



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:37 pm BST

PDB ID : 1NYR  
Title : Structure of Staphylococcus aureus threonyl-tRNA synthetase complexed with ATP  
Authors : Torres-Larios, A.; Sankaranarayanan, R.; Rees, B.; Dock-Bregeon, A.C.; Moras, D.  
Deposited on : 2003-02-13  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

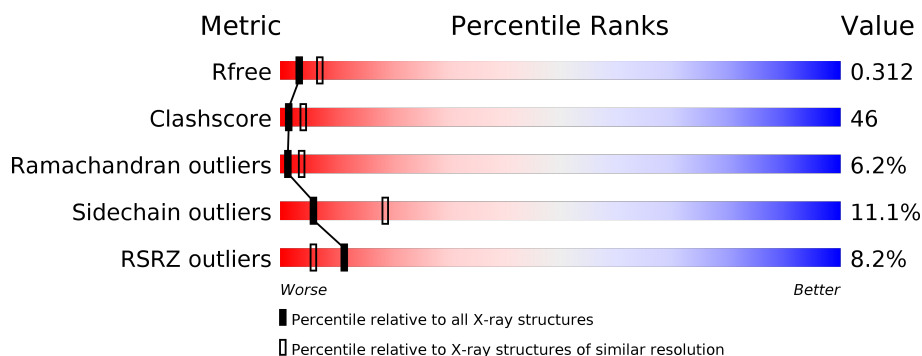
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	645	
1	B	645	

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
4	THR	A	1004	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10684 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

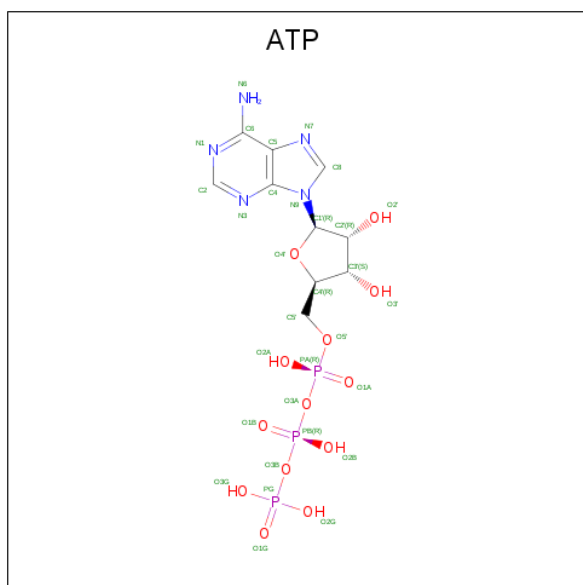
- Molecule 1 is a protein called threonyl-tRNA synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5216	3296	894	1003	23			
1	B	637	Total	C	N	O	S	0	0	0
			5171	3265	888	994	24			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

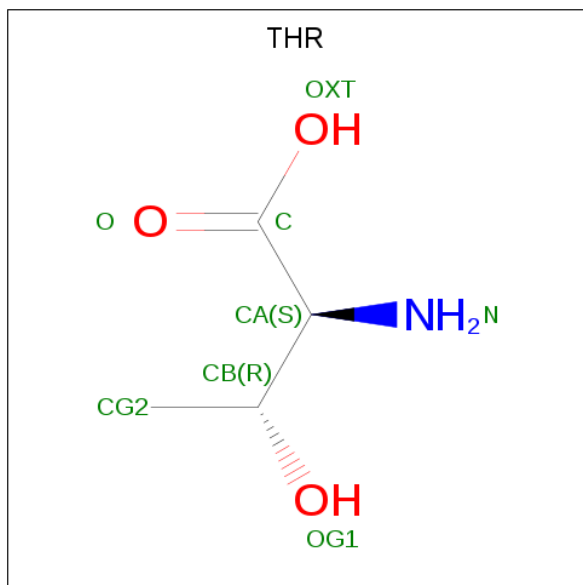
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is THREONINE (three-letter code: THR) (formula:  $C_4H_9NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

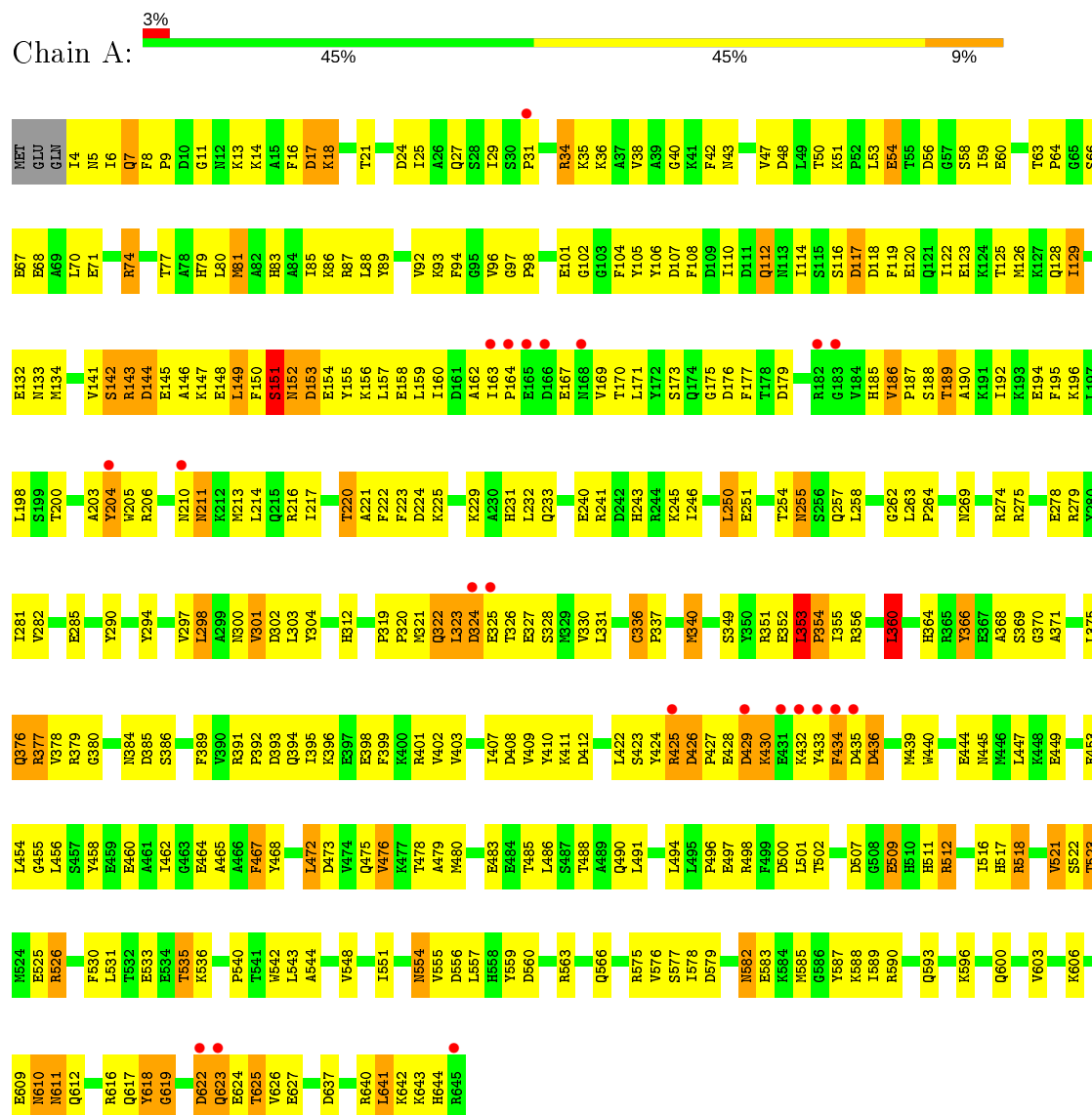
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	97	Total	O	0	0
			97	97		

### 3 Residue-property plots [i](#)

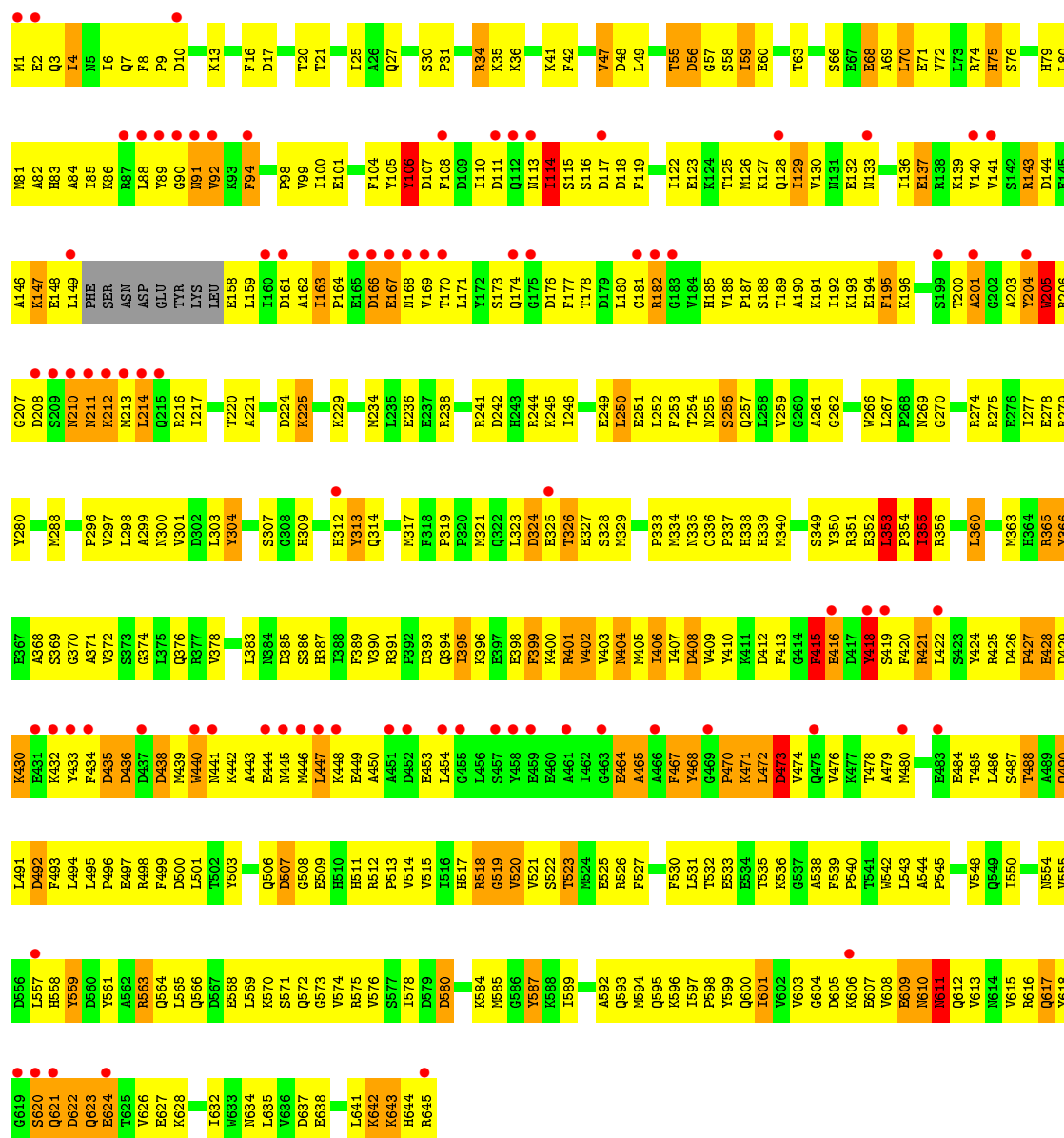
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: threonyl-tRNA synthetase 1



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.13Å 122.52Å 148.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.80) 98.8 (14.99-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.313 0.239 , 0.312	Depositor DCC
$R_{free}$ test set	2311 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 80.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	0/5325	0.84	11/7182 (0.2%)
1	B	0.51	0/5277	0.75	4/7115 (0.1%)
All	All	0.56	0/10602	0.80	15/14297 (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
1	B	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	353	LEU	C-N-CA	-6.53	94.58	122.00
1	A	557	LEU	CA-CB-CG	6.33	129.85	115.30
1	A	353	LEU	N-CA-C	6.28	127.95	111.00
1	A	619	GLY	N-CA-C	6.12	128.40	113.10
1	A	353	LEU	C-N-CD	5.72	140.41	128.40
1	A	425	ARG	N-CA-C	5.64	126.22	111.00
1	B	447	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	360	LEU	N-CA-C	-5.52	96.11	111.00
1	A	472	LEU	N-CA-C	-5.49	96.17	111.00
1	A	625	THR	N-CA-C	-5.48	96.20	111.00
1	B	355	ILE	N-CA-C	5.31	125.33	111.00
1	A	275	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	360	LEU	N-CA-C	-5.13	97.14	111.00
1	B	415	PHE	N-CA-C	5.08	124.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	PRO	N-CA-C	-5.07	98.93	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	TYR	Sidechain
1	B	418	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	A	5216	0	5104	386	0
1	B	5171	0	5067	567	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	3	0
3	B	31	0	12	3	0
4	A	8	0	5	4	0
4	B	8	0	5	2	0
5	A	119	0	0	9	0
5	B	97	0	0	15	0
All	All	10684	0	10205	952	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 46.

