



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YP3
Title : Crystal structure of potato tuber ADP-glucose pyrophosphorylase in complex with ATP
Authors : Jin, X.; Ballicora, M.A.; Preiss, J.; Geiger, J.H.
Deposited on : 2005-01-29
Resolution : 2.60 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

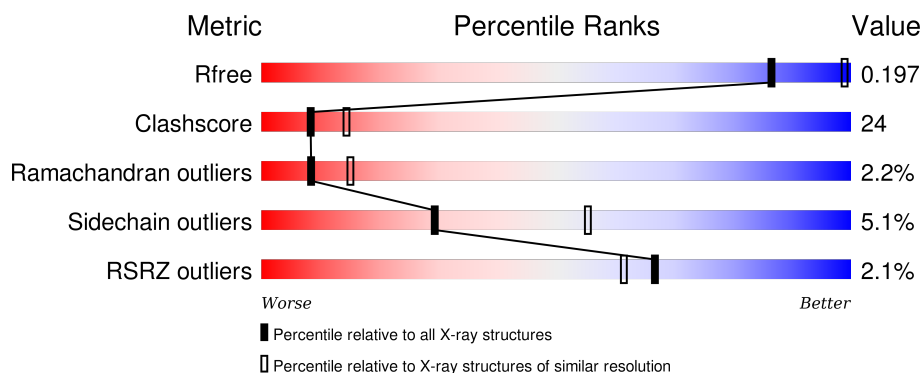
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	451	 53% 39% 2% 5% 2%
1	B	451	 50% 42% 2% 2% 4%
1	C	451	 62% 34% 2% 2% 2%
1	D	451	 42% 47% 5% 5% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13765 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 Glucose-1-phosphate adenylyltransferase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3369	2143	570	640	16			
1	B	432	Total	C	N	O	S	0	0	0
			3340	2120	568	636	16			
1	C	435	Total	C	N	O	S	0	0	0
			3380	2149	572	643	16			
1	D	425	Total	C	N	O	S	0	0	0
			3295	2096	558	626	15			

There are 4 discrepancies between the modelled and reference sequences:

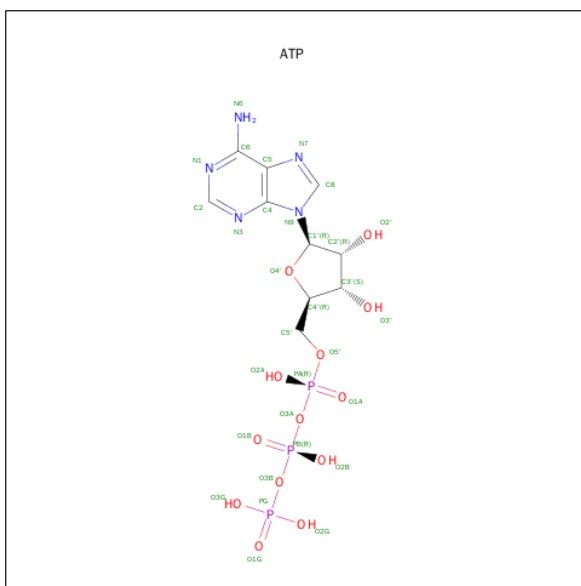
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P23509
B	1	MET	-	INITIATING METHIONINE	UNP P23509
C	1	MET	-	INITIATING METHIONINE	UNP P23509
D	1	MET	-	INITIATING METHIONINE	UNP P23509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$$\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3).$$


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

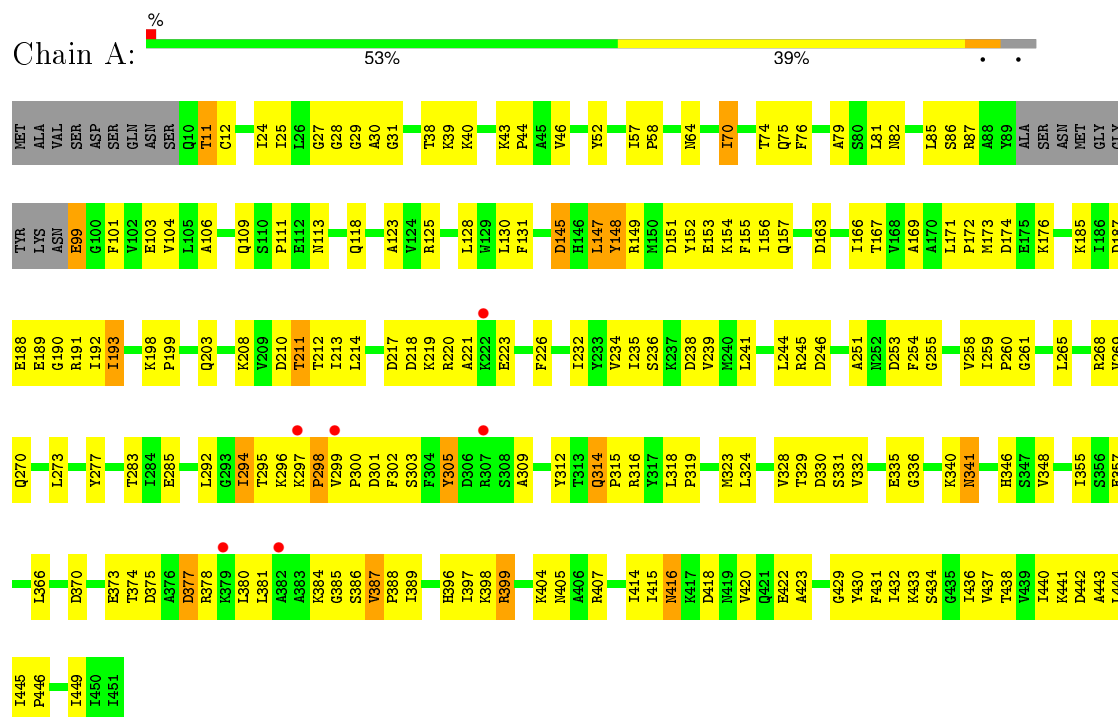
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0
4	B	58	Total O 58 58	0	0
4	C	97	Total O 97 97	0	0
4	D	33	Total O 33 33	0	0

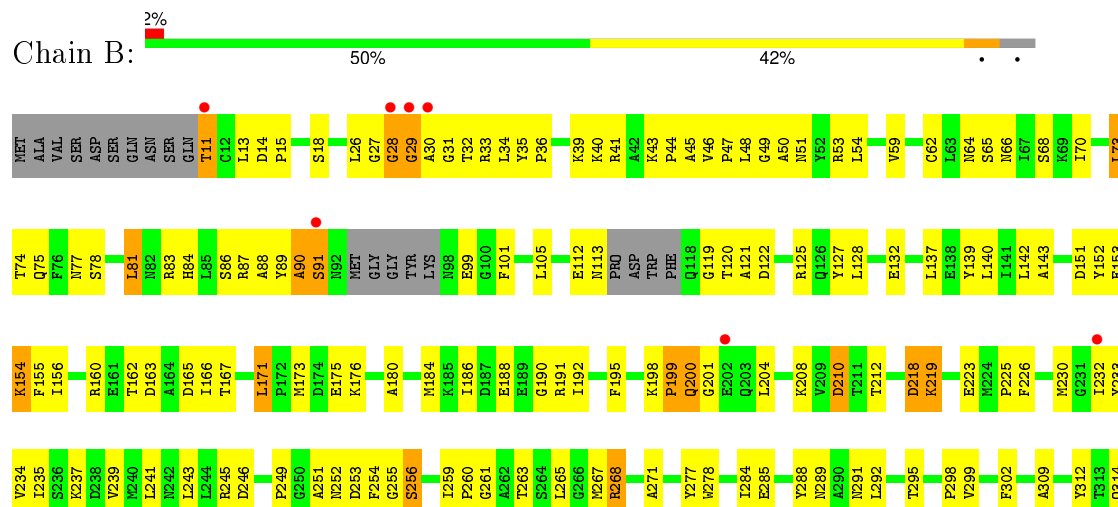
3 Residue-property plots

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: Glucose-1-phosphate adenylyltransferase small subunit



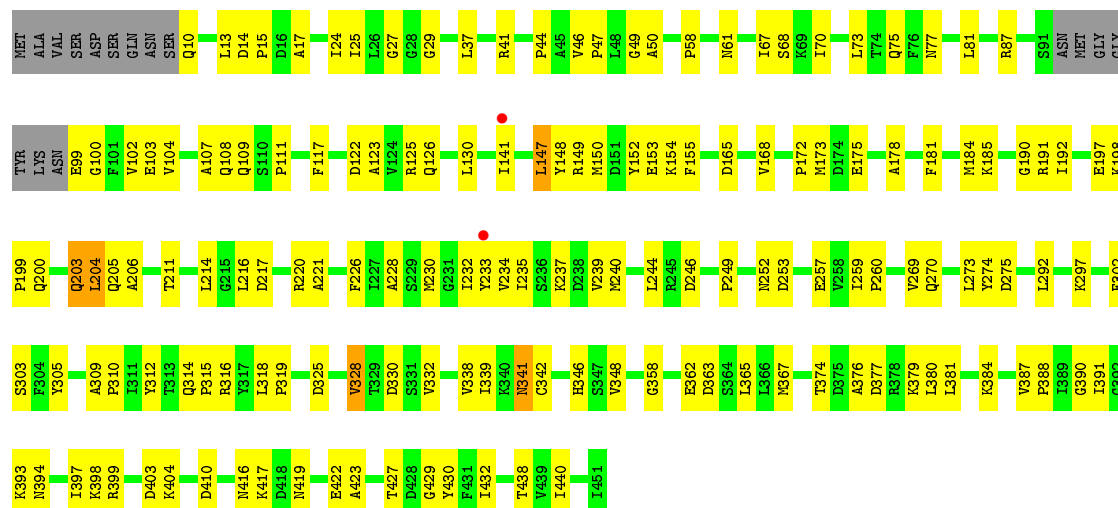
- Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit





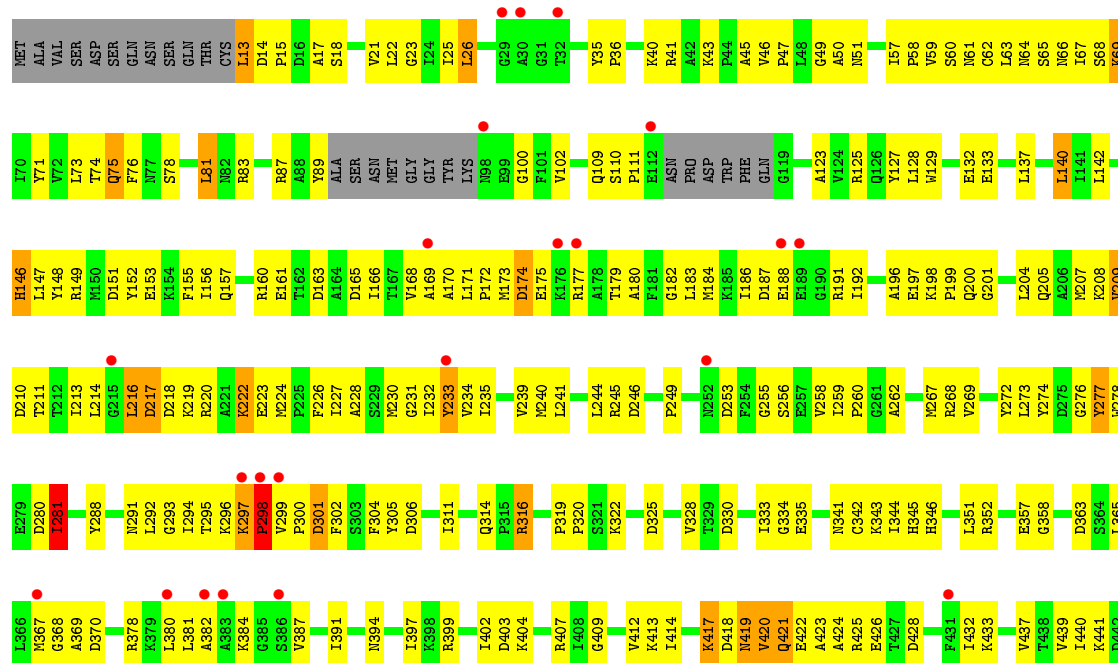
• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

Chain C: 62% 34%



• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

Chain D: 5% 42% 47% 5% 6%



I443	I444	I445	P446	I449	I450	I451
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.58Å 142.96Å 90.44Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 26.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.97-2.60) 99.8 (26.14-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.175 , 0.255 0.204 , 0.197	Depositor DCC
R_{free} test set	2886 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.4	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 56946 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13765	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: SO4, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3433	0.64	0/4646
1	B	0.36	0/3399	0.63	0/4597
1	C	0.38	0/3444	0.66	0/4661
1	D	0.34	0/3354	0.60	0/4535
All	All	0.36	0/13630	0.63	0/18439

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	TYR	Sidechain
1	B	430	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	3369	0	3380	159	0
1	B	3340	0	3356	165	0
1	C	3380	0	3390	122	0
1	D	3295	0	3318	227	0
2	A	20	0	0	0	0
2	B	15	0	0	2	0
2	C	20	0	0	1	0
2	D	10	0	0	1	0
3	A	31	0	12	3	0
3	C	31	0	12	0	0
4	A	66	0	0	3	0
4	B	58	0	0	3	0
4	C	97	0	0	7	0
4	D	33	0	0	4	0
All	All	13765	0	13468	654	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 24.

