



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:05 AM UTC

PDB ID : 1DV2 / pdb_00001dv2
Title : The structure of biotin carboxylase, mutant E288K, complexed with ATP
Authors : Thoden, J.B.; Blanchard, C.Z.; Holden, H.M.; Waldrop, G.L.
Deposited on : 2000-01-19
Resolution : 2.50 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

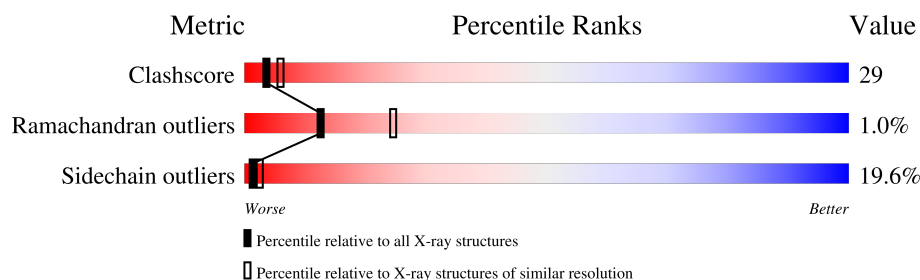
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	452	
1	B	452	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	1000	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7113 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 BIOTIN CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	1	0
			3469	2184	624	639	22			
1	B	448	Total	C	N	O	S	0	0	0
			3452	2175	619	636	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1A	HIS	-	insertion	UNP P24182
A	1B	SER	-	insertion	UNP P24182
A	1C	GLY	-	insertion	UNP P24182
B	1A	HIS	-	insertion	UNP P24182
B	1B	SER	-	insertion	UNP P24182
B	1C	GLY	-	insertion	UNP P24182
A	288	LYS	GLU	engineered mutation	UNP P24182
B	288	LYS	GLU	engineered mutation	UNP P24182

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	B	48	Total O 48 48	0	0

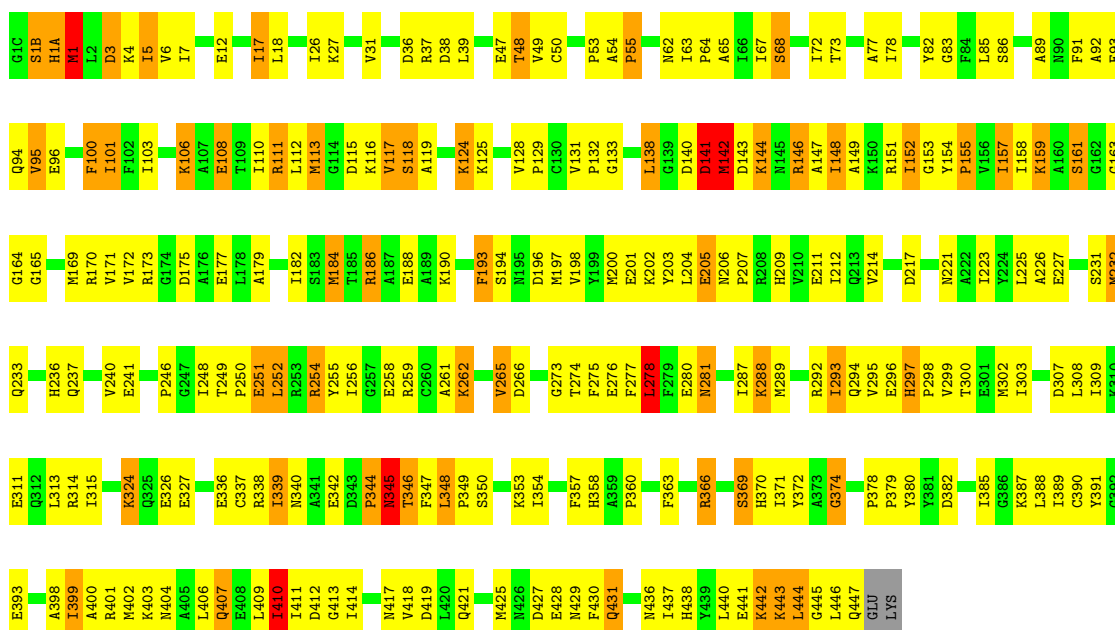
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

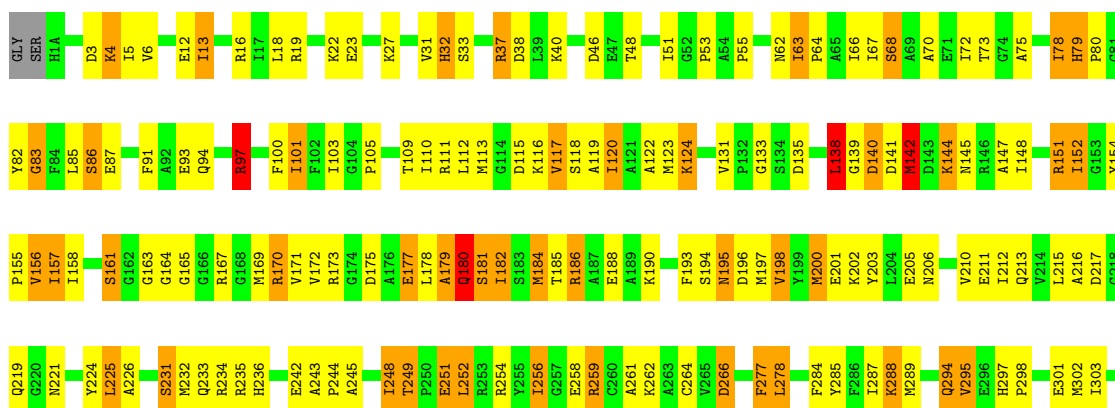
- Molecule 1: BIOTIN CARBOXYLASE

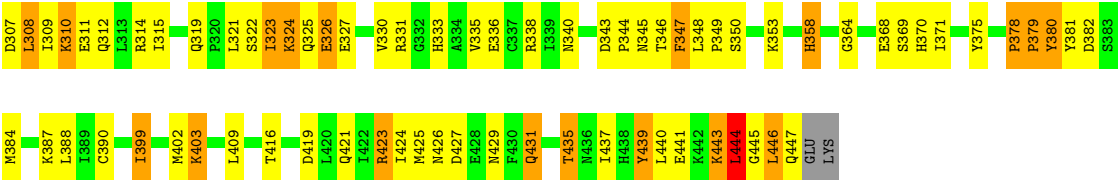
Chain A: 44% 42% 12%



- Molecule 1: BIOTIN CARBOXYLASE

Chain B: 47% 37% 14% ..





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.30Å 115.50Å 122.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.6 (30.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.171 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7113	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.19	1/3537 (0.0%)	1.76	52/4771 (1.1%)
1	B	1.10	0/3516	1.66	38/4744 (0.8%)
All	All	1.15	1/7053 (0.0%)	1.71	90/9515 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	ILE	CA-CB	-5.16	1.48	1.54