All (952) 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:A:426:ASP:HB3	1:A:427:PRO:HD2	1.31	1.11
1:B:518:ARG:HG3	1:B:518:ARG:HH11	1.12	1.09
1:B:471:LYS:HB3	1:B:490:GLN:HB3	1.32	1.09
1:B:606:LYS:HA	1:B:609:GLU:HB2	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:HG2	1:A:435:ASP:HB3	1.34	1.05
1:A:322:GLN:HG3	1:A:323:LEU:H	1.18	1.04
1:B:82:ALA:HB2	1:B:106:TYR:HE1	1.21	1.03
1:A:449:GLU:O	1:A:453:GLU:HG3	1.62	1.00
1:B:353:LEU:O	1:B:353:LEU:HD13	1.63	0.97
1:B:82:ALA:HB2	1:B:106:TYR:CE1	1.97	0.97
1:B:589:ILE:H	1:B:589:ILE:HD12	1.28	0.97
1:B:6:ILE:HD13	1:B:25:ILE:HD11	1.47	0.96
1:B:418:TYR:H	1:B:418:TYR:HD2	1.12	0.94
1:B:444:GLU:HB2	1:B:448:LYS:HE2	1.49	0.93
1:B:410:TYR:OH	1:B:486:LEU:HD23	1.69	0.92
1:B:430:LYS:NZ	1:B:497:GLU:HG3	1.87	0.90
1:B:616:ARG:NH1	1:B:622:ASP:HB3	1.86	0.90
1:A:371:ALA:HB1	1:A:377:ARG:HD3	1.53	0.88
1:B:354:PRO:HG3	1:B:394:GLN:HE22	1.36	0.88
1:A:94:PHE:HB2	1:A:156:LYS:HE3	1.54	0.88
1:B:349:SER:OG	1:B:351:ARG:HG3	1.73	0.88
1:B:446:MET:HA	1:B:449:GLU:HG3	1.56	0.88
1:A:110:ILE:HD12	1:A:114:ILE:HD11	1.53	0.87
1:A:319:PRO:HG2	1:B:321:MET:HB2	1.55	0.87
1:B:465:ALA:HA	1:B:471:LYS:HE2	1.56	0.87
1:A:158:GLU:HB3	1:A:206:ARG:NH2	1.90	0.87
1:A:322:GLN:CG	1:A:323:LEU:H	1.85	0.86
1:A:322:GLN:HG3	1:A:323:LEU:N	1.90	0.86
1:B:617:GLN:HE22	1:B:645:ARG:HD3	1.39	0.86
1:B:592:ALA:HB3	1:B:600:GLN:HE21	1.40	0.86
1:A:322:GLN:HG2	1:A:327:GLU:HB2	1.55	0.86
1:A:554:ASN:HD21	1:A:556:ASP:HB2	1.38	0.86
1:A:428:GLU:CG	1:A:435:ASP:HB3	2.05	0.86
1:B:337:PRO:HG2	5:B:2007:HOH:O	1.75	0.86
1:B:428:GLU:HB3	1:B:440:TRP:HE1	1.40	0.86
1:B:442:LYS:NZ	1:B:446:MET:HB2	1.90	0.85
1:B:406:ILE:HD11	1:B:487:SER:OG	1.74	0.85
1:B:4:ILE:HG22	1:B:16:PHE:O	1.76	0.85
1:B:422:LEU:HD22	1:B:448:LYS:HG2	1.59	0.85
1:A:554:ASN:HD22	1:A:556:ASP:H	1.25	0.84
1:B:426:ASP:CG	1:B:427:PRO:HD2	1.98	0.83
1:B:490:GLN:HG3	1:B:517:HIS:HB2	1.60	0.83
1:A:426:ASP:HB3	1:A:427:PRO:CD	2.09	0.83
1:A:616:ARG:NH1	1:A:619:GLY:H	1.77	0.82
1:B:80:LEU:HG	1:B:126:MET:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:ALA:O	1:B:575:ARG:NH1	2.13	0.82
1:B:621:GLN:HE21	1:B:623:GLN:HG2	1.44	0.82
1:A:523:THR:HG22	1:A:526:ARG:HB3	1.59	0.82
1:A:554:ASN:ND2	1:A:556:ASP:HB2	1.94	0.82
1:B:169:VAL:HG12	1:B:170:THR:H	1.42	0.82
1:B:429:ASP:HB3	1:B:494:LEU:HD21	1.61	0.82
1:B:585:MET:SD	1:B:589:ILE:HD11	2.20	0.82
1:B:212:LYS:H	1:B:212:LYS:HD2	1.43	0.81
1:B:643:LYS:HG2	1:B:644:HIS:H	1.44	0.81
1:B:450:ALA:HA	1:B:453:GLU:HG2	1.62	0.81
1:A:70:LEU:O	1:A:74:ARG:HG3	1.81	0.81
1:B:500:ASP:HA	1:B:512:ARG:NH2	1.96	0.81
1:B:163:ILE:H	1:B:164:PRO:HD3	1.46	0.80
1:B:443:ALA:O	1:B:447:LEU:HB2	1.81	0.80
1:A:246:ILE:HG23	1:A:250:LEU:HD22	1.64	0.80
1:B:354:PRO:HG3	1:B:394:GLN:NE2	1.97	0.80
1:B:340:MET:HE3	1:B:495:LEU:HD13	1.64	0.79
1:B:85:ILE:HG22	1:B:92:VAL:HG21	1.64	0.79
1:B:261:ALA:HB1	1:B:372:VAL:HG11	1.65	0.79
1:B:403:VAL:O	1:B:403:VAL:HG12	1.81	0.79
1:B:323:LEU:HD12	1:B:329:MET:HG3	1.63	0.79
1:A:436:ASP:HB3	1:A:439:MET:HB3	1.64	0.79
1:B:390:VAL:HG12	1:B:391:ARG:H	1.46	0.79
1:A:5:ASN:H	1:A:56:ASP:HB3	1.48	0.78
1:B:84:ALA:HB2	1:B:126:MET:HB3	1.66	0.78
1:B:523:THR:CG2	1:B:526:ARG:H	1.96	0.78
1:B:507:ASP:O	1:B:509:GLU:HG2	1.83	0.78
1:B:445:ASN:O	1:B:449:GLU:HG2	1.83	0.78
1:B:89:TYR:CD2	1:B:92:VAL:HG11	2.19	0.78
1:A:153:ASP:HB3	1:A:156:LYS:HB2	1.66	0.77
1:B:336:CYS:HA	1:B:387:HIS:CE1	2.19	0.77
1:A:132:GLU:OE1	1:A:134:MET:HE2	1.84	0.77
1:A:440:TRP:O	1:A:444:GLU:HG3	1.84	0.77
1:A:141:VAL:HB	1:A:145:GLU:HB2	1.67	0.77
1:A:340:MET:HG3	1:A:501:LEU:HD11	1.66	0.77
1:A:610:ASN:HB2	1:A:612:GLN:NE2	2.00	0.77
1:B:606:LYS:HA	1:B:609:GLU:CB	2.11	0.77
1:B:474:VAL:HG21	1:B:487:SER:HB2	1.65	0.77
1:A:337:PRO:HG2	5:A:1009:HOH:O	1.85	0.76
1:B:443:ALA:O	1:B:470:PRO:HG3	1.85	0.76
1:B:446:MET:HA	1:B:449:GLU:CG	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:CD1	1:A:114:ILE:HD11	2.15	0.76
1:B:340:MET:CE	1:B:495:LEU:HD13	2.16	0.76
1:B:85:ILE:HB	5:B:2021:HOH:O	1.84	0.76
1:B:106:TYR:HB3	1:B:108:PHE:CE1	2.21	0.75
1:A:93:LYS:HD3	1:A:155:TYR:HE1	1.50	0.75
1:B:114:ILE:HD12	1:B:217:ILE:HD11	1.66	0.75
1:B:126:MET:O	1:B:130:VAL:HG23	1.87	0.75
1:B:161:ASP:O	1:B:164:PRO:HD3	1.86	0.75
1:B:430:LYS:HZ2	1:B:497:GLU:HG3	1.52	0.75
1:B:55:THR:OG1	1:B:56:ASP:N	2.21	0.74
1:B:604:GLY:H	1:B:607:GLU:HB2	1.52	0.74
1:B:395:ILE:HD11	1:B:514:VAL:HG11	1.68	0.74
1:B:205:TRP:H	1:B:214:LEU:HG	1.52	0.74
1:B:83:HIS:HE1	1:B:176:ASP:HB2	1.53	0.74
1:B:169:VAL:HG12	1:B:170:THR:N	2.02	0.74
1:B:559:TYR:HE2	1:B:563:ARG:HG2	1.53	0.74
1:A:110:ILE:HG22	1:A:112:GLN:H	1.53	0.73
1:B:118:ASP:O	1:B:122:ILE:HG13	1.89	0.73
1:A:141:VAL:HG21	1:A:146:ALA:HB2	1.70	0.73
1:A:579:ASP:OD1	1:A:588:LYS:HG2	1.89	0.73
1:B:518:ARG:CG	1:B:518:ARG:HH11	1.94	0.73
1:A:27:GLN:HE22	1:A:31:PRO:HG3	1.53	0.73
1:B:471:LYS:CB	1:B:490:GLN:HB3	2.14	0.72
1:A:428:GLU:CG	1:A:440:TRP:HE1	2.02	0.72
1:A:152:ASN:N	1:A:152:ASN:HD22	1.86	0.72
1:B:422:LEU:HD23	1:B:447:LEU:HD12	1.71	0.72
1:B:523:THR:HG22	1:B:526:ARG:HB3	1.71	0.72
1:A:18:LYS:HG3	1:A:54:GLU:O	1.88	0.72
1:B:512:ARG:HH11	1:B:512:ARG:HG3	1.55	0.72
1:A:107:ASP:OD2	1:A:216:ARG:HB2	1.89	0.71
1:B:616:ARG:HH12	1:B:622:ASP:HB3	1.52	0.71
1:A:436:ASP:HB3	1:A:439:MET:CB	2.20	0.71
1:A:622:ASP:O	1:A:624:GLU:N	2.18	0.71
1:A:38:VAL:O	1:A:187:PRO:HD3	1.90	0.71
1:B:632:ILE:HD12	5:B:2070:HOH:O	1.91	0.71
1:B:420:PHE:CE2	1:B:474:VAL:HG22	2.26	0.70
1:B:68:GLU:HA	1:B:71:GLU:HG3	1.71	0.70
1:B:601:ILE:HD11	1:B:615:VAL:HG12	1.72	0.70
1:B:89:TYR:HD2	1:B:92:VAL:HG11	1.55	0.70
4:A:1004:THR:OXT	4:A:1004:THR:HG22	1.91	0.70
1:A:428:GLU:OE1	1:A:435:ASP:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:VAL:HG23	1:B:328:SER:O	1.92	0.69
1:A:428:GLU:HA	1:A:467:PHE:O	1.92	0.69
1:A:622:ASP:C	1:A:624:GLU:H	1.95	0.69
1:A:102:GLY:O	1:A:220:THR:HG23	1.92	0.69
1:B:47:VAL:HG23	1:B:48:ASP:O	1.93	0.69
1:B:100:ILE:HG13	1:B:104:PHE:HA	1.75	0.69
1:B:31:PRO:O	1:B:35:LYS:HG3	1.93	0.69
1:B:205:TRP:HB3	1:B:211:ASN:CG	2.13	0.69
1:A:427:PRO:O	1:A:467:PHE:HA	1.93	0.68
1:A:200:THR:HG22	1:A:217:ILE:HG12	1.74	0.68
1:B:395:ILE:HD13	1:B:491:LEU:HD21	1.75	0.68
1:B:390:VAL:HG12	1:B:394:GLN:HB2	1.76	0.68
1:B:396:LYS:O	1:B:400:LYS:HG3	1.94	0.68
1:A:298:LEU:HD12	1:A:298:LEU:H	1.59	0.68
1:B:174:GLN:HG2	1:B:177:PHE:HB3	1.76	0.68
1:A:301:VAL:HG23	1:A:328:SER:O	1.94	0.68
1:B:66:SER:HB3	1:B:69:ALA:HB2	1.76	0.68
1:A:66:SER:OG	1:A:68:GLU:HG3	1.94	0.68
1:A:186:VAL:HG22	1:A:187:PRO:HD2	1.76	0.67
1:A:97:GLY:HA3	1:A:106:TYR:CD2	2.29	0.67
1:B:644:HIS:O	1:B:645:ARG:HG3	1.93	0.67
1:B:98:PRO:HD2	1:B:105:TYR:CE1	2.29	0.67
1:A:83:HIS:CE1	1:A:129:ILE:HD13	2.29	0.67
1:A:298:LEU:HD12	1:A:298:LEU:N	2.10	0.67
1:A:554:ASN:ND2	1:A:556:ASP:H	1.90	0.67
1:B:163:ILE:H	1:B:164:PRO:CD	2.06	0.67
1:A:157:LEU:HA	1:A:160:ILE:HG22	1.77	0.67
1:B:376:GLN:OE1	1:B:478:THR:HB	1.95	0.67
1:B:390:VAL:HG12	1:B:391:ARG:N	2.09	0.67
1:A:384:ASN:HD22	1:A:521:VAL:H	1.43	0.67
1:B:596:LYS:HD3	1:B:618:TYR:CZ	2.30	0.67
1:B:589:ILE:N	1:B:589:ILE:HD12	2.06	0.67
1:B:430:LYS:HZ1	1:B:497:GLU:HG3	1.59	0.66
4:A:1004:THR:CG2	4:A:1004:THR:OXT	2.43	0.66
1:A:326:THR:HG22	1:A:327:GLU:HG3	1.77	0.66
1:B:119:PHE:CD1	1:B:122:ILE:HD12	2.30	0.66
1:B:485:THR:HB	5:B:2068:HOH:O	1.96	0.66
1:A:377:ARG:NH2	3:A:1003:ATP:O3G	2.29	0.66
1:A:410:TYR:OH	1:A:486:LEU:HD23	1.96	0.66
1:B:262:GLY:N	1:B:372:VAL:HG13	2.10	0.66
1:B:471:LYS:HA	1:B:490:GLN:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:N	1:B:164:PRO:CD	2.58	0.65
1:B:433:TYR:C	1:B:435:ASP:H	2.00	0.65
1:B:563:ARG:HG3	1:B:563:ARG:HH11	1.61	0.65
1:A:110:ILE:HD12	1:A:114:ILE:CD1	2.24	0.65
1:A:395:ILE:CG2	1:A:491:LEU:HD21	2.26	0.65
1:B:584:LYS:N	1:B:584:LYS:HD3	2.10	0.65
1:A:154:GLU:O	1:A:158:GLU:HG3	1.96	0.65
1:A:5:ASN:O	1:A:6:ILE:HD13	1.96	0.65
1:B:350:TYR:CE2	1:B:506:GLN:HA	2.32	0.65
1:B:119:PHE:HD1	1:B:122:ILE:HD12	1.60	0.65
1:B:643:LYS:HG2	1:B:644:HIS:N	2.12	0.65
1:A:87:ARG:NE	1:A:176:ASP:OD2	2.29	0.65
1:B:167:GLU:C	1:B:168:ASN:HD22	1.99	0.65
1:A:34:ARG:HG3	1:A:35:LYS:N	2.13	0.64
1:A:476:VAL:HG13	1:A:530:PHE:CE1	2.31	0.64
1:A:118:ASP:O	1:A:122:ILE:HG13	1.97	0.64
1:B:428:GLU:HB3	1:B:440:TRP:NE1	2.12	0.64
1:B:133:ASN:HA	1:B:190:ALA:HB2	1.79	0.64
1:A:518:ARG:HD3	1:A:518:ARG:C	2.17	0.64
1:B:6:ILE:HD12	1:B:16:PHE:CD1	2.33	0.64
1:B:3:GLN:O	1:B:4:ILE:HB	1.98	0.64
1:A:322:GLN:CG	1:A:323:LEU:N	2.51	0.64
1:B:492:ASP:OD1	1:B:495:LEU:HD12	1.98	0.63
1:B:554:ASN:HB3	1:B:557:LEU:HB2	1.80	0.63
1:A:157:LEU:O	1:A:160:ILE:HG22	1.99	0.63
1:B:621:GLN:NE2	1:B:623:GLN:HG2	2.12	0.63
1:A:616:ARG:HH12	1:A:619:GLY:H	1.45	0.63
1:B:236:GLU:C	1:B:238:ARG:H	2.02	0.63
1:B:420:PHE:O	1:B:421:ARG:HB3	1.98	0.63
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.64	0.63
1:B:75:HIS:HB2	1:B:99:VAL:HG22	1.81	0.63
1:B:129:ILE:O	1:B:132:GLU:HB2	1.98	0.63
1:B:146:ALA:C	1:B:148:GLU:H	2.02	0.63
1:A:153:ASP:O	1:A:157:LEU:HB2	1.99	0.63
1:B:242:ASP:OD1	1:B:244:ARG:HB2	1.97	0.63
1:A:17:ASP:N	1:A:17:ASP:OD2	2.31	0.63
1:A:96:VAL:O	1:A:98:PRO:HD3	1.99	0.62
1:B:616:ARG:HG2	1:B:616:ARG:O	1.99	0.62
1:A:143:ARG:O	1:A:144:ASP:HB2	1.98	0.62
1:B:507:ASP:O	1:B:509:GLU:N	2.32	0.62
1:B:565:LEU:CD2	1:B:601:ILE:HG21	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:SER:O	1:B:488:THR:HB	1.99	0.62
1:B:83:HIS:CE1	1:B:176:ASP:HB2	2.33	0.62
1:A:155:TYR:O	1:A:159:LEU:HB2	1.99	0.62
1:A:323:LEU:HG	1:A:326:THR:HB	1.80	0.62
1:A:5:ASN:O	1:A:56:ASP:HB2	2.00	0.62
1:B:407:ILE:HG23	1:B:408:ASP:OD2	2.00	0.62
1:A:5:ASN:N	1:A:56:ASP:HB3	2.15	0.62
1:B:403:VAL:CG1	1:B:403:VAL:O	2.48	0.62
1:A:158:GLU:HB3	1:A:206:ARG:HH21	1.63	0.62
1:A:14:LYS:HE3	1:A:16:PHE:CZ	2.35	0.62
1:A:433:TYR:CG	1:A:434:PHE:N	2.68	0.62
1:B:402:VAL:O	1:B:406:ILE:HG22	2.00	0.62
1:A:303:LEU:HD21	1:A:337:PRO:HB2	1.82	0.61
1:A:473:ASP:HB3	1:A:485:THR:HG23	1.80	0.61
1:B:74:ARG:C	1:B:76:SER:H	2.04	0.61
1:B:288:MET:HE3	1:B:405:MET:HB2	1.81	0.61
1:A:500:ASP:OD1	1:A:512:ARG:NH2	2.31	0.61
1:B:205:TRP:HB3	1:B:211:ASN:ND2	2.15	0.61
1:A:105:TYR:HA	1:A:217:ILE:O	2.00	0.61
1:A:353:LEU:O	1:A:355:ILE:N	2.34	0.61
1:B:234:MET:SD	1:B:234:MET:C	2.78	0.61
1:B:288:MET:SD	1:B:405:MET:SD	2.98	0.61
1:B:159:LEU:HD11	1:B:162:ALA:HB3	1.82	0.61
1:A:297:VAL:O	1:A:297:VAL:HG22	2.00	0.61
1:A:303:LEU:CD2	1:A:337:PRO:HB2	2.31	0.61
1:A:141:VAL:CG2	1:A:146:ALA:HB2	2.31	0.61
1:B:105:TYR:HA	1:B:217:ILE:O	2.00	0.61
