



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 04:22 PM EDT

PDB ID : 11KK / pdb_000011kk
Title : Crystal structure of HerA Like Helicae YjgR with NTPase fold from Escherchia coli
Authors : Kim, Y.; Maltseva, N.; Endres, M.; Joachimiak, A.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2026-03-01
Resolution : 2.90 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:

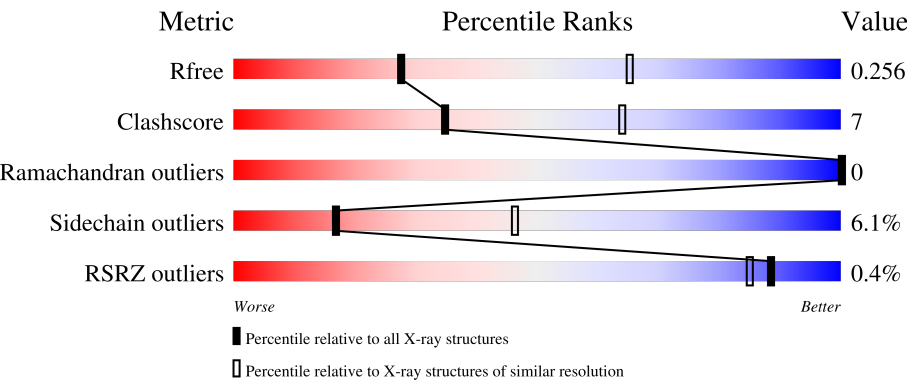
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	503	<div><div></div><div>74%20%• 5%</div></div>
1	B	503	<div><div></div><div>72%22%• •</div></div>
1	C	503	<div><div>%</div><div>77%17%• 5%</div></div>
1	D	503	<div><div></div><div>75%20%• •</div></div>

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Mol	Chain	Length	Quality of chain
1	E	503	<div><div></div><div>73%</div><div>18%</div><div>• 7%</div></div>
1	F	503	<div><div></div><div>69%</div><div>25%</div><div>• 5%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22184 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 HerA like helicase YjgR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	Se	0	0	0
			3660	2320	635	693	1	11			
1	B	481	Total	C	N	O	S	Se	0	0	0
			3687	2336	642	697	1	11			
1	C	480	Total	C	N	O	S	Se	0	0	0
			3675	2329	637	695	1	13			
1	D	486	Total	C	N	O	S	Se	0	0	0
			3722	2356	648	705	1	12			
1	E	470	Total	C	N	O	S	Se	0	0	0
			3597	2282	621	682	1	11			
1	F	478	Total	C	N	O	S	Se	0	0	0
			3670	2325	638	694	1	12			

There are 18 discrepancies between the modelled and reference sequences:

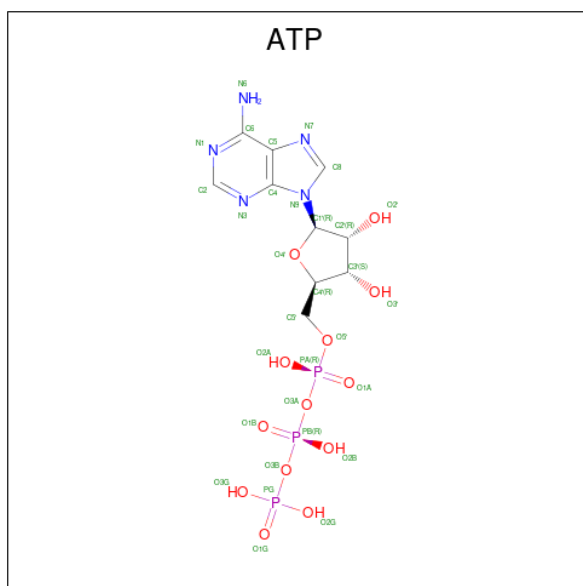
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P39342
A	-1	ASN	-	expression tag	UNP P39342
A	0	ALA	-	expression tag	UNP P39342
B	-2	SER	-	expression tag	UNP P39342
B	-1	ASN	-	expression tag	UNP P39342
B	0	ALA	-	expression tag	UNP P39342
C	-2	SER	-	expression tag	UNP P39342
C	-1	ASN	-	expression tag	UNP P39342
C	0	ALA	-	expression tag	UNP P39342
D	-2	SER	-	expression tag	UNP P39342
D	-1	ASN	-	expression tag	UNP P39342
D	0	ALA	-	expression tag	UNP P39342
E	-2	SER	-	expression tag	UNP P39342
E	-1	ASN	-	expression tag	UNP P39342
E	0	ALA	-	expression tag	UNP P39342
F	-2	SER	-	expression tag	UNP P39342
F	-1	ASN	-	expression tag	UNP P39342

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP P39342

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

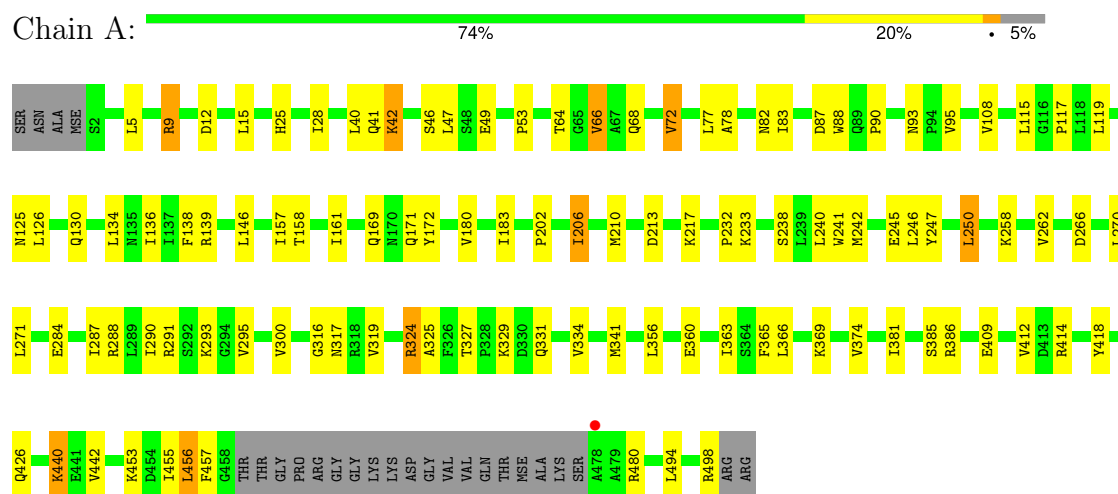
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			1	1		