All (654) 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:D:297:LYS:HB3	1:D:298:PRO:HD2	1.10	1.09
1:C:211:THR:HG21	1:C:216:LEU:HD22	1.39	1.04
1:D:420:VAL:HG12	1:D:421:GLN:H	1.24	0.98
1:D:22:LEU:HD22	1:D:69:LYS:HB3	1.48	0.95
1:D:297:LYS:HB3	1:D:298:PRO:CD	2.01	0.91
1:D:297:LYS:CB	1:D:298:PRO:HD2	2.01	0.91
1:B:33:ARG:HB2	1:B:33:ARG:HH11	1.36	0.90
1:A:341:ASN:HB3	1:A:357:GLU:OE2	1.71	0.90
1:D:146:HIS:HB3	1:D:280:ASP:HA	1.53	0.90
1:D:422:GLU:HG3	1:D:433:LYS:HD2	1.55	0.89
1:B:192:ILE:HD11	1:B:271:ALA:HB2	1.55	0.87
1:D:367:MET:HG3	1:D:403:ASP:HA	1.57	0.86
1:B:243:LEU:HD21	1:B:267:MET:HE1	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:H	1:A:113:ASN:HD21	1.24	0.84
1:D:387:VAL:HG23	1:D:407:ARG:HB3	1.56	0.84
1:D:173:MET:HA	1:D:224:MET:HE1	1.58	0.83
1:C:316:ARG:HB3	1:C:318:LEU:HD13	1.59	0.82
1:C:259:ILE:HB	1:C:260:PRO:HD3	1.61	0.82
1:D:240:MET:HE1	4:D:1037:HOH:O	1.78	0.82
1:B:40:LYS:HD2	1:B:441:LYS:HB3	1.62	0.82
1:C:367:MET:HG3	1:C:403:ASP:HA	1.58	0.82
1:D:200:GLN:HA	1:D:204:LEU:HD12	1.62	0.81
1:B:259:ILE:HB	1:B:260:PRO:HD3	1.62	0.81
1:D:246:ASP:O	1:D:249:PRO:HD3	1.81	0.81
1:D:241:LEU:O	1:D:245:ARG:HG2	1.80	0.81
1:D:214:LEU:HB3	1:D:273:LEU:HB2	1.64	0.80
1:A:99:GLU:N	1:D:87:ARG:HH22	1.80	0.80
1:D:449:ILE:HD13	1:D:450:ILE:H	1.48	0.79
1:D:216:LEU:HD22	1:D:220:ARG:HG2	1.62	0.78
1:A:399:ARG:HH21	1:A:399:ARG:HG2	1.48	0.78
1:A:259:ILE:HB	1:A:260:PRO:HD3	1.65	0.77
1:A:295:THR:HG22	1:A:332:VAL:HG13	1.67	0.77
1:A:147:LEU:O	1:A:148:TYR:HB3	1.82	0.77
1:D:296:LYS:CG	1:D:300:PRO:HA	2.15	0.77
1:B:28:GLY:HA3	1:B:74:THR:HA	1.66	0.76
1:A:82:ASN:O	1:A:86:SER:HB2	1.84	0.76
1:A:378:ARG:HG2	1:A:378:ARG:HH21	1.51	0.76
1:C:125:ARG:HD2	4:C:1077:HOH:O	1.85	0.76
1:B:33:ARG:HB2	1:B:33:ARG:NH1	2.01	0.76
1:C:384:LYS:HA	1:C:384:LYS:HE2	1.68	0.76
1:A:128:LEU:HD21	1:A:241:LEU:HA	1.69	0.75
1:A:99:GLU:HB3	1:D:87:ARG:HH12	1.50	0.75
1:A:152:TYR:O	1:A:156:ILE:HG12	1.85	0.75
1:C:77:ASN:HD22	1:C:109:GLN:NE2	1.85	0.74
1:A:423:ALA:HB3	1:A:432:ILE:HB	1.68	0.74
1:B:40:LYS:HG3	1:B:441:LYS:HD3	1.70	0.74
1:A:155:PHE:CE2	1:A:234:VAL:HG23	2.23	0.74
1:C:149:ARG:NH1	1:C:303:SER:O	2.21	0.73
1:C:346:HIS:O	1:C:363:ASP:HA	1.88	0.73
1:B:261:GLY:O	1:B:265:LEU:HD13	1.87	0.73
1:D:425:ARG:HB3	1:D:428:ASP:HB2	1.71	0.73
1:D:132:GLU:HG2	1:D:241:LEU:HD21	1.70	0.72
1:D:22:LEU:HD13	1:D:23:GLY:N	2.04	0.72
1:D:273:LEU:HD13	1:D:274:TYR:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LYS:HA	1:D:219:LYS:HE2	1.70	0.72
1:B:26:LEU:HD22	1:B:143:ALA:HB2	1.70	0.72
1:B:420:VAL:HG12	1:B:421:GLN:H	1.53	0.72
1:B:35:TYR:OH	1:B:39:LYS:HE2	1.90	0.71
1:C:211:THR:CG2	1:C:216:LEU:HD22	2.19	0.71
1:D:75:GLN:HA	1:D:75:GLN:HE21	1.56	0.71
1:B:43:LYS:O	1:B:46:VAL:HG23	1.90	0.71
1:C:24:ILE:HB	1:C:141:ILE:HD13	1.73	0.71
1:D:449:ILE:CD1	1:D:450:ILE:H	2.04	0.70
1:D:43:LYS:O	1:D:46:VAL:HG23	1.91	0.70
1:D:41:ARG:HH12	1:D:441:LYS:HD2	1.56	0.70
1:B:127:TYR:CZ	1:C:109:GLN:HG2	2.26	0.70
1:A:189:GLU:OE2	1:A:189:GLU:HA	1.92	0.70
1:D:155:PHE:CZ	1:D:234:VAL:HG23	2.26	0.69
1:B:376:ALA:O	1:B:380:LEU:HD22	1.92	0.69
1:D:420:VAL:HG12	1:D:421:GLN:N	2.04	0.69
1:D:173:MET:SD	1:D:177:ARG:HB3	2.32	0.69
1:A:166:ILE:HG12	1:A:235:ILE:HG12	1.74	0.69
1:C:230:MET:HE2	1:C:232:ILE:HD12	1.74	0.69
1:A:25:ILE:HD12	1:A:70:ILE:HD13	1.75	0.69
1:B:351:LEU:H	1:B:351:LEU:HD23	1.56	0.69
1:D:166:ILE:HG21	1:D:259:ILE:HD12	1.76	0.68
1:C:390:GLY:HA2	4:C:1116:HOH:O	1.93	0.68
1:C:391:ILE:HD12	1:C:397:ILE:HD12	1.75	0.68
1:D:68:SER:HB3	1:D:100:GLY:HA3	1.75	0.68
1:D:51:ASN:HD21	1:D:335:GLU:H	1.41	0.68
1:D:300:PRO:O	1:D:301:ASP:HB2	1.93	0.67
1:A:397:ILE:HD12	1:A:414:ILE:HD12	1.76	0.67
1:B:323:MET:CE	1:B:333:ILE:HD13	2.25	0.67
1:B:128:LEU:HD11	1:B:241:LEU:HD12	1.75	0.67
1:A:171:LEU:HD23	1:A:173:MET:CE	2.25	0.67
1:A:185:LYS:O	1:A:193:ILE:HD13	1.94	0.67
1:C:13:LEU:H	1:C:13:LEU:HD22	1.60	0.67
1:B:31:GLY:H	1:B:33:ARG:HH22	1.44	0.66
1:A:340:LYS:HG2	1:A:355:ILE:O	1.95	0.66
1:D:370:ASP:OD1	1:D:404:LYS:HD3	1.95	0.66
1:B:387:VAL:HG11	1:B:409:GLY:HA2	1.75	0.66
1:B:341:ASN:OD1	1:B:357:GLU:HG3	1.96	0.66
1:D:87:ARG:HB3	1:D:314:GLN:HG3	1.78	0.66
1:D:26:LEU:N	1:D:26:LEU:HD12	2.11	0.65
1:C:339:ILE:HG23	1:C:342:CYS:SG	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:MET:CG	1:D:403:ASP:HA	2.26	0.65
1:D:235:ILE:HG21	1:D:240:MET:HB2	1.79	0.65
1:D:165:ASP:HB3	1:D:239:VAL:HG21	1.78	0.65
1:B:323:MET:HE2	1:B:333:ILE:HD13	1.78	0.65
1:A:328:VAL:CG1	1:A:331:SER:HB2	2.26	0.65
1:D:255:GLY:O	1:D:260:PRO:HD3	1.96	0.64
1:C:305:TYR:HB2	1:D:319:PRO:HD3	1.78	0.64
1:D:218:ASP:O	1:D:222:LYS:HD3	1.97	0.64
1:D:125:ARG:HA	1:D:128:LEU:HG	1.80	0.64
1:B:78:SER:HB3	1:B:81:LEU:HB2	1.79	0.64
1:A:149:ARG:NH1	1:A:303:SER:O	2.31	0.64
1:A:40:LYS:H	1:A:113:ASN:ND2	1.96	0.63
1:A:414:ILE:CG2	1:A:437:VAL:HG11	2.27	0.63
1:D:277:TYR:CD2	1:D:302:PHE:HB2	2.33	0.63
1:B:288:TYR:O	1:B:292:LEU:HD23	1.99	0.63
1:D:291:ASN:O	1:D:294:ILE:HG12	1.98	0.63
1:A:330:ASP:O	1:A:346:HIS:HA	1.98	0.63
1:C:77:ASN:HD22	1:C:109:GLN:HE22	1.43	0.63
1:A:31:GLY:HA3	1:A:38:THR:HG21	1.78	0.63
1:A:29:GLY:HA2	1:A:75:GLN:HB2	1.79	0.63
1:B:420:VAL:HG12	1:B:421:GLN:N	2.14	0.63
1:D:299:VAL:HG12	1:D:301:ASP:H	1.64	0.63
1:D:417:LYS:HB2	1:D:417:LYS:NZ	2.13	0.63
1:B:208:LYS:HG3	1:B:225:PRO:HB2	1.81	0.62
1:D:231:GLY:C	1:D:232:ILE:HD12	2.19	0.62
1:A:324:LEU:O	1:B:329:THR:HA	2.00	0.62
1:A:446:PRO:O	1:A:449:ILE:HG12	1.99	0.62
1:B:49:GLY:O	1:B:50:ALA:HB3	1.98	0.62
1:D:157:GLN:O	1:D:161:GLU:HG3	1.99	0.62
1:D:296:LYS:HG2	1:D:300:PRO:HA	1.82	0.62
1:D:174:ASP:CG	1:D:175:GLU:H	2.02	0.62
1:C:27:GLY:HA3	1:C:44:PRO:HG3	1.80	0.62
1:B:73:LEU:HD12	1:B:105:LEU:HB2	1.82	0.62
1:A:99:GLU:HB2	4:D:1013:HOH:O	1.99	0.62
1:A:163:ASP:O	1:A:268:ARG:HD2	1.99	0.62
1:A:43:LYS:O	1:A:46:VAL:HG23	2.00	0.62
1:A:384:LYS:HD2	1:A:384:LYS:O	2.00	0.62
1:C:297:LYS:HD2	1:C:330:ASP:OD1	2.00	0.61
1:A:40:LYS:HB3	1:A:40:LYS:NZ	2.15	0.61
1:A:416:ASN:HD21	1:A:420:VAL:H	1.48	0.61
1:B:31:GLY:H	1:B:33:ARG:NH2	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HD12	1:D:13:LEU:N	2.14	0.61
1:D:75:GLN:HA	1:D:75:GLN:NE2	2.14	0.61
1:C:150:MET:HE3	1:C:232:ILE:HD13	1.81	0.61
1:B:199:PRO:HG2	1:B:204:LEU:HD13	1.82	0.61
1:D:21:VAL:HG21	1:D:156:ILE:HD13	1.82	0.61
1:D:235:ILE:CG2	1:D:240:MET:HB2	2.31	0.61
1:C:24:ILE:HB	1:C:141:ILE:CD1	2.31	0.61
1:B:298:PRO:HG2	1:B:299:VAL:HG23	1.83	0.61
1:B:325:ASP:HB3	1:B:341:ASN:HB3	1.83	0.60
1:D:180:ALA:O	1:D:198:LYS:HG2	2.00	0.60
1:D:173:MET:HA	1:D:224:MET:CE	2.30	0.60
1:A:323:MET:SD	1:B:328:VAL:HG21	2.41	0.60
1:A:99:GLU:CB	1:D:87:ARG:HH12	2.15	0.60
1:C:332:VAL:HG13	1:D:320:PRO:HB2	1.82	0.60
1:D:184:MET:SD	1:D:192:ILE:HD13	2.41	0.60
1:B:192:ILE:CD1	1:B:271:ALA:HB2	2.31	0.60
1:D:450:ILE:HG22	1:D:451:ILE:N	2.17	0.60
1:C:155:PHE:CE2	1:C:234:VAL:HG23	2.36	0.60
1:D:168:VAL:HG13	1:D:233:TYR:CD2	2.37	0.60
1:D:75:GLN:CA	1:D:75:GLN:HE21	2.14	0.60
1:D:110:SER:OG	1:D:111:PRO:HD2	2.00	0.60
1:A:430:TYR:HA	1:A:440:ILE:HG13	1.84	0.60
1:C:185:LYS:HE2	1:C:206:ALA:O	2.01	0.60
1:C:203:GLN:HG2	4:C:1096:HOH:O	2.01	0.60
1:C:117:PHE:HA	4:C:1035:HOH:O	2.01	0.60
1:D:41:ARG:NE	1:D:47:PRO:HD3	2.16	0.59
1:D:220:ARG:HG2	1:D:220:ARG:HH11	1.67	0.59
1:C:319:PRO:HD3	1:D:305:TYR:HB2	1.83	0.59
1:B:30:ALA:HB1	1:B:43:LYS:NZ	2.18	0.59
1:A:414:ILE:HG23	1:A:437:VAL:HG11	1.84	0.59
1:D:73:LEU:N	1:D:73:LEU:HD12	2.18	0.59
1:B:152:TYR:O	1:B:156:ILE:HG12	2.03	0.59
1:D:345:HIS:HB3	4:D:1033:HOH:O	2.02	0.59
1:C:380:LEU:HD22	1:C:380:LEU:H	1.66	0.59
1:B:219:LYS:HE2	1:B:223:GLU:OE1	2.03	0.59
1:B:34:LEU:HD12	1:B:43:LYS:HE3	1.84	0.59
1:B:112:GLU:O	1:B:113:ASN:CB	2.51	0.59
1:D:413:LYS:HB2	1:D:450:ILE:HG23	1.84	0.58
1:D:365:LEU:HD21	1:D:367:MET:HE1	1.85	0.58
1:A:277:TYR:CD2	1:A:302:PHE:HB2	2.38	0.58
1:A:255:GLY:HA2	1:A:259:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ARG:HG2	4:D:1038:HOH:O	2.03	0.58
1:A:377:ASP:O	1:A:381:LEU:HG	2.04	0.58
1:D:137:LEU:HD12	1:D:160:ARG:NH2	2.18	0.58
1:D:277:TYR:CD1	1:D:301:ASP:HB3	2.38	0.57
1:B:199:PRO:HG2	1:B:204:LEU:CD1	2.35	0.57
1:C:330:ASP:O	1:C:346:HIS:HA	2.03	0.57
1:D:352:ARG:HD2	1:D:369:ALA:O	2.04	0.57
1:A:318:LEU:HD12	1:A:335:GLU:HG3	1.86	0.57
1:D:76:PHE:CD2	1:D:111:PRO:HA	2.40	0.57
1:D:41:ARG:HE	1:D:47:PRO:HD3	1.70	0.57
1:C:391:ILE:HD12	1:C:397:ILE:CD1	2.34	0.57
1:B:120:THR:OG1	1:B:253:ASP:HA	2.05	0.56
1:B:416:ASN:OD1	1:B:420:VAL:HG23	2.05	0.56
1:B:151:ASP:OD2	1:B:153:GLU:HB2	2.05	0.56
1:D:22:LEU:CD2	1:D:69:LYS:HB3	2.30	0.56
1:D:102:VAL:HG13	1:D:102:VAL:O	2.05	0.56
1:B:358:GLY:O	1:B:394:ASN:HA	2.06	0.56
1:A:145:ASP:HB2	3:A:757:ATP:O3'	2.05	0.56
1:B:88:ALA:HB2	1:B:314:GLN:HA	1.86	0.56
1:A:214:LEU:HB3	1:A:273:LEU:HB2	1.88	0.56
1:C:381:LEU:HD23	1:C:388:PRO:HA	1.88	0.56
1:B:40:LYS:O	1:B:41:ARG:HB3	2.06	0.55
1:D:387:VAL:HG11	1:D:409:GLY:CA	2.36	0.55
1:D:449:ILE:HG23	1:D:450:ILE:N	2.21	0.55
1:A:25:ILE:CD1	1:A:70:ILE:HD13	2.36	0.55
1:B:446:PRO:HD2	1:B:449:ILE:HD12	1.87	0.55
1:D:41:ARG:NH1	1:D:441:LYS:HD2	2.20	0.55
1:B:128:LEU:O	1:B:132:GLU:HG2	2.06	0.55
1:D:17:ALA:HB1	1:D:67:ILE:HD13	1.88	0.55
1:C:150:MET:HE2	1:C:274:TYR:CE2	2.42	0.55
1:A:149:ARG:NH2	1:A:309:ALA:O	2.38	0.55
1:D:232:ILE:HD12	1:D:232:ILE:N	2.22	0.55
1:D:14:ASP:HA	1:D:15:PRO:C	2.27	0.55
1:B:119:GLY:O	1:B:122:ASP:HB2	2.07	0.55
1:D:128:LEU:O	1:D:132:GLU:HG3	2.07	0.55
1:A:378:ARG:CG	1:A:378:ARG:HH21	2.19	0.55
1:B:30:ALA:HB3	1:B:43:LYS:HD2	1.89	0.55
1:C:253:ASP:O	1:C:257:GLU:HB2	2.07	0.55
1:A:370:ASP:H	1:A:405:ASN:HD21	1.53	0.55
1:C:191:ARG:HG2	1:C:191:ARG:HH21	1.71	0.55
