



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:46 AM UTC

PDB ID : 3ND6 / pdb_00003nd6
Title : Crystal structure of phosphopantetheine adenylyltransferase (PPAT) in complex with ATP from *Enterococcus faecalis*
Authors : Yoon, H.J.; Lee, H.H.; Suh, S.W.
Deposited on : 2010-06-07
Resolution : 2.30 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

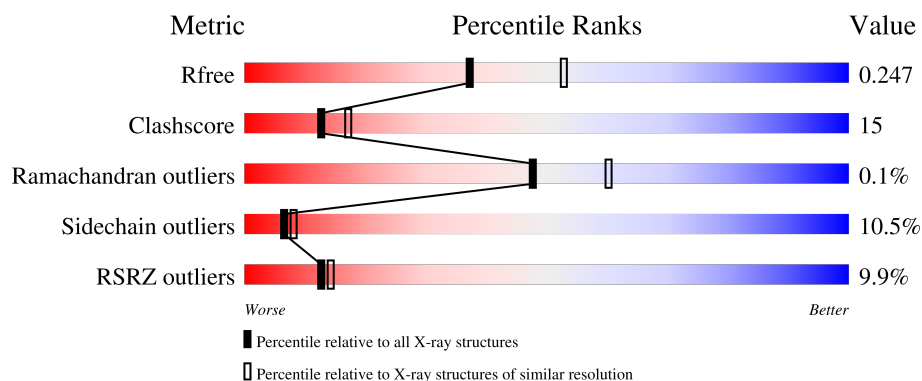
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	171	5% 64% 21% • 11%
1	B	171	7% 62% 20% 6% 11%
1	C	171	12% 61% 22% 6% 11%
1	D	171	12% 62% 21% 6% 11%
1	E	171	5% 64% 20% • 11%

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Mol	Chain	Length	Quality of chain
1	F	171	12% 62% 22% • • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7943 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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	B	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	C	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	D	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	E	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	F	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			

There are 48 discrepancies between the modelled and reference sequences:

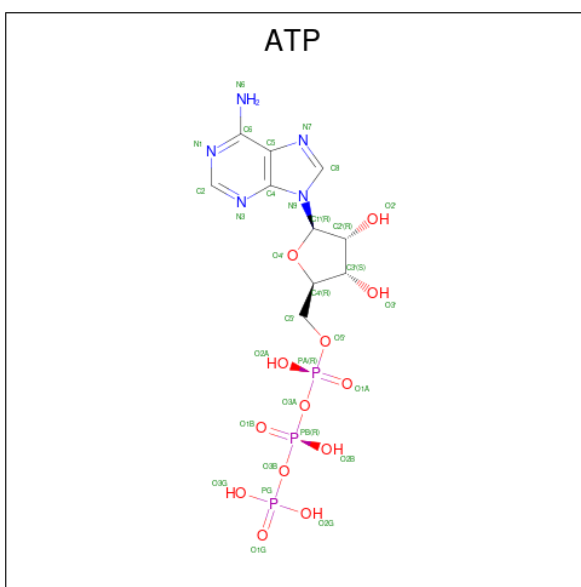
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	LEU	-	expression tag	UNP Q831P9
A	165	GLU	-	expression tag	UNP Q831P9
A	166	HIS	-	expression tag	UNP Q831P9
A	167	HIS	-	expression tag	UNP Q831P9
A	168	HIS	-	expression tag	UNP Q831P9
A	169	HIS	-	expression tag	UNP Q831P9
A	170	HIS	-	expression tag	UNP Q831P9
A	171	HIS	-	expression tag	UNP Q831P9
B	164	LEU	-	expression tag	UNP Q831P9
B	165	GLU	-	expression tag	UNP Q831P9
B	166	HIS	-	expression tag	UNP Q831P9
B	167	HIS	-	expression tag	UNP Q831P9
B	168	HIS	-	expression tag	UNP Q831P9
B	169	HIS	-	expression tag	UNP Q831P9
B	170	HIS	-	expression tag	UNP Q831P9
B	171	HIS	-	expression tag	UNP Q831P9
C	164	LEU	-	expression tag	UNP Q831P9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	GLU	-	expression tag	UNP Q831P9
C	166	HIS	-	expression tag	UNP Q831P9
C	167	HIS	-	expression tag	UNP Q831P9
C	168	HIS	-	expression tag	UNP Q831P9
C	169	HIS	-	expression tag	UNP Q831P9
C	170	HIS	-	expression tag	UNP Q831P9
C	171	HIS	-	expression tag	UNP Q831P9
D	164	LEU	-	expression tag	UNP Q831P9
D	165	GLU	-	expression tag	UNP Q831P9
D	166	HIS	-	expression tag	UNP Q831P9
D	167	HIS	-	expression tag	UNP Q831P9
D	168	HIS	-	expression tag	UNP Q831P9
D	169	HIS	-	expression tag	UNP Q831P9
D	170	HIS	-	expression tag	UNP Q831P9
D	171	HIS	-	expression tag	UNP Q831P9
E	164	LEU	-	expression tag	UNP Q831P9
E	165	GLU	-	expression tag	UNP Q831P9
E	166	HIS	-	expression tag	UNP Q831P9
E	167	HIS	-	expression tag	UNP Q831P9
E	168	HIS	-	expression tag	UNP Q831P9
E	169	HIS	-	expression tag	UNP Q831P9
E	170	HIS	-	expression tag	UNP Q831P9
E	171	HIS	-	expression tag	UNP Q831P9
F	164	LEU	-	expression tag	UNP Q831P9
F	165	GLU	-	expression tag	UNP Q831P9
F	166	HIS	-	expression tag	UNP Q831P9
F	167	HIS	-	expression tag	UNP Q831P9
F	168	HIS	-	expression tag	UNP Q831P9
F	169	HIS	-	expression tag	UNP Q831P9
F	170	HIS	-	expression tag	UNP Q831P9
F	171	HIS	-	expression tag	UNP Q831P9

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



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

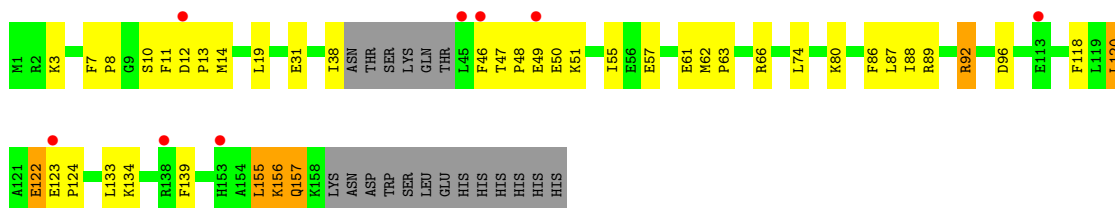
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	89	Total O 89 89	0	0
3	B	78	Total O 78 78	0	0
3	C	53	Total O 53 53	0	0
3	D	71	Total O 71 71	0	0
3	E	64	Total O 64 64	0	0
3	F	58	Total O 58 58	0	0

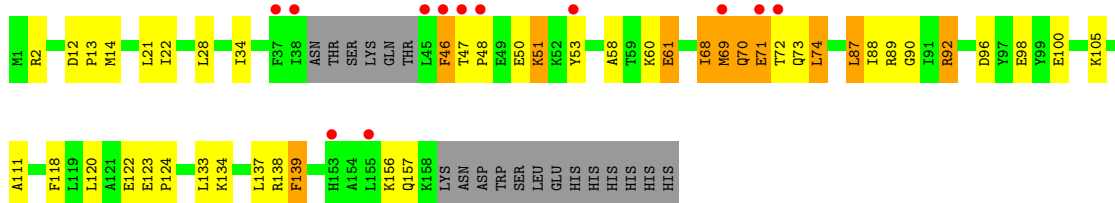
3 Residue-property plots [i](#)

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.

