



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:09 AM GMT

PDB ID : 3O8L
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

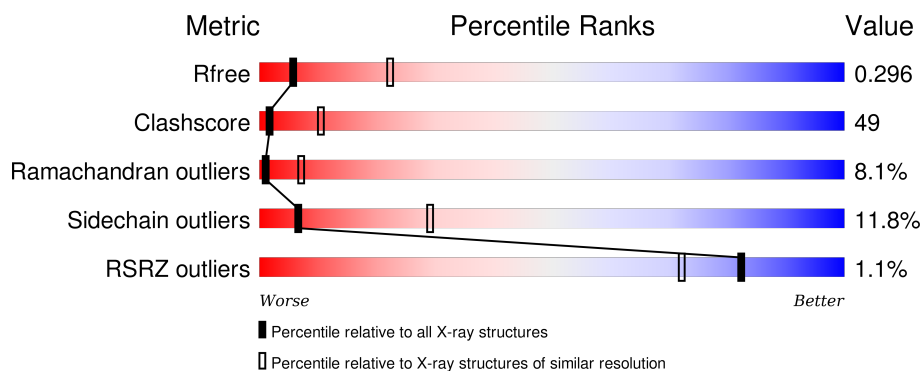
1 Overall quality at a glance ⓘ

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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

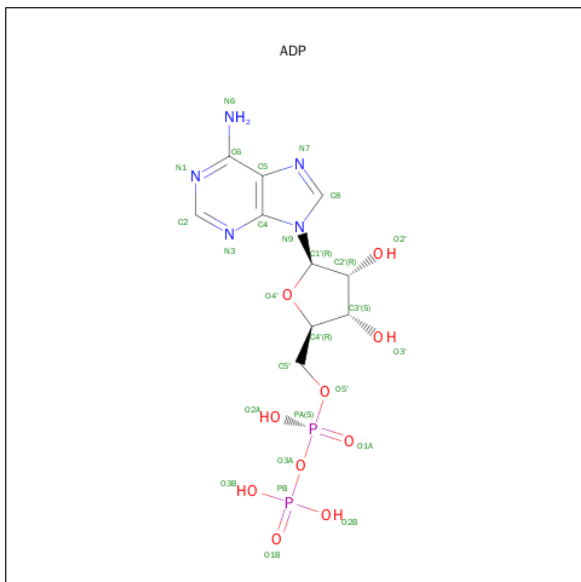
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	762	 36% 50% 11% 2%
1	B	762	 35% 52% 11% 2%

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:

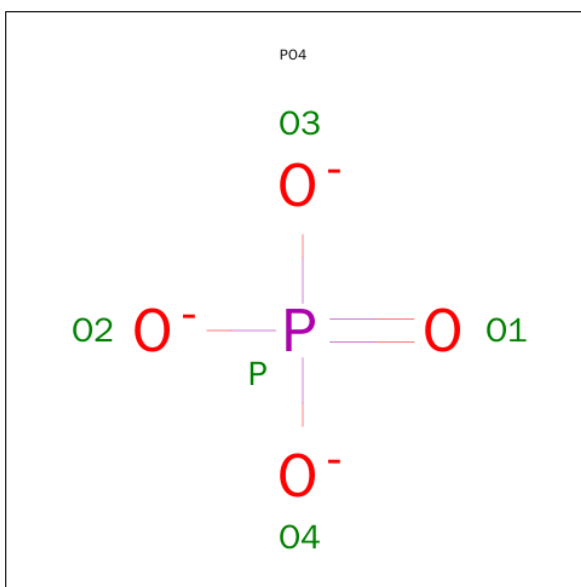
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	764	-	-	-	X
3	ADP	B	764	-	-	-	X
4	PO4	A	766	-	-	-	X
4	PO4	A	767	-	-	-	X
4	PO4	B	767	-	-	-	X

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

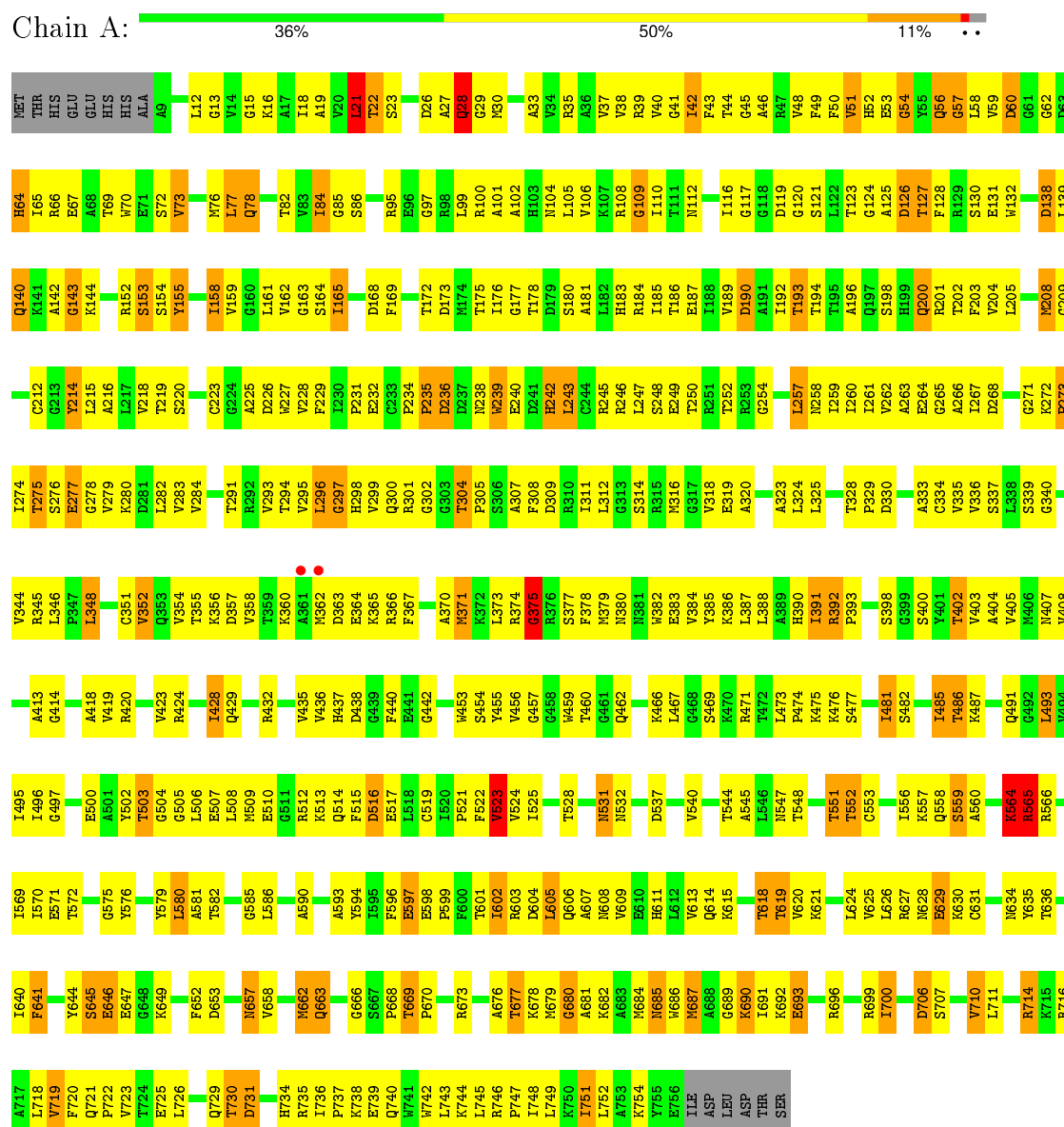


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

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 errors 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, α , β , γ	163.68Å 163.68Å 356.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.00 – 3.20 45.54 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.00-3.20) 100.0 (45.54-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.302 0.235 , 0.296	Depositor DCC
R_{free} test set	2361 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 113.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 47369 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11646	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ATP, 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	0.59	0/5819	0.83	3/7859 (0.0%)
1	B	0.61	0/5819	0.80	1/7859 (0.0%)
All	All	0.60	0/11638	0.81	4/15718 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	505	GLY	N-CA-C	-6.49	96.87	113.10
1	A	523	VAL	CB-CA-C	-6.48	99.09	111.40
1	A	21	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	375	GLY	N-CA-C	5.07	125.78	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	482	0
1	B	5719	0	5742	564	0
2	A	62	0	24	5	0
2	B	62	0	24	1	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	15	0	0	1	0
4	B	15	0	0	1	0
All	All	11646	0	11556	1037	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 49.

