



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 03:17 PM UTC

PDB ID : 8ZI0 / pdb_00008zi0
EMDB ID : EMD-60117
Title : Cryo-EM reveals transition states of the *Acinetobacter baumannii* F1-ATPase rotary subunits gamma and epsilon and novel compound targets - Conformation 1
Authors : Le, K.C.M.; Wong, C.F.; Gruber, G.
Deposited on : 2024-05-12
Resolution : 3.18 Å (reported)
Based on initial model : 7YRY

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

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

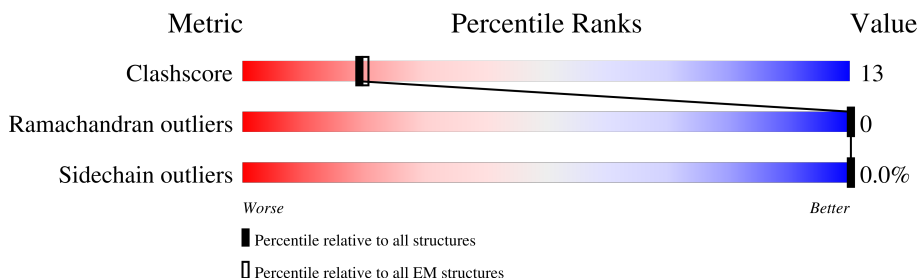
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	514	79% 16% 5%
1	B	514	77% 18% 5%
1	C	514	79% 16% 5%
2	D	464	83% 17%
2	E	464	70% 29%
2	F	464	77% 23%
3	e	133	55% 44% .
4	g	289	58% 41%

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
5	ATP	B	601	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25014 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	489	Total	C	N	O	S	0	0
			3702	2333	635	719	15		
1	B	489	Total	C	N	O	S	0	0
			3703	2333	635	720	15		
1	C	489	Total	C	N	O	S	0	0
			3703	2333	635	720	15		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	463	Total	C	N	O	S	0	0
			3525	2223	602	687	13		
2	E	463	Total	C	N	O	S	0	0
			3525	2223	602	687	13		
2	F	463	Total	C	N	O	S	0	0
			3525	2223	602	687	13		

- Molecule 3 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	132	Total	C	N	O	S	0	0
			959	601	163	192	3		

- Molecule 4 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	288	Total	C	N	O	S	0	0
			2243	1411	400	420	12		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

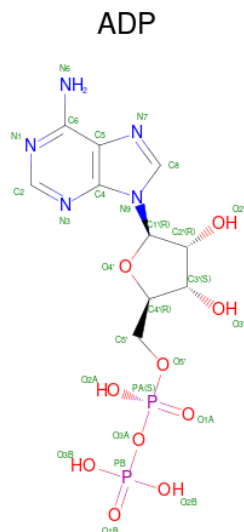


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	C	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

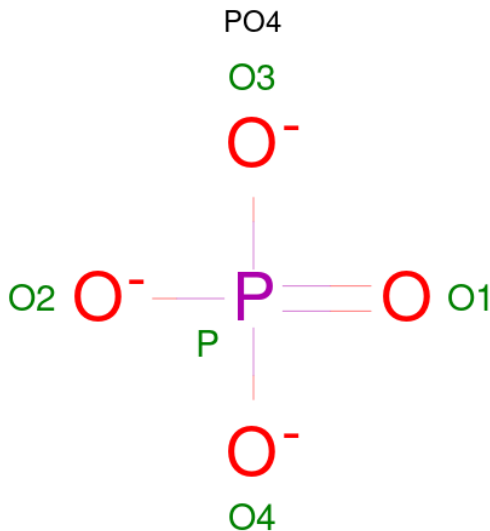
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Mg 1 1	0
6	B	1	Total Mg 1 1	0
6	C	1	Total Mg 1 1	0
6	D	1	Total Mg 1 1	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

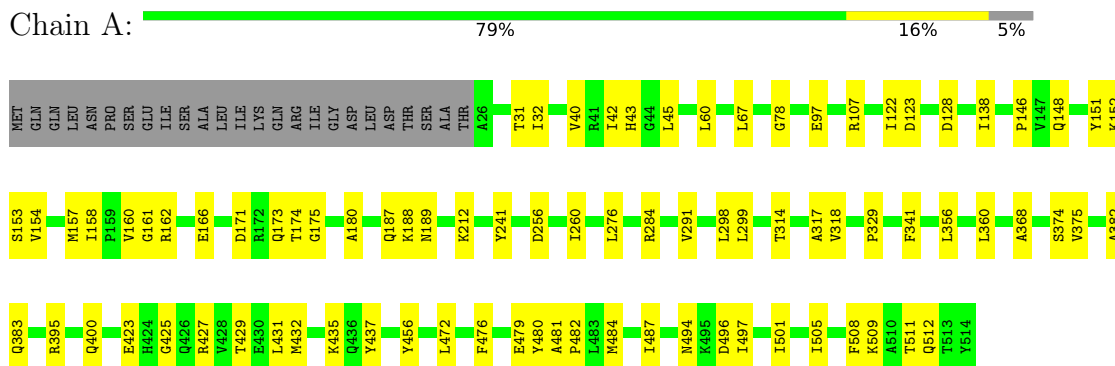


Mol	Chain	Residues	Atoms			AltConf
8	E	1	Total	O	P	0
			5	4	1	

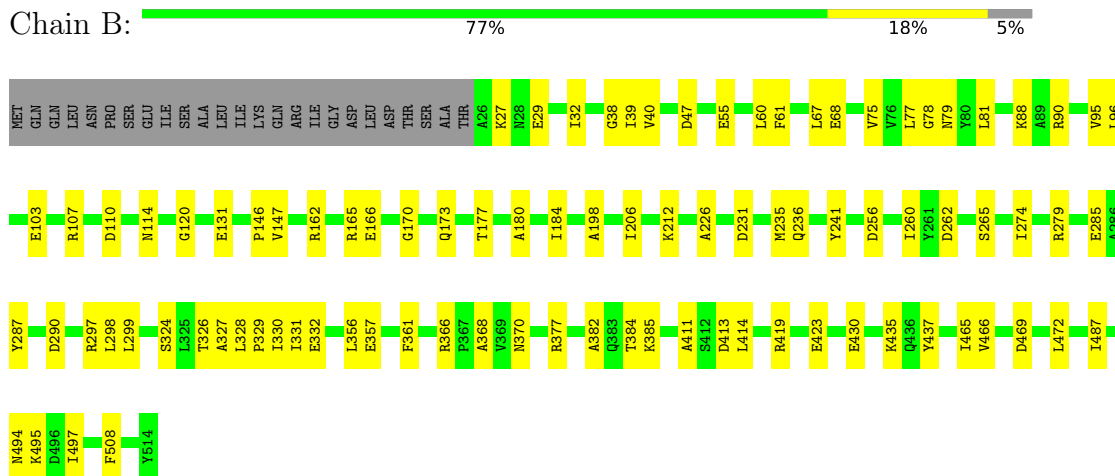
3 Residue-property plots

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.

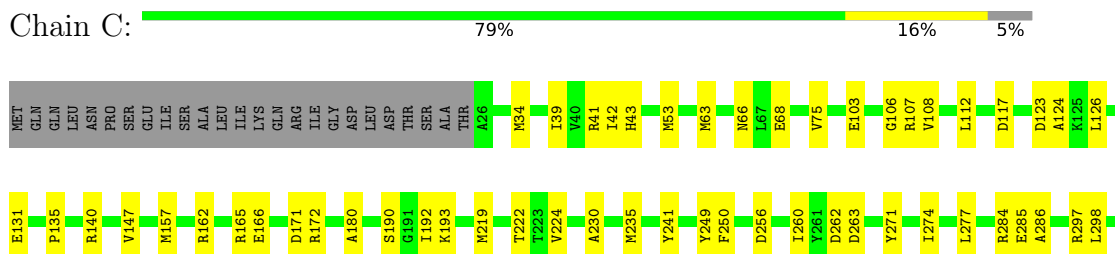
- Molecule 1: ATP synthase subunit alpha



- Molecule 1: ATP synthase subunit alpha

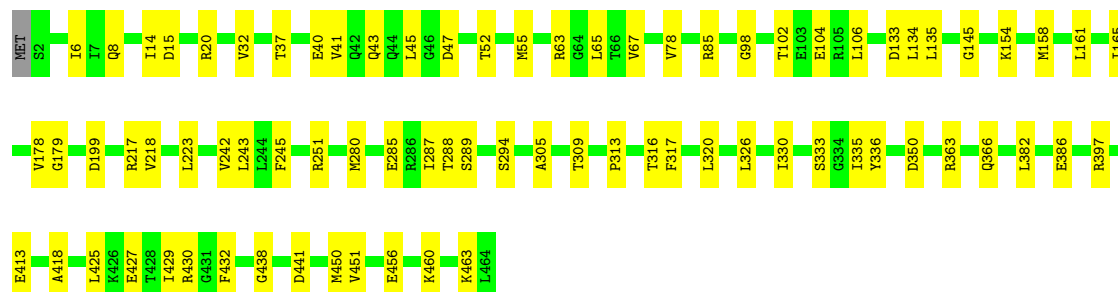
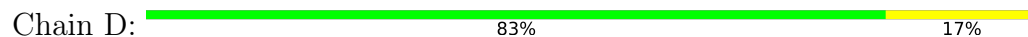


- Molecule 1: ATP synthase subunit alpha

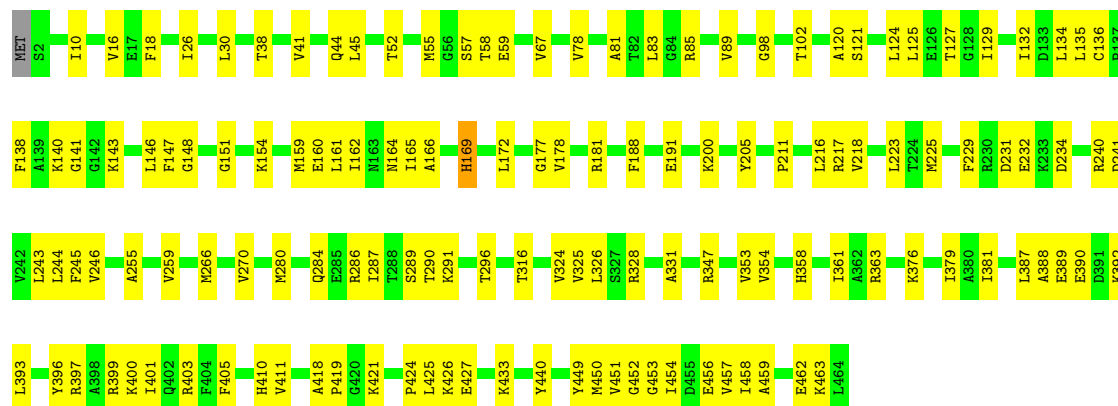




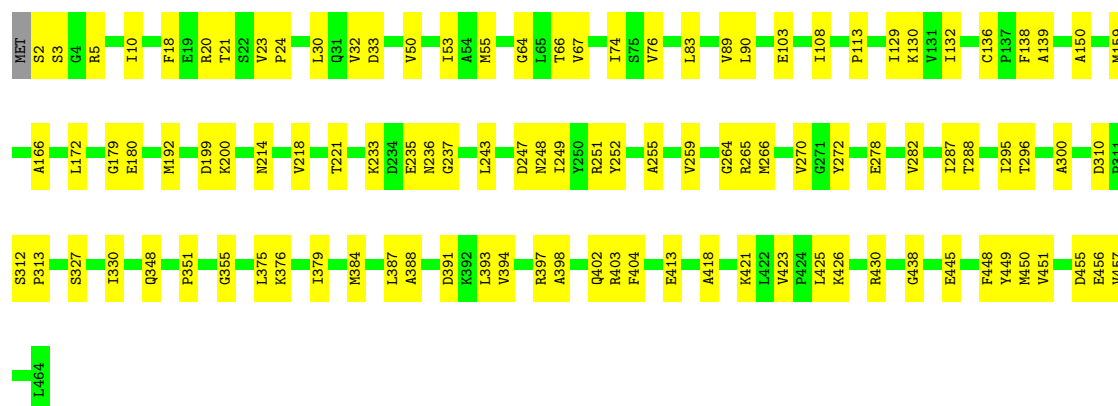
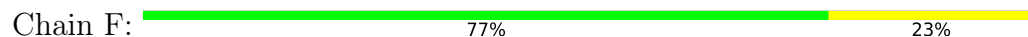
• Molecule 2: ATP synthase subunit beta



