



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:29 pm BST

PDB ID : 3O8N  
Title : Structure of phosphofructokinase from rabbit skeletal muscle  
Authors : Banaszak, K.; Chang, S.H.; Rypniewski, W.  
Deposited on : 2010-08-03  
Resolution : 3.20 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

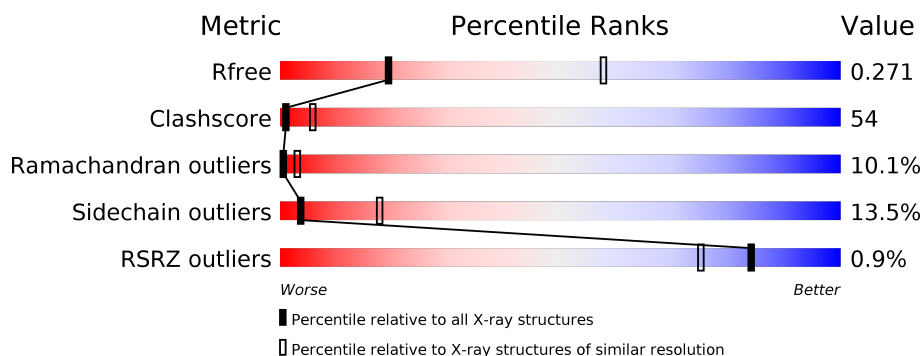
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	762	<div> <div></div> <div>31%</div> <div>52%</div> <div>14%</div> <div>..</div> </div>
1	B	762	<div> <div></div> <div>29%</div> <div>54%</div> <div>15%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	767	-	X	-	-
3	PO4	A	768	-	X	-	-
3	PO4	B	766	-	X	-	-
3	PO4	B	767	-	X	-	-
3	PO4	B	768	-	X	-	-

## 2 Entry composition [i](#)

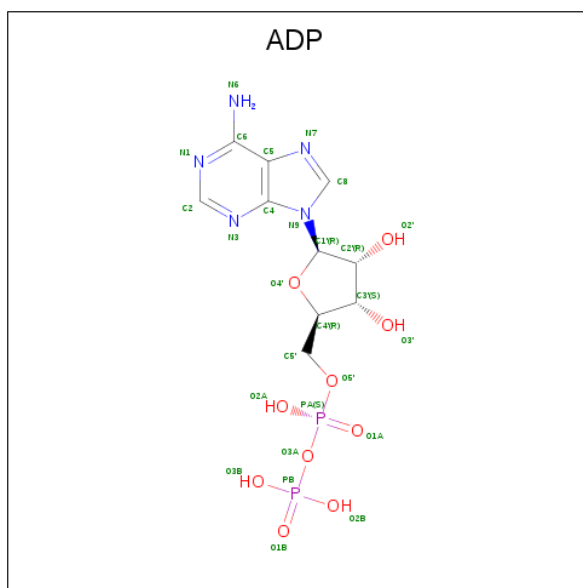
There are 3 unique types of molecules in this entry. The entry contains 11630 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-phosphofructokinase, muscle type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	276	0	0
			5719	3583	1031	1068	37			
1	B	748	Total	C	N	O	S	259	0	0
			5719	3583	1031	1068	37			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

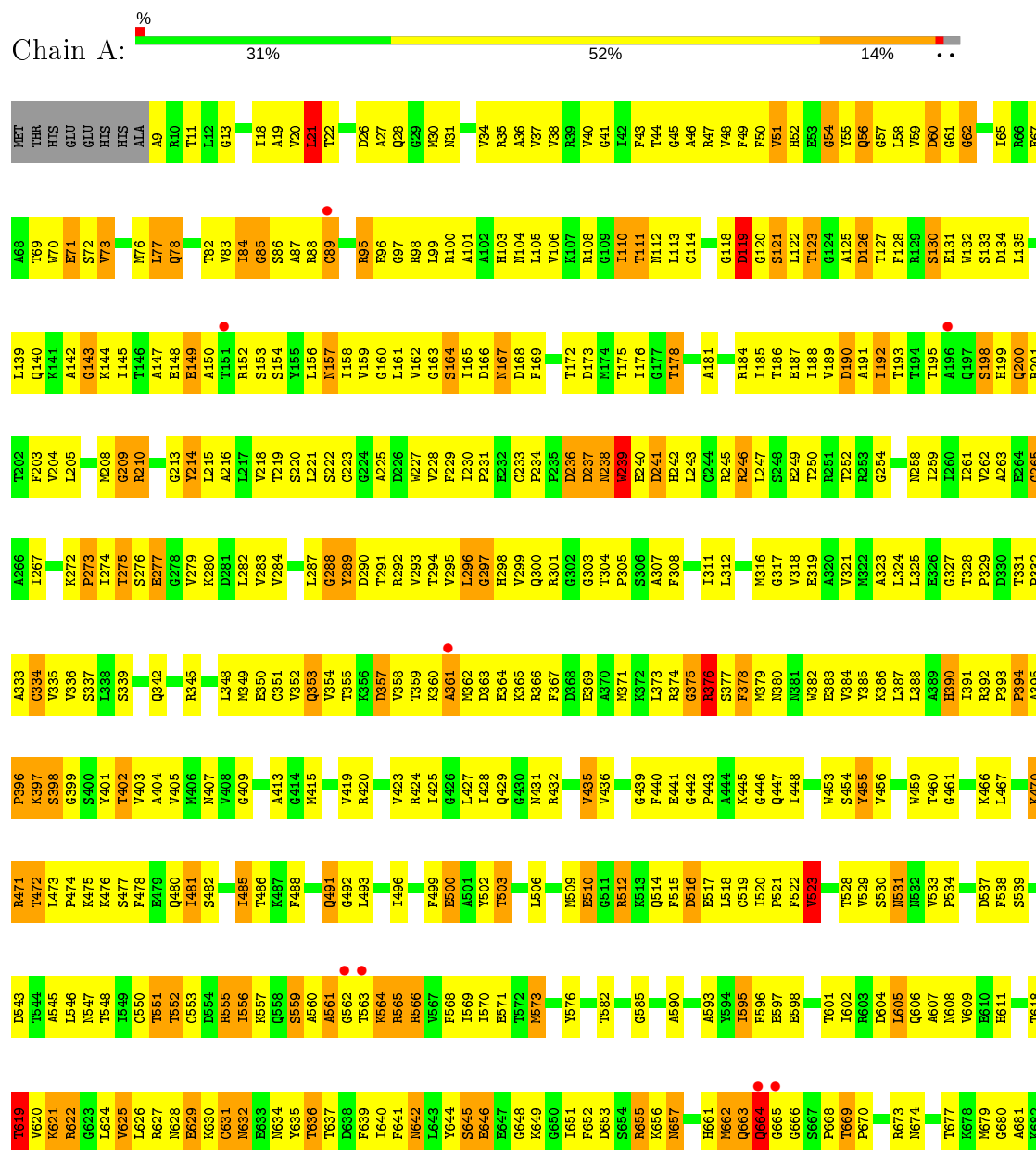


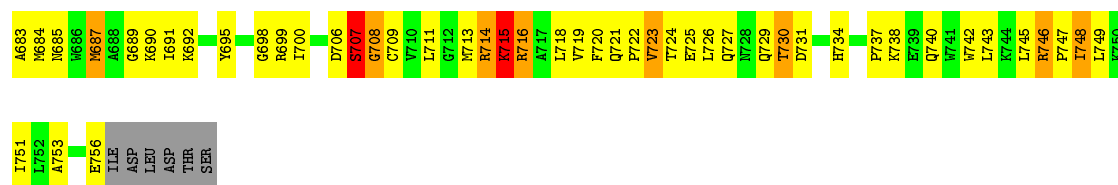
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

### 3 Residue-property plots

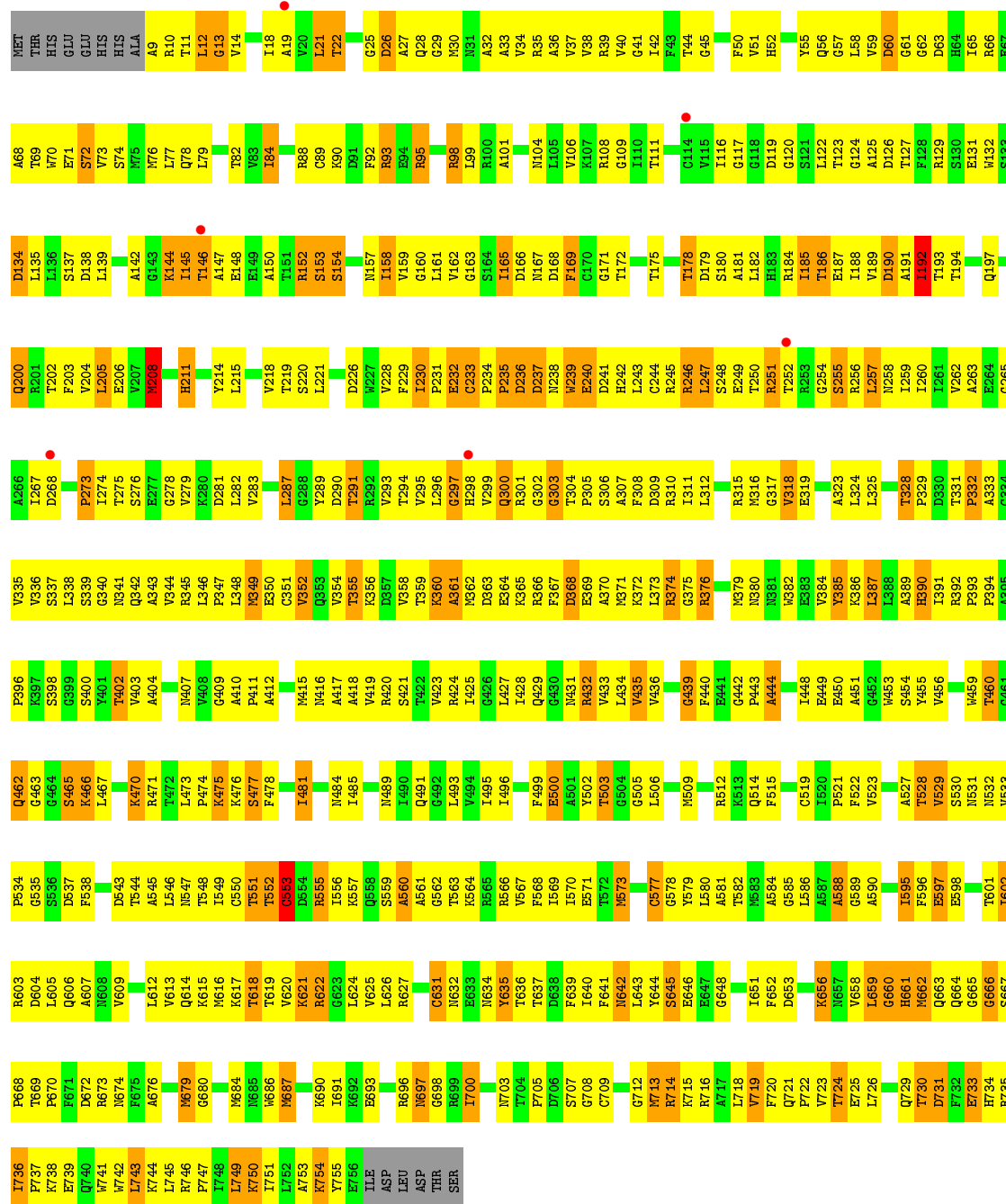
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 6-phosphofructokinase, muscle type





- Molecule 1: 6-phosphofructokinase, muscle type



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.29 Å   163.29 Å   356.94 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.87 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 100.0 (29.87-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 3.18 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229   ,   0.302 0.206   ,   0.271	Depositor DCC
$R_{free}$ test set	2353 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.4	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 105.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: PO4, ADP

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	0.64	1/5819 (0.0%)	0.86	3/7859 (0.0%)
1	B	0.63	1/5819 (0.0%)	0.83	2/7859 (0.0%)
All	All	0.63	2/11638 (0.0%)	0.84	5/15718 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	709	CYS	CB-SG	-6.18	1.71	1.82
1	B	577	CYS	CB-SG	-5.10	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	VAL	CB-CA-C	-6.50	99.05	111.40
1	A	303	GLY	N-CA-C	-5.95	98.22	113.10
1	B	505	GLY	N-CA-C	-5.36	99.71	113.10
1	B	553	CYS	CA-CB-SG	5.15	123.28	114.00
1	A	21	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	576	TYR	Sidechain
1	B	385	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	5719	0	5742	574	0
1	B	5719	0	5742	620	0
2	A	81	0	36	6	0
2	B	81	0	36	7	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
All	All	11630	0	11556	1183	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 54.

