:TRP:N	2.47	0.46
3:A:438:GLU:CD	3:A:463:ARG:HH21	2.19	0.46
3:A:484:LEU:C	3:A:486:LEU:N	2.68	0.46
4:B:31:ILE:O	4:B:32:LYS:C	2.54	0.46
4:B:80:LEU:O	4:B:80:LEU:HD12	2.15	0.46
5:L:61:ARG:CB	5:L:76:SER:HB3	2.44	0.46
3:A:96:HIS:ND1	3:A:97:PRO:CD	2.79	0.46
3:A:121:ASP:OD1	3:A:123:ASP:N	2.48	0.46
3:A:257:ILE:O	3:A:261:VAL:HG12	2.16	0.46
4:B:414:TRP:CD1	4:B:414:TRP:C	2.89	0.46
5:L:112:ALA:HB1	5:L:113:PRO:HD2	1.97	0.46
6:H:68:ARG:NH2	6:H:88:GLU:OE2	2.48	0.46
3:A:477:THR:O	3:A:480:GLN:HB3	2.16	0.46
4:B:12:LEU:H	4:B:12:LEU:CD1	2.13	0.46
4:B:75:VAL:HG11	4:B:77:PHE:CE2	2.50	0.46
4:B:366:LYS:HA	4:B:405:TYR:CD2	2.50	0.46
3:A:454:LYS:HB2	3:A:454:LYS:NZ	2.30	0.46
5:L:140:TYR:CD2	5:L:141:PRO:HA	2.50	0.46
2:P:806:DT:C2	2:P:807:DC:C5	3.03	0.46
3:A:50:ILE:CG2	3:A:145:GLN:HB3	2.45	0.46
3:A:442:VAL:HG12	3:A:481:ALA:HB1	1.98	0.46
3:A:509:GLN:N	3:A:510:PRO:CD	2.79	0.46
4:B:106:VAL:HG13	4:B:234:LEU:CB	2.41	0.46
4:B:207:GLN:C	4:B:209:LEU:N	2.69	0.46
4:B:219:LYS:HB3	4:B:232:TYR:CE2	2.51	0.46
5:L:61:ARG:HG2	5:L:61:ARG:HH11	1.80	0.46
4:B:356:ARG:HG2	4:B:357:MET:N	2.30	0.46
6:H:165:ASN:HB3	6:H:168:SER:HB2	1.98	0.46
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.51	0.46
3:A:377:THR:O	3:A:381:VAL:HG23	2.16	0.46
4:B:34:LEU:HD21	4:B:60:VAL:HG23	1.96	0.46
1:T:715:DA:H2"	1:T:716:DA:H8	1.81	0.46
3:A:280:SER:C	3:A:282:LEU:N	2.68	0.46
4:B:108:VAL:HG23	4:B:108:VAL:O	2.16	0.46
5:L:28:ASP:C	5:L:30:SER:H	2.18	0.46
5:L:189:HIS:O	5:L:211:ARG:NE	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:812:DT:C2'	2:P:813:DT:H71	2.46	0.46
3:A:20:LYS:HG2	3:A:55:PRO:O	2.16	0.46
3:A:23:GLN:HG2	3:A:133:PRO:HD3	1.97	0.46
3:A:199:ARG:HH21	3:A:202:ILE:HG21	1.81	0.46
3:A:475:GLN:HB3	3:A:501:TYR:HE2	1.78	0.46
4:B:329:ILE:O	4:B:392:PRO:CG	2.64	0.46
3:A:90:VAL:CG1	4:B:141:GLY:H	2.29	0.46
3:A:253:THR:HA	3:A:292:VAL:HA	1.97	0.46
3:A:353:LYS:HD2	3:A:353:LYS:O	2.15	0.46
4:B:131:THR:CG2	4:B:132:ILE:N	2.79	0.46
5:L:150:ILE:O	5:L:151:ASP:C	2.52	0.46
3:A:219:LYS:HE2	3:A:219:LYS:HB3	1.72	0.45
3:A:247:PRO:HD2	3:A:260:LEU:CD1	2.42	0.45
4:B:340:GLN:HG3	4:B:351:THR:CG2	2.37	0.45
3:A:5:ILE:HG12	3:A:212:TRP:CE3	2.51	0.45
3:A:163:SER:O	3:A:167:ILE:HG13	2.16	0.45
3:A:342:TYR:HD2	3:A:344:GLU:O	1.99	0.45
5:L:60:SER:C	5:L:62:PHE:N	2.68	0.45
5:L:115:VAL:CG1	5:L:116:SER:N	2.79	0.45
5:L:162:SER:OG	6:H:177:PRO:HG2	2.15	0.45
3:A:156:SER:HB3	3:A:157:PRO:HD3	1.98	0.45
3:A:278:GLN:C	3:A:280:SER:H	2.20	0.45
3:A:278:GLN:CB	3:A:302:GLU:CB	2.94	0.45
3:A:531:VAL:HG12	3:A:532:TYR:N	2.31	0.45
4:B:77:PHE:O	4:B:81:ASN:ND2	2.49	0.45
4:B:207:GLN:O	4:B:210:LEU:N	2.49	0.45
4:B:380:ILE:O	4:B:384:GLY:HA2	2.16	0.45
6:H:59:ASN:N	6:H:59:ASN:HD22	2.13	0.45
6:H:104:SER:HB3	6:H:107:ASP:OD2	2.16	0.45
3:A:103:LYS:O	3:A:104:LYS:C	2.54	0.45
3:A:125:ARG:HB3	3:A:145:GLN:CG	2.46	0.45
3:A:473:THR:CG2	3:A:474:ASN:N	2.74	0.45
4:B:153:TRP:CZ3	4:B:155:GLY:HA3	2.52	0.45
4:B:239:TRP:CH2	4:B:378:GLU:HA	2.52	0.45
4:B:354:TYR:OH	4:B:357:MET:HG3	2.16	0.45
5:L:49:TYR:CD2	5:L:49:TYR:N	2.85	0.45
5:L:90:GLN:CD	5:L:90:GLN:O	2.54	0.45
5:L:95:PRO:HB3	6:H:63:PRO:HD3	1.99	0.45
5:L:116:SER:O	5:L:134:CYS:HA	2.16	0.45
5:L:66:GLY:HA3	5:L:71:TYR:CG	2.51	0.45
5:L:89:GLN:HA	5:L:97:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:823:ATM:H2'	3:A:115:TYR:CD2	2.51	0.45
3:A:274:ILE:O	3:A:275:LYS:C	2.55	0.45
3:A:550:LYS:NZ	3:A:553:SER:HB2	2.32	0.45
4:B:178:ILE:HD11	4:B:201:LYS:CG	2.41	0.45
4:B:205:LEU:C	4:B:207:GLN:N	2.68	0.45
6:H:61:TYR:N	6:H:61:TYR:CD1	2.85	0.45
3:A:329:ILE:C	3:A:330:GLN:NE2	2.70	0.45
3:A:442:VAL:HG22	3:A:495:ILE:HG22	1.97	0.45
3:A:454:LYS:HZ1	3:A:554:ALA:HB3	1.81	0.45
4:B:277:ARG:C	4:B:279:LEU:N	2.70	0.45
4:B:285:GLY:N	4:B:287:LYS:NZ	2.64	0.45
4:B:286:THR:O	4:B:286:THR:OG1	2.34	0.45
4:B:368:LEU:O	4:B:372:VAL:HG23	2.16	0.45
5:L:17:ASP:HB2	5:L:78:LEU:HD12	1.99	0.45
5:L:140:TYR:CD2	5:L:141:PRO:CA	3.00	0.45
5:L:179:LEU:HG	5:L:181:LEU:HD11	1.99	0.45
3:A:135:ILE:HG12	3:A:136:ASN:H	1.77	0.45
3:A:227:PHE:O	3:A:233:GLU:HA	2.16	0.45
3:A:261:VAL:HG13	3:A:262:GLY:N	2.32	0.45
3:A:270:ILE:HG23	3:A:271:TYR:N	2.31	0.45
5:L:18:ARG:HA	5:L:76:SER:O	2.16	0.45
5:L:73:LEU:HD12	5:L:74:THR:H	1.81	0.45
6:H:6:GLU:HB3	6:H:117:THR:OG1	2.16	0.45
3:A:27:THR:O	3:A:31:ILE:HG13	2.17	0.45
3:A:494:ASN:HB3	4:B:289:LEU:CD1	2.47	0.45
4:B:65:LYS:HE2	4:B:67:ASP:HB3	1.98	0.45
4:B:207:GLN:O	4:B:208:HIS:C	2.55	0.45
4:B:369:THR:O	4:B:373:GLN:HG3	2.16	0.45
5:L:147:LYS:HB3	5:L:195:GLU:HB2	1.99	0.45
6:H:77:ASN:O	6:H:78:ASN:HB2	2.16	0.45
6:H:148:LEU:CD2	6:H:220:ILE:HG21	2.36	0.45
1:T:715:DA:H2"	1:T:716:DA:C8	2.51	0.45
3:A:90:VAL:HG13	4:B:141:GLY:H	1.82	0.45
3:A:485:ALA:O	3:A:489:SER:HB2	2.17	0.45