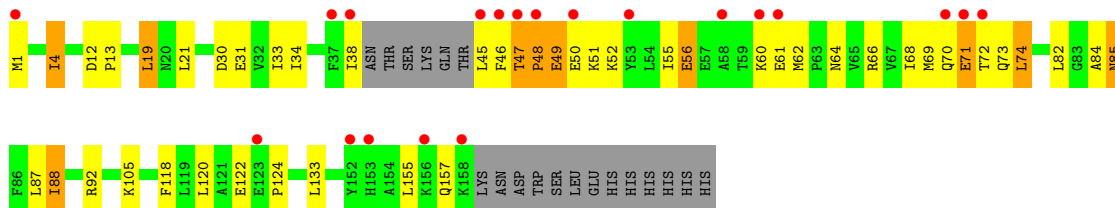
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase

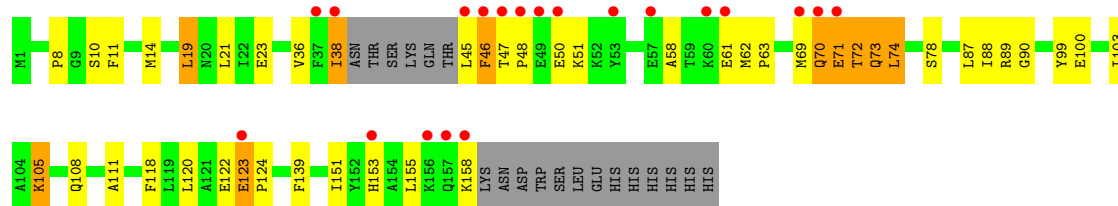


- Molecule 1: Phosphopantetheine adenylyltransferase

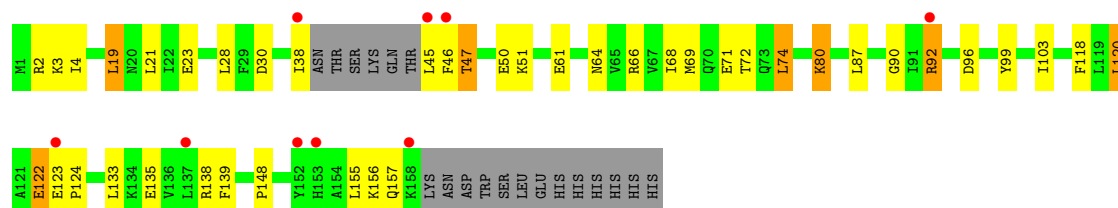


- Molecule 1: Phosphopantetheine adenylyltransferase

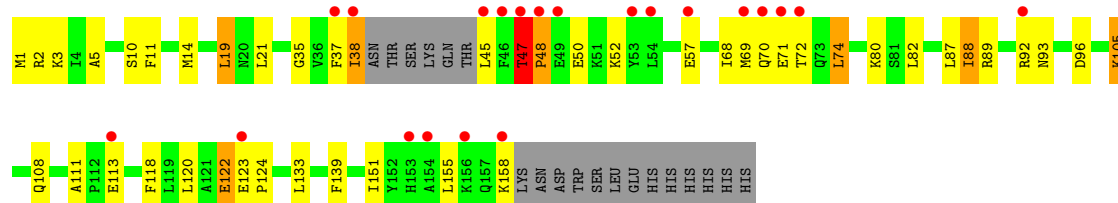




● Molecule 1: Phosphopantetheine adenylyltransferase



● Molecule 1: Phosphopantetheine adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.79Å 123.91Å 124.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.30) 98.7 (20.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.62 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.245 0.210 , 0.247	Depositor DCC
R_{free} test set	3865 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7943	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 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	0.51	0/1248	0.85	2/1683 (0.1%)
1	B	0.58	0/1248	0.91	6/1683 (0.4%)
1	C	0.60	0/1248	0.98	3/1683 (0.2%)
1	D	0.56	0/1248	0.85	3/1683 (0.2%)
1	E	0.53	0/1248	0.79	0/1683
1	F	0.47	0/1248	0.82	5/1683 (0.3%)
All	All	0.54	0/7488	0.87	19/10098 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	GLU	N-CA-C	-14.14	89.73	110.23
1	D	71	GLU	N-CA-C	-9.82	96.99	110.35
1	C	62	MET	CA-C-N	6.11	125.33	118.97
1	C	62	MET	C-N-CA	6.11	125.33	118.97
1	B	47	THR	CA-C-N	5.91	127.22	119.84
1	B	47	THR	C-N-CA	5.91	127.22	119.84
1	F	88	ILE	CB-CA-C	-5.82	103.00	110.98
1	B	111	ALA	CA-C-N	5.33	125.00	119.56
1	B	111	ALA	C-N-CA	5.33	125.00	119.56
1	F	47	THR	CA-C-N	5.27	126.43	119.84
1	F	47	THR	C-N-CA	5.27	126.43	119.84
1	B	87	LEU	CA-C-N	-5.25	116.67	123.19
1	B	87	LEU	C-N-CA	-5.25	116.67	123.19
1	D	111	ALA	CA-C-N	5.14	124.80	119.56
1	D	111	ALA	C-N-CA	5.14	124.80	119.56
1	F	111	ALA	CA-C-N	5.09	124.75	119.56
1	F	111	ALA	C-N-CA	5.09	124.75	119.56
1	A	7	PHE	CA-C-N	5.05	125.44	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	PHE	C-N-CA	5.05	125.44	119.99

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	1224	0	1246	29	0
1	B	1224	0	1246	52	0
1	C	1224	0	1246	54	0
1	D	1224	0	1246	41	0
1	E	1224	0	1246	37	0
1	F	1224	0	1246	42	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	0	0
3	A	89	0	0	4	0
3	B	78	0	0	4	0
3	C	53	0	0	2	0
3	D	71	0	0	0	0
3	E	64	0	0	1	0
3	F	58	0	0	2	0
All	All	7943	0	7548	229	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 15.