1:B:7:GLN:O	1:B:58:SER:HA	2.00	0.61
1:B:143:ARG:N	1:B:168:ASN:HB3	2.16	0.60
1:B:386:SER:HB3	1:B:518:ARG:HG2	1.83	0.60
1:A:246:ILE:CG2	1:A:250:LEU:HD22	2.31	0.60
1:A:488:THR:O	1:A:518:ARG:HA	2.01	0.60
1:B:317:MET:HG2	1:B:333:PRO:HB3	1.84	0.60
1:B:612:GLN:HG2	1:B:627:GLU:HA	1.82	0.60
1:A:554:ASN:HD22	1:A:556:ASP:N	1.97	0.60
1:B:518:ARG:HG3	1:B:518:ARG:NH1	1.94	0.60
1:A:433:TYR:CE2	1:A:434:PHE:HB2	2.37	0.60
1:B:80:LEU:CG	1:B:126:MET:HB2	2.31	0.60
1:B:304:TYR:HA	1:B:307:SER:HG	1.67	0.59
1:B:478:THR:HG21	1:B:484:GLU:HG3	1.84	0.59
1:B:589:ILE:CD1	1:B:589:ILE:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:OE2	1:A:428:GLU:N	2.35	0.59
1:B:442:LYS:HZ2	1:B:446:MET:HB2	1.63	0.59
1:B:447:LEU:HD11	1:B:471:LYS:O	2.02	0.59
1:B:406:ILE:HD11	1:B:487:SER:CB	2.31	0.59
1:A:392:PRO:HD2	5:A:1025:HOH:O	2.02	0.59
1:B:312:HIS:HD2	1:B:427:PRO:HB2	1.67	0.59
1:B:430:LYS:HB3	1:B:436:ASP:HB2	1.84	0.59
1:B:453:GLU:O	1:B:454:LEU:HD13	2.03	0.59
1:A:433:TYR:CD2	1:A:434:PHE:N	2.70	0.59
1:B:27:GLN:OE1	1:B:34:ARG:HD3	2.02	0.59
1:A:257:GLN:HG3	1:A:258:LEU:H	1.66	0.59
1:A:321:MET:O	1:A:322:GLN:HB2	2.03	0.59
1:A:523:THR:CG2	1:A:526:ARG:H	2.16	0.59
1:B:454:LEU:HD22	1:B:454:LEU:N	2.18	0.59
1:A:158:GLU:HB3	1:A:206:ARG:HH22	1.66	0.58
1:A:399:PHE:O	1:A:403:VAL:HG23	2.02	0.58
1:B:254:THR:HG23	1:B:267:LEU:HD11	1.85	0.58
1:A:85:ILE:HD11	1:A:122:ILE:HD13	1.85	0.58
1:B:80:LEU:HD11	1:B:129:ILE:HG21	1.84	0.58
1:A:241:ARG:HD2	1:A:536:LYS:NZ	2.18	0.58
1:B:107:ASP:OD2	1:B:216:ARG:HB2	2.03	0.58
1:A:324:ASP:C	1:A:326:THR:H	2.06	0.58
1:A:428:GLU:CB	1:A:440:TRP:HE1	2.16	0.58
1:B:110:ILE:HG22	1:B:111:ASP:N	2.19	0.58
1:B:125:THR:C	1:B:127:LYS:H	2.06	0.58
1:A:445:ASN:HB3	5:A:1031:HOH:O	2.03	0.58
1:B:82:ALA:CB	1:B:106:TYR:HE1	2.07	0.58
1:A:478:THR:CG2	1:A:479:ALA:N	2.67	0.58
1:A:582:ASN:HD22	1:A:582:ASN:C	2.04	0.58
1:A:585:MET:HG3	1:A:589:ILE:HD13	1.85	0.58
1:B:114:ILE:CD1	1:B:217:ILE:HD11	2.33	0.58
1:A:152:ASN:N	1:A:152:ASN:ND2	2.52	0.58
1:B:430:LYS:HG2	1:B:436:ASP:OD1	2.03	0.58
1:A:196:LYS:HD3	1:A:232:LEU:HD11	1.85	0.58
1:B:300:ASN:HD21	1:B:327:GLU:CD	2.06	0.58
1:A:7:GLN:HG2	1:A:13:LYS:CD	2.33	0.57
1:A:143:ARG:H	1:A:169:VAL:HG22	1.67	0.57
1:B:262:GLY:N	1:B:372:VAL:CG1	2.67	0.57
1:A:324:ASP:O	1:A:326:THR:N	2.37	0.57
1:B:82:ALA:HB1	1:B:177:PHE:CZ	2.38	0.57
1:B:425:ARG:HD2	1:B:425:ARG:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:O	1:A:323:LEU:HG	2.03	0.57
1:B:522:SER:OG	1:B:523:THR:N	2.36	0.57
1:B:441:ASN:O	1:B:445:ASN:ND2	2.38	0.57
1:B:488:THR:O	1:B:518:ARG:HA	2.04	0.57
1:A:87:ARG:HH21	1:A:176:ASP:CB	2.16	0.57
1:B:395:ILE:CD1	1:B:514:VAL:HG11	2.34	0.57
1:B:56:ASP:C	1:B:56:ASP:OD2	2.42	0.57
1:B:606:LYS:CA	1:B:609:GLU:HB2	2.20	0.57
1:B:182:ARG:HD2	1:B:182:ARG:N	2.20	0.57
1:B:404:ASN:O	1:B:407:ILE:CG2	2.52	0.57
1:A:454:LEU:HB3	1:A:456:LEU:HD13	1.87	0.57
1:A:531:LEU:O	1:A:535:THR:HB	2.04	0.57
1:B:105:TYR:HD1	1:B:106:TYR:N	2.03	0.57
1:B:169:VAL:CG1	1:B:170:THR:H	2.13	0.57
1:B:453:GLU:CB	1:B:454:LEU:HD22	2.34	0.57
1:B:429:ASP:O	1:B:430:LYS:HB2	2.04	0.57
1:A:323:LEU:O	1:A:324:ASP:O	2.23	0.57
1:A:427:PRO:O	1:A:467:PHE:O	2.22	0.57
1:B:422:LEU:HD23	1:B:447:LEU:CD1	2.35	0.56
1:A:4:ILE:N	1:A:16:PHE:O	2.39	0.56
1:B:604:GLY:O	1:B:608:VAL:HG23	2.05	0.56
1:A:617:GLN:O	1:A:618:TYR:C	2.43	0.56
1:B:404:ASN:O	1:B:407:ILE:HG22	2.04	0.56
1:B:570:LYS:C	1:B:572:GLN:H	2.08	0.56
1:A:110:ILE:HG22	1:A:112:GLN:N	2.20	0.56
1:A:399:PHE:O	1:A:402:VAL:CG1	2.52	0.56
1:A:423:SER:HB3	1:A:464:GLU:HB2	1.88	0.56
1:B:353:LEU:CD1	1:B:353:LEU:O	2.45	0.56
1:A:304:TYR:HE2	1:A:337:PRO:HG3	1.70	0.56
1:A:566:GLN:NE2	1:A:578:ILE:HG13	2.21	0.56
1:B:83:HIS:ND1	1:B:177:PHE:HB2	2.21	0.56
1:B:403:VAL:C	5:B:2026:HOH:O	2.43	0.56
1:B:565:LEU:HD21	1:B:601:ILE:HG21	1.87	0.56
1:B:601:ILE:HG22	1:B:601:ILE:O	2.03	0.56
1:B:86:LYS:O	1:B:86:LYS:HG2	2.05	0.56
1:B:386:SER:HB2	1:B:518:ARG:NH1	2.20	0.56
1:B:492:ASP:OD2	1:B:492:ASP:C	2.43	0.56
1:A:351:ARG:HH22	1:B:580:ASP:HB3	1.70	0.56
1:A:97:GLY:HA2	1:A:105:TYR:O	2.06	0.56
1:B:98:PRO:HD2	1:B:105:TYR:CZ	2.41	0.56
1:B:496:PRO:HG3	1:B:515:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD11	1:A:220:THR:OG1	2.05	0.56
1:A:312:HIS:ND1	1:A:427:PRO:HB2	2.20	0.56
1:A:163:ILE:N	1:A:164:PRO:HD3	2.21	0.56
1:A:122:ILE:O	1:A:126:MET:HG2	2.06	0.55
1:A:279:ARG:HH11	1:A:279:ARG:HG3	1.70	0.55
1:A:436:ASP:CB	1:A:439:MET:HB3	2.34	0.55
1:A:617:GLN:HG2	1:A:623:GLN:CD	2.27	0.55
1:B:229:LYS:HA	1:B:229:LYS:HE2	1.88	0.55
1:B:621:GLN:O	1:B:623:GLN:N	2.34	0.55
1:A:254:THR:HG22	1:A:255:ASN:O	2.06	0.55
1:B:416:GLU:CD	1:B:416:GLU:O	2.44	0.55
1:B:558:HIS:CD2	1:B:604:GLY:HA2	2.42	0.55
1:B:336:CYS:HB2	1:B:337:PRO:CD	2.35	0.55
1:A:428:GLU:HB3	1:A:440:TRP:HE1	1.71	0.55
1:B:338:HIS:HD2	5:B:2007:HOH:O	1.89	0.55
1:B:4:ILE:HG22	1:B:16:PHE:H	1.70	0.55
1:B:144:ASP:HA	1:B:147:LYS:HG3	1.89	0.55
1:B:195:PHE:N	1:B:195:PHE:HD1	2.05	0.55
1:B:471:LYS:HD3	1:B:490:GLN:NE2	2.22	0.55
1:B:496:PRO:HG3	1:B:515:VAL:HG23	1.89	0.55
1:B:520:VAL:HG12	1:B:521:VAL:N	2.21	0.55
1:A:214:LEU:N	1:A:214:LEU:HD12	2.22	0.55
1:A:399:PHE:O	1:A:402:VAL:HG13	2.07	0.55
1:A:81:MET:HE2	1:A:104:PHE:HE2	1.72	0.55
1:B:490:GLN:CG	1:B:517:HIS:HB2	2.33	0.55
1:B:604:GLY:H	1:B:607:GLU:CB	2.18	0.55
1:A:163:ILE:HG22	1:A:163:ILE:O	2.07	0.54
1:A:322:GLN:HB3	1:A:327:GLU:O	2.07	0.54
1:A:494:LEU:HD11	1:A:498:ARG:HD3	1.90	0.54
1:A:622:ASP:C	1:A:624:GLU:N	2.59	0.54
1:A:89:TYR:O	1:A:92:VAL:HG23	2.07	0.54
1:A:467:PHE:CD1	1:A:467:PHE:C	2.80	0.54
1:B:110:ILE:HG22	1:B:111:ASP:H	1.71	0.54
1:B:83:HIS:CG	1:B:177:PHE:HB2	2.43	0.54
1:B:195:PHE:N	1:B:195:PHE:CD1	2.75	0.54
1:B:621:GLN:O	1:B:623:GLN:HG3	2.07	0.54
1:A:152:ASN:H	1:A:152:ASN:ND2	2.05	0.54
1:B:303:LEU:HD11	1:B:337:PRO:HB2	1.88	0.54
1:B:548:VAL:O	1:B:576:VAL:HG23	2.07	0.54
1:B:592:ALA:HB3	1:B:600:GLN:NE2	2.19	0.54
1:A:157:LEU:C	1:A:159:LEU:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASP:OD2	1:B:438:ASP:HB3	2.08	0.54
1:B:100:ILE:HG22	1:B:101:GLU:N	2.22	0.54
1:B:169:VAL:CG1	1:B:170:THR:N	2.71	0.54
1:B:304:TYR:HA	1:B:307:SER:OG	2.08	0.54
1:B:323:LEU:HD12	1:B:329:MET:CG	2.34	0.54
1:B:440:TRP:CE3	1:B:440:TRP:HA	2.42	0.54
1:B:523:THR:HG22	1:B:526:ARG:H	1.73	0.54
1:A:150:PHE:O	1:A:157:LEU:HD13	2.07	0.54
1:B:312:HIS:O	1:B:314:GLN:N	2.41	0.54
1:B:41:LYS:HB3	1:B:60:GLU:HB2	1.88	0.54
1:B:442:LYS:HZ1	1:B:446:MET:HB2	1.71	0.54
1:A:304:TYR:CE2	1:A:337:PRO:HG3	2.43	0.54
1:B:159:LEU:O	1:B:159:LEU:HD13	2.08	0.54
1:B:535:THR:O	1:B:536:LYS:HB2	2.07	0.54
1:A:93:LYS:HD3	1:A:155:TYR:CE1	2.38	0.54
1:A:42:PHE:CD2	1:A:53:LEU:HD22	2.43	0.54
1:B:404:ASN:ND2	1:B:404:ASN:O	2.41	0.54
1:A:59:ILE:HG13	1:A:60:GLU:H	1.74	0.53
1:B:566:GLN:HG3	1:B:576:VAL:HG13	1.90	0.53
1:B:407:ILE:HG23	1:B:408:ASP:H	1.74	0.53
1:B:472:LEU:O	1:B:472:LEU:HG	2.07	0.53
1:B:146:ALA:O	1:B:148:GLU:N	2.40	0.53
1:B:274:ARG:O	1:B:278:GLU:HG3	2.08	0.53
1:B:339:HIS:ND1	1:B:387:HIS:ND1	2.53	0.53
1:B:426:ASP:OD2	1:B:427:PRO:HD2	2.08	0.53
1:B:512:ARG:NH1	1:B:512:ARG:HG3	2.23	0.53
1:B:125:THR:C	1:B:127:LYS:N	2.59	0.53
1:B:200:THR:O	1:B:201:ALA:O	2.26	0.53
1:A:395:ILE:HG21	1:A:491:LEU:HD21	1.90	0.53
1:A:521:VAL:HG13	1:A:521:VAL:O	2.08	0.53
1:A:43:ASN:ND2	1:A:58:SER:H	2.07	0.53
1:B:143:ARG:HB2	1:B:168:ASN:HA	1.90	0.53
1:A:323:LEU:CG	1:A:323:LEU:O	2.56	0.53
1:B:212:LYS:HD2	1:B:212:LYS:N	2.21	0.53
1:B:299:ALA:HB1	1:B:303:LEU:HD23	1.90	0.53
1:B:406:ILE:CD1	1:B:487:SER:HB3	2.38	0.53
1:B:436:ASP:OD2	1:B:439:MET:HG2	2.08	0.53
1:B:472:LEU:O	1:B:473:ASP:O	2.27	0.53
1:B:395:ILE:HD11	1:B:514:VAL:HG21	1.90	0.53
1:A:210:ASN:HD22	1:A:210:ASN:N	2.06	0.53
1:B:144:ASP:OD1	1:B:147:LYS:HE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:LYS:O	1:B:610:ASN:OD1	2.27	0.53
1:B:611:ASN:H	1:B:611:ASN:HD22	1.57	0.53
1:B:205:TRP:C	1:B:205:TRP:CE3	2.83	0.53
1:B:7:GLN:N	1:B:57:GLY:O	2.35	0.53
1:A:133:ASN:HD22	1:A:189:THR:HG22	1.73	0.53
1:A:589:ILE:HG23	1:A:600:GLN:HE22	1.74	0.53
1:B:139:LYS:HG2	1:B:140:VAL:N	2.23	0.53
1:B:593:GLN:HG3	1:B:600:GLN:HE22	1.74	0.53
1:A:123:GLU:HA	1:A:126:MET:HG2	1.91	0.52
1:A:86:LYS:HD3	1:A:177:PHE:HD1	1.74	0.52
1:A:368:ALA:HA	5:B:2010:HOH:O	2.09	0.52
1:A:264:PRO:HG3	1:A:375:LEU:HD23	1.90	0.52
1:A:59:ILE:HG13	1:A:60:GLU:N	2.25	0.52
1:B:391:ARG:HD3	1:B:503:TYR:CE2	2.44	0.52
1:B:540:PRO:HG2	1:B:543:LEU:HD12	1.91	0.52
1:A:455:GLY:O	1:A:456:LEU:HD12	2.09	0.52
1:B:532:THR:HG1	1:B:539:PHE:HZ	1.56	0.52
1:A:304:TYR:HE2	1:A:337:PRO:CG	2.21	0.52
1:A:428:GLU:HG3	1:A:440:TRP:HE1	1.72	0.52
1:B:323:LEU:CD1	1:B:329:MET:HG3	2.35	0.52
1:B:407:ILE:HG23	1:B:408:ASP:N	2.25	0.52
1:B:641:LEU:O	1:B:642:LYS:HB2	2.10	0.52
1:B:74:ARG:O	1:B:76:SER:N	2.42	0.52
1:A:386:SER:HB3	1:A:518:ARG:HD2	1.90	0.52
1:B:144:ASP:HA	1:B:147:LYS:HE2	1.92	0.52
1:B:159:LEU:HD21	1:B:162:ALA:HB3	1.91	0.52
1:B:390:VAL:CG1	1:B:394:GLN:HB2	2.39	0.52
1:B:542:TRP:CH2	1:B:543:LEU:HD21	2.45	0.52
1:A:478:THR:HG22	1:A:479:ALA:N	2.24	0.52
1:B:521:VAL:O	1:B:522:SER:HB3	2.09	0.52
1:B:428:GLU:HG2	1:B:429:ASP:N	2.25	0.52
1:A:433:TYR:CZ	1:A:434:PHE:HB2	2.45	0.51
1:B:617:GLN:NE2	1:B:645:ARG:HD3	2.16	0.51
1:A:68:GLU:HA	1:A:71:GLU:HG3	1.92	0.51
1:B:404:ASN:C	1:B:407:ILE:HG22	2.30	0.51
1:B:444:GLU:HB2	1:B:448:LYS:CE	2.33	0.51
1:B:251:GLU:O	1:B:269:ASN:HB2	2.10	0.51
1:A:490:GLN:O	1:A:516:ILE:HA	2.11	0.51
1:A:544:ALA:O	1:A:575:ARG:NH1	2.43	0.51
1:B:80:LEU:HD11	1:B:129:ILE:CG2	2.41	0.51
1:B:335:ASN:HB2	1:B:385:ASP:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LYS:O	1:B:435:ASP:N	2.44	0.51
1:B:542:TRP:CZ2	1:B:543:LEU:HD21	2.46	0.51
1:B:80:LEU:CD1	1:B:129:ILE:HD13	2.40	0.51
1:A:157:LEU:C	1:A:159:LEU:N	2.63	0.51
1:B:564:GLN:O	1:B:568:GLU:HG3	2.11	0.51
1:A:7:GLN:HE22	1:A:11:GLY:HA2	1.76	0.51
1:A:424:TYR:C	1:A:462:ILE:HD12	2.31	0.50
1:B:213:MET:HE3	1:B:213:MET:HA	1.93	0.50
1:A:7:GLN:HG2	1:A:13:LYS:HD2	1.92	0.50
1:B:105:TYR:CD1	1:B:106:TYR:N	2.79	0.50
1:B:415:PHE:CZ	1:B:530:PHE:CE2	2.99	0.50
1:B:200:THR:O	1:B:200:THR:HG22	2.10	0.50
1:A:392:PRO:O	1:A:395:ILE:HG13	2.11	0.50
1:A:79:HIS:CD2	1:A:185:HIS:NE2	2.79	0.50
1:A:312:HIS:CE1	1:A:428:GLU:O	2.65	0.50
1:A:555:VAL:HG23	1:A:555:VAL:O	2.12	0.50
1:A:579:ASP:OD2	1:A:588:LYS:HE2	2.11	0.50
1:A:643:LYS:HG2	1:A:644:HIS:N	2.27	0.50
1:A:8:PHE:HB3	1:A:9:PRO:HD2	1.93	0.50
1:B:478:THR:O	1:B:480:MET:N	2.45	0.50
1:B:497:GLU:HA	1:B:512:ARG:HE	1.76	0.50