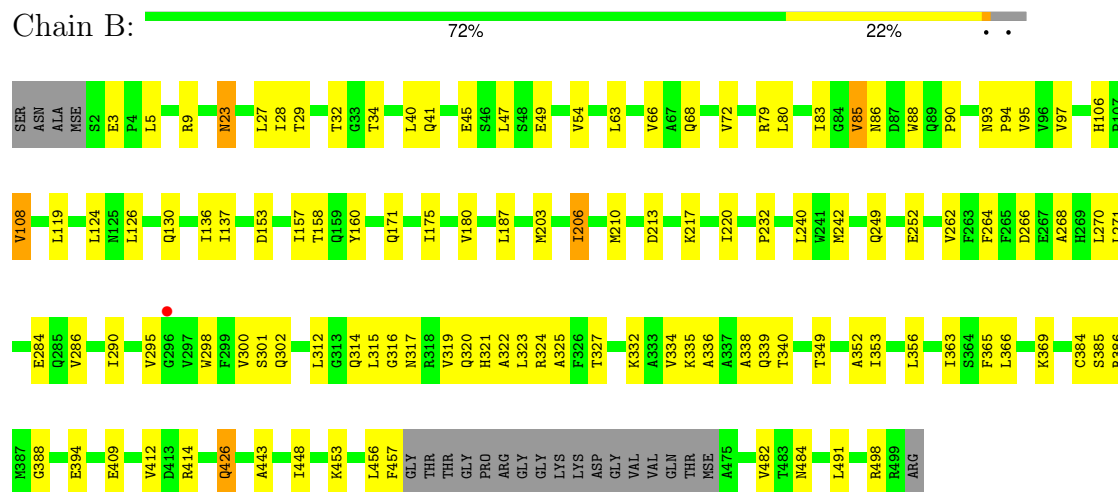
3 Residue-property plots

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

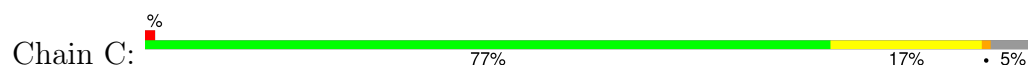
• Molecule 1: HerA like helicase YjgR

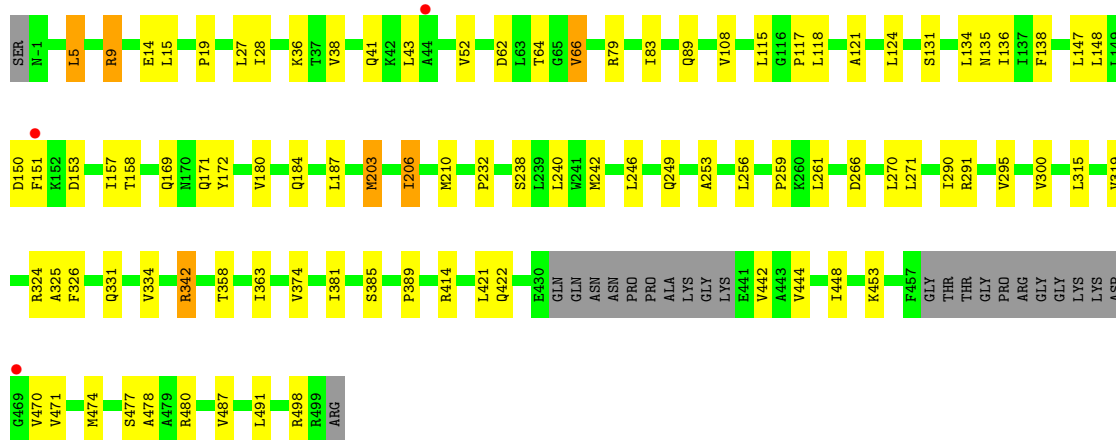


• Molecule 1: HerA like helicase YjgR



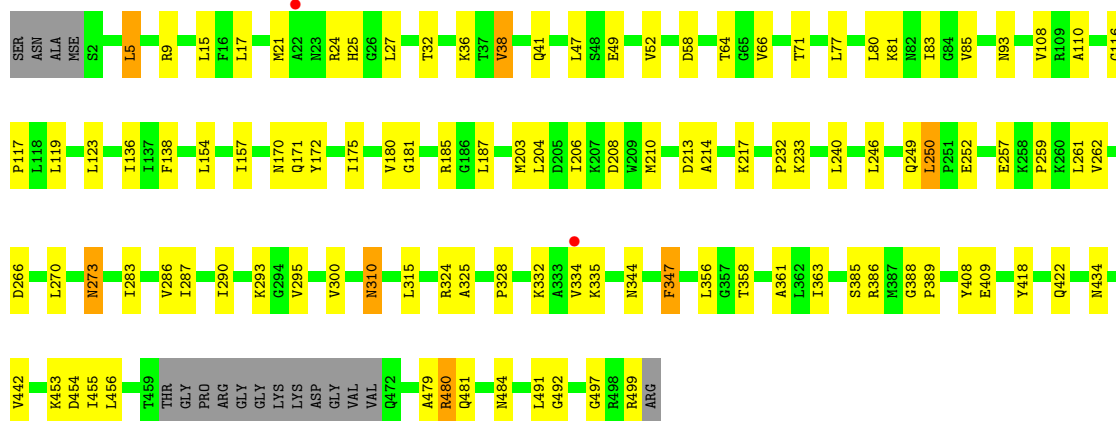
• Molecule 1: HerA like helicase YjgR





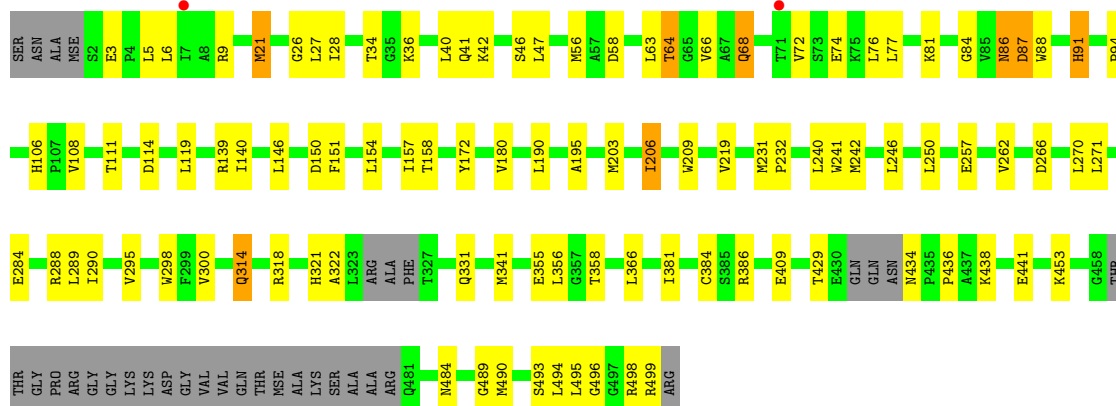
- Molecule 1: HerA like helicase YjgR

Chain D: 75% 20%



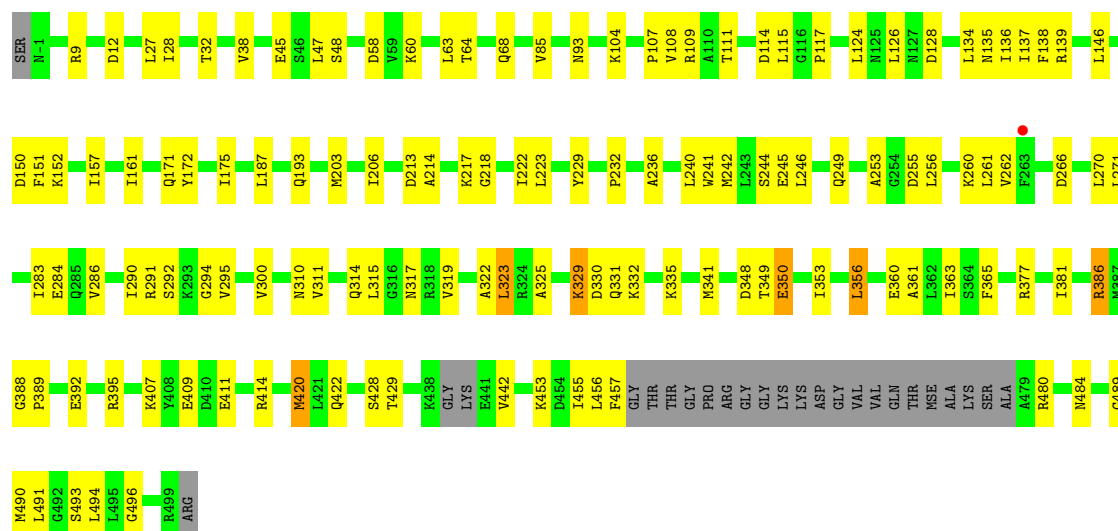
- Molecule 1: HerA like helicase YjgR

Chain E: 73% 18% 7%



- Molecule 1: HerA like helicase YjgR

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.64Å 229.36Å 99.53Å 90.00° 112.88° 90.00°	Depositor
Resolution (Å)	47.04 – 2.90 47.04 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.04-2.90) 98.7 (47.04-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.216 , 0.256 0.216 , 0.256	Depositor DCC
R_{free} test set	3575 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22184	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: 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	0.10	0/3713	0.26	0/5010
1	B	0.09	0/3740	0.25	0/5045
1	C	0.11	0/3723	0.26	0/5017
1	D	0.10	0/3774	0.28	0/5089
1	E	0.10	0/3647	0.25	0/4918
1	F	0.11	0/3721	0.27	1/5018 (0.0%)
All	All	0.10	0/22318	0.26	1/30097 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	311	VAL	N-CA-C	-5.41	107.55	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3660	0	3697	53	0
1	B	3687	0	3729	62	0
1	C	3675	0	3721	48	0
1	D	3722	0	3763	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3597	0	3636	51	0
1	F	3670	0	3708	68	0
2	A	27	0	12	0	0
2	B	31	0	12	0	0
2	C	27	0	12	1	0
2	D	31	0	12	2	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	D	1	0	0	0	0
All	All	22184	0	22326	332	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 7.