• Molecule 2: ATP synthase subunit beta

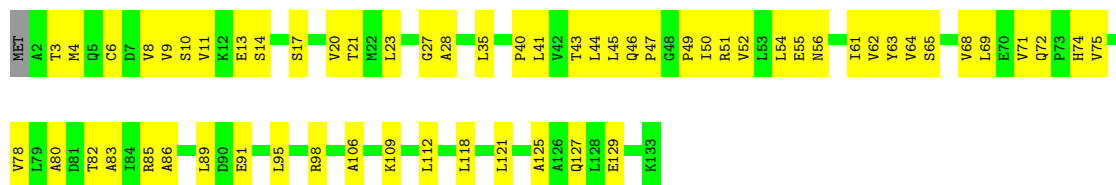


• Molecule 2: ATP synthase subunit beta



• Molecule 3: ATP synthase epsilon chain

Chain e:  55% 44%



● Molecule 4: ATP synthase gamma chain

Chain g:  58% 41%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	160000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: ADP, ATP, MG, PO4

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	0.41	0/3758	0.57	0/5086
1	B	0.51	0/3759	0.70	0/5086
1	C	0.53	0/3759	0.69	0/5086
2	D	0.45	0/3582	0.64	0/4854
2	E	0.55	0/3582	0.79	0/4854
2	F	0.55	0/3582	0.77	0/4854
3	e	0.63	0/967	0.81	0/1317
4	g	0.55	0/2273	0.75	0/3062
All	All	0.51	0/25262	0.71	0/34199

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3702	0	3729	74	0
1	B	3703	0	3729	90	0
1	C	3703	0	3728	59	0
2	D	3525	0	3555	61	0
2	E	3525	0	3555	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3525	0	3555	77	0
3	e	959	0	992	74	0
4	g	2243	0	2294	107	0
5	A	31	0	12	4	0
5	B	31	0	12	14	0
5	C	31	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	D	27	0	12	0	0
8	E	5	0	0	0	0
All	All	25014	0	25185	637	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 13.

