



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:13 AM GMT

PDB ID : 3LC6
Title : The alternative conformation structure of isocitrate dehydrogenase kinase/phosphatase from E. Coli
Authors : Zheng, J.; Jia, Z.
Deposited on : 2010-01-09
Resolution : 3.10 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

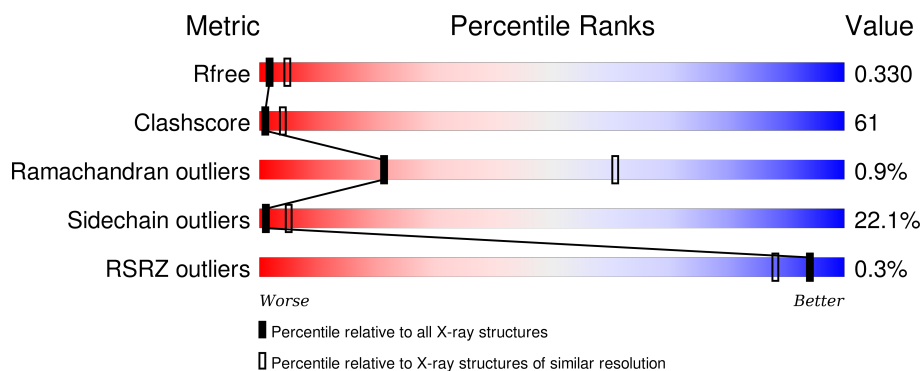
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	578	<div> <div></div> <div>24% 56% 14% • 5%</div> </div>
1	B	578	<div> <div></div> <div>27% 52% 14% 7%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9107 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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4526	2906	800	799	21			
1	B	539	Total	C	N	O	S	0	0	0
			4454	2861	785	788	20			

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

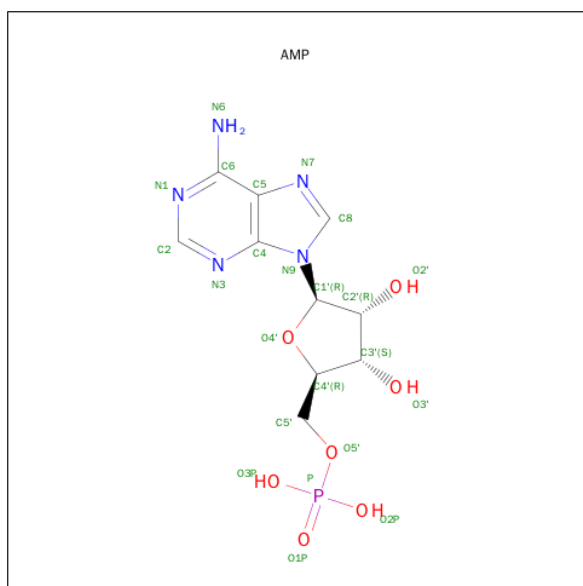


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	45	Total	O	0	0
			45	45		

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: Isocitrate dehydrogenase kinase/phosphatase



F518	B519	H520	W521	L522		D525		I528	G529	F530	F531	F532		M535	H536	A537	D538	L539	F540	D541	D542	Y544	W545	B546	A547	L548	Q549	N550	R551	I552	R553	B554	G555	W556	W557	B558	D559	V560	Y561	A562	Y563	R564	R565	R566	R568	F569	W570	V571	B572	Y573	G574	GLU	MET	LEU	PHE					
I453	F454	P455		N458	L459	F460	K461	M462	F463	G464	V465	T466	R467		R470	V471	V472	F473	Y474	D475	D476	D477	E478	I479	G480	Y481	M482	T483	E484	V485		D489	I490	PRO	PRO	PRO	ARG	TTR	PRO	GLU	ASP	GLU	LEU	ALA	SER	GLU	PRO	TRP	SER	VAL	SER	PRO	G511		F514	P515	E516	E517		
L392	L393	L394	Q395	E396	F397	A398	E399	K400	I401	D402	D403	L404		Q407	I408	V409	I410	R411	H412	L413	Y414	I415	E416	R417	R418	M419	V420	F421	L422	N423	I424	W425	L426	E427	Q428	V429	E430	G431	Q432	Q433	L434	R435	D436	A437	I438	E439	E440	Y441	G442	M443	A444	I445	R446	Q447	L448	A449	A450	A451	N452	
F331	D332	R333	V334	F335	K336	R337	I338	K339	I340	K341	F342	ALA	PRO	GLN	LYS	GLU	MET	SER	ALA	A351	R352	V353	R354	A355	C356	Y357	Q358	L359	V360	K361	R362	R363	R364	V365	G366	G367	R368	K369	A370	D371	T372	Q373	E374	F375	R376	F377	F378	V379	L380	E381	R382	R383	R384		P387	A388	L389	K390	E391	
V268	E269	W270	L271		I274	L275	P276	G277	T278	T279	T280	A281	E282	L283	Y284	M285	A286	I287	G288	C289	Q290	K291	H292	A293	K294	T295	E296	S297	Y298	R299	E300	Y301	Y304	L305	T242	T243	A244	E245	A246	S247	T248	V249	F250	G251	F252	A253	R254	S255	Y256	R257	K258	V259	K323	L324	V325	F326	T327	L328	P329	G330
N204		W208	L209		K212	L213	T214	T215	D216	S217	G218	T219	L220	P221	F222	L223			T226	H227	Q228	T229	D230	D231	G232	E233	L234	T236	D237	T238	C239	L240	T241	T242	T243	A244	E245	A246	S247	T248	V249	F250	G251	F252	A253	R254	S255	Y256	R257	K258	V259	K323	L324	V325	F326	T327	L328	P329	G330	
T134	I135	P136	R137	P138	L139	A140	K141	D142	F143	H144	P145		W149		L152	L153	M154	R155	Y156	I157	S158	D159	L160	P161	L162	L164		M168	K169	S170	R171	D172	H174	Y175	I176	I177	R178	H179	L180	T181		P186		L189		S192	H193	L194	S195	V196	A197	N198	E199	L200	Y201	F202	R203			
Q72		D75		F78	L79	L80	R81	W82		B85		B86	T87	R88	L89	L90	P91	D92	Y93	F94	R95	F96	T98	E97	A99	E100	S101	F102	F103	N104	S105	V106	Y107	C108	R109	L110	PHE	D112	H113	R114	S115	L116	F117	P118	E119	R120	F121	F122	L123	F124	S125	S126	Q127	P128	GLU	ARG	ARG	PHE	ARG	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 133.76Å 187.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (10.00-3.10) 83.7 (10.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.46 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.287 , 0.332 0.292 , 0.330	Depositor DCC
R_{free} test set	1191 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 24325 reflections	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	9107	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: AMP, MG, 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	0.62	2/4643 (0.0%)	0.80	7/6283 (0.1%)
1	B	0.57	1/4567 (0.0%)	0.77	1/6179 (0.0%)
All	All	0.60	3/9210 (0.0%)	0.79	8/12462 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	5
1	B	0	2
All	All	1	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	CYS	CB-SG	-6.93	1.70	1.82
1	A	511	GLY	N-CA	6.30	1.55	1.46
1	A	356	CYS	CB-SG	-5.39	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	N-CA-C	-8.62	89.69	112.10
1	A	239	CYS	N-CA-C	7.35	130.85	111.00
1	A	509	SER	N-CA-CB	-6.98	100.02	110.50
1	A	238	THR	N-CA-C	6.78	129.31	111.00
1	B	240	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	75	ASP	N-CA-C	-6.36	93.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	PRO	N-CA-C	5.33	125.96	112.10
1	A	117	THR	C-N-CD	-5.26	109.03	120.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	239	CYS	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	128	PRO	Peptide
1	A	230	ASP	Peptide
1	A	350	ALA	Peptide
1	A	510	PRO	Peptide
1	B	117	THR	Peptide
1	B	278	LYS	Peptide

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	4526	0	4449	592	7
1	B	4454	0	4376	518	7
2	A	27	0	12	5	0
3	A	1	0	0	0	0
4	B	23	0	12	2	0
5	A	31	0	0	12	0
5	B	45	0	0	11	0
All	All	9107	0	8849	1095	7

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 61.

