



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 AM UTC

PDB ID : 7DY2 / pdb_00007dy2
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors : Furuike, Y.; Akiyama, S.
Deposited on : 2021-01-20
Resolution : 3.04 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

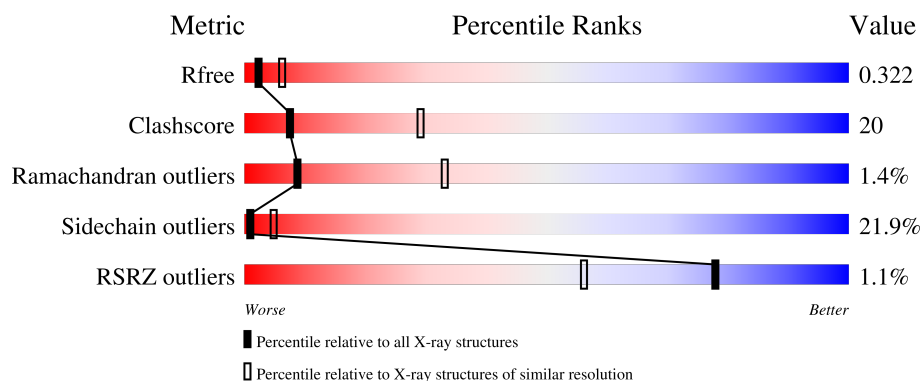
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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.



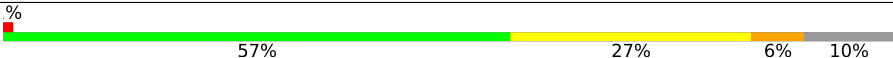
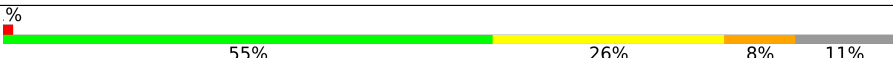
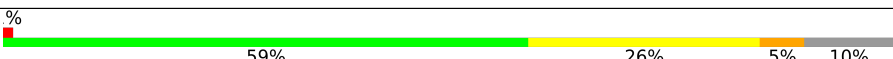
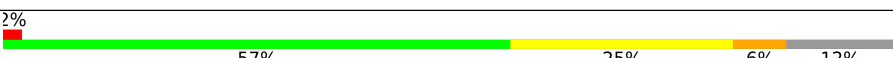
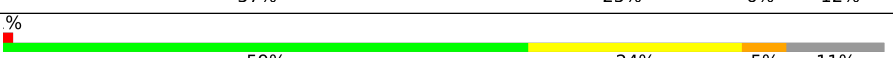
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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 $\leq 5\%$. 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	519	 57% 26% 6% 11%
1	B	519	 57% 26% 6% 11%
1	C	519	 54% 28% 7% 11%
1	D	519	 53% 29% 6% 12%
1	E	519	 54% 29% 7% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	519	
1	G	519	
1	I	519	
1	J	519	
1	K	519	
1	L	519	
2	H	519	

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
1	SEP	K	431	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 39277 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.

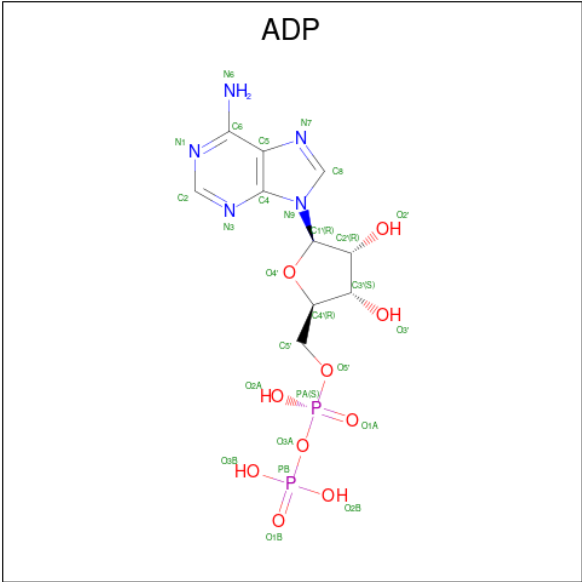
- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	P	S	0	0	0
			3300	2058	575	653	1	13			
1	B	461	Total	C	N	O	P	S	0	0	0
			3204	1995	566	631	1	11			
1	E	464	Total	C	N	O	P	S	0	0	0
			3287	2046	580	647	1	13			
1	F	467	Total	C	N	O	P	S	0	0	0
			3245	2013	575	644	1	12			
1	C	462	Total	C	N	O	P	S	0	0	0
			3236	2016	563	644	1	12			
1	D	458	Total	C	N	O	P	S	0	0	0
			3173	1958	567	634	1	13			
1	G	459	Total	C	N	O	P	S	0	0	0
			3000	1835	546	607	1	11			
1	K	465	Total	C	N	O	P	S	0	0	0
			3132	1933	563	623	1	12			
1	L	457	Total	C	N	O	P	S	0	0	0
			3082	1905	548	617	1	11			
1	I	467	Total	C	N	O	P	S	0	0	0
			3349	2087	585	662	1	14			
1	J	464	Total	C	N	O	P	S	0	0	0
			3342	2098	581	648	1	14			

- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

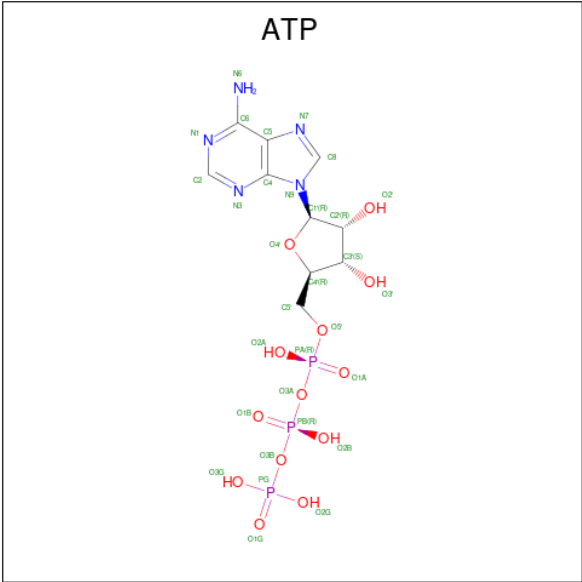
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	460	Total	C	N	O	S	0	0	0
			3197	1998	553	634	12			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	E	2	Total Mg 2 2	0	0
5	F	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	K	1	Total Mg 1 1	0	0
5	L	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0

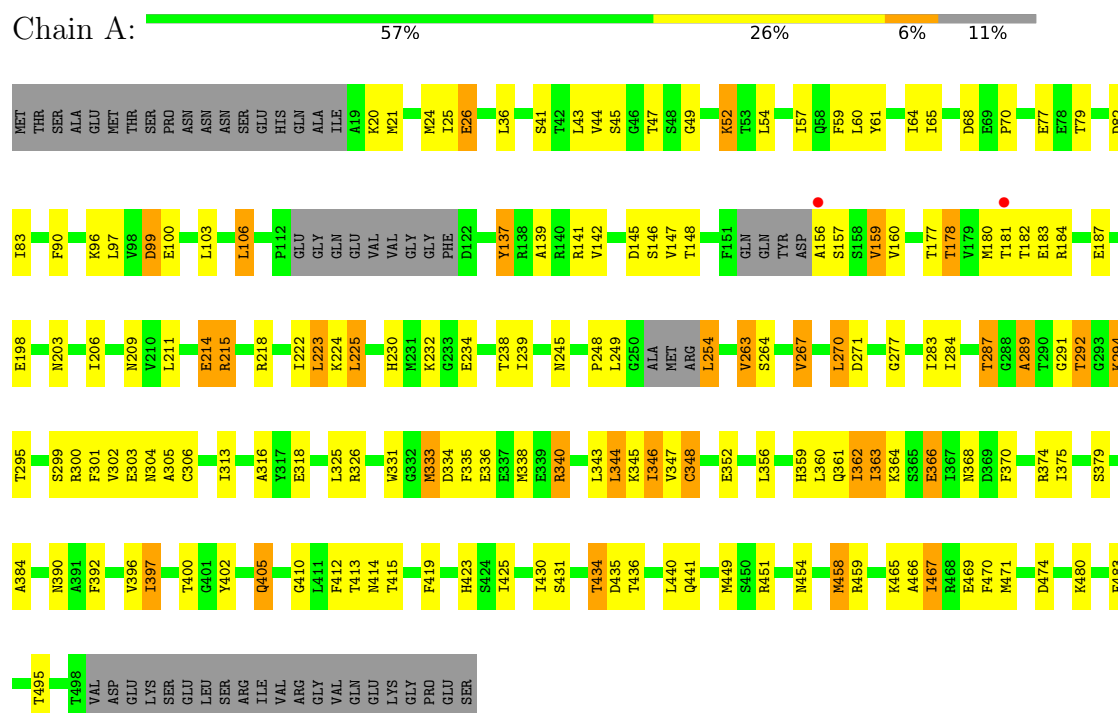
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0
6	F	2	Total O 2 2	0	0
6	D	1	Total O 1 1	0	0
6	G	2	Total O 2 2	0	0
6	H	4	Total O 4 4	0	0
6	K	1	Total O 1 1	0	0
6	I	2	Total O 2 2	0	0

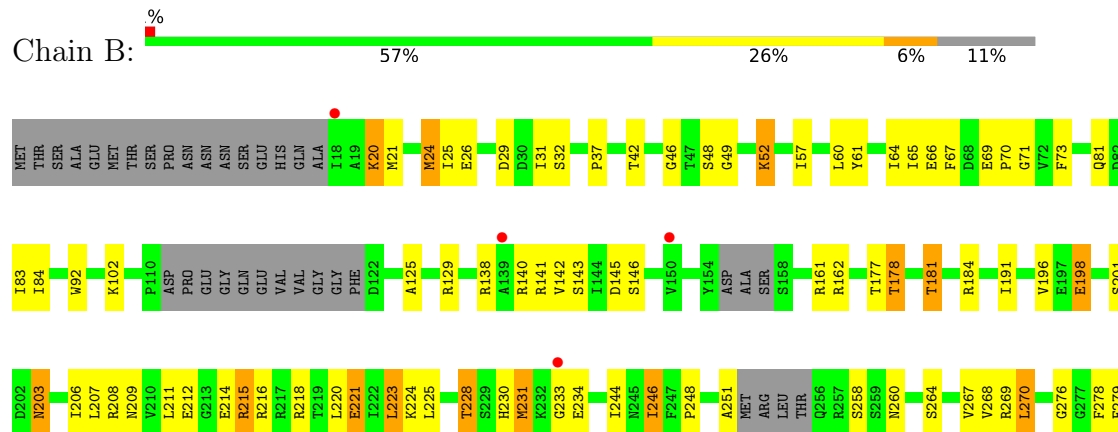
3 Residue-property plots

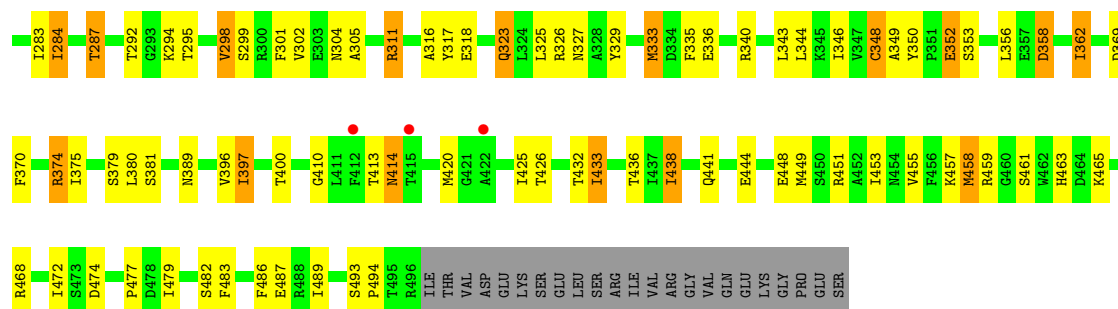
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

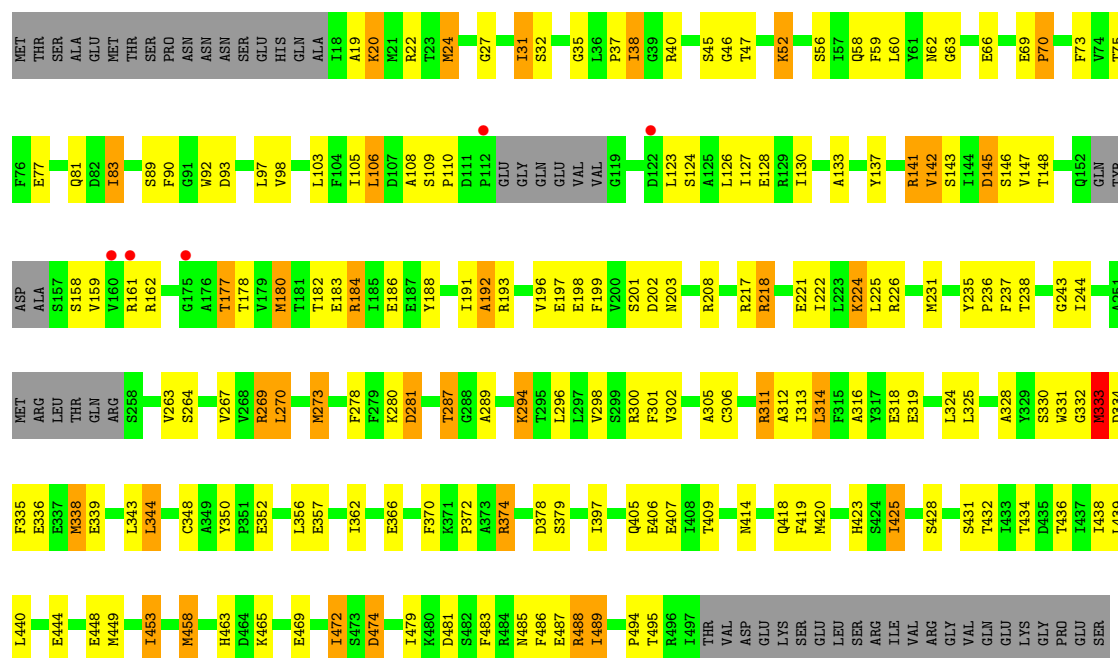


• Molecule 1: Circadian clock protein kinase KaiC

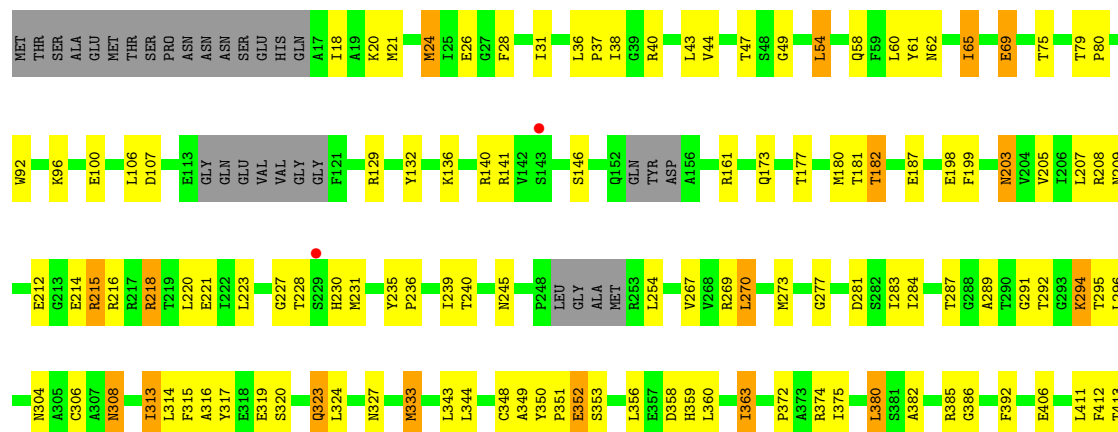


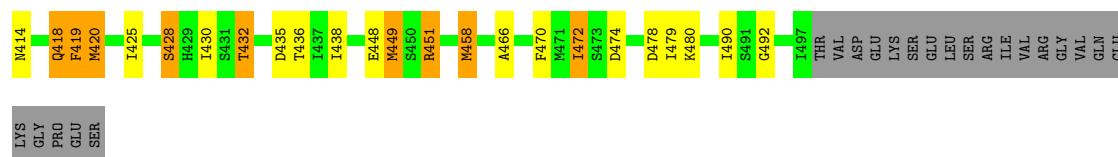


• Molecule 1: Circadian clock protein kinase KaiC

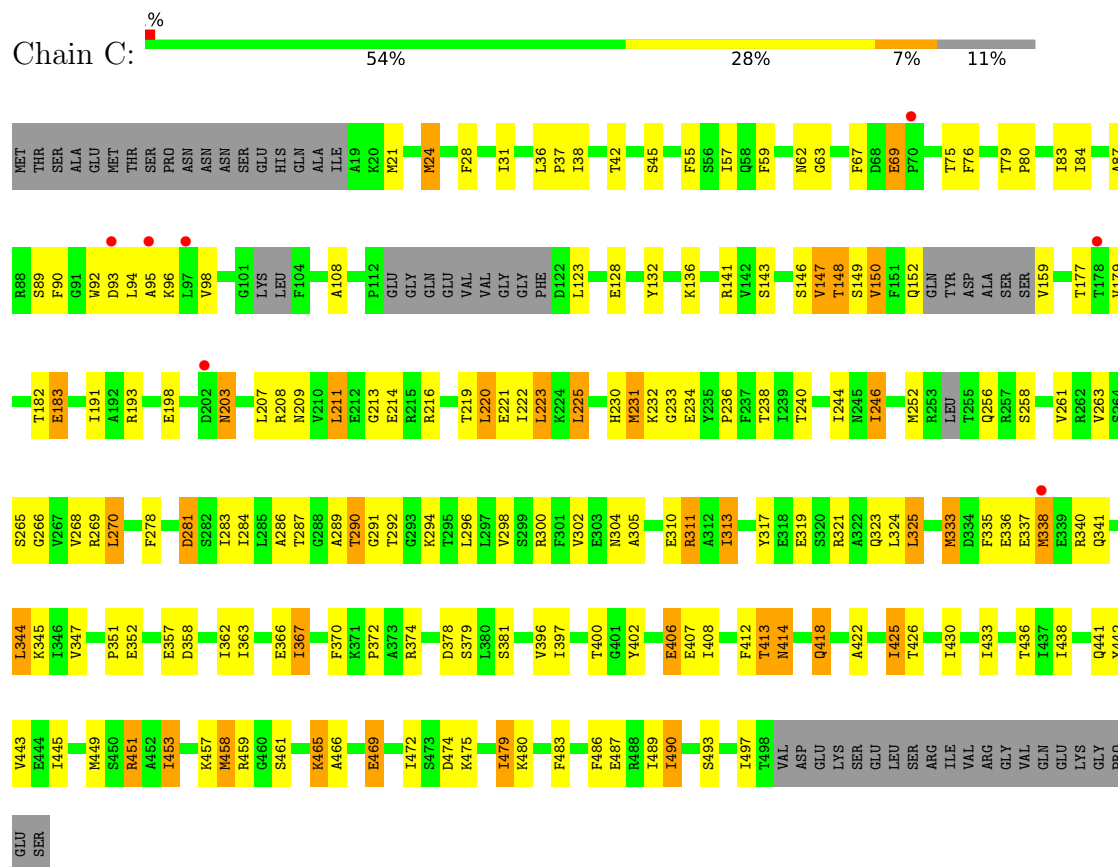


• Molecule 1: Circadian clock protein kinase KaiC

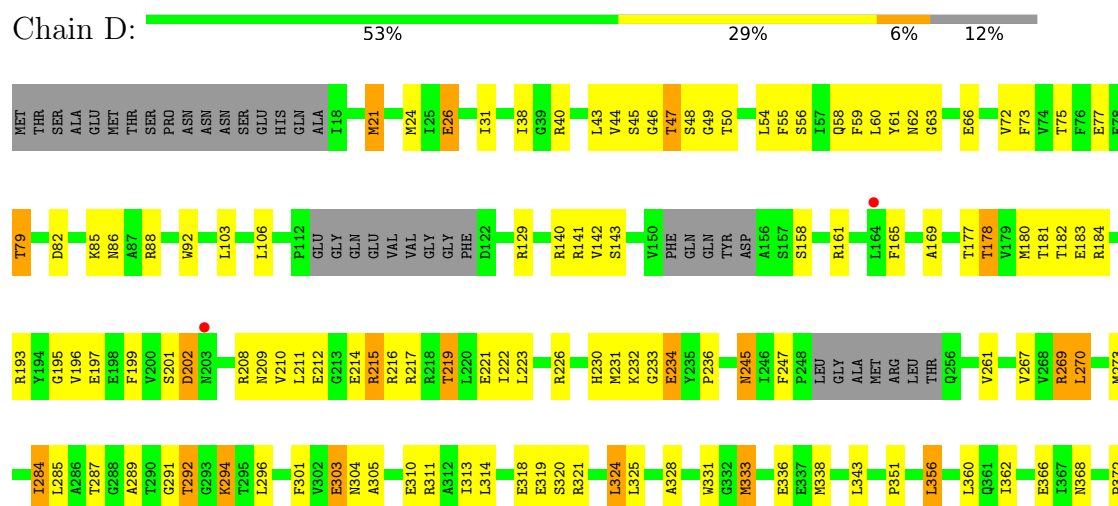


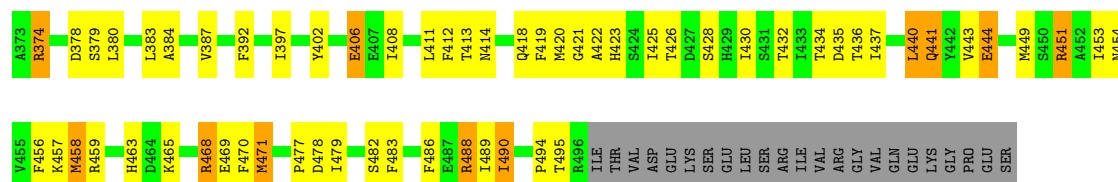


• Molecule 1: Circadian clock protein kinase KaiC

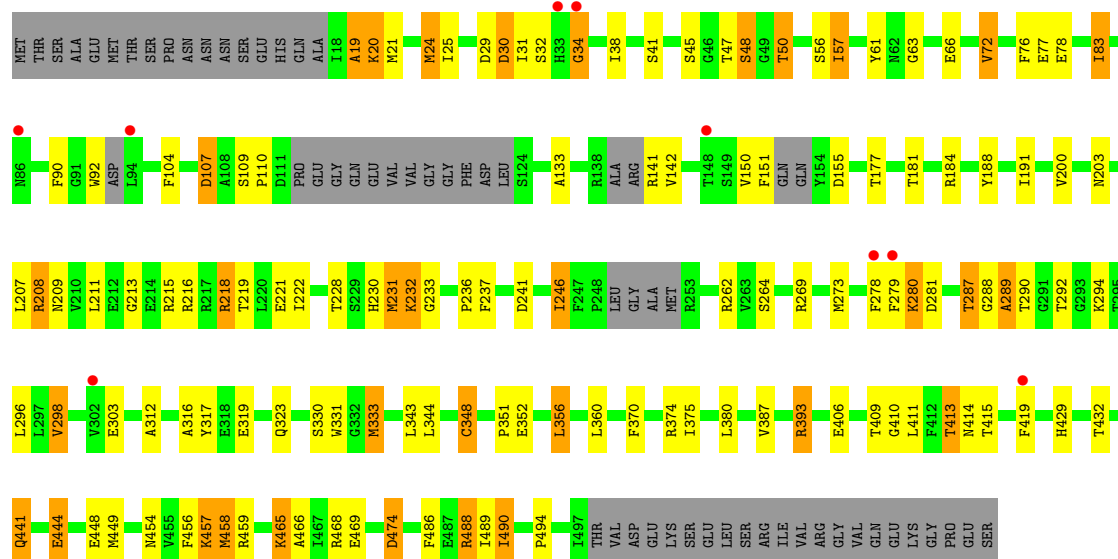


• Molecule 1: Circadian clock protein kinase KaiC

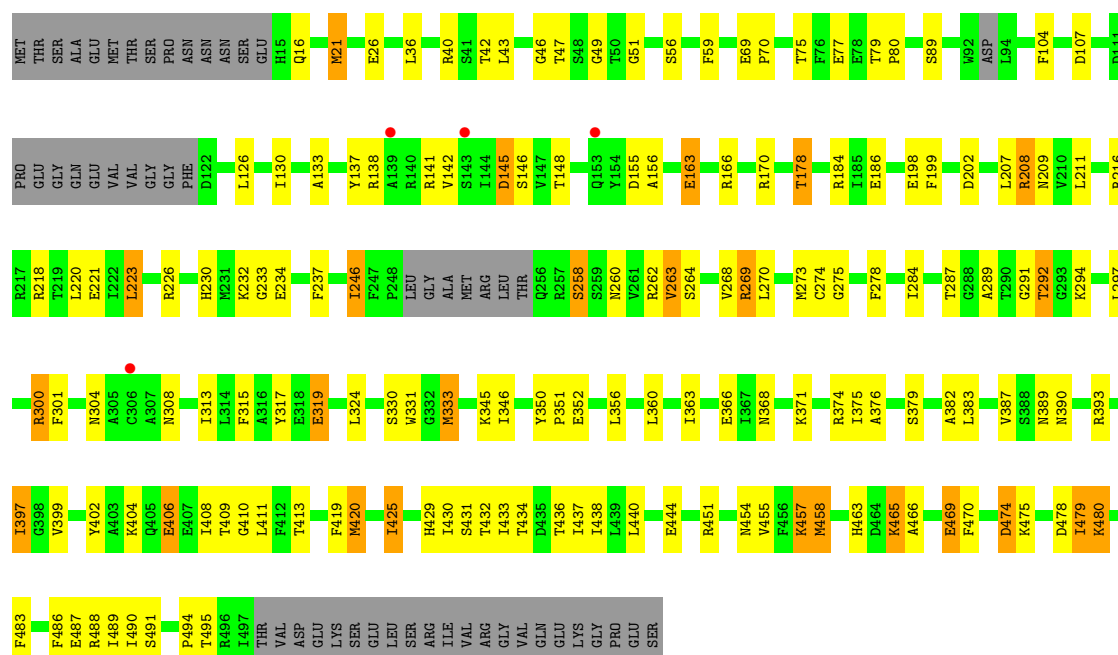




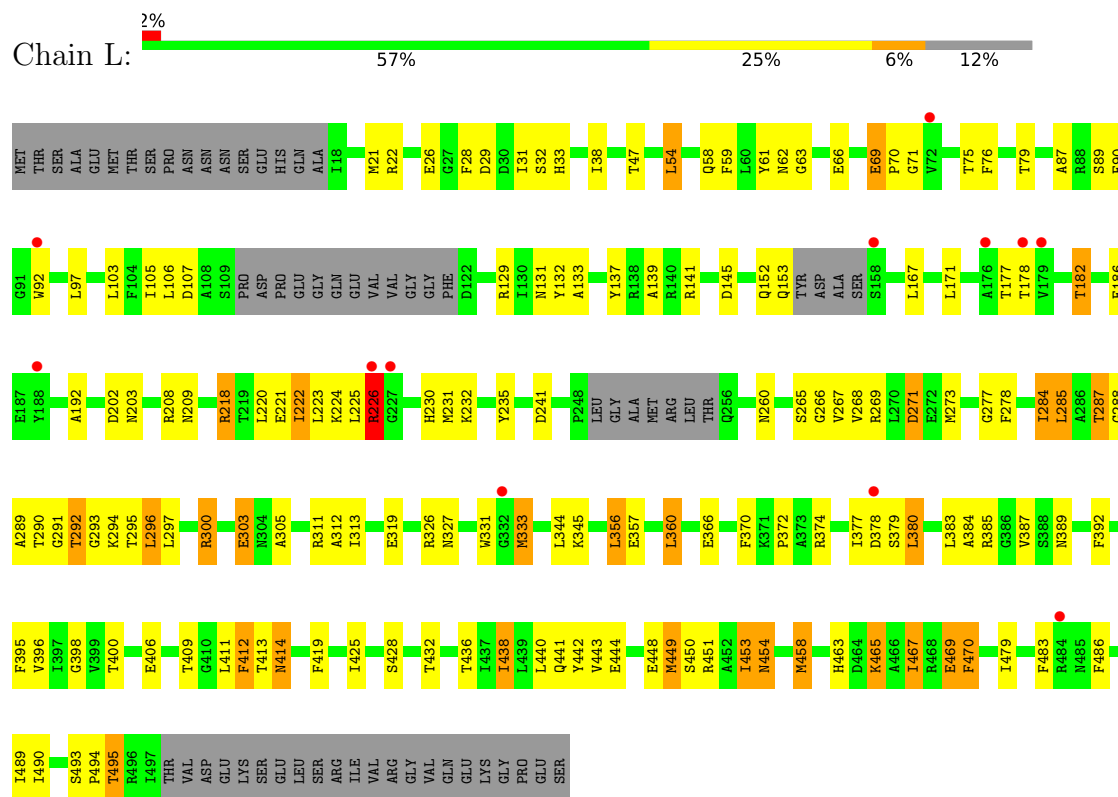
• Molecule 1: Circadian clock protein kinase KaiC



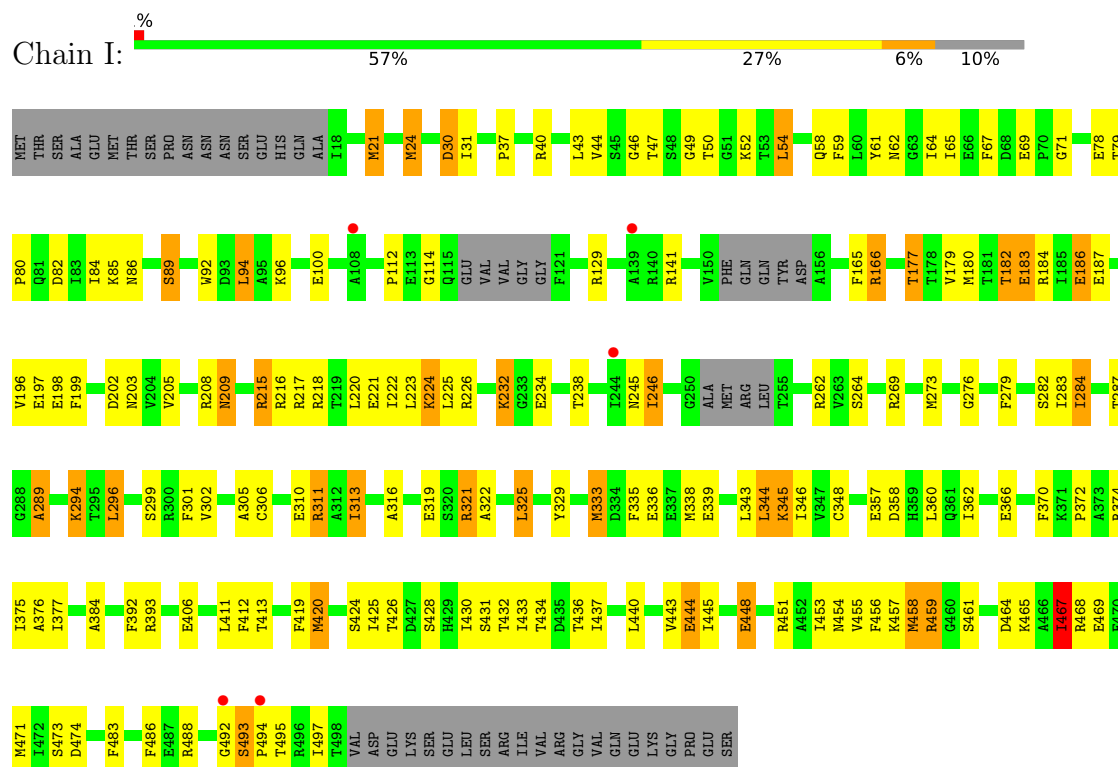
• Molecule 1: Circadian clock protein kinase KaiC



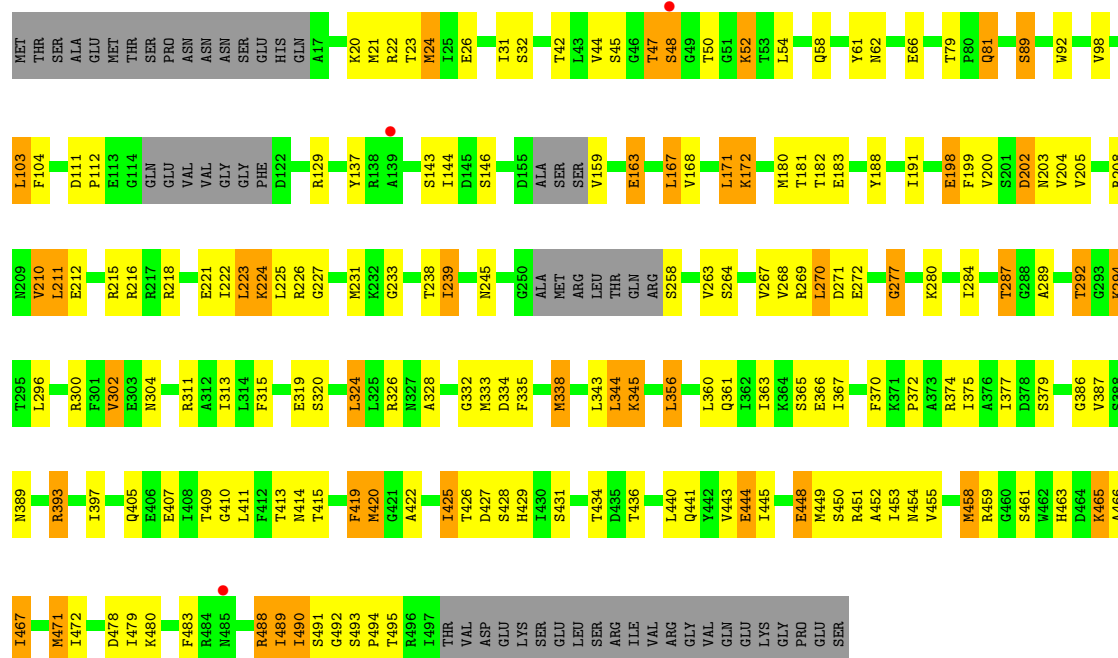
- Molecule 1: Circadian clock protein kinase KaiC



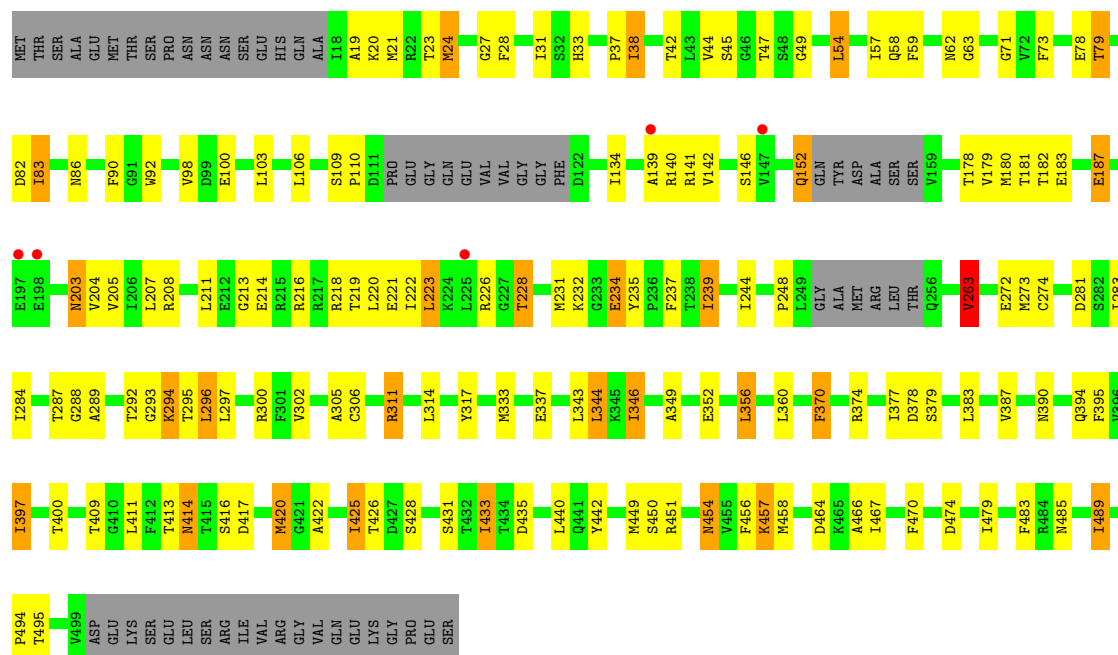
- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC



• Molecule 2: Circadian clock protein kinase KaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.80Å 206.60Å 168.38Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	49.24 – 3.04 49.24 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.24-3.04) 99.1 (49.24-3.04)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.263 , 0.326 0.261 , 0.322	Depositor DCC
R_{free} test set	6048 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	39277	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ADP, SEP, MG, 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	1.04	0/3342	1.46	0/4539
1	B	1.06	0/3244	1.48	0/4413
1	C	1.05	0/3275	1.46	0/4450
1	D	1.06	0/3213	1.47	0/4366
1	E	1.06	0/3330	1.49	0/4516
1	F	1.06	0/3286	1.48	1/4465 (0.0%)
1	G	1.10	0/3032	1.54	0/4131
1	I	1.04	0/3394	1.46	0/4600
1	J	1.03	0/3388	1.44	1/4597 (0.0%)
1	K	1.08	0/3171	1.50	1/4311 (0.0%)
1	L	1.08	0/3119	1.50	0/4249
2	H	1.06	0/3251	1.47	0/4424
All	All	1.06	0/39045	1.48	3/53061 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	233	GLY	CA-C-O	-5.67	118.32	122.23
1	J	277	GLY	CA-C-O	-5.36	118.29	122.52
1	F	277	GLY	CA-C-O	-5.10	118.20	122.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	155	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	2905	141	0
1	B	3204	0	2737	130	0
1	C	3236	0	2796	134	0
1	D	3173	0	2656	127	0
1	E	3287	0	2870	163	0
1	F	3245	0	2754	118	0
1	G	3000	0	2290	94	0
1	I	3349	0	2937	142	0
1	J	3342	0	2999	153	0
1	K	3132	0	2520	113	0
1	L	3082	0	2480	144	0
2	H	3197	0	2704	135	0
3	A	27	0	12	3	0
3	C	27	0	12	3	0
3	D	54	0	24	2	0
3	F	27	0	12	3	0
3	G	27	0	12	0	0
3	H	27	0	12	3	0
3	I	54	0	24	3	0
3	K	27	0	12	3	0
3	L	27	0	12	3	0
4	A	31	0	12	3	0
4	B	62	0	24	2	0
4	C	31	0	12	2	0
4	E	62	0	24	3	0
4	F	31	0	12	2	0
4	G	31	0	12	1	0
4	H	31	0	12	2	0
4	J	62	0	24	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	31	0	12	0	0
4	L	31	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	4	0	0	0	0
6	I	2	0	0	0	0
6	K	1	0	0	0	0
All	All	39277	0	32936	1466	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 20.