All (637) 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:366:ARG:HB3	5:B:601:ATP:N1	1.55	1.18
3:e:28:ALA:HB3	3:e:43:THR:HG21	1.19	1.17
3:e:8:VAL:HG23	3:e:78:VAL:N	1.61	1.16
3:e:8:VAL:HG23	3:e:78:VAL:H	1.12	1.14
3:e:8:VAL:HG21	3:e:78:VAL:HB	1.29	1.13
3:e:47:PRO:HA	3:e:65:SER:HA	1.39	1.03
2:E:392:LYS:HG2	2:E:396:TYR:HE2	1.19	1.02
3:e:28:ALA:HB3	3:e:43:THR:CG2	1.90	1.01
2:E:392:LYS:CG	2:E:396:TYR:HE2	1.75	0.99
4:g:106:GLN:HB3	4:g:111:ILE:HB	1.45	0.97
1:A:511:THR:O	1:A:512:GLN:HG2	1.65	0.96
2:E:392:LYS:HG2	2:E:396:TYR:CE2	2.01	0.95
1:B:366:ARG:CG	5:B:601:ATP:C2	2.49	0.95
1:B:366:ARG:HB3	5:B:601:ATP:C2	2.01	0.94
1:A:175:GLY:HA2	5:A:601:ATP:H5'2	1.51	0.93
1:B:366:ARG:HD3	5:B:601:ATP:C2	2.06	0.91
3:e:8:VAL:CG2	3:e:78:VAL:HB	2.00	0.90
3:e:43:THR:HG22	3:e:44:LEU:H	1.39	0.88
2:E:161:LEU:O	2:E:165:ILE:HG12	1.75	0.86
4:g:74:LYS:O	4:g:166:ASP:HB3	1.75	0.85
1:B:27:LYS:HD2	1:B:47:ASP:CG	2.01	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:GLY:HA3	2:D:251:ARG:HG3	1.58	0.85
3:e:28:ALA:CB	3:e:43:THR:CG2	2.54	0.85
1:B:27:LYS:HD2	1:B:47:ASP:OD2	1.76	0.84
1:B:366:ARG:CB	5:B:601:ATP:C2	2.61	0.84
2:F:451:VAL:HG21	2:F:457:VAL:HG22	1.58	0.83
3:e:11:VAL:HG22	4:g:45:TYR:CE2	2.14	0.82
1:C:192:ILE:HG22	1:C:256:ASP:HB2	1.60	0.82
2:F:264:GLY:O	2:F:265:ARG:HG2	1.79	0.82
3:e:28:ALA:CB	3:e:43:THR:HG21	2.06	0.82
2:E:165:ILE:HG21	2:E:243:LEU:HD22	1.61	0.82
1:B:472:LEU:HD13	1:B:508:PHE:CD2	2.16	0.81
3:e:43:THR:HG22	3:e:44:LEU:N	1.94	0.81
1:B:366:ARG:HG2	5:B:601:ATP:H2	1.46	0.81
1:B:413:ASP:O	1:B:414:LEU:HG	1.81	0.80
2:F:449:TYR:CE2	2:F:450:MET:HG2	2.16	0.80
1:B:180:ALA:HB1	1:B:260:ILE:HG21	1.63	0.80
1:A:291:VAL:HG11	1:A:341:PHE:HE2	1.44	0.80
1:A:511:THR:O	1:A:512:GLN:CG	2.29	0.80
2:F:449:TYR:CD2	2:F:450:MET:HG2	2.18	0.79
1:B:366:ARG:HG2	5:B:601:ATP:C2	2.15	0.79
2:E:421:LYS:HZ3	2:E:452:GLY:HA3	1.48	0.78
1:B:366:ARG:CD	5:B:601:ATP:C2	2.65	0.78
2:F:379:ILE:HD11	2:F:384:MET:HG3	1.63	0.78
2:E:354:VAL:HG12	2:E:358:HIS:HB3	1.65	0.78
3:e:43:THR:HA	4:g:212:PRO:HG3	1.65	0.78
1:A:456:TYR:HB3	1:A:509:LYS:HE3	1.62	0.78
2:E:169:HIS:HE1	2:E:241:ASP:HB3	1.46	0.77
2:F:214:ASN:O	2:F:218:VAL:HG23	1.85	0.77
3:e:49:PRO:HA	3:e:63:TYR:HA	1.66	0.77
3:e:8:VAL:HG21	3:e:78:VAL:CB	2.11	0.77
1:B:198:ALA:HA	1:B:262:ASP:HB2	1.69	0.75
2:E:421:LYS:NZ	2:E:452:GLY:HA3	2.01	0.74
3:e:43:THR:CG2	3:e:44:LEU:H	1.98	0.74
1:C:284:ARG:HG2	2:E:270:VAL:O	1.87	0.73
4:g:52:VAL:O	4:g:56:LEU:HD13	1.88	0.73
2:F:451:VAL:HG21	2:F:457:VAL:CG2	2.18	0.73
1:A:400:GLN:NE2	2:D:333:SER:O	2.23	0.72
3:e:6:CYS:SG	3:e:20:VAL:CG2	2.77	0.72
2:E:134:LEU:HG	2:E:135:LEU:HD12	1.71	0.72
1:A:42:ILE:HG21	1:A:45:LEU:CD1	2.19	0.71
2:F:55:MET:HB3	2:F:214:ASN:HD21	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:392:LYS:CG	2:E:396:TYR:CE2	2.66	0.71
2:D:451:VAL:CG1	2:D:456:GLU:HB3	2.21	0.71
3:e:8:VAL:CG2	3:e:78:VAL:N	2.49	0.71
2:F:10:ILE:HG13	2:F:10:ILE:O	1.92	0.70
4:g:171:VAL:HG22	4:g:185:VAL:HG13	1.73	0.70
2:D:161:LEU:O	2:D:165:ILE:HD12	1.92	0.70
3:e:8:VAL:HG23	3:e:78:VAL:CA	2.21	0.70
2:E:172:LEU:HD11	2:E:240:ARG:NH1	2.07	0.69
2:E:143:LYS:NZ	2:E:284:GLN:O	2.21	0.69
3:e:64:VAL:HG13	3:e:83:ALA:HB2	1.73	0.69
2:E:169:HIS:CE1	2:E:241:ASP:CB	2.75	0.69
2:E:81:ALA:HB3	2:E:102:THR:HB	1.75	0.69
1:B:411:ALA:H	3:e:112:LEU:HD11	1.56	0.68
3:e:40:PRO:HB3	3:e:72:GLN:CG	2.23	0.68
1:B:173:GLN:N	5:B:601:ATP:O1G	2.24	0.68
3:e:40:PRO:HB3	3:e:72:GLN:HG2	1.75	0.68
2:E:178:VAL:HB	2:E:218:VAL:HG11	1.76	0.68
2:E:169:HIS:CE1	2:E:241:ASP:HB3	2.29	0.68
3:e:127:GLN:O	4:g:10:LYS:NZ	2.26	0.68
4:g:218:LEU:HD12	4:g:219:ASN:N	2.10	0.67
2:F:53:ILE:CD1	2:F:259:VAL:HG13	2.24	0.67
2:D:363:ARG:NH1	2:D:366:GLN:OE1	2.28	0.67
1:C:284:ARG:CG	2:E:270:VAL:O	2.43	0.67
3:e:68:VAL:HG12	3:e:69:LEU:N	2.09	0.67
3:e:45:LEU:HD13	3:e:69:LEU:HD23	1.78	0.66
1:C:476:PHE:HB3	1:C:484:MET:HE3	1.77	0.66
1:A:148:GLN:O	1:A:187:GLN:NE2	2.28	0.66
2:D:32:VAL:HG12	2:D:67:VAL:HG22	1.77	0.66
2:D:223:LEU:HD11	2:D:287:ILE:HG12	1.77	0.66
1:C:157:MET:HE1	1:C:395:ARG:HA	1.78	0.66
3:e:43:THR:O	3:e:68:VAL:HG13	1.96	0.65
2:E:146:LEU:HD12	2:E:324:VAL:O	1.96	0.65
4:g:46:ALA:HA	4:g:49:MET:HB2	1.78	0.65
4:g:211:GLU:N	4:g:212:PRO:HD2	2.11	0.65
4:g:241:GLU:OE1	4:g:242:GLN:NE2	2.29	0.65
1:A:173:GLN:N	5:A:601:ATP:O2B	2.29	0.65
5:B:601:ATP:O2A	2:E:347:ARG:NH1	2.27	0.65
2:D:336:TYR:HB2	2:D:450:MET:HE1	1.78	0.64
2:D:386:GLU:OE1	2:D:386:GLU:N	2.29	0.64
2:E:229:PHE:O	2:E:232:GLU:HB2	1.98	0.64
1:B:131:GLU:OE2	1:B:297:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TYR:HE1	1:A:298:LEU:HB2	1.61	0.64
2:E:58:THR:HG23	2:E:58:THR:O	1.96	0.63
2:E:169:HIS:CE1	2:E:241:ASP:HB2	2.33	0.63
2:F:5:ARG:NH1	2:F:64:GLY:O	2.32	0.63
1:B:366:ARG:HD3	5:B:601:ATP:N3	2.13	0.63
4:g:81:VAL:HG11	4:g:234:VAL:HG12	1.78	0.63
2:D:397:ARG:HH12	2:D:438:GLY:HA2	1.63	0.63
2:E:85:ARG:NH2	2:E:98:GLY:O	2.21	0.63
4:g:4:LEU:HB3	4:g:5:LYS:HE2	1.80	0.63
2:D:242:VAL:O	2:D:243:LEU:HD12	1.98	0.63
2:F:136:CYS:O	2:F:136:CYS:SG	2.56	0.63
4:g:56:LEU:HD21	4:g:221:LEU:HB3	1.81	0.63
2:D:242:VAL:C	2:D:243:LEU:HD12	2.23	0.62
4:g:5:LYS:HZ3	4:g:8:ARG:HH12	1.48	0.62
1:C:171:ASP:OD1	1:C:172:ARG:N	2.30	0.62
3:e:91:GLU:O	3:e:91:GLU:HG2	1.98	0.62
1:B:357:GLU:OE2	1:B:370:ASN:ND2	2.32	0.61
1:B:413:ASP:O	1:B:414:LEU:CG	2.48	0.61
2:E:381:ILE:HD11	4:g:85:ARG:HH22	1.64	0.61
1:A:42:ILE:HG21	1:A:45:LEU:HD11	1.80	0.61
3:e:6:CYS:SG	3:e:20:VAL:HG22	2.41	0.61
2:E:127:THR:HG22	2:E:129:ILE:H	1.65	0.61
1:B:162:ARG:NH1	1:B:256:ASP:OD2	2.33	0.61
1:A:511:THR:O	1:A:512:GLN:NE2	2.34	0.61
1:B:180:ALA:HB1	1:B:260:ILE:HD13	1.82	0.60
3:e:45:LEU:HD21	3:e:50:ILE:HD11	1.83	0.60
4:g:104:LYS:HA	4:g:107:GLN:HB3	1.81	0.60
1:C:106:GLY:N	1:C:222:THR:O	2.34	0.60
2:E:353:VAL:HG23	2:E:354:VAL:HG23	1.83	0.60
2:F:287:ILE:HG23	2:F:295:ILE:HG22	1.83	0.60
4:g:50:ARG:O	4:g:53:ILE:HG13	2.00	0.60
2:F:76:VAL:HG11	2:F:221:THR:HG23	1.82	0.60
2:F:233:LYS:HB3	2:F:237:GLY:HA2	1.84	0.60
1:C:230:ALA:HB2	2:D:285:GLU:HG3	1.83	0.60
1:B:107:ARG:NH2	1:B:120:GLY:O	2.27	0.60
1:B:413:ASP:C	1:B:414:LEU:HG	2.26	0.60
3:e:86:ALA:HB1	3:e:91:GLU:CD	2.26	0.60
2:D:451:VAL:HG21	2:D:460:LYS:HD2	1.83	0.60
2:E:454:ILE:O	2:E:457:VAL:HG12	2.02	0.60
2:E:354:VAL:CG1	2:E:358:HIS:ND1	2.64	0.60
1:B:32:ILE:HG23	1:B:40:VAL:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:103:GLU:HG3	2:F:103:GLU:O	2.03	0.59
1:A:42:ILE:HG21	1:A:45:LEU:HD12	1.83	0.59
2:D:427:GLU:OE1	2:D:430:ARG:NH2	2.35	0.59
3:e:13:GLU:HG2	3:e:14:SER:N	2.17	0.59
1:A:31:THR:O	1:A:42:ILE:HG23	2.02	0.59
2:F:397:ARG:HH12	2:F:438:GLY:HA2	1.67	0.59
3:e:71:VAL:O	3:e:72:GLN:HG2	2.03	0.59
1:A:435:LYS:HA	5:A:601:ATP:HN62	1.68	0.59
2:F:89:VAL:HG13	2:F:90:LEU:HD12	1.83	0.59
4:g:140:ILE:HG13	4:g:141:GLY:N	2.17	0.59
1:A:42:ILE:CG2	1:A:45:LEU:HD12	2.33	0.59
2:F:247:ASP:OD1	2:F:248:ASN:N	2.36	0.59
2:D:451:VAL:HG13	2:D:456:GLU:HB3	1.85	0.59
2:E:16:VAL:HG11	2:E:67:VAL:HG11	1.85	0.59
2:F:166:ALA:HB3	2:F:200:LYS:HD3	1.85	0.59
1:A:487:ILE:HD11	1:A:497:ILE:HD12	1.85	0.58
1:B:38:GLY:O	1:B:39:ILE:HD13	2.03	0.58
1:C:135:PRO:O	1:C:140:ARG:NH1	2.35	0.58
1:B:60:LEU:HD23	1:B:78:GLY:HA3	1.84	0.58
1:B:384:THR:HG22	1:B:385:LYS:N	2.16	0.58
2:E:78:VAL:HG23	2:E:225:MET:HG2	1.85	0.58
4:g:48:ASN:HA	4:g:51:ARG:HD2	1.85	0.58
4:g:71:ARG:NH1	4:g:163:GLY:HA2	2.18	0.58
1:B:472:LEU:CD1	1:B:508:PHE:CD2	2.86	0.58
1:C:343:PRO:HA	1:C:346:VAL:HG22	1.86	0.58
3:e:8:VAL:CG2	3:e:78:VAL:CB	2.76	0.58
1:A:511:THR:C	1:A:512:GLN:HG2	2.29	0.58
4:g:71:ARG:HH12	4:g:163:GLY:CA	2.17	0.58
2:F:247:ASP:O	2:F:300:ALA:HB3	2.04	0.57
2:E:172:LEU:CD1	2:E:240:ARG:HH11	2.17	0.57
1:B:27:LYS:HD2	1:B:47:ASP:CB	2.35	0.57
2:D:41:VAL:HA	2:D:52:THR:HG22	1.86	0.57
2:E:354:VAL:HG12	2:E:358:HIS:CB	2.34	0.57
1:A:161:GLY:HA3	1:A:382:ALA:HB1	1.87	0.57
1:C:75:VAL:HG11	1:C:274:ILE:HD11	1.85	0.57
3:e:8:VAL:CG2	3:e:78:VAL:CA	2.83	0.57
4:g:60:ASN:HB3	4:g:63:TYR:HB3	1.87	0.57
1:B:146:PRO:HB3	1:B:382:ALA:O	2.05	0.57
1:B:290:ASP:OD1	1:B:290:ASP:N	2.38	0.57
2:D:161:LEU:O	2:D:165:ILE:CD1	2.53	0.57
2:E:326:LEU:C	2:E:326:LEU:HD12	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:63:TYR:CE1	3:e:89:LEU:HD13	2.40	0.57
2:E:89:VAL:HG22	2:E:218:VAL:HG22	1.86	0.57
2:D:32:VAL:HG21	2:D:37:THR:HB	1.86	0.56
2:F:403:ARG:NH1	2:F:445:GLU:OE1	2.38	0.56
1:B:361:PHE:HE1	5:B:601:ATP:N3	2.03	0.56
1:C:241:TYR:HE1	1:C:298:LEU:HB2	1.70	0.56
4:g:71:ARG:HH12	4:g:163:GLY:HA2	1.70	0.56
2:E:326:LEU:HD12	2:E:326:LEU:O	2.06	0.56
2:E:451:VAL:HG11	2:E:457:VAL:HB	1.87	0.56
2:F:310:ASP:HB3	2:F:313:PRO:HD2	1.88	0.56
1:A:97:GLU:HB2	1:A:128:ASP:O	2.04	0.56
2:F:20:ARG:HG3	2:F:21:THR:N	2.21	0.56
2:D:134:LEU:HD13	2:D:429:ILE:HD13	1.86	0.56
2:D:178:VAL:HG22	2:D:218:VAL:HG13	1.87	0.56
2:F:130:LYS:HE3	2:F:404:PHE:O	2.05	0.56
3:e:68:VAL:HG12	3:e:69:LEU:H	1.69	0.56
2:E:410:HIS:CD2	2:E:418:ALA:HB1	2.41	0.56
1:B:326:THR:HG22	1:B:327:ALA:N	2.21	0.56
2:F:387:LEU:HB3	2:F:391:ASP:OD1	2.04	0.56
4:g:75:ARG:HG3	4:g:164:GLU:O	2.05	0.55
2:E:151:GLY:O	2:E:154:LYS:NZ	2.37	0.55
1:A:360:LEU:HB2	1:A:368:ALA:HB1	1.87	0.55
3:e:95:LEU:HA	3:e:98:ARG:HE	1.71	0.55
3:e:125:ALA:O	3:e:129:GLU:N	2.39	0.55
1:A:160:VAL:HG12	1:A:161:GLY:H	1.72	0.55
1:A:494:ASN:OD1	1:A:496:ASP:HB2	2.07	0.55
2:E:440:TYR:CE2	2:E:454:ILE:HD11	2.42	0.55
4:g:104:LYS:O	4:g:108:GLU:N	2.39	0.55
1:A:511:THR:O	1:A:512:GLN:CD	2.50	0.55
2:E:38:THR:HB	2:E:55:MET:HB2	1.89	0.55
2:E:449:TYR:CE2	2:E:450:MET:HG2	2.42	0.55
4:g:39:MET:CE	4:g:236:GLU:HB2	2.36	0.55
4:g:67:TYR:OH	4:g:157:LEU:HD12	2.07	0.55
1:C:391:SER:OG	1:C:395:ARG:NH2	2.39	0.54
2:F:83:LEU:HD11	2:F:172:LEU:HD13	1.90	0.54
2:F:264:GLY:O	2:F:265:ARG:CG	2.53	0.54
1:C:162:ARG:NH1	1:C:256:ASP:OD2	2.39	0.54
3:e:3:THR:HA	3:e:21:THR:HG22	1.89	0.54
1:B:231:ASP:O	1:B:236:GLN:NE2	2.41	0.54
1:B:147:VAL:HG23	1:B:162:ARG:HG2	1.89	0.54
1:B:77:LEU:HB3	1:B:235:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:VAL:HG12	1:B:96:LEU:N	2.22	0.54
2:D:32:VAL:CG2	2:D:37:THR:HB	2.38	0.54
3:e:40:PRO:HB3	3:e:72:GLN:CD	2.33	0.54
1:A:162:ARG:NH1	1:A:256:ASP:OD2	2.41	0.54
2:D:313:PRO:O	2:D:317:PHE:CD2	2.61	0.54
1:C:126:LEU:HD12	1:C:249:TYR:HE1	1.73	0.54
3:e:62:VAL:HG22	3:e:85:ARG:HA	1.90	0.54
1:A:291:VAL:HG11	1:A:341:PHE:CE2	2.35	0.54
2:D:134:LEU:HG	2:D:135:LEU:HD12	1.88	0.54
2:E:124:LEU:HD22	2:E:138:PHE:O	2.07	0.54
1:A:188:LYS:O	1:A:189:ASN:HB2	2.08	0.53
4:g:132:LYS:NZ	4:g:133:VAL:O	2.41	0.53
1:C:68:GLU:OE1	2:E:10:ILE:HD11	2.07	0.53
1:C:330:ILE:O	1:C:331:ILE:HD13	2.08	0.53
2:E:18:PHE:HZ	2:E:30:LEU:HD13	1.72	0.53
4:g:74:LYS:O	4:g:166:ASP:CB	2.52	0.53
1:B:279:ARG:HA	2:E:266:MET:HE1	1.91	0.53
1:B:413:ASP:O	1:B:413:ASP:OD1	2.26	0.53
4:g:220:GLY:O	4:g:224:ARG:HD3	2.07	0.53
1:B:212:LYS:HG2	1:B:437:TYR:CZ	2.44	0.53
1:C:126:LEU:CD1	1:C:249:TYR:HE1	2.22	0.53
2:E:172:LEU:CD1	2:E:240:ARG:NH1	2.71	0.53
1:C:389:LYS:O	1:C:389:LYS:NZ	2.30	0.53
2:E:57:SER:HA	2:E:211:PRO:HG2	1.91	0.53
2:E:136:CYS:SG	2:E:136:CYS:O	2.67	0.53
4:g:246:MET:HG3	4:g:247:VAL:N	2.23	0.53
1:A:146:PRO:HB3	1:A:383:GLN:HA	1.90	0.53
1:A:511:THR:O	1:A:511:THR:HG22	2.09	0.53
1:B:147:VAL:CG2	1:B:162:ARG:HG2	2.39	0.53
1:A:42:ILE:HG22	1:A:43:HIS:N	2.24	0.53
1:A:60:LEU:HD11	1:A:78:GLY:HA3	1.91	0.53
1:B:29:GLU:HG3	1:B:88:LYS:NZ	2.24	0.53
2:F:199:ASP:CG	2:F:199:ASP:O	2.51	0.53
1:B:110:ASP:OD1	1:B:114:ASN:N	2.41	0.52
3:e:106:ALA:HA	3:e:109:LYS:HG2	1.91	0.52
2:D:451:VAL:HG21	2:D:460:LYS:CD	2.40	0.52
2:E:354:VAL:CG1	2:E:358:HIS:CG	2.93	0.52
2:E:453:GLY:H	2:E:456:GLU:HB3	1.74	0.52
2:D:134:LEU:HD22	2:D:432:PHE:CD2	2.45	0.52
2:E:147:PHE:HB2	2:E:325:VAL:HG22	1.92	0.52
4:g:43:ARG:HB3	4:g:44:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:188:LEU:HG	4:g:226:ILE:HD11	1.92	0.52
2:D:280:MET:SD	2:D:316:THR:OG1	2.61	0.52
3:e:9:VAL:HB	3:e:14:SER:HA	1.92	0.52
3:e:21:THR:HG21	3:e:55:GLU:HG3	1.92	0.52
1:A:314:THR:HG21	1:A:318:VAL:HG12	1.90	0.52
1:C:126:LEU:HD12	1:C:249:TYR:CE1	2.45	0.52
2:E:328:ARG:HA	2:E:331:ALA:HB3	1.92	0.52
2:F:18:PHE:HZ	2:F:30:LEU:HD21	1.74	0.52
3:e:6:CYS:O	3:e:17:SER:HA	2.10	0.52
3:e:68:VAL:CG1	3:e:69:LEU:N	2.73	0.52
3:e:86:ALA:HB1	3:e:91:GLU:OE1	2.09	0.52
4:g:211:GLU:N	4:g:212:PRO:CD	2.73	0.52
1:C:117:ASP:N	1:C:117:ASP:OD1	2.38	0.51
2:F:179:GLY:O	2:F:251:ARG:NE	2.42	0.51
4:g:74:LYS:HG2	4:g:75:ARG:N	2.25	0.51
1:B:166:GLU:HB3	1:B:328:LEU:CD2	2.40	0.51
2:E:172:LEU:HD13	2:E:229:PHE:CD1	2.44	0.51
2:F:270:VAL:HG13	2:F:272:TYR:CE2	2.46	0.51
4:g:48:ASN:O	4:g:52:VAL:HG23	2.10	0.51
1:A:284:ARG:NH2	2:D:305:ALA:CB	2.73	0.51
1:B:377:ARG:HH21	2:F:150:ALA:HB3	1.75	0.51
2:E:424:PRO:HG2	2:E:427:GLU:HB2	1.92	0.51
2:F:243:LEU:HD23	2:F:296:THR:HB	1.93	0.51
2:E:459:ALA:O	2:E:463:LYS:HG2	2.10	0.51
4:g:32:MET:HG2	4:g:33:ARG:NH1	2.25	0.51
1:B:366:ARG:CG	5:B:601:ATP:H2	2.06	0.51
4:g:158:ASP:O	4:g:162:LYS:NZ	2.42	0.51
1:B:39:ILE:CD1	1:B:75:VAL:HG12	2.41	0.51
1:C:370:ASN:O	1:C:374:SER:OG	2.24	0.51
2:D:154:LYS:HG2	2:D:326:LEU:HD12	1.93	0.51
4:g:120:GLN:O	4:g:123:VAL:HG12	2.11	0.51
1:B:27:LYS:HD2	1:B:47:ASP:HB2	1.92	0.50
1:B:173:GLN:O	1:B:173:GLN:HG2	2.11	0.50
2:E:26:ILE:HD11	2:E:44:GLN:HG3	1.93	0.50
4:g:16:SER:O	4:g:20:ILE:HG23	2.11	0.50
3:e:9:VAL:HG23	4:g:45:TYR:HD1	1.75	0.50
3:e:13:GLU:HG2	3:e:14:SER:H	1.75	0.50
2:D:382:LEU:HD23	2:D:386:GLU:HG3	1.92	0.50
2:E:387:LEU:HB3	2:E:390:GLU:HB2	1.94	0.50
1:B:27:LYS:CD	1:B:47:ASP:OD2	2.53	0.50
2:E:165:ILE:HG21	2:E:243:LEU:CD2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:ALA:CB	2:F:200:LYS:HD3	2.42	0.50
2:F:255:ALA:O	2:F:259:VAL:HG23	2.11	0.50
1:A:123:ASP:N	1:A:123:ASP:OD1	2.42	0.50
2:E:134:LEU:CG	2:E:135:LEU:HD12	2.42	0.50
2:F:50:VAL:HG23	2:F:50:VAL:O	2.11	0.50
3:e:23:LEU:HB2	3:e:52:VAL:HG12	1.94	0.50
2:F:132:ILE:HG23	2:F:138:PHE:CE1	2.47	0.50
4:g:93:ILE:HG13	4:g:94:ASN:N	2.26	0.50
1:B:419:ARG:O	1:B:423:GLU:HG2	2.12	0.50
2:D:330:ILE:HG22	2:D:335:ILE:HB	1.94	0.50
2:F:448:PHE:O	2:F:451:VAL:HG22	2.11	0.50
4:g:81:VAL:HB	4:g:237:ASN:HD22	1.77	0.49
1:A:501:ILE:O	1:A:505:ILE:HG12	2.12	0.49
1:C:66:ASN:HB3	1:C:68:GLU:OE2	2.12	0.49
1:C:413:ASP:O	1:C:414:LEU:HG	2.11	0.49
1:A:423:GLU:O	1:A:427:ARG:HG2	2.11	0.49
2:E:134:LEU:HD23	2:E:135:LEU:CD1	2.41	0.49
3:e:68:VAL:CG1	3:e:69:LEU:H	2.25	0.49
1:A:212:LYS:HE2	1:A:437:TYR:CZ	2.47	0.49
4:g:140:ILE:HG13	4:g:141:GLY:H	1.78	0.49
1:B:165:ARG:NH1	1:B:299:LEU:O	2.38	0.49
4:g:47:ASP:O	4:g:51:ARG:HG3	2.12	0.49
1:A:171:ASP:O	1:A:174:THR:HG22	2.13	0.49
1:A:276:LEU:HD22	2:F:266:MET:SD	2.53	0.49
1:B:39:ILE:HD12	1:B:75:VAL:HG12	1.94	0.49
1:B:466:VAL:O	1:B:469:ASP:HB3	2.13	0.49
2:E:172:LEU:HB3	2:E:229:PHE:CD2	2.47	0.49
2:E:399:ARG:O	2:E:403:ARG:HG2	2.12	0.49
3:e:71:VAL:C	3:e:72:GLN:CG	2.86	0.49
4:g:45:TYR:O	4:g:49:MET:N	2.39	0.49
2:E:216:LEU:HG	2:E:217:ARG:HG2	1.95	0.49
4:g:53:ILE:HA	4:g:56:LEU:HD22	1.95	0.49
2:E:424:PRO:HG2	2:E:427:GLU:CB	2.43	0.49
2:D:55:MET:HE1	2:D:217:ARG:HG3	1.94	0.49
2:F:393:LEU:HD21	2:F:397:ARG:HH21	1.77	0.49
1:A:67:LEU:HB3	2:D:63:ARG:HH11	1.77	0.48
2:E:454:ILE:O	2:E:458:ILE:HG13	2.12	0.48
1:B:241:TYR:HE1	1:B:298:LEU:HB2	1.78	0.48
1:B:411:ALA:H	3:e:112:LEU:CD1	2.23	0.48
2:E:141:GLY:HA3	2:E:289:SER:HB3	1.94	0.48
2:E:347:ARG:O	2:E:347:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HG13	1:C:277:LEU:HB3	1.95	0.48
2:D:40:GLU:OE1	2:D:217:ARG:NE	2.44	0.48
2:E:393:LEU:HD21	2:E:397:ARG:HH21	1.78	0.48
2:F:449:TYR:O	2:F:451:VAL:HG13	2.13	0.48
3:e:50:ILE:HG22	3:e:51:ARG:N	2.28	0.48
4:g:245:ARG:O	4:g:249:MET:HG2	2.14	0.48
1:B:206:ILE:HD13	1:B:226:ALA:HB1	1.96	0.48
1:B:494:ASN:OD1	1:B:494:ASN:O	2.31	0.48
2:F:249:ILE:O	2:F:252:TYR:HB3	2.12	0.48
1:C:34:MET:HB3	1:C:41:ARG:HB2	1.95	0.48
1:C:180:ALA:HB1	1:C:260:ILE:HD13	1.94	0.48
2:F:159:MET:HE1	2:F:192:MET:HE2	1.95	0.48
3:e:4:MET:HB3	3:e:20:VAL:O	2.13	0.48
4:g:71:ARG:NH1	4:g:163:GLY:CA	2.77	0.48
2:D:313:PRO:O	2:D:317:PHE:HD2	1.96	0.48
2:E:125:LEU:HD23	2:E:125:LEU:O	2.13	0.48
1:A:107:ARG:HB3	1:A:122:ILE:HD11	1.95	0.47
2:E:162:ILE:HD13	2:E:245:PHE:CE1	2.48	0.47
4:g:33:ARG:O	4:g:37:GLU:HG2	2.14	0.47
4:g:35:ALA:HB1	4:g:239:ALA:HB2	1.95	0.47
1:B:75:VAL:HG11	1:B:274:ILE:HD11	1.96	0.47
2:D:85:ARG:NH2	2:D:98:GLY:O	2.46	0.47
2:E:162:ILE:O	2:E:166:ALA:N	2.47	0.47
4:g:3:ASN:HB3	4:g:6:GLU:HG3	1.95	0.47
4:g:32:MET:HG3	4:g:33:ARG:N	2.30	0.47
4:g:188:LEU:CD2	4:g:226:ILE:HD11	2.43	0.47
1:C:423:GLU:O	1:C:427:ARG:HG2	2.15	0.47
4:g:66:ARG:NH2	4:g:161:ASP:OD1	2.47	0.47
4:g:218:LEU:HD12	4:g:218:LEU:C	2.40	0.47
1:A:425:GLY:O	1:A:429:THR:OG1	2.28	0.47
1:C:112:LEU:HD11	1:C:235:MET:HE1	1.97	0.47
2:E:83:LEU:HD22	2:E:200:LYS:HA	1.96	0.47
2:E:449:TYR:CD2	2:E:450:MET:HG2	2.49	0.47
1:A:166:GLU:O	1:A:329:PRO:HD2	2.15	0.47
1:A:479:GLU:O	1:A:480:TYR:C	2.56	0.47
4:g:65:HIS:CD2	4:g:67:TYR:CD2	3.03	0.47
4:g:76:VAL:HG13	4:g:111:ILE:CG2	2.43	0.47
1:A:291:VAL:CG1	1:A:341:PHE:HE2	2.22	0.47
2:E:58:THR:O	2:E:58:THR:CG2	2.63	0.47
2:F:33:ASP:HB2	2:F:66:THR:HG23	1.97	0.47
3:e:46:GLN:HB3	3:e:47:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:78:TYR:OH	4:g:106:GLN:HG3	2.13	0.47
1:B:67:LEU:O	1:B:68:GLU:HG3	2.15	0.47
2:D:158:MET:HE2	2:D:245:PHE:HB3	1.95	0.47
2:E:148:GLY:HA3	2:E:326:LEU:H	1.80	0.47
1:B:166:GLU:O	1:B:329:PRO:HD2	2.15	0.46
2:F:113:PRO:HG3	2:F:288:THR:HG21	1.97	0.46
3:e:51:ARG:NH1	3:e:51:ARG:HA	2.30	0.46
1:C:219:MET:O	1:C:219:MET:HG3	2.15	0.46
4:g:145:SER:OG	4:g:147:GLU:HG3	2.14	0.46
4:g:188:LEU:HD21	4:g:226:ILE:CD1	2.45	0.46
2:D:102:THR:HG22	2:D:104:GLU:H	1.81	0.46
2:E:354:VAL:HG12	2:E:358:HIS:CG	2.50	0.46
1:B:384:THR:CG2	1:B:385:LYS:N	2.78	0.46
2:D:78:VAL:HG11	2:D:106:LEU:HD12	1.96	0.46
1:A:374:SER:O	1:A:395:ARG:HD2	2.16	0.46
1:B:184:ILE:HG13	1:B:260:ILE:HD12	1.97	0.46
1:C:284:ARG:CD	2:E:270:VAL:O	2.63	0.46
1:C:496:ASP:OD1	1:C:497:ILE:N	2.49	0.46
4:g:71:ARG:HB3	4:g:72:PRO:HD2	1.97	0.46
1:A:153:SER:O	1:A:157:MET:HB2	2.16	0.46
1:C:343:PRO:HA	1:C:346:VAL:CG2	2.45	0.46
2:E:216:LEU:HG	2:E:217:ARG:N	2.31	0.46
1:C:53:MET:HE1	1:C:63:MET:HG3	1.98	0.46
1:C:356:LEU:HA	1:C:368:ALA:O	2.16	0.46
1:C:334:GLN:HB3	2:D:309:THR:HG23	1.97	0.46
2:F:129:ILE:O	2:F:130:LYS:HB3	2.16	0.46
1:A:42:ILE:CG2	1:A:43:HIS:H	2.29	0.46
1:B:487:ILE:HD11	1:B:497:ILE:HG23	1.97	0.46
3:e:51:ARG:HH22	3:e:61:ILE:HD12	1.81	0.46
4:g:46:ALA:O	4:g:50:ARG:HG3	2.15	0.46
4:g:48:ASN:OD1	4:g:51:ARG:NH1	2.49	0.46
2:E:223:LEU:HD21	2:E:286:ARG:HB2	1.97	0.45
1:A:107:ARG:HG3	1:A:122:ILE:HG12	1.99	0.45
1:B:177:THR:O	1:B:180:ALA:N	2.49	0.45
2:D:451:VAL:CG1	2:D:456:GLU:CB	2.92	0.45
2:E:255:ALA:O	2:E:259:VAL:HG23	2.16	0.45
2:E:376:LYS:HB2	2:E:379:ILE:HG12	1.98	0.45
3:e:3:THR:HA	3:e:21:THR:HA	1.98	0.45
4:g:117:LEU:HD22	4:g:123:VAL:HA	1.97	0.45
1:C:107:ARG:HA	1:C:107:ARG:HD3	1.75	0.45
1:C:147:VAL:HG23	1:C:162:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LYS:HG2	1:C:250:PHE:CE2	2.51	0.45
2:E:388:ALA:C	2:E:390:GLU:H	2.24	0.45
4:g:221:LEU:HA	4:g:224:ARG:HB2	1.98	0.45
1:A:479:GLU:C	1:A:481:ALA:N	2.73	0.45
1:B:95:VAL:CG1	1:B:96:LEU:N	2.79	0.45
1:B:494:ASN:OD1	1:B:497:ILE:HG13	2.16	0.45
2:D:363:ARG:HD3	2:D:363:ARG:HA	1.55	0.45
1:C:262:ASP:O	1:C:263:ASP:OD1	2.34	0.45
2:E:451:VAL:HG21	2:E:457:VAL:HG23	1.98	0.45
4:g:221:LEU:O	4:g:225:TYR:N	2.39	0.45
1:A:494:ASN:OD1	1:A:494:ASN:C	2.60	0.45
2:F:53:ILE:HD11	2:F:259:VAL:HG13	1.97	0.45
4:g:227:GLU:HA	4:g:230:VAL:HG22	1.99	0.45
2:D:382:LEU:HD11	3:e:121:LEU:HD13	1.99	0.45
3:e:9:VAL:HG23	4:g:45:TYR:CD1	2.52	0.45
3:e:27:GLY:HA3	3:e:45:LEU:HD12	1.99	0.45
4:g:74:LYS:HA	4:g:111:ILE:HG23	1.98	0.45
2:E:41:VAL:HA	2:E:52:THR:HG22	1.99	0.45
4:g:250:LYS:O	4:g:253:THR:OG1	2.33	0.45
1:B:262:ASP:O	1:B:330:ILE:HB	2.17	0.44
1:B:361:PHE:CZ	5:B:601:ATP:H1'	2.52	0.44
2:E:162:ILE:HD13	2:E:245:PHE:HE1	1.83	0.44
2:E:234:ASP:OD1	2:E:234:ASP:N	2.50	0.44
2:F:2:SER:OG	2:F:3:SER:N	2.49	0.44
4:g:33:ARG:O	4:g:34:ARG:C	2.59	0.44
4:g:71:ARG:O	4:g:72:PRO:C	2.60	0.44
1:A:160:VAL:HG12	1:A:161:GLY:N	2.32	0.44
1:B:103:GLU:H	1:B:103:GLU:HG2	1.58	0.44
1:B:435:LYS:HE2	1:B:435:LYS:HB2	1.88	0.44
2:E:392:LYS:HG3	2:E:396:TYR:HE2	1.74	0.44
2:F:248:ASN:HA	2:F:300:ALA:O	2.17	0.44
4:g:214:ALA:HA	4:g:217:LEU:HB3	1.98	0.44
1:B:413:ASP:O	1:B:414:LEU:CD2	2.65	0.44
4:g:7:ILE:HG21	4:g:267:TYR:HB2	2.00	0.44
1:C:351:ASP:O	1:C:377:ARG:HG2	2.18	0.44
1:C:398:LEU:HD23	1:C:398:LEU:HA	1.81	0.44
2:D:134:LEU:CD1	2:D:429:ILE:HD13	2.48	0.44
1:A:314:THR:HG23	1:A:317:ALA:H	1.80	0.44
2:E:44:GLN:O	2:E:45:LEU:HD23	2.17	0.44
2:E:243:LEU:HG	2:E:296:THR:HG23	1.99	0.44
2:E:381:ILE:HD11	4:g:85:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:HIS:HA	2:E:419:PRO:HD2	2.00	0.44
2:F:388:ALA:N	2:F:391:ASP:OD2	2.50	0.44
4:g:79:ILE:CG2	4:g:170:LEU:HA	2.48	0.44
1:A:481:ALA:N	1:A:482:PRO:CD	2.81	0.44
2:F:130:LYS:CE	2:F:404:PHE:O	2.66	0.44
4:g:141:GLY:O	4:g:144:PRO:HD3	2.18	0.44
1:B:55:GLU:HB3	1:B:61:PHE:HE1	1.82	0.44
1:C:108:VAL:HG22	1:C:224:VAL:HB	2.00	0.44
1:C:407:PHE:HE1	3:e:118:LEU:HB3	1.82	0.44
2:E:280:MET:HE1	2:E:316:THR:HA	2.00	0.44
4:g:39:MET:HE2	4:g:236:GLU:HB2	2.00	0.44
4:g:68:MET:HG2	4:g:191:LEU:HD23	2.00	0.44
4:g:106:GLN:O	4:g:110:SER:N	2.51	0.44
1:A:472:LEU:HD13	1:A:508:PHE:CD2	2.53	0.43
2:E:290:THR:HG22	2:E:291:LYS:H	1.83	0.43
2:E:361:ILE:HD12	2:E:433:LYS:HG3	1.99	0.43
2:F:32:VAL:HG22	2:F:67:VAL:HG22	2.00	0.43
3:e:10:SER:HA	3:e:80:ALA:HB3	2.00	0.43
4:g:56:LEU:HD21	4:g:221:LEU:CB	2.46	0.43
2:E:244:LEU:HD21	2:E:246:VAL:HG23	1.99	0.43
4:g:53:ILE:HA	4:g:56:LEU:HB2	2.00	0.43
4:g:134:LEU:H	4:g:134:LEU:HD23	1.83	0.43
1:C:131:GLU:OE2	1:C:297:ARG:NH2	2.52	0.43
1:C:165:ARG:HG2	1:C:302:ALA:HB3	1.99	0.43
2:D:145:GLY:HA3	2:D:320:LEU:HD13	2.01	0.43
2:D:285:GLU:O	2:D:288:THR:OG1	2.37	0.43
2:E:161:LEU:HA	2:E:164:ASN:HD21	1.83	0.43
4:g:39:MET:HE1	4:g:236:GLU:HB2	1.99	0.43
2:F:426:LYS:O	2:F:430:ARG:HG3	2.18	0.43
3:e:41:LEU:HD23	3:e:41:LEU:HA	1.84	0.43
2:E:129:ILE:HB	2:E:132:ILE:HG22	2.00	0.43
2:E:354:VAL:HG12	2:E:354:VAL:O	2.18	0.43
1:A:42:ILE:HG22	1:A:43:HIS:H	1.81	0.43
1:A:431:LEU:HD23	1:A:432:MET:SD	2.59	0.43
1:C:123:ASP:O	1:C:124:ALA:C	2.61	0.43
2:F:455:ASP:O	2:F:456:GLU:C	2.62	0.43
4:g:229:MET:HE3	4:g:229:MET:HB3	1.80	0.43
2:D:43:GLN:OE1	2:D:45:LEU:HD21	2.19	0.43
2:E:459:ALA:O	2:E:462:GLU:HG3	2.19	0.43
4:g:78:TYR:CD1	4:g:169:TYR:HB3	2.53	0.43
1:A:42:ILE:CG2	1:A:43:HIS:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:74:HIS:ND1	3:e:75:VAL:HG23	2.34	0.43
1:C:385:LYS:HE3	1:C:493:TYR:H	1.83	0.43
2:F:74:ILE:HB	2:F:108:ILE:HD11	2.00	0.43
2:F:421:LYS:HA	2:F:421:LYS:HD3	1.86	0.43
4:g:20:ILE:HG13	4:g:21:THR:N	2.33	0.43
4:g:37:GLU:O	4:g:41:GLN:HG2	2.19	0.43
4:g:145:SER:OG	4:g:147:GLU:OE2	2.35	0.43
1:C:284:ARG:HD2	2:E:270:VAL:O	2.18	0.42
2:E:363:ARG:HD3	2:E:363:ARG:HA	1.74	0.42
3:e:35:LEU:C	3:e:35:LEU:HD12	2.44	0.42
1:B:79:ASN:OD1	1:B:81:LEU:HB2	2.20	0.42
2:D:350:ASP:OD1	2:D:350:ASP:N	2.51	0.42
2:E:397:ARG:HA	2:E:400:LYS:HE3	2.01	0.42
2:E:425:LEU:HG	2:E:426:LYS:N	2.34	0.42
1:C:190:SER:OG	1:C:192:ILE:HG12	2.19	0.42
1:C:192:ILE:CG2	1:C:256:ASP:HB2	2.41	0.42
2:D:413:GLU:HG2	2:D:418:ALA:O	2.19	0.42
2:E:159:MET:HG3	2:E:191:GLU:HG2	2.01	0.42
4:g:168:ILE:O	4:g:187:GLN:NE2	2.52	0.42
4:g:220:GLY:HA2	4:g:223:VAL:HG22	2.00	0.42
4:g:231:TYR:O	4:g:235:ILE:HG12	2.19	0.42
4:g:54:ALA:O	4:g:57:VAL:HG22	2.18	0.42
4:g:76:VAL:HG13	4:g:111:ILE:HG21	2.01	0.42
1:B:472:LEU:HD13	1:B:508:PHE:CE2	2.53	0.42
2:D:20:ARG:NH2	2:D:47:ASP:OD1	2.53	0.42
2:F:413:GLU:HB3	2:F:418:ALA:O	2.19	0.42
3:e:85:ARG:O	3:e:85:ARG:HG2	2.20	0.42
1:A:171:ASP:O	1:A:174:THR:CG2	2.67	0.42
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.84	0.42
2:E:401:ILE:HG22	2:E:405:PHE:CZ	2.54	0.42
2:F:180:GLU:OE1	2:F:251:ARG:NH2	2.53	0.42
2:F:312:SER:HB3	2:F:313:PRO:HD3	2.01	0.42
3:e:69:LEU:HD12	3:e:69:LEU:O	2.20	0.42
4:g:213:GLU:HG3	4:g:215:GLU:HB3	2.01	0.42
1:B:326:THR:HG22	1:B:327:ALA:H	1.85	0.42
2:F:398:ALA:O	2:F:402:GLN:HG3	2.20	0.42
1:A:375:VAL:HG12	1:A:395:ARG:CZ	2.50	0.42
1:C:42:ILE:HG22	1:C:43:HIS:O	2.20	0.42
1:C:271:TYR:HA	1:C:274:ILE:HG22	2.02	0.42
2:D:441:ASP:N	2:D:441:ASP:OD1	2.50	0.42
2:E:161:LEU:HA	2:E:164:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:423:VAL:O	2:F:423:VAL:HG13	2.19	0.42
1:A:276:LEU:CD2	2:F:266:MET:SD	3.08	0.42
2:E:159:MET:HE1	2:E:188:PHE:CE2	2.55	0.42
2:E:177:GLY:O	2:E:205:TYR:HA	2.19	0.42
2:F:18:PHE:CZ	2:F:30:LEU:HD21	2.53	0.42
3:e:6:CYS:SG	3:e:20:VAL:HG21	2.58	0.42
4:g:240:CYS:O	4:g:243:SER:OG	2.31	0.42
2:E:143:LYS:HD3	2:E:287:ILE:HB	2.01	0.42
2:E:421:LYS:HD3	2:E:452:GLY:HA3	2.01	0.42
2:F:139:ALA:HB2	2:F:348:GLN:HG2	2.02	0.42
2:F:351:PRO:HA	2:F:355:GLY:O	2.20	0.42
4:g:50:ARG:HA	4:g:53:ILE:HG13	2.00	0.42
4:g:66:ARG:HH22	4:g:161:ASP:HA	1.85	0.42
4:g:127:LYS:HD2	4:g:127:LYS:HA	1.78	0.42
1:B:170:GLY:O	1:B:332:GLU:HA	2.20	0.41
1:B:256:ASP:OD1	1:B:256:ASP:N	2.50	0.41
2:D:133:ASP:HB3	2:D:425:LEU:HD13	2.02	0.41
2:E:148:GLY:HA3	2:E:326:LEU:HG	2.01	0.41
1:B:430:GLU:HB3	1:B:465:ILE:HG21	2.02	0.41
2:E:148:GLY:CA	2:E:326:LEU:H	2.33	0.41
2:F:278:GLU:O	2:F:282:VAL:HG13	2.20	0.41
2:E:120:ALA:O	2:E:121:SER:HB3	2.20	0.41
1:A:158:ILE:HD13	1:A:374:SER:HB3	2.02	0.41
1:B:67:LEU:C	1:B:68:GLU:HG3	2.45	0.41
1:C:366:ARG:HH12	2:D:363:ARG:HD2	1.83	0.41
2:D:134:LEU:CD1	2:D:429:ILE:CD1	2.98	0.41
2:D:463:LYS:HE3	2:D:463:LYS:HB2	1.85	0.41
2:E:140:LYS:NZ	2:E:241:ASP:OD2	2.45	0.41
2:E:421:LYS:NZ	2:E:452:GLY:CA	2.78	0.41
2:F:327:SER:OG	2:F:330:ILE:HG13	2.19	0.41
3:e:54:LEU:HG	3:e:56:ASN:H	1.85	0.41
1:A:299:LEU:HD21	1:A:329:PRO:HG3	2.02	0.41
1:B:356:LEU:HA	1:B:368:ALA:O	2.20	0.41
2:D:451:VAL:CG2	2:D:460:LYS:HD2	2.49	0.41
2:E:57:SER:O	2:E:59:GLU:OE1	2.38	0.41
1:A:138:ILE:HD12	1:A:138:ILE:HA	1.88	0.41
2:D:289:SER:HB2	2:D:294:SER:HA	2.01	0.41
1:B:256:ASP:HA	1:B:324:SER:O	2.20	0.41
1:B:279:ARG:HA	2:E:266:MET:CE	2.50	0.41
1:B:285:GLU:C	1:B:287:TYR:H	2.29	0.41
1:B:384:THR:HG22	1:B:385:LYS:H	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:ILE:HD12	2:D:65:LEU:HB2	2.03	0.41
2:F:391:ASP:O	2:F:394:VAL:HB	2.21	0.41
4:g:50:ARG:HA	4:g:53:ILE:CG1	2.51	0.41
1:A:151:TYR:HB2	1:A:154:VAL:HG12	2.01	0.41
1:A:476:PHE:O	1:A:484:MET:HG3	2.21	0.41
1:B:326:THR:CG2	1:B:327:ALA:N	2.84	0.41
1:B:494:ASN:O	1:B:495:LYS:C	2.64	0.41
1:C:166:GLU:O	1:C:329:PRO:HD2	2.21	0.41
2:E:160:GLU:OE2	2:E:411:VAL:HB	2.20	0.41
2:E:231:ASP:O	2:E:232:GLU:C	2.62	0.41
2:F:235:GLU:O	2:F:236:ASN:HB3	2.21	0.41
2:F:375:LEU:CD2	2:F:391:ASP:HB2	2.51	0.41
3:e:28:ALA:HB2	3:e:44:LEU:O	2.21	0.41
4:g:71:ARG:HH12	4:g:163:GLY:HA3	1.85	0.41
4:g:105:ALA:O	4:g:108:GLU:HB3	2.21	0.41
1:A:356:LEU:HA	1:A:368:ALA:O	2.21	0.41
4:g:220:GLY:O	4:g:223:VAL:HG22	2.21	0.41
4:g:228:SER:O	4:g:232:GLN:HG2	2.21	0.41
1:A:152:LYS:HB2	1:A:152:LYS:HE3	1.81	0.40
2:D:14:ILE:O	2:D:52:THR:OG1	2.35	0.40
2:E:389:GLU:H	2:E:392:LYS:HB3	1.86	0.40
2:F:376:LYS:O	2:F:379:ILE:HG22	2.21	0.40
1:A:180:ALA:HB1	1:A:260:ILE:HG21	2.03	0.40
1:C:103:GLU:OE1	1:C:124:ALA:HA	2.21	0.40
2:F:425:LEU:HB3	2:F:426:LYS:NZ	2.36	0.40
1:A:32:ILE:HG23	1:A:40:VAL:HG13	2.03	0.40
1:A:175:GLY:CA	5:A:601:ATP:H5'2	2.35	0.40
1:A:241:TYR:CE1	1:A:298:LEU:HB2	2.50	0.40
1:C:377:ARG:HH12	2:E:181:ARG:NH2	2.19	0.40
1:C:423:GLU:OE2	1:C:427:ARG:NH1	2.55	0.40
2:D:8:GLN:HB3	2:D:15:ASP:OD1	2.21	0.40
2:F:132:ILE:CG2	2:F:138:PHE:CZ	3.04	0.40
3:e:65:SER:OG	3:e:82:THR:HB	2.21	0.40
4:g:200:LEU:HD23	4:g:200:LEU:HA	1.90	0.40
1:B:55:GLU:HG3	1:B:90:ARG:HB3	2.03	0.40
2:D:199:ASP:OD1	2:D:199:ASP:N	2.53	0.40
2:F:83:LEU:HD21	2:F:172:LEU:HD22	2.04	0.40
1:A:107:ARG:CB	1:A:122:ILE:HD11	2.50	0.40
1:B:265:SER:OG	1:B:331:ILE:HG23	2.21	0.40
1:C:285:GLU:O	1:C:286:ALA:HB3	2.21	0.40
2:F:23:VAL:O	2:F:24:PRO:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:393:LEU:HD11	2:F:397:ARG:CZ	2.51	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 PDB entries followed by that with respect to all EM entries.