1:B:484:GLU:HB3	1:B:526:ARG:HD3	1.93	0.50
1:B:277:ILE:HD13	1:B:527:PHE:CD2	2.47	0.50
1:A:156:LYS:HE2	1:A:179:ASP:OD2	2.12	0.50
1:A:494:LEU:O	1:A:497:GLU:HB2	2.12	0.50
1:A:566:GLN:NE2	1:A:577:SER:HA	2.26	0.50
1:B:299:ALA:CB	1:B:303:LEU:HD23	2.41	0.50
1:B:439:MET:HE1	1:B:494:LEU:HB2	1.94	0.50
1:B:499:PHE:HB3	1:B:501:LEU:HD21	1.93	0.50
1:A:143:ARG:CZ	1:A:163:ILE:HG23	2.42	0.50
1:A:143:ARG:N	1:A:169:VAL:HG22	2.25	0.50
1:A:67:GLU:O	1:A:71:GLU:HG2	2.12	0.50
1:B:254:THR:CG2	1:B:267:LEU:HD11	2.42	0.50
1:B:559:TYR:HE2	1:B:563:ARG:CG	2.22	0.50
1:A:143:ARG:HD3	1:A:163:ILE:HG12	1.93	0.50
1:B:187:PRO:HD2	1:B:191:LYS:HD2	1.94	0.50
1:B:404:ASN:HD22	1:B:407:ILE:HG21	1.77	0.50
1:A:153:ASP:CB	1:A:156:LYS:HB2	2.39	0.50
1:A:399:PHE:HE2	1:A:472:LEU:HD12	1.77	0.50
1:A:294:TYR:HB2	1:B:266:TRP:HB2	1.92	0.50
1:B:403:VAL:HA	1:B:406:ILE:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:TYR:HE1	1:B:512:ARG:O	1.95	0.50
1:A:525:GLU:H	1:A:525:GLU:CD	2.14	0.49
1:A:637:ASP:O	1:A:641:LEU:HB2	2.11	0.49
1:B:550:ILE:CD1	1:B:565:LEU:HD23	2.42	0.49
1:A:274:ARG:O	1:A:278:GLU:HG3	2.13	0.49
1:A:428:GLU:OE1	1:A:435:ASP:CB	2.59	0.49
1:B:163:ILE:HG12	1:B:163:ILE:O	2.12	0.49
1:B:312:HIS:CD2	1:B:427:PRO:HB2	2.47	0.49
1:A:426:ASP:CB	1:A:427:PRO:HD2	2.22	0.49
1:B:42:PHE:CB	1:B:47:VAL:HG11	2.42	0.49
1:B:521:VAL:O	1:B:521:VAL:HG12	2.11	0.49
1:B:643:LYS:NZ	1:B:645:ARG:HD2	2.28	0.49
1:A:257:GLN:HG3	1:A:258:LEU:N	2.28	0.49
1:B:419:SER:C	1:B:420:PHE:CD1	2.86	0.49
1:A:155:TYR:HD2	1:A:205:TRP:CE2	2.30	0.49
1:A:326:THR:HG22	1:A:327:GLU:CG	2.42	0.49
1:B:41:LYS:HD2	1:B:60:GLU:CD	2.32	0.49
1:B:442:LYS:CE	1:B:446:MET:HB2	2.42	0.49
1:B:499:PHE:HB3	1:B:501:LEU:CD2	2.42	0.49
1:B:7:GLN:HA	1:B:13:LYS:CB	2.43	0.49
1:A:376:GLN:HE22	1:A:526:ARG:HD2	1.76	0.49
1:B:336:CYS:CA	1:B:387:HIS:CE1	2.94	0.49
1:B:443:ALA:HA	1:B:493:PHE:HE2	1.77	0.49
1:B:545:PRO:O	1:B:575:ARG:HD2	2.12	0.49
1:B:585:MET:CE	1:B:589:ILE:HD11	2.42	0.49
1:A:194:GLU:HB2	1:A:222:PHE:O	2.12	0.49
1:B:550:ILE:HD13	1:B:565:LEU:HD23	1.95	0.49
1:A:205:TRP:HB3	1:A:211:ASN:HB3	1.94	0.49
1:A:391:ARG:NH1	1:A:393:ASP:OD2	2.45	0.49
1:B:171:LEU:HD21	1:B:178:THR:CG2	2.43	0.49
1:B:424:TYR:N	1:B:424:TYR:CD1	2.80	0.49
1:B:386:SER:HB3	1:B:518:ARG:CG	2.43	0.49
1:B:616:ARG:CZ	1:B:622:ASP:HB3	2.43	0.49
1:A:143:ARG:H	1:A:169:VAL:CG2	2.25	0.49
1:A:4:ILE:HG13	1:A:56:ASP:CA	2.42	0.49
1:A:583:GLU:HG3	1:A:587:TYR:CE2	2.47	0.49
1:B:4:ILE:HG12	1:B:56:ASP:HB2	1.94	0.49
1:A:194:GLU:OE2	1:A:225:LYS:HE3	2.12	0.48
1:A:540:PRO:HG2	1:A:543:LEU:HD12	1.95	0.48
1:B:391:ARG:HB2	1:B:394:GLN:HG3	1.95	0.48
1:A:160:ILE:HD11	1:A:169:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:O	1:A:285:GLU:HG3	2.13	0.48
1:A:353:LEU:HD13	1:A:353:LEU:O	2.13	0.48
1:A:385:ASP:OD2	1:A:386:SER:N	2.46	0.48
1:A:593:GLN:HE22	1:A:616:ARG:NH1	2.11	0.48
1:B:1:MET:O	1:B:2:GLU:HG2	2.13	0.48
1:B:521:VAL:O	1:B:521:VAL:CG1	2.60	0.48
1:B:610:ASN:OD1	1:B:610:ASN:N	2.46	0.48
1:A:110:ILE:C	1:A:112:GLN:H	2.16	0.48
1:A:616:ARG:NH1	1:A:619:GLY:N	2.56	0.48
1:B:125:THR:O	1:B:128:GLN:N	2.35	0.48
1:B:494:LEU:CD1	1:B:498:ARG:HG3	2.44	0.48
1:A:157:LEU:CA	1:A:160:ILE:HG22	2.42	0.48
1:B:59:ILE:H	1:B:59:ILE:HD12	1.78	0.48
1:A:290:TYR:HA	1:A:356:ARG:HB2	1.95	0.48
1:B:173:SER:OG	1:B:174:GLN:N	2.47	0.48
1:B:262:GLY:CA	1:B:372:VAL:HG13	2.42	0.48
1:A:263:LEU:O	1:B:296:PRO:HG2	2.14	0.48
1:B:395:ILE:HD11	1:B:514:VAL:CG1	2.42	0.48
1:B:563:ARG:HG3	1:B:563:ARG:NH1	2.25	0.48
1:B:635:LEU:O	1:B:638:GLU:N	2.47	0.48
1:A:596:LYS:HD3	1:A:618:TYR:CZ	2.48	0.48
1:A:262:GLY:O	1:A:263:LEU:HD23	2.13	0.48
1:B:277:ILE:HD13	1:B:527:PHE:HD2	1.78	0.48
1:B:241:ARG:HH22	1:B:536:LYS:HZ2	1.61	0.48
1:B:561:TYR:HD2	1:B:603:VAL:CG1	2.26	0.48
1:B:92:VAL:HB	1:B:110:ILE:CD1	2.43	0.48
1:A:319:PRO:HA	1:A:320:PRO:HD3	1.67	0.48
1:A:396:LYS:HE2	1:A:449:GLU:HB2	1.96	0.48
1:A:517:HIS:HB3	4:A:1004:THR:OG1	2.14	0.48
1:A:610:ASN:CB	1:A:612:GLN:NE2	2.73	0.48
1:B:229:LYS:CA	1:B:229:LYS:HE2	2.43	0.48
1:A:389:PHE:N	1:A:389:PHE:CD1	2.81	0.48
1:A:409:VAL:O	1:A:412:ASP:HB2	2.14	0.48
1:A:384:ASN:ND2	1:A:521:VAL:H	2.09	0.48
1:B:126:MET:HE2	1:B:195:PHE:HE2	1.79	0.48
1:B:180:LEU:HD23	1:B:180:LEU:C	2.34	0.48
1:B:536:LYS:O	1:B:596:LYS:NZ	2.47	0.48
1:A:222:PHE:HZ	1:A:231:HIS:CD2	2.31	0.48
1:A:38:VAL:HG21	1:A:223:PHE:HZ	1.79	0.48
1:A:610:ASN:O	1:A:611:ASN:C	2.51	0.48
1:B:622:ASP:O	1:B:623:GLN:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:O	1:A:35:LYS:HG3	2.14	0.47
1:A:38:VAL:HG21	1:A:223:PHE:CZ	2.49	0.47
1:A:189:THR:HG21	5:A:1028:HOH:O	2.14	0.47
1:A:322:GLN:CG	1:A:327:GLU:HB2	2.35	0.47
1:B:368:ALA:C	1:B:370:GLY:H	2.16	0.47
1:B:398:GLU:O	1:B:401:ARG:N	2.39	0.47
1:B:439:MET:O	1:B:443:ALA:N	2.47	0.47
1:B:585:MET:O	1:B:589:ILE:CD1	2.62	0.47
1:A:142:SER:O	1:A:143:ARG:HB3	2.13	0.47
1:B:428:GLU:H	1:B:428:GLU:CD	2.18	0.47
1:B:472:LEU:O	1:B:472:LEU:CG	2.63	0.47
1:B:487:SER:HA	1:B:519:GLY:O	2.14	0.47
1:A:589:ILE:HG22	1:A:590:ARG:N	2.29	0.47
1:A:63:THR:HB	1:A:64:PRO:HD2	1.96	0.47
1:B:386:SER:CB	1:B:518:ARG:NH1	2.78	0.47
1:B:559:TYR:HD2	1:B:559:TYR:C	2.18	0.47
1:A:143:ARG:HD3	1:A:163:ILE:CD1	2.44	0.47
1:A:353:LEU:HD22	1:A:353:LEU:HA	1.55	0.47
1:A:616:ARG:HH12	1:A:619:GLY:N	2.11	0.47
1:B:187:PRO:CG	1:B:191:LYS:HD2	2.43	0.47
1:B:433:TYR:C	1:B:435:ASP:N	2.63	0.47
1:A:154:GLU:HG3	1:A:155:TYR:CD1	2.50	0.47
1:A:195:PHE:HA	1:A:221:ALA:HA	1.96	0.47
1:A:54:GLU:OE1	1:A:54:GLU:HA	2.15	0.47
1:B:7:GLN:HA	1:B:13:LYS:HB3	1.97	0.47
1:B:174:GLN:HG3	1:B:174:GLN:O	2.14	0.47
1:B:450:ALA:CA	1:B:453:GLU:HG2	2.41	0.47
1:B:70:LEU:C	1:B:72:VAL:N	2.66	0.47
1:B:8:PHE:N	1:B:8:PHE:CD1	2.83	0.47
1:B:136:ILE:HD12	1:B:136:ILE:N	2.28	0.47
1:B:604:GLY:N	1:B:607:GLU:HB2	2.26	0.47
1:B:620:SER:O	1:B:621:GLN:C	2.53	0.47
1:B:196:LYS:O	1:B:220:THR:N	2.40	0.47
1:B:204:TYR:HA	1:B:214:LEU:HG	1.96	0.47
1:B:476:VAL:CG1	1:B:484:GLU:HB2	2.45	0.47
1:B:75:HIS:O	1:B:75:HIS:CD2	2.68	0.47
1:B:8:PHE:C	1:B:10:ASP:H	2.17	0.47
1:A:429:ASP:O	1:A:430:LYS:HB2	2.14	0.47
1:B:181:CYS:SG	1:B:185:HIS:NE2	2.85	0.47
1:B:205:TRP:N	1:B:214:LEU:HG	2.25	0.47
1:A:279:ARG:NH1	1:A:279:ARG:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLN:NE2	1:A:526:ARG:HD2	2.30	0.46
1:A:398:GLU:OE1	1:A:401:ARG:NH2	2.42	0.46
1:B:518:ARG:CG	1:B:518:ARG:NH1	2.63	0.46
1:B:559:TYR:CD2	1:B:559:TYR:C	2.88	0.46
1:A:108:PHE:O	1:A:214:LEU:HB3	2.14	0.46
1:B:7:GLN:CB	1:B:13:LYS:HB3	2.45	0.46
1:B:389:PHE:N	1:B:389:PHE:CD1	2.84	0.46
1:B:509:GLU:O	1:B:511:HIS:ND1	2.48	0.46
1:B:644:HIS:O	1:B:645:ARG:CG	2.63	0.46
1:A:360:LEU:HB2	5:A:1088:HOH:O	2.16	0.46
1:A:464:GLU:OE1	1:A:464:GLU:HA	2.15	0.46
1:B:210:ASN:ND2	1:B:210:ASN:O	2.48	0.46
1:B:241:ARG:NH2	1:B:536:LYS:HZ2	2.13	0.46
1:A:119:PHE:O	1:A:123:GLU:HB2	2.16	0.46
1:A:518:ARG:O	1:A:518:ARG:HD3	2.15	0.46
1:B:129:ILE:HD11	1:B:189:THR:HG21	1.97	0.46
1:B:355:ILE:HG13	1:B:356:ARG:N	2.30	0.46
1:B:617:GLN:O	1:B:618:TYR:C	2.54	0.46
1:A:157:LEU:O	1:A:159:LEU:N	2.48	0.46
1:A:42:PHE:O	1:A:43:ASN:HB2	2.14	0.46
1:A:70:LEU:HD13	1:A:74:ARG:NH2	2.31	0.46
1:A:7:GLN:HG2	1:A:13:LYS:HD3	1.97	0.46
1:A:92:VAL:HG12	1:A:93:LYS:O	2.16	0.46
1:B:114:ILE:HD12	1:B:217:ILE:CD1	2.40	0.46
1:B:204:TYR:O	1:B:205:TRP:C	2.53	0.46
1:B:521:VAL:HG13	1:B:527:PHE:CD2	2.51	0.46
1:B:56:ASP:OD2	1:B:56:ASP:O	2.32	0.46
1:B:415:PHE:CZ	1:B:530:PHE:HE2	2.34	0.46
1:B:123:GLU:C	1:B:125:THR:H	2.19	0.46
1:B:167:GLU:C	1:B:168:ASN:ND2	2.68	0.46
1:B:418:TYR:CD2	1:B:418:TYR:N	2.65	0.46
1:B:470:PRO:O	1:B:490:GLN:HB2	2.16	0.46
1:A:467:PHE:CD1	1:A:468:TYR:N	2.84	0.46
1:B:146:ALA:C	1:B:148:GLU:N	2.69	0.46
1:B:159:LEU:CD1	1:B:162:ALA:HB3	2.45	0.46
1:B:42:PHE:HB3	1:B:47:VAL:HG11	1.97	0.46
1:B:474:VAL:O	1:B:485:THR:HA	2.16	0.46
1:B:515:VAL:O	1:B:515:VAL:HG12	2.14	0.46
1:A:456:LEU:O	1:A:458:TYR:CD2	2.68	0.46
1:B:214:LEU:N	1:B:214:LEU:HD22	2.30	0.46
1:B:471:LYS:HB2	1:B:472:LEU:H	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:PRO:HA	1:B:618:TYR:HB2	1.98	0.46
1:B:363:MET:HA	5:B:2022:HOH:O	2.15	0.45
1:B:390:VAL:CG1	1:B:391:ARG:H	2.23	0.45
1:B:420:PHE:CD2	1:B:474:VAL:HG22	2.51	0.45
1:B:74:ARG:C	1:B:76:SER:N	2.68	0.45
1:A:40:GLY:O	1:A:47:VAL:HG22	2.16	0.45
1:A:428:GLU:O	1:A:435:ASP:OD2	2.35	0.45
1:B:245:LYS:HD3	1:B:245:LYS:HA	1.86	0.45
1:B:430:LYS:HD3	1:B:439:MET:SD	2.56	0.45
1:A:80:LEU:CD2	1:A:192:ILE:HG21	2.46	0.45
1:A:224:ASP:N	1:A:224:ASP:OD1	2.49	0.45
1:B:206:ARG:HG3	1:B:208:ASP:OD1	2.17	0.45
1:B:213:MET:HA	1:B:213:MET:CE	2.46	0.45
1:B:394:GLN:O	1:B:396:LYS:N	2.49	0.45
1:B:523:THR:HG22	1:B:526:ARG:CB	2.43	0.45
1:B:616:ARG:NH1	1:B:622:ASP:CB	2.71	0.45
1:A:424:TYR:CE2	1:A:444:GLU:HB3	2.52	0.45
1:B:105:TYR:O	1:B:106:TYR:HB2	2.15	0.45
1:B:7:GLN:O	1:B:58:SER:CA	2.64	0.45
1:B:641:LEU:O	1:B:642:LYS:CB	2.62	0.45
1:A:526:ARG:NH2	3:A:1003:ATP:H2'	2.30	0.45
1:A:210:ASN:ND2	1:A:210:ASN:N	2.64	0.45
1:A:229:LYS:O	1:A:233:GLN:HG3	2.17	0.45
1:A:97:GLY:HA2	1:A:106:TYR:HA	1.99	0.45
1:B:194:GLU:OE1	1:B:225:LYS:HG3	2.17	0.45
1:B:439:MET:CE	1:B:494:LEU:HB2	2.46	0.45
1:B:80:LEU:CD1	1:B:129:ILE:HG21	2.46	0.45
1:B:88:LEU:O	1:B:88:LEU:HG	2.16	0.45
1:A:423:SER:HB3	1:A:464:GLU:CB	2.46	0.45
1:B:402:VAL:CG2	1:B:403:VAL:N	2.79	0.45
1:B:443:ALA:O	1:B:447:LEU:CB	2.59	0.45
1:A:523:THR:HG21	3:A:1003:ATP:N3	2.32	0.45
1:A:282:VAL:CG2	1:A:360:LEU:CD2	2.95	0.45
1:A:282:VAL:CG2	1:A:360:LEU:HD21	2.46	0.45
1:B:607:GLU:C	5:B:2040:HOH:O	2.54	0.45
1:A:349:SER:O	1:A:352:GLU:HG2	2.17	0.45
1:A:476:VAL:CG1	1:A:530:PHE:CE1	2.99	0.45
1:A:498:ARG:HG2	1:A:498:ARG:H	1.47	0.45
1:A:606:LYS:CE	1:A:625:THR:HG21	2.47	0.45
1:B:395:ILE:HD13	1:B:491:LEU:CD2	2.46	0.45
1:A:142:SER:O	1:A:143:ARG:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:MET:CA	1:B:126:MET:HE3	2.47	0.45
1:B:406:ILE:CD1	1:B:487:SER:CB	2.94	0.45
1:B:569:LEU:HD22	1:B:574:VAL:HG21	1.98	0.45
1:B:587:TYR:CD1	1:B:587:TYR:C	2.90	0.45
1:B:597:ILE:O	1:B:597:ILE:HG22	2.17	0.45
1:A:364:HIS:CD2	1:A:380:GLY:HA2	2.52	0.45
1:A:473:ASP:HB3	1:A:475:GLN:NE2	2.32	0.45
1:A:606:LYS:HE3	1:A:625:THR:HG21	1.99	0.45
1:A:6:ILE:O	1:A:13:LYS:HA	2.17	0.45
1:B:113:ASN:O	1:B:114:ILE:HG23	2.17	0.45
1:B:589:ILE:O	1:B:600:GLN:NE2	2.50	0.45
1:A:321:MET:O	1:A:321:MET:CG	2.64	0.44
1:B:561:TYR:CD2	1:B:608:VAL:HG22	2.53	0.44
1:B:82:ALA:HB2	1:B:106:TYR:CD1	2.50	0.44
1:B:595:GLN:HB3	1:B:597:ILE:HD13	1.98	0.44