All (1095) 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:279:THR:OG1	1:A:282:GLU:HG3	1.16	1.29
1:A:200:LEU:HD23	1:A:201:PHE:N	1.48	1.29
1:A:128:PRO:HB2	1:A:129:GLU:CA	1.56	1.29
1:B:550:ASN:O	1:B:554:GLU:HG3	1.31	1.29
1:A:23:ARG:O	1:A:27:VAL:HG23	1.37	1.25
1:A:128:PRO:CB	1:A:129:GLU:HA	1.57	1.24
1:B:434:LEU:O	1:B:438:ILE:HG23	1.38	1.24
1:B:376:GLU:O	1:B:411:ARG:HA	1.38	1.23
1:A:200:LEU:HD23	1:A:200:LEU:C	1.56	1.23
1:A:8:LEU:HD12	5:A:596:HOH:O	1.33	1.21
1:A:416:GLU:OE2	2:A:1762:ADP:N6	1.71	1.21
1:B:5:LEU:O	1:B:9:ILE:CG2	1.89	1.20
1:B:228:GLN:HB2	1:B:233:GLU:O	1.37	1.20
1:A:279:THR:OG1	1:A:282:GLU:CG	1.90	1.17
1:A:311:GLN:NE2	5:A:590:HOH:O	1.74	1.17
1:B:237:ASP:O	1:B:238:THR:HG22	1.41	1.16
1:B:124:PHE:HB2	1:B:299:ARG:CG	1.75	1.16
1:B:382:LYS:NZ	1:B:403:ASP:OD1	1.79	1.16
1:A:240:LEU:CD2	1:A:245:GLU:HG3	1.75	1.15
1:B:124:PHE:HB2	1:B:299:ARG:HG2	1.28	1.14
1:B:117:THR:OG1	1:B:118:PRO:HA	1.45	1.12
1:B:5:LEU:O	1:B:9:ILE:HG22	0.95	1.11
1:A:107:TYR:HE2	1:A:115:SER:HB3	1.16	1.10
1:B:304:TYR:CD2	1:B:305:LEU:HD12	1.88	1.08
1:B:413:LEU:HD23	1:B:413:LEU:O	1.54	1.07
1:B:203:ARG:NH2	1:B:254:ARG:HD2	1.70	1.07
1:A:308:CYS:C	1:A:309:ASN:HD22	1.56	1.07
1:A:168:ASN:HD22	1:A:171:ARG:HB2	1.18	1.07
1:B:124:PHE:CB	1:B:299:ARG:HG2	1.84	1.06
1:A:30:GLY:O	1:A:34:ARG:HG3	1.55	1.06
1:B:253:ALA:CB	1:B:367:GLY:HA2	1.87	1.05
1:B:178:ARG:HA	1:B:181:THR:HG22	1.07	1.04
1:B:304:TYR:HD2	1:B:305:LEU:CD1	1.69	1.04
1:A:155:ARG:O	1:A:159:ASP:OD2	1.74	1.04
1:B:253:ALA:HB3	1:B:367:GLY:HA2	1.35	1.03
1:B:127:GLN:HB3	1:B:128:PRO:HD3	1.38	1.03
1:A:189:LEU:C	1:A:189:LEU:HD23	1.79	1.03
1:B:304:TYR:CD2	1:B:305:LEU:CD1	2.42	1.03
1:A:126:SER:O	1:A:128:PRO:HD3	1.57	1.02
1:A:167:GLN:HG2	1:A:233:GLU:HB2	1.39	1.01
1:B:257:PHE:HB2	1:B:286:ALA:O	1.58	1.01
1:A:168:ASN:ND2	1:A:171:ARG:HB2	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:CD2	1:A:200:LEU:C	2.29	0.99
1:A:240:LEU:HD22	1:A:245:GLU:HG3	1.39	0.99
1:A:189:LEU:O	1:A:189:LEU:HD23	1.60	0.99
1:B:404:LEU:HB2	1:B:407:GLN:HE21	1.28	0.99
1:A:238:THR:HG23	1:A:238:THR:O	1.63	0.99
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.44	0.99
1:B:538:ASP:OD1	5:B:580:HOH:O	1.82	0.97
1:B:178:ARG:HA	1:B:181:THR:CG2	1.95	0.97
1:A:101:SER:HA	1:A:104:ASN:ND2	1.79	0.97
1:A:8:LEU:CD1	5:A:596:HOH:O	1.99	0.97
1:A:429:VAL:HG12	1:A:433:GLN:OE1	1.64	0.97
1:A:430:GLU:OE2	1:A:527:ARG:NH1	1.97	0.96
1:A:107:TYR:CE2	1:A:115:SER:HB3	2.00	0.96
1:B:61:VAL:O	1:B:65:LEU:N	1.96	0.96
1:A:546:ARG:O	1:A:550:ASN:HB2	1.66	0.95
1:B:516:GLU:O	1:B:519:ARG:HG2	1.64	0.95
1:B:296:GLU:O	1:B:300:GLU:HG3	1.66	0.95
1:B:338:ILE:HG12	1:B:353:VAL:HG21	1.49	0.95
1:A:96:PHE:CE1	1:A:128:PRO:CG	2.51	0.94
1:B:24:PHE:O	1:B:28:THR:OG1	1.86	0.94
1:B:366:VAL:HG11	1:B:447:GLN:HG2	1.47	0.94
1:B:404:LEU:O	1:B:407:GLN:NE2	2.01	0.93
1:B:108:CYS:HB3	1:B:113:HIS:CE1	2.03	0.93
1:B:327:THR:CG2	1:B:328:LEU:H	1.82	0.92
1:B:541:ARG:NH2	1:B:544:TYR:HB2	1.84	0.92
1:A:305:LEU:HD13	1:A:305:LEU:H	1.30	0.92
1:B:201:PHE:HB3	1:B:257:PHE:CE1	2.04	0.92
1:B:117:THR:OG1	1:B:118:PRO:CA	2.18	0.92
1:B:442:GLY:HA3	1:B:536:HIS:CD2	2.04	0.92
1:B:361:LYS:HE2	1:B:372:THR:O	1.69	0.91
1:A:105:SER:O	1:A:109:ARG:HG2	1.69	0.91
1:A:86:TYR:OH	1:A:99:ALA:O	1.88	0.91
1:B:455:PRO:HB2	1:B:458:MET:HB3	1.53	0.91
1:B:267:LEU:O	1:B:271:LEU:HD12	1.70	0.91
1:B:253:ALA:HB1	1:B:367:GLY:C	1.91	0.91
1:A:135:ILE:HG12	1:A:266:ALA:HB1	1.52	0.90
1:B:327:THR:HG22	1:B:328:LEU:H	1.35	0.90
1:A:192:SER:HB2	1:A:214:ILE:O	1.71	0.90
1:A:356:CYS:HB2	1:A:476:TYR:O	1.71	0.90
1:A:125:SER:CB	1:A:129:GLU:HG3	2.02	0.90
1:A:189:LEU:HD23	1:A:190:SER:OG	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HG23	5:B:601:HOH:O	1.69	0.89
1:B:178:ARG:CA	1:B:181:THR:HG22	1.98	0.89
1:A:454:PHE:HB2	1:A:482:MET:SD	2.13	0.89
1:A:96:PHE:CE1	1:A:128:PRO:HG2	2.08	0.89
1:B:81:ARG:HH21	1:B:81:ARG:HG2	1.37	0.89
1:B:310:GLU:HG3	1:B:328:LEU:HD23	1.54	0.88
1:B:450:ALA:HB1	1:B:558:GLU:CG	2.03	0.88
1:B:228:GLN:CB	1:B:233:GLU:O	2.21	0.88
1:A:193:HIS:NE2	1:A:214:ILE:HG21	1.88	0.88
1:B:304:TYR:HD2	1:B:305:LEU:HD12	1.28	0.88
1:B:551:ARG:O	1:B:556:HIS:HB3	1.72	0.88
1:A:309:ASN:HD22	1:A:309:ASN:N	1.68	0.88
1:B:535:MET:O	5:B:580:HOH:O	1.92	0.88
1:A:65:LEU:O	1:A:69:THR:OG1	1.90	0.88
1:A:356:CYS:CB	1:A:476:TYR:O	2.22	0.88
1:B:137:ARG:HB3	1:B:138:PRO:HD2	1.54	0.87
1:A:193:HIS:CD2	1:A:214:ILE:HG21	2.09	0.87
1:A:132:PHE:O	1:A:134:THR:HG23	1.74	0.87
1:B:382:LYS:HZ3	1:B:403:ASP:CG	1.76	0.87
1:B:336:LYS:HD2	1:B:416:GLU:OE2	1.74	0.87
1:B:327:THR:HG22	1:B:328:LEU:N	1.87	0.87
1:A:23:ARG:O	1:A:27:VAL:CG2	2.23	0.86
1:A:75:ASP:HB2	1:A:77:GLU:HG2	1.53	0.86
1:A:443:ASN:O	1:A:447:GLN:HG3	1.76	0.86
1:A:126:SER:C	1:A:128:PRO:CD	2.43	0.86
1:A:381:GLU:O	1:A:385:ILE:HG12	1.74	0.86
1:B:284:TYR:CE1	1:B:292:HIS:HD2	1.93	0.86
1:A:489:ASP:HA	1:A:514:PHE:CD1	2.11	0.86
1:A:252:PHE:CE2	1:A:417:ARG:HD2	2.11	0.85
1:A:221:PRO:O	1:A:241:THR:HG23	1.77	0.85
1:A:96:PHE:CE1	1:A:128:PRO:HG3	2.11	0.85
1:A:294:LYS:HG3	1:A:373:GLN:HG2	1.59	0.85
1:B:5:LEU:C	1:B:9:ILE:HG22	1.97	0.84
1:B:127:GLN:HB3	1:B:128:PRO:CD	2.07	0.84
1:A:167:GLN:OE1	1:A:167:GLN:HA	1.77	0.84
1:A:240:LEU:HD22	1:A:245:GLU:CG	2.07	0.83
1:B:90:LEU:HD22	1:B:96:PHE:HB2	1.58	0.83
1:A:444:ALA:O	1:A:448:LEU:HD22	1.78	0.83
1:B:253:ALA:CB	1:B:367:GLY:CA	2.56	0.83
1:A:465:VAL:HA	1:A:470:ARG:O	1.79	0.82
1:A:113:HIS:HB2	1:A:376:GLU:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASP:HB3	1:A:528:ILE:HG12	1.61	0.82
1:A:192:SER:CB	1:A:214:ILE:O	2.27	0.82
1:B:7:LEU:O	1:B:11:GLN:HG2	1.79	0.82
5:A:596:HOH:O	1:B:60:LEU:HD11	1.78	0.82
1:A:335:PHE:HB3	1:A:413:LEU:HD11	1.60	0.82
1:A:125:SER:HB3	1:A:129:GLU:HG3	1.62	0.82
1:B:124:PHE:CB	1:B:299:ARG:CG	2.52	0.82
1:A:489:ASP:OD1	1:A:516:GLU:HB3	1.80	0.82
1:B:108:CYS:HB3	1:B:113:HIS:ND1	1.95	0.81
1:A:257:PHE:N	1:A:286:ALA:O	2.10	0.81
1:B:482:MET:O	1:B:549:GLN:NE2	2.13	0.81
1:B:95:ARG:HH22	1:B:262:PRO:HB3	1.43	0.81
1:A:332:ASP:OD1	1:A:333:ARG:HG3	1.80	0.81
1:A:338:ILE:HD12	1:A:338:ILE:N	1.96	0.81
1:A:338:ILE:O	1:A:400:LYS:HD2	1.80	0.81
1:A:107:TYR:HE2	1:A:115:SER:CB	1.94	0.81
1:A:20:GLN:HA	1:A:57:HIS:CD2	2.16	0.81
1:A:325:VAL:HG11	2:A:1762:ADP:O4'	1.80	0.80
1:B:538:ASP:HB3	1:B:541:ARG:NH2	1.95	0.80
1:A:294:LYS:HG3	1:A:373:GLN:CG	2.10	0.80
1:A:203:ARG:O	5:A:594:HOH:O	1.99	0.80
1:B:450:ALA:HB1	1:B:558:GLU:HG2	1.64	0.80
1:A:382:LYS:HB3	1:A:406:GLU:O	1.82	0.80
1:A:96:PHE:HE1	1:A:128:PRO:HG2	1.43	0.80
1:A:366:VAL:HG13	1:A:560:VAL:HB	1.64	0.80
1:A:252:PHE:CD2	1:A:417:ARG:HD2	2.17	0.80
1:A:126:SER:C	1:A:128:PRO:HD2	2.02	0.80
1:B:153:LEU:O	1:B:157:ILE:HD12	1.82	0.80
1:A:238:THR:CG2	1:A:238:THR:O	2.29	0.80
1:A:47:MET:SD	1:A:362:GLU:O	2.40	0.80
1:B:245:GLU:O	1:B:248:ILE:HG22	1.82	0.79
1:A:167:GLN:CG	1:A:233:GLU:HB2	2.13	0.79
1:B:438:ILE:HG13	1:B:439:GLU:N	1.97	0.79
1:A:189:LEU:O	1:A:189:LEU:CD2	2.30	0.79
1:B:201:PHE:HB3	1:B:257:PHE:CD1	2.17	0.79
1:B:366:VAL:CG1	1:B:447:GLN:HG2	2.11	0.79
1:A:126:SER:O	1:A:128:PRO:CD	2.30	0.79
1:A:400:LYS:NZ	1:A:412:HIS:NE2	2.31	0.79
1:A:268:VAL:HG13	1:A:283:LEU:HB3	1.63	0.79
1:B:100:GLU:O	1:B:104:ASN:ND2	2.16	0.79
1:B:32:GLN:OE1	5:B:615:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:TRP:CE3	1:B:223:LEU:HD22	2.18	0.78
1:B:97:GLU:O	1:B:100:GLU:HG2	1.82	0.78
1:B:317:GLY:HA2	1:B:424:ILE:HD11	1.64	0.78
1:A:108:CYS:O	1:A:113:HIS:N	2.15	0.78
1:A:189:LEU:CD2	1:A:190:SER:OG	2.30	0.78
1:A:509:SER:N	1:A:510:PRO:CD	2.47	0.78
1:A:279:THR:OG1	1:A:282:GLU:CD	2.21	0.78
1:A:47:MET:HG3	1:A:48:LYS:H	1.48	0.78
1:A:167:GLN:OE1	1:A:167:GLN:CA	2.30	0.78
1:B:322:VAL:HG11	1:B:475:ASP:OD2	1.85	0.77
1:A:305:LEU:CD1	1:A:305:LEU:H	1.96	0.77
1:A:340:ASP:OD1	1:A:400:LYS:HG3	1.84	0.77
1:B:208:TRP:CE3	1:B:223:LEU:CD2	2.68	0.77
1:B:237:ASP:O	1:B:238:THR:CG2	2.29	0.77
1:B:304:TYR:HD2	1:B:305:LEU:HD13	1.48	0.77
1:B:387:PRO:HA	1:B:390:MET:CB	2.14	0.77
1:B:366:VAL:HG11	1:B:447:GLN:CG	2.14	0.77
1:A:128:PRO:HB2	1:A:129:GLU:HA	0.80	0.77
1:B:61:VAL:HG23	1:B:62:VAL:N	2.00	0.77
1:B:304:TYR:CD2	1:B:305:LEU:HD13	2.20	0.77
1:B:29:SER:HB3	1:B:260:TYR:CD1	2.20	0.77
1:B:550:ASN:O	1:B:554:GLU:CG	2.24	0.77
1:B:117:THR:HG1	1:B:118:PRO:HA	1.49	0.77
1:A:488:ARG:O	1:A:514:PHE:CE1	2.37	0.77
1:A:47:MET:HG3	1:A:48:LYS:N	2.00	0.77
1:A:139:LEU:C	1:A:198:ASN:OD1	2.24	0.76
1:B:427:GLU:C	1:B:429:VAL:H	1.83	0.76
1:A:125:SER:HB2	1:A:129:GLU:HG3	1.67	0.76
1:B:368:ARG:NH1	5:B:590:HOH:O	2.17	0.76
1:A:381:GLU:HB2	1:A:384:HIS:HB2	1.67	0.76
1:B:89:LEU:C	1:B:91:PRO:HD3	2.05	0.76
1:B:203:ARG:HH21	1:B:254:ARG:HD2	1.49	0.76
1:B:418:ARG:HG3	1:B:418:ARG:O	1.84	0.76
1:B:68:ILE:HG13	1:B:69:THR:H	1.51	0.75
1:A:137:ARG:NH2	1:B:199:GLU:OE1	2.19	0.75
1:A:423:ASN:OD1	1:A:461:LYS:CB	2.35	0.75
1:B:296:GLU:O	1:B:300:GLU:CG	2.35	0.75
1:B:90:LEU:N	1:B:91:PRO:HD3	2.02	0.75
1:A:304:TYR:CE2	1:A:328:LEU:HD21	2.21	0.74
1:A:268:VAL:HG13	1:A:283:LEU:CB	2.17	0.74
1:B:95:ARG:NH2	1:B:262:PRO:HB3	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ARG:HH21	1:B:564:ARG:HG3	1.52	0.74
1:B:253:ALA:HB3	1:B:367:GLY:CA	2.13	0.74
1:B:326:PHE:HE2	1:B:337:VAL:HG12	1.52	0.74
1:B:81:ARG:HH21	1:B:81:ARG:CG	2.00	0.74
1:B:450:ALA:CB	1:B:558:GLU:HG2	2.17	0.74
1:A:292:HIS:CD2	1:A:296:GLU:HG2	2.23	0.74
1:A:76:ALA:HA	1:A:79:LEU:HB2	1.68	0.74
1:B:275:LEU:O	1:B:277:GLY:N	2.21	0.74
1:B:376:GLU:HA	1:B:412:HIS:H	1.52	0.73
1:A:108:CYS:HB3	1:A:113:HIS:CD2	2.23	0.73
1:B:25:LEU:HB3	1:B:260:TYR:CE1	2.23	0.73
1:A:128:PRO:CG	1:A:129:GLU:HA	2.18	0.73
1:A:304:TYR:HE2	1:A:328:LEU:HD21	1.53	0.73
1:A:420:VAL:O	1:A:420:VAL:HG23	1.86	0.73
1:B:482:MET:HE2	1:B:545:TRP:HZ3	1.52	0.73
1:A:361:LYS:NZ	1:A:372:THR:OG1	2.22	0.73
1:B:525:ASP:HB3	1:B:528:ILE:HD12	1.70	0.73
1:B:541:ARG:HH22	1:B:544:TYR:HB2	1.51	0.73
1:A:101:SER:HA	1:A:104:ASN:HD22	1.52	0.73
1:A:90:LEU:N	1:A:91:PRO:HD3	2.03	0.73
1:B:387:PRO:HA	1:B:390:MET:HB2	1.69	0.73
1:A:338:ILE:HD12	1:A:338:ILE:H	1.54	0.73
1:A:107:TYR:CE2	1:A:115:SER:CB	2.71	0.72
1:A:192:SER:HB3	1:A:215:THR:HA	1.71	0.72
1:A:452:ASN:O	1:A:453:ILE:HD13	1.89	0.72
1:A:452:ASN:OD1	1:A:552:ILE:HG21	1.89	0.72
1:A:429:VAL:CG1	1:A:433:GLN:OE1	2.37	0.72
1:A:440:GLU:HB3	1:A:471:VAL:HG23	1.71	0.72
1:B:397:ALA:O	1:B:401:ILE:HD12	1.89	0.72
1:B:399:GLU:OE2	5:B:617:HOH:O	2.06	0.72
1:B:242:THR:O	1:B:245:GLU:HG3	1.88	0.72
1:A:254:ARG:C	1:A:365:ARG:NH2	2.43	0.72
1:B:118:PRO:HD2	1:B:119:GLU:H	1.55	0.72
1:B:413:LEU:HD23	1:B:413:LEU:C	2.10	0.72
1:B:323:MET:SD	1:B:338:ILE:HG13	2.29	0.72
1:B:372:THR:HA	1:B:415:ILE:O	1.90	0.72
1:A:549:GLN:O	1:A:553:ARG:HG3	1.90	0.72
1:B:438:ILE:CG1	1:B:439:GLU:N	2.53	0.71
1:B:253:ALA:HB1	1:B:367:GLY:CA	2.20	0.71
1:B:275:LEU:O	1:B:275:LEU:HG	1.88	0.71
1:A:454:PHE:CZ	1:A:513:VAL:HG11	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:O	1:A:514:PHE:CD1	2.43	0.71
1:A:488:ARG:HH21	1:A:490:ILE:HB	1.54	0.71
1:B:215:THR:O	1:B:218:GLY:O	2.09	0.71
1:A:524:ALA:O	1:A:526:PRO:HD3	1.90	0.71
1:B:229:THR:N	1:B:233:GLU:OE2	2.23	0.71
1:A:227:HIS:O	1:A:234:LEU:HB2	1.91	0.71
1:A:328:LEU:HD12	1:A:329:PRO:CD	2.18	0.71
1:B:122:PHE:CD2	1:B:122:PHE:N	2.58	0.70
1:B:352:HIS:O	1:B:356:CYS:HB2	1.91	0.70
1:A:430:GLU:HA	1:A:434:LEU:HB2	1.72	0.70
1:A:461:LYS:H	1:A:461:LYS:HD3	1.56	0.70
1:B:229:THR:HG22	1:B:233:GLU:OE2	1.90	0.70
1:A:30:GLY:O	1:A:34:ARG:CG	2.38	0.70
1:A:97:GLU:OE2	1:A:265:ALA:HB2	1.92	0.70
1:B:354:ARG:NE	1:B:374:GLU:OE2	2.25	0.70
1:A:48:LYS:HG2	1:A:362:GLU:HB2	1.72	0.70
1:A:463:PHE:HB3	1:A:471:VAL:HG12	1.72	0.70
1:A:322:VAL:O	1:A:339:LYS:HG3	1.91	0.70
1:A:77:GLU:HG3	1:A:78:PHE:N	2.06	0.70
1:B:208:TRP:HE3	1:B:223:LEU:CD2	2.03	0.70
1:B:48:LYS:HE2	1:B:362:GLU:CD	2.12	0.70
1:B:122:PHE:H	1:B:122:PHE:HD2	1.38	0.69
1:A:166:TRP:C	1:A:167:GLN:OE1	2.30	0.69
1:A:228:GLN:HA	1:A:234:LEU:HA	1.74	0.69
1:B:438:ILE:HD13	1:B:531:LEU:HB3	1.72	0.69
1:A:281:ALA:O	1:A:285:MET:HG3	1.92	0.69
1:A:357:TYR:CE1	1:A:476:TYR:HD2	2.09	0.69