4:B:295:LEU:HD22	4:B:300:GLU:CA	2.47	0.45
4:B:373:GLN:HE22	4:B:406:TRP:HA	1.82	0.45
5:L:181:LEU:HD23	5:L:185:GLU:HG2	1.98	0.45
5:L:197:THR:HG23	5:L:204:PRO:HG3	1.99	0.45
6:H:27:PHE:CZ	6:H:99:GLN:HG3	2.52	0.45
1:T:705:DA:H2'	1:T:706:DT:H5'	1.94	0.44
1:T:714:DG:H2"	1:T:715:DA:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:120:LEU:HB2	3:A:148:VAL:O	2.18	0.44
3:A:276:VAL:O	3:A:276:VAL:CG1	2.64	0.44
3:A:344:GLU:HG3	3:A:345:PRO:HD2	1.99	0.44
3:A:417:VAL:HG22	3:A:419:THR:HG22	1.98	0.44
3:A:492:GLU:HA	3:A:530:LYS:O	2.17	0.44
4:B:48:SER:OG	4:B:147:ASN:ND2	2.41	0.44
4:B:197:GLN:O	4:B:200:THR:HB	2.17	0.44
4:B:393:ILE:CG1	4:B:394:GLN:N	2.80	0.44
6:H:34:ILE:HG23	6:H:35:GLY:N	2.25	0.44
6:H:133:PRO:HD3	6:H:218:LYS:CD	2.47	0.44
3:A:194:GLU:C	3:A:196:GLY:N	2.71	0.44
3:A:443:ASP:O	3:A:481:ALA:HB2	2.17	0.44
3:A:550:LYS:HA	3:A:550:LYS:NZ	2.32	0.44
4:B:314:VAL:CG1	4:B:315:HIS:N	2.78	0.44
5:L:140:TYR:CE2	5:L:141:PRO:HG3	2.51	0.44
3:A:441:TYR:CD2	3:A:544:GLY:C	2.91	0.44
4:B:10:VAL:HG22	4:B:87:PHE:CZ	2.53	0.44
4:B:221:HIS:HB3	4:B:229:TRP:CE2	2.52	0.44
5:L:148:TRP:CD2	5:L:179:LEU:HD13	2.53	0.44
6:H:150:CYS:HB2	6:H:164:TRP:CZ2	2.51	0.44
6:H:152:VAL:HB	6:H:187:LEU:CD1	2.47	0.44
6:H:221:VAL:O	6:H:221:VAL:HG23	2.18	0.44
3:A:46:LYS:HD2	3:A:116:PHE:HB3	1.98	0.44
3:A:96:HIS:CG	3:A:97:PRO:HD2	2.52	0.44
4:B:200:THR:O	4:B:204:GLU:HG3	2.18	0.44
5:L:135:PHE:C	5:L:136:LEU:HD12	2.38	0.44
6:H:2:ILE:HG21	6:H:112:HIS:HD2	1.83	0.44
6:H:73:LYS:HD2	6:H:75:THR:OG1	2.17	0.44
6:H:157:PRO:HD2	6:H:211:ALA:CB	2.48	0.44
3:A:278:GLN:C	3:A:280:SER:N	2.71	0.44
4:B:254:VAL:HG21	4:B:288:ALA:O	2.16	0.44
4:B:299:ALA:C	4:B:301:LEU:N	2.68	0.44
5:L:92:SER:O	5:L:93:LYS:HB2	2.17	0.44
5:L:148:TRP:CG	5:L:179:LEU:HD13	2.52	0.44
6:H:62:ASN:HD22	6:H:64:SER:N	2.15	0.44
6:H:126:THR:O	6:H:126:THR:CG2	2.66	0.44
3:A:27:THR:HG1	3:A:30:LYS:HG3	1.82	0.44
3:A:439:THR:HA	3:A:494:ASN:HB2	2.00	0.44
4:B:118:VAL:O	4:B:148:VAL:HG23	2.18	0.44
4:B:169:GLU:N	4:B:170:PRO:CD	2.80	0.44
6:H:88:GLU:O	6:H:121:VAL:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:GLY:HA3	3:A:56:TYR:CE2	2.53	0.44
4:B:112:GLY:HA3	4:B:151:GLN:HE21	1.82	0.44
4:B:327:ALA:HA	4:B:340:GLN:O	2.18	0.44
3:A:49:LYS:HB2	3:A:49:LYS:HZ3	1.79	0.44
3:A:279:LEU:C	3:A:282:LEU:HG	2.37	0.44
4:B:252:TRP:CD1	4:B:252:TRP:N	2.85	0.44
4:B:391:LEU:O	4:B:393:ILE:N	2.48	0.44
5:L:160:LEU:O	5:L:161:ASN:ND2	2.51	0.44
3:A:265:ASN:O	3:A:268:SER:N	2.49	0.43
3:A:325:LEU:HD21	3:A:383:TRP:CD2	2.52	0.43
4:B:24:TRP:CZ3	4:B:59:PRO:HG3	2.53	0.43
5:L:4:MET:SD	5:L:25:ALA:HA	2.58	0.43
5:L:117:ILE:HD12	5:L:133:VAL:O	2.18	0.43
1:T:707:DG:C2'	1:T:708:DG:C5'	2.95	0.43
3:A:226:PRO:HG3	3:A:235:HIS:NE2	2.33	0.43
3:A:295:LEU:HB3	3:A:300:GLU:OE2	2.17	0.43
3:A:395:LYS:O	3:A:399:GLU:HG3	2.19	0.43
4:B:197:GLN:NE2	4:B:197:GLN:HA	2.30	0.43
3:A:130:PHE:CE2	3:A:144:TYR:CB	3.01	0.43
3:A:497:THR:HG22	3:A:498:ASP:N	2.25	0.43
3:A:499:SER:OG	3:A:502:ALA:CB	2.66	0.43
4:B:34:LEU:HA	4:B:34:LEU:HD12	1.80	0.43
4:B:37:ILE:O	4:B:37:ILE:CG1	2.66	0.43
4:B:67:ASP:OD2	4:B:219:LYS:HG2	2.18	0.43
4:B:304:ALA:O	4:B:307:ARG:CG	2.63	0.43
3:A:183:TYR:O	3:A:184:MET:HB3	2.19	0.43
3:A:494:ASN:CB	4:B:289:LEU:HD12	2.49	0.43
4:B:88:TRP:CG	4:B:154:LYS:HB3	2.53	0.43
4:B:99:GLY:HA2	4:B:102:LYS:HD2	2.00	0.43
4:B:281:LYS:C	4:B:283:LEU:N	2.72	0.43
4:B:330:GLN:N	4:B:330:GLN:OE1	2.51	0.43
5:L:117:ILE:HG13	5:L:118:PHE:N	2.32	0.43
6:H:34:ILE:N	6:H:34:ILE:CD1	2.81	0.43
1:T:703:DG:H1'	3:A:61:PHE:HE1	1.83	0.43
3:A:427:TYR:HE1	3:A:510:PRO:O	2.01	0.43
4:B:253:THR:O	4:B:257:ILE:HG12	2.19	0.43
4:B:266:TRP:CZ3	4:B:423:VAL:HG23	2.52	0.43
5:L:189:HIS:O	5:L:211:ARG:CD	2.67	0.43
6:H:13:GLN:O	6:H:16:GLN:HB2	2.19	0.43
6:H:54:TRP:CE3	6:H:55:TRP:HZ3	2.36	0.43
1:T:708:DG:OP1	3:A:89:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:297:GLU:O	3:A:300:GLU:HB2	2.18	0.43
3:A:523:GLU:OE2	3:A:523:GLU:CA	2.64	0.43
4:B:312:GLU:OE1	4:B:313:PRO:HD2	2.18	0.43
5:L:19:VAL:CG1	5:L:20:THR:H	2.32	0.43
5:L:191:SER:HB2	5:L:210:ASN:HD21	1.84	0.43
6:H:12:VAL:HG12	6:H:13:GLN:N	2.32	0.43
6:H:197:THR:O	6:H:201:GLU:N	2.48	0.43
3:A:83:ARG:NH1	3:A:83:ARG:HG2	2.34	0.43
3:A:363:ASN:O	3:A:367:GLN:HG3	2.17	0.43
3:A:393:ILE:H	3:A:416:PHE:HD1	1.66	0.43
4:B:107:THR:HG22	4:B:108:VAL:N	2.33	0.43
4:B:260:LEU:O	4:B:260:LEU:HD12	2.19	0.43
4:B:355:ALA:O	4:B:356:ARG:HB2	2.17	0.43
5:L:46:LEU:HB3	5:L:55:HIS:ND1	2.34	0.43
3:A:454:LYS:NZ	3:A:554:ALA:HB3	2.34	0.43
3:A:83:ARG:HG2	3:A:83:ARG:HH11	1.84	0.43
3:A:111:VAL:HG11	3:A:214:LEU:CD1	2.38	0.43
3:A:329:ILE:O	3:A:330:GLN:NE2	2.52	0.43
3:A:365:VAL:O	3:A:366:LYS:C	2.57	0.43
5:L:121:SER:O	5:L:122:SER:C	2.57	0.43