All (1183) 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:634:ASN:HD22	1:B:646:GLU:HG2	1.15	1.11
1:A:247:LEU:HD23	1:A:258:ASN:HD22	1.07	1.08
1:A:646:GLU:HG2	1:B:634:ASN:HD22	1.13	1.06
1:A:69:THR:HG22	1:A:72:SER:HB3	1.35	1.06
1:A:113:LEU:HB3	1:A:158:ILE:HG22	1.38	1.05
1:A:485:ILE:HD12	1:A:517:GLU:HB3	1.39	1.04
1:B:609:VAL:HG22	1:B:644:TYR:CE2	1.94	1.03
1:A:247:LEU:CD2	1:A:258:ASN:HD22	1.70	1.03
1:B:700:ILE:HD13	1:B:700:ILE:H	1.22	1.01
1:A:512:ARG:HD3	1:A:519:CYS:HA	1.42	1.00
1:A:376:ARG:HA	1:A:376:ARG:HH21	1.22	1.00
1:B:566:ARG:HG2	1:B:653:ASP:HB3	1.44	1.00
1:B:275:THR:HG23	1:B:278:GLY:H	1.25	1.00
1:B:339:SER:HB3	1:B:344:VAL:HG11	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HG21	1:B:318:VAL:HG13	1.45	0.98
1:A:379:MET:O	1:A:383:GLU:HG2	1.65	0.96
1:A:380:ASN:O	1:A:384:VAL:HG23	1.65	0.95
1:A:238:ASN:O	1:A:239:TRP:HB3	1.66	0.95
1:B:35:ARG:NH1	1:B:77:LEU:HD13	1.82	0.94
1:A:73:VAL:HG12	1:A:76:MET:SD	2.09	0.93
1:A:275:THR:OG1	1:A:277:GLU:HG2	1.69	0.93
1:B:250:THR:HG22	1:B:255:SER:HB3	1.50	0.93
1:B:126:ASP:O	1:B:129:ARG:HG3	1.70	0.92
1:B:551:THR:O	1:B:553:CYS:N	2.03	0.92
1:A:214:TYR:CE2	1:A:218:VAL:HG21	2.05	0.91
1:A:214:TYR:HE2	1:A:218:VAL:HG21	1.36	0.91
1:A:58:LEU:HG	1:A:101:ALA:HB1	1.53	0.90
1:B:603:ARG:NH1	1:B:603:ARG:HB2	1.87	0.90
1:A:173:ASP:HB3	2:A:764:ADP:H5'1	1.53	0.90
1:B:436:VAL:HG22	1:B:448:ILE:HG12	1.51	0.89
1:B:296:LEU:HD12	1:B:296:LEU:H	1.36	0.89
1:B:41:GLY:O	1:B:44:THR:HG22	1.73	0.89
1:A:566:ARG:HH21	1:A:566:ARG:HG3	1.34	0.89
1:A:247:LEU:HD23	1:A:258:ASN:ND2	1.88	0.88
1:A:595:ILE:HD12	1:A:746:ARG:CZ	2.05	0.86
1:B:595:ILE:HD12	1:B:746:ARG:NH1	1.90	0.86
1:B:667:SER:OG	1:B:668:PRO:HD2	1.74	0.86
1:B:658:VAL:O	1:B:658:VAL:HG12	1.75	0.86
1:A:123:THR:O	1:A:127:THR:HG22	1.74	0.86
1:B:84:ILE:HD12	1:B:84:ILE:H	1.39	0.86
1:B:481:ILE:O	1:B:481:ILE:HD12	1.75	0.85
1:B:419:VAL:O	1:B:423:VAL:HG23	1.77	0.85
1:B:39:ARG:HD2	1:B:70:TRP:CZ2	2.10	0.84
1:B:101:ALA:HA	1:B:104:ASN:HD22	1.37	0.84
1:B:297:GLY:O	1:B:299:VAL:N	2.09	0.84
1:B:84:ILE:HD12	1:B:84:ILE:N	1.93	0.84
1:A:634:ASN:ND2	1:B:646:GLU:HG2	1.92	0.84
1:A:387:LEU:O	1:A:390:HIS:HB2	1.78	0.83
1:B:509:MET:O	1:B:512:ARG:HB2	1.77	0.83
1:B:215:LEU:O	1:B:219:THR:HG22	1.79	0.83
1:B:146:THR:HG23	1:B:147:ALA:H	1.41	0.83
1:B:200:GLN:HB3	1:B:251:ARG:NH2	1.94	0.82
1:A:297:GLY:O	1:A:299:VAL:N	2.12	0.82
1:B:641:PHE:CD2	1:B:656:LYS:HG2	2.15	0.82
1:B:603:ARG:HB2	1:B:603:ARG:HH11	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HG12	1:A:147:ALA:H	1.43	0.82
1:B:551:THR:HG22	1:B:552:THR:N	1.92	0.81
1:B:567:VAL:HG23	1:B:616:MET:HE1	1.63	0.81
1:A:376:ARG:HA	1:A:376:ARG:NH2	1.93	0.81
1:B:502:TYR:OH	1:B:730:THR:HG21	1.81	0.81
1:B:175:THR:O	1:B:178:THR:HG22	1.80	0.81
1:A:165:ILE:HD11	1:A:208:MET:SD	2.20	0.81
1:B:116:ILE:HG12	1:B:161:LEU:HD13	1.61	0.80
1:A:41:GLY:O	1:A:44:THR:HG22	1.80	0.80
1:B:617:LYS:HG3	1:B:651:ILE:HG21	1.64	0.80
1:A:646:GLU:HG2	1:B:634:ASN:ND2	1.96	0.80
1:B:621:LYS:O	1:B:622:ARG:HD2	1.82	0.80
1:B:13:GLY:HA3	1:B:44:THR:HG23	1.62	0.79
1:B:192:ILE:HD13	1:B:203:PHE:CD2	2.17	0.79
1:A:646:GLU:CG	1:B:634:ASN:HD22	1.92	0.79
1:A:719:VAL:HG23	1:A:721:GLN:HG3	1.64	0.79
1:A:119:ASP:O	1:A:123:THR:HG22	1.84	0.79
1:B:240:GLU:HG3	1:B:282:LEU:HD22	1.64	0.78
1:B:532:ASN:O	1:B:737:PRO:HD3	1.83	0.78
1:B:185:ILE:O	1:B:189:VAL:HG23	1.83	0.78
1:B:493:LEU:HD23	1:B:495:ILE:HD11	1.66	0.78
1:B:509:MET:SD	1:B:512:ARG:NH1	2.56	0.78
1:B:352:VAL:O	1:B:355:THR:HG22	1.83	0.78
1:B:386:LYS:HE3	2:B:765:ADP:H2'	1.64	0.77
1:B:27:ALA:O	1:B:30:MET:HG3	1.84	0.77
1:A:228:VAL:HG12	1:A:229:PHE:H	1.49	0.77
1:A:402:THR:HB	1:A:432:ARG:HB3	1.67	0.77
1:A:240:GLU:HG3	1:A:282:LEU:HD22	1.66	0.77
1:B:708:GLY:O	1:B:723:VAL:HG22	1.84	0.77
1:A:570:ILE:HB	1:A:626:LEU:CD2	2.15	0.77
1:B:184:ARG:NH1	1:B:303:GLY:HA3	2.00	0.76
1:B:101:ALA:HA	1:B:104:ASN:ND2	2.01	0.76
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.48	0.76
1:A:167:ASN:HB2	1:A:178:THR:HG21	1.68	0.76
1:B:419:VAL:HG21	1:B:467:LEU:HD12	1.65	0.76
1:B:339:SER:HB3	1:B:344:VAL:CG1	2.16	0.76
1:B:35:ARG:HH11	1:B:77:LEU:HD13	1.51	0.76
1:A:49:PHE:CE1	1:A:110:ILE:HD11	2.21	0.75
1:B:687:MET:HE3	1:B:687:MET:O	1.85	0.75
1:A:208:MET:HB2	1:A:300:GLN:OE1	1.86	0.75
1:B:38:VAL:O	1:B:42:ILE:HG12	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:PRO:O	1:B:484:ASN:ND2	2.19	0.75
1:A:247:LEU:CD2	1:A:258:ASN:ND2	2.47	0.75
1:A:551:THR:HG22	1:A:552:THR:N	2.01	0.75
1:A:726:LEU:O	1:A:730:THR:HG22	1.85	0.75
1:A:35:ARG:HD3	1:A:77:LEU:HD13	1.68	0.75
1:B:192:ILE:O	1:B:192:ILE:HD12	1.85	0.75
1:A:506:LEU:HD23	1:A:723:VAL:HB	1.68	0.74
1:B:416:ASN:HB3	1:B:459:TRP:HB3	1.69	0.74
1:B:537:ASP:HB3	1:B:741:TRP:NE1	2.01	0.74
1:B:240:GLU:HG3	1:B:282:LEU:CD2	2.16	0.74
1:A:748:ILE:HD13	1:A:748:ILE:C	2.07	0.74
1:B:471:ARG:HB2	1:B:500:GLU:HG2	1.67	0.74
1:B:669:THR:O	1:B:673:ARG:HG3	1.86	0.74
1:A:172:THR:HB	1:A:337:SER:OG	1.87	0.74
1:B:234:PRO:HG3	1:B:367:PHE:CE1	2.22	0.74
1:B:279:VAL:O	1:B:283:VAL:HG23	1.88	0.74
1:A:609:VAL:C	1:A:611:HIS:H	1.91	0.74
1:B:232:GLU:O	1:B:233:CYS:HB2	1.87	0.74
1:B:90:LYS:HG3	1:B:93:ARG:HD3	1.70	0.74
1:A:642:ASN:HD22	1:A:642:ASN:N	1.85	0.73
1:A:55:TYR:O	1:A:59:VAL:HG23	1.88	0.73
1:B:257:LEU:HD12	1:B:258:ASN:N	2.02	0.73
1:B:627:ARG:HD2	1:B:640:ILE:HD12	1.70	0.73
1:B:104:ASN:O	1:B:108:ARG:HG2	1.89	0.73
1:A:132:TRP:O	1:A:135:LEU:HB2	1.88	0.73
1:A:279:VAL:O	1:A:283:VAL:HG12	1.86	0.73
1:A:502:TYR:OH	1:A:730:THR:HG21	1.88	0.73
1:A:642:ASN:HD22	1:A:642:ASN:H	1.37	0.73
1:A:561:ALA:HA	1:A:622:ARG:CZ	2.19	0.73
1:A:561:ALA:HA	1:A:622:ARG:NH2	2.04	0.73
1:B:393:PRO:HB3	1:B:453:TRP:CE3	2.23	0.72
1:A:364:GLU:O	1:A:366:ARG:N	2.21	0.72
1:B:189:VAL:O	1:B:193:THR:HG22	1.89	0.72
1:B:726:LEU:HD23	1:B:729:GLN:OE1	1.89	0.72
1:A:188:ILE:HD13	1:A:296:LEU:HD22	1.69	0.72
1:A:334:CYS:SG	1:A:345:ARG:HB3	2.29	0.72
1:B:267:ILE:HA	1:B:273:PRO:HA	1.69	0.72
1:A:131:GLU:O	1:A:135:LEU:HG	1.89	0.72
1:A:441:GLU:HG3	1:A:472:THR:HG21	1.71	0.72
1:B:473:LEU:HD21	1:B:503:THR:HG22	1.71	0.72
1:B:700:ILE:N	1:B:700:ILE:HD13	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ARG:HG3	1:A:566:ARG:NH2	2.05	0.72
1:B:376:ARG:HH21	1:B:376:ARG:HG3	1.55	0.72
1:A:216:ALA:O	1:A:219:THR:HG22	1.90	0.72
1:A:296:LEU:HD12	1:A:300:GLN:HE21	1.54	0.71
1:A:259:ILE:HG22	1:A:261:ILE:CD1	2.20	0.71
1:B:84:ILE:CD1	1:B:84:ILE:H	2.02	0.71
1:A:742:TRP:CE3	1:A:743:LEU:HD22	2.25	0.71
1:B:425:ILE:O	1:B:429:GLN:HG3	1.90	0.71
1:A:609:VAL:HG22	1:A:644:TYR:CZ	2.26	0.71
1:B:234:PRO:HB3	1:B:267:ILE:HD12	1.72	0.71
1:B:402:THR:HG23	1:B:491:GLN:OE1	1.90	0.71
1:B:506:LEU:HD23	1:B:723:VAL:HB	1.72	0.71
1:B:595:ILE:H	1:B:595:ILE:HD13	1.55	0.71
1:A:715:LYS:O	1:A:716:ARG:CB	2.38	0.70
1:A:423:VAL:HG12	1:A:427:LEU:HD11	1.74	0.70
1:A:621:LYS:O	1:A:622:ARG:HD2	1.90	0.70
1:B:231:PRO:O	1:B:233:CYS:N	2.24	0.70
1:A:423:VAL:O	1:A:427:LEU:HD12	1.92	0.70
1:A:145:ILE:HG23	1:A:148:GLU:H	1.56	0.70
1:B:585:GLY:HA2	1:B:626:LEU:HD12	1.74	0.70
1:A:742:TRP:CZ3	1:A:743:LEU:HD22	2.27	0.70
1:B:122:LEU:O	1:B:125:ALA:HB3	1.92	0.70
1:B:634:ASN:O	1:B:636:THR:HG23	1.91	0.70
1:B:90:LYS:NZ	1:B:93:ARG:NH1	2.39	0.70
1:A:78:GLN:N	1:A:78:GLN:OE1	2.25	0.70
1:A:167:ASN:HB3	1:A:214:TYR:HD1	1.56	0.70
1:B:215:LEU:O	1:B:219:THR:CG2	2.39	0.70
1:B:567:VAL:HG23	1:B:616:MET:CE	2.20	0.70
1:B:146:THR:HA	1:B:150:ALA:HB3	1.74	0.69
1:B:21:LEU:HD23	1:B:21:LEU:O	1.92	0.69
1:B:549:ILE:O	1:B:553:CYS:HB3	1.91	0.69
1:B:61:GLY:O	1:B:63:ASP:N	2.25	0.69
1:B:423:VAL:HG12	1:B:427:LEU:HD12	1.74	0.69
1:B:382:TRP:CZ2	1:B:386:LYS:HD2	2.27	0.69
1:B:531:ASN:HD21	1:B:538:PHE:HA	1.56	0.69
1:A:740:GLN:HB2	1:A:743:LEU:HD23	1.74	0.69
1:A:470:LYS:HE2	1:A:470:LYS:HA	1.72	0.69
1:A:157:ASN:HD22	1:A:157:ASN:H	1.40	0.69
1:A:71:GLU:CD	1:A:71:GLU:H	1.95	0.69
1:B:307:ALA:H	1:B:547:ASN:HD21	1.39	0.69
1:A:126:ASP:HB2	1:A:348:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:THR:HB	1:B:329:PRO:CD	2.23	0.69
1:A:482:SER:HA	1:A:485:ILE:HG23	1.75	0.68
1:A:56:GLN:HG3	1:A:89:CYS:HB2	1.73	0.68
1:A:18:ILE:HG12	1:A:48:VAL:HG22	1.74	0.68
1:A:714:ARG:HE	1:A:714:ARG:HA	1.59	0.68
1:B:228:VAL:HG12	1:B:229:PHE:N	2.09	0.68
1:B:700:ILE:CD1	1:B:700:ILE:H	2.03	0.68
1:B:35:ARG:HH12	1:B:77:LEU:HD22	1.56	0.68
1:B:696:ARG:O	1:B:698:GLY:N	2.24	0.68
1:B:179:ASP:HB3	1:B:309:ASP:OD2	1.94	0.68
1:B:275:THR:HG23	1:B:278:GLY:N	2.03	0.68
1:A:38:VAL:HA	1:A:48:VAL:HG11	1.74	0.68
1:A:71:GLU:N	1:A:71:GLU:OE1	2.21	0.68
1:B:470:LYS:HE2	1:B:471:ARG:H	1.58	0.68
1:A:397:LYS:O	1:A:398:SER:HB3	1.93	0.68
1:B:333:ALA:O	1:B:348:LEU:N	2.27	0.68
1:B:256:ARG:O	1:B:257:LEU:HB3	1.94	0.68
1:B:387:LEU:HD21	1:B:428:ILE:HG21	1.76	0.67
1:B:387:LEU:O	1:B:390:HIS:HB2	1.94	0.67
1:B:419:VAL:HG11	1:B:467:LEU:HD11	1.75	0.67
1:B:22:THR:CG2	1:B:84:ILE:HB	2.24	0.67
1:A:157:ASN:N	1:A:157:ASN:HD22	1.88	0.67
1:A:22:THR:O	1:A:54:GLY:HA2	1.93	0.67
1:B:358:VAL:HG22	1:B:373:LEU:HB3	1.76	0.67
1:A:307:ALA:O	1:A:311:ILE:HG13	1.94	0.67
1:A:548:THR:O	1:A:552:THR:HG23	1.95	0.67
1:A:239:TRP:CD1	1:A:239:TRP:C	2.68	0.67
1:B:551:THR:HG22	1:B:552:THR:H	1.60	0.67
1:B:232:GLU:O	1:B:371:MET:HG2	1.95	0.67
1:A:636:THR:HG23	1:A:639:PHE:H	1.61	0.66
1:A:595:ILE:HD12	1:A:746:ARG:NH1	2.10	0.66
1:B:229:PHE:HD1	1:B:262:VAL:HG22	1.60	0.66
1:A:491:GLN:O	1:A:691:ILE:HD12	1.94	0.66
1:A:485:ILE:CD1	1:A:517:GLU:HB3	2.20	0.66
1:B:12:LEU:HG	1:B:325:LEU:HD13	1.77	0.66
1:B:470:LYS:HE2	1:B:470:LYS:HA	1.77	0.66
1:B:350:GLU:O	1:B:354:VAL:HG23	1.95	0.66
1:B:412:ALA:O	1:B:415:MET:HG3	1.96	0.66
1:A:595:ILE:HG23	1:A:746:ARG:HH12	1.60	0.66
1:B:435:VAL:CG1	1:B:467:LEU:HD21	2.26	0.65
1:A:521:PRO:HB3	1:A:707:SER:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:O	1:A:189:VAL:HG23	1.95	0.65
1:A:228:VAL:HG12	1:A:229:PHE:N	2.11	0.65
1:A:284:VAL:HA	1:A:288:GLY:HA2	1.79	0.65
1:B:90:LYS:HZ3	1:B:93:ARG:HH12	1.45	0.65
1:B:90:LYS:HZ2	1:B:93:ARG:NH1	1.94	0.65
1:A:297:GLY:O	1:A:299:VAL:HG13	1.97	0.65
1:A:756:GLU:O	1:A:756:GLU:HG2	1.96	0.65
1:B:552:THR:HG22	1:B:555:ARG:HH22	1.60	0.65
1:B:185:ILE:HD12	1:B:185:ILE:O	1.96	0.65
1:A:56:GLN:NE2	1:A:87:ALA:HB1	2.12	0.65
1:B:502:TYR:OH	1:B:730:THR:CG2	2.45	0.65
1:B:658:VAL:CG1	1:B:658:VAL:O	2.45	0.65
1:A:167:ASN:HB3	1:A:214:TYR:CD1	2.32	0.65
1:A:394:PRO:O	1:A:396:PRO:HD3	1.97	0.65
1:A:521:PRO:HB3	1:A:707:SER:CB	2.27	0.65
1:A:711:LEU:HD11	1:A:718:LEU:HB3	1.79	0.64
1:B:619:THR:HG23	1:B:620:VAL:H	1.62	0.64
1:A:570:ILE:HB	1:A:626:LEU:HD23	1.79	0.64
1:A:69:THR:CG2	1:A:72:SER:HB3	2.19	0.64
1:B:159:VAL:HG23	1:B:324:LEU:CD2	2.28	0.64
1:A:49:PHE:CD1	1:A:110:ILE:HD11	2.33	0.64
1:B:641:PHE:CG	1:B:656:LYS:HG2	2.32	0.64
1:B:506:LEU:CD2	1:B:723:VAL:HB	2.28	0.64
1:B:731:ASP:OD1	1:B:731:ASP:O	2.16	0.64
1:A:308:PHE:CZ	1:A:312:LEU:HD22	2.31	0.64
1:A:364:GLU:C	1:A:366:ARG:H	2.01	0.64
1:B:624:LEU:HD12	1:B:625:VAL:N	2.12	0.64
1:B:90:LYS:NZ	1:B:93:ARG:HH12	1.96	0.64
1:B:168:ASP:OD1	1:B:169:PHE:N	2.31	0.64
1:B:12:LEU:HG	1:B:325:LEU:CD1	2.28	0.64
1:B:723:VAL:HG23	1:B:724:THR:H	1.63	0.64
1:A:657:ASN:HD22	1:A:657:ASN:N	1.95	0.63
1:B:44:THR:HG21	1:B:325:LEU:HD11	1.79	0.63
1:B:465:SER:O	1:B:466:LYS:HB2	1.96	0.63
1:B:535:GLY:O	1:B:712:GLY:HA3	1.97	0.63
1:A:262:VAL:HG12	1:A:263:ALA:O	1.97	0.63
1:B:409:GLY:HA2	1:B:471:ARG:HB3	1.81	0.63
1:B:60:ASP:N	1:B:60:ASP:OD1	2.29	0.63
1:A:98:ARG:O	1:A:99:LEU:C	2.36	0.63
1:A:22:THR:HG21	1:A:82:THR:OG1	1.99	0.63
1:B:459:TRP:HA	1:B:462:GLN:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG21	1:A:318:VAL:HG22	1.81	0.63
1:A:595:ILE:HD12	1:A:746:ARG:NH2	2.14	0.63
1:B:58:LEU:HA	1:B:65:ILE:HD11	1.81	0.63
1:A:393:PRO:HG3	1:A:453:TRP:CE3	2.34	0.63
1:B:229:PHE:CD1	1:B:262:VAL:HG22	2.33	0.63
1:B:402:THR:HG21	1:B:489:ASN:HD22	1.63	0.63
1:A:745:LEU:C	1:A:747:PRO:HD2	2.20	0.62
1:A:103:HIS:CE1	1:A:144:LYS:HG2	2.33	0.62
1:A:352:VAL:HA	1:A:355:THR:HG22	1.80	0.62
1:A:715:LYS:O	1:A:716:ARG:HB3	1.99	0.62
1:B:713:MET:CG	1:B:718:LEU:HD12	2.30	0.62
1:B:566:ARG:CG	1:B:653:ASP:HB3	2.26	0.62
1:A:21:LEU:HD23	1:A:21:LEU:O	1.99	0.62
1:A:731:ASP:OD1	1:A:731:ASP:C	2.38	0.62
1:B:713:MET:HG3	1:B:718:LEU:HD12	1.81	0.62
1:A:485:ILE:HD13	1:A:485:ILE:C	2.20	0.62
1:A:512:ARG:CD	1:A:519:CYS:HA	2.26	0.61
1:A:168:ASP:OD2	1:A:169:PHE:N	2.32	0.61
1:A:65:ILE:HB	1:A:108:ARG:HH12	1.64	0.61
1:B:250:THR:HG22	1:B:255:SER:CB	2.29	0.61
1:B:393:PRO:HB3	1:B:453:TRP:HE3	1.66	0.61
1:B:456:VAL:O	1:B:459:TRP:CD1	2.53	0.61
1:A:745:LEU:O	1:A:746:ARG:C	2.39	0.61
1:A:409:GLY:HA2	1:A:471:ARG:HB3	1.81	0.61
1:B:188:ILE:O	1:B:192:ILE:HG23	2.00	0.61
1:B:475:LYS:O	1:B:477:SER:N	2.34	0.61
1:B:531:ASN:HD21	1:B:538:PHE:CA	2.12	0.61
1:B:585:GLY:CA	1:B:626:LEU:HD12	2.31	0.61
1:A:601:THR:HG22	1:A:604:ASP:OD2	2.01	0.61
1:B:307:ALA:H	1:B:547:ASN:ND2	1.98	0.61
1:B:577:CYS:HA	1:B:597:GLU:OE2	2.01	0.61
1:A:234:PRO:HG2	1:A:367:PHE:CE1	2.35	0.61
1:A:646:GLU:HA	1:A:649:LYS:HD3	1.82	0.61
1:B:234:PRO:HB3	1:B:267:ILE:CD1	2.30	0.61
1:B:297:GLY:O	1:B:299:VAL:HG13	2.01	0.61
1:B:753:ALA:O	1:B:754:LYS:HB2	2.00	0.61
1:B:367:PHE:O	1:B:370:ALA:N	2.33	0.61
1:B:624:LEU:HD12	1:B:625:VAL:H	1.64	0.61
1:A:21:LEU:HD23	1:A:21:LEU:C	2.21	0.61
1:B:364:GLU:C	1:B:366:ARG:H	2.04	0.61
1:B:39:ARG:CD	1:B:70:TRP:CE2	2.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:CYS:O	1:B:355:THR:HB	2.00	0.61
1:B:145:ILE:HG22	1:B:145:ILE:O	2.00	0.60
1:B:192:ILE:HD13	1:B:203:PHE:CE2	2.35	0.60
1:B:275:THR:O	1:B:279:VAL:HG23	2.01	0.60
1:B:618:THR:HG22	1:B:619:THR:N	2.16	0.60
1:A:56:GLN:O	1:A:59:VAL:N	2.33	0.60
1:A:31:ASN:HD21	1:A:83:VAL:HG23	1.66	0.60
1:B:34:VAL:O	1:B:38:VAL:HG23	2.01	0.60
1:B:262:VAL:HG12	1:B:263:ALA:O	2.00	0.60
1:B:131:GLU:C	1:B:135:LEU:HG	2.22	0.60
1:A:173:ASP:OD2	1:A:339:SER:HA	2.02	0.60
1:A:420:ARG:HD2	1:A:456:VAL:O	2.02	0.60
1:A:461:GLY:HA2	1:A:673:ARG:NH1	2.17	0.60
1:A:646:GLU:HG3	1:B:634:ASN:HB2	1.82	0.60
1:A:352:VAL:C	1:A:354:VAL:H	2.03	0.60
1:A:387:LEU:CD2	1:A:428:ILE:HG21	2.32	0.60
1:B:366:ARG:HH11	1:B:366:ARG:HB3	1.65	0.60
1:A:323:ALA:HA	1:A:345:ARG:NH1	2.17	0.60
1:A:204:VAL:HB	1:A:293:VAL:HG22	1.84	0.59
1:A:645:SER:O	1:A:646:GLU:C	2.40	0.59
2:B:765:ADP:H5'1	2:B:765:ADP:O1B	2.02	0.59
1:A:49:PHE:CE2	1:A:67:GLU:HG3	2.38	0.59
1:A:69:THR:HG23	1:A:72:SER:H	1.67	0.59
1:A:157:ASN:ND2	1:A:157:ASN:H	1.99	0.59
2:B:763:ADP:H5'2	2:B:763:ADP:C8	2.38	0.59
1:B:95:ARG:HA	1:B:98:ARG:CG	2.33	0.59
1:B:204:VAL:C	1:B:205:LEU:HD23	2.23	0.59
1:B:208:MET:HA	1:B:208:MET:HE2	1.85	0.59
1:A:714:ARG:O	1:A:715:LYS:C	2.40	0.59
1:A:726:LEU:HD23	1:A:729:GLN:OE1	2.02	0.59
1:B:200:GLN:HB3	1:B:251:ARG:CZ	2.32	0.59
1:B:299:VAL:O	1:B:302:GLY:N	2.28	0.59
1:B:531:ASN:ND2	1:B:538:PHE:HA	2.17	0.59
1:B:627:ARG:HG2	1:B:627:ARG:HH11	1.68	0.59
1:A:441:GLU:CG	1:A:472:THR:HG21	2.32	0.59
1:B:605:LEU:O	1:B:609:VAL:HG23	2.03	0.59
1:A:70:TRP:HB3	1:A:71:GLU:OE1	2.03	0.59
1:B:182:LEU:HD11	1:B:218:VAL:HG11	1.85	0.58
1:B:221:LEU:HD13	1:B:385:TYR:HB2	1.85	0.58
1:B:71:GLU:O	1:B:74:SER:HB3	2.02	0.58
1:A:419:VAL:O	1:A:423:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:VAL:HG12	1:A:534:PRO:O	2.02	0.58
1:A:634:ASN:HB2	1:B:646:GLU:CG	2.33	0.58
1:A:657:ASN:N	1:A:657:ASN:ND2	2.50	0.58
1:B:595:ILE:HD12	1:B:746:ARG:HH12	1.67	0.58
1:A:361:ALA:HB1	1:A:369:GLU:HG3	1.84	0.58
1:A:376:ARG:HH21	1:A:376:ARG:CA	2.06	0.58
1:A:573:MET:HE3	1:A:661:HIS:HA	1.85	0.58
1:A:50:PHE:O	1:A:51:VAL:HB	2.04	0.58
1:A:563:THR:O	1:A:564:LYS:O	2.21	0.58
1:A:609:VAL:C	1:A:611:HIS:N	2.57	0.58
1:B:22:THR:HG21	1:B:82:THR:OG1	2.02	0.58
1:A:595:ILE:CG2	1:A:746:ARG:HH12	2.16	0.58
1:B:9:ALA:C	1:B:11:THR:H	2.07	0.58
1:A:201:ARG:HG2	1:A:290:ASP:OD2	2.04	0.58
1:A:327:GLY:O	1:A:328:THR:HG22	2.03	0.58
1:B:493:LEU:CD2	1:B:495:ILE:HD11	2.33	0.58
1:B:523:VAL:HG22	1:B:686:TRP:CZ3	2.38	0.58
1:B:744:LYS:O	1:B:747:PRO:HD2	2.04	0.58
1:A:358:VAL:HG22	1:A:373:LEU:HB3	1.86	0.58
1:B:355:THR:CG2	1:B:356:LYS:N	2.66	0.58
1:B:549:ILE:O	1:B:553:CYS:CB	2.51	0.58
1:A:191:ALA:O	1:A:193:THR:N	2.36	0.58
1:A:582:THR:OG1	1:A:746:ARG:NH1	2.35	0.58
1:B:643:LEU:O	1:B:643:LEU:HD12	2.03	0.58
1:A:123:THR:HA	1:A:126:ASP:HB3	1.86	0.57
1:B:218:VAL:HG13	1:B:674:ASN:HD21	1.68	0.57
1:A:407:ASN:HA	1:A:496:ILE:O	2.03	0.57
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.86	0.57
1:A:605:LEU:HD21	1:A:640:ILE:HD13	1.86	0.57
1:B:336:VAL:HG23	1:B:336:VAL:O	2.04	0.57
1:A:58:LEU:HD11	1:A:105:LEU:HD21	1.86	0.57
1:A:159:VAL:HG23	1:A:324:LEU:CD2	2.34	0.57
1:B:349:MET:O	1:B:352:VAL:HG23	2.04	0.57
1:A:352:VAL:O	1:A:354:VAL:N	2.37	0.57
1:B:211:HIS:HB3	1:B:362:MET:HE1	1.87	0.57
1:B:39:ARG:HD2	1:B:70:TRP:CH2	2.39	0.57
1:B:184:ARG:HA	1:B:187:GLU:OE2	2.05	0.57
1:B:566:ARG:O	1:B:616:MET:HE1	2.04	0.57
1:A:145:ILE:CD1	1:A:147:ALA:HB3	2.35	0.57
1:A:172:THR:CB	1:A:337:SER:OG	2.52	0.57
1:B:214:TYR:CZ	1:B:218:VAL:HG21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLY:O	1:B:662:MET:N	2.38	0.57
1:A:158:ILE:HD12	1:A:158:ILE:O	2.05	0.57
1:A:312:LEU:HD12	1:A:312:LEU:O	2.04	0.57
1:B:247:LEU:HD11	1:B:260:ILE:HD11	1.87	0.57
1:A:331:THR:HG23	1:A:332:PRO:HD2	1.87	0.56
1:A:413:ALA:HB1	1:A:668:PRO:HA	1.87	0.56
1:B:669:THR:HB	1:B:670:PRO:HD2	1.85	0.56