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	PRO	CA-C-N	9.61	129.35	119.64
1	B	378	PRO	C-N-CA	9.61	129.35	119.64
1	A	347	PHE	CA-CB-CG	-8.13	105.67	113.80
1	A	380	TYR	N-CA-C	7.88	119.95	111.36
1	A	281	ASN	CB-CA-C	-7.74	100.74	111.73
1	B	379	PRO	CB-CA-C	-6.86	100.27	111.31
1	A	124	LYS	CA-C-N	6.82	129.97	120.29
1	A	124	LYS	C-N-CA	6.82	129.97	120.29
1	A	419	ASP	CA-CB-CG	-6.64	105.96	112.60
1	B	350	SER	N-CA-CB	6.60	121.41	110.99
1	B	97	ARG	NE-CZ-NH1	6.59	128.09	121.50
1	A	83	GLY	N-CA-C	6.57	124.10	115.36
1	A	155	PRO	N-CA-CB	6.56	109.82	102.60
1	A	246	PRO	CB-CA-C	-6.51	103.06	111.46
1	A	83	GLY	CA-C-N	-6.50	109.12	121.54
1	A	83	GLY	C-N-CA	-6.50	109.12	121.54
1	A	265	VAL	O-C-N	6.50	128.18	121.87
1	B	79	HIS	CA-CB-CG	-6.45	107.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	N-CA-CB	6.30	120.99	110.53
1	B	175	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	344	PRO	N-CA-CB	6.21	109.42	103.52
1	A	17	ILE	CB-CA-C	-6.17	103.81	112.14
1	A	346	THR	CA-CB-OG1	6.14	118.81	109.60
1	A	350	SER	CA-C-N	6.12	126.30	120.31
1	A	350	SER	C-N-CA	6.12	126.30	120.31
1	B	195	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	349	PRO	N-CA-CB	6.05	108.57	103.25
1	B	142	MET	N-CA-C	6.04	120.38	112.89
1	A	308	LEU	CB-CA-C	6.00	120.45	110.92
1	A	442	LYS	N-CA-C	5.92	117.74	111.28
1	A	128	VAL	CB-CA-C	5.77	117.13	110.89
1	A	1	MET	CA-C-N	5.74	128.91	120.82
1	A	1	MET	C-N-CA	5.74	128.91	120.82
1	A	3	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	347	PHE	N-CA-C	-5.70	106.27	113.23
1	B	380	TYR	N-CA-C	5.70	118.43	111.82
1	A	100	PHE	CA-CB-CG	-5.69	108.11	113.80
1	A	390	CYS	N-CA-CB	5.64	120.65	110.83
1	B	13	ILE	N-CA-CB	5.63	117.51	110.47
1	B	439	TYR	N-CA-C	5.61	117.84	111.11
1	A	407	GLN	CA-CB-CG	-5.61	102.88	114.10
1	B	78	ILE	N-CA-CB	-5.60	104.20	111.82
1	A	152	ILE	CB-CA-C	-5.56	103.25	112.26
1	B	277	PHE	CA-CB-CG	5.55	119.35	113.80
1	B	83	GLY	N-CA-C	5.54	126.31	113.18
1	B	38	ASP	CA-CB-CG	-5.51	107.09	112.60
1	B	266	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	410	ILE	CB-CA-C	-5.49	103.01	110.42
1	A	117	VAL	O-C-N	5.48	127.42	121.94
1	B	382	ASP	N-CA-CB	5.46	117.72	110.29
1	A	278	LEU	N-CA-C	-5.40	101.73	110.32
1	A	366	ARG	CD-NE-CZ	-5.39	116.85	124.40
1	A	345	ASN	N-CA-CB	5.38	118.54	110.14
1	B	180	GLN	O-C-N	5.37	127.61	122.07
1	B	138	LEU	CA-C-N	5.37	126.60	120.53
1	B	138	LEU	C-N-CA	5.37	126.60	120.53
1	B	206	ASN	N-CA-C	5.32	118.31	108.94
1	A	418	VAL	N-CA-C	5.32	115.94	110.36
1	B	32	HIS	CA-CB-CG	-5.30	108.50	113.80
1	A	124	LYS	O-C-N	5.30	127.73	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ALA	CA-C-N	5.29	127.23	120.56
1	A	398	ALA	C-N-CA	5.29	127.23	120.56
1	B	87	GLU	N-CA-C	5.29	119.33	111.87
1	A	308	LEU	N-CA-C	5.27	117.45	111.02
1	A	400	ALA	O-C-N	5.27	127.57	122.09
1	B	347	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	374	GLY	N-CA-C	-5.26	107.54	115.32
1	B	97	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	B	375	TYR	CA-C-N	-5.23	115.63	123.00
1	B	375	TYR	C-N-CA	-5.23	115.63	123.00
1	A	288	LYS	N-CA-C	5.21	114.71	107.73
1	B	139	GLY	CA-C-N	5.20	128.22	120.31
1	B	139	GLY	C-N-CA	5.20	128.22	120.31
1	A	55	PRO	CA-C-N	5.19	127.55	120.54
1	A	55	PRO	C-N-CA	5.19	127.55	120.54
1	A	113	MET	N-CA-C	-5.19	106.95	113.28
1	B	46	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	358	HIS	N-CA-CB	5.15	118.86	110.77
1	B	140	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	256	ILE	N-CA-C	5.11	118.22	111.17
1	A	412	ASP	CB-CA-C	-5.10	100.88	109.50
1	A	337	CYS	CA-C-N	-5.08	114.16	121.42
1	A	337	CYS	C-N-CA	-5.08	114.16	121.42
1	A	297	HIS	CA-C-N	-5.06	113.43	119.05
1	A	297	HIS	C-N-CA	-5.06	113.43	119.05
1	B	117	VAL	N-CA-CB	5.06	116.47	110.55
1	B	248	ILE	N-CA-C	5.06	115.62	107.73
1	A	95	VAL	N-CA-C	-5.02	105.50	110.62
1	B	295	VAL	N-CA-CB	-5.01	105.36	110.62
1	A	175	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

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	3469	0	3498	199	0
1	B	3452	0	3481	212	0
2	A	31	0	12	10	0
2	B	31	0	12	8	0
3	A	82	0	0	3	0
3	B	48	0	0	4	0
All	All	7113	0	7003	410	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 29.