2:P:823:ATM:H2'	3:A:115:TYR:HD2	1.83	0.43
3:A:254:VAL:CG1	3:A:255:ASN:N	2.81	0.43
3:A:406:TRP:HE1	4:B:418:ASN:HD22	1.66	0.43
3:A:459:THR:CG2	3:A:463:ARG:CB	2.88	0.43
4:B:7:THR:HG23	4:B:7:THR:O	2.19	0.43
4:B:113:ASP:C	4:B:115:TYR:H	2.21	0.43
5:L:122:SER:O	5:L:126:THR:N	2.50	0.43
6:H:14:PRO:O	6:H:15:SER:HB2	2.19	0.43
6:H:18:PHE:HE1	6:H:20:LEU:HG	1.84	0.43
3:A:170:PRO:HG2	3:A:171:PHE:N	2.31	0.42
3:A:386:THR:HG22	3:A:387:PRO:HD2	1.99	0.42
3:A:398:TRP:O	3:A:401:TRP:N	2.52	0.42
5:L:36:TYR:CE1	5:L:46:LEU:CD1	3.02	0.42
6:H:94:ILE:HA	6:H:117:THR:O	2.19	0.42
4:B:77:PHE:O	4:B:81:ASN:HB2	2.19	0.42
4:B:258:GLN:O	4:B:261:VAL:N	2.51	0.42
4:B:422:LEU:HD23	4:B:422:LEU:HA	1.80	0.42
6:H:17:PRO:HB3	6:H:85:MET:CE	2.50	0.42
3:A:166:LYS:NZ	3:A:166:LYS:HB3	2.35	0.42
3:A:484:LEU:O	3:A:485:ALA:C	2.57	0.42
4:B:26:LEU:HG	4:B:133:PRO:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:39:THR:O	4:B:42:GLU:HB3	2.19	0.42
4:B:47:ILE:CD1	4:B:146:TYR:HA	2.49	0.42
4:B:205:LEU:O	4:B:205:LEU:HD12	2.19	0.42
4:B:210:LEU:HD12	4:B:210:LEU:HA	1.77	0.42
5:L:131:SER:HA	5:L:179:LEU:O	2.19	0.42
5:L:144:ILE:CG2	5:L:145:ASN:N	2.81	0.42
5:L:147:LYS:HZ1	5:L:154:GLU:HB2	1.84	0.42
5:L:161:ASN:CB	5:L:163:TRP:CH2	3.03	0.42
3:A:49:LYS:HB2	3:A:49:LYS:HZ2	1.82	0.42
3:A:76:ASP:OD1	3:A:76:ASP:C	2.58	0.42
3:A:288:ALA:HB3	3:A:291:GLU:CB	2.45	0.42
4:B:266:TRP:CE3	4:B:423:VAL:HG23	2.54	0.42
4:B:292:VAL:HG12	4:B:292:VAL:O	2.20	0.42
4:B:396:GLU:CD	4:B:396:GLU:H	2.22	0.42
5:L:48:ILE:CD1	5:L:73:LEU:HD13	2.48	0.42
5:L:73:LEU:HD12	5:L:74:THR:N	2.35	0.42
1:T:713:DC:H2"	1:T:714:DG:C5'	2.49	0.42
3:A:171:PHE:O	3:A:175:ASN:ND2	2.53	0.42
3:A:463:ARG:CG	3:A:464:GLN:N	2.82	0.42
3:A:545:ASN:O	3:A:547:GLN:N	2.52	0.42
4:B:72:ARG:HH11	4:B:72:ARG:CG	2.32	0.42
4:B:221:HIS:HB3	4:B:229:TRP:CD2	2.54	0.42
4:B:295:LEU:HD22	4:B:300:GLU:H	1.83	0.42
4:B:360:ALA:O	4:B:362:THR:N	2.53	0.42
5:L:63:SER:OG	5:L:74:THR:HB	2.20	0.42
5:L:138:ASN:HA	5:L:172:THR:OG1	2.20	0.42
6:H:34:ILE:HD12	6:H:34:ILE:H	1.85	0.42
6:H:34:ILE:CD1	6:H:34:ILE:H	2.31	0.42
3:A:112:GLY:O	3:A:215:THR:HG23	2.20	0.42
3:A:221:HIS:HB2	3:A:227:PHE:CD2	2.54	0.42
3:A:486:LEU:HA	3:A:528:LYS:NZ	2.34	0.42
4:B:156:SER:HB2	4:B:157:PRO:CD	2.49	0.42
4:B:388:LYS:HA	4:B:413:GLU:O	2.20	0.42
5:L:32:TYR:C	5:L:91:TYR:CE2	2.93	0.42
5:L:159:VAL:HG22	5:L:179:LEU:HD12	2.01	0.42
6:H:156:PHE:HA	6:H:157:PRO:HA	1.64	0.42
6:H:169:LEU:HD23	6:H:191:VAL:HG21	2.00	0.42
6:H:174:HIS:O	6:H:190:SER:N	2.47	0.42
1:T:724:DT:H5'	3:A:448:ARG:HH21	1.84	0.42
3:A:389:PHE:HB2	3:A:414:TRP:HB3	2.01	0.42
3:A:460:ASN:HD22	4:B:288:ALA:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:314:VAL:HB	4:B:317:VAL:HG23	2.01	0.42
5:L:106:ILE:HG13	5:L:106:ILE:H	1.67	0.42
5:L:190:ASN:OD1	5:L:210:ASN:HB3	2.20	0.42
3:A:84:THR:O	3:A:154:LYS:NZ	2.50	0.42
3:A:90:VAL:CG1	4:B:140:PRO:CB	2.95	0.42
3:A:138:GLU:CG	3:A:139:THR:N	2.76	0.42
3:A:473:THR:O	3:A:476:LYS:HB2	2.20	0.42
4:B:228:LEU:C	4:B:230:MET:H	2.23	0.42
4:B:239:TRP:CZ2	4:B:378:GLU:HG2	2.55	0.42
5:L:146:VAL:CG2	5:L:175:MET:CE	2.96	0.42
6:H:56:ASP:OD2	6:H:58:ASP:N	2.52	0.42
3:A:124:PHE:CD1	3:A:127:TYR:HD2	2.38	0.42
3:A:222:GLN:O	3:A:223:LYS:C	2.58	0.42
3:A:339:TYR:CD2	3:A:375:ILE:HD11	2.55	0.42
3:A:405:TYR:CD1	3:A:406:TRP:N	2.88	0.42
3:A:516:GLU:O	3:A:517:LEU:C	2.58	0.42
4:B:225:PRO:HB2	4:B:226:PRO:CD	2.37	0.42
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.67	0.42
6:H:24:PHE:CE1	6:H:78:ASN:HB3	2.55	0.42
3:A:188:TYR:CD1	3:A:188:TYR:O	2.73	0.42
3:A:221:HIS:CD2	3:A:221:HIS:H	2.36	0.42
3:A:262:GLY:HA2	3:A:265:ASN:HD22	1.85	0.42
3:A:420:PRO:HA	3:A:422:LEU:N	2.35	0.42
3:A:532:TYR:C	3:A:532:TYR:CD2	2.93	0.42
5:L:90:GLN:CD	5:L:90:GLN:C	2.78	0.42
3:A:2:ILE:HG22	3:A:3:SER:N	2.35	0.41
3:A:128:THR:HB	3:A:146:TYR:HB2	2.02	0.41
3:A:279:LEU:N	3:A:279:LEU:CD2	2.82	0.41
3:A:439:THR:HG21	4:B:289:LEU:HG	2.01	0.41
4:B:148:VAL:O	4:B:149:LEU:C	2.58	0.41
4:B:424:LYS:HD2	4:B:424:LYS:HA	1.89	0.41
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.55	0.41
2:P:812:DT:H2"	2:P:813:DT:H71	2.02	0.41
3:A:68:SER:O	3:A:69:THR:CB	2.68	0.41
3:A:155:GLY:O	3:A:156:SER:C	2.58	0.41
3:A:486:LEU:HD21	3:A:495:ILE:CD1	2.46	0.41
4:B:42:GLU:HA	4:B:47:ILE:HG22	2.02	0.41
6:H:37:THR:HG23	6:H:52:THR:OG1	2.20	0.41
3:A:68:SER:O	3:A:69:THR:HB	2.21	0.41
3:A:87:PHE:HE2	3:A:154:LYS:HD2	1.85	0.41
4:B:112:GLY:CA	4:B:151:GLN:HE21	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:175:MET:HE3	5:L:177:SER:HB2	2.02	0.41
6:H:30:SER:O	6:H:31:THR:C	2.59	0.41
6:H:169:LEU:HD12	6:H:169:LEU:HA	1.90	0.41
3:A:27:THR:OG1	3:A:29:GLU:HB3	2.21	0.41
3:A:95:PRO:HD2	3:A:230:MET:HE2	2.03	0.41
4:B:21:VAL:CG1	4:B:59:PRO:HD3	2.49	0.41