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	487/514 (95%)	474 (97%)	13 (3%)	0	100	100
1	B	487/514 (95%)	471 (97%)	16 (3%)	0	100	100
1	C	487/514 (95%)	478 (98%)	9 (2%)	0	100	100
2	D	461/464 (99%)	444 (96%)	17 (4%)	0	100	100
2	E	461/464 (99%)	441 (96%)	20 (4%)	0	100	100
2	F	461/464 (99%)	445 (96%)	16 (4%)	0	100	100
3	e	130/133 (98%)	128 (98%)	2 (2%)	0	100	100
4	g	286/289 (99%)	281 (98%)	5 (2%)	0	100	100
All	All	3260/3356 (97%)	3162 (97%)	98 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	384/406 (95%)	384 (100%)	0	100	100
1	B	384/406 (95%)	384 (100%)	0	100	100
1	C	384/406 (95%)	384 (100%)	0	100	100
2	D	378/379 (100%)	378 (100%)	0	100	100
2	E	378/379 (100%)	377 (100%)	1 (0%)	86	86
2	F	378/379 (100%)	378 (100%)	0	100	100
3	e	101/102 (99%)	101 (100%)	0	100	100
4	g	235/236 (100%)	235 (100%)	0	100	100
All	All	2622/2693 (97%)	2621 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	169	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	B	164	GLN
1	B	203	GLN
2	E	109	HIS
2	E	164	ASN
2	E	236	ASN
2	E	319	HIS
2	E	402	GLN
2	F	111	GLN
2	F	273	GLN
2	F	348	GLN
3	e	46	GLN
3	e	56	ASN
4	g	41	GLN
4	g	94	ASN
4	g	101	GLN
4	g	120	GLN
4	g	177	ASN
4	g	264	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
5	ATP	A	601	6	32,33,33	1.39	4 (12%)	48,52,52	1.73	9 (18%)
5	ATP	B	601	6	32,33,33	1.40	4 (12%)	48,52,52	1.74	9 (18%)
5	ATP	C	602	6	32,33,33	0.57	1 (3%)	48,52,52	0.29	0
7	ADP	D	502	6	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)
8	PO4	E	601	-	4,4,4	0.99	0	6,6,6	0.48	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
7	ADP	D	502	6	-	1/16/32/32	0/3/3/3
5	ATP	A	601	6	-	4/22/38/38	0/3/3/3
5	ATP	C	602	6	-	8/22/38/38	0/3/3/3
5	ATP	B	601	6	-	4/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	ATP	C5-C4	4.68	1.47	1.39
5	A	601	ATP	C5-C4	4.68	1.47	1.39
7	D	502	ADP	C5-C4	4.68	1.47	1.39
5	B	601	ATP	C5-C6	2.76	1.48	1.41
7	D	502	ADP	C5-C6	2.73	1.48	1.41
5	A	601	ATP	C5-C6	2.72	1.48	1.41
5	C	602	ATP	PA-O3A	-2.48	1.56	1.59
7	D	502	ADP	C8-N7	2.34	1.36	1.31
5	B	601	ATP	C8-N7	2.33	1.36	1.31
7	D	502	ADP	C5-N7	-2.29	1.34	1.39
5	A	601	ATP	C8-N7	2.28	1.36	1.31
5	A	601	ATP	C5-N7	-2.27	1.34	1.39
5	B	601	ATP	C5-N7	-2.26	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	502	ADP	C5-C4-N3	-5.74	118.82	126.72
5	A	601	ATP	C5-C4-N3	-5.73	118.83	126.72
5	B	601	ATP	C5-C4-N3	-5.64	118.94	126.72
5	A	601	ATP	N3-C4-N9	4.59	134.97	127.17
7	D	502	ADP	N3-C4-N9	4.57	134.94	127.17
5	B	601	ATP	N3-C4-N9	4.42	134.69	127.17
5	B	601	ATP	C4-C5-N7	-3.68	106.38	110.58
7	D	502	ADP	C2-N3-C4	3.66	120.77	111.83
5	A	601	ATP	C2-N3-C4	3.60	120.63	111.83
5	B	601	ATP	C2-N3-C4	3.60	120.62	111.83
7	D	502	ADP	C4-C5-N7	-3.42	106.67	110.58
5	A	601	ATP	C4-C5-N7	-3.38	106.72	110.58
7	D	502	ADP	N3-C2-N1	-3.16	123.80	128.58
5	A	601	ATP	N3-C2-N1	-3.12	123.86	128.58
5	B	601	ATP	N3-C2-N1	-3.10	123.89	128.58
5	B	601	ATP	C4-N9-C8	2.82	108.70	105.74
5	B	601	ATP	C5-N7-C8	2.72	107.73	103.45
7	D	502	ADP	C4-N9-C8	2.70	108.57	105.74
5	A	601	ATP	C4-N9-C8	2.66	108.53	105.74
7	D	502	ADP	C5-N7-C8	2.49	107.36	103.45
5	A	601	ATP	C5-N7-C8	2.47	107.33	103.45
5	A	601	ATP	C3'-C2'-C1'	2.47	106.13	101.46
7	D	502	ADP	C3'-C2'-C1'	2.28	105.78	101.46
5	B	601	ATP	C6-C5-N7	2.25	136.43	132.09
5	B	601	ATP	N9-C8-N7	-2.20	110.82	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	502	ADP	C6-C5-N7	2.09	136.12	132.09
5	A	601	ATP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	ATP	C5'-O5'-PA-O1A
5	B	601	ATP	C5'-O5'-PA-O1A
5	B	601	ATP	C5'-O5'-PA-O2A
5	B	601	ATP	C5'-O5'-PA-O3A
5	C	602	ATP	C5'-O5'-PA-O2A
5	C	602	ATP	C5'-O5'-PA-O3A
5	C	602	ATP	C3'-C4'-C5'-O5'
5	C	602	ATP	O4'-C4'-C5'-O5'
5	A	601	ATP	O4'-C4'-C5'-O5'
5	A	601	ATP	C3'-C4'-C5'-O5'
7	D	502	ADP	C5'-O5'-PA-O1A
5	A	601	ATP	C4'-C5'-O5'-PA
5	C	602	ATP	PB-O3B-PG-O1G
5	C	602	ATP	PB-O3B-PG-O2G
5	C	602	ATP	PB-O3B-PG-O3G
5	B	601	ATP	C2'-C1'-N9-C8
5	C	602	ATP	PG-O3B-PB-O2B