All (410) 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:B:179:ALA:HB3	1:B:180:GLN:HE21	1.19	1.00
1:B:440:LEU:HG	1:B:444:LEU:HD22	1.40	0.97
1:B:131:VAL:HG22	1:B:285:TYR:HB3	1.45	0.95
1:B:169:MET:HE1	2:B:1001:ATP:H5'1	1.46	0.95
1:B:278:LEU:HD22	1:B:287:ILE:HD11	1.51	0.93
1:B:278:LEU:HD13	1:B:287:ILE:HD11	1.52	0.91
1:A:117:VAL:HG21	1:A:197:MET:HE3	1.53	0.89
1:A:54:ALA:HB3	1:A:55:PRO:HD3	1.54	0.89
1:A:133:GLY:HA2	1:A:152:ILE:HD11	1.55	0.87
1:B:236:HIS:CE1	2:B:1001:ATP:H5'2	2.11	0.85
1:B:72:ILE:HD12	1:B:73:THR:HG23	1.58	0.84
1:B:154:TYR:HE1	1:B:172:VAL:HG12	1.41	0.84
1:B:72:ILE:CD1	1:B:73:THR:HG23	2.06	0.84
1:B:133:GLY:HA2	1:B:152:ILE:HD11	1.60	0.84
1:A:169:MET:HE1	2:A:1000:ATP:H5'1	1.58	0.83
1:A:72:ILE:HD12	1:A:73:THR:N	1.94	0.83
1:A:72:ILE:CD1	1:A:73:THR:HG23	2.09	0.83
1:B:440:LEU:HG	1:B:444:LEU:CD2	2.07	0.83
1:B:419:ASP:HB3	1:B:423:ARG:NH1	1.94	0.82
1:A:112:LEU:HG	1:A:113:MET:HE2	1.59	0.82
1:B:142:MET:HA	1:B:145:ASN:HB2	1.62	0.82
1:B:154:TYR:CE1	1:B:172:VAL:HG12	2.16	0.81
1:B:340:ASN:HD22	1:B:384:MET:HA	1.44	0.81
1:A:133:GLY:HA2	1:A:152:ILE:CD1	2.12	0.79
1:B:297:HIS:CG	1:B:298:PRO:HD3	2.17	0.79
1:B:323:ILE:HD12	1:B:323:ILE:H	1.48	0.78
1:B:179:ALA:HB3	1:B:180:GLN:NE2	1.96	0.77
1:B:369:SER:OG	1:B:371:ILE:HG12	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:THR:OG1	1:B:251:GLU:HG2	1.85	0.76
1:B:151:ARG:HG2	1:B:152:ILE:N	1.99	0.76
1:B:236:HIS:HE1	2:B:1001:ATP:H5'2	1.48	0.75
1:B:278:LEU:CD2	1:B:287:ILE:HD11	2.16	0.75
1:A:298:PRO:O	1:A:302:MET:HG2	1.88	0.74
1:A:142:MET:HE3	1:A:179:ALA:HA	1.70	0.73
1:B:278:LEU:HD13	1:B:287:ILE:CD1	2.17	0.73
1:A:91:PHE:O	1:A:95:VAL:HG23	1.88	0.73
1:B:278:LEU:CD1	1:B:287:ILE:HD11	2.18	0.72
1:A:309:ILE:O	1:A:313:LEU:HG	1.89	0.72
1:B:278:LEU:HD22	1:B:287:ILE:CD1	2.19	0.72
1:A:117:VAL:CG2	1:A:197:MET:HE3	2.20	0.71
1:B:217:ASP:OD2	1:B:221:ASN:HB2	1.90	0.71
1:A:250:PRO:O	1:A:254:ARG:HD3	1.89	0.71
1:A:370:HIS:CD2	1:A:370:HIS:H	2.07	0.71
1:B:37:ARG:HG3	1:B:37:ARG:HH11	1.55	0.70
1:B:441:GLU:HG2	1:B:446:LEU:HD13	1.73	0.70
1:A:72:ILE:HD12	1:A:73:THR:HG23	1.72	0.70
1:A:36:ASP:HB3	1:A:39:LEU:CD1	2.22	0.69
1:A:324:LYS:HB2	1:A:327:GLU:OE2	1.92	0.69
1:A:372:TYR:HB3	1:B:358:HIS:CE1	2.27	0.69
1:A:112:LEU:HG	1:A:113:MET:CE	2.22	0.69
1:A:345:ASN:N	1:A:345:ASN:HD22	1.89	0.69
1:A:295:VAL:O	1:A:387:LYS:HE3	1.91	0.69
1:B:435:THR:HB	3:B:1316:HOH:O	1.92	0.69
1:B:217:ASP:CG	1:B:221:ASN:HB2	2.18	0.68
1:B:72:ILE:HD12	1:B:73:THR:N	2.09	0.68
1:B:346:THR:OG1	1:B:348:LEU:HD12	1.94	0.67
1:B:419:ASP:O	1:B:423:ARG:HD2	1.94	0.67
1:B:323:ILE:HD12	1:B:323:ILE:N	2.09	0.67
1:A:278:LEU:N	1:A:287:ILE:HD11	2.10	0.66
1:B:252:LEU:HD22	1:B:284:PHE:HE1	1.59	0.66
1:A:427:ASP:OD2	1:A:429:ASN:HB2	1.96	0.66
1:A:440:LEU:HG	1:A:444:LEU:HD22	1.78	0.65
1:B:256:ILE:HD11	1:B:277:PHE:CE2	2.31	0.65
1:B:184:MET:O	1:B:188:GLU:HG3	1.96	0.65
1:A:82:TYR:CZ	1:A:295:VAL:HG22	2.32	0.65
1:A:93:GLU:OE1	1:A:111:ARG:NH1	2.29	0.65
1:A:63:ILE:HB	1:A:64:PRO:HD3	1.78	0.64
1:A:138:LEU:HD21	1:A:200:MET:HB2	1.79	0.64
1:B:288:LYS:NZ	2:B:1001:ATP:O3G	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:O	1:A:407:GLN:HG3	1.98	0.64
1:B:112:LEU:HG	1:B:113:MET:CE	2.27	0.64
1:A:231:SER:O	1:A:437:ILE:HA	1.96	0.64
1:B:80:PRO:HB2	1:B:86:SER:HA	1.80	0.63
1:A:274:THR:CB	1:A:294:GLN:HE21	2.10	0.63
1:B:113:MET:CE	1:B:119:ALA:HA	2.29	0.62
1:B:133:GLY:CA	1:B:152:ILE:HD11	2.29	0.62
1:B:116:LYS:O	1:B:120:ILE:HG13	1.99	0.62
1:A:311:GLU:OE2	1:A:314:ARG:NH1	2.33	0.61
1:A:203:TYR:C	1:A:204:LEU:HD12	2.25	0.61
1:A:207:PRO:CA	1:A:280:GLU:HG3	2.29	0.61
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.65	0.61
1:A:169:MET:HE1	2:A:1000:ATP:C5'	2.30	0.61
1:B:138:LEU:HD23	1:B:182:ILE:HG12	1.82	0.61
1:B:242:GLU:OE2	1:B:333:HIS:NE2	2.32	0.61
1:B:4:LYS:HB2	1:B:27:LYS:HB2	1.82	0.61
1:B:53:PRO:HB2	1:B:55:PRO:HD2	1.83	0.61
1:A:112:LEU:CD2	1:A:113:MET:HE3	2.31	0.60
1:B:186:ARG:HG2	1:B:198:VAL:HG13	1.83	0.60
1:A:36:ASP:HB3	1:A:39:LEU:HD12	1.83	0.60
1:B:427:ASP:OD1	1:B:443:LYS:HE2	2.01	0.60
1:A:184:MET:O	1:A:188:GLU:HG3	2.02	0.60
1:B:212:ILE:HD12	1:B:212:ILE:N	2.17	0.60
1:A:115:ASP:HB3	1:A:118:SER:OG	2.02	0.60
1:B:245:ALA:HB3	1:B:248:ILE:HG13	1.83	0.60
1:A:206:ASN:HD22	1:A:436:ASN:ND2	2.00	0.60
1:A:190:LYS:O	1:A:194:SER:HA	2.00	0.60
1:A:288:LYS:NZ	2:A:1000:ATP:O3G	2.31	0.60
1:B:154:TYR:HE1	1:B:172:VAL:CG1	2.14	0.59
1:B:19:ARG:HD2	3:B:1307:HOH:O	2.01	0.59
1:B:298:PRO:O	1:B:302:MET:HG2	2.03	0.59
1:A:5:ILE:HG23	1:A:26:ILE:CG2	2.32	0.59
1:B:124:LYS:NZ	1:B:135:ASP:OD2	2.29	0.59
1:B:425:MET:O	1:B:431:GLN:NE2	2.36	0.59
1:B:427:ASP:OD2	1:B:429:ASN:HB2	2.03	0.59
1:B:200:MET:HG3	1:B:201:GLU:N	2.17	0.58
1:B:112:LEU:HG	1:B:113:MET:HE2	1.83	0.58
1:B:441:GLU:O	1:B:446:LEU:HB2	2.02	0.58
1:A:249:THR:OG1	1:A:251:GLU:HG2	2.03	0.58
1:A:339:ILE:C	1:A:340:ASN:HD22	2.11	0.58
1:B:115:ASP:HB3	1:B:118:SER:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:O	1:A:258:GLU:HG3	2.04	0.58
1:A:358:HIS:O	1:A:409:LEU:HD12	2.04	0.58
1:A:112:LEU:HD23	1:A:113:MET:HE3	1.86	0.58
1:A:164:GLY:CA	1:A:193:PHE:HE2	2.17	0.58
1:A:379:PRO:HD3	3:A:1228:HOH:O	2.03	0.58
1:B:344:PRO:HG3	1:B:416:THR:O	2.04	0.58
1:A:154:TYR:HB3	1:A:155:PRO:HA	1.85	0.58
1:B:145:ASN:HD22	1:B:182:ILE:HD13	1.67	0.58
1:B:232:MET:HE2	3:B:1316:HOH:O	2.02	0.58
1:B:346:THR:CB	1:B:348:LEU:HD12	2.34	0.58
1:A:164:GLY:HA3	1:A:193:PHE:CE2	2.39	0.58
1:B:148:ILE:HA	1:B:151:ARG:HD2	1.86	0.58
1:A:63:ILE:CB	1:A:64:PRO:HD3	2.34	0.57
1:B:145:ASN:ND2	1:B:182:ILE:HD13	2.18	0.57
1:B:172:VAL:HG13	1:B:177:GLU:HB2	1.85	0.57
1:A:236:HIS:NE2	2:A:1000:ATP:O2G	2.37	0.57
1:A:275:PHE:CE1	1:A:289:MET:HE3	2.39	0.57
1:A:148:ILE:O	1:A:151:ARG:HB3	2.02	0.57
1:A:214:VAL:HG22	1:A:273:GLY:O	2.04	0.57
1:B:256:ILE:HD11	1:B:277:PHE:CZ	2.39	0.57
1:A:149:ALA:O	1:A:153:GLY:N	2.34	0.57
1:B:133:GLY:HA2	1:B:152:ILE:CD1	2.32	0.57
1:B:259:ARG:HH11	1:B:259:ARG:CG	2.16	0.57
1:B:370:HIS:CD2	1:B:370:HIS:H	2.22	0.57
1:B:72:ILE:HD12	1:B:72:ILE:C	2.30	0.57
1:A:53:PRO:HB2	1:A:55:PRO:HD2	1.87	0.57
1:A:141:ASP:O	1:A:144:LYS:HD2	2.05	0.57