All (1037) 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	0.99	1.09
1:A:646:GLU:HG2	1:B:634:ASN:HD22	1.22	1.03
1:A:296:LEU:HD12	1:A:296:LEU:H	1.23	1.02
1:A:751:ILE:HD13	1:A:752:LEU:N	1.75	1.00
1:B:609:VAL:HG22	1:B:644:TYR:CE2	1.95	0.99
1:B:283:VAL:HG21	1:B:291:THR:HG21	1.45	0.98
1:A:634:ASN:ND2	1:B:646:GLU:HG2	1.79	0.98
1:B:35:ARG:HH11	1:B:77:LEU:HD13	1.25	0.96
1:A:391:ILE:HD12	1:A:392:ARG:H	1.29	0.96
1:A:28:GLN:HE21	1:A:28:GLN:H	1.11	0.96
1:A:257:LEU:HD12	1:A:259:ILE:HD11	1.46	0.95
1:B:514:GLN:HE21	1:B:514:GLN:H	1.12	0.91
1:B:221:LEU:HD23	1:B:674:ASN:ND2	1.85	0.91
1:A:334:CYS:SG	1:A:345:ARG:HB3	2.10	0.91
1:A:392:ARG:HB3	1:A:393:PRO:CA	2.01	0.90
1:B:39:ARG:HD2	1:B:70:TRP:CZ2	2.06	0.90
1:A:259:ILE:HG22	1:A:261:ILE:CD1	2.01	0.90
1:B:734:HIS:O	1:B:736:ILE:HG23	1.72	0.90
1:B:159:VAL:HG23	1:B:324:LEU:HD23	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:HB3	1:A:393:PRO:HA	1.53	0.89
1:A:257:LEU:H	1:A:257:LEU:HD23	1.38	0.89
1:B:296:LEU:HD12	1:B:296:LEU:H	1.36	0.88
1:B:549:ILE:HD12	1:B:659:LEU:HD13	1.56	0.88
1:B:509:MET:SD	1:B:512:ARG:NH1	2.48	0.87
1:A:491:GLN:HB3	1:A:700:ILE:HD11	1.55	0.87
1:B:664:GLN:C	1:B:666:GLY:H	1.73	0.87
1:A:44:THR:HG21	1:A:325:LEU:HD11	1.56	0.86
1:A:18:ILE:HG22	1:A:112:ASN:HB2	1.57	0.86
1:B:520:ILE:HG22	1:B:700:ILE:HD11	1.56	0.86
1:B:416:ASN:OD1	1:B:466:LYS:HB2	1.74	0.86
1:B:275:THR:HG23	1:B:278:GLY:HA3	1.58	0.85
1:B:419:VAL:O	1:B:423:VAL:HG23	1.77	0.85
1:A:66:ARG:HA	1:A:66:ARG:NE	1.90	0.84
1:A:280:LYS:HG2	1:A:291:THR:CG2	2.07	0.84
1:A:392:ARG:CB	1:A:393:PRO:HA	2.06	0.84
1:B:221:LEU:HD23	1:B:674:ASN:HD22	1.37	0.84
1:B:120:GLY:O	1:B:123:THR:HG22	1.77	0.84
1:A:245:ARG:O	1:A:249:GLU:HG3	1.77	0.83
1:B:184:ARG:NH1	1:B:303:GLY:HA3	1.94	0.83
1:A:58:LEU:HG	1:A:101:ALA:HB1	1.59	0.83
1:B:348:LEU:O	1:B:352:VAL:HG23	1.77	0.82
1:A:165:ILE:O	1:A:215:LEU:HD11	1.78	0.82
1:B:595:ILE:H	1:B:595:ILE:HD13	1.43	0.81
1:A:646:GLU:HG2	1:B:634:ASN:HB2	1.62	0.81
1:B:35:ARG:HH12	1:B:77:LEU:HD22	1.42	0.81
1:B:618:THR:HG22	1:B:619:THR:N	1.95	0.81
1:A:40:VAL:HG21	1:A:318:VAL:HG22	1.61	0.81
1:A:296:LEU:CD1	1:A:296:LEU:H	1.94	0.81
1:B:514:GLN:HE21	1:B:514:GLN:N	1.78	0.81
1:A:391:ILE:HD11	2:A:765:ATP:O2G	1.79	0.81
1:B:663:GLN:C	1:B:665:GLY:H	1.84	0.80
1:B:208:MET:HB2	1:B:300:GLN:OE1	1.81	0.80
1:B:382:TRP:CZ2	1:B:386:LYS:HD2	2.16	0.80
1:B:641:PHE:CD2	1:B:656:LYS:HD3	2.17	0.80
1:A:491:GLN:HB3	1:A:700:ILE:CD1	2.10	0.80
1:A:243:LEU:HD12	1:A:243:LEU:O	1.82	0.80
1:A:391:ILE:HD11	2:A:765:ATP:PG	2.22	0.80
1:B:419:VAL:HG11	1:B:467:LEU:HD11	1.62	0.80
1:A:364:GLU:O	1:A:366:ARG:N	2.15	0.80
1:A:646:GLU:HG2	1:B:634:ASN:ND2	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:HD11	1:B:333:ALA:HB2	1.65	0.79
1:B:687:MET:HE3	1:B:687:MET:O	1.81	0.79
1:B:41:GLY:O	1:B:44:THR:HG22	1.81	0.79
1:B:35:ARG:NH1	1:B:77:LEU:HD13	1.96	0.79
1:A:646:GLU:CG	1:B:634:ASN:HB2	2.13	0.78
1:B:440:PHE:O	1:B:443:PRO:HD2	1.83	0.78
1:A:246:ARG:O	1:A:250:THR:HG22	1.84	0.78
1:A:268:ASP:HB3	1:A:274:ILE:HD11	1.65	0.78
1:B:509:MET:O	1:B:512:ARG:HB2	1.83	0.78
1:A:259:ILE:HG22	1:A:261:ILE:HD12	1.66	0.78
1:A:354:VAL:HA	1:A:357:ASP:OD2	1.83	0.78
1:A:280:LYS:HG2	1:A:291:THR:HG22	1.64	0.77
1:B:436:VAL:HG22	1:B:448:ILE:HD12	1.64	0.77
1:A:696:ARG:HG3	1:A:696:ARG:HH11	1.50	0.77
1:A:208:MET:HB2	1:A:300:GLN:OE1	1.84	0.77
1:B:658:VAL:O	1:B:658:VAL:HG12	1.83	0.77
1:A:172:THR:OG1	1:A:337:SER:HB2	1.83	0.76
1:B:350:GLU:O	1:B:354:VAL:HG23	1.85	0.76
1:A:380:ASN:O	1:A:384:VAL:HG23	1.85	0.76
1:B:441:GLU:OE2	1:B:472:THR:HG21	1.83	0.76
1:B:470:LYS:HE2	1:B:471:ARG:H	1.50	0.76
1:A:335:VAL:HG23	1:A:348:LEU:HG	1.67	0.76
1:B:664:GLN:C	1:B:666:GLY:N	2.38	0.76
1:B:412:ALA:O	1:B:415:MET:HG3	1.86	0.76
1:A:312:LEU:O	1:A:316:MET:HG2	1.84	0.76
1:A:391:ILE:HD12	1:A:392:ARG:N	2.01	0.76
1:B:257:LEU:HD12	1:B:259:ILE:HD11	1.68	0.76
1:A:120:GLY:O	1:A:123:THR:HG22	1.84	0.76
1:B:443:PRO:O	1:B:484:ASN:ND2	2.18	0.75
1:A:516:ASP:O	1:A:519:CYS:HB2	1.87	0.75
1:A:348:LEU:O	1:A:352:VAL:HG23	1.86	0.75
1:B:420:ARG:HH11	1:B:460:THR:HB	1.52	0.74
1:A:33:ALA:O	1:A:37:VAL:HG23	1.87	0.74
1:A:296:LEU:HD12	1:A:296:LEU:N	1.99	0.74
1:B:418:ALA:HB2	1:B:676:ALA:HB1	1.68	0.74
1:A:734:HIS:O	1:A:736:ILE:HG23	1.86	0.74
1:A:601:THR:HG22	1:A:604:ASP:OD2	1.87	0.74
1:A:590:ALA:HB2	1:A:624:LEU:HD23	1.69	0.74
1:B:618:THR:HG22	1:B:619:THR:H	1.52	0.74
1:A:551:THR:HG22	1:A:552:THR:N	2.00	0.74
1:B:642:ASN:HD22	1:B:642:ASN:N	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:THR:HG23	1:B:72:SER:HB3	1.70	0.73
1:A:192:ILE:HG22	1:A:193:THR:N	2.02	0.73
1:B:459:TRP:H	1:B:459:TRP:HD1	1.34	0.73
1:B:40:VAL:HG22	1:B:751:ILE:HD11	1.71	0.72
1:A:120:GLY:HA2	1:A:123:THR:HG22	1.70	0.72
1:A:668:PRO:HG2	1:A:673:ARG:HE	1.54	0.72
1:A:548:THR:O	1:A:552:THR:HG23	1.88	0.72
1:B:124:GLY:HA2	1:B:127:THR:HG22	1.70	0.72
1:A:275:THR:HG23	1:A:278:GLY:HA3	1.72	0.72
1:B:316:MET:HE3	1:B:337:SER:HA	1.72	0.72
1:B:296:LEU:CD1	1:B:296:LEU:H	2.03	0.72
1:A:605:LEU:HD11	1:A:640:ILE:HD12	1.72	0.72
1:A:82:THR:HG21	1:A:86:SER:HB2	1.72	0.72
1:A:609:VAL:C	1:A:611:HIS:H	1.93	0.72
1:B:39:ARG:HD2	1:B:70:TRP:CE2	2.24	0.71
1:B:656:LYS:O	1:B:656:LYS:HG3	1.87	0.71
1:B:275:THR:O	1:B:279:VAL:HG23	1.90	0.71
1:A:58:LEU:HD11	1:A:105:LEU:HD21	1.70	0.71
1:A:220:SER:HB3	1:A:225:ALA:HB3	1.72	0.71
1:B:744:LYS:O	1:B:747:PRO:HD2	1.89	0.71
1:B:47:ARG:HD2	1:B:67:GLU:OE1	1.90	0.71
1:B:281:ASP:O	1:B:284:VAL:N	2.24	0.71
1:B:215:LEU:O	1:B:219:THR:CG2	2.38	0.71
1:B:595:ILE:HD12	1:B:746:ARG:NH1	2.05	0.71
1:A:387:LEU:HD23	1:A:428:ILE:HD13	1.71	0.71
1:B:679:MET:HE1	1:B:718:LEU:HD11	1.71	0.71
1:B:283:VAL:HG23	1:B:284:VAL:N	2.05	0.71
1:B:159:VAL:HG23	1:B:324:LEU:CD2	2.20	0.71
1:B:528:THR:HG23	1:B:531:ASN:H	1.56	0.70
1:B:663:GLN:O	1:B:665:GLY:N	2.24	0.70
1:B:95:ARG:HA	1:B:98:ARG:HD2	1.72	0.70
1:A:679:MET:HE3	1:A:718:LEU:HD11	1.73	0.70
1:B:231:PRO:O	1:B:233:CYS:N	2.25	0.70
1:A:297:GLY:O	1:A:299:VAL:HG13	1.91	0.69
1:B:205:LEU:HD22	1:B:296:LEU:HD11	1.73	0.69
1:B:232:GLU:HG2	1:B:374:ARG:HG2	1.74	0.69
1:A:190:ASP:O	1:A:193:THR:HG22	1.92	0.69
1:B:69:THR:CG2	1:B:72:SER:HB3	2.22	0.69
1:A:275:THR:OG1	1:A:277:GLU:HG2	1.92	0.69
1:B:38:VAL:O	1:B:42:ILE:HG12	1.94	0.68
1:B:605:LEU:HD21	1:B:640:ILE:HD13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:CB	1:A:393:PRO:CA	2.66	0.68
1:B:160:GLY:O	1:B:335:VAL:HG13	1.93	0.68
1:B:679:MET:CE	1:B:718:LEU:HD11	2.22	0.68
1:B:328:THR:HB	1:B:329:PRO:CD	2.23	0.68
1:A:521:PRO:HB3	1:A:707:SER:HB2	1.76	0.68
1:A:280:LYS:HG3	1:A:293:VAL:HG23	1.76	0.68
1:A:69:THR:HG23	1:A:72:SER:H	1.57	0.68
1:B:205:LEU:HD23	1:B:294:THR:HB	1.74	0.68
1:B:247:LEU:HD23	1:B:258:ASN:ND2	2.08	0.68
1:B:35:ARG:NH1	1:B:77:LEU:HD22	2.08	0.68
1:B:731:ASP:OD1	1:B:731:ASP:O	2.12	0.68
1:B:158:ILE:HD11	1:B:333:ALA:CB	2.22	0.68
1:B:61:GLY:O	1:B:63:ASP:N	2.26	0.68
1:B:551:THR:HG22	1:B:552:THR:N	2.08	0.68
1:A:257:LEU:HD12	1:A:259:ILE:CD1	2.23	0.67
1:B:481:ILE:O	1:B:485:ILE:HG23	1.95	0.67
1:A:364:GLU:C	1:A:366:ARG:H	1.97	0.67
1:B:435:VAL:CG1	1:B:467:LEU:HD21	2.24	0.67
1:A:268:ASP:HB3	1:A:274:ILE:CD1	2.24	0.67
1:B:281:ASP:O	1:B:283:VAL:N	2.27	0.67
1:B:493:LEU:HD23	1:B:495:ILE:HD11	1.77	0.67
1:B:531:ASN:HD21	1:B:538:PHE:HA	1.59	0.67
1:A:27:ALA:O	1:A:30:MET:HG3	1.94	0.67
1:A:259:ILE:HG22	1:A:261:ILE:HD11	1.76	0.66
1:A:262:VAL:HG12	1:A:263:ALA:O	1.95	0.66
1:A:51:VAL:O	1:A:51:VAL:HG12	1.95	0.66
1:B:609:VAL:HG13	1:B:644:TYR:CD2	2.30	0.66
1:B:456:VAL:O	1:B:459:TRP:CD1	2.49	0.66
1:B:459:TRP:CD2	1:B:466:LYS:NZ	2.63	0.66
1:B:247:LEU:CD2	1:B:258:ASN:HD22	2.08	0.66
1:A:726:LEU:O	1:A:730:THR:HG22	1.95	0.66
1:A:258:ASN:C	1:A:259:ILE:HD12	2.16	0.66
1:A:711:LEU:HD11	1:A:718:LEU:HG	1.78	0.66
1:B:722:PRO:HG2	1:B:725:GLU:HB2	1.77	0.66
1:B:595:ILE:HD13	1:B:595:ILE:N	2.11	0.66
1:A:481:ILE:HG12	1:A:482:SER:N	2.10	0.66
1:A:601:THR:O	1:A:604:ASP:N	2.27	0.65
1:B:502:TYR:OH	1:B:730:THR:HG21	1.96	0.65
1:A:619:THR:HG23	1:A:620:VAL:H	1.61	0.65
1:B:510:GLU:O	1:B:512:ARG:N	2.29	0.65
1:B:65:ILE:HG22	1:B:65:ILE:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:O	1:A:299:VAL:N	2.30	0.65
1:B:402:THR:HG21	1:B:432:ARG:NH2	2.12	0.65
1:A:312:LEU:HD11	1:A:316:MET:HE2	1.79	0.65
1:B:247:LEU:HA	1:B:250:THR:HG22	1.79	0.65
1:A:420:ARG:HA	1:A:456:VAL:HG11	1.78	0.65
1:A:528:THR:HG23	1:A:531:ASN:H	1.61	0.65
1:B:473:LEU:HD21	1:B:503:THR:HG22	1.78	0.65
1:B:419:VAL:HG21	1:B:467:LEU:HD12	1.79	0.65
1:A:228:VAL:HG12	1:A:229:PHE:N	2.12	0.65
1:B:495:ILE:HG22	1:B:501:ALA:HB1	1.79	0.65
1:B:514:GLN:NE2	1:B:514:GLN:H	1.90	0.65
1:B:39:ARG:CD	1:B:70:TRP:CE2	2.79	0.65
1:B:512:ARG:HH22	1:B:707:SER:HB2	1.60	0.65
1:B:345:ARG:O	1:B:346:LEU:HD23	1.96	0.65
1:A:419:VAL:O	1:A:423:VAL:HG23	1.97	0.65
1:A:646:GLU:CG	1:B:634:ASN:HD22	2.04	0.64
1:A:66:ARG:HH21	1:A:108:ARG:NH2	1.95	0.64
1:A:333:ALA:HB1	1:A:348:LEU:HD12	1.78	0.64
1:A:387:LEU:HD22	1:A:428:ILE:HG21	1.79	0.64
1:B:296:LEU:HD12	1:B:296:LEU:N	2.11	0.64
1:A:296:LEU:O	1:A:297:GLY:O	2.14	0.64
1:A:159:VAL:HG23	1:A:324:LEU:CD2	2.28	0.64
1:A:39:ARG:HD2	1:A:70:TRP:CE2	2.32	0.64
1:A:586:LEU:O	1:A:586:LEU:HD12	1.96	0.64
1:A:123:THR:O	1:A:127:THR:HG22	1.96	0.64
1:B:247:LEU:HA	1:B:250:THR:CG2	2.28	0.64
1:B:726:LEU:HD23	1:B:729:GLN:OE1	1.97	0.64
1:B:387:LEU:CD2	1:B:428:ILE:HD13	2.27	0.64
1:B:112:ASN:OD1	1:B:157:ASN:HB2	1.98	0.64
1:B:21:LEU:HD23	1:B:21:LEU:O	1.97	0.64
1:B:577:CYS:HA	1:B:597:GLU:OE2	1.97	0.63
1:A:475:LYS:O	1:A:477:SER:N	2.31	0.63
1:B:567:VAL:HG22	1:B:616:MET:HE1	1.80	0.63
1:B:110:ILE:H	1:B:110:ILE:HD12	1.62	0.63
1:B:686:TRP:HZ2	1:B:709:CYS:HG	1.46	0.63
1:A:569:ILE:HD12	1:A:641:PHE:HA	1.79	0.63
1:A:159:VAL:HG23	1:A:324:LEU:HD23	1.79	0.63
1:B:585:GLY:HA2	1:B:626:LEU:HD12	1.80	0.63
1:B:228:VAL:HG12	1:B:229:PHE:N	2.13	0.63
1:B:334:CYS:HA	1:B:346:LEU:O	1.98	0.63
1:B:9:ALA:HB1	1:B:11:THR:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ARG:HG3	1:B:456:VAL:HB	1.81	0.63
1:B:612:LEU:O	1:B:616:MET:HG2	1.99	0.63
1:A:280:LYS:O	1:A:284:VAL:HG23	1.99	0.63
1:B:481:ILE:HD12	1:B:481:ILE:O	1.99	0.63
1:A:609:VAL:C	1:A:611:HIS:N	2.51	0.63
1:B:232:GLU:O	1:B:371:MET:HG2	1.98	0.63
1:A:102:ALA:O	1:A:106:VAL:HG23	1.99	0.63
1:B:182:LEU:HD11	1:B:218:VAL:HG11	1.80	0.63
1:B:193:THR:HG23	1:B:194:THR:N	2.13	0.63
1:B:428:ILE:HG13	1:B:453:TRP:HZ3	1.62	0.63
1:B:724:THR:HA	1:B:727:GLN:HE21	1.63	0.62
1:B:624:LEU:HD12	1:B:625:VAL:N	2.14	0.62
1:A:503:THR:HG22	1:A:504:GLY:N	2.15	0.62
1:A:22:THR:HG21	1:A:82:THR:OG1	1.99	0.62
1:B:481:ILE:C	1:B:481:ILE:HD12	2.18	0.62
1:B:249:GLU:HA	1:B:252:THR:HG22	1.82	0.62
1:B:101:ALA:HA	1:B:104:ASN:HD22	1.64	0.62
1:B:436:VAL:HG22	1:B:448:ILE:CD1	2.29	0.62
1:A:35:ARG:HD3	1:A:77:LEU:HD13	1.82	0.62
1:A:731:ASP:OD1	1:A:731:ASP:C	2.37	0.62
1:A:56:GLN:O	1:A:59:VAL:N	2.32	0.62
1:A:202:THR:HG22	1:A:202:THR:O	2.00	0.61
1:B:605:LEU:HD11	1:B:640:ILE:HD12	1.82	0.61
1:B:669:THR:O	1:B:673:ARG:HG3	2.00	0.61
1:A:496:ILE:CD1	1:A:525:ILE:HD12	2.30	0.61
1:A:49:PHE:CD1	1:A:110:ILE:HD11	2.34	0.61
1:A:565:ARG:HH21	1:A:565:ARG:HG2	1.65	0.61
1:B:376:ARG:HH21	1:B:376:ARG:HB3	1.65	0.61
1:B:634:ASN:O	1:B:636:THR:HG23	2.01	0.61
1:B:514:GLN:NE2	1:B:514:GLN:N	2.46	0.61
1:A:185:ILE:HD11	1:A:215:LEU:HD23	1.82	0.61
1:A:259:ILE:CG2	1:A:261:ILE:HD11	2.31	0.61
