



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:16 PM UTC

PDB ID : 4DUG / pdb_00004dug
Title : Crystal Structure of Circadian Clock Protein KaiC E318A Mutant
Authors : Egli, M.; Mori, T.; Pattanayek, R.; Xu, Y.; Qin, X.; Johnson, C.H.
Deposited on : 2012-02-21
Resolution : 3.29 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

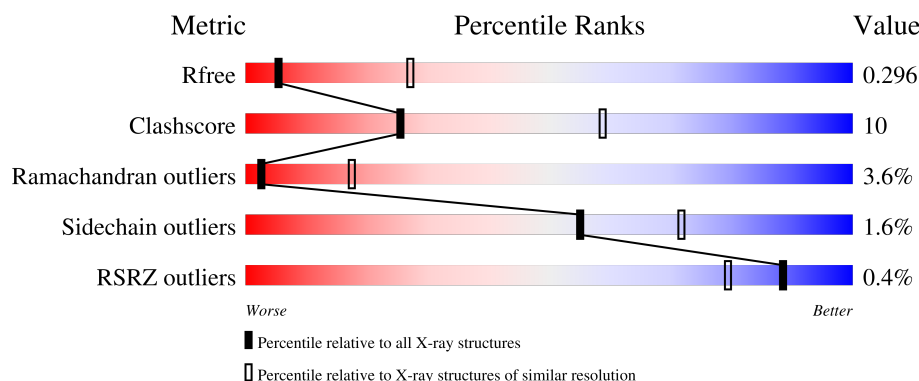
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	% 74% 22% ..
1	B	519	% 66% 29% ..
1	C	519	 72% 22% ..
1	E	519	 67% 28% ..
1	F	519	 68% 28% ..

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Mol	Chain	Length	Quality of chain
2	D	519	73% 21%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24157 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	506	Total	C	N	O	P	S	0	0	0
			3986	2507	701	762	1	15			
1	B	498	Total	C	N	O	P	S	0	0	0
			3925	2471	691	747	1	15			
1	C	497	Total	C	N	O	P	S	0	0	0
			3921	2469	690	746	1	15			
1	E	501	Total	C	N	O	P	S	0	0	0
			3944	2483	692	753	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3986	2507	701	762	1	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ALA	GLU	engineered mutation	UNP Q79PF4
B	318	ALA	GLU	engineered mutation	UNP Q79PF4
C	318	ALA	GLU	engineered mutation	UNP Q79PF4
E	318	ALA	GLU	engineered mutation	UNP Q79PF4
F	318	ALA	GLU	engineered mutation	UNP Q79PF4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	500	Total	C	N	O	S	0	0	0
			3937	2481	694	747	15			

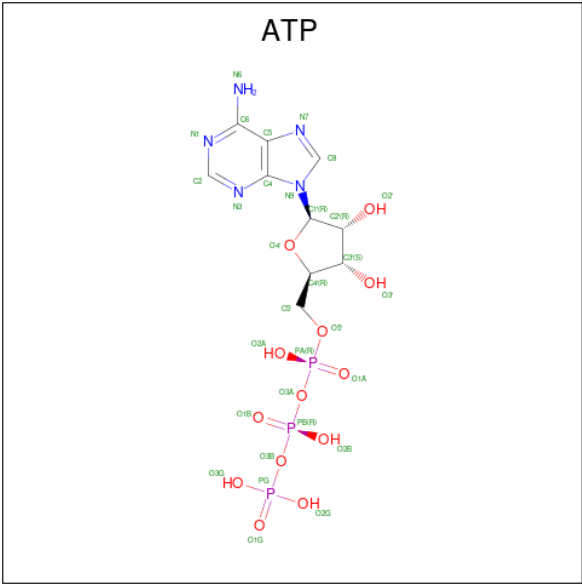
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	318	ALA	GLU	engineered mutation	UNP Q79PF4

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		

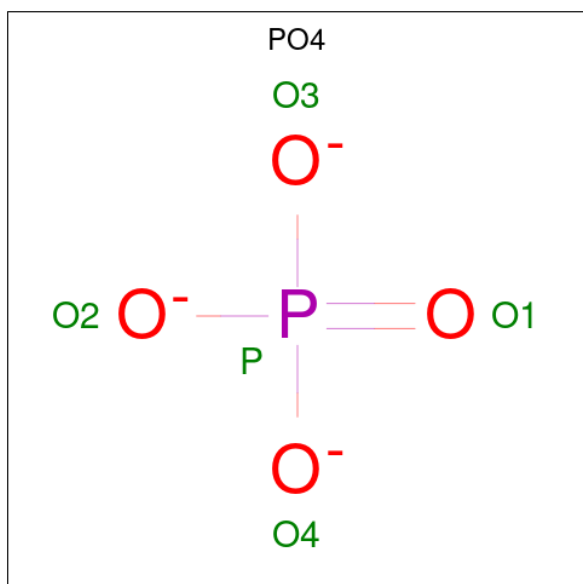
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	B	11	Total	O	0	0
			11	11		

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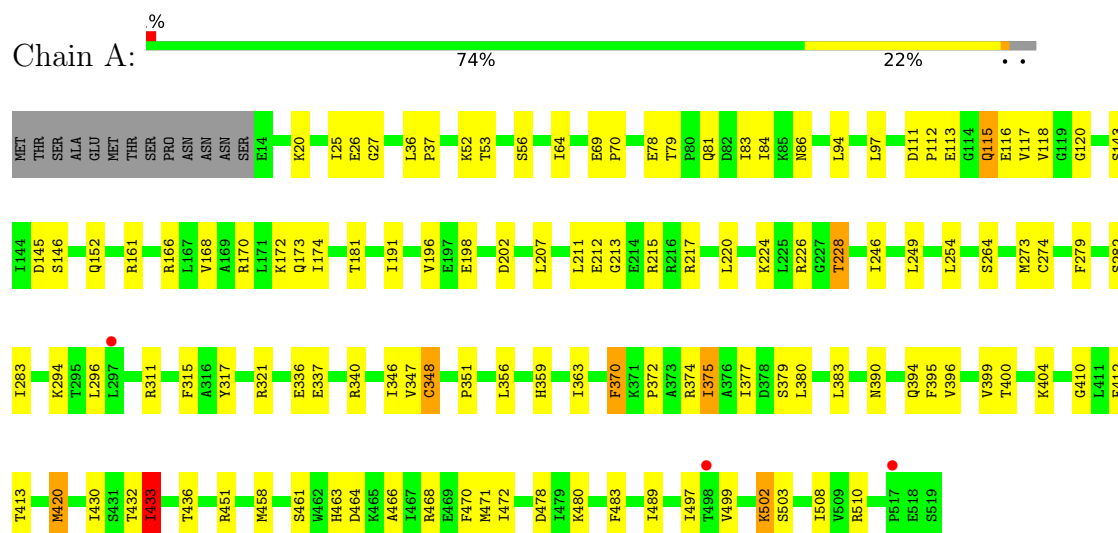
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	12	Total 12	O 12	0	0
6	D	14	Total 14	O 14	0	0
6	E	15	Total 15	O 15	0	0
6	F	5	Total 5	O 5	0	0

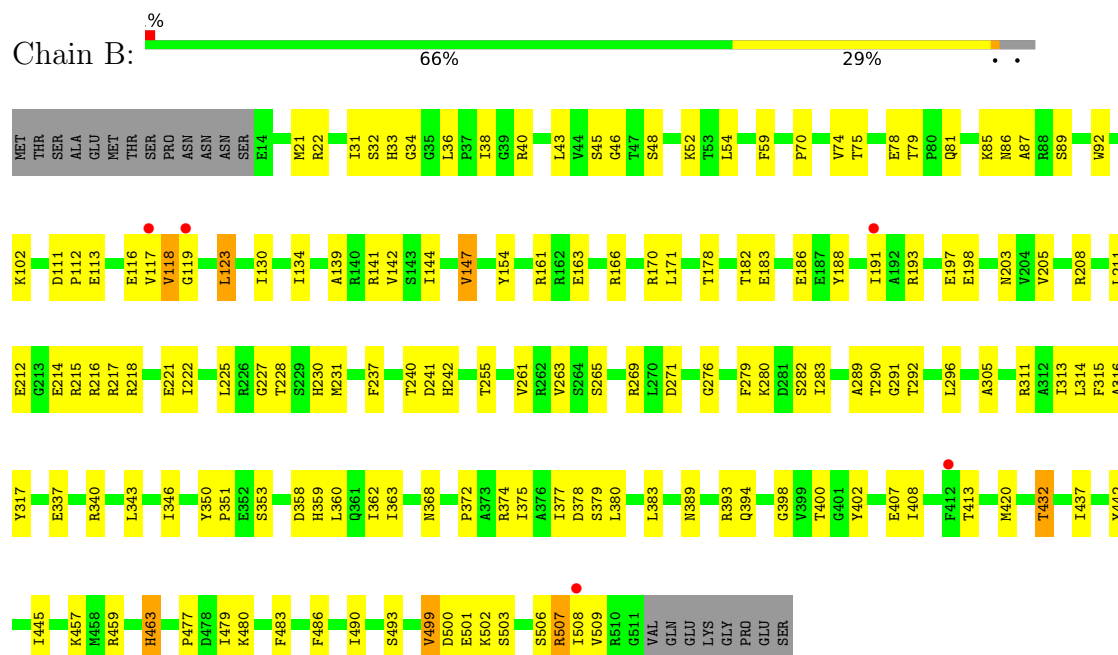
3 Residue-property plots

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

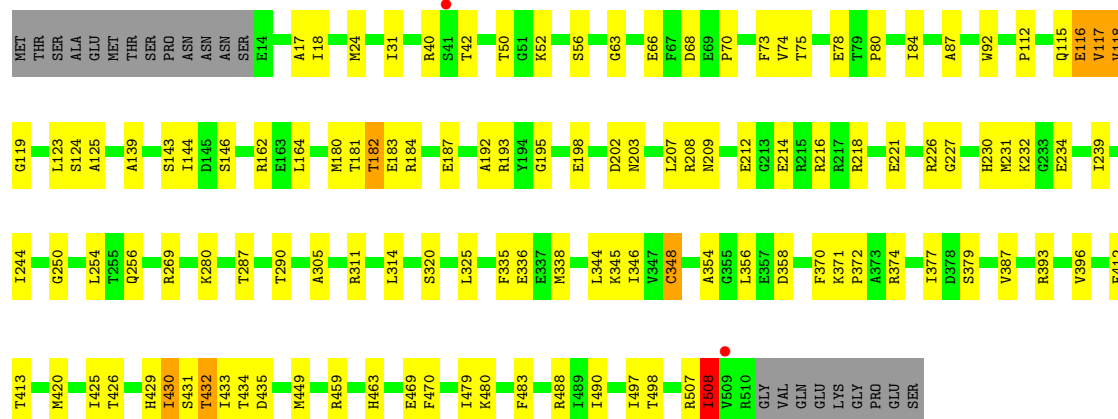


- Molecule 1: Circadian clock protein kinase kaiC



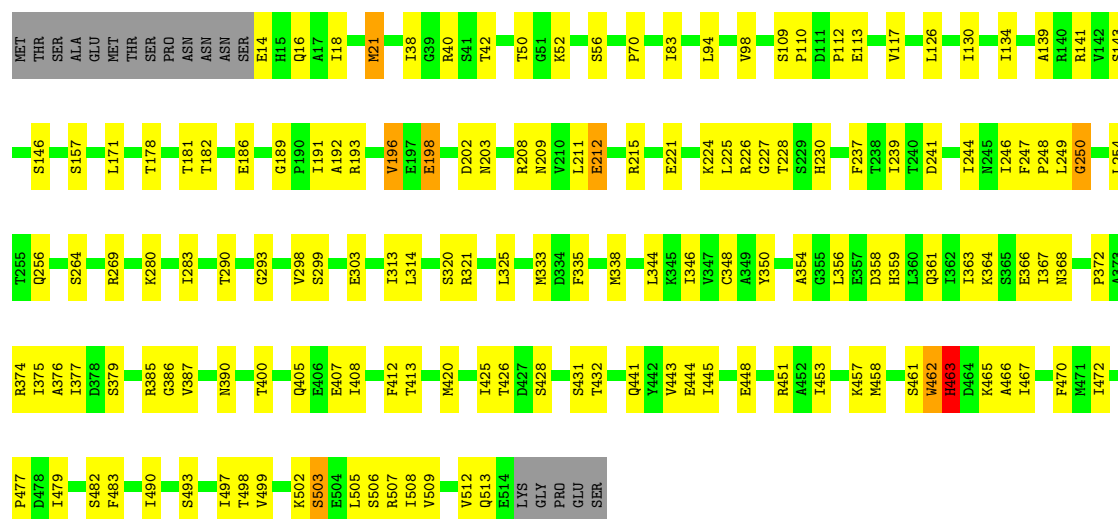
- Molecule 1: Circadian clock protein kinase kaiC

Chain C:  72% 22%



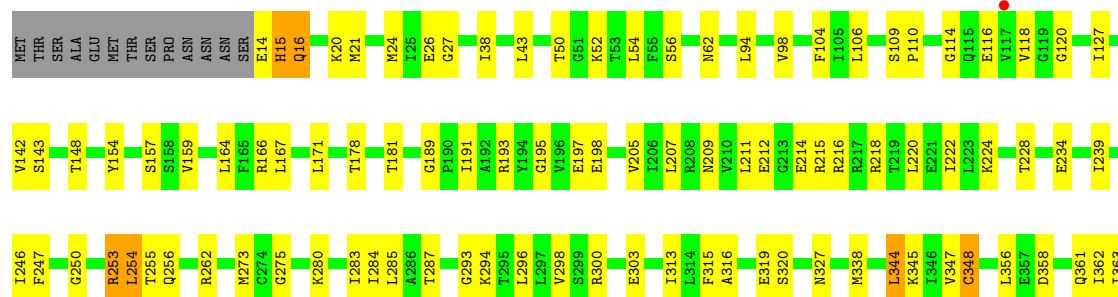
• Molecule 1: Circadian clock protein kinase kaiC

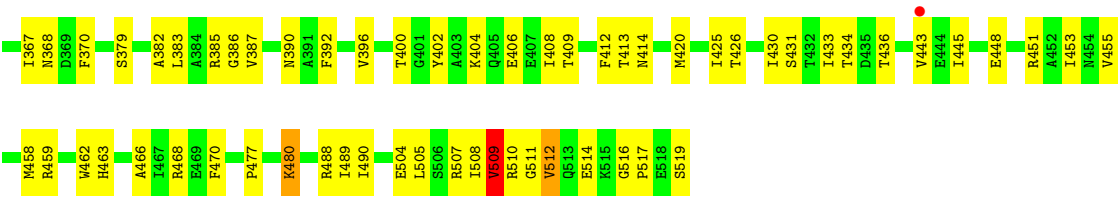
Chain E:  67% 28%



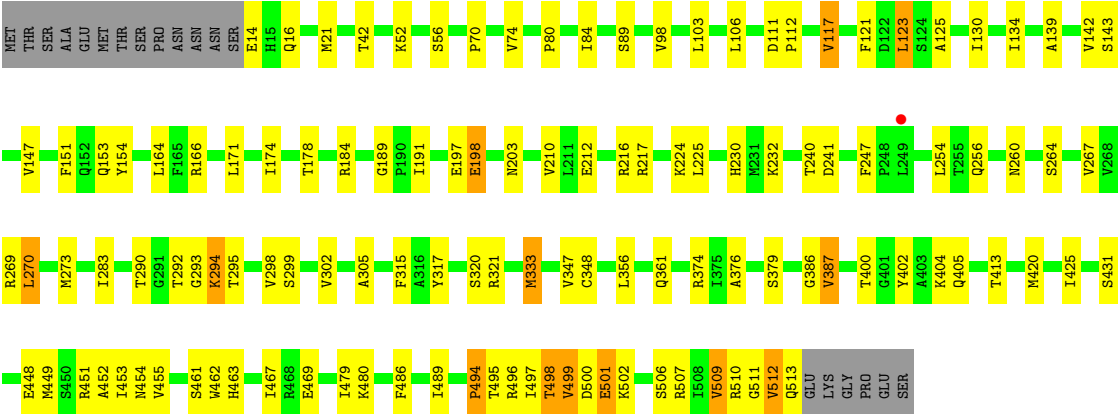
• Molecule 1: Circadian clock protein kinase kaiC