All (229) 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:C:38:ILE:CD1	1:C:48:PRO:HB3	1.57	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:THR:HG21	1:C:50:GLU:CD	1.65	1.21
1:C:38:ILE:HD13	1:C:48:PRO:HB3	1.22	1.12
1:C:47:THR:CG2	1:C:50:GLU:CD	2.22	1.12
1:C:47:THR:CG2	1:C:50:GLU:OE2	2.02	1.05
1:C:1:MET:HE2	1:C:85:ASN:HD22	1.21	0.99
1:F:92:ARG:HG2	1:F:96:ASP:OD2	1.63	0.98
1:C:38:ILE:CD1	1:C:48:PRO:CB	2.41	0.98
1:A:92:ARG:HG2	1:A:96:ASP:OD2	1.65	0.96
1:B:138:ARG:HE	1:B:139:PHE:HE2	1.15	0.94
1:C:47:THR:HG23	1:C:50:GLU:HB2	1.45	0.94
1:C:73:GLN:NE2	3:C:227:HOH:O	2.02	0.93
1:B:92:ARG:HG2	1:B:96:ASP:OD1	1.71	0.91
1:E:92:ARG:HG3	1:E:92:ARG:HH11	1.38	0.87
1:D:70:GLN:HE21	1:D:70:GLN:HA	1.41	0.86
1:A:92:ARG:CZ	3:A:304:HOH:O	2.24	0.83
1:E:123:GLU:HG2	1:F:105:LYS:HE2	1.61	0.82
1:B:71:GLU:O	1:B:73:GLN:HG2	1.78	0.82
1:C:47:THR:HG23	1:C:50:GLU:CB	2.10	0.81
1:C:38:ILE:HD11	1:C:48:PRO:HB3	1.61	0.80
1:C:38:ILE:HD11	1:C:48:PRO:CB	2.11	0.79
1:A:92:ARG:NH1	3:A:223:HOH:O	2.19	0.76
1:C:47:THR:HG23	1:C:50:GLU:OE2	1.86	0.75
1:F:52:LYS:HB2	1:F:69:MET:SD	2.25	0.75
1:E:120:LEU:HD22	1:F:118:PHE:CE2	2.20	0.75
1:D:123:GLU:HG3	1:D:124:PRO:HD3	1.68	0.75
1:B:70:GLN:HA	1:B:70:GLN:NE2	2.00	0.74
1:C:4:ILE:HG13	1:C:84:ALA:HA	1.70	0.73
1:A:92:ARG:NE	3:A:304:HOH:O	2.21	0.73
1:E:92:ARG:HG3	1:E:92:ARG:NH1	2.01	0.72
1:C:47:THR:OG1	1:C:48:PRO:HD2	1.91	0.70
1:A:120:LEU:HD22	1:B:118:PHE:CE2	2.28	0.69
1:B:89:ARG:HD3	1:B:100:GLU:OE1	1.93	0.68
1:F:38:ILE:HG12	1:F:48:PRO:HG3	1.75	0.68
1:C:47:THR:CG2	1:C:50:GLU:CG	2.71	0.68
1:D:38:ILE:HD13	1:D:38:ILE:H	1.58	0.68
1:E:123:GLU:HG2	1:F:105:LYS:CE	2.24	0.67
1:E:92:ARG:HG2	1:E:96:ASP:OD1	1.94	0.67
1:B:70:GLN:HA	1:B:70:GLN:HE21	1.59	0.67
1:B:138:ARG:C	1:B:139:PHE:HD2	2.04	0.66
1:D:123:GLU:N	1:D:124:PRO:HD2	2.11	0.65
1:D:151:ILE:O	1:D:155:LEU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:H	1:A:49:GLU:CD	2.05	0.65
1:C:47:THR:HG23	1:C:50:GLU:CD	2.17	0.65
1:C:88:ILE:C	1:C:88:ILE:HD13	2.22	0.64
1:D:36:VAL:HG11	1:D:51:LYS:HD2	1.80	0.64
1:C:30:ASP:O	1:C:64:ASN:HB2	1.98	0.63
1:D:70:GLN:HA	1:D:70:GLN:NE2	2.13	0.63
1:B:69:MET:O	1:B:70:GLN:NE2	2.27	0.63
1:D:123:GLU:OE1	1:E:123:GLU:HB3	1.98	0.63
1:C:47:THR:HG21	1:C:50:GLU:CG	2.28	0.62
1:C:47:THR:HG22	1:C:50:GLU:OE2	1.96	0.62
1:A:3:LYS:HE3	1:B:28:LEU:O	1.99	0.62
1:D:70:GLN:HE21	1:D:70:GLN:CA	2.10	0.62
1:C:47:THR:HG23	1:C:50:GLU:CG	2.30	0.62
1:B:71:GLU:O	1:B:71:GLU:HG3	2.00	0.61
1:F:38:ILE:HD12	1:F:38:ILE:H	1.65	0.60
1:A:123:GLU:HG3	1:F:123:GLU:HG2	1.83	0.60
1:D:38:ILE:HD11	1:D:71:GLU:HA	1.82	0.60
1:F:122:GLU:C	1:F:124:PRO:HD2	2.27	0.60
1:D:123:GLU:HG3	1:D:124:PRO:CD	2.31	0.60
1:A:88:ILE:O	1:A:89:ARG:HD2	2.03	0.59
1:E:46:PHE:CZ	1:E:155:LEU:HD13	2.38	0.59
1:A:38:ILE:HD12	1:A:48:PRO:HG3	1.83	0.59
1:C:1:MET:HE2	1:C:85:ASN:ND2	2.06	0.58
1:E:66:ARG:HD2	1:E:68:ILE:HD11	1.85	0.58
1:B:92:ARG:NH1	1:B:92:ARG:HG3	2.18	0.58
1:E:19:LEU:HD22	1:E:23:GLU:OE2	2.04	0.57
1:B:92:ARG:HG3	1:B:92:ARG:HH11	1.68	0.57
1:C:52:LYS:HZ1	1:C:56:GLU:CD	2.12	0.56
1:E:99:TYR:CZ	1:E:103:ILE:HD11	2.40	0.56
1:C:48:PRO:HG2	1:C:49:GLU:N	2.20	0.56
1:C:4:ILE:HD11	1:C:33:ILE:HD12	1.89	0.55
1:F:14:MET:CE	1:F:19:LEU:HG	2.36	0.55
1:E:123:GLU:N	1:E:124:PRO:HD2	2.22	0.54
1:F:70:GLN:NE2	1:F:70:GLN:HA	2.21	0.54
1:D:21:LEU:HD11	1:D:90:GLY:HA3	1.90	0.54
1:E:135:GLU:O	1:E:138:ARG:HG2	2.07	0.54
1:C:31:GLU:OE2	1:C:66:ARG:HD3	2.08	0.54
1:F:88:ILE:O	1:F:89:ARG:HD2	2.08	0.54
1:E:122:GLU:C	1:E:124:PRO:HD2	2.33	0.54
1:B:139:PHE:HB2	1:D:74:LEU:HD13	1.90	0.53
1:F:151:ILE:O	1:F:155:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:PRO:HG2	1:C:49:GLU:H	1.72	0.53
1:D:139:PHE:HB2	1:F:74:LEU:HD13	1.90	0.53
1:E:21:LEU:HD11	1:E:90:GLY:HA3	1.91	0.53
1:F:123:GLU:N	1:F:124:PRO:HD2	2.23	0.53
1:D:70:GLN:HG2	1:D:78:SER:HB2	1.91	0.53
1:B:92:ARG:NH2	3:B:177:HOH:O	2.42	0.52
1:B:122:GLU:C	1:B:124:PRO:HD2	2.34	0.52
1:C:4:ILE:HD11	1:C:33:ILE:CD1	2.40	0.52
1:E:38:ILE:O	1:E:72:THR:HG23	2.09	0.52
1:B:14:MET:HE1	1:B:58:ALA:CB	2.39	0.52
1:C:38:ILE:HD13	1:C:48:PRO:CB	2.14	0.52
1:B:14:MET:HE1	1:B:58:ALA:HB3	1.91	0.52
1:A:123:GLU:N	1:A:124:PRO:CD	2.73	0.51
1:E:46:PHE:HB2	1:E:51:LYS:HG3	1.92	0.51
1:C:85:ASN:OD1	1:C:85:ASN:N	2.35	0.51
1:F:123:GLU:N	1:F:124:PRO:CD	2.74	0.51
1:B:48:PRO:HA	1:B:51:LYS:CB	2.41	0.50
1:B:123:GLU:N	1:B:124:PRO:CD	2.74	0.50
1:A:12:ASP:O	1:A:134:LYS:HE3	2.11	0.50
1:B:12:ASP:HB3	1:B:51:LYS:NZ	2.26	0.50
1:C:48:PRO:CG	1:C:49:GLU:N	2.74	0.50
1:C:92:ARG:NE	3:C:303:HOH:O	2.38	0.50
1:A:122:GLU:C	1:A:124:PRO:HD2	2.37	0.50
1:D:88:ILE:O	1:D:89:ARG:HD2	2.12	0.49
1:C:70:GLN:OE1	1:C:73:GLN:OE1	2.30	0.49
1:F:48:PRO:HB3	1:F:69:MET:HE2	1.95	0.49
1:C:74:LEU:HD13	1:E:139:PHE:CB	2.43	0.48
1:A:31:GLU:OE1	1:A:66:ARG:NH1	2.47	0.48
1:D:122:GLU:C	1:D:124:PRO:HD2	2.39	0.48
1:F:80:LYS:HE2	1:F:113:GLU:OE1	2.13	0.48
1:C:70:GLN:O	1:C:71:GLU:C	2.55	0.48
1:B:98:GLU:OE1	1:F:93:ASN:HB2	2.13	0.47
1:E:30:ASP:O	1:E:64:ASN:HB2	2.14	0.47
1:C:155:LEU:HD12	1:C:155:LEU:HA	1.78	0.47
1:F:68:ILE:HD11	1:F:82:LEU:HD11	1.97	0.47
1:A:86:PHE:CE2	1:B:28:LEU:HD13	2.50	0.47
1:A:139:PHE:HB2	1:E:74:LEU:HD13	1.95	0.47
1:A:66:ARG:HD3	3:A:254:HOH:O	2.13	0.47
1:D:139:PHE:CB	1:F:74:LEU:HD13	2.44	0.47
1:E:38:ILE:HD11	1:E:69:MET:CE	2.45	0.47