1:A:50:PHE:CE2	1:A:84:ILE:HD11	2.36	0.61
1:A:19:ALA:HA	1:A:49:PHE:O	2.01	0.61
1:B:283:VAL:HG23	1:B:284:VAL:H	1.65	0.61
1:B:485:ILE:HG12	1:B:517:GLU:HB3	1.82	0.61
1:B:481:ILE:HD11	1:B:518:LEU:HD21	1.82	0.61
1:B:126:ASP:HB2	1:B:348:LEU:HD22	1.81	0.61
1:B:316:MET:HE1	1:B:338:LEU:HB2	1.82	0.61
1:A:35:ARG:HH12	1:A:752:LEU:HD13	1.66	0.60
1:B:228:VAL:HG12	1:B:229:PHE:H	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:PRO:HB2	1:B:673:ARG:HG2	1.83	0.60
1:B:601:THR:O	1:B:603:ARG:N	2.34	0.60
1:A:722:PRO:HG2	1:A:725:GLU:HG3	1.82	0.60
1:A:308:PHE:CZ	1:A:312:LEU:HD22	2.36	0.60
1:B:495:ILE:CG2	1:B:501:ALA:HB1	2.32	0.60
1:B:307:ALA:H	1:B:547:ASN:HD21	1.47	0.60
1:B:627:ARG:NH2	1:B:636:THR:HA	2.17	0.60
1:A:609:VAL:O	1:A:611:HIS:N	2.30	0.60
1:B:604:ASP:O	1:B:607:ALA:N	2.33	0.60
1:B:333:ALA:HB1	1:B:348:LEU:HD12	1.84	0.60
1:A:52:HIS:HA	1:A:84:ILE:O	2.02	0.60
1:A:183:HIS:O	1:A:187:GLU:HG3	2.01	0.60
1:A:99:LEU:HD12	1:A:100:ARG:N	2.17	0.60
1:A:28:GLN:NE2	1:A:28:GLN:H	1.93	0.59
1:A:590:ALA:HA	1:A:624:LEU:HB3	1.83	0.59
1:B:18:ILE:HD12	1:B:324:LEU:HD12	1.84	0.59
1:B:456:VAL:HA	1:B:459:TRP:NE1	2.17	0.59
1:A:280:LYS:HG2	1:A:291:THR:HG21	1.83	0.59
1:B:185:ILE:HD12	1:B:219:THR:HB	1.85	0.59
1:A:120:GLY:CA	1:A:123:THR:HG22	2.32	0.59
1:B:425:ILE:O	1:B:429:GLN:HG3	2.02	0.59
1:B:459:TRP:N	1:B:459:TRP:CD1	2.64	0.59
1:B:185:ILE:O	1:B:189:VAL:HG23	2.00	0.59
1:B:687:MET:HE1	1:B:691:ILE:HD11	1.83	0.59
1:A:78:GLN:OE1	1:A:78:GLN:N	2.35	0.59
1:A:66:ARG:CZ	1:A:66:ARG:HA	2.32	0.59
1:A:593:ALA:HA	1:A:626:LEU:O	2.02	0.59
1:B:416:ASN:HB3	1:B:459:TRP:HB3	1.84	0.59
1:B:660:GLY:C	1:B:662:MET:H	2.06	0.59
1:B:675:PHE:HA	1:B:678:LYS:HE2	1.85	0.59
2:A:763:ATP:O2A	2:A:763:ATP:O2B	2.21	0.59
1:B:595:ILE:HD12	1:B:746:ARG:HH12	1.65	0.59
1:B:404:ALA:HB2	1:B:490:ILE:HD12	1.84	0.59
1:B:532:ASN:O	1:B:737:PRO:HD3	2.02	0.59
1:B:700:ILE:HG13	1:B:700:ILE:O	2.02	0.58
1:B:166:ASP:OD1	1:B:209:GLY:HA2	2.02	0.58
1:B:314:SER:O	1:B:318:VAL:HG23	2.03	0.58
1:B:481:ILE:HD11	1:B:518:LEU:CD2	2.33	0.58
1:A:459:TRP:HA	1:A:462:GLN:HG3	1.85	0.58
1:B:306:SER:O	1:B:310:ARG:HG3	2.04	0.58
1:B:713:MET:HG3	1:B:718:LEU:HD12	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HA	1:A:273:PRO:HA	1.84	0.58
1:A:726:LEU:HD23	1:A:729:GLN:OE1	2.03	0.58
1:B:416:ASN:OD1	1:B:466:LYS:CB	2.49	0.58
1:B:535:GLY:O	1:B:712:GLY:HA3	2.03	0.58
1:B:663:GLN:C	1:B:665:GLY:N	2.51	0.58
1:A:398:SER:C	1:A:400:SER:H	2.07	0.58
1:B:215:LEU:O	1:B:219:THR:HG22	2.03	0.58
1:A:751:ILE:HD13	1:A:751:ILE:C	2.23	0.57
1:B:216:ALA:O	1:B:219:THR:HG23	2.04	0.57
1:A:646:GLU:HG2	1:B:634:ASN:CB	2.32	0.57
1:B:319:GLU:OE2	1:B:345:ARG:NE	2.37	0.57
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.69	0.57
1:A:268:ASP:CB	1:A:274:ILE:HD11	2.34	0.57
1:B:9:ALA:C	1:B:11:THR:H	2.06	0.57
1:A:153:SER:O	1:A:155:TYR:N	2.26	0.57
1:A:524:VAL:CG1	1:A:710:VAL:HG22	2.34	0.57
1:B:369:GLU:O	1:B:373:LEU:HB2	2.03	0.57
1:B:158:ILE:HD13	1:B:158:ILE:H	1.70	0.57
1:B:323:ALA:HA	1:B:345:ARG:HH12	1.70	0.57
1:A:15:GLY:O	1:A:16:LYS:HG2	2.05	0.57
1:A:116:ILE:HG12	1:A:161:LEU:HD13	1.86	0.57
1:A:243:LEU:HD12	1:A:247:LEU:HD12	1.87	0.57
1:B:435:VAL:HB	1:B:467:LEU:HD21	1.87	0.57
1:B:40:VAL:HG21	1:B:318:VAL:HG13	1.85	0.57
1:A:95:ARG:C	1:A:97:GLY:H	2.07	0.57
1:A:42:ILE:HD13	1:A:48:VAL:HG23	1.87	0.57
1:A:371:MET:SD	1:A:378:PHE:CE2	2.98	0.56
1:B:611:HIS:CE1	1:B:754:LYS:HB3	2.40	0.56
1:A:50:PHE:O	1:A:51:VAL:HG23	2.05	0.56
1:B:387:LEU:HD22	1:B:428:ILE:HD13	1.86	0.56
1:A:219:THR:O	1:A:223:CYS:SG	2.57	0.56
1:A:312:LEU:HD11	1:A:316:MET:CE	2.35	0.56
1:A:564:LYS:HA	1:A:564:LYS:HE2	1.86	0.56
1:B:485:ILE:O	1:B:485:ILE:HD12	2.05	0.56
1:A:523:VAL:HG22	1:A:686:TRP:CZ3	2.39	0.56
1:B:609:VAL:HG13	1:B:644:TYR:HD2	1.70	0.56
1:B:642:ASN:N	1:B:642:ASN:ND2	2.53	0.56
1:A:682:LYS:HG2	1:A:718:LEU:HD23	1.87	0.56
1:B:669:THR:HB	1:B:670:PRO:HD2	1.86	0.56
1:B:169:PHE:CE2	1:B:351:CYS:HB3	2.40	0.56
1:B:221:LEU:CD2	1:B:674:ASN:HD22	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ARG:HE	1:A:714:ARG:HA	1.71	0.56
1:A:352:VAL:HA	1:A:355:THR:HG22	1.86	0.56
1:B:247:LEU:HD23	1:B:258:ASN:HD22	1.70	0.56
1:A:532:ASN:O	1:A:737:PRO:HD3	2.05	0.56
1:A:471:ARG:HB3	1:A:500:GLU:HG3	1.87	0.56
1:B:556:ILE:HG22	1:B:568:PHE:CD2	2.40	0.56
1:B:543:ASP:HB3	1:B:672:ASP:OD2	2.06	0.56
1:B:275:THR:HG23	1:B:278:GLY:CA	2.32	0.56
1:B:292:ARG:O	1:B:293:VAL:HG23	2.06	0.55
1:B:257:LEU:O	1:B:257:LEU:HG	2.06	0.55
1:B:372:LYS:HA	1:B:379:MET:HE1	1.88	0.55
1:B:281:ASP:O	1:B:282:LEU:C	2.43	0.55
1:B:235:PRO:HD2	1:B:267:ILE:O	2.07	0.55
1:B:611:HIS:HE1	1:B:754:LYS:HB3	1.70	0.55
1:A:177:GLY:N	1:A:309:ASP:OD1	2.37	0.55
1:A:26:ASP:O	1:A:301:ARG:NH1	2.39	0.55
1:B:190:ASP:O	1:B:194:THR:HG23	2.07	0.55
1:B:745:LEU:O	1:B:748:ILE:HG12	2.06	0.55
1:B:124:GLY:CA	1:B:127:THR:HG22	2.37	0.55
1:A:686:TRP:CZ3	1:A:687:MET:HG2	2.41	0.55
1:A:153:SER:C	1:A:155:TYR:H	2.08	0.55
1:A:391:ILE:HD12	1:A:391:ILE:H	1.71	0.55
1:A:408:VAL:O	1:A:497:GLY:HA3	2.06	0.55
1:A:101:ALA:HA	1:A:104:ASN:HD22	1.71	0.55
1:B:708:GLY:O	1:B:723:VAL:HG22	2.05	0.55
1:B:299:VAL:HG23	1:B:300:GLN:N	2.22	0.55
1:A:335:VAL:CG2	1:A:348:LEU:HG	2.37	0.55
1:A:605:LEU:HD21	1:A:640:ILE:HD13	1.88	0.55
1:A:168:ASP:OD2	1:A:169:PHE:N	2.39	0.55
1:A:696:ARG:NH1	1:A:696:ARG:HG3	2.21	0.55
1:B:537:ASP:HB3	1:B:741:TRP:NE1	2.20	0.55
1:B:535:GLY:O	1:B:714:ARG:HD2	2.06	0.55
1:A:294:THR:HG22	1:A:295:VAL:N	2.22	0.55
1:B:562:GLY:C	1:B:564:LYS:H	2.08	0.55
1:A:646:GLU:HG3	1:B:634:ASN:HB2	1.86	0.55
1:A:726:LEU:O	1:A:730:THR:CG2	2.54	0.55
1:A:569:ILE:HG12	1:A:625:VAL:HB	1.88	0.55
1:A:627:ARG:NH2	1:A:636:THR:HA	2.21	0.55
1:A:402:THR:HB	1:A:432:ARG:HB3	1.89	0.55
1:B:240:GLU:OE1	1:B:240:GLU:N	2.40	0.55
1:B:441:GLU:OE2	1:B:472:THR:CG2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLY:O	1:B:335:VAL:HA	2.07	0.55
1:B:18:ILE:HD12	1:B:324:LEU:CD1	2.38	0.54
1:B:641:PHE:CG	1:B:656:LYS:HD3	2.42	0.54
1:A:387:LEU:CD2	1:A:428:ILE:HG21	2.37	0.54
1:B:485:ILE:C	1:B:485:ILE:HD12	2.28	0.54
1:A:275:THR:O	1:A:279:VAL:HG23	2.07	0.54
1:A:275:THR:HG23	1:A:278:GLY:CA	2.37	0.54
1:B:402:THR:HG23	1:B:491:GLN:HE21	1.72	0.54
1:B:471:ARG:HB2	1:B:500:GLU:HG2	1.90	0.54
1:A:551:THR:CG2	1:A:552:THR:N	2.68	0.54
1:B:289:TYR:C	1:B:291:THR:H	2.11	0.54
1:A:271:GLY:O	1:A:273:PRO:HD3	2.07	0.54
1:B:565:ARG:HH11	1:B:565:ARG:HG3	1.73	0.54
1:B:551:THR:O	1:B:552:THR:C	2.46	0.54
1:B:193:THR:C	1:B:195:THR:H	2.11	0.54
1:A:679:MET:O	1:A:681:ALA:N	2.40	0.54
1:B:523:VAL:HG22	1:B:686:TRP:CZ3	2.42	0.54
1:A:271:GLY:O	1:A:273:PRO:CD	2.55	0.54
1:A:231:PRO:O	1:A:234:PRO:HD3	2.07	0.54
1:A:513:LYS:HB2	1:A:514:GLN:NE2	2.23	0.54
1:B:609:VAL:HA	1:B:644:TYR:HE2	1.72	0.54
1:A:204:VAL:O	1:A:204:VAL:HG12	2.07	0.54
1:A:403:VAL:HG12	1:A:404:ALA:N	2.23	0.54
1:A:340:GLY:HA2	1:A:716:ARG:HA	1.90	0.54
1:B:119:ASP:OD1	1:B:120:GLY:N	2.38	0.54
1:B:267:ILE:HA	1:B:273:PRO:HA	1.88	0.54
1:A:53:GLU:O	1:A:54:GLY:O	2.26	0.54
1:B:420:ARG:HH11	1:B:460:THR:CB	2.20	0.54
1:A:721:GLN:NE2	1:A:726:LEU:HD21	2.23	0.54
1:B:376:ARG:CB	1:B:376:ARG:NH2	2.70	0.54
1:A:29:GLY:HA3	1:A:176:ILE:CG2	2.38	0.54
1:B:605:LEU:HG	1:B:643:LEU:HD23	1.90	0.54
1:B:382:TRP:CE2	1:B:386:LYS:HD2	2.43	0.54
1:B:21:LEU:HD23	1:B:21:LEU:C	2.28	0.54
1:B:175:THR:O	1:B:178:THR:HG22	2.08	0.54
1:B:364:GLU:O	1:B:366:ARG:N	2.41	0.54
1:B:726:LEU:O	1:B:729:GLN:HB2	2.08	0.53
1:A:722:PRO:HG2	1:A:725:GLU:CG	2.37	0.53
1:B:409:GLY:HA2	1:B:471:ARG:HB3	1.89	0.53
1:B:11:THR:O	1:B:13:GLY:N	2.42	0.53
1:A:436:VAL:HG13	1:A:442:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HA	1:A:73:VAL:HG11	1.89	0.53
1:B:459:TRP:CE2	1:B:466:LYS:NZ	2.77	0.53
1:B:185:ILE:HG12	1:B:185:ILE:O	2.08	0.53
1:A:375:GLY:HA2	1:A:379:MET:CE	2.39	0.53
1:B:34:VAL:O	1:B:38:VAL:HG23	2.07	0.53
1:B:21:LEU:HD12	1:B:51:VAL:HG11	1.90	0.53
1:B:667:SER:OG	1:B:668:PRO:HD2	2.08	0.53
1:A:435:VAL:HG13	1:A:467:LEU:CD2	2.39	0.53
1:B:283:VAL:CG2	1:B:284:VAL:N	2.72	0.53
1:B:182:LEU:CD1	1:B:218:VAL:HG11	2.38	0.53
1:A:189:VAL:O	1:A:193:THR:HB	2.09	0.53
1:B:124:GLY:HA2	1:B:127:THR:CG2	2.38	0.53
1:B:231:PRO:C	1:B:233:CYS:H	2.11	0.53
1:B:402:THR:HG21	1:B:432:ARG:HH21	1.71	0.53
1:A:738:LYS:O	1:A:739:GLU:HB2	2.09	0.53
1:A:748:ILE:CG1	1:A:749:LEU:N	2.71	0.53
1:A:59:VAL:O	1:A:60:ASP:O	2.26	0.53
1:B:184:ARG:HA	1:B:187:GLU:OE2	2.09	0.53
1:A:120:GLY:O	1:A:123:THR:CG2	2.54	0.53
1:A:711:LEU:HD22	1:A:720:PHE:CZ	2.44	0.53
1:A:500:GLU:OE2	1:A:735:ARG:NH2	2.40	0.53
1:B:407:ASN:O	1:B:439:GLY:HA2	2.09	0.53
1:B:549:ILE:O	1:B:553:CYS:HB2	2.09	0.53
1:B:709:CYS:HA	1:B:722:PRO:HA	1.89	0.53
1:A:124:GLY:O	1:A:127:THR:HG23	2.09	0.53
1:B:213:GLY:HA3	1:B:230:ILE:HG22	1.89	0.53
1:B:84:ILE:HD12	1:B:84:ILE:N	2.24	0.53
1:A:35:ARG:HD3	1:A:77:LEU:CD1	2.38	0.53
1:B:738:LYS:O	1:B:739:GLU:HB2	2.08	0.53
1:A:436:VAL:CG1	1:A:442:GLY:HA3	2.38	0.53
1:B:407:ASN:HA	1:B:496:ILE:O	2.09	0.53
1:A:572:THR:O	1:A:629:GLU:HB3	2.08	0.53
1:A:57:GLY:HA2	1:A:64:HIS:CD2	2.44	0.53
1:A:751:ILE:HD13	1:A:752:LEU:H	1.67	0.53
1:B:470:LYS:HG3	1:B:472:THR:HG23	1.90	0.53
1:B:319:GLU:HG2	1:B:343:ALA:HB1	1.90	0.53
1:B:632:ASN:C	1:B:632:ASN:OD1	2.47	0.52
1:B:41:GLY:O	1:B:44:THR:CG2	2.53	0.52
1:A:746:ARG:N	1:A:747:PRO:HD2	2.24	0.52
1:B:569:ILE:HD12	1:B:641:PHE:HA	1.91	0.52
1:B:257:LEU:H	1:B:257:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLY:O	1:A:267:ILE:HG23	2.08	0.52
1:B:402:THR:CB	1:B:432:ARG:HH21	2.22	0.52
1:B:358:VAL:HA	1:B:373:LEU:HD13	1.91	0.52
1:A:239:TRP:CD1	1:A:240:GLU:N	2.78	0.52
1:A:379:MET:O	1:A:383:GLU:HG2	2.09	0.52
1:A:509:MET:O	1:A:512:ARG:HB2	2.09	0.52
1:A:604:ASP:O	1:A:607:ALA:N	2.43	0.52
1:A:360:LYS:O	1:A:363:ASP:N	2.42	0.52
1:A:165:ILE:N	1:A:165:ILE:HD13	2.23	0.52
1:A:371:MET:CE	1:A:382:TRP:CD1	2.93	0.52
1:B:649:LYS:C	1:B:651:ILE:H	2.13	0.52
1:A:706:ASP:N	1:A:706:ASP:OD1	2.41	0.52
1:A:228:VAL:CG1	1:A:229:PHE:N	2.71	0.52
1:A:380:ASN:HD22	1:A:678:LYS:HE2	1.75	0.52
1:A:485:ILE:HG13	1:A:485:ILE:O	2.08	0.52
1:B:126:ASP:O	1:B:129:ARG:HG3	2.09	0.52
1:A:185:ILE:O	1:A:189:VAL:HG23	2.10	0.52
1:A:364:GLU:C	1:A:366:ARG:N	2.62	0.52
1:A:437:HIS:O	1:A:438:ASP:HB2	2.10	0.52
1:A:506:LEU:CD2	1:A:723:VAL:HB	2.39	0.52
1:A:247:LEU:HA	1:A:250:THR:CG2	2.40	0.52
1:A:374:ARG:HG2	1:A:378:PHE:CD2	2.45	0.51
1:A:689:GLY:O	1:A:692:LYS:N	2.43	0.51
1:B:664:GLN:O	1:B:666:GLY:N	2.43	0.51
1:B:459:TRP:O	1:B:462:GLN:HG3	2.09	0.51
1:B:419:VAL:HG11	1:B:467:LEU:CD1	2.37	0.51
1:B:687:MET:O	1:B:691:ILE:HG12	2.10	0.51
1:B:55:TYR:O	1:B:58:LEU:N	2.42	0.51
1:B:145:ILE:C	1:B:147:ALA:H	2.13	0.51
1:B:214:TYR:CZ	1:B:218:VAL:HG21	2.46	0.51
1:B:713:MET:HG3	1:B:718:LEU:CD1	2.40	0.51
1:B:9:ALA:HB3	1:B:12:LEU:H	1.76	0.51
1:B:262:VAL:HG12	1:B:263:ALA:O	2.10	0.51
1:A:138:ASP:C	1:A:140:GLN:H	2.14	0.51
1:A:139:LEU:O	1:A:143:GLY:HA3	2.10	0.51
1:B:731:ASP:C	1:B:731:ASP:OD1	2.47	0.51
1:B:212:CYS:HA	1:B:232:GLU:OE2	2.11	0.51
1:A:39:ARG:HD2	1:A:70:TRP:CZ2	2.44	0.51
1:A:748:ILE:HG12	1:A:749:LEU:N	2.26	0.51
1:A:557:LYS:O	1:A:558:GLN:NE2	2.44	0.51
1:B:153:SER:O	1:B:155:TYR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB3	1:A:116:ILE:HD13	1.92	0.51
1:B:110:ILE:CD1	1:B:110:ILE:H	2.22	0.51
1:B:624:LEU:HD12	1:B:625:VAL:H	1.73	0.51
1:A:601:THR:O	1:A:601:THR:HG23	2.09	0.51
1:B:11:THR:HA	1:B:14:VAL:HG23	1.92	0.51