All (332) 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:E:72:VAL:HG12	1:E:77:LEU:HD11	1.74	0.69
1:A:171:GLN:HG2	1:A:442:VAL:HG13	1.79	0.64
1:C:325:ALA:HB2	1:C:334:VAL:HG21	1.81	0.62
1:E:47:LEU:HD13	1:E:262:VAL:HG21	1.83	0.60
1:A:325:ALA:HB2	1:A:334:VAL:HG21	1.84	0.60
1:A:240:LEU:HD22	1:A:271:LEU:HD11	1.84	0.59
1:C:470:VAL:HG12	1:C:474:MSE:HE2	1.85	0.59
1:D:249:GLN:HG3	1:D:497:GLY:HA3	1.84	0.59
1:D:52:VAL:HG11	1:D:259:PRO:HD2	1.85	0.58
1:F:284:GLU:HB2	1:F:310:ASN:HD22	1.67	0.58
1:D:41:GLN:HG3	1:D:66:VAL:HG22	1.85	0.58
1:E:40:LEU:HD23	1:E:63:LEU:HD21	1.86	0.58
1:F:9:ARG:HG2	1:F:381:ILE:HD11	1.85	0.58
1:D:32:THR:OG1	1:F:291:ARG:NH2	2.36	0.58
1:E:284:GLU:OE2	1:E:288:ARG:NH2	2.37	0.58
1:A:49:GLU:HA	1:A:217:LYS:HD2	1.85	0.58
1:C:158:THR:HG22	1:C:180:VAL:HG13	1.86	0.58
1:D:453:LYS:HE2	1:D:481:GLN:HE22	1.67	0.58
1:B:157:ILE:HD11	1:B:456:LEU:HG	1.86	0.58
1:D:171:GLN:HG2	1:D:442:VAL:HG13	1.86	0.58
1:F:27:LEU:HB2	1:F:315:LEU:HD13	1.86	0.57
1:F:244:SER:HB3	1:F:491:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ARG:HB3	1:C:326:PHE:CE2	2.40	0.57
1:E:438:LYS:HB3	1:E:441:GLU:HB2	1.87	0.56
1:F:266:ASP:HA	1:F:300:VAL:HB	1.86	0.56
1:A:41:GLN:HE21	1:A:385:SER:HB2	1.70	0.56
1:B:41:GLN:HG3	1:B:66:VAL:HG22	1.87	0.56
1:D:119:LEU:HD21	1:D:240:LEU:HD22	1.88	0.56
1:D:116:GLY:HA3	1:D:492:GLY:HA3	1.87	0.56
1:D:175:ILE:HD12	1:D:180:VAL:HG21	1.87	0.56
1:E:58:ASP:OD2	1:E:64:THR:OG1	2.23	0.56
1:A:210:MSE:HE1	1:A:250:LEU:HD21	1.89	0.55
1:F:150:ASP:OD1	1:F:151:PHE:N	2.38	0.55
1:A:41:GLN:HG3	1:A:66:VAL:HG22	1.88	0.55
1:A:158:THR:HG22	1:A:180:VAL:HG13	1.87	0.55
1:E:266:ASP:HA	1:E:300:VAL:HB	1.87	0.55
1:A:319:VAL:HG22	1:A:363:ILE:HG13	1.89	0.55
1:F:322:ALA:N	1:F:356:LEU:HD11	2.22	0.54
1:F:429:THR:HB	1:F:484:ASN:HB2	1.89	0.54
1:B:47:LEU:HD13	1:B:262:VAL:HG21	1.88	0.54
1:C:203:MSE:SE	1:C:498:ARG:HG3	2.58	0.54
1:A:202:PRO:HD3	1:A:412:VAL:HG23	1.89	0.54
1:B:27:LEU:HB2	1:B:315:LEU:HD13	1.89	0.54
1:D:434:ASN:O	1:E:139:ARG:NH2	2.41	0.54
1:C:124:LEU:HD21	1:C:187:LEU:HD23	1.90	0.54
1:B:108:VAL:HG21	1:B:242:MSE:HE3	1.89	0.53
1:C:266:ASP:HA	1:C:300:VAL:HB	1.90	0.53
1:C:136:ILE:HG23	1:C:172:TYR:HB3	1.89	0.53
1:B:232:PRO:HB3	1:B:270:LEU:HD22	1.90	0.53
1:D:21:MSE:SE	1:D:24:ARG:HE	2.41	0.53
1:A:126:LEU:HB3	1:A:130:GLN:HB2	1.90	0.53
1:E:209:TRP:HH2	1:E:242:MSE:HB3	1.74	0.53
1:E:87:ASP:OD1	1:E:87:ASP:N	2.42	0.53
1:C:471:VAL:HA	1:C:474:MSE:HE3	1.91	0.53
1:F:392:GLU:HG2	1:F:395:ARG:HH22	1.73	0.53
1:D:232:PRO:HB3	1:D:270:LEU:HD22	1.91	0.52
1:E:158:THR:HG22	1:E:180:VAL:HG13	1.89	0.52
1:C:79:ARG:O	1:C:83:ILE:HG12	2.10	0.52
1:F:386:ARG:HG3	1:F:388:GLY:H	1.74	0.52
1:B:349:THR:O	1:B:353:ILE:HG12	2.10	0.52
1:F:325:ALA:HA	1:F:330:ASP:HB3	1.91	0.52
1:A:414:ARG:NH1	1:A:418:TYR:OH	2.43	0.52
1:B:171:GLN:HB2	1:B:443:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ILE:HG23	1:D:172:TYR:HB3	1.92	0.52
1:B:332:LYS:O	1:B:336:ALA:N	2.32	0.51
1:C:5:LEU:HD21	1:C:19:PRO:HG3	1.92	0.51
1:D:110:ALA:HA	1:D:203:MSE:HG3	1.92	0.51
1:E:3:GLU:N	1:E:3:GLU:OE1	2.43	0.51
1:A:266:ASP:HA	1:A:300:VAL:HB	1.90	0.51
1:A:15:LEU:HD13	1:A:363:ILE:HB	1.91	0.51
1:C:150:ASP:OD1	1:C:151:PHE:N	2.40	0.51
1:D:213:ASP:OD1	1:D:214:ALA:N	2.41	0.51
1:D:286:VAL:HG21	1:D:491:LEU:HD11	1.93	0.51
1:D:344:ASN:HB3	1:D:347:PHE:CE1	2.45	0.51
1:D:58:ASP:OD2	1:D:64:THR:OG1	2.25	0.51
1:E:106:HIS:ND1	1:E:409:GLU:OE2	2.44	0.51
1:F:45:GLU:HG3	1:F:93:ASN:HD21	1.76	0.51
1:B:203:MSE:SE	1:B:498:ARG:HG3	2.61	0.51
1:D:356:LEU:HD13	1:D:361:ALA:HA	1.93	0.51
1:F:48:SER:OG	1:F:218:GLY:O	2.26	0.51
1:B:80:LEU:HB3	1:B:85:VAL:HG22	1.94	0.50
1:B:136:ILE:HG21	1:B:175:ILE:HD11	1.92	0.50
1:A:136:ILE:HG23	1:A:172:TYR:HB3	1.92	0.50
1:A:210:MSE:HE3	1:A:246:LEU:HD11	1.93	0.50
1:E:119:LEU:HD13	1:E:241:TRP:HB2	1.93	0.50
1:B:213:ASP:N	1:B:217:LYS:O	2.38	0.50
1:E:232:PRO:HB3	1:E:270:LEU:HD13	1.94	0.50
1:B:386:ARG:HG2	1:B:388:GLY:H	1.76	0.50
1:C:27:LEU:HB2	1:C:315:LEU:HD13	1.94	0.50
1:B:3:GLU:N	1:B:3:GLU:OE1	2.44	0.50
1:C:342:ARG:HG2	1:C:374:VAL:HA	1.94	0.50
1:C:118:LEU:HD23	1:C:491:LEU:HA	1.94	0.50
1:E:6:LEU:HD21	1:E:9:ARG:HB3	1.94	0.50
1:B:106:HIS:ND1	1:B:409:GLU:OE2	2.36	0.49
1:F:489:GLY:N	1:F:493:SER:O	2.41	0.49
1:A:117:PRO:HG3	1:A:138:PHE:HB2	1.94	0.49
1:D:266:ASP:HA	1:D:300:VAL:HB	1.94	0.49
1:D:273:ASN:HD22	1:D:273:ASN:C	2.21	0.49
1:E:72:VAL:HG22	1:E:88:TRP:HZ3	1.77	0.49
1:A:47:LEU:HD13	1:A:262:VAL:HG21	1.94	0.49
1:F:240:LEU:HD21	1:F:283:ILE:HD11	1.93	0.49
1:F:420:MSE:H	1:F:420:MSE:HG2	1.43	0.49
1:B:240:LEU:HD22	1:B:271:LEU:HD11	1.94	0.49
1:F:353:ILE:HA	1:F:356:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ILE:HG12	1:C:295:VAL:HB	1.94	0.49
1:D:25:HIS:NE2	1:D:287:ILE:O	2.44	0.49
1:B:29:THR:OG1	1:B:320:GLN:NE2	2.46	0.49
1:D:157:ILE:HD11	1:D:456:LEU:HG	1.95	0.49
1:D:386:ARG:NH1	1:D:389:PRO:O	2.45	0.49
1:F:260:LYS:N	1:F:294:GLY:O	2.44	0.48
1:A:139:ARG:NH1	1:B:484:ASN:OD1	2.42	0.48
1:B:268:ALA:HB3	1:B:301:SER:HB2	1.95	0.48
1:E:429:THR:CG2	1:E:484:ASN:HB2	2.44	0.48
1:F:229:TYR:HE1	1:F:270:LEU:HD11	1.78	0.48
1:D:117:PRO:HG3	1:D:138:PHE:CG	2.49	0.48
1:A:9:ARG:HD3	1:A:83:ILE:HG22	1.94	0.48
1:B:95:VAL:HG22	1:B:220:ILE:HB	1.95	0.48
1:A:72:VAL:HG23	1:A:77:LEU:HD11	1.95	0.48
1:E:146:LEU:HD21	1:E:453:LYS:HG2	1.96	0.48
1:F:115:LEU:HD23	1:F:115:LEU:H	1.79	0.48
1:F:136:ILE:HG23	1:F:172:TYR:HB3	1.96	0.48
1:F:213:ASP:N	1:F:217:LYS:O	2.46	0.48
1:B:316:GLY:HA3	1:B:366:LEU:HD11	1.95	0.48
1:E:9:ARG:HG2	1:E:381:ILE:HD11	1.94	0.48
1:E:489:GLY:N	1:E:493:SER:O	2.45	0.48
1:F:47:LEU:HD13	1:F:262:VAL:HG21	1.95	0.48
1:B:28:ILE:HG12	1:B:300:VAL:HG22	1.96	0.48
1:D:49:GLU:HA	1:D:217:LYS:HD2	1.96	0.48
1:F:58:ASP:OD2	1:F:64:THR:OG1	2.30	0.47
1:F:349:THR:O	1:F:353:ILE:HG12	2.14	0.47
1:C:319:VAL:HG22	1:C:363:ILE:HG13	1.96	0.47
1:C:246:LEU:HD21	1:C:261:LEU:HD22	1.96	0.47
1:F:157:ILE:O	1:F:161:ILE:HG12	2.14	0.47
1:C:324:ARG:HE	1:C:326:PHE:HE2	1.62	0.47
1:B:317:ASN:HB3	1:B:365:PHE:HD1	1.79	0.47
1:B:319:VAL:HG22	1:B:363:ILE:HG23	1.97	0.47
1:F:232:PRO:HB3	1:F:270:LEU:HD22	1.97	0.47
1:B:41:GLN:HE21	1:B:385:SER:HB2	1.78	0.47
1:D:80:LEU:HB3	1:D:85:VAL:HB	1.97	0.47
1:E:42:LYS:NZ	1:E:46:SER:OG	2.47	0.47
1:F:360:GLU:CD	1:F:377:ARG:HE	2.22	0.47
1:B:72:VAL:HG22	1:B:88:TRP:HZ3	1.80	0.47
1:A:494:LEU:HD23	1:A:498:ARG:HG2	1.97	0.47
1:B:286:VAL:HG21	1:B:491:LEU:HG	1.96	0.47
1:F:124:LEU:HD21	1:F:187:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:TYR:CE1	1:F:270:LEU:HD11	2.50	0.47
1:F:319:VAL:HG22	1:F:363:ILE:HG12	1.97	0.47
1:C:253:ALA:HB3	1:C:256:LEU:HD11	1.97	0.46
1:F:111:THR:OG1	1:F:114:ASP:OD2	2.31	0.46
1:D:386:ARG:HG3	1:D:388:GLY:H	1.80	0.46
1:E:26:GLY:HA3	1:E:298:TRP:CD2	2.51	0.46
1:F:392:GLU:HG2	1:F:395:ARG:NH2	2.30	0.46
1:D:15:LEU:HD13	1:D:363:ILE:HB	1.97	0.46
1:E:150:ASP:OD1	1:E:151:PHE:N	2.40	0.46
1:B:34:THR:HG21	1:B:322:ALA:H	1.80	0.46
1:B:158:THR:HG22	1:B:180:VAL:HG13	1.96	0.46
1:B:264:PHE:CD1	1:B:298:TRP:HB2	2.51	0.46
1:B:426:GLN:HG2	1:B:482:VAL:HG12	1.97	0.46
1:F:107:PRO:HG2	1:F:409:GLU:HA	1.98	0.46
1:E:436:PRO:HA	1:E:484:ASN:HA	1.98	0.46
1:A:66:VAL:HG12	1:A:93:ASN:HB2	1.98	0.46
1:A:68:GLN:HG3	1:A:386:ARG:NH2	2.31	0.46
1:B:290:ILE:HG12	1:B:295:VAL:HB	1.97	0.46
1:D:154:LEU:HD23	1:D:187:LEU:HD21	1.98	0.46
1:C:15:LEU:HD23	1:C:363:ILE:HB	1.96	0.46
1:C:240:LEU:HD22	1:C:271:LEU:HD11	1.97	0.46
1:D:484:ASN:OD1	1:E:139:ARG:NH1	2.43	0.46
1:E:289:LEU:HD12	1:E:490:MSE:HE1	1.98	0.46
1:C:41:GLN:HG3	1:C:66:VAL:HG22	1.97	0.46
1:C:203:MSE:HE2	1:C:203:MSE:HB3	1.80	0.46
1:E:27:LEU:HB3	1:E:318:ARG:HD3	1.98	0.46
1:E:86:ASN:O	1:E:86:ASN:ND2	2.40	0.46
1:F:236:ALA:HB1	1:F:271:LEU:HD13	1.97	0.46
1:F:317:ASN:HB3	1:F:365:PHE:HD1	1.81	0.45