All (1466) 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:K:207:LEU:HD21	1:K:220:LEU:HD12	1.30	1.10
1:C:311:ARG:HD3	1:C:370:PHE:CE2	1.90	1.07
1:L:384:ALA:HB2	1:L:392:PHE:CE1	1.92	1.04
1:F:352:GLU:OE2	1:F:385:ARG:NH2	1.91	1.03
1:J:52:LYS:HB3	1:J:181:THR:HG23	1.38	1.03
1:C:147:VAL:O	1:C:150:VAL:HG12	1.59	1.03
1:B:225:LEU:HB2	1:B:230:HIS:HD2	1.21	1.02
1:A:156:ALA:HB1	1:A:159:VAL:CG2	1.90	1.01
1:A:156:ALA:HB1	1:A:159:VAL:HG21	1.44	1.00
4:A:602:ATP:H3'	1:B:458:MET:O	1.59	1.00
1:E:203:ASN:HB3	1:E:225:LEU:CD2	1.92	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.26	0.98
1:G:457:LYS:NZ	4:L:602:ATP:O3G	1.96	0.98
1:G:230:HIS:O	1:G:232:LYS:NZ	1.99	0.95
1:K:483:PHE:HB2	1:K:489:ILE:HD11	1.47	0.94
1:G:24:MET:HA	1:G:24:MET:HE3	1.48	0.94
1:A:249:LEU:HD13	1:F:353:SER:HA	1.48	0.93
1:G:393:ARG:NH1	1:G:429:HIS:O	2.02	0.93
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.50	0.92
1:K:21:MET:SD	1:K:141:ARG:NE	2.42	0.92
1:E:440:LEU:HD21	1:E:453:ILE:HD12	1.52	0.92
1:F:207:LEU:CD2	1:F:220:LEU:HD12	2.01	0.90
1:A:64:ILE:HG21	1:A:97:LEU:CD2	2.01	0.90
1:B:49:GLY:O	1:B:218:ARG:NH2	2.03	0.90
1:B:325:LEU:CD2	1:B:335:PHE:HB2	2.01	0.90
2:H:449:MET:HE2	1:I:467:ILE:HD11	1.52	0.90
1:A:287:THR:HG21	1:A:425:ILE:O	1.71	0.90
1:I:431:SEP:O	1:I:434:THR:HG22	1.72	0.89
1:I:284:ILE:HG23	1:I:436:THR:HB	1.51	0.89
1:K:483:PHE:HB2	1:K:489:ILE:CD1	2.02	0.88
1:L:294:LYS:NZ	4:L:602:ATP:O1B	2.06	0.88
1:J:471:MET:HG2	1:J:480:LYS:HE2	1.54	0.88
1:B:225:LEU:HB2	1:B:230:HIS:CD2	2.08	0.87
1:G:262:ARG:HA	1:G:278:PHE:O	1.74	0.87
1:I:82:ASP:OD2	1:J:172:LYS:HE2	1.75	0.87
1:F:37:PRO:HG2	1:F:203:ASN:OD1	1.74	0.87
1:C:84:ILE:CB	1:C:95:ALA:HA	2.04	0.87
1:B:21:MET:HE1	1:B:177:THR:HB	1.57	0.86
1:I:61:TYR:O	1:I:65:ILE:HG12	1.75	0.86
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.58	0.86
1:J:284:ILE:HB	1:J:411:LEU:HD12	1.57	0.86
1:I:306:CYS:SG	1:I:338:MET:HE1	2.15	0.86
1:D:26:GLU:CB	1:D:245:ASN:HA	2.06	0.86
1:I:306:CYS:SG	1:I:338:MET:CE	2.64	0.85
1:A:249:LEU:CD1	1:F:353:SER:HA	2.05	0.85
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.58	0.85
1:C:311:ARG:HD3	1:C:370:PHE:CZ	2.10	0.85
1:E:281:ASP:CG	1:E:407:GLU:OE2	2.20	0.85
1:E:31:ILE:HA	1:E:231:MET:HG3	1.57	0.84
1:A:291:GLY:O	1:A:451:ARG:NH1	2.11	0.83
1:D:356:LEU:CD2	1:D:387:VAL:HG11	2.09	0.83
1:A:64:ILE:HG21	1:A:97:LEU:HD21	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.09	0.83
1:D:425:ILE:HD11	1:D:456:PHE:CE2	2.14	0.83
1:L:292:THR:OG1	1:L:442:TYR:CE1	2.31	0.82
1:E:52:LYS:HE3	4:E:601:ATP:O2B	1.80	0.82
1:K:40:ARG:NH1	1:K:226:ARG:O	2.11	0.82
1:B:323:GLN:HE22	1:C:459:ARG:HD2	1.44	0.82
1:E:318:GLU:HG2	1:F:432:THR:OG1	1.79	0.82
1:B:325:LEU:HD23	1:B:335:PHE:HB2	1.59	0.82
1:C:286:ALA:HB3	1:C:413:THR:HG22	1.60	0.82
1:A:294:LYS:HG2	1:A:413:THR:HG23	1.62	0.81
1:F:96:LYS:O	1:F:100:GLU:HG3	1.80	0.81
1:C:286:ALA:HB3	1:C:413:THR:CG2	2.10	0.81
1:E:431:SEP:O	1:E:434:THR:HG22	1.80	0.81
1:A:64:ILE:CG2	1:A:97:LEU:HD21	2.10	0.81
1:K:420:MET:HE2	1:L:490:ILE:HG13	1.61	0.81
1:I:448:GLU:HG3	1:J:465:LYS:O	1.81	0.81
1:J:52:LYS:HB3	1:J:181:THR:CG2	2.10	0.81
1:E:338:MET:HB3	1:E:344:LEU:HB2	1.63	0.80
1:D:31:ILE:HA	1:D:231:MET:HG3	1.63	0.80
1:G:72:VAL:HG13	1:G:104:PHE:CD2	2.17	0.80
2:H:420:MET:HE1	2:H:449:MET:HE1	1.61	0.80
1:G:221:GLU:HG3	1:G:233:GLY:O	1.81	0.80
1:F:24:MET:HB2	1:F:62:ASN:HB3	1.63	0.80
1:K:207:LEU:CD2	1:K:220:LEU:HD12	2.11	0.80
1:I:325:LEU:CD2	1:I:336:GLU:HG2	2.11	0.80
1:E:483:PHE:HB2	1:E:489:ILE:CD1	2.12	0.80
1:B:301:PHE:O	1:B:374:ARG:NH1	2.15	0.80
1:A:146:SER:HA	1:A:181:THR:HG22	1.64	0.80
2:H:146:SER:HA	2:H:181:THR:O	1.81	0.79
1:B:21:MET:HE1	1:B:177:THR:CB	2.12	0.79
1:K:300:ARG:NH1	1:K:475:LYS:O	2.15	0.79
1:D:418:GLN:NE2	1:D:422:ALA:HA	1.97	0.79
1:I:419:PHE:CD2	1:J:425:ILE:HD13	2.17	0.78
1:K:425:ILE:HG12	1:J:419:PHE:CE2	2.19	0.78
3:I:602:ADP:H3'	1:J:458:MET:O	1.82	0.78
1:E:90:PHE:CE2	1:E:243:GLY:HA2	2.18	0.78
1:E:287:THR:CG2	1:E:414:ASN:HD22	1.95	0.78
1:A:146:SER:HB3	1:A:181:THR:HG21	1.65	0.77
1:E:301:PHE:O	1:E:374:ARG:NH1	2.17	0.77
2:H:58:GLN:HG3	2:H:92:TRP:HH2	1.46	0.77
1:L:384:ALA:CB	1:L:392:PHE:CE1	2.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:ASN:O	1:J:66:GLU:HB2	1.84	0.77
2:H:284:ILE:HB	2:H:411:LEU:HD12	1.65	0.77
1:K:209:ASN:OD1	1:K:216:ARG:HD2	1.84	0.77
1:B:221:GLU:HB2	1:B:234:GLU:HA	1.66	0.77
1:C:287:THR:HG23	1:C:414:ASN:HD21	1.50	0.77
1:G:356:LEU:HD21	1:G:387:VAL:HG11	1.64	0.77
1:E:73:PHE:CE2	1:E:83:ILE:HD12	2.18	0.77
1:A:289:ALA:O	1:A:294:LYS:NZ	2.17	0.77
1:F:287:THR:HG22	1:F:414:ASN:HD22	1.50	0.77
1:K:104:PHE:HE2	1:K:133:ALA:HB2	1.49	0.77
1:G:290:THR:HG21	2:H:425:ILE:HD13	1.67	0.77
1:F:146:SER:HA	1:F:181:THR:O	1.85	0.76
1:G:459:ARG:HB2	1:L:327:ASN:HD21	1.48	0.76
1:B:57:ILE:HD11	1:B:83:ILE:HG23	1.67	0.76
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.50	0.76
1:I:329:TYR:HA	1:I:333:MET:O	1.84	0.76
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.65	0.76
2:H:58:GLN:HG3	2:H:92:TRP:CH2	2.20	0.76
1:C:337:GLU:O	1:C:341:GLN:HG3	1.86	0.76
1:L:58:GLN:HG3	1:L:92:TRP:CH2	2.20	0.76
1:E:311:ARG:NH1	1:E:370:PHE:O	2.18	0.75
4:C:602:ATP:H3'	1:D:458:MET:O	1.86	0.75
1:I:492:GLY:O	1:I:494:PRO:HD3	1.86	0.75
1:I:31:ILE:HG22	1:I:222:ILE:HD11	1.67	0.75
1:C:311:ARG:CD	1:C:370:PHE:CE2	2.70	0.75
1:I:21:MET:HE1	1:I:177:THR:HB	1.68	0.75
1:C:214:GLU:OE2	1:D:217:ARG:NH1	2.16	0.74
1:E:73:PHE:HE2	1:E:83:ILE:HD12	1.51	0.74
1:D:202:ASP:HA	1:D:226:ARG:HD2	1.68	0.74
2:H:397:ILE:HG22	2:H:433:ILE:HD13	1.66	0.74
1:L:292:THR:OG1	1:L:442:TYR:HE1	1.68	0.74
1:L:436:THR:OG1	1:L:458:MET:HE3	1.86	0.74
1:I:425:ILE:HD11	1:I:456:PHE:CE2	2.22	0.74
1:E:161:ARG:CB	1:E:196:VAL:CB	2.65	0.74
1:J:335:PHE:HA	1:J:338:MET:HG3	1.70	0.74
1:D:440:LEU:HD21	1:D:470:PHE:CZ	2.23	0.74
1:J:441:GLN:HE22	1:J:490:ILE:HA	1.50	0.74
1:D:301:PHE:O	1:D:374:ARG:NH1	2.20	0.74
1:L:294:LYS:HB3	1:L:413:THR:HG23	1.69	0.73
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.69	0.73
1:J:471:MET:HG2	1:J:480:LYS:CE	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:PHE:O	1:I:141:ARG:NH1	2.22	0.73
2:H:356:LEU:HD22	2:H:387:VAL:HG11	1.69	0.73
1:A:146:SER:CB	1:A:181:THR:CG2	2.66	0.73
1:I:419:PHE:CD2	1:J:425:ILE:CD1	2.71	0.73
2:H:425:ILE:HG22	2:H:426:THR:HG23	1.69	0.72
1:J:52:LYS:HE2	1:J:181:THR:CG2	2.18	0.72
1:E:287:THR:HG21	1:E:425:ILE:O	1.88	0.72
1:E:182:THR:HG21	1:E:197:GLU:HG2	1.69	0.72
1:C:183:GLU:HB2	1:D:199:PHE:CE1	2.24	0.72
1:E:59:PHE:O	1:E:141:ARG:NH1	2.23	0.72
1:D:267:VAL:HG22	1:D:477:PRO:HG3	1.71	0.72
1:F:451:ARG:HB2	1:F:470:PHE:CE2	2.25	0.72
1:J:375:ILE:O	1:J:410:GLY:HA2	1.88	0.72
1:G:72:VAL:HG13	1:G:104:PHE:HD2	1.54	0.72
1:A:64:ILE:HG21	1:A:97:LEU:HD22	1.70	0.72
1:A:45:SER:CB	1:A:182:THR:HB	2.20	0.71
1:F:315:PHE:HE1	1:F:375:ILE:CG2	2.03	0.71
1:G:211:LEU:HD12	1:G:216:ARG:HG2	1.72	0.71
1:E:59:PHE:C	1:E:141:ARG:NH1	2.48	0.71
1:A:264:SER:O	1:A:374:ARG:NH2	2.23	0.71
1:A:423:HIS:O	1:F:418:GLN:HA	1.89	0.71
2:H:294:LYS:HB3	2:H:413:THR:CG2	2.20	0.71
2:H:467:ILE:HD12	2:H:467:ILE:H	1.54	0.71
1:D:294:LYS:HB3	1:D:413:THR:HG23	1.71	0.71
1:C:183:GLU:OE2	1:D:161:ARG:NH2	2.22	0.71
1:B:325:LEU:HD21	1:B:335:PHE:HB2	1.71	0.71
1:L:451:ARG:CB	1:L:470:PHE:HE2	2.04	0.71
1:I:31:ILE:HG22	1:I:222:ILE:CD1	2.21	0.71
1:J:203:ASN:HB3	1:J:225:LEU:HD23	1.71	0.71
1:D:356:LEU:HD22	1:D:387:VAL:HG11	1.72	0.70
1:G:24:MET:HA	1:G:24:MET:CE	2.19	0.70
1:A:59:PHE:O	1:A:141:ARG:NH1	2.24	0.70
1:D:486:PHE:HA	1:D:495:THR:O	1.90	0.70
2:H:287:THR:HG21	2:H:425:ILE:O	1.91	0.70
1:J:203:ASN:HB3	1:J:225:LEU:CD2	2.21	0.70
1:B:468:ARG:HA	1:B:482:SER:HA	1.73	0.70
1:D:61:TYR:CZ	1:D:92:TRP:CD1	2.79	0.70
1:G:459:ARG:HB2	1:L:327:ASN:ND2	2.06	0.70
2:H:31:ILE:HA	2:H:231:MET:HG3	1.73	0.70
1:J:52:LYS:HE2	1:J:181:THR:HG22	1.73	0.70
1:A:21:MET:HE1	1:A:177:THR:HB	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:ASN:O	1:G:216:ARG:NH1	2.22	0.70
1:I:279:PHE:HB2	1:I:282:SER:HB3	1.72	0.70
1:F:28:PHE:CE2	1:F:36:LEU:HD21	2.27	0.70
1:A:206:ILE:HD11	1:A:223:LEU:HG	1.74	0.69
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.74	0.69
1:J:458:MET:HG3	1:J:463:HIS:HB3	1.75	0.69
1:B:248:PRO:HB2	1:B:251:ALA:HB2	1.74	0.69
1:B:203:ASN:HB3	1:B:225:LEU:CD2	2.22	0.69
1:E:60:LEU:HD23	1:E:141:ARG:HD3	1.75	0.69
1:K:436:THR:HG23	1:K:458:MET:HG2	1.74	0.69
1:A:336:GLU:O	1:A:340:ARG:HG3	1.92	0.68
1:L:225:LEU:HD12	1:L:230:HIS:HB3	1.75	0.68
1:E:37:PRO:O	1:E:177:THR:CG2	2.42	0.68
1:I:313:ILE:HG13	1:I:372:PRO:HG3	1.75	0.68
1:E:425:ILE:HD13	1:D:419:PHE:CE2	2.29	0.68
1:C:458:MET:HG2	1:C:461:SER:HB3	1.76	0.68
1:G:375:ILE:O	1:G:410:GLY:HA2	1.94	0.68
1:E:58:GLN:HG3	1:E:92:TRP:CH2	2.28	0.68
1:C:236:PRO:HB2	1:C:357:GLU:HG3	1.73	0.68
1:F:37:PRO:HG2	1:F:203:ASN:CG	2.19	0.68
2:H:21:MET:HE3	2:H:141:ARG:NE	2.08	0.68
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.73	0.67
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.77	0.67
1:E:89:SER:CB	1:F:227:GLY:O	2.42	0.67
1:A:245:ASN:HB3	1:A:361:GLN:HE22	1.60	0.67
1:F:352:GLU:CD	1:F:385:ARG:HH21	2.00	0.67
1:A:292:THR:HB	1:A:440:LEU:HB3	1.77	0.67
1:L:454:ASN:HB2	1:L:467:ILE:HA	1.76	0.67
1:F:313:ILE:HG13	1:F:372:PRO:HG3	1.75	0.67
1:E:463:HIS:O	1:E:465:LYS:NZ	2.27	0.67
2:H:356:LEU:CD2	2:H:387:VAL:HG11	2.23	0.67
1:A:214:GLU:HG3	1:B:234:GLU:HG3	1.77	0.67
1:I:24:MET:HB2	1:I:62:ASN:HB3	1.77	0.67
1:A:344:LEU:CD1	1:A:346:ILE:HD11	2.25	0.67
1:J:263:VAL:CG2	1:J:280:LYS:HA	2.25	0.67
1:A:156:ALA:HB1	1:A:159:VAL:HG23	1.77	0.66
1:C:45:SER:OG	1:C:191:ILE:O	2.12	0.66
2:H:397:ILE:HG22	2:H:433:ILE:CD1	2.25	0.66
1:J:449:MET:HA	1:J:449:MET:HE2	1.78	0.66
1:I:486:PHE:CD2	1:I:494:PRO:HB2	2.30	0.66
3:A:601:ADP:O3'	1:B:224:LYS:HB2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLN:HE21	1:B:327:ASN:HD21	1.44	0.66
1:D:267:VAL:HG22	1:D:477:PRO:CG	2.26	0.66
1:B:31:ILE:HA	1:B:231:MET:HG3	1.76	0.65
1:K:420:MET:CE	1:L:490:ILE:HG13	2.25	0.65
2:H:374:ARG:HA	2:H:409:THR:O	1.97	0.65
1:A:45:SER:HB3	1:A:182:THR:HB	1.79	0.65
1:A:254:LEU:HD12	1:F:320:SER:HB3	1.79	0.65
1:J:191:ILE:HB	1:J:198:GLU:HG2	1.78	0.65
2:H:283:ILE:CD1	2:H:400:THR:HG23	2.26	0.65
1:L:384:ALA:CA	1:L:392:PHE:CE1	2.80	0.65
1:J:146:SER:H	1:J:181:THR:HB	1.62	0.65
1:A:222:ILE:CG2	1:A:225:LEU:HD12	2.27	0.65
1:D:488:ARG:HH11	1:D:488:ARG:HB2	1.60	0.65
1:I:80:PRO:O	1:I:84:ILE:HG13	1.97	0.65
1:A:146:SER:CB	1:A:181:THR:HG21	2.26	0.65
1:K:269:ARG:O	1:K:273:MET:HG3	1.96	0.65
1:F:304:ASN:O	1:F:308:ASN:ND2	2.30	0.64
1:L:292:THR:CG2	1:L:440:LEU:HB3	2.26	0.64
1:E:440:LEU:CD2	1:E:453:ILE:HD12	2.27	0.64
1:C:321:ARG:O	1:C:325:LEU:HB2	1.97	0.64
2:H:71:GLY:HA2	2:H:141:ARG:O	1.97	0.64
1:L:292:THR:HG21	1:L:440:LEU:CB	2.27	0.64
1:D:79:THR:HG23	1:D:82:ASP:HB2	1.80	0.64
1:B:279:PHE:CE1	1:B:461:SER:HB2	2.32	0.64
1:K:483:PHE:CB	1:K:489:ILE:HD11	2.25	0.64
1:E:124:SER:O	1:E:128:GLU:HG3	1.98	0.64
1:E:483:PHE:HB2	1:E:489:ILE:HD12	1.79	0.64
1:L:294:LYS:HB3	1:L:413:THR:CG2	2.27	0.64
1:L:377:ILE:HD12	1:L:412:PHE:CE2	2.31	0.64
1:I:283:ILE:HG23	1:I:412:PHE:HE1	1.61	0.64
1:J:374:ARG:HA	1:J:409:THR:O	1.97	0.64
1:A:326:ARG:HG3	1:B:260:ASN:HD21	1.62	0.64
1:B:215:ARG:HE	1:B:215:ARG:HA	1.62	0.64
1:C:325:LEU:HD23	1:C:335:PHE:HB2	1.78	0.64
1:K:292:THR:HB	1:K:440:LEU:HB2	1.78	0.64
1:L:38:ILE:HA	1:L:177:THR:HG22	1.79	0.64
1:I:419:PHE:HD2	1:J:425:ILE:HD13	1.63	0.64
1:F:269:ARG:HG2	1:F:479:ILE:CB	2.27	0.64
1:L:230:HIS:CD2	1:L:232:LYS:HE3	2.33	0.64
1:J:269:ARG:HG2	1:J:479:ILE:HB	1.78	0.64
1:J:445:ILE:HD11	1:J:494:PRO:HG2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.33	0.64
1:K:278:PHE:CE1	1:K:284:ILE:HG21	2.33	0.64
1:I:299:SER:HB3	1:I:333:MET:HE3	1.80	0.64
1:A:294:LYS:HG2	1:A:413:THR:CG2	2.27	0.63
1:D:296:LEU:HD13	1:D:331:TRP:CD2	2.32	0.63
1:I:24:MET:CB	1:I:62:ASN:HB3	2.28	0.63
1:E:158:SER:O	1:E:162:ARG:CB	2.46	0.63
1:C:287:THR:HG23	1:C:414:ASN:ND2	2.13	0.63
1:C:283:ILE:HG23	1:C:412:PHE:CE1	2.33	0.63
1:K:218:ARG:HB2	1:K:237:PHE:O	1.98	0.63
1:L:208:ARG:O	1:L:218:ARG:HA	1.98	0.63
1:E:325:LEU:HD23	1:E:335:PHE:CB	2.28	0.63
1:G:208:ARG:O	1:G:218:ARG:HA	1.98	0.63
1:K:466:ALA:HA	1:J:448:GLU:HA	1.80	0.63
1:K:429:HIS:HA	1:K:431:SEP:O1P	1.98	0.63
1:J:31:ILE:HG23	1:J:231:MET:HB2	1.79	0.63
1:G:303:GLU:CB	1:G:333:MET:CE	2.77	0.63
1:J:292:THR:HG22	1:J:440:LEU:HB3	1.81	0.63
1:I:313:ILE:HG13	1:I:372:PRO:CG	2.29	0.63
1:E:350:TYR:CZ	1:F:254:LEU:HD12	2.34	0.63
1:K:223:LEU:HD13	1:J:48:SER:HB3	1.80	0.63
1:K:269:ARG:HB3	1:K:479:ILE:HG13	1.81	0.63
1:J:263:VAL:HG21	1:J:280:LYS:HA	1.80	0.63
1:E:218:ARG:HB2	1:E:237:PHE:CE2	2.34	0.63
1:D:291:GLY:O	1:D:451:ARG:NH1	2.32	0.62
1:G:289:ALA:O	1:G:294:LYS:NZ	2.33	0.62
1:A:313:ILE:HD11	1:A:370:PHE:HB3	1.81	0.62
1:B:305:ALA:HB2	1:B:374:ARG:HD3	1.81	0.62
1:B:311:ARG:HA	1:B:343:LEU:O	1.99	0.62
1:C:290:THR:HG22	1:D:456:PHE:HE2	1.64	0.62
1:D:356:LEU:HD21	1:D:387:VAL:HG11	1.79	0.62
1:L:269:ARG:HB3	1:L:479:ILE:HD12	1.81	0.62
1:I:59:PHE:CD2	1:I:179:VAL:HG21	2.34	0.62
1:F:304:ASN:HB3	1:F:374:ARG:HH12	1.62	0.62
1:L:292:THR:HG1	1:L:442:TYR:HE1	1.33	0.62
1:B:61:TYR:CE1	1:B:92:TRP:HB3	2.35	0.62
1:B:375:ILE:O	1:B:410:GLY:HA2	2.00	0.62
2:H:294:LYS:HB3	2:H:413:THR:HG23	1.80	0.62
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.62	0.62
1:B:449:MET:HE2	1:C:490:ILE:HD12	1.81	0.62
1:G:312:ALA:N	1:G:343:LEU:O	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:LEU:CD2	2:H:90:PHE:CZ	2.83	0.62
1:J:263:VAL:HG12	1:J:374:ARG:NH2	2.15	0.62
1:C:396:VAL:O	1:C:400:THR:HG23	2.00	0.62
1:D:406:GLU:HB3	1:D:408:ILE:HG13	1.82	0.62
1:L:87:ALA:HB1	1:L:92:TRP:HB2	1.80	0.62
1:I:444:GLU:O	1:I:494:PRO:HD2	1.98	0.61
1:F:267:VAL:HB	1:F:270:LEU:HB2	1.80	0.61
1:L:21:MET:CE	1:L:177:THR:HG21	2.29	0.61
1:J:345:LYS:NZ	1:J:366:GLU:OE1	2.28	0.61
1:A:215:ARG:HG2	1:A:215:ARG:HH21	1.63	0.61
1:G:393:ARG:HH21	1:L:385:ARG:CB	2.13	0.61
1:K:300:ARG:HA	1:K:333:MET:HE1	1.82	0.61
1:L:384:ALA:N	1:L:392:PHE:HE1	1.98	0.61
1:C:311:ARG:CD	1:C:370:PHE:CZ	2.83	0.61
1:L:230:HIS:NE2	1:L:232:LYS:HE3	2.16	0.61
1:I:82:ASP:OD2	1:J:172:LYS:CE	2.47	0.61
1:E:436:THR:CG2	1:E:458:MET:HE3	2.31	0.61
2:H:24:MET:HB3	2:H:62:ASN:ND2	2.16	0.61
1:L:208:ARG:NH2	1:L:221:GLU:OE2	2.34	0.61
1:E:483:PHE:CB	1:E:489:ILE:CD1	2.78	0.61
1:D:471:MET:HG3	1:D:478:ASP:HB3	1.82	0.61
1:G:303:GLU:HB2	1:G:333:MET:CE	2.30	0.61
1:A:436:THR:OG1	1:A:458:MET:HE3	2.00	0.61
2:H:314:LEU:HD23	2:H:346:ILE:HG23	1.83	0.61
1:E:289:ALA:CB	1:E:419:PHE:HA	2.31	0.61
1:G:279:PHE:CB	1:L:326:ARG:HH12	2.14	0.61
1:B:316:ALA:O	1:B:348:CYS:HA	2.01	0.60
1:E:73:PHE:HE2	1:E:83:ILE:CD1	2.14	0.60
1:I:313:ILE:HG13	1:I:372:PRO:HB3	1.83	0.60
1:A:45:SER:HB2	1:A:182:THR:HB	1.82	0.60
1:B:323:GLN:HE22	1:C:459:ARG:CD	2.14	0.60
1:D:285:LEU:HB3	1:D:434:THR:HG21	1.83	0.60
1:B:458:MET:HG3	1:B:463:HIS:HB3	1.83	0.60
1:F:43:LEU:HD11	1:F:182:THR:OG1	2.01	0.60
1:C:79:THR:OG1	1:C:80:PRO:CD	2.49	0.60
1:L:75:THR:HG22	1:L:107:ASP:HA	1.81	0.60
1:L:458:MET:HB2	1:L:463:HIS:CD2	2.36	0.60
1:B:444:GLU:CB	1:C:490:ILE:HD11	2.31	0.60
2:H:49:GLY:O	2:H:218:ARG:NH2	2.35	0.60
1:L:384:ALA:HA	1:L:392:PHE:CD1	2.36	0.60
1:C:146:SER:O	1:C:149:SER:OG	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:SER:HB3	2:H:223:LEU:CD1	2.31	0.60
2:H:311:ARG:HG2	2:H:370:PHE:CE2	2.36	0.60
1:J:443:VAL:HG12	1:J:445:ILE:HG12	1.83	0.60
1:C:152:GLN:HA	1:D:158:SER:CB	2.32	0.60
2:H:283:ILE:HG13	2:H:400:THR:HG23	1.81	0.60
1:K:351:PRO:HG2	1:K:382:ALA:HB1	1.84	0.60
1:I:313:ILE:HD11	1:I:370:PHE:HB3	1.83	0.60
1:C:443:VAL:HG12	1:C:445:ILE:HG12	1.84	0.60
1:D:418:GLN:NE2	1:D:422:ALA:CA	2.64	0.60
1:C:87:ALA:HB1	1:C:94:LEU:CB	2.32	0.60
1:K:304:ASN:O	1:K:308:ASN:ND2	2.35	0.60
1:F:28:PHE:CZ	1:F:36:LEU:HD21	2.36	0.60
1:F:75:THR:HG22	1:F:107:ASP:HA	1.84	0.60
1:I:322:ALA:HB1	1:J:258:SER:N	2.16	0.60
1:A:21:MET:CE	1:A:177:THR:HB	2.31	0.60
1:B:436:THR:OG1	1:B:458:MET:CE	2.49	0.60
1:E:296:LEU:HD23	1:E:472:ILE:HD13	1.84	0.60
1:I:67:PHE:HB2	1:I:69:GLU:HG3	1.84	0.60
1:I:306:CYS:SG	1:I:338:MET:HE2	2.42	0.60
1:I:384:ALA:HB2	1:I:392:PHE:CE2	2.37	0.60
1:F:207:LEU:HD22	1:F:220:LEU:HD12	1.82	0.59
1:C:37:PRO:HD3	1:C:225:LEU:HD21	1.83	0.59
1:C:90:PHE:CZ	3:C:601:ADP:N7	2.70	0.59
1:C:263:VAL:HG13	1:C:374:ARG:NH2	2.15	0.59
1:L:89:SER:CB	3:L:601:ADP:HN61	2.14	0.59
1:J:211:LEU:HB2	1:J:216:ARG:HD3	1.84	0.59
1:B:451:ARG:NH2	4:B:701:ATP:O2'	2.35	0.59
2:H:297:LEU:HD11	2:H:440:LEU:HD11	1.85	0.59
1:B:295:THR:HA	1:B:298:VAL:HG23	1.83	0.59
1:C:287:THR:HG21	1:C:425:ILE:O	2.02	0.59
1:K:284:ILE:HB	1:K:411:LEU:HD12	1.83	0.59
1:B:215:ARG:HA	1:B:215:ARG:NE	2.16	0.59
1:A:459:ARG:HG3	1:F:323:GLN:HE22	1.67	0.59
1:E:318:GLU:CG	1:F:432:THR:OG1	2.50	0.59
1:D:380:LEU:HD12	1:D:412:PHE:HB3	1.85	0.59
2:H:58:GLN:CG	2:H:92:TRP:CH2	2.85	0.59
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.83	0.59
1:G:356:LEU:CD2	1:G:387:VAL:HG11	2.32	0.59
1:L:266:GLY:HA3	1:L:300:ARG:CG	2.32	0.59
1:L:290:THR:O	1:L:442:TYR:OH	2.13	0.59
1:C:317:TYR:HB3	1:C:351:PRO:HG3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:292:THR:HG21	1:L:440:LEU:HB2	1.85	0.59
1:F:18:ILE:HB	1:F:228:THR:CG2	2.33	0.59
1:K:356:LEU:HD21	1:K:387:VAL:HG11	1.85	0.59
1:G:316:ALA:O	1:G:348:CYS:HA	2.02	0.59
1:A:146:SER:HA	1:A:181:THR:CG2	2.32	0.59
1:L:71:GLY:O	1:L:103:LEU:HA	2.03	0.59
1:A:325:LEU:CD2	1:A:335:PHE:HB2	2.33	0.58
1:A:435:ASP:HA	1:A:459:ARG:HG2	1.85	0.58
1:G:20:LYS:NZ	1:G:32:SER:O	2.35	0.58
1:L:225:LEU:HD12	1:L:230:HIS:CB	2.33	0.58
1:I:221:GLU:HB2	1:I:234:GLU:HB3	1.85	0.58
1:B:455:VAL:HG11	1:B:463:HIS:HB2	1.85	0.58
1:E:208:ARG:O	1:E:218:ARG:HA	2.03	0.58
1:C:191:ILE:CD1	1:C:223:LEU:HD12	2.34	0.58
1:L:288:GLY:HA3	1:L:440:LEU:O	2.04	0.58
1:G:151:PHE:CB	1:G:155:ASP:CB	2.82	0.58
1:J:221:GLU:HG3	1:J:233:GLY:C	2.27	0.58
1:G:72:VAL:CG1	1:G:104:PHE:CD2	2.86	0.58
2:H:305:ALA:HB2	2:H:374:ARG:HD2	1.84	0.58
1:L:483:PHE:HB3	1:L:486:PHE:HB2	1.85	0.58
1:A:316:ALA:O	1:A:348:CYS:HA	2.03	0.58
1:A:471:MET:CB	1:A:480:LYS:NZ	2.67	0.58
1:D:420:MET:O	1:D:422:ALA:N	2.36	0.58
1:E:224:LYS:HB2	3:D:601:ADP:H3'	1.86	0.58
1:C:418:GLN:HB3	1:D:423:HIS:O	2.03	0.58
1:G:57:ILE:HD11	1:G:83:ILE:HG23	1.86	0.58
2:H:311:ARG:HG2	2:H:370:PHE:CD2	2.38	0.58
1:K:21:MET:SD	1:K:141:ARG:CG	2.92	0.58
1:K:237:PHE:HB3	1:K:246:ILE:HG23	1.84	0.58
1:I:372:PRO:HB2	1:I:374:ARG:O	2.03	0.58
1:B:52:LYS:HB2	4:B:702:ATP:O1B	2.04	0.58
1:E:406:GLU:O	1:E:406:GLU:HG3	2.04	0.58
1:E:448:GLU:HA	1:F:466:ALA:HA	1.85	0.58
1:C:79:THR:OG1	1:C:80:PRO:HD2	2.04	0.58
1:C:300:ARG:NH1	1:C:475:LYS:O	2.35	0.58
1:D:458:MET:HG3	1:D:463:HIS:HB3	1.85	0.58
1:B:302:VAL:CG1	1:B:344:LEU:HD13	2.33	0.58
1:I:58:GLN:HG3	1:I:92:TRP:CH2	2.39	0.58
1:J:284:ILE:CB	1:J:411:LEU:HD12	2.33	0.58
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.69	0.58
1:A:364:LYS:O	1:A:368:ASN:ND2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:MET:HA	1:E:338:MET:CE	2.32	0.58
1:B:57:ILE:CD1	1:B:83:ILE:HG23	2.31	0.58
1:E:281:ASP:OD1	1:E:407:GLU:OE2	2.20	0.58
1:K:36:LEU:HD12	1:K:59:PHE:CE1	2.39	0.58
1:B:71:GLY:HA2	1:B:141:ARG:O	2.03	0.57
1:C:338:MET:HB3	1:C:344:LEU:HB2	1.86	0.57
1:D:418:GLN:HE22	1:D:422:ALA:HA	1.65	0.57
1:L:225:LEU:CD1	1:L:230:HIS:HB3	2.33	0.57
1:L:384:ALA:CA	1:L:392:PHE:HE1	2.17	0.57
1:E:192:ALA:HB1	1:E:197:GLU:HB2	1.86	0.57
1:C:191:ILE:HD13	1:C:223:LEU:HD12	1.86	0.57
2:H:54:LEU:HD22	2:H:90:PHE:CZ	2.40	0.57
1:I:436:THR:OG1	1:I:458:MET:HE3	2.05	0.57
1:J:42:THR:HG23	1:J:203:ASN:HB2	1.87	0.57
1:A:222:ILE:HG21	1:A:225:LEU:CD1	2.34	0.57
1:L:58:GLN:HG3	1:L:92:TRP:HH2	1.65	0.57
1:I:321:ARG:HG2	1:I:321:ARG:HH21	1.68	0.57
1:B:279:PHE:HE1	1:B:461:SER:HB2	1.67	0.57
1:C:266:GLY:HA2	1:C:304:ASN:HD22	1.68	0.57
1:D:267:VAL:CG2	1:D:477:PRO:HG3	2.33	0.57
1:K:406:GLU:HB3	1:K:408:ILE:HG13	1.86	0.57
1:E:350:TYR:CZ	1:F:254:LEU:CD1	2.87	0.57
1:C:87:ALA:CB	1:C:94:LEU:CB	2.82	0.57
1:C:193:ARG:NH2	1:D:195:GLY:O	2.34	0.57
2:H:302:VAL:HG11	2:H:344:LEU:HD21	1.86	0.57
1:K:104:PHE:CE2	1:K:133:ALA:HB2	2.36	0.57
1:K:258:SER:OG	1:J:326:ARG:NH1	2.36	0.57
1:J:271:ASP:HA	1:J:277:GLY:HA2	1.86	0.57
1:B:397:ILE:HD13	1:B:433:ILE:HD13	1.85	0.57
1:K:104:PHE:CD2	1:K:133:ALA:HB1	2.39	0.57
1:K:163:GLU:OE2	1:K:163:GLU:HA	2.04	0.57
1:K:263:VAL:N	1:K:278:PHE:O	2.36	0.57
1:B:350:TYR:HE1	1:C:252:MET:CB	2.17	0.57
1:B:425:ILE:HG22	1:B:426:THR:HG23	1.86	0.57
1:E:311:ARG:HG3	1:E:372:PRO:HA	1.87	0.57
1:F:294:LYS:HD3	4:F:602:ATP:O2B	2.04	0.57
1:C:379:SER:HB2	1:C:413:THR:O	2.04	0.57
1:I:166:ARG:HH11	1:I:166:ARG:HB3	1.70	0.57
1:L:293:GLY:O	1:L:297:LEU:HG	2.05	0.56
1:F:106:LEU:HD11	1:F:129:ARG:NE	2.20	0.56
2:H:183:GLU:HB3	1:I:199:PHE:CE1	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ARG:HB3	1:I:166:ARG:NH1	2.20	0.56
1:I:284:ILE:HG23	1:I:436:THR:CB	2.31	0.56
1:F:209:ASN:O	1:F:216:ARG:NH1	2.33	0.56
1:G:459:ARG:C	1:L:327:ASN:HD21	2.13	0.56
2:H:297:LEU:CD1	2:H:440:LEU:HD11	2.35	0.56
1:K:297:LEU:HD12	1:K:440:LEU:HD11	1.88	0.56
1:J:202:ASP:O	1:J:224:LYS:HD2	2.04	0.56
1:J:268:VAL:O	1:J:272:GLU:HG3	2.06	0.56
1:J:287:THR:HG21	1:J:425:ILE:O	2.04	0.56
1:E:62:ASN:O	1:E:66:GLU:HB2	2.04	0.56
1:G:222:ILE:HG22	1:G:230:HIS:CE1	2.40	0.56
1:E:269:ARG:HH11	1:E:269:ARG:HG3	1.67	0.56
1:C:311:ARG:NE	1:C:370:PHE:CE1	2.73	0.56
1:D:46:GLY:HA2	1:D:184:ARG:HD3	1.88	0.56
1:D:285:LEU:CB	1:D:434:THR:HG21	2.35	0.56
2:H:207:LEU:HD21	2:H:220:LEU:HD12	1.86	0.56
1:K:431:SEP:O	1:K:434:THR:HG22	2.06	0.56
1:J:361:GLN:O	1:J:365:SER:HB2	2.05	0.56
1:A:21:MET:SD	1:A:141:ARG:NE	2.78	0.56
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.88	0.56
1:I:325:LEU:CD2	1:I:336:GLU:CG	2.82	0.56
1:F:436:THR:HG23	1:F:458:MET:HG2	1.87	0.56
1:C:313:ILE:HG13	1:C:372:PRO:HG3	1.86	0.56
1:K:294:LYS:HB3	1:K:413:THR:CG2	2.35	0.56
1:B:206:ILE:HD11	1:B:223:LEU:HG	1.88	0.56
1:B:225:LEU:CB	1:B:230:HIS:HD2	2.05	0.56
1:E:52:LYS:CE	4:E:601:ATP:O2B	2.54	0.56
1:E:63:GLY:HA3	1:E:141:ARG:NE	2.20	0.56
1:K:133:ALA:O	1:K:137:TYR:HD1	1.89	0.56
1:L:291:GLY:C	1:L:442:TYR:OH	2.48	0.56
1:L:305:ALA:CB	1:L:312:ALA:HB2	2.36	0.56
1:J:221:GLU:HG3	1:J:233:GLY:O	2.06	0.56
1:C:183:GLU:CB	1:D:199:PHE:CE1	2.89	0.56
1:C:270:LEU:HD21	1:C:438:ILE:HD12	1.88	0.56
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.71	0.55
1:E:93:ASP:O	1:E:97:LEU:HD23	2.05	0.55
1:F:54:LEU:N	3:F:601:ADP:O1A	2.37	0.55
1:C:345:LYS:HB2	1:C:370:PHE:CZ	2.41	0.55
3:C:601:ADP:O2'	1:D:230:HIS:NE2	2.38	0.55
1:K:269:ARG:CB	1:K:479:ILE:HG13	2.36	0.55
1:I:313:ILE:HG13	1:I:372:PRO:CB	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:O	1:A:100:GLU:HG3	2.06	0.55
1:F:287:THR:HG22	1:F:414:ASN:ND2	2.20	0.55
1:K:351:PRO:HB3	1:K:383:LEU:HD23	1.87	0.55
1:I:325:LEU:HD21	1:I:336:GLU:HG2	1.85	0.55
1:J:44:VAL:HG22	1:J:205:VAL:HB	1.87	0.55
1:A:451:ARG:NH2	4:A:602:ATP:O2'	2.39	0.55
1:E:419:PHE:CD2	1:F:425:ILE:HG12	2.40	0.55
1:I:202:ASP:HA	1:I:226:ARG:HD2	1.87	0.55
1:B:323:GLN:NE2	1:B:327:ASN:HD21	2.04	0.55
1:E:280:LYS:O	1:E:409:THR:OG1	2.22	0.55
1:C:92:TRP:C	1:C:94:LEU:H	2.15	0.55
2:H:86:ASN:OD1	1:I:40:ARG:NH2	2.40	0.55
1:L:59:PHE:O	1:L:141:ARG:NH1	2.40	0.55
1:K:104:PHE:CE2	1:K:133:ALA:CB	2.89	0.55
1:L:305:ALA:HB3	1:L:312:ALA:HB2	1.89	0.55
1:F:284:ILE:HB	1:F:411:LEU:HD12	1.88	0.55
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.89	0.55
1:G:323:GLN:NE2	2:H:435:ASP:OD2	2.40	0.55
2:H:305:ALA:HB2	2:H:374:ARG:CD	2.36	0.55
1:K:104:PHE:HE2	1:K:133:ALA:CB	2.18	0.55
1:J:313:ILE:CD1	1:J:372:PRO:HG3	2.37	0.55
1:B:244:ILE:HG22	1:B:246:ILE:HD12	1.89	0.55
1:E:338:MET:HB3	1:E:344:LEU:CB	2.33	0.55
2:H:57:ILE:HD11	2:H:83:ILE:CG2	2.37	0.55
1:I:269:ARG:O	1:I:273:MET:HG3	2.07	0.55
1:E:311:ARG:CG	1:E:372:PRO:HA	2.37	0.55
1:I:262:ARG:NH1	1:I:461:SER:OG	2.40	0.55
1:G:90:PHE:HB3	1:G:241:ASP:O	2.07	0.54
1:K:390:ASN:OD1	1:J:386:GLY:HA3	2.07	0.54
1:D:38:ILE:HA	1:D:177:THR:OG1	2.07	0.54
2:H:24:MET:HB3	2:H:62:ASN:CG	2.32	0.54
1:I:43:LEU:HD11	1:I:182:THR:OG1	2.07	0.54
1:I:59:PHE:CD2	1:I:179:VAL:CG2	2.90	0.54
1:A:345:LYS:NZ	1:A:366:GLU:HG3	2.23	0.54
1:B:486:PHE:CD2	1:B:494:PRO:HB2	2.41	0.54
1:F:380:LEU:HG	1:F:412:PHE:HB3	1.89	0.54
1:D:425:ILE:HG22	1:D:426:THR:HG23	1.90	0.54
1:D:444:GLU:O	1:D:494:PRO:HD2	2.08	0.54
1:G:466:ALA:HA	1:L:448:GLU:HA	1.87	0.54
1:I:203:ASN:HB3	1:I:225:LEU:CD2	2.37	0.54
1:J:444:GLU:HB2	1:J:449:MET:CE	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD13	1:F:353:SER:CA	2.29	0.54
1:E:148:THR:HG23	1:E:193:ARG:HD2	1.88	0.54
1:D:468:ARG:HA	1:D:482:SER:HA	1.89	0.54
1:K:470:PHE:HA	1:K:478:ASP:O	2.07	0.54
1:J:280:LYS:O	1:J:409:THR:OG1	2.12	0.54
1:A:294:LYS:HB3	1:A:413:THR:CG2	2.38	0.54
1:B:436:THR:CG2	1:B:458:MET:HE3	2.38	0.54
1:I:220:LEU:C	1:I:220:LEU:HD23	2.32	0.54
1:E:294:LYS:O	1:E:298:VAL:HG23	2.07	0.54
4:E:601:ATP:O2'	1:F:230:HIS:NE2	2.39	0.54
1:C:24:MET:HB2	1:C:62:ASN:CB	2.37	0.54
1:D:451:ARG:NH2	3:D:602:ADP:O2'	2.41	0.54
1:G:444:GLU:OE2	2:H:489:ILE:HG22	2.08	0.54
1:J:24:MET:HB2	1:J:62:ASN:HB3	1.88	0.54
1:G:30:ASP:OD2	1:G:30:ASP:N	2.41	0.54
1:K:319:GLU:HG3	1:K:324:LEU:HD21	1.89	0.54
1:J:356:LEU:CD2	1:J:387:VAL:HG11	2.38	0.54
1:E:224:LYS:HB3	1:D:49:GLY:HA3	1.89	0.54
1:C:290:THR:HG22	1:D:456:PHE:CE2	2.42	0.54
1:D:436:THR:OG1	1:D:458:MET:HE3	2.07	0.54
1:K:292:THR:HB	1:K:440:LEU:CB	2.37	0.54
1:B:438:ILE:CG2	1:B:453:ILE:HD11	2.38	0.54
1:G:31:ILE:O	1:G:231:MET:HG3	2.07	0.54
2:H:274:CYS:O	2:H:458:MET:HE2	2.07	0.54
1:L:63:GLY:O	1:L:69:GLU:HG3	2.07	0.54
1:L:266:GLY:HA3	1:L:300:ARG:HG2	1.89	0.54
1:B:278:PHE:CE1	1:B:284:ILE:HG21	2.43	0.54
1:C:453:ILE:HG21	1:C:479:ILE:HD13	1.89	0.54
1:L:54:LEU:C	1:L:54:LEU:HD12	2.32	0.54
1:A:390:ASN:HD21	1:F:386:GLY:HA3	1.73	0.53
1:E:270:LEU:HD21	1:E:438:ILE:HD12	1.88	0.53
1:D:319:GLU:HB2	1:D:324:LEU:HD21	1.89	0.53
1:I:289:ALA:HB2	1:I:419:PHE:HA	1.90	0.53
1:A:222:ILE:CG2	1:A:225:LEU:CD1	2.86	0.53
1:E:263:VAL:N	1:E:278:PHE:O	2.40	0.53
1:C:209:ASN:O	1:C:216:ARG:NH1	2.38	0.53
1:I:59:PHE:CE2	1:I:179:VAL:HG23	2.43	0.53
1:C:220:LEU:HD23	1:C:220:LEU:C	2.34	0.53
1:D:21:MET:HE1	1:D:177:THR:HB	1.89	0.53
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.91	0.53
1:J:356:LEU:HD22	1:J:387:VAL:HG11	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ARG:NH2	1:C:221:GLU:OE2	2.41	0.53
1:D:209:ASN:O	1:D:216:ARG:NH1	2.39	0.53
1:D:289:ALA:O	1:D:292:THR:OG1	2.25	0.53
1:B:311:ARG:HB2	1:B:370:PHE:CE2	2.42	0.53
1:F:28:PHE:CE2	1:F:36:LEU:CD2	2.92	0.53
1:F:470:PHE:HA	1:F:478:ASP:O	2.09	0.53
1:C:469:GLU:HB3	1:C:483:PHE:CZ	2.44	0.53
1:D:311:ARG:HA	1:D:343:LEU:O	2.09	0.53
1:K:488:ARG:N	1:J:444:GLU:OE2	2.41	0.53
1:A:303:GLU:HG3	1:A:338:MET:HE1	1.91	0.53
1:A:362:ILE:N	1:A:362:ILE:HD13	2.23	0.53
1:C:291:GLY:O	1:C:451:ARG:NH1	2.42	0.53
2:H:219:THR:HB	2:H:234:GLU:HB2	1.90	0.53
1:L:171:LEU:HD22	1:L:178:THR:CB	2.39	0.53
1:E:203:ASN:HB3	1:E:225:LEU:HD22	1.82	0.53
1:E:267:VAL:HB	1:E:270:LEU:HB2	1.91	0.53
1:F:420:MET:HE3	1:F:492:GLY:CA	2.39	0.53
1:D:418:GLN:HB2	1:D:422:ALA:HB2	1.91	0.53
2:H:284:ILE:CB	2:H:411:LEU:HD12	2.37	0.53
1:K:317:TYR:HB3	1:K:351:PRO:HG3	1.90	0.53
1:A:306:CYS:SG	1:A:344:LEU:HB2	2.48	0.53
1:B:358:ASP:O	1:B:362:ILE:HG13	2.08	0.53
1:F:269:ARG:O	1:F:273:MET:HG3	2.09	0.53
1:F:315:PHE:HE1	1:F:375:ILE:HG23	1.73	0.53
1:G:218:ARG:HD2	1:G:237:PHE:CE1	2.44	0.53
1:K:301:PHE:CZ	1:K:374:ARG:HD3	2.44	0.53
1:L:384:ALA:HB2	1:L:392:PHE:CD1	2.39	0.53
1:B:60:LEU:HD11	1:B:143:SER:HB2	1.89	0.53
1:E:335:PHE:HA	1:E:338:MET:HG3	1.90	0.53
1:F:218:ARG:HH11	1:F:239:ILE:HB	1.72	0.53
2:H:283:ILE:CG1	2:H:400:THR:HG23	2.39	0.53
2:H:417:ASP:O	1:I:424:SER:HB3	2.09	0.53
1:I:443:VAL:HG13	1:I:494:PRO:HD3	1.90	0.53
1:J:300:ARG:HD2	1:J:333:MET:CE	2.39	0.53
1:B:142:VAL:O	1:B:178:THR:HA	2.09	0.52
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.41	0.52
1:L:21:MET:HE3	1:L:177:THR:HG21	1.90	0.52
1:L:303:GLU:CB	1:L:333:MET:CE	2.87	0.52
1:L:89:SER:CB	3:L:601:ADP:N6	2.72	0.52
1:J:89:SER:HB3	4:J:702:ATP:HN61	1.74	0.52
1:B:436:THR:HG23	1:B:458:MET:HE3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:166:ARG:O	1:K:170:ARG:N	2.38	0.52
1:J:208:ARG:NH2	1:J:221:GLU:OE2	2.42	0.52
1:A:375:ILE:O	1:A:410:GLY:HA2	2.08	0.52
1:F:291:GLY:O	1:F:451:ARG:NH1	2.43	0.52
1:G:290:THR:CG2	2:H:425:ILE:HD13	2.38	0.52
1:G:312:ALA:O	1:G:344:LEU:HA	2.10	0.52
1:K:284:ILE:HG23	1:K:436:THR:HB	1.90	0.52
1:A:211:LEU:HD12	1:A:215:ARG:O	2.10	0.52
1:C:220:LEU:HD22	1:C:246:ILE:HG21	1.91	0.52
1:D:267:VAL:HB	1:D:270:LEU:HB2	1.92	0.52
1:G:298:VAL:HG21	1:G:413:THR:CG2	2.40	0.52
2:H:54:LEU:HD21	2:H:90:PHE:CZ	2.43	0.52
1:L:384:ALA:CB	1:L:392:PHE:CD1	2.93	0.52
1:J:429:HIS:HA	1:J:431:SEP:O1P	2.10	0.52
1:C:37:PRO:HG2	1:C:203:ASN:OD1	2.10	0.52
1:K:393:ARG:O	1:K:397:ILE:HG12	2.10	0.52
1:A:334:ASP:O	1:A:338:MET:HG3	2.10	0.52
3:A:601:ADP:HO3'	1:B:224:LYS:HB2	1.73	0.52
1:C:286:ALA:O	1:C:413:THR:HG22	2.10	0.52
1:K:202:ASP:HA	1:K:226:ARG:NH1	2.24	0.52
1:A:271:ASP:O	1:A:277:GLY:N	2.42	0.52
1:B:264:SER:OG	1:B:304:ASN:ND2	2.43	0.52
1:E:425:ILE:HD11	1:E:439:LEU:HD22	1.91	0.52
1:G:273:MET:HE3	1:G:468:ARG:HD2	1.92	0.52
1:J:440:LEU:CD2	1:J:453:ILE:HG13	2.39	0.52
1:A:99:ASP:OD1	1:A:99:ASP:N	2.42	0.52
1:A:254:LEU:CD1	1:F:320:SER:HB3	2.39	0.52
1:K:490:ILE:CB	1:J:420:MET:CE	2.88	0.52
1:B:215:ARG:NH2	1:B:352:GLU:O	2.43	0.51
1:C:191:ILE:HB	1:C:198:GLU:HG2	1.91	0.51
1:G:218:ARG:NH2	2:H:232:LYS:HE3	2.25	0.51
1:J:443:VAL:N	1:J:450:SER:O	2.39	0.51
1:A:331:TRP:HA	1:A:474:ASP:O	2.10	0.51
1:F:319:GLU:OE1	1:F:327:ASN:ND2	2.42	0.51
1:D:31:ILE:HA	1:D:231:MET:CG	2.36	0.51
1:D:60:LEU:HD12	1:D:73:PHE:HB2	1.92	0.51
1:A:146:SER:CA	1:A:181:THR:HG22	2.37	0.51
1:C:325:LEU:CD2	1:C:335:PHE:HB2	2.40	0.51
1:G:104:PHE:CE2	1:G:133:ALA:HB1	2.46	0.51
2:H:78:GLU:OE1	2:H:86:ASN:ND2	2.43	0.51
1:K:356:LEU:HD21	1:K:387:VAL:CG1	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:483:PHE:HB3	1:K:486:PHE:HB2	1.91	0.51
1:I:443:VAL:HG13	1:I:492:GLY:O	2.10	0.51
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.76	0.51
1:E:289:ALA:O	1:E:294:LYS:NZ	2.44	0.51
1:C:90:PHE:HE2	1:C:240:THR:O	1.93	0.51
1:D:453:ILE:HG21	1:D:479:ILE:HG12	1.91	0.51
2:H:293:GLY:O	2:H:296:LEU:HB3	2.10	0.51
1:L:131:ASN:C	1:L:133:ALA:H	2.17	0.51
1:L:311:ARG:CB	1:L:372:PRO:HA	2.40	0.51
1:B:70:PRO:HG2	1:B:138:ARG:O	2.10	0.51
1:E:436:THR:HG23	1:E:458:MET:HE3	1.92	0.51
1:E:458:MET:HG3	1:E:463:HIS:HB3	1.93	0.51
1:D:62:ASN:O	1:D:66:GLU:HB2	2.10	0.51
1:G:449:MET:HE2	2:H:467:ILE:HD11	1.93	0.51
2:H:294:LYS:HB3	2:H:413:THR:HG21	1.92	0.51
1:K:36:LEU:HD22	1:K:42:THR:HG21	1.92	0.51
1:I:37:PRO:HG2	1:I:203:ASN:OD1	2.09	0.51
1:I:306:CYS:HB2	1:I:338:MET:CE	2.41	0.51
1:A:224:LYS:HB3	1:F:49:GLY:HA3	1.92	0.51
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.40	0.51
1:B:264:SER:O	1:B:374:ARG:NH2	2.42	0.51
1:E:487:GLU:O	1:E:494:PRO:HA	2.11	0.51
1:G:50:THR:HB	1:G:207:LEU:HB3	1.92	0.51
1:G:489:ILE:N	1:L:444:GLU:OE1	2.43	0.51
2:H:214:GLU:CD	1:I:217:ARG:HH11	2.18	0.51
1:J:379:SER:HB2	1:J:413:THR:O	2.11	0.51
1:A:215:ARG:HE	1:B:233:GLY:HA3	1.75	0.51
1:B:20:LYS:HE3	1:B:228:THR:HG21	1.92	0.51
1:E:31:ILE:HG23	1:E:231:MET:HB2	1.92	0.51
1:C:191:ILE:CD1	1:C:223:LEU:CD1	2.89	0.51
1:C:281:ASP:OD1	1:C:281:ASP:N	2.44	0.51
1:D:45:SER:HB3	1:D:182:THR:HB	1.93	0.51
2:H:295:THR:OG1	2:H:378:ASP:OD1	2.28	0.51
2:H:302:VAL:CG1	2:H:344:LEU:HD21	2.40	0.51
1:A:471:MET:CB	1:A:480:LYS:HZ2	2.23	0.51
1:B:302:VAL:HG11	1:B:344:LEU:HD13	1.93	0.51
1:E:73:PHE:CE2	1:E:83:ILE:CD1	2.92	0.51
1:C:59:PHE:O	1:C:141:ARG:NH1	2.42	0.51
1:D:294:LYS:HB3	1:D:413:THR:CG2	2.39	0.51
1:I:86:ASN:O	1:I:89:SER:HB3	2.10	0.51
1:I:306:CYS:CB	1:I:338:MET:CE	2.88	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ILE:HG22	3:F:601:ADP:N3	2.26	0.51
1:D:43:LEU:HA	1:D:180:MET:HB2	1.93	0.51
1:K:199:PHE:CE1	1:J:183:GLU:CB	2.94	0.51
1:I:302:VAL:HG13	1:I:344:LEU:HD23	1.93	0.51
1:J:440:LEU:HD23	1:J:453:ILE:HG13	1.91	0.51
1:C:313:ILE:HD11	1:C:372:PRO:HD3	1.92	0.50
1:D:486:PHE:CD2	1:D:494:PRO:HB2	2.46	0.50
1:J:188:TYR:HE1	1:J:210:VAL:CG1	2.24	0.50
1:J:294:LYS:HE3	1:J:413:THR:CG2	2.41	0.50
1:J:393:ARG:O	1:J:397:ILE:HG12	2.11	0.50
1:C:67:PHE:HB3	1:C:69:GLU:CG	2.42	0.50
1:K:104:PHE:HD2	1:K:133:ALA:HB1	1.77	0.50
1:K:331:TRP:HA	1:K:474:ASP:O	2.10	0.50
1:L:331:TRP:CZ2	4:L:602:ATP:C8	3.00	0.50
1:L:440:LEU:CD2	1:L:453:ILE:HG13	2.42	0.50
1:A:344:LEU:HD11	1:A:346:ILE:HD11	1.94	0.50
1:A:466:ALA:HA	1:F:448:GLU:HA	1.94	0.50
1:C:191:ILE:HD11	1:C:223:LEU:HD11	1.93	0.50
1:D:21:MET:CE	1:D:177:THR:HB	2.42	0.50
1:K:278:PHE:CD1	1:K:284:ILE:HG13	2.47	0.50
1:J:315:PHE:HE1	1:J:375:ILE:HG23	1.76	0.50
1:E:183:GLU:HB2	1:F:199:PHE:CE1	2.47	0.50
1:G:19:ALA:O	1:G:38:ILE:N	2.44	0.50
1:G:280:LYS:C	1:G:409:THR:HG1	2.18	0.50
1:F:24:MET:CB	1:F:62:ASN:HB3	2.38	0.50
1:F:161:ARG:NH2	1:F:199:PHE:HB2	2.26	0.50
2:H:420:MET:CE	2:H:449:MET:HE1	2.37	0.50
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.76	0.50
2:H:451:ARG:NH2	4:H:602:ATP:O2'	2.44	0.50
1:K:294:LYS:HB3	1:K:413:THR:HG23	1.93	0.50
1:K:431:SEP:C	1:K:434:THR:HG22	2.41	0.50
1:L:285:LEU:HA	1:L:412:PHE:O	2.11	0.50
1:A:423:HIS:C	1:F:419:PHE:CE2	2.90	0.50
1:E:287:THR:HG23	1:E:414:ASN:ND2	2.11	0.50
1:D:351:PRO:HB3	1:D:383:LEU:HD23	1.94	0.50
2:H:239:ILE:N	2:H:239:ILE:HD13	2.26	0.50
1:J:52:LYS:CB	1:J:181:THR:HG23	2.26	0.50
1:E:483:PHE:HB3	1:E:486:PHE:HB2	1.93	0.50
1:D:305:ALA:O	1:D:310:GLU:HB2	2.11	0.50
1:D:320:SER:O	1:D:324:LEU:HD23	2.12	0.50
1:K:376:ALA:HA	1:K:411:LEU:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:292:THR:CG2	1:L:440:LEU:CB	2.87	0.50
1:I:296:LEU:HD12	1:I:296:LEU:C	2.36	0.50
1:E:60:LEU:HD23	1:E:141:ARG:CD	2.40	0.50
1:C:300:ARG:HA	1:C:333:MET:HE1	1.93	0.50
1:D:165:PHE:O	1:D:169:ALA:N	2.44	0.50
1:G:232:LYS:H	1:G:232:LYS:HD2	1.77	0.50
2:H:20:LYS:NZ	2:H:228:THR:CG2	2.75	0.50
1:K:431:SEP:HA	1:K:434:THR:HG22	1.94	0.50
1:J:264:SER:O	1:J:374:ARG:NH1	2.42	0.50
1:J:483:PHE:HB2	1:J:489:ILE:CD1	2.42	0.50
1:A:142:VAL:O	1:A:178:THR:HA	2.13	0.49
1:A:215:ARG:HG2	1:A:215:ARG:NH2	2.24	0.49
1:B:295:THR:HA	1:B:298:VAL:CG2	2.41	0.49
1:E:318:GLU:HG2	1:F:432:THR:HG1	1.76	0.49
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.94	0.49
1:D:284:ILE:HG23	1:D:436:THR:HB	1.94	0.49
1:L:356:LEU:CD2	1:L:387:VAL:HG11	2.41	0.49
1:I:301:PHE:O	1:I:374:ARG:NH1	2.45	0.49
1:A:294:LYS:HB3	1:A:413:THR:HG21	1.95	0.49
1:E:183:GLU:HB2	1:F:199:PHE:CZ	2.47	0.49
1:J:54:LEU:HD23	1:J:239:ILE:CD1	2.42	0.49
1:B:358:ASP:OD2	1:B:358:ASP:N	2.45	0.49
1:E:148:THR:HG21	1:E:193:ARG:HD2	1.89	0.49
2:H:110:PRO:HD2	1:I:165:PHE:HE2	1.78	0.49
1:L:463:HIS:CE1	1:L:465:LYS:HD3	2.47	0.49
1:A:83:ILE:HD12	1:A:83:ILE:N	2.27	0.49
1:A:396:VAL:O	1:A:400:THR:HB	2.12	0.49
1:E:188:TYR:HE2	1:D:211:LEU:CD2	2.25	0.49
1:E:306:CYS:CB	1:E:338:MET:CE	2.90	0.49
1:G:298:VAL:HG21	1:G:413:THR:HG21	1.94	0.49
1:K:21:MET:SD	1:K:141:ARG:HG2	2.51	0.49
1:J:48:SER:HA	4:J:702:ATP:O1G	2.13	0.49
1:C:363:ILE:O	1:C:367:ILE:HG13	2.13	0.49
2:H:317:TYR:HA	2:H:349:ALA:O	2.12	0.49
1:K:284:ILE:HB	1:K:411:LEU:CD1	2.43	0.49
1:K:375:ILE:O	1:K:410:GLY:HA2	2.11	0.49
1:J:163:GLU:OE2	1:J:163:GLU:HA	2.12	0.49
1:B:379:SER:HB2	1:B:413:THR:HB	1.94	0.49
1:B:436:THR:OG1	1:B:458:MET:HE3	2.13	0.49
1:C:92:TRP:C	1:C:94:LEU:N	2.71	0.49
1:G:48:SER:HB3	2:H:223:LEU:HD13	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:601:ADP:O3'	1:I:225:LEU:N	2.43	0.49
1:K:304:ASN:OD1	1:K:374:ARG:NH2	2.45	0.49
1:K:330:SER:O	1:K:474:ASP:HA	2.12	0.49
1:E:294:LYS:HB2	1:E:294:LYS:HE2	1.62	0.49
1:E:338:MET:CB	1:E:344:LEU:CB	2.90	0.49
1:F:283:ILE:N	1:F:435:ASP:OD2	2.27	0.49
1:F:308:ASN:HD22	1:F:308:ASN:N	2.10	0.49
1:D:321:ARG:O	1:D:325:LEU:HG	2.13	0.49
1:B:444:GLU:HB2	1:C:490:ILE:HD11	1.94	0.49
1:G:29:ASP:O	1:G:34:GLY:N	2.45	0.49
2:H:37:PRO:HG2	2:H:203:ASN:OD1	2.12	0.49
1:L:269:ARG:O	1:L:273:MET:HG3	2.12	0.49
1:J:294:LYS:HE3	1:J:413:THR:HG23	1.94	0.49
1:J:389:ASN:HD21	1:J:428:SER:HA	1.78	0.49
1:B:29:ASP:HA	1:B:32:SER:OG	2.13	0.49
1:E:425:ILE:HD13	1:D:419:PHE:CD2	2.48	0.49
1:F:132:TYR:O	1:F:136:LYS:N	2.45	0.49
1:I:436:THR:OG1	1:I:458:MET:CE	2.61	0.49
1:B:329:TYR:HA	1:B:333:MET:O	2.13	0.49
1:E:296:LEU:HD23	1:E:472:ILE:CD1	2.42	0.49
1:L:167:LEU:O	1:L:171:LEU:HD12	2.13	0.49
1:I:305:ALA:HB2	1:I:374:ARG:HD3	1.94	0.49
1:E:46:GLY:HA2	1:E:184:ARG:HD2	1.93	0.48
1:C:132:TYR:O	1:C:136:LYS:N	2.41	0.48
1:C:219:THR:HG22	1:C:236:PRO:HA	1.94	0.48
1:I:197:GLU:OE2	1:I:197:GLU:N	2.43	0.48
1:I:437:ILE:CD1	1:I:457:LYS:HE2	2.43	0.48
1:I:440:LEU:CD2	1:I:453:ILE:HG13	2.43	0.48
1:E:306:CYS:HB3	1:E:338:MET:CE	2.42	0.48
1:C:298:VAL:O	1:C:302:VAL:HG23	2.12	0.48
1:L:76:PHE:HD1	1:L:145:ASP:O	1.96	0.48
1:L:440:LEU:HD21	1:L:453:ILE:HG13	1.95	0.48
1:I:40:ARG:HH12	1:I:226:ARG:HB3	1.77	0.48
1:A:146:SER:CA	1:A:181:THR:CG2	2.90	0.48
1:A:234:GLU:HB2	1:F:214:GLU:HB3	1.95	0.48
1:A:465:LYS:O	1:F:449:MET:N	2.43	0.48
2:H:239:ILE:HD12	2:H:244:ILE:HG12	1.94	0.48
1:E:60:LEU:HA	1:E:141:ARG:CD	2.44	0.48
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.95	0.48
1:E:338:MET:HA	1:E:338:MET:HE3	1.96	0.48
1:F:58:GLN:HG3	1:F:92:TRP:CH2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:443:VAL:CG1	1:L:494:PRO:HG3	2.43	0.48
1:J:294:LYS:NZ	1:J:415:THR:OG1	2.45	0.48
1:J:483:PHE:HB2	1:J:489:ILE:HD12	1.95	0.48
1:A:156:ALA:CB	1:A:159:VAL:HG21	2.31	0.48
1:E:59:PHE:C	1:E:141:ARG:HH12	2.21	0.48
1:E:63:GLY:HA3	1:E:141:ARG:HE	1.77	0.48
1:E:235:TYR:CZ	1:D:215:ARG:NH1	2.82	0.48
2:H:211:LEU:HD13	2:H:216:ARG:NE	2.28	0.48
1:L:62:ASN:O	1:L:66:GLU:HB2	2.14	0.48
1:L:202:ASP:OD1	1:L:226:ARG:NH2	2.43	0.48
1:I:289:ALA:CB	1:I:419:PHE:HA	2.43	0.48
1:I:325:LEU:HD23	1:I:336:GLU:CG	2.43	0.48
1:A:36:LEU:HD12	1:A:59:PHE:CE1	2.49	0.48
1:C:483:PHE:HB2	1:C:489:ILE:HD11	1.95	0.48
1:D:221:GLU:HG3	1:D:233:GLY:C	2.39	0.48
2:H:211:LEU:HD13	2:H:216:ARG:CD	2.44	0.48
1:L:289:ALA:HB2	1:L:419:PHE:HA	1.94	0.48
1:J:171:LEU:H	1:J:171:LEU:HD12	1.79	0.48
1:B:248:PRO:HB2	1:B:251:ALA:CB	2.42	0.48
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.42	0.48
1:E:264:SER:O	1:E:374:ARG:NH2	2.46	0.48
1:G:296:LEU:HA	1:G:331:TRP:CZ3	2.49	0.48
1:I:215:ARG:NH1	1:J:233:GLY:HA3	2.29	0.48
1:I:313:ILE:HD11	1:I:372:PRO:HD3	1.96	0.48
1:B:207:LEU:CD2	1:B:220:LEU:HD12	2.44	0.48
1:B:246:ILE:HD12	1:B:246:ILE:N	2.29	0.48
1:B:278:PHE:CZ	1:B:284:ILE:HG21	2.48	0.48
1:B:486:PHE:HD2	1:B:494:PRO:HB2	1.79	0.48
1:E:40:ARG:O	1:E:177:THR:HG22	2.14	0.48
1:D:368:ASN:OD1	1:D:402:TYR:OH	2.32	0.48
1:D:313:ILE:HG13	1:D:372:PRO:HG3	1.95	0.48
2:H:63:GLY:HA3	2:H:141:ARG:CZ	2.44	0.48
2:H:294:LYS:HG2	2:H:413:THR:HG23	1.96	0.48
1:L:297:LEU:N	1:L:297:LEU:HD23	2.28	0.48
1:I:469:GLU:HB2	1:I:483:PHE:CZ	2.48	0.48
1:A:64:ILE:CG2	1:A:97:LEU:CD2	2.76	0.48
1:E:420:MET:HE1	1:F:490:ILE:HB	1.96	0.48
2:H:467:ILE:HG21	2:H:489:ILE:HD11	1.95	0.48
1:I:37:PRO:HD2	1:I:203:ASN:ND2	2.29	0.48
1:I:273:MET:HE2	1:I:455:VAL:HG23	1.96	0.48
1:J:313:ILE:HD11	1:J:372:PRO:HG3	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:471:MET:HE2	1:J:478:ASP:HB3	1.96	0.47
1:D:59:PHE:O	1:D:141:ARG:NH1	2.47	0.47
1:D:303:GLU:HG3	1:D:333:MET:HE2	1.96	0.47
2:H:20:LYS:HE2	2:H:33:HIS:O	2.14	0.47
1:L:451:ARG:CB	1:L:470:PHE:CE2	2.92	0.47
1:I:283:ILE:HG23	1:I:412:PHE:CE1	2.45	0.47
1:J:52:LYS:N	4:J:702:ATP:O2B	2.46	0.47
1:L:22:ARG:NH2	1:L:29:ASP:OD2	2.47	0.47
1:J:98:VAL:HA	1:J:103:LEU:O	2.14	0.47
1:F:289:ALA:CB	1:F:419:PHE:HA	2.44	0.47
1:G:269:ARG:O	1:G:273:MET:HG3	2.14	0.47
2:H:237:PHE:HE1	2:H:239:ILE:HD11	1.79	0.47
3:H:601:ADP:O3'	1:I:224:LYS:HB2	2.13	0.47
1:L:70:PRO:HG2	1:L:139:ALA:HA	1.95	0.47
1:L:284:ILE:HD13	1:L:284:ILE:N	2.29	0.47
1:L:384:ALA:HA	1:L:392:PHE:HD1	1.76	0.47
1:I:21:MET:HE1	1:I:177:THR:CB	2.41	0.47
1:B:244:ILE:HG22	1:B:246:ILE:CD1	2.43	0.47
1:E:20:LYS:HG2	1:E:35:GLY:O	2.13	0.47
1:E:106:LEU:C	1:E:106:LEU:HD12	2.39	0.47
1:E:423:HIS:CE1	1:D:420:MET:CB	2.97	0.47
1:F:313:ILE:HG13	1:F:372:PRO:CG	2.43	0.47
1:C:302:VAL:HG11	1:C:344:LEU:HD21	1.96	0.47
1:D:324:LEU:HD23	1:D:324:LEU:N	2.30	0.47
2:H:27:GLY:HA3	2:H:248:PRO:HD3	1.97	0.47
1:K:374:ARG:HA	1:K:409:THR:O	2.14	0.47
1:I:208:ARG:NH2	1:I:221:GLU:OE2	2.47	0.47
1:J:455:VAL:HG11	1:J:463:HIS:HB2	1.95	0.47
1:E:142:VAL:O	1:E:178:THR:HA	2.15	0.47
1:E:281:ASP:OD2	1:E:407:GLU:OE2	2.33	0.47
4:G:602:ATP:O3G	2:H:457:LYS:NZ	2.47	0.47
2:H:467:ILE:HG21	2:H:489:ILE:CD1	2.44	0.47
2:H:489:ILE:HA	2:H:494:PRO:HB3	1.96	0.47
1:K:315:PHE:CE2	1:K:363:ILE:HA	2.50	0.47
1:J:455:VAL:HG11	1:J:463:HIS:CB	2.45	0.47
1:A:451:ARG:HB2	1:A:470:PHE:CE2	2.50	0.47
1:B:209:ASN:O	1:B:216:ARG:NH1	2.39	0.47
1:F:28:PHE:HE2	1:F:36:LEU:CD2	2.27	0.47
1:G:21:MET:SD	1:G:141:ARG:NE	2.88	0.47
1:G:279:PHE:CB	1:L:326:ARG:NH1	2.78	0.47
1:L:90:PHE:CE2	3:L:601:ADP:C6	3.02	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:264:SER:O	1:I:374:ARG:NH2	2.48	0.47
1:I:376:ALA:HA	1:I:411:LEU:O	2.15	0.47
1:J:58:GLN:O	1:J:62:ASN:ND2	2.48	0.47
1:J:203:ASN:CB	1:J:225:LEU:HD23	2.42	0.47
1:J:471:MET:HG2	1:J:480:LYS:NZ	2.30	0.47
1:D:58:GLN:HG3	1:D:92:TRP:CH2	2.49	0.47
1:D:197:GLU:OE2	1:D:197:GLU:N	2.44	0.47
1:D:236:PRO:HG2	1:D:247:PHE:CE1	2.49	0.47
1:G:298:VAL:CG2	1:G:413:THR:CG2	2.93	0.47
1:I:443:VAL:CG1	1:I:494:PRO:HD3	2.45	0.47
1:I:459:ARG:HD2	1:I:459:ARG:HA	1.66	0.47
1:J:313:ILE:HG23	1:J:345:LYS:HB3	1.97	0.47
1:B:336:GLU:O	1:B:340:ARG:HG3	2.14	0.47
1:D:45:SER:HA	1:D:182:THR:O	2.14	0.47
2:H:20:LYS:NZ	2:H:228:THR:HG21	2.30	0.47
1:J:414:ASN:CG	1:J:426:THR:HG22	2.39	0.47
1:E:24:MET:HB2	1:E:62:ASN:HB3	1.97	0.47
1:E:40:ARG:NH2	1:D:86:ASN:OD1	2.47	0.47
1:E:296:LEU:HD13	1:E:331:TRP:CE3	2.50	0.47
1:F:382:ALA:HA	1:F:385:ARG:HD3	1.97	0.47
1:G:488:ARG:NH2	1:L:495:THR:OG1	2.46	0.47
1:K:379:SER:HB2	1:K:413:THR:HB	1.97	0.47
1:J:471:MET:CG	1:J:480:LYS:HE2	2.35	0.47
1:A:283:ILE:HD12	1:A:412:PHE:CE1	2.49	0.46
1:A:379:SER:HB2	1:A:413:THR:O	2.15	0.46
1:B:146:SER:H	1:B:181:THR:HB	1.80	0.46
1:C:323:GLN:HE22	1:D:435:ASP:CG	2.23	0.46
1:D:440:LEU:CD2	1:D:470:PHE:CZ	2.97	0.46
2:H:311:ARG:HG3	2:H:343:LEU:HA	1.96	0.46
1:I:96:LYS:O	1:I:100:GLU:HG3	2.15	0.46
1:J:52:LYS:CB	1:J:181:THR:CG2	2.87	0.46
1:J:311:ARG:HA	1:J:343:LEU:O	2.15	0.46
1:B:214:GLU:HG2	1:C:234:GLU:HG3	1.97	0.46
2:H:23:THR:HG21	2:H:28:PHE:CE2	2.49	0.46
2:H:45:SER:HA	2:H:182:THR:O	2.15	0.46
2:H:454:ASN:HB2	2:H:467:ILE:HA	1.97	0.46
1:J:284:ILE:HB	1:J:411:LEU:CD1	2.36	0.46
1:J:292:THR:HG22	1:J:440:LEU:CB	2.45	0.46
1:A:203:ASN:HB3	1:A:225:LEU:HG	1.96	0.46
1:E:338:MET:HA	1:E:338:MET:HE2	1.97	0.46
4:C:602:ATP:O2G	1:D:457:LYS:NZ	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LEU:O	1:D:58:GLN:HB2	2.15	0.46
2:H:134:ILE:HA	2:H:139:ALA:HB2	1.98	0.46
2:H:152:GLN:HA	2:H:152:GLN:HE21	1.80	0.46
1:K:142:VAL:CB	1:K:178:THR:HG23	2.45	0.46
1:L:436:THR:HG1	1:L:458:MET:HE3	1.80	0.46
1:I:464:ASP:OD2	1:I:468:ARG:NE	2.47	0.46
1:A:344:LEU:HD13	1:A:346:ILE:HD11	1.96	0.46
1:E:312:ALA:HA	1:E:374:ARG:O	2.15	0.46
1:F:287:THR:HG22	1:F:414:ASN:HB3	1.98	0.46
1:F:392:PHE:HE2	1:F:428:SER:HB2	1.81	0.46
1:C:63:GLY:O	1:C:67:PHE:HB2	2.15	0.46
2:H:289:ALA:O	2:H:294:LYS:NZ	2.47	0.46
1:A:21:MET:CE	1:A:177:THR:CB	2.92	0.46
1:B:396:VAL:O	1:B:400:THR:CB	2.64	0.46
1:E:199:PHE:CE1	1:D:183:GLU:CB	2.99	0.46
1:G:25:ILE:HG22	1:G:246:ILE:HD12	1.97	0.46
3:H:601:ADP:HO3'	1:I:225:LEU:N	2.14	0.46
1:L:438:ILE:HD13	1:L:438:ILE:N	2.30	0.46
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.81	0.46
1:F:294:LYS:HB3	1:F:413:THR:HG23	1.98	0.46
1:C:358:ASP:O	1:C:362:ILE:HG12	2.15	0.46
1:C:379:SER:CB	1:C:413:THR:O	2.64	0.46
1:D:384:ALA:HB2	1:D:392:PHE:CZ	2.49	0.46
2:H:302:VAL:CG1	2:H:344:LEU:CD2	2.93	0.46
2:H:383:LEU:HD13	2:H:395:PHE:CZ	2.50	0.46
1:L:59:PHE:HZ	1:L:177:THR:OG1	1.99	0.46
1:L:177:THR:O	1:L:177:THR:OG1	2.29	0.46
1:K:216:ARG:HA	1:K:216:ARG:HD3	1.82	0.46
1:K:350:TYR:HA	1:K:351:PRO:HD3	1.82	0.46
1:I:220:LEU:HD13	1:I:246:ILE:CD1	2.46	0.46
1:I:321:ARG:HH21	1:I:321:ARG:CG	2.28	0.46
1:J:215:ARG:HG2	1:J:215:ARG:HH21	1.81	0.46
1:E:123:LEU:O	1:E:127:ILE:HG13	2.16	0.46
1:E:202:ASP:HA	1:E:226:ARG:HE	1.81	0.46
1:C:402:TYR:O	1:C:406:GLU:HB2	2.16	0.46
1:L:21:MET:HE2	1:L:177:THR:HG21	1.97	0.46
1:A:234:GLU:O	1:F:215:ARG:NH2	2.49	0.46
1:F:317:TYR:HB3	1:F:351:PRO:HG3	1.98	0.46
1:G:208:ARG:HE	1:G:208:ARG:HB2	1.59	0.46
2:H:142:VAL:HB	2:H:178:THR:HG23	1.97	0.46
1:K:291:GLY:O	1:K:451:ARG:NH1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:469:GLU:HG2	1:K:480:LYS:HB2	1.97	0.46
1:E:306:CYS:HB3	1:E:338:MET:HE2	1.97	0.46
1:C:430:ILE:O	1:C:430:ILE:HD12	2.16	0.46
2:H:79:THR:HG22	2:H:82:ASP:CG	2.41	0.46
3:K:601:ADP:O3'	1:L:224:LYS:HA	2.16	0.46
1:L:21:MET:CE	1:L:177:THR:CG2	2.93	0.46
1:L:266:GLY:HA3	1:L:300:ARG:HG3	1.97	0.46
1:L:303:GLU:HG3	1:L:333:MET:HE3	1.97	0.46
1:L:383:LEU:HD13	1:L:395:PHE:CZ	2.51	0.46
1:I:296:LEU:HD12	1:I:296:LEU:O	2.15	0.46
1:J:104:PHE:HB2	1:J:137:TYR:CE2	2.50	0.46
1:J:188:TYR:HE1	1:J:210:VAL:HG13	1.81	0.46
1:B:317:TYR:HA	1:B:349:ALA:O	2.16	0.45
1:D:328:ALA:O	1:D:333:MET:HG3	2.16	0.45
2:H:21:MET:HE3	2:H:141:ARG:CZ	2.47	0.45
1:K:466:ALA:CB	1:J:448:GLU:HG3	2.46	0.45
1:L:182:THR:HG21	1:L:192:ALA:HB1	1.98	0.45
1:J:61:TYR:CZ	1:J:92:TRP:CD1	3.04	0.45
1:J:372:PRO:HG3	1:J:375:ILE:HD11	1.97	0.45
1:F:333:MET:HE2	1:F:333:MET:HB3	1.79	0.45
1:G:219:THR:HG22	1:G:236:PRO:HA	1.98	0.45
1:G:465:LYS:HB2	1:L:449:MET:O	2.15	0.45
1:I:49:GLY:O	1:I:218:ARG:NH2	2.49	0.45
1:I:54:LEU:HD12	1:I:54:LEU:O	2.16	0.45
1:I:64:ILE:HD11	1:I:71:GLY:H	1.81	0.45
1:I:166:ARG:H	1:I:166:ARG:HG2	1.60	0.45
1:J:31:ILE:HA	1:J:231:MET:HG3	1.98	0.45
1:C:483:PHE:HB3	1:C:486:PHE:CD1	2.51	0.45
2:H:110:PRO:HD2	1:I:165:PHE:CE2	2.51	0.45
1:J:443:VAL:HG13	1:J:494:PRO:CG	2.46	0.45
1:J:455:VAL:CG1	1:J:463:HIS:HB2	2.47	0.45
1:B:61:TYR:C	1:B:61:TYR:CD2	2.94	0.45
1:E:305:ALA:HB2	1:E:374:ARG:CD	2.35	0.45
1:F:69:GLU:OE1	1:F:141:ARG:NE	2.49	0.45
1:C:90:PHE:HZ	3:C:601:ADP:N7	2.13	0.45
1:C:265:SER:HB3	1:C:278:PHE:CE1	2.52	0.45
1:G:107:ASP:C	1:G:109:SER:H	2.24	0.45
2:H:467:ILE:HD12	2:H:467:ILE:N	2.27	0.45
1:K:488:ARG:O	1:K:491:SER:OG	2.28	0.45
1:I:420:MET:HE2	1:I:492:GLY:HA3	1.99	0.45
1:E:314:LEU:HD12	1:E:314:LEU:C	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:TRP:HA	1:E:474:ASP:O	2.16	0.45
2:H:19:ALA:C	2:H:38:ILE:HG13	2.42	0.45
2:H:204:VAL:HG12	2:H:223:LEU:HB2	1.98	0.45
1:K:379:SER:CB	1:K:413:THR:HB	2.46	0.45
1:J:289:ALA:O	1:J:292:THR:OG1	2.33	0.45
1:A:146:SER:HB2	1:A:181:THR:CG2	2.45	0.45
1:A:180:MET:HE2	1:A:180:MET:HB3	1.78	0.45
1:B:318:GLU:OE2	1:B:379:SER:OG	2.27	0.45
1:C:214:GLU:HA	1:D:234:GLU:HG3	1.98	0.45
1:C:296:LEU:HD12	1:C:296:LEU:O	2.16	0.45
1:D:314:LEU:HD21	1:D:324:LEU:CD1	2.47	0.45
1:J:168:VAL:HA	1:J:171:LEU:CD1	2.47	0.45
1:J:292:THR:HG21	1:J:440:LEU:C	2.41	0.45
1:A:52:LYS:HE2	3:A:601:ADP:O1B	2.17	0.45
1:A:454:ASN:HB2	1:A:467:ILE:HA	1.99	0.45
1:E:147:VAL:HG11	1:E:180:MET:HG3	1.98	0.45
1:D:142:VAL:O	1:D:178:THR:HA	2.15	0.45
1:G:289:ALA:HB2	1:G:419:PHE:HA	1.98	0.45
1:K:356:LEU:N	1:K:356:LEU:HD22	2.32	0.45
1:L:384:ALA:CA	1:L:392:PHE:CD1	3.00	0.45
1:J:300:ARG:CD	1:J:333:MET:CE	2.95	0.45
1:A:289:ALA:O	1:A:415:THR:HG23	2.17	0.45
1:E:324:LEU:O	1:E:328:ALA:CB	2.65	0.45
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.84	0.45
1:G:289:ALA:CB	1:G:419:PHE:HA	2.46	0.45
2:H:306:CYS:SG	2:H:344:LEU:HB2	2.57	0.45
1:L:345:LYS:HD2	1:L:370:PHE:CD1	2.52	0.45
1:I:30:ASP:OD2	1:I:30:ASP:N	2.49	0.45
1:I:44:VAL:HA	1:I:205:VAL:O	2.17	0.45
1:I:262:ARG:HB3	1:I:276:GLY:O	2.17	0.45
1:J:419:PHE:CD2	1:J:419:PHE:N	2.84	0.45
1:J:488:ARG:O	1:J:491:SER:OG	2.34	0.45
1:A:302:VAL:CG1	1:A:344:LEU:HG	2.47	0.45
1:B:441:GLN:NE2	1:B:489:ILE:O	2.48	0.45
1:F:316:ALA:O	1:F:348:CYS:HA	2.17	0.45
1:C:21:MET:HE1	1:C:141:ARG:HG2	1.99	0.45
1:C:42:THR:HG23	1:C:203:ASN:HB2	1.99	0.45
2:H:451:ARG:HH11	2:H:451:ARG:HG2	1.82	0.45
1:L:296:LEU:HD12	1:L:296:LEU:C	2.42	0.45
1:L:489:ILE:HD13	1:L:494:PRO:HB3	1.98	0.45
1:E:425:ILE:CD1	1:D:419:PHE:CE2	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ILE:HG23	1:C:412:PHE:HE1	1.78	0.45
1:G:486:PHE:CD2	1:G:494:PRO:HB2	2.52	0.45
2:H:71:GLY:CA	2:H:141:ARG:O	2.65	0.45
2:H:223:LEU:HD23	2:H:223:LEU:HA	1.87	0.45
1:L:291:GLY:O	1:L:442:TYR:OH	2.35	0.45
1:J:436:THR:OG1	1:J:458:MET:HE3	2.17	0.45
1:B:207:LEU:HD22	1:B:220:LEU:HD12	2.00	0.44
1:L:61:TYR:CE2	1:L:92:TRP:CD1	3.05	0.44
1:J:167:LEU:O	1:J:171:LEU:HD12	2.17	0.44
2:H:207:LEU:CD2	2:H:220:LEU:HD12	2.47	0.44
1:K:198:GLU:HG3	1:K:199:PHE:CD2	2.51	0.44
1:B:294:LYS:CB	1:B:413:THR:CG2	2.95	0.44
1:B:299:SER:O	1:B:333:MET:HE1	2.17	0.44
1:E:235:TYR:HA	1:E:236:PRO:HD2	1.89	0.44
1:E:269:ARG:O	1:E:273:MET:HG3	2.17	0.44
1:E:465:LYS:O	1:D:449:MET:N	2.47	0.44
1:F:37:PRO:HB2	1:F:40:ARG:HB2	1.98	0.44
1:I:294:LYS:HB3	1:I:413:THR:HG23	1.99	0.44
1:J:61:TYR:CE1	1:J:92:TRP:CD1	3.05	0.44
1:A:294:LYS:HE2	4:A:602:ATP:O1B	2.18	0.44
1:B:31:ILE:HD12	1:B:246:ILE:HG21	1.98	0.44
1:C:28:PHE:CE1	1:C:55:PHE:CZ	3.05	0.44
1:C:221:GLU:HG3	1:C:233:GLY:O	2.17	0.44
1:C:311:ARG:CD	1:C:370:PHE:CD2	3.00	0.44
1:G:45:SER:OG	1:G:191:ILE:O	2.31	0.44
1:C:337:GLU:HG3	1:C:341:GLN:OE1	2.17	0.44
1:G:448:GLU:HA	2:H:466:ALA:HA	1.98	0.44
1:K:221:GLU:HB2	1:K:234:GLU:HA	1.99	0.44
1:A:147:VAL:CB	1:A:180:MET:CE	2.96	0.44
1:F:31:ILE:HG23	1:F:231:MET:HB2	1.99	0.44
1:K:274:CYS:SG	1:K:278:PHE:HE2	2.41	0.44
1:L:287:THR:HG21	1:L:425:ILE:O	2.17	0.44
1:I:358:ASP:O	1:I:362:ILE:HG13	2.18	0.44
1:A:97:LEU:HB3	1:A:103:LEU:HB3	2.00	0.44
1:E:126:LEU:O	1:E:130:ILE:HG13	2.18	0.44
1:E:333:MET:HE3	1:E:333:MET:HB2	1.79	0.44
1:G:61:TYR:CE1	1:G:92:TRP:HB3	2.52	0.44
1:J:345:LYS:HB2	1:J:370:PHE:CE2	2.53	0.44
1:A:61:TYR:CZ	1:A:65:ILE:HG13	2.53	0.44
1:A:183:GLU:CD	1:B:161:ARG:HH22	2.25	0.44
1:B:325:LEU:HD21	1:B:335:PHE:CB	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ARG:HG2	1:B:451:ARG:NH1	2.32	0.44
1:F:44:VAL:HA	1:F:205:VAL:O	2.17	0.44
1:F:295:THR:OG1	4:F:602:ATP:O1B	2.34	0.44
1:D:294:LYS:HE2	1:D:413:THR:CG2	2.48	0.44
1:G:290:THR:CG2	2:H:456:PHE:CE2	3.01	0.44
2:H:395:PHE:CD2	2:H:395:PHE:C	2.96	0.44
1:L:220:LEU:C	1:L:220:LEU:HD23	2.43	0.44
1:B:37:PRO:HD2	1:B:203:ASN:ND2	2.32	0.44
1:B:287:THR:HG23	1:B:414:ASN:ND2	2.28	0.44
1:E:32:SER:HB2	1:E:35:GLY:O	2.18	0.44
1:E:182:THR:CG2	1:E:197:GLU:HG2	2.43	0.44
1:E:313:ILE:HG13	1:E:372:PRO:HB3	2.00	0.44
1:F:296:LEU:O	1:F:296:LEU:HD12	2.17	0.44
1:I:24:MET:HB3	1:I:62:ASN:ND2	2.33	0.44
1:J:211:LEU:HB2	1:J:216:ARG:CD	2.47	0.44
1:A:148:THR:HG21	1:A:183:GLU:HB2	1.99	0.43
1:F:412:PHE:N	1:F:412:PHE:CD1	2.86	0.43
1:C:28:PHE:HB2	1:C:246:ILE:HD13	1.99	0.43
1:D:106:LEU:HD11	1:D:129:ARG:NE	2.32	0.43
1:K:368:ASN:ND2	1:K:402:TYR:OH	2.48	0.43
1:K:466:ALA:HB2	1:J:448:GLU:HG3	2.00	0.43
1:I:209:ASN:O	1:I:216:ARG:NH1	2.47	0.43
1:A:49:GLY:O	1:A:218:ARG:NH2	2.50	0.43
1:A:431:SEP:HA	1:A:434:THR:HG22	2.00	0.43
1:C:381:SER:HB3	1:C:414:ASN:HB2	1.99	0.43
1:D:378:ASP:HA	1:D:379:SER:HA	1.75	0.43
1:G:262:ARG:CA	1:G:278:PHE:O	2.55	0.43
1:G:290:THR:CG2	2:H:425:ILE:CD1	2.96	0.43
1:K:487:GLU:O	1:K:494:PRO:HA	2.18	0.43
1:L:356:LEU:HD21	1:L:387:VAL:HG11	2.00	0.43
1:J:445:ILE:HD11	1:J:494:PRO:CG	2.48	0.43
1:J:452:ALA:HB1	1:J:467:ILE:CG2	2.48	0.43
1:A:469:GLU:HB3	1:A:483:PHE:CZ	2.54	0.43
1:E:316:ALA:HB3	1:E:348:CYS:SG	2.59	0.43
1:E:316:ALA:HB2	1:E:324:LEU:HD11	2.00	0.43
1:F:54:LEU:HD12	1:F:54:LEU:C	2.44	0.43
1:I:306:CYS:HB2	1:I:338:MET:HE3	2.00	0.43
1:I:335:PHE:HA	1:I:338:MET:HG3	2.00	0.43
3:I:601:ADP:N7	1:J:227:GLY:O	2.51	0.43
1:J:20:LYS:HE2	1:J:32:SER:O	2.18	0.43
1:J:490:ILE:HA	1:J:490:ILE:HD13	1.73	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PHE:CE2	1:B:145:ASP:CB	3.02	0.43
1:F:317:TYR:HA	1:F:349:ALA:O	2.18	0.43
1:C:263:VAL:N	1:C:278:PHE:O	2.48	0.43
1:K:274:CYS:HG	1:K:278:PHE:HE2	1.64	0.43
1:I:434:THR:CG2	1:I:437:ILE:HD11	2.48	0.43
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.54	0.43
1:A:145:ASP:HA	1:A:146:SER:HA	1.77	0.43
1:A:302:VAL:HG11	1:A:344:LEU:HD21	2.01	0.43
1:A:359:HIS:O	1:A:363:ILE:HG13	2.19	0.43
1:B:267:VAL:HB	1:B:270:LEU:HB2	2.01	0.43
1:B:487:GLU:O	1:B:494:PRO:HA	2.18	0.43
1:E:22:ARG:NH1	1:E:24:MET:SD	2.91	0.43
1:E:350:TYR:CE1	1:F:254:LEU:CD1	3.02	0.43
1:F:31:ILE:O	1:F:231:MET:N	2.42	0.43
1:C:37:PRO:CG	1:C:225:LEU:CD2	2.97	0.43
2:H:187:GLU:OE2	2:H:187:GLU:HA	2.18	0.43
2:H:283:ILE:HD12	2:H:400:THR:HG23	2.00	0.43
1:I:338:MET:HE2	1:I:338:MET:HB3	1.75	0.43
1:J:328:ALA:O	1:J:332:GLY:O	2.36	0.43
1:J:420:MET:HG3	1:J:492:GLY:HA3	2.00	0.43
1:A:318:GLU:OE2	1:B:432:THR:HG21	2.18	0.43
1:B:42:THR:HG23	1:B:203:ASN:HB2	1.99	0.43
1:E:45:SER:HA	1:E:182:THR:O	2.17	0.43
1:E:334:ASP:O	1:E:338:MET:HG2	2.19	0.43
1:F:296:LEU:HD12	1:F:296:LEU:C	2.44	0.43
1:D:441:GLN:HE22	1:D:490:ILE:HA	1.84	0.43
1:D:488:ARG:HH11	1:D:488:ARG:CB	2.28	0.43
1:G:290:THR:O	2:H:456:PHE:HE2	2.02	0.43
1:G:456:PHE:CZ	1:L:419:PHE:HB2	2.53	0.43
1:L:469:GLU:HB3	1:L:483:PHE:CZ	2.53	0.43
1:B:267:VAL:CG2	1:B:477:PRO:HG3	2.49	0.43
1:E:145:ASP:HA	1:E:146:SER:HA	1.69	0.43
1:E:350:TYR:CE1	1:F:254:LEU:HD12	2.54	0.43
2:H:44:VAL:HA	2:H:205:VAL:O	2.18	0.43
1:K:49:GLY:HA2	3:K:601:ADP:H5'2	2.00	0.43
1:K:208:ARG:NH2	1:K:221:GLU:OE2	2.52	0.43
1:C:37:PRO:HD2	1:C:203:ASN:ND2	2.34	0.43
1:C:152:GLN:CA	1:D:158:SER:CB	2.96	0.43
1:G:21:MET:HE1	1:G:177:THR:CB	2.48	0.43
1:K:145:ASP:HA	1:K:146:SER:HA	1.65	0.43
1:K:211:LEU:CD1	1:K:216:ARG:HE	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:406:GLU:HB3	1:K:408:ILE:CG1	2.49	0.43
1:A:57:ILE:HD11	1:A:83:ILE:HG23	2.01	0.43
1:B:287:THR:HG21	1:B:425:ILE:O	2.19	0.43
1:E:109:SER:HA	1:E:110:PRO:HD2	1.92	0.43
1:E:133:ALA:O	1:E:137:TYR:HD1	2.02	0.43
1:F:420:MET:HE3	1:F:420:MET:HB3	1.81	0.43
1:D:296:LEU:HD13	1:D:331:TRP:CE2	2.52	0.43
2:H:263:VAL:CG1	2:H:374:ARG:NH2	2.82	0.43
1:J:191:ILE:HD13	1:J:223:LEU:HD12	2.01	0.43
1:F:18:ILE:HB	1:F:228:THR:HG21	2.01	0.43
1:C:325:LEU:HD21	1:C:336:GLU:N	2.34	0.43
1:G:218:ARG:HB2	1:G:237:PHE:CE2	2.54	0.43
1:L:265:SER:HB3	1:L:278:PHE:CE1	2.54	0.43
1:L:384:ALA:HA	1:L:392:PHE:CE1	2.51	0.43
1:I:436:THR:CG2	1:I:458:MET:HE3	2.49	0.43
1:J:296:LEU:HD23	1:J:472:ILE:HG12	2.01	0.43
1:B:125:ALA:O	1:B:129:ARG:HG3	2.19	0.42
1:B:146:SER:HA	1:B:181:THR:HG22	2.01	0.42
1:D:44:VAL:O	1:D:181:THR:HA	2.19	0.42
1:D:267:VAL:CG2	1:D:477:PRO:CG	2.94	0.42
1:D:437:ILE:HD12	1:D:457:LYS:HG2	2.00	0.42
1:G:264:SER:O	1:G:374:ARG:NH1	2.49	0.42
1:G:323:GLN:HE22	2:H:435:ASP:CG	2.27	0.42
2:H:54:LEU:HD12	2:H:54:LEU:O	2.19	0.42
1:I:61:TYR:CE2	1:I:92:TRP:CD1	3.07	0.42
1:J:292:THR:CG2	1:J:440:LEU:CB	2.96	0.42
1:A:45:SER:OG	1:A:184:ARG:HD2	2.19	0.42
1:A:54:LEU:HD13	1:A:90:PHE:CE1	2.53	0.42
1:B:31:ILE:HG23	1:B:231:MET:HB2	2.01	0.42
1:F:18:ILE:HG13	1:F:228:THR:CG2	2.49	0.42
1:D:31:ILE:CA	1:D:231:MET:HG3	2.43	0.42
1:D:269:ARG:O	1:D:273:MET:HG3	2.19	0.42
2:H:283:ILE:HG13	2:H:400:THR:CG2	2.46	0.42
1:L:271:ASP:HA	1:L:277:GLY:HA2	2.01	0.42
1:I:183:GLU:OE2	1:J:199:PHE:CD2	2.73	0.42
1:I:186:GLU:OE1	1:I:187:GLU:N	2.52	0.42
1:A:397:ILE:HD12	1:F:352:GLU:OE2	2.19	0.42
1:B:24:MET:SD	1:B:67:PHE:HE1	2.43	0.42
1:E:98:VAL:HA	1:E:103:LEU:O	2.19	0.42
2:H:288:GLY:HA2	2:H:440:LEU:O	2.19	0.42
1:J:79:THR:HG23	1:J:81:GLN:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ALA:HB2	1:A:392:PHE:CE2	2.54	0.42
1:B:397:ILE:CD1	1:B:433:ILE:HD13	2.49	0.42
1:E:267:VAL:HB	1:E:270:LEU:CB	2.49	0.42
1:C:335:PHE:HA	1:C:338:MET:HG3	2.01	0.42
1:D:318:GLU:OE2	1:D:379:SER:OG	2.30	0.42
2:H:467:ILE:H	2:H:467:ILE:CD1	2.29	0.42
1:L:28:PHE:O	1:L:32:SER:OG	2.33	0.42
1:L:449:MET:HE2	1:L:449:MET:HB3	1.89	0.42
1:I:338:MET:HE2	1:I:344:LEU:HB2	2.00	0.42
1:A:436:THR:OG1	1:A:458:MET:CE	2.67	0.42
1:B:221:GLU:HG3	1:B:233:GLY:O	2.20	0.42
1:I:299:SER:HB3	1:I:333:MET:CE	2.49	0.42
1:B:333:MET:HE3	1:B:333:MET:HB3	1.79	0.42
1:E:306:CYS:CB	1:E:338:MET:HE1	2.49	0.42
1:G:63:GLY:CA	1:G:141:ARG:NH1	2.82	0.42
2:H:54:LEU:HD23	2:H:239:ILE:CG2	2.49	0.42
1:K:444:GLU:CD	1:L:489:ILE:H	2.28	0.42
1:L:222:ILE:CG2	1:L:230:HIS:ND1	2.82	0.42
1:L:331:TRP:HZ2	4:L:602:ATP:C8	2.38	0.42
1:J:54:LEU:HD23	1:J:239:ILE:HD12	2.01	0.42
1:J:451:ARG:NH2	4:J:701:ATP:O2'	2.52	0.42
1:B:326:ARG:NH1	1:C:258:SER:OG	2.46	0.42
1:E:184:ARG:HH21	1:E:191:ILE:HA	1.84	0.42
1:C:75:THR:O	1:C:108:ALA:HB3	2.20	0.42
1:C:225:LEU:HB2	1:C:230:HIS:CD2	2.54	0.42
1:C:244:ILE:CG2	1:C:246:ILE:HG13	2.49	0.42
1:G:441:GLN:NE2	1:G:489:ILE:O	2.52	0.42
1:G:457:LYS:HB2	1:L:291:GLY:HA3	2.02	0.42
2:H:420:MET:HE1	2:H:449:MET:CE	2.42	0.42
2:H:470:PHE:CD1	2:H:470:PHE:C	2.97	0.42
1:K:458:MET:HB2	1:K:463:HIS:CD2	2.54	0.42
1:L:313:ILE:HD11	1:L:370:PHE:HB3	2.01	0.42
1:L:383:LEU:HD13	1:L:395:PHE:CE2	2.55	0.42
1:A:44:VAL:O	1:A:181:THR:HA	2.19	0.42
1:A:402:TYR:HA	1:A:405:GLN:HG2	2.02	0.42
2:H:208:ARG:NH2	2:H:221:GLU:OE2	2.52	0.42
1:K:51:GLY:HA2	3:K:601:ADP:O2A	2.20	0.42
1:K:264:SER:O	1:K:374:ARG:NH2	2.52	0.42
1:K:434:THR:CG2	1:K:437:ILE:HD11	2.50	0.42
1:L:38:ILE:HA	1:L:177:THR:CG2	2.50	0.42
1:L:294:LYS:CB	1:L:413:THR:CG2	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:396:VAL:O	1:L:400:THR:OG1	2.19	0.42
1:J:23:THR:O	1:J:62:ASN:ND2	2.53	0.42
1:A:344:LEU:HD22	1:A:344:LEU:C	2.45	0.42
1:B:448:GLU:HA	1:C:466:ALA:HA	2.02	0.42
1:E:335:PHE:HA	1:E:338:MET:CG	2.48	0.42
1:C:290:THR:O	1:C:442:TYR:OH	2.32	0.42
1:G:21:MET:HE3	1:G:177:THR:HG21	2.01	0.42
2:H:42:THR:HG23	2:H:203:ASN:HB2	2.02	0.42
2:H:263:VAL:HG12	2:H:374:ARG:NH2	2.35	0.42
2:H:442:TYR:CE2	2:H:451:ARG:NH1	2.88	0.42
1:K:46:GLY:HA2	1:K:184:ARG:HD3	2.02	0.42
1:K:230:HIS:CD2	4:J:702:ATP:O2'	2.73	0.42
1:L:333:MET:H	1:L:333:MET:HG2	1.66	0.42
1:L:356:LEU:HD12	1:L:356:LEU:HA	1.89	0.42
1:J:431:SEP:HA	1:J:434:THR:HG22	2.02	0.42
1:A:345:LYS:HZ1	1:A:366:GLU:HG3	1.84	0.42
1:E:338:MET:CB	1:E:344:LEU:HB2	2.41	0.42
1:F:287:THR:HA	1:F:414:ASN:O	2.20	0.42
1:F:296:LEU:CD2	1:F:472:ILE:HG23	2.49	0.42
1:C:31:ILE:HA	1:C:231:MET:SD	2.60	0.42
1:D:325:LEU:HD13	1:D:336:GLU:HG3	2.01	0.42
1:G:317:TYR:HB3	1:G:351:PRO:HG3	2.01	0.42
2:H:214:GLU:HG2	1:I:234:GLU:HG3	2.01	0.42
2:H:414:ASN:ND2	2:H:414:ASN:C	2.78	0.42
1:L:287:THR:HA	1:L:414:ASN:O	2.20	0.42
1:L:380:LEU:HG	1:L:412:PHE:HB3	2.01	0.42
1:I:21:MET:HE2	1:I:21:MET:HB2	1.82	0.42
1:I:311:ARG:HG3	1:I:343:LEU:HA	2.02	0.42
1:J:304:ASN:OD1	1:J:374:ARG:NH2	2.53	0.42
1:A:230:HIS:CE1	3:F:601:ADP:O2'	2.73	0.41
1:A:301:PHE:O	1:A:374:ARG:NH1	2.53	0.41
2:H:57:ILE:HD11	2:H:83:ILE:HG22	2.01	0.41
2:H:284:ILE:O	2:H:411:LEU:HA	2.20	0.41
1:K:126:LEU:O	1:K:130:ILE:N	2.52	0.41
1:I:294:LYS:HG3	1:I:440:LEU:HD12	2.01	0.41
1:J:45:SER:HA	1:J:182:THR:O	2.20	0.41
1:A:106:LEU:C	1:A:106:LEU:HD12	2.46	0.41
1:B:46:GLY:H	1:B:184:ARG:HG3	1.84	0.41
1:E:75:THR:O	1:E:108:ALA:HB3	2.20	0.41
1:F:350:TYR:HA	1:F:351:PRO:HD3	1.91	0.41
1:C:211:LEU:HB2	1:C:216:ARG:CZ	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:284:ILE:HG23	1:L:436:THR:HB	2.02	0.41
1:L:360:LEU:HD23	1:L:360:LEU:HA	1.88	0.41
1:A:137:TYR:CD1	1:A:137:TYR:N	2.88	0.41
1:E:69:GLU:HA	1:E:70:PRO:HD2	1.87	0.41
1:F:146:SER:CA	1:F:181:THR:O	2.62	0.41
1:D:55:PHE:C	1:D:55:PHE:CD2	2.98	0.41
1:D:436:THR:OG1	1:D:458:MET:CE	2.68	0.41
2:H:73:PHE:O	2:H:106:LEU:N	2.52	0.41
1:L:443:VAL:HG13	1:L:494:PRO:CD	2.50	0.41
1:I:78:GLU:OE1	1:I:86:ASN:ND2	2.53	0.41
1:J:324:LEU:HD23	1:J:324:LEU:HA	1.80	0.41
1:J:379:SER:CB	1:J:413:THR:HG22	2.51	0.41
1:J:444:GLU:O	1:J:494:PRO:HD2	2.21	0.41
1:B:225:LEU:HD23	1:B:225:LEU:HA	1.92	0.41
1:E:27:GLY:O	1:E:31:ILE:HG13	2.20	0.41
1:C:57:ILE:HD11	1:C:83:ILE:HG23	2.01	0.41
1:C:345:LYS:HB2	1:C:370:PHE:CE2	2.54	0.41
1:C:490:ILE:H	1:C:490:ILE:HG12	1.67	0.41
1:G:213:GLY:C	1:G:215:ARG:H	2.29	0.41
2:H:394:GLN:O	2:H:397:ILE:HG13	2.20	0.41
1:L:106:LEU:C	1:L:106:LEU:HD12	2.45	0.41
1:I:448:GLU:HA	1:J:466:ALA:HA	2.02	0.41
1:I:451:ARG:NH1	1:I:451:ARG:HG2	2.35	0.41
1:J:223:LEU:HD23	1:J:223:LEU:HA	1.92	0.41
1:J:289:ALA:HB2	1:J:419:PHE:HA	2.02	0.41
1:B:31:ILE:HD11	1:B:248:PRO:HG3	2.03	0.41
1:E:311:ARG:HA	1:E:343:LEU:O	2.20	0.41
1:F:18:ILE:HB	1:F:228:THR:HG22	2.03	0.41
1:C:37:PRO:CD	1:C:225:LEU:HD21	2.49	0.41
1:C:465:LYS:H	1:C:465:LYS:HG2	1.78	0.41
2:H:59:PHE:O	2:H:141:ARG:NH1	2.50	0.41
1:A:60:LEU:CD2	1:A:141:ARG:HB3	2.50	0.41
1:B:295:THR:CA	1:B:298:VAL:HG23	2.50	0.41
1:B:449:MET:CE	1:C:490:ILE:HD12	2.48	0.41
1:E:338:MET:CE	1:E:338:MET:CA	2.98	0.41
1:E:488:ARG:CB	1:E:488:ARG:HH11	2.33	0.41
1:F:37:PRO:HD2	1:F:203:ASN:ND2	2.35	0.41
1:C:211:LEU:HD12	1:C:216:ARG:HG2	2.01	0.41
1:D:269:ARG:HD3	1:D:269:ARG:HA	1.87	0.41
1:D:285:LEU:HA	1:D:412:PHE:O	2.20	0.41
1:D:304:ASN:HB3	1:D:374:ARG:HH22	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:GLU:HB2	1:G:333:MET:HE2	2.01	0.41
2:H:218:ARG:HH11	1:I:232:LYS:HE2	1.86	0.41
2:H:378:ASP:HA	2:H:379:SER:HA	1.77	0.41
1:K:457:LYS:NZ	4:J:701:ATP:O3G	2.52	0.41
1:L:289:ALA:O	1:L:294:LYS:NZ	2.51	0.41
1:I:287:THR:HG21	1:I:425:ILE:O	2.21	0.41
1:I:311:ARG:HA	1:I:343:LEU:O	2.21	0.41
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.93	0.41
1:E:60:LEU:HA	1:E:141:ARG:HD3	2.03	0.41
1:K:262:ARG:HH12	1:K:275:GLY:C	2.29	0.41
1:L:374:ARG:HA	1:L:409:THR:O	2.21	0.41
1:I:279:PHE:O	1:I:282:SER:OG	2.27	0.41
1:I:451:ARG:HG2	1:I:451:ARG:HH11	1.85	0.41
1:I:473:SER:HA	3:I:602:ADP:C2	2.55	0.41
1:J:302:VAL:CG1	1:J:344:LEU:HD21	2.50	0.41
1:A:289:ALA:HB1	1:A:419:PHE:HA	2.01	0.41
1:A:384:ALA:HB2	1:A:392:PHE:CZ	2.56	0.41
1:E:105:ILE:N	1:E:105:ILE:HD12	2.36	0.41
1:E:488:ARG:HH11	1:E:488:ARG:HB3	1.85	0.41
1:F:359:HIS:O	1:F:363:ILE:HG13	2.20	0.41
1:C:191:ILE:HD11	1:C:223:LEU:CD1	2.51	0.41
1:C:305:ALA:O	1:C:310:GLU:HB2	2.21	0.41
1:D:208:ARG:HB2	1:D:219:THR:OG1	2.20	0.41
1:G:188:TYR:CE2	1:G:208:ARG:HD2	2.55	0.41
2:H:231:MET:HB3	2:H:235:TYR:OH	2.21	0.41
1:K:289:ALA:HB2	1:K:419:PHE:HA	2.03	0.41
1:L:292:THR:HG21	1:L:440:LEU:HB3	1.90	0.41
1:L:412:PHE:N	1:L:412:PHE:CD1	2.88	0.41
1:I:46:GLY:HA2	1:I:184:ARG:HD3	2.02	0.41
1:I:339:GLU:CD	1:I:346:ILE:HD12	2.46	0.41
1:A:41:SER:HB2	1:A:178:THR:HB	2.03	0.41
1:A:60:LEU:HD23	1:A:141:ARG:HB3	2.03	0.41
1:B:64:ILE:HD13	1:B:102:LYS:CB	2.51	0.41
1:F:18:ILE:HG13	1:F:228:THR:HG23	2.02	0.41
1:F:231:MET:HB3	1:F:235:TYR:OH	2.21	0.41
1:F:306:CYS:SG	1:F:343:LEU:O	2.74	0.41
1:C:90:PHE:CE2	1:C:240:THR:O	2.72	0.41
1:C:406:GLU:HB3	1:C:408:ILE:HG13	2.03	0.41
1:D:60:LEU:CD1	1:D:73:PHE:HB2	2.51	0.41
1:D:273:MET:O	1:D:463:HIS:HA	2.20	0.41
1:D:294:LYS:CB	1:D:413:THR:HG23	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:THR:HA	1:G:414:ASN:O	2.21	0.41
2:H:274:CYS:HB3	2:H:458:MET:HE1	2.03	0.41
2:H:296:LEU:HD12	2:H:296:LEU:O	2.21	0.41
1:K:425:ILE:HG12	1:J:419:PHE:HE2	1.77	0.41
1:L:31:ILE:HG23	1:L:231:MET:HB2	2.02	0.41
1:L:33:HIS:HD2	1:L:230:HIS:HA	1.86	0.41
1:L:470:PHE:CD2	1:L:470:PHE:C	2.99	0.41
1:J:191:ILE:HG21	1:J:204:VAL:HG11	2.02	0.41
1:B:350:TYR:HB2	1:B:353:SER:HB3	2.03	0.41
1:E:58:GLN:HG3	1:E:92:TRP:HH2	1.85	0.41
1:E:378:ASP:HA	1:E:379:SER:HA	1.73	0.41
1:F:21:MET:HE1	1:F:177:THR:OG1	2.21	0.41
1:D:489:ILE:HA	1:D:494:PRO:HG3	2.01	0.41
1:L:231:MET:HB3	1:L:235:TYR:OH	2.21	0.41
1:B:191:ILE:CB	1:B:198:GLU:HG2	2.51	0.40
1:E:217:ARG:NH1	1:D:214:GLU:OE1	2.49	0.40
1:C:296:LEU:HD12	1:C:296:LEU:C	2.46	0.40
1:D:61:TYR:OH	1:D:92:TRP:CD1	2.73	0.40
1:G:441:GLN:HE22	1:G:490:ILE:HA	1.86	0.40
4:H:602:ATP:H3'	1:I:458:MET:O	2.21	0.40
1:K:313:ILE:HA	1:K:345:LYS:O	2.21	0.40
1:I:37:PRO:HB2	1:I:203:ASN:HD21	1.86	0.40
1:F:61:TYR:CD2	1:F:65:ILE:HG13	2.56	0.40
1:C:284:ILE:HG23	1:C:436:THR:HB	2.03	0.40
1:D:63:GLY:HA3	1:D:141:ARG:NH1	2.37	0.40
1:G:330:SER:O	1:G:474:ASP:HA	2.21	0.40
1:K:75:THR:CG2	1:K:107:ASP:HA	2.51	0.40
1:K:465:LYS:O	1:J:449:MET:N	2.50	0.40
1:J:111:ASP:HA	1:J:112:PRO:HD3	1.97	0.40
1:J:267:VAL:HB	1:J:270:LEU:HB2	2.02	0.40
1:C:207:LEU:HD22	1:C:220:LEU:HB2	2.02	0.40
1:D:180:MET:HE3	1:D:180:MET:HB3	1.91	0.40
1:G:456:PHE:HZ	1:L:419:PHE:HB2	1.86	0.40
2:H:54:LEU:HD21	2:H:90:PHE:CE2	2.56	0.40
1:I:344:LEU:HD22	1:I:345:LYS:N	2.36	0.40
1:J:320:SER:O	1:J:324:LEU:N	2.54	0.40
1:A:294:LYS:HE2	1:A:294:LYS:HB2	1.67	0.40
1:B:346:ILE:HG22	1:B:348:CYS:SG	2.62	0.40
1:E:19:ALA:C	1:E:38:ILE:HG13	2.46	0.40
1:E:325:LEU:HD22	1:E:336:GLU:HG2	2.04	0.40
1:E:332:GLY:O	1:E:333:MET:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:TYR:HA	1:F:236:PRO:HD2	1.90	0.40
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.61	0.40
1:C:378:ASP:HA	1:C:379:SER:HA	1.66	0.40
1:G:31:ILE:HA	1:G:231:MET:HG3	2.03	0.40
2:H:109:SER:HA	2:H:110:PRO:HD3	1.93	0.40
1:K:70:PRO:HG2	1:K:138:ARG:O	2.22	0.40
1:K:80:PRO:CG	1:K:107:ASP:HB2	2.52	0.40
1:L:378:ASP:HA	1:L:379:SER:HA	1.75	0.40
1:A:299:SER:CB	1:A:333:MET:HE2	2.51	0.40
1:A:435:ASP:CA	1:A:459:ARG:HG2	2.51	0.40
1:B:64:ILE:HG12	1:B:69:GLU:O	2.22	0.40
1:B:301:PHE:O	1:B:301:PHE:CG	2.75	0.40
1:B:449:MET:HE2	1:C:490:ILE:CD1	2.50	0.40
1:F:308:ASN:ND2	1:F:308:ASN:N	2.70	0.40
1:D:45:SER:CB	1:D:182:THR:HB	2.51	0.40
1:G:288:GLY:C	1:G:294:LYS:HZ2	2.29	0.40
1:L:458:MET:HG3	1:L:463:HIS:HB3	2.03	0.40
1:I:84:ILE:HG23	1:I:94:LEU:HB2	2.04	0.40
1:I:316:ALA:O	1:I:348:CYS:HA	2.20	0.40
1:J:379:SER:HB3	1:J:413:THR:HG22	2.04	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	455/519 (88%)	409 (90%)	42 (9%)	4 (1%)	14	44
1	B	452/519 (87%)	401 (89%)	46 (10%)	5 (1%)	11	39
1	C	451/519 (87%)	399 (88%)	41 (9%)	11 (2%)	4	21
1	D	449/519 (86%)	392 (87%)	50 (11%)	7 (2%)	7	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	455/519 (88%)	411 (90%)	40 (9%)	4 (1%)	14	44
1	F	458/519 (88%)	404 (88%)	51 (11%)	3 (1%)	18	49
1	G	446/519 (86%)	372 (83%)	60 (14%)	14 (3%)	3	16
1	I	458/519 (88%)	410 (90%)	41 (9%)	7 (2%)	8	32
1	J	455/519 (88%)	410 (90%)	41 (9%)	4 (1%)	14	44
1	K	456/519 (88%)	413 (91%)	40 (9%)	3 (1%)	18	49
1	L	448/519 (86%)	393 (88%)	45 (10%)	10 (2%)	5	23
2	H	452/519 (87%)	411 (91%)	35 (8%)	6 (1%)	9	35
All	All	5435/6228 (87%)	4825 (89%)	532 (10%)	78 (1%)	9	33