1:B:515:PHE:N	1:B:515:PHE:CD1	2.78	0.51
1:B:615:LYS:HB3	1:B:620:VAL:HG21	1.93	0.51
1:B:433:VAL:C	1:B:434:LEU:HD12	2.30	0.51
1:B:234:PRO:HG3	1:B:367:PHE:CZ	2.45	0.51
1:B:551:THR:O	1:B:554:ASP:N	2.42	0.51
1:B:415:MET:O	1:B:419:VAL:HG23	2.10	0.51
1:B:595:ILE:N	1:B:595:ILE:CD1	2.74	0.51
1:B:311:ILE:HG23	1:B:586:LEU:HD23	1.93	0.51
2:A:763:ATP:O5'	2:A:763:ATP:H8	1.93	0.51
1:A:259:ILE:CG2	1:A:261:ILE:CD1	2.82	0.50
1:B:665:GLY:O	1:B:666:GLY:O	2.28	0.50
1:B:435:VAL:HG22	1:B:451:ALA:HB2	1.92	0.50
1:A:227:TRP:CD1	1:A:228:VAL:N	2.79	0.50
1:A:316:MET:HE3	1:A:337:SER:HA	1.92	0.50
1:B:328:THR:HB	1:B:329:PRO:HD2	1.93	0.50
1:A:66:ARG:HH21	1:A:108:ARG:HH22	1.56	0.50
1:B:165:ILE:HD11	1:B:208:MET:HG2	1.93	0.50
1:A:214:TYR:O	1:A:218:VAL:HG23	2.12	0.50
1:B:731:ASP:OD2	1:B:734:HIS:HD2	1.94	0.50
1:B:435:VAL:CB	1:B:467:LEU:HD21	2.41	0.50
1:A:165:ILE:H	1:A:165:ILE:CD1	2.24	0.50
1:A:392:ARG:HB2	1:A:393:PRO:HA	1.87	0.50
1:B:294:THR:HG22	1:B:295:VAL:N	2.27	0.50
1:B:729:GLN:O	1:B:738:LYS:HG3	2.12	0.50
1:B:248:SER:O	1:B:252:THR:HG22	2.10	0.50
1:A:95:ARG:C	1:A:97:GLY:N	2.65	0.50
1:B:568:PHE:N	1:B:568:PHE:CD1	2.78	0.50
1:B:281:ASP:C	1:B:283:VAL:N	2.63	0.50
1:A:371:MET:SD	1:A:378:PHE:HE2	2.35	0.50
1:A:601:THR:O	1:A:603:ARG:N	2.44	0.50
1:B:63:ASP:C	1:B:65:ILE:H	2.15	0.50
1:A:576:TYR:HD2	1:A:596:PHE:CD1	2.28	0.50
1:A:645:SER:O	1:A:646:GLU:C	2.49	0.50
1:A:596:PHE:C	1:A:596:PHE:CD2	2.84	0.50
1:B:423:VAL:HG12	1:B:427:LEU:CD1	2.42	0.50
1:A:189:VAL:HG22	1:A:205:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:PHE:O	1:A:598:GLU:N	2.45	0.50
1:B:38:VAL:HG21	1:B:73:VAL:HG11	1.94	0.50
1:B:403:VAL:HG12	1:B:404:ALA:N	2.27	0.50
1:B:192:ILE:HG23	1:B:203:PHE:CE2	2.47	0.50
1:A:23:SER:HB3	1:A:121:SER:HB3	1.94	0.50
1:A:387:LEU:HD23	1:A:428:ILE:CD1	2.42	0.50
1:B:496:ILE:HG12	1:B:525:ILE:HD12	1.94	0.50
1:B:289:TYR:O	1:B:291:THR:N	2.45	0.49
1:B:280:LYS:HB2	1:B:293:VAL:HG21	1.93	0.49
1:A:120:GLY:HA2	1:A:123:THR:CG2	2.40	0.49
1:B:531:ASN:HD21	1:B:538:PHE:CA	2.25	0.49
1:A:481:ILE:O	1:A:485:ILE:HG23	2.12	0.49
1:A:628:ASN:HB3	1:A:631:CYS:HB3	1.94	0.49
1:B:344:VAL:HG23	1:B:344:VAL:O	2.11	0.49
1:B:47:ARG:HD2	1:B:67:GLU:CD	2.32	0.49
1:B:421:SER:O	1:B:425:ILE:N	2.39	0.49
1:B:741:TRP:CG	1:B:742:TRP:N	2.80	0.49
1:A:295:VAL:HG12	1:A:295:VAL:O	2.10	0.49
1:A:393:PRO:HB3	1:A:453:TRP:CE3	2.47	0.49
1:B:159:VAL:CG2	1:B:324:LEU:HD23	2.34	0.49
1:B:562:GLY:O	1:B:564:LYS:N	2.45	0.49
1:B:234:PRO:HB2	1:B:268:ASP:C	2.33	0.49
1:A:50:PHE:CZ	1:A:84:ILE:HD11	2.47	0.49
1:B:9:ALA:C	1:B:11:THR:N	2.65	0.49
1:B:564:LYS:O	1:B:565:ARG:C	2.50	0.49
1:A:388:LEU:CD2	1:A:424:ARG:HB2	2.42	0.49
1:A:482:SER:HA	1:A:485:ILE:HG23	1.94	0.49
1:A:418:ALA:HB2	1:A:676:ALA:HB1	1.94	0.49
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.93	0.49
1:A:65:ILE:HB	1:A:108:ARG:HH12	1.78	0.49
1:B:618:THR:CG2	1:B:619:THR:H	2.16	0.49
1:B:41:GLY:C	1:B:44:THR:HG22	2.33	0.49
1:A:125:ALA:O	1:A:128:PHE:HB3	2.13	0.49
1:B:169:PHE:CZ	1:B:351:CYS:HB3	2.48	0.49
1:B:456:VAL:HA	1:B:459:TRP:CE2	2.48	0.49
1:A:70:TRP:CZ2	1:A:754:LYS:HB2	2.48	0.49
1:A:130:SER:C	1:A:132:TRP:H	2.17	0.49
1:A:328:THR:C	1:A:330:ASP:H	2.16	0.49
1:B:352:VAL:O	1:B:355:THR:HB	2.12	0.49
1:A:714:ARG:HG3	1:A:719:VAL:HG13	1.95	0.49
1:A:169:PHE:CZ	1:A:351:CYS:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:NH2	1:A:108:ARG:NH2	2.61	0.48
1:A:336:VAL:HA	1:A:344:VAL:O	2.13	0.48
1:B:283:VAL:CG2	1:B:284:VAL:H	2.26	0.48
1:A:367:PHE:O	1:A:370:ALA:HB3	2.14	0.48
1:B:360:LYS:O	1:B:363:ASP:N	2.44	0.48
1:B:734:HIS:O	1:B:736:ILE:N	2.46	0.48
1:B:193:THR:CG2	1:B:194:THR:N	2.76	0.48
1:B:510:GLU:OE1	1:B:510:GLU:HA	2.13	0.48
1:A:216:ALA:O	1:A:219:THR:HG22	2.14	0.48
1:A:696:ARG:HH11	1:A:696:ARG:CG	2.21	0.48
1:B:231:PRO:C	1:B:233:CYS:N	2.67	0.48
1:B:424:ARG:HD2	1:B:453:TRP:CZ2	2.48	0.48
1:A:407:ASN:HA	1:A:496:ILE:O	2.12	0.48
1:B:400:SER:HB2	1:B:431:ASN:HA	1.94	0.48
1:A:669:THR:HB	1:A:670:PRO:HD2	1.96	0.48
1:B:69:THR:HG23	1:B:72:SER:CB	2.41	0.48
1:A:696:ARG:NH1	1:A:696:ARG:CG	2.76	0.48
1:B:679:MET:O	1:B:680:GLY:C	2.51	0.48
1:B:567:VAL:HG22	1:B:616:MET:CE	2.42	0.48
1:B:41:GLY:HA2	1:B:44:THR:HG22	1.94	0.48
1:B:247:LEU:CA	1:B:250:THR:HG22	2.43	0.48
1:B:426:GLY:HA2	1:B:684:MET:HE2	1.94	0.48
1:A:73:VAL:HG12	1:A:76:MET:SD	2.53	0.48
1:B:435:VAL:HG12	1:B:467:LEU:HD21	1.95	0.48
1:A:82:THR:HG21	1:A:86:SER:CB	2.41	0.48
1:A:635:TYR:CD2	1:A:635:TYR:N	2.79	0.48
1:A:65:ILE:HB	1:A:108:ARG:NH1	2.29	0.48
1:A:239:TRP:O	1:A:242:HIS:HB3	2.14	0.48
1:B:751:ILE:HD11	1:B:752:LEU:HD23	1.95	0.48
1:B:747:PRO:O	1:B:751:ILE:HG23	2.14	0.48
1:A:679:MET:CE	1:A:718:LEU:HD11	2.44	0.48
1:B:21:LEU:HB2	1:B:51:VAL:HB	1.94	0.48
1:B:122:LEU:O	1:B:125:ALA:HB3	2.13	0.48
1:A:304:THR:OG1	1:A:305:PRO:HD2	2.14	0.48
1:B:741:TRP:CD2	1:B:742:TRP:N	2.82	0.48
1:B:751:ILE:CD1	1:B:752:LEU:HD23	2.43	0.48
1:B:376:ARG:HH21	1:B:376:ARG:CB	2.26	0.48
1:B:307:ALA:H	1:B:547:ASN:ND2	2.10	0.48
1:B:111:THR:O	1:B:156:LEU:HD12	2.13	0.48
1:B:450:GLU:HG3	1:B:451:ALA:N	2.24	0.48
1:B:312:LEU:O	1:B:316:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:O	1:A:72:SER:OG	2.30	0.48
1:B:547:ASN:O	1:B:550:CYS:N	2.47	0.48
1:A:319:GLU:HG3	1:A:336:VAL:CG1	2.44	0.48
1:A:282:LEU:HG	1:A:283:VAL:N	2.28	0.48
1:A:580:LEU:O	1:A:581:ALA:C	2.51	0.48
1:B:165:ILE:HB	1:B:181:ALA:HB2	1.96	0.47
1:B:214:TYR:O	1:B:216:ALA:N	2.46	0.47
1:B:470:LYS:HE2	1:B:471:ARG:N	2.26	0.47
1:A:391:ILE:CD1	1:A:392:ARG:N	2.73	0.47
1:A:49:PHE:CD1	1:A:110:ILE:CD1	2.97	0.47
1:B:560:ALA:C	1:B:622:ARG:HH22	2.18	0.47
1:B:116:ILE:HG12	1:B:161:LEU:HB3	1.95	0.47
1:A:391:ILE:O	1:A:392:ARG:O	2.32	0.47
1:B:205:LEU:CD2	1:B:294:THR:HB	2.42	0.47
1:A:42:ILE:O	1:A:45:GLY:N	2.47	0.47
1:A:104:ASN:O	1:A:108:ARG:HG2	2.13	0.47
1:B:84:ILE:CD1	1:B:84:ILE:N	2.78	0.47
1:A:275:THR:HG23	1:A:278:GLY:H	1.80	0.47
1:B:364:GLU:C	1:B:366:ARG:H	2.17	0.47
1:B:30:MET:O	1:B:34:VAL:HG23	2.14	0.47
1:A:475:LYS:C	1:A:477:SER:H	2.18	0.47
1:A:440:PHE:C	1:A:442:GLY:N	2.65	0.47
1:A:212:CYS:SG	1:A:214:TYR:HB2	2.54	0.47
1:B:360:LYS:O	1:B:362:MET:N	2.48	0.47
1:A:742:TRP:CZ3	1:A:743:LEU:HG	2.50	0.47
1:A:570:ILE:HA	1:A:657:ASN:O	2.14	0.47
1:B:549:ILE:CD1	1:B:659:LEU:HD13	2.38	0.47
1:A:440:PHE:C	1:A:442:GLY:H	2.14	0.47
1:B:512:ARG:NH2	1:B:707:SER:HB2	2.27	0.47
1:A:66:ARG:NH1	1:A:67:GLU:H	2.11	0.47
1:A:239:TRP:CH2	1:A:274:ILE:HD12	2.49	0.47
1:B:370:ALA:O	1:B:374:ARG:N	2.48	0.47
1:B:247:LEU:CD2	1:B:258:ASN:ND2	2.72	0.47
1:B:477:SER:O	1:B:481:ILE:HG23	2.14	0.47
1:B:402:THR:CG2	1:B:491:GLN:HE21	2.28	0.47
1:B:403:VAL:HG21	1:B:684:MET:HE3	1.97	0.47
1:B:234:PRO:HG3	1:B:367:PHE:CE1	2.49	0.47
1:B:578:GLY:H	1:B:597:GLU:CD	2.18	0.47
1:A:335:VAL:HG23	1:A:348:LEU:CG	2.39	0.47
1:A:565:ARG:NH1	1:A:618:THR:O	2.47	0.47
1:A:435:VAL:CG1	1:A:467:LEU:CD2	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:GLY:O	1:A:691:ILE:N	2.48	0.47
1:B:153:SER:C	1:B:155:TYR:N	2.68	0.47
1:A:457:GLY:HA2	4:A:767:PO4:O3	2.15	0.47
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.72	0.47
1:A:120:GLY:C	1:A:123:THR:HG22	2.35	0.47
1:A:475:LYS:C	1:A:477:SER:N	2.69	0.47
1:B:11:THR:HG23	1:B:12:LEU:N	2.30	0.47
1:B:100:ARG:O	1:B:104:ASN:ND2	2.47	0.47
1:B:562:GLY:C	1:B:564:LYS:N	2.68	0.47
1:B:756:GLU:HG2	1:B:756:GLU:O	2.14	0.47
1:A:613:VAL:C	1:A:615:LYS:H	2.17	0.47
1:A:679:MET:O	1:A:680:GLY:C	2.51	0.47
1:B:27:ALA:O	1:B:30:MET:HG3	2.15	0.47
1:A:571:GLU:HB3	1:A:658:VAL:HG22	1.97	0.47
1:B:149:GLU:O	1:B:153:SER:HB3	2.15	0.47
1:B:610:GLU:O	1:B:614:GLN:HG2	2.15	0.47
1:A:424:ARG:HD2	1:A:453:TRP:CE2	2.50	0.46
1:A:193:THR:CG2	1:A:194:THR:N	2.78	0.46
1:B:595:ILE:HD11	1:B:598:GLU:HB3	1.97	0.46
1:B:531:ASN:ND2	1:B:538:PHE:HA	2.28	0.46
1:B:605:LEU:O	1:B:609:VAL:HG23	2.15	0.46
1:B:420:ARG:NH1	1:B:460:THR:HG21	2.30	0.46
1:A:473:LEU:HD22	1:A:474:PRO:HD2	1.97	0.46
1:B:279:VAL:O	1:B:281:ASP:N	2.47	0.46
1:B:214:TYR:C	1:B:216:ALA:H	2.18	0.46
1:A:382:TRP:CE2	1:A:386:LYS:HD2	2.50	0.46
1:A:714:ARG:HG3	1:A:719:VAL:CG1	2.46	0.46
1:B:402:THR:HG21	1:B:489:ASN:HD22	1.81	0.46
1:B:358:VAL:HG12	1:B:358:VAL:O	2.15	0.46
1:A:435:VAL:HG13	1:A:467:LEU:HD22	1.97	0.46
1:B:340:GLY:O	1:B:342:GLN:HG3	2.16	0.46
1:A:35:ARG:CD	1:A:77:LEU:HD13	2.45	0.46
1:B:605:LEU:HA	1:B:605:LEU:HD12	1.75	0.46
1:B:279:VAL:O	1:B:283:VAL:HG13	2.16	0.46
1:A:393:PRO:HB3	1:A:453:TRP:CZ3	2.50	0.46
1:B:308:PHE:CZ	1:B:312:LEU:HD22	2.51	0.46
1:B:566:ARG:CD	1:B:653:ASP:HB3	2.45	0.46
1:B:660:GLY:O	1:B:662:MET:N	2.47	0.46
1:B:560:ALA:O	1:B:622:ARG:NH2	2.47	0.46
1:A:117:GLY:O	1:A:163:GLY:N	2.46	0.46
1:B:249:GLU:O	1:B:253:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:THR:O	1:B:604:ASP:N	2.42	0.46
1:B:378:PHE:CD2	1:B:378:PHE:C	2.89	0.46
1:A:235:PRO:O	1:A:236:ASP:C	2.53	0.46
1:B:277:GLU:O	1:B:280:LYS:HB3	2.16	0.46
1:B:509:MET:CE	1:B:705:PRO:HA	2.45	0.46
1:B:658:VAL:CG1	1:B:658:VAL:O	2.54	0.46
1:A:517:GLU:C	1:A:519:CYS:H	2.18	0.46
1:A:719:VAL:HG22	1:A:721:GLN:HG2	1.98	0.46
1:B:323:ALA:HA	1:B:345:ARG:NH1	2.31	0.46
1:B:387:LEU:CD2	1:B:428:ILE:HG21	2.45	0.46
1:A:628:ASN:O	1:A:630:LYS:N	2.49	0.46
2:B:763:ATP:O5'	2:B:763:ATP:H8	1.98	0.46
1:B:512:ARG:HG2	1:B:519:CYS:SG	2.56	0.46
1:B:459:TRP:CG	1:B:466:LYS:NZ	2.83	0.46
1:A:58:LEU:CD1	1:A:105:LEU:HD21	2.40	0.46
1:B:302:GLY:O	1:B:303:GLY:O	2.33	0.46
1:B:618:THR:CG2	1:B:619:THR:N	2.64	0.46
1:B:687:MET:C	1:B:687:MET:HE3	2.36	0.46
1:A:239:TRP:CD1	1:A:239:TRP:C	2.89	0.46
1:B:387:LEU:HD23	1:B:428:ILE:HD13	1.98	0.46
1:A:243:LEU:CD1	1:A:247:LEU:HD12	2.46	0.46
1:B:336:VAL:HG23	1:B:336:VAL:O	2.16	0.46
1:B:192:ILE:HG23	1:B:203:PHE:CZ	2.50	0.46
1:A:594:TYR:OH	1:A:608:ASN:ND2	2.46	0.46
1:A:673:ARG:O	1:A:677:THR:HB	2.15	0.46
1:A:50:PHE:CD2	1:A:84:ILE:HD11	2.51	0.46
1:A:742:TRP:C	1:A:744:LYS:N	2.69	0.46
1:B:342:GLN:NE2	1:B:715:LYS:HD2	2.31	0.46
1:B:214:TYR:C	1:B:216:ALA:N	2.69	0.46
1:A:165:ILE:N	1:A:165:ILE:CD1	2.79	0.46
1:B:621:LYS:O	1:B:622:ARG:HD2	2.16	0.46
1:B:565:ARG:HA	1:B:621:LYS:O	2.16	0.45
1:A:662:MET:O	1:A:663:GLN:C	2.54	0.45
1:A:56:GLN:O	1:A:58:LEU:N	2.50	0.45
1:B:364:GLU:C	1:B:366:ARG:N	2.70	0.45
1:A:328:THR:O	1:A:330:ASP:N	2.49	0.45
1:B:609:VAL:HG22	1:B:644:TYR:CD2	2.48	0.45
1:B:184:ARG:HD3	1:B:187:GLU:OE2	2.16	0.45
1:A:371:MET:HE2	1:A:382:TRP:CD1	2.52	0.45
1:B:601:THR:O	1:B:602:ILE:C	2.54	0.45
1:B:560:ALA:C	1:B:562:GLY:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD23	1:A:325:LEU:HD13	1.98	0.45
1:A:42:ILE:O	1:A:44:THR:N	2.49	0.45
1:B:299:VAL:O	1:B:302:GLY:N	2.37	0.45
1:A:748:ILE:HG12	1:A:749:LEU:H	1.82	0.45
1:A:506:LEU:HD23	1:A:723:VAL:HB	1.98	0.45
1:A:556:ILE:O	1:A:558:GLN:N	2.45	0.45
1:A:392:ARG:HB3	1:A:393:PRO:C	2.36	0.45
1:B:484:ASN:C	1:B:486:THR:N	2.69	0.45
1:A:606:GLN:OE1	1:B:606:GLN:OE1	2.35	0.45
1:B:748:ILE:O	1:B:752:LEU:HG	2.16	0.45
1:B:566:ARG:O	1:B:616:MET:HE1	2.17	0.45
1:B:404:ALA:HB2	1:B:490:ILE:CD1	2.46	0.45
1:B:380:ASN:O	1:B:381:ASN:C	2.55	0.45
1:A:21:LEU:HD23	1:A:22:THR:N	2.32	0.45
1:A:339:SER:OG	1:A:344:VAL:HG11	2.16	0.45
1:A:280:LYS:HB2	1:A:293:VAL:CG2	2.47	0.45
1:A:564:LYS:O	1:A:565:ARG:O	2.35	0.45
1:B:376:ARG:HB3	1:B:376:ARG:NH2	2.31	0.45
1:A:690:LYS:HE3	1:A:706:ASP:HB2	1.98	0.45
1:B:552:THR:HG21	1:B:659:LEU:CD2	2.47	0.45
1:B:459:TRP:N	1:B:459:TRP:HD1	2.05	0.45
1:B:502:TYR:OH	1:B:730:THR:CG2	2.64	0.45