Chain F:  68% 28%





● Molecule 2: Circadian clock protein kinase kaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.71Å 135.06Å 204.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.05 – 3.29 30.05 – 3.29	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.05-3.29) 83.2 (30.05-3.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.245 , 0.303 0.237 , 0.296	Depositor DCC
R_{free} test set	2549 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24157	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, ATP, MG, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/4040	0.74	0/5440
1	B	0.28	0/3978	0.74	0/5358
1	C	0.27	0/3974	0.72	0/5353
1	E	0.28	0/3997	0.74	0/5385
1	F	0.27	0/4040	0.73	0/5440
2	D	0.29	0/4002	0.75	0/5393
All	All	0.28	0/24031	0.74	0/32369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3986	0	3982	73	0
1	B	3925	0	3926	103	0
1	C	3921	0	3922	71	0
1	E	3944	0	3937	84	0
1	F	3986	0	3982	91	0
2	D	3937	0	3943	85	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	62	0	24	5	0
4	B	62	0	24	3	0
4	C	62	0	24	1	0
4	D	62	0	24	4	0
4	E	62	0	24	3	0
4	F	62	0	24	5	0
5	C	5	0	0	0	0
6	A	12	0	0	0	0
6	B	11	0	0	0	0
6	C	12	0	0	0	0
6	D	14	0	0	0	0
6	E	15	0	0	0	0
6	F	5	0	0	1	0
All	All	24157	0	23836	459	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 10.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:THR:HG23	1:B:242:HIS:H	1.12	1.11
1:B:240:THR:HG23	1:B:242:HIS:N	1.88	0.89
2:D:379:SER:H	2:D:413:THR:HB	1.40	0.87
1:E:379:SER:H	1:E:413:THR:HB	1.40	0.86
1:B:502:LYS:H	1:B:503:SER:HA	1.40	0.82
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.66	0.76
1:C:379:SER:H	1:C:413:THR:HB	1.49	0.76
1:E:458:MET:HG2	1:E:461:SER:HB3	1.66	0.76
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.66	0.76
1:E:512:VAL:HA	1:E:513:GLN:HB2	1.69	0.74
1:E:146:SER:H	1:E:181:THR:HB	1.53	0.73
2:D:500:ASP:H	2:D:501:GLU:HA	1.54	0.72
1:B:506:SER:HA	1:B:507:ARG:HB2	1.72	0.71
1:E:303:GLU:HG3	1:E:338:MET:HE1	1.73	0.70
1:B:171:LEU:HD13	1:B:178:THR:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:ARG:HH21	1:F:239:ILE:H	1.39	0.69
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.74	0.69
2:D:453:ILE:HG21	2:D:479:ILE:HD12	1.75	0.68
1:A:321:ARG:HD2	1:B:255:THR:HG23	1.75	0.68
1:F:209:ASN:O	1:F:216:ARG:NH1	2.26	0.68
1:A:466:ALA:HA	1:F:448:GLU:HA	1.74	0.68
1:E:256:GLN:HG3	1:E:405:GLN:HB3	1.76	0.68
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.76	0.67
1:B:86:ASN:HA	1:C:18:ILE:HD11	1.76	0.67
2:D:321:ARG:NH1	2:D:347:VAL:O	2.28	0.67
1:F:142:VAL:HB	1:F:178:THR:HG22	1.77	0.67
1:E:364:LYS:O	1:E:368:ASN:ND2	2.28	0.66
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.77	0.66
1:C:123:LEU:O	1:C:125:ALA:N	2.28	0.66
2:D:290:THR:HG21	1:E:431:SER:HB2	1.77	0.65
2:D:495:THR:HG22	2:D:497:ILE:H	1.61	0.65
2:D:171:LEU:HD13	2:D:178:THR:HG21	1.79	0.65
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.29	0.65
1:E:40:ARG:NH1	1:E:226:ARG:O	2.30	0.64
1:B:379:SER:H	1:B:413:THR:HB	1.62	0.64
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.79	0.64
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.81	0.63
1:E:453:ILE:HG21	1:E:479:ILE:HD12	1.80	0.63
1:F:287:THR:HG21	1:F:425:ILE:HG23	1.80	0.63
1:A:170:ARG:NH1	1:A:173:GLN:OE1	2.31	0.63
1:B:316:ALA:HA	1:B:378:ASP:HB3	1.81	0.63
1:B:372:PRO:HG2	1:B:408:ILE:HD13	1.80	0.62
1:B:280:LYS:NZ	1:B:407:GLU:OE2	2.32	0.62
2:D:509:VAL:HG22	2:D:510:ARG:HB3	1.81	0.62
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.81	0.62
1:C:425:ILE:HG22	1:C:426:THR:HG23	1.82	0.62
1:F:468:ARG:NH1	1:F:480:LYS:O	2.34	0.61
1:C:497:ILE:HG23	1:C:498:THR:H	1.65	0.61
1:F:171:LEU:HD13	1:F:178:THR:HG21	1.81	0.61
1:B:493:SER:HB3	1:C:488:ARG:HG2	1.82	0.61
1:B:315:PHE:HE2	1:B:375:ILE:HD11	1.65	0.61
1:A:20:LYS:HE3	1:A:228:THR:HG21	1.82	0.61
2:D:512:VAL:HA	2:D:513:GLN:HB2	1.82	0.60
2:D:449:MET:HG2	1:E:467:ILE:HD11	1.83	0.60
1:A:283:ILE:HG12	1:A:404:LYS:HE3	1.83	0.60
1:E:482:SER:OG	1:E:483:PHE:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:451:ARG:NH2	4:D:602:ATP:O2'	2.34	0.60
1:F:453:ILE:HG13	1:F:470:PHE:CD1	2.37	0.59
1:E:14:GLU:HG3	1:E:16:GLN:H	1.68	0.59
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.83	0.59
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.85	0.59
1:C:146:SER:H	1:C:181:THR:HB	1.67	0.59
4:D:603:ATP:O3G	1:E:224:LYS:NZ	2.36	0.59
2:D:500:ASP:H	2:D:502:LYS:HB2	1.68	0.58
1:E:290:THR:HG21	1:F:431:SER:HB2	1.84	0.58
1:F:379:SER:H	1:F:413:THR:HB	1.68	0.58
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.84	0.58
1:B:32:SER:O	1:B:34:GLY:N	2.37	0.57
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.36	0.57
2:D:501:GLU:HA	2:D:502:LYS:HB2	1.84	0.57
1:C:432:TPO:O	1:C:434:THR:N	2.38	0.57
1:E:56:SER:HB2	1:E:143:SER:HB3	1.87	0.57
1:F:294:LYS:N	4:F:602:ATP:O2B	2.38	0.57
1:B:368:ASN:ND2	1:B:402:TYR:OH	2.33	0.57
1:C:396:VAL:HG11	1:C:430:ILE:HG21	1.85	0.57
1:C:508:ILE:HG21	1:E:512:VAL:HB	1.85	0.57
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.70	0.57
1:E:448:GLU:HG2	1:F:466:ALA:HA	1.86	0.56
1:F:14:GLU:N	6:F:702:HOH:O	2.38	0.56
1:F:256:GLN:HG2	1:F:404:LYS:HB3	1.87	0.56
1:F:21:MET:HB2	1:F:38:ILE:HG12	1.86	0.56
1:C:42:THR:HA	1:C:203:ASN:HB2	1.87	0.56
1:A:346:ILE:HG22	1:A:348:CYS:HB2	1.87	0.56
1:F:283:ILE:HG13	1:F:400:THR:HG23	1.88	0.56
1:B:227:GLY:O	1:B:228:THR:HG23	2.05	0.56
1:B:315:PHE:HB2	1:B:377:ILE:HD13	1.87	0.56
1:F:382:ALA:HA	1:F:385:ARG:HE	1.71	0.56
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.88	0.56
1:A:52:LYS:N	4:A:803:ATP:O2B	2.40	0.55
1:B:111:ASP:O	1:B:113:GLU:N	2.40	0.55
2:D:298:VAL:O	2:D:302:VAL:HG23	2.06	0.55
1:C:182:THR:HG22	1:C:183:GLU:H	1.71	0.55
1:E:359:HIS:O	1:E:363:ILE:HG12	2.06	0.55
1:C:344:LEU:HD22	1:C:345:LYS:N	2.22	0.55
1:A:118:VAL:O	1:A:118:VAL:HG23	2.07	0.55
1:B:263:VAL:HB	1:B:374:ARG:HH21	1.72	0.55
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:VAL:HB	2:D:178:THR:HG22	1.89	0.54
1:A:79:THR:HG22	1:A:81:GLN:HG2	1.89	0.54
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.89	0.54
1:B:87:ALA:HB1	1:B:92:TRP:HE1	1.72	0.54
1:C:344:LEU:HD22	1:C:345:LYS:H	1.72	0.54
2:D:294:LYS:HG2	2:D:413:THR:HG23	1.88	0.54
2:D:500:ASP:N	2:D:501:GLU:HA	2.21	0.54
1:A:471:MET:HG2	1:A:478:ASP:HB3	1.88	0.54
1:F:20:LYS:HE3	1:F:228:THR:HG21	1.90	0.54
1:E:502:LYS:HG3	1:E:503:SER:H	1.73	0.54
1:A:146:SER:H	1:A:181:THR:HB	1.73	0.54
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.90	0.54
1:B:216:ARG:NE	1:C:221:GLU:OE1	2.36	0.54
1:C:24:MET:HE2	1:C:66:GLU:HG3	1.89	0.53
1:B:240:THR:HG23	1:B:241:ASP:N	2.24	0.53
1:E:375:ILE:HG12	1:E:408:ILE:HG21	1.89	0.53
1:B:291:GLY:O	1:B:442:TYR:OH	2.24	0.53
1:B:290:THR:HG21	1:C:431:SER:HB2	1.90	0.53
1:A:217:ARG:NE	1:F:214:GLU:OE2	2.41	0.53
1:B:240:THR:CG2	1:B:242:HIS:H	2.02	0.53
1:B:502:LYS:N	1:B:503:SER:HA	2.10	0.53
2:D:14:GLU:HG3	2:D:16:GLN:H	1.74	0.53
1:E:283:ILE:HG12	1:E:400:THR:HG23	1.90	0.53
1:A:451:ARG:NH2	4:A:802:ATP:O2'	2.41	0.53
2:D:240:THR:OG1	2:D:241:ASP:N	2.41	0.52
2:D:451:ARG:HH21	1:E:465:LYS:HE3	1.74	0.52
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.92	0.52
1:B:350:TYR:O	1:B:353:SER:OG	2.25	0.52
1:E:215:ARG:NH2	1:F:234:GLU:O	2.43	0.52
1:F:509:VAL:O	1:F:511:GLY:N	2.43	0.52
1:F:253:ARG:O	1:F:255:THR:N	2.41	0.52
1:B:86:ASN:OD1	1:C:40:ARG:NH2	2.41	0.52
1:B:205:VAL:HG22	1:B:222:ILE:HG12	1.91	0.52
1:C:31:ILE:HG23	1:C:231:MET:HB2	1.91	0.52
4:A:802:ATP:O2'	1:B:463:HIS:NE2	2.42	0.52
1:E:248:PRO:O	1:E:250:GLY:N	2.42	0.52
1:E:280:LYS:NZ	1:E:407:GLU:OE1	2.40	0.52
1:B:337:GLU:HA	1:B:340:ARG:HD2	1.90	0.52
1:E:193:ARG:NH2	1:F:195:GLY:O	2.28	0.52
4:A:802:ATP:O3G	1:B:459:ARG:NH2	2.38	0.52
4:C:603:ATP:O3G	2:D:224:LYS:NZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:THR:HG23	1:A:458:MET:HG2	1.92	0.52
1:C:393:ARG:HH21	1:C:429:HIS:HB2	1.75	0.52
1:C:214:GLU:OE2	2:D:217:ARG:NH1	2.43	0.51
2:D:452:ALA:HA	2:D:469:GLU:HA	1.92	0.51
1:B:182:THR:HG22	1:B:183:GLU:H	1.75	0.51
1:B:314:LEU:HB3	1:B:346:ILE:HG22	1.92	0.51
1:F:157:SER:O	1:F:159:VAL:N	2.41	0.51
1:B:85:LYS:HE3	1:C:18:ILE:HG13	1.93	0.51
1:C:449:MET:HE2	2:D:467:ILE:HD11	1.92	0.51
1:A:86:ASN:OD1	1:B:40:ARG:NH2	2.44	0.51
1:A:254:LEU:HG	1:F:320:SER:HA	1.92	0.51
1:B:393:ARG:NH2	1:B:432:TPO:O2P	2.43	0.51
2:D:121:PHE:HD1	2:D:125:ALA:HB2	1.76	0.51
1:F:430:ILE:HG23	1:F:433:ILE:HD12	1.93	0.51
1:B:87:ALA:HB1	1:B:92:TRP:NE1	2.26	0.51
2:D:425:ILE:HD12	2:D:425:ILE:H	1.75	0.51
1:A:264:SER:O	1:A:374:ARG:NH2	2.44	0.51
1:E:126:LEU:O	1:E:130:ILE:HG12	2.11	0.51
1:B:225:LEU:HB3	1:B:228:THR:OG1	2.10	0.50
1:B:43:LEU:O	1:B:205:VAL:N	2.38	0.50
2:D:42:THR:HA	2:D:203:ASN:HB2	1.93	0.50
1:B:186:GLU:HG3	1:B:188:TYR:H	1.76	0.50
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.77	0.50
1:E:507:ARG:HG2	1:E:508:ILE:H	1.76	0.50
1:F:451:ARG:NH2	4:F:602:ATP:O3'	2.44	0.50
1:A:27:GLY:HA3	1:A:246:ILE:HB	1.93	0.50
1:A:396:VAL:HG21	1:A:430:ILE:HG21	1.93	0.50
1:A:84:ILE:HG12	1:A:94:LEU:HB2	1.94	0.50
1:B:111:ASP:C	1:B:113:GLU:H	2.19	0.50
2:D:247:PHE:HZ	2:D:361:GLN:HB2	1.76	0.50
1:E:505:LEU:HB3	1:E:506:SER:HB2	1.94	0.50
1:A:379:SER:H	1:A:413:THR:HB	1.76	0.50
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.94	0.50
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.77	0.49
1:C:116:GLU:O	1:C:118:VAL:N	2.39	0.49
2:D:256:GLN:HG3	2:D:404:LYS:HB3	1.93	0.49
1:F:303:GLU:HG3	1:F:338:MET:HE1	1.93	0.49
1:A:315:PHE:HB2	1:A:377:ILE:HG13	1.95	0.49
1:C:230:HIS:CE1	1:C:232:LYS:HG3	2.47	0.49
1:E:320:SER:HA	1:F:254:LEU:HG	1.93	0.49
1:F:54:LEU:HD23	1:F:239:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:ILE:HD12	1:F:412:PHE:HE2	1.77	0.49
1:B:360:LEU:HD11	1:B:398:GLY:HA3	1.93	0.49
1:A:224:LYS:NZ	4:F:603:ATP:O1G	2.32	0.49
1:B:89:SER:HB2	4:B:603:ATP:HN61	1.77	0.49
1:C:75:THR:OG1	1:C:78:GLU:O	2.29	0.49
1:F:443:VAL:HG12	1:F:445:ILE:HG13	1.95	0.49
1:C:348:CYS:HB3	2:D:254:LEU:HB2	1.94	0.49
1:E:182:THR:HG21	1:E:192:ALA:HB1	1.93	0.49
1:B:227:GLY:O	1:B:228:THR:CG2	2.60	0.49
1:C:469:GLU:HG3	1:C:480:LYS:HE3	1.95	0.49
1:E:363:ILE:O	1:E:367:ILE:HG12	2.12	0.49
1:F:262:ARG:NH1	1:F:275:GLY:O	2.46	0.49
4:B:602:ATP:O3G	1:C:459:ARG:NH2	2.46	0.49
1:F:396:VAL:HG11	1:F:430:ILE:HG21	1.95	0.49
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.94	0.49
1:E:264:SER:O	1:E:374:ARG:NH2	2.44	0.49
1:A:64:ILE:HD12	1:A:97:LEU:HD13	1.95	0.48
1:B:79:THR:OG1	1:B:81:GLN:OE1	2.31	0.48
1:B:45:SER:HB3	1:B:182:THR:HB	1.94	0.48
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.77	0.48
2:D:320:SER:HA	1:E:254:LEU:HG	1.94	0.48
4:E:603:ATP:O1G	1:F:224:LYS:NZ	2.46	0.48
1:F:56:SER:HB2	1:F:143:SER:HB3	1.95	0.48
1:E:313:ILE:HG13	1:E:372:PRO:HB3	1.95	0.48
1:F:414:ASN:HD22	1:F:426:THR:HG22	1.79	0.48
1:F:16:GLN:HB3	1:F:228:THR:HG22	1.95	0.48
1:F:296:LEU:N	4:F:602:ATP:O1A	2.46	0.48
1:C:354:ALA:HB1	1:C:358:ASP:HB2	1.95	0.48
1:F:363:ILE:O	1:F:367:ILE:HG12	2.13	0.48
2:D:509:VAL:HG13	2:D:510:ARG:HG2	1.96	0.48
1:F:247:PHE:HZ	1:F:361:GLN:HB2	1.78	0.48
2:D:216:ARG:NE	1:E:221:GLU:OE1	2.34	0.48
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.95	0.48
2:D:123:LEU:HD12	2:D:166:ARG:HD2	1.96	0.47
1:A:56:SER:HB2	1:A:143:SER:HB3	1.95	0.47
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.96	0.47
1:B:191:ILE:HB	1:B:198:GLU:HG2	1.95	0.47
1:E:502:LYS:HD2	1:E:502:LYS:HA	1.72	0.47
1:B:437:ILE:HD13	1:B:457:LYS:HD3	1.96	0.47
1:C:239:ILE:HG12	1:C:244:ILE:HD13	1.97	0.47
2:D:486:PHE:CE1	2:D:496:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ASP:OD1	4:E:603:ATP:N6	2.44	0.47
1:E:377:ILE:HD12	1:E:412:PHE:HE1	1.78	0.47
1:B:507:ARG:HG3	1:B:508:ILE:HG12	1.95	0.47
1:E:298:VAL:HG13	1:E:376:ALA:HB1	1.95	0.47
1:C:449:MET:HG3	2:D:454:ASN:HD21	1.79	0.47
1:B:389:ASN:O	1:B:393:ARG:N	2.41	0.47
1:C:325:LEU:HD11	1:C:336:GLU:HG3	1.96	0.47
1:A:152:GLN:HG3	1:B:161:ARG:HH11	1.80	0.47
2:D:130:ILE:O	2:D:134:ILE:HG12	2.14	0.47
1:C:50:THR:HB	1:C:207:LEU:HB3	1.97	0.47
1:C:56:SER:HB2	1:C:143:SER:HB3	1.97	0.47
1:A:359:HIS:O	1:A:363:ILE:HG12	2.15	0.46
1:B:46:GLY:N	1:B:52:LYS:HD3	2.30	0.46
1:C:87:ALA:HB1	1:C:92:TRP:CD1	2.50	0.46
1:E:18:ILE:HB	1:E:228:THR:HG23	1.96	0.46
4:E:602:ATP:H2	1:F:462:TRP:HD1	1.62	0.46
1:F:434:THR:O	1:F:459:ARG:NH2	2.47	0.46
1:B:116:GLU:C	1:B:118:VAL:H	2.23	0.46
1:B:116:GLU:OE1	1:C:162:ARG:NH2	2.47	0.46
1:B:279:PHE:O	1:B:282:SER:OG	2.28	0.46
1:B:296:LEU:HD21	1:B:477:PRO:HB3	1.96	0.46
1:E:325:LEU:HD22	1:E:335:PHE:HB2	1.97	0.46
1:F:27:GLY:HA3	1:F:246:ILE:HB	1.97	0.46
1:F:316:ALA:HB3	1:F:348:CYS:SG	2.55	0.46
1:B:217:ARG:NH2	1:B:394:GLN:OE1	2.48	0.46
1:B:445:ILE:HD13	1:B:483:PHE:HE2	1.80	0.46
1:E:321:ARG:O	1:E:325:LEU:HG	2.16	0.46
2:D:489:ILE:HD13	2:D:494:PRO:HB3	1.97	0.46
1:A:363:ILE:HG21	1:A:399:VAL:HG13	1.98	0.46
1:A:470:PHE:HE2	1:A:472:ILE:HD11	1.81	0.46
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.98	0.46
1:E:443:VAL:HG12	1:E:445:ILE:HG12	1.97	0.46
1:E:451:ARG:HB3	1:E:470:PHE:CE1	2.50	0.46
1:B:123:LEU:HG	1:B:163:GLU:HB3	1.97	0.46
1:C:63:GLY:O	1:C:68:ASP:N	2.49	0.46
1:E:354:ALA:HB1	1:E:358:ASP:HB2	1.96	0.46
4:A:802:ATP:HO2'	1:B:463:HIS:CD2	2.33	0.46
2:D:273:MET:SD	2:D:479:ILE:HG21	2.56	0.46
1:E:426:THR:HG22	1:E:428:SER:H	1.81	0.46
1:B:197:GLU:OE2	1:B:197:GLU:N	2.34	0.46
2:D:290:THR:OG1	1:E:457:LYS:NZ	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:VAL:HB	2:D:270:LEU:HB2	1.98	0.46
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.97	0.46
1:A:78:GLU:HB3	1:A:83:ILE:HD11	1.98	0.45
1:F:358:ASP:O	1:F:362:ILE:HG12	2.17	0.45
1:F:396:VAL:HG21	1:F:430:ILE:HD13	1.98	0.45
1:B:134:ILE:HA	1:B:139:ALA:HB3	1.98	0.45
1:B:215:ARG:NH2	1:C:234:GLU:O	2.49	0.45
1:F:284:ILE:HG13	1:F:436:THR:HB	1.98	0.45
1:F:458:MET:HE2	1:F:458:MET:HB3	1.90	0.45
1:B:499:VAL:C	1:B:501:GLU:H	2.24	0.45
1:C:470:PHE:HA	1:C:480:LYS:HE2	1.97	0.45
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.99	0.45
1:F:104:PHE:CE2	1:F:106:LEU:HB3	2.51	0.45
1:F:211:LEU:HD12	1:F:215:ARG:O	2.16	0.45
1:A:249:LEU:HD12	1:A:394:GLN:HG3	1.97	0.45
1:A:375:ILE:HG22	1:A:410:GLY:HA2	1.97	0.45
1:B:313:ILE:HB	1:B:375:ILE:HG13	1.99	0.45
1:E:225:LEU:HD12	1:E:230:HIS:HB3	1.99	0.45
1:F:300:ARG:HH21	1:F:477:PRO:HD2	1.82	0.45
1:A:84:ILE:HG23	1:A:94:LEU:H	1.81	0.45
2:D:184:ARG:HH11	2:D:191:ILE:HA	1.81	0.45
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.87	0.45
1:E:130:ILE:O	1:E:134:ILE:HG12	2.17	0.45
1:A:166:ARG:NH2	1:F:114:GLY:O	2.50	0.44
1:F:24:MET:HB2	1:F:62:ASN:HB3	1.99	0.44
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.98	0.44
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.99	0.44
1:F:356:LEU:HD11	1:F:387:VAL:HG11	1.99	0.44
1:A:111:ASP:C	1:A:113:GLU:H	2.25	0.44
2:D:283:ILE:HG12	2:D:400:THR:HG23	1.99	0.44
2:D:386:GLY:HA2	1:E:390:ASN:OD1	2.17	0.44
1:E:344:LEU:HD21	1:E:346:ILE:HD11	1.98	0.44
1:A:53:THR:O	1:A:56:SER:OG	2.34	0.44
1:A:274:CYS:O	1:A:461:SER:OG	2.25	0.44
1:A:296:LEU:HD13	1:A:472:ILE:HD12	2.00	0.44
1:B:311:ARG:HG2	1:B:343:LEU:HA	1.98	0.44
2:D:56:SER:HB2	2:D:143:SER:HB3	1.99	0.44
1:F:294:LYS:O	1:F:298:VAL:HG23	2.18	0.44
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.53	0.44
1:A:168:VAL:O	1:A:172:LYS:HG3	2.18	0.44
1:B:214:GLU:HB3	1:C:234:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:PHE:CD1	2:D:125:ALA:HB2	2.51	0.44
1:B:130:ILE:O	1:B:134:ILE:HG13	2.18	0.44
1:E:186:GLU:HG3	1:E:189:GLY:N	2.32	0.44
1:F:514:GLU:OE1	1:F:514:GLU:N	2.50	0.44
1:B:225:LEU:HD12	1:B:230:HIS:HB3	2.00	0.44
1:B:265:SER:N	1:B:271:ASP:OD1	2.51	0.44
1:C:490:ILE:HD12	1:C:490:ILE:H	1.83	0.44
1:E:21:MET:HE1	1:E:141:ARG:HG2	2.00	0.44
1:E:247:PHE:HZ	1:E:361:GLN:HB2	1.83	0.44
1:F:15:HIS:HB3	1:F:16:GLN:H	1.54	0.44
1:A:115:GLN:HB3	1:A:116:GLU:H	1.67	0.43
1:A:321:ARG:NH2	1:A:347:VAL:O	2.46	0.43
1:A:483:PHE:HB2	1:A:489:ILE:HD13	2.00	0.43
2:D:469:GLU:HG3	2:D:480:LYS:HE3	2.00	0.43
1:E:42:THR:HA	1:E:203:ASN:HB2	2.00	0.43
1:F:280:LYS:O	1:F:409:THR:HB	2.18	0.43
1:C:314:LEU:HB3	1:C:346:ILE:HD13	2.00	0.43
1:C:356:LEU:HD13	1:C:387:VAL:HG21	2.00	0.43
1:E:314:LEU:HB3	1:E:346:ILE:HD13	2.00	0.43
1:E:506:SER:OG	1:E:507:ARG:N	2.51	0.43
1:F:285:LEU:HB2	1:F:434:THR:HG21	2.00	0.43
1:F:514:GLU:HG3	1:F:519:SER:HB3	2.00	0.43
1:C:290:THR:HG21	2:D:431:SER:HB3	2.00	0.43
1:F:368:ASN:OD1	1:F:402:TYR:OH	2.37	0.43
1:A:464:ASP:OD2	1:A:468:ARG:NH1	2.52	0.43
1:B:358:ASP:O	1:B:362:ILE:HG12	2.19	0.43
1:E:239:ILE:HG12	1:E:244:ILE:HD13	1.99	0.43
1:F:205:VAL:HG22	1:F:222:ILE:HG13	2.01	0.43
1:B:31:ILE:HG23	1:B:231:MET:HB2	2.01	0.43
1:B:87:ALA:HB1	1:B:92:TRP:CD1	2.54	0.43
1:B:359:HIS:O	1:B:363:ILE:HG12	2.19	0.43
1:C:209:ASN:O	1:C:216:ARG:NH1	2.51	0.43
2:D:80:PRO:O	2:D:84:ILE:HG12	2.18	0.43
2:D:264:SER:O	2:D:374:ARG:NH2	2.42	0.43
1:C:182:THR:HG21	1:C:192:ALA:HB1	2.01	0.43
1:F:316:ALA:O	1:F:348:CYS:HA	2.19	0.43
1:B:74:VAL:HB	1:B:144:ILE:HG23	2.01	0.43
2:D:299:SER:O	2:D:333:MET:HE1	2.19	0.43
1:E:283:ILE:HG13	1:E:412:PHE:HE2	1.84	0.43
1:B:350:TYR:CZ	1:C:254:LEU:HD13	2.54	0.42
1:C:52:LYS:HE3	1:C:52:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ARG:HH22	1:C:208:ARG:HG2	1.84	0.42
1:C:218:ARG:HH12	2:D:232:LYS:HE2	1.84	0.42
1:E:52:LYS:HB2	1:E:52:LYS:HE3	1.86	0.42
1:A:145:ASP:HA	1:A:181:THR:HB	2.01	0.42
2:D:89:SER:HB2	1:E:227:GLY:O	2.18	0.42
2:D:451:ARG:NH2	4:D:602:ATP:HO2'	2.17	0.42
1:E:462:TRP:CG	1:E:463:HIS:N	2.87	0.42
2:D:134:ILE:HG21	2:D:174:ILE:HG21	2.01	0.42
1:F:283:ILE:HG23	1:F:412:PHE:HE2	1.84	0.42
1:A:213:GLY:C	1:A:215:ARG:H	2.27	0.42
1:A:400:THR:HG21	1:A:433:ILE:HG22	2.00	0.42
1:B:54:LEU:N	4:B:603:ATP:O1A	2.52	0.42
1:B:142:VAL:O	1:B:178:THR:HA	2.20	0.42
1:F:109:SER:HA	1:F:110:PRO:HD3	1.90	0.42
1:B:289:ALA:O	1:B:292:THR:OG1	2.31	0.42
2:D:98:VAL:HA	2:D:103:LEU:O	2.19	0.42
1:A:294:LYS:HE2	1:A:294:LYS:HB2	1.75	0.42
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.55	0.42
1:A:468:ARG:HD2	1:A:480:LYS:O	2.20	0.42
1:B:21:MET:SD	1:B:141:ARG:NE	2.92	0.42
2:D:448:GLU:HG2	1:E:466:ALA:HA	2.00	0.42
1:E:21:MET:HB2	1:E:38:ILE:HG12	2.02	0.42
1:E:237:PHE:HB3	1:E:246:ILE:HG23	2.01	0.42
1:B:193:ARG:NH2	1:C:195:GLY:O	2.51	0.42
1:B:227:GLY:C	1:B:228:THR:HG23	2.44	0.42
2:D:269:ARG:HG2	2:D:479:ILE:HB	2.00	0.42
1:E:109:SER:HA	1:E:110:PRO:HD3	1.94	0.42
1:A:273:MET:O	1:A:464:ASP:N	2.41	0.42
1:A:279:PHE:HB2	1:A:282:SER:HB3	2.01	0.42
1:A:337:GLU:OE1	1:A:340:ARG:NH1	2.53	0.42
1:C:73:PHE:HD1	1:C:143:SER:HB2	1.84	0.42
2:D:52:LYS:HE3	2:D:52:LYS:HB2	1.84	0.42
1:F:94:LEU:O	1:F:98:VAL:HG23	2.19	0.42
1:A:470:PHE:CE2	1:A:472:ILE:HD11	2.54	0.42
1:C:320:SER:HA	2:D:254:LEU:HB3	2.01	0.42
1:E:171:LEU:HD13	1:E:178:THR:HG21	2.00	0.42
1:E:493:SER:HB3	1:F:488:ARG:HA	2.00	0.42
1:A:207:LEU:HD21	1:A:220:LEU:HD12	2.01	0.42
1:C:80:PRO:O	1:C:84:ILE:HG12	2.20	0.42
1:F:313:ILE:HD12	1:F:367:ILE:HD13	2.02	0.42
1:F:319:GLU:OE1	1:F:327:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ASN:HB3	1:B:225:LEU:HD23	2.01	0.41
1:B:483:PHE:HB3	1:B:486:PHE:HB2	2.02	0.41
1:C:202:ASP:HA	1:C:226:ARG:HD2	2.01	0.41
1:C:335:PHE:HA	1:C:338:MET:HE3	2.02	0.41
1:F:273:MET:HE2	1:F:455:VAL:HG23	2.02	0.41
1:A:380:LEU:HD11	1:A:412:PHE:HD2	1.85	0.41
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.56	0.41
1:B:218:ARG:HB3	1:B:237:PHE:CZ	2.55	0.41
1:C:74:VAL:HB	1:C:144:ILE:HA	2.03	0.41
2:D:510:ARG:H	2:D:511:GLY:C	2.29	0.41
1:F:218:ARG:NH2	1:F:239:ILE:H	2.12	0.41
2:D:74:VAL:HG22	2:D:106:LEU:HD23	2.02	0.41
1:E:350:TYR:CE2	1:F:254:LEU:HD13	2.56	0.41
1:F:164:LEU:HD11	1:F:197:GLU:HG3	2.03	0.41
1:A:420:MET:HE1	1:B:490:ILE:HG21	2.03	0.41
1:C:435:ASP:HA	1:C:459:ARG:HH11	1.85	0.41
2:D:512:VAL:HA	2:D:513:GLN:CB	2.46	0.41
1:E:112:PRO:O	1:F:166:ARG:HG3	2.20	0.41
1:F:191:ILE:HG21	1:F:198:GLU:HG3	2.02	0.41
1:F:383:LEU:HB2	1:F:392:PHE:HE1	1.85	0.41
1:A:202:ASP:HA	1:A:226:ARG:NH1	2.35	0.41
1:B:317:TYR:CZ	1:B:383:LEU:HD11	2.55	0.41
1:C:184:ARG:NH1	1:C:187:GLU:O	2.53	0.41
1:C:254:LEU:HD12	1:C:256:GLN:HE22	1.86	0.41
2:D:171:LEU:HA	2:D:174:ILE:HD12	2.03	0.41
2:D:298:VAL:HG13	2:D:376:ALA:HB1	2.02	0.41
2:D:511:GLY:HA3	2:D:513:GLN:HG3	2.03	0.41
1:F:382:ALA:HB1	1:F:385:ARG:HH21	1.86	0.41
1:A:25:ILE:O	1:A:27:GLY:N	2.54	0.41
1:B:75:THR:OG1	1:B:78:GLU:O	2.34	0.41
1:C:311:ARG:HB3	1:C:370:PHE:CE2	2.55	0.41
2:D:111:ASP:HA	2:D:112:PRO:HD3	1.85	0.41
1:E:94:LEU:O	1:E:98:VAL:HG23	2.20	0.41
1:F:215:ARG:HH11	1:F:215:ARG:HA	1.86	0.41
1:F:489:ILE:HG22	1:F:490:ILE:HD13	2.02	0.41
1:A:69:GLU:HA	1:A:70:PRO:HD3	1.88	0.41
1:A:336:GLU:O	1:A:340:ARG:HG3	2.20	0.41
1:A:356:LEU:HD23	1:A:395:PHE:HB2	2.03	0.41
1:B:22:ARG:O	1:B:141:ARG:NH2	2.54	0.41
1:B:70:PRO:HG3	1:B:102:LYS:HD2	2.03	0.41
1:B:166:ARG:O	1:B:170:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:MET:HE2	2:D:21:MET:HB3	1.90	0.41
2:D:273:MET:HE2	2:D:455:VAL:HG23	2.03	0.41
2:D:498:THR:HB	2:D:499:VAL:HA	2.02	0.41
1:F:52:LYS:HB3	1:F:181:THR:HG23	2.03	0.41
1:F:344:LEU:HD22	1:F:345:LYS:N	2.36	0.41
1:A:226:ARG:HH21	4:F:603:ATP:PG	2.44	0.41
2:D:461:SER:OG	2:D:462:TRP:N	2.53	0.41
1:F:283:ILE:HG23	1:F:412:PHE:CE2	2.56	0.41
1:A:390:ASN:OD1	1:F:386:GLY:HA3	2.21	0.40
1:B:351:PRO:HB3	1:B:383:LEU:HD23	2.02	0.40
2:D:293:GLY:O	2:D:295:THR:N	2.54	0.40
2:D:402:TYR:HA	2:D:405:GLN:HG2	2.03	0.40
1:C:164:LEU:HD11	1:C:180:MET:HE1	2.03	0.40
2:D:184:ARG:HD3	2:D:191:ILE:O	2.21	0.40
1:E:50:THR:HG22	1:E:209:ASN:HB2	2.03	0.40
1:A:52:LYS:HB2	1:A:52:LYS:HE3	1.89	0.40
1:A:508:ILE:HG13	1:A:510:ARG:H	1.86	0.40
1:B:48:SER:OG	1:C:198:GLU:O	2.36	0.40
1:B:89:SER:HB3	1:C:227:GLY:O	2.21	0.40
1:C:377:ILE:HD12	1:C:412:PHE:HE1	1.86	0.40
2:D:151:PHE:C	2:D:153:GLN:H	2.29	0.40
1:F:406:GLU:HB3	1:F:408:ILE:HG12	2.04	0.40
1:A:170:ARG:O	1:A:174:ILE:HG12	2.22	0.40
1:A:202:ASP:HA	1:A:226:ARG:HH11	1.86	0.40
1:B:144:ILE:HG22	1:B:147:VAL:HG12	2.04	0.40
1:B:261:VAL:O	1:B:279:PHE:HA	2.20	0.40
1:C:70:PRO:HB2	1:C:139:ALA:HA	2.04	0.40
1:C:469:GLU:HB3	1:C:483:PHE:CZ	2.56	0.40
1:C:117:VAL:C	1:C:119:GLY:H	2.30	0.40
2:D:499:VAL:HA	2:D:500:ASP:HA	1.63	0.40
2:D:509:VAL:HA	2:D:510:ARG:HB3	2.03	0.40
4:D:602:ATP:C2	1:E:462:TRP:HA	2.56	0.40
1:E:299:SER:C	1:E:333:MET:HE1	2.46	0.40
1:E:386:GLY:HA3	1:F:390:ASN:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/519 (97%)	424 (84%)	64 (13%)	15 (3%)	3	20
1	B	495/519 (95%)	425 (86%)	55 (11%)	15 (3%)	3	20
1	C	494/519 (95%)	425 (86%)	51 (10%)	18 (4%)	2	17
1	E	498/519 (96%)	434 (87%)	44 (9%)	20 (4%)	2	15
1	F	503/519 (97%)	427 (85%)	50 (10%)	26 (5%)	1	11
2	D	498/519 (96%)	436 (88%)	47 (9%)	15 (3%)	3	20
All	All	2991/3114 (96%)	2571 (86%)	311 (10%)	109 (4%)	2	17