1:A:560:ALA:C	1:A:562:GLY:H	2.08	0.56
1:B:243:LEU:O	1:B:243:LEU:HD12	2.04	0.56
1:B:315:ARG:O	1:B:318:VAL:HG23	2.05	0.56
1:B:455:TYR:HE2	1:B:459:TRP:CZ2	2.23	0.56
1:A:113:LEU:HB3	1:A:158:ILE:CG2	2.25	0.56
1:B:323:ALA:N	1:B:345:ARG:HH21	2.04	0.56
1:B:440:PHE:O	1:B:443:PRO:HD2	2.05	0.56
1:A:108:ARG:HB2	1:A:110:ILE:HD13	1.87	0.56
1:A:239:TRP:HA	1:A:242:HIS:HB2	1.87	0.56
1:A:259:ILE:HG22	1:A:261:ILE:HD12	1.87	0.56
1:A:424:ARG:HD2	1:A:453:TRP:CE2	2.40	0.56
1:B:729:GLN:O	1:B:738:LYS:HG3	2.06	0.56
1:A:491:GLN:HA	1:A:520:ILE:HG21	1.86	0.56
1:B:203:PHE:HB3	1:B:205:LEU:HD21	1.88	0.56
1:B:296:LEU:CD1	1:B:296:LEU:H	2.13	0.56
1:B:481:ILE:C	1:B:481:ILE:HD12	2.25	0.56
1:A:249:GLU:O	1:A:252:THR:HG22	2.06	0.56
1:A:52:HIS:HA	1:A:84:ILE:HD12	1.86	0.56
1:B:595:ILE:HD11	1:B:598:GLU:HB3	1.87	0.56
1:A:331:THR:HG22	1:A:332:PRO:O	2.06	0.56
1:A:374:ARG:HG2	1:A:378:PHE:CD2	2.41	0.56
1:B:455:TYR:CE2	1:B:459:TRP:CZ2	2.94	0.56
1:B:473:LEU:HD21	1:B:503:THR:CG2	2.35	0.56
1:A:163:GLY:HA2	1:A:176:ILE:HB	1.87	0.56
1:A:398:SER:OG	1:A:399:GLY:N	2.38	0.56
1:B:299:VAL:C	1:B:301:ARG:N	2.59	0.56
1:A:500:GLU:N	1:A:500:GLU:OE1	2.39	0.55
1:B:172:THR:HB	1:B:337:SER:HB2	1.89	0.55
1:B:208:MET:HB2	1:B:300:GLN:OE1	2.06	0.55
1:B:473:LEU:CD2	1:B:503:THR:HG22	2.36	0.55
2:B:764:ADP:H2'	2:B:764:ADP:N3	2.20	0.55
1:A:214:TYR:CE2	1:A:218:VAL:CG2	2.87	0.55
1:A:267:ILE:HA	1:A:273:PRO:HA	1.87	0.55
1:A:646:GLU:CG	1:B:634:ASN:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLU:HB3	1:B:135:LEU:HD21	1.88	0.55
1:B:475:LYS:C	1:B:477:SER:H	2.09	0.55
1:B:95:ARG:HA	1:B:98:ARG:HG3	1.87	0.55
1:A:169:PHE:CZ	1:A:351:CYS:HB3	2.41	0.55
1:A:186:THR:HG22	1:A:190:ASP:OD2	2.05	0.55
1:A:514:GLN:HB3	1:A:515:PHE:CE1	2.41	0.55
1:B:190:ASP:O	1:B:194:THR:HG23	2.07	0.55
1:B:361:ALA:HB1	1:B:369:GLU:HB3	1.86	0.55
1:B:456:VAL:HA	1:B:459:TRP:CE2	2.41	0.55
1:A:111:THR:O	1:A:156:LEU:HA	2.07	0.55
1:A:352:VAL:HG23	1:A:353:GLN:H	1.71	0.55
1:A:446:GLY:C	1:A:448:ILE:HD12	2.27	0.55
1:A:566:ARG:HG3	1:A:653:ASP:HB3	1.89	0.55
1:B:218:VAL:HG13	1:B:674:ASN:ND2	2.22	0.55
1:A:265:GLY:O	1:A:267:ILE:HG23	2.07	0.55
1:A:655:ARG:HG2	1:A:655:ARG:NH2	2.22	0.55
1:A:689:GLY:O	1:A:692:LYS:N	2.40	0.55
1:A:436:VAL:HG11	1:A:443:PRO:HD3	1.88	0.55
1:A:595:ILE:HD11	1:A:598:GLU:HB3	1.87	0.55
1:B:470:LYS:HE2	1:B:470:LYS:CA	2.36	0.55
1:A:441:GLU:HG3	1:A:472:THR:CG2	2.34	0.55
1:A:56:GLN:HE21	1:A:89:CYS:H	1.53	0.55
1:A:715:LYS:O	1:A:715:LYS:HG2	2.06	0.55
1:B:348:LEU:HD23	1:B:352:VAL:HG22	1.88	0.55
1:B:456:VAL:HA	1:B:459:TRP:NE1	2.22	0.55
1:B:642:ASN:HD22	1:B:642:ASN:N	2.04	0.55
1:A:715:LYS:O	1:A:715:LYS:CG	2.52	0.55
1:B:713:MET:HG3	1:B:718:LEU:CD1	2.37	0.55
1:A:521:PRO:HG2	1:A:691:ILE:HD13	1.88	0.55
1:B:28:GLN:HB3	1:B:305:PRO:HB3	1.88	0.55
1:B:470:LYS:HE2	1:B:471:ARG:N	2.21	0.55
1:A:239:TRP:CD1	1:A:240:GLU:N	2.75	0.55
1:B:625:VAL:HG11	1:B:644:TYR:HE1	1.71	0.54
1:A:371:MET:SD	1:A:378:PHE:HE2	2.30	0.54
1:B:543:ASP:HB3	1:B:672:ASP:OD2	2.07	0.54
1:A:43:PHE:C	1:A:45:GLY:H	2.11	0.54
1:A:747:PRO:O	1:A:751:ILE:HG12	2.08	0.54
1:B:450:GLU:HG2	1:B:451:ALA:H	1.71	0.54
1:B:455:TYR:CE2	1:B:459:TRP:HZ2	2.25	0.54
1:A:349:MET:O	1:A:350:GLU:C	2.45	0.54
1:A:620:VAL:CG1	1:A:621:LYS:N	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:HA	1:B:45:GLY:O	2.07	0.54
1:A:352:VAL:HG23	1:A:353:GLN:N	2.23	0.54
1:A:546:LEU:O	1:A:546:LEU:HG	2.06	0.54
1:B:131:GLU:O	1:B:135:LEU:HG	2.08	0.54
1:B:191:ALA:C	1:B:193:THR:H	2.10	0.54
1:B:39:ARG:HD2	1:B:70:TRP:CE2	2.43	0.54
1:A:440:PHE:C	1:A:442:GLY:N	2.60	0.54
1:A:492:GLY:HA3	1:A:687:MET:HE1	1.90	0.54
1:B:230:ILE:HD13	1:B:230:ILE:N	2.22	0.54
1:B:319:GLU:HG2	1:B:343:ALA:HB1	1.88	0.54
1:A:275:THR:HG1	1:A:277:GLU:HG2	1.72	0.54
1:A:172:THR:HB	1:A:337:SER:HG	1.73	0.54
1:A:522:PHE:CD2	1:A:708:GLY:HA2	2.43	0.54
1:A:729:GLN:C	1:A:738:LYS:HD3	2.27	0.54
1:B:588:ALA:O	1:B:590:ALA:N	2.40	0.54
1:B:745:LEU:C	1:B:747:PRO:HD2	2.28	0.54
1:A:296:LEU:O	1:A:297:GLY:O	2.24	0.54
1:A:619:THR:HG23	1:A:620:VAL:H	1.73	0.54
1:A:413:ALA:HB1	1:A:668:PRO:CA	2.38	0.54
1:B:555:ARG:HH11	1:B:555:ARG:HB2	1.72	0.54
1:B:644:TYR:O	1:B:645:SER:C	2.45	0.54
1:B:709:CYS:HA	1:B:722:PRO:HA	1.90	0.54
1:B:34:VAL:HG21	1:B:84:ILE:CD1	2.38	0.54
1:A:280:LYS:O	1:A:284:VAL:HG23	2.08	0.54
1:A:593:ALA:HA	1:A:626:LEU:O	2.07	0.54
1:A:642:ASN:ND2	1:A:642:ASN:H	2.05	0.54
1:A:609:VAL:HG22	1:A:644:TYR:CE2	2.42	0.54
1:B:182:LEU:CD1	1:B:218:VAL:HG11	2.38	0.54
1:B:364:GLU:O	1:B:366:ARG:N	2.40	0.54
1:A:656:LYS:HD2	1:A:656:LYS:O	2.08	0.54
1:B:55:TYR:O	1:B:57:GLY:N	2.41	0.54
1:B:664:GLN:C	1:B:666:GLY:H	2.12	0.54
1:A:27:ALA:O	1:A:30:MET:HG3	2.09	0.53
1:B:230:ILE:H	1:B:230:ILE:HD13	1.72	0.53
1:A:113:LEU:CB	1:A:158:ILE:HG22	2.26	0.53
1:A:220:SER:HB3	1:A:225:ALA:HB3	1.89	0.53
1:A:551:THR:CG2	1:A:552:THR:N	2.71	0.53
1:B:235:PRO:HD2	1:B:267:ILE:O	2.08	0.53
1:B:459:TRP:N	1:B:459:TRP:CD1	2.75	0.53
1:B:679:MET:O	1:B:680:GLY:C	2.44	0.53
1:B:734:HIS:HB2	1:B:736:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:O	1:B:98:ARG:NE	2.38	0.53
1:B:228:VAL:HG12	1:B:229:PHE:H	1.72	0.53
1:A:514:GLN:HB3	1:A:515:PHE:CD1	2.43	0.53
1:B:239:TRP:CG	1:B:240:GLU:N	2.76	0.53
1:B:235:PRO:HG3	1:B:274:ILE:CD1	2.38	0.53
1:A:445:LYS:HB3	1:A:447:GLN:NE2	2.23	0.53
1:A:88:ARG:HH11	1:A:88:ARG:HG2	1.74	0.53
1:B:205:LEU:N	1:B:205:LEU:HD23	2.24	0.53
1:B:450:GLU:HG2	1:B:451:ALA:N	2.23	0.53
1:B:294:THR:HG22	1:B:295:VAL:N	2.24	0.53
1:B:573:MET:HG2	1:B:661:HIS:HA	1.91	0.53
1:B:722:PRO:HG2	1:B:725:GLU:HB2	1.91	0.53
1:B:304:THR:OG1	1:B:305:PRO:HD2	2.08	0.53
1:B:335:VAL:CG2	1:B:348:LEU:HA	2.38	0.53
1:A:163:GLY:O	1:A:164:SER:HB2	2.08	0.53
1:A:240:GLU:OE1	1:A:240:GLU:N	2.40	0.53
1:A:695:TYR:CZ	1:A:698:GLY:HA2	2.43	0.53
1:B:124:GLY:O	1:B:127:THR:HG22	2.09	0.53
1:B:203:PHE:H	1:B:203:PHE:HD1	1.55	0.53
1:B:255:SER:C	1:B:257:LEU:H	2.12	0.53
1:B:569:ILE:HG22	1:B:569:ILE:O	2.09	0.53
1:A:118:GLY:CA	2:A:763:ADP:O3B	2.56	0.53
1:B:21:LEU:HB2	1:B:51:VAL:HB	1.91	0.53
1:B:547:ASN:O	1:B:548:THR:C	2.48	0.53
1:A:655:ARG:HH21	1:A:655:ARG:HG2	1.73	0.53
1:A:523:VAL:HG21	1:A:683:ALA:HB1	1.91	0.53
1:B:38:VAL:HG21	1:B:73:VAL:HG11	1.90	0.53
1:B:389:ALA:O	1:B:390:HIS:O	2.27	0.53
1:B:578:GLY:H	1:B:597:GLU:CD	2.11	0.53
1:A:167:ASN:HA	1:A:175:THR:OG1	2.09	0.52
1:A:238:ASN:O	1:A:239:TRP:CB	2.49	0.52
1:B:243:LEU:HD11	1:B:247:LEU:HD11	1.91	0.52
1:B:535:GLY:C	1:B:714:ARG:HD2	2.28	0.52
1:A:139:LEU:O	1:A:143:GLY:HA3	2.10	0.52
1:B:311:ILE:HG12	1:B:586:LEU:HD23	1.90	0.52
1:B:33:ALA:O	1:B:37:VAL:HG23	2.10	0.52
1:B:435:VAL:HG11	1:B:467:LEU:HD21	1.89	0.52
1:A:382:TRP:CE2	1:A:386:LYS:HD2	2.44	0.52
1:A:435:VAL:HG13	1:A:467:LEU:HD22	1.90	0.52
1:A:531:ASN:ND2	1:A:539:SER:H	2.06	0.52
1:B:206:GLU:OE2	1:B:276:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:HA	1:A:242:HIS:CB	2.39	0.52
1:A:375:GLY:O	1:A:376:ARG:O	2.27	0.52
1:B:239:TRP:CD2	1:B:240:GLU:OE1	2.63	0.52
1:B:595:ILE:HD13	1:B:595:ILE:N	2.23	0.52
1:A:191:ALA:C	1:A:193:THR:N	2.60	0.52
1:A:726:LEU:O	1:A:729:GLN:HB2	2.09	0.52
1:B:39:ARG:NH1	1:B:39:ARG:HG3	2.22	0.52
1:B:432:ARG:HG2	1:B:432:ARG:HH11	1.74	0.52
1:A:173:ASP:HB3	2:A:764:ADP:C5'	2.34	0.52
1:A:360:LYS:O	1:A:364:GLU:OE2	2.27	0.52
1:A:566:ARG:HH21	1:A:566:ARG:CG	2.12	0.52
1:B:132:TRP:HZ2	1:B:153:SER:O	1.93	0.52
1:B:296:LEU:O	1:B:297:GLY:O	2.28	0.52
1:B:39:ARG:NE	1:B:70:TRP:CE2	2.77	0.52
1:A:140:GLN:NE2	1:A:144:LYS:O	2.43	0.52
1:B:158:ILE:HD13	1:B:158:ILE:O	2.10	0.52
1:B:184:ARG:HE	1:B:187:GLU:CD	2.13	0.52
1:B:231:PRO:C	1:B:233:CYS:H	2.12	0.52
1:A:634:ASN:HB2	1:B:646:GLU:HG2	1.92	0.52
1:A:239:TRP:O	1:A:240:GLU:C	2.48	0.52
1:A:435:VAL:HG13	1:A:467:LEU:CD2	2.40	0.52
1:A:35:ARG:CD	1:A:77:LEU:HD13	2.39	0.52
1:A:126:ASP:HB2	1:A:348:LEU:CD2	2.39	0.52
1:B:69:THR:O	1:B:72:SER:OG	2.27	0.52
1:A:392:ARG:HG2	1:A:393:PRO:HD3	1.92	0.52
1:A:88:ARG:NH1	1:A:88:ARG:HG2	2.24	0.52
1:B:267:ILE:HD12	1:B:268:ASP:O	2.09	0.52
1:B:299:VAL:C	1:B:301:ARG:H	2.12	0.52
1:A:18:ILE:HG22	1:A:112:ASN:HB2	1.92	0.51
1:B:477:SER:O	1:B:481:ILE:HG23	2.10	0.51
1:B:648:GLY:HA3	1:B:652:PHE:CZ	2.45	0.51
1:B:119:ASP:OD1	1:B:120:GLY:N	2.43	0.51
1:B:342:GLN:NE2	1:B:715:LYS:HG2	2.25	0.51
1:A:636:THR:HG23	1:A:639:PHE:N	2.23	0.51
1:B:560:ALA:HB3	1:B:622:ARG:HH22	1.74	0.51
1:A:746:ARG:N	1:A:747:PRO:HD2	2.26	0.51
1:B:120:GLY:O	1:B:123:THR:N	2.44	0.51
1:B:560:ALA:HB1	1:B:563:THR:HB	1.92	0.51
1:A:189:VAL:HG13	1:A:259:ILE:HD13	1.92	0.51
1:A:203:PHE:CD1	1:A:203:PHE:N	2.78	0.51
1:A:473:LEU:HD21	1:A:503:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ASN:HB2	1:B:646:GLU:HG3	1.93	0.51
1:B:190:ASP:O	1:B:193:THR:HG23	2.10	0.51
1:A:481:ILE:CG1	1:A:482:SER:N	2.73	0.51
1:B:237:ASP:O	1:B:239:TRP:N	2.43	0.51
1:B:312:LEU:O	1:B:316:MET:HG2	2.10	0.51
1:B:364:GLU:C	1:B:366:ARG:N	2.64	0.51
1:B:634:ASN:O	1:B:636:THR:N	2.44	0.51
1:A:82:THR:HG23	1:A:85:GLY:HA2	1.93	0.51
1:B:299:VAL:O	1:B:301:ARG:N	2.44	0.51
1:A:110:ILE:CD1	1:A:110:ILE:N	2.73	0.51
1:A:13:GLY:O	1:A:46:ALA:CA	2.59	0.51
1:A:333:ALA:HB1	1:A:348:LEU:HD12	1.92	0.51
1:B:59:VAL:HA	1:B:101:ALA:HB2	1.93	0.51
1:A:352:VAL:C	1:A:354:VAL:N	2.65	0.51
1:A:537:ASP:OD1	1:A:714:ARG:NH2	2.37	0.51
1:B:129:ARG:NH1	1:B:349:MET:SD	2.84	0.51
1:B:470:LYS:CE	1:B:470:LYS:HA	2.40	0.51
1:B:521:PRO:HA	1:B:707:SER:O	2.10	0.51
1:A:555:ARG:O	1:A:556:ILE:C	2.48	0.50
1:B:117:GLY:O	1:B:163:GLY:N	2.44	0.50
1:B:376:ARG:HG3	1:B:376:ARG:NH2	2.24	0.50
1:B:459:TRP:H	1:B:459:TRP:HD1	1.59	0.50
1:B:569:ILE:HD11	1:B:644:TYR:CD1	2.46	0.50
1:B:605:LEU:HD21	1:B:640:ILE:HG12	1.92	0.50
1:B:658:VAL:O	1:B:659:LEU:C	2.48	0.50
1:B:686:TRP:CG	1:B:720:PHE:CE2	2.99	0.50
1:A:642:ASN:ND2	1:A:642:ASN:N	2.57	0.50
1:B:219:THR:HG23	1:B:220:SER:N	2.25	0.50
1:B:609:VAL:HA	1:B:644:TYR:HE2	1.76	0.50
1:A:154:SER:O	1:A:329:PRO:HB3	2.12	0.50
1:A:606:GLN:CD	1:B:606:GLN:OE1	2.50	0.50
1:B:700:ILE:CD1	1:B:700:ILE:N	2.68	0.50
1:B:726:LEU:O	1:B:729:GLN:HB2	2.12	0.50
1:A:128:PHE:C	1:A:130:SER:N	2.64	0.50
1:A:335:VAL:O	1:A:335:VAL:HG12	2.11	0.50
1:A:670:PRO:HA	1:A:673:ARG:HD2	1.93	0.50
1:B:750:LYS:O	1:B:755:TYR:HB2	2.11	0.50
1:A:353:GLN:O	1:A:357:ASP:OD1	2.29	0.50
1:A:402:THR:HG21	1:A:432:ARG:HH21	1.76	0.50
1:A:711:LEU:HD22	1:A:720:PHE:CE2	2.47	0.50
1:B:392:ARG:HB3	1:B:393:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:O	1:A:113:LEU:HD12	2.11	0.50
1:B:124:GLY:HA2	1:B:127:THR:HG22	1.92	0.50
1:B:203:PHE:N	1:B:203:PHE:CD1	2.79	0.50
1:B:417:ALA:O	1:B:420:ARG:HB3	2.12	0.50
1:A:239:TRP:CG	1:A:240:GLU:N	2.80	0.50
1:A:283:VAL:HG23	1:A:289:TYR:HE1	1.77	0.50
1:A:312:LEU:O	1:A:316:MET:HG2	2.12	0.50
1:A:360:LYS:O	1:A:362:MET:N	2.45	0.50
1:B:658:VAL:O	1:B:660:GLY:N	2.44	0.50
1:B:665:GLY:O	1:B:666:GLY:C	2.48	0.50
1:A:366:ARG:O	1:A:369:GLU:HB3	2.12	0.50
1:A:377:SER:O	1:A:380:ASN:N	2.44	0.50
1:A:590:ALA:HA	1:A:624:LEU:HB3	1.94	0.50
1:B:402:THR:HG21	1:B:489:ASN:ND2	2.27	0.50
1:A:454:SER:O	1:A:455:TYR:C	2.51	0.49
1:B:101:ALA:O	1:B:104:ASN:HB2	2.10	0.49
1:B:731:ASP:OD1	1:B:731:ASP:C	2.50	0.49
1:A:88:ARG:O	2:A:763:ADP:H3'	2.12	0.49
1:B:202:THR:O	1:B:202:THR:HG22	2.12	0.49
1:B:738:LYS:O	1:B:739:GLU:HB2	2.11	0.49
1:B:73:VAL:HA	1:B:76:MET:SD	2.51	0.49
1:A:711:LEU:HD11	1:A:718:LEU:HD23	1.93	0.49
1:B:254:GLY:O	1:B:255:SER:C	2.50	0.49
1:A:184:ARG:HA	1:A:187:GLU:OE2	2.13	0.49
1:B:567:VAL:CG2	1:B:616:MET:HE1	2.38	0.49
1:B:88:ARG:O	2:B:763:ADP:H3'	2.11	0.49
1:A:502:TYR:CE2	1:A:534:PRO:HG2	2.48	0.49
1:A:604:ASP:O	1:A:605:LEU:C	2.50	0.49
1:A:632:ASN:C	1:A:632:ASN:OD1	2.50	0.49
1:B:159:VAL:HG21	1:B:324:LEU:HG	1.95	0.49
1:A:475:LYS:O	1:A:477:SER:N	2.46	0.49
1:A:521:PRO:HA	1:A:707:SER:HB2	1.95	0.49
1:A:657:ASN:ND2	1:A:657:ASN:H	2.11	0.49
1:B:535:GLY:HA2	1:B:714:ARG:HH11	1.77	0.49
1:A:415:MET:O	1:A:419:VAL:HG23	2.13	0.49
1:B:299:VAL:CG2	1:B:300:GLN:N	2.75	0.49
1:B:50:PHE:N	1:B:66:ARG:O	2.45	0.49
1:A:55:TYR:OH	1:A:125:ALA:HB2	2.13	0.49
1:B:21:LEU:HD23	1:B:21:LEU:C	2.32	0.49
1:B:239:TRP:CD1	1:B:240:GLU:N	2.80	0.49
1:B:359:THR:OG1	1:B:360:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HD12	1:A:158:ILE:C	2.33	0.49
1:A:261:ILE:HD12	1:A:261:ILE:N	2.26	0.49
1:A:319:GLU:HG3	1:A:336:VAL:CG1	2.43	0.49
1:A:448:ILE:HD13	1:A:488:PHE:CE1	2.48	0.49
1:B:275:THR:CG2	1:B:278:GLY:H	2.12	0.49
1:B:481:ILE:O	1:B:485:ILE:HG13	2.13	0.49
1:B:529:VAL:HG13	1:B:545:ALA:HB2	1.94	0.49
1:A:241:ASP:O	1:A:242:HIS:C	2.51	0.48
1:A:59:VAL:O	1:A:60:ASP:O	2.31	0.48
1:B:65:ILE:CG2	1:B:108:ARG:NH1	2.76	0.48
1:B:509:MET:O	1:B:512:ARG:CB	2.55	0.48
1:B:551:THR:CG2	1:B:552:THR:N	2.64	0.48
1:B:569:ILE:HD11	1:B:644:TYR:HD1	1.79	0.48
1:A:510:GLU:OE1	1:A:510:GLU:HA	2.12	0.48
1:A:646:GLU:O	1:A:649:LYS:HB2	2.12	0.48
1:B:59:VAL:HA	1:B:101:ALA:CB	2.43	0.48
1:B:239:TRP:CH2	1:B:274:ILE:HD13	2.48	0.48
1:A:20:VAL:HG23	1:A:114:CYS:SG	2.54	0.48
1:A:51:VAL:O	1:A:51:VAL:HG12	2.11	0.48
1:B:211:HIS:HB3	1:B:362:MET:CE	2.43	0.48
1:B:306:SER:O	1:B:310:ARG:HG3	2.13	0.48
2:B:763:ADP:H8	2:B:763:ADP:H5'2	1.79	0.48
1:A:247:LEU:HD22	1:A:258:ASN:ND2	2.29	0.48
1:A:335:VAL:CG2	1:A:348:LEU:HG	2.43	0.48
1:A:401:TYR:O	1:A:431:ASN:HB3	2.14	0.48
1:A:628:ASN:HB3	1:A:631:CYS:HB3	1.96	0.48
1:B:289:TYR:O	1:B:291:THR:OG1	2.29	0.48
1:B:302:GLY:O	1:B:303:GLY:O	2.32	0.48
1:B:55:TYR:O	1:B:58:LEU:N	2.43	0.48
1:A:522:PHE:CD2	1:A:522:PHE:C	2.86	0.48
1:A:56:GLN:O	1:A:58:LEU:N	2.46	0.48
1:B:157:ASN:OD1	1:B:324:LEU:HD23	2.13	0.48
1:B:371:MET:CE	1:B:379:MET:HG2	2.44	0.48
1:A:371:MET:SD	1:A:378:PHE:CE2	3.06	0.48
1:A:689:GLY:O	1:A:690:LYS:C	2.52	0.48
1:A:97:GLY:O	1:A:100:ARG:HB3	2.13	0.48
1:B:18:ILE:HG22	1:B:19:ALA:N	2.29	0.48
1:B:228:VAL:CG1	1:B:229:PHE:N	2.76	0.48
1:B:251:ARG:HE	1:B:251:ARG:HA	1.78	0.48
1:B:281:ASP:O	1:B:282:LEU:C	2.51	0.48
1:A:209:GLY:O	1:A:210:ARG:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ILE:HD11	1:A:518:LEU:HD21	1.94	0.48
1:B:22:THR:HG22	1:B:84:ILE:HB	1.95	0.48
1:A:327:GLY:C	1:A:328:THR:CG2	2.82	0.48
1:A:543:ASP:O	1:A:547:ASN:HB2	2.14	0.48
1:B:287:LEU:HB3	1:B:289:TYR:CE2	2.49	0.48
1:B:289:TYR:O	1:B:291:THR:N	2.47	0.48
1:B:424:ARG:HD2	1:B:453:TRP:CZ2	2.49	0.48
1:B:555:ARG:HG2	1:B:556:ILE:N	2.29	0.48
1:B:741:TRP:CD2	1:B:742:TRP:N	2.82	0.48
1:A:349:MET:HA	1:A:352:VAL:CG2	2.44	0.47
1:A:561:ALA:HA	1:A:622:ARG:NH1	2.29	0.47
1:A:403:VAL:HG21	1:A:684:MET:HE3	1.95	0.47
1:B:144:LYS:O	1:B:145:ILE:HB	2.14	0.47
1:A:145:ILE:HD13	1:A:147:ALA:HB3	1.96	0.47
1:B:239:TRP:C	1:B:239:TRP:CD1	2.87	0.47
1:B:30:MET:O	1:B:34:VAL:HG23	2.14	0.47
1:A:132:TRP:HA	1:A:135:LEU:HD12	1.95	0.47
1:A:239:TRP:O	1:A:242:HIS:N	2.47	0.47
1:B:65:ILE:HG22	1:B:65:ILE:O	2.15	0.47
1:B:35:ARG:HH11	1:B:77:LEU:HB2	1.80	0.47
1:A:199:HIS:O	1:A:201:ARG:N	2.36	0.47
1:A:246:ARG:HB3	1:A:246:ARG:HE	1.51	0.47
1:B:308:PHE:CZ	1:B:312:LEU:HD22	2.50	0.47
1:B:546:LEU:CD1	1:B:584:ALA:HB2	2.43	0.47
1:A:652:PHE:HD1	1:A:653:ASP:O	1.96	0.47
1:B:167:ASN:HA	1:B:175:THR:OG1	2.14	0.47
1:B:36:ALA:HB3	1:B:317:GLY:HA3	1.95	0.47
1:B:499:PHE:CZ	1:B:735:ARG:HA	2.50	0.47
1:B:687:MET:HE2	1:B:687:MET:HB3	1.70	0.47
1:B:687:MET:HE3	1:B:691:ILE:HG13	1.97	0.47
1:A:191:ALA:C	1:A:193:THR:H	2.17	0.47
1:B:512:ARG:HG2	1:B:519:CYS:SG	2.55	0.47
1:A:606:GLN:NE2	1:B:602:ILE:HG23	2.28	0.47
1:A:292:ARG:HG2	1:A:293:VAL:N	2.30	0.47
1:A:360:LYS:O	1:A:363:ASP:N	2.47	0.47
1:A:424:ARG:HD2	1:A:453:TRP:CD2	2.50	0.47
1:B:660:GLY:O	1:B:661:HIS:C	2.53	0.47
1:B:723:VAL:HG23	1:B:724:THR:N	2.28	0.47
1:A:167:ASN:CB	1:A:178:THR:HG21	2.42	0.47
1:A:631:CYS:O	1:A:632:ASN:HB2	2.15	0.47
1:A:706:ASP:C	1:A:707:SER:O	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:VAL:HB	1:B:293:VAL:HG22	1.97	0.47
1:B:319:GLU:HA	1:B:319:GLU:OE1	2.11	0.47
1:B:387:LEU:CD2	1:B:428:ILE:HG21	2.43	0.47
1:A:221:LEU:HD13	1:A:385:TYR:HB2	1.96	0.47
1:A:61:GLY:O	1:A:62:GLY:C	2.53	0.47
1:B:632:ASN:OD1	1:B:634:ASN:N	2.48	0.47
1:A:407:ASN:O	1:A:439:GLY:HA2	2.14	0.47
1:A:18:ILE:N	1:A:47:ARG:O	2.37	0.47
1:A:679:MET:O	1:A:681:ALA:N	2.48	0.47
1:A:695:TYR:OH	1:A:698:GLY:HA2	2.15	0.47
1:B:627:ARG:NH1	1:B:627:ARG:HG2	2.28	0.47
1:A:601:THR:O	1:A:604:ASP:HB2	2.15	0.47
1:A:164:SER:O	1:A:178:THR:HG22	2.15	0.46
1:A:246:ARG:O	1:A:250:THR:HG22	2.14	0.46
1:A:642:ASN:HB3	1:B:634:ASN:HB3	1.97	0.46
1:B:13:GLY:N	1:B:325:LEU:HD13	2.30	0.46
1:B:362:MET:HG3	1:B:367:PHE:CD2	2.50	0.46
1:B:36:ALA:CB	1:B:317:GLY:HA3	2.45	0.46
1:B:417:ALA:HA	1:B:460:THR:HA	1.97	0.46
1:B:55:TYR:C	1:B:57:GLY:H	2.17	0.46
1:A:545:ALA:HA	1:A:663:GLN:OE1	2.16	0.46
1:A:629:GLU:O	1:A:630:LYS:HG3	2.15	0.46
1:A:641:PHE:CD2	1:A:656:LYS:HG2	2.50	0.46
1:A:683:ALA:C	1:A:685:ASN:N	2.68	0.46
1:B:124:GLY:C	1:B:127:THR:HG22	2.35	0.46
1:B:555:ARG:CG	1:B:556:ILE:N	2.78	0.46
1:B:571:GLU:OE2	1:B:637:THR:OG1	2.25	0.46
1:B:662:MET:O	1:B:662:MET:HG2	2.15	0.46
1:A:287:LEU:HB3	1:A:289:TYR:CZ	2.49	0.46
1:A:295:VAL:HG12	1:A:295:VAL:O	2.15	0.46
1:A:44:THR:OG1	1:A:325:LEU:HD13	2.14	0.46
1:A:20:VAL:O	1:A:50:PHE:O	2.33	0.46
1:A:531:ASN:HD21	1:A:538:PHE:HA	1.80	0.46
1:B:632:ASN:C	1:B:632:ASN:OD1	2.53	0.46
1:A:470:LYS:HE2	1:A:471:ARG:H	1.80	0.46
1:B:338:LEU:HA	1:B:342:GLN:O	2.14	0.46
1:B:465:SER:O	1:B:466:LYS:CB	2.64	0.46