1:A:142:MET:HE1	1:A:182:ILE:HD12	1.86	0.57
1:A:164:GLY:N	1:A:193:PHE:HE2	2.03	0.57
1:A:348:LEU:HD12	1:A:349:PRO:HD2	1.87	0.57
1:B:185:THR:O	1:B:188:GLU:N	2.38	0.57
1:A:296:GLU:OE2	1:A:296:GLU:N	2.37	0.56
1:B:37:ARG:HH11	1:B:37:ARG:CG	2.18	0.56
1:B:147:ALA:O	1:B:151:ARG:HB3	2.06	0.56
1:B:340:ASN:HD22	1:B:384:MET:CA	2.15	0.56
1:B:210:VAL:O	1:B:277:PHE:HB2	2.06	0.56
1:A:207:PRO:HB3	1:A:280:GLU:HG3	1.88	0.56
1:B:123:MET:HA	1:B:123:MET:HE2	1.87	0.56
1:B:278:LEU:HD22	1:B:287:ILE:CG1	2.35	0.55
1:A:277:PHE:C	1:A:287:ILE:HD11	2.32	0.55
1:A:421:GLN:HA	1:A:421:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:HB2	1:A:389:ILE:HG12	1.89	0.55
1:B:170:ARG:HE	1:B:181:SER:HA	1.71	0.55
1:B:216:ALA:O	1:B:315:ILE:HD13	2.07	0.55
1:B:63:ILE:HB	1:B:64:PRO:HD3	1.87	0.55
1:A:207:PRO:HA	1:A:280:GLU:HG3	1.88	0.55
1:B:141:ASP:OD1	1:B:144:LYS:HD2	2.08	0.55
1:A:12:GLU:OE2	1:A:387:LYS:NZ	2.34	0.54
1:B:105:PRO:HG2	1:B:110:ILE:CG1	2.37	0.54
1:B:164:GLY:N	1:B:193:PHE:HE2	2.05	0.54
1:A:72:ILE:HD12	1:A:72:ILE:C	2.32	0.54
1:A:274:THR:HG21	1:A:294:GLN:NE2	2.22	0.54
1:A:212:ILE:HD13	1:A:277:PHE:CD1	2.43	0.54
1:B:186:ARG:HG2	1:B:198:VAL:CG1	2.37	0.54
1:A:369:SER:HB2	1:A:385:ILE:O	2.07	0.54
1:A:236:HIS:CE1	2:A:1000:ATP:H5'2	2.42	0.54
1:B:75:ALA:O	1:B:100:PHE:HE1	1.91	0.54
1:B:163:GLY:C	1:B:193:PHE:HE2	2.15	0.54
1:A:54:ALA:HB3	1:A:55:PRO:CD	2.33	0.54
1:B:169:MET:HE1	2:B:1001:ATP:C5'	2.29	0.54
1:A:38:ASP:HB2	3:A:1327:HOH:O	2.08	0.54
1:A:106:LYS:HB2	1:A:108:GLU:HG3	1.90	0.53
1:B:62:ASN:OD1	1:B:64:PRO:HD2	2.08	0.53
1:B:165:GLY:HA2	2:B:1001:ATP:O3B	2.08	0.53
1:A:357:PHE:HA	1:A:410:ILE:O	2.08	0.53
1:A:443:LYS:C	1:A:445:GLY:H	2.15	0.53
1:B:388:LEU:O	1:B:402:MET:HE1	2.09	0.53
1:A:252:LEU:O	1:A:255:TYR:HB3	2.09	0.53
1:A:276:GLU:OE1	1:A:288:LYS:HE3	2.07	0.53
1:A:346:THR:HB	1:A:348:LEU:HB2	1.89	0.53
1:B:278:LEU:CG	1:B:287:ILE:HD11	2.38	0.53
1:A:402:MET:O	1:A:406:LEU:HG	2.09	0.53
1:B:190:LYS:O	1:B:194:SER:HA	2.08	0.53
1:A:261:ALA:O	1:A:265:VAL:HG23	2.09	0.53
1:B:152:ILE:CD1	1:B:200:MET:HG2	2.38	0.53
1:A:1:MET:HE1	1:A:314:ARG:HG2	1.91	0.52
1:A:129:PRO:HG2	1:A:256:ILE:CD1	2.39	0.52
1:A:143:ASP:OD2	1:A:146:ARG:NH1	2.43	0.52
1:B:211:GLU:C	1:B:212:ILE:HD12	2.33	0.52
1:A:193:PHE:CD1	1:A:193:PHE:N	2.76	0.52
1:A:227:GLU:H	1:A:227:GLU:CD	2.18	0.52
1:B:19:ARG:O	1:B:23:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:HB3	1:B:437:ILE:HG22	1.90	0.52
1:A:425:MET:O	1:A:431:GLN:NE2	2.43	0.52
1:B:93:GLU:O	1:B:97:ARG:HB2	2.09	0.52
1:A:68:SER:O	1:A:72:ILE:HG13	2.08	0.52
1:A:165:GLY:N	2:A:1000:ATP:O1B	2.43	0.52
1:B:346:THR:HB	1:B:348:LEU:HD12	1.91	0.52
1:A:411:ILE:HG22	1:A:411:ILE:O	2.10	0.52
1:A:421:GLN:O	1:A:425:MET:HG2	2.10	0.52
1:B:145:ASN:HD22	1:B:182:ILE:CD1	2.22	0.52
1:A:413:GLY:O	1:A:414:ILE:HG23	2.10	0.52
1:B:441:GLU:CG	1:B:446:LEU:HD13	2.40	0.52
1:A:206:ASN:N	1:A:280:GLU:OE2	2.43	0.52
1:B:261:ALA:O	1:B:264:CYS:HB2	2.09	0.52
1:B:314:ARG:O	1:B:319:GLN:HB2	2.09	0.52
1:B:101:ILE:O	1:B:101:ILE:HG22	2.09	0.51
1:B:195:ASN:C	1:B:197:MET:H	2.16	0.51
1:B:85:LEU:HB3	1:B:91:PHE:CD1	2.45	0.51
1:B:109:THR:O	1:B:112:LEU:HB3	2.11	0.51
1:A:133:GLY:HA3	1:A:200:MET:O	2.11	0.51
1:B:297:HIS:CD2	1:B:298:PRO:HD3	2.44	0.51
1:A:360:PRO:HD3	1:A:409:LEU:HD13	1.92	0.51
1:B:164:GLY:HA3	1:B:193:PHE:CE2	2.46	0.51
1:A:353:LYS:HE3	1:A:374:GLY:HA2	1.93	0.51
1:B:346:THR:HB	1:B:348:LEU:CD1	2.41	0.51
1:A:164:GLY:HA3	1:A:193:PHE:HE2	1.76	0.50
1:B:224:TYR:C	1:B:225:LEU:HG	2.36	0.50
1:B:440:LEU:O	1:B:444:LEU:HD22	2.12	0.50
1:A:204:LEU:HD12	1:A:204:LEU:N	2.25	0.50
1:A:388:LEU:O	1:A:402:MET:HE1	2.11	0.50
1:B:4:LYS:HD2	1:B:75:ALA:HA	1.93	0.50
1:B:6:VAL:HB	1:B:78:ILE:HG12	1.93	0.50
1:A:391:TYR:O	1:A:401:ARG:NH1	2.41	0.50
1:A:399:ILE:HD13	1:A:430:PHE:CE1	2.47	0.50
1:B:113:MET:HE2	1:B:119:ALA:HA	1.94	0.50
1:B:297:HIS:N	1:B:298:PRO:HD2	2.27	0.50
1:A:158:ILE:HD11	1:A:200:MET:HE2	1.94	0.50
1:B:148:ILE:HG22	1:B:152:ILE:HD12	1.93	0.49
1:A:203:TYR:CD1	2:A:1000:ATP:C2	3.00	0.49
1:A:340:ASN:HD22	1:A:340:ASN:N	2.08	0.49
1:B:343:ASP:O	1:B:347:PHE:N	2.45	0.49
1:A:164:GLY:CA	1:A:193:PHE:CE2	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ILE:HG22	1:B:324:LYS:N	2.27	0.49
1:B:427:ASP:OD2	1:B:429:ASN:N	2.44	0.49
1:A:251:GLU:CD	1:A:251:GLU:H	2.20	0.49
1:B:105:PRO:HG2	1:B:110:ILE:HG13	1.94	0.49
1:B:325:GLN:O	1:B:327:GLU:N	2.46	0.49
1:B:346:THR:O	1:B:347:PHE:HB2	2.13	0.49
1:B:419:ASP:HB3	1:B:423:ARG:HH11	1.76	0.49
1:A:201:GLU:OE2	2:A:1000:ATP:N6	2.38	0.49
1:A:207:PRO:CB	1:A:280:GLU:HG3	2.43	0.49
1:A:249:THR:HG23	1:A:252:LEU:HD12	1.95	0.49
1:B:358:HIS:O	1:B:409:LEU:HA	2.13	0.49
1:A:302:MET:HE3	1:A:391:TYR:HB2	1.95	0.49
1:A:370:HIS:CD2	1:A:370:HIS:N	2.80	0.49
1:A:399:ILE:HD13	1:A:430:PHE:HE1	1.78	0.49
1:A:241:GLU:OE1	1:A:338:ARG:NE	2.41	0.48
1:B:297:HIS:ND1	1:B:298:PRO:HD3	2.28	0.48
1:A:196:ASP:O	1:A:198:VAL:HG13	2.14	0.48
1:A:236:HIS:HE2	2:A:1000:ATP:PG	2.37	0.48
1:B:154:TYR:HA	1:B:155:PRO:C	2.39	0.48
1:A:217:ASP:OD1	1:A:221:ASN:HB2	2.14	0.48
1:B:233:GLN:O	1:B:440:LEU:HB3	2.13	0.48
1:B:133:GLY:C	1:B:152:ILE:HD11	2.39	0.48
1:B:62:ASN:O	1:B:66:ILE:HG13	2.14	0.48
1:B:13:ILE:HD12	1:B:13:ILE:HA	1.63	0.48
1:A:204:LEU:N	1:A:204:LEU:CD1	2.76	0.47
1:A:62:ASN:ND2	1:A:65:ALA:HB2	2.29	0.47
1:A:186:ARG:HG2	1:A:196:ASP:O	2.14	0.47
1:A:133:GLY:HA2	1:A:152:ILE:HD13	1.95	0.47
1:B:16:ARG:HA	3:B:1307:HOH:O	2.14	0.47
1:B:301:GLU:CG	1:B:308:LEU:HD12	2.45	0.47
1:B:16:ARG:CZ	1:B:309:ILE:HG13	2.45	0.47
1:B:156:VAL:HG13	1:B:157:ILE:N	2.29	0.47
1:A:211:GLU:C	1:A:212:ILE:HD12	2.40	0.47
1:B:37:ARG:CG	1:B:37:ARG:NH1	2.78	0.47
1:B:64:PRO:O	1:B:68:SER:HB2	2.15	0.47
1:B:133:GLY:HA2	1:B:201:GLU:HA	1.97	0.46
1:B:297:HIS:N	1:B:298:PRO:CD	2.79	0.46
1:A:206:ASN:HD22	1:A:436:ASN:HD21	1.61	0.46
1:B:113:MET:HE1	1:B:119:ALA:HA	1.98	0.46
1:B:252:LEU:HD22	1:B:284:PHE:CE1	2.46	0.46
1:A:92:ALA:O	1:A:96:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG13	1:A:100:PHE:HB2	1.96	0.46
1:B:440:LEU:O	1:B:444:LEU:HB2	2.15	0.46
1:A:196:ASP:N	1:A:196:ASP:OD2	2.46	0.46
1:B:113:MET:HE1	1:B:122:ALA:HB3	1.97	0.46