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	LYS
1	B	33	HIS
1	B	117	VAL
1	C	124	SER
1	C	212	GLU
1	C	433	ILE
1	C	507	ARG
1	C	508	ILE
2	D	333	MET
2	D	498	THR
1	E	462	TRP
1	F	254	LEU
1	F	509	VAL
1	F	517	PRO
1	A	26	GLU
1	A	211	LEU
1	A	463	HIS
1	B	112	PRO
1	B	211	LEU
1	B	212	GLU

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Mol	Chain	Res	Type
1	B	420	MET
1	B	463	HIS
1	B	507	ARG
1	C	193	ARG
1	C	463	HIS
2	D	154	TYR
2	D	294	LYS
2	D	463	HIS
2	D	512	VAL
1	E	113	GLU
1	E	211	LEU
1	E	212	GLU
1	E	249	LEU
1	E	463	HIS
1	F	26	GLU
1	F	120	GLY
1	F	154	TYR
1	F	212	GLU
1	F	510	ARG
1	A	420	MET
1	C	17	ALA
1	C	115	GLN
1	C	116	GLU
1	C	250	GLY
1	C	348	CYS
1	C	420	MET
2	D	292	THR
2	D	348	CYS
1	E	348	CYS
1	F	15	HIS
1	F	16	GLN
1	F	250	GLY
1	F	348	CYS
1	F	463	HIS
1	F	507	ARG
1	F	516	GLY
1	A	212	GLU
1	A	348	CYS
1	B	154	TYR
1	B	276	GLY
1	C	118	VAL
2	D	420	MET

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Mol	Chain	Res	Type
2	D	506	SER
1	E	157	SER
1	E	385	ARG
1	E	420	MET
1	E	498	THR
1	F	116	GLU
1	F	189	GLY
1	F	370	PHE
1	F	504	GLU
1	F	508	ILE
1	A	117	VAL
1	A	120	GLY
1	A	370	PHE
1	A	372	PRO
1	A	499	VAL
1	B	480	LYS
1	B	499	VAL
1	C	372	PRO
2	D	212	GLU
2	D	507	ARG
1	E	497	ILE
1	E	503	SER
1	F	253	ARG
1	F	420	MET
1	A	503	SER
1	B	118	VAL
1	B	500	ASP
1	E	117	VAL
1	F	480	LYS
1	F	505	LEU
1	C	371	LYS
1	E	425	ILE
1	E	509	VAL
1	A	112	PRO
1	A	433	ILE
1	C	117	VAL
1	E	250	GLY
1	E	293	GLY
2	D	117	VAL
2	D	189	GLY
1	E	477	PRO
1	B	119	GLY