4:B:78:ARG:CZ	4:B:411:ILE:CG2	2.98	0.41
4:B:376:THR:O	4:B:380:ILE:HG13	2.20	0.41
4:B:81:ASN:OD1	4:B:154:LYS:HG2	2.21	0.41
4:B:153:TRP:O	4:B:155:GLY:N	2.53	0.41
4:B:171:PHE:HE1	4:B:205:LEU:CA	2.28	0.41
4:B:312:GLU:HB3	4:B:313:PRO:HD2	2.02	0.41
6:H:164:TRP:CZ3	6:H:205:CYS:HB2	2.55	0.41
3:A:86:ASP:O	4:B:55:PRO:HB3	2.21	0.41
3:A:261:VAL:O	3:A:264:LEU:HB2	2.21	0.41
3:A:407:GLN:NE2	4:B:394:GLN:HE21	2.18	0.41
4:B:42:GLU:O	4:B:45:GLY:HA2	2.20	0.41
4:B:74:LEU:HA	4:B:74:LEU:HD23	1.81	0.41
4:B:97:PRO:CD	4:B:181:TYR:CD1	3.02	0.41
4:B:171:PHE:CE1	4:B:205:LEU:CA	3.00	0.41
4:B:189:VAL:HB	4:B:202:ILE:HD11	2.02	0.41
6:H:29:LEU:HD23	6:H:29:LEU:HA	1.85	0.41
3:A:320:ASP:OD1	3:A:320:ASP:C	2.59	0.41
3:A:350:LYS:HG2	3:A:351:THR:N	2.35	0.41
3:A:364:ASP:HB3	3:A:423:VAL:HG13	2.01	0.41
3:A:380:ILE:O	3:A:384:GLY:HA2	2.21	0.41
3:A:460:ASN:HD22	4:B:288:ALA:CA	2.33	0.41
3:A:543:GLY:C	3:A:545:ASN:N	2.72	0.41
4:B:37:ILE:O	4:B:37:ILE:HG13	2.21	0.41
4:B:94:ILE:HD11	4:B:161:GLN:HB2	2.03	0.41
4:B:195:ILE:O	4:B:199:ARG:HD3	2.21	0.41
4:B:200:THR:O	4:B:203:GLU:N	2.54	0.41
4:B:260:LEU:HD11	4:B:264:LEU:HD11	2.02	0.41
4:B:329:ILE:HD11	4:B:375:ILE:CD1	2.50	0.41
4:B:401:TRP:O	4:B:402:TRP:C	2.58	0.41
5:L:36:TYR:CE1	5:L:46:LEU:HD13	2.55	0.41
3:A:70:LYS:HB3	3:A:70:LYS:HE2	1.90	0.41
3:A:271:TYR:HA	3:A:272:PRO:HD3	1.89	0.41
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.55	0.41
3:A:373:GLN:NE2	4:B:397:THR:CG2	2.65	0.41
4:B:417:VAL:HG23	4:B:417:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:9:SER:O	5:L:102:THR:HA	2.21	0.41
5:L:25:ALA:HB2	5:L:29:ILE:HD13	2.02	0.41
5:L:149:LYS:HD2	5:L:195:GLU:OE2	2.21	0.41
3:A:3:SER:HA	3:A:4:PRO:HD3	1.72	0.41
3:A:38:CYS:HB3	3:A:144:TYR:CE2	2.56	0.41
3:A:53:GLU:OE1	3:A:53:GLU:N	2.45	0.41
3:A:160:PHE:CE2	3:A:185:ASP:HB3	2.56	0.41
3:A:164:MET:CE	3:A:185:ASP:HA	2.50	0.41
3:A:266:TRP:O	3:A:269:GLN:HG2	2.20	0.41
3:A:455:ALA:HA	3:A:552:VAL:HG11	2.02	0.41
3:A:486:LEU:HA	3:A:528:LYS:HZ2	1.85	0.41
3:A:507:GLN:C	3:A:509:GLN:H	2.23	0.41
4:B:37:ILE:CD1	4:B:73:LYS:HB2	2.51	0.41
4:B:47:ILE:CG2	4:B:144:TYR:CD1	3.04	0.41
4:B:132:ILE:HA	4:B:133:PRO:HD3	1.70	0.41
4:B:171:PHE:CZ	4:B:205:LEU:HB2	2.56	0.41
4:B:266:TRP:HH2	4:B:422:LEU:HD22	1.85	0.41
5:L:36:TYR:HE1	5:L:46:LEU:HD13	1.86	0.41
5:L:39:LYS:HB3	5:L:39:LYS:HZ2	1.85	0.41
5:L:48:ILE:HG21	5:L:51:THR:O	2.20	0.41
3:A:24:TRP:HZ3	3:A:61:PHE:HB3	1.86	0.41
3:A:280:SER:C	3:A:282:LEU:H	2.25	0.41
4:B:214:LEU:N	4:B:214:LEU:HD12	2.36	0.41
5:L:147:LYS:HZ2	5:L:149:LYS:CE	2.24	0.41
1:T:719:DG:H2"	1:T:720:DG:OP2	2.21	0.40
1:T:724:DT:H2"	1:T:725:DG:C8	2.57	0.40
2:P:822:DA:H2"	2:P:823:ATM:C5'	2.52	0.40
3:A:440:PHE:HE2	3:A:489:SER:OG	2.00	0.40
3:A:447:ASN:HD21	3:A:449:GLU:HB2	1.86	0.40
3:A:459:THR:HG23	3:A:461:LYS:H	1.86	0.40
4:B:37:ILE:O	4:B:41:MET:HG3	2.20	0.40
4:B:254:VAL:O	4:B:255:ASN:C	2.60	0.40
4:B:337:TRP:CD1	4:B:337:TRP:N	2.89	0.40
4:B:339:TYR:C	4:B:339:TYR:HD1	2.24	0.40
4:B:363:ASN:HD21	4:B:365:VAL:HB	1.87	0.40
6:H:54:TRP:HB3	6:H:55:TRP:CE3	2.55	0.40
6:H:84:MET:HG2	6:H:87:VAL:CG1	2.48	0.40
3:A:135:ILE:HG12	3:A:136:ASN:ND2	2.36	0.40
3:A:525:LEU:N	3:A:525:LEU:CD1	2.84	0.40
4:B:80:LEU:HD12	4:B:84:THR:HG23	2.03	0.40
4:B:222:GLN:HG3	4:B:223:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:372:VAL:HG13	4:B:389:PHE:CD2	2.56	0.40
5:L:14:SER:O	5:L:15:LEU:C	2.59	0.40
5:L:181:LEU:N	5:L:181:LEU:CD1	2.84	0.40
6:H:148:LEU:HD23	6:H:148:LEU:HA	1.85	0.40
6:H:164:TRP:HD1	6:H:173:VAL:HG11	1.86	0.40
1:T:709:DC:H2"	1:T:710:DG:H5'	2.03	0.40
3:A:50:ILE:CG1	3:A:143:ARG:HB3	2.51	0.40
3:A:164:MET:HE3	3:A:185:ASP:HA	2.04	0.40
3:A:241:VAL:O	3:A:242:GLN:C	2.59	0.40
3:A:247:PRO:O	3:A:252:TRP:CH2	2.71	0.40
4:B:257:ILE:C	4:B:261:VAL:HG23	2.38	0.40
3:A:80:LEU:HA	3:A:80:LEU:HD23	1.85	0.40
3:A:131:THR:HG22	3:A:132:ILE:N	2.36	0.40
3:A:365:VAL:O	3:A:368:LEU:N	2.55	0.40
3:A:543:GLY:C	3:A:545:ASN:H	2.25	0.40
3:A:545:ASN:O	3:A:548:VAL:HG23	2.22	0.40
4:B:284:ARG:N	4:B:287:LYS:HZ1	2.19	0.40
5:L:21:ILE:HD13	5:L:102:THR:CG2	2.51	0.40
5:L:151:ASP:OD2	5:L:189:HIS:ND1	2.55	0.40
5:L:206:VAL:CG1	5:L:207:LYS:N	2.84	0.40
3:A:276:VAL:C	3:A:278:GLN:N	2.73	0.40
3:A:344:GLU:HB3	3:A:345:PRO:CD	2.34	0.40
3:A:457:TYR:CD2	3:A:457:TYR:C	2.95	0.40
4:B:23:GLN:NE2	4:B:60:VAL:O	2.52	0.40
4:B:245:VAL:CG2	4:B:246:LEU:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	556/558 (100%)	408 (73%)	110 (20%)	38 (7%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	B	427/430 (99%)	333 (78%)	62 (14%)	32 (8%)	1 5
5	L	209/211 (99%)	167 (80%)	31 (15%)	11 (5%)	2 11
6	H	223/225 (99%)	187 (84%)	30 (14%)	6 (3%)	5 26
All	All	1415/1424 (99%)	1095 (77%)	233 (16%)	87 (6%)	1 8