1:A:376:GLU:O	1:A:411:ARG:HA	1.90	0.69
1:B:220:LEU:HD12	1:B:221:PRO:HD2	1.74	0.69
1:A:95:ARG:NH2	1:B:26:GLU:HG2	2.06	0.69
1:B:412:HIS:O	1:B:412:HIS:CG	2.46	0.69
1:B:48:LYS:O	1:B:52:HIS:ND1	2.25	0.69
1:B:87:THR:CG2	1:B:122:PHE:HE1	2.05	0.69
1:B:270:TRP:CE3	1:B:271:LEU:HG	2.28	0.69
1:B:274:ILE:HG13	1:B:275:LEU:H	1.56	0.69
1:A:93:TYR:O	1:A:96:PHE:HB3	1.91	0.69
1:B:68:ILE:HG13	1:B:69:THR:N	2.05	0.69
1:B:253:ALA:CB	1:B:367:GLY:C	2.62	0.69
1:A:153:LEU:CD2	1:A:176:ILE:HG21	2.23	0.69
1:A:136:PRO:O	1:B:163:ARG:NH1	2.25	0.69
1:A:139:LEU:O	1:A:198:ASN:OD1	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:HA	1:A:365:ARG:HH21	1.58	0.68
1:A:200:LEU:HD23	1:A:201:PHE:CA	2.22	0.68
1:A:292:HIS:O	1:A:292:HIS:HD2	1.76	0.68
1:B:544:TYR:O	1:B:548:LEU:HB3	1.94	0.68
1:B:334:VAL:O	1:B:415:ILE:HG23	1.94	0.68
1:A:454:PHE:HZ	1:A:513:VAL:HG11	1.59	0.68
1:B:324:LEU:O	1:B:337:VAL:HG13	1.94	0.68
1:A:94:PRO:HB2	1:A:263:LEU:HD21	1.76	0.68
1:B:21:TYR:O	1:B:24:PHE:HB3	1.94	0.68
1:B:152:LEU:HD22	1:B:152:LEU:N	2.08	0.68
1:B:124:PHE:CB	1:B:299:ARG:HD3	2.25	0.67
1:B:137:ARG:HB3	1:B:138:PRO:CD	2.23	0.67
1:A:58:VAL:O	1:A:62:VAL:HB	1.93	0.67
1:A:371:ASP:CG	1:A:372:THR:H	1.98	0.67
1:B:54:TYR:OH	1:B:102:PHE:HA	1.93	0.67
1:B:93:TYR:HB3	1:B:96:PHE:HB3	1.75	0.67
1:B:118:PRO:CD	1:B:119:GLU:H	2.08	0.67
1:B:107:TYR:OH	1:B:115:SER:O	2.10	0.67
1:B:203:ARG:NH2	1:B:254:ARG:CD	2.53	0.67
1:A:95:ARG:NH2	1:B:26:GLU:OE1	2.27	0.67
1:A:343:ALA:HB3	1:A:344:PRO:HD3	1.76	0.67
1:A:52:HIS:NE2	1:A:362:GLU:OE1	2.26	0.67
1:B:97:GLU:OE1	1:B:265:ALA:HB2	1.95	0.67
1:B:376:GLU:O	1:B:411:ARG:CA	2.31	0.67
1:A:255:SER:HA	1:A:365:ARG:NH2	2.11	0.66
1:B:323:MET:HG3	1:B:338:ILE:HA	1.77	0.66
1:B:274:ILE:HG13	1:B:275:LEU:N	2.09	0.66
1:A:411:ARG:O	1:A:412:HIS:CD2	2.48	0.66
1:A:434:LEU:HD11	1:A:528:ILE:HG22	1.78	0.66
1:A:55:ASP:HA	1:A:58:VAL:CG1	2.25	0.66
1:B:65:LEU:O	1:B:68:ILE:HG12	1.96	0.66
1:B:448:LEU:HD13	1:B:453:ILE:CG2	2.26	0.66
1:A:222:PHE:O	1:A:222:PHE:HD2	1.79	0.66
1:A:462:ASN:CG	1:A:475:ASP:OD2	2.34	0.66
1:A:97:GLU:HB2	1:A:292:HIS:HE1	1.60	0.66
1:A:279:THR:CB	1:A:282:GLU:HG3	2.26	0.66
1:A:254:ARG:O	1:A:365:ARG:NH2	2.29	0.66
1:A:451:ALA:O	1:A:453:ILE:N	2.29	0.66
1:A:139:LEU:HD21	1:A:267:LEU:HD13	1.78	0.65
1:A:404:LEU:N	1:A:407:GLN:O	2.28	0.65
1:A:167:GLN:OE1	1:A:167:GLN:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HG	1:A:221:PRO:HD3	1.78	0.65
1:B:123:ILE:O	1:B:123:ILE:HG12	1.95	0.65
1:B:366:VAL:HG12	1:B:366:VAL:O	1.96	0.65
1:A:337:VAL:HG22	1:A:413:LEU:HD13	1.77	0.65
1:A:199:GLU:N	1:A:199:GLU:OE1	2.30	0.65
1:A:95:ARG:CZ	1:B:26:GLU:HG2	2.26	0.65
1:A:202:TYR:O	1:A:257:PHE:HD1	1.80	0.65
1:A:95:ARG:NE	1:A:262:PRO:O	2.29	0.65
1:A:157:ILE:CG2	1:A:169:LYS:HD2	2.26	0.65
1:A:332:ASP:O	1:A:418:ARG:N	2.26	0.65
1:A:220:LEU:HG	1:A:221:PRO:CD	2.27	0.65
1:A:420:VAL:CG2	1:A:465:VAL:HB	2.27	0.65
1:B:427:GLU:C	1:B:429:VAL:N	2.51	0.65
1:A:101:SER:CA	1:A:104:ASN:ND2	2.59	0.65
1:A:377:ASN:ND2	1:A:411:ARG:HG2	2.12	0.65
1:A:150:GLU:OE1	1:A:173:ILE:HD12	1.97	0.65
1:A:132:PHE:C	1:A:134:THR:HG23	2.18	0.64
1:A:200:LEU:HD11	1:A:207:ALA:HB1	1.78	0.64
1:A:516:GLU:OE1	1:A:540:PHE:HD1	1.80	0.64
1:A:371:ASP:O	1:A:416:GLU:HB2	1.97	0.64
1:B:310:GLU:HG2	1:B:311:GLN:N	2.12	0.64
1:A:77:GLU:HG3	1:A:78:PHE:H	1.63	0.64
1:A:279:THR:HG1	1:A:282:GLU:CD	2.00	0.64
1:A:282:GLU:OE2	1:A:417:ARG:NH2	2.30	0.64
1:B:529:GLY:O	1:B:532:PHE:HB2	1.96	0.64
1:A:292:HIS:O	1:A:292:HIS:CD2	2.50	0.64
1:A:264:PRO:HB3	1:A:287:ILE:HD12	1.80	0.64
1:A:151:SER:O	1:A:154:MET:HB2	1.97	0.64
1:A:128:PRO:HB2	1:A:129:GLU:C	2.16	0.63
1:B:253:ALA:CB	1:B:367:GLY:O	2.46	0.63
1:B:284:TYR:CE1	1:B:292:HIS:CD2	2.83	0.63
1:A:33:GLN:O	1:A:37:GLN:HB2	1.98	0.63
1:B:305:LEU:N	1:B:305:LEU:HD13	2.12	0.63
1:A:308:CYS:C	1:A:309:ASN:ND2	2.41	0.63
1:A:152:LEU:O	1:A:155:ARG:HB2	1.98	0.63
1:A:229:THR:HB	1:A:233:GLU:HG2	1.78	0.63
1:B:420:VAL:HG13	1:B:465:VAL:HB	1.79	0.63
1:A:104:ASN:OD1	1:A:122:PHE:O	2.17	0.63
1:A:519:ARG:HD3	1:A:540:PHE:HB2	1.79	0.63
1:A:529:GLY:O	1:A:532:PHE:HB2	1.99	0.63
1:B:108:CYS:CB	1:B:113:HIS:ND1	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:HH	1:B:102:PHE:HA	1.63	0.63
1:A:489:ASP:CA	1:A:514:PHE:CD1	2.82	0.62
1:A:420:VAL:O	1:A:420:VAL:CG2	2.45	0.62
1:B:370:ALA:N	1:B:476:TYR:OH	2.28	0.62
1:A:145:PRO:HD2	1:A:193:HIS:HA	1.80	0.62
1:A:143:PHE:O	1:A:194:LEU:N	2.31	0.62
1:A:438:ILE:O	1:A:536:HIS:HE1	1.83	0.62
1:A:154:MET:O	1:A:158:SER:OG	2.16	0.62
1:B:61:VAL:CG2	1:B:62:VAL:N	2.62	0.62
1:A:309:ASN:N	1:A:309:ASN:ND2	2.43	0.62
1:A:206:ALA:HB3	5:A:594:HOH:O	1.99	0.62
1:B:245:GLU:O	1:B:248:ILE:CG2	2.47	0.62
1:B:338:ILE:HD11	1:B:414:TYR:HD2	1.64	0.62
1:B:58:VAL:O	1:B:61:VAL:HG22	2.00	0.62
1:A:304:TYR:CE2	1:A:328:LEU:CD2	2.82	0.62
1:A:292:HIS:HD2	1:A:296:GLU:HG2	1.63	0.62
1:A:54:TYR:O	1:A:58:VAL:HG12	1.99	0.62
1:A:200:LEU:CD2	1:A:201:PHE:N	2.43	0.61
1:B:102:PHE:O	1:B:106:VAL:HG23	2.00	0.61
1:B:124:PHE:HB2	1:B:299:ARG:CD	2.29	0.61
1:A:365:ARG:HB3	1:A:369:MET:HB2	1.83	0.61
1:A:516:GLU:OE1	1:A:540:PHE:CD1	2.53	0.61
1:B:220:LEU:HD12	1:B:221:PRO:CD	2.30	0.61
1:A:422:LEU:HB3	1:A:460:PHE:O	2.01	0.61
1:A:75:ASP:CB	1:A:77:GLU:HG2	2.27	0.61
1:A:414:TYR:C	1:A:415:ILE:HD12	2.19	0.61
1:A:509:SER:N	1:A:510:PRO:HD2	2.13	0.61
1:A:170:SER:O	1:A:173:ILE:HG12	2.00	0.61
1:B:124:PHE:HB2	1:B:299:ARG:HG3	1.80	0.61
1:A:240:LEU:HD23	1:A:245:GLU:HG3	1.75	0.61
1:B:253:ALA:HB1	1:B:367:GLY:O	2.00	0.61
1:B:215:THR:C	1:B:217:SER:H	2.04	0.61
1:B:228:GLN:HE21	1:B:232:GLY:HA2	1.64	0.61
1:B:413:LEU:O	1:B:413:LEU:CD2	2.41	0.61
1:A:423:ASN:OD1	1:A:461:LYS:HB2	2.00	0.61
1:A:127:GLN:N	1:A:128:PRO:CD	2.61	0.61
1:B:448:LEU:HD13	1:B:453:ILE:HG22	1.82	0.61
1:A:69:THR:HG22	1:A:73:SER:OG	2.01	0.61
1:A:119:GLU:OE1	1:A:119:GLU:N	2.34	0.61
1:A:133:ARG:HG3	1:A:133:ARG:O	2.01	0.61
1:A:208:TRP:CZ3	1:A:225:PRO:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:C	1:A:134:THR:H	2.02	0.60
1:A:108:CYS:SG	1:A:113:HIS:HA	2.40	0.60
1:B:391:GLU:HA	1:B:394:LEU:HB3	1.83	0.60
1:B:389:LEU:O	1:B:389:LEU:HG	2.00	0.60
1:B:95:ARG:NH2	1:B:262:PRO:O	2.25	0.60
1:B:265:ALA:O	1:B:269:GLU:HB2	2.01	0.60
1:A:101:SER:HA	1:A:104:ASN:HD21	1.63	0.60
1:A:86:TYR:O	1:A:90:LEU:CD1	2.50	0.60
1:A:132:PHE:O	1:A:134:THR:N	2.28	0.60
1:A:324:LEU:N	1:A:337:VAL:O	2.29	0.60
1:A:264:PRO:O	1:A:268:VAL:HG23	2.01	0.60
1:A:420:VAL:HG22	1:A:465:VAL:HB	1.84	0.60
1:A:127:GLN:N	1:A:128:PRO:HD2	2.17	0.60
1:A:266:ALA:O	1:A:269:GLU:HB3	2.02	0.60
1:A:557:VAL:CG1	1:A:557:VAL:O	2.49	0.60
1:A:126:SER:O	1:A:127:GLN:HB3	2.01	0.60
1:B:315:ALA:HB3	1:B:325:VAL:HG11	1.84	0.60
1:A:229:THR:N	1:A:233:GLU:O	2.33	0.60
1:B:514:PHE:HD2	1:B:517:GLU:HB2	1.66	0.60
1:B:270:TRP:HE3	1:B:271:LEU:HG	1.66	0.60
1:B:525:ASP:CB	1:B:528:ILE:HD12	2.32	0.59
1:A:331:PHE:HD1	1:A:332:ASP:H	1.49	0.59
1:A:116:LEU:HD12	1:A:117:THR:H	1.66	0.59
1:A:463:PHE:HB3	1:A:471:VAL:CG1	2.31	0.59
1:A:488:ARG:O	1:A:514:PHE:HE1	1.83	0.59
1:B:108:CYS:CB	1:B:113:HIS:HD1	2.15	0.59
1:A:458:MET:HE2	5:A:601:HOH:O	2.02	0.59
1:A:357:TYR:CE1	1:A:476:TYR:CD2	2.89	0.59
1:A:305:LEU:HD13	1:A:305:LEU:N	2.07	0.59
1:A:351:ALA:HB3	1:A:354:ARG:HG3	1.83	0.59
1:A:86:TYR:O	1:A:90:LEU:HD12	2.03	0.59
1:A:213:LEU:O	1:A:213:LEU:HG	2.01	0.59
1:B:124:PHE:CB	1:B:299:ARG:CD	2.80	0.59
1:B:482:MET:CE	1:B:545:TRP:HZ3	2.16	0.59
1:B:420:VAL:HG21	1:B:425:TRP:HD1	1.67	0.59
1:A:458:MET:CE	5:A:601:HOH:O	2.50	0.59
1:B:104:ASN:HB2	4:B:1604:AMP:O3'	2.03	0.59
1:B:261:ALA:HB2	1:B:267:LEU:HD22	1.84	0.59
1:B:359:LEU:O	1:B:363:HIS:HB2	2.01	0.59
1:A:19:ALA:O	1:A:22:GLY:N	2.36	0.59
1:A:489:ASP:HB3	1:A:514:PHE:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HD13	1:A:86:TYR:OH	2.01	0.58
1:A:58:VAL:HG23	1:A:106:VAL:HG22	1.84	0.58
1:B:116:LEU:C	1:B:117:THR:HG22	2.23	0.58
1:A:61:VAL:O	1:A:65:LEU:HB2	2.03	0.58
1:A:109:ARG:NH1	1:A:374:GLU:OE1	2.36	0.58
1:A:161:PRO:HB3	1:B:138:PRO:HB3	1.84	0.58
1:A:252:PHE:O	1:A:365:ARG:NH1	2.37	0.58
1:A:301:TYR:HA	1:A:331:PHE:HZ	1.67	0.58
1:B:208:TRP:CZ3	1:B:223:LEU:HD22	2.38	0.58
1:B:370:ALA:H	1:B:476:TYR:HH	1.51	0.58
1:B:433:GLN:HA	1:B:433:GLN:OE1	2.04	0.58
1:B:310:GLU:CG	1:B:328:LEU:HD23	2.31	0.58
1:B:220:LEU:CD1	1:B:221:PRO:HD2	2.34	0.58
1:A:335:PHE:N	1:A:335:PHE:CD2	2.71	0.58
1:A:101:SER:CA	1:A:104:ASN:HD22	2.16	0.58
1:A:245:GLU:O	1:A:249:VAL:HG12	2.03	0.58
1:A:304:TYR:HE2	1:A:328:LEU:CD2	2.15	0.58
1:B:442:GLY:O	1:B:446:ARG:HG3	2.04	0.58
1:B:95:ARG:NH2	1:B:262:PRO:CB	2.67	0.58
1:B:295:THR:HG22	1:B:296:GLU:N	2.16	0.58
1:B:221:PRO:HG3	1:B:274:ILE:O	2.03	0.58
1:B:541:ARG:O	1:B:541:ARG:HG2	2.04	0.58
1:A:39:ASP:O	1:A:42:ALA:HB3	2.04	0.57
1:B:32:GLN:HE22	1:B:161:PRO:HB3	1.69	0.57
1:B:327:THR:OG1	1:B:334:VAL:HA	2.04	0.57
1:B:253:ALA:HA	1:B:369:MET:O	2.05	0.57
1:B:450:ALA:HB1	1:B:558:GLU:CB	2.34	0.57
1:A:358:GLN:C	1:A:360:VAL:H	2.06	0.57
1:A:340:ASP:OD1	1:A:400:LYS:CG	2.53	0.57
1:A:325:VAL:HG11	2:A:1762:ADP:C1'	2.34	0.57
1:B:78:PHE:O	1:B:82:VAL:HG23	2.04	0.57
1:A:48:LYS:O	1:A:52:HIS:ND1	2.37	0.57
1:B:354:ARG:HE	1:B:412:HIS:CD2	2.23	0.57
1:B:124:PHE:HB3	1:B:299:ARG:HG2	1.82	0.57
1:A:215:THR:O	1:A:218:GLY:O	2.23	0.57
1:A:292:HIS:CD2	1:A:296:GLU:CG	2.88	0.57
1:A:145:PRO:CD	1:A:193:HIS:HA	2.35	0.57
1:A:449:ALA:CB	1:A:548:LEU:HD13	2.35	0.57
1:A:222:PHE:O	1:A:222:PHE:CD2	2.58	0.56
1:B:356:CYS:SG	1:B:479:ILE:HG22	2.45	0.56
1:A:222:PHE:HE2	1:A:224:LEU:HD12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HB3	1:A:53:LEU:HD22	1.87	0.56
1:A:315:ALA:HB3	1:A:325:VAL:HG13	1.87	0.56
1:B:334:VAL:HB	1:B:418:ARG:HB3	1.87	0.56
1:A:294:LYS:HG3	1:A:373:GLN:HG3	1.87	0.56
1:B:179:HIS:CD2	1:B:241:THR:OG1	2.57	0.56
1:A:380:LEU:HD13	1:A:410:ILE:HG21	1.86	0.56
1:A:425:TRP:O	1:A:429:VAL:HG22	2.05	0.56
1:A:568:ARG:CG	1:A:571:VAL:HG12	2.35	0.56
1:A:489:ASP:HA	1:A:514:PHE:CE1	2.39	0.56
1:A:68:ILE:HG13	1:B:67:CYS:SG	2.45	0.56
1:B:9:ILE:HG21	1:B:82:VAL:HG22	1.87	0.56
1:B:93:TYR:HB3	1:B:96:PHE:CB	2.35	0.56
1:B:325:VAL:HG22	1:B:334:VAL:HG22	1.87	0.56
1:A:113:HIS:CB	1:A:376:GLU:HB3	2.35	0.56
1:A:325:VAL:O	1:A:325:VAL:HG13	2.06	0.56
1:A:442:GLY:HA3	1:A:536:HIS:NE2	2.21	0.56
1:B:326:PHE:CE2	1:B:337:VAL:HG12	2.36	0.56
1:B:327:THR:CG2	1:B:328:LEU:N	2.46	0.55
1:A:308:CYS:SG	1:A:309:ASN:N	2.78	0.55
1:A:449:ALA:HB1	1:A:548:LEU:HD13	1.88	0.55
1:A:237:ASP:C	1:A:237:ASP:OD1	2.43	0.55
1:A:408:ILE:O	1:A:408:ILE:HG12	2.05	0.55
1:A:299:ARG:O	1:A:303:VAL:HG23	2.06	0.55
1:B:411:ARG:O	1:B:412:HIS:HB3	2.06	0.55
1:B:54:TYR:HH	1:B:105:SER:HG	1.54	0.55
1:B:149:TRP:HB3	1:B:177:ILE:HD11	1.87	0.55
1:A:488:ARG:NH2	1:A:490:ILE:HB	2.21	0.55
1:B:95:ARG:NH1	5:B:603:HOH:O	2.02	0.55
1:A:423:ASN:OD1	1:A:461:LYS:HB3	2.06	0.55
1:B:318:ILE:HB	1:B:461:LYS:CE	2.37	0.55
1:A:108:CYS:CB	1:A:113:HIS:HA	2.36	0.55
1:B:394:LEU:HA	1:B:401:ILE:HD13	1.88	0.55
1:B:529:GLY:O	1:B:532:PHE:N	2.27	0.55
1:B:107:TYR:HE2	1:B:116:LEU:HA	1.72	0.55
1:B:171:ARG:O	1:B:175:TYR:HD2	1.90	0.55
1:A:244:ALA:O	1:A:248:ILE:HG12	2.06	0.55
1:B:51:ILE:HD11	1:B:256:TYR:HD2	1.72	0.55
1:A:23:ARG:HB3	1:A:53:LEU:CD2	2.37	0.55
1:B:441:TYR:O	1:B:444:ALA:HB3	2.06	0.55
1:A:127:GLN:O	1:A:128:PRO:C	2.42	0.55
1:A:250:PHE:HB2	1:A:275:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:THR:HG22	1:B:415:ILE:O	2.07	0.55
1:A:209:LEU:HB3	1:A:224:LEU:HB2	1.89	0.55
1:A:20:GLN:C	1:A:20:GLN:NE2	2.61	0.55
1:A:153:LEU:HD21	1:A:176:ILE:HG21	1.87	0.55
1:A:201:PHE:O	1:A:208:TRP:HB2	2.07	0.54
1:A:255:SER:CA	1:A:365:ARG:HH21	2.18	0.54
1:A:371:ASP:CG	1:A:372:THR:N	2.60	0.54
1:B:312:PHE:CD2	1:B:384:HIS:HB3	2.42	0.54
1:A:189:LEU:O	1:A:190:SER:CB	2.55	0.54
1:B:134:THR:O	1:B:134:THR:HG22	2.06	0.54
1:B:338:ILE:HG22	1:B:339:LYS:O	2.08	0.54
1:B:61:VAL:CG2	1:B:62:VAL:H	2.20	0.54
1:B:237:ASP:OD2	1:B:563:TYR:OH	2.22	0.54
1:B:324:LEU:HD13	1:B:393:LEU:HD12	1.89	0.54
1:A:25:LEU:O	1:A:29:SER:HB3	2.06	0.54
1:B:231:ASP:OD1	1:B:231:ASP:N	2.29	0.54