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Mol	Chain	Res	Type
2	D	494	PRO
1	E	196	VAL
1	F	293	GLY
1	F	512	VAL
1	C	112	PRO

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	430/442 (97%)	424 (99%)	6 (1%)	59	73
1	B	423/442 (96%)	419 (99%)	4 (1%)	70	78
1	C	423/442 (96%)	418 (99%)	5 (1%)	63	75
1	E	425/442 (96%)	415 (98%)	10 (2%)	43	65
1	F	430/442 (97%)	425 (99%)	5 (1%)	63	75
2	D	426/443 (96%)	415 (97%)	11 (3%)	40	64
All	All	2557/2653 (96%)	2516 (98%)	41 (2%)	55	72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	228	THR
1	A	375	ILE
1	A	433	ILE
1	A	497	ILE
1	A	502	LYS
1	B	123	LEU
1	B	147	VAL
1	B	380	LEU
1	B	509	VAL
1	C	182	THR
1	C	280	LYS
1	C	287	THR

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Mol	Chain	Res	Type
1	C	430	ILE
1	C	508	ILE
2	D	117	VAL
2	D	123	LEU
2	D	147	VAL
2	D	198	GLU
2	D	210	VAL
2	D	260	ASN
2	D	270	LEU
2	D	387	VAL
2	D	499	VAL
2	D	501	GLU
2	D	509	VAL
1	E	21	MET
1	E	83	ILE
1	E	196	VAL
1	E	198	GLU
1	E	212	GLU
1	E	366	GLU
1	E	444	GLU
1	E	463	HIS
1	E	472	ILE
1	E	499	VAL
1	F	43	LEU
1	F	118	VAL
1	F	344	LEU
1	F	509	VAL
1	F	512	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	HIS
1	A	454	ASN
1	A	513	GLN
1	B	131	ASN
1	B	323	GLN
1	B	327	ASN
1	B	342	ASN
1	C	454	ASN
2	D	15	HIS
2	D	203	ASN

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Mol	Chain	Res	Type
2	D	245	ASN
2	D	308	ASN
1	E	62	ASN
1	E	394	GLN
1	E	441	GLN
1	F	327	ASN
1	F	418	GLN
1	F	441	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	TPO	F	432	1	8,10,11	0.83	0	10,14,16	1.25	0
1	TPO	A	432	1	8,10,11	0.84	0	10,14,16	1.26	1 (10%)
1	TPO	B	432	1	8,10,11	0.88	0	10,14,16	1.41	1 (10%)
1	TPO	E	432	1	8,10,11	0.83	0	10,14,16	1.23	1 (10%)
1	TPO	C	432	1	8,10,11	1.03	0	10,14,16	1.61	3 (30%)

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	TPO	F	432	1	-	2/9/11/13	-
1	TPO	A	432	1	-	3/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	432	1	-	5/9/11/13	-
1	TPO	E	432	1	-	4/9/11/13	-
1	TPO	C	432	1	-	7/9/11/13	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	TPO	CG2-CB-CA	-2.78	107.84	113.26
1	C	432	TPO	P-OG1-CB	-2.77	115.79	123.33
1	B	432	TPO	P-OG1-CB	-2.32	117.02	123.33
1	A	432	TPO	P-OG1-CB	-2.25	117.20	123.33
1	C	432	TPO	O-C-CA	-2.14	119.25	124.77
1	E	432	TPO	P-OG1-CB	-2.03	117.80	123.33

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	432	TPO	O-C-CA-CB
1	B	432	TPO	C-CA-CB-CG2
1	C	432	TPO	N-CA-CB-OG1
1	C	432	TPO	C-CA-CB-CG2
1	E	432	TPO	O-C-CA-CB
1	F	432	TPO	N-CA-CB-OG1
1	A	432	TPO	CB-OG1-P-O1P
1	C	432	TPO	N-CA-CB-CG2
1	F	432	TPO	CB-OG1-P-O1P
1	B	432	TPO	CB-OG1-P-O2P
1	B	432	TPO	N-CA-CB-CG2
1	B	432	TPO	CB-OG1-P-O1P
1	C	432	TPO	CB-OG1-P-O1P
1	E	432	TPO	CB-OG1-P-O1P
1	B	432	TPO	CB-OG1-P-O3P
1	C	432	TPO	CB-OG1-P-O2P
1	C	432	TPO	CB-OG1-P-O3P
1	E	432	TPO	CB-OG1-P-O2P
1	E	432	TPO	CB-OG1-P-O3P
1	C	432	TPO	O-C-CA-CB
1	A	432	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	432	TPO	1	0
1	C	432	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	E	602	3	32,33,33	1.44	6 (18%)	48,52,52	1.72	10 (20%)
4	ATP	F	602	3	32,33,33	1.42	4 (12%)	48,52,52	1.74	9 (18%)
4	ATP	D	602	3	32,33,33	1.40	5 (15%)	48,52,52	1.76	9 (18%)
4	ATP	A	803	3	32,33,33	1.41	4 (12%)	48,52,52	1.75	9 (18%)
4	ATP	B	602	3	32,33,33	1.48	7 (21%)	48,52,52	1.77	9 (18%)
4	ATP	C	602	3	32,33,33	1.41	5 (15%)	48,52,52	1.79	8 (16%)
4	ATP	A	802	3	32,33,33	1.39	4 (12%)	48,52,52	1.80	9 (18%)
4	ATP	E	603	3	32,33,33	1.42	5 (15%)	48,52,52	1.78	11 (22%)
5	PO4	C	605	-	4,4,4	0.95	0	6,6,6	0.47	0
4	ATP	D	603	3	32,33,33	1.43	4 (12%)	48,52,52	1.78	10 (20%)
4	ATP	C	603	3	32,33,33	1.41	4 (12%)	48,52,52	1.78	9 (18%)
4	ATP	B	603	3	32,33,33	1.44	6 (18%)	48,52,52	1.76	9 (18%)
4	ATP	F	603	3	32,33,33	1.43	6 (18%)	48,52,52	1.79	10 (20%)

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	E	602	3	-	1/22/38/38	0/3/3/3
4	ATP	F	602	3	-	4/22/38/38	0/3/3/3
4	ATP	D	602	3	-	6/22/38/38	0/3/3/3
4	ATP	A	803	3	-	5/22/38/38	0/3/3/3
4	ATP	B	602	3	-	2/22/38/38	0/3/3/3
4	ATP	C	602	3	-	5/22/38/38	0/3/3/3
4	ATP	A	802	3	-	4/22/38/38	0/3/3/3
4	ATP	E	603	3	-	7/22/38/38	0/3/3/3
4	ATP	D	603	3	-	8/22/38/38	0/3/3/3
4	ATP	C	603	3	-	5/22/38/38	0/3/3/3
4	ATP	B	603	3	-	6/22/38/38	0/3/3/3
4	ATP	F	603	3	-	4/22/38/38	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	ATP	C5-C4	4.79	1.47	1.39
4	B	602	ATP	C5-C4	4.78	1.47	1.39
4	D	603	ATP	C5-C4	4.76	1.47	1.39
4	C	603	ATP	C5-C4	4.75	1.47	1.39
4	B	603	ATP	C5-C4	4.74	1.47	1.39
4	F	602	ATP	C5-C4	4.74	1.47	1.39
4	A	802	ATP	C5-C4	4.73	1.47	1.39
4	C	602	ATP	C5-C4	4.70	1.47	1.39
4	E	602	ATP	C5-C4	4.70	1.47	1.39
4	F	603	ATP	C5-C4	4.70	1.47	1.39
4	D	602	ATP	C5-C4	4.69	1.47	1.39
4	E	603	ATP	C5-C4	4.66	1.47	1.39
4	D	603	ATP	C5-C6	2.81	1.48	1.41
4	F	602	ATP	C5-C6	2.79	1.48	1.41
4	B	603	ATP	C5-C6	2.79	1.48	1.41
4	A	802	ATP	C5-C6	2.78	1.48	1.41
4	F	603	ATP	C5-C6	2.78	1.48	1.41
4	E	602	ATP	C5-C6	2.76	1.48	1.41
4	B	602	ATP	C5-C6	2.75	1.48	1.41
4	E	603	ATP	C5-C6	2.74	1.48	1.41
4	C	603	ATP	C5-C6	2.74	1.48	1.41
4	A	803	ATP	C5-C6	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	ATP	C5-C6	2.72	1.48	1.41
4	C	602	ATP	C5-C6	2.67	1.48	1.41
4	D	603	ATP	C8-N7	2.44	1.36	1.31
4	F	603	ATP	C8-N7	2.44	1.36	1.31
4	B	602	ATP	PA-O3A	2.43	1.62	1.59
4	E	603	ATP	C8-N7	2.42	1.36	1.31
4	F	602	ATP	C8-N7	2.41	1.36	1.31
4	A	802	ATP	C8-N7	2.41	1.36	1.31
4	E	602	ATP	C8-N7	2.41	1.36	1.31
4	B	602	ATP	C8-N7	2.37	1.36	1.31
4	A	803	ATP	C8-N7	2.36	1.36	1.31
4	C	603	ATP	C8-N7	2.35	1.36	1.31
4	B	603	ATP	C8-N7	2.35	1.36	1.31
4	D	602	ATP	C8-N7	2.32	1.36	1.31
4	D	602	ATP	C5-N7	-2.31	1.34	1.39
4	C	602	ATP	C5-N7	-2.31	1.34	1.39
4	B	602	ATP	C5-N7	-2.27	1.34	1.39
4	B	603	ATP	C5-N7	-2.26	1.35	1.39
4	C	602	ATP	C8-N7	2.24	1.36	1.31
4	C	603	ATP	C5-N7	-2.22	1.35	1.39
4	B	602	ATP	PB-O3B	2.22	1.61	1.59
4	E	602	ATP	C5-N7	-2.21	1.35	1.39
4	F	603	ATP	PA-O3A	2.21	1.61	1.59
4	E	602	ATP	PB-O3A	2.21	1.61	1.59
4	A	803	ATP	C5-N7	-2.20	1.35	1.39
4	A	802	ATP	C5-N7	-2.19	1.35	1.39
4	B	603	ATP	PA-O3A	2.19	1.61	1.59
4	F	603	ATP	C5-N7	-2.18	1.35	1.39
4	D	603	ATP	C5-N7	-2.18	1.35	1.39
4	B	602	ATP	PB-O3A	2.17	1.61	1.59
4	F	602	ATP	C5-N7	-2.17	1.35	1.39
4	E	603	ATP	C5-N7	-2.16	1.35	1.39
4	E	603	ATP	PA-O3A	2.16	1.61	1.59
4	F	603	ATP	PB-O3B	2.06	1.61	1.59
4	B	603	ATP	PB-O3B	2.06	1.61	1.59
4	E	602	ATP	PA-O3A	2.06	1.61	1.59
4	D	602	ATP	PA-O3A	2.04	1.61	1.59
4	C	602	ATP	PB-O3B	2.03	1.61	1.59

All (112) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	ATP	C5-C4-N3	-5.97	118.50	126.72
4	B	603	ATP	C5-C4-N3	-5.96	118.51	126.72
4	B	602	ATP	C5-C4-N3	-5.95	118.53	126.72
4	C	603	ATP	C5-C4-N3	-5.94	118.54	126.72
4	D	603	ATP	C5-C4-N3	-5.91	118.58	126.72
4	F	602	ATP	C5-C4-N3	-5.90	118.60	126.72
4	F	603	ATP	C5-C4-N3	-5.87	118.64	126.72
4	D	602	ATP	C5-C4-N3	-5.87	118.64	126.72
4	C	602	ATP	C5-C4-N3	-5.83	118.68	126.72
4	A	803	ATP	C5-C4-N3	-5.80	118.73	126.72
4	E	602	ATP	C5-C4-N3	-5.74	118.82	126.72
4	E	603	ATP	C5-C4-N3	-5.69	118.89	126.72
4	C	602	ATP	N3-C4-N9	4.84	135.40	127.17
4	B	603	ATP	N3-C4-N9	4.69	135.15	127.17
4	D	602	ATP	N3-C4-N9	4.66	135.09	127.17
4	B	602	ATP	N3-C4-N9	4.64	135.07	127.17
4	C	603	ATP	N3-C4-N9	4.63	135.04	127.17
4	A	803	ATP	N3-C4-N9	4.61	135.00	127.17
4	A	802	ATP	N3-C4-N9	4.60	134.99	127.17
4	D	603	ATP	N3-C4-N9	4.59	134.97	127.17
4	F	602	ATP	N3-C4-N9	4.54	134.89	127.17
4	E	602	ATP	N3-C4-N9	4.46	134.75	127.17
4	F	603	ATP	N3-C4-N9	4.45	134.73	127.17
4	E	603	ATP	N3-C4-N9	4.34	134.54	127.17
4	B	603	ATP	C2-N3-C4	3.76	121.01	111.83
4	B	602	ATP	C2-N3-C4	3.74	120.96	111.83
4	D	603	ATP	C2-N3-C4	3.73	120.95	111.83
4	A	802	ATP	C2-N3-C4	3.72	120.91	111.83
4	F	602	ATP	C2-N3-C4	3.71	120.89	111.83
4	C	603	ATP	C2-N3-C4	3.71	120.88	111.83
4	F	603	ATP	C4-C5-N7	-3.70	106.35	110.58
4	F	603	ATP	C2-N3-C4	3.70	120.86	111.83
4	E	603	ATP	C2-N3-C4	3.69	120.83	111.83
4	D	602	ATP	C2-N3-C4	3.67	120.81	111.83
4	A	803	ATP	C2-N3-C4	3.67	120.80	111.83
4	C	602	ATP	C2-N3-C4	3.67	120.79	111.83
4	E	603	ATP	C4-C5-N7	-3.66	106.39	110.58
4	C	603	ATP	C4-C5-N7	-3.64	106.42	110.58
4	F	602	ATP	C4-C5-N7	-3.63	106.44	110.58
4	E	602	ATP	C2-N3-C4	3.61	120.65	111.83
4	D	603	ATP	C4-C5-N7	-3.61	106.46	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	ATP	C4-C5-N7	-3.55	106.52	110.58
4	A	802	ATP	C4-C5-N7	-3.54	106.53	110.58
4	A	803	ATP	C4-C5-N7	-3.50	106.58	110.58
4	B	603	ATP	C4-C5-N7	-3.49	106.59	110.58
4	B	602	ATP	C4-C5-N7	-3.49	106.59	110.58
4	D	602	ATP	C4-C5-N7	-3.39	106.71	110.58
4	E	603	ATP	N3-C2-N1	-3.28	123.61	128.58
4	B	603	ATP	N3-C2-N1	-3.22	123.72	128.58
4	D	603	ATP	N3-C2-N1	-3.21	123.72	128.58
4	C	602	ATP	N3-C2-N1	-3.21	123.72	128.58
4	B	602	ATP	N3-C2-N1	-3.21	123.73	128.58
4	C	602	ATP	C4-C5-N7	-3.17	106.95	110.58
4	A	803	ATP	N3-C2-N1	-3.16	123.80	128.58
4	F	603	ATP	N3-C2-N1	-3.16	123.80	128.58
4	C	603	ATP	N3-C2-N1	-3.14	123.83	128.58
4	F	602	ATP	N3-C2-N1	-3.14	123.83	128.58
4	A	802	ATP	N3-C2-N1	-3.12	123.86	128.58
4	D	602	ATP	N3-C2-N1	-3.11	123.88	128.58
4	E	602	ATP	N3-C2-N1	-3.06	123.95	128.58
4	C	602	ATP	C4-N9-C8	2.83	108.71	105.74
4	A	802	ATP	C3'-C2'-C1'	2.72	106.60	101.46
4	E	602	ATP	C4-N9-C8	2.67	108.54	105.74
4	A	803	ATP	C4-N9-C8	2.67	108.54	105.74
4	C	603	ATP	C5-N7-C8	2.65	107.61	103.45
4	F	603	ATP	C5-N7-C8	2.64	107.60	103.45
4	F	602	ATP	C5-N7-C8	2.61	107.56	103.45
4	E	603	ATP	C4-N9-C8	2.61	108.48	105.74
4	D	603	ATP	C5-N7-C8	2.60	107.54	103.45
4	C	602	ATP	C3'-C2'-C1'	2.60	106.38	101.46
4	E	603	ATP	C5-N7-C8	2.60	107.53	103.45
4	B	603	ATP	C5-N7-C8	2.59	107.52	103.45
4	E	602	ATP	C5-N7-C8	2.58	107.51	103.45
4	D	602	ATP	C4-N9-C8	2.57	108.44	105.74
4	A	803	ATP	C5-N7-C8	2.57	107.49	103.45
4	C	603	ATP	C4-N9-C8	2.56	108.43	105.74
4	B	602	ATP	C3'-C2'-C1'	2.55	106.29	101.46
4	A	802	ATP	C5-N7-C8	2.53	107.43	103.45
4	B	602	ATP	C5-N7-C8	2.53	107.42	103.45
4	D	602	ATP	C5-N7-C8	2.51	107.39	103.45
4	D	603	ATP	C4-N9-C8	2.51	108.37	105.74
4	B	603	ATP	C4-N9-C8	2.48	108.35	105.74
4	F	602	ATP	C4-N9-C8	2.48	108.35	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	603	ATP	C4-N9-C8	2.44	108.30	105.74
4	C	602	ATP	C5-N7-C8	2.43	107.27	103.45
4	B	602	ATP	C4-N9-C8	2.42	108.28	105.74
4	A	802	ATP	C4-N9-C8	2.42	108.28	105.74
4	C	603	ATP	C3'-C2'-C1'	2.42	106.04	101.46
4	D	602	ATP	C3'-C2'-C1'	2.38	105.97	101.46
4	A	803	ATP	C3'-C2'-C1'	2.35	105.90	101.46
4	F	603	ATP	O4'-C1'-N9	2.31	112.53	108.09
4	D	603	ATP	C3'-C2'-C1'	2.31	105.83	101.46
4	E	603	ATP	C6-C5-N7	2.27	136.47	132.09
4	F	602	ATP	C3'-C2'-C1'	2.26	105.74	101.46
4	B	603	ATP	C3'-C2'-C1'	2.26	105.74	101.46
4	E	602	ATP	C3'-C2'-C1'	2.23	105.69	101.46
4	F	603	ATP	C6-C5-N7	2.20	136.34	132.09
4	F	602	ATP	C6-C5-N7	2.16	136.26	132.09
4	E	603	ATP	C3'-C2'-C1'	2.16	105.55	101.46
4	E	603	ATP	O4'-C1'-N9	2.15	112.22	108.09
4	D	603	ATP	C6-C5-N7	2.15	136.23	132.09
4	E	602	ATP	C6-C5-N7	2.15	136.23	132.09
4	A	803	ATP	C6-C5-N7	2.13	136.20	132.09
4	C	603	ATP	C6-C5-N7	2.13	136.19	132.09
4	A	802	ATP	C6-C5-N7	2.09	136.12	132.09
4	E	602	ATP	N9-C8-N7	-2.07	111.00	113.94
4	E	603	ATP	N9-C8-N7	-2.05	111.03	113.94
4	B	603	ATP	C6-C5-N7	2.05	136.04	132.09
4	B	602	ATP	C6-C5-N7	2.03	136.01	132.09
4	F	603	ATP	C3'-C2'-C1'	2.02	105.29	101.46
4	D	603	ATP	O4'-C1'-N9	2.02	111.97	108.09
4	D	602	ATP	C6-C5-N7	2.00	135.96	132.09