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ALA
1	F	26	GLU
1	C	422	ALA
1	D	421	GLY
1	G	200	VAL
1	G	281	ASP
2	H	422	ALA
1	K	156	ALA
1	A	248	PRO
1	E	70	PRO
1	E	333	MET
1	C	76	PHE
1	C	93	ASP
1	C	123	LEU
1	C	289	ALA
1	D	26	GLU
1	D	47	THR
1	D	196	VAL
1	G	34	GLY
1	G	66	GLU
1	G	107	ASP
1	G	289	ALA
1	L	152	GLN
1	L	467	ILE
1	I	114	GLY
1	A	157	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	66	GLU
1	E	77	GLU
1	E	192	ALA
1	F	140	ARG
1	D	77	GLU
1	G	19	ALA
1	G	77	GLU
1	G	370	PHE
2	H	140	ARG
2	H	483	PHE
1	K	26	GLU
1	L	26	GLU
1	L	105	ILE
1	L	226	ARG
1	L	267	VAL
1	I	467	ILE
1	I	493	SER
1	J	422	ALA
1	A	26	GLU
1	B	140	ARG
1	B	196	VAL
1	C	213	GLY
1	D	459	ARG
1	G	319	GLU
2	H	213	GLY
2	H	485	ASN
1	K	16	GLN
1	L	132	TYR
1	I	289	ALA
1	J	334	ASP
1	C	96	LYS
1	C	98	VAL
1	C	148	THR
1	C	425	ILE
1	D	140	ARG
1	G	150	VAL
1	G	458	MET
2	H	263	VAL
1	L	137	TYR
1	G	280	LYS
1	I	196	VAL
1	J	47	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	80	PRO
1	G	110	PRO
1	L	398	GLY
1	I	112	PRO
1	B	65	ILE
1	I	433	ILE
1	C	147	VAL
1	L	268	VAL
1	J	467	ILE
1	B	276	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	297/443 (67%)	238 (80%)	59 (20%)	1	6
1	B	272/443 (61%)	215 (79%)	57 (21%)	1	5
1	C	282/443 (64%)	213 (76%)	69 (24%)	1	3
1	D	266/443 (60%)	202 (76%)	64 (24%)	1	3
1	E	290/443 (66%)	224 (77%)	66 (23%)	1	4
1	F	275/443 (62%)	222 (81%)	53 (19%)	1	7
1	G	213/443 (48%)	165 (78%)	48 (22%)	1	4
1	I	301/443 (68%)	236 (78%)	65 (22%)	1	5
1	J	307/443 (69%)	238 (78%)	69 (22%)	1	4
1	K	240/443 (54%)	186 (78%)	54 (22%)	1	4
1	L	239/443 (54%)	186 (78%)	53 (22%)	1	4
2	H	273/444 (62%)	218 (80%)	55 (20%)	1	6
All	All	3255/5317 (61%)	2543 (78%)	712 (22%)	1	5