1:A:442:GLY:HA3	1:A:536:HIS:CE1	2.43	0.54
1:A:221:PRO:HB3	1:A:274:ILE:HG23	1.90	0.54
1:A:128:PRO:CB	1:A:129:GLU:CA	2.38	0.54
1:B:255:SER:OG	1:B:364:ASP:OD1	2.26	0.54
1:B:195:GLN:O	1:B:212:LYS:N	2.33	0.54
1:A:97:GLU:HB2	1:A:292:HIS:CE1	2.42	0.54
1:A:170:SER:O	1:A:173:ILE:CG1	2.56	0.54
1:A:456:GLY:HA3	1:A:478:GLU:O	2.08	0.54
1:B:462:ASN:HB3	1:B:475:ASP:HB2	1.90	0.54
1:A:372:THR:HA	1:A:415:ILE:O	2.08	0.54
1:B:403:ASP:C	1:B:404:LEU:HD23	2.28	0.54
1:B:290:GLN:HA	1:B:293:ALA:HB3	1.90	0.54
1:A:359:LEU:O	1:A:359:LEU:HD23	2.08	0.54
1:B:118:PRO:CD	1:B:119:GLU:N	2.71	0.53
1:B:538:ASP:N	1:B:538:ASP:OD1	2.41	0.53
1:B:327:THR:C	1:B:328:LEU:HD12	2.29	0.53
1:B:353:VAL:O	1:B:357:TYR:HB2	2.09	0.53
1:B:375:PHE:HE2	1:B:415:ILE:HD12	1.73	0.53
1:A:366:VAL:O	1:A:366:VAL:HG12	2.09	0.53
1:B:287:ILE:O	1:B:287:ILE:HG22	2.08	0.53
1:B:280:THR:O	1:B:284:TYR:HD2	1.90	0.53
1:B:465:VAL:HA	1:B:470:ARG:O	2.08	0.53
1:A:490:ILE:O	1:A:491:PRO:O	2.25	0.53
1:A:279:THR:OG1	1:A:282:GLU:OE1	2.26	0.53
1:A:96:PHE:CZ	1:A:128:PRO:CG	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:TYR:HB3	1:B:563:TYR:CE1	2.43	0.53
1:A:449:ALA:O	1:A:451:ALA:O	2.25	0.53
1:A:292:HIS:HD2	1:A:296:GLU:CG	2.21	0.53
1:A:483:THR:HG23	1:A:553:ARG:HD3	1.91	0.53
1:A:194:LEU:CD2	1:A:195:GLN:N	2.72	0.53
1:A:358:GLN:O	1:A:361:LYS:N	2.38	0.53
1:B:556:HIS:CE1	5:B:579:HOH:O	2.60	0.53
1:A:488:ARG:HB2	1:A:546:ARG:HH22	1.73	0.53
1:A:489:ASP:HB3	1:A:514:PHE:CB	2.39	0.53
1:A:490:ILE:O	1:A:491:PRO:C	2.46	0.53
1:B:427:GLU:O	1:B:429:VAL:N	2.39	0.53
1:B:48:LYS:NZ	5:B:610:HOH:O	2.30	0.53
1:A:200:LEU:HD23	1:A:200:LEU:O	2.05	0.53
1:B:313:ILE:O	1:B:327:THR:N	2.40	0.53
1:B:79:LEU:HD12	1:B:120:ARG:HB3	1.90	0.53
1:A:200:LEU:CD2	1:A:200:LEU:O	2.55	0.53
1:A:78:PHE:C	1:A:80:LEU:H	2.11	0.53
1:B:294:LYS:HG3	1:B:373:GLN:OE1	2.09	0.53
1:A:194:LEU:HD23	1:A:195:GLN:H	1.73	0.53
1:A:334:VAL:O	1:A:415:ILE:HA	2.08	0.52
1:B:251:GLY:O	1:B:254:ARG:HB2	2.09	0.52
1:B:127:GLN:CB	1:B:128:PRO:HD3	2.26	0.52
1:B:85:HIS:O	1:B:88:ARG:HG2	2.08	0.52
1:B:338:ILE:HG21	1:B:353:VAL:HG11	1.90	0.52
1:A:359:LEU:HD21	1:A:481:TYR:CE1	2.44	0.52
1:A:317:GLY:HA2	1:A:424:ILE:HD11	1.91	0.52
1:B:448:LEU:HD12	1:B:455:PRO:HG3	1.91	0.52
1:B:177:ILE:O	1:B:181:THR:N	2.43	0.52
1:B:294:LYS:NZ	4:B:1604:AMP:O3P	2.30	0.52
1:A:40:TRP:HD1	1:A:43:VAL:HB	1.74	0.52
1:B:286:ALA:O	1:B:287:ILE:HD12	2.09	0.52
1:A:264:PRO:CB	1:A:287:ILE:HD12	2.40	0.52
1:B:63:GLU:O	1:B:67:CYS:HB2	2.10	0.52
1:B:278:LYS:HB2	1:B:282:GLU:OE2	2.10	0.52
1:A:200:LEU:CD2	1:A:201:PHE:C	2.78	0.52
1:A:95:ARG:NH2	1:B:26:GLU:CG	2.72	0.52
1:B:186:PRO:HA	1:B:189:LEU:HD22	1.90	0.52
1:A:445:ILE:HG22	1:A:445:ILE:O	2.10	0.52
1:B:552:ILE:C	1:B:554:GLU:H	2.10	0.52
1:B:338:ILE:HG12	1:B:353:VAL:CG2	2.33	0.52
1:B:80:LEU:HD11	1:B:119:GLU:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:SER:HA	1:B:104:ASN:ND2	2.25	0.52
1:A:323:MET:HE2	1:A:336:LYS:HB3	1.92	0.52
1:B:124:PHE:HB3	1:B:299:ARG:HD3	1.90	0.52
1:B:482:MET:CE	1:B:545:TRP:CZ3	2.92	0.52
1:A:33:GLN:O	1:A:37:GLN:N	2.40	0.52
1:B:176:ILE:HD11	1:B:236:ILE:HD12	1.92	0.52
1:A:200:LEU:HD23	1:A:201:PHE:C	2.29	0.52
1:B:569:PHE:O	1:B:573:TYR:O	2.28	0.52
1:A:336:LYS:HD2	1:A:416:GLU:OE1	2.09	0.52
1:B:438:ILE:HB	1:B:532:PHE:CE2	2.45	0.51
1:A:358:GLN:HA	1:A:361:LYS:HB2	1.92	0.51
1:B:54:TYR:OH	1:B:105:SER:OG	2.25	0.51
1:A:127:GLN:O	1:A:128:PRO:O	2.29	0.51
1:B:514:PHE:CD2	1:B:517:GLU:HB2	2.45	0.51
1:A:380:LEU:HD13	1:A:410:ILE:CG2	2.40	0.51
1:B:222:PHE:O	1:B:222:PHE:CD2	2.63	0.51
1:A:237:ASP:OD1	1:A:238:THR:N	2.43	0.51
1:B:564:ARG:NH2	1:B:564:ARG:HG3	2.24	0.51
1:A:194:LEU:CD2	1:A:195:GLN:H	2.23	0.51
1:B:204:ASN:ND2	1:B:560:VAL:HG11	2.24	0.51
1:A:194:LEU:HD22	1:A:195:GLN:N	2.25	0.51
1:B:40:TRP:HD1	1:B:43:VAL:HG21	1.76	0.51
1:B:430:GLU:N	1:B:430:GLU:OE2	2.44	0.51
1:B:374:GLU:HB2	1:B:414:TYR:CE1	2.46	0.51
1:A:189:LEU:O	1:A:190:SER:HB2	2.10	0.51
1:A:57:HIS:O	1:A:61:VAL:CG1	2.58	0.51
1:A:74:THR:HA	1:A:78:PHE:HE1	1.76	0.51
1:B:62:VAL:HG21	1:B:109:ARG:HB3	1.93	0.51
1:B:515:PRO:HB3	1:B:545:TRP:NE1	2.25	0.51
1:B:154:MET:HG3	1:B:173:ILE:HG21	1.92	0.51
1:A:462:ASN:HB3	1:A:475:ASP:HB2	1.93	0.51
1:B:569:PHE:O	1:B:573:TYR:HB2	2.11	0.51
1:A:33:GLN:HE22	1:B:134:THR:HG23	1.75	0.51
1:A:81:ARG:O	1:A:85:HIS:CD2	2.63	0.51
1:A:138:PRO:HB2	1:A:140:ALA:O	2.11	0.51
1:B:81:ARG:NH2	1:B:81:ARG:CG	2.66	0.51
1:B:116:LEU:O	1:B:117:THR:HG22	2.11	0.51
1:B:312:PHE:HD2	1:B:384:HIS:HB3	1.74	0.51
1:A:449:ALA:HB1	1:A:482:MET:CE	2.40	0.51
1:A:32:GLN:OE1	1:B:138:PRO:HD3	2.11	0.51
1:B:422:LEU:O	1:B:425:TRP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:CYS:O	1:A:360:VAL:HG23	2.11	0.51
1:B:327:THR:HG23	1:B:328:LEU:H	1.73	0.51
1:B:280:THR:HG22	1:B:284:TYR:CE2	2.46	0.51
1:A:336:LYS:HB2	1:A:414:TYR:HB2	1.93	0.51
1:B:559:ASP:HB3	1:B:561:TYR:CE2	2.46	0.51
1:B:382:LYS:HG3	1:B:408:ILE:HG12	1.92	0.51
1:B:95:ARG:HD3	1:B:262:PRO:O	2.11	0.51
1:A:268:VAL:HG13	1:A:283:LEU:HB2	1.93	0.51
1:A:53:LEU:HA	1:A:56:HIS:HB3	1.93	0.50
1:B:96:PHE:CD1	1:B:96:PHE:C	2.84	0.50
1:A:260:TYR:O	1:A:260:TYR:CD2	2.64	0.50
1:B:54:TYR:CG	1:B:291:LYS:HD3	2.46	0.50
1:B:525:ASP:HB3	1:B:528:ILE:CD1	2.40	0.50
1:B:334:VAL:CG1	1:B:416:GLU:HG3	2.41	0.50
1:A:439:GLU:HG3	1:A:535:MET:HG3	1.94	0.50
1:B:518:PHE:O	1:B:522:LEU:HB2	2.11	0.50
1:B:315:ALA:HB3	1:B:325:VAL:CG1	2.41	0.50
1:A:149:TRP:CD1	1:A:189:LEU:HG	2.47	0.50
1:B:29:SER:HB3	1:B:260:TYR:HD1	1.75	0.50
1:A:55:ASP:HA	1:A:58:VAL:HG13	1.93	0.50
1:B:353:VAL:O	1:B:354:ARG:C	2.50	0.50
1:B:241:THR:N	1:B:245:GLU:OE1	2.37	0.50
1:B:368:ARG:O	1:B:473:PHE:HB3	2.11	0.50
1:B:318:ILE:HB	1:B:461:LYS:HE2	1.94	0.50
1:B:239:CYS:HB2	1:B:569:PHE:HZ	1.77	0.50
1:A:414:TYR:O	1:A:415:ILE:HD12	2.11	0.50
1:B:61:VAL:HG23	1:B:62:VAL:H	1.73	0.50
1:B:194:LEU:HD12	1:B:213:LEU:HA	1.94	0.50
1:A:95:ARG:NH2	1:B:26:GLU:CD	2.65	0.50
1:B:21:TYR:O	1:B:24:PHE:CB	2.59	0.50
1:B:448:LEU:HD13	1:B:453:ILE:HG21	1.94	0.49
1:A:519:ARG:HD3	1:A:540:PHE:CB	2.42	0.49
1:A:20:GLN:NE2	1:A:20:GLN:O	2.45	0.49
1:A:375:PHE:O	1:A:412:HIS:HA	2.12	0.49
1:A:198:ASN:OD1	1:A:198:ASN:O	2.30	0.49
1:B:287:ILE:O	1:B:287:ILE:CG2	2.60	0.49
1:B:366:VAL:CG1	1:B:366:VAL:O	2.59	0.49
1:B:275:LEU:C	1:B:277:GLY:N	2.65	0.49
1:B:176:ILE:HD11	1:B:236:ILE:CD1	2.41	0.49
1:B:339:LYS:HD3	1:B:342:PHE:HA	1.93	0.49
1:B:376:GLU:HA	1:B:412:HIS:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:O	1:A:77:GLU:C	2.50	0.49
1:A:382:LYS:CB	1:A:406:GLU:O	2.58	0.49
1:B:196:VAL:HG13	1:B:209:LEU:HD21	1.93	0.49
1:A:107:TYR:CZ	1:A:120:ARG:HG3	2.48	0.49
1:B:310:GLU:OE2	1:B:384:HIS:CE1	2.66	0.49
1:A:328:LEU:CD1	1:A:329:PRO:HD2	2.31	0.49
1:B:476:TYR:HB3	1:B:479:ILE:HD12	1.94	0.49
1:A:449:ALA:HB1	1:A:482:MET:HE2	1.93	0.49
1:A:411:ARG:O	1:A:412:HIS:HD2	1.93	0.49
1:B:223:LEU:HD13	1:B:249:VAL:HG11	1.94	0.49
1:A:157:ILE:HG22	1:A:169:LYS:HD2	1.92	0.49
1:A:197:ALA:HB3	1:A:210:VAL:CG1	2.43	0.49
1:A:525:ASP:CB	1:A:528:ILE:HG12	2.39	0.49
1:A:470:ARG:HB3	1:A:470:ARG:CZ	2.43	0.49
1:A:48:LYS:O	1:A:52:HIS:CE1	2.65	0.49
1:B:322:VAL:HG23	1:B:323:MET:N	2.26	0.49
1:A:305:LEU:HD23	1:A:381:GLU:OE2	2.12	0.49
1:B:387:PRO:HA	1:B:390:MET:HB3	1.92	0.49
1:A:40:TRP:CD1	1:A:43:VAL:HB	2.48	0.49
1:A:125:SER:HB2	1:A:129:GLU:CG	2.40	0.49
1:B:124:PHE:CD2	1:B:299:ARG:HD3	2.47	0.49
1:A:249:VAL:HG13	1:A:250:PHE:HD2	1.78	0.49
1:B:539:LEU:O	1:B:545:TRP:NE1	2.43	0.49
1:A:339:LYS:HD2	1:A:396:GLU:OE1	2.12	0.49
1:A:355:ALA:O	1:A:359:LEU:HB2	2.13	0.49
1:A:7:LEU:O	1:A:11:GLN:HB2	2.13	0.49
1:A:453:ILE:HG23	1:A:479:ILE:HD12	1.95	0.49
1:A:461:LYS:CD	1:A:461:LYS:H	2.24	0.49
1:B:304:TYR:HB3	1:B:305:LEU:HD13	1.95	0.48
1:A:165:HIS:H	1:A:165:HIS:CD2	2.30	0.48
1:A:333:ARG:HA	1:A:418:ARG:H	1.79	0.48
1:B:328:LEU:HB3	1:B:329:PRO:HD2	1.96	0.48
1:A:441:TYR:O	1:A:444:ALA:HB3	2.13	0.48
1:A:338:ILE:CD1	1:A:338:ILE:H	2.24	0.48
1:B:95:ARG:HH22	1:B:262:PRO:CB	2.20	0.48
1:B:338:ILE:HD11	1:B:414:TYR:CD2	2.46	0.48
1:A:240:LEU:HD22	1:A:245:GLU:CB	2.43	0.48
1:A:132:PHE:C	1:A:134:THR:N	2.66	0.48
1:A:338:ILE:CD1	1:A:338:ILE:N	2.67	0.48
1:B:168:ASN:C	1:B:170:SER:H	2.16	0.48
1:A:336:LYS:N	1:A:414:TYR:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:CYS:O	1:A:309:ASN:ND2	2.45	0.48
1:A:368:ARG:HH22	1:A:440:GLU:HG3	1.78	0.48
1:A:222:PHE:HE2	1:A:224:LEU:CD1	2.26	0.48
1:A:457:ASP:OD1	1:A:457:ASP:C	2.52	0.48
1:B:47:MET:O	1:B:47:MET:HG3	2.14	0.48
1:B:340:ASP:N	1:B:340:ASP:OD1	2.40	0.48
1:A:356:CYS:HB3	1:A:476:TYR:O	2.10	0.48
1:A:68:ILE:O	1:A:68:ILE:HG22	2.14	0.48
1:B:85:HIS:HA	1:B:88:ARG:HD3	1.96	0.48
1:B:438:ILE:CD1	1:B:531:LEU:HB3	2.41	0.48
1:A:302:LEU:O	1:A:306:GLN:HB2	2.14	0.48
1:A:116:LEU:CD1	1:A:117:THR:H	2.27	0.48
1:B:116:LEU:O	1:B:117:THR:CB	2.56	0.48
1:B:251:GLY:O	1:B:254:ARG:CG	2.62	0.48
1:B:304:TYR:CE2	1:B:305:LEU:HD12	2.45	0.48
1:A:241:THR:O	1:A:241:THR:HG22	2.13	0.48
1:B:203:ARG:NH1	1:B:255:SER:O	2.47	0.48
1:A:189:LEU:HD21	1:A:190:SER:OG	2.13	0.48
1:B:538:ASP:HA	1:B:541:ARG:HD3	1.95	0.48
1:A:335:PHE:CB	1:A:413:LEU:HD11	2.37	0.48
1:B:222:PHE:C	1:B:222:PHE:CD2	2.87	0.48
1:A:452:ASN:OD1	1:A:552:ILE:CG2	2.60	0.47
1:A:281:ALA:HB2	1:A:296:GLU:HB3	1.95	0.47
1:B:7:LEU:HD22	1:B:8:LEU:N	2.28	0.47
1:B:108:CYS:HB3	1:B:113:HIS:HD1	1.74	0.47
1:A:450:ALA:O	1:A:557:VAL:CG2	2.63	0.47
1:B:16:GLY:O	1:B:20:GLN:HB2	2.14	0.47
1:B:327:THR:HG21	1:B:418:ARG:HD3	1.96	0.47
1:A:447:GLN:NE2	5:A:580:HOH:O	2.47	0.47
1:A:25:LEU:HB2	1:A:260:TYR:CE1	2.49	0.47
1:B:375:PHE:CE2	1:B:415:ILE:HD12	2.49	0.47
1:A:97:GLU:HG2	1:A:98:ILE:N	2.30	0.47
1:A:305:LEU:HD22	1:A:306:GLN:N	2.29	0.47
1:B:145:PRO:HB3	1:B:149:TRP:CD1	2.49	0.47
1:B:122:PHE:HB3	1:B:127:GLN:HB2	1.96	0.47
1:B:259:VAL:HG11	1:B:267:LEU:HD21	1.95	0.47
1:A:25:LEU:HD13	5:B:603:HOH:O	2.14	0.47
1:B:420:VAL:CG2	1:B:425:TRP:HD1	2.28	0.47
1:A:255:SER:CA	1:A:365:ARG:NH2	2.76	0.47
1:A:100:GLU:O	1:A:103:PHE:HB3	2.15	0.47
1:A:460:PHE:HZ	1:A:522:LEU:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:C	1:B:217:SER:N	2.66	0.47
1:A:156:VAL:O	1:A:160:LEU:HG	2.13	0.47
1:A:189:LEU:HD23	1:A:190:SER:CB	2.44	0.47
1:A:488:ARG:HD2	1:A:546:ARG:HH22	1.79	0.47
1:B:259:VAL:CG1	1:B:267:LEU:HD21	2.45	0.47
1:A:544:TYR:CE2	1:A:548:LEU:HD11	2.49	0.47
1:A:65:LEU:HD22	1:A:110:LEU:HD11	1.97	0.47
1:B:90:LEU:N	1:B:91:PRO:CD	2.74	0.47
1:B:290:GLN:O	1:B:294:LYS:N	2.41	0.47
1:A:462:ASN:ND2	1:A:475:ASP:OD2	2.48	0.47
1:B:378:PHE:HE2	1:B:380:LEU:HD21	1.80	0.47
1:B:539:LEU:O	1:B:539:LEU:HD23	2.15	0.47
1:B:90:LEU:HD21	1:B:99:ALA:CB	2.45	0.47
1:B:58:VAL:HG23	1:B:59:GLY:N	2.30	0.47
1:A:304:TYR:CD2	1:A:328:LEU:HD23	2.49	0.47
1:A:32:GLN:NE2	1:B:138:PRO:HD3	2.30	0.47
1:A:557:VAL:HG12	1:A:557:VAL:O	2.15	0.47
1:B:376:GLU:CA	1:B:412:HIS:H	2.24	0.46
1:B:203:ARG:HH22	1:B:254:ARG:HG3	1.80	0.46
1:A:422:LEU:HD13	1:A:471:VAL:HG13	1.97	0.46
1:B:137:ARG:CB	1:B:138:PRO:CD	2.89	0.46
1:A:326:PHE:HE2	1:A:337:VAL:HG21	1.80	0.46
1:B:246:ALA:HA	1:B:249:VAL:CG1	2.45	0.46
1:B:380:LEU:CD1	1:B:410:ILE:HD11	2.45	0.46
1:B:257:PHE:CB	1:B:286:ALA:O	2.46	0.46
1:A:430:GLU:HG3	1:A:431:GLY:N	2.30	0.46
1:A:145:PRO:HB3	1:A:148:GLY:HA2	1.96	0.46
1:B:189:LEU:C	1:B:189:LEU:HD23	2.36	0.46
1:A:84:GLU:HG3	1:A:85:HIS:N	2.27	0.46
1:B:295:THR:O	1:B:298:TYR:N	2.46	0.46
1:A:86:TYR:CD2	1:A:90:LEU:HD11	2.50	0.46
1:B:271:LEU:O	1:B:274:ILE:HG23	2.14	0.46
1:B:173:ILE:N	5:B:601:HOH:O	2.48	0.46
1:A:480:CYS:HB2	1:A:484:GLU:OE1	2.16	0.46
1:A:5:LEU:O	1:A:9:ILE:HG13	2.16	0.46
1:B:368:ARG:C	1:B:369:MET:HG2	2.35	0.46
1:A:228:GLN:HG2	1:A:229:THR:N	2.29	0.46
1:A:448:LEU:O	1:A:451:ALA:O	2.32	0.46
1:A:441:TYR:OH	1:A:458:MET:O	2.30	0.46
1:B:334:VAL:HB	1:B:418:ARG:CB	2.45	0.46
1:A:304:TYR:CD2	1:A:328:LEU:CD2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HD2	1:A:163:ARG:HA	1.66	0.46
1:B:304:TYR:C	1:B:304:TYR:CD2	2.89	0.46
1:B:149:TRP:HH2	1:B:194:LEU:HD13	1.80	0.46
1:A:516:GLU:C	1:A:518:PHE:N	2.69	0.46