1:B:40:LEU:HD13	1:B:300:VAL:HG21	1.98	0.45
1:D:36:LYS:HB2	1:D:36:LYS:HE3	1.75	0.45
1:D:77:LEU:O	1:D:81:LYS:HG3	2.17	0.45
1:D:208:ASP:OD2	1:D:408:TYR:OH	2.26	0.45
1:D:27:LEU:HB2	1:D:315:LEU:HD13	1.97	0.45
1:A:316:GLY:HA3	1:A:366:LEU:HD11	1.99	0.45
1:F:152:LYS:NZ	1:F:414:ARG:HD3	2.32	0.45
1:A:134:LEU:HD13	1:A:183:ILE:HD13	1.98	0.45
1:B:93:ASN:ND2	1:B:385:SER:OG	2.50	0.45
1:B:49:GLU:HA	1:B:217:LYS:HD2	1.98	0.45
1:A:146:LEU:HD11	1:A:453:LYS:HG2	1.98	0.44
1:A:440:LYS:HE2	1:A:440:LYS:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:ARG:NH1	1:F:389:PRO:O	2.45	0.44
1:C:41:GLN:HE21	1:C:385:SER:HB2	1.82	0.44
1:D:210:MSE:HE3	1:D:250:LEU:HD21	1.99	0.44
1:E:290:ILE:HG12	1:E:295:VAL:HB	1.98	0.44
1:B:325:ALA:HB2	1:B:334:VAL:HG21	1.98	0.44
1:E:190:LEU:HB3	1:E:195:ALA:HB3	2.00	0.44
1:D:283:ILE:O	1:D:287:ILE:HG12	2.17	0.44
1:D:328:PRO:O	1:D:332:LYS:HG3	2.17	0.44
1:A:456:LEU:HD13	1:A:480:ARG:HG2	1.99	0.44
1:C:117:PRO:HG3	1:C:138:PHE:HB2	2.00	0.44
1:E:9:ARG:HD3	1:E:84:GLY:HA3	2.00	0.44
1:E:322:ALA:HA	1:E:356:LEU:HD21	1.99	0.44
1:C:422:GLN:NE2	1:C:478:ALA:O	2.51	0.44
1:D:325:ALA:HB2	1:D:334:VAL:HG11	1.99	0.44
1:B:284:GLU:HG3	1:B:314:GLN:HE22	1.83	0.44
1:D:181:GLY:O	1:D:185:ARG:HG3	2.17	0.44
1:F:249:GLN:HG2	1:F:496:GLY:O	2.18	0.44
1:F:428:SER:OG	1:F:494:LEU:HD21	2.18	0.44
1:A:290:ILE:HG12	1:A:295:VAL:HB	2.00	0.43
1:B:153:ASP:OD1	1:B:414:ARG:NH2	2.50	0.43
1:E:36:LYS:HG2	1:E:321:HIS:CD2	2.53	0.43
1:E:111:THR:OG1	1:E:114:ASP:OD2	2.33	0.43
1:A:42:LYS:HE2	1:A:46:SER:OG	2.17	0.43
1:A:53:PRO:HG2	1:A:210:MSE:HA	1.99	0.43
1:A:238:SER:O	1:A:242:MSE:HG3	2.18	0.43
1:C:9:ARG:HG2	1:C:381:ILE:HD11	2.00	0.43
1:C:89:GLN:OE1	1:C:89:GLN:N	2.47	0.43
1:A:453:LYS:HB3	1:A:457:PHE:CE2	2.54	0.43
1:B:338:ALA:HA	1:B:349:THR:HG21	2.00	0.43
1:C:9:ARG:NH2	1:C:14:GLU:OE2	2.51	0.43
1:D:233:LYS:HD2	1:D:233:LYS:HA	1.85	0.43
1:F:150:ASP:HB3	1:F:152:LYS:HG2	2.00	0.43
1:A:247:TYR:O	1:A:293:LYS:NZ	2.36	0.43
1:A:284:GLU:OE2	1:A:288:ARG:NH2	2.52	0.43
1:C:206:ILE:H	1:C:206:ILE:HG13	1.63	0.43
1:E:91:HIS:HD2	1:E:384:CYS:HB2	1.83	0.43
1:F:253:ALA:HB3	1:F:256:LEU:HD11	2.00	0.43
1:B:124:LEU:HD21	1:B:187:LEU:HD23	2.00	0.43
1:C:153:ASP:OD1	1:C:414:ARG:NH2	2.51	0.43
1:F:135:ASN:O	1:F:139:ARG:HB2	2.18	0.43
1:B:32:THR:HB	1:C:291:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:PRO:HG3	1:B:213:ASP:HB2	2.01	0.43
1:B:335:LYS:O	1:B:339:GLN:HG2	2.19	0.43
1:D:358:THR:HG22	2:D:601:ATP:C8	2.54	0.43
1:E:41:GLN:HG3	1:E:66:VAL:HG12	1.99	0.43
1:E:429:THR:HG22	1:E:484:ASN:HB2	1.99	0.43
1:A:78:ALA:O	1:A:82:ASN:ND2	2.37	0.43
1:B:160:TYR:OH	1:B:448:ILE:O	2.35	0.43
1:C:28:ILE:HD11	1:C:43:LEU:HD12	2.01	0.43
1:F:104:LYS:HE3	1:F:395:ARG:NH2	2.33	0.43
1:A:457:PHE:CE1	1:A:480:ARG:HB3	2.54	0.43
1:B:126:LEU:HB3	1:B:130:GLN:HB2	2.01	0.43
1:F:117:PRO:HG3	1:F:138:PHE:HB2	2.01	0.43
1:B:352:ALA:O	1:B:356:LEU:HD22	2.19	0.43
1:C:38:VAL:HG21	2:C:601:ATP:C5	2.54	0.43
1:C:442:VAL:C	1:C:444:VAL:H	2.27	0.43
1:E:34:THR:C	1:E:358:THR:HG23	2.44	0.43
1:A:232:PRO:HB3	1:A:270:LEU:HD22	2.01	0.42
1:B:79:ARG:O	1:B:83:ILE:HG12	2.19	0.42
1:B:317:ASN:HB3	1:B:365:PHE:CD1	2.54	0.42
1:F:203:MSE:HE3	1:F:241:TRP:HZ2	1.84	0.42
1:F:457:PHE:HE2	1:F:480:ARG:H	1.67	0.42
1:A:157:ILE:O	1:A:161:ILE:HG12	2.18	0.42
1:B:63:LEU:O	1:B:66:VAL:HG23	2.18	0.42
1:C:238:SER:O	1:C:242:MSE:HG3	2.19	0.42
1:A:25:HIS:NE2	1:A:287:ILE:O	2.45	0.42
1:C:121:ALA:HB2	1:C:134:LEU:HD23	2.02	0.42
1:E:140:ILE:HG12	1:E:172:TYR:CE2	2.53	0.42
1:B:45:GLU:HG3	1:B:93:ASN:HD21	1.84	0.42
1:F:124:LEU:HB2	1:F:126:LEU:HG	2.01	0.42
1:F:246:LEU:HD21	1:F:261:LEU:HD22	2.00	0.42
1:D:246:LEU:HD21	1:D:261:LEU:HD23	2.01	0.42
1:E:154:LEU:HA	1:E:157:ILE:HG22	2.01	0.42
1:F:206:ILE:HD11	1:F:249:GLN:HB2	2.02	0.42
1:F:245:GLU:OE1	1:F:249:GLN:NE2	2.46	0.42
1:A:324:ARG:HD3	1:A:324:ARG:HA	1.46	0.42
1:B:9:ARG:HD3	1:B:83:ILE:HG22	2.02	0.42
1:C:131:SER:O	1:C:135:ASN:ND2	2.49	0.42
1:A:246:LEU:O	1:A:250:LEU:HD12	2.20	0.42
1:B:68:GLN:HE21	1:B:394:GLU:HB3	1.84	0.42
1:E:94:PRO:HG2	1:E:219:VAL:HA	2.01	0.42
1:E:240:LEU:HD22	1:E:271:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:LEU:HD13	1:F:361:ALA:HA	2.01	0.42
1:F:68:GLN:HB2	1:F:386:ARG:HB3	2.02	0.42
1:A:317:ASN:HB3	1:A:365:PHE:HD1	1.84	0.42
1:D:38:VAL:HG21	2:D:601:ATP:C5	2.55	0.41
1:D:310:ASN:OD1	1:D:310:ASN:N	2.46	0.41
1:E:206:ILE:H	1:E:206:ILE:HG13	1.61	0.41
1:E:68:GLN:HG3	1:E:386:ARG:HH21	1.84	0.41
1:F:223:LEU:HD22	1:F:242:MSE:HE1	2.03	0.41
1:B:453:LYS:HB3	1:B:457:PHE:CE2	2.56	0.41
1:F:146:LEU:HD21	1:F:453:LYS:HG2	2.02	0.41
1:F:350:GLU:CD	1:F:350:GLU:H	2.28	0.41
1:B:23:ASN:OD1	1:B:23:ASN:N	2.52	0.41
1:B:34:THR:HG21	1:B:321:HIS:HB3	2.03	0.41
1:D:252:GLU:OE1	1:D:293:LYS:HG2	2.20	0.41
1:F:286:VAL:HG22	1:F:490:MSE:HE3	2.02	0.41
1:A:213:ASP:HB2	1:A:217:LYS:HB2	2.02	0.41
1:C:62:ASP:OD1	1:C:389:PRO:HG3	2.21	0.41
1:D:47:LEU:HD13	1:D:262:VAL:HG21	2.03	0.41
1:E:88:TRP:NE1	1:E:384:CYS:HA	2.36	0.41
1:D:93:ASN:OD1	1:D:385:SER:OG	2.39	0.41
1:E:288:ARG:CZ	1:E:314:GLN:HE22	2.34	0.41
1:A:88:TRP:CZ3	1:A:90:PRO:HG3	2.56	0.41
1:B:266:ASP:HA	1:B:300:VAL:HB	2.02	0.41
1:C:147:LEU:HD13	1:C:421:LEU:HG	2.02	0.41
1:F:152:LYS:HZ1	1:F:414:ARG:HD3	1.85	0.41
1:F:323:LEU:HD12	1:F:323:LEU:HA	1.90	0.41
1:B:206:ILE:H	1:B:206:ILE:HG13	1.57	0.41
1:C:28:ILE:HG22	1:C:36:LYS:HD2	2.03	0.41
1:C:232:PRO:HB3	1:C:270:LEU:HD22	2.02	0.41
1:D:203:MSE:HG2	1:D:204:LEU:N	2.35	0.41
1:B:90:PRO:HA	1:B:384:CYS:HB3	2.02	0.41
1:D:240:LEU:HD21	1:D:491:LEU:HD22	2.03	0.41
1:D:335:LYS:HD2	1:D:335:LYS:HA	1.92	0.41
1:F:213:ASP:OD1	1:F:214:ALA:N	2.50	0.41
1:A:25:HIS:CE1	1:A:291:ARG:HB3	2.56	0.40
1:A:87:ASP:OD1	1:A:87:ASP:N	2.52	0.40
1:A:247:TYR:HB2	1:A:290:ILE:HD12	2.02	0.40
1:C:158:THR:HB	1:C:184:GLN:NE2	2.36	0.40
1:D:290:ILE:HG12	1:D:295:VAL:HB	2.03	0.40
1:D:418:TYR:HB3	1:D:479:ALA:O	2.20	0.40
1:D:479:ALA:H	1:D:480:ARG:HE	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:LEU:O	1:E:250:LEU:HG	2.21	0.40
1:E:429:THR:HG23	1:E:434:ASN:OD1	2.21	0.40
1:F:290:ILE:HG12	1:F:295:VAL:HB	2.03	0.40
1:F:329:LYS:HE2	1:F:329:LYS:HB3	1.93	0.40
1:F:456:LEU:O	1:F:480:ARG:NH1	2.54	0.40
1:A:241:TRP:CZ2	1:A:245:GLU:HG3	2.55	0.40
1:A:356:LEU:HD13	1:A:360:GLU:O	2.21	0.40
1:C:148:LEU:HD21	1:C:157:ILE:HG13	2.03	0.40
1:F:134:LEU:HA	1:F:137:ILE:HD12	2.02	0.40
1:F:171:GLN:HG2	1:F:442:VAL:HG13	2.02	0.40
1:A:206:ILE:H	1:A:206:ILE:HG13	1.55	0.40
1:B:28:ILE:HG22	1:B:319:VAL:HB	2.04	0.40
1:B:54:VAL:HG22	1:B:262:VAL:HB	2.04	0.40
1:C:52:VAL:HG21	1:C:259:PRO:HD2	2.03	0.40
1:D:456:LEU:HD23	1:D:456:LEU:HA	1.88	0.40
1:A:125:ASN:HB2	1:A:233:LYS:HE2	2.02	0.40
1:B:32:THR:HB	1:C:291:ARG:NH2	2.36	0.40
1:C:249:GLN:HE21	1:C:249:GLN:HB2	1.75	0.40
1:D:5:LEU:HD11	1:D:17:LEU:HD23	2.02	0.40
1:D:32:THR:HG21	1:F:314:GLN:HG2	2.04	0.40
1:E:21:MSE:HG2	1:E:366:LEU:HB2	2.02	0.40
1:E:496:GLY:O	1:E:499:ARG:NH1	2.55	0.40
1:F:64:THR:HA	1:F:222:ILE:HD13	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	474/503 (94%)	460 (97%)	14 (3%)	0	100	100
1	B	477/503 (95%)	459 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	474/503 (94%)	456 (96%)	18 (4%)	0	100	100
1	D	482/503 (96%)	459 (95%)	23 (5%)	0	100	100
1	E	462/503 (92%)	446 (96%)	16 (4%)	0	100	100
1	F	472/503 (94%)	450 (95%)	22 (5%)	0	100	100
All	All	2841/3018 (94%)	2730 (96%)	111 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	390/396 (98%)	360 (92%)	30 (8%)	12	35
1	B	393/396 (99%)	372 (95%)	21 (5%)	20	52
1	C	392/396 (99%)	373 (95%)	19 (5%)	23	55
1	D	397/396 (100%)	376 (95%)	21 (5%)	20	52
1	E	385/396 (97%)	361 (94%)	24 (6%)	16	46
1	F	392/396 (99%)	363 (93%)	29 (7%)	13	38
All	All	2349/2376 (99%)	2205 (94%)	144 (6%)	17	46