1:C:246:ASP:O	1:C:249:PRO:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LYS:HG2	1:A:298:PRO:HD2	1.89	0.54
1:C:103:GLU:HG3	1:C:104:VAL:N	2.21	0.54
1:B:155:PHE:HE1	1:B:167:THR:HG22	1.73	0.54
1:B:139:TYR:CE1	1:B:237:LYS:HA	2.42	0.54
1:A:192:ILE:HD12	1:A:269:VAL:HG12	1.88	0.54
1:D:253:ASP:O	1:D:258:VAL:HG23	2.08	0.54
1:A:171:LEU:HD23	1:A:173:MET:HE1	1.90	0.54
1:A:405:ASN:N	1:A:405:ASN:ND2	2.54	0.54
1:C:348:VAL:HB	1:C:365:LEU:HD12	1.90	0.54
1:B:64:ASN:ND2	1:B:312:TYR:OH	2.40	0.54
1:A:154:LYS:NZ	1:A:157:GLN:HE22	2.05	0.54
1:D:346:HIS:O	1:D:363:ASP:HA	2.08	0.54
1:B:89:TYR:O	1:B:91:SER:N	2.41	0.53
1:C:305:TYR:CB	1:D:319:PRO:HD3	2.38	0.53
1:A:444:LEU:HD23	1:A:444:LEU:C	2.28	0.53
1:C:376:ALA:O	1:C:379:LYS:HB3	2.08	0.53
1:C:310:PRO:HG2	1:C:312:TYR:CE2	2.44	0.53
1:A:27:GLY:CA	1:A:44:PRO:HG3	2.39	0.53
1:D:397:ILE:HG21	1:D:402:ILE:HD11	1.89	0.53
1:A:25:ILE:HD12	1:A:70:ILE:CD1	2.37	0.53
1:A:283:THR:HG22	1:A:285:GLU:N	2.23	0.53
1:B:137:LEU:HD12	1:B:160:ARG:NH2	2.24	0.53
1:D:89:TYR:HB2	1:D:102:VAL:HG11	1.91	0.53
1:D:399:ARG:HG2	1:D:399:ARG:O	2.09	0.53
1:D:146:HIS:HA	1:D:281:ILE:HG12	1.91	0.53
1:A:125:ARG:NH1	1:A:251:ALA:O	2.42	0.53
1:B:328:VAL:HA	1:B:344:ILE:O	2.09	0.53
1:D:343:LYS:O	1:D:344:ILE:HD13	2.08	0.53
1:A:28:GLY:O	1:A:74:THR:HA	2.09	0.52
1:A:405:ASN:HD22	1:A:405:ASN:N	2.06	0.52
1:A:199:PRO:HB3	1:A:203:GLN:HG3	1.91	0.52
1:D:288:TYR:O	1:D:292:LEU:HD22	2.08	0.52
1:A:29:GLY:O	1:A:30:ALA:HB3	2.09	0.52
1:A:283:THR:HG22	1:A:285:GLU:H	1.74	0.52
1:B:51:ASN:ND2	1:B:335:GLU:HG2	2.23	0.52
1:C:13:LEU:HD22	1:C:13:LEU:N	2.23	0.52
1:D:294:ILE:HG21	1:D:304:PHE:HE1	1.74	0.52
1:D:387:VAL:HG11	1:D:409:GLY:HA3	1.92	0.52
1:A:305:TYR:HB2	1:B:319:PRO:HD3	1.92	0.52
1:D:169:ALA:HB3	1:D:230:MET:HB2	1.92	0.52
1:A:57:ILE:HB	1:A:58:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HD21	1:C:302:PHE:CE2	2.44	0.52
1:B:184:MET:HE2	1:B:192:ILE:HG21	1.91	0.52
1:A:255:GLY:HA2	1:A:259:ILE:CG1	2.39	0.52
1:B:29:GLY:HA2	1:B:75:GLN:HG2	1.92	0.52
1:B:83:ARG:O	1:B:87:ARG:HB2	2.09	0.52
1:A:373:GLU:OE2	1:A:407:ARG:NH1	2.38	0.52
1:A:375:ASP:O	1:A:378:ARG:HB3	2.10	0.52
1:C:168:VAL:HG11	1:C:184:MET:HE1	1.92	0.52
1:D:78:SER:HB3	1:D:81:LEU:HB2	1.91	0.52
1:A:399:ARG:NH2	1:A:399:ARG:HG2	2.22	0.52
1:D:174:ASP:CG	1:D:175:GLU:N	2.62	0.52
1:C:147:LEU:O	1:C:148:TYR:HB3	2.09	0.52
1:A:70:ILE:O	1:A:70:ILE:HG13	2.09	0.51
1:D:149:ARG:HB2	1:D:149:ARG:NH2	2.24	0.51
1:B:62:CYS:CB	1:B:70:ILE:HD11	2.40	0.51
1:D:168:VAL:HG13	1:D:233:TYR:HD2	1.74	0.51
1:A:24:ILE:HD12	1:A:131:PHE:CZ	2.46	0.51
1:C:68:SER:HB2	1:C:100:GLY:HA3	1.92	0.51
1:B:86:SER:O	1:B:90:ALA:HB3	2.11	0.51
1:B:444:LEU:O	1:B:446:PRO:HD3	2.11	0.51
1:B:370:ASP:OD1	1:B:404:LYS:HE2	2.11	0.51
1:D:417:LYS:HB2	1:D:417:LYS:HZ2	1.76	0.51
1:D:132:GLU:HG2	1:D:241:LEU:CD2	2.39	0.51
1:A:153:GLU:O	1:A:157:GLN:HB2	2.10	0.51
1:C:150:MET:HE3	1:C:232:ILE:CD1	2.40	0.51
1:C:348:VAL:HB	1:C:365:LEU:CD1	2.41	0.51
1:C:29:GLY:HA2	1:C:75:GLN:HB2	1.93	0.51
1:D:298:PRO:O	1:D:300:PRO:HD3	2.11	0.51
1:D:292:LEU:H	1:D:292:LEU:HD22	1.76	0.51
1:A:101:PHE:HD1	1:A:103:GLU:HG3	1.76	0.51
1:B:101:PHE:CD1	1:B:101:PHE:C	2.84	0.50
1:A:314:GLN:O	1:A:316:ARG:HG3	2.11	0.50
1:A:245:ARG:HD2	1:A:246:ASP:OD1	2.11	0.50
1:D:36:PRO:HB2	1:D:440:ILE:HG13	1.92	0.50
1:D:391:ILE:HD12	1:D:391:ILE:N	2.26	0.50
1:D:378:ARG:O	1:D:381:LEU:HB2	2.11	0.50
1:D:417:LYS:HG3	1:D:418:ASP:H	1.77	0.50
1:B:27:GLY:O	1:B:29:GLY:N	2.45	0.50
1:D:179:THR:OG1	1:D:200:GLN:HG2	2.11	0.50
1:B:68:SER:N	4:B:1059:HOH:O	2.43	0.50
1:B:387:VAL:HG23	1:B:444:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ILE:C	1:D:26:LEU:HD12	2.32	0.50
1:C:387:VAL:HG12	1:C:388:PRO:O	2.12	0.50
1:D:256:SER:O	1:D:260:PRO:HG2	2.12	0.50
1:B:14:ASP:HA	1:B:15:PRO:C	2.31	0.50
1:B:32:THR:HG22	4:B:1045:HOH:O	2.11	0.50
1:B:232:ILE:O	1:B:232:ILE:HG13	2.11	0.50
1:D:73:LEU:HD23	1:D:123:ALA:HB1	1.92	0.50
1:B:230:MET:HE2	1:B:278:TRP:CZ3	2.47	0.50
1:C:25:ILE:HD13	1:C:58:PRO:HB2	1.92	0.50
1:B:336:GLY:O	1:B:352:ARG:HA	2.12	0.50
1:B:328:VAL:HG12	1:B:344:ILE:HB	1.93	0.50
1:B:330:ASP:O	1:B:346:HIS:HA	2.12	0.49
1:D:219:LYS:O	1:D:223:GLU:HG3	2.13	0.49
1:A:298:PRO:HG2	1:A:299:VAL:H	1.77	0.49
1:A:422:GLU:OE2	1:A:433:LYS:HD2	2.11	0.49
1:D:322:LYS:HB3	1:D:322:LYS:NZ	2.27	0.49
1:B:31:GLY:C	1:B:33:ARG:H	2.14	0.49
1:D:450:ILE:HG22	1:D:451:ILE:H	1.77	0.49
1:A:396:HIS:C	1:A:397:ILE:HD13	2.32	0.49
1:C:200:GLN:O	1:C:203:GLN:HB3	2.12	0.49
1:C:190:GLY:C	1:C:270:GLN:NE2	2.66	0.49
1:C:429:GLY:C	1:C:440:ILE:HD12	2.33	0.49
1:C:367:MET:CG	1:C:403:ASP:HA	2.37	0.49
1:C:217:ASP:OD1	1:C:220:ARG:HD3	2.13	0.49
1:B:285:GLU:HG2	1:B:289:ASN:ND2	2.28	0.49
1:A:40:LYS:N	1:A:113:ASN:HD21	2.03	0.49
1:D:214:LEU:CD1	1:D:227:ILE:HG21	2.42	0.49
1:D:424:ALA:O	1:D:425:ARG:HG2	2.12	0.49
1:B:246:ASP:O	1:B:249:PRO:HD3	2.12	0.49
1:C:328:VAL:HG22	1:C:328:VAL:O	2.12	0.49
1:A:380:LEU:HD23	1:A:380:LEU:C	2.32	0.49
1:B:260:PRO:O	1:B:263:THR:HB	2.12	0.49
1:B:295:THR:HG22	1:B:332:VAL:HG13	1.94	0.49
1:C:362:GLU:O	1:C:398:LYS:HA	2.12	0.49
1:A:219:LYS:C	1:A:221:ALA:H	2.16	0.49
1:B:34:LEU:HD12	1:B:43:LYS:CE	2.42	0.48
1:C:319:PRO:HD3	1:D:305:TYR:CB	2.43	0.48
1:C:197:GLU:OE2	1:C:198:LYS:HG3	2.13	0.48
1:A:433:LYS:HB2	4:A:1083:HOH:O	2.13	0.48
1:B:30:ALA:HB1	1:B:43:LYS:HZ2	1.78	0.48
1:A:446:PRO:HD2	1:A:449:ILE:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ASP:HA	1:B:378:ARG:NH2	2.28	0.48
1:D:140:LEU:HD22	1:D:142:LEU:HG	1.95	0.48
1:A:441:LYS:O	1:A:442:ASP:HB2	2.14	0.48
1:C:173:MET:SD	1:C:178:ALA:HA	2.53	0.48
1:D:186:ILE:HA	1:D:191:ARG:O	2.12	0.48
1:D:418:ASP:O	1:D:420:VAL:N	2.46	0.48
1:D:175:GLU:OE1	1:D:175:GLU:HA	2.13	0.48
1:D:62:CYS:HB3	1:D:67:ILE:HB	1.95	0.48
1:A:151:ASP:OD1	1:A:153:GLU:HB2	2.13	0.48
1:B:121:ALA:N	1:B:252:ASN:O	2.47	0.48
1:D:83:ARG:O	1:D:87:ARG:HB2	2.14	0.48
1:D:304:PHE:O	1:D:311:ILE:HG12	2.14	0.48
1:B:396:HIS:C	1:B:397:ILE:HD12	2.34	0.48
1:B:165:ASP:HB3	1:B:239:VAL:HG21	1.96	0.48
1:A:429:GLY:O	1:A:430:TYR:HB3	2.14	0.48
1:B:440:ILE:HG22	1:B:441:LYS:N	2.29	0.48
1:C:339:ILE:N	1:C:339:ILE:HD12	2.29	0.48
1:A:217:ASP:HB3	1:A:220:ARG:HB2	1.95	0.48
1:B:387:VAL:CG1	1:B:409:GLY:HA2	2.44	0.47
1:C:417:LYS:C	1:C:419:ASN:H	2.15	0.47
1:D:345:HIS:O	1:D:346:HIS:C	2.52	0.47
1:C:376:ALA:O	1:C:380:LEU:HD22	2.13	0.47
1:D:151:ASP:OD1	1:D:153:GLU:HB2	2.14	0.47
1:A:370:ASP:OD1	1:A:404:LYS:HE2	2.14	0.47
1:A:125:ARG:HD3	1:A:244:LEU:O	2.14	0.47
1:D:382:ALA:C	1:D:384:LYS:H	2.16	0.47
1:A:399:ARG:HH21	1:A:399:ARG:CG	2.21	0.47
1:D:26:LEU:CD1	1:D:26:LEU:N	2.76	0.47
1:D:418:ASP:O	1:D:419:ASN:C	2.52	0.47
1:C:70:ILE:O	1:C:102:VAL:HA	2.14	0.47
1:A:430:TYR:HE1	1:A:432:ILE:HD11	1.79	0.47
1:D:240:MET:HG2	1:D:244:LEU:HD12	1.97	0.47
1:D:245:ARG:NH1	1:D:246:ASP:OD2	2.47	0.47
1:A:295:THR:CG2	1:A:332:VAL:HG13	2.40	0.47
1:C:77:ASN:O	1:C:111:PRO:HA	2.14	0.47
1:A:416:ASN:ND2	1:A:420:VAL:H	2.11	0.47
1:C:155:PHE:CE2	1:C:234:VAL:CG2	2.97	0.47
1:A:28:GLY:HA2	3:A:757:ATP:H1'	1.96	0.47
1:D:201:GLY:O	1:D:205:GLN:HG2	2.13	0.47
1:A:111:PRO:HG3	1:D:129:TRP:CE3	2.49	0.47
1:B:210:ASP:OD2	1:B:212:THR:OG1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ILE:HB	1:D:58:PRO:HD3	1.97	0.47
1:B:166:ILE:HG12	1:B:235:ILE:HG23	1.97	0.47
1:A:118:GLN:NE2	1:A:123:ALA:HA	2.28	0.47
1:C:154:LYS:NZ	4:C:1066:HOH:O	2.47	0.47
1:D:208:LYS:HG2	1:D:226:PHE:CZ	2.50	0.47
1:D:424:ALA:C	1:D:425:ARG:HG2	2.35	0.47
1:D:169:ALA:CB	1:D:230:MET:HB2	2.45	0.47
1:C:165:ASP:HB3	1:C:239:VAL:HG21	1.97	0.47
1:A:236:SER:HB2	1:A:239:VAL:HG23	1.97	0.47
1:D:296:LYS:O	1:D:297:LYS:O	2.33	0.47
1:D:367:MET:HG3	1:D:403:ASP:OD1	2.15	0.47
1:D:152:TYR:O	1:D:156:ILE:HG13	2.15	0.47
1:A:398:LYS:HB3	1:A:415:ILE:HG22	1.97	0.47
1:D:163:ASP:OD1	1:D:163:ASP:O	2.33	0.46
1:A:172:PRO:HA	1:A:226:PHE:O	2.15	0.46
1:A:101:PHE:CD1	1:A:103:GLU:HG3	2.51	0.46
1:B:180:ALA:O	1:B:198:LYS:HE3	2.15	0.46
1:A:81:LEU:CD1	1:A:104:VAL:HG21	2.45	0.46
1:C:214:LEU:HB3	1:C:273:LEU:HB2	1.97	0.46
1:C:325:ASP:O	1:C:341:ASN:HA	2.14	0.46
1:A:378:ARG:CG	1:A:378:ARG:NH2	2.78	0.46
1:D:74:THR:HG22	1:D:75:GLN:N	2.30	0.46
1:D:169:ALA:HB1	1:D:230:MET:SD	2.56	0.46
1:A:87:ARG:HD3	1:A:314:GLN:OE1	2.16	0.46
1:A:191:ARG:N	1:A:270:GLN:NE2	2.63	0.46
1:D:267:MET:O	1:D:269:VAL:HG23	2.15	0.46
1:A:261:GLY:O	1:A:265:LEU:HG	2.16	0.46
1:C:367:MET:HB3	1:C:404:LYS:HD3	1.98	0.46
1:C:190:GLY:C	1:C:270:GLN:HE22	2.18	0.46
1:B:243:LEU:HD21	1:B:267:MET:CE	2.39	0.46
1:A:277:TYR:CE2	1:A:302:PHE:HB2	2.51	0.46
1:A:214:LEU:N	1:A:214:LEU:HD22	2.30	0.46
1:D:41:ARG:NH2	1:D:403:ASP:OD1	2.49	0.46
1:D:259:ILE:HB	1:D:260:PRO:HD3	1.97	0.46
1:D:380:LEU:O	1:D:384:LYS:HE3	2.15	0.46
1:C:108:GLN:HG3	4:C:1037:HOH:O	2.16	0.46
1:D:49:GLY:O	1:D:50:ALA:HB3	2.16	0.46
1:B:195:PHE:CD1	1:B:195:PHE:N	2.84	0.46
1:C:184:MET:HE2	1:C:192:ILE:HD13	1.98	0.46
1:A:79:ALA:CB	1:D:133:GLU:HG3	2.46	0.46
1:C:211:THR:HG21	1:C:216:LEU:CD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASP:OD2	1:A:212:THR:HB	2.15	0.46
1:D:147:LEU:O	1:D:148:TYR:HB3	2.16	0.46
1:B:127:TYR:OH	1:C:109:GLN:HG2	2.15	0.45
1:A:445:ILE:HG22	1:A:449:ILE:HB	1.97	0.45
1:B:50:ALA:HB2	1:B:348:VAL:HG12	1.98	0.45
1:D:330:ASP:O	1:D:346:HIS:HA	2.16	0.45
1:C:123:ALA:O	1:C:126:GLN:HB3	2.16	0.45
1:D:65:SER:O	1:D:66:ASN:HB2	2.15	0.45
1:B:47:PRO:HB2	1:B:367:MET:CE	2.46	0.45
1:C:13:LEU:H	1:C:13:LEU:CD2	2.27	0.45
1:C:319:PRO:HD3	1:D:305:TYR:CG	2.50	0.45
1:B:51:ASN:HD21	1:B:335:GLU:HG2	1.81	0.45
1:B:65:SER:O	1:B:66:ASN:HB3	2.17	0.45
1:B:66:ASN:O	1:B:66:ASN:OD1	2.34	0.45
1:C:41:ARG:NH1	2:C:1002:SO4:O1	2.49	0.45
1:B:35:TYR:CG	1:B:36:PRO:HA	2.51	0.45