1:A:458:MET:HB2	5:A:601:HOH:O	2.14	0.46
1:A:412:HIS:CG	1:A:412:HIS:O	2.69	0.46
1:A:160:LEU:C	1:A:162:LEU:H	2.19	0.46
1:A:101:SER:C	1:A:104:ASN:HD22	2.18	0.46
1:A:438:ILE:CD1	1:A:531:LEU:HD23	2.45	0.46
1:B:290:GLN:O	1:B:293:ALA:HB3	2.15	0.46
1:A:151:SER:O	1:A:154:MET:CB	2.62	0.46
1:B:204:ASN:HD22	1:B:560:VAL:CG1	2.28	0.46
1:A:365:ARG:O	1:A:366:VAL:HB	2.15	0.46
1:B:78:PHE:HD1	1:B:81:ARG:NH2	2.13	0.46
1:B:402:THR:O	1:B:408:ILE:HG22	2.16	0.46
1:A:552:ILE:HA	1:A:556:HIS:O	2.16	0.46
1:B:450:ALA:HB1	1:B:558:GLU:CD	2.36	0.46
1:A:401:ILE:HA	1:A:409:VAL:O	2.15	0.46
1:A:208:TRP:CE3	1:A:225:PRO:HG3	2.51	0.46
1:B:334:VAL:HG12	1:B:416:GLU:HG3	1.96	0.46
1:B:173:ILE:HG13	1:B:174:HIS:N	2.31	0.46
1:B:72:GLN:HG3	1:B:72:GLN:H	1.34	0.46
1:B:434:LEU:O	1:B:438:ILE:CG2	2.33	0.46
1:B:299:ARG:HD2	1:B:299:ARG:HA	1.32	0.46
1:A:86:TYR:O	1:A:90:LEU:HD11	2.16	0.46
1:B:450:ALA:HB1	1:B:558:GLU:HB2	1.98	0.46
1:A:114:ARG:C	1:A:114:ARG:HD3	2.36	0.46
1:B:458:MET:O	1:B:458:MET:HG3	2.16	0.45
1:A:228:GLN:OE1	1:A:231:ASP:HA	2.16	0.45
1:A:481:TYR:HB2	1:A:484:GLU:HG3	1.97	0.45
1:B:323:MET:CG	1:B:338:ILE:HA	2.44	0.45
1:B:301:TYR:O	1:B:305:LEU:HD22	2.15	0.45
1:B:33:GLN:O	1:B:33:GLN:HG3	2.16	0.45
1:B:376:GLU:OE2	1:B:411:ARG:NH2	2.48	0.45
1:B:454:PHE:HD1	1:B:482:MET:HE2	1.81	0.45
1:A:488:ARG:HB2	1:A:546:ARG:NH2	2.30	0.45
1:B:66:ARG:O	1:B:69:THR:O	2.33	0.45
1:A:227:HIS:O	1:A:234:LEU:CB	2.62	0.45
1:A:134:THR:OG1	1:A:134:THR:O	2.29	0.45
1:A:78:PHE:C	1:A:80:LEU:N	2.68	0.45
1:A:337:VAL:HG22	1:A:413:LEU:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:O	1:A:156:VAL:HG22	2.16	0.45
1:A:245:GLU:OE1	1:A:245:GLU:HA	2.17	0.45
1:A:90:LEU:N	1:A:91:PRO:CD	2.78	0.45
1:A:464:GLY:O	1:A:471:VAL:HA	2.16	0.45
1:A:568:ARG:HG3	1:A:571:VAL:HG12	1.98	0.45
1:B:312:PHE:N	1:B:384:HIS:O	2.38	0.45
1:A:222:PHE:CD2	1:A:222:PHE:C	2.90	0.45
1:B:75:ASP:O	1:B:79:LEU:HB2	2.16	0.45
1:A:366:VAL:O	1:A:366:VAL:CG1	2.64	0.45
1:B:125:SER:HA	1:B:296:GLU:CG	2.47	0.45
1:B:274:ILE:CG1	1:B:275:LEU:H	2.25	0.45
1:A:57:HIS:O	1:A:61:VAL:HG13	2.17	0.45
1:B:37:GLN:O	1:B:38:ALA:HB3	2.17	0.45
1:B:310:GLU:OE2	1:B:384:HIS:ND1	2.49	0.45
1:A:173:ILE:HG13	1:A:174:HIS:N	2.32	0.45
1:A:357:TYR:CD1	1:A:476:TYR:HD2	2.35	0.45
1:A:430:GLU:HG3	1:A:431:GLY:H	1.82	0.45
1:A:13:ILE:HA	1:A:61:VAL:HG21	1.98	0.45
1:A:203:ARG:HB2	1:A:257:PHE:CE1	2.52	0.45
1:A:47:MET:O	1:A:50:ARG:N	2.48	0.45
1:A:126:SER:O	1:A:127:GLN:CB	2.63	0.45
1:B:466:THR:CG2	1:B:467:ARG:N	2.79	0.45
1:B:420:VAL:O	1:B:465:VAL:N	2.40	0.44
1:B:481:TYR:C	1:B:483:THR:H	2.21	0.44
1:B:382:LYS:NZ	1:B:403:ASP:CG	2.54	0.44
1:A:296:GLU:O	1:A:300:GLU:HG3	2.17	0.44
1:A:36:GLU:HA	1:A:164:LEU:HD11	1.98	0.44
1:A:371:ASP:OD2	1:A:372:THR:N	2.51	0.44
1:A:234:LEU:O	1:A:234:LEU:HD22	2.16	0.44
1:B:544:TYR:O	1:B:548:LEU:CB	2.64	0.44
1:A:47:MET:CG	1:A:48:LYS:N	2.77	0.44
1:B:162:LEU:H	1:B:162:LEU:HD22	1.81	0.44
1:B:226:ILE:CG2	1:B:234:LEU:HD22	2.47	0.44
1:B:338:ILE:CG1	1:B:353:VAL:HG21	2.35	0.44
1:A:301:TYR:HA	1:A:331:PHE:CZ	2.51	0.44
1:A:103:PHE:C	1:A:103:PHE:CD2	2.91	0.44
1:A:368:ARG:HB2	1:A:448:LEU:HD13	2.00	0.44
1:A:153:LEU:HD11	1:A:224:LEU:HD11	2.00	0.44
1:B:196:VAL:CG1	1:B:209:LEU:HD21	2.48	0.44
1:A:139:LEU:O	1:A:139:LEU:HD23	2.18	0.44
1:A:255:SER:N	1:A:365:ARG:NH2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD12	1:A:117:THR:N	2.32	0.44
1:B:298:TYR:HA	1:B:301:TYR:HB3	1.99	0.44
1:B:87:THR:HG22	1:B:122:PHE:HE1	1.80	0.44
1:A:100:GLU:O	1:A:104:ASN:ND2	2.51	0.44
1:A:135:ILE:HG22	1:A:137:ARG:O	2.16	0.44
1:B:565:ARG:O	1:B:567:GLN:N	2.51	0.44
1:A:127:GLN:O	1:A:127:GLN:HG3	2.17	0.44
1:B:375:PHE:O	1:B:413:LEU:N	2.50	0.44
1:B:387:PRO:HA	1:B:390:MET:H	1.83	0.44
1:B:152:LEU:N	1:B:152:LEU:CD2	2.79	0.44
1:B:323:MET:HE3	1:B:323:MET:HB2	1.95	0.44
1:A:474:TYR:OH	2:A:1762:ADP:H2'	2.18	0.44
1:B:164:LEU:CD1	1:B:228:GLN:HE22	2.31	0.44
1:B:80:LEU:CD1	1:B:119:GLU:O	2.66	0.44
1:B:290:GLN:HB3	1:B:290:GLN:HE21	1.46	0.44
1:A:153:LEU:HD22	1:A:176:ILE:HG21	1.99	0.44
1:A:17:PHE:CG	1:A:18:ASP:N	2.85	0.44
1:A:155:ARG:C	1:A:159:ASP:OD2	2.52	0.44
1:B:32:GLN:O	1:B:36:GLU:HB2	2.18	0.44
1:B:564:ARG:HH21	1:B:564:ARG:CG	2.25	0.44
1:B:152:LEU:H	1:B:152:LEU:HD22	1.82	0.44
1:A:394:LEU:HD23	1:A:401:ILE:HD11	2.00	0.44
1:B:565:ARG:C	1:B:567:GLN:N	2.71	0.44
1:B:121:LEU:C	1:B:121:LEU:HD12	2.38	0.44
1:B:5:LEU:HB2	1:B:78:PHE:CZ	2.53	0.43
1:B:454:PHE:HA	1:B:455:PRO:HD3	1.87	0.43
1:A:255:SER:N	1:A:365:ARG:HH21	2.17	0.43
1:A:23:ARG:HE	1:A:53:LEU:HD11	1.83	0.43
1:A:361:LYS:HZ3	1:A:372:THR:HG1	1.58	0.43
1:B:297:SER:HA	1:B:300:GLU:HG3	2.01	0.43
1:A:309:ASN:HA	1:A:310:GLU:HA	1.86	0.43
1:A:23:ARG:CD	1:A:53:LEU:HD21	2.48	0.43
1:B:5:LEU:HA	1:B:8:LEU:HB3	2.00	0.43
1:B:274:ILE:CG1	1:B:275:LEU:N	2.80	0.43
1:A:458:MET:HE3	5:A:601:HOH:O	2.17	0.43
1:B:246:ALA:HA	1:B:249:VAL:HG13	2.00	0.43
1:B:305:LEU:CD1	1:B:305:LEU:N	2.80	0.43
1:B:370:ALA:N	1:B:476:TYR:HH	2.14	0.43
1:B:430:GLU:N	1:B:430:GLU:CD	2.72	0.43
1:B:288:GLY:O	1:B:290:GLN:N	2.42	0.43
1:B:438:ILE:HB	1:B:532:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:VAL:O	1:A:515:PRO:HD3	2.19	0.43
1:A:256:TYR:HB3	1:A:286:ALA:O	2.19	0.43
1:A:172:ASP:HA	1:A:175:TYR:HD2	1.84	0.43
1:A:432:GLN:HB3	5:A:607:HOH:O	2.18	0.43
1:A:371:ASP:OD2	1:A:372:THR:O	2.36	0.43
1:B:204:ASN:ND2	1:B:560:VAL:CG1	2.82	0.43
1:A:81:ARG:O	1:A:85:HIS:HB2	2.19	0.43
1:A:18:ASP:HB3	1:B:19:ALA:HA	1.99	0.43
1:B:434:LEU:HD11	1:B:528:ILE:HG23	2.00	0.43
1:B:448:LEU:HD11	1:B:473:PHE:CD2	2.53	0.43
1:A:490:ILE:HG23	1:A:491:PRO:HD3	2.00	0.43
1:A:32:GLN:HE22	1:B:138:PRO:HD3	1.83	0.43
1:A:113:HIS:CG	1:A:376:GLU:HB3	2.53	0.43
1:A:385:ILE:HG22	1:A:386:SER:O	2.19	0.43
1:A:116:LEU:O	1:A:120:ARG:HB3	2.19	0.43
1:A:193:HIS:CE1	1:A:214:ILE:HG21	2.50	0.43
1:B:49:ASN:O	1:B:52:HIS:HB2	2.19	0.43
1:B:123:ILE:O	1:B:123:ILE:HG23	2.19	0.43
1:B:441:TYR:CD2	1:B:441:TYR:C	2.91	0.43
1:A:253:ALA:O	1:A:367:GLY:N	2.50	0.43
1:A:301:TYR:HD1	1:A:331:PHE:HE2	1.67	0.43
1:B:382:LYS:CE	1:B:403:ASP:OD1	2.64	0.43
1:A:202:TYR:O	1:A:257:PHE:CD1	2.67	0.43
1:B:564:ARG:CG	1:B:564:ARG:NH2	2.82	0.43
1:A:170:SER:HA	1:A:173:ILE:HG12	1.99	0.43
1:A:23:ARG:HD3	1:A:53:LEU:HD21	2.01	0.42
1:B:149:TRP:HZ2	1:B:192:SER:O	2.01	0.42
1:A:368:ARG:NH2	1:A:440:GLU:HG3	2.33	0.42
1:A:397:ALA:HB1	1:A:400:LYS:HB2	2.00	0.42
1:A:139:LEU:O	1:A:139:LEU:CD2	2.68	0.42
1:A:408:ILE:O	1:A:408:ILE:CG1	2.67	0.42
1:A:535:MET:HE3	1:A:535:MET:O	2.18	0.42
1:B:139:LEU:O	1:B:198:ASN:OD1	2.36	0.42
1:A:211:GLY:HA2	1:A:270:TRP:HH2	1.84	0.42
1:A:193:HIS:CD2	1:A:214:ILE:CG2	2.93	0.42
1:B:101:SER:C	1:B:104:ASN:HD22	2.22	0.42
1:B:9:ILE:HG13	1:B:65:LEU:HD21	2.02	0.42
1:B:301:TYR:O	1:B:305:LEU:CD2	2.67	0.42
1:A:112:ASP:O	1:A:113:HIS:C	2.57	0.42
1:B:363:HIS:CE1	1:B:451:ALA:O	2.71	0.42
1:A:197:ALA:HB3	1:A:210:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:HB3	1:A:569:PHE:CZ	2.53	0.42
1:B:331:PHE:CE2	1:B:333:ARG:HG2	2.54	0.42
1:B:422:LEU:O	1:B:423:ASN:C	2.57	0.42
1:A:549:GLN:HG3	1:A:553:ARG:HE	1.83	0.42
1:A:311:GLN:HB3	1:A:384:HIS:O	2.19	0.42
1:A:440:GLU:O	1:A:444:ALA:HB2	2.20	0.42
1:A:79:LEU:HD11	1:A:111:PHE:CZ	2.55	0.42
1:B:543:ASP:O	1:B:547:ALA:HB3	2.19	0.42
1:A:334:VAL:HG22	1:A:418:ARG:HA	2.01	0.42
1:A:116:LEU:HB3	1:A:120:ARG:NH1	2.34	0.42
1:B:448:LEU:O	1:B:453:ILE:N	2.51	0.42
1:B:442:GLY:CA	1:B:536:HIS:CD2	2.88	0.42
1:A:221:PRO:HD2	1:A:241:THR:O	2.19	0.42
1:A:221:PRO:O	1:A:241:THR:CG2	2.60	0.42
1:A:465:VAL:HG12	1:A:466:THR:N	2.34	0.42
1:A:143:PHE:N	1:A:194:LEU:O	2.53	0.42
1:B:143:PHE:N	1:B:143:PHE:CD2	2.88	0.42
1:B:450:ALA:HB3	1:B:558:GLU:HG2	1.98	0.42
1:A:488:ARG:O	1:A:514:PHE:HD1	1.95	0.42
1:B:89:LEU:C	1:B:91:PRO:CD	2.84	0.42
1:A:157:ILE:HG21	1:A:169:LYS:HG3	2.02	0.42
1:A:489:ASP:CB	1:A:514:PHE:CD1	3.02	0.42
1:B:226:ILE:HG22	1:B:234:LEU:HD22	2.02	0.42
1:B:121:LEU:O	1:B:121:LEU:HD12	2.20	0.42
1:B:459:LEU:O	1:B:463:PHE:HD2	2.03	0.42
1:A:200:LEU:HD21	1:A:208:TRP:H	1.85	0.41
1:B:403:ASP:O	1:B:404:LEU:HD23	2.19	0.41
1:A:32:GLN:HG3	1:A:202:TYR:OH	2.20	0.41
1:B:48:LYS:HE2	1:B:362:GLU:CG	2.49	0.41
1:A:315:ALA:HB3	1:A:325:VAL:CG1	2.50	0.41
1:A:80:LEU:CD2	1:A:119:GLU:O	2.68	0.41
1:A:196:VAL:HG13	1:A:209:LEU:HD23	2.02	0.41
1:A:379:VAL:O	1:A:379:VAL:HG13	2.21	0.41
1:A:325:VAL:CG1	2:A:1762:ADP:O4'	2.61	0.41
1:A:358:GLN:C	1:A:360:VAL:N	2.72	0.41
1:B:32:GLN:O	1:B:36:GLU:CB	2.68	0.41
1:B:168:ASN:C	1:B:170:SER:N	2.73	0.41
1:A:390:MET:O	1:A:394:LEU:N	2.35	0.41
1:B:466:THR:HG23	1:B:467:ARG:N	2.34	0.41
1:B:285:MET:HB2	1:B:285:MET:HE3	1.95	0.41
1:B:354:ARG:HA	1:B:354:ARG:HD3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:O	1:B:369:MET:HG2	2.19	0.41
1:A:79:LEU:HD11	1:A:111:PHE:CE1	2.55	0.41
1:B:514:PHE:CD2	1:B:517:GLU:OE2	2.73	0.41
1:B:318:ILE:O	1:B:319:ARG:C	2.59	0.41
1:A:564:ARG:C	1:A:566:ARG:H	2.23	0.41
1:A:69:THR:O	1:A:73:SER:HB2	2.21	0.41
1:B:280:THR:HG22	1:B:284:TYR:HE2	1.85	0.41
1:B:93:TYR:CB	1:B:96:PHE:HB3	2.48	0.41
1:A:113:HIS:O	1:A:377:ASN:HB2	2.20	0.41
1:A:54:TYR:OH	1:A:102:PHE:HA	2.20	0.41
1:A:157:ILE:CG2	1:A:169:LYS:CD	2.96	0.41
1:B:432:GLN:O	1:B:436:ASP:N	2.34	0.41
1:B:525:ASP:CB	1:B:528:ILE:CD1	2.99	0.41
1:A:334:VAL:HG23	1:A:416:GLU:O	2.20	0.41
1:B:68:ILE:CG1	1:B:69:THR:H	2.26	0.41
1:B:78:PHE:CD1	1:B:81:ARG:NH2	2.88	0.41
1:A:362:GLU:HG2	1:A:362:GLU:H	1.73	0.41
1:A:355:ALA:O	1:A:359:LEU:CB	2.68	0.41
1:B:340:ASP:OD1	1:B:396:GLU:O	2.37	0.41
1:A:222:PHE:CE2	1:A:224:LEU:CD1	3.03	0.41
1:B:525:ASP:CG	1:B:528:ILE:HD12	2.40	0.41
1:B:549:GLN:C	1:B:551:ARG:N	2.74	0.41
1:A:438:ILE:O	1:A:441:TYR:HB3	2.21	0.41
1:B:58:VAL:HG11	1:B:105:SER:HB2	2.03	0.41
1:B:116:LEU:H	1:B:116:LEU:HG	1.64	0.41
1:B:253:ALA:O	1:B:365:ARG:HB3	2.21	0.41
1:A:166:TRP:O	1:A:167:GLN:OE1	2.38	0.41
1:B:541:ARG:HH22	1:B:544:TYR:CB	2.26	0.41
1:A:204:ASN:C	1:A:206:ALA:H	2.24	0.41
1:A:204:ASN:HB3	1:A:205:LYS:H	1.53	0.41
1:A:509:SER:N	1:A:510:PRO:HD3	2.33	0.41
1:A:198:ASN:HA	1:A:199:GLU:HA	1.71	0.41
1:A:157:ILE:HG21	1:A:169:LYS:CD	2.51	0.41
1:B:565:ARG:C	1:B:567:GLN:H	2.24	0.41
1:B:57:HIS:O	1:B:61:VAL:HG13	2.21	0.41
1:B:68:ILE:CG1	1:B:69:THR:N	2.79	0.41
1:A:305:LEU:C	1:A:307:GLY:H	2.24	0.41
1:A:389:LEU:O	1:A:392:LEU:HD23	2.21	0.41
1:B:529:GLY:O	1:B:532:PHE:CB	2.66	0.40
1:B:559:ASP:HB3	1:B:561:TYR:HE2	1.86	0.40
1:A:240:LEU:HD22	1:A:245:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TYR:OH	1:A:120:ARG:CG	2.69	0.40
1:A:234:LEU:H	1:A:234:LEU:HD13	1.87	0.40
1:A:161:PRO:CB	1:B:138:PRO:HB3	2.49	0.40
1:A:134:THR:H	1:A:134:THR:HG23	1.51	0.40
1:A:143:PHE:O	1:A:194:LEU:O	2.39	0.40
1:A:9:ILE:O	1:A:12:THR:HB	2.22	0.40
1:A:474:TYR:CD1	1:A:474:TYR:C	2.95	0.40
1:A:250:PHE:CB	1:A:275:LEU:HD21	2.51	0.40
1:B:334:VAL:HG12	1:B:416:GLU:O	2.21	0.40
1:B:24:PHE:CE1	1:B:50:ARG:HG2	2.56	0.40
1:B:271:LEU:HB2	1:B:283:LEU:HD11	2.02	0.40
1:B:200:LEU:HB3	1:B:208:TRP:O	2.21	0.40
1:B:34:ARG:HA	1:B:34:ARG:HD2	1.93	0.40
1:B:203:ARG:NH2	1:B:254:ARG:CG	2.83	0.40
1:B:425:TRP:CZ3	1:B:429:VAL:HG21	2.56	0.40
1:B:433:GLN:CA	1:B:433:GLN:OE1	2.68	0.40
1:A:172:ASP:OD1	1:A:236:ILE:HB	2.21	0.40
1:B:155:ARG:HA	1:B:155:ARG:HD3	1.91	0.40
1:A:305:LEU:CD1	1:A:305:LEU:N	2.72	0.40
1:B:126:SER:O	1:B:127:GLN:C	2.58	0.40
1:A:229:THR:HB	1:A:233:GLU:CG	2.50	0.40
1:A:516:GLU:O	1:A:517:GLU:C	2.60	0.40
1:A:48:LYS:CG	1:A:362:GLU:HB2	2.45	0.40
1:B:101:SER:HA	1:B:104:ASN:HD22	1.85	0.40
1:B:195:GLN:HB2	1:B:214:ILE:HD11	2.04	0.40
1:A:107:TYR:OH	1:A:120:ARG:HG3	2.21	0.40
1:A:220:LEU:HG	1:A:221:PRO:HD2	1.99	0.40
1:A:226:ILE:HG23	1:A:236:ILE:HG12	2.02	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASN:ND2	1:B:427:GLU:CD[2_455]	1.48	0.72
1:A:423:ASN:CG	1:B:427:GLU:OE2[2_455]	1.55	0.65
1:A:423:ASN:ND2	1:B:427:GLU:OE1[2_455]	1.74	0.46
1:A:423:ASN:ND2	1:B:427:GLU:OE2[2_455]	1.98	0.22
1:A:423:ASN:CG	1:B:427:GLU:CD[2_455]	2.01	0.19
1:A:423:ASN:OD1	1:B:427:GLU:OE2[2_455]	2.09	0.11
1:A:423:ASN:CB	1:B:427:GLU:OE2[2_455]	2.13	0.07