1:B:139:PHE:CE1	1:D:72:THR:HG23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:ARG:NE	3:F:373:HOH:O	2.25	0.47
1:B:139:PHE:HD2	1:B:139:PHE:N	2.11	0.47
1:B:12:ASP:HA	1:B:13:PRO:HA	1.66	0.47
1:B:139:PHE:CB	1:D:74:LEU:HD13	2.45	0.47
1:A:123:GLU:N	1:A:124:PRO:HD2	2.30	0.47
1:C:33:ILE:HG21	1:C:82:LEU:HD13	1.96	0.47
1:E:19:LEU:HD12	1:E:148:PRO:HG3	1.96	0.47
1:B:139:PHE:N	1:B:139:PHE:CD2	2.82	0.46
1:E:80:LYS:HB2	1:E:80:LYS:NZ	2.29	0.46
1:F:38:ILE:HG12	1:F:48:PRO:CG	2.42	0.46
1:B:12:ASP:CG	1:B:12:ASP:O	2.57	0.46
1:B:60:LYS:HG3	1:B:61:GLU:OE2	2.15	0.46
1:D:14:MET:HE2	1:D:151:ILE:CD1	2.46	0.46
1:D:89:ARG:HB2	1:D:118:PHE:CD1	2.51	0.46
1:E:46:PHE:HZ	1:E:155:LEU:HD13	1.80	0.46
1:A:49:GLU:CD	1:A:49:GLU:N	2.73	0.46
1:A:12:ASP:HA	1:A:13:PRO:HA	1.67	0.46
1:C:48:PRO:CG	1:C:49:GLU:H	2.29	0.45
1:C:21:LEU:HD11	2:C:963:ATP:N3	2.32	0.45
1:D:99:TYR:CZ	1:D:103:ILE:HD11	2.51	0.45
1:D:100:GLU:HB3	1:D:118:PHE:HE1	1.81	0.45
1:B:48:PRO:HA	1:B:51:LYS:HB2	1.97	0.45
1:B:138:ARG:C	1:B:139:PHE:CD2	2.92	0.45
1:C:122:GLU:C	1:C:124:PRO:HD2	2.42	0.45
1:B:12:ASP:HB3	1:B:51:LYS:HZ1	1.80	0.45
1:C:12:ASP:HA	1:C:13:PRO:HA	1.78	0.45
1:B:74:LEU:HD13	1:F:139:PHE:HB2	1.99	0.45
1:C:60:LYS:HG3	1:C:61:GLU:N	2.32	0.45
1:C:74:LEU:HD13	1:E:139:PHE:HB2	1.98	0.45
1:E:123:GLU:HG2	1:F:105:LYS:NZ	2.32	0.45
1:D:19:LEU:HD13	1:D:23:GLU:OE2	2.16	0.45
1:D:153:HIS:C	1:D:155:LEU:H	2.26	0.45
1:C:118:PHE:CE2	1:D:120:LEU:HG	2.52	0.44
1:F:68:ILE:CD1	1:F:82:LEU:HD11	2.46	0.44
1:D:74:LEU:HD12	1:D:74:LEU:HA	1.85	0.44
1:F:71:GLU:O	1:F:72:THR:C	2.60	0.44
1:D:105:LYS:HD3	1:D:105:LYS:HA	1.43	0.44
1:F:108:GLN:HE21	1:F:108:GLN:HB3	1.58	0.44
1:C:51:LYS:O	1:C:55:ILE:HG13	2.17	0.43
1:D:10:SER:O	1:D:11:PHE:C	2.61	0.43
1:C:49:GLU:H	1:C:49:GLU:HG2	1.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ILE:HD11	1:E:69:MET:HE3	1.99	0.43
1:A:46:PHE:CZ	1:A:155:LEU:HD13	2.53	0.43
1:C:69:MET:HE2	1:C:69:MET:HB3	1.85	0.43
1:D:123:GLU:N	1:D:124:PRO:CD	2.81	0.43
1:E:156:LYS:O	1:E:156:LYS:HG3	2.19	0.43
1:E:28:LEU:O	1:F:3:LYS:CE	2.67	0.43
1:D:99:TYR:CZ	1:D:103:ILE:CD1	3.02	0.43
1:B:22:ILE:HD13	1:B:34:ILE:HD11	1.99	0.43
1:B:2:ARG:NH1	3:B:200:HOH:O	2.52	0.43
1:B:72:THR:HB	1:F:139:PHE:CE1	2.54	0.43
1:D:8:PRO:HD2	1:D:89:ARG:NH1	2.34	0.43
1:F:35:GLY:O	1:F:37:PHE:HD2	2.01	0.43
1:F:47:THR:OG1	1:F:50:GLU:CD	2.62	0.43
1:A:156:LYS:HB2	1:A:156:LYS:NZ	2.34	0.43
1:E:123:GLU:N	1:E:124:PRO:CD	2.82	0.43
1:B:68:ILE:HD11	3:B:318:HOH:O	2.19	0.43
1:B:123:GLU:N	1:B:124:PRO:HD2	2.33	0.42
1:E:118:PHE:CE2	1:F:120:LEU:HG	2.53	0.42
1:F:5:ALA:HB1	1:F:88:ILE:HG13	2.01	0.42
1:A:14:MET:HE1	1:A:55:ILE:HG23	2.01	0.42
1:F:38:ILE:CG2	1:F:48:PRO:HG3	2.49	0.42
1:C:52:LYS:HB2	1:C:69:MET:HE1	2.02	0.42
1:B:46:PHE:O	1:B:48:PRO:HD3	2.19	0.42
1:C:34:ILE:N	1:C:34:ILE:HD12	2.35	0.42
1:A:8:PRO:HD2	1:A:89:ARG:NH1	2.35	0.42
1:B:48:PRO:HA	1:B:51:LYS:HB3	2.02	0.42
1:B:105:LYS:HA	1:B:105:LYS:HD3	1.80	0.42
1:B:22:ILE:HD13	1:B:34:ILE:CD1	2.50	0.42
1:B:92:ARG:CZ	3:B:177:HOH:O	2.66	0.42
1:E:2:ARG:HE	1:E:4:ILE:HD11	1.85	0.42
1:A:118:PHE:CE2	1:B:120:LEU:HG	2.55	0.42
1:E:99:TYR:CZ	1:E:103:ILE:CD1	3.02	0.41
1:C:45:LEU:C	1:C:45:LEU:HD23	2.45	0.41
1:A:62:MET:HA	1:A:63:PRO:HD3	1.91	0.41
1:A:156:LYS:O	1:A:157:GLN:C	2.63	0.41
1:B:68:ILE:CG2	1:B:70:GLN:HG2	2.50	0.41
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.89	0.41
1:D:36:VAL:CG1	1:D:51:LYS:HD2	2.49	0.41
1:E:71:GLU:HG2	3:E:249:HOH:O	2.20	0.41
1:F:38:ILE:HG21	1:F:48:PRO:HG3	2.01	0.41
1:B:21:LEU:HD11	1:B:90:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:THR:HG23	1:E:50:GLU:CD	2.46	0.41
1:E:74:LEU:HD12	1:E:74:LEU:HA	1.86	0.41
1:C:47:THR:O	1:C:50:GLU:HB2	2.20	0.41
1:A:10:SER:O	1:A:11:PHE:C	2.64	0.41
1:A:47:THR:HG23	1:A:50:GLU:OE1	2.20	0.41
1:B:138:ARG:NE	1:B:139:PHE:HE2	1.97	0.41
1:C:120:LEU:HG	1:D:118:PHE:CE2	2.55	0.41
1:D:46:PHE:O	1:D:47:THR:C	2.63	0.41
1:D:48:PRO:C	1:D:50:GLU:N	2.78	0.41
1:F:1:MET:O	1:F:3:LYS:HD3	2.21	0.41
1:B:50:GLU:HA	1:B:53:TYR:HB3	2.02	0.41
1:B:72:THR:HB	1:F:139:PHE:HE1	1.86	0.41
1:F:10:SER:O	1:F:11:PHE:C	2.63	0.41
1:D:73:GLN:HG2	1:D:74:LEU:N	2.36	0.40
1:F:2:ARG:NH2	3:F:373:HOH:O	2.48	0.40
1:F:88:ILE:C	1:F:89:ARG:HD2	2.46	0.40
1:D:45:LEU:N	1:D:45:LEU:HD22	2.36	0.40
1:B:46:PHE:HB3	1:B:51:LYS:HG3	2.03	0.40
1:D:14:MET:HE1	1:D:58:ALA:CB	2.52	0.40
1:B:70:GLN:NE2	1:B:70:GLN:CA	2.78	0.40
1:D:62:MET:HA	1:D:63:PRO:HD3	1.85	0.40
1:F:74:LEU:HD12	1:F:74:LEU:HA	1.85	0.40
1:E:3:LYS:HB2	1:E:30:ASP:H	1.86	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	148/171 (86%)	142 (96%)	6 (4%)	0	100	100
1	B	148/171 (86%)	141 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	148/171 (86%)	144 (97%)	4 (3%)	0	100	100
1	D	148/171 (86%)	142 (96%)	6 (4%)	0	100	100
1	E	148/171 (86%)	146 (99%)	2 (1%)	0	100	100
1	F	148/171 (86%)	143 (97%)	4 (3%)	1 (1%)	18	23
All	All	888/1026 (86%)	858 (97%)	29 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	48	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	135/154 (88%)	121 (90%)	14 (10%)	7	8
1	B	135/154 (88%)	118 (87%)	17 (13%)	4	5
1	C	135/154 (88%)	119 (88%)	16 (12%)	5	6
1	D	135/154 (88%)	121 (90%)	14 (10%)	7	8
1	E	135/154 (88%)	123 (91%)	12 (9%)	9	12
1	F	135/154 (88%)	123 (91%)	12 (9%)	9	12
All	All	810/924 (88%)	725 (90%)	85 (10%)	6	8