1:B:556:ILE:HG22	1:B:568:PHE:CD2	2.51	0.46
1:B:687:MET:O	1:B:691:ILE:HG13	2.14	0.46
1:B:50:PHE:CD1	1:B:68:ALA:HB2	2.50	0.46
1:A:135:LEU:O	1:A:139:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:HB2	1:A:178:THR:CG2	2.41	0.46
1:A:30:MET:O	1:A:34:VAL:HG23	2.16	0.46
1:A:425:ILE:O	1:A:429:GLN:HG3	2.16	0.46
1:A:506:LEU:CD2	1:A:723:VAL:HB	2.43	0.46
1:B:161:LEU:HD12	1:B:161:LEU:N	2.31	0.46
1:B:367:PHE:O	1:B:369:GLU:N	2.48	0.46
1:B:747:PRO:O	1:B:751:ILE:HG13	2.16	0.46
1:A:349:MET:HA	1:A:352:VAL:HG22	1.97	0.46
1:A:440:PHE:C	1:A:442:GLY:H	2.18	0.46
1:A:560:ALA:O	1:A:562:GLY:N	2.49	0.46
1:B:366:ARG:NH1	1:B:366:ARG:HB3	2.30	0.46
1:A:560:ALA:C	1:A:562:GLY:N	2.69	0.46
1:B:382:TRP:CE2	1:B:386:LYS:HD2	2.51	0.46
1:B:641:PHE:CE2	1:B:656:LYS:HG2	2.51	0.46
1:A:104:ASN:O	1:A:108:ARG:HG2	2.16	0.46
1:A:13:GLY:O	1:A:46:ALA:HA	2.16	0.46
1:A:429:GLN:HE22	1:A:685:ASN:HA	1.80	0.46
1:A:748:ILE:CD1	1:A:748:ILE:C	2.81	0.46
1:B:191:ALA:O	1:B:193:THR:N	2.49	0.46
1:B:355:THR:HG22	1:B:356:LYS:N	2.31	0.46
1:B:407:ASN:O	1:B:439:GLY:HA2	2.16	0.46
1:B:467:LEU:HD23	1:B:467:LEU:HA	1.83	0.46
1:B:69:THR:CG2	1:B:72:SER:OG	2.63	0.46
1:A:565:ARG:HA	1:A:621:LYS:O	2.16	0.46
1:B:235:PRO:HG3	1:B:274:ILE:HD11	1.98	0.46
1:B:283:VAL:O	1:B:287:LEU:HB2	2.15	0.46
1:A:602:ILE:HD12	1:B:643:LEU:HD13	1.96	0.46
1:A:13:GLY:O	1:A:46:ALA:HB2	2.16	0.45
1:A:531:ASN:HA	1:A:531:ASN:HD22	1.57	0.45
1:A:635:TYR:CD2	1:A:635:TYR:N	2.78	0.45
1:A:627:ARG:NH1	1:A:637:THR:N	2.64	0.45
1:B:246:ARG:O	1:B:248:SER:N	2.49	0.45
1:B:403:VAL:HG12	1:B:404:ALA:N	2.30	0.45
1:A:316:MET:HA	1:A:316:MET:CE	2.46	0.45
1:A:234:PRO:HD2	1:A:367:PHE:CD1	2.51	0.45
1:A:605:LEU:HA	1:A:605:LEU:HD12	1.84	0.45
1:B:122:LEU:HD12	1:B:169:PHE:CE1	2.51	0.45
1:A:47:ARG:HD2	1:A:67:GLU:OE1	2.17	0.45
1:A:499:PHE:O	1:A:503:THR:HB	2.16	0.45
1:A:645:SER:O	1:A:648:GLY:N	2.35	0.45
1:A:715:LYS:O	1:A:716:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:TYR:C	1:B:291:THR:N	2.70	0.45
1:B:13:GLY:N	1:B:44:THR:O	2.49	0.45
1:A:289:TYR:O	1:A:290:ASP:C	2.54	0.45
1:A:475:LYS:HA	1:A:478:PHE:CE1	2.51	0.45
1:B:137:SER:C	1:B:139:LEU:H	2.20	0.45
1:B:152:ARG:O	1:B:154:SER:N	2.49	0.45
1:B:52:HIS:HD1	1:B:52:HIS:H	1.65	0.45
1:B:421:SER:OG	1:B:680:GLY:HA3	2.16	0.45
1:A:110:ILE:HD12	1:A:110:ILE:N	2.31	0.45
1:A:149:GLU:O	1:A:150:ALA:C	2.55	0.45
1:A:198:SER:O	1:A:199:HIS:HB2	2.16	0.45
1:A:529:VAL:HG12	1:A:530:SER:N	2.31	0.45
1:A:543:ASP:O	1:A:547:ASN:N	2.46	0.45
1:A:555:ARG:O	1:A:559:SER:HB3	2.17	0.45
1:B:257:LEU:CD1	1:B:259:ILE:HG13	2.46	0.45
1:B:360:LYS:O	1:B:363:ASP:N	2.44	0.45
1:B:473:LEU:HB3	1:B:474:PRO:HD2	1.97	0.45
1:B:605:LEU:HA	1:B:605:LEU:HD12	1.64	0.45
1:B:38:VAL:HG21	1:B:73:VAL:CG1	2.46	0.45
1:A:165:ILE:HB	1:A:181:ALA:HB2	1.96	0.45
1:A:252:THR:C	1:A:254:GLY:H	2.19	0.45
1:A:294:THR:HG22	1:A:295:VAL:N	2.31	0.45
1:A:37:VAL:HA	1:A:321:VAL:CG2	2.46	0.45
1:B:165:ILE:HB	1:B:181:ALA:HB2	1.98	0.45
1:B:443:PRO:HA	1:B:448:ILE:HD11	1.99	0.45
1:B:625:VAL:HG11	1:B:644:TYR:CE1	2.51	0.45
1:A:454:SER:O	1:A:456:VAL:N	2.50	0.45
1:B:101:ALA:CA	1:B:104:ASN:HD22	2.18	0.45
1:B:428:ILE:HD11	1:B:453:TRP:CH2	2.52	0.45
1:B:547:ASN:O	1:B:550:CYS:N	2.50	0.45
1:B:418:ALA:HB2	1:B:676:ALA:HB1	1.99	0.45
1:A:388:LEU:CD2	1:A:424:ARG:HB2	2.47	0.45
1:A:560:ALA:C	1:A:622:ARG:HH22	2.20	0.45
1:A:56:GLN:HE21	1:A:89:CYS:N	2.15	0.45
1:B:380:ASN:O	1:B:384:VAL:HG23	2.17	0.45
1:B:55:TYR:C	1:B:57:GLY:N	2.70	0.45
1:A:43:PHE:C	1:A:45:GLY:N	2.70	0.45
1:A:531:ASN:ND2	1:A:539:SER:N	2.65	0.45
1:B:239:TRP:O	1:B:242:HIS:N	2.50	0.45
1:B:249:GLU:HA	1:B:252:THR:HG22	1.99	0.45
1:B:566:ARG:O	1:B:616:MET:CE	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ARG:CZ	1:B:603:ARG:HB2	2.43	0.45
1:A:233:CYS:N	1:A:234:PRO:HD3	2.31	0.45
1:A:26:ASP:O	1:A:301:ARG:HG2	2.16	0.45
1:A:604:ASP:O	1:A:607:ALA:N	2.50	0.45
1:B:242:HIS:ND1	1:B:245:ARG:NH2	2.64	0.45
1:B:475:LYS:HA	1:B:478:PHE:CZ	2.52	0.45
1:A:304:THR:OG1	1:A:305:PRO:HD2	2.16	0.44
1:A:459:TRP:CZ3	1:A:466:LYS:HB2	2.52	0.44
1:A:719:VAL:HG23	1:A:719:VAL:O	2.17	0.44
1:B:117:GLY:O	1:B:162:VAL:HA	2.18	0.44
1:B:234:PRO:O	1:B:236:ASP:N	2.49	0.44
1:B:696:ARG:HB3	1:B:697:ASN:H	1.57	0.44
1:A:559:SER:C	1:A:561:ALA:N	2.68	0.44
1:A:596:PHE:C	1:A:598:GLU:H	2.21	0.44
1:B:122:LEU:O	1:B:125:ALA:CB	2.64	0.44
1:B:146:THR:HG23	1:B:147:ALA:N	2.21	0.44
1:B:509:MET:CE	1:B:705:PRO:HA	2.48	0.44
1:A:125:ALA:O	1:A:128:PHE:HB3	2.17	0.44
1:A:630:LYS:O	1:A:632:ASN:N	2.50	0.44
1:A:724:THR:H	1:A:724:THR:HG23	1.45	0.44
1:B:240:GLU:HG3	1:B:282:LEU:HD21	1.97	0.44
1:B:332:PRO:HB2	1:B:333:ALA:H	1.63	0.44
1:B:571:GLU:O	1:B:571:GLU:HG2	2.17	0.44
1:B:609:VAL:HG22	1:B:644:TYR:CD2	2.46	0.44
1:A:261:ILE:N	1:A:261:ILE:CD1	2.80	0.44
1:A:335:VAL:CG2	1:A:348:LEU:HA	2.47	0.44
1:A:358:VAL:HG12	1:A:358:VAL:O	2.17	0.44
1:A:401:TYR:OH	1:A:692:LYS:HA	2.17	0.44
1:B:25:GLY:O	1:B:26:ASP:C	2.55	0.44
1:B:393:PRO:HG3	1:B:453:TRP:HB2	1.99	0.44
1:B:481:ILE:CD1	1:B:485:ILE:HD11	2.48	0.44
1:B:76:MET:HA	1:B:79:LEU:HD12	1.98	0.44
1:B:35:ARG:NH1	1:B:77:LEU:HB2	2.32	0.44
1:A:403:VAL:HG12	1:A:404:ALA:N	2.32	0.44
1:A:218:VAL:HG13	1:A:674:ASN:ND2	2.33	0.44
1:B:339:SER:CB	1:B:344:VAL:HG11	2.29	0.44
1:B:347:PRO:O	1:B:348:LEU:C	2.54	0.44
1:B:459:TRP:O	1:B:462:GLN:HG3	2.18	0.44
1:B:617:LYS:HG3	1:B:651:ILE:CG2	2.40	0.44
1:B:52:HIS:HA	1:B:84:ILE:O	2.17	0.44
1:A:213:GLY:O	1:A:216:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:O	1:A:237:ASP:O	2.36	0.44
1:B:234:PRO:HB2	1:B:268:ASP:C	2.38	0.44
1:B:635:TYR:N	1:B:635:TYR:CD2	2.84	0.44
1:B:502:TYR:CZ	1:B:730:THR:HG21	2.52	0.44
1:A:189:VAL:HA	1:A:192:ILE:HB	1.98	0.44
1:A:245:ARG:O	1:A:249:GLU:N	2.42	0.44
1:A:528:THR:HG23	1:A:531:ASN:H	1.83	0.44
1:A:730:THR:N	1:A:738:LYS:HD3	2.33	0.44
1:B:190:ASP:O	1:B:193:THR:CG2	2.66	0.44
1:B:257:LEU:HD11	1:B:259:ILE:HG13	1.99	0.44
1:B:335:VAL:HG23	1:B:348:LEU:HA	1.98	0.44
1:B:527:ALA:C	1:B:528:THR:HG22	2.38	0.44
1:B:731:ASP:OD2	1:B:734:HIS:HD2	2.00	0.44
1:A:441:GLU:OE2	1:A:472:THR:HG21	2.17	0.44
1:B:145:ILE:O	1:B:147:ALA:N	2.51	0.44
1:B:475:LYS:C	1:B:477:SER:N	2.70	0.44
1:B:552:THR:HG22	1:B:555:ARG:NH2	2.31	0.44
1:B:586:LEU:HB2	1:B:749:LEU:HD22	2.00	0.44
1:B:95:ARG:HA	1:B:98:ARG:HG2	1.99	0.44
1:A:20:VAL:HA	1:A:114:CYS:HB3	1.98	0.44
1:A:665:GLY:O	1:A:666:GLY:C	2.56	0.44
1:B:159:VAL:HG23	1:B:324:LEU:HD23	1.96	0.44
1:B:289:TYR:C	1:B:291:THR:H	2.20	0.44
1:B:455:TYR:CD2	1:B:455:TYR:C	2.91	0.44
1:B:341:ASN:ND2	1:B:538:PHE:CZ	2.86	0.44
1:A:161:LEU:HD12	1:A:161:LEU:N	2.33	0.43
1:A:287:LEU:CB	1:A:289:TYR:OH	2.66	0.43
1:A:59:VAL:C	1:A:60:ASP:O	2.53	0.43
1:B:407:ASN:HA	1:B:496:ILE:O	2.17	0.43
1:B:709:CYS:HA	1:B:721:GLN:O	2.18	0.43
1:A:201:ARG:HB3	1:A:203:PHE:CE1	2.52	0.43
1:A:239:TRP:CH2	1:A:274:ILE:CD1	3.01	0.43
1:A:376:ARG:NH2	1:A:376:ARG:CA	2.72	0.43
1:A:393:PRO:HA	1:A:394:PRO:HD3	1.66	0.43
1:A:480:GLN:H	1:A:480:GLN:CD	2.21	0.43
1:A:641:PHE:CG	1:A:656:LYS:HG2	2.53	0.43
1:B:248:SER:O	1:B:252:THR:HG22	2.18	0.43
1:B:360:LYS:O	1:B:362:MET:N	2.51	0.43
1:B:370:ALA:O	1:B:372:LYS:N	2.51	0.43
1:B:715:LYS:HB3	1:B:716:ARG:H	1.61	0.43
1:A:360:LYS:O	1:A:361:ALA:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ASP:O	1:A:519:CYS:HB2	2.18	0.43
1:A:534:PRO:HA	1:A:737:PRO:HB3	1.99	0.43
1:A:605:LEU:HD11	1:A:640:ILE:HD12	1.99	0.43
1:B:255:SER:C	1:B:257:LEU:N	2.72	0.43
1:B:370:ALA:C	1:B:372:LYS:N	2.68	0.43
1:B:618:THR:HG22	1:B:619:THR:H	1.83	0.43
1:A:149:GLU:CD	1:A:149:GLU:C	2.76	0.43
1:A:219:THR:O	1:A:223:CYS:SG	2.74	0.43
1:A:722:PRO:O	1:A:725:GLU:HB2	2.19	0.43
1:A:50:PHE:HB3	1:A:84:ILE:HD11	2.00	0.43
1:B:194:THR:O	1:B:197:GLN:HG3	2.17	0.43
1:A:103:HIS:HE1	1:A:144:LYS:HG2	1.80	0.43
1:A:214:TYR:HE2	1:A:218:VAL:CG2	2.19	0.43
1:A:377:SER:O	1:A:378:PHE:C	2.57	0.43
1:A:571:GLU:HA	1:A:627:ARG:O	2.18	0.43
1:A:731:ASP:N	1:A:738:LYS:HG3	2.33	0.43
1:A:95:ARG:O	1:A:96:GLU:C	2.54	0.43
1:B:134:ASP:O	1:B:137:SER:HB3	2.17	0.43
1:A:213:GLY:HA3	1:A:230:ILE:HG22	1.99	0.43
1:A:159:VAL:HG13	1:A:334:CYS:HB3	2.01	0.43
1:B:400:SER:HB2	1:B:431:ASN:HA	2.00	0.43
1:B:433:VAL:C	1:B:434:LEU:HD12	2.39	0.43
1:B:741:TRP:CG	1:B:742:TRP:N	2.87	0.43
1:A:239:TRP:CH2	1:A:274:ILE:HD13	2.54	0.43
1:A:292:ARG:CG	1:A:293:VAL:N	2.82	0.43
1:A:36:ALA:HB3	1:A:317:GLY:HA3	1.99	0.43
1:A:380:ASN:C	1:A:384:VAL:HG23	2.34	0.43
1:A:473:LEU:HA	1:A:473:LEU:HD23	1.70	0.43
1:A:18:ILE:CG1	1:A:48:VAL:HG22	2.48	0.43
1:A:605:LEU:O	1:A:609:VAL:HG23	2.18	0.43
1:B:146:THR:HA	1:B:150:ALA:CB	2.46	0.43
1:B:186:THR:O	1:B:187:GLU:C	2.57	0.43
1:B:188:ILE:HG22	1:B:189:VAL:N	2.34	0.43
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.82	0.43
1:B:546:LEU:HD11	1:B:584:ALA:CA	2.48	0.43
1:B:573:MET:HE2	1:B:661:HIS:CD2	2.54	0.43
2:B:764:ADP:O1B	2:B:764:ADP:O2A	2.36	0.43
1:A:252:THR:C	1:A:254:GLY:N	2.72	0.43
1:A:374:ARG:CG	1:A:378:PHE:CD2	3.01	0.43
1:A:606:GLN:HE21	1:B:602:ILE:CG2	2.32	0.43
1:A:711:LEU:HD22	1:A:720:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:SER:OG	1:B:228:VAL:HG22	2.18	0.43
1:B:596:PHE:O	1:B:598:GLU:N	2.51	0.43
1:A:165:ILE:O	1:A:215:LEU:HD11	2.19	0.43
1:B:29:GLY:O	1:B:32:ALA:HB3	2.19	0.43
1:A:475:LYS:C	1:A:477:SER:H	2.23	0.43
1:A:502:TYR:CD1	1:A:723:VAL:HG12	2.54	0.43
1:B:370:ALA:O	1:B:374:ARG:HB2	2.19	0.43
1:B:515:PHE:N	1:B:515:PHE:CD1	2.87	0.43
1:B:612:LEU:O	1:B:616:MET:HG2	2.18	0.43
1:B:713:MET:C	1:B:714:ARG:HG2	2.39	0.43
1:B:733:GLU:HG2	1:B:734:HIS:CE1	2.54	0.43
1:A:392:ARG:CB	1:A:393:PRO:CD	2.97	0.42
1:B:139:LEU:HD13	1:B:142:ALA:HB3	2.01	0.42
1:B:18:ILE:HG23	1:B:324:LEU:HD13	2.00	0.42
1:B:573:MET:HE3	1:B:661:HIS:HA	2.01	0.42
1:A:167:ASN:O	1:A:167:ASN:ND2	2.49	0.42
1:A:604:ASP:O	1:A:606:GLN:N	2.51	0.42
1:A:746:ARG:O	1:A:749:LEU:HB3	2.19	0.42
1:B:459:TRP:N	1:B:459:TRP:HD1	2.17	0.42
1:B:690:LYS:HA	1:B:690:LYS:HD3	1.80	0.42
1:A:319:GLU:OE2	1:A:345:ARG:NE	2.45	0.42
1:A:402:THR:HB	1:A:432:ARG:HE	1.84	0.42
1:A:481:ILE:O	1:A:485:ILE:HG22	2.18	0.42
1:A:679:MET:C	1:A:681:ALA:N	2.73	0.42
1:B:159:VAL:HG12	1:B:160:GLY:N	2.34	0.42
1:B:267:ILE:CD1	1:B:268:ASP:O	2.68	0.42
1:B:604:ASP:O	1:B:607:ALA:N	2.52	0.42
1:A:348:LEU:O	1:A:352:VAL:HG22	2.20	0.42
1:A:359:THR:O	1:A:360:LYS:C	2.57	0.42
1:A:424:ARG:HD2	1:A:453:TRP:CZ2	2.54	0.42
1:A:65:ILE:O	1:A:108:ARG:NH2	2.52	0.42
1:B:538:PHE:CE2	1:B:741:TRP:HZ2	2.36	0.42
1:A:120:GLY:O	1:A:121:SER:C	2.57	0.42
1:A:312:LEU:HD12	1:A:316:MET:HG2	2.01	0.42
1:A:669:THR:O	1:A:670:PRO:C	2.56	0.42
1:B:34:VAL:HG21	1:B:84:ILE:HD13	2.01	0.42
1:B:348:LEU:CD2	1:B:352:VAL:CG2	2.98	0.42
1:B:367:PHE:C	1:B:369:GLU:N	2.73	0.42
1:B:502:TYR:CE2	1:B:730:THR:HG21	2.54	0.42
1:A:189:VAL:HG22	1:A:205:LEU:CD1	2.50	0.42
1:A:420:ARG:HA	1:A:456:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:PHE:CD2	1:A:522:PHE:O	2.73	0.42
1:A:608:ASN:O	1:A:611:HIS:HB3	2.19	0.42
1:A:566:ARG:NH2	1:A:653:ASP:OD2	2.52	0.42
2:A:764:ADP:O3B	2:A:764:ADP:O5'	2.38	0.42
1:B:182:LEU:HA	1:B:185:ILE:HG23	2.00	0.42
1:B:123:THR:HA	1:B:352:VAL:HG11	2.01	0.42
1:B:475:LYS:HA	1:B:478:PHE:CE1	2.54	0.42
1:B:59:VAL:O	1:B:59:VAL:HG12	2.19	0.42
1:B:570:ILE:CG2	1:B:659:LEU:HG	2.49	0.42
1:A:227:TRP:CD1	1:A:228:VAL:N	2.88	0.42
1:A:28:GLN:HB3	1:A:305:PRO:HB3	2.01	0.42
1:A:392:ARG:HG2	1:A:393:PRO:CD	2.50	0.42
1:A:515:PHE:N	1:A:515:PHE:CD1	2.88	0.42
1:B:366:ARG:NH1	1:B:366:ARG:CB	2.82	0.42
1:B:560:ALA:O	1:B:562:GLY:N	2.52	0.42
1:A:272:LYS:HA	1:A:273:PRO:HD2	1.63	0.42
1:A:352:VAL:O	1:A:355:THR:HG22	2.20	0.42
1:A:382:TRP:CD2	1:A:386:LYS:HD2	2.55	0.42
1:A:387:LEU:HD21	1:A:428:ILE:HG21	2.02	0.42
1:A:441:GLU:O	1:A:445:LYS:HB2	2.19	0.42
1:A:475:LYS:HA	1:A:478:PHE:CZ	2.55	0.42
1:A:679:MET:HE3	1:A:718:LEU:HD21	2.01	0.42
1:A:745:LEU:O	1:A:748:ILE:N	2.53	0.42
1:B:124:GLY:CA	1:B:127:THR:HG22	2.50	0.42
1:B:339:SER:O	1:B:340:GLY:C	2.58	0.42
1:B:585:GLY:HA2	1:B:626:LEU:CD1	2.47	0.42
1:B:613:VAL:HG12	1:B:614:GLN:N	2.34	0.42
1:B:509:MET:HE3	1:B:705:PRO:HA	2.01	0.42
1:A:218:VAL:HG13	1:A:674:ASN:HD21	1.85	0.42
1:B:208:MET:HE3	1:B:300:GLN:OE1	2.19	0.42
1:B:44:THR:CG2	1:B:325:LEU:HD11	2.46	0.42
1:B:221:LEU:CD1	1:B:385:TYR:HB2	2.49	0.42
1:B:582:THR:OG1	1:B:746:ARG:HD3	2.20	0.42
1:A:13:GLY:HA3	1:A:325:LEU:HD22	2.01	0.42
1:A:470:LYS:HE2	1:A:470:LYS:CA	2.44	0.42
1:A:50:PHE:O	1:A:51:VAL:CB	2.68	0.42
1:A:618:THR:HB	1:A:619:THR:H	1.55	0.42
1:B:229:PHE:HB2	1:B:262:VAL:HA	2.02	0.42
1:B:597:GLU:HB3	1:B:743:LEU:HD11	2.01	0.42
1:B:684:MET:HG3	1:B:684:MET:O	2.20	0.42
1:B:573:MET:HG3	1:B:573:MET:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:LEU:O	1:B:581:ALA:C	2.55	0.41
1:A:113:LEU:HA	1:A:113:LEU:HD12	1.86	0.41
1:A:350:GLU:O	1:A:354:VAL:HG23	2.21	0.41
1:A:651:ILE:HG12	1:A:651:ILE:H	1.64	0.41
1:A:664:GLN:HB2	1:A:664:GLN:HE21	1.66	0.41
1:A:668:PRO:O	1:A:673:ARG:NE	2.50	0.41
1:B:135:LEU:C	1:B:137:SER:H	2.23	0.41
1:B:159:VAL:CG2	1:B:324:LEU:HG	2.50	0.41
1:B:328:THR:CB	1:B:329:PRO:CD	2.95	0.41
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.74	0.41
1:B:71:GLU:N	1:B:71:GLU:OE1	2.34	0.41
1:A:35:ARG:HD3	1:A:77:LEU:CD1	2.44	0.41
1:B:350:GLU:O	1:B:354:VAL:N	2.50	0.41
1:B:443:PRO:O	1:B:444:ALA:C	2.58	0.41
1:A:606:GLN:OE1	1:B:606:GLN:OE1	2.38	0.41
1:B:687:MET:CE	1:B:691:ILE:HG13	2.51	0.41
1:A:335:VAL:O	1:A:336:VAL:C	2.58	0.41
1:A:595:ILE:CD1	1:A:598:GLU:HB3	2.49	0.41
1:A:606:GLN:HE21	1:B:602:ILE:HG23	1.86	0.41
1:A:726:LEU:O	1:A:730:THR:CG2	2.61	0.41
1:A:534:PRO:CG	1:A:730:THR:HB	2.50	0.41
2:A:765:ADP:O2B	2:A:765:ADP:H5'1	2.21	0.41
1:B:139:LEU:CD1	1:B:142:ALA:HB3	2.50	0.41
1:B:385:TYR:CD2	1:B:385:TYR:C	2.94	0.41
1:B:560:ALA:HB1	1:B:563:THR:CB	2.51	0.41
1:A:168:ASP:O	1:A:169:PHE:C	2.59	0.41
1:A:191:ALA:O	1:A:192:ILE:C	2.58	0.41
1:A:364:GLU:C	1:A:366:ARG:N	2.67	0.41
1:A:387:LEU:HD22	1:A:428:ILE:HG21	2.03	0.41
1:A:470:LYS:HA	1:A:470:LYS:CE	2.45	0.41
1:A:625:VAL:HG11	1:A:644:TYR:CE1	2.55	0.41
1:A:56:GLN:HE22	1:A:87:ALA:HB1	1.82	0.41
1:B:124:GLY:HA2	1:B:127:THR:CG2	2.50	0.41
1:B:348:LEU:CD2	1:B:352:VAL:HG22	2.51	0.41
1:B:595:ILE:HD12	1:B:746:ARG:CZ	2.46	0.41
1:A:159:VAL:HG12	1:A:160:GLY:N	2.36	0.41
1:A:289:TYR:O	1:A:291:THR:N	2.53	0.41
1:A:606:GLN:C	1:A:608:ASN:N	2.73	0.41
1:A:585:GLY:HA2	1:A:626:LEU:HD12	2.01	0.41
1:A:690:LYS:HD2	1:A:690:LYS:HA	1.74	0.41
1:A:749:LEU:O	1:A:749:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LYS:C	1:B:362:MET:H	2.24	0.41
1:B:433:VAL:O	1:B:434:LEU:HD12	2.20	0.41
1:B:402:THR:CG2	1:B:489:ASN:ND2	2.84	0.41
1:B:533:VAL:CG1	1:B:534:PRO:N	2.83	0.41
1:B:718:LEU:C	1:B:719:VAL:HG12	2.40	0.41
1:A:446:GLY:HA2	1:A:448:ILE:HD11	2.02	0.41
1:B:529:VAL:HG13	1:B:545:ALA:CB	2.51	0.41
1:A:639:PHE:CE1	1:B:639:PHE:CE1	3.08	0.41
1:A:230:ILE:HA	1:A:231:PRO:HD3	1.87	0.41
1:A:325:LEU:C	1:A:327:GLY:H	2.24	0.41
1:A:556:ILE:HG22	1:A:568:PHE:CD2	2.55	0.41
1:A:76:MET:O	1:A:77:LEU:C	2.59	0.41
1:B:175:THR:O	1:B:178:THR:CG2	2.60	0.41
1:B:598:GLU:OE1	1:B:746:ARG:NE	2.54	0.41
1:B:656:LYS:HD2	1:B:656:LYS:O	2.21	0.41
1:A:628:ASN:C	1:A:630:LYS:H	2.23	0.41
1:A:687:MET:O	1:A:691:ILE:HG12	2.21	0.41
1:B:440:PHE:C	1:B:442:GLY:N	2.73	0.41
1:B:705:PRO:O	1:B:722:PRO:HB3	2.21	0.41
1:B:499:PHE:CE2	1:B:735:ARG:HG2	2.55	0.41
1:A:9:ALA:C	1:A:11:THR:H	2.24	0.41
1:A:122:LEU:HD11	1:A:162:VAL:HG22	2.02	0.41
1:B:323:ALA:HA	1:B:345:ARG:NH2	2.36	0.41
1:B:171:GLY:HA3	1:B:346:LEU:HD12	2.03	0.41
1:B:544:THR:HA	1:B:669:THR:HG23	2.03	0.41
1:B:601:THR:O	1:B:602:ILE:C	2.57	0.41
1:A:352:VAL:HA	1:A:355:THR:CG2	2.50	0.40
1:A:662:MET:O	1:A:663:GLN:HG2	2.21	0.40
1:B:231:PRO:HG3	1:B:265:GLY:O	2.20	0.40
1:B:376:ARG:CG	1:B:376:ARG:NH2	2.84	0.40
1:B:35:ARG:HE	1:B:39:ARG:NH1	2.19	0.40
1:B:59:VAL:C	1:B:60:ASP:OD1	2.59	0.40
1:A:294:THR:CG2	1:A:295:VAL:N	2.84	0.40
1:A:383:GLU:H	1:A:383:GLU:HG2	1.64	0.40
1:B:293:VAL:HG12	1:B:293:VAL:O	2.21	0.40
1:B:358:VAL:HA	1:B:373:LEU:HD13	2.03	0.40
1:B:570:ILE:HB	1:B:626:LEU:HD23	2.03	0.40
1:A:407:ASN:O	1:A:439:GLY:CA	2.69	0.40
1:A:569:ILE:HA	1:A:625:VAL:O	2.22	0.40
1:B:184:ARG:HA	1:B:184:ARG:HD3	1.80	0.40
1:B:522:PHE:O	1:B:522:PHE:CD2	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:GLU:CG	1:B:734:HIS:CE1	3.05	0.40
1:A:509:MET:O	1:A:510:GLU:C	2.58	0.40
1:A:662:MET:HB3	1:A:663:GLN:H	1.48	0.40
1:A:731:ASP:OD2	1:A:734:HIS:CD2	2.75	0.40
1:A:77:LEU:HA	1:A:77:LEU:HD12	1.95	0.40
1:B:106:VAL:O	1:B:109:GLY:N	2.54	0.40
1:B:191:ALA:C	1:B:193:THR:N	2.71	0.40
1:B:328:THR:HB	1:B:329:PRO:HD3	2.03	0.40
1:B:403:VAL:O	1:B:434:LEU:N	2.47	0.40
1:B:436:VAL:CG2	1:B:448:ILE:HG12	2.37	0.40
1:A:164:SER:OG	1:A:166:ASP:OD1	2.40	0.40
1:A:239:TRP:O	1:A:243:LEU:N	2.43	0.40
1:A:36:ALA:CB	1:A:317:GLY:HA3	2.52	0.40
1:A:395:ALA:HA	1:A:396:PRO:HD2	1.89	0.40
1:A:528:THR:HG22	1:A:539:SER:CB	2.52	0.40
1:A:746:ARG:O	1:A:747:PRO:C	2.58	0.40
1:A:751:ILE:C	1:A:753:ALA:N	2.75	0.40
1:B:101:ALA:O	1:B:104:ASN:N	2.54	0.40
1:B:244:CYS:O	1:B:245:ARG:C	2.59	0.40
1:B:546:LEU:HD11	1:B:584:ALA:N	2.37	0.40
1:B:613:VAL:C	1:B:615:LYS:N	2.75	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	746/762 (98%)	560 (75%)	117 (16%)	69 (9%)	1	3
1	B	746/762 (98%)	542 (73%)	122 (16%)	82 (11%)	0	2
All	All	1492/1524 (98%)	1102 (74%)	239 (16%)	151 (10%)	0	3