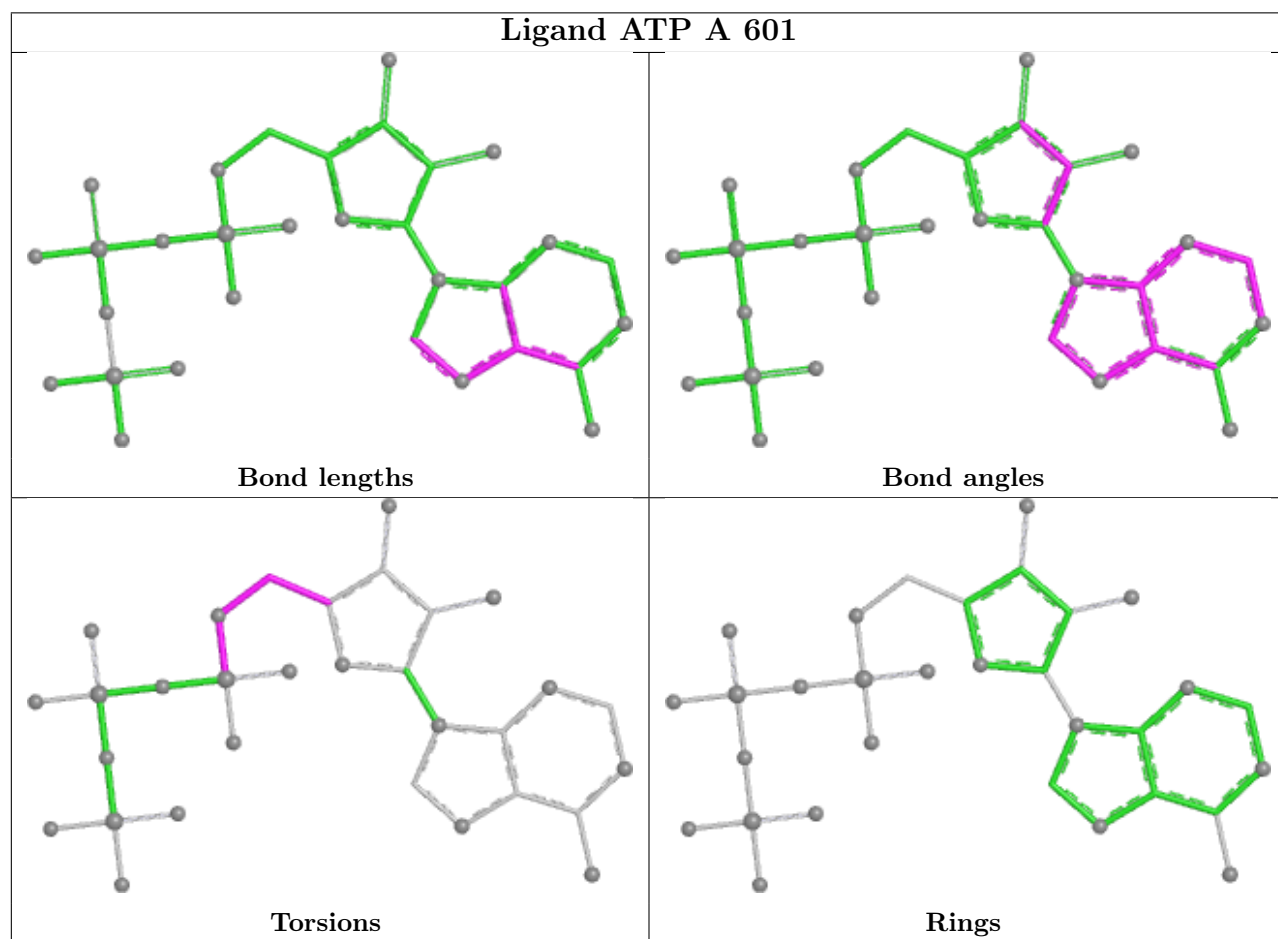
There are no ring outliers.