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	51	LYS
1	A	57	GLU
1	A	61	GLU
1	A	74	LEU
1	A	80	LYS

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Mol	Chain	Res	Type
1	A	87	LEU
1	A	92	ARG
1	A	120	LEU
1	A	122	GLU
1	A	133	LEU
1	A	155	LEU
1	A	156	LYS
1	A	157	GLN
1	B	46	PHE
1	B	51	LYS
1	B	61	GLU
1	B	68	ILE
1	B	69	MET
1	B	70	GLN
1	B	71	GLU
1	B	74	LEU
1	B	87	LEU
1	B	88	ILE
1	B	92	ARG
1	B	133	LEU
1	B	134	LYS
1	B	137	LEU
1	B	139	PHE
1	B	156	LYS
1	B	157	GLN
1	C	4	ILE
1	C	19	LEU
1	C	46	PHE
1	C	47	THR
1	C	48	PRO
1	C	49	GLU
1	C	56	GLU
1	C	68	ILE
1	C	72	THR
1	C	74	LEU
1	C	85	ASN
1	C	87	LEU
1	C	88	ILE
1	C	105	LYS
1	C	133	LEU
1	C	157	GLN
1	D	19	LEU

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Mol	Chain	Res	Type
1	D	38	ILE
1	D	46	PHE
1	D	61	GLU
1	D	69	MET
1	D	70	GLN
1	D	72	THR
1	D	73	GLN
1	D	74	LEU
1	D	87	LEU
1	D	105	LYS
1	D	108	GLN
1	D	123	GLU
1	D	158	LYS
1	E	19	LEU
1	E	45	LEU
1	E	47	THR
1	E	61	GLU
1	E	74	LEU
1	E	80	LYS
1	E	87	LEU
1	E	92	ARG
1	E	120	LEU
1	E	122	GLU
1	E	133	LEU
1	E	157	GLN
1	F	19	LEU
1	F	21	LEU
1	F	38	ILE
1	F	45	LEU
1	F	47	THR
1	F	57	GLU
1	F	74	LEU
1	F	87	LEU
1	F	105	LYS
1	F	122	GLU
1	F	133	LEU
1	F	158	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	GLN

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Mol	Chain	Res	Type
1	B	109	HIS
1	C	73	GLN
1	D	70	GLN
1	E	70	GLN
1	E	73	GLN
1	E	85	ASN
1	E	157	GLN
1	F	73	GLN
1	F	85	ASN
1	F	108	GLN
1	F	109	HIS