1:B:380:TYR:HB2	1:B:381:TYR:CE1	2.51	0.46
1:A:443:LYS:C	1:A:445:GLY:N	2.73	0.46
1:B:63:ILE:N	1:B:64:PRO:CD	2.79	0.46
1:A:4:LYS:HE2	1:A:47:GLU:OE2	2.16	0.46
1:A:85:LEU:HB3	1:A:91:PHE:CD1	2.51	0.46
1:A:159:LYS:HE3	2:A:1000:ATP:N7	2.31	0.46
1:A:399:ILE:CD1	1:A:430:PHE:CE1	2.98	0.46
1:B:180:GLN:HB3	1:B:184:MET:SD	2.56	0.46
1:A:163:GLY:C	1:A:193:PHE:HE2	2.24	0.46
1:A:232:MET:CB	1:A:240:VAL:HB	2.46	0.46
1:B:112:LEU:HG	1:B:113:MET:HE3	1.97	0.46
1:B:152:ILE:HG21	1:B:156:VAL:HG22	1.97	0.46
1:B:295:VAL:HG11	1:B:338:ARG:CZ	2.46	0.46
1:A:131:VAL:HG12	1:A:132:PRO:N	2.31	0.46
1:A:117:VAL:HG23	1:A:161:SER:OG	2.17	0.45
1:A:225:LEU:O	1:A:226:ALA:HB3	2.14	0.45
1:A:297:HIS:N	1:A:298:PRO:CD	2.79	0.45
1:B:18:LEU:C	1:B:18:LEU:HD23	2.40	0.45
1:A:62:ASN:HB3	1:A:65:ALA:HB3	1.98	0.45
1:A:193:PHE:HD1	1:A:193:PHE:H	1.63	0.45
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.82	0.45
1:B:335:VAL:HG12	1:B:336:GLU:N	2.31	0.45
1:B:309:ILE:O	1:B:312:GLN:HB2	2.17	0.45
1:A:5:ILE:HG23	1:A:26:ILE:HG21	1.97	0.45
1:A:37:ARG:NH2	1:A:50:CYS:SG	2.89	0.45
1:A:212:ILE:HD13	1:A:277:PHE:CE1	2.51	0.45
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.46	0.45
1:A:274:THR:CB	1:A:294:GLN:NE2	2.79	0.45
1:A:292:ARG:HG3	1:A:293:ILE:O	2.17	0.45
1:B:152:ILE:HG21	1:B:156:VAL:CG2	2.46	0.45
1:B:443:LYS:C	1:B:445:GLY:H	2.24	0.45
1:B:165:GLY:N	2:B:1001:ATP:O1B	2.48	0.45
1:B:301:GLU:HG3	1:B:308:LEU:HD12	1.98	0.45
1:A:348:LEU:HD12	1:A:348:LEU:HA	1.79	0.45
1:B:303:ILE:HD12	1:B:330:VAL:HG22	1.99	0.45
1:B:138:LEU:HD12	1:B:138:LEU:HA	1.75	0.45
1:B:142:MET:N	1:B:142:MET:SD	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:ILE:HG22	1:B:403:LYS:HD2	1.99	0.44
1:B:307:ASP:O	1:B:311:GLU:HG2	2.18	0.44
1:B:259:ARG:CG	1:B:259:ARG:NH1	2.78	0.44
1:B:315:ILE:HD11	1:B:321:LEU:HD21	1.99	0.44
1:A:77:ALA:HB2	1:A:101:ILE:HB	2.00	0.44
1:A:89:ALA:O	1:A:93:GLU:HB2	2.18	0.44
1:A:363:PHE:O	1:A:401:ARG:HD3	2.16	0.44
1:B:164:GLY:CA	1:B:193:PHE:CE2	3.00	0.44
1:B:200:MET:CG	1:B:201:GLU:N	2.80	0.44
1:B:378:PRO:HA	1:B:379:PRO:HD3	1.77	0.44
1:A:307:ASP:O	1:A:311:GLU:HG2	2.16	0.44
1:A:233:GLN:O	1:A:440:LEU:HB3	2.18	0.44
1:A:278:LEU:HD22	1:A:287:ILE:HG12	1.99	0.44
1:A:340:ASN:H	1:A:417:ASN:CG	2.23	0.44
1:B:32:HIS:HE1	1:B:37:ARG:HH11	1.66	0.44
1:A:144:LYS:O	1:A:147:ALA:HB3	2.18	0.43
1:B:427:ASP:OD1	1:B:439:TYR:OH	2.30	0.43
1:B:403:LYS:HG3	1:B:425:MET:HB3	2.00	0.43
1:B:421:GLN:O	1:B:425:MET:HG2	2.19	0.43
1:B:193:PHE:O	1:B:194:SER:HB2	2.18	0.43
1:A:197:MET:C	1:A:198:VAL:HG13	2.42	0.43
1:A:212:ILE:HD12	1:A:212:ILE:N	2.32	0.43
1:A:427:ASP:HB3	1:A:430:PHE:CB	2.49	0.43
1:A:116:LYS:O	1:A:119:ALA:HB3	2.19	0.43
1:A:278:LEU:HD12	1:A:278:LEU:HA	1.83	0.43
1:B:195:ASN:OD1	1:B:197:MET:HB2	2.18	0.43
1:A:444:LEU:HA	1:A:444:LEU:HD12	1.40	0.43
1:A:348:LEU:HA	1:A:349:PRO:HD2	1.76	0.43
1:A:440:LEU:HD12	1:A:440:LEU:HA	1.78	0.43
1:B:156:VAL:HG11	1:B:200:MET:SD	2.58	0.43
1:A:108:GLU:H	1:A:108:GLU:HG2	1.21	0.43
1:A:110:ILE:HD13	1:A:110:ILE:HG21	1.73	0.43
1:B:164:GLY:CA	1:B:193:PHE:HE2	2.31	0.43
1:A:232:MET:CG	1:A:240:VAL:HB	2.49	0.42
1:A:217:ASP:HA	1:A:315:ILE:HG12	2.00	0.42
1:B:67:ILE:O	1:B:70:ALA:HB3	2.19	0.42
1:B:212:ILE:N	1:B:212:ILE:CD1	2.82	0.42
1:A:298:PRO:HB3	1:A:366:ARG:CZ	2.49	0.42
1:B:117:VAL:HG23	1:B:161:SER:OG	2.18	0.42
1:B:294:GLN:HE21	1:B:294:GLN:HB3	1.49	0.42
1:A:48:THR:C	1:A:49:VAL:HG23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:C	1:A:207:PRO:HD3	2.45	0.42
1:B:157:ILE:HB	1:B:203:TYR:HB2	2.02	0.42
1:B:243:ALA:HA	1:B:244:PRO:C	2.44	0.42
1:A:280:GLU:O	1:A:281:ASN:HB2	2.20	0.42
1:A:298:PRO:HB3	1:A:366:ARG:NH1	2.34	0.42
1:B:40:LYS:HA	1:B:40:LYS:HD3	1.81	0.42
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.80	0.42
1:B:424:ILE:C	1:B:426:ASN:N	2.74	0.42
1:A:342:GLU:O	1:A:344:PRO:HD3	2.20	0.42
1:B:33:SER:HB2	1:B:53:PRO:O	2.19	0.42
1:B:256:ILE:HD13	1:B:284:PHE:CG	2.54	0.42
1:B:325:GLN:C	1:B:327:GLU:H	2.28	0.42
1:A:1(A):HIS:HA	3:A:1239:HOH:O	2.19	0.42
1:A:17:ILE:O	1:A:17:ILE:HG22	2.15	0.42
1:A:31:VAL:O	1:A:31:VAL:HG23	2.18	0.42
1:A:436:ASN:C	1:A:438:HIS:H	2.26	0.42
1:B:133:GLY:HA3	1:B:200:MET:O	2.20	0.41
1:B:213:GLN:O	1:B:225:LEU:HD12	2.19	0.41
1:A:78:ILE:C	1:A:103:ILE:HD12	2.45	0.41
1:A:209:HIS:CD2	1:A:209:HIS:C	2.98	0.41
1:B:364:GLY:O	1:B:390:CYS:HA	2.20	0.41
1:A:354:ILE:O	1:A:374:GLY:N	2.47	0.41
1:B:101:ILE:HG21	1:B:101:ILE:HD13	1.80	0.41
1:B:236:HIS:HE2	2:B:1001:ATP:PG	2.44	0.41
1:A:410:ILE:O	1:A:410:ILE:HG22	2.12	0.41
1:B:200:MET:HE2	1:B:200:MET:HB2	1.55	0.41
1:B:116:LYS:O	1:B:119:ALA:HB3	2.20	0.41
1:B:368:GLU:HB2	1:B:387:LYS:HB2	2.03	0.41
1:A:6:VAL:HG12	1:A:7:ILE:N	2.34	0.41
1:B:31:VAL:HB	1:B:51:ILE:CG2	2.51	0.41
1:B:419:ASP:HB3	1:B:423:ARG:HH12	1.81	0.41
1:B:217:ASP:OD1	1:B:221:ASN:HB2	2.21	0.41
1:A:1(B):SER:C	1:A:1(A):HIS:CD2	2.98	0.41
1:A:152:ILE:HD13	1:A:152:ILE:HG21	1.62	0.41
1:A:262:LYS:HE2	1:A:266:ASP:OD1	2.21	0.41
1:A:63:ILE:CB	1:A:64:PRO:CD	2.99	0.41
1:A:157:ILE:HG13	1:A:171:VAL:HG22	2.03	0.41
1:A:296:GLU:O	1:A:299:VAL:HG22	2.20	0.41
1:A:393:GLU:OE2	1:A:393:GLU:N	2.43	0.41
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.91	0.41
1:A:427:ASP:HB3	1:A:430:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PRO:HG2	1:A:256:ILE:HD11	2.03	0.40
1:B:23:GLU:OE1	1:B:310:LYS:HE3	2.20	0.40
1:B:12:GLU:OE2	1:B:387:LYS:NZ	2.53	0.40
1:B:152:ILE:CG2	1:B:156:VAL:CG2	2.99	0.40
1:A:142:MET:CE	1:A:179:ALA:HA	2.47	0.40
1:A:152:ILE:CG2	1:A:202:LYS:HB2	2.52	0.40
1:A:193:PHE:O	1:A:194:SER:HB2	2.21	0.40
1:B:343:ASP:O	1:B:347:PHE:HA	2.22	0.40
1:A:54:ALA:CB	1:A:55:PRO:HD3	2.36	0.40
1:B:79:HIS:ND1	1:B:79:HIS:C	2.80	0.40
1:B:254:ARG:O	1:B:258:GLU:HB2	2.22	0.40
1:B:323:ILE:H	1:B:323:ILE:CD1	2.25	0.40
1:B:325:GLN:C	1:B:327:GLU:N	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/452 (99%)	406 (90%)	41 (9%)	2 (0%)	30	49
1	B	446/452 (99%)	407 (91%)	32 (7%)	7 (2%)	7	14
All	All	895/904 (99%)	813 (91%)	73 (8%)	9 (1%)	12	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	MET
1	B	181	SER
1	B	179	ALA
1	B	196	ASP
1	B	226	ALA