All (712) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	24	MET
1	A	25	ILE
1	A	26	GLU
1	A	43	LEU
1	A	47	THR
1	A	52	LYS
1	A	68	ASP
1	A	77	GLU
1	A	79	THR
1	A	82	ASP
1	A	99	ASP
1	A	106	LEU
1	A	137	TYR
1	A	159	VAL
1	A	160	VAL
1	A	178	THR
1	A	187	GLU
1	A	198	GLU
1	A	209	ASN
1	A	214	GLU
1	A	215	ARG
1	A	223	LEU
1	A	225	LEU
1	A	232	LYS
1	A	238	THR
1	A	239	ILE
1	A	254	LEU
1	A	263	VAL
1	A	267	VAL
1	A	270	LEU
1	A	284	ILE
1	A	287	THR
1	A	292	THR
1	A	294	LYS
1	A	295	THR
1	A	300	ARG
1	A	333	MET
1	A	340	ARG
1	A	343	LEU
1	A	344	LEU
1	A	346	ILE
1	A	347	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	CYS
1	A	352	GLU
1	A	356	LEU
1	A	360	LEU
1	A	362	ILE
1	A	363	ILE
1	A	366	GLU
1	A	397	ILE
1	A	405	GLN
1	A	430	ILE
1	A	434	THR
1	A	441	GLN
1	A	449	MET
1	A	458	MET
1	A	467	ILE
1	A	495	THR
1	B	20	LYS
1	B	24	MET
1	B	25	ILE
1	B	26	GLU
1	B	48	SER
1	B	52	LYS
1	B	81	GLN
1	B	84	ILE
1	B	162	ARG
1	B	178	THR
1	B	181	THR
1	B	198	GLU
1	B	201	SER
1	B	203	ASN
1	B	211	LEU
1	B	212	GLU
1	B	215	ARG
1	B	221	GLU
1	B	223	LEU
1	B	228	THR
1	B	231	MET
1	B	246	ILE
1	B	258	SER
1	B	268	VAL
1	B	270	LEU
1	B	283	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	284	ILE
1	B	287	THR
1	B	292	THR
1	B	298	VAL
1	B	311	ARG
1	B	323	GLN
1	B	333	MET
1	B	348	CYS
1	B	352	GLU
1	B	356	LEU
1	B	358	ASP
1	B	362	ILE
1	B	369	ASP
1	B	374	ARG
1	B	380	LEU
1	B	381	SER
1	B	389	ASN
1	B	397	ILE
1	B	414	ASN
1	B	420	MET
1	B	433	ILE
1	B	438	ILE
1	B	457	LYS
1	B	458	MET
1	B	459	ARG
1	B	465	LYS
1	B	472	ILE
1	B	474	ASP
1	B	479	ILE
1	B	483	PHE
1	B	493	SER
1	E	20	LYS
1	E	24	MET
1	E	31	ILE
1	E	38	ILE
1	E	47	THR
1	E	52	LYS
1	E	56	SER
1	E	81	GLN
1	E	83	ILE
1	E	106	LEU
1	E	141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	142	VAL
1	E	143	SER
1	E	145	ASP
1	E	159	VAL
1	E	177	THR
1	E	180	MET
1	E	184	ARG
1	E	186	GLU
1	E	198	GLU
1	E	201	SER
1	E	218	ARG
1	E	222	ILE
1	E	224	LYS
1	E	238	THR
1	E	244	ILE
1	E	269	ARG
1	E	270	LEU
1	E	273	MET
1	E	281	ASP
1	E	287	THR
1	E	294	LYS
1	E	300	ARG
1	E	302	VAL
1	E	311	ARG
1	E	314	LEU
1	E	319	GLU
1	E	330	SER
1	E	333	MET
1	E	338	MET
1	E	339	GLU
1	E	344	LEU
1	E	352	GLU
1	E	356	LEU
1	E	357	GLU
1	E	362	ILE
1	E	366	GLU
1	E	374	ARG
1	E	397	ILE
1	E	405	GLN
1	E	418	GLN
1	E	425	ILE
1	E	428	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	432	THR
1	E	444	GLU
1	E	449	MET
1	E	453	ILE
1	E	458	MET
1	E	469	GLU
1	E	472	ILE
1	E	474	ASP
1	E	481	ASP
1	E	485	ASN
1	E	488	ARG
1	E	489	ILE
1	E	495	THR
1	F	20	LYS
1	F	24	MET
1	F	38	ILE
1	F	47	THR
1	F	54	LEU
1	F	60	LEU
1	F	65	ILE
1	F	69	GLU
1	F	79	THR
1	F	173	GLN
1	F	180	MET
1	F	182	THR
1	F	187	GLU
1	F	198	GLU
1	F	203	ASN
1	F	208	ARG
1	F	212	GLU
1	F	215	ARG
1	F	218	ARG
1	F	221	GLU
1	F	223	LEU
1	F	240	THR
1	F	245	ASN
1	F	270	LEU
1	F	281	ASP
1	F	292	THR
1	F	294	LYS
1	F	308	ASN
1	F	313	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	314	LEU
1	F	323	GLN
1	F	324	LEU
1	F	333	MET
1	F	352	GLU
1	F	356	LEU
1	F	358	ASP
1	F	360	LEU
1	F	363	ILE
1	F	380	LEU
1	F	406	GLU
1	F	418	GLN
1	F	419	PHE
1	F	420	MET
1	F	428	SER
1	F	430	ILE
1	F	432	THR
1	F	438	ILE
1	F	449	MET
1	F	451	ARG
1	F	458	MET
1	F	472	ILE
1	F	474	ASP
1	F	480	LYS
1	C	24	MET
1	C	36	LEU
1	C	38	ILE
1	C	69	GLU
1	C	89	SER
1	C	128	GLU
1	C	143	SER
1	C	148	THR
1	C	150	VAL
1	C	159	VAL
1	C	177	THR
1	C	179	VAL
1	C	182	THR
1	C	183	GLU
1	C	203	ASN
1	C	211	LEU
1	C	220	LEU
1	C	222	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	223	LEU
1	C	225	LEU
1	C	231	MET
1	C	232	LYS
1	C	238	THR
1	C	246	ILE
1	C	256	GLN
1	C	261	VAL
1	C	268	VAL
1	C	269	ARG
1	C	270	LEU
1	C	281	ASP
1	C	290	THR
1	C	292	THR
1	C	294	LYS
1	C	311	ARG
1	C	313	ILE
1	C	319	GLU
1	C	325	LEU
1	C	333	MET
1	C	338	MET
1	C	340	ARG
1	C	344	LEU
1	C	347	VAL
1	C	352	GLU
1	C	366	GLU
1	C	367	ILE
1	C	397	ILE
1	C	406	GLU
1	C	407	GLU
1	C	413	THR
1	C	414	ASN
1	C	418	GLN
1	C	426	THR
1	C	433	ILE
1	C	441	GLN
1	C	449	MET
1	C	451	ARG
1	C	453	ILE
1	C	457	LYS
1	C	458	MET
1	C	465	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	469	GLU
1	C	472	ILE
1	C	474	ASP
1	C	479	ILE
1	C	480	LYS
1	C	487	GLU
1	C	490	ILE
1	C	493	SER
1	C	497	ILE
1	D	21	MET
1	D	24	MET
1	D	40	ARG
1	D	47	THR
1	D	48	SER
1	D	50	THR
1	D	56	SER
1	D	72	VAL
1	D	75	THR
1	D	79	THR
1	D	85	LYS
1	D	88	ARG
1	D	103	LEU
1	D	143	SER
1	D	178	THR
1	D	193	ARG
1	D	201	SER
1	D	202	ASP
1	D	210	VAL
1	D	212	GLU
1	D	215	ARG
1	D	219	THR
1	D	222	ILE
1	D	223	LEU
1	D	232	LYS
1	D	234	GLU
1	D	245	ASN
1	D	261	VAL
1	D	269	ARG
1	D	270	LEU
1	D	284	ILE
1	D	287	THR
1	D	292	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	294	LYS
1	D	303	GLU
1	D	324	LEU
1	D	333	MET
1	D	338	MET
1	D	356	LEU
1	D	360	LEU
1	D	362	ILE
1	D	366	GLU
1	D	374	ARG
1	D	397	ILE
1	D	406	GLU
1	D	411	LEU
1	D	414	ASN
1	D	428	SER
1	D	430	ILE
1	D	432	THR
1	D	440	LEU
1	D	441	GLN
1	D	443	VAL
1	D	444	GLU
1	D	451	ARG
1	D	454	ASN
1	D	458	MET
1	D	465	LYS
1	D	468	ARG
1	D	469	GLU
1	D	471	MET
1	D	483	PHE
1	D	488	ARG
1	D	490	ILE
1	G	20	LYS
1	G	24	MET
1	G	30	ASP
1	G	41	SER
1	G	47	THR
1	G	48	SER
1	G	50	THR
1	G	56	SER
1	G	57	ILE
1	G	72	VAL
1	G	76	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	78	GLU
1	G	83	ILE
1	G	142	VAL
1	G	181	THR
1	G	184	ARG
1	G	203	ASN
1	G	208	ARG
1	G	218	ARG
1	G	228	THR
1	G	231	MET
1	G	232	LYS
1	G	246	ILE
1	G	287	THR
1	G	292	THR
1	G	298	VAL
1	G	333	MET
1	G	348	CYS
1	G	352	GLU
1	G	356	LEU
1	G	360	LEU
1	G	380	LEU
1	G	393	ARG
1	G	406	GLU
1	G	411	LEU
1	G	413	THR
1	G	415	THR
1	G	432	THR
1	G	441	GLN
1	G	444	GLU
1	G	454	ASN
1	G	457	LYS
1	G	458	MET
1	G	465	LYS
1	G	469	GLU
1	G	474	ASP
1	G	488	ARG
1	G	490	ILE
2	H	24	MET
2	H	38	ILE
2	H	47	THR
2	H	54	LEU
2	H	79	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	83	ILE
2	H	98	VAL
2	H	100	GLU
2	H	103	LEU
2	H	152	GLN
2	H	179	VAL
2	H	180	MET
2	H	187	GLU
2	H	203	ASN
2	H	222	ILE
2	H	223	LEU
2	H	226	ARG
2	H	228	THR
2	H	234	GLU
2	H	239	ILE
2	H	263	VAL
2	H	272	GLU
2	H	273	MET
2	H	281	ASP
2	H	292	THR
2	H	294	LYS
2	H	296	LEU
2	H	300	ARG
2	H	311	ARG
2	H	333	MET
2	H	337	GLU
2	H	344	LEU
2	H	346	ILE
2	H	352	GLU
2	H	356	LEU
2	H	360	LEU
2	H	370	PHE
2	H	377	ILE
2	H	390	ASN
2	H	397	ILE
2	H	414	ASN
2	H	416	SER
2	H	420	MET
2	H	425	ILE
2	H	428	SER
2	H	431	SER
2	H	433	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	450	SER
2	H	454	ASN
2	H	457	LYS
2	H	464	ASP
2	H	474	ASP
2	H	479	ILE
2	H	489	ILE
2	H	495	THR
1	K	21	MET
1	K	43	LEU
1	K	47	THR
1	K	56	SER
1	K	69	GLU
1	K	77	GLU
1	K	79	THR
1	K	89	SER
1	K	145	ASP
1	K	148	THR
1	K	163	GLU
1	K	178	THR
1	K	186	GLU
1	K	208	ARG
1	K	223	LEU
1	K	232	LYS
1	K	246	ILE
1	K	258	SER
1	K	260	ASN
1	K	263	VAL
1	K	268	VAL
1	K	269	ARG
1	K	270	LEU
1	K	287	THR
1	K	292	THR
1	K	300	ARG
1	K	319	GLU
1	K	333	MET
1	K	346	ILE
1	K	352	GLU
1	K	360	LEU
1	K	366	GLU
1	K	371	LYS
1	K	389	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	397	ILE
1	K	399	VAL
1	K	404	LYS
1	K	406	GLU
1	K	420	MET
1	K	425	ILE
1	K	430	ILE
1	K	432	THR
1	K	433	ILE
1	K	438	ILE
1	K	454	ASN
1	K	455	VAL
1	K	457	LYS
1	K	458	MET
1	K	465	LYS
1	K	469	GLU
1	K	474	ASP
1	K	479	ILE
1	K	480	LYS
1	K	495	THR
1	L	47	THR
1	L	54	LEU
1	L	69	GLU
1	L	79	THR
1	L	97	LEU
1	L	129	ARG
1	L	153	GLN
1	L	182	THR
1	L	186	GLU
1	L	203	ASN
1	L	209	ASN
1	L	218	ARG
1	L	222	ILE
1	L	223	LEU
1	L	226	ARG
1	L	241	ASP
1	L	260	ASN
1	L	271	ASP
1	L	284	ILE
1	L	285	LEU
1	L	287	THR
1	L	292	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	295	THR
1	L	296	LEU
1	L	300	ARG
1	L	303	GLU
1	L	319	GLU
1	L	333	MET
1	L	344	LEU
1	L	356	LEU
1	L	357	GLU
1	L	360	LEU
1	L	366	GLU
1	L	380	LEU
1	L	389	ASN
1	L	406	GLU
1	L	411	LEU
1	L	412	PHE
1	L	414	ASN
1	L	428	SER
1	L	432	THR
1	L	438	ILE
1	L	441	GLN
1	L	449	MET
1	L	450	SER
1	L	453	ILE
1	L	454	ASN
1	L	458	MET
1	L	465	LYS
1	L	469	GLU
1	L	470	PHE
1	L	493	SER
1	L	495	THR
1	I	21	MET
1	I	24	MET
1	I	30	ASP
1	I	47	THR
1	I	50	THR
1	I	52	LYS
1	I	54	LEU
1	I	79	THR
1	I	85	LYS
1	I	89	SER
1	I	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	129	ARG
1	I	166	ARG
1	I	177	THR
1	I	180	MET
1	I	182	THR
1	I	183	GLU
1	I	186	GLU
1	I	198	GLU
1	I	209	ASN
1	I	215	ARG
1	I	223	LEU
1	I	224	LYS
1	I	232	LYS
1	I	238	THR
1	I	245	ASN
1	I	246	ILE
1	I	284	ILE
1	I	294	LYS
1	I	296	LEU
1	I	310	GLU
1	I	311	ARG
1	I	313	ILE
1	I	319	GLU
1	I	321	ARG
1	I	325	LEU
1	I	333	MET
1	I	344	LEU
1	I	345	LYS
1	I	357	GLU
1	I	360	LEU
1	I	366	GLU
1	I	375	ILE
1	I	377	ILE
1	I	393	ARG
1	I	406	GLU
1	I	420	MET
1	I	426	THR
1	I	428	SER
1	I	430	ILE
1	I	432	THR
1	I	444	GLU
1	I	445	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	448	GLU
1	I	454	ASN
1	I	458	MET
1	I	459	ARG
1	I	465	LYS
1	I	467	ILE
1	I	471	MET
1	I	474	ASP
1	I	488	ARG
1	I	493	SER
1	I	495	THR
1	I	497	ILE
1	J	21	MET
1	J	22	ARG
1	J	24	MET
1	J	26	GLU
1	J	47	THR
1	J	48	SER
1	J	50	THR
1	J	52	LYS
1	J	81	GLN
1	J	89	SER
1	J	103	LEU
1	J	129	ARG
1	J	143	SER
1	J	144	ILE
1	J	159	VAL
1	J	163	GLU
1	J	167	LEU
1	J	171	LEU
1	J	172	LYS
1	J	180	MET
1	J	198	GLU
1	J	200	VAL
1	J	202	ASP
1	J	210	VAL
1	J	211	LEU
1	J	212	GLU
1	J	218	ARG
1	J	222	ILE
1	J	223	LEU
1	J	224	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	226	ARG
1	J	238	THR
1	J	239	ILE
1	J	245	ASN
1	J	270	LEU
1	J	287	THR
1	J	292	THR
1	J	294	LYS
1	J	302	VAL
1	J	319	GLU
1	J	324	LEU
1	J	338	MET
1	J	344	LEU
1	J	345	LYS
1	J	356	LEU
1	J	360	LEU
1	J	363	ILE
1	J	367	ILE
1	J	377	ILE
1	J	393	ARG
1	J	405	GLN
1	J	407	GLU
1	J	419	PHE
1	J	420	MET
1	J	425	ILE
1	J	427	ASP
1	J	444	GLU
1	J	448	GLU
1	J	454	ASN
1	J	458	MET
1	J	459	ARG
1	J	461	SER
1	J	465	LYS
1	J	471	MET
1	J	488	ARG
1	J	489	ILE
1	J	490	ILE
1	J	493	SER
1	J	495	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	209	ASN
1	A	230	HIS
1	A	327	ASN
1	A	368	ASN
1	A	414	ASN
1	A	418	GLN
1	B	33	HIS
1	B	203	ASN
1	B	209	ASN
1	B	260	ASN
1	B	304	ASN
1	B	308	ASN
1	B	323	GLN
1	B	341	GLN
1	B	389	ASN
1	B	414	ASN
1	E	81	GLN
1	E	203	ASN
1	E	260	ASN
1	E	359	HIS
1	E	389	ASN
1	E	405	GLN
1	E	414	ASN
1	E	418	GLN
1	E	423	HIS
1	F	173	GLN
1	F	203	ASN
1	F	209	ASN
1	F	308	ASN
1	F	323	GLN
1	F	414	ASN
1	F	418	GLN
1	F	429	HIS
1	C	260	ASN
1	C	304	ASN
1	C	323	GLN
1	C	361	GLN
1	C	389	ASN
1	C	414	ASN
1	C	418	GLN
1	D	209	ASN
1	D	323	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	389	ASN
1	D	394	GLN
1	D	414	ASN
1	D	418	GLN
1	D	441	GLN
1	G	341	GLN
1	G	441	GLN
2	H	152	GLN
2	H	209	ASN
2	H	245	ASN
2	H	389	ASN
2	H	414	ASN
2	H	429	HIS
2	H	454	ASN
1	K	260	ASN
1	K	308	ASN
1	K	389	ASN
1	K	414	ASN
1	K	418	GLN
1	L	33	HIS
1	L	203	ASN
1	L	323	GLN
1	L	359	HIS
1	L	414	ASN
1	L	418	GLN
1	L	441	GLN
1	L	454	ASN
1	I	203	ASN
1	I	209	ASN
1	I	342	ASN
1	I	414	ASN
1	I	418	GLN
1	I	429	HIS
1	I	454	ASN
1	J	209	ASN
1	J	308	ASN
1	J	389	ASN
1	J	390	ASN
1	J	414	ASN
1	J	441	GLN
1	J	454	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	B	431	1	8,9,10	0.59	0	7,12,14	0.60	0
1	SEP	J	431	1	8,9,10	0.56	0	7,12,14	0.79	0
1	SEP	C	431	1	8,9,10	0.61	0	7,12,14	0.66	0
1	SEP	L	431	1	8,9,10	0.62	0	7,12,14	0.74	0
1	SEP	G	431	1	8,9,10	0.72	0	7,12,14	0.79	0
1	SEP	K	431	1	8,9,10	0.63	0	7,12,14	0.64	0
1	SEP	I	431	1	8,9,10	0.60	0	7,12,14	0.62	0
1	SEP	F	431	1	8,9,10	0.60	0	7,12,14	0.65	0
1	SEP	A	431	1	8,9,10	0.61	0	7,12,14	0.71	0
1	SEP	E	431	1	8,9,10	0.64	0	7,12,14	0.71	0
1	SEP	D	431	1	8,9,10	0.60	0	7,12,14	0.79	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
1	SEP	B	431	1	-	2/6/8/10	-
1	SEP	J	431	1	-	3/6/8/10	-
1	SEP	C	431	1	-	3/6/8/10	-
1	SEP	L	431	1	-	1/6/8/10	-
1	SEP	G	431	1	-	2/6/8/10	-
1	SEP	K	431	1	-	2/6/8/10	-
1	SEP	I	431	1	-	5/6/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	F	431	1	-	2/6/8/10	-
1	SEP	A	431	1	-	2/6/8/10	-
1	SEP	E	431	1	-	2/6/8/10	-
1	SEP	D	431	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	431	SEP	N-CA-CB-OG
1	B	431	SEP	N-CA-CB-OG
1	B	431	SEP	C-CA-CB-OG
1	F	431	SEP	N-CA-CB-OG
1	F	431	SEP	C-CA-CB-OG
1	C	431	SEP	N-CA-CB-OG
1	D	431	SEP	N-CA-CB-OG
1	G	431	SEP	N-CA-CB-OG
1	K	431	SEP	N-CA-CB-OG
1	K	431	SEP	C-CA-CB-OG
1	L	431	SEP	N-CA-CB-OG
1	I	431	SEP	N-CA-CB-OG
1	I	431	SEP	C-CA-CB-OG
1	I	431	SEP	CB-OG-P-O1P
1	I	431	SEP	CB-OG-P-O2P
1	J	431	SEP	N-CA-CB-OG
1	J	431	SEP	C-CA-CB-OG
1	C	431	SEP	CB-OG-P-O1P
1	E	431	SEP	CA-CB-OG-P
1	J	431	SEP	CA-CB-OG-P
1	E	431	SEP	N-CA-CB-OG
1	C	431	SEP	CB-OG-P-O2P
1	I	431	SEP	CB-OG-P-O3P
1	G	431	SEP	CA-CB-OG-P
1	A	431	SEP	C-CA-CB-OG