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	D	964	-	32,33,33	1.42	6 (18%)	48,52,52	1.87	10 (20%)
2	ATP	B	962	-	32,33,33	1.35	5 (15%)	48,52,52	1.89	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	961	-	32,33,33	1.48	7 (21%)	48,52,52	1.77	11 (22%)
2	ATP	E	965	-	32,33,33	1.39	6 (18%)	48,52,52	1.81	9 (18%)
2	ATP	F	966	-	32,33,33	1.46	8 (25%)	48,52,52	1.79	9 (18%)
2	ATP	C	963	-	32,33,33	1.46	6 (18%)	48,52,52	1.77	9 (18%)

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	964	-	-	3/22/38/38	0/3/3/3
2	ATP	B	962	-	-	3/22/38/38	0/3/3/3
2	ATP	A	961	-	-	6/22/38/38	0/3/3/3
2	ATP	E	965	-	-	5/22/38/38	0/3/3/3
2	ATP	F	966	-	-	7/22/38/38	0/3/3/3
2	ATP	C	963	-	-	6/22/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	963	ATP	C5-C4	4.61	1.47	1.39
2	F	966	ATP	C5-C4	4.44	1.47	1.39
2	A	961	ATP	C5-C4	4.40	1.46	1.39
2	E	965	ATP	C5-C4	4.37	1.46	1.39
2	D	964	ATP	C5-C4	4.22	1.46	1.39
2	B	962	ATP	C5-C4	3.64	1.45	1.39
2	A	961	ATP	PB-O3A	3.60	1.63	1.59
2	C	963	ATP	PB-O3A	3.00	1.62	1.59
2	B	962	ATP	PB-O3A	2.95	1.62	1.59
2	D	964	ATP	C5-C6	2.94	1.49	1.41
2	E	965	ATP	C5-C6	2.73	1.48	1.41
2	A	961	ATP	C5-C6	2.70	1.48	1.41
2	C	963	ATP	PB-O3B	2.67	1.62	1.59
2	C	963	ATP	C5-C6	2.58	1.48	1.41
2	B	962	ATP	C5-C6	2.57	1.48	1.41
2	D	964	ATP	PB-O3A	2.57	1.62	1.59
2	E	965	ATP	PB-O3B	2.48	1.62	1.59
2	F	966	ATP	C5-C6	2.47	1.47	1.41
2	D	964	ATP	PB-O3B	2.46	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	964	ATP	C8-N7	2.44	1.36	1.31
2	F	966	ATP	PA-O3A	2.42	1.62	1.59
2	A	961	ATP	PB-O3B	2.37	1.62	1.59
2	F	966	ATP	C5-N7	-2.35	1.34	1.39
2	A	961	ATP	C8-N7	2.35	1.36	1.31
2	B	962	ATP	C4-N9	-2.35	1.32	1.37
2	B	962	ATP	C5-N7	-2.30	1.34	1.39
2	C	963	ATP	C8-N7	2.24	1.36	1.31
2	F	966	ATP	C4-N9	-2.24	1.33	1.37
2	C	963	ATP	C5-N7	-2.22	1.35	1.39
2	E	965	ATP	PB-O3A	2.22	1.61	1.59
2	E	965	ATP	C8-N7	2.19	1.35	1.31
2	F	966	ATP	PB-O3B	2.12	1.61	1.59
2	F	966	ATP	PB-O3A	2.11	1.61	1.59
2	A	961	ATP	C4-N9	-2.08	1.33	1.37
2	A	961	ATP	C5-N7	-2.06	1.35	1.39
2	E	965	ATP	C5-N7	-2.02	1.35	1.39
2	D	964	ATP	C5-N7	-2.02	1.35	1.39
2	F	966	ATP	C8-N7	2.01	1.35	1.31

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	963	ATP	C5-C4-N3	-5.74	118.81	126.72
2	E	965	ATP	C5-C4-N3	-5.72	118.84	126.72
2	D	964	ATP	C5-C4-N3	-5.66	118.93	126.72
2	A	961	ATP	C5-C4-N3	-5.53	119.11	126.72
2	F	966	ATP	C5-C4-N3	-5.27	119.46	126.72
2	B	962	ATP	C5-C4-N3	-5.19	119.57	126.72
2	C	963	ATP	N3-C4-N9	4.84	135.40	127.17
2	E	965	ATP	N3-C4-N9	4.66	135.09	127.17
2	F	966	ATP	N3-C4-N9	4.58	134.96	127.17
2	D	964	ATP	N3-C4-N9	4.39	134.64	127.17
2	A	961	ATP	N3-C4-N9	4.38	134.62	127.17
2	B	962	ATP	N3-C4-N9	4.28	134.44	127.17
2	E	965	ATP	C2-N3-C4	3.91	121.38	111.83
2	D	964	ATP	C4-C5-N7	-3.89	106.13	110.58
2	B	962	ATP	C4-N9-C8	3.79	109.72	105.74
2	E	965	ATP	N3-C2-N1	-3.78	122.87	128.58
2	D	964	ATP	C2-N3-C4	3.72	120.92	111.83
2	C	963	ATP	C2-N3-C4	3.62	120.68	111.83
2	B	962	ATP	C4-C5-N7	-3.59	106.48	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	962	ATP	C2-N3-C4	3.59	120.59	111.83
2	A	961	ATP	C2-N3-C4	3.55	120.50	111.83
2	F	966	ATP	C2-N3-C4	3.50	120.38	111.83
2	F	966	ATP	N3-C2-N1	-3.46	123.34	128.58
2	B	962	ATP	N3-C2-N1	-3.43	123.39	128.58
2	E	965	ATP	C4-C5-N7	-3.36	106.74	110.58
2	D	964	ATP	N3-C2-N1	-3.34	123.52	128.58
2	D	964	ATP	C4-N9-C8	3.28	109.18	105.74
2	F	966	ATP	C4-N9-C8	3.28	109.18	105.74
2	C	963	ATP	N3-C2-N1	-3.27	123.62	128.58
2	D	964	ATP	C5-N7-C8	3.26	108.58	103.45
2	A	961	ATP	C4-C5-N7	-3.21	106.92	110.58
2	A	961	ATP	N3-C2-N1	-3.12	123.86	128.58
2	B	962	ATP	N9-C8-N7	-3.07	109.58	113.94
2	B	962	ATP	C5-N7-C8	3.04	108.22	103.45
2	E	965	ATP	C4-N9-C8	3.02	108.91	105.74
2	D	964	ATP	N9-C8-N7	-3.00	109.67	113.94
2	C	963	ATP	C4-C5-N7	-2.99	107.17	110.58
2	F	966	ATP	C4-C5-N7	-2.94	107.22	110.58
2	A	961	ATP	C4-N9-C8	2.87	108.75	105.74
2	C	963	ATP	C4-N9-C8	2.77	108.65	105.74
2	E	965	ATP	C5-N7-C8	2.73	107.74	103.45
2	A	961	ATP	O2B-PB-O3B	2.68	114.53	107.27
2	F	966	ATP	O2B-PB-O3A	2.62	114.36	107.27
2	B	962	ATP	O2B-PB-O3A	2.60	114.29	107.27
2	B	962	ATP	C6-C5-N7	2.46	136.83	132.09
2	D	964	ATP	C6-C5-N7	2.45	136.82	132.09
2	D	964	ATP	O3A-PA-O1A	-2.41	103.46	110.70
2	E	965	ATP	N9-C8-N7	-2.40	110.54	113.94
2	F	966	ATP	O2A-PA-O3A	2.32	113.56	107.27
2	A	961	ATP	C5-N7-C8	2.32	107.09	103.45
2	E	965	ATP	C6-C5-N7	2.28	136.48	132.09
2	C	963	ATP	C5-N7-C8	2.27	107.01	103.45
2	C	963	ATP	O2B-PB-O1B	2.23	122.83	112.44
2	F	966	ATP	C5-N7-C8	2.19	106.89	103.45
2	B	962	ATP	O3G-PG-O2G	2.15	115.86	107.80
2	C	963	ATP	O3G-PG-O2G	2.12	115.76	107.80
2	A	961	ATP	C6-C5-N7	2.10	136.14	132.09
2	A	961	ATP	N9-C8-N7	-2.09	110.98	113.94
2	B	962	ATP	C2'-C1'-N9	-2.05	108.21	113.30
2	A	961	ATP	O3G-PG-O2G	2.00	115.32	107.80