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	541/578 (94%)	470 (87%)	65 (12%)	6 (1%)	17	55
1	B	529/578 (92%)	457 (86%)	68 (13%)	4 (1%)	24	63
All	All	1070/1156 (93%)	927 (87%)	133 (12%)	10 (1%)	21	61

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	GLY
1	A	366	VAL
1	A	511	GLY
1	B	118	PRO
1	B	566	ARG
1	A	264	PRO
1	A	351	ALA
1	B	90	LEU
1	B	216	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	480/508 (94%)	382 (80%)	98 (20%)	1	6
1	B	472/508 (93%)	360 (76%)	112 (24%)	1	3
All	All	952/1016 (94%)	742 (78%)	210 (22%)	1	5

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	17	PHE
1	A	18	ASP
1	A	20	GLN
1	A	25	LEU
1	A	29	SER
1	A	37	GLN
1	A	50	ARG
1	A	58	VAL
1	A	61	VAL
1	A	62	VAL
1	A	65	LEU
1	A	70	ASN
1	A	72	GLN
1	A	78	PHE
1	A	84	GLU
1	A	87	THR
1	A	93	TYR
1	A	114	ARG
1	A	115	SER
1	A	134	THR
1	A	135	ILE
1	A	151	SER
1	A	154	MET
1	A	158	SER
1	A	163	ARG
1	A	167	GLN
1	A	176	ILE
1	A	179	HIS
1	A	181	THR
1	A	189	LEU
1	A	194	LEU
1	A	199	GLU
1	A	209	LEU
1	A	214	ILE
1	A	215	THR
1	A	217	SER
1	A	219	THR
1	A	222	PHE
1	A	234	LEU
1	A	238	THR