1:B:70:LEU:C	1:B:72:VAL:H	2.21	0.44
1:A:88:LEU:HD11	1:A:125:THR:OG1	2.17	0.44
1:B:186:VAL:HG13	1:B:187:PRO:N	2.32	0.44
1:B:439:MET:O	1:B:443:ALA:HB2	2.17	0.44
1:B:494:LEU:HD12	1:B:498:ARG:HG3	1.99	0.44
1:B:570:LYS:C	1:B:572:GLN:N	2.70	0.44
1:A:81:MET:CE	1:A:104:PHE:HE2	2.31	0.44
1:A:422:LEU:HD12	1:A:458:TYR:CE1	2.53	0.44
1:A:439:MET:HE2	1:A:494:LEU:N	2.33	0.44
1:A:36:LYS:HG2	1:A:64:PRO:HD2	1.98	0.44
1:B:419:SER:O	1:B:474:VAL:HG13	2.17	0.44
1:B:186:VAL:HG11	1:B:191:LYS:HB3	1.99	0.44
1:B:236:GLU:C	1:B:238:ARG:N	2.71	0.44
1:B:420:PHE:CE1	1:B:474:VAL:HG13	2.52	0.44
1:B:587:TYR:HD1	1:B:587:TYR:C	2.20	0.44
1:A:336:CYS:SG	4:A:1004:THR:N	2.91	0.44
1:A:4:ILE:HD11	1:A:56:ASP:N	2.32	0.44
1:B:81:MET:HA	1:B:126:MET:HE3	2.00	0.44
1:B:166:ASP:O	1:B:167:GLU:HG3	2.18	0.44
1:B:470:PRO:O	1:B:490:GLN:CB	2.66	0.44
1:B:21:THR:HB	1:B:49:LEU:O	2.18	0.44
1:A:472:LEU:C	1:A:472:LEU:HD23	2.38	0.44
1:A:566:GLN:HE21	1:A:577:SER:HA	1.83	0.44
1:B:186:VAL:HG13	1:B:187:PRO:CD	2.47	0.44
1:B:309:HIS:CE1	1:B:467:PHE:CD2	3.06	0.44
1:B:402:VAL:C	1:B:404:ASN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD11	1:A:56:ASP:H	1.83	0.44
1:B:275:ARG:HD2	5:B:2006:HOH:O	2.18	0.44
1:B:570:LYS:O	1:B:572:GLN:N	2.51	0.44
1:A:14:LYS:HE3	1:A:16:PHE:CE1	2.52	0.44
1:A:303:LEU:HG	1:A:337:PRO:HB2	2.00	0.44
1:A:354:PRO:HD3	1:A:394:GLN:HE22	1.83	0.44
1:A:582:ASN:ND2	1:A:582:ASN:C	2.71	0.44
1:A:637:ASP:OD2	1:A:640:ARG:NH2	2.50	0.44
1:B:177:PHE:CD2	1:B:178:THR:N	2.85	0.44
1:B:194:GLU:HG3	1:B:224:ASP:C	2.38	0.44
1:B:523:THR:HG23	1:B:525:GLU:N	2.33	0.44
1:B:601:ILE:HG13	1:B:613:VAL:HB	1.99	0.44
1:B:94:PHE:HE2	5:B:2021:HOH:O	2.00	0.44
1:A:117:ASP:N	1:A:117:ASP:OD1	2.49	0.43
1:A:158:GLU:CB	1:A:206:ARG:HH21	2.29	0.43
1:B:365:ARG:HG2	1:B:365:ARG:HH11	1.82	0.43
1:B:535:THR:HB	1:B:538:ALA:O	2.18	0.43
1:B:644:HIS:O	1:B:645:ARG:CB	2.66	0.43
1:A:576:VAL:HG22	1:A:577:SER:N	2.32	0.43
1:B:186:VAL:CG1	1:B:191:LYS:HB3	2.49	0.43
3:B:2003:ATP:C5'	4:B:2004:THR:OXT	2.66	0.43
1:B:366:TYR:CD1	1:B:366:TYR:C	2.91	0.43
1:B:558:HIS:O	1:B:559:TYR:C	2.57	0.43
1:B:637:ASP:OD2	1:B:641:LEU:HD23	2.18	0.43
1:A:399:PHE:O	1:A:402:VAL:HG12	2.17	0.43
1:A:243:HIS:HB3	1:A:533:GLU:HG3	2.00	0.43
1:A:559:TYR:OH	1:A:563:ARG:NH1	2.45	0.43
1:B:467:PHE:HD2	1:B:468:TYR:HD1	1.66	0.43
1:B:531:LEU:HD21	1:B:543:LEU:HD13	2.01	0.43
1:A:146:ALA:O	1:A:147:LYS:C	2.56	0.43
1:A:497:GLU:CD	1:A:512:ARG:HH11	2.22	0.43
1:B:17:ASP:O	1:B:20:THR:OG1	2.28	0.43
4:B:2004:THR:N	5:B:2016:HOH:O	2.51	0.43
1:B:404:ASN:HD22	1:B:407:ILE:CG2	2.30	0.43
1:B:408:ASP:N	1:B:408:ASP:OD2	2.50	0.43
1:B:428:GLU:OE2	1:B:435:ASP:HB3	2.17	0.43
1:B:443:ALA:HB1	1:B:470:PRO:CD	2.47	0.43
1:B:241:ARG:HH12	1:B:536:LYS:HZ2	1.67	0.43
1:B:85:ILE:O	1:B:89:TYR:CB	2.66	0.43
1:A:106:TYR:HB3	1:A:108:PHE:CE1	2.53	0.43
1:A:116:SER:HA	1:A:119:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:SER:HA	1:B:31:PRO:HD3	1.82	0.43
1:B:333:PRO:HG2	1:B:334:MET:HG2	1.99	0.43
1:B:353:LEU:N	1:B:354:PRO:CD	2.82	0.43
1:B:372:VAL:HG12	5:B:2013:HOH:O	2.18	0.43
1:B:74:ARG:NH1	1:B:221:ALA:O	2.51	0.43
1:A:143:ARG:HD3	1:A:163:ILE:HD11	2.00	0.43
1:A:107:ASP:HB3	1:A:214:LEU:HD22	2.00	0.43
1:B:371:ALA:O	1:B:372:VAL:C	2.57	0.43
1:B:391:ARG:O	1:B:394:GLN:HB2	2.19	0.43
1:B:468:TYR:HB2	1:B:492:ASP:CG	2.38	0.43
1:B:66:SER:HB3	1:B:69:ALA:CB	2.45	0.43
1:B:418:TYR:HD2	1:B:418:TYR:N	1.94	0.43
1:B:75:HIS:HB2	1:B:99:VAL:CG2	2.48	0.43
1:B:634:ASN:O	1:B:638:GLU:HB2	2.19	0.43
1:A:141:VAL:CB	1:A:145:GLU:HB2	2.45	0.43
1:A:478:THR:CG2	1:A:480:MET:HG2	2.48	0.43
1:B:206:ARG:HD2	1:B:206:ARG:O	2.19	0.43
1:B:425:ARG:C	1:B:425:ARG:HD2	2.40	0.43
1:A:321:MET:HB2	1:B:319:PRO:HG2	2.00	0.43
1:A:551:ILE:HG23	1:A:588:LYS:HD3	2.01	0.43
1:A:641:LEU:HD13	5:A:1050:HOH:O	2.19	0.43
1:A:643:LYS:HG2	1:A:644:HIS:H	1.84	0.43
1:B:212:LYS:O	1:B:214:LEU:HD22	2.18	0.43
1:B:253:PHE:O	1:B:254:THR:HG22	2.19	0.43
1:B:405:MET:C	1:B:407:ILE:H	2.21	0.43
1:B:421:ARG:O	1:B:421:ARG:HG3	2.19	0.43
1:A:149:LEU:HD23	1:A:171:LEU:HD21	2.01	0.42
1:A:157:LEU:HA	1:A:160:ILE:CG2	2.47	0.42
1:A:424:TYR:HE1	1:A:460:GLU:OE2	2.02	0.42
1:B:192:ILE:C	1:B:193:LYS:HD2	2.40	0.42
1:A:27:GLN:NE2	1:A:31:PRO:HG3	2.29	0.42
1:A:376:GLN:NE2	5:A:1101:HOH:O	2.35	0.42
1:A:392:PRO:CD	5:A:1025:HOH:O	2.66	0.42
1:A:50:THR:O	1:A:51:LYS:C	2.55	0.42
1:B:612:GLN:HB3	1:B:626:VAL:O	2.19	0.42
1:B:36:LYS:HE3	1:B:63:THR:CG2	2.49	0.42
1:B:6:ILE:O	1:B:13:LYS:HA	2.19	0.42
1:A:322:GLN:HE21	1:A:323:LEU:HB3	1.84	0.42
1:A:375:LEU:HB3	1:A:525:GLU:HB2	2.00	0.42
1:A:70:LEU:O	1:A:74:ARG:CG	2.60	0.42
1:A:80:LEU:HD23	1:A:192:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:C	1:B:171:LEU:HD13	2.40	0.42
1:A:331:LEU:HD11	1:B:298:LEU:HD21	2.01	0.42
1:B:420:PHE:CE2	1:B:474:VAL:CG2	3.01	0.42
1:B:70:LEU:HD22	1:B:74:ARG:HG3	2.00	0.42
1:A:83:HIS:ND1	1:A:129:ILE:HD13	2.34	0.42
1:A:85:ILE:HG21	1:A:108:PHE:CD2	2.54	0.42
1:B:391:ARG:NH1	1:B:393:ASP:OD2	2.52	0.42
1:B:471:LYS:NZ	5:B:2091:HOH:O	2.53	0.42
1:B:574:VAL:HG12	1:B:575:ARG:N	2.34	0.42
1:B:7:GLN:HG3	1:B:13:LYS:HB3	2.01	0.42
1:B:84:ALA:CB	1:B:126:MET:HB3	2.44	0.42
1:B:299:ALA:O	1:B:329:MET:HA	2.20	0.42
1:A:204:TYR:HE1	5:A:1064:HOH:O	2.03	0.42
1:A:203:ALA:O	1:A:213:MET:HG3	2.19	0.42
1:A:54:GLU:OE1	1:A:54:GLU:CA	2.68	0.42
1:A:4:ILE:HG13	1:A:56:ASP:HB3	2.02	0.42
1:A:606:LYS:O	1:A:609:GLU:HB2	2.20	0.42
1:A:626:VAL:HG12	1:A:627:GLU:O	2.19	0.42
1:B:204:TYR:HA	1:B:214:LEU:HD23	2.02	0.42
1:B:241:ARG:NH1	1:B:536:LYS:HZ2	2.18	0.42
1:B:378:VAL:H	3:B:2003:ATP:HN62	1.68	0.42
1:B:439:MET:HE3	1:B:494:LEU:N	2.35	0.42
1:B:86:LYS:HE3	1:B:91:ASN:HA	2.01	0.42
1:B:324:ASP:O	1:B:326:THR:N	2.45	0.42
1:B:4:ILE:O	1:B:4:ILE:HG23	2.20	0.42
1:B:610:ASN:O	1:B:611:ASN:C	2.57	0.42
1:A:151:SER:HB2	1:A:152:ASN:H	1.72	0.42
1:A:303:LEU:CG	1:A:337:PRO:HB2	2.49	0.42
1:A:360:LEU:HA	1:A:360:LEU:HD13	1.92	0.42
1:B:141:VAL:HG11	1:B:146:ALA:HB2	2.02	0.42
1:B:171:LEU:O	1:B:171:LEU:HD13	2.19	0.42
1:B:438:ASP:CG	1:B:439:MET:N	2.73	0.42
1:A:203:ALA:O	1:A:214:LEU:N	2.53	0.42
1:A:25:ILE:O	1:A:29:ILE:HG13	2.20	0.42
1:A:444:GLU:O	1:A:445:ASN:C	2.58	0.42
1:B:137:GLU:H	1:B:137:GLU:HG2	1.51	0.42
3:B:2003:ATP:O2B	3:B:2003:ATP:O2A	2.38	0.42
1:B:492:ASP:OD1	1:B:495:LEU:HB2	2.20	0.42
1:B:74:ARG:HH11	1:B:74:ARG:CG	2.29	0.42
1:B:8:PHE:O	1:B:10:ASP:N	2.51	0.42
1:A:152:ASN:H	1:A:152:ASN:HD22	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:C	1:A:190:ALA:H	2.23	0.41
1:A:254:THR:HG22	1:A:255:ASN:N	2.35	0.41
1:A:456:LEU:O	1:A:458:TYR:HD2	2.03	0.41
1:B:4:ILE:HG22	1:B:16:PHE:C	2.39	0.41
1:B:241:ARG:HH12	1:B:536:LYS:NZ	2.16	0.41
1:B:616:ARG:CZ	1:B:622:ASP:CB	2.98	0.41
1:A:143:ARG:NH1	1:A:163:ILE:HG23	2.35	0.41
1:A:251:GLU:O	1:A:269:ASN:HB2	2.20	0.41
1:A:340:MET:CE	1:A:389:PHE:CE2	3.03	0.41
1:A:262:GLY:O	1:A:378:VAL:HB	2.20	0.41
1:A:486:LEU:O	1:A:522:SER:HB2	2.20	0.41
1:B:80:LEU:HD13	1:B:129:ILE:HD13	2.03	0.41
1:B:186:VAL:HG13	1:B:187:PRO:HD2	2.01	0.41
1:B:559:TYR:O	1:B:559:TYR:HD2	2.02	0.41
1:A:480:MET:HG3	1:A:480:MET:O	2.21	0.41
1:A:509:GLU:CD	1:A:509:GLU:H	2.24	0.41
1:B:474:VAL:O	1:B:486:LEU:N	2.52	0.41
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.87	0.41
1:A:240:GLU:HA	1:A:245:LYS:HE2	2.02	0.41
1:A:300:ASN:O	1:A:302:ASP:N	2.54	0.41
1:A:340:MET:CG	1:A:501:LEU:HD11	2.45	0.41
1:B:204:TYR:O	1:B:207:GLY:N	2.53	0.41
1:B:255:ASN:HD21	1:B:374:GLY:HA2	1.86	0.41
1:B:474:VAL:HG21	1:B:487:SER:CB	2.45	0.41
1:B:501:LEU:O	1:B:512:ARG:HG2	2.19	0.41
1:B:115:SER:HA	1:B:200:THR:HG21	2.03	0.41
1:B:212:LYS:H	1:B:212:LYS:CD	2.25	0.41
1:B:429:ASP:HA	1:B:435:ASP:OD2	2.20	0.41
1:B:444:GLU:O	1:B:448:LYS:HG3	2.20	0.41
1:B:453:GLU:HB2	1:B:454:LEU:HD22	2.00	0.41
1:B:383:LEU:HA	1:B:523:THR:HA	2.02	0.41
1:B:4:ILE:CG2	1:B:16:PHE:O	2.60	0.41
1:B:280:TYR:OH	1:B:409:VAL:HA	2.20	0.41
1:B:262:GLY:H	1:B:372:VAL:HG13	1.81	0.41
1:B:399:PHE:O	1:B:403:VAL:HB	2.21	0.41
1:B:47:VAL:HG23	1:B:48:ASP:N	2.35	0.41
1:B:4:ILE:O	1:B:4:ILE:CG2	2.68	0.41
1:A:502:THR:HA	1:A:511:HIS:O	2.21	0.41
1:B:246:ILE:HG22	1:B:250:LEU:HD22	2.03	0.41
1:B:252:LEU:O	1:B:270:GLY:HA3	2.21	0.41
1:B:584:LYS:O	1:B:585:MET:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:GLN:O	1:B:624:GLU:O	2.39	0.41
1:A:428:GLU:HG3	1:A:440:TRP:NE1	2.35	0.41
1:A:542:TRP:CE3	1:A:642:LYS:HE3	2.56	0.41
1:A:21:THR:O	1:A:24:ASP:HB2	2.20	0.41
1:A:282:VAL:HG23	1:A:360:LEU:HD21	2.03	0.41
1:A:548:VAL:HB	1:A:576:VAL:HG23	2.03	0.41
1:A:603:VAL:O	1:A:603:VAL:HG12	2.20	0.41
1:B:100:ILE:HG22	1:B:101:GLU:H	1.85	0.41
1:B:186:VAL:CG1	1:B:188:SER:O	2.69	0.41
1:B:211:ASN:HB2	1:B:214:LEU:HD21	2.03	0.41
1:B:486:LEU:HB3	1:B:487:SER:H	1.57	0.41
1:A:143:ARG:HD3	1:A:163:ILE:CG1	2.51	0.41
1:A:340:MET:HE2	1:A:389:PHE:CE2	2.56	0.41
1:B:182:ARG:HD2	1:B:182:ARG:H	1.82	0.41
1:B:400:LYS:O	1:B:404:ASN:HB2	2.21	0.41
1:B:241:ARG:O	1:B:533:GLU:HG2	2.21	0.41
1:A:97:GLY:CA	1:A:105:TYR:O	2.69	0.41
1:A:408:ASP:HA	1:A:411:LYS:HE3	2.02	0.41
1:B:191:LYS:O	1:B:191:LYS:CG	2.70	0.41
1:B:256:SER:OG	1:B:259:VAL:HG23	2.21	0.41
1:A:368:ALA:O	1:A:370:GLY:N	2.54	0.40
1:A:364:HIS:HA	1:A:379:ARG:O	2.22	0.40
1:A:434:PHE:HD2	1:A:434:PHE:HA	1.63	0.40
1:A:583:GLU:HG3	1:A:587:TYR:CD2	2.56	0.40
1:B:430:LYS:CB	1:B:436:ASP:HB2	2.49	0.40
1:B:540:PRO:CG	1:B:543:LEU:HD12	2.51	0.40
1:B:585:MET:O	1:B:589:ILE:HD12	2.21	0.40
1:B:561:TYR:HD2	1:B:603:VAL:HG11	1.85	0.40
1:A:585:MET:O	1:A:588:LYS:HB2	2.22	0.40
1:B:204:TYR:CD1	1:B:204:TYR:N	2.90	0.40
1:B:554:ASN:CG	1:B:557:LEU:HD12	2.41	0.40
1:B:563:ARG:HA	1:B:578:ILE:HD11	2.02	0.40
1:B:598:PRO:C	1:B:599:TYR:CD1	2.95	0.40
1:A:13:LYS:HE3	1:A:13:LYS:HB3	1.91	0.40
1:B:114:ILE:HG22	1:B:118:ASP:OD2	2.22	0.40
1:B:129:ILE:CD1	1:B:174:GLN:HE22	2.35	0.40
1:B:245:LYS:O	1:B:249:GLU:HB2	2.22	0.40
1:B:6:ILE:HA	1:B:57:GLY:O	2.21	0.40
1:A:106:TYR:O	1:A:108:PHE:CE1	2.74	0.40
1:A:93:LYS:CD	1:A:155:TYR:HE1	2.25	0.40
1:A:77:THR:HA	1:A:80:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:HIS:CD2	1:B:174:GLN:OE1	2.74	0.40
1:B:288:MET:CE	1:B:405:MET:HB2	2.51	0.40
1:A:407:ILE:O	1:A:410:TYR:HB2	2.21	0.40
1:B:573:GLY:O	5:B:2093:HOH:O	2.22	0.40
1:B:616:ARG:O	1:B:617:GLN:C	2.58	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/645 (99%)	552 (86%)	62 (10%)	26 (4%)	3	9
1	B	633/645 (98%)	466 (74%)	114 (18%)	53 (8%)	1	2
All	All	1273/1290 (99%)	1018 (80%)	176 (14%)	79 (6%)	1	4