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Mol	Chain	Res	Type
1	A	382	ASP
1	B	326	GLU
1	B	444	LEU
1	B	83	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	362/363 (100%)	295 (82%)	67 (18%)	1	3
1	B	360/363 (99%)	286 (79%)	74 (21%)	1	2
All	All	722/726 (99%)	581 (80%)	141 (20%)	1	2

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(B)	SER
1	A	1(A)	HIS
1	A	1	MET
1	A	3	ASP
1	A	5	ILE
1	A	18	LEU
1	A	27	LYS
1	A	48	THR
1	A	67	ILE
1	A	68	SER
1	A	86	SER
1	A	94	GLN
1	A	101	ILE
1	A	106	LYS
1	A	108	GLU
1	A	111	ARG
1	A	118	SER
1	A	124	LYS
1	A	125	LYS

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Mol	Chain	Res	Type
1	A	138	LEU
1	A	140	ASP
1	A	141	ASP
1	A	142	MET
1	A	144	LYS
1	A	146	ARG
1	A	148	ILE
1	A	157	ILE
1	A	159	LYS
1	A	161	SER
1	A	170	ARG
1	A	172	VAL
1	A	173	ARG
1	A	177	GLU
1	A	184	MET
1	A	186	ARG
1	A	193	PHE
1	A	205	GLU
1	A	223	ILE
1	A	232	MET
1	A	237	GLN
1	A	248	ILE
1	A	251	GLU
1	A	252	LEU
1	A	254	ARG
1	A	259	ARG
1	A	262	LYS
1	A	278	LEU
1	A	293	ILE
1	A	300	THR
1	A	303	ILE
1	A	324	LYS
1	A	326	GLU
1	A	345	ASN
1	A	348	LEU
1	A	369	SER
1	A	371	ILE
1	A	399	ILE
1	A	404	ASN
1	A	410	ILE
1	A	428	GLU
1	A	431	GLN