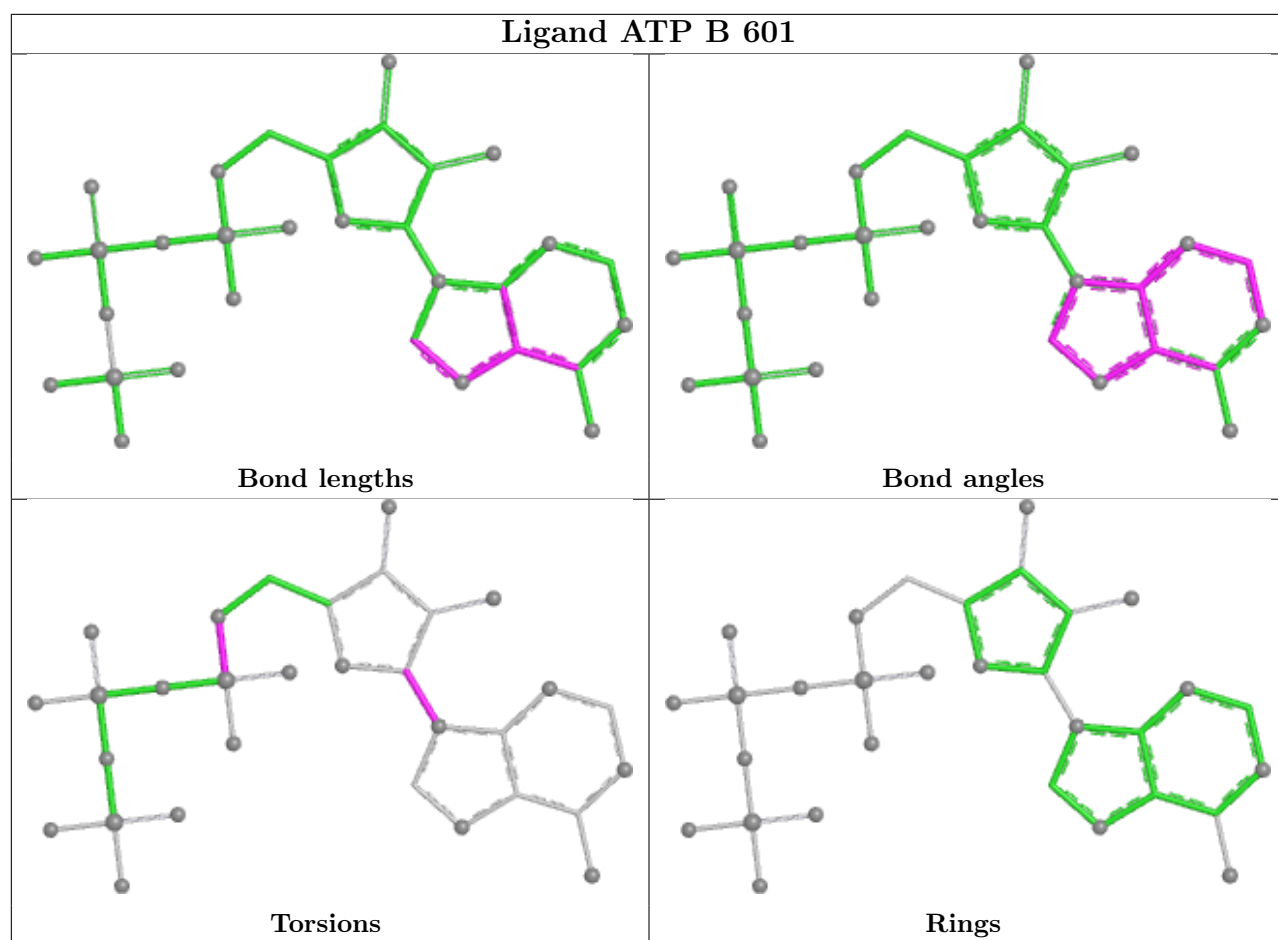
2 monomers are involved in 18 short contacts:

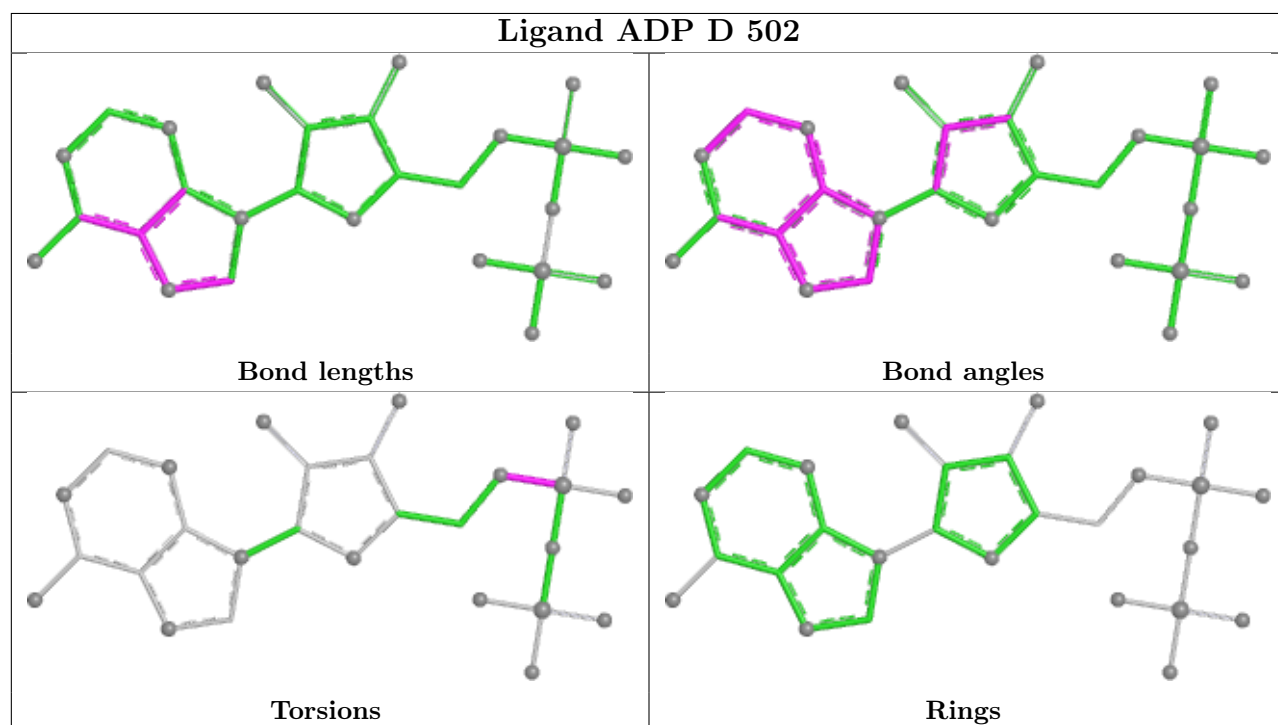
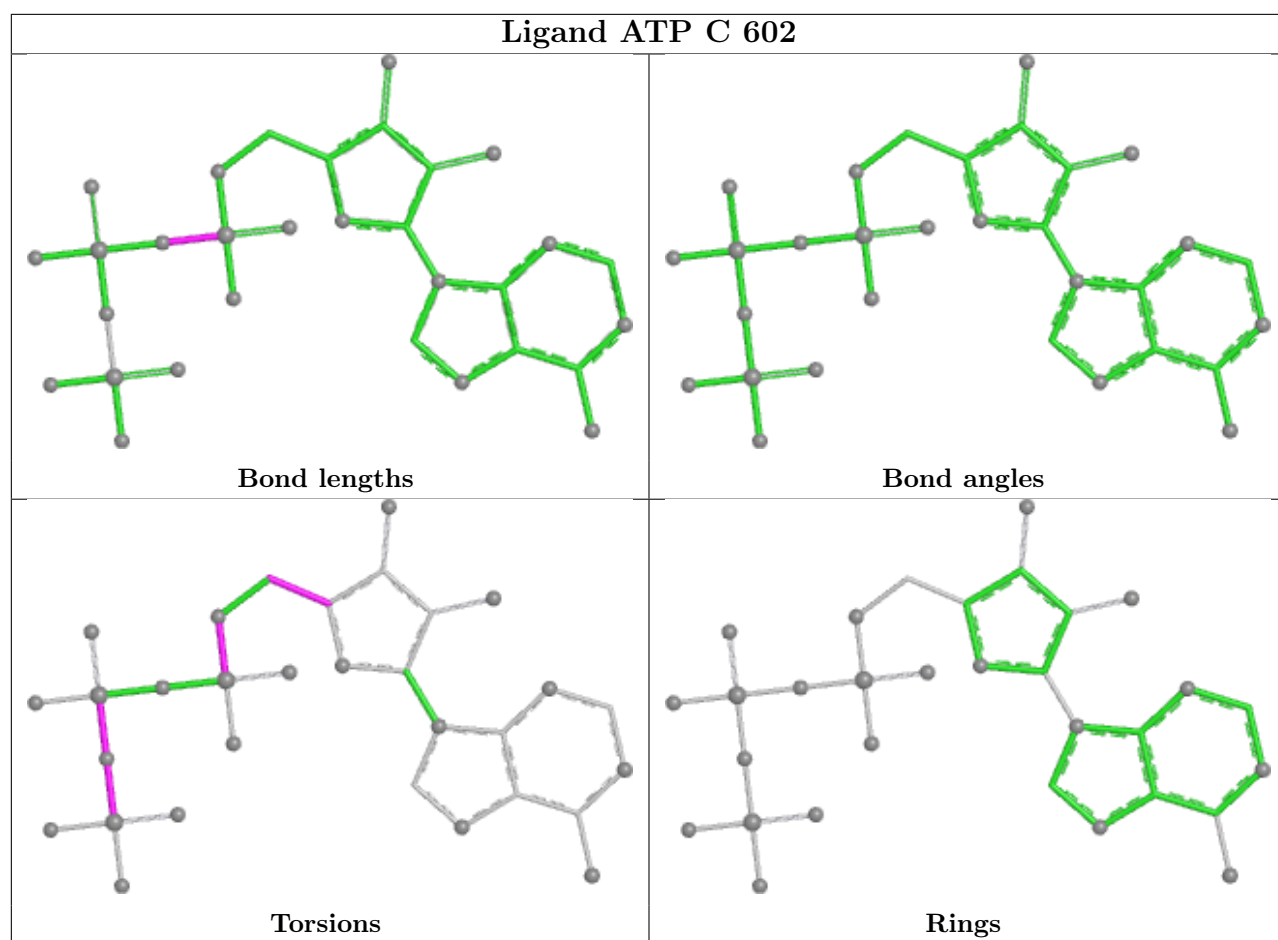
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	ATP	4	0
5	B	601	ATP	14	0