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	A	324	ASP
1	A	425	ARG
1	A	430	LYS
1	A	432	LYS
1	A	465	ALA
1	B	4	ILE
1	B	90	GLY
1	B	91	ASN
1	B	147	LYS
1	B	167	GLU
1	B	201	ALA
1	B	205	TRP

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Mol	Chain	Res	Type
1	B	313	TYR
1	B	324	ASP
1	B	325	GLU
1	B	415	PHE
1	B	421	ARG
1	B	430	LYS
1	B	465	ALA
1	B	473	ASP
1	B	479	ALA
1	B	508	GLY
1	B	605	ASP
1	B	617	GLN
1	B	621	GLN
1	B	624	GLU
1	A	18	LYS
1	A	143	ARG
1	A	144	ASP
1	A	151	SER
1	A	175	GLY
1	A	322	GLN
1	A	325	GLU
1	A	436	ASP
1	A	618	TYR
1	A	623	GLN
1	B	75	HIS
1	B	106	TYR
1	B	114	ILE
1	B	355	ILE
1	B	464	GLU
1	B	488	THR
1	B	520	VAL
1	B	611	ASN
1	A	149	LEU
1	A	189	THR
1	B	9	PRO
1	B	143	ARG
1	B	166	ASP
1	B	203	ALA
1	B	369	SER
1	B	395	ILE
1	B	436	ASP
1	B	471	LYS