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	89	CYS
1	A	143	GLY
1	A	152	ARG
1	A	153	SER
1	A	198	SER
1	A	210	ARG
1	A	237	ASP
1	A	239	TRP
1	A	297	GLY
1	A	298	HIS
1	A	365	LYS
1	A	376	ARG
1	A	390	HIS
1	A	564	LYS
1	A	645	SER
1	B	12	LEU
1	B	62	GLY
1	B	144	LYS
1	B	146	THR
1	B	154	SER
1	B	169	PHE
1	B	232	GLU
1	B	233	CYS
1	B	236	ASP
1	B	237	ASP
1	B	238	ASN
1	B	255	SER
1	B	291	THR
1	B	298	HIS
1	B	303	GLY
1	B	375	GLY
1	B	390	HIS
1	B	476	LYS
1	B	551	THR
1	B	552	THR
1	B	560	ALA
1	B	589	GLY
1	B	661	HIS
1	B	697	ASN
1	A	54	GLY
1	A	56	GLN

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Mol	Chain	Res	Type
1	A	57	GLY
1	A	62	GLY
1	A	130	SER
1	A	133	SER
1	A	200	GLN
1	A	265	GLY
1	A	273	PRO
1	A	288	GLY
1	A	353	GLN
1	A	375	GLY
1	A	391	ILE
1	A	397	LYS
1	A	476	LYS
1	A	561	ALA
1	A	619	THR
1	A	664	GLN
1	A	708	GLY
1	A	716	ARG
1	B	26	ASP
1	B	56	GLN
1	B	89	CYS
1	B	152	ARG
1	B	153	SER
1	B	247	LEU
1	B	297	GLY
1	B	360	LYS
1	B	365	LYS
1	B	368	ASP
1	B	465	SER
1	B	466	LYS
1	B	553	CYS
1	B	559	SER
1	B	561	ALA
1	B	564	LYS
1	B	579	TYR
1	B	597	GLU
1	B	660	GLY
1	A	119	ASP
1	A	142	ALA
1	A	164	SER
1	A	192	ILE
1	A	209	GLY