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Mol	Chain	Res	Type
1	A	239	CYS
1	A	242	THR
1	A	254	ARG
1	A	263	LEU
1	A	271	LEU
1	A	273	GLU
1	A	279	THR
1	A	280	THR
1	A	290	GLN
1	A	301	TYR
1	A	305	LEU
1	A	308	CYS
1	A	309	ASN
1	A	310	GLU
1	A	322	VAL
1	A	324	LEU
1	A	328	LEU
1	A	331	PHE
1	A	334	VAL
1	A	335	PHE
1	A	337	VAL
1	A	338	ILE
1	A	342	PHE
1	A	349	SER
1	A	361	LYS
1	A	362	GLU
1	A	374	GLU
1	A	378	PHE
1	A	380	LEU
1	A	383	ARG
1	A	386	SER
1	A	392	LEU
1	A	408	ILE
1	A	410	ILE
1	A	416	GLU
1	A	438	ILE
1	A	448	LEU
1	A	458	MET
1	A	461	LYS
1	A	474	TYR
1	A	485	VAL
1	A	521	TRP

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Mol	Chain	Res	Type
1	A	522	LEU
1	A	525	ASP
1	A	532	PHE
1	A	534	GLU
1	A	540	PHE
1	A	541	ARG
1	A	544	TYR
1	A	548	LEU
1	A	549	GLN
1	A	550	ASN
1	A	554	GLU
1	A	557	VAL
1	A	563	TYR
1	A	564	ARG
1	B	3	ARG
1	B	5	LEU
1	B	6	GLU
1	B	7	LEU
1	B	33	GLN
1	B	35	PHE
1	B	44	GLN
1	B	47	MET
1	B	53	LEU
1	B	67	CYS
1	B	72	GLN
1	B	79	LEU
1	B	80	LEU
1	B	81	ARG
1	B	89	LEU
1	B	93	TYR
1	B	95	ARG
1	B	96	PHE
1	B	109	ARG
1	B	112	ASP
1	B	113	HIS
1	B	116	LEU
1	B	117	THR
1	B	121	LEU
1	B	122	PHE
1	B	124	PHE
1	B	134	THR
1	B	136	PRO