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	ARG
1	A	12	ASP
1	A	28	ILE
1	A	40	LEU
1	A	42	LYS
1	A	64	THR
1	A	66	VAL
1	A	72	VAL

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Mol	Chain	Res	Type
1	A	95	VAL
1	A	108	VAL
1	A	115	LEU
1	A	119	LEU
1	A	169	GLN
1	A	206	ILE
1	A	250	LEU
1	A	258	LYS
1	A	324	ARG
1	A	327	THR
1	A	329	LYS
1	A	331	GLN
1	A	341	MSE
1	A	369	LYS
1	A	374	VAL
1	A	381	ILE
1	A	409	GLU
1	A	426	GLN
1	A	440	LYS
1	A	455	ILE
1	A	456	LEU
1	B	5	LEU
1	B	23	ASN
1	B	85	VAL
1	B	86	ASN
1	B	97	VAL
1	B	108	VAL
1	B	119	LEU
1	B	137	ILE
1	B	206	ILE
1	B	210	MSE
1	B	249	GLN
1	B	252	GLU
1	B	302	GLN
1	B	312	LEU
1	B	323	LEU
1	B	324	ARG
1	B	327	THR
1	B	340	THR
1	B	369	LYS
1	B	412	VAL
1	B	426	GLN

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Mol	Chain	Res	Type
1	C	5	LEU
1	C	9	ARG
1	C	64	THR
1	C	66	VAL
1	C	108	VAL
1	C	115	LEU
1	C	169	GLN
1	C	171	GLN
1	C	203	MSE
1	C	206	ILE
1	C	210	MSE
1	C	331	GLN
1	C	342	ARG
1	C	358	THR
1	C	448	ILE
1	C	453	LYS
1	C	477	SER
1	C	480	ARG
1	C	487	VAL
1	D	5	LEU
1	D	9	ARG
1	D	38	VAL
1	D	71	THR
1	D	83	ILE
1	D	108	VAL
1	D	123	LEU
1	D	170	ASN
1	D	206	ILE
1	D	250	LEU
1	D	257	GLU
1	D	273	ASN
1	D	310	ASN
1	D	324	ARG
1	D	347	PHE
1	D	409	GLU
1	D	422	GLN
1	D	454	ASP
1	D	455	ILE
1	D	480	ARG
1	D	499	ARG
1	E	5	LEU
1	E	21	MSE

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Mol	Chain	Res	Type
1	E	28	ILE
1	E	56	MSE
1	E	64	THR
1	E	68	GLN
1	E	74	GLU
1	E	76	LEU
1	E	81	LYS
1	E	86	ASN
1	E	87	ASP
1	E	91	HIS
1	E	108	VAL
1	E	203	MSE
1	E	206	ILE
1	E	231	MSE
1	E	257	GLU
1	E	314	GLN
1	E	331	GLN
1	E	341	MSE
1	E	355	GLU
1	E	494	LEU
1	E	495	LEU
1	E	498	ARG
1	F	12	ASP
1	F	28	ILE
1	F	32	THR
1	F	38	VAL
1	F	60	LYS
1	F	63	LEU
1	F	85	VAL
1	F	108	VAL
1	F	109	ARG
1	F	128	ASP
1	F	175	ILE
1	F	193	GLN
1	F	255	ASP
1	F	292	SER
1	F	323	LEU
1	F	329	LYS
1	F	331	GLN
1	F	332	LYS
1	F	335	LYS
1	F	341	MSE

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Mol	Chain	Res	Type
1	F	348	ASP
1	F	350	GLU
1	F	356	LEU
1	F	386	ARG
1	F	407	LYS
1	F	411	GLU
1	F	420	MSE
1	F	422	GLN
1	F	455	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	41	GLN
1	A	285	GLN
1	A	331	GLN
1	B	41	GLN
1	B	302	GLN
1	B	314	GLN
1	B	320	GLN
1	C	-1	ASN
1	C	41	GLN
1	C	82	ASN
1	C	164	ASN
1	C	193	GLN
1	C	303	ASN
1	D	170	ASN
1	D	193	GLN
1	D	230	GLN
1	D	481	GLN
1	E	23	ASN
1	E	41	GLN
1	E	68	GLN
1	E	82	ASN
1	E	269	HIS
1	E	314	GLN
1	E	396	ASN
1	E	400	ASN
1	E	422	GLN
1	F	93	ASN
1	F	331	GLN

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Mol	Chain	Res	Type
1	F	481	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	D	601	3	32,33,33	0.27	0	48,52,52	0.32	0
2	ATP	F	601	-	28,29,33	0.36	0	43,45,52	0.34	0
2	ATP	E	601	-	28,29,33	0.35	0	43,45,52	0.37	0
2	ATP	A	601	-	28,29,33	0.36	0	43,45,52	0.37	0
2	ATP	B	601	3	32,33,33	0.26	0	48,52,52	0.33	0
2	ATP	C	601	-	28,29,33	0.34	0	43,45,52	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	601	3	-	1/22/38/38	0/3/3/3
2	ATP	F	601	-	-	2/16/32/38	0/3/3/3
2	ATP	E	601	-	-	0/16/32/38	0/3/3/3
2	ATP	A	601	-	-	0/16/32/38	0/3/3/3
2	ATP	B	601	3	-	1/22/38/38	0/3/3/3
2	ATP	C	601	-	-	0/16/32/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

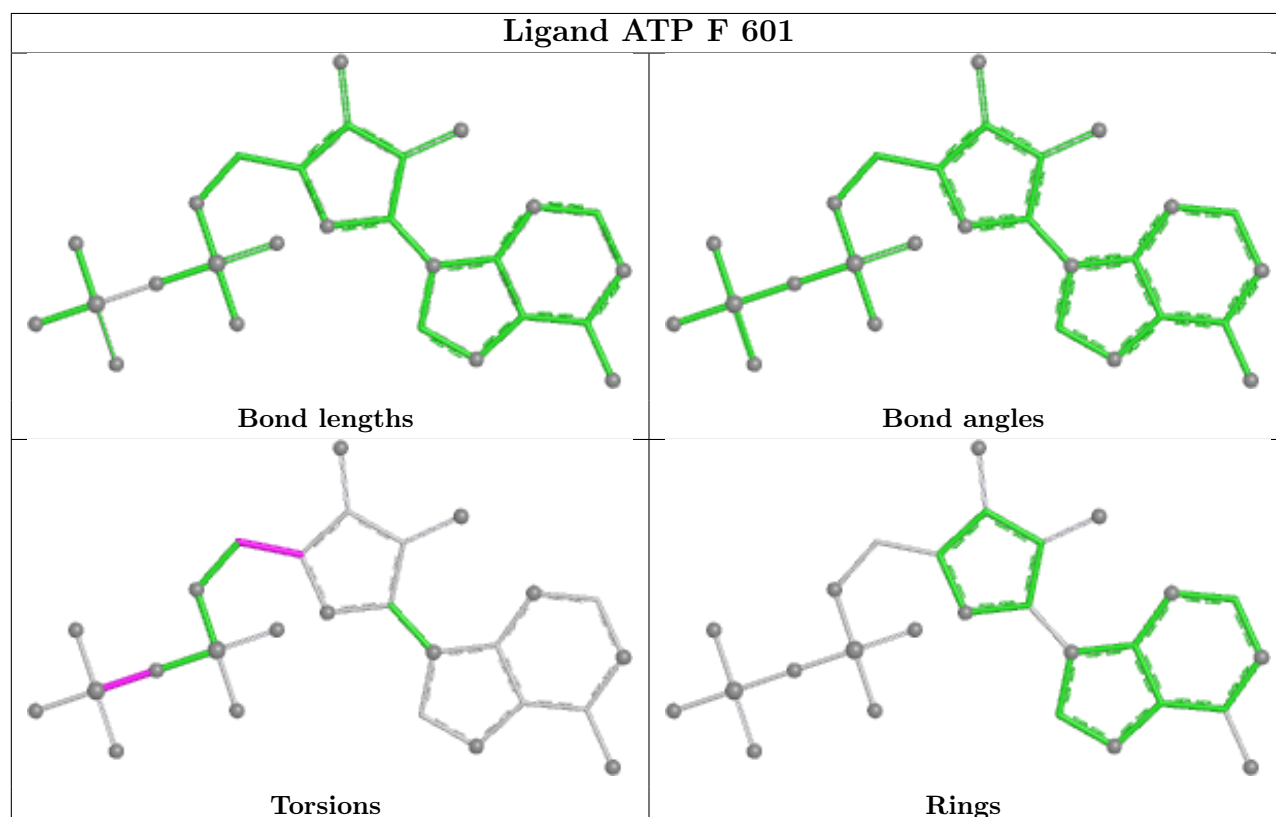
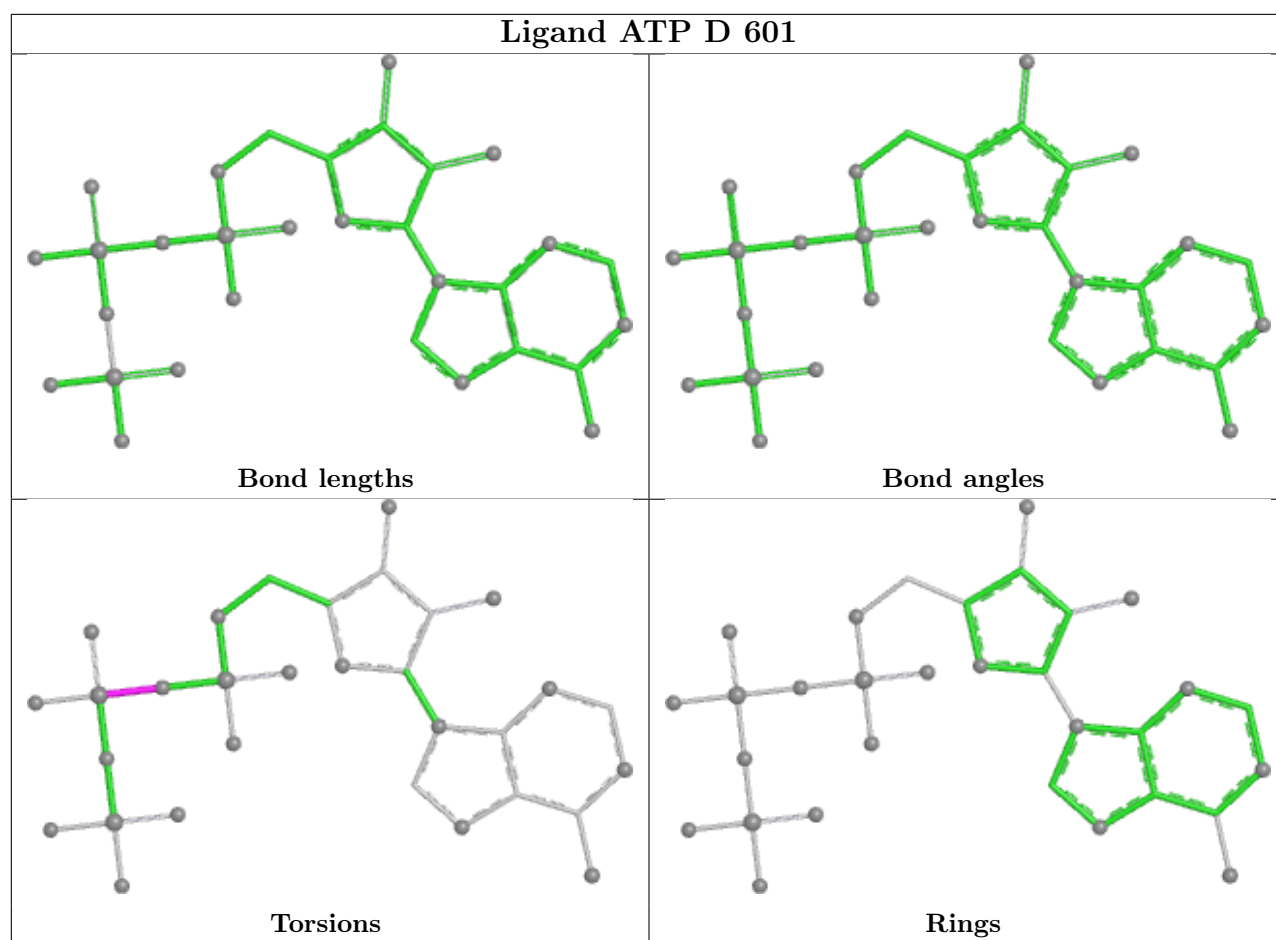
Mol	Chain	Res	Type	Atoms
2	F	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	PA-O3A-PB-O1B
2	F	601	ATP	PA-O3A-PB-O2B
2	D	601	ATP	PA-O3A-PB-O2B

There are no ring outliers.