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	961	ATP	PB-O3B-PG-O3G
2	A	961	ATP	C5'-O5'-PA-O1A
2	A	961	ATP	C5'-O5'-PA-O2A
2	A	961	ATP	C5'-O5'-PA-O3A
2	B	962	ATP	C5'-O5'-PA-O2A
2	B	962	ATP	C5'-O5'-PA-O3A
2	C	963	ATP	C5'-O5'-PA-O1A
2	C	963	ATP	C5'-O5'-PA-O2A
2	C	963	ATP	C5'-O5'-PA-O3A
2	D	964	ATP	C5'-O5'-PA-O2A
2	D	964	ATP	C5'-O5'-PA-O3A
2	E	965	ATP	C5'-O5'-PA-O1A
2	E	965	ATP	C5'-O5'-PA-O2A
2	E	965	ATP	C5'-O5'-PA-O3A
2	F	966	ATP	C5'-O5'-PA-O1A
2	F	966	ATP	C5'-O5'-PA-O2A
2	F	966	ATP	C5'-O5'-PA-O3A
2	F	966	ATP	C3'-C4'-C5'-O5'
2	F	966	ATP	O4'-C4'-C5'-O5'
2	C	963	ATP	PB-O3B-PG-O1G
2	C	963	ATP	PB-O3B-PG-O3G
2	F	966	ATP	PB-O3A-PA-O2A
2	A	961	ATP	PB-O3B-PG-O1G
2	A	961	ATP	PB-O3A-PA-O2A
2	E	965	ATP	PB-O3A-PA-O1A
2	F	966	ATP	PB-O3A-PA-O1A
2	B	962	ATP	PA-O3A-PB-O2B
2	C	963	ATP	PB-O3A-PA-O2A
2	D	964	ATP	PG-O3B-PB-O2B
2	E	965	ATP	PB-O3A-PA-O2A

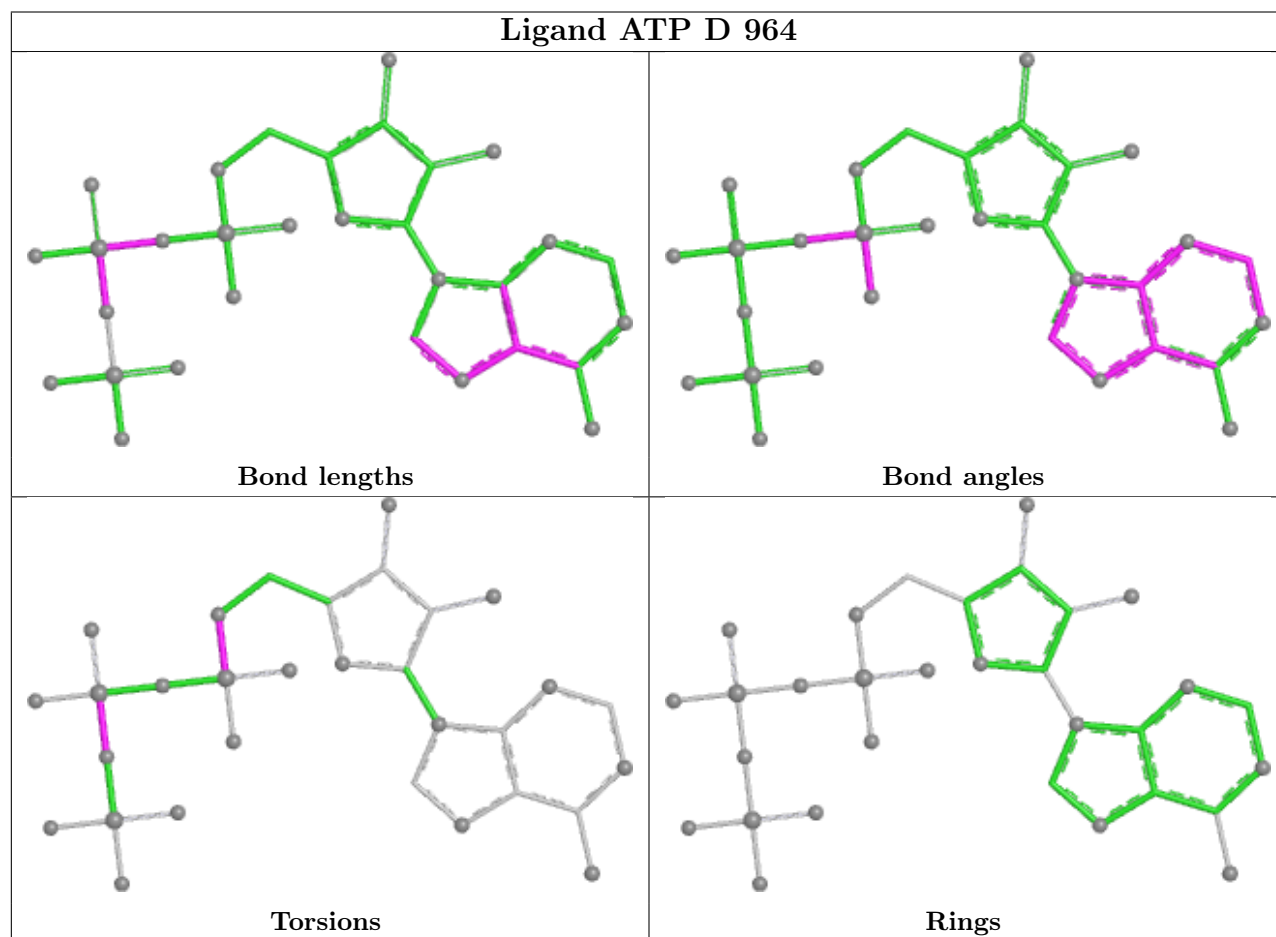
There are no ring outliers.