1:D:258:VAL:O	1:D:262:ALA:HB2	2.16	0.45
1:A:314:GLN:NE2	1:A:316:ARG:HG2	2.32	0.45
1:A:217:ASP:HB3	1:A:220:ARG:HE	1.81	0.45
1:D:209:VAL:O	1:D:210:ASP:HB3	2.15	0.45
1:C:10:GLN:N	4:C:1068:HOH:O	2.49	0.45
1:D:140:LEU:HD11	1:D:152:TYR:CG	2.51	0.45
1:B:323:MET:HE1	1:B:333:ILE:HD13	1.95	0.45
1:B:186:ILE:HB	1:B:190:GLY:HA2	1.99	0.45
1:D:423:ALA:HB3	1:D:432:ILE:HB	1.98	0.45
1:D:22:LEU:HD11	1:D:71:TYR:HD1	1.82	0.45
1:D:214:LEU:HD11	1:D:227:ILE:HG21	1.98	0.45
1:B:375:ASP:HA	1:B:378:ARG:HH22	1.82	0.45
1:D:35:TYR:HE2	1:D:426:GLU:OE2	2.00	0.45
1:B:11:THR:HB	1:B:154:LYS:HZ3	1.82	0.45
1:A:319:PRO:O	1:A:336:GLY:HA2	2.17	0.45
1:B:441:LYS:O	1:B:442:ASP:HB2	2.17	0.45
1:C:13:LEU:HD21	1:C:153:GLU:HB3	1.99	0.45
1:A:314:GLN:HA	1:A:315:PRO:HD3	1.85	0.45
1:D:187:ASP:OD1	1:D:191:ARG:HB3	2.16	0.45
1:D:60:SER:O	1:D:64:ASN:ND2	2.50	0.45
1:D:444:LEU:O	1:D:446:PRO:HD3	2.17	0.45
1:D:199:PRO:O	1:D:204:LEU:HG	2.16	0.45
1:B:13:LEU:HD22	1:B:160:ARG:NH1	2.32	0.45
1:B:18:SER:N	1:B:66:ASN:OD1	2.50	0.45
1:C:61:ASN:HB3	1:C:152:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HB3	1:B:44:PRO:HD3	1.99	0.44
1:C:380:LEU:HD22	1:C:380:LEU:N	2.32	0.44
1:B:62:CYS:HB2	1:B:70:ILE:HD11	2.00	0.44
1:D:403:ASP:HB3	1:D:441:LYS:HA	1.99	0.44
1:D:205:GLN:C	1:D:207:MET:H	2.21	0.44
1:B:416:ASN:H	1:B:451:ILE:C	2.20	0.44
1:C:155:PHE:CZ	1:C:234:VAL:HG23	2.52	0.44
1:A:198:LYS:N	1:A:199:PRO:CD	2.81	0.44
1:D:420:VAL:CG1	1:D:421:GLN:H	2.07	0.44
1:B:415:ILE:O	1:B:416:ASN:C	2.56	0.44
1:D:295:THR:O	1:D:330:ASP:OD1	2.34	0.44
1:A:167:THR:HA	1:A:270:GLN:O	2.18	0.44
1:C:314:GLN:HA	1:C:315:PRO:HD3	1.81	0.44
1:A:106:ALA:HB3	1:A:109:GLN:OE1	2.17	0.44
1:D:421:GLN:O	1:D:432:ILE:HG22	2.18	0.44
1:B:31:GLY:N	1:B:33:ARG:NH2	2.65	0.44
1:D:200:GLN:CA	1:D:204:LEU:HB2	2.47	0.44
1:A:433:LYS:O	1:A:434:SER:C	2.55	0.44
1:B:309:ALA:HB1	4:B:1022:HOH:O	2.17	0.44
1:B:49:GLY:O	1:B:50:ALA:CB	2.65	0.44
1:D:57:ILE:N	1:D:58:PRO:HD2	2.31	0.44
1:D:444:LEU:C	1:D:444:LEU:HD23	2.38	0.44
1:C:422:GLU:HA	1:C:432:ILE:O	2.17	0.44
1:C:358:GLY:O	1:C:394:ASN:HA	2.18	0.44
1:C:338:VAL:O	1:C:338:VAL:HG12	2.18	0.44
1:D:78:SER:HB3	1:D:81:LEU:CB	2.48	0.44
1:C:14:ASP:N	1:C:15:PRO:O	2.50	0.44
1:B:255:GLY:O	1:B:256:SER:HB3	2.18	0.44
1:D:208:LYS:HG2	1:D:226:PHE:CE1	2.53	0.44
1:D:68:SER:HB3	1:D:100:GLY:CA	2.46	0.44
1:B:49:GLY:H	1:B:291:ASN:HD21	1.66	0.44
1:B:171:LEU:HB2	1:B:230:MET:HG3	2.00	0.44
1:D:183:LEU:HB2	1:D:207:MET:HE2	2.00	0.43
1:D:182:GLY:HA2	1:D:196:ALA:O	2.18	0.43
1:D:188:GLU:HA	1:D:213:ILE:HD13	2.00	0.43
1:B:31:GLY:HA3	1:B:33:ARG:NH2	2.34	0.43
1:B:160:ARG:C	1:B:162:THR:H	2.21	0.43
1:C:244:LEU:HD23	1:C:244:LEU:HA	1.86	0.43
1:D:293:GLY:O	1:D:296:LYS:HG2	2.18	0.43
1:D:277:TYR:CE2	1:D:302:PHE:HB2	2.54	0.43
1:A:43:LYS:HB3	1:A:44:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ARG:NE	2:D:1011:SO4:O1	2.50	0.43
1:D:328:VAL:HG13	1:D:344:ILE:HB	2.00	0.43
1:B:154:LYS:HB2	1:B:154:LYS:HZ2	1.83	0.43
1:C:237:LYS:O	1:C:240:MET:HB3	2.19	0.43
1:C:122:ASP:OD1	1:C:252:ASN:ND2	2.52	0.43
1:B:399:ARG:NH2	1:B:435:GLY:HA3	2.34	0.43
1:D:170:ALA:HB3	1:D:272:TYR:O	2.18	0.43
1:C:393:LYS:HB2	1:C:410:ASP:OD2	2.19	0.43
1:C:175:GLU:HA	1:C:226:PHE:CE1	2.53	0.43
1:D:276:GLY:O	1:D:277:TYR:C	2.56	0.43
1:A:187:ASP:C	1:A:187:ASP:OD2	2.57	0.43
1:B:268:ARG:HH21	1:B:268:ARG:HG2	1.84	0.43
1:D:59:VAL:O	1:D:63:LEU:HG	2.19	0.43
1:A:432:ILE:HA	1:A:436:ILE:O	2.18	0.43
1:A:154:LYS:HA	1:A:154:LYS:HD3	1.82	0.43
1:C:154:LYS:HD3	1:C:154:LYS:HA	1.82	0.43
1:D:439:VAL:CG1	1:D:443:ALA:HB3	2.49	0.43
1:C:363:ASP:O	1:C:399:ARG:HA	2.18	0.43
1:B:351:LEU:O	1:B:352:ARG:HB2	2.18	0.43
1:C:192:ILE:HD12	1:C:269:VAL:HG12	1.99	0.43
1:B:121:ALA:HA	1:B:254:PHE:CE1	2.54	0.43
1:A:292:LEU:HD23	1:A:348:VAL:HG23	2.01	0.43
1:B:48:LEU:HD22	1:B:54:LEU:HD23	2.00	0.43
1:A:378:ARG:HG2	1:A:378:ARG:NH2	2.27	0.43
1:C:149:ARG:NH2	1:C:309:ALA:O	2.51	0.43
1:B:314:GLN:NE2	2:B:1009:SO4:S	2.92	0.43
1:A:389:ILE:HG21	1:A:405:ASN:HA	2.00	0.43
1:C:172:PRO:HA	1:C:226:PHE:O	2.19	0.43
1:C:181:PHE:HB3	1:C:228:ALA:HB1	2.01	0.43
1:B:377:ASP:C	1:B:379:LYS:N	2.72	0.43
1:D:73:LEU:CD1	1:D:73:LEU:N	2.82	0.43
1:B:84:HIS:HA	1:B:314:GLN:NE2	2.34	0.43
1:D:341:ASN:O	1:D:342:CYS:HB3	2.19	0.43
1:D:305:TYR:CG	1:D:306:ASP:N	2.87	0.43
1:B:142:LEU:HD11	1:B:152:TYR:CE1	2.54	0.43
1:A:220:ARG:HA	1:A:223:GLU:OE1	2.19	0.43
1:A:210:ASP:O	1:A:213:ILE:HD12	2.19	0.43
1:A:366:LEU:HB3	4:A:1039:HOH:O	2.19	0.43
1:C:46:VAL:HA	1:C:47:PRO:HD3	1.80	0.43
1:B:45:ALA:O	1:B:53:ARG:NH1	2.48	0.43
1:D:294:ILE:HA	1:D:300:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PHE:O	1:A:258:VAL:HB	2.19	0.42
1:A:174:ASP:N	1:A:174:ASP:OD2	2.42	0.42
1:D:171:LEU:HD23	1:D:172:PRO:O	2.19	0.42
1:A:440:ILE:O	1:A:443:ALA:CB	2.67	0.42
1:C:211:THR:HG22	1:C:216:LEU:HB2	2.00	0.42
1:D:451:ILE:HG22	1:D:451:ILE:OXT	2.19	0.42
1:C:27:GLY:CA	1:C:44:PRO:HG3	2.48	0.42
1:D:325:ASP:HB3	1:D:341:ASN:OD1	2.20	0.42
1:B:417:LYS:C	1:B:419:ASN:H	2.22	0.42
1:C:211:THR:HB	1:C:221:ALA:CB	2.50	0.42
1:C:430:TYR:HB2	1:C:438:THR:O	2.20	0.42
1:D:333:ILE:HG22	1:D:334:GLY:O	2.18	0.42
1:C:87:ARG:HG2	1:C:87:ARG:NH2	2.33	0.42
1:D:368:GLY:O	1:D:404:LYS:HA	2.19	0.42
1:D:280:ASP:O	1:D:281:ILE:HG23	2.19	0.42
1:D:412:VAL:HG12	1:D:413:LYS:N	2.33	0.42
1:C:374:THR:N	1:C:377:ASP:OD2	2.53	0.42
1:D:278:TRP:C	1:D:278:TRP:CD1	2.91	0.42
1:A:176:LYS:HD2	1:A:176:LYS:N	2.35	0.42
1:C:37:LEU:HD22	1:C:367:MET:CE	2.50	0.42
1:D:412:VAL:CG1	1:D:413:LYS:N	2.83	0.42
1:A:190:GLY:C	1:A:270:GLN:NE2	2.73	0.42
1:A:64:ASN:ND2	1:A:312:TYR:OH	2.48	0.42
1:B:277:TYR:CE2	1:B:302:PHE:HB2	2.55	0.42
1:D:173:MET:CE	1:D:228:ALA:HB3	2.49	0.42
1:B:62:CYS:HB3	1:B:70:ILE:HD11	2.02	0.42
1:D:57:ILE:HB	1:D:58:PRO:CD	2.50	0.42
1:B:399:ARG:NH2	1:B:434:SER:O	2.51	0.42
1:C:204:LEU:CD2	1:C:226:PHE:CE2	3.03	0.42
1:C:41:ARG:HH22	1:C:403:ASP:CG	2.23	0.42
1:D:204:LEU:HD23	1:D:226:PHE:CE2	2.54	0.42
1:B:451:ILE:HG22	1:B:451:ILE:O	2.19	0.42
1:B:51:ASN:HD21	1:B:335:GLU:H	1.66	0.42
1:D:57:ILE:O	1:D:61:ASN:ND2	2.53	0.42
1:A:109:GLN:NE2	1:D:127:TYR:OH	2.53	0.42
1:B:347:SER:HB3	1:B:364:SER:O	2.20	0.42
1:A:386:SER:O	1:A:387:VAL:HB	2.20	0.42
1:D:449:ILE:HD13	1:D:450:ILE:N	2.27	0.42
1:C:230:MET:CE	1:C:232:ILE:HD12	2.47	0.42
1:D:14:ASP:OD1	1:D:14:ASP:C	2.58	0.42
1:A:389:ILE:CG2	1:A:405:ASN:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ILE:HA	1:D:451:ILE:HB	2.02	0.41
1:A:169:ALA:HB3	1:A:232:ILE:HB	2.01	0.41
1:A:11:THR:HB	1:A:157:GLN:NE2	2.34	0.41
1:C:429:GLY:HA2	1:C:440:ILE:HD12	2.02	0.41
1:C:423:ALA:HB3	1:C:432:ILE:HB	2.02	0.41
1:D:341:ASN:O	1:D:357:GLU:HA	2.20	0.41
1:B:284:ILE:HD13	1:B:284:ILE:HA	1.94	0.41
1:D:188:GLU:HA	1:D:213:ILE:CD1	2.50	0.41
1:B:239:VAL:HG12	1:B:243:LEU:HD12	2.01	0.41
1:B:387:VAL:CG1	1:B:388:PRO:HD2	2.51	0.41
1:B:325:ASP:O	1:B:341:ASN:HA	2.19	0.41
1:B:13:LEU:HD22	1:B:160:ARG:HH11	1.85	0.41
1:A:210:ASP:HB3	1:A:213:ILE:HD12	2.02	0.41
1:B:191:ARG:HD2	1:B:268:ARG:NH2	2.36	0.41
1:D:450:ILE:CG2	1:D:451:ILE:N	2.83	0.41
1:A:335:GLU:H	1:A:335:GLU:HG2	1.66	0.41
1:A:253:ASP:HB3	3:A:757:ATP:O3G	2.20	0.41
1:A:219:LYS:C	1:A:221:ALA:N	2.73	0.41
1:A:399:ARG:NH2	1:A:399:ARG:CG	2.80	0.41
1:A:199:PRO:CB	1:A:203:GLN:HG3	2.50	0.41
1:C:75:GLN:O	1:C:107:ALA:HB3	2.20	0.41
1:B:175:GLU:HB3	1:B:226:PHE:HE2	1.85	0.41
1:D:387:VAL:CG2	1:D:407:ARG:HB3	2.39	0.41
1:B:441:LYS:HE3	2:B:1001:SO4:O1	2.20	0.41
1:C:199:PRO:HB2	1:C:203:GLN:HG3	2.01	0.41
1:B:155:PHE:CE2	1:B:234:VAL:HG23	2.56	0.41
1:D:45:ALA:HB2	1:D:81:LEU:HG	2.01	0.41
1:B:125:ARG:NH1	1:B:251:ALA:O	2.44	0.41
1:A:259:ILE:CB	1:A:260:PRO:HD3	2.44	0.41
1:B:446:PRO:HD2	1:B:449:ILE:CD1	2.50	0.41
1:B:83:ARG:HH21	1:B:83:ARG:HG3	1.86	0.41
1:B:87:ARG:NH2	1:B:314:GLN:HG2	2.36	0.41
1:D:17:ALA:O	1:D:18:SER:C	2.60	0.41
1:A:208:LYS:HG3	1:A:226:PHE:CZ	2.56	0.41
1:B:331:SER:HB3	1:B:347:SER:O	2.21	0.41
1:A:329:THR:HA	1:B:324:LEU:O	2.21	0.41
1:B:195:PHE:CZ	1:B:260:PRO:HA	2.56	0.41
1:A:294:ILE:HD13	1:A:300:PRO:CB	2.51	0.41
1:A:431:PHE:C	1:A:432:ILE:HG13	2.42	0.41
1:B:325:ASP:HB3	1:B:341:ASN:CB	2.50	0.41
1:D:182:GLY:HA2	1:D:197:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ALA:HB1	1:C:67:ILE:HG12	2.03	0.41
1:D:437:VAL:HG11	1:D:451:ILE:HG21	2.03	0.40
1:B:420:VAL:HG12	1:B:422:GLU:H	1.86	0.40
1:B:13:LEU:HD11	1:B:156:ILE:HB	2.03	0.40
1:B:87:ARG:HD3	1:C:99:GLU:OE2	2.22	0.40
1:A:187:ASP:HB2	4:A:1084:HOH:O	2.21	0.40
1:D:171:LEU:HD23	1:D:171:LEU:C	2.41	0.40
1:C:49:GLY:O	1:C:50:ALA:HB3	2.20	0.40
1:A:155:PHE:CE2	1:A:232:ILE:HG22	2.56	0.40
1:B:278:TRP:CD1	1:B:278:TRP:O	2.74	0.40
1:A:210:ASP:O	1:A:212:THR:N	2.54	0.40
1:B:173:MET:O	1:B:226:PHE:HB2	2.21	0.40
1:B:366:LEU:N	1:B:366:LEU:HD23	2.36	0.40
1:D:41:ARG:HH22	1:D:403:ASP:CG	2.25	0.40
1:D:200:GLN:C	1:D:204:LEU:HB2	2.42	0.40
1:D:449:ILE:HD12	1:D:450:ILE:O	2.21	0.40
1:A:294:ILE:CG2	1:A:332:VAL:HG11	2.52	0.40
1:D:187:ASP:CG	1:D:191:ARG:HB3	2.41	0.40
1:B:387:VAL:HG11	1:B:409:GLY:CA	2.48	0.40
1:C:234:VAL:O	1:C:235:ILE:HG13	2.20	0.40
1:A:154:LYS:HZ2	1:A:157:GLN:HE22	1.68	0.40
1:B:11:THR:HB	1:B:154:LYS:HE2	2.04	0.40
1:A:328:VAL:HG12	1:A:331:SER:HB2	2.02	0.40
1:B:59:VAL:HG11	1:B:89:TYR:CE1	2.56	0.40
1:D:397:ILE:CG2	1:D:402:ILE:HD11	2.52	0.40
1:A:388:PRO:HA	1:A:407:ARG:NH2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/451 (95%)	375 (87%)	47 (11%)	7 (2%)	12	24
1	B	426/451 (94%)	365 (86%)	47 (11%)	14 (3%)	5	7
1	C	431/451 (96%)	393 (91%)	36 (8%)	2 (0%)	34	60
1	D	419/451 (93%)	337 (80%)	68 (16%)	14 (3%)	5	7
All	All	1705/1804 (94%)	1470 (86%)	198 (12%)	37 (2%)	8	15