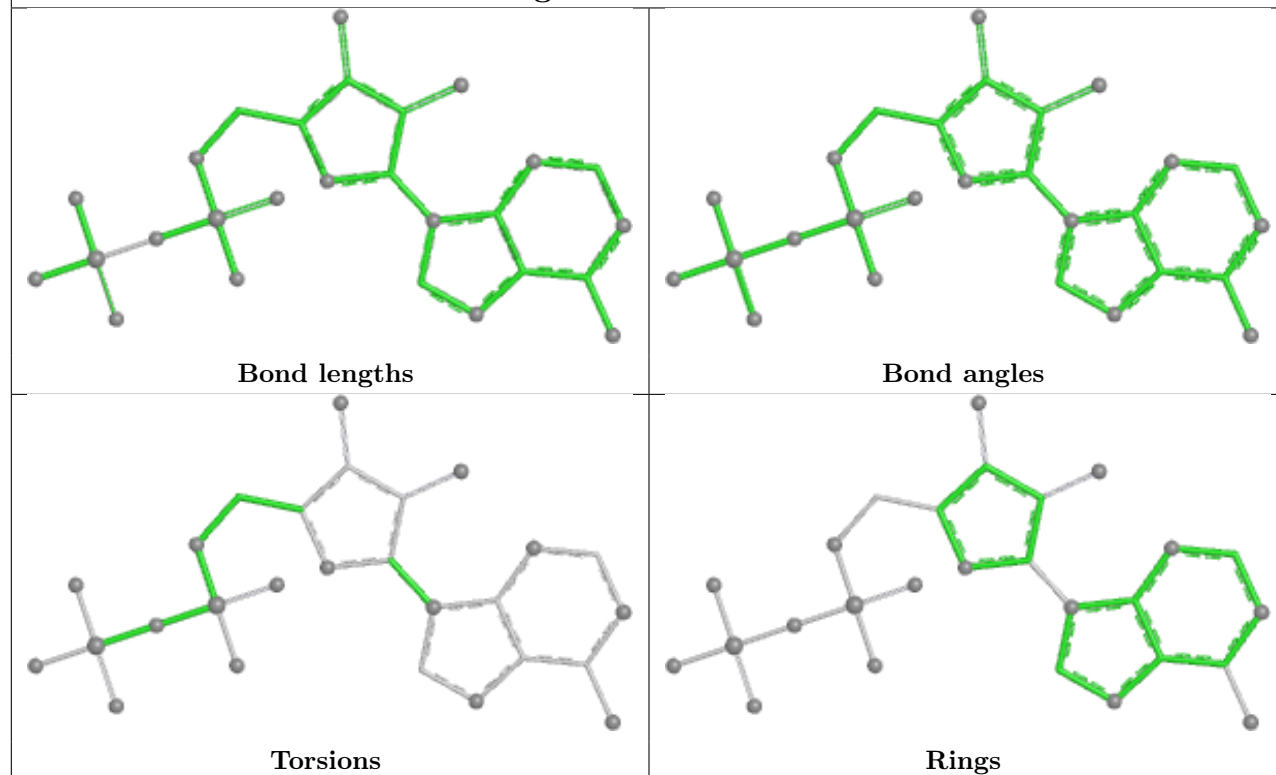
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	ATP	2	0
2	C	601	ATP	1	0

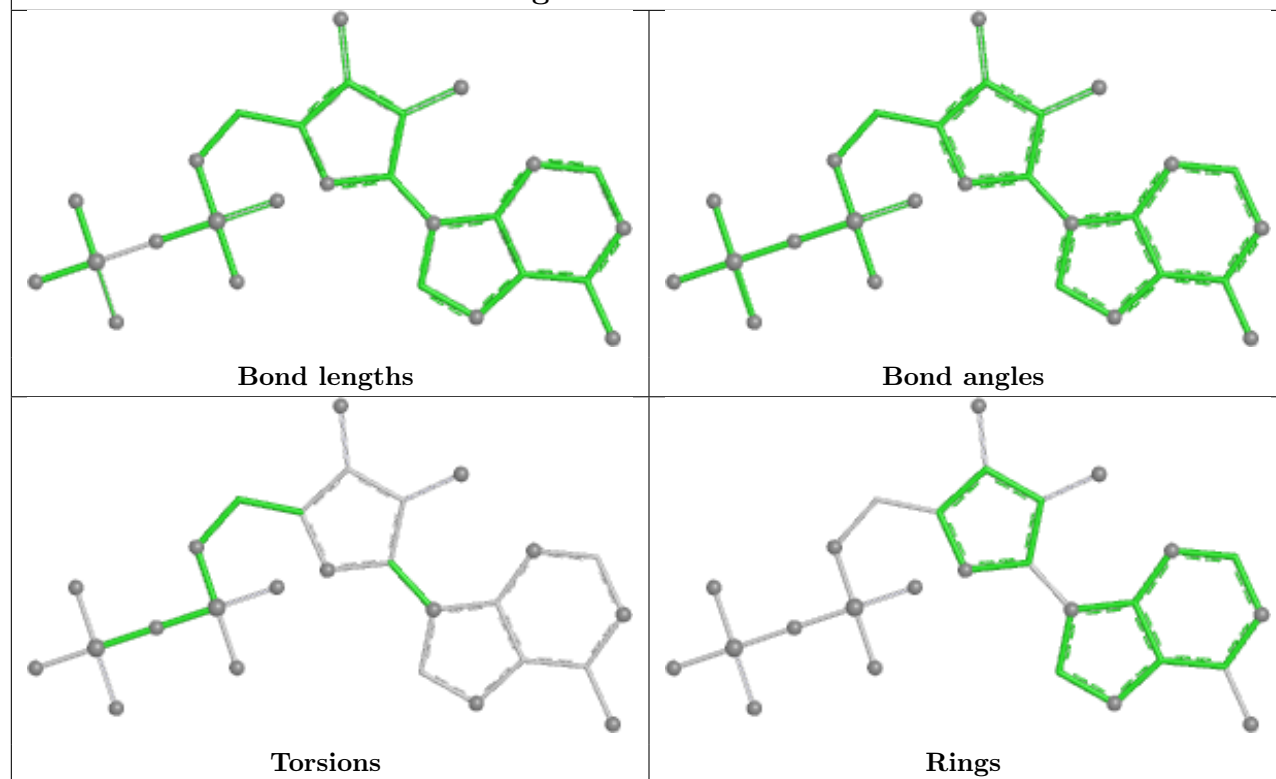
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