1:B:376:ARG:NH2	1:B:376:ARG:HB2	2.32	0.45
1:A:414:GLY:HA3	1:A:540:VAL:CG1	2.46	0.45
1:B:734:HIS:O	1:B:735:ARG:C	2.54	0.45
1:B:508:LEU:O	1:B:509:MET:C	2.55	0.45
1:A:413:ALA:HB1	1:A:668:PRO:HA	1.98	0.45
1:B:403:VAL:HG21	1:B:684:MET:CE	2.46	0.45
1:B:340:GLY:O	1:B:342:GLN:N	2.51	0.45
1:B:638:ASP:N	1:B:638:ASP:OD1	2.49	0.45
1:A:391:ILE:CD1	2:A:765:ATP:PG	3.02	0.44
1:B:551:THR:HG22	1:B:552:THR:H	1.80	0.44
1:A:502:TYR:OH	1:A:730:THR:HG21	2.17	0.44
1:B:83:VAL:HG12	1:B:84:ILE:HD12	1.99	0.44
1:A:652:PHE:HD1	1:A:653:ASP:O	1.99	0.44
1:A:486:THR:HG22	1:A:487:LYS:N	2.32	0.44
1:A:203:PHE:CD1	1:A:203:PHE:N	2.85	0.44
1:B:333:ALA:HB3	1:B:348:LEU:HB2	1.99	0.44
1:A:500:GLU:CD	1:A:735:ARG:HH21	2.19	0.44
1:A:571:GLU:HA	1:A:627:ARG:O	2.17	0.44
1:A:319:GLU:HG3	1:A:336:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:ARG:HB3	1:B:697:ASN:H	1.51	0.44
1:B:69:THR:O	1:B:70:TRP:C	2.55	0.44
1:B:659:LEU:HD23	1:B:659:LEU:HA	1.73	0.44
1:A:407:ASN:HB3	1:A:469:SER:HB3	1.99	0.44
1:B:433:VAL:O	1:B:434:LEU:HD12	2.17	0.44
1:A:596:PHE:C	1:A:598:GLU:H	2.21	0.44
1:B:644:TYR:O	1:B:645:SER:C	2.54	0.44
1:A:159:VAL:HG11	1:A:320:ALA:HA	1.99	0.44
1:A:711:LEU:CD1	1:A:718:LEU:HG	2.46	0.44
1:B:84:ILE:HG22	1:B:84:ILE:O	2.17	0.44
1:A:745:LEU:C	1:A:747:PRO:HD2	2.37	0.44
1:A:13:GLY:O	1:A:46:ALA:HA	2.17	0.44
1:B:215:LEU:O	1:B:219:THR:HG21	2.16	0.44
1:A:354:VAL:C	1:A:356:LYS:N	2.71	0.44
1:A:375:GLY:HA2	1:A:379:MET:HE2	2.00	0.44
1:B:190:ASP:O	1:B:193:THR:HG22	2.17	0.44
1:A:537:ASP:OD1	1:A:714:ARG:NH2	2.37	0.44
1:A:629:GLU:O	1:A:630:LYS:HG3	2.17	0.44
1:B:279:VAL:C	1:B:281:ASP:N	2.70	0.44
1:B:185:ILE:C	1:B:185:ILE:HD13	2.37	0.44
1:A:165:ILE:HD13	1:A:165:ILE:H	1.82	0.44
1:A:377:SER:O	1:A:378:PHE:C	2.55	0.44
1:A:459:TRP:NE1	1:A:466:LYS:NZ	2.65	0.44
1:A:742:TRP:CE3	1:A:743:LEU:HG	2.53	0.44
1:A:524:VAL:HB	1:A:710:VAL:CG2	2.47	0.44
1:A:294:THR:CG2	1:A:295:VAL:N	2.81	0.44
1:A:582:THR:OG1	1:A:746:ARG:NH1	2.50	0.44
1:A:745:LEU:O	1:A:746:ARG:C	2.55	0.44
1:A:252:THR:C	1:A:254:GLY:H	2.20	0.44
1:B:56:GLN:O	1:B:60:ASP:OD2	2.36	0.44
1:A:41:GLY:O	1:A:44:THR:HG22	2.17	0.44
1:B:416:ASN:O	1:B:417:ALA:C	2.55	0.44
1:B:180:SER:O	1:B:181:ALA:C	2.56	0.44
1:B:730:THR:O	1:B:738:LYS:HD2	2.17	0.44
1:B:754:LYS:O	1:B:755:TYR:O	2.36	0.44
1:A:408:VAL:O	1:A:497:GLY:CA	2.66	0.44
1:A:579:TYR:HD1	1:A:742:TRP:CD1	2.36	0.44
1:B:696:ARG:O	1:B:698:GLY:N	2.50	0.44
1:B:245:ARG:HG2	1:B:245:ARG:HH11	1.83	0.44
1:A:371:MET:O	1:A:379:MET:HE2	2.18	0.43
1:A:232:GLU:OE2	1:A:374:ARG:NE	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ALA:CB	1:B:490:ILE:HD12	2.47	0.43
1:B:555:ARG:HG2	1:B:556:ILE:N	2.34	0.43
1:A:435:VAL:CG1	1:A:467:LEU:HD22	2.48	0.43
1:A:360:LYS:C	1:A:362:MET:N	2.71	0.43
1:A:140:GLN:NE2	1:A:144:LYS:O	2.51	0.43
1:B:78:GLN:CD	1:B:78:GLN:H	2.20	0.43
1:B:205:LEU:HB2	1:B:261:ILE:HD13	2.00	0.43
1:B:352:VAL:HA	1:B:355:THR:HB	1.99	0.43
1:B:393:PRO:HD3	1:B:453:TRP:CD2	2.53	0.43
1:A:598:GLU:HA	1:A:599:PRO:HD2	1.83	0.43
1:A:613:VAL:C	1:A:615:LYS:N	2.71	0.43
1:A:239:TRP:CG	1:A:240:GLU:N	2.86	0.43
1:B:193:THR:HA	1:B:257:LEU:HD11	2.00	0.43
1:A:413:ALA:HB1	1:A:668:PRO:CA	2.49	0.43
1:A:387:LEU:CD2	1:A:428:ILE:HD13	2.45	0.43
1:B:240:GLU:CG	1:B:282:LEU:HD22	2.49	0.43
1:A:257:LEU:N	1:A:257:LEU:HD23	2.20	0.43
1:A:21:LEU:HD23	1:A:21:LEU:C	2.38	0.43
1:B:528:THR:O	1:B:528:THR:HG23	2.19	0.43
1:B:481:ILE:HD12	1:B:485:ILE:HG23	2.00	0.43
1:B:307:ALA:O	1:B:311:ILE:HG12	2.18	0.43
1:A:509:MET:O	1:A:512:ARG:N	2.50	0.43
1:B:576:TYR:CE1	1:B:630:LYS:HD2	2.53	0.43
1:A:358:VAL:HG22	1:A:373:LEU:HB3	2.00	0.43
1:B:609:VAL:HG22	1:B:644:TYR:CZ	2.50	0.43
1:A:186:THR:HG22	1:A:190:ASP:OD2	2.18	0.43
1:B:742:TRP:C	1:B:744:LYS:H	2.21	0.43
1:B:485:ILE:CG1	1:B:517:GLU:HB3	2.48	0.43
1:B:424:ARG:HD2	1:B:453:TRP:CH2	2.54	0.43
1:B:109:GLY:O	1:B:110:ILE:C	2.57	0.43
1:A:686:TRP:HZ3	1:A:687:MET:HG2	1.82	0.43
1:B:243:LEU:HD12	1:B:243:LEU:O	2.17	0.43
1:A:679:MET:HG2	1:A:718:LEU:HD21	2.01	0.43
1:A:38:VAL:O	1:A:42:ILE:HG12	2.19	0.43
1:B:355:THR:HG22	1:B:356:LYS:N	2.34	0.43
1:A:185:ILE:CD1	1:A:215:LEU:HD23	2.49	0.43
1:B:193:THR:O	1:B:195:THR:N	2.52	0.43
1:B:566:ARG:HD2	1:B:653:ASP:OD2	2.18	0.43
1:B:547:ASN:O	1:B:548:THR:C	2.57	0.43
1:B:615:LYS:HB3	1:B:620:VAL:CG2	2.48	0.43
1:A:258:ASN:O	1:A:259:ILE:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:VAL:O	1:B:296:LEU:C	2.54	0.43
1:B:510:GLU:C	1:B:512:ARG:N	2.72	0.43
1:A:13:GLY:CA	1:A:44:THR:O	2.66	0.43
1:A:558:GLN:O	1:A:559:SER:O	2.37	0.43
1:B:414:GLY:HA3	1:B:540:VAL:CG1	2.49	0.43
1:B:113:LEU:O	1:B:158:ILE:HA	2.19	0.43
1:A:544:THR:OG1	1:A:669:THR:HG23	2.19	0.43
1:B:78:GLN:N	1:B:78:GLN:OE1	2.37	0.43
1:A:684:MET:O	1:A:684:MET:HG3	2.19	0.43
1:B:510:GLU:C	1:B:512:ARG:H	2.22	0.42
1:B:520:ILE:HA	1:B:521:PRO:HD3	1.84	0.42
1:A:275:THR:HG23	1:A:278:GLY:N	2.34	0.42
1:B:402:THR:CG2	1:B:432:ARG:HH21	2.30	0.42
1:A:503:THR:CG2	1:A:504:GLY:N	2.79	0.42
1:B:200:GLN:HA	1:B:256:ARG:O	2.19	0.42
1:A:679:MET:C	1:A:681:ALA:N	2.72	0.42
1:A:564:LYS:CA	1:A:564:LYS:HE2	2.50	0.42
1:A:234:PRO:HG3	1:A:367:PHE:CZ	2.53	0.42
1:A:742:TRP:C	1:A:744:LYS:H	2.21	0.42
1:B:242:HIS:O	1:B:246:ARG:HG2	2.19	0.42
1:B:89:CYS:O	1:B:89:CYS:SG	2.77	0.42
1:A:634:ASN:HB2	1:B:646:GLU:CG	2.48	0.42
1:A:112:ASN:HB3	1:A:324:LEU:HD13	2.01	0.42
1:B:218:VAL:HG12	1:B:219:THR:N	2.35	0.42
1:B:328:THR:CB	1:B:329:PRO:CD	2.93	0.42
1:A:669:THR:CB	1:A:670:PRO:HD2	2.49	0.42
1:A:307:ALA:O	1:A:311:ILE:HG13	2.19	0.42
1:B:549:ILE:HD12	1:B:659:LEU:CD1	2.37	0.42
1:A:120:GLY:O	1:A:121:SER:C	2.58	0.42
1:A:604:ASP:O	1:A:606:GLN:N	2.52	0.42
1:A:564:LYS:HB3	1:A:565:ARG:H	1.72	0.42
1:B:319:GLU:HG3	1:B:336:VAL:HB	2.01	0.42
1:A:319:GLU:CG	1:A:336:VAL:HB	2.50	0.42
1:B:359:THR:O	1:B:362:MET:HB2	2.19	0.42
1:A:158:ILE:H	1:A:158:ILE:HD13	1.84	0.42
1:A:429:GLN:HE22	1:A:685:ASN:HA	1.85	0.42
1:B:554:ASP:O	1:B:557:LYS:HB3	2.19	0.42
1:B:185:ILE:CD1	1:B:219:THR:HB	2.49	0.42
1:A:227:TRP:HB3	1:A:260:ILE:HG23	2.00	0.42
1:B:29:GLY:HA3	1:B:176:ILE:CG2	2.49	0.42
1:A:76:MET:O	1:A:77:LEU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:VAL:HA	1:B:288:GLY:HA2	2.02	0.42
1:A:388:LEU:HD23	1:A:424:ARG:CB	2.49	0.42
1:A:491:GLN:CB	1:A:700:ILE:HD11	2.39	0.42
1:A:65:ILE:O	1:A:65:ILE:HG22	2.19	0.42
1:A:751:ILE:HD11	1:A:752:LEU:HD23	2.02	0.42
1:B:240:GLU:HG2	1:B:282:LEU:HD22	2.02	0.42
1:B:509:MET:HE3	1:B:705:PRO:HA	2.02	0.42
1:A:193:THR:CG2	1:A:194:THR:HG23	2.50	0.42
1:A:352:VAL:O	1:A:355:THR:HG22	2.20	0.42
1:B:481:ILE:HD12	1:B:485:ILE:CG2	2.50	0.42
1:B:192:ILE:HD13	1:B:192:ILE:N	2.34	0.42
1:B:132:TRP:CE3	1:B:156:LEU:HD22	2.55	0.42
1:B:204:VAL:HB	1:B:293:VAL:HG22	2.01	0.42
1:A:13:GLY:N	1:A:44:THR:O	2.53	0.42
1:A:18:ILE:CG2	1:A:112:ASN:HB2	2.41	0.42
1:B:502:TYR:O	1:B:505:GLY:N	2.42	0.42
1:A:575:GLY:HA2	1:A:630:LYS:HE2	2.02	0.42
1:A:360:LYS:O	1:A:362:MET:N	2.52	0.42
1:A:261:ILE:HD12	1:A:261:ILE:N	2.35	0.42
1:B:110:ILE:N	1:B:110:ILE:HD12	2.33	0.42
1:A:328:THR:C	1:A:330:ASP:N	2.73	0.42
1:B:342:GLN:HE21	1:B:715:LYS:HD2	1.84	0.42
1:B:628:ASN:HB3	1:B:631:CYS:HB3	2.01	0.42
1:B:280:LYS:C	1:B:283:VAL:HG22	2.40	0.42
1:A:248:SER:O	1:A:249:GLU:C	2.59	0.42
1:B:184:ARG:HA	1:B:184:ARG:HD3	1.76	0.42
1:A:193:THR:HG23	1:A:194:THR:HG23	2.01	0.42
1:A:375:GLY:HA2	1:A:379:MET:HE3	2.02	0.42
1:A:565:ARG:HH21	1:A:565:ARG:CG	2.32	0.42
1:B:228:VAL:HG23	1:B:385:TYR:CE2	2.55	0.42
1:B:84:ILE:O	1:B:84:ILE:CG2	2.68	0.42
1:A:344:VAL:HG23	1:A:346:LEU:HG	2.01	0.42
1:A:634:ASN:HB2	1:B:646:GLU:HG2	2.02	0.41
1:A:323:ALA:HA	1:A:345:ARG:NH1	2.35	0.41
1:A:604:ASP:O	1:A:605:LEU:C	2.57	0.41
1:A:509:MET:O	1:A:510:GLU:C	2.59	0.41
1:B:280:LYS:HB2	1:B:293:VAL:CG2	2.50	0.41
1:A:377:SER:O	1:A:380:ASN:N	2.53	0.41
1:B:475:LYS:C	1:B:477:SER:H	2.23	0.41
1:B:585:GLY:CA	1:B:626:LEU:HD12	2.47	0.41
1:A:524:VAL:HB	1:A:710:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:O	1:A:158:ILE:HD13	2.20	0.41
1:A:264:GLU:C	1:A:266:ALA:H	2.23	0.41
1:B:69:THR:O	1:B:72:SER:N	2.41	0.41
1:B:41:GLY:CA	1:B:44:THR:HG22	2.49	0.41
1:B:742:TRP:C	1:B:744:LYS:N	2.74	0.41
1:A:39:ARG:CD	1:A:70:TRP:CE2	3.02	0.41
1:A:22:THR:HG23	1:A:85:GLY:O	2.21	0.41
1:B:59:VAL:HA	1:B:101:ALA:HB2	2.03	0.41
1:B:132:TRP:CD2	1:B:156:LEU:HD22	2.56	0.41
1:B:627:ARG:HG2	1:B:627:ARG:HH11	1.85	0.41
1:B:578:GLY:HA3	1:B:595:ILE:HB	2.02	0.41
1:A:618:THR:HG22	1:A:619:THR:N	2.35	0.41
1:B:251:ARG:C	1:B:253:ARG:H	2.23	0.41
1:B:426:GLY:CA	1:B:684:MET:HE2	2.50	0.41
1:A:505:GLY:O	1:A:508:LEU:N	2.42	0.41
1:B:520:ILE:CG2	1:B:700:ILE:HD11	2.40	0.41
1:B:181:ALA:O	1:B:185:ILE:HG22	2.21	0.41
1:A:609:VAL:HG22	1:A:644:TYR:CZ	2.55	0.41
1:B:63:ASP:O	1:B:65:ILE:N	2.53	0.41
1:A:50:PHE:O	1:A:51:VAL:CG2	2.67	0.41
1:B:101:ALA:O	1:B:104:ASN:HB2	2.21	0.41
1:A:169:PHE:CE2	1:A:351:CYS:HB3	2.56	0.41
1:A:435:VAL:CG1	1:A:467:LEU:HD21	2.51	0.41
1:A:544:THR:O	1:A:545:ALA:C	2.56	0.41
1:A:581:ALA:O	1:A:585:GLY:N	2.50	0.41
1:B:244:CYS:C	1:B:246:ARG:N	2.74	0.41
1:A:454:SER:O	1:A:455:TYR:C	2.59	0.41
1:A:597:GLU:H	1:A:597:GLU:CD	2.21	0.41
1:B:551:THR:CG2	1:B:552:THR:N	2.78	0.41
1:B:193:THR:HA	1:B:257:LEU:CD1	2.50	0.41
1:B:124:GLY:C	1:B:127:THR:HG22	2.41	0.41
1:B:402:THR:HB	1:B:432:ARG:HE	1.85	0.41
1:A:515:PHE:CD1	1:A:515:PHE:N	2.89	0.41
1:B:632:ASN:OD1	1:B:634:ASN:N	2.54	0.41
1:B:419:VAL:CG1	1:B:467:LEU:HD11	2.43	0.41
1:A:215:LEU:O	1:A:219:THR:HB	2.21	0.41
1:A:517:GLU:C	1:A:519:CYS:N	2.74	0.41
1:A:473:LEU:HA	1:A:473:LEU:HD23	1.63	0.41
1:A:162:VAL:CG1	1:A:175:THR:HG22	2.50	0.41
1:B:524:VAL:HB	1:B:710:VAL:HG22	2.02	0.41
1:B:39:ARG:NH1	1:B:39:ARG:HG3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLN:HE21	1:A:700:ILE:HD13	1.86	0.41
1:B:423:VAL:HG12	1:B:427:LEU:HD11	2.02	0.41
1:B:299:VAL:CG2	1:B:300:GLN:N	2.84	0.41
1:A:181:ALA:O	1:A:185:ILE:HG13	2.21	0.41
1:A:247:LEU:HD11	1:A:260:ILE:HD11	2.03	0.41
1:B:251:ARG:C	1:B:253:ARG:N	2.75	0.41
1:A:596:PHE:C	1:A:598:GLU:N	2.74	0.41
1:B:22:THR:HG21	1:B:82:THR:OG1	2.20	0.41
1:A:388:LEU:HD23	1:A:424:ARG:HB2	2.02	0.41
1:B:440:PHE:C	1:B:443:PRO:HD2	2.40	0.41
1:B:471:ARG:NH2	4:B:768:PO4:O1	2.53	0.41
1:B:230:ILE:HA	1:B:231:PRO:HD3	1.87	0.41
1:B:679:MET:HE3	1:B:718:LEU:HD11	2.01	0.40
1:B:229:PHE:HZ	1:B:239:TRP:CZ3	2.39	0.40
1:A:153:SER:C	1:A:155:TYR:N	2.70	0.40
1:A:403:VAL:CG1	1:A:404:ALA:N	2.84	0.40
1:A:414:GLY:HA3	1:A:540:VAL:HG11	2.03	0.40
1:A:493:LEU:O	1:A:522:PHE:HA	2.21	0.40
1:A:101:ALA:O	1:A:104:ASN:HB2	2.22	0.40
1:A:208:MET:CG	1:A:209:GLY:H	2.33	0.40
1:B:723:VAL:HG23	1:B:724:THR:H	1.86	0.40
1:A:473:LEU:HB3	1:A:474:PRO:HD2	2.03	0.40
1:A:184:ARG:HD2	1:A:302:GLY:O	2.21	0.40
1:A:602:ILE:HG13	1:A:602:ILE:O	2.21	0.40
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.94	0.40
1:A:473:LEU:HD22	1:A:504:GLY:HA2	2.02	0.40
1:B:649:LYS:HD2	1:B:649:LYS:HA	1.88	0.40
1:B:377:SER:O	1:B:380:ASN:N	2.52	0.40
1:A:186:THR:O	1:A:190:ASP:HB2	2.21	0.40
1:B:235:PRO:HB2	1:B:239:TRP:CB	2.52	0.40
1:A:109:GLY:C	1:A:110:ILE:HG12	2.41	0.40
1:B:193:THR:C	1:B:195:THR:N	2.75	0.40
1:B:403:VAL:HG12	1:B:404:ALA:H	1.85	0.40
1:A:173:ASP:HB3	3:A:764:ADP:H4'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	746/762 (98%)	564 (76%)	123 (16%)	59 (8%)	1	8
1	B	746/762 (98%)	565 (76%)	119 (16%)	62 (8%)	1	7
All	All	1492/1524 (98%)	1129 (76%)	242 (16%)	121 (8%)	1	7