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Mol	Chain	Res	Type
1	B	472	LEU
1	B	571	SER
1	B	620	SER
1	B	628	LYS
1	A	211	ASN
1	A	301	VAL
1	A	366	TYR
1	A	369	SER
1	B	163	ILE
1	B	623	GLN
1	B	643	LYS
1	A	162	ALA
1	A	429	ASP
1	A	611	ASN
1	B	353	LEU
1	B	622	ASP
1	B	642	LYS
1	B	116	SER
1	B	427	PRO
1	B	406	ILE
1	B	470	PRO
1	B	513	PRO
1	B	519	GLY
1	A	426	ASP

### 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	
1	A	567/570 (100%)	512 (90%)	55 (10%)	8	24
1	B	562/570 (99%)	491 (87%)	71 (13%)	4	14
All	All	1129/1140 (99%)	1003 (89%)	126 (11%)	6	18

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	17	ASP
1	A	34	ARG
1	A	48	ASP
1	A	54	GLU
1	A	74	ARG
1	A	81	MET
1	A	101	GLU
1	A	112	GLN
1	A	117	ASP
1	A	120	GLU
1	A	128	GLN
1	A	129	ILE
1	A	148	GLU
1	A	151	SER
1	A	152	ASN
1	A	153	ASP
1	A	167	GLU
1	A	170	THR
1	A	173	SER
1	A	186	VAL
1	A	204	TYR
1	A	220	THR
1	A	250	LEU
1	A	255	ASN
1	A	298	LEU
1	A	323	LEU
1	A	330	VAL
1	A	336	CYS
1	A	340	MET
1	A	353	LEU
1	A	360	LEU
1	A	366	TYR
1	A	376	GLN
1	A	377	ARG
1	A	434	PHE
1	A	447	LEU
1	A	467	PHE
1	A	476	VAL
1	A	483	GLU
1	A	496	PRO
1	A	507	ASP
1	A	509	GLU

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Mol	Chain	Res	Type
1	A	512	ARG
1	A	518	ARG
1	A	521	VAL
1	A	523	THR
1	A	526	ARG
1	A	535	THR
1	A	554	ASN
1	A	560	ASP
1	A	582	ASN
1	A	610	ASN
1	A	622	ASP
1	A	641	LEU
1	B	34	ARG
1	B	47	VAL
1	B	55	THR
1	B	56	ASP
1	B	59	ILE
1	B	68	GLU
1	B	70	LEU
1	B	92	VAL
1	B	94	PHE
1	B	106	TYR
1	B	114	ILE
1	B	117	ASP
1	B	129	ILE
1	B	137	GLU
1	B	149	LEU
1	B	158	GLU
1	B	182	ARG
1	B	195	PHE
1	B	204	TYR
1	B	205	TRP
1	B	210	ASN
1	B	211	ASN
1	B	212	LYS
1	B	214	LEU
1	B	225	LYS
1	B	250	LEU
1	B	256	SER
1	B	257	GLN
1	B	279	ARG
1	B	297	VAL

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Mol	Chain	Res	Type
1	B	313	TYR
1	B	326	THR
1	B	352	GLU
1	B	353	LEU
1	B	355	ILE
1	B	360	LEU
1	B	365	ARG
1	B	366	TYR
1	B	399	PHE
1	B	401	ARG
1	B	402	VAL
1	B	404	ASN
1	B	408	ASP
1	B	412	ASP
1	B	413	PHE
1	B	416	GLU
1	B	418	TYR
1	B	428	GLU
1	B	434	PHE
1	B	435	ASP
1	B	438	ASP
1	B	440	TRP
1	B	464	GLU
1	B	467	PHE
1	B	468	TYR
1	B	473	ASP
1	B	490	GLN
1	B	492	ASP
1	B	507	ASP
1	B	518	ARG
1	B	523	THR
1	B	555	VAL
1	B	559	TYR
1	B	563	ARG
1	B	580	ASP
1	B	587	TYR
1	B	594	MET
1	B	601	ILE
1	B	609	GLU
1	B	610	ASN
1	B	611	ASN

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	43	ASN
1	A	133	ASN
1	A	152	ASN
1	A	210	ASN
1	A	231	HIS
1	A	233	GLN
1	A	322	GLN
1	A	345	ASN
1	A	364	HIS
1	A	376	GLN
1	A	384	ASN
1	A	475	GLN
1	A	490	GLN
1	A	554	ASN
1	A	566	GLN
1	A	582	ASN
1	A	593	GLN
1	A	600	GLN
1	A	612	GLN
1	A	617	GLN
1	B	12	ASN
1	B	79	HIS
1	B	83	HIS
1	B	121	GLN
1	B	128	GLN
1	B	174	GLN
1	B	210	ASN
1	B	211	ASN
1	B	255	ASN
1	B	309	HIS
1	B	404	ASN
1	B	490	GLN
1	B	506	GLN
1	B	572	GLN
1	B	595	GLN
1	B	600	GLN
1	B	611	ASN
1	B	612	GLN
1	B	617	GLN
1	B	621	GLN
1	B	634	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z  > 2$
3	ATP	A	1003	-	26,33,33	0.78	0	31,52,52	1.16	4 (12%)
3	ATP	B	2003	-	26,33,33	0.73	0	31,52,52	1.20	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1003	-	-	5/18/38/38	0/3/3/3
3	ATP	B	2003	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	ATP	PB-O3B-PG	-3.28	121.56	132.83
3	B	2003	ATP	PA-O3A-PB	-2.93	122.77	132.83
3	A	1003	ATP	PB-O3B-PG	-2.92	122.80	132.83
3	A	1003	ATP	PA-O3A-PB	-2.88	122.94	132.83
3	A	1003	ATP	C5-C6-N6	2.40	124.00	120.35
3	B	2003	ATP	C5-C6-N6	2.38	123.97	120.35
3	A	1003	ATP	O2G-PG-O1G	2.38	120.00	110.68
3	B	2003	ATP	O2G-PG-O1G	2.31	119.72	110.68

There are no chirality outliers.

All (10) torsion outliers are listed below:

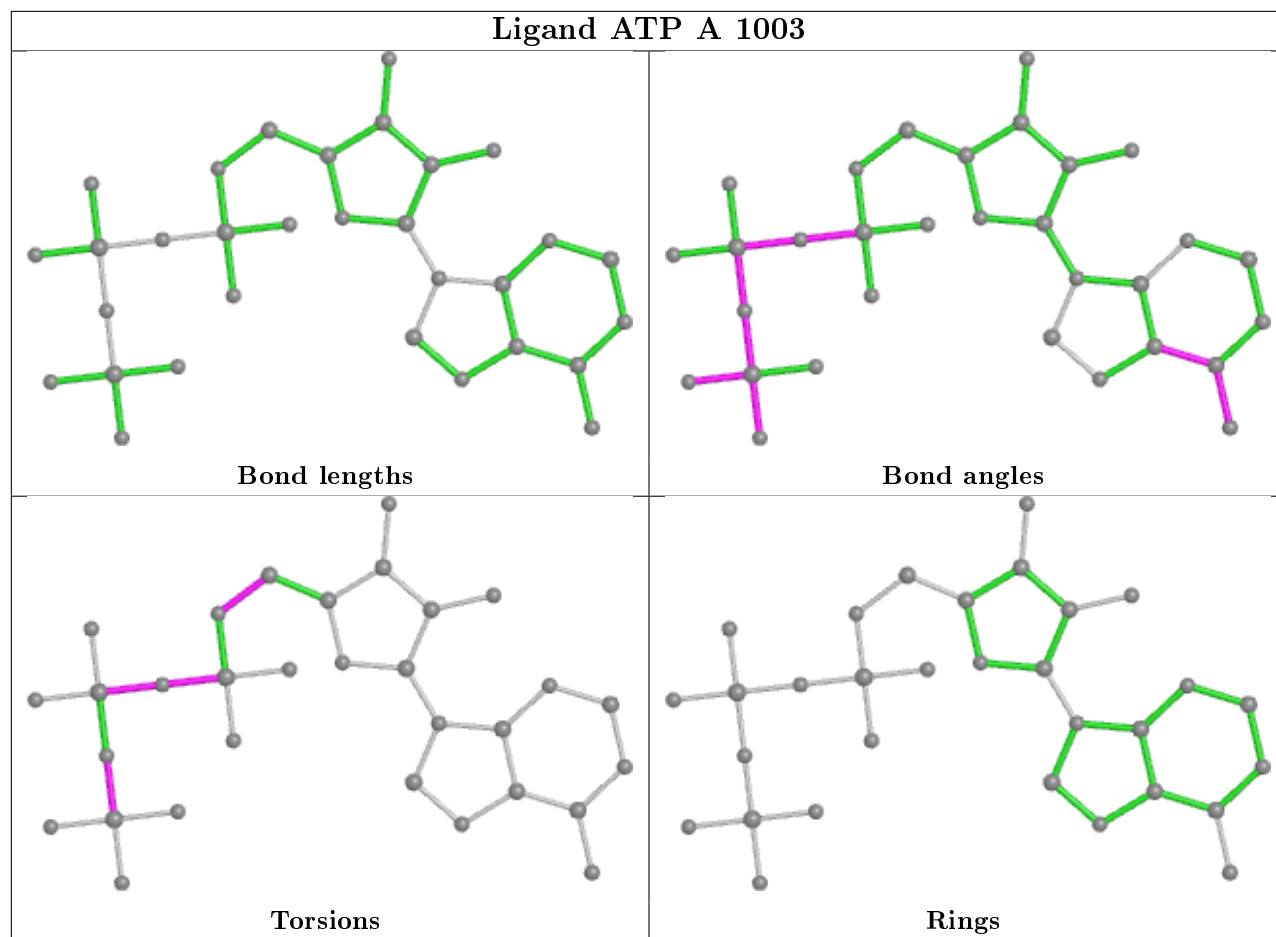
Mol	Chain	Res	Type	Atoms
3	B	2003	ATP	C5'-O5'-PA-O1A
3	B	2003	ATP	C5'-O5'-PA-O2A
3	B	2003	ATP	C5'-O5'-PA-O3A
3	B	2003	ATP	PA-O3A-PB-O2B
3	A	1003	ATP	PA-O3A-PB-O2B
3	B	2003	ATP	PB-O3A-PA-O2A
3	A	1003	ATP	PB-O3A-PA-O2A
3	A	1003	ATP	C4'-C5'-O5'-PA
3	A	1003	ATP	PB-O3B-PG-O3G
3	A	1003	ATP	PA-O3A-PB-O1B