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	66	LYS
3	A	195	ILE
3	A	278	GLN
3	A	345	PRO
3	A	393	ILE
3	A	485	ALA
3	A	544	GLY
4	B	2	ILE
4	B	225	PRO
4	B	292	VAL
4	B	426	TRP
5	L	51	THR
5	L	78	LEU
5	L	143	ASP
3	A	273	GLY
3	A	281	LYS
3	A	284	ARG
3	A	323	LYS
3	A	324	ASP
3	A	490	GLY
3	A	543	GLY
4	B	77	PHE
4	B	95	PRO
4	B	154	LYS
4	B	270	ILE
4	B	278	GLN
4	B	282	LEU
4	B	286	THR
4	B	300	GLU
4	B	361	HIS
4	B	395	LYS
4	B	423	VAL
4	B	424	LYS

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Mol	Chain	Res	Type
5	L	28	ASP
5	L	61	ARG
6	H	144	SER
6	H	211	ALA
3	A	60	VAL
3	A	104	LYS
3	A	217	PRO
3	A	279	LEU
3	A	429	LEU
3	A	443	ASP
3	A	449	GLU
4	B	28	GLU
4	B	53	GLU
4	B	116	PHE
4	B	290	THR
4	B	331	LYS
4	B	421	PRO
5	L	29	ILE
5	L	76	SER
6	H	32	SER
3	A	123	ASP
3	A	156	SER
3	A	184	MET
3	A	321	PRO
3	A	463	ARG
3	A	484	LEU
3	A	505	ILE
3	A	538	ALA
3	A	546	GLU
4	B	87	PHE
4	B	114	ALA
4	B	208	HIS
4	B	247	PRO
4	B	427	TYR
5	L	17	ASP
6	H	139	ALA
3	A	85	GLN
3	A	542	ILE
4	B	29	GLU
4	B	404	GLU
5	L	93	LYS
6	H	210	PRO