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	51	VAL
1	A	54	GLY
1	A	60	ASP
1	A	153	SER
1	A	198	SER
1	A	214	TYR
1	A	238	ASN
1	A	297	GLY
1	A	298	HIS
1	A	365	LYS
1	A	375	GLY
1	A	392	ARG
1	A	559	SER
1	A	565	ARG
1	B	60	ASP
1	B	62	GLY
1	B	232	GLU
1	B	291	THR
1	B	303	GLY
1	B	390	HIS
1	B	445	LYS
1	B	466	LYS
1	B	602	ILE
1	B	645	SER

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Mol	Chain	Res	Type
1	B	664	GLN
1	B	735	ARG
1	B	753	ALA
1	A	56	GLN
1	A	57	GLY
1	A	142	ALA
1	A	143	GLY
1	A	152	ARG
1	A	154	SER
1	A	196	ALA
1	A	236	ASP
1	A	476	LYS
1	A	564	LYS
1	A	629	GLU
1	A	647	GLU
1	A	663	GLN
1	A	666	GLY
1	A	680	GLY
1	A	690	LYS
1	B	12	LEU
1	B	64	HIS
1	B	107	LYS
1	B	110	ILE
1	B	154	SER
1	B	194	THR
1	B	201	ARG
1	B	208	MET
1	B	237	ASP
1	B	247	LEU
1	B	280	LYS
1	B	282	LEU
1	B	290	ASP
1	B	332	PRO
1	B	341	ASN
1	B	361	ALA
1	B	365	LYS
1	B	397	LYS
1	B	465	SER
1	B	476	LYS
1	B	511	GLY
1	B	551	THR
1	B	563	THR