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	431	SEP	2	0
1	K	431	SEP	4	0
1	I	431	SEP	1	0
1	A	431	SEP	1	0
1	E	431	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	$\# Z > 2$
4	ATP	J	701	5	32,33,33	0.57	0	48,52,52	0.55	0
3	ADP	K	601	-	28,29,29	0.52	0	43,45,45	0.52	0
4	ATP	F	602	5	32,33,33	0.52	0	48,52,52	0.57	0
4	ATP	L	602	-	32,33,33	0.49	0	48,52,52	0.62	0
3	ADP	D	601	-	28,29,29	0.50	0	43,45,45	0.51	0
3	ADP	I	602	-	28,29,29	0.37	0	43,45,45	0.57	0
3	ADP	C	601	-	28,29,29	0.49	0	43,45,45	0.42	0
3	ADP	G	601	-	28,29,29	0.48	0	43,45,45	0.52	0
3	ADP	I	601	-	28,29,29	0.47	0	43,45,45	0.51	0
4	ATP	B	701	5	32,33,33	0.55	0	48,52,52	0.71	1 (2%)
3	ADP	F	601	-	28,29,29	0.47	0	43,45,45	0.47	0
4	ATP	K	602	5	32,33,33	0.54	0	48,52,52	0.56	0
3	ADP	D	602	-	28,29,29	0.45	0	43,45,45	0.50	0
4	ATP	G	602	5	32,33,33	0.53	0	48,52,52	0.56	0
4	ATP	E	601	5	32,33,33	0.52	0	48,52,52	0.61	0
4	ATP	A	602	5	32,33,33	0.48	0	48,52,52	0.66	0
4	ATP	H	602	5	32,33,33	0.50	0	48,52,52	0.58	0
4	ATP	C	602	5	32,33,33	0.50	0	48,52,52	0.56	0
3	ADP	L	601	-	28,29,29	0.42	0	43,45,45	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	B	702	-	32,33,33	0.51	0	48,52,52	0.64	0
4	ATP	E	602	5	32,33,33	0.53	0	48,52,52	0.61	0
3	ADP	A	601	-	28,29,29	0.41	0	43,45,45	0.50	0
4	ATP	J	702	-	32,33,33	0.55	0	48,52,52	0.54	0
3	ADP	H	601	-	28,29,29	0.47	0	43,45,45	0.49	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
4	ATP	J	701	5	-	7/22/38/38	0/3/3/3
3	ADP	K	601	-	-	5/16/32/32	0/3/3/3
4	ATP	F	602	5	-	6/22/38/38	0/3/3/3
4	ATP	L	602	-	-	0/22/38/38	0/3/3/3
3	ADP	D	601	-	-	8/16/32/32	0/3/3/3
3	ADP	I	602	-	-	2/16/32/32	0/3/3/3
3	ADP	C	601	-	-	3/16/32/32	0/3/3/3
3	ADP	G	601	-	-	4/16/32/32	0/3/3/3
3	ADP	I	601	-	-	6/16/32/32	0/3/3/3
4	ATP	B	701	5	-	4/22/38/38	0/3/3/3
3	ADP	F	601	-	-	6/16/32/32	0/3/3/3
4	ATP	K	602	5	-	1/22/38/38	0/3/3/3
3	ADP	D	602	-	-	2/16/32/32	0/3/3/3
4	ATP	G	602	5	-	6/22/38/38	0/3/3/3
4	ATP	E	601	5	-	7/22/38/38	0/3/3/3
4	ATP	A	602	5	-	3/22/38/38	0/3/3/3
4	ATP	H	602	5	-	5/22/38/38	0/3/3/3
4	ATP	C	602	5	-	6/22/38/38	0/3/3/3
3	ADP	L	601	-	-	4/16/32/32	0/3/3/3
4	ATP	B	702	-	-	5/22/38/38	0/3/3/3
4	ATP	E	602	5	-	5/22/38/38	0/3/3/3
3	ADP	A	601	-	-	5/16/32/32	0/3/3/3
4	ATP	J	702	-	-	5/22/38/38	0/3/3/3
3	ADP	H	601	-	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	ATP	C3'-C2'-C1'	2.03	105.30	101.46

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O2A
3	A	601	ADP	C5'-O5'-PA-O3A
3	F	601	ADP	C5'-O5'-PA-O1A
3	F	601	ADP	C5'-O5'-PA-O2A
3	F	601	ADP	C5'-O5'-PA-O3A
3	C	601	ADP	C5'-O5'-PA-O1A
3	C	601	ADP	C5'-O5'-PA-O2A
3	C	601	ADP	C5'-O5'-PA-O3A
3	D	601	ADP	PA-O3A-PB-O3B
3	D	601	ADP	C5'-O5'-PA-O1A
3	D	601	ADP	C5'-O5'-PA-O3A
3	G	601	ADP	C5'-O5'-PA-O1A
3	G	601	ADP	C5'-O5'-PA-O2A
3	G	601	ADP	C5'-O5'-PA-O3A
3	H	601	ADP	C5'-O5'-PA-O1A
3	H	601	ADP	C5'-O5'-PA-O2A
3	H	601	ADP	C5'-O5'-PA-O3A
3	K	601	ADP	C5'-O5'-PA-O2A
3	I	601	ADP	C5'-O5'-PA-O3A
3	I	602	ADP	PA-O3A-PB-O3B
4	B	701	ATP	PB-O3B-PG-O2G
4	B	702	ATP	C5'-O5'-PA-O1A
4	E	601	ATP	C5'-O5'-PA-O1A
4	E	601	ATP	C5'-O5'-PA-O2A
4	E	601	ATP	C5'-O5'-PA-O3A
4	F	602	ATP	C5'-O5'-PA-O1A
4	F	602	ATP	C5'-O5'-PA-O3A
4	C	602	ATP	PB-O3B-PG-O3G
4	G	602	ATP	PB-O3B-PG-O3G
4	G	602	ATP	C5'-O5'-PA-O3A
4	H	602	ATP	C4'-C5'-O5'-PA
4	J	701	ATP	PB-O3B-PG-O2G
4	J	702	ATP	C5'-O5'-PA-O2A
4	J	702	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	601	ADP	O4'-C4'-C5'-O5'
4	F	602	ATP	O4'-C4'-C5'-O5'
3	D	601	ADP	C3'-C4'-C5'-O5'
3	L	601	ADP	O4'-C4'-C5'-O5'
3	L	601	ADP	C3'-C4'-C5'-O5'
4	F	602	ATP	C3'-C4'-C5'-O5'
3	I	601	ADP	O4'-C4'-C5'-O5'
4	B	702	ATP	O4'-C4'-C5'-O5'
4	B	702	ATP	C3'-C4'-C5'-O5'
3	F	601	ADP	C3'-C4'-C5'-O5'
3	K	601	ADP	C3'-C4'-C5'-O5'
3	I	601	ADP	C3'-C4'-C5'-O5'
4	H	602	ATP	C3'-C4'-C5'-O5'
4	J	702	ATP	O4'-C4'-C5'-O5'
4	J	702	ATP	C3'-C4'-C5'-O5'
3	D	602	ADP	C3'-C4'-C5'-O5'
4	H	602	ATP	O4'-C4'-C5'-O5'
3	D	601	ADP	O4'-C4'-C5'-O5'
4	G	602	ATP	O4'-C4'-C5'-O5'
3	I	602	ADP	PA-O3A-PB-O1B
3	D	601	ADP	PA-O3A-PB-O2B
4	E	602	ATP	PB-O3B-PG-O2G
3	A	601	ADP	PB-O3A-PA-O2A
3	F	601	ADP	PB-O3A-PA-O2A
3	L	601	ADP	PB-O3A-PA-O2A
4	F	602	ATP	PB-O3A-PA-O1A
4	C	602	ATP	PA-O3A-PB-O1B
3	D	602	ADP	O4'-C4'-C5'-O5'
3	D	601	ADP	C5'-O5'-PA-O2A
3	K	601	ADP	C5'-O5'-PA-O1A
3	K	601	ADP	C5'-O5'-PA-O3A
3	I	601	ADP	C5'-O5'-PA-O1A
4	G	602	ATP	C5'-O5'-PA-O1A
4	E	601	ATP	O4'-C4'-C5'-O5'
4	G	602	ATP	C3'-C4'-C5'-O5'
3	I	601	ADP	PB-O3A-PA-O1A
4	J	702	ATP	PB-O3A-PA-O2A
3	G	601	ADP	C3'-C4'-C5'-O5'
4	C	602	ATP	PB-O3B-PG-O1G
4	E	601	ATP	C3'-C4'-C5'-O5'
3	F	601	ADP	PB-O3A-PA-O1A
4	B	701	ATP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	602	ATP	PG-O3B-PB-O2B
4	J	701	ATP	PG-O3B-PB-O1B
4	J	701	ATP	PG-O3B-PB-O2B
4	E	601	ATP	C4'-C5'-O5'-PA
3	D	601	ADP	PA-O3A-PB-O1B
4	B	701	ATP	PB-O3B-PG-O1G
4	J	701	ATP	PB-O3B-PG-O1G
4	E	602	ATP	PB-O3B-PG-O3G
4	C	602	ATP	PB-O3B-PG-O2G
4	H	602	ATP	PB-O3B-PG-O3G
4	J	701	ATP	PB-O3B-PG-O3G
3	L	601	ADP	PB-O3A-PA-O1A
3	I	601	ADP	PB-O3A-PA-O2A
4	A	602	ATP	PA-O3A-PB-O1B
4	B	702	ATP	PB-O3A-PA-O1A
4	E	602	ATP	PA-O3A-PB-O1B
4	F	602	ATP	PB-O3A-PA-O2A
4	K	602	ATP	PB-O3A-PA-O1A
4	J	701	ATP	PB-O3A-PA-O1A
4	J	701	ATP	PB-O3A-PA-O2A
4	H	602	ATP	PB-O3B-PG-O1G
3	A	601	ADP	PB-O3A-PA-O1A
4	A	602	ATP	PG-O3B-PB-O2B
4	A	602	ATP	PA-O3A-PB-O2B
4	B	701	ATP	PB-O3A-PA-O1A
4	B	702	ATP	PB-O3A-PA-O2A
4	E	601	ATP	PG-O3B-PB-O2B
4	E	602	ATP	PG-O3B-PB-O1B
4	C	602	ATP	PG-O3B-PB-O2B
4	C	602	ATP	PA-O3A-PB-O2B
4	G	602	ATP	PA-O3A-PB-O2B

There are no ring outliers.

21 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	701	ATP	2	0
3	K	601	ADP	3	0
4	F	602	ATP	2	0
4	L	602	ATP	4	0
3	D	601	ADP	1	0
3	I	602	ADP	2	0

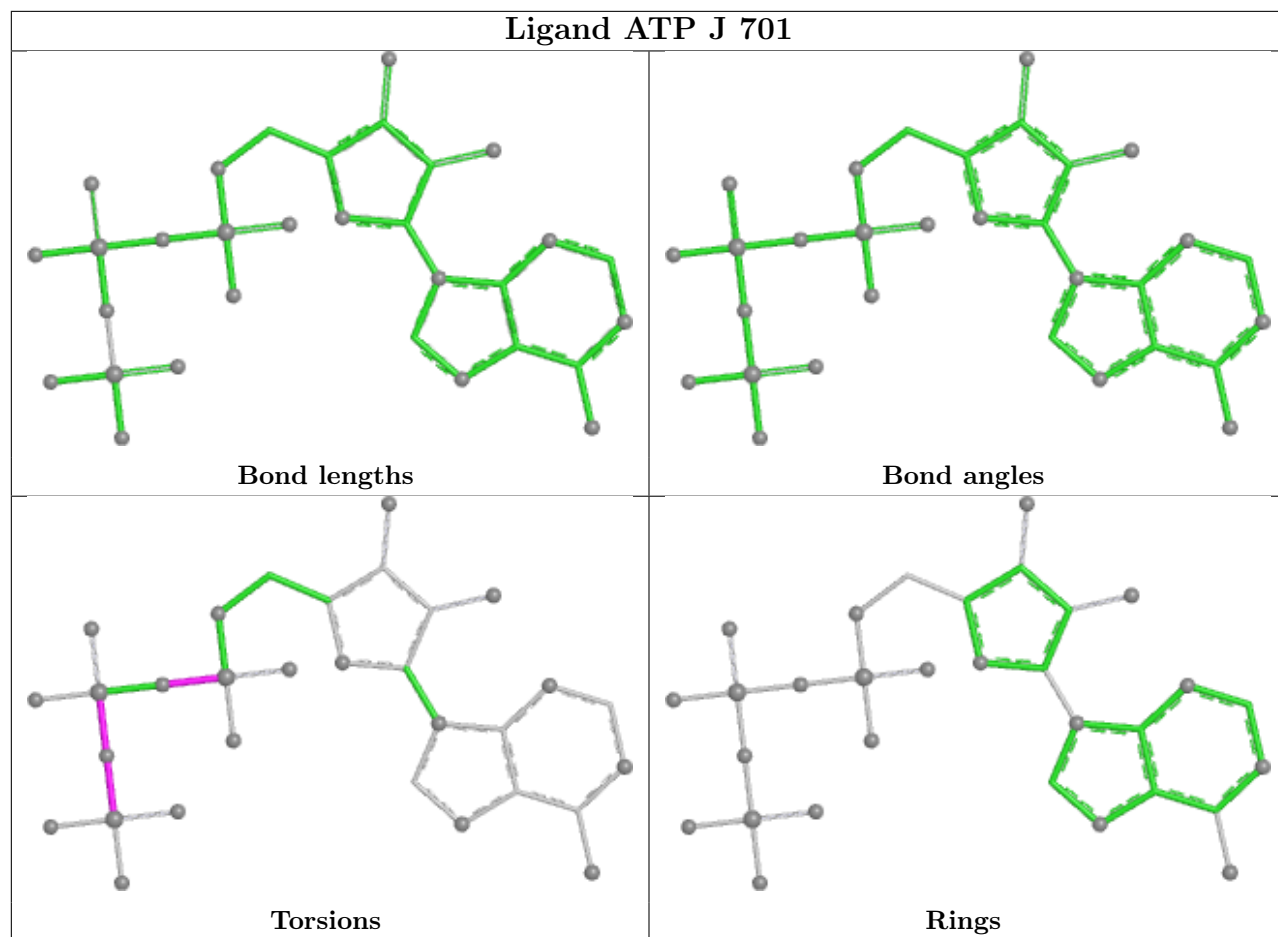
Continued on next page...