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Mol	Chain	Res	Type
3	A	114	ALA
3	A	137	ASN
4	B	170	PRO
4	B	355	ALA
6	H	75	THR
3	A	135	ILE
3	A	555	GLY
5	L	120	PRO
3	A	140	PRO
5	L	40	PRO
4	B	111	VAL
3	A	139	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	485/498 (97%)	416 (86%)	69 (14%)	3 16
4	B	388/392 (99%)	328 (84%)	60 (16%)	2 13
5	L	190/190 (100%)	167 (88%)	23 (12%)	5 21
6	H	196/196 (100%)	169 (86%)	27 (14%)	3 17
All	All	1259/1276 (99%)	1080 (86%)	179 (14%)	3 16

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	VAL
3	A	22	LYS
3	A	24	TRP
3	A	37	ILE
3	A	40	GLU
3	A	61	PHE
3	A	64	LYS
3	A	67	ASP
3	A	78	ARG

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Mol	Chain	Res	Type
3	A	80	LEU
3	A	85	GLN
3	A	86	ASP
3	A	87	PHE
3	A	94	ILE
3	A	110	ASP
3	A	135	ILE
3	A	136	ASN
3	A	175	ASN
3	A	177	ASP
3	A	188	TYR
3	A	199	ARG
3	A	215	THR
3	A	219	LYS
3	A	220	LYS
3	A	221	HIS
3	A	240	THR
3	A	245	VAL
3	A	246	LEU
3	A	250	ASP
3	A	253	THR
3	A	279	LEU
3	A	283	LEU
3	A	290	THR
3	A	309	ILE
3	A	325	LEU
3	A	334	GLN
3	A	342	TYR
3	A	353	LYS
3	A	361	HIS
3	A	362	THR
3	A	365	VAL
3	A	373	GLN
3	A	374	LYS
3	A	385	LYS
3	A	387	PRO
3	A	397	THR
3	A	401	TRP
3	A	405	TYR
3	A	407	GLN
3	A	409	THR
3	A	415	GLU