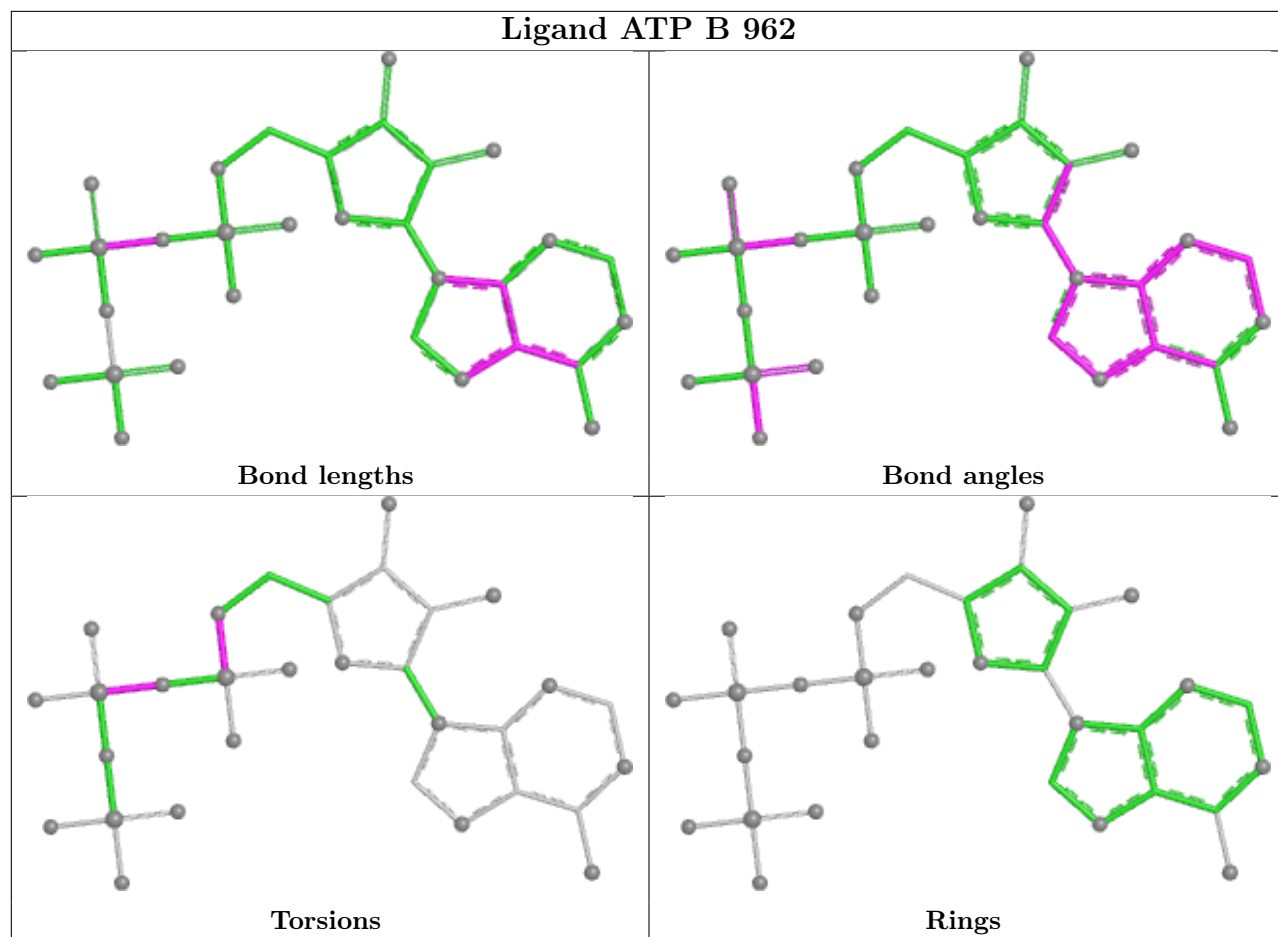
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	963	ATP	1	0

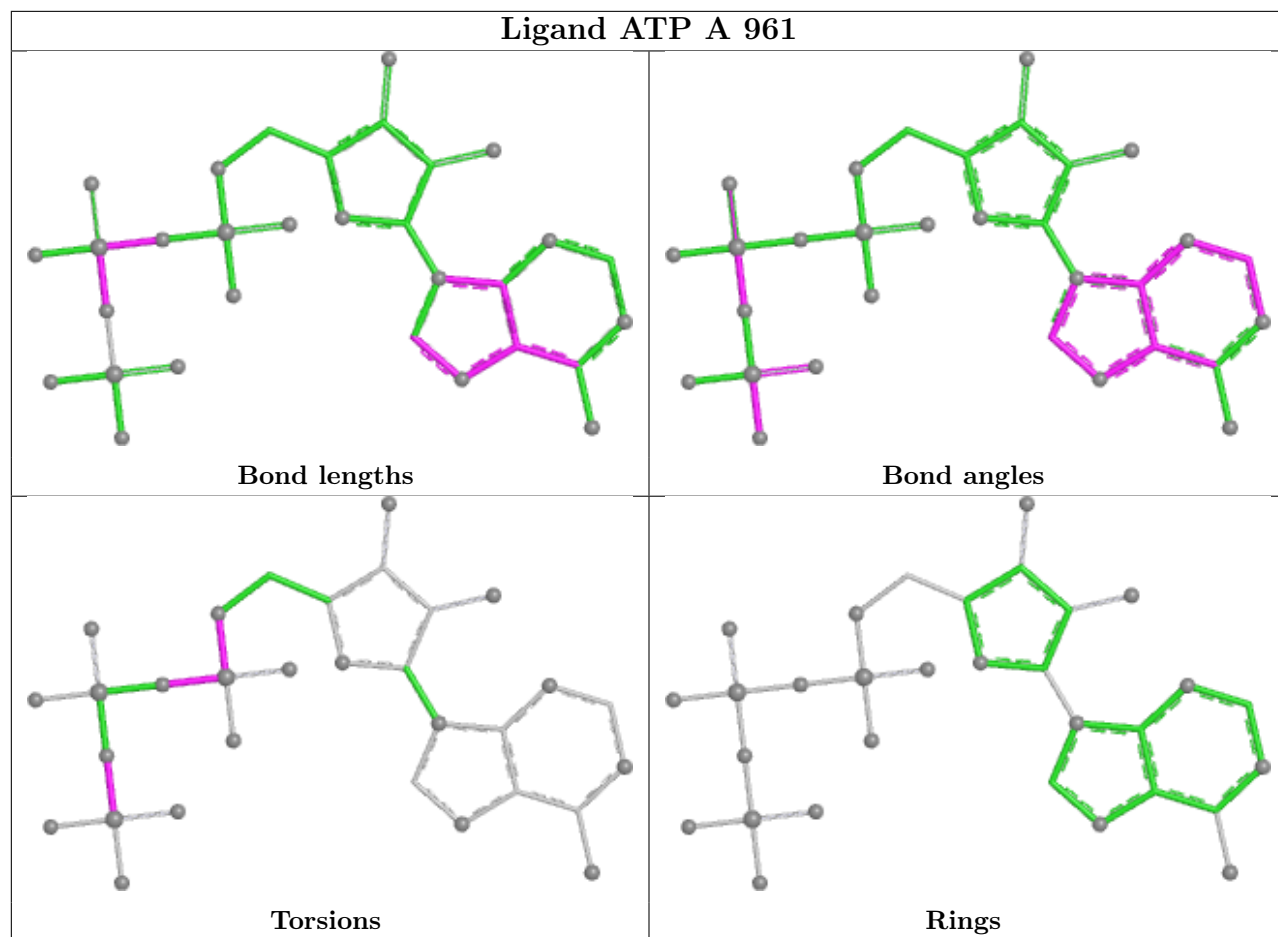
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