Continued from previous page...

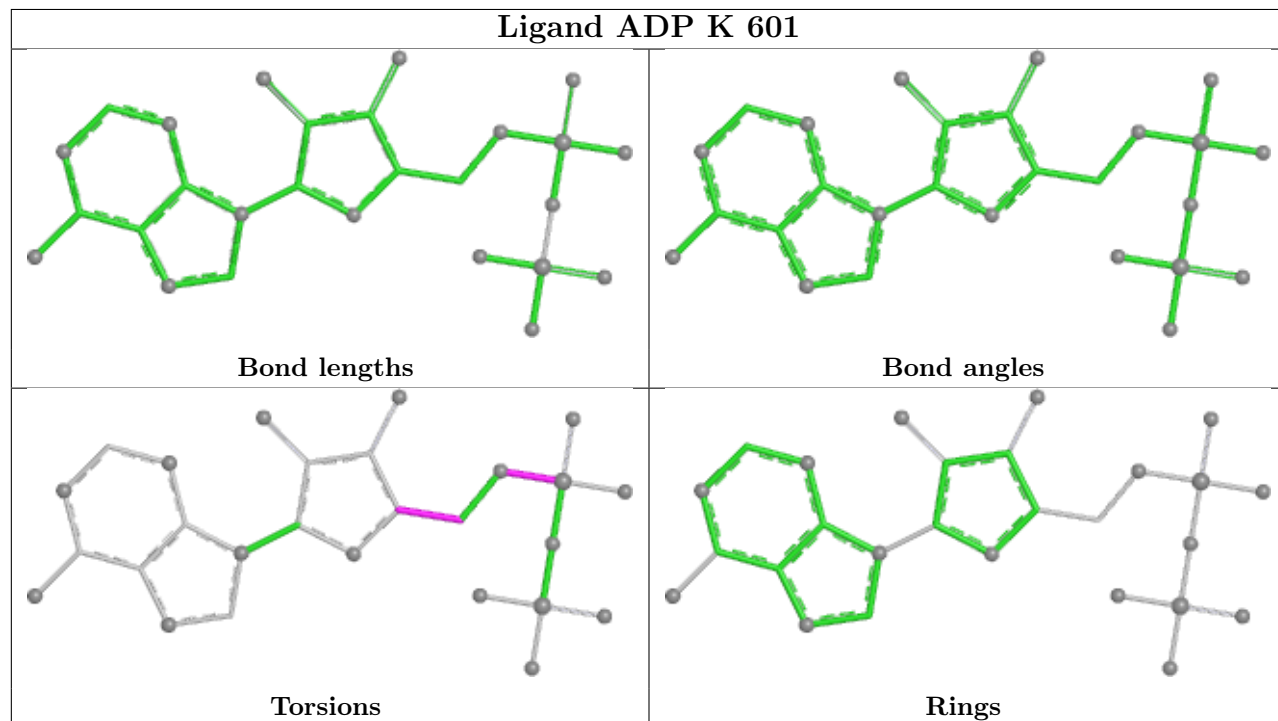
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	ADP	3	0
3	I	601	ADP	1	0
4	B	701	ATP	1	0
3	F	601	ADP	3	0
3	D	602	ADP	1	0
4	G	602	ATP	1	0
4	E	601	ATP	3	0
4	A	602	ATP	3	0
4	H	602	ATP	2	0
4	C	602	ATP	2	0
3	L	601	ADP	3	0
4	B	702	ATP	1	0
3	A	601	ADP	3	0
4	J	702	ATP	4	0
3	H	601	ADP	3	0

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.

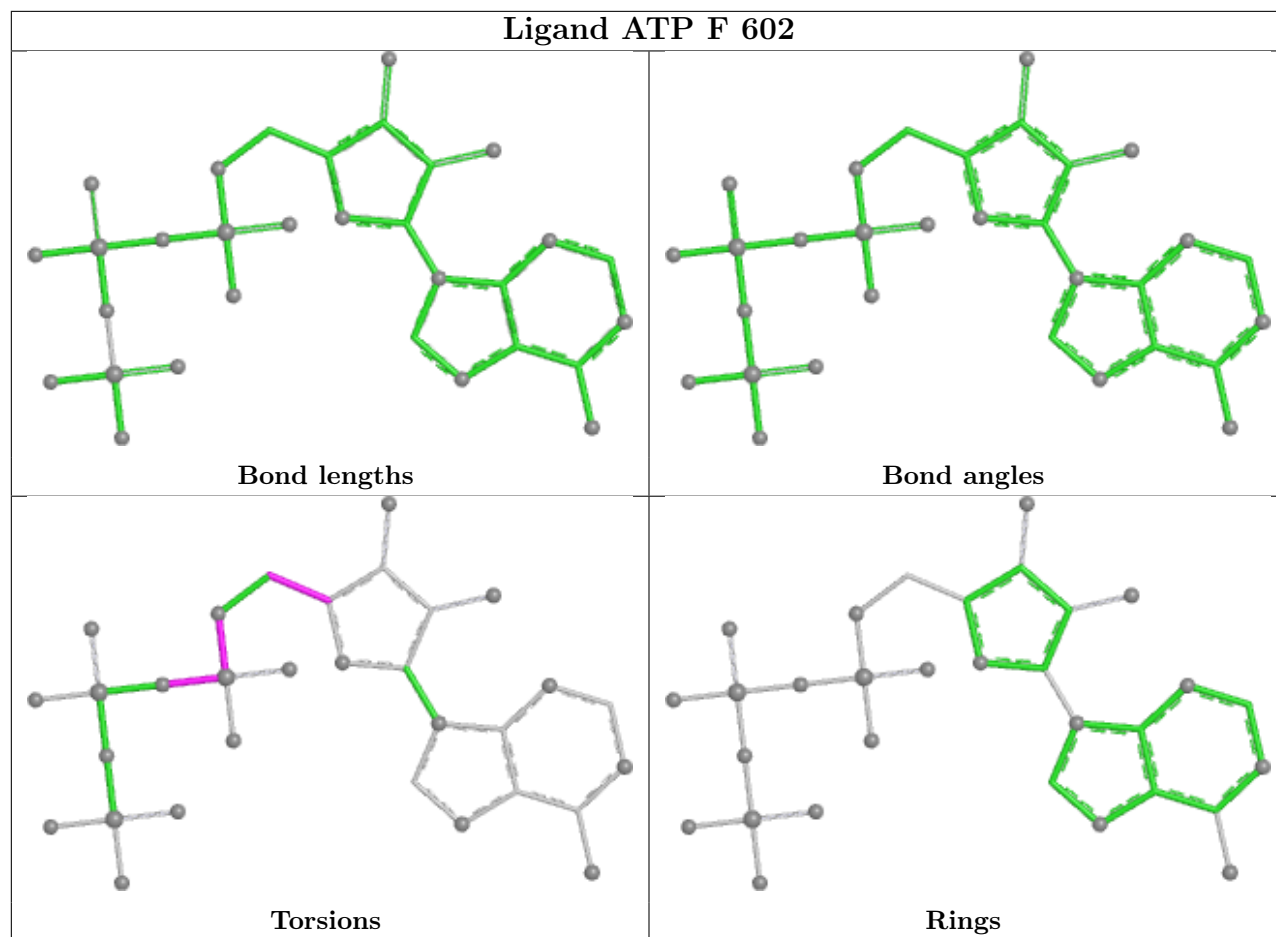
Ligand ATP J 701



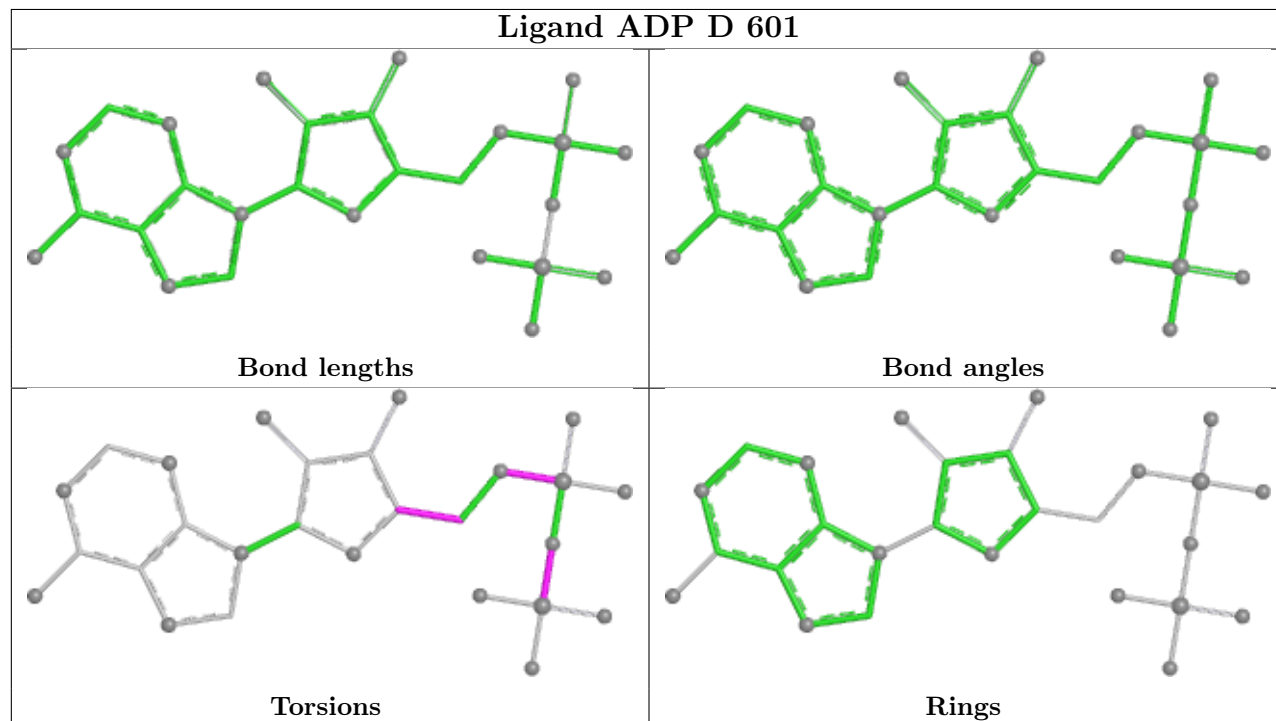
Ligand ADP K 601



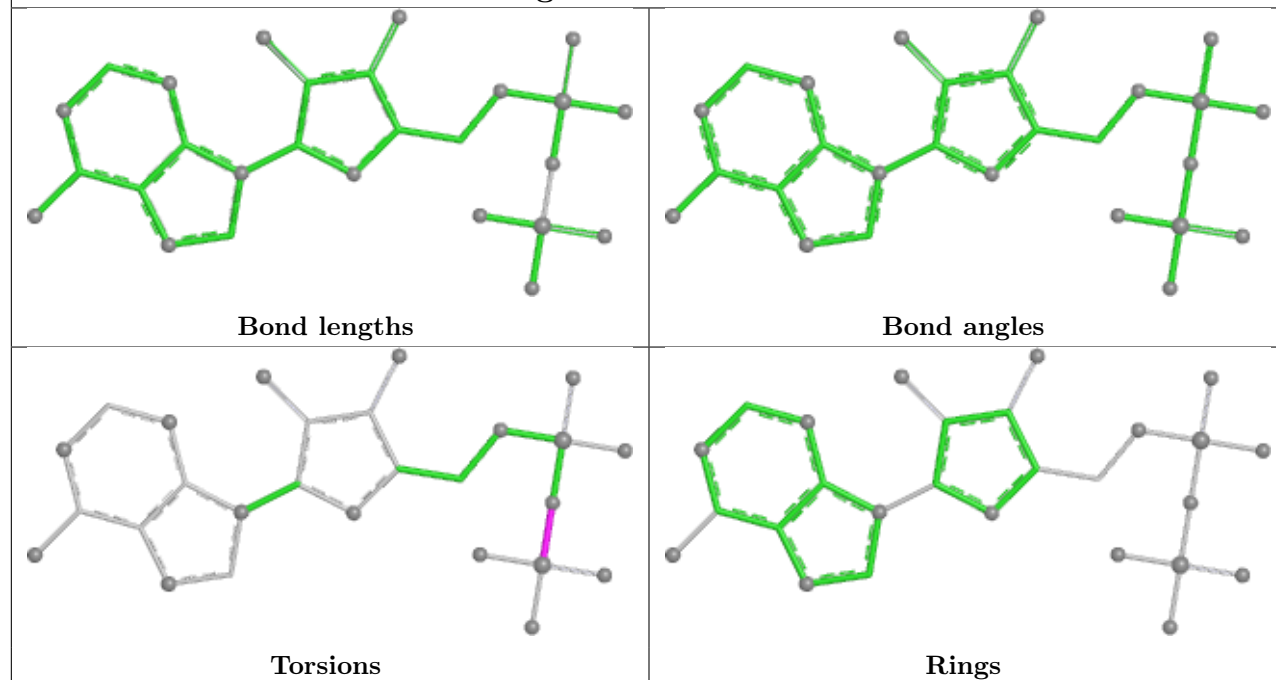
Ligand ATP F 602



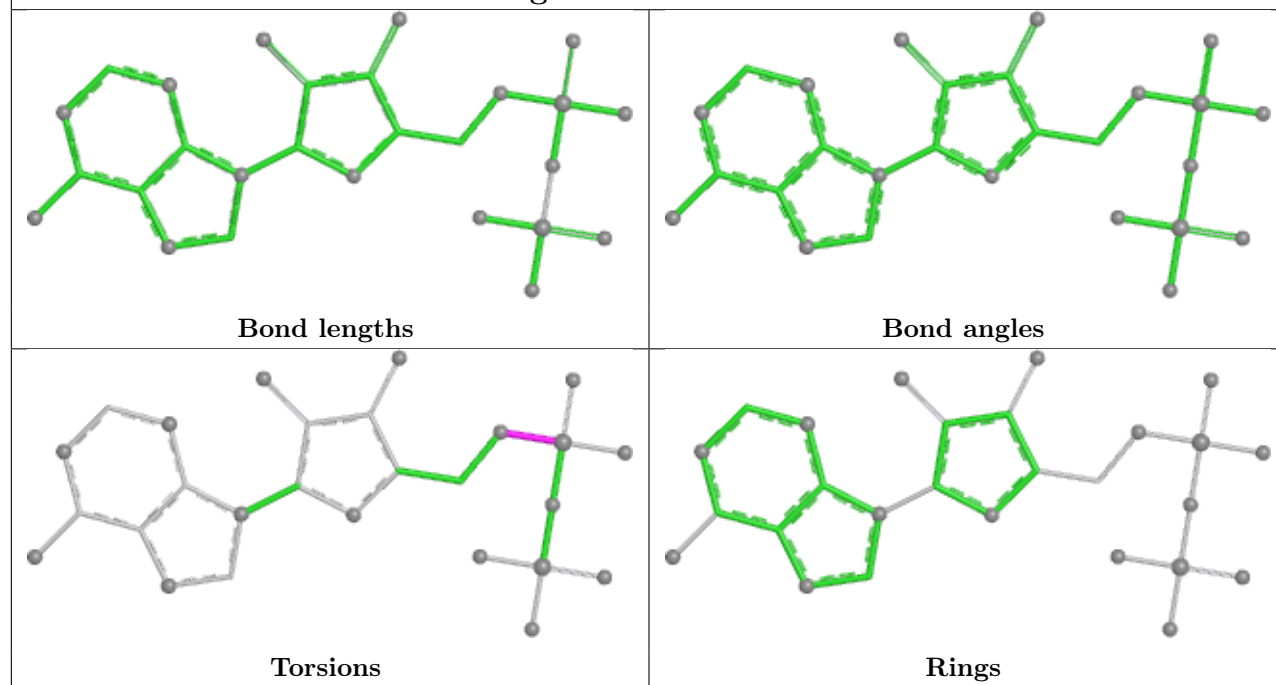
Ligand ADP D 601

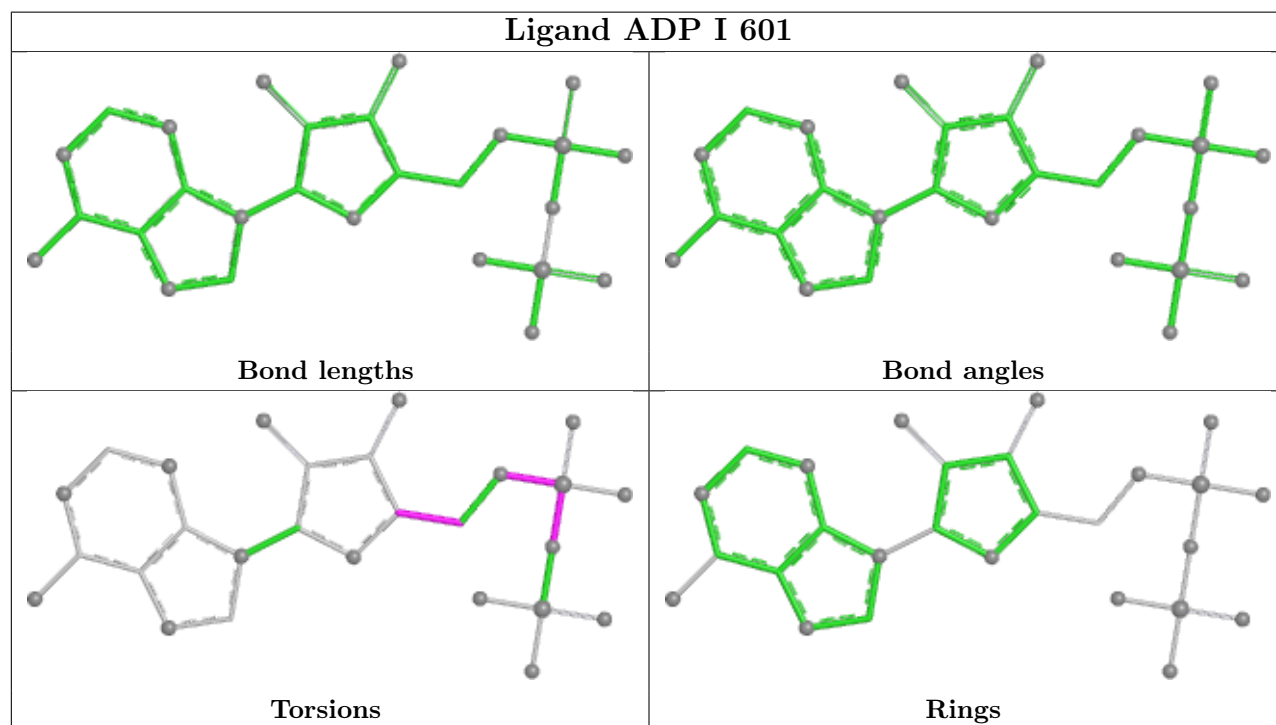
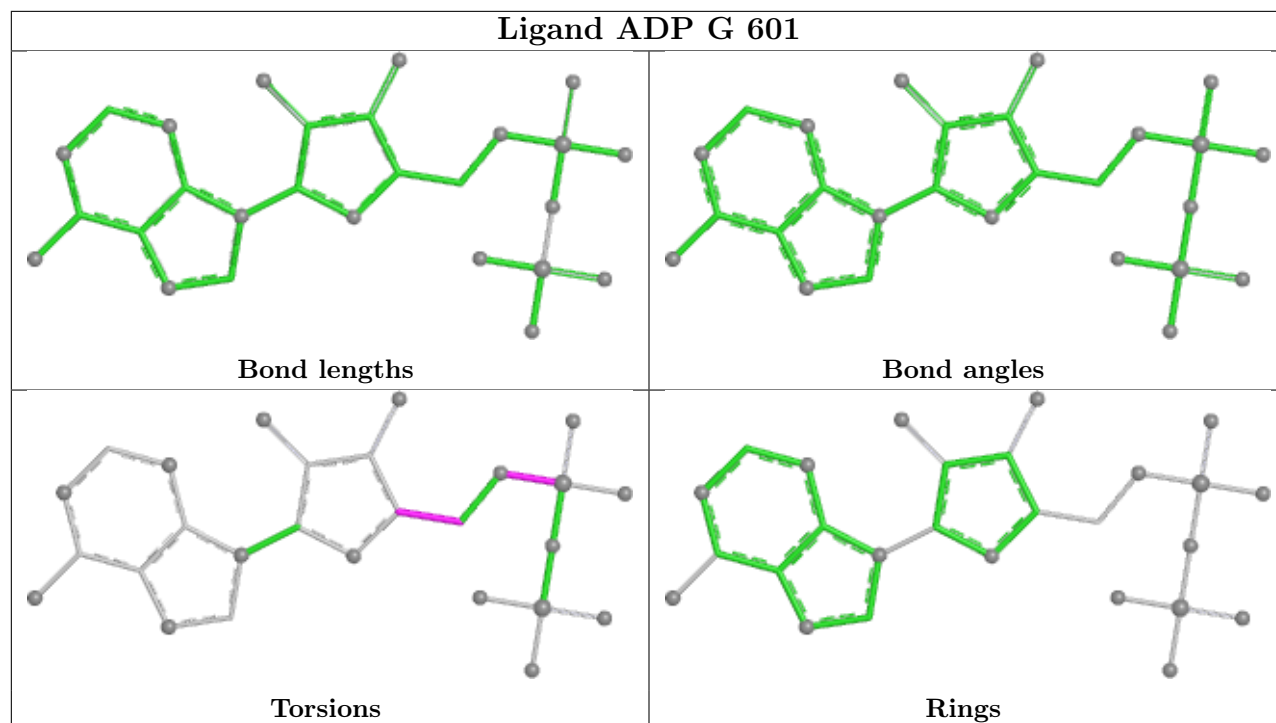