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Mol	Chain	Res	Type
3	A	419	THR
3	A	425	LEU
3	A	442	VAL
3	A	451	LYS
3	A	464	GLN
3	A	465	LYS
3	A	469	LEU
3	A	478	GLU
3	A	497	THR
3	A	500	GLN
3	A	511	ASP
3	A	519	ASN
3	A	525	LEU
3	A	532	TYR
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	5	ILE
4	B	12	LEU
4	B	27	THR
4	B	37	ILE
4	B	42	GLU
4	B	47	ILE
4	B	55	PRO
4	B	74	LEU
4	B	87	PHE
4	B	100	LEU
4	B	103	LYS
4	B	109	LEU
4	B	148	VAL
4	B	169	GLU
4	B	175	ASN
4	B	193	LEU
4	B	197	GLN
4	B	199	ARG
4	B	212	TRP
4	B	215	THR
4	B	218	ASP
4	B	220	LYS

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Mol	Chain	Res	Type
4	B	221	HIS
4	B	225	PRO
4	B	242	GLN
4	B	244	ILE
4	B	246	LEU
4	B	250	ASP
4	B	266	TRP
4	B	271	TYR
4	B	276	VAL
4	B	277	ARG
4	B	282	LEU
4	B	286	THR
4	B	295	LEU
4	B	301	LEU
4	B	305	GLU
4	B	315	HIS
4	B	318	TYR
4	B	324	ASP
4	B	330	GLN
4	B	339	TYR
4	B	347	LYS
4	B	348	ASN
4	B	351	THR
4	B	353	LYS
4	B	357	MET
4	B	363	ASN
4	B	364	ASP
4	B	401	TRP
4	B	407	GLN
4	B	410	TRP
4	B	413	GLU
4	B	418	ASN
4	B	419	THR
4	B	424	LYS
4	B	425	LEU
4	B	427	TYR
5	L	7	THR
5	L	10	SER
5	L	11	LEU
5	L	15	LEU
5	L	33	LEU
5	L	39	LYS