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ALA
1	B	99	GLU
1	B	256	SER
1	D	174	ASP
1	D	297	LYS
1	D	298	PRO
1	D	419	ASN
1	D	420	VAL
1	A	298	PRO
1	A	385	GLY
1	B	91	SER
1	B	200	GLN
1	B	201	GLY
1	B	403	ASP
1	D	211	THR
1	A	39	LYS
1	A	148	TYR
1	B	28	GLY
1	B	176	LYS
1	C	205	GLN
1	C	416	ASN
1	A	211	THR
1	A	387	VAL
1	B	218	ASP
1	D	216	LEU
1	D	217	ASP
1	D	268	ARG
1	D	277	TYR
1	D	281	ILE
1	D	421	GLN
1	B	219	LYS
1	B	416	ASN
1	D	394	ASN

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Mol	Chain	Res	Type
1	A	297	LYS
1	B	199	PRO
1	D	358	GLY
1	B	29	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/375 (96%)	336 (93%)	25 (7%)	19	38
1	B	357/375 (95%)	341 (96%)	16 (4%)	34	62
1	C	362/375 (96%)	350 (97%)	12 (3%)	45	73
1	D	352/375 (94%)	332 (94%)	20 (6%)	25	49
All	All	1432/1500 (96%)	1359 (95%)	73 (5%)	29	55