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Mol	Chain	Res	Type
1	A	357	ASP
1	A	361	ALA
1	A	396	PRO
1	A	398	SER
1	A	605	LEU
1	A	631	CYS
1	A	632	ASN
1	A	646	GLU
1	A	715	LYS
1	B	98	ARG
1	B	246	ARG
1	B	257	LEU
1	B	290	ASP
1	B	332	PRO
1	B	349	MET
1	B	361	ALA
1	B	376	ARG
1	B	529	VAL
1	B	618	THR
1	B	631	CYS
1	B	635	TYR
1	B	659	LEU
1	B	666	GLY
1	B	754	LYS
1	A	51	VAL
1	A	214	TYR
1	A	296	LEU
1	A	474	PRO
1	A	555	ARG
1	A	556	ILE
1	A	557	LYS
1	A	629	GLU
1	A	707	SER
1	B	13	GLY
1	B	138	ASP
1	B	145	ILE
1	B	235	PRO
1	B	240	GLU
1	B	398	SER
1	B	444	ALA
1	B	588	ALA
1	B	645	SER

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Mol	Chain	Res	Type
1	A	85	GLY
1	A	236	ASP
1	A	238	ASN
1	A	246	ARG
1	A	455	TYR
1	A	597	GLU
1	B	95	ARG
1	B	99	LEU
1	B	148	GLU
1	B	208	MET
1	B	273	PRO
1	B	300	GLN
1	B	475	LYS
1	A	378	PHE
1	A	394	PRO
1	B	192	ILE
1	B	328	THR
1	B	602	ILE
1	B	439	GLY
1	B	463	GLY
1	B	391	ILE
1	B	394	PRO
1	A	746	ARG
1	B	396	PRO
1	A	680	GLY

### 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	605/618 (98%)	520 (86%)	85 (14%)	3	16
1	B	605/618 (98%)	527 (87%)	78 (13%)	4	19
All	All	1210/1236 (98%)	1047 (86%)	163 (14%)	4	18

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	71	GLU
1	A	73	VAL
1	A	77	LEU
1	A	78	GLN
1	A	84	ILE
1	A	86	SER
1	A	95	ARG
1	A	106	VAL
1	A	110	ILE
1	A	111	THR
1	A	119	ASP
1	A	121	SER
1	A	123	THR
1	A	126	ASP
1	A	134	ASP
1	A	149	GLU
1	A	157	ASN
1	A	167	ASN
1	A	178	THR
1	A	190	ASP
1	A	195	THR
1	A	200	GLN
1	A	222	SER
1	A	239	TRP
1	A	241	ASP
1	A	275	THR
1	A	276	SER
1	A	277	GLU
1	A	289	TYR
1	A	334	CYS
1	A	342	GLN
1	A	376	ARG
1	A	402	THR
1	A	405	VAL
1	A	435	VAL
1	A	460	THR
1	A	470	LYS
1	A	471	ARG
1	A	472	THR
1	A	481	ILE
1	A	485	ILE
1	A	486	THR

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Mol	Chain	Res	Type
1	A	491	GLN
1	A	493	LEU
1	A	500	GLU
1	A	503	THR
1	A	510	GLU
1	A	512	ARG
1	A	516	ASP
1	A	523	VAL
1	A	531	ASN
1	A	550	CYS
1	A	551	THR
1	A	552	THR
1	A	553	CYS
1	A	559	SER
1	A	565	ARG
1	A	566	ARG
1	A	573	MET
1	A	595	ILE
1	A	619	THR
1	A	621	LYS
1	A	622	ARG
1	A	625	VAL
1	A	636	THR
1	A	642	ASN
1	A	655	ARG
1	A	657	ASN
1	A	662	MET
1	A	663	GLN
1	A	664	GLN
1	A	669	THR
1	A	677	THR
1	A	687	MET
1	A	699	ARG
1	A	700	ILE
1	A	707	SER
1	A	713	MET
1	A	714	ARG
1	A	715	LYS
1	A	723	VAL
1	A	727	GLN
1	A	730	THR
1	A	748	ILE