Ligand ADP I 602

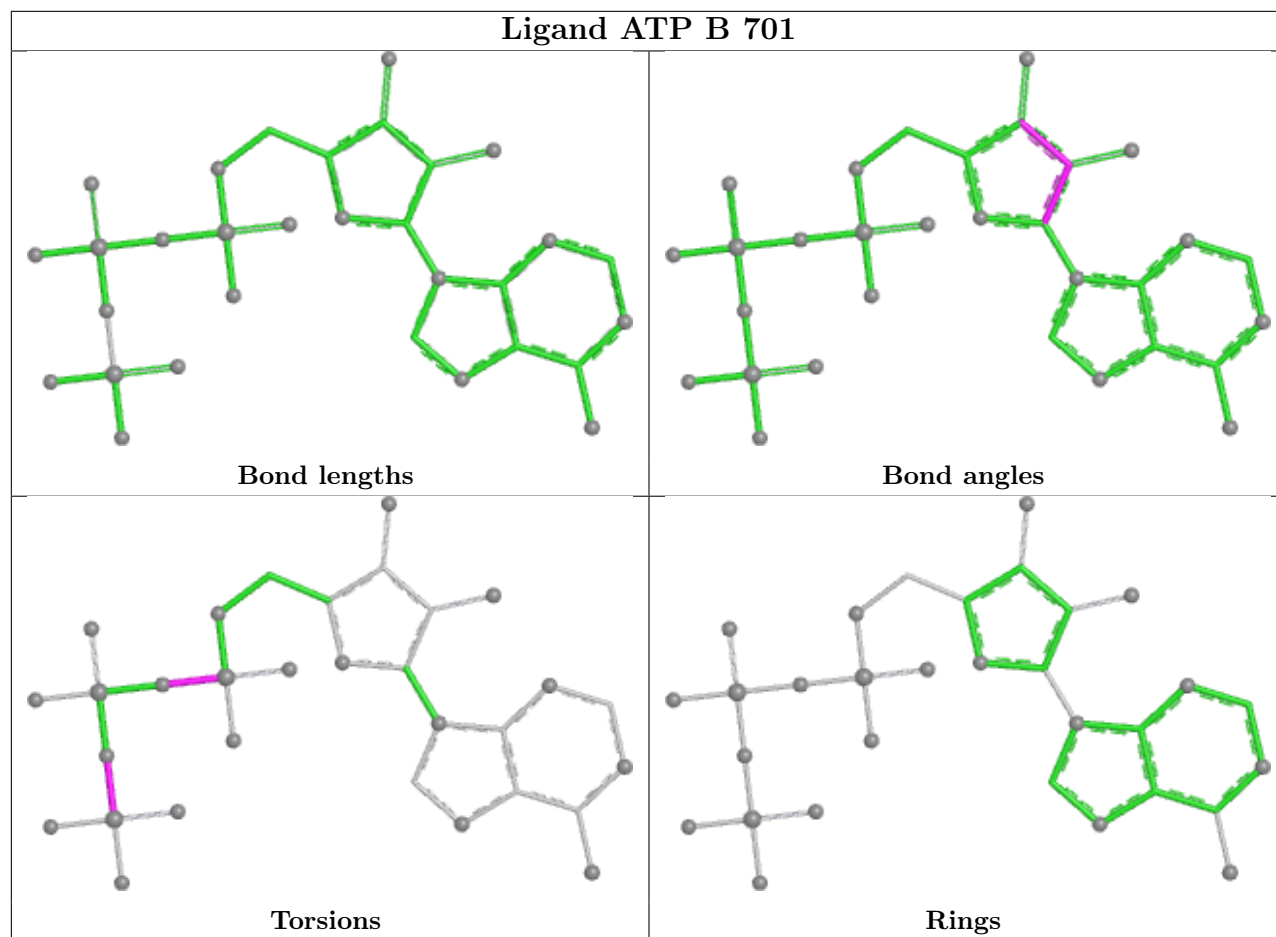


Ligand ADP C 601

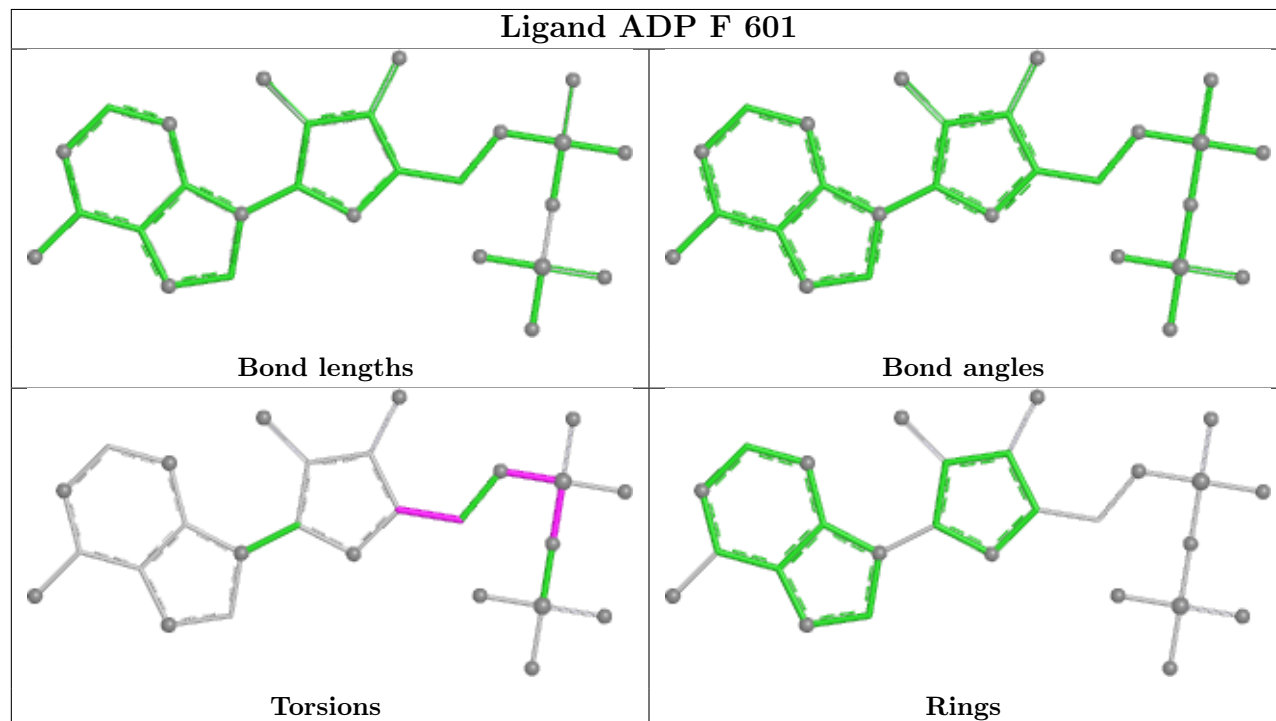




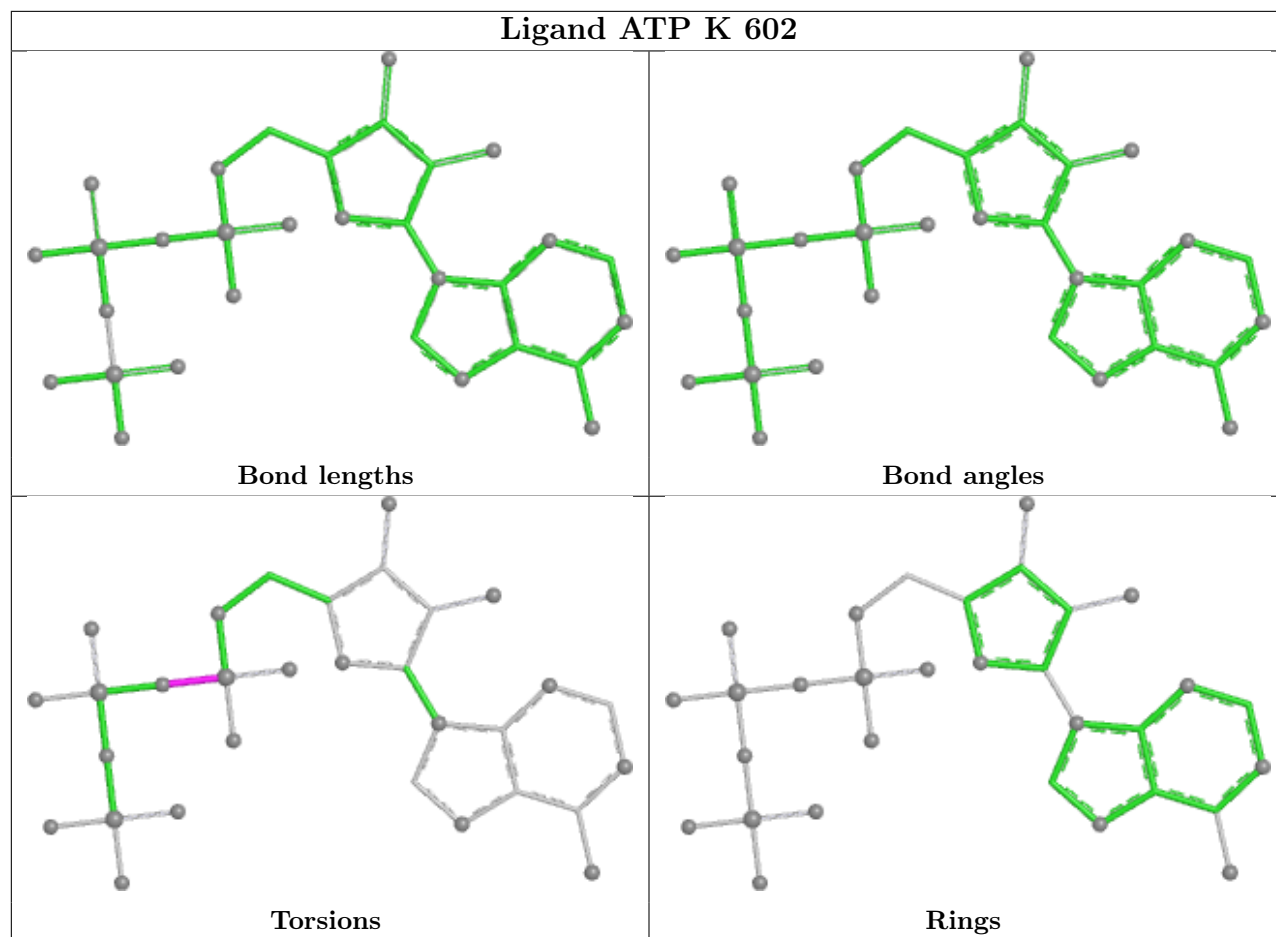
Ligand ATP B 701



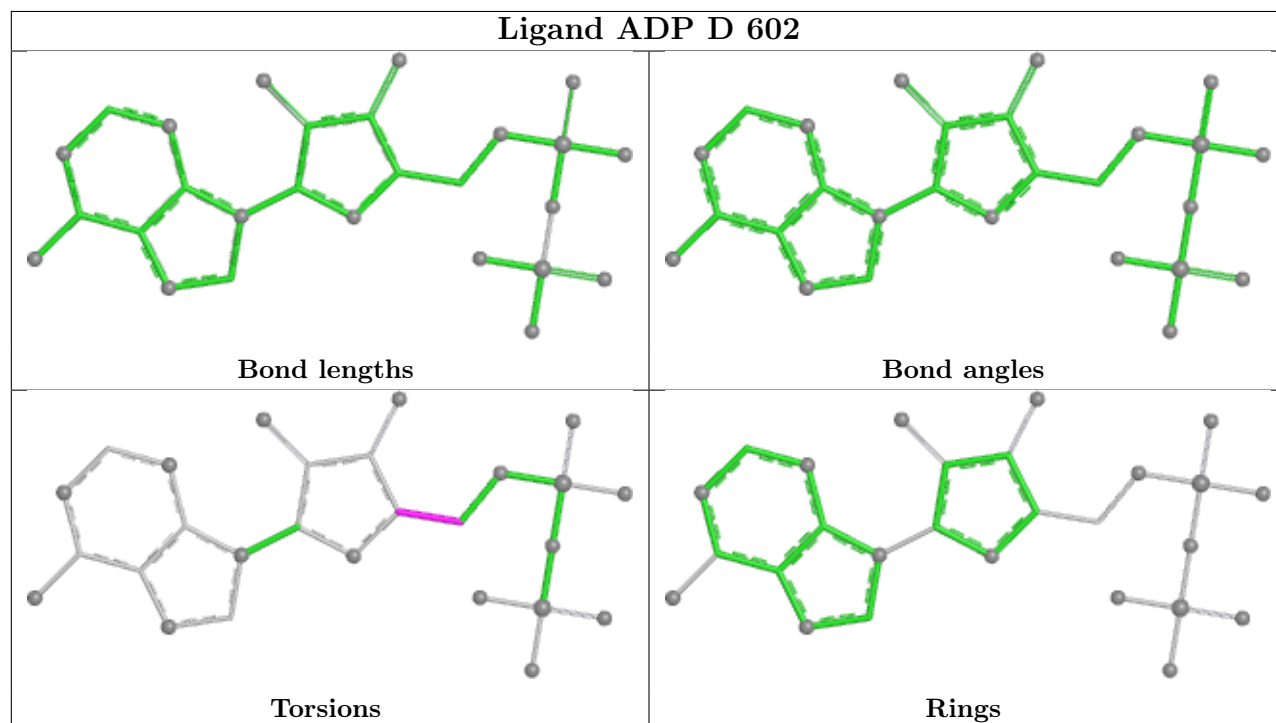
Ligand ADP F 601

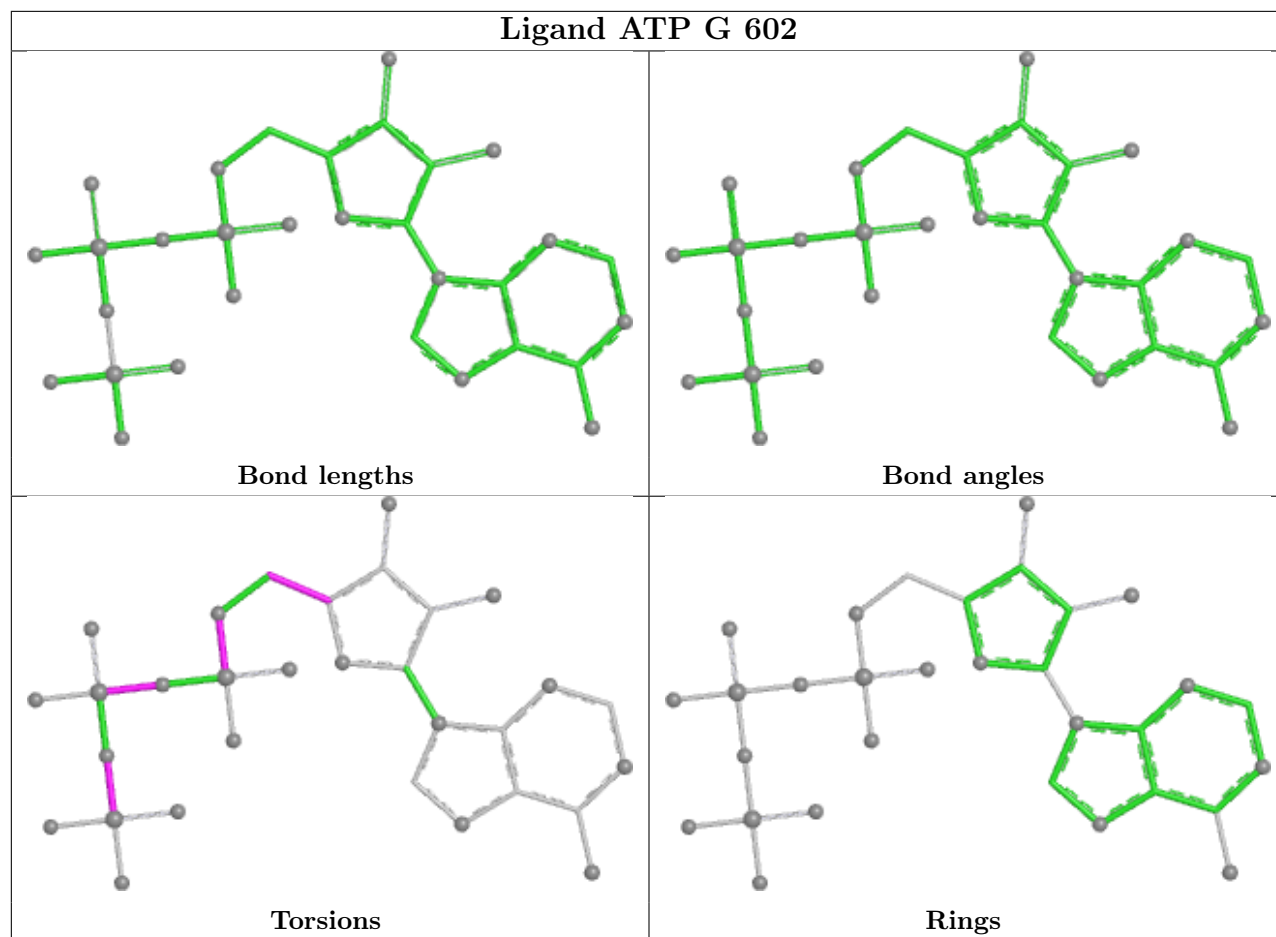


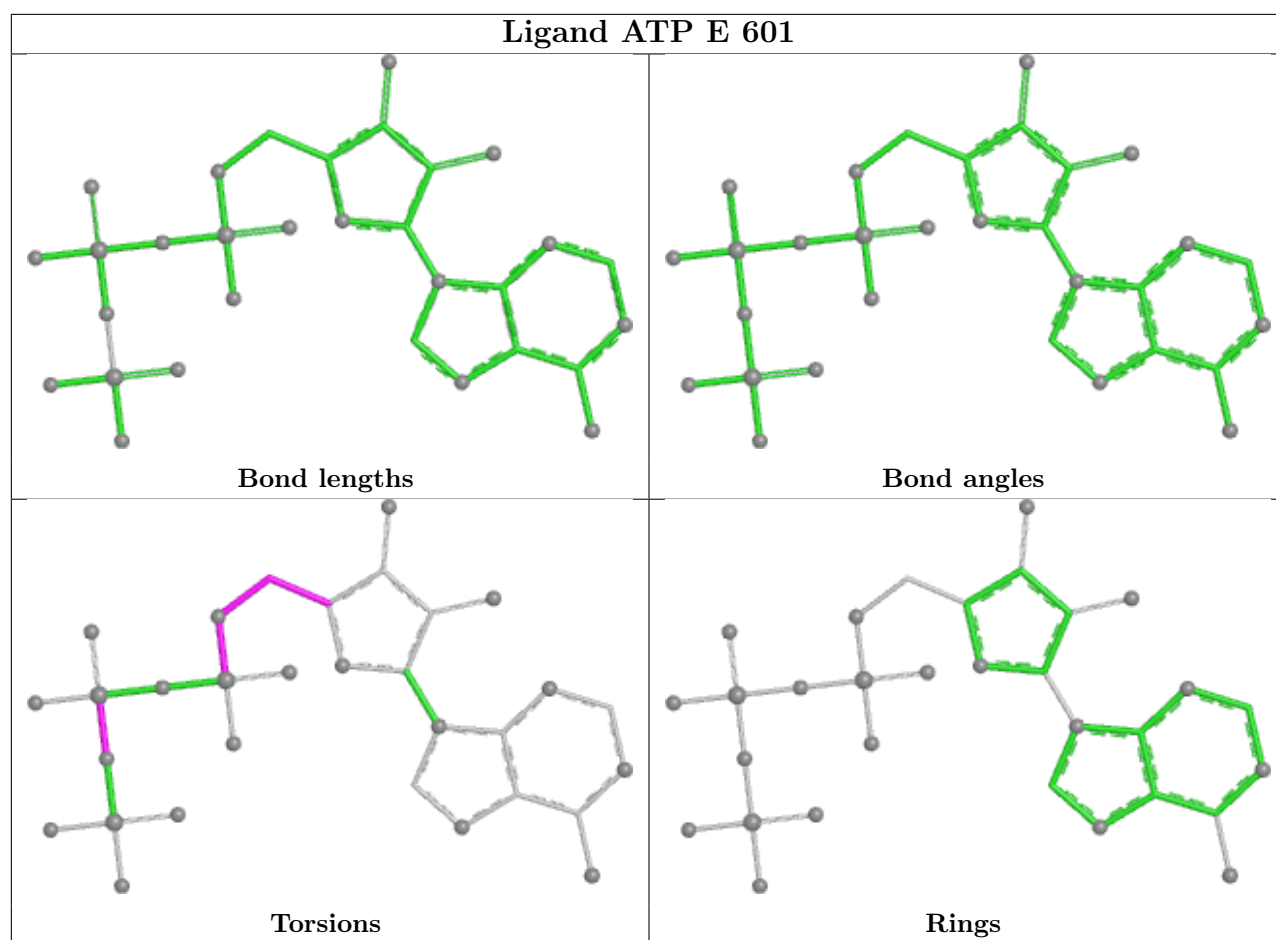
Ligand ATP K 602

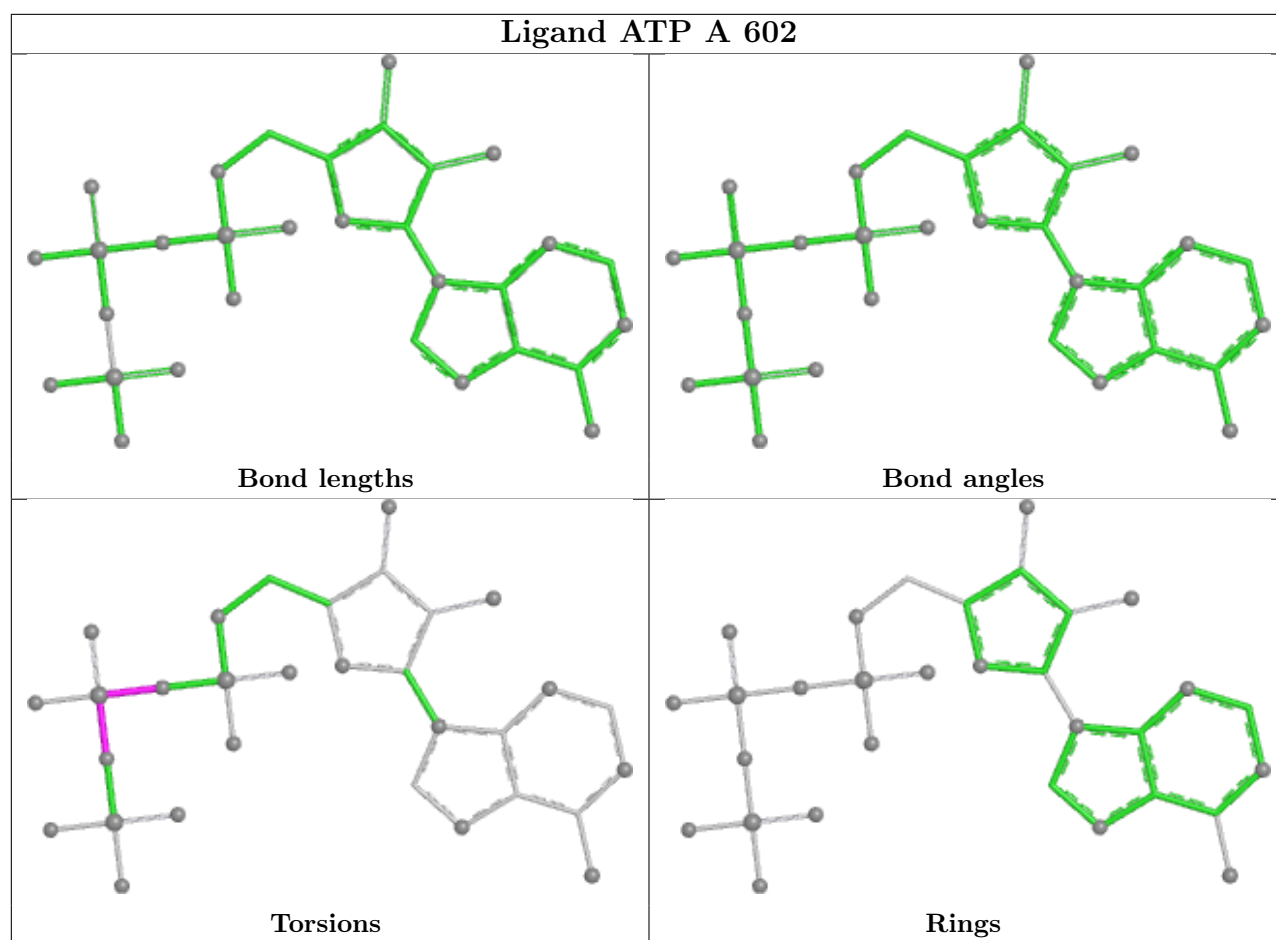


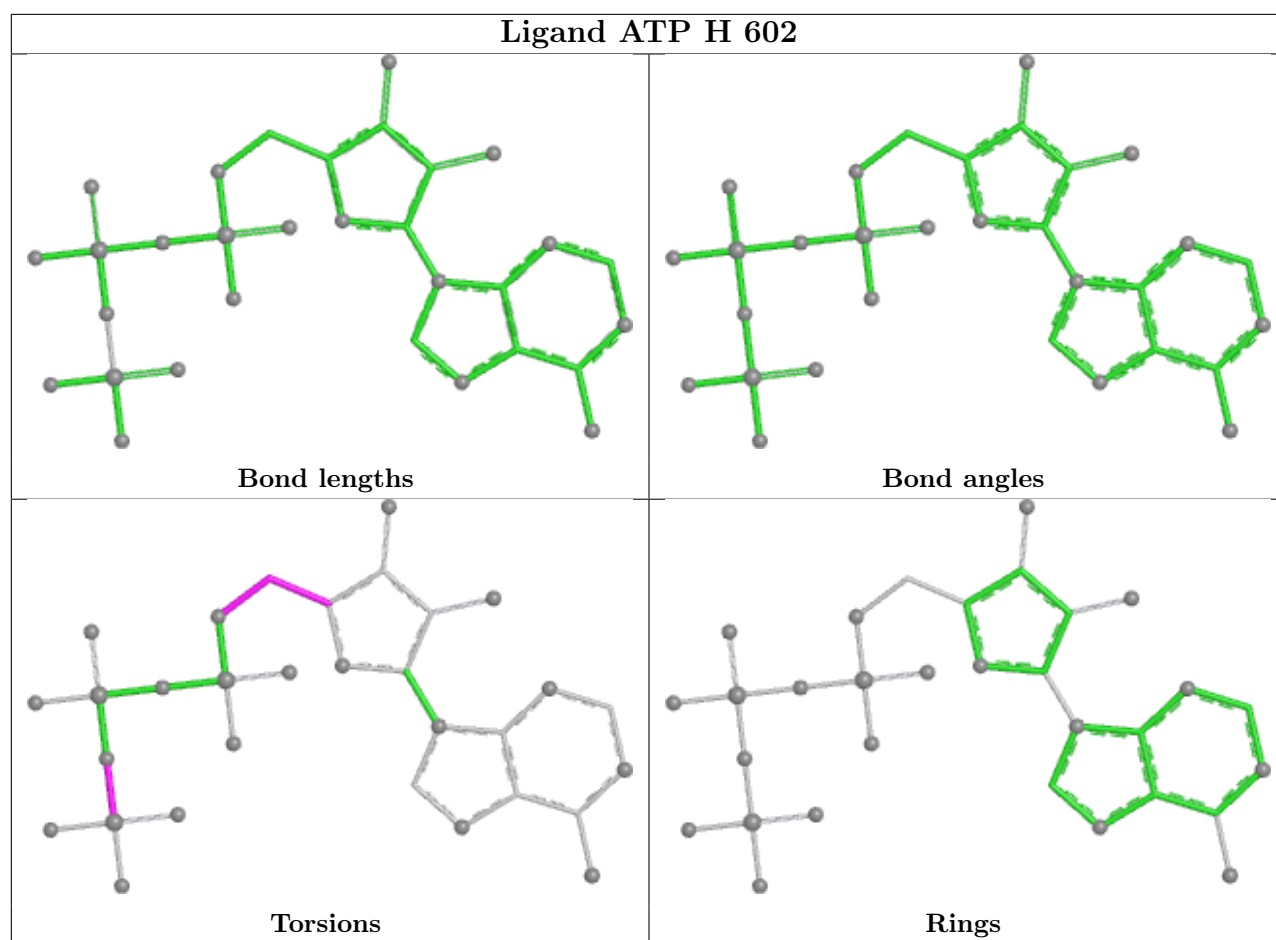
Ligand ADP D 602



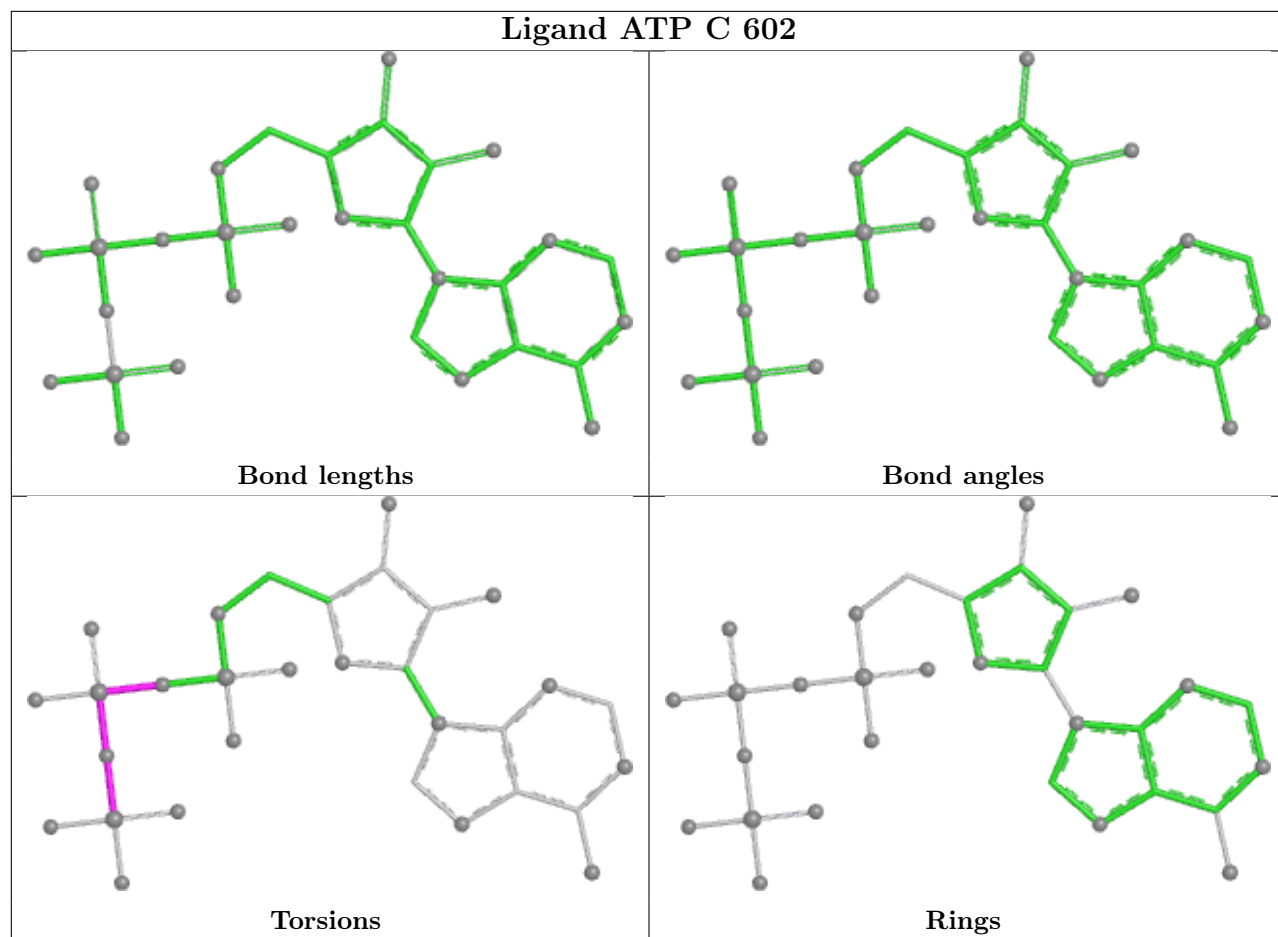




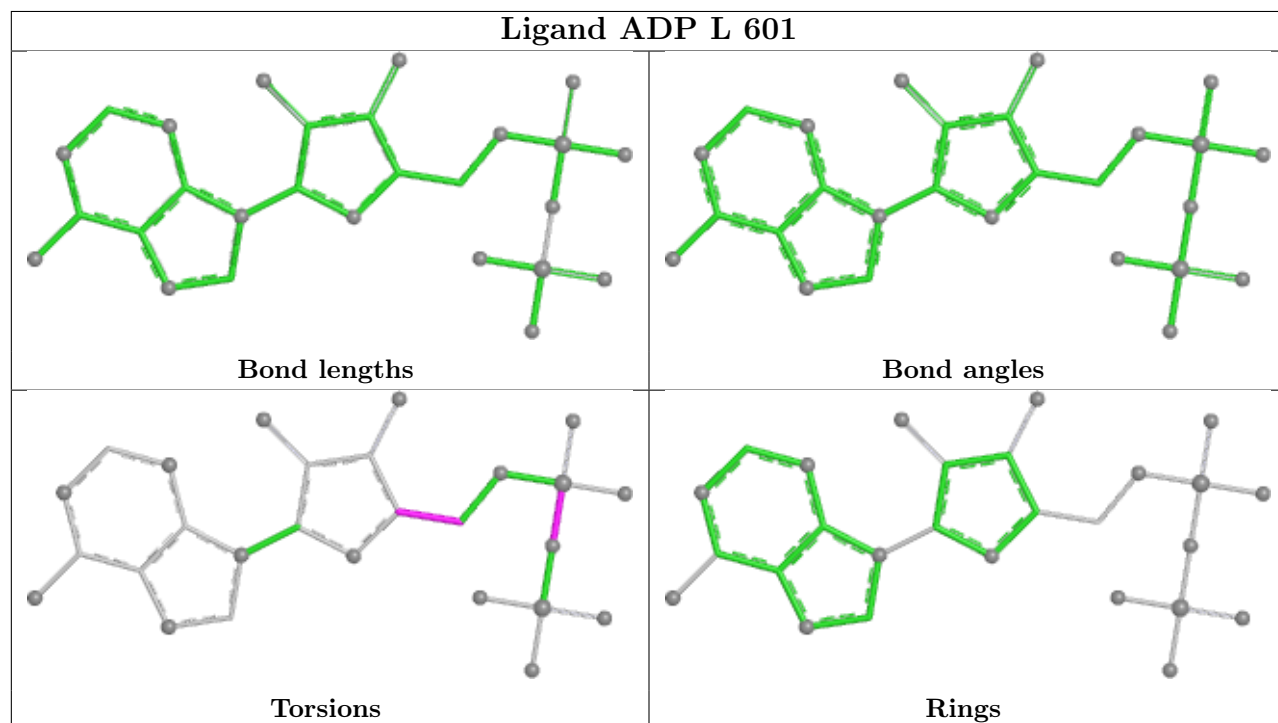


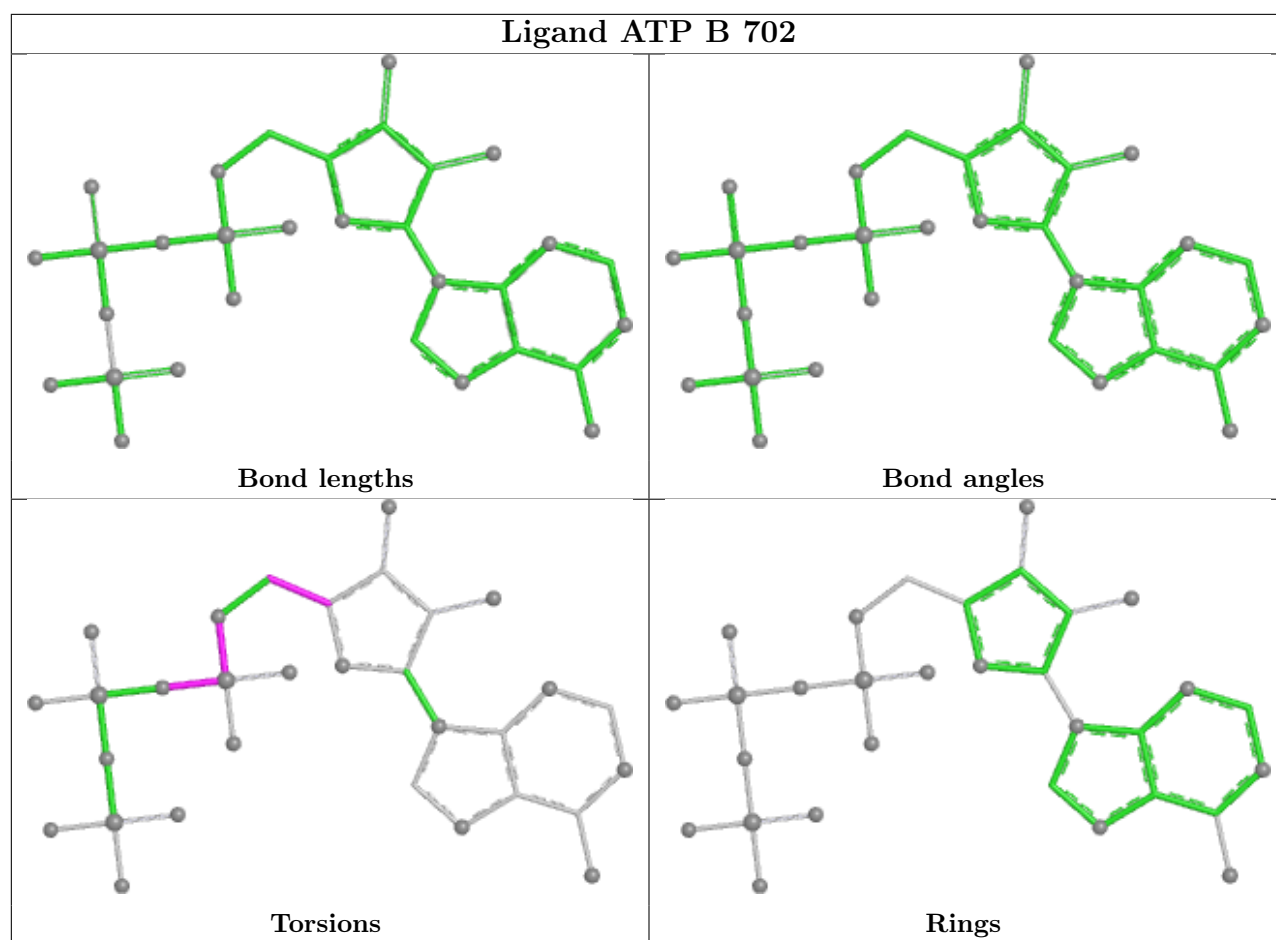


Ligand ATP C 602

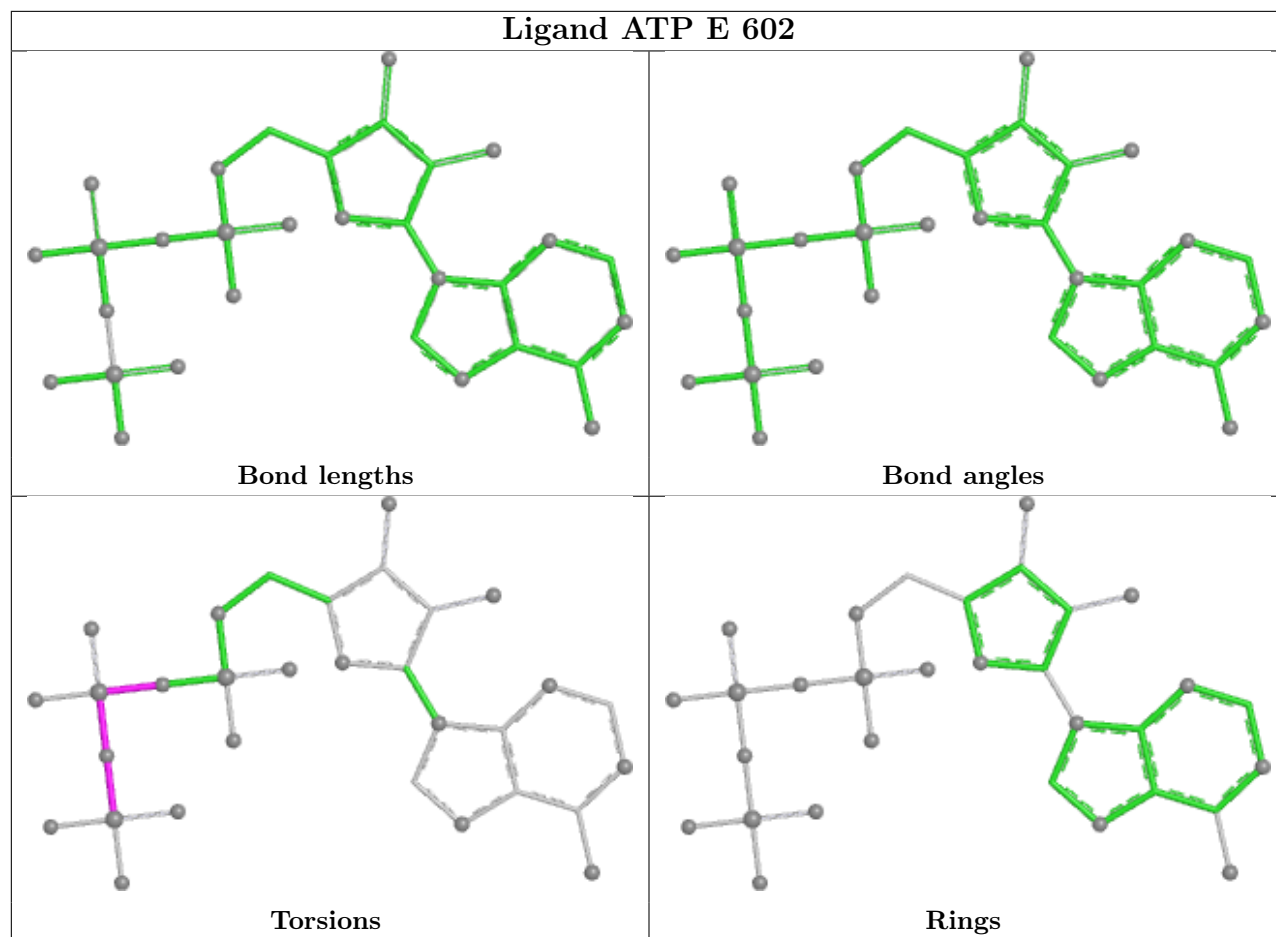


Ligand ADP L 601

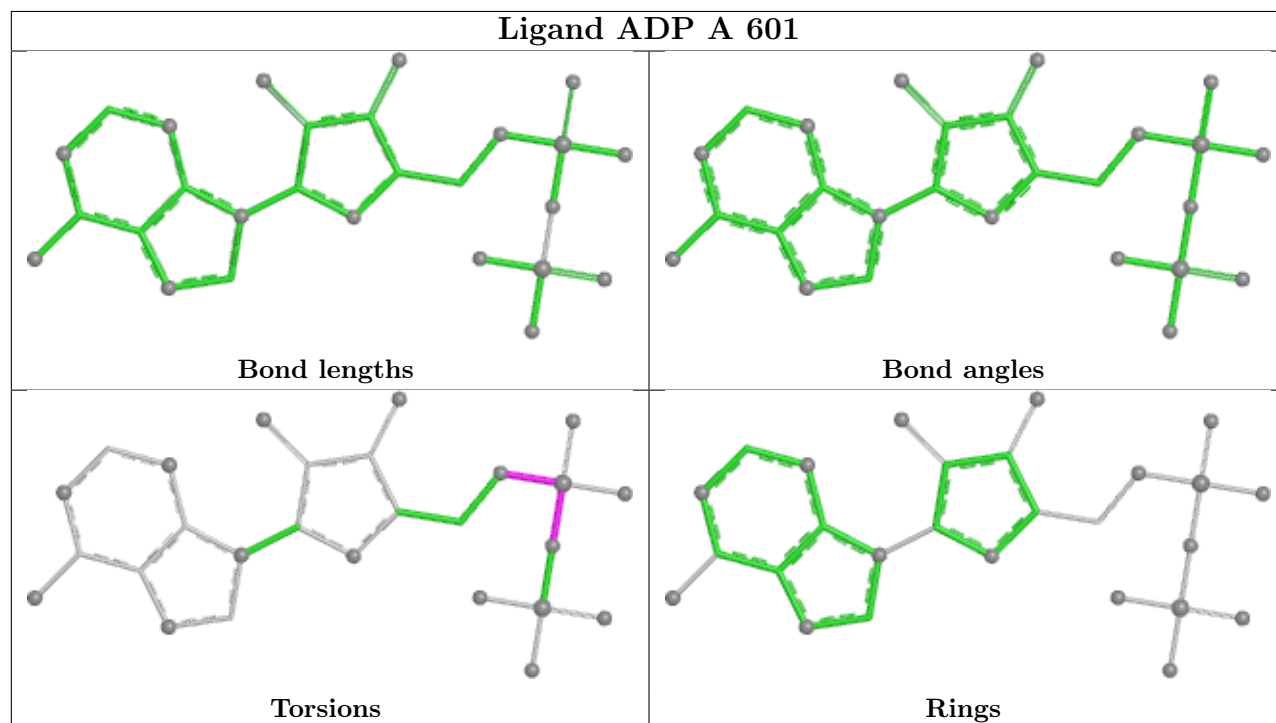




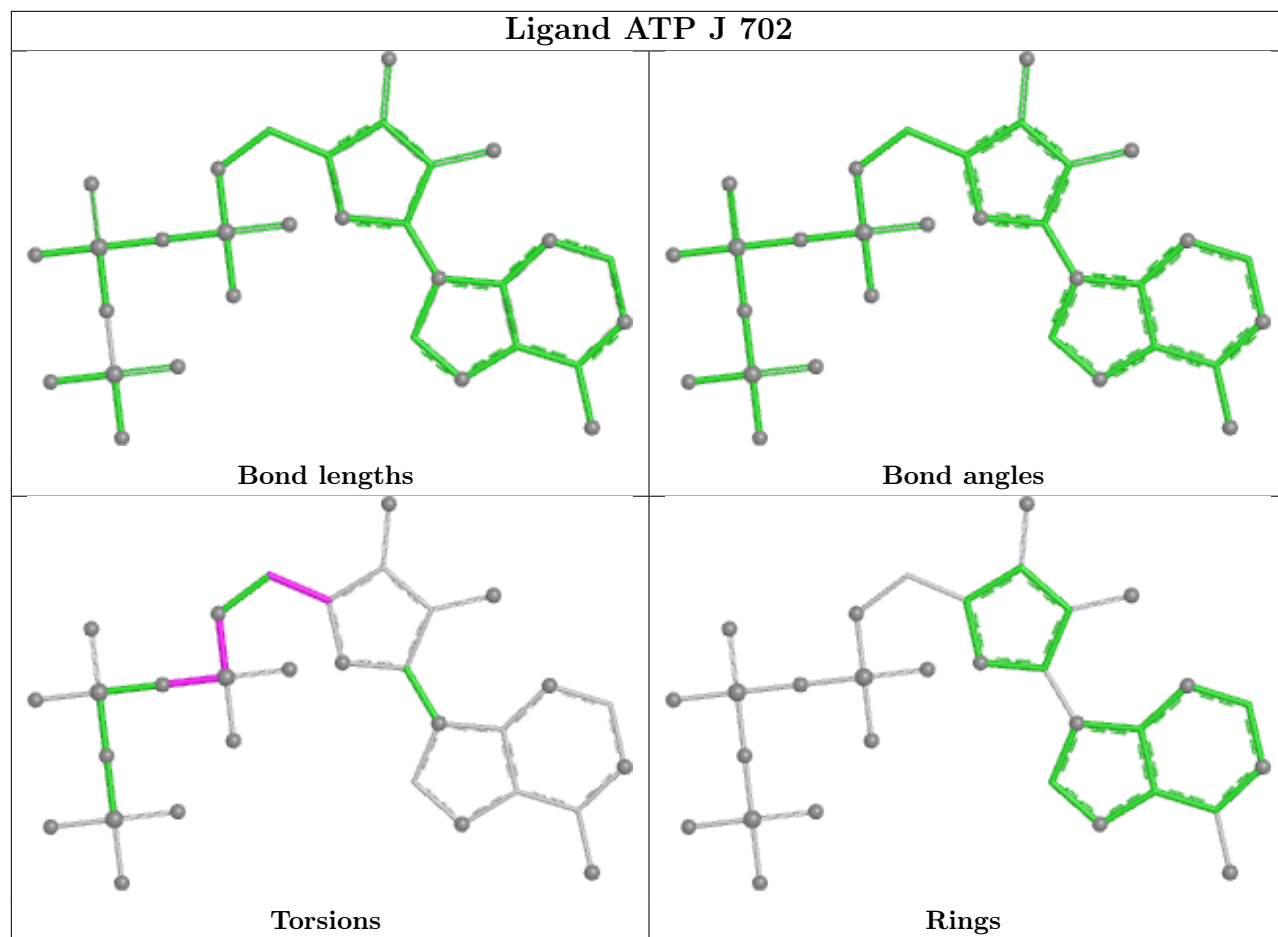
Ligand ATP E 602



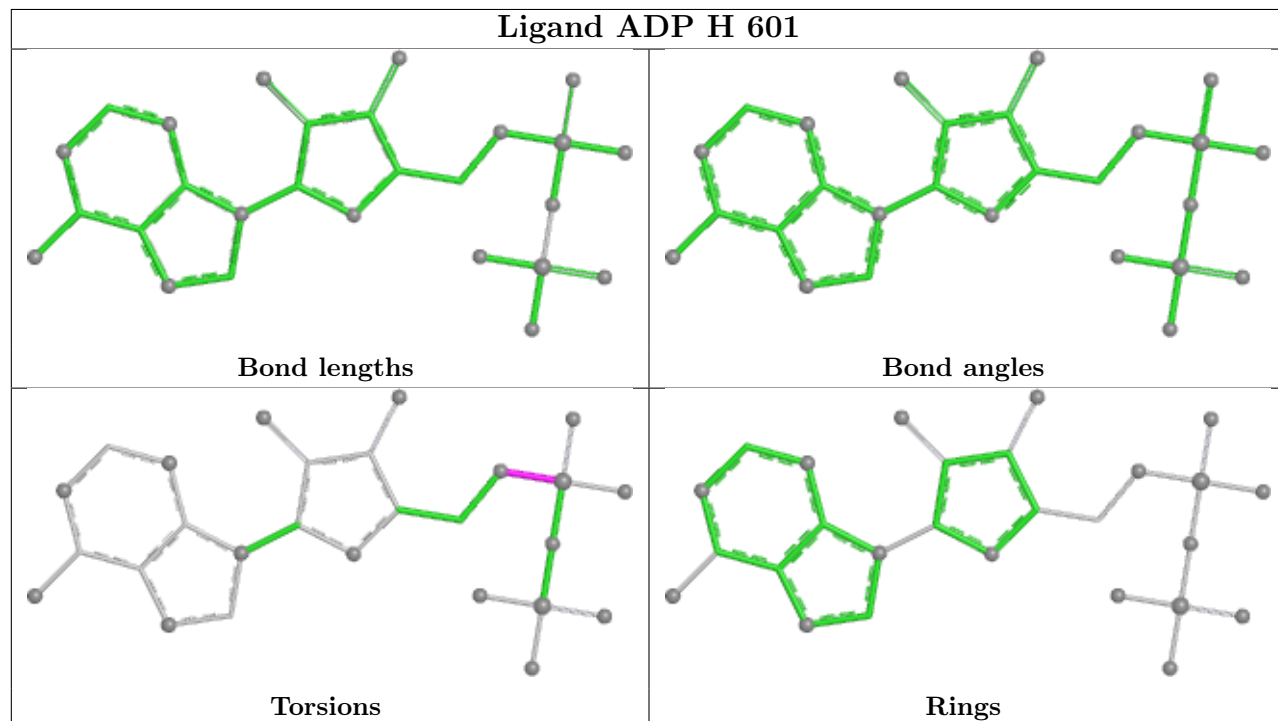
Ligand ADP A 601



Ligand ATP J 702



Ligand ADP H 601



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 ⓘ

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	463/519 (89%)	0.18	2 (0%) 88 76	48, 69, 111, 145	0
1	B	460/519 (88%)	0.23	7 (1%) 72 48	51, 77, 107, 125	0
1	C	461/519 (88%)	0.19	7 (1%) 72 48	46, 69, 113, 153	0
1	D	457/519 (88%)	0.19	2 (0%) 88 76	45, 70, 104, 122	0
1	E	463/519 (89%)	0.13	5 (1%) 78 56	44, 71, 95, 126	0
1	F	466/519 (89%)	0.09	2 (0%) 88 76	46, 71, 100, 125	0
1	G	458/519 (88%)	0.31	9 (1%) 65 41	56, 82, 129, 145	0
1	I	466/519 (89%)	0.14	5 (1%) 78 56	44, 65, 94, 119	0
1	J	463/519 (89%)	0.09	3 (0%) 85 69	44, 62, 92, 159	0
1	K	464/519 (89%)	0.26	4 (0%) 81 60	56, 78, 124, 145	0
1	L	456/519 (87%)	0.40	12 (2%) 57 33	62, 88, 119, 144	0
2	H	460/519 (88%)	0.18	5 (1%) 78 56	48, 70, 99, 124	0
All	All	5537/6228 (88%)	0.20	63 (1%) 78 56	44, 72, 111, 159	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	LEU	5.1
1	C	95	ALA	4.1
1	G	278	PHE	4.0
1	K	139	ALA	3.9
1	I	494	PRO	3.3
1	I	492	GLY	3.2
1	I	139	ALA	3.0
1	K	153	GLN	3.0
1	B	150	VAL	2.9
1	J	48	SER	2.9
1	A	181	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	233	GLY	2.7
1	L	378	ASP	2.7
1	L	158	SER	2.6
1	L	178	THR	2.6
1	J	139	ALA	2.6
2	H	147	VAL	2.6
1	G	419	PHE	2.6
1	B	422	ALA	2.6
1	C	178	THR	2.6
1	E	160	VAL	2.5
1	I	244	ILE	2.5
1	K	143	SER	2.5
1	L	179	VAL	2.4
1	E	161	ARG	2.4
1	K	306	CYS	2.4
1	L	92	TRP	2.4
1	I	108	ALA	2.4
1	G	34	GLY	2.3
1	L	188	TYR	2.3
1	G	94	LEU	2.3
1	G	148	THR	2.3
1	D	203	ASN	2.3
1	C	70	PRO	2.3
1	G	302	VAL	2.3
1	L	72	VAL	2.3
2	H	198	GLU	2.3
1	G	279	PHE	2.2
2	H	197	GLU	2.2
2	H	139	ALA	2.2
1	C	93	ASP	2.2
1	A	156	ALA	2.2
1	L	332	GLY	2.2
1	G	86	ASN	2.2
1	D	164	LEU	2.2
1	E	175	GLY	2.2
1	B	412	PHE	2.2
1	J	485	ASN	2.2
1	E	112	PRO	2.2
1	E	122	ASP	2.2
1	B	18	ILE	2.1
1	L	484	ARG	2.1
1	F	143	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	139	ALA	2.1
1	L	227	GLY	2.1
1	L	226	ARG	2.1
1	C	202	ASP	2.1
1	C	338	MET	2.0
1	B	415	THR	2.0
1	L	176	ALA	2.0
2	H	225	LEU	2.0
1	F	229	SER	2.0
1	G	33	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
1	SEP	L	431	10/11	0.85	0.12	78,80,84,84	0
1	SEP	K	431	10/11	0.87	0.13	63,65,70,70	0
1	SEP	G	431	10/11	0.87	0.14	61,62,62,62	4
1	SEP	D	431	10/11	0.89	0.12	73,76,78,78	0
1	SEP	B	431	10/11	0.89	0.12	67,68,72,72	0
1	SEP	J	431	10/11	0.90	0.10	63,67,73,73	0
1	SEP	A	431	10/11	0.92	0.12	65,67,68,68	4
1	SEP	C	431	10/11	0.93	0.09	63,64,65,66	0
1	SEP	F	431	10/11	0.93	0.10	59,60,64,65	0
1	SEP	E	431	10/11	0.95	0.07	74,77,79,80	0
1	SEP	I	431	10/11	0.96	0.10	62,63,63,63	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