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	12	CYS
1	A	52	TYR
1	A	70	ILE
1	A	76	PHE
1	A	85	LEU
1	A	99	GLU
1	A	130	LEU
1	A	145	ASP
1	A	147	LEU
1	A	188	GLU
1	A	193	ILE
1	A	211	THR
1	A	218	ASP
1	A	238	ASP
1	A	294	ILE
1	A	301	ASP

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Mol	Chain	Res	Type
1	A	314	GLN
1	A	341	ASN
1	A	374	THR
1	A	377	ASP
1	A	399	ARG
1	A	416	ASN
1	A	418	ASP
1	A	438	THR
1	B	11	THR
1	B	73	LEU
1	B	77	ASN
1	B	81	LEU
1	B	140	LEU
1	B	154	LYS
1	B	163	ASP
1	B	171	LEU
1	B	188	GLU
1	B	200	GLN
1	B	210	ASP
1	B	218	ASP
1	B	233	TYR
1	B	245	ARG
1	B	268	ARG
1	B	426	GLU
1	C	73	LEU
1	C	81	LEU
1	C	130	LEU
1	C	147	LEU
1	C	203	GLN
1	C	204	LEU
1	C	233	TYR
1	C	275	ASP
1	C	292	LEU
1	C	328	VAL
1	C	341	ASN
1	C	427	THR
1	D	13	LEU
1	D	26	LEU
1	D	40	LYS
1	D	69	LYS
1	D	75	GLN
1	D	81	LEU