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Mol	Chain	Res	Type
1	B	10	ARG
1	B	21	LEU
1	B	22	THR
1	B	60	ASP
1	B	72	SER
1	B	78	GLN
1	B	84	ILE
1	B	93	ARG
1	B	111	THR
1	B	134	ASP
1	B	158	ILE
1	B	165	ILE
1	B	166	ASP
1	B	178	THR
1	B	180	SER
1	B	185	ILE
1	B	186	THR
1	B	190	ASP
1	B	192	ILE
1	B	200	GLN
1	B	205	LEU
1	B	208	MET
1	B	211	HIS
1	B	226	ASP
1	B	230	ILE
1	B	239	TRP
1	B	241	ASP
1	B	251	ARG
1	B	287	LEU
1	B	318	VAL
1	B	331	THR
1	B	352	VAL
1	B	355	THR
1	B	368	ASP
1	B	374	ARG
1	B	387	LEU
1	B	402	THR
1	B	432	ARG
1	B	435	VAL
1	B	449	GLU
1	B	454	SER
1	B	460	THR

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Mol	Chain	Res	Type
1	B	462	GLN
1	B	470	LYS
1	B	477	SER
1	B	481	ILE
1	B	500	GLU
1	B	503	THR
1	B	514	GLN
1	B	528	THR
1	B	530	SER
1	B	555	ARG
1	B	557	LYS
1	B	573	MET
1	B	595	ILE
1	B	621	LYS
1	B	622	ARG
1	B	631	CYS
1	B	642	ASN
1	B	656	LYS
1	B	662	MET
1	B	663	GLN
1	B	679	MET
1	B	687	MET
1	B	693	GLU
1	B	700	ILE
1	B	703	ASN
1	B	713	MET
1	B	714	ARG
1	B	719	VAL
1	B	724	THR
1	B	730	THR
1	B	731	ASP
1	B	733	GLU
1	B	736	ILE
1	B	743	LEU
1	B	749	LEU
1	B	750	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	64	HIS

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Mol	Chain	Res	Type
1	A	112	ASN
1	A	157	ASN
1	A	258	ASN
1	A	390	HIS
1	A	429	GLN
1	A	431	ASN
1	A	437	HIS
1	A	447	GLN
1	A	462	GLN
1	A	484	ASN
1	A	489	ASN
1	A	531	ASN
1	A	611	HIS
1	A	628	ASN
1	A	634	ASN
1	A	642	ASN
1	A	657	ASN
1	A	661	HIS
1	A	664	GLN
1	A	674	ASN
1	A	703	ASN
1	A	721	GLN
1	A	727	GLN
1	B	104	ASN
1	B	183	HIS
1	B	342	GLN
1	B	431	ASN
1	B	462	GLN
1	B	489	ASN
1	B	514	GLN
1	B	531	ASN
1	B	547	ASN
1	B	634	ASN
1	B	642	ASN
1	B	674	ASN
1	B	703	ASN
1	B	734	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands 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	ADP	A	764	-	24,29,29	0.98	1 (4%)	29,45,45	2.00	9 (31%)
3	PO4	A	767	-	4,4,4	1.96	3 (75%)	6,6,6	1.22	1 (16%)
3	PO4	B	767	-	4,4,4	1.97	3 (75%)	6,6,6	1.20	1 (16%)
2	ADP	B	764	-	24,29,29	0.99	1 (4%)	29,45,45	1.51	3 (10%)
3	PO4	B	766	-	4,4,4	1.98	3 (75%)	6,6,6	1.18	1 (16%)
2	ADP	A	765	-	24,29,29	0.94	1 (4%)	29,45,45	1.32	3 (10%)
2	ADP	B	763	-	24,29,29	0.96	1 (4%)	29,45,45	1.55	4 (13%)
3	PO4	A	766	-	4,4,4	1.98	2 (50%)	6,6,6	1.39	1 (16%)
3	PO4	A	768	-	4,4,4	1.96	3 (75%)	6,6,6	1.34	1 (16%)
2	ADP	A	763	-	24,29,29	0.95	1 (4%)	29,45,45	1.57	5 (17%)
2	ADP	B	765	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
3	PO4	B	768	-	4,4,4	1.97	3 (75%)	6,6,6	1.15	1 (16%)

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	ADP	A	764	-	-	2/12/32/32	0/3/3/3
2	ADP	B	764	-	-	4/12/32/32	0/3/3/3
2	ADP	A	765	-	-	1/12/32/32	0/3/3/3
2	ADP	B	763	-	-	5/12/32/32	0/3/3/3
2	ADP	A	763	-	-	2/12/32/32	0/3/3/3
2	ADP	B	765	-	-	1/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	764	ADP	O4'-C1'	2.63	1.44	1.41
2	B	763	ADP	O4'-C1'	2.45	1.44	1.41
2	A	764	ADP	O4'-C1'	2.40	1.44	1.41
3	A	766	PO4	P-O2	2.35	1.61	1.54
3	B	766	PO4	P-O2	2.31	1.61	1.54
3	A	766	PO4	P-O3	2.30	1.61	1.54
3	B	766	PO4	P-O3	2.29	1.61	1.54
3	B	767	PO4	P-O3	2.26	1.61	1.54
3	B	767	PO4	P-O2	2.26	1.61	1.54
3	A	767	PO4	P-O3	2.24	1.61	1.54
2	A	763	ADP	O4'-C1'	2.23	1.44	1.41
3	B	768	PO4	P-O2	2.22	1.61	1.54
3	A	767	PO4	P-O2	2.22	1.61	1.54
3	B	768	PO4	P-O3	2.22	1.61	1.54
3	A	768	PO4	P-O3	2.20	1.61	1.54
3	A	768	PO4	P-O2	2.20	1.61	1.54
2	B	765	ADP	O4'-C1'	2.17	1.44	1.41
3	B	768	PO4	P-O4	-2.13	1.48	1.54
3	A	768	PO4	P-O4	-2.11	1.48	1.54
3	B	767	PO4	P-O4	-2.09	1.48	1.54
3	A	767	PO4	P-O4	-2.07	1.48	1.54
2	A	765	ADP	O4'-C1'	2.07	1.44	1.41
3	B	766	PO4	P-O4	-2.05	1.48	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	764	ADP	PA-O3A-PB	-4.74	116.56	132.83
2	A	763	ADP	N3-C2-N1	-4.53	121.59	128.68
2	B	763	ADP	N3-C2-N1	-4.46	121.71	128.68
2	A	765	ADP	N3-C2-N1	-4.41	121.79	128.68
2	B	764	ADP	N3-C2-N1	-4.37	121.85	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	765	ADP	N3-C2-N1	-4.32	121.92	128.68
2	B	763	ADP	PA-O3A-PB	-4.30	118.08	132.83
2	A	764	ADP	N3-C2-N1	-4.23	122.06	128.68
2	A	763	ADP	PA-O3A-PB	-4.04	118.97	132.83
2	A	764	ADP	O2B-PB-O3A	-3.92	91.48	104.64
2	A	764	ADP	C2'-C3'-C4'	-3.90	95.06	102.64
2	A	764	ADP	PA-O3A-PB	-3.87	119.54	132.83
2	B	765	ADP	PA-O3A-PB	-3.29	121.52	132.83
2	A	765	ADP	O4'-C1'-C2'	-3.22	102.22	106.93
2	A	764	ADP	O2B-PB-O1B	3.08	122.75	110.68
2	B	763	ADP	O2A-PA-O5'	-2.98	93.89	107.75
2	A	764	ADP	O3B-PB-O3A	-2.98	94.63	104.64
2	B	764	ADP	C2'-C3'-C4'	-2.83	97.13	102.64
2	B	765	ADP	O4'-C1'-C2'	-2.76	102.90	106.93
2	A	764	ADP	O3B-PB-O1B	2.73	121.38	110.68
2	B	765	ADP	C3'-C2'-C1'	-2.70	96.91	100.98
2	A	763	ADP	O2A-PA-O5'	-2.60	95.68	107.75
3	A	766	PO4	O4-P-O1	2.56	120.25	110.89
2	A	765	ADP	PA-O3A-PB	-2.53	124.13	132.83
3	A	768	PO4	O4-P-O1	2.52	120.13	110.89
2	A	763	ADP	O5'-PA-O1A	-2.34	99.92	109.07
2	A	764	ADP	O3A-PB-O1B	-2.30	98.42	111.19
3	A	767	PO4	O4-P-O1	2.29	119.27	110.89
3	B	767	PO4	O4-P-O1	2.27	119.21	110.89
2	A	763	ADP	O2A-PA-O1A	2.13	122.78	112.24
2	B	763	ADP	O5'-PA-O1A	-2.11	100.81	109.07
3	B	766	PO4	O4-P-O1	2.10	118.57	110.89
2	A	764	ADP	O4'-C4'-C3'	-2.05	101.06	105.11
3	B	768	PO4	O4-P-O1	2.03	118.33	110.89

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	764	ADP	C5'-O5'-PA-O2A
2	A	764	ADP	C5'-O5'-PA-O3A
2	B	764	ADP	C5'-O5'-PA-O2A
2	B	763	ADP	C5'-O5'-PA-O1A
2	B	763	ADP	C4'-C5'-O5'-PA
2	A	763	ADP	O4'-C4'-C5'-O5'
2	A	763	ADP	C3'-C4'-C5'-O5'
2	A	765	ADP	PB-O3A-PA-O5'

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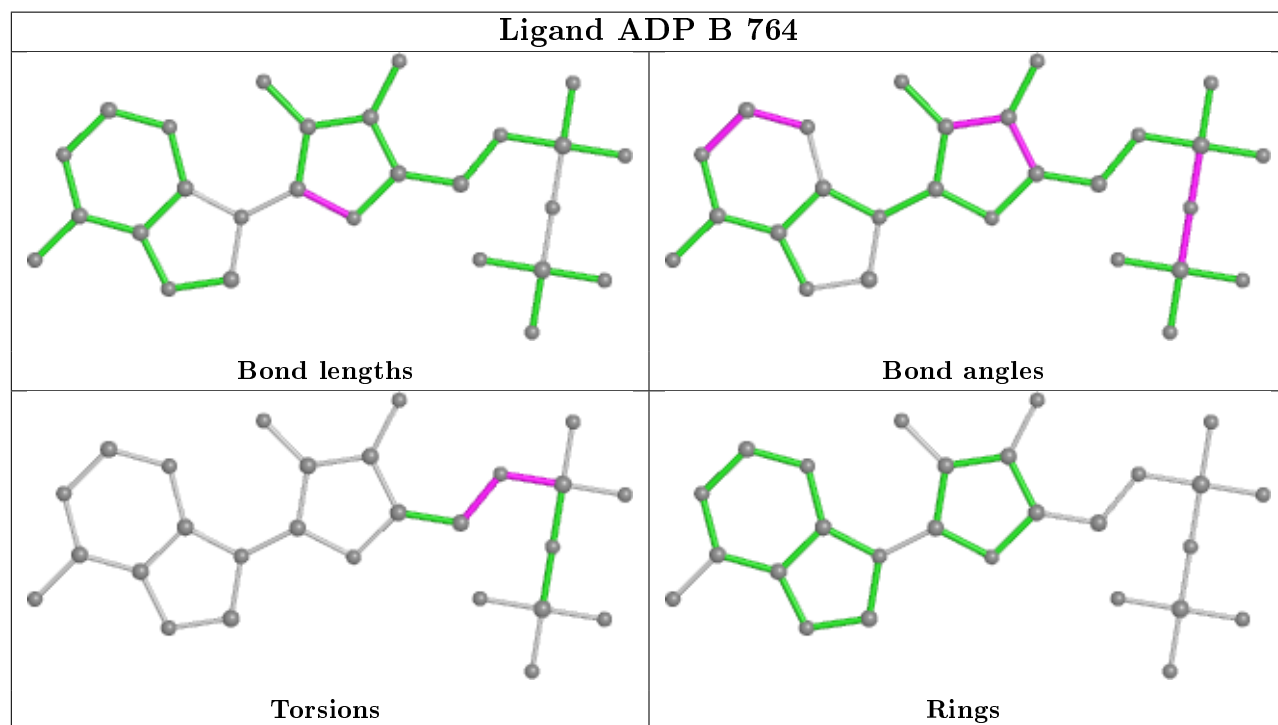
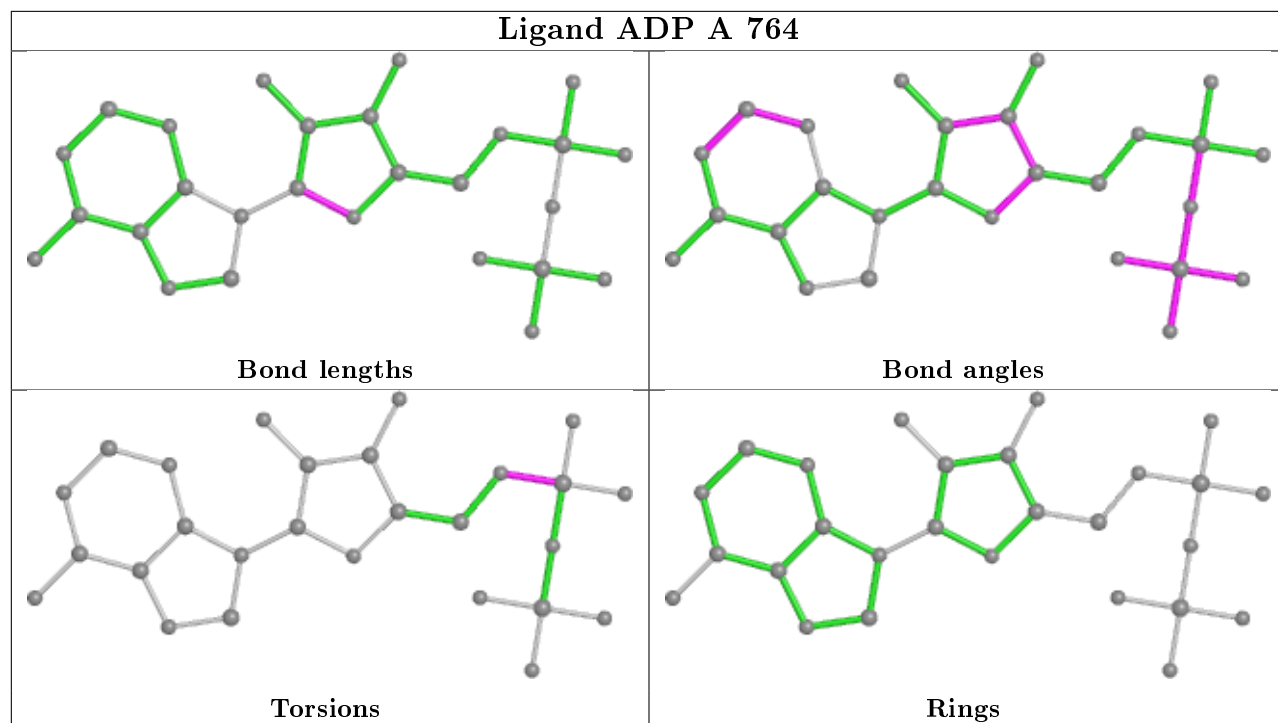
Mol	Chain	Res	Type	Atoms
2	B	765	ADP	PB-O3A-PA-O5'
2	B	764	ADP	C5'-O5'-PA-O3A
2	B	764	ADP	C4'-C5'-O5'-PA
2	B	764	ADP	C5'-O5'-PA-O1A
2	B	763	ADP	C5'-O5'-PA-O2A
2	B	763	ADP	C5'-O5'-PA-O3A
2	B	763	ADP	PB-O3A-PA-O1A

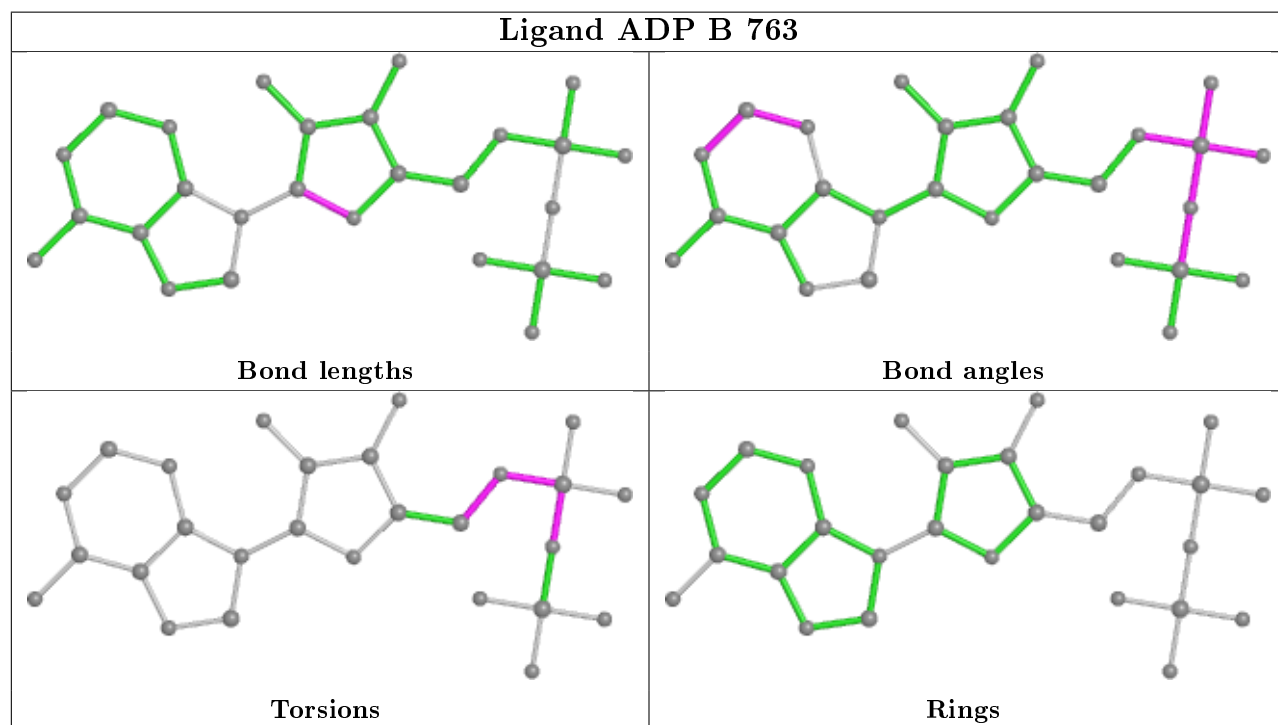
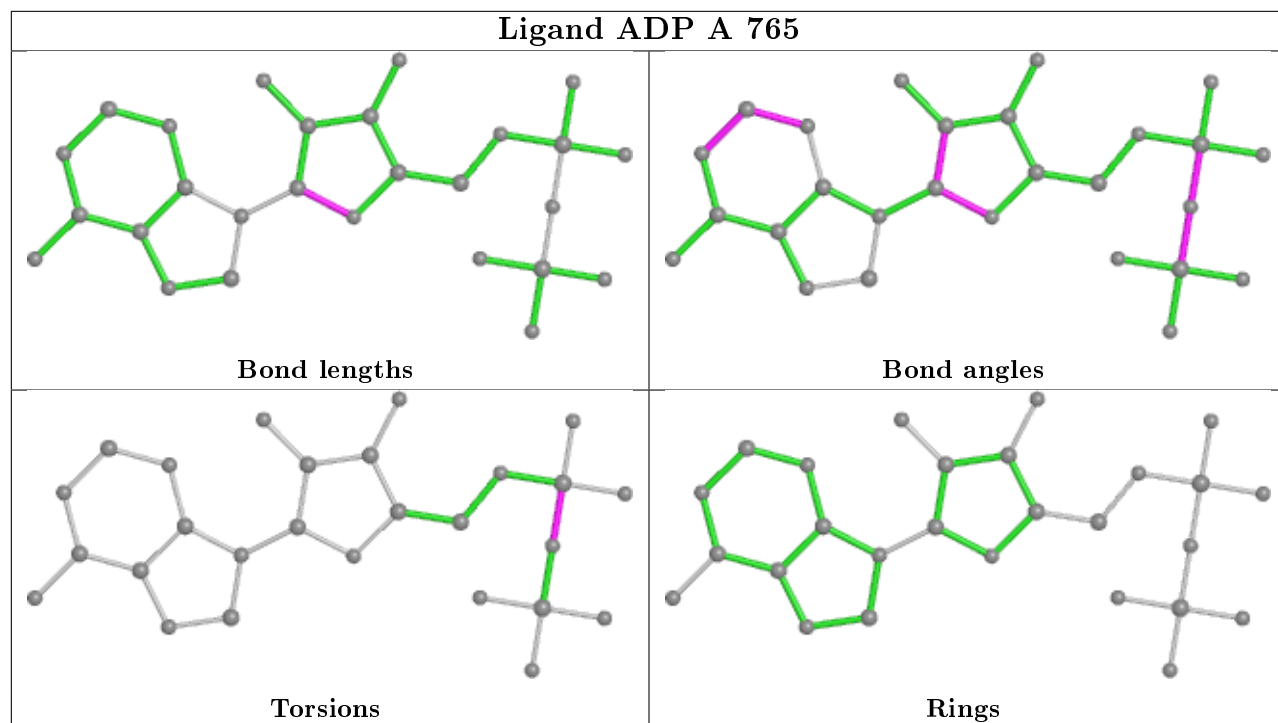
There are no ring outliers.