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Mol	Chain	Res	Type
5	L	49	TYR
5	L	67	SER
5	L	75	ILE
5	L	76	SER
5	L	77	ASN
5	L	83	ILE
5	L	89	GLN
5	L	90	GLN
5	L	91	TYR
5	L	106	ILE
5	L	110	ASP
5	L	142	LYS
5	L	143	ASP
5	L	144	ILE
5	L	173	TYR
5	L	180	THR
5	L	197	THR
6	H	1	GLN
6	H	3	THR
6	H	7	SER
6	H	11	ILE
6	H	17	PRO
6	H	25	SER
6	H	31	THR
6	H	43	SER
6	H	59	ASN
6	H	62	ASN
6	H	72	SER
6	H	81	PHE
6	H	82	LEU
6	H	88	GLU
6	H	107	ASP
6	H	126	THR
6	H	141	GLN
6	H	145	MET
6	H	152	VAL
6	H	159	PRO
6	H	160	VAL
6	H	187	LEU
6	H	192	THR
6	H	210	PRO
6	H	216	VAL

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Mol	Chain	Res	Type
6	H	218	LYS
6	H	225	CYS

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

Mol	Chain	Res	Type
3	A	23	GLN
3	A	91	GLN
3	A	136	ASN
3	A	175	ASN
3	A	207	GLN
3	A	221	HIS
3	A	255	ASN
3	A	269	GLN
3	A	306	ASN
3	A	330	GLN
3	A	447	ASN
3	A	480	GLN
3	A	494	ASN
3	A	500	GLN
3	A	520	GLN
3	A	539	HIS
3	A	545	ASN
4	B	57	ASN
4	B	91	GLN
4	B	137	ASN
4	B	151	GLN
4	B	161	GLN
4	B	235	HIS
4	B	242	GLN
4	B	255	ASN
4	B	278	GLN
4	B	348	ASN
4	B	363	ASN
4	B	394	GLN
4	B	418	ASN
5	L	77	ASN
5	L	89	GLN
5	L	90	GLN
5	L	138	ASN
5	L	190	ASN
5	L	210	ASN

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Mol	Chain	Res	Type
6	H	59	ASN
6	H	62	ASN
6	H	79	GLN
6	H	174	HIS
6	H	181	GLN
6	H	206	ASN
6	H	209	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	3,1,2	22,28,29	2.25	3 (13%)	23,39,42	4.05	11 (47%)
2	ATM	P	823	1,2	16,23,24	1.46	4 (25%)	17,32,35	3.21	3 (17%)

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	3,1,2	-	2/8/26/27	0/3/3/3
2	ATM	P	823	1,2	-	2/7/24/25	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	817	MRG	C2-N2	7.29	1.45	1.34
2	P	817	MRG	C21-N2	-5.56	1.34	1.45
2	P	823	ATM	N4'-N3'	3.07	1.31	1.23
2	P	823	ATM	C3'-N3'	-2.56	1.41	1.48
2	P	823	ATM	C4-N3	2.44	1.37	1.33
2	P	817	MRG	C8-N7	-2.21	1.30	1.34
2	P	823	ATM	C6-C5	2.20	1.46	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	817	MRG	C21-N2-C2	-14.08	99.41	123.75
2	P	823	ATM	C4-N3-C2	11.80	125.11	115.14
2	P	817	MRG	C5-C6-N1	-7.75	112.83	123.43
2	P	817	MRG	C6-N1-C2	5.85	125.65	115.18
2	P	817	MRG	C23-C22-C21	-4.18	99.22	112.65
2	P	817	MRG	C2-N3-C4	-4.07	110.66	115.28
2	P	823	ATM	C5A-C5-C4	3.53	127.70	121.37
2	P	817	MRG	N2-C2-N3	3.09	122.53	117.19
2	P	817	MRG	N2-C2-N1	-2.55	112.78	117.19
2	P	817	MRG	C2'-C1'-N9	-2.38	108.77	114.27
2	P	823	ATM	C3'-C2'-C1'	2.37	105.79	103.25
2	P	817	MRG	C22-C21-N2	2.26	117.57	111.49
2	P	817	MRG	C22-C23-S24	2.17	119.94	112.96
2	P	817	MRG	C4-C5-N7	2.01	111.49	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	817	MRG	N2-C21-C22-C23
2	P	823	ATM	C3'-N3'-N4'-N5'
2	P	823	ATM	O4'-C1'-N1-C6
2	P	817	MRG	C21-C22-C23-S24

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	817	MRG	1	0
2	P	823	ATM	8	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	425:LEU	C	426:TRP	N	1.16

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	T	23/27 (85%)	0.02	1 (4%) 35 13	57, 99, 110, 121	0
2	P	19/22 (86%)	-0.06	0 100 100	74, 88, 106, 110	0
3	A	556/558 (99%)	-0.06	15 (2%) 54 26	35, 80, 110, 110	1 (0%)
4	B	428/430 (99%)	-0.27	3 (0%) 87 69	27, 62, 108, 110	1 (0%)
5	L	211/211 (100%)	-0.24	0 100 100	39, 71, 106, 110	0
6	H	225/225 (100%)	-0.34	1 (0%) 92 79	35, 62, 99, 110	0
All	All	1462/1473 (99%)	-0.19	20 (1%) 75 49	27, 71, 109, 121	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	283	LEU	3.8
4	B	315	HIS	3.5
3	A	252	TRP	3.1
3	A	448	ARG	2.9
3	A	2	ILE	2.8
3	A	64	LYS	2.8
1	T	703	DG	2.8
3	A	222	GLN	2.8
3	A	67	ASP	2.6
3	A	1	PRO	2.6
6	H	138	SER	2.6
3	A	286	THR	2.5
3	A	295	LEU	2.5
3	A	71	TRP	2.4
3	A	223	LYS	2.4
4	B	303	LEU	2.2
3	A	68	SER	2.1
3	A	282	LEU	2.1
4	B	252	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	293	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MRG	P	817	26/27	0.91	0.16	79,79,79,80	0
2	ATM	P	823	22/23	0.94	0.16	62,68,81,86	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	A	1002	1/1	0.70	0.43	58,58,58,58	0
7	MG	A	1001	1/1	0.98	0.35	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.