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	ATP	PB-O3A-PA-O5'
4	A	802	ATP	C5'-O5'-PA-O1A
4	A	802	ATP	C5'-O5'-PA-O3A
4	A	803	ATP	C5'-O5'-PA-O2A
4	B	603	ATP	C5'-O5'-PA-O1A
4	B	603	ATP	C5'-O5'-PA-O2A
4	B	603	ATP	C5'-O5'-PA-O3A
4	C	602	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	C	602	ATP	PB-O3B-PG-O3G
4	D	602	ATP	C5'-O5'-PA-O1A
4	D	602	ATP	C5'-O5'-PA-O2A
4	D	602	ATP	C5'-O5'-PA-O3A
4	D	603	ATP	C5'-O5'-PA-O2A
4	E	603	ATP	C5'-O5'-PA-O1A
4	E	603	ATP	C5'-O5'-PA-O2A
4	E	603	ATP	C5'-O5'-PA-O3A
4	F	603	ATP	C5'-O5'-PA-O1A
4	F	603	ATP	C5'-O5'-PA-O2A
4	F	603	ATP	C5'-O5'-PA-O3A
4	C	602	ATP	O4'-C4'-C5'-O5'
4	C	602	ATP	C3'-C4'-C5'-O5'
4	D	603	ATP	C3'-C4'-C5'-O5'
4	B	602	ATP	PB-O3A-PA-O1A
4	D	602	ATP	PB-O3A-PA-O1A
4	A	803	ATP	PB-O3A-PA-O5'
4	D	603	ATP	PB-O3A-PA-O5'
4	E	602	ATP	PB-O3A-PA-O5'
4	E	603	ATP	PB-O3A-PA-O5'
4	F	602	ATP	PB-O3A-PA-O5'
4	F	603	ATP	PB-O3A-PA-O5'
4	D	603	ATP	PG-O3B-PB-O2B
4	E	603	ATP	PG-O3B-PB-O2B
4	A	802	ATP	C5'-O5'-PA-O2A
4	A	803	ATP	C5'-O5'-PA-O3A
4	D	603	ATP	C5'-O5'-PA-O1A
4	D	603	ATP	C5'-O5'-PA-O3A
4	C	603	ATP	PA-O3A-PB-O2B
4	F	602	ATP	PB-O3B-PG-O1G
4	E	603	ATP	PB-O3A-PA-O1A
4	B	602	ATP	PB-O3A-PA-O5'
4	D	602	ATP	PB-O3A-PA-O5'
4	A	803	ATP	PB-O3B-PG-O1G
4	A	803	ATP	PB-O3B-PG-O3G
4	F	602	ATP	PB-O3B-PG-O2G
4	F	602	ATP	PB-O3B-PG-O3G
4	C	603	ATP	O4'-C4'-C5'-O5'
4	C	603	ATP	C3'-C4'-C5'-O5'
4	B	603	ATP	PG-O3B-PB-O1B
4	C	603	ATP	PG-O3B-PB-O1B
4	C	603	ATP	PG-O3B-PB-O2B

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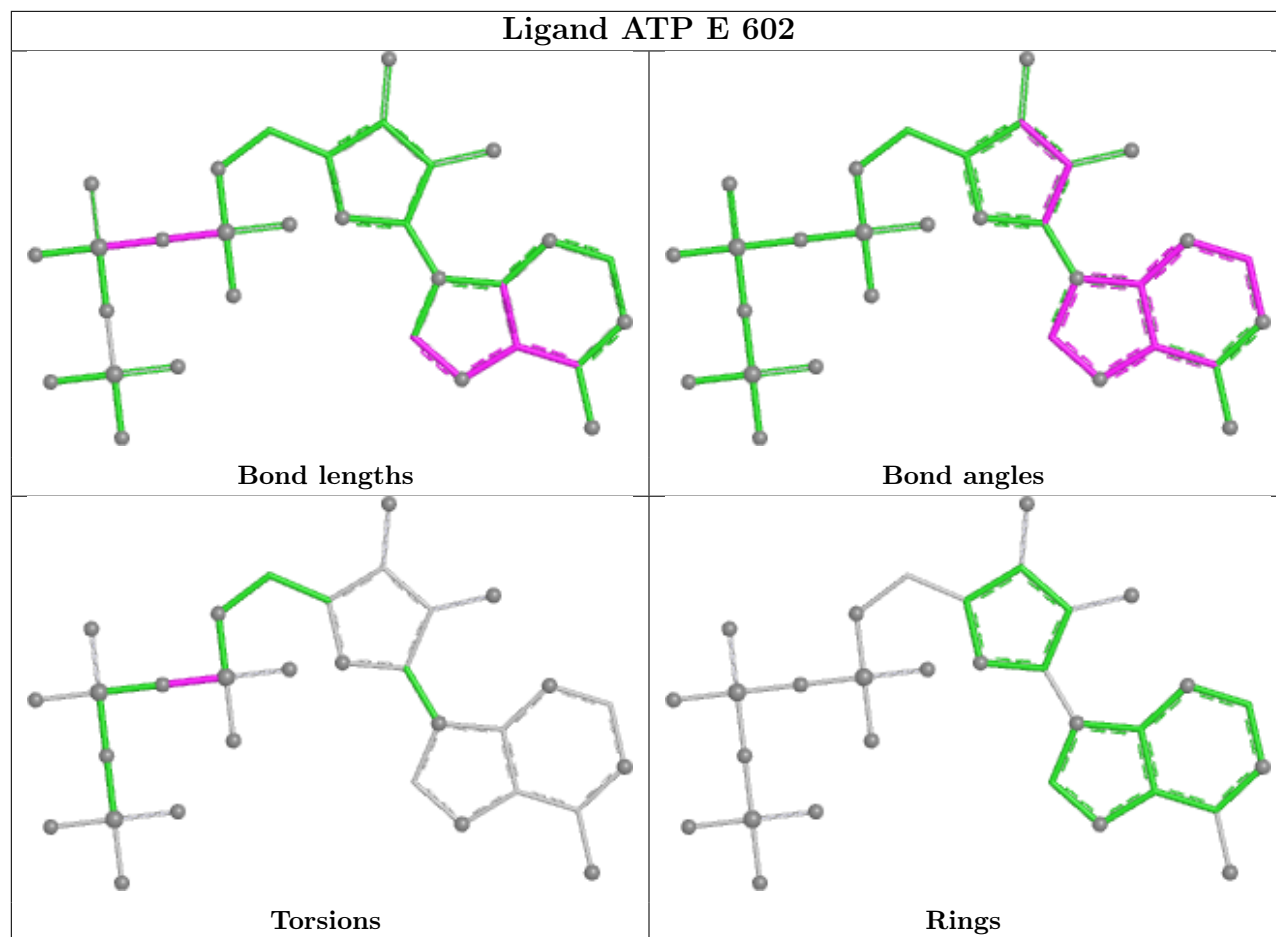
Mol	Chain	Res	Type	Atoms
4	D	602	ATP	PA-O3A-PB-O1B
4	D	603	ATP	PG-O3B-PB-O1B
4	C	602	ATP	PB-O3B-PG-O1G
4	B	603	ATP	PG-O3B-PB-O2B
4	B	603	ATP	PA-O3A-PB-O2B
4	E	603	ATP	PG-O3B-PB-O1B
4	D	603	ATP	O4'-C4'-C5'-O5'

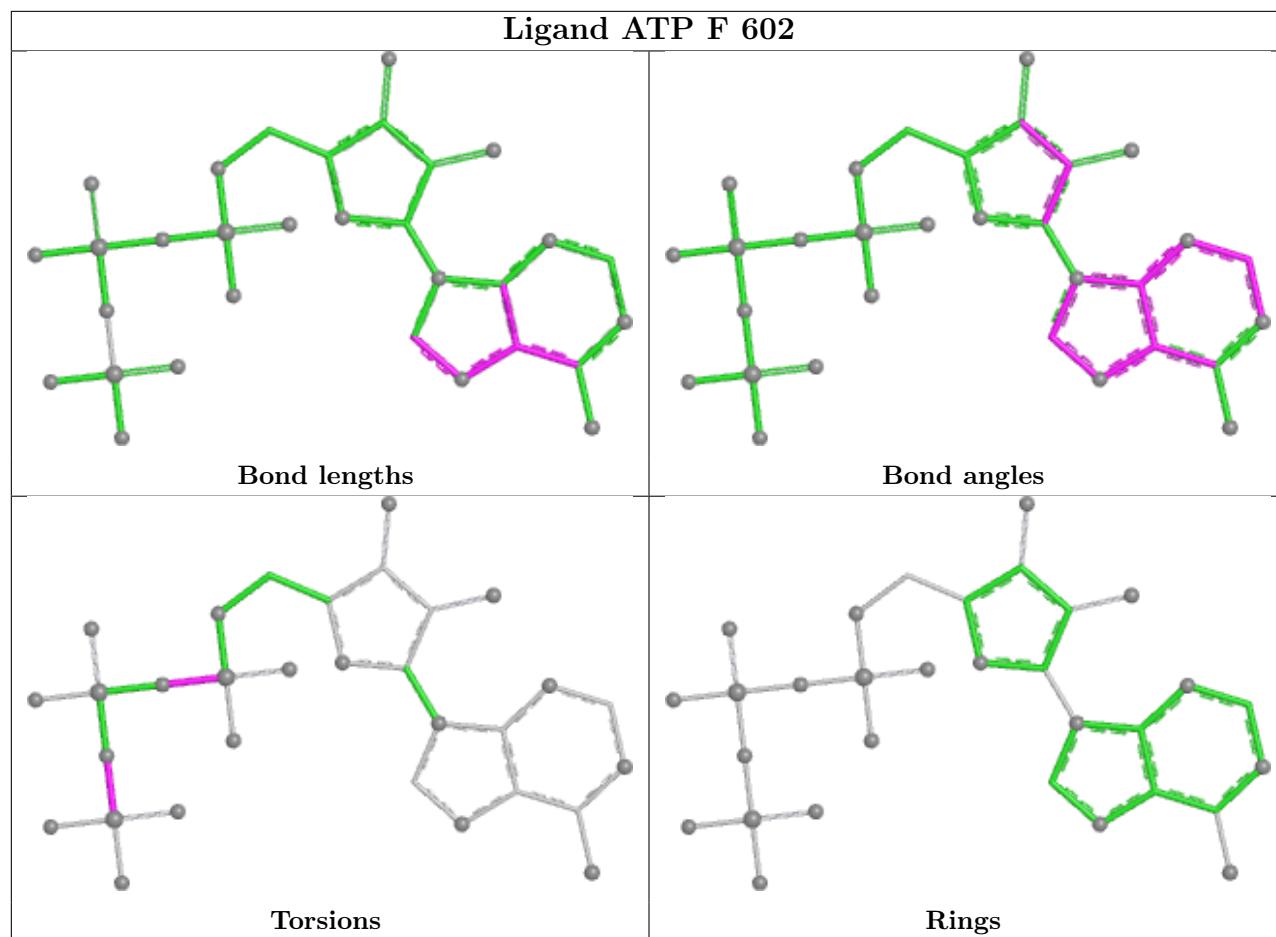
There are no ring outliers.

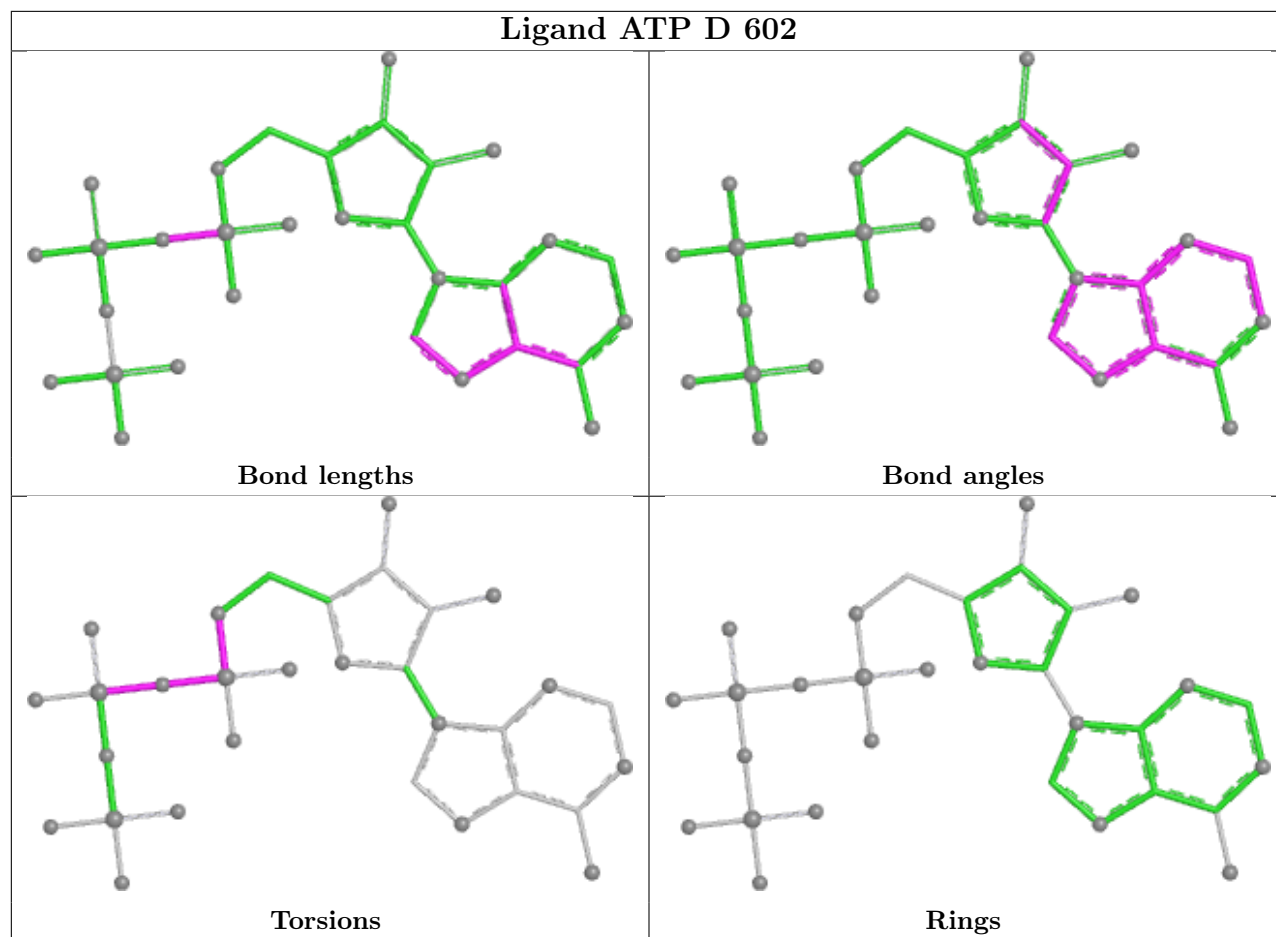
11 monomers are involved in 21 short contacts:

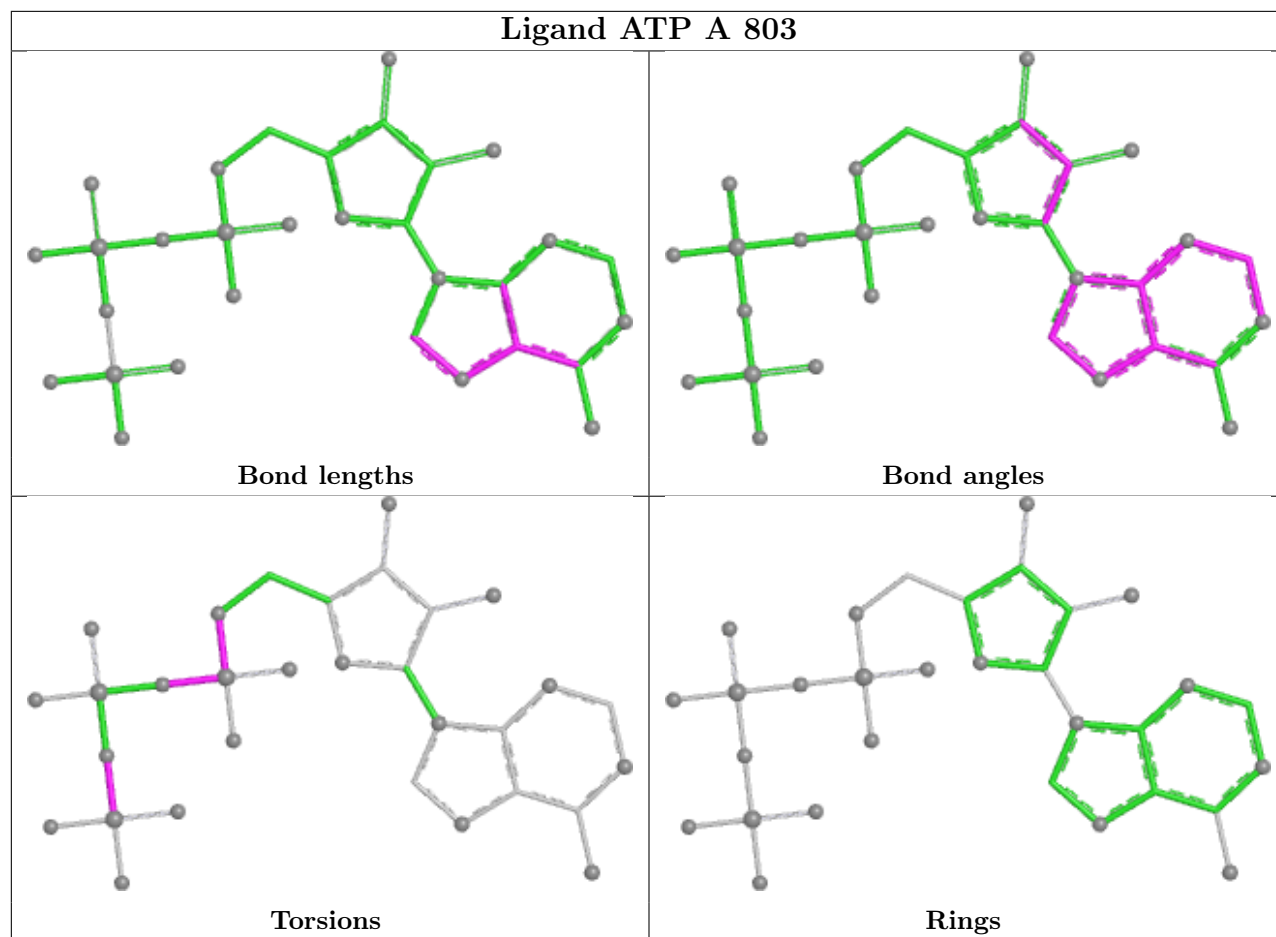
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	602	ATP	1	0
4	F	602	ATP	3	0
4	D	602	ATP	3	0
4	A	803	ATP	1	0
4	B	602	ATP	1	0
4	A	802	ATP	4	0
4	E	603	ATP	2	0
4	D	603	ATP	1	0
4	C	603	ATP	1	0
4	B	603	ATP	2	0
4	F	603	ATP	2	0