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Mol	Chain	Res	Type
1	A	441	GLU
1	A	442	LYS
1	A	443	LYS
1	A	444	LEU
1	A	446	LEU
1	A	447	GLN
1	B	3	ASP
1	B	4	LYS
1	B	5	ILE
1	B	22	LYS
1	B	37	ARG
1	B	48	THR
1	B	63	ILE
1	B	68	SER
1	B	82	TYR
1	B	86	SER
1	B	94	GLN
1	B	97	ARG
1	B	101	ILE
1	B	103	ILE
1	B	111	ARG
1	B	120	ILE
1	B	124	LYS
1	B	138	LEU
1	B	140	ASP
1	B	142	MET
1	B	144	LYS
1	B	151	ARG
1	B	152	ILE
1	B	156	VAL
1	B	157	ILE
1	B	158	ILE
1	B	161	SER
1	B	167	ARG
1	B	170	ARG
1	B	171	VAL
1	B	173	ARG
1	B	177	GLU
1	B	178	LEU
1	B	180	GLN
1	B	182	ILE
1	B	184	MET

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Mol	Chain	Res	Type
1	B	186	ARG
1	B	198	VAL
1	B	200	MET
1	B	202	LYS
1	B	205	GLU
1	B	219	GLN
1	B	225	LEU
1	B	231	SER
1	B	234	ARG
1	B	235	ARG
1	B	249	THR
1	B	251	GLU
1	B	252	LEU
1	B	259	ARG
1	B	262	LYS
1	B	266	ASP
1	B	278	LEU
1	B	288	LYS
1	B	289	MET
1	B	294	GLN
1	B	308	LEU
1	B	310	LYS
1	B	322	SER
1	B	323	ILE
1	B	324	LYS
1	B	326	GLU
1	B	331	ARG
1	B	345	ASN
1	B	353	LYS
1	B	399	ILE
1	B	403	LYS
1	B	423	ARG
1	B	431	GLN
1	B	435	THR
1	B	443	LYS
1	B	444	LEU
1	B	446	LEU
1	B	447	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1(A)	HIS
1	A	206	ASN
1	A	294	GLN
1	A	319	GLN
1	A	340	ASN
1	A	345	ASN
1	A	370	HIS
1	A	447	GLN
1	B	94	GLN
1	B	145	ASN
1	B	180	GLN
1	B	209	HIS
1	B	219	GLN
1	B	281	ASN
1	B	319	GLN
1	B	340	ASN
1	B	345	ASN
1	B	358	HIS
1	B	370	HIS
1	B	404	ASN
1	B	426	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	1000	-	32,33,33	2.19	5 (15%)	48,52,52	1.35	7 (14%)
2	ATP	B	1001	-	32,33,33	2.12	5 (15%)	48,52,52	1.20	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	1000	-	-	3/22/38/38	0/3/3/3
2	ATP	B	1001	-	-	7/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	ATP	C2'-C3'	-8.60	1.30	1.53
2	B	1001	ATP	C2'-C3'	-8.08	1.31	1.53
2	A	1000	ATP	PA-O3A	-6.33	1.52	1.59
2	B	1001	ATP	PB-O3A	6.04	1.66	1.59
2	B	1001	ATP	PA-O3A	-3.17	1.56	1.59
2	B	1001	ATP	PB-O3B	-2.44	1.56	1.59
2	A	1000	ATP	C2-N3	-2.39	1.29	1.33
2	A	1000	ATP	PB-O3A	2.33	1.62	1.59
2	B	1001	ATP	C2-N3	-2.12	1.30	1.33
2	A	1000	ATP	PB-O3B	-2.05	1.57	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ATP	O3B-PB-O1B	4.56	124.42	110.70
2	A	1000	ATP	C3'-C2'-C1'	3.72	108.50	101.46
2	B	1001	ATP	C3'-C2'-C1'	3.64	108.34	101.46
2	B	1001	ATP	C2'-C3'-C4'	3.23	108.85	102.61
2	B	1001	ATP	O2A-PA-O3A	2.54	114.14	107.27
2	A	1000	ATP	O2B-PB-O3B	2.51	114.07	107.27
2	B	1001	ATP	O4'-C1'-N9	2.40	112.69	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ATP	O2B-PB-O3B	2.36	113.65	107.27
2	A	1000	ATP	O4'-C4'-C3'	-2.22	100.75	105.15
2	A	1000	ATP	O4'-C1'-C2'	-2.14	102.03	106.62
2	A	1000	ATP	O3G-PG-O3B	2.06	111.56	104.64
2	A	1000	ATP	O2A-PA-O3A	2.01	112.72	107.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