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Mol	Chain	Res	Type
1	B	141	LYS
1	B	152	LEU
1	B	158	SER
1	B	159	ASP
1	B	171	ARG
1	B	174	HIS
1	B	189	LEU
1	B	212	LYS
1	B	215	THR
1	B	219	THR
1	B	222	PHE
1	B	223	LEU
1	B	231	ASP
1	B	233	GLU
1	B	241	THR
1	B	243	THR
1	B	245	GLU
1	B	247	SER
1	B	249	VAL
1	B	257	PHE
1	B	258	MET
1	B	263	LEU
1	B	275	LEU
1	B	280	THR
1	B	287	ILE
1	B	290	GLN
1	B	291	LYS
1	B	294	LYS
1	B	295	THR
1	B	299	ARG
1	B	305	LEU
1	B	306	GLN
1	B	309	ASN
1	B	321	MET
1	B	324	LEU
1	B	325	VAL
1	B	329	PRO
1	B	337	VAL
1	B	341	LYS
1	B	352	HIS
1	B	353	VAL
1	B	354	ARG

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Mol	Chain	Res	Type
1	B	356	CYS
1	B	357	TYR
1	B	359	LEU
1	B	360	VAL
1	B	364	ASP
1	B	368	ARG
1	B	372	THR
1	B	376	GLU
1	B	379	VAL
1	B	383	ARG
1	B	392	LEU
1	B	400	LYS
1	B	401	ILE
1	B	402	THR
1	B	404	LEU
1	B	408	ILE
1	B	411	ARG
1	B	413	LEU
1	B	417	ARG
1	B	418	ARG
1	B	420	VAL
1	B	425	TRP
1	B	426	LEU
1	B	427	GLU
1	B	428	GLN
1	B	430	GLU
1	B	433	GLN
1	B	459	LEU
1	B	466	THR
1	B	472	VAL
1	B	474	TYR
1	B	478	GLU
1	B	479	ILE
1	B	485	VAL
1	B	489	ASP
1	B	514	PHE
1	B	516	GLU
1	B	521	TRP
1	B	531	LEU
1	B	538	ASP
1	B	559	ASP
1	B	571	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	33	GLN
1	A	45	GLN
1	A	64	GLN
1	A	72	GLN
1	A	85	HIS
1	A	104	ASN
1	A	165	HIS
1	A	168	ASN
1	A	227	HIS
1	A	292	HIS
1	A	309	ASN
1	A	407	GLN
1	A	447	GLN
1	A	536	HIS
1	A	550	ASN
1	B	32	GLN
1	B	64	GLN
1	B	72	GLN
1	B	168	ASN
1	B	179	HIS
1	B	204	ASN
1	B	228	GLN
1	B	290	GLN
1	B	292	HIS
1	B	309	ASN
1	B	363	HIS
1	B	407	GLN
1	B	412	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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	1762	3	22,29,29	0.86	1 (4%)	27,45,45	2.79	5 (18%)
4	AMP	B	1604	-	20,25,25	1.05	1 (5%)	22,38,38	2.37	6 (27%)

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	1762	3	-	0/12/32/32	0/3/3/3
4	AMP	B	1604	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1762	ADP	C5-C4	2.57	1.46	1.40
4	B	1604	AMP	C5-C4	3.07	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1762	ADP	N3-C2-N1	-8.70	122.23	128.89
2	A	1762	ADP	C2'-C1'-N9	-8.67	101.05	114.29
4	B	1604	AMP	N3-C2-N1	-8.11	122.69	128.89
2	A	1762	ADP	PA-O3A-PB	-4.26	118.39	132.67
4	B	1604	AMP	C4-C5-N7	-3.91	105.88	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1604	AMP	C2'-C1'-N9	-3.74	108.58	114.29
2	A	1762	ADP	C4-C5-N7	-3.15	106.58	109.48
2	A	1762	ADP	C1'-N9-C4	-2.49	123.18	126.94
4	B	1604	AMP	C1'-N9-C4	-2.07	123.81	126.94
4	B	1604	AMP	O3P-P-O2P	2.03	115.10	107.38
4	B	1604	AMP	O4'-C1'-N9	2.27	112.85	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1762	ADP	5	0
4	B	1604	AMP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	547/578 (94%)	-0.23	3 (0%) 91 83	2, 15, 29, 37	0
1	B	539/578 (93%)	-0.16	0 100 100	4, 18, 28, 34	0
All	All	1086/1156 (93%)	-0.19	3 (0%) 94 88	2, 17, 29, 37	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	THR	3.4
1	A	158	SER	2.3
1	A	146	ASP	2.3

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(\AA^2)	Q<0.9
2	ADP	A	1762	27/27	0.95	0.15	-0.90	6,10,11,12	0
4	AMP	B	1604	23/23	0.93	0.17	-1.26	23,25,31,34	0
3	MG	A	579	1/1	0.98	0.20	-	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.