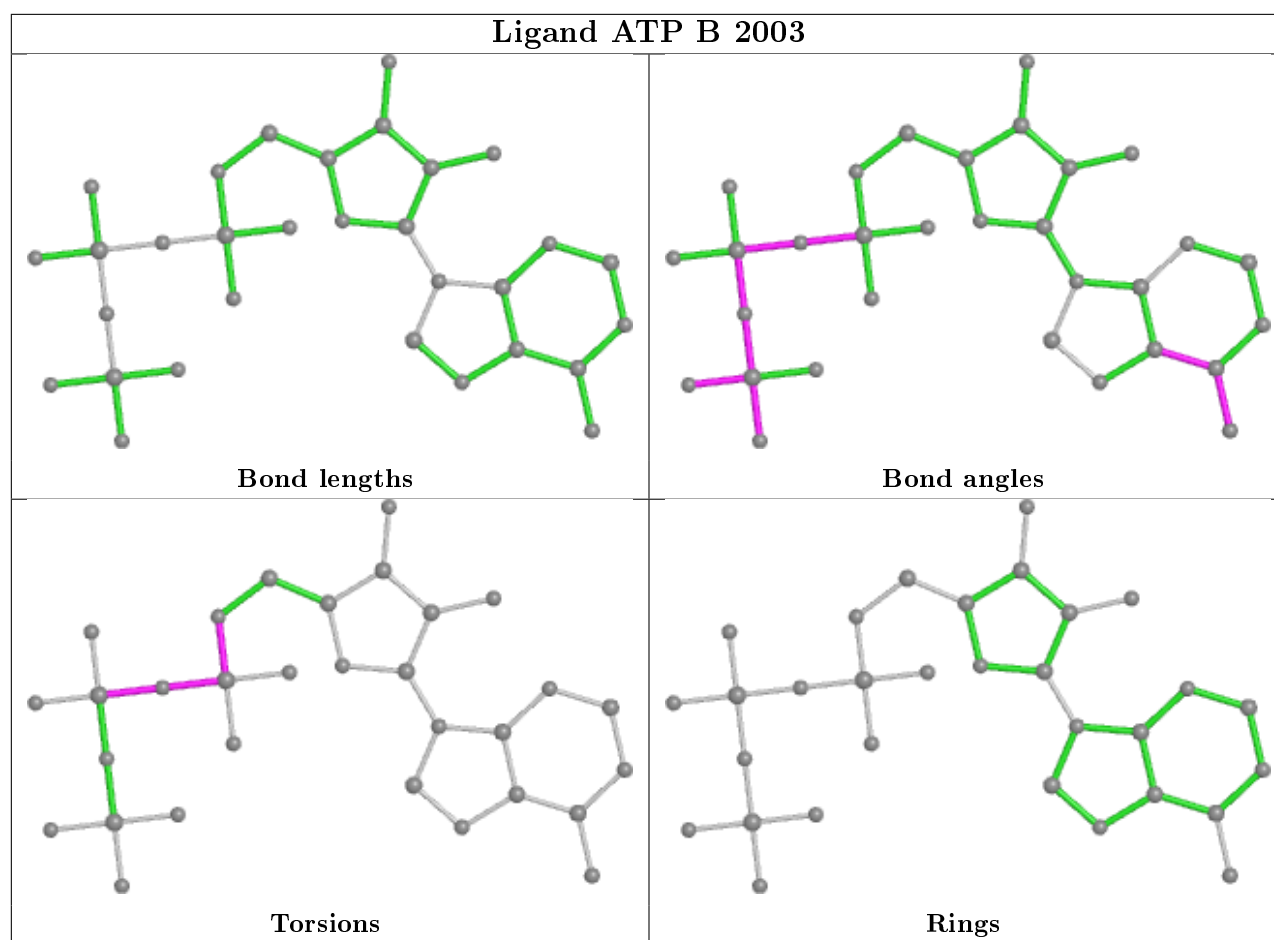
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	ATP	3	0
3	B	2003	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	642/645 (99%)	-0.10	22 (3%) 45 35	24, 58, 103, 134	0
1	B	637/645 (98%)	0.51	83 (13%) 3 2	29, 79, 143, 157	0
All	All	1279/1290 (99%)	0.20	105 (8%) 11 6	24, 67, 135, 157	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	TYR	6.8
1	B	111	ASP	5.9
1	B	212	LYS	5.8
1	B	88	LEU	5.7
1	B	90	GLY	5.3
1	B	166	ASP	5.2
1	A	434	PHE	5.1
1	A	432	LYS	5.0
1	B	455	GLY	5.0
1	B	113	ASN	4.9
1	A	204	TYR	4.7
1	B	447	LEU	4.7
1	B	441	ASN	4.6
1	A	431	GLU	4.6
1	B	170	THR	4.5
1	A	166	ASP	4.5
1	B	209	SER	4.5
1	A	433	TYR	4.4
1	B	210	ASN	4.4
1	A	325	GLU	4.3
1	B	161	ASP	4.1
1	B	208	ASP	4.1
1	B	459	GLU	4.1
1	B	94	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	619	GLY	4.1
1	B	168	ASN	4.0
1	B	445	ASN	4.0
1	B	183	GLY	4.0
1	A	163	ILE	3.9
1	A	164	PRO	3.9
1	B	457	SER	3.9
1	B	211	ASN	3.9
1	A	623	GLN	3.8
1	A	429	ASP	3.8
1	B	91	ASN	3.8
1	B	117	ASP	3.7
1	B	87	ARG	3.6
1	B	440	TRP	3.6
1	B	2	GLU	3.4
1	B	160	ILE	3.4
1	B	92	VAL	3.4
1	B	1	MET	3.3
1	B	454	LEU	3.3
1	B	446	MET	3.3
1	B	165	GLU	3.2
1	B	204	TYR	3.2
1	B	645	ARG	3.2
1	B	112	GLN	3.1
1	B	431	GLU	3.1
1	B	169	VAL	3.1
1	B	458	TYR	3.1
1	B	182	ARG	3.1
1	A	182	ARG	3.1
1	B	167	GLU	3.1
1	B	199	SER	3.1
1	B	175	GLY	3.0
1	B	434	PHE	3.0
1	B	557	LEU	3.0
1	B	181	CYS	2.9
1	A	324	ASP	2.9
1	B	141	VAL	2.9
1	B	133	ASN	2.8
1	B	213	MET	2.8
1	B	312	HIS	2.8
1	A	210	ASN	2.7
1	B	140	VAL	2.7

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	10	ASP	2.6
1	B	214	LEU	2.6
1	B	89	TYR	2.6
1	A	168	ASN	2.5
1	A	165	GLU	2.5
1	B	466	ALA	2.4
1	B	437	ASP	2.4
1	A	645	ARG	2.4
1	B	416	GLU	2.4
1	A	31	PRO	2.4
1	A	183	GLY	2.3
1	B	149	LEU	2.3
1	B	606	LYS	2.3
1	B	174	GLN	2.3
1	B	452	ASP	2.3
1	B	422	LEU	2.3
1	B	451	ALA	2.3
1	B	480	MET	2.3
1	B	475	GLN	2.3
1	A	622	ASP	2.3
1	B	624	GLU	2.3
1	B	201	ALA	2.2
1	B	448	LYS	2.2
1	B	215	GLN	2.2
1	A	435	ASP	2.2
1	A	425	ARG	2.2
1	B	419	SER	2.2
1	B	432	LYS	2.2
1	B	463	GLY	2.2
1	B	444	GLU	2.2
1	B	108	PHE	2.1
1	B	418	TYR	2.1
1	B	461	ALA	2.1
1	B	325	GLU	2.1
1	B	469	GLY	2.0
1	B	621	GLN	2.0
1	B	483	GLU	2.0
1	B	620	SER	2.0
1	B	128	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

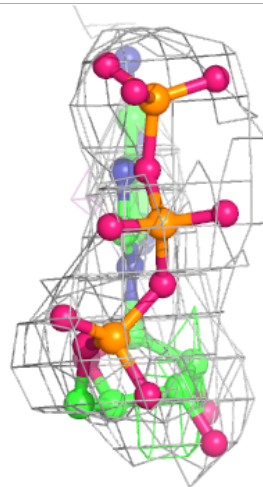
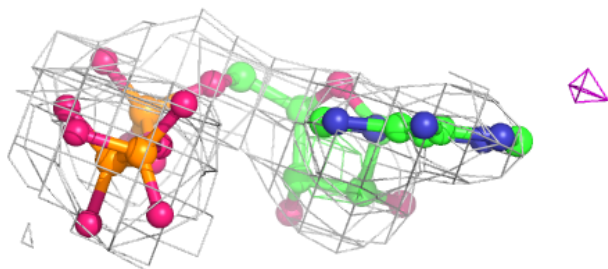
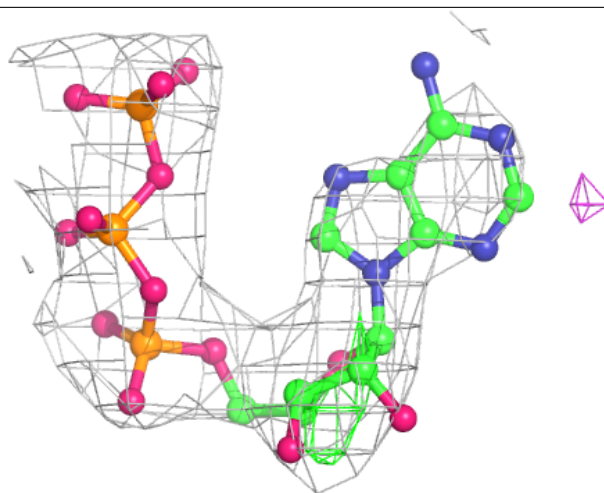
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	B	2003	31/31	0.81	0.25	119,121,141,141	0
3	ATP	A	1003	31/31	0.89	0.22	56,63,88,91	0
4	THR	B	2004	8/8	0.97	0.21	113,114,114,115	0
4	THR	A	1004	8/8	0.98	0.18	75,75,77,77	0
2	ZN	A	1002	1/1	0.98	0.03	93,93,93,93	0
2	ZN	B	2001	1/1	0.99	0.10	70,70,70,70	0
2	ZN	A	1001	1/1	0.99	0.08	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



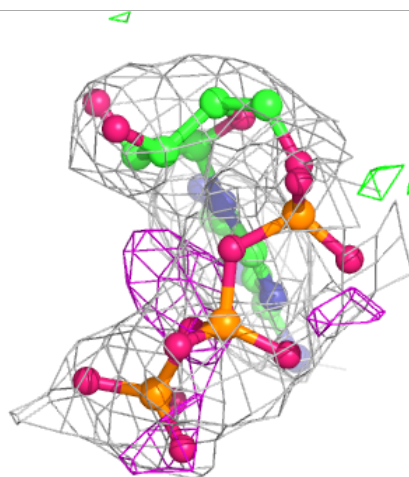
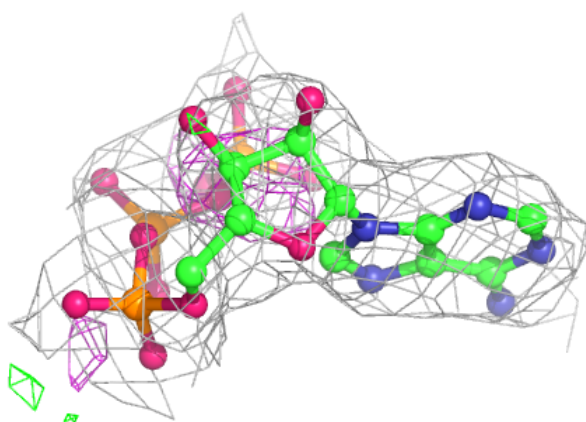
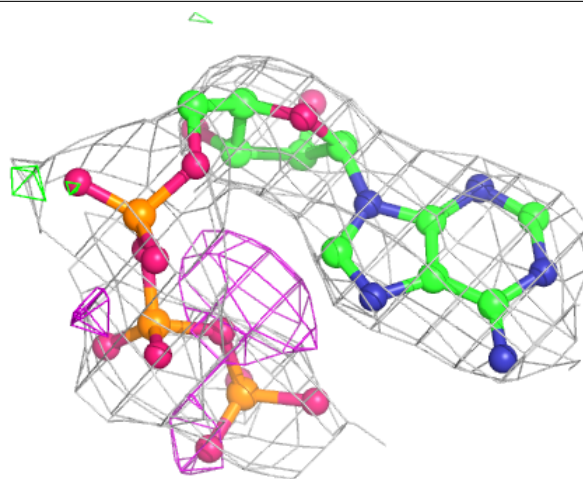
**Electron density around ATP B 2003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP A 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.