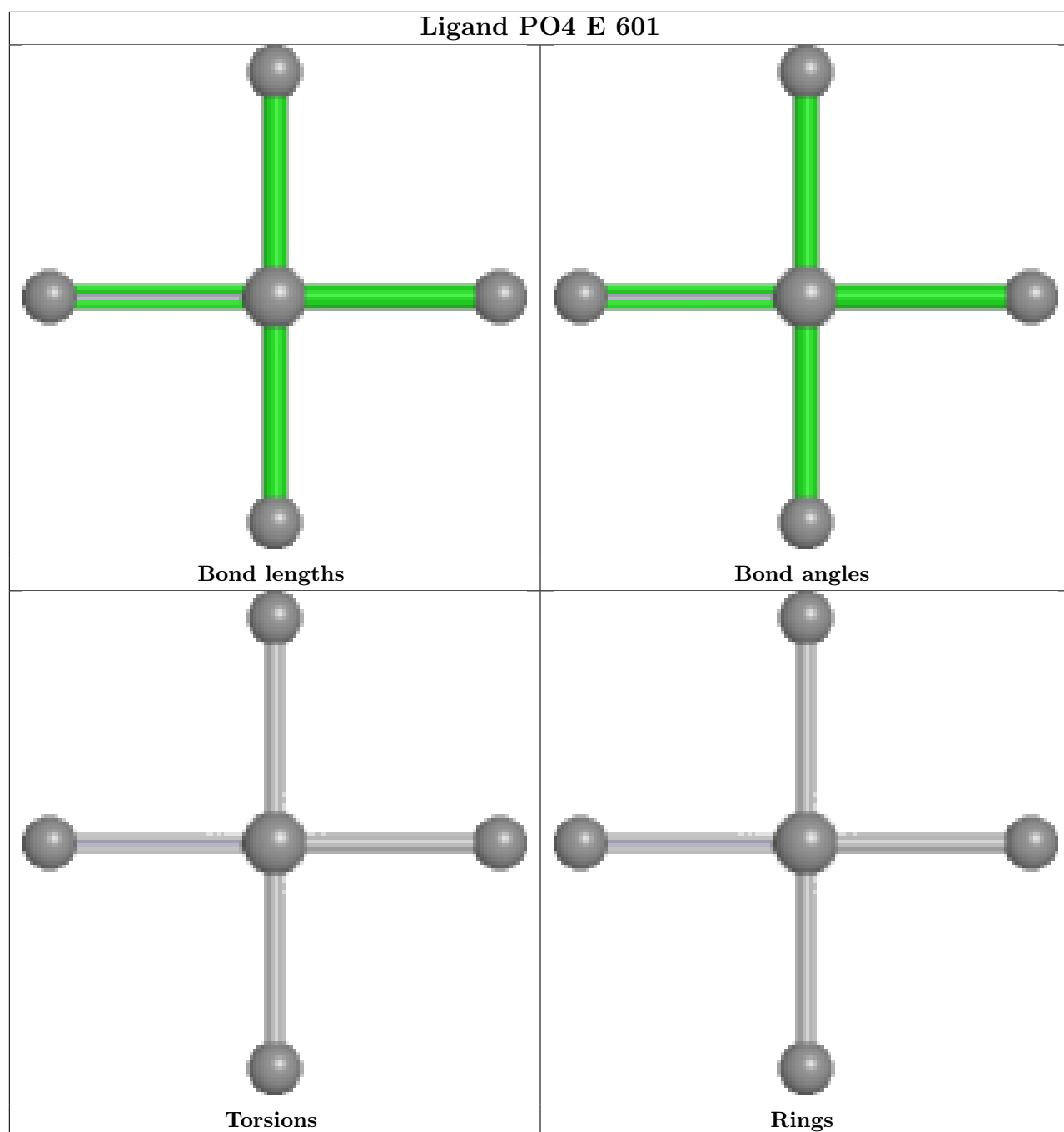
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.