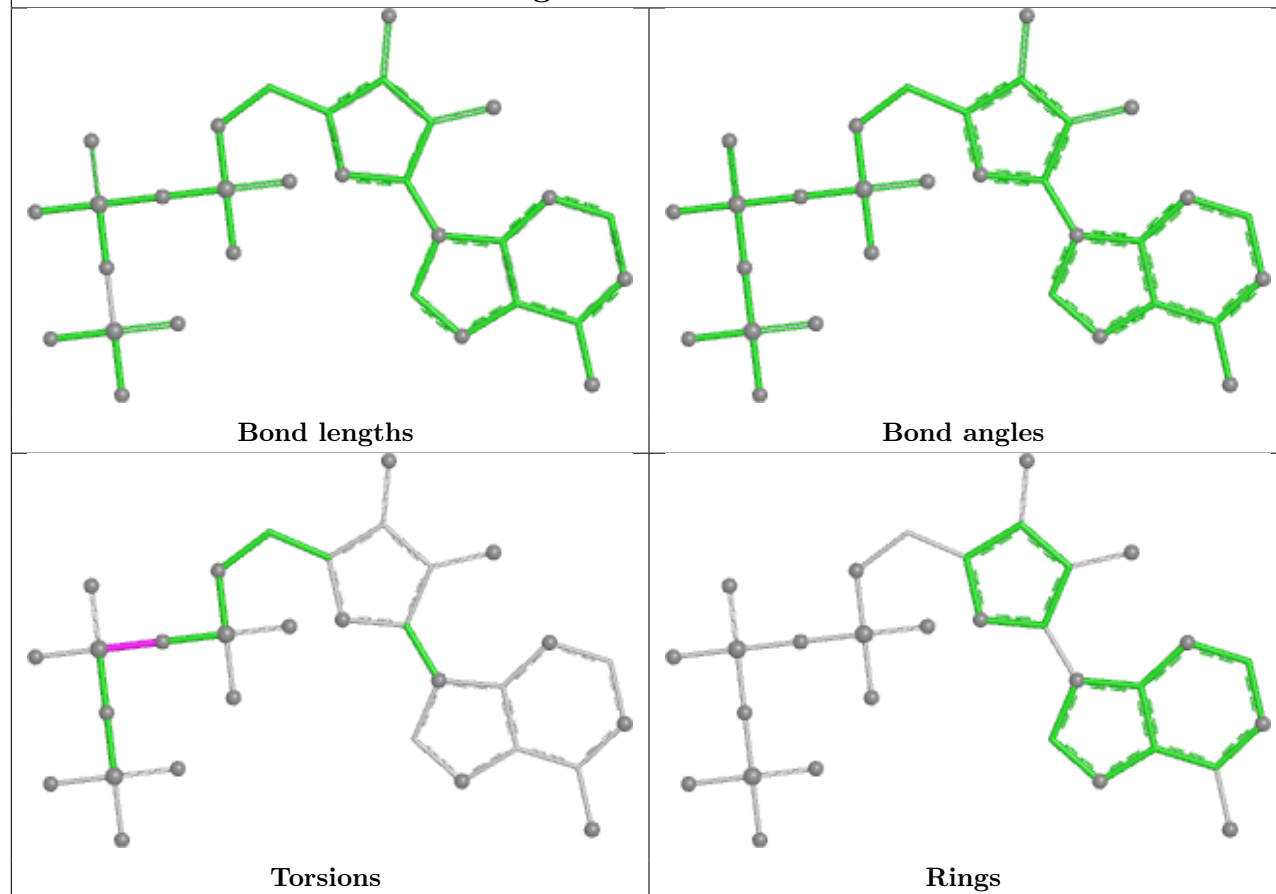
Ligand ATP E 601



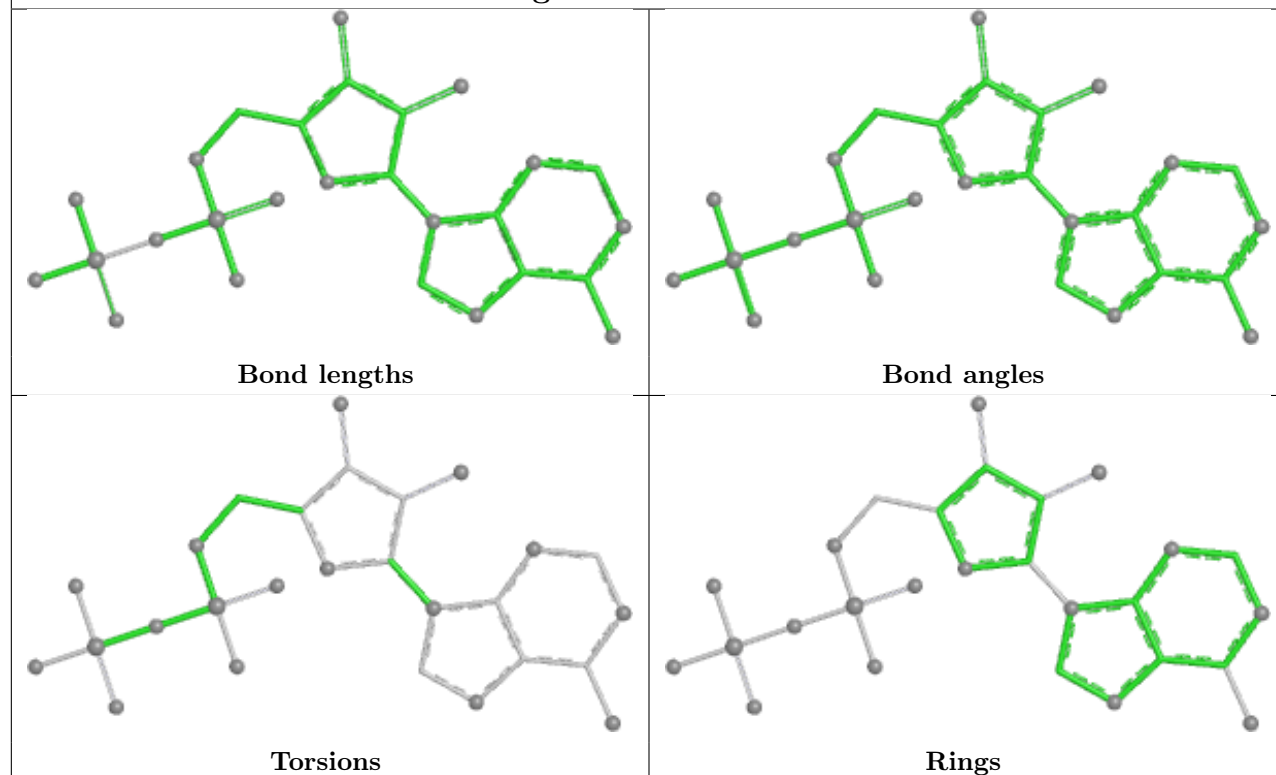
Ligand ATP A 601



Ligand ATP B 601



Ligand ATP C 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/503 (92%)	-0.29	1 (0%) 91 89	54, 72, 100, 123	0
1	B	470/503 (93%)	-0.28	1 (0%) 91 89	54, 77, 108, 128	0
1	C	467/503 (92%)	-0.23	3 (0%) 85 81	53, 75, 110, 138	0
1	D	474/503 (94%)	-0.27	2 (0%) 88 85	55, 79, 113, 136	0
1	E	459/503 (91%)	-0.17	2 (0%) 88 85	56, 91, 130, 156	0
1	F	466/503 (92%)	-0.13	1 (0%) 91 89	67, 100, 133, 150	0
All	All	2803/3018 (92%)	-0.23	10 (0%) 88 85	53, 82, 123, 156	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	ALA	2.8
1	C	151	PHE	2.6
1	E	7	ILE	2.6
1	A	478	ALA	2.5
1	D	334	VAL	2.3
1	F	263	PHE	2.3
1	C	469	GLY	2.2
1	D	22	ALA	2.2
1	B	296	GLY	2.1
1	E	71	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

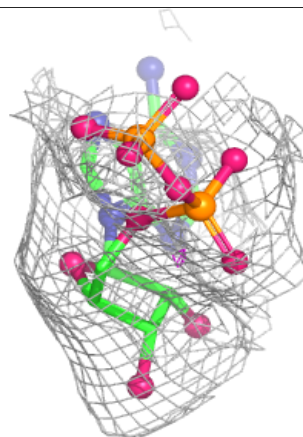
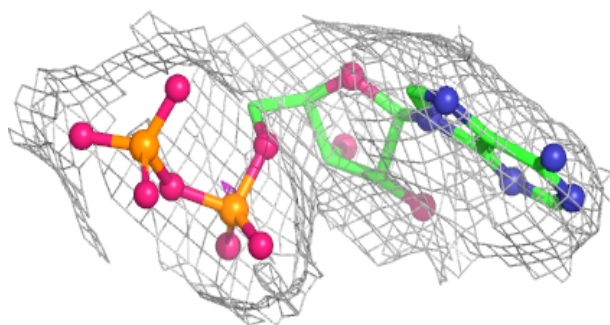
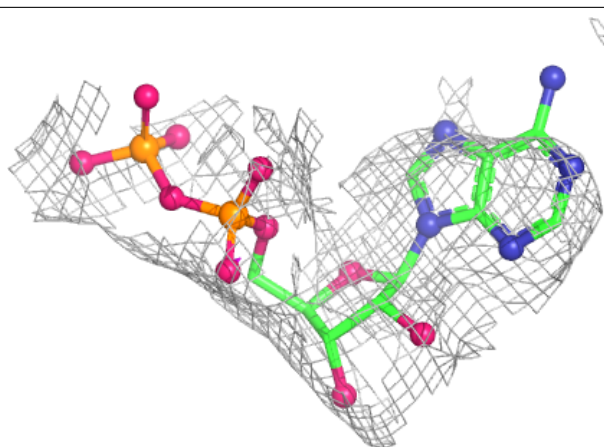
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	E	601	27/31	0.83	0.08	109,113,121,123	0
2	ATP	F	601	27/31	0.84	0.09	94,103,108,111	0
3	MG	D	602	1/1	0.88	0.14	70,70,70,70	0
2	ATP	C	601	27/31	0.91	0.06	72,77,92,94	0
3	MG	B	602	1/1	0.93	0.10	61,61,61,61	0
2	ATP	D	601	31/31	0.93	0.07	66,70,74,83	0
2	ATP	A	601	27/31	0.94	0.05	71,77,87,90	0
2	ATP	B	601	31/31	0.96	0.05	54,61,69,72	0

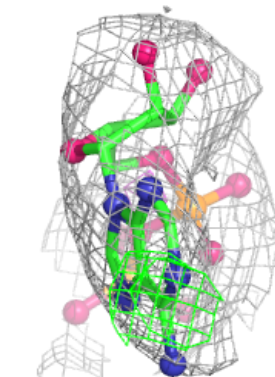
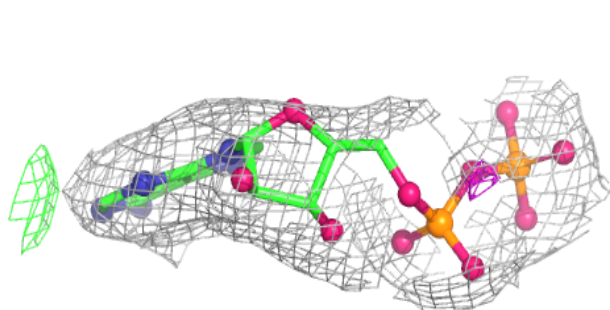
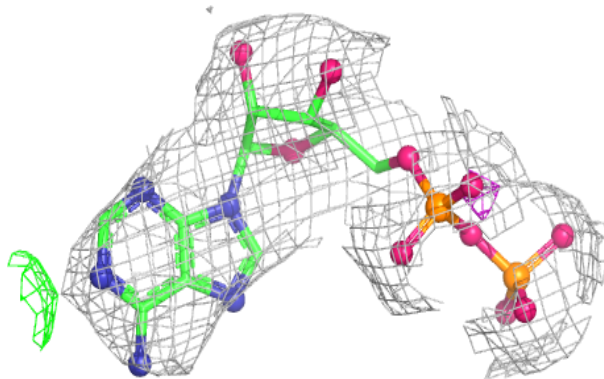
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

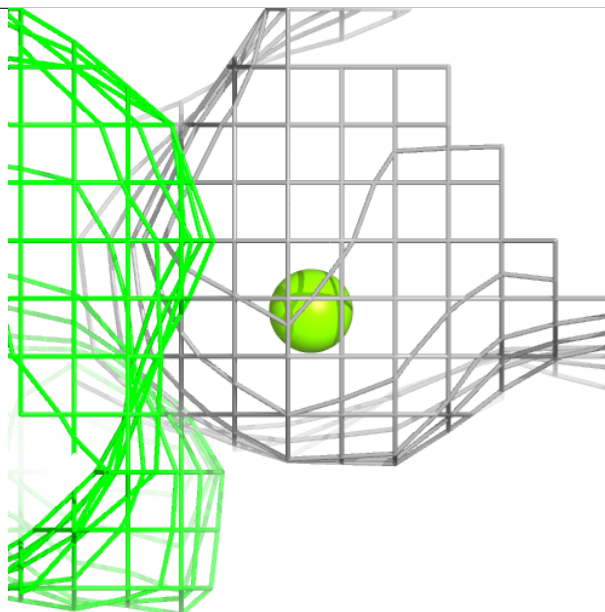
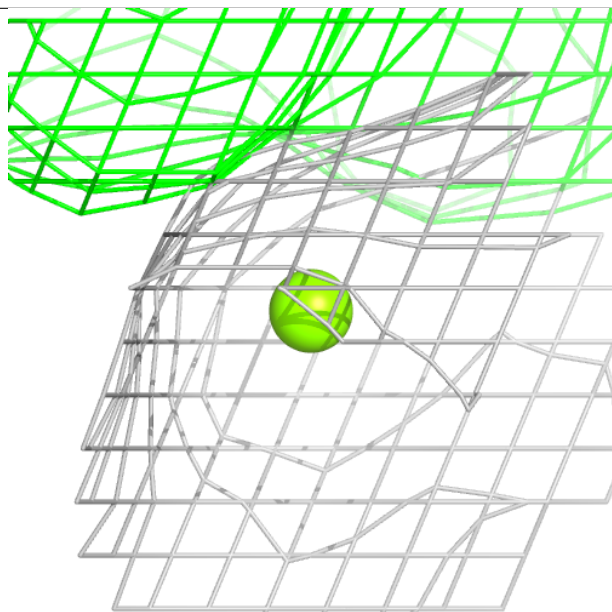
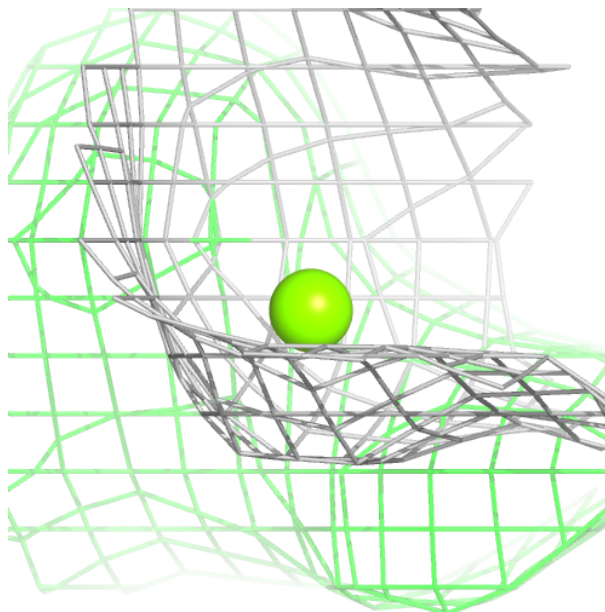
**Electron density around ATP F 601:**

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



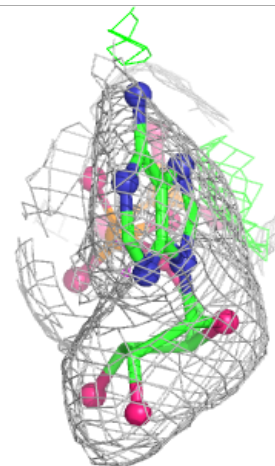
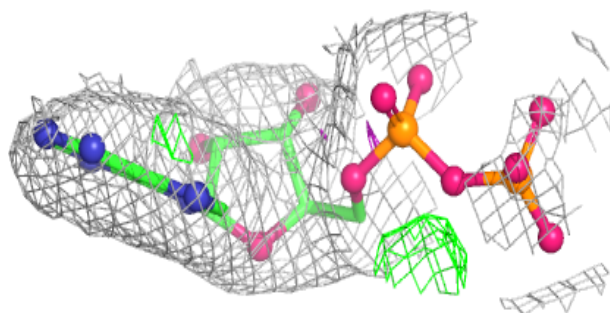
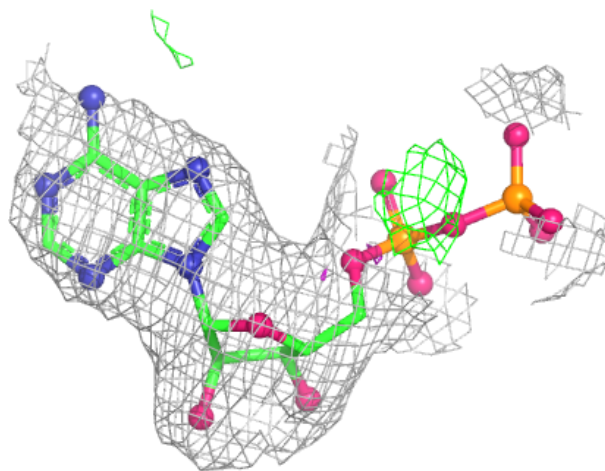
Electron density around MG D 602:

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



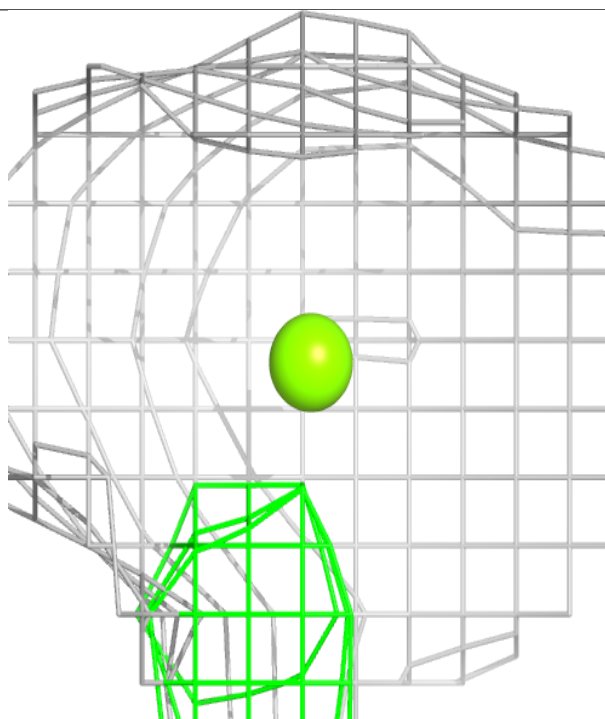
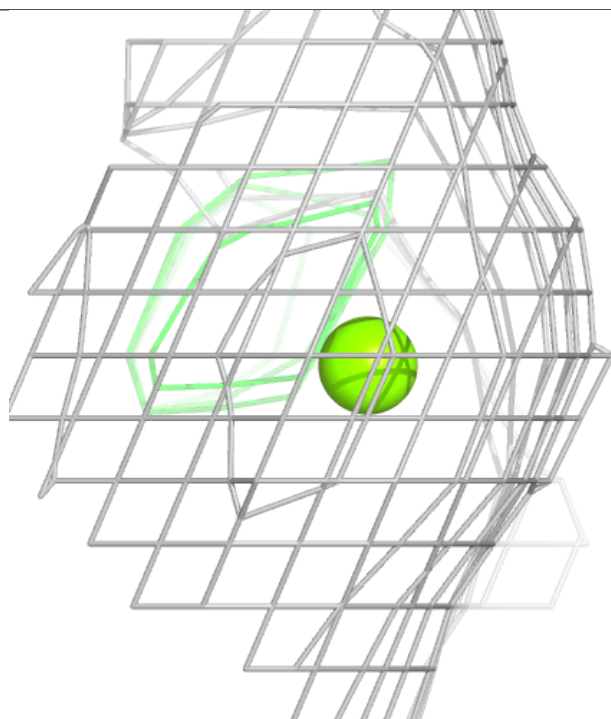
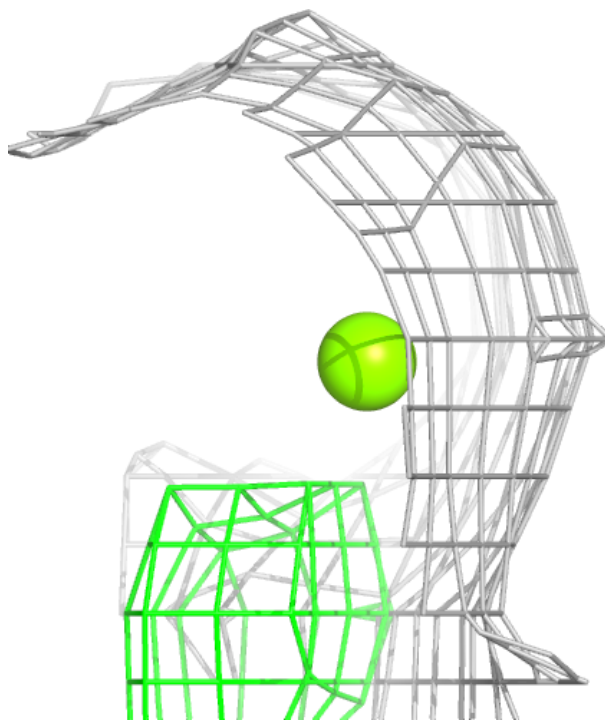
Electron density around ATP C 601:

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



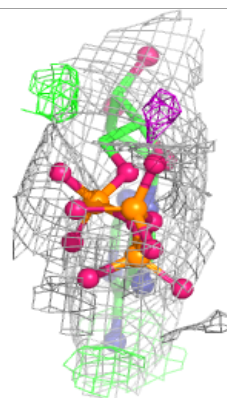
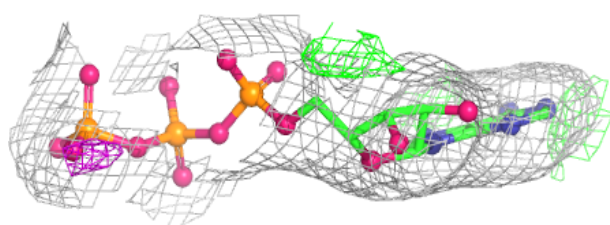
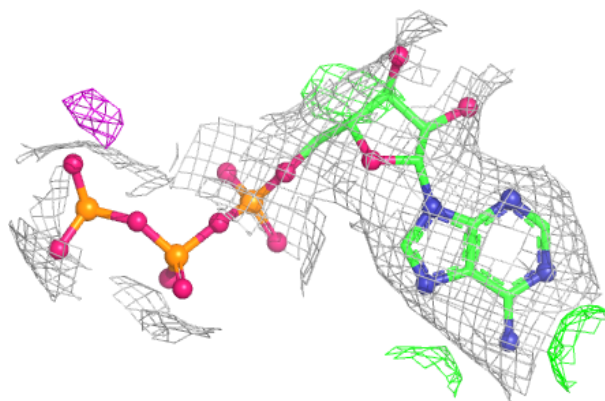
Electron density around MG B 602:

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

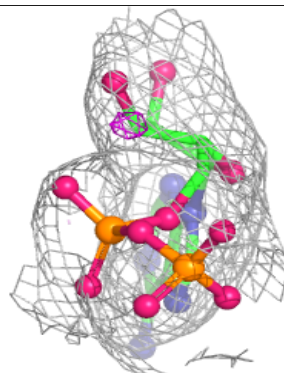
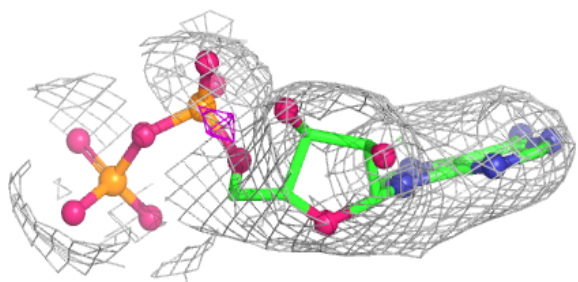
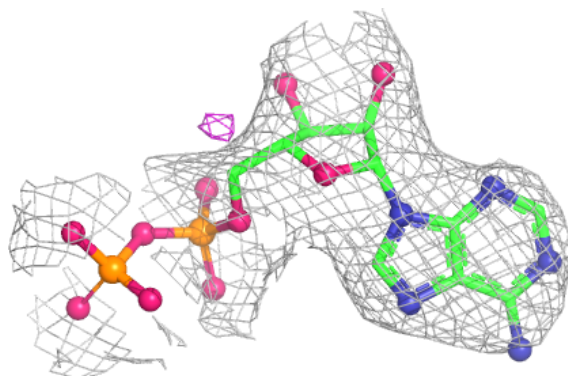


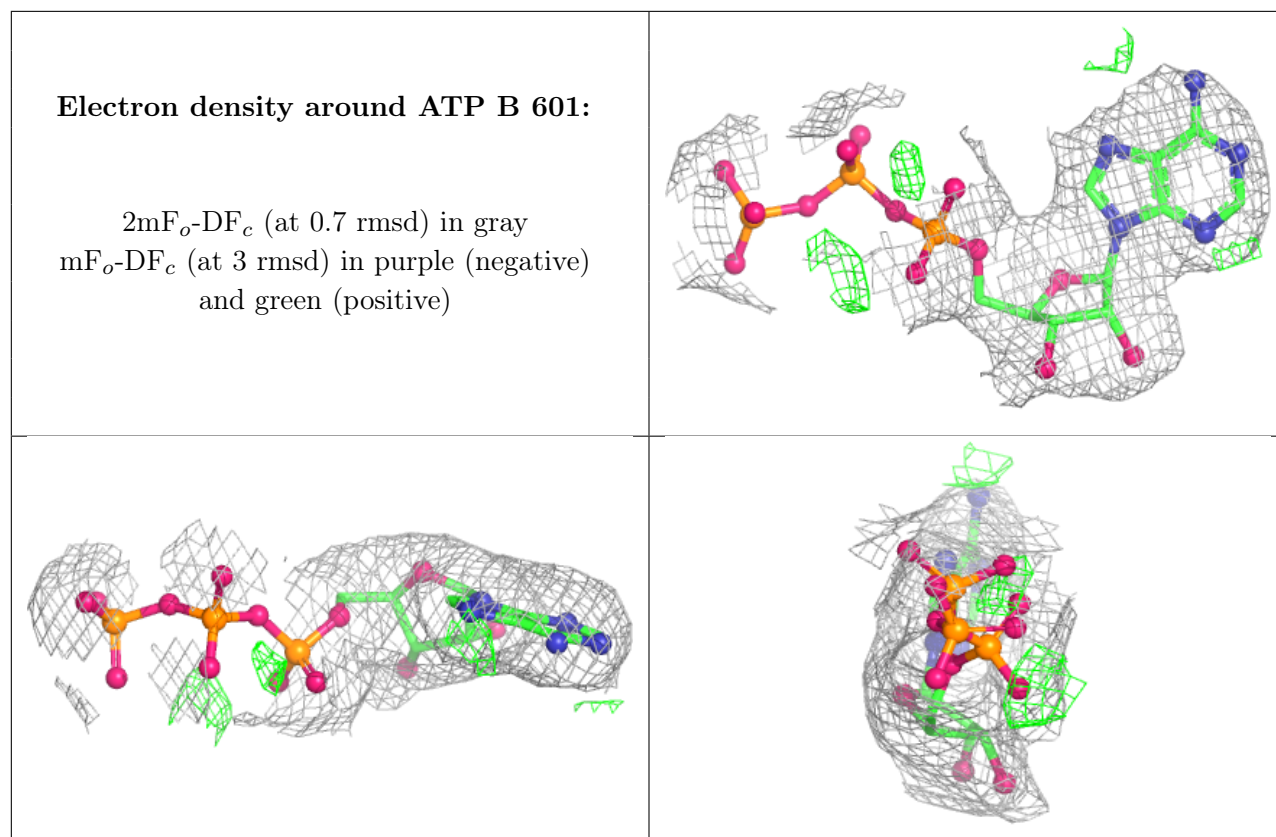
Electron density around ATP D 601:

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

**Electron density around ATP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.