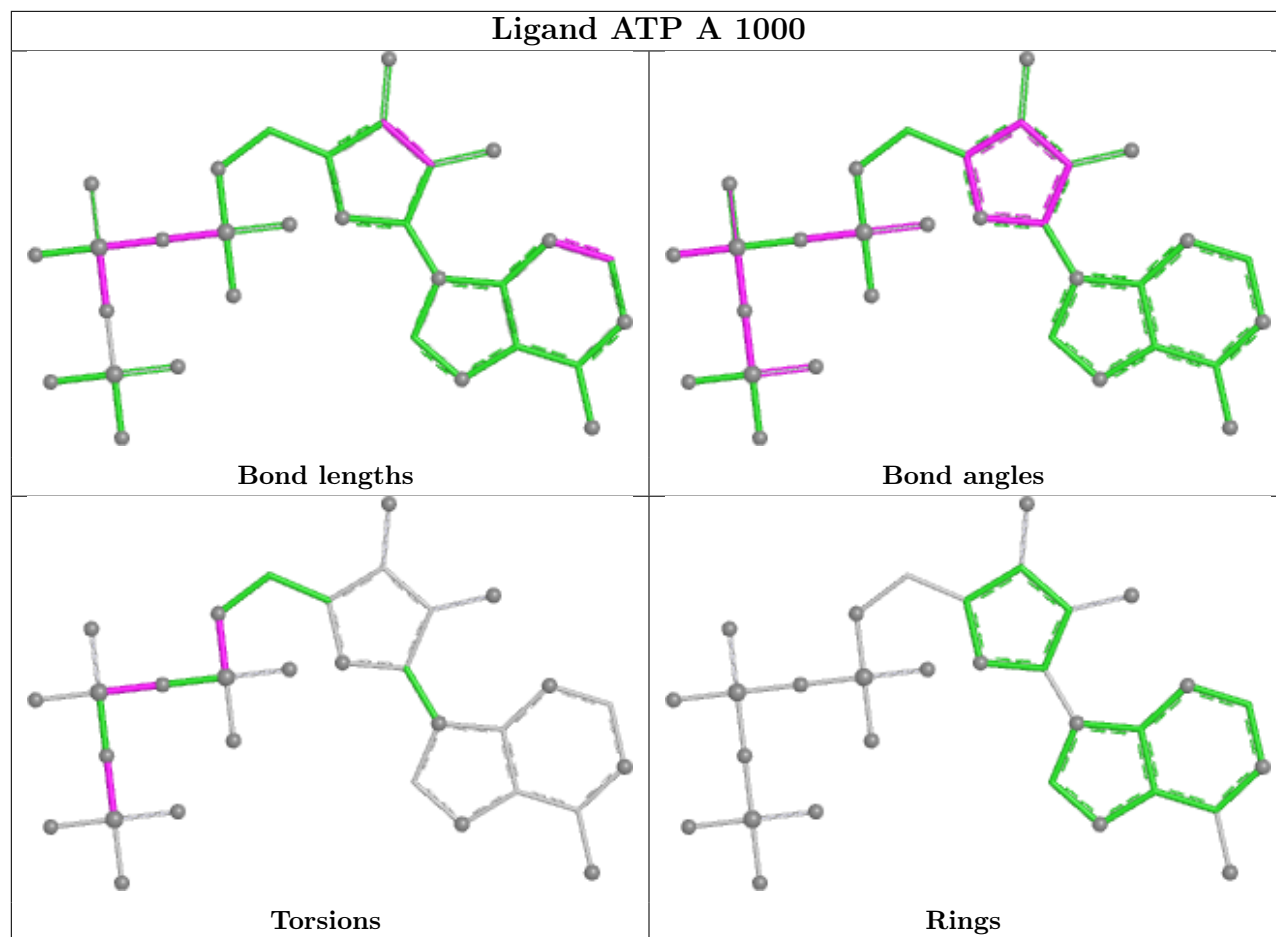
Mol	Chain	Res	Type	Atoms
2	A	1000	ATP	C5'-O5'-PA-O3A
2	B	1001	ATP	C5'-O5'-PA-O2A
2	A	1000	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PA-O3A-PB-O2B
2	B	1001	ATP	C5'-O5'-PA-O1A
2	B	1001	ATP	C5'-O5'-PA-O3A
2	B	1001	ATP	PG-O3B-PB-O2B
2	A	1000	ATP	PB-O3B-PG-O2G
2	B	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PG-O3B-PB-O1B

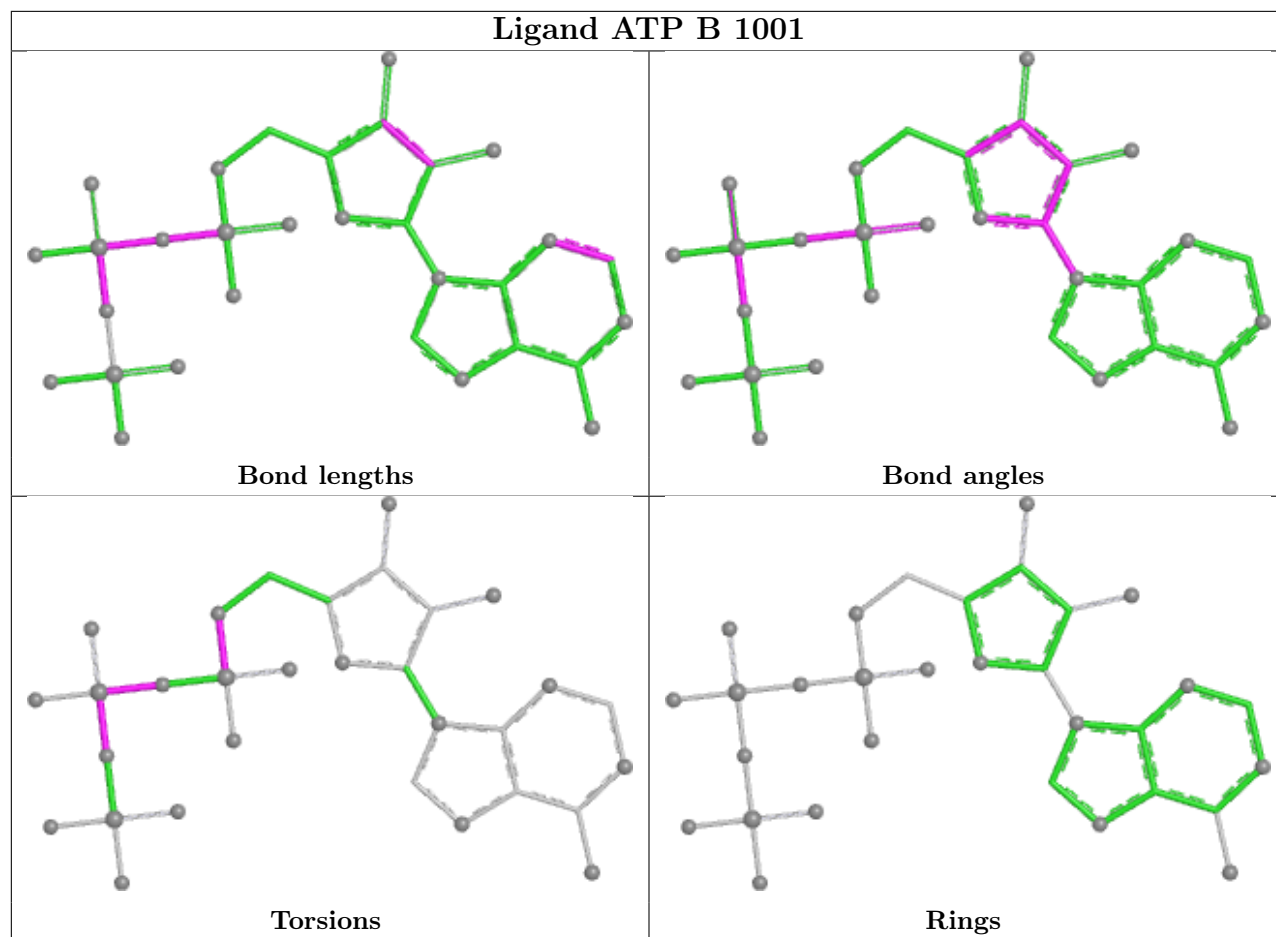
There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	ATP	10	0
2	B	1001	ATP	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.