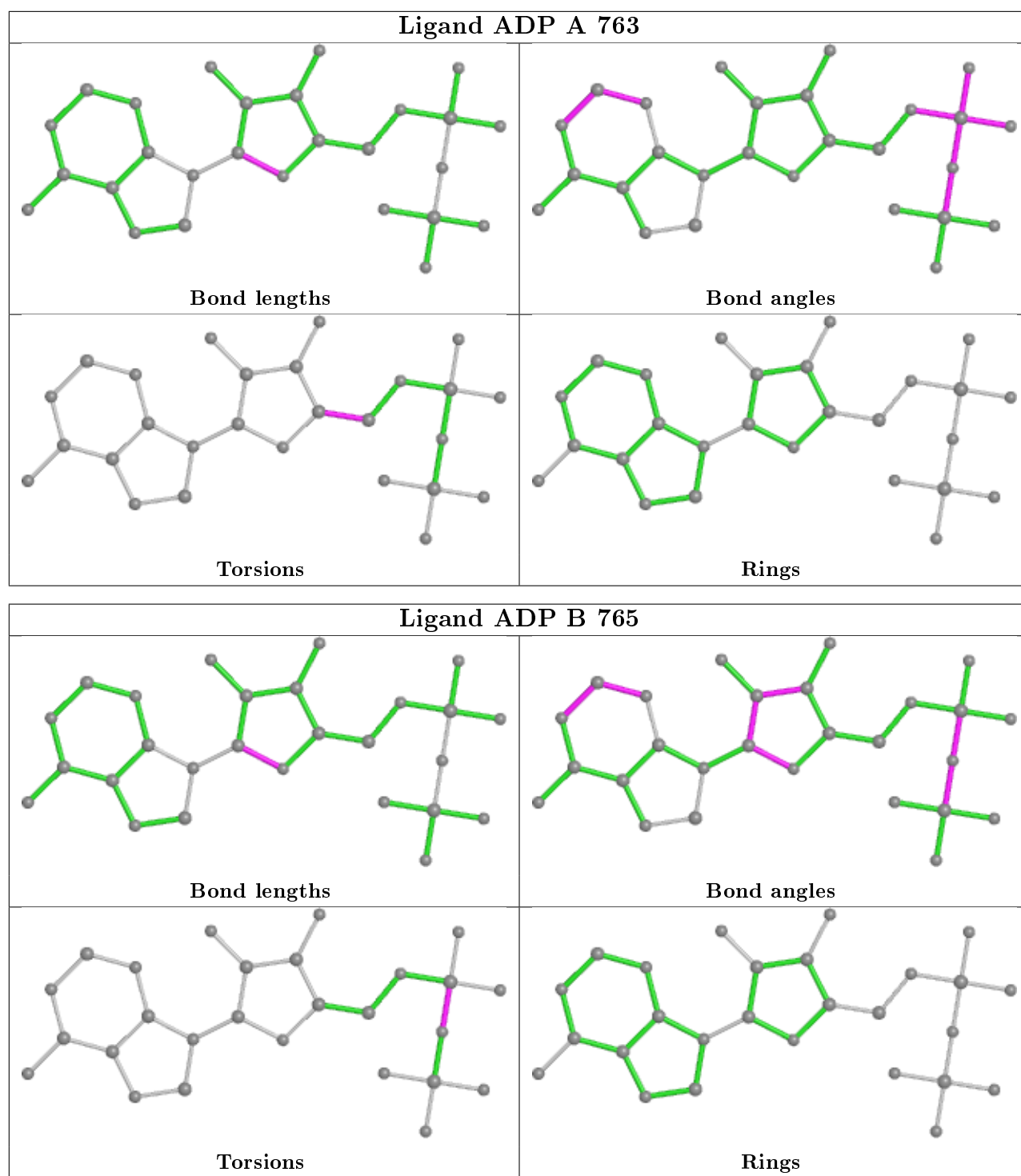
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	764	ADP	3	0
2	B	764	ADP	2	0
2	A	765	ADP	1	0
2	B	763	ADP	3	0
2	A	763	ADP	2	0
2	B	765	ADP	2	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 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, 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	748/762 (98%)	-0.56	8 (1%) 80 69	14, 54, 136, 202	58 (7%)
1	B	748/762 (98%)	-0.41	6 (0%) 86 78	8, 59, 152, 201	58 (7%)
All	All	1496/1524 (98%)	-0.48	14 (0%) 84 75	8, 56, 146, 202	116 (7%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	THR	3.5
1	A	563	THR	2.9
1	A	562	GLY	2.6
1	B	146	THR	2.5
1	B	114	CYS	2.3
1	A	361	ALA	2.3
1	B	19	ALA	2.3
1	A	151	THR	2.3
1	A	664	GLN	2.2
1	B	298	HIS	2.1
1	A	665	GLY	2.1
1	A	89	CYS	2.0
1	B	268	ASP	2.0
1	A	196	ALA	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

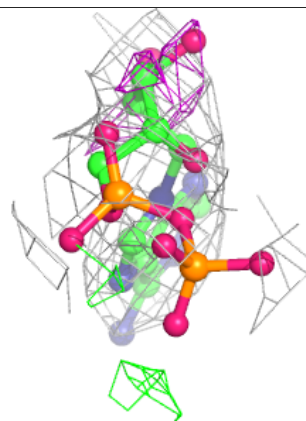
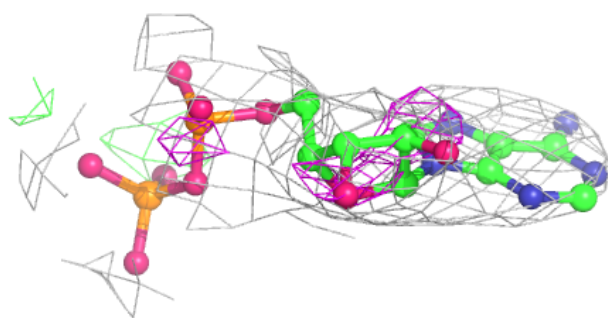
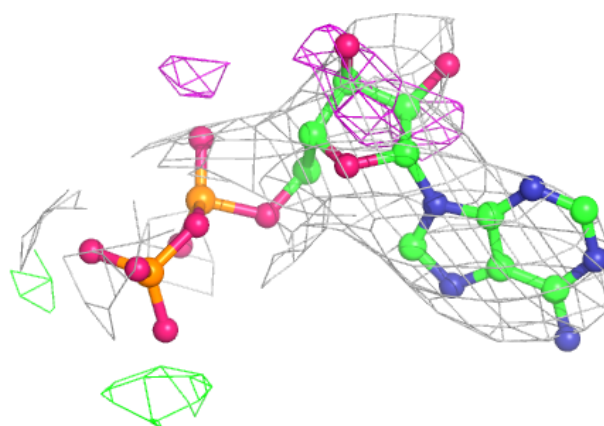
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	B	763	27/27	0.83	0.31	70,86,86,86	0
3	PO4	A	766	5/5	0.84	0.33	84,85,86,86	0
2	ADP	B	765	27/27	0.86	0.20	70,86,86,86	0
2	ADP	A	763	27/27	0.88	0.24	70,85,86,86	0
3	PO4	B	766	5/5	0.91	0.29	83,84,86,86	0
2	ADP	A	765	27/27	0.91	0.17	70,79,86,86	0
2	ADP	A	764	27/27	0.91	0.20	70,84,86,86	0
3	PO4	B	767	5/5	0.93	0.33	81,81,83,84	0
2	ADP	B	764	27/27	0.93	0.18	70,85,86,86	0
3	PO4	A	767	5/5	0.97	0.28	67,69,70,71	0
3	PO4	A	768	5/5	0.98	0.21	67,68,69,71	0
3	PO4	B	768	5/5	0.99	0.24	69,70,72,72	0

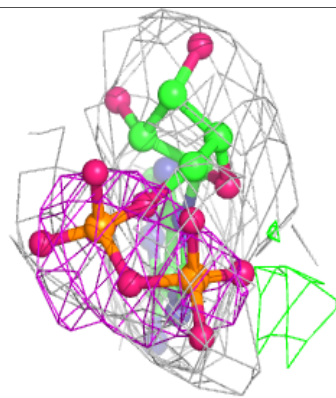
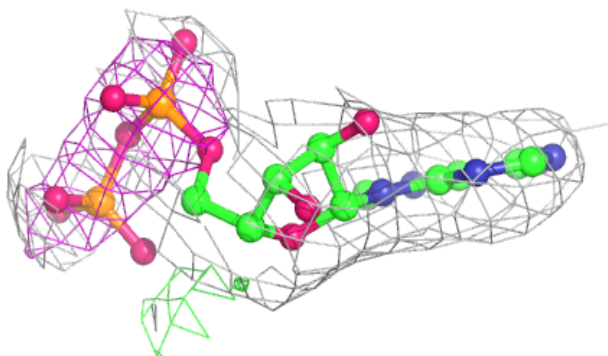
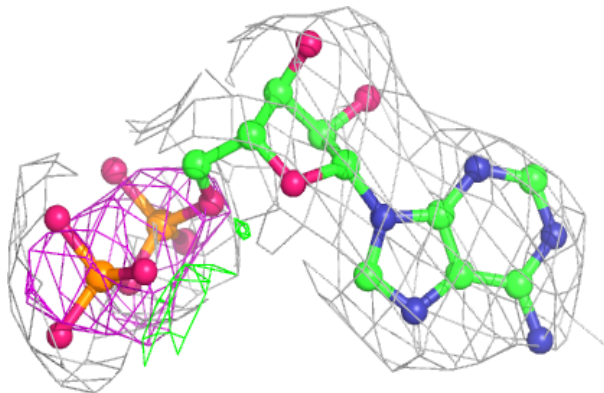
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP B 763:**

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

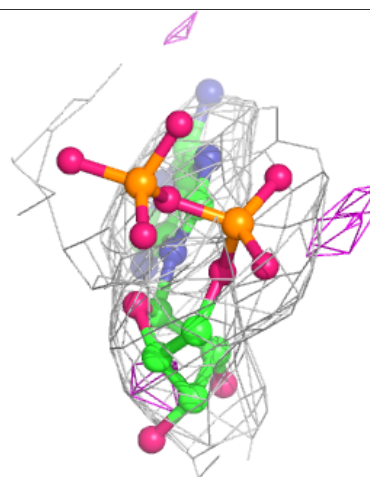
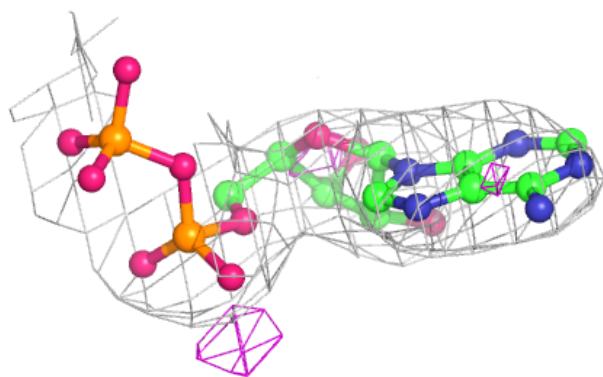
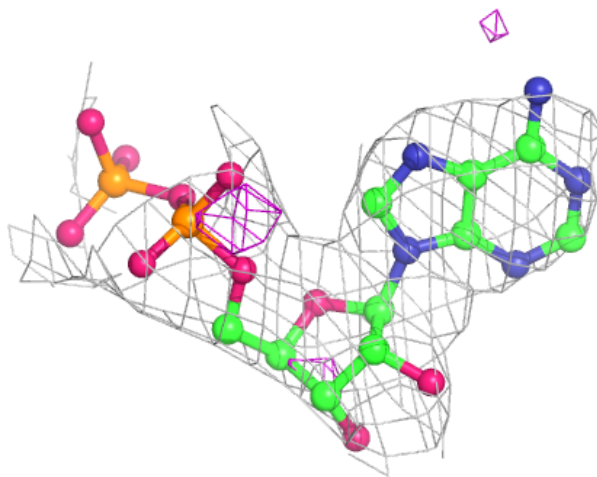
**Electron density around ADP B 765:**

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



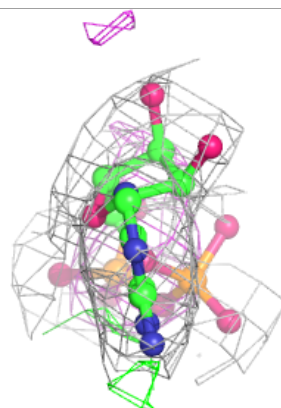
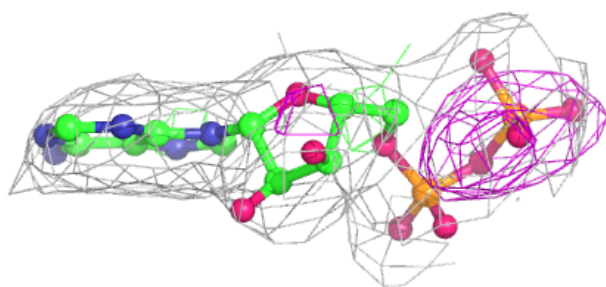
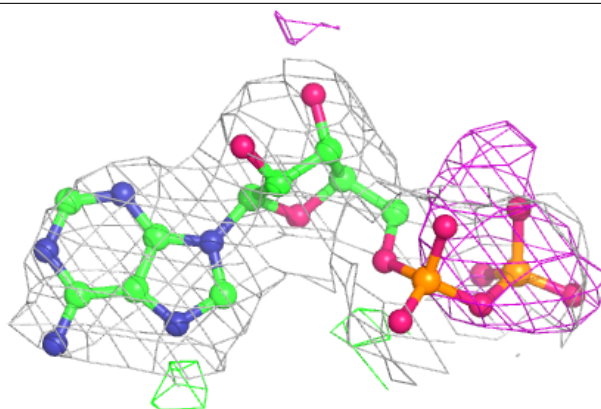
**Electron density around ADP A 763:**

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

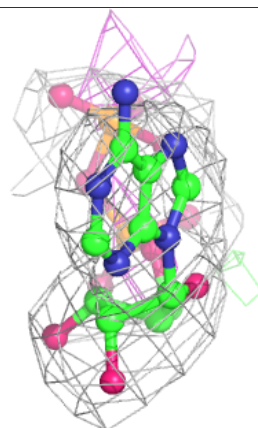
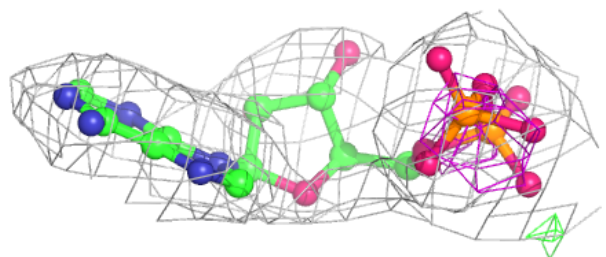
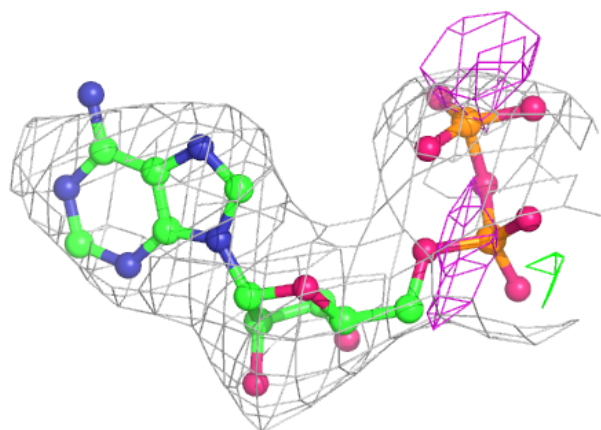


**Electron density around ADP A 765:**

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

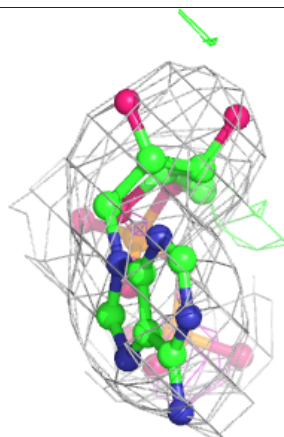
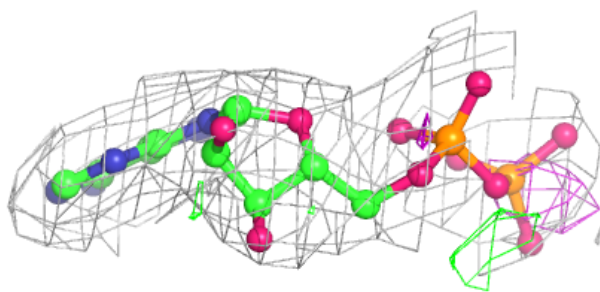
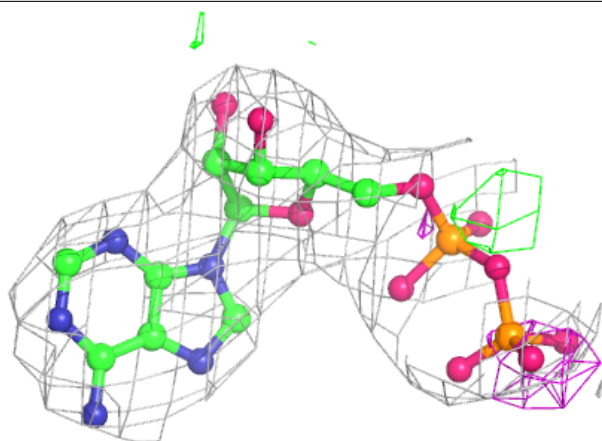
**Electron density around ADP A 764:**

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



**Electron density around ADP B 764:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.