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Mol	Chain	Res	Type
1	D	109	GLN
1	D	140	LEU
1	D	146	HIS
1	D	209	VAL
1	D	217	ASP
1	D	222	LYS
1	D	233	TYR
1	D	281	ILE
1	D	298	PRO
1	D	301	ASP
1	D	316	ARG
1	D	351	LEU
1	D	417	LYS
1	D	449	ILE

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	51	ASN
1	A	64	ASN
1	A	82	ASN
1	A	113	ASN
1	A	126	GLN
1	A	146	HIS
1	A	157	GLN
1	A	270	GLN
1	A	314	GLN
1	A	341	ASN
1	A	405	ASN
1	A	416	ASN
1	B	51	ASN
1	B	64	ASN
1	B	252	ASN
1	B	270	GLN
1	B	289	ASN
1	B	291	ASN
1	B	419	ASN
1	B	421	GLN
1	C	10	GLN
1	C	51	ASN
1	C	64	ASN
1	C	82	ASN

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Mol	Chain	Res	Type
1	C	109	GLN
1	C	242	ASN
1	C	252	ASN
1	C	270	GLN
1	C	345	HIS
1	C	346	HIS
1	C	396	HIS
1	D	51	ASN
1	D	66	ASN
1	D	75	GLN
1	D	82	ASN
1	D	252	ASN
1	D	314	GLN
1	D	396	HIS
1	D	419	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	SO4	A	1000	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	A	1007	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	1008	-	4,4,4	0.30	0	6,6,6	0.18	0
2	SO4	A	1020	-	4,4,4	0.21	0	6,6,6	0.21	0
3	ATP	A	757	-	24,33,33	1.17	3 (12%)	31,52,52	2.75	7 (22%)
2	SO4	B	1001	-	4,4,4	0.21	0	6,6,6	0.31	0
2	SO4	B	1006	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	B	1009	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	C	1002	-	4,4,4	0.15	0	6,6,6	0.26	0
2	SO4	C	1005	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	C	1010	-	4,4,4	0.22	0	6,6,6	0.06	0
2	SO4	C	1022	-	4,4,4	0.32	0	6,6,6	0.15	0
3	ATP	C	758	-	24,33,33	1.20	2 (8%)	31,52,52	2.66	7 (22%)
2	SO4	D	1003	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	D	1011	-	4,4,4	0.20	0	6,6,6	0.19	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	SO4	A	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1020	-	-	0/0/0/0	0/0/0/0
3	ATP	A	757	-	-	0/18/38/38	0/3/3/3
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1009	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1010	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1022	-	-	0/0/0/0	0/0/0/0
3	ATP	C	758	-	-	0/18/38/38	0/3/3/3
2	SO4	D	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1011	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	757	ATP	O4'-C4'	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	757	ATP	C2-N1	2.26	1.38	1.33
3	C	758	ATP	C2-N1	2.45	1.38	1.33
3	A	757	ATP	C2-N3	3.35	1.38	1.32
3	C	758	ATP	C2-N3	3.37	1.38	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	757	ATP	N3-C2-N1	-11.72	119.92	128.89
3	C	758	ATP	N3-C2-N1	-11.54	120.06	128.89
3	C	758	ATP	C4-C5-N7	-4.93	104.94	109.48
3	A	757	ATP	C4-C5-N7	-4.44	105.40	109.48
3	A	757	ATP	O4'-C1'-N9	-3.97	99.78	108.10
3	C	758	ATP	O4'-C1'-N9	-3.30	101.19	108.10
3	C	758	ATP	N6-C6-N1	-2.33	114.21	119.20
3	C	758	ATP	PB-O3B-PG	-2.33	124.86	132.67
3	A	757	ATP	N6-C6-N1	-2.32	114.23	119.20
3	A	757	ATP	PB-O3B-PG	-2.22	125.22	132.67
3	C	758	ATP	O2'-C2'-C3'	2.27	119.20	111.83
3	A	757	ATP	O2'-C2'-C3'	2.30	119.29	111.83
3	C	758	ATP	C2'-C1'-N9	3.88	120.22	114.29
3	A	757	ATP	C2'-C1'-N9	4.91	121.80	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	757	ATP	3	0
2	B	1001	SO4	1	0
2	B	1009	SO4	1	0
2	C	1002	SO4	1	0
2	D	1011	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	433/451 (96%)	-0.24	6 (1%) 78 74	21, 42, 75, 91	0
1	B	432/451 (95%)	-0.15	7 (1%) 74 69	19, 44, 83, 91	0
1	C	435/451 (96%)	-0.36	2 (0%) 91 90	15, 36, 64, 80	0
1	D	425/451 (94%)	0.20	22 (5%) 31 24	19, 59, 90, 91	0
All	All	1725/1804 (95%)	-0.14	37 (2%) 67 61	15, 44, 83, 91	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	ASN	4.8
1	B	30	ALA	4.5
1	D	380	LEU	4.1
1	D	383	ALA	3.7
1	D	30	ALA	3.6
1	D	382	ALA	3.5
1	D	299	VAL	3.2
1	D	177	ARG	3.1
1	A	307	ARG	3.0
1	D	233	TYR	2.9
1	B	11	THR	2.8
1	B	28	GLY	2.6
1	B	29	GLY	2.6
1	D	297	LYS	2.6
1	D	431	PHE	2.6
1	B	202	GLU	2.5
1	A	297	LYS	2.5
1	D	188	GLU	2.5
1	A	382	ALA	2.5
1	D	252	ASN	2.5
1	D	29	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	189	GLU	2.4
1	D	215	GLY	2.3
1	B	232	ILE	2.2
1	D	32	THR	2.2
1	D	112	GLU	2.2
1	B	91	SER	2.2
1	D	386	SER	2.2
1	A	222	LYS	2.2
1	D	298	PRO	2.1
1	A	379	LYS	2.1
1	A	299	VAL	2.1
1	C	233	TYR	2.1
1	D	169	ALA	2.1
1	D	176	LYS	2.0
1	C	141	ILE	2.0
1	D	367	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
2	SO4	A	1020	5/5	0.90	0.19	1.11	76,78,79,80	0
2	SO4	B	1006	5/5	0.92	0.18	0.49	86,87,87,88	0
2	SO4	C	1022	5/5	0.89	0.18	0.35	76,76,78,79	0
3	ATP	C	758	31/31	0.88	0.18	0.27	40,57,81,82	0
2	SO4	C	1010	5/5	0.96	0.15	-0.03	56,57,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	C	1005	5/5	0.96	0.15	-0.06	82,82,83,84	0
2	SO4	B	1001	5/5	0.98	0.13	-0.42	43,46,48,52	0
2	SO4	B	1009	5/5	0.91	0.13	-0.45	66,66,68,68	0
2	SO4	A	1007	5/5	0.94	0.12	-0.46	89,89,90,91	0
2	SO4	D	1003	5/5	0.97	0.14	-0.63	56,59,59,60	0
2	SO4	C	1002	5/5	0.99	0.13	-0.67	27,28,31,32	0
3	ATP	A	757	31/31	0.91	0.14	-0.74	50,62,81,83	0
2	SO4	D	1011	5/5	0.95	0.12	-0.74	62,66,66,67	0
2	SO4	A	1000	5/5	0.99	0.11	-0.80	36,37,37,39	0
2	SO4	A	1008	5/5	0.97	0.12	-1.24	49,52,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.