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Mol	Chain	Res	Type
1	B	565	ARG
1	B	589	GLY
1	B	597	GLU
1	B	618	THR
1	B	661	HIS
1	B	666	GLY
1	B	755	TYR
1	A	126	ASP
1	A	208	MET
1	A	235	PRO
1	A	272	LYS
1	A	273	PRO
1	A	296	LEU
1	A	390	HIS
1	A	560	ALA
1	A	597	GLU
1	A	602	ILE
1	A	605	LEU
1	A	645	SER
1	B	16	LYS
1	B	75	MET
1	B	141	LYS
1	B	146	THR
1	B	555	ARG
1	B	559	SER
1	B	564	LYS
1	B	662	MET
1	A	28	GLN
1	A	109	GLY
1	A	131	GLU
1	A	619	THR
1	A	646	GLU
1	B	198	SER
1	B	215	LEU
1	B	382	TRP
1	B	510	GLU
1	B	697	ASN
1	A	200	GLN
1	A	371	MET
1	A	580	LEU
1	A	618	THR
1	A	641	PHE

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Mol	Chain	Res	Type
1	A	662	MET
1	A	693	GLU
1	B	199	HIS
1	B	396	PRO
1	B	561	ALA
1	B	579	TYR
1	A	201	ARG
1	B	446	GLY
1	A	42	ILE
1	B	698	GLY
1	A	62	GLY
1	A	329	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	605/618 (98%)	530 (88%)	75 (12%)	6	27
1	B	605/618 (98%)	537 (89%)	68 (11%)	7	32
All	All	1210/1236 (98%)	1067 (88%)	143 (12%)	6	29