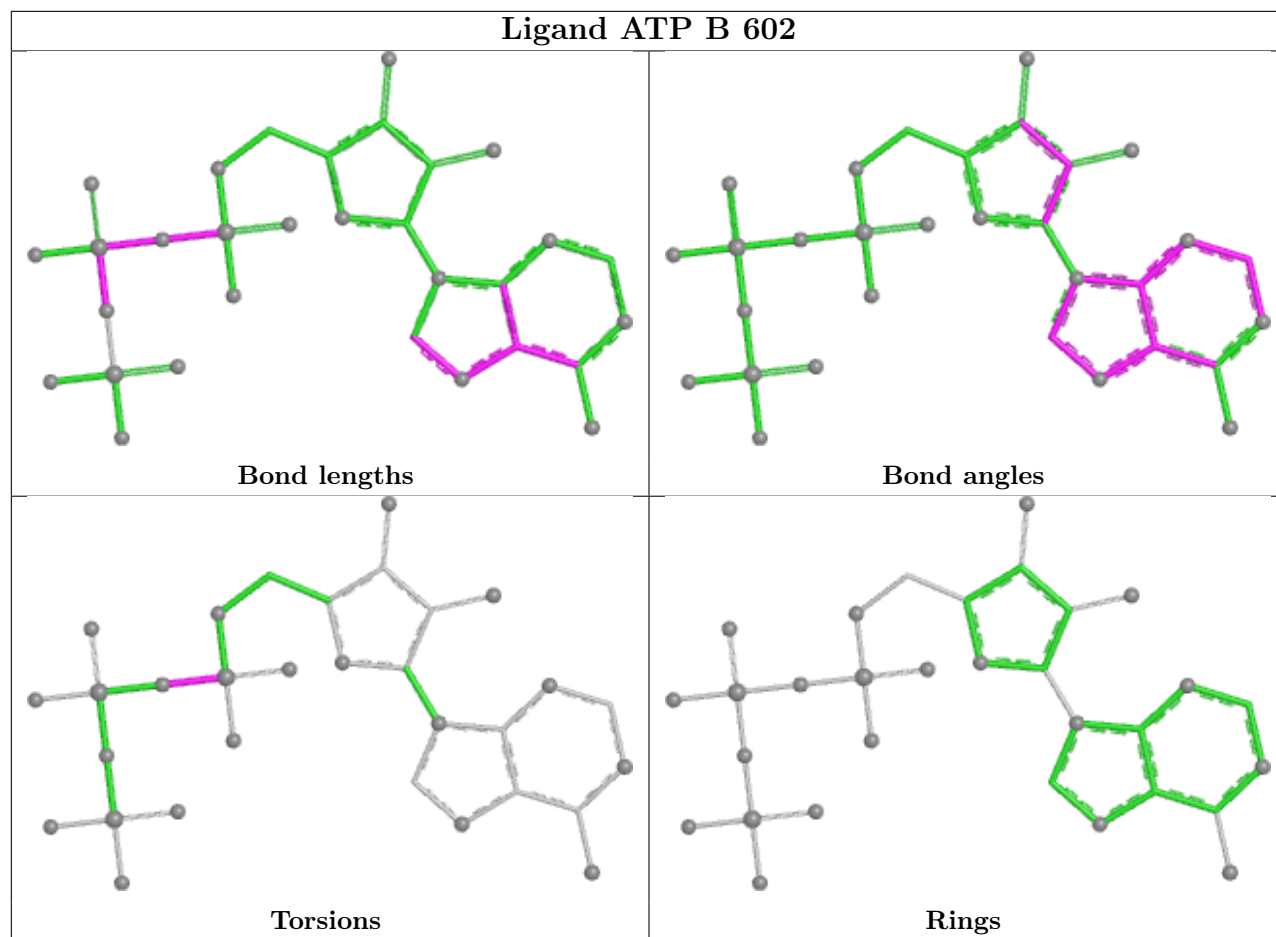
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