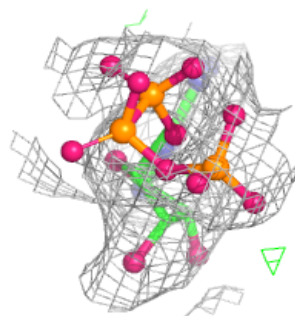
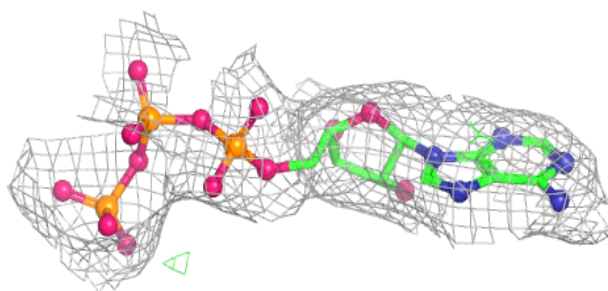
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	703	1/1	0.83	0.16	60,60,60,60	0
5	MG	K	603	1/1	0.83	0.14	84,84,84,84	0
5	MG	J	703	1/1	0.84	0.09	83,83,83,83	0
5	MG	L	603	1/1	0.85	0.09	73,73,73,73	0
5	MG	E	603	1/1	0.88	0.09	59,59,59,59	0
4	ATP	E	601	31/31	0.89	0.10	78,79,93,94	0
3	ADP	D	601	27/27	0.89	0.10	68,73,74,75	0
3	ADP	L	601	27/27	0.89	0.11	82,86,87,89	0
4	ATP	B	702	31/31	0.90	0.09	75,77,81,83	0
4	ATP	J	702	31/31	0.91	0.08	70,72,82,83	0
3	ADP	K	601	27/27	0.91	0.08	83,87,89,90	0
4	ATP	G	602	31/31	0.91	0.10	74,76,80,80	0
3	ADP	C	601	27/27	0.92	0.09	74,79,83,84	0
4	ATP	H	602	31/31	0.92	0.09	68,71,78,78	0
3	ADP	I	602	27/27	0.93	0.08	37,42,46,47	0
5	MG	E	604	1/1	0.93	0.08	84,84,84,84	0
5	MG	F	603	1/1	0.93	0.19	76,76,76,76	0
3	ADP	A	601	27/27	0.93	0.08	67,70,72,73	0
3	ADP	G	601	27/27	0.93	0.08	64,70,76,78	0
4	ATP	C	602	31/31	0.93	0.08	63,66,70,71	0
4	ATP	K	602	31/31	0.94	0.08	70,72,75,76	0
4	ATP	L	602	31/31	0.94	0.07	74,76,84,84	0
5	MG	C	603	1/1	0.94	0.07	73,73,73,73	0
4	ATP	B	701	31/31	0.94	0.07	61,66,71,71	0
3	ADP	F	601	27/27	0.94	0.07	60,61,62,63	0
3	ADP	D	602	27/27	0.94	0.08	53,59,63,64	0
4	ATP	J	701	31/31	0.95	0.07	65,68,72,73	0
3	ADP	I	601	27/27	0.95	0.07	46,47,49,50	0
4	ATP	E	602	31/31	0.95	0.07	59,60,72,73	0
4	ATP	F	602	31/31	0.95	0.07	59,60,62,63	0
4	ATP	A	602	31/31	0.95	0.08	59,63,67,68	0
3	ADP	H	601	27/27	0.96	0.07	49,50,52,52	0
5	MG	H	603	1/1	0.97	0.04	48,48,48,48	0
5	MG	D	603	1/1	0.97	0.08	49,49,49,49	0
5	MG	A	603	1/1	0.99	0.03	68,68,68,68	0
5	MG	G	603	1/1	0.99	0.04	41,41,41,41	0

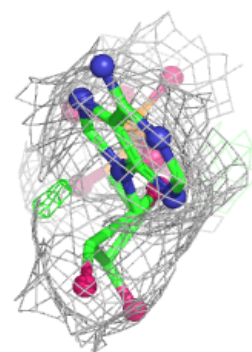
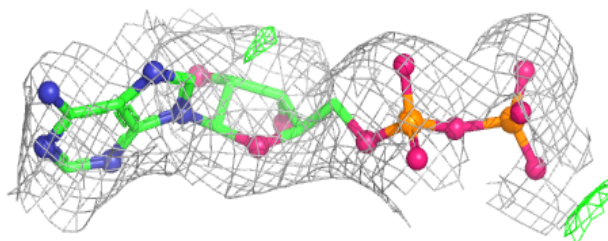
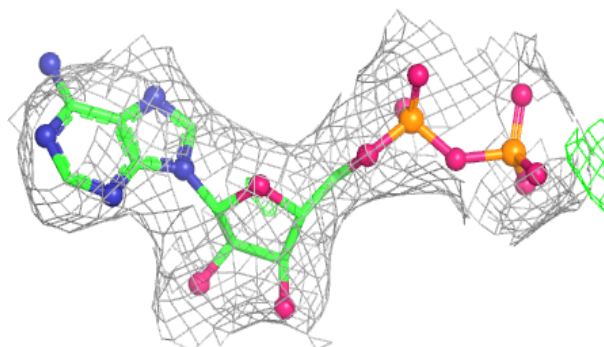
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP E 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

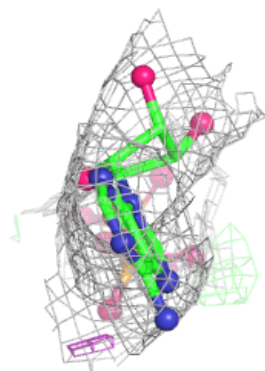
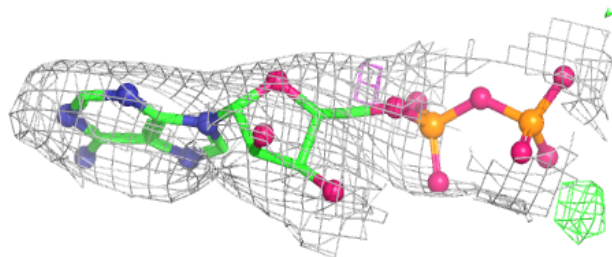
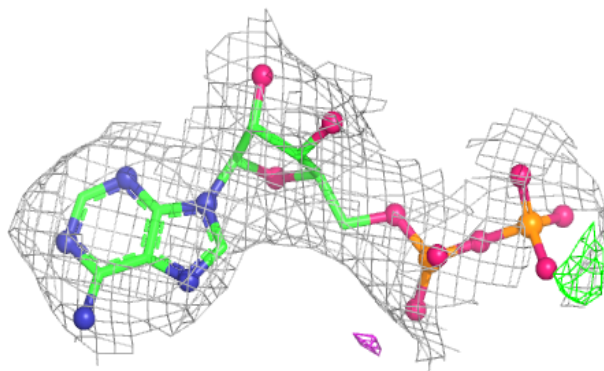
**Electron density around ADP D 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

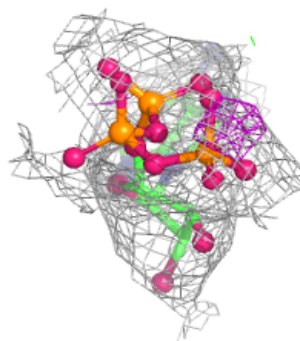
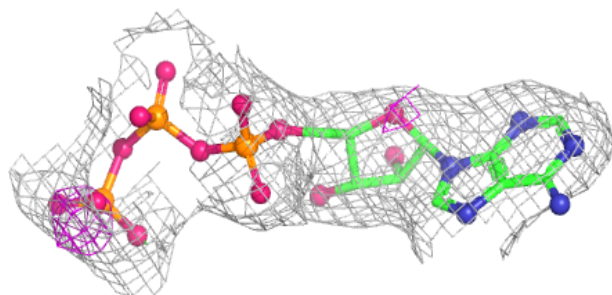
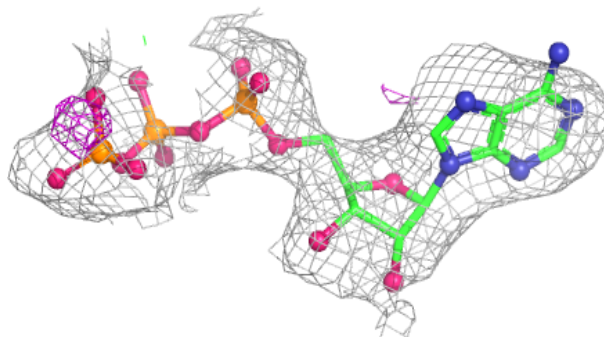


Electron density around ADP L 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

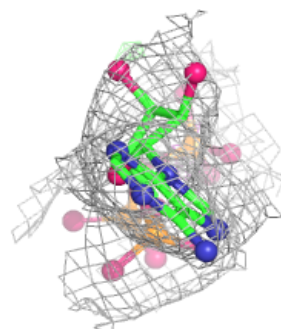
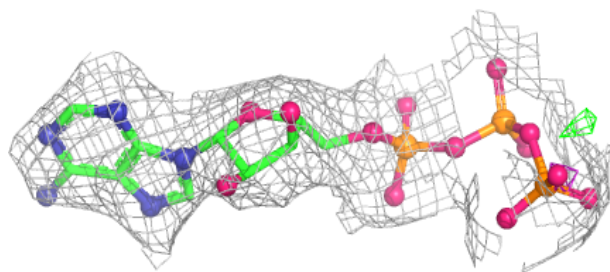
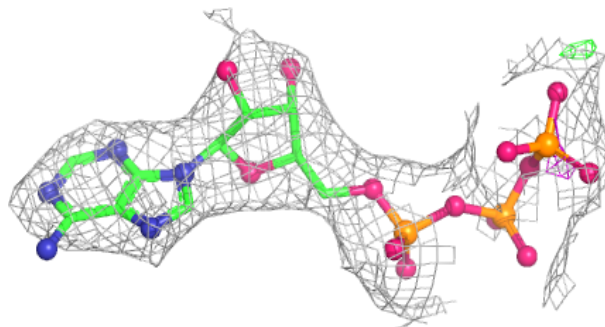
**Electron density around ATP B 702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

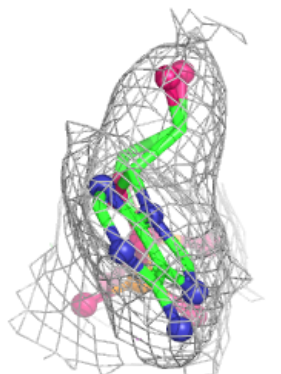
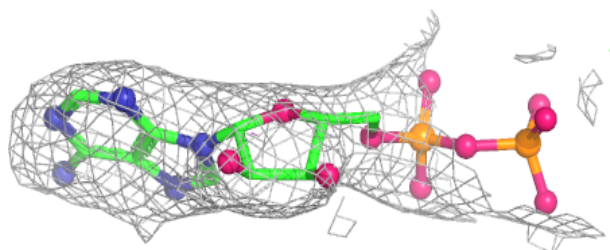
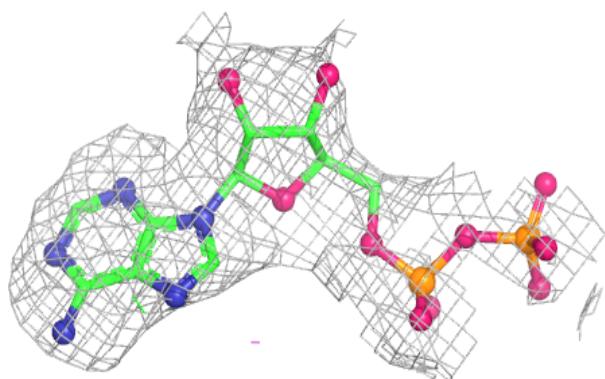


Electron density around ATP J 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

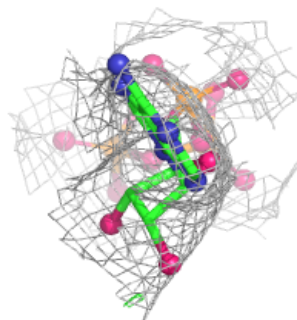
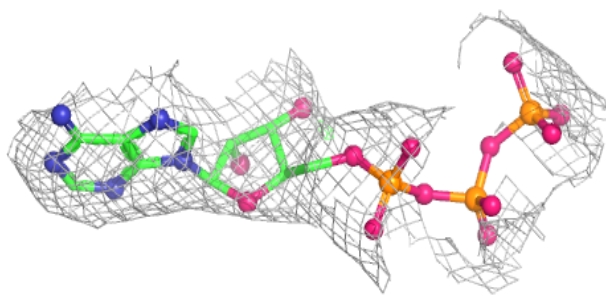
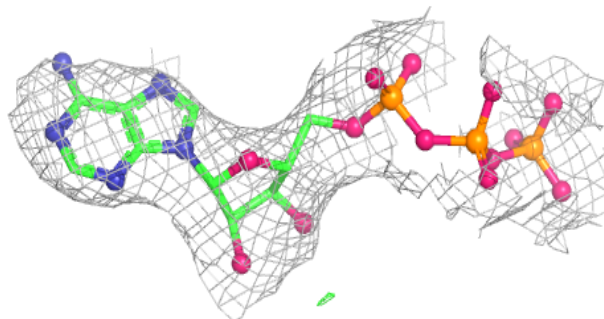
**Electron density around ADP K 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

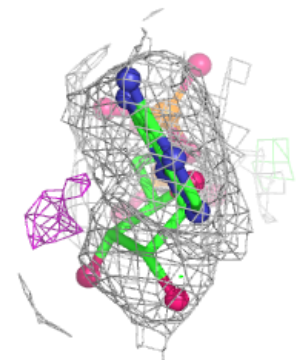
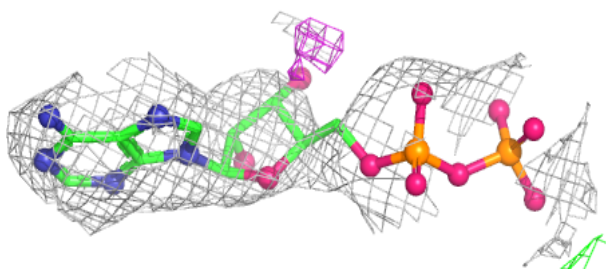
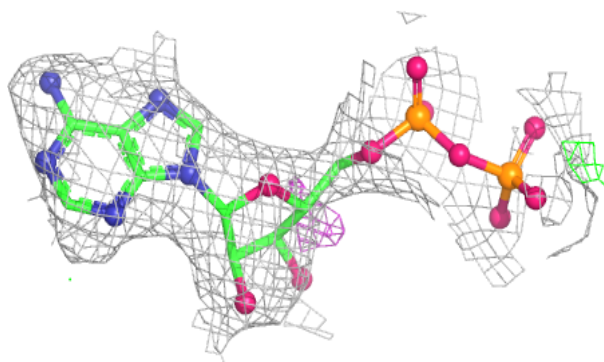


Electron density around ATP G 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

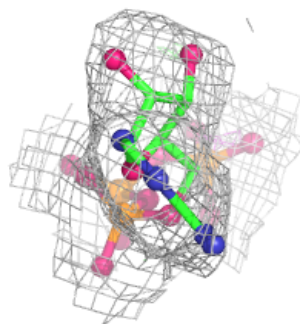
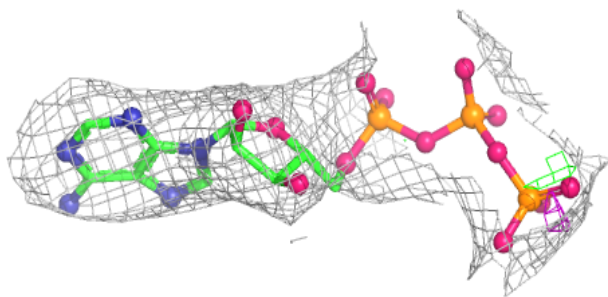
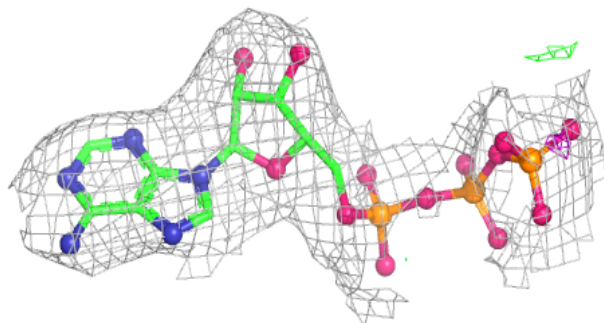
**Electron density around ADP C 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

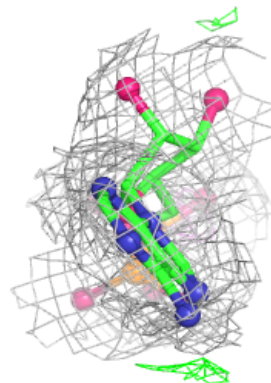
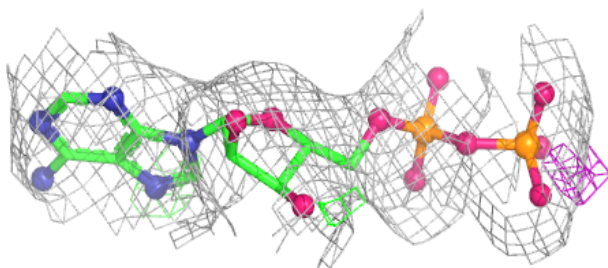
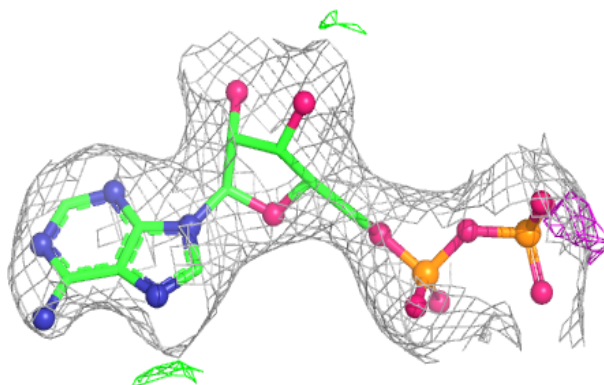


Electron density around ATP H 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

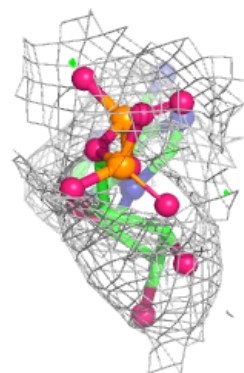
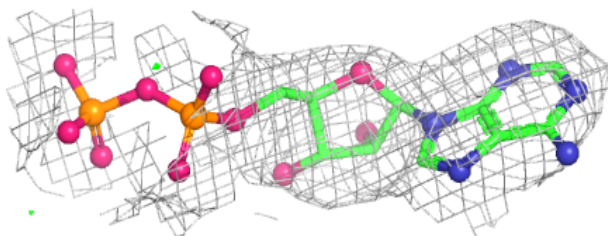
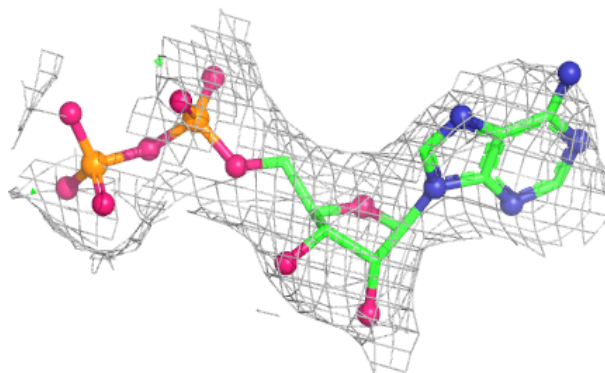
**Electron density around ADP I 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

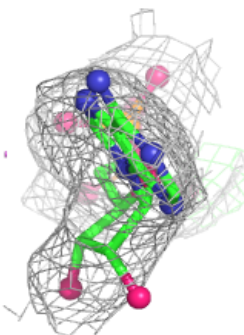
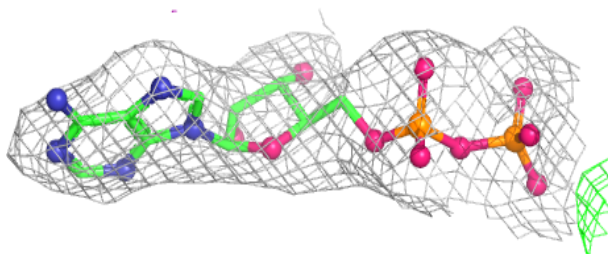
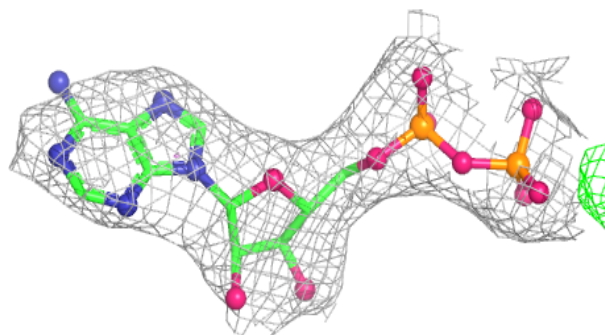


Electron density around ADP A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

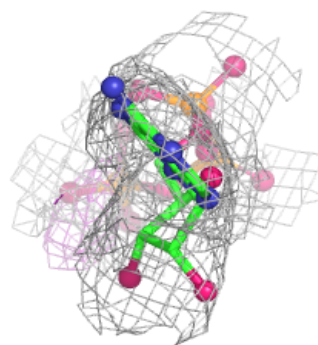
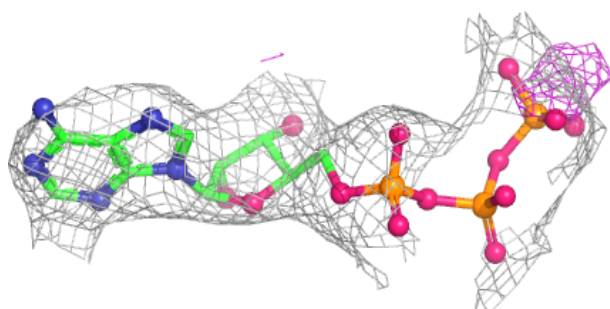
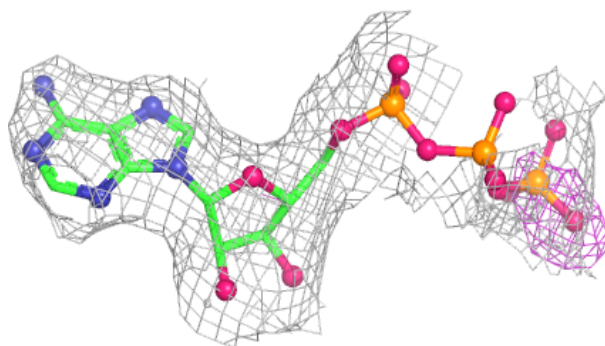
**Electron density around ADP G 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

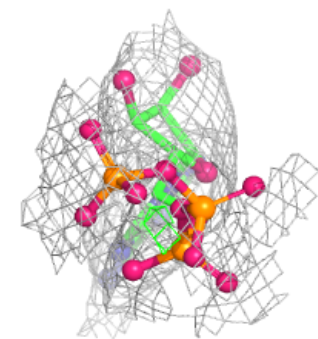
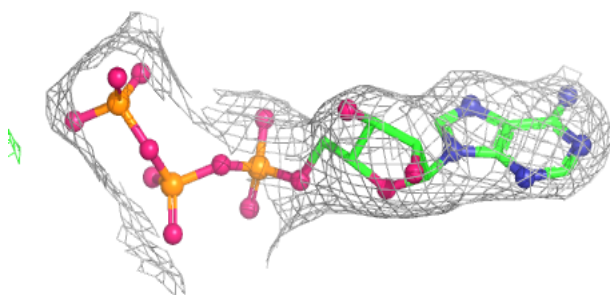
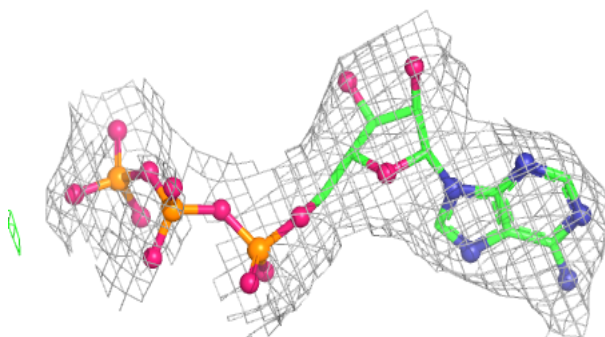


Electron density around ATP C 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

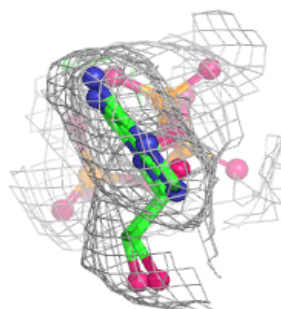
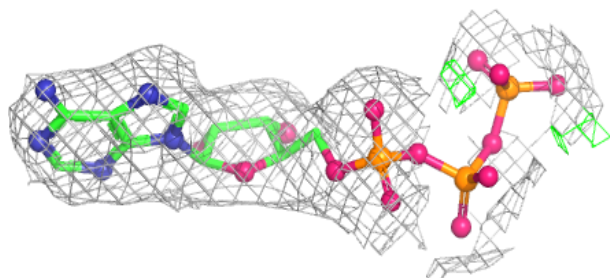
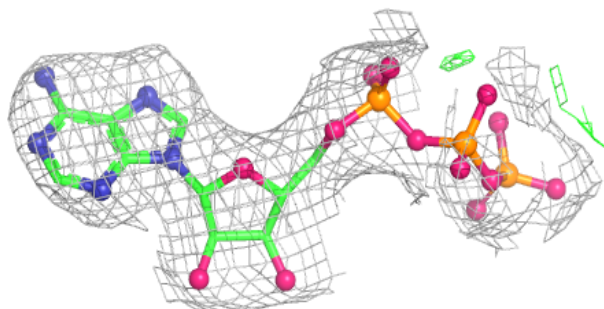
**Electron density around ATP K 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

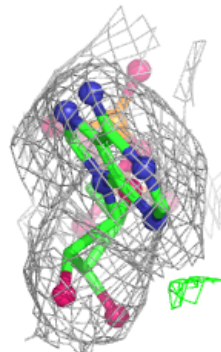
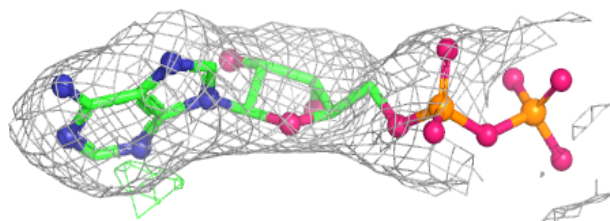
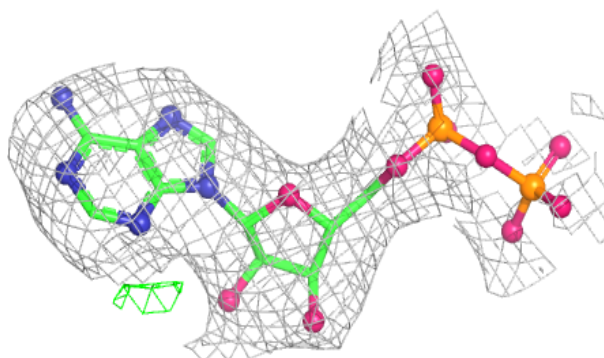


Electron density around ATP B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

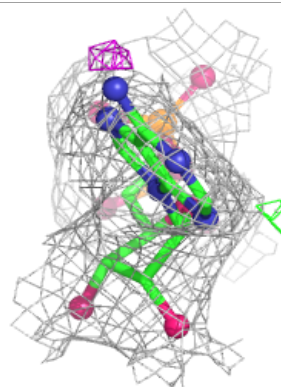
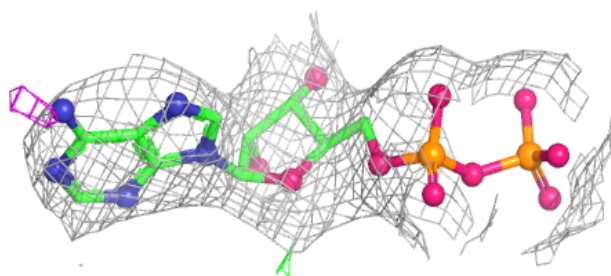
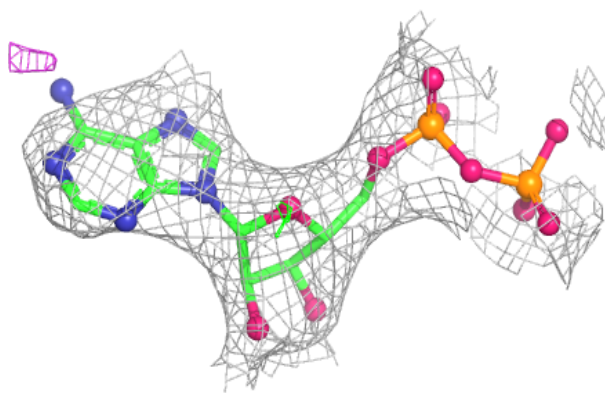
**Electron density around ADP F 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

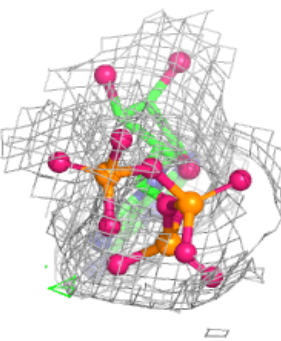
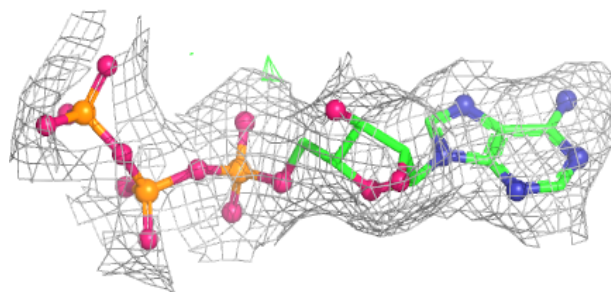
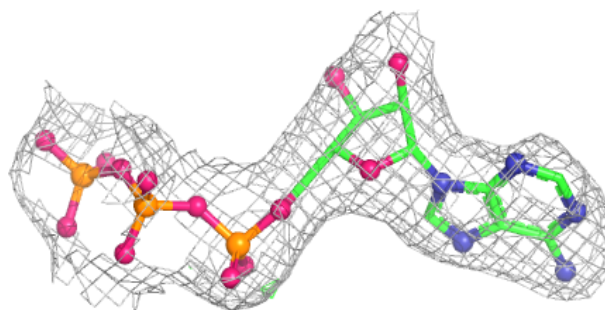


Electron density around ADP D 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

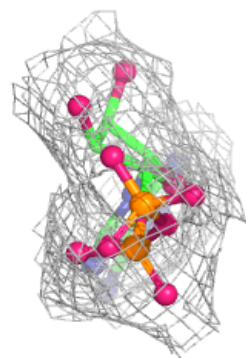
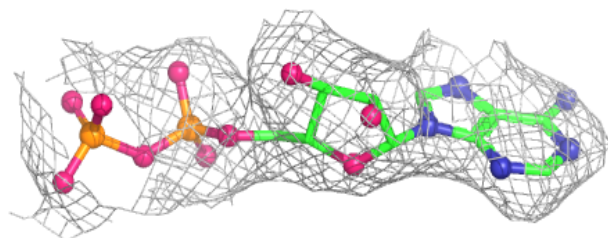
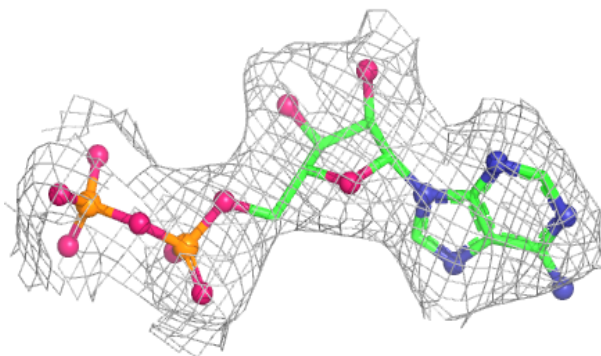
**Electron density around ATP J 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

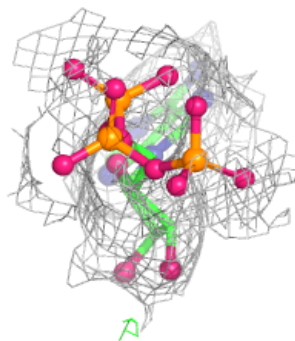
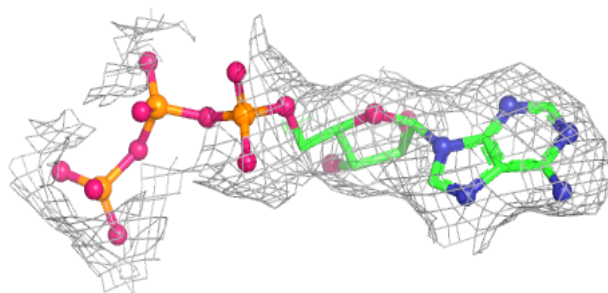
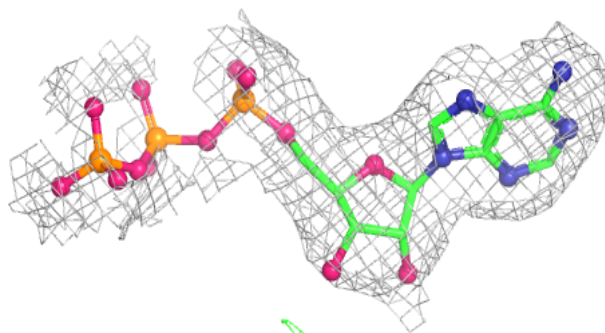


Electron density around ADP I 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

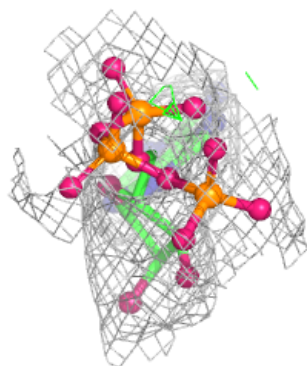
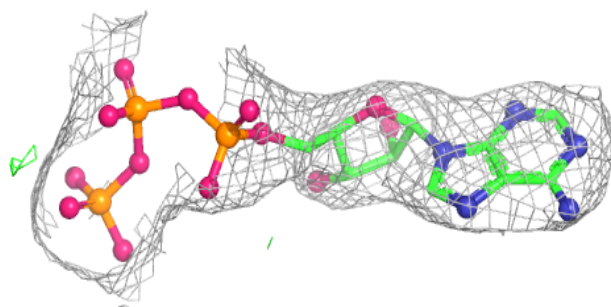
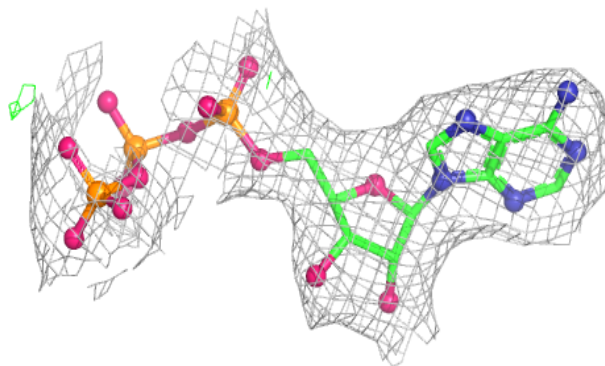
**Electron density around ATP E 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

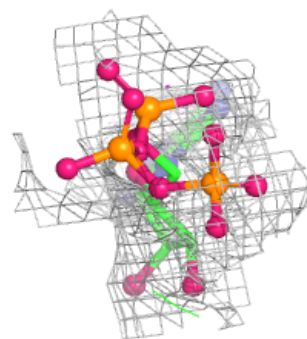
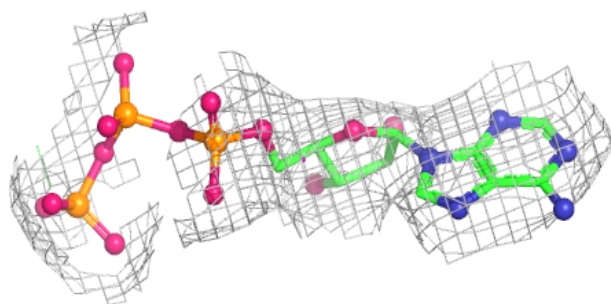
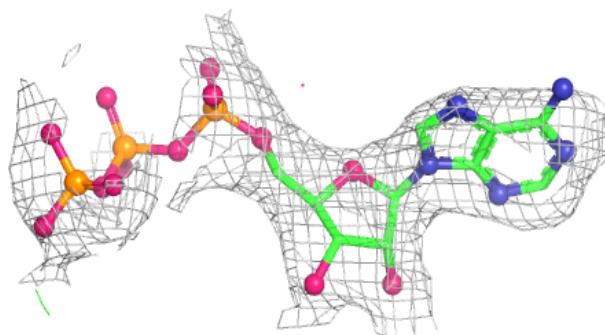


Electron density around ATP F 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

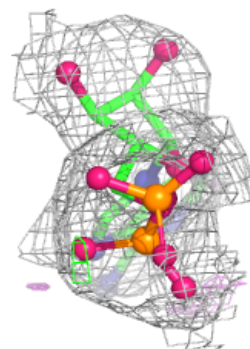
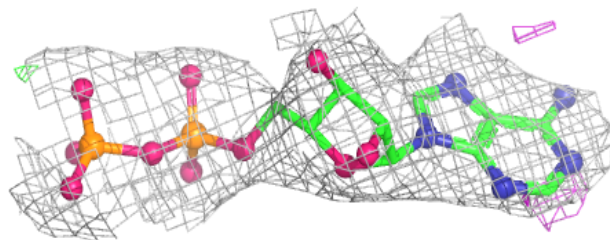
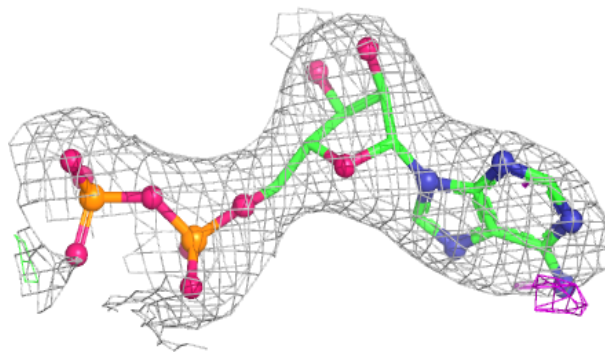
**Electron density around ATP A 602:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP H 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.