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	22	THR
1	A	28	GLN
1	A	64	HIS
1	A	73	VAL
1	A	77	LEU
1	A	78	GLN
1	A	84	ILE
1	A	119	ASP
1	A	126	ASP
1	A	127	THR

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Mol	Chain	Res	Type
1	A	138	ASP
1	A	140	GLN
1	A	155	TYR
1	A	158	ILE
1	A	164	SER
1	A	165	ILE
1	A	178	THR
1	A	180	SER
1	A	190	ASP
1	A	193	THR
1	A	200	GLN
1	A	226	ASP
1	A	239	TRP
1	A	242	HIS
1	A	243	LEU
1	A	257	LEU
1	A	275	THR
1	A	276	SER
1	A	277	GLU
1	A	304	THR
1	A	314	SER
1	A	348	LEU
1	A	352	VAL
1	A	391	ILE
1	A	402	THR
1	A	405	VAL
1	A	428	ILE
1	A	460	THR
1	A	481	ILE
1	A	485	ILE
1	A	486	THR
1	A	493	LEU
1	A	495	ILE
1	A	503	THR
1	A	507	GLU
1	A	516	ASP
1	A	523	VAL
1	A	531	ASN
1	A	547	ASN
1	A	551	THR
1	A	552	THR
1	A	553	CYS

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Mol	Chain	Res	Type
1	A	564	LYS
1	A	565	ARG
1	A	566	ARG
1	A	614	GLN
1	A	621	LYS
1	A	649	LYS
1	A	657	ASN
1	A	669	THR
1	A	677	THR
1	A	685	ASN
1	A	687	MET
1	A	693	GLU
1	A	699	ARG
1	A	700	ILE
1	A	706	ASP
1	A	710	VAL
1	A	714	ARG
1	A	719	VAL
1	A	730	THR
1	A	731	ASP
1	A	740	GLN
1	A	751	ILE
1	B	18	ILE
1	B	21	LEU
1	B	22	THR
1	B	26	ASP
1	B	69	THR
1	B	78	GLN
1	B	89	CYS
1	B	129	ARG
1	B	138	ASP
1	B	158	ILE
1	B	165	ILE
1	B	173	ASP
1	B	178	THR
1	B	185	ILE
1	B	189	VAL
1	B	200	GLN
1	B	208	MET
1	B	210	ARG
1	B	219	THR
1	B	238	ASN

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Mol	Chain	Res	Type
1	B	253	ARG
1	B	274	ILE
1	B	275	THR
1	B	348	LEU
1	B	368	ASP
1	B	373	LEU
1	B	374	ARG
1	B	402	THR
1	B	411	PRO
1	B	420	ARG
1	B	435	VAL
1	B	450	GLU
1	B	454	SER
1	B	460	THR
1	B	462	GLN
1	B	466	LYS
1	B	467	LEU
1	B	470	LYS
1	B	481	ILE
1	B	485	ILE
1	B	500	GLU
1	B	503	THR
1	B	509	MET
1	B	512	ARG
1	B	514	GLN
1	B	517	GLU
1	B	530	SER
1	B	550	CYS
1	B	553	CYS
1	B	566	ARG
1	B	573	MET
1	B	595	ILE
1	B	621	LYS
1	B	622	ARG
1	B	638	ASP
1	B	642	ASN
1	B	703	ASN
1	B	707	SER
1	B	713	MET
1	B	714	ARG
1	B	719	VAL
1	B	723	VAL

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Mol	Chain	Res	Type
1	B	724	THR
1	B	730	THR
1	B	731	ASP
1	B	743	LEU
1	B	749	LEU
1	B	754	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	28	GLN
1	A	64	HIS
1	A	104	ASN
1	A	380	ASN
1	A	429	GLN
1	A	431	ASN
1	A	437	HIS
1	A	447	GLN
1	A	462	GLN
1	A	489	ASN
1	A	491	GLN
1	A	514	GLN
1	A	531	ASN
1	A	608	ASN
1	A	634	ASN
1	A	642	ASN
1	A	661	HIS
1	A	674	ASN
1	A	703	ASN
1	A	734	HIS
1	A	740	GLN
1	B	104	ASN
1	B	183	HIS
1	B	242	HIS
1	B	258	ASN
1	B	342	GLN
1	B	431	ASN
1	B	437	HIS
1	B	489	ASN
1	B	491	GLN
1	B	514	GLN
1	B	531	ASN

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Mol	Chain	Res	Type
1	B	547	ASN
1	B	634	ASN
1	B	642	ASN
1	B	674	ASN
1	B	703	ASN
1	B	727	GLN
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 ⓘ

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 ⓘ

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	ATP	A	763	-	24,33,33	1.06	1 (4%)	31,52,52	2.25	5 (16%)
3	ADP	A	764	-	22,29,29	1.03	1 (4%)	27,45,45	2.48	7 (25%)
2	ATP	A	765	-	24,33,33	1.04	1 (4%)	31,52,52	2.81	14 (45%)
4	PO4	A	766	-	4,4,4	1.78	2 (50%)	6,6,6	0.30	0
4	PO4	A	767	-	4,4,4	1.75	2 (50%)	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	768	-	4,4,4	1.76	2 (50%)	6,6,6	0.31	0
2	ATP	B	763	-	24,33,33	1.03	1 (4%)	31,52,52	2.16	5 (16%)
3	ADP	B	764	-	22,29,29	1.01	1 (4%)	27,45,45	2.14	4 (14%)
2	ATP	B	765	-	24,33,33	1.00	1 (4%)	31,52,52	2.73	9 (29%)
4	PO4	B	766	-	4,4,4	1.80	2 (50%)	6,6,6	0.29	0
4	PO4	B	767	-	4,4,4	1.77	2 (50%)	6,6,6	0.28	0
4	PO4	B	768	-	4,4,4	1.76	2 (50%)	6,6,6	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	763	-	-	0/18/38/38	0/3/3/3
3	ADP	A	764	-	-	0/12/32/32	0/3/3/3
2	ATP	A	765	-	-	0/18/38/38	0/3/3/3
4	PO4	A	766	-	-	0/0/0/0	0/0/0/0
4	PO4	A	767	-	-	0/0/0/0	0/0/0/0
4	PO4	A	768	-	-	0/0/0/0	0/0/0/0
2	ATP	B	763	-	-	0/18/38/38	0/3/3/3
3	ADP	B	764	-	-	0/12/32/32	0/3/3/3
2	ATP	B	765	-	-	0/18/38/38	0/3/3/3
4	PO4	B	766	-	-	0/0/0/0	0/0/0/0
4	PO4	B	767	-	-	0/0/0/0	0/0/0/0
4	PO4	B	768	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	765	ATP	O4'-C1'	2.06	1.43	1.41
4	A	768	PO4	P-O2	2.16	1.61	1.53
4	B	768	PO4	P-O3	2.18	1.61	1.53
4	A	767	PO4	P-O2	2.19	1.61	1.53
4	A	767	PO4	P-O3	2.20	1.61	1.53
4	B	768	PO4	P-O2	2.20	1.61	1.53
4	B	767	PO4	P-O3	2.20	1.61	1.53
4	B	767	PO4	P-O2	2.22	1.61	1.53
4	A	766	PO4	P-O2	2.23	1.61	1.53
4	A	768	PO4	P-O3	2.24	1.61	1.53
4	A	766	PO4	P-O3	2.25	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	766	PO4	P-O3	2.26	1.61	1.53
4	B	766	PO4	P-O2	2.26	1.61	1.53
2	A	765	ATP	O4'-C1'	2.37	1.44	1.41
3	B	764	ADP	O4'-C1'	2.40	1.44	1.41
3	A	764	ADP	O4'-C1'	2.46	1.44	1.41
2	B	763	ATP	O4'-C1'	2.51	1.44	1.41
2	A	763	ATP	O4'-C1'	2.59	1.44	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	763	ATP	N3-C2-N1	-9.51	121.61	128.89
2	B	765	ATP	N3-C2-N1	-9.43	121.68	128.89
3	A	764	ADP	N3-C2-N1	-9.35	121.73	128.89
2	B	763	ATP	N3-C2-N1	-9.27	121.79	128.89
3	B	764	ADP	N3-C2-N1	-9.22	121.83	128.89
2	A	765	ATP	N3-C2-N1	-9.06	121.95	128.89
2	B	765	ATP	O3A-PA-O5'	-5.43	88.52	102.94
2	B	765	ATP	PA-O3A-PB	-5.09	118.44	132.73
2	A	765	ATP	PA-O3A-PB	-4.89	119.00	132.73
2	B	765	ATP	C4'-O4'-C1'	-4.67	104.59	109.72
2	B	763	ATP	PB-O3B-PG	-4.30	118.24	132.67
2	A	763	ATP	C2'-C1'-N9	-4.16	107.93	114.29
2	A	763	ATP	PB-O3B-PG	-4.16	118.72	132.67
2	A	765	ATP	O3A-PA-O5'	-4.12	92.00	102.94
2	B	763	ATP	PA-O3A-PB	-4.02	121.43	132.73
2	B	765	ATP	PB-O3B-PG	-3.99	119.27	132.67
2	A	765	ATP	O2A-PA-O5'	-3.82	89.19	108.46
2	A	763	ATP	PA-O3A-PB	-3.64	122.50	132.73
3	B	764	ADP	PA-O3A-PB	-3.62	120.53	132.67
2	A	765	ATP	PB-O3B-PG	-3.60	120.59	132.67
2	B	765	ATP	O2A-PA-O5'	-3.42	91.22	108.46
2	B	765	ATP	O5'-PA-O1A	-3.40	96.42	109.62
3	A	764	ADP	PA-O3A-PB	-3.40	121.27	132.67
2	A	765	ATP	O5'-PA-O1A	-3.19	97.25	109.62
2	A	765	ATP	C5'-C4'-C3'	-2.92	103.63	115.21
2	A	765	ATP	O2G-PG-O3B	-2.76	92.59	105.09
2	A	765	ATP	O3G-PG-O3B	-2.60	93.29	105.09
3	A	764	ADP	O2B-PB-O3A	-2.58	93.39	105.09
3	A	764	ADP	O3B-PB-O3A	-2.57	93.43	105.09
3	B	764	ADP	C2'-C1'-N9	-2.53	110.42	114.29
3	A	764	ADP	C4-C5-N7	-2.34	107.33	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	763	ATP	C2'-C1'-N9	-2.28	110.81	114.29
2	B	765	ATP	C4-C5-N7	-2.27	107.39	109.48
2	A	763	ATP	C2'-C3'-C4'	-2.16	98.17	102.61
3	B	764	ADP	C4-C5-N7	-2.16	107.50	109.48
2	A	765	ATP	C4'-O4'-C1'	-2.15	107.36	109.72
2	A	765	ATP	C4-C5-N7	-2.14	107.51	109.48
2	B	763	ATP	C4-C5-N7	-2.06	107.58	109.48
2	B	765	ATP	O2A-PA-O3A	2.45	116.20	105.09
2	A	765	ATP	O2A-PA-O3A	2.65	117.13	105.09
2	A	765	ATP	O3G-PG-O1G	3.36	121.40	110.58
3	A	764	ADP	O2B-PB-O1B	3.50	121.84	110.58
3	A	764	ADP	O3B-PB-O1B	3.60	122.16	110.58
2	A	765	ATP	O2G-PG-O1G	3.84	122.93	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	763	ATP	2	0
3	A	764	ADP	1	0
2	A	765	ATP	3	0
4	A	767	PO4	1	0
2	B	763	ATP	1	0
4	B	768	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	739/762 (96%)	-0.43	2 (0%) 94 93	14, 57, 138, 202	76 (10%)
1	B	745/762 (97%)	-0.23	14 (1%) 70 55	7, 59, 148, 202	86 (11%)
All	All	1484/1524 (97%)	-0.33	16 (1%) 82 72	7, 58, 144, 202	162 (10%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	SER	6.7
1	B	142	ALA	6.3
1	B	92	PHE	4.0
1	B	59	VAL	4.0
1	B	154	SER	3.5
1	B	291	THR	3.0
1	B	556	ILE	3.0
1	B	143	GLY	2.8
1	B	58	LEU	2.4
1	B	101	ALA	2.4
1	B	153	SER	2.3
1	B	110	ILE	2.2
1	A	361	ALA	2.2
1	B	127	THR	2.1
1	B	294	THR	2.1
1	A	362	MET	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ADP	A	764	27/27	0.86	0.29	3.36	135,138,144,144	0
4	PO4	B	767	5/5	0.89	0.32	3.28	66,66,69,71	0
4	PO4	A	766	5/5	0.88	0.32	2.87	99,99,100,101	0
3	ADP	B	764	27/27	0.82	0.26	2.81	145,148,154,154	0
4	PO4	A	767	5/5	0.94	0.28	2.08	60,60,61,63	0
4	PO4	B	766	5/5	0.91	0.32	1.81	91,92,93,94	0
4	PO4	A	768	5/5	0.97	0.17	0.44	55,56,57,58	0
2	ATP	A	763	31/31	0.85	0.22	0.35	82,87,97,98	0
2	ATP	A	765	31/31	0.93	0.20	0.05	58,63,77,78	0
4	PO4	B	768	5/5	0.99	0.15	-0.09	52,53,55,55	0
2	ATP	B	763	31/31	0.87	0.19	-0.46	98,100,101,101	0
2	ATP	B	765	31/31	0.96	0.12	-1.89	72,77,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.