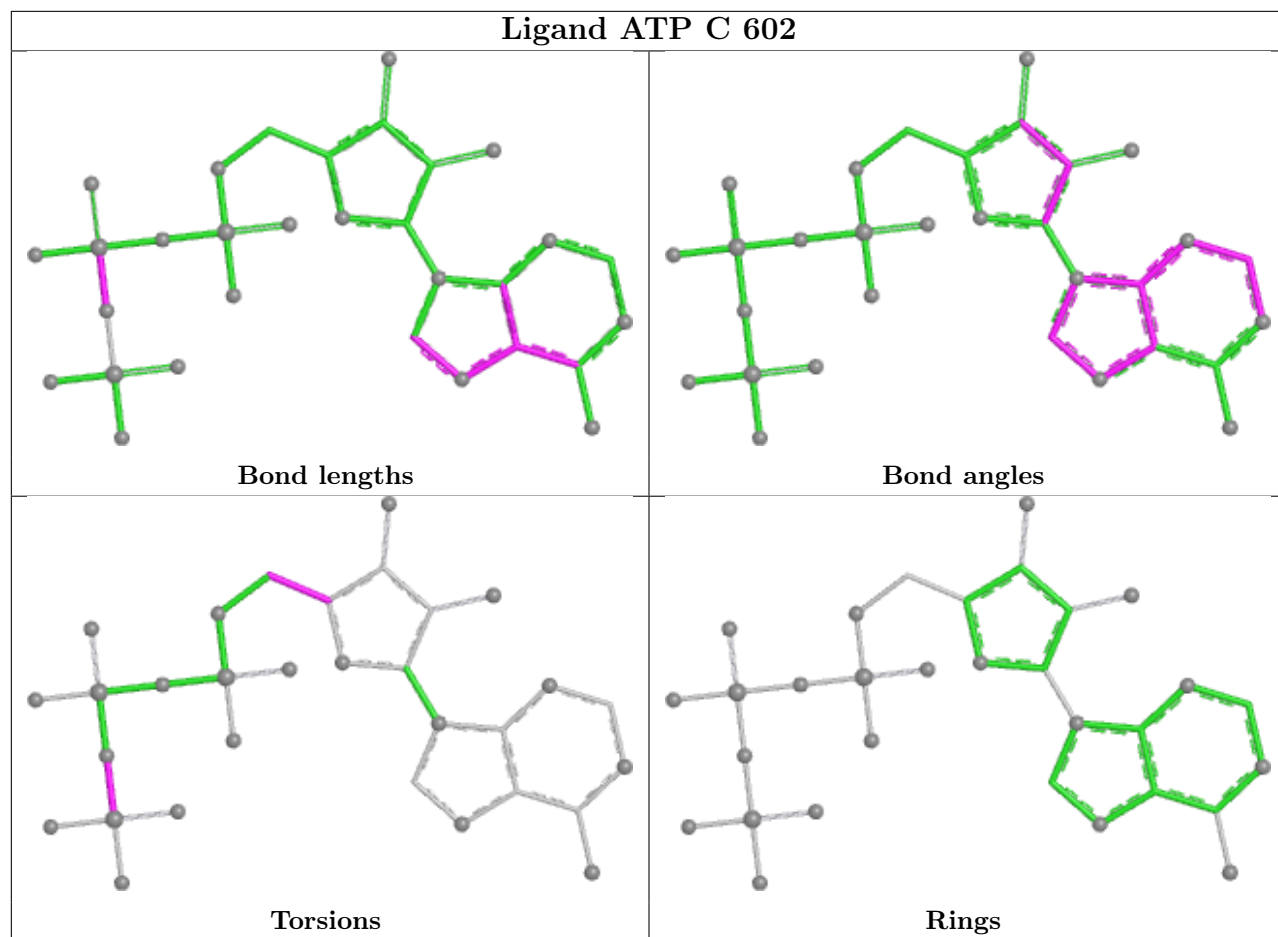


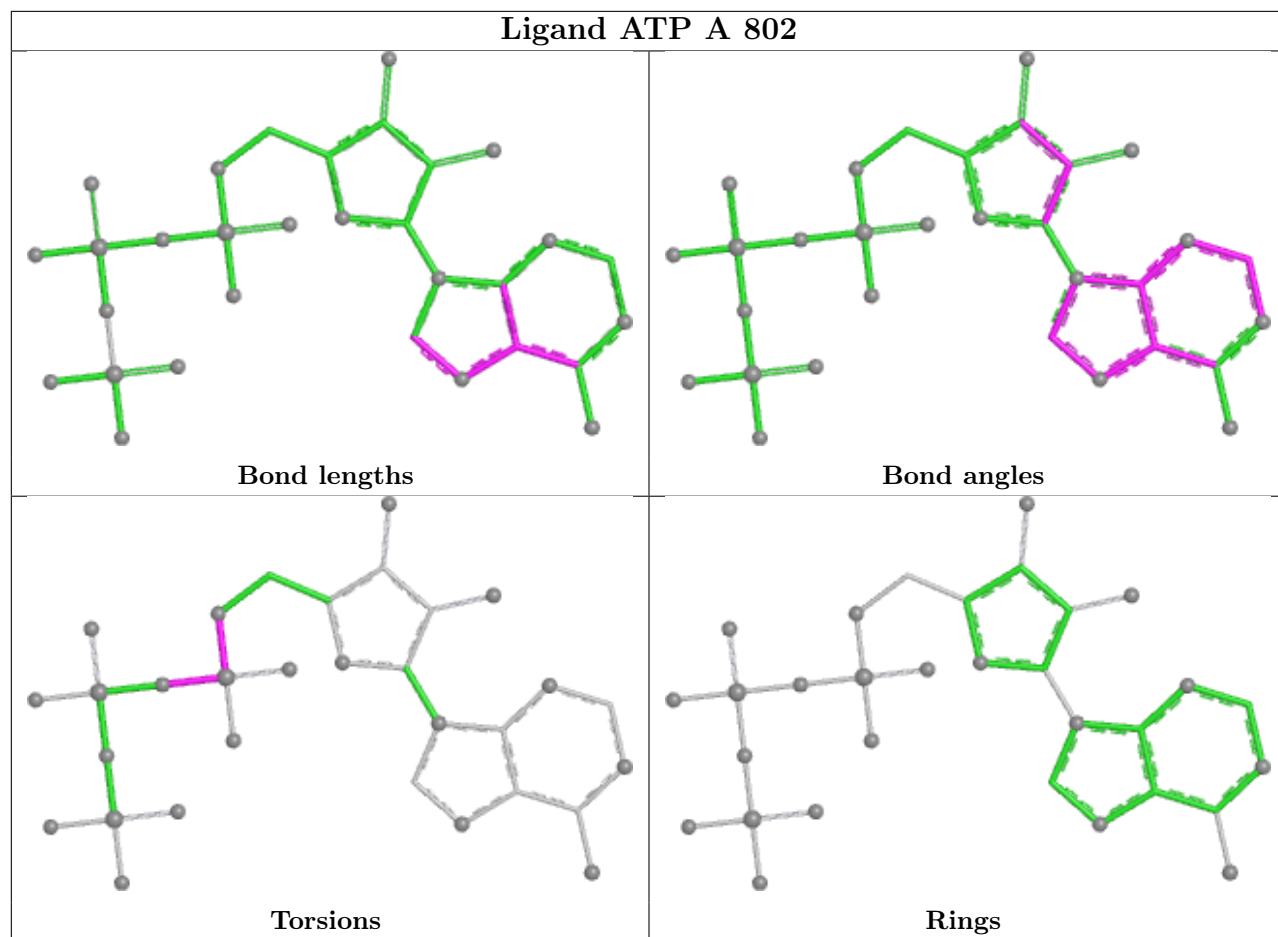


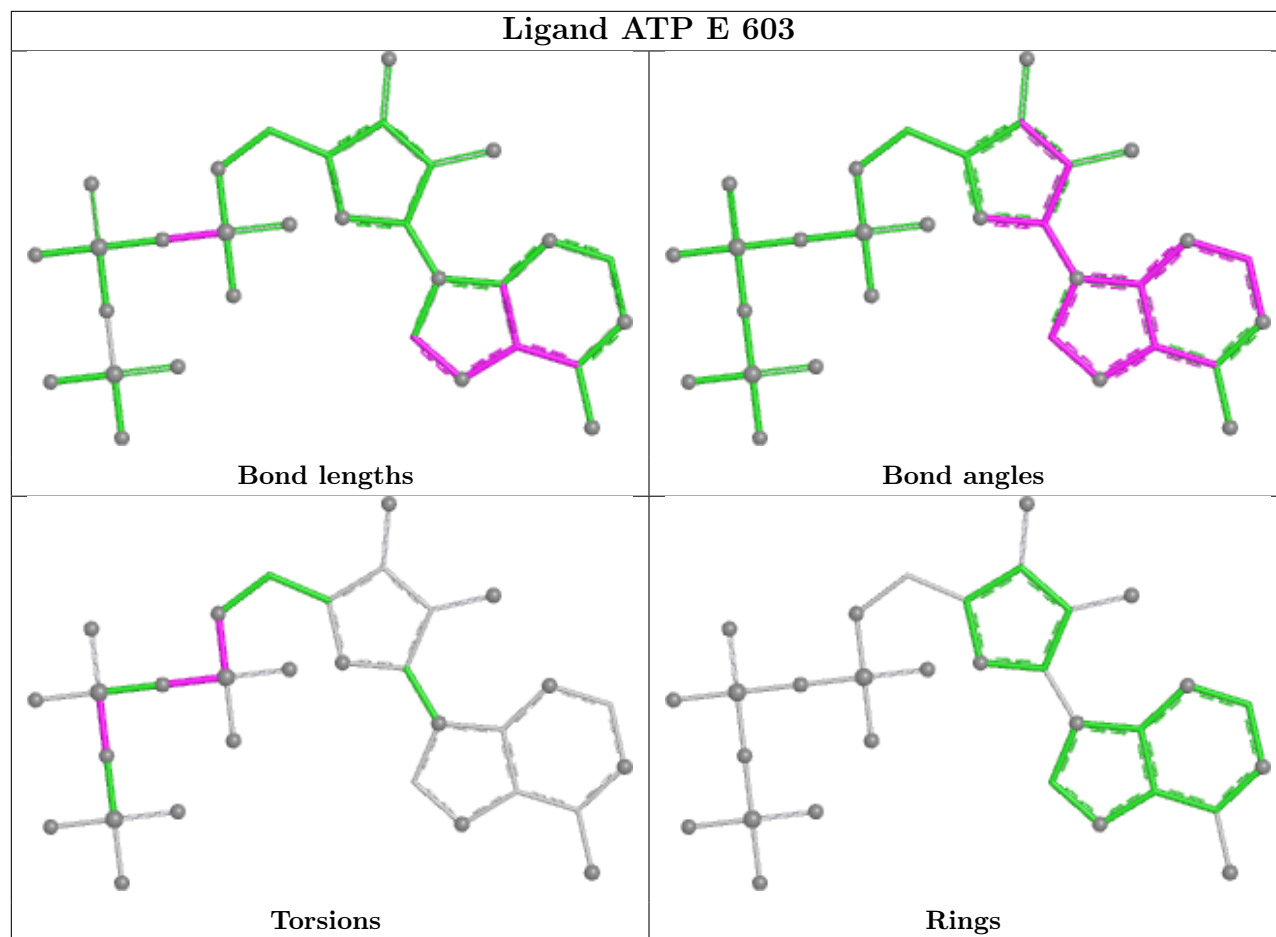


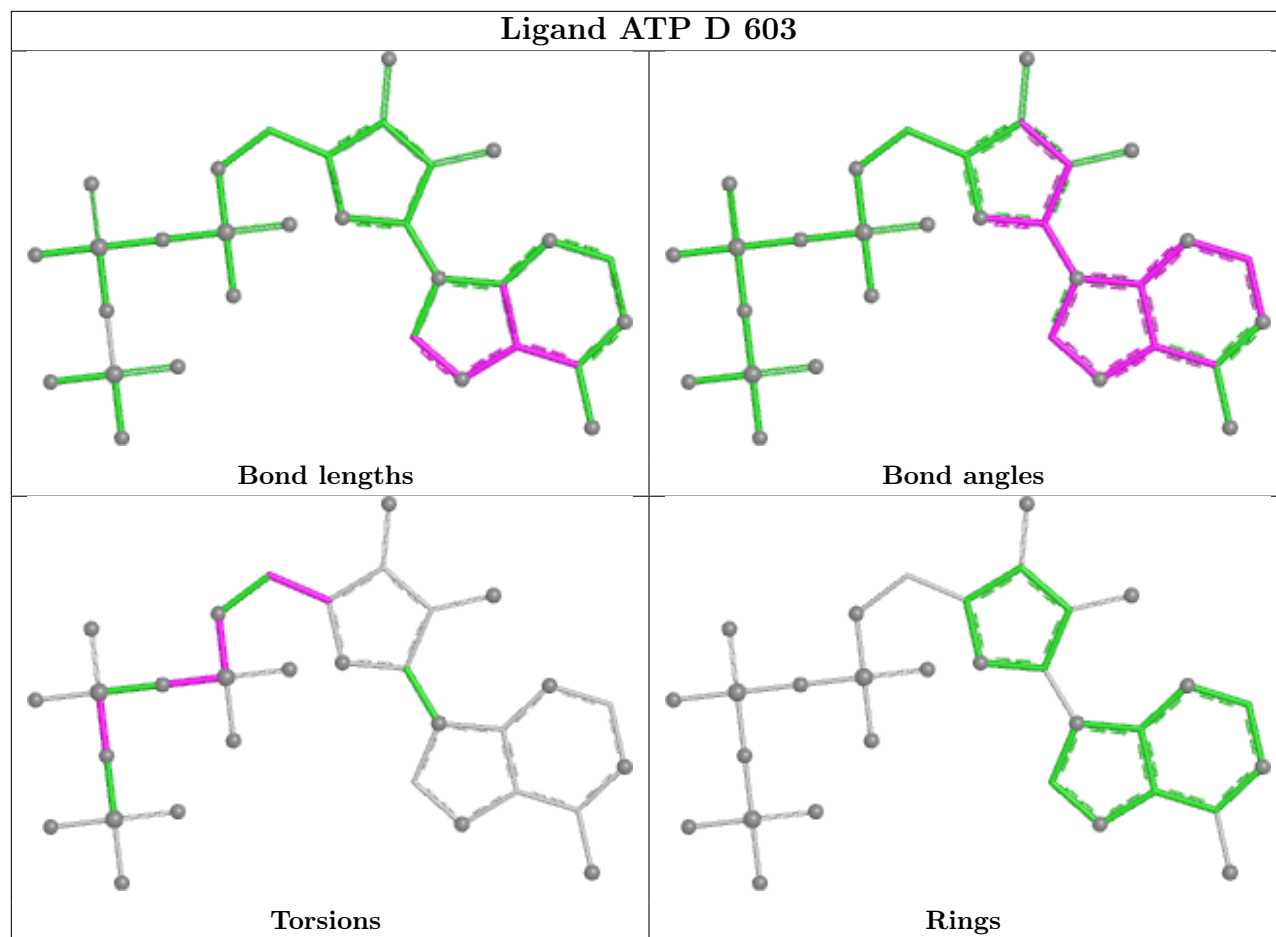


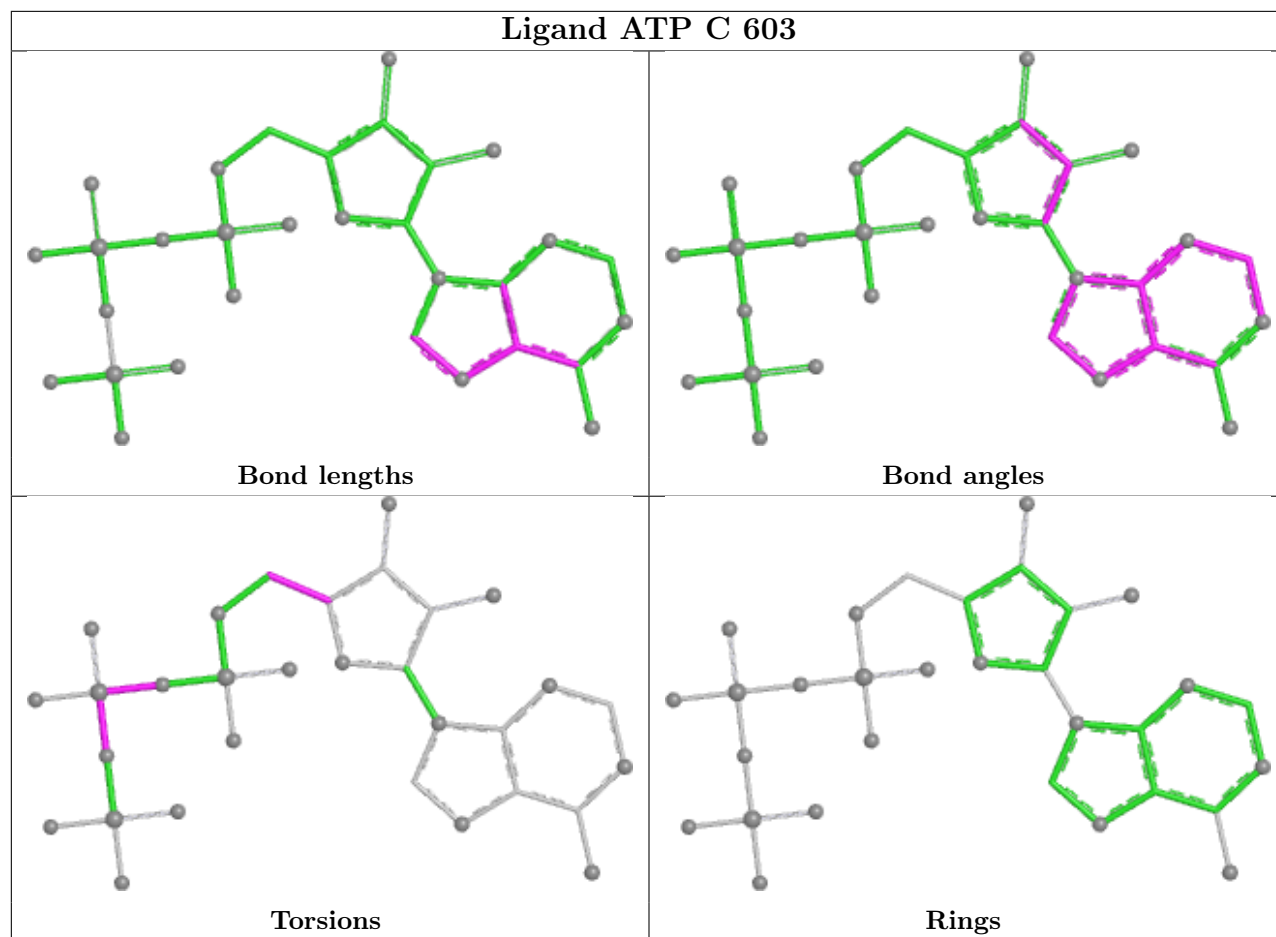


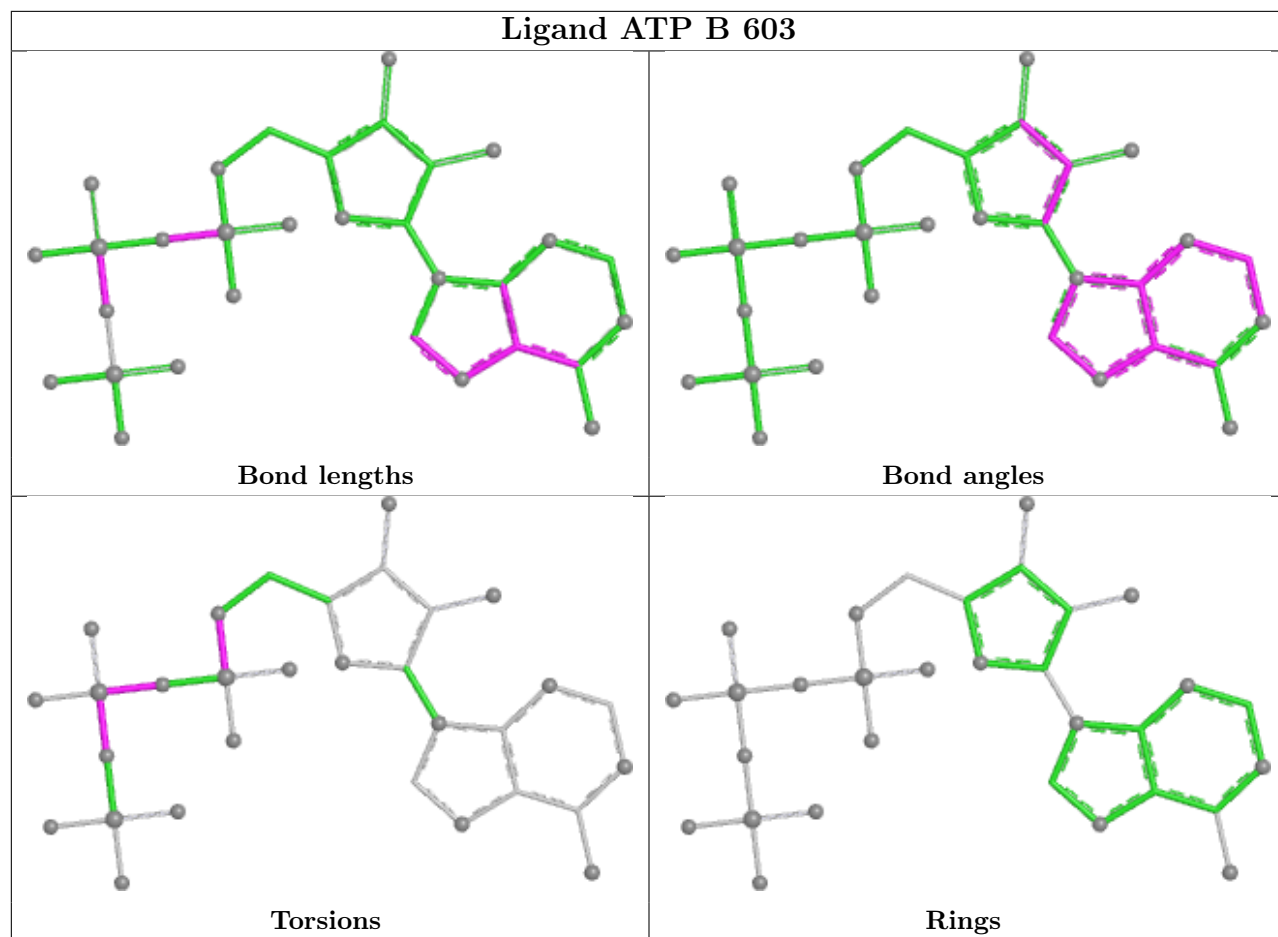


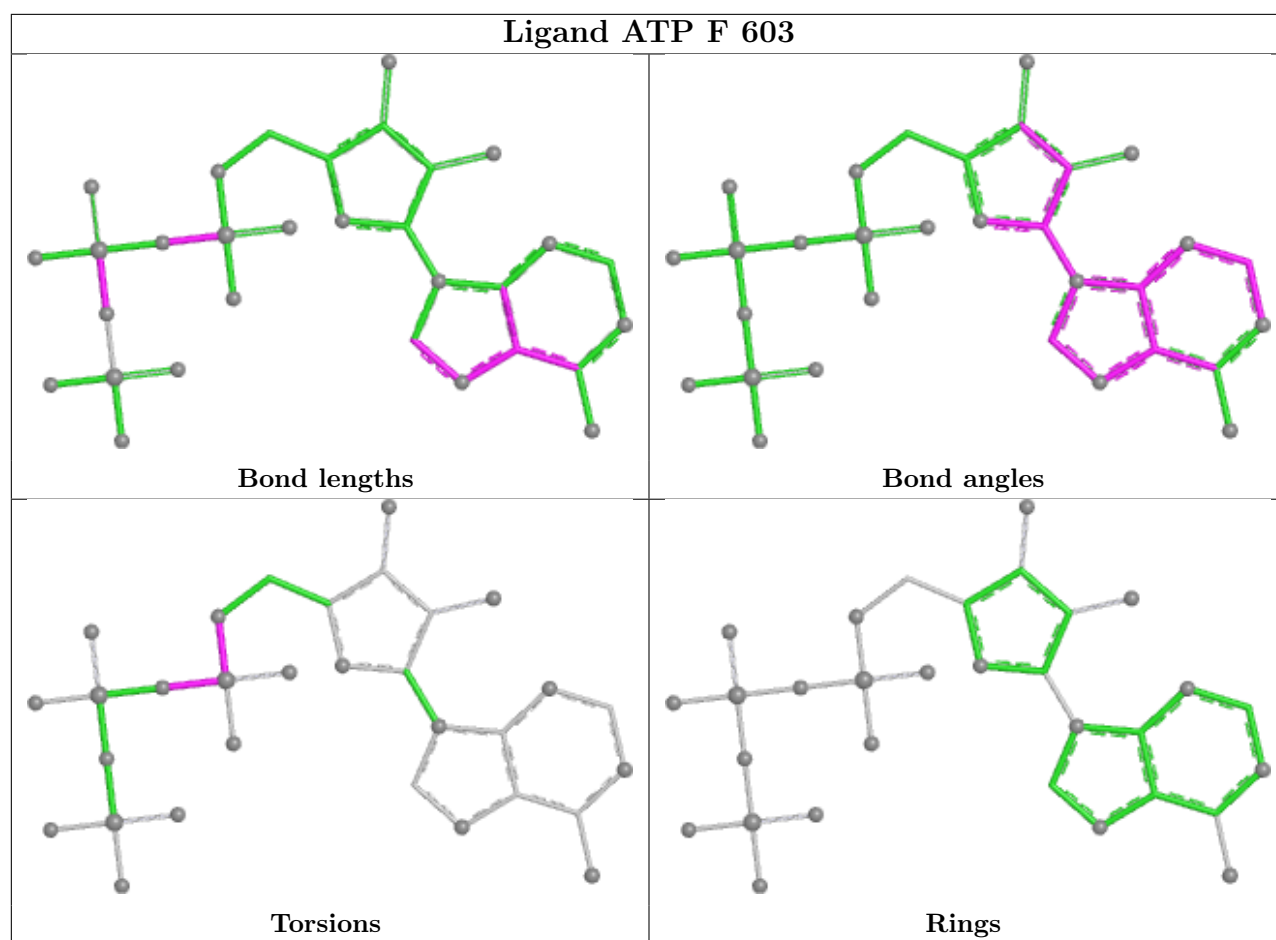












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	505/519 (97%)	0.13	3 (0%) 85 73	66, 113, 156, 183	0
1	B	497/519 (95%)	0.20	5 (1%) 79 63	75, 115, 154, 195	0
1	C	496/519 (95%)	0.04	2 (0%) 88 79	57, 101, 149, 191	0
1	E	500/519 (96%)	-0.10	0 100 100	41, 87, 140, 176	0
1	F	505/519 (97%)	-0.02	2 (0%) 88 79	42, 99, 150, 174	0
2	D	500/519 (96%)	-0.14	1 (0%) 91 86	50, 83, 139, 186	0
All	All	3003/3114 (96%)	0.02	13 (0%) 88 79	41, 101, 151, 195	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	SER	3.2
1	B	412	PHE	2.5
1	B	119	GLY	2.4
2	D	249	LEU	2.4
1	A	297	LEU	2.3
1	F	443	VAL	2.3
1	B	508	ILE	2.2
1	A	498	THR	2.1
1	B	117	VAL	2.1
1	F	117	VAL	2.1
1	C	509	VAL	2.1
1	A	517	PRO	2.1
1	B	191	ILE	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	TPO	F	432	11/12	0.65	0.15	102,112,126,149	0
1	TPO	B	432	11/12	0.75	0.11	109,120,131,144	0
1	TPO	A	432	11/12	0.80	0.10	104,112,128,135	0
1	TPO	C	432	11/12	0.86	0.09	83,101,125,141	0
1	TPO	E	432	11/12	0.88	0.11	76,87,116,130	0

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(Å ²)	Q<0.9
3	MG	B	601	1/1	0.65	0.15	114,114,114,114	0
3	MG	D	601	1/1	0.80	0.21	112,112,112,112	0
3	MG	F	604	1/1	0.82	0.10	68,68,68,68	0
3	MG	C	604	1/1	0.84	0.09	101,101,101,101	0
5	PO4	C	605	5/5	0.84	0.19	104,105,118,130	0
3	MG	F	601	1/1	0.85	0.14	100,100,100,100	0
4	ATP	F	602	31/31	0.86	0.11	99,116,132,134	0
4	ATP	B	603	31/31	0.86	0.11	97,110,121,126	0
4	ATP	A	803	31/31	0.87	0.10	81,96,117,121	0
3	MG	D	604	1/1	0.87	0.12	87,87,87,87	0
3	MG	C	601	1/1	0.88	0.08	77,77,77,77	0
3	MG	E	601	1/1	0.88	0.11	85,85,85,85	0
3	MG	A	801	1/1	0.89	0.08	110,110,110,110	0
4	ATP	A	802	31/31	0.89	0.10	96,115,126,130	0
4	ATP	B	602	31/31	0.90	0.09	79,96,105,109	0
4	ATP	E	602	31/31	0.91	0.10	78,104,118,124	0
4	ATP	D	602	31/31	0.92	0.10	76,85,93,98	0
3	MG	B	604	1/1	0.92	0.07	114,114,114,114	0
4	ATP	E	603	31/31	0.93	0.09	51,59,75,89	0
3	MG	E	604	1/1	0.94	0.09	71,71,71,71	0
4	ATP	D	603	31/31	0.94	0.08	50,58,75,91	0

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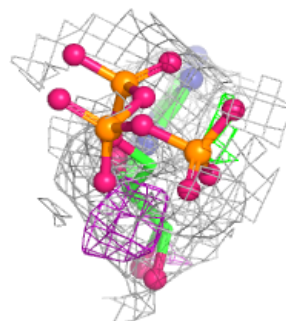
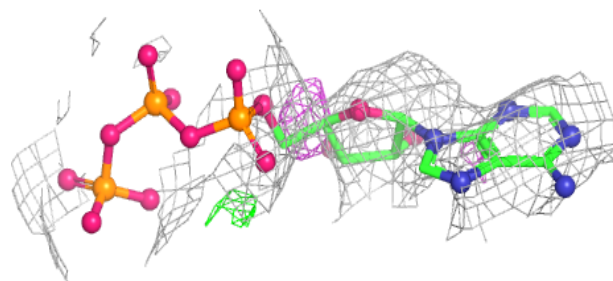
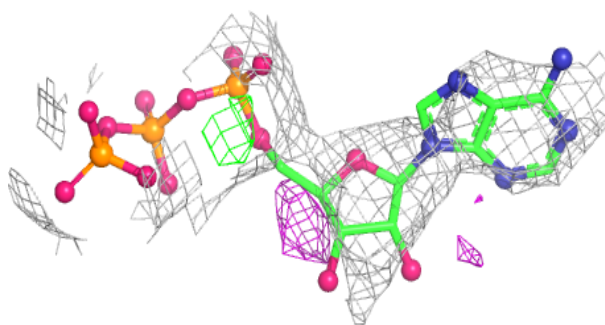
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	F	603	31/31	0.94	0.09	61,71,80,84	0
4	ATP	C	602	31/31	0.94	0.07	62,75,86,94	0
4	ATP	C	603	31/31	0.95	0.07	65,80,96,108	0
3	MG	A	804	1/1	0.98	0.06	80,80,80,80	0

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.

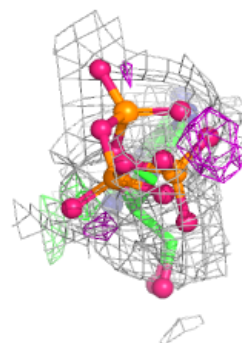
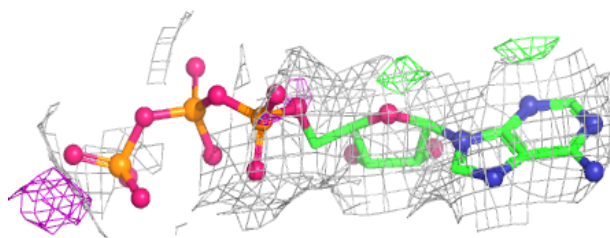
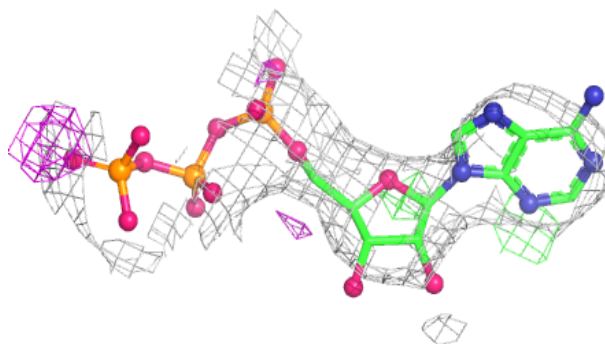
Electron density around ATP F 602:

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

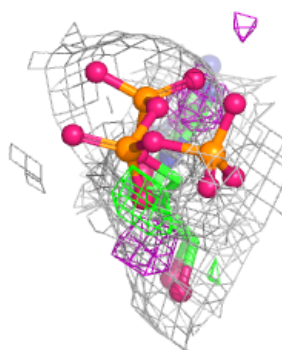
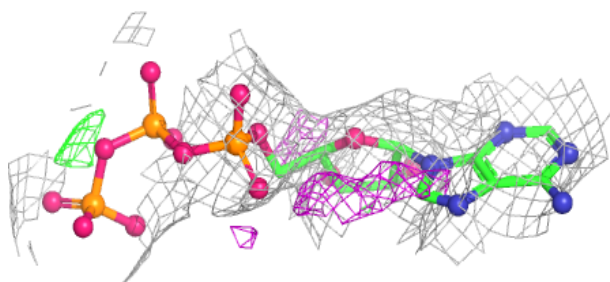
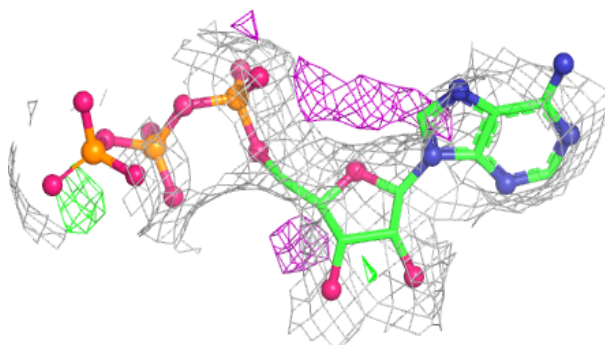


Electron density around ATP B 603:

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

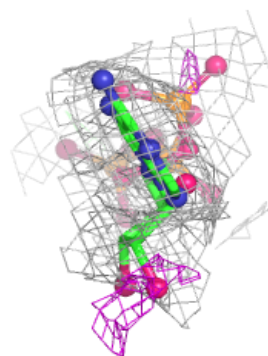
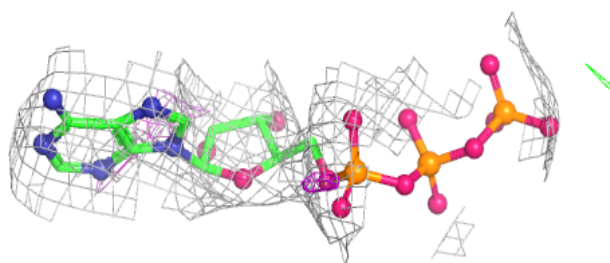
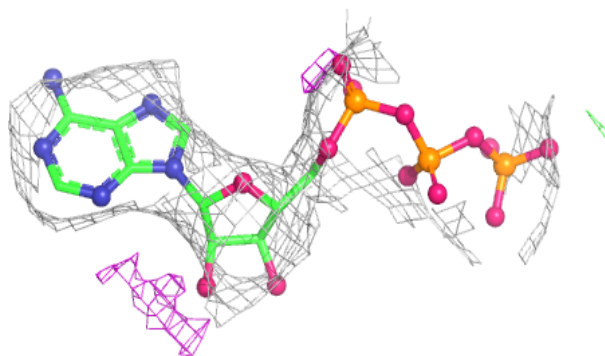
**Electron density around ATP A 803:**

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and green (positive)

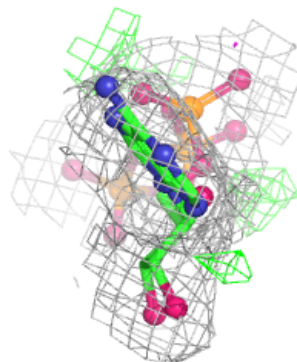
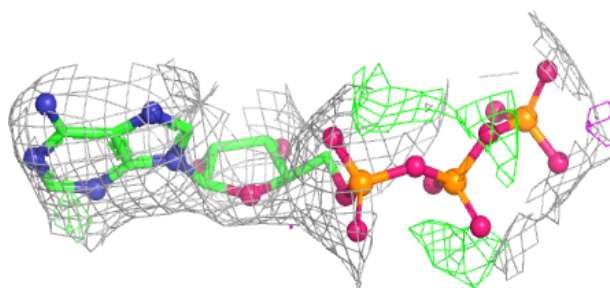
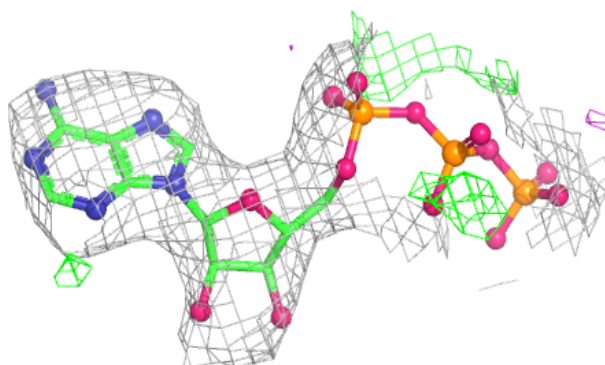


Electron density around ATP A 802:

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and green (positive)

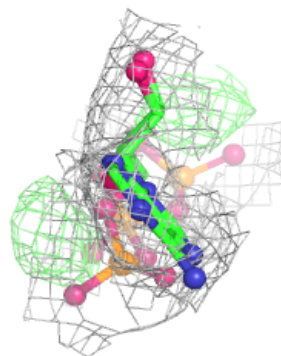
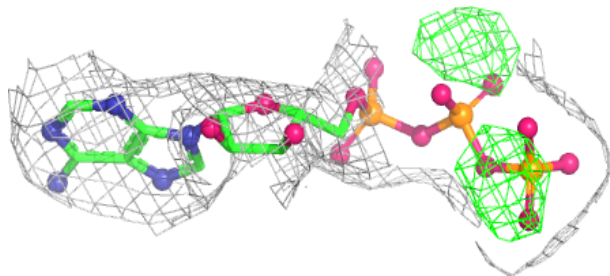
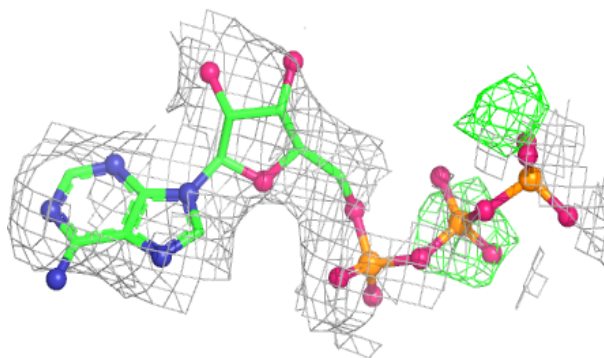
**Electron density around ATP B 602:**

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and green (positive)

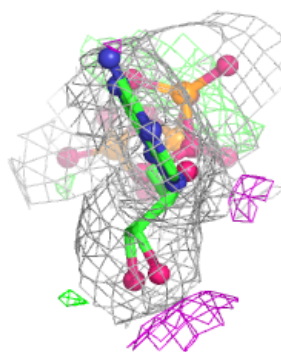
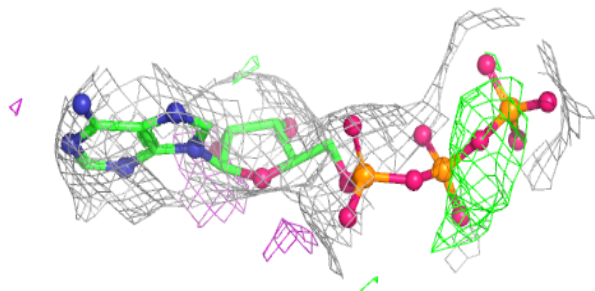
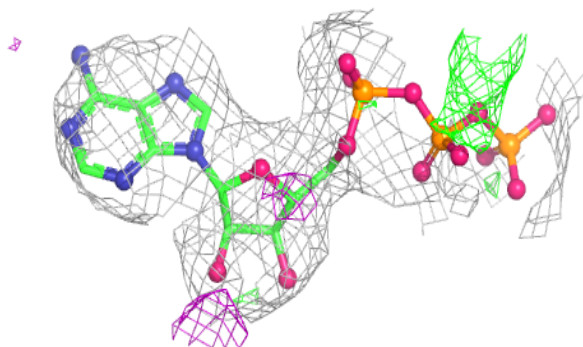


Electron density around ATP E 602:

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and green (positive)

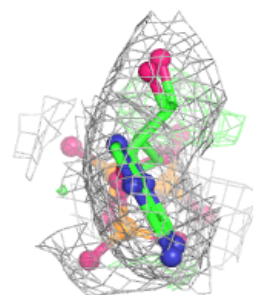
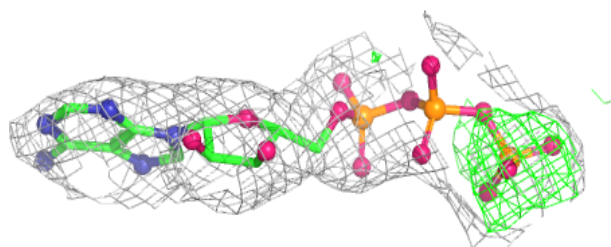
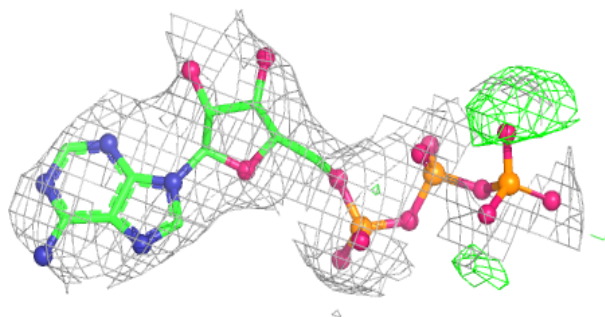
**Electron density around ATP D 602:**

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and green (positive)

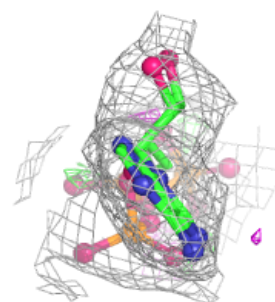
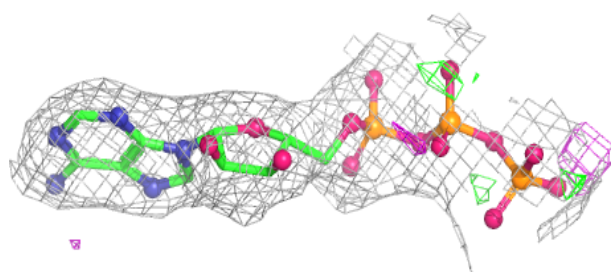
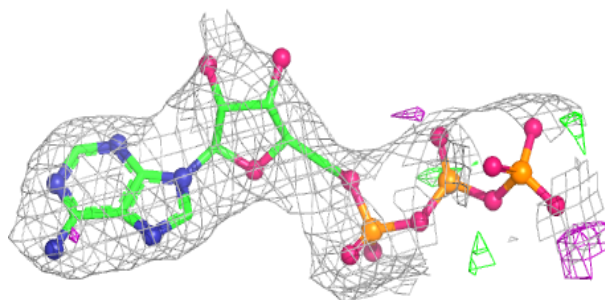


Electron density around ATP E 603:

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and green (positive)

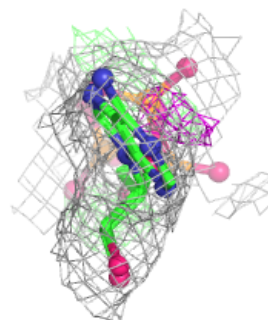
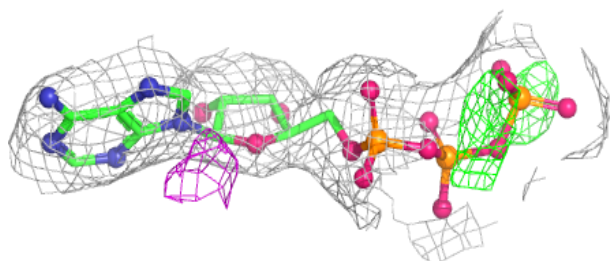
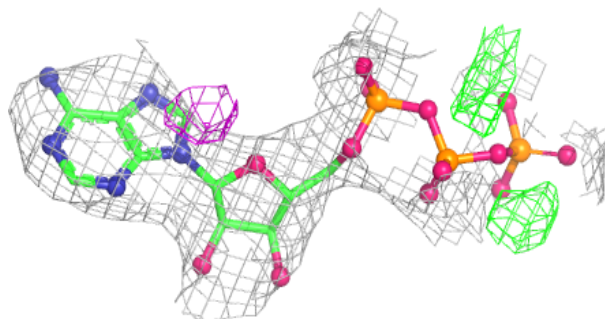
**Electron density around ATP D 603:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

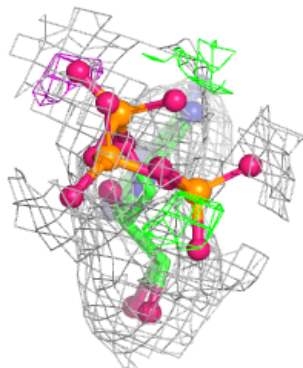
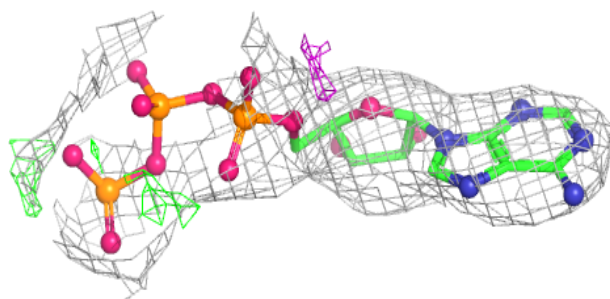
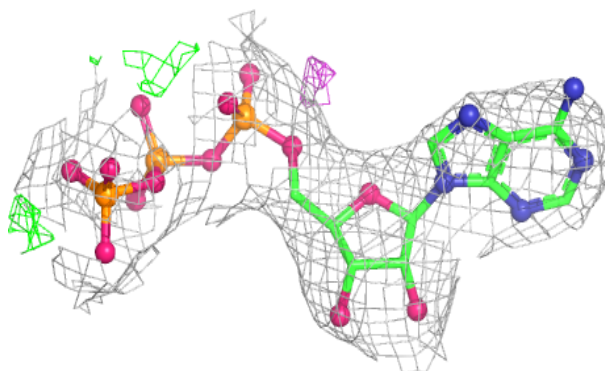


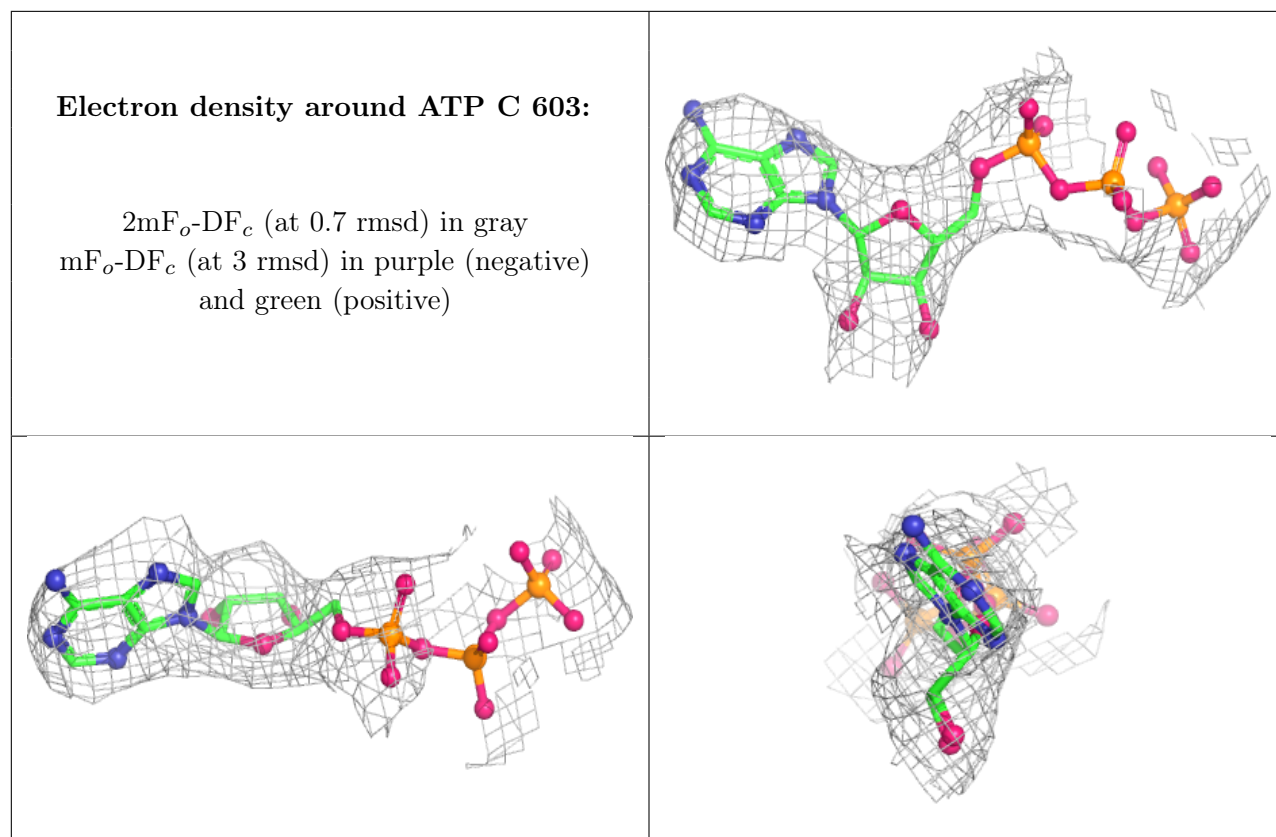
Electron density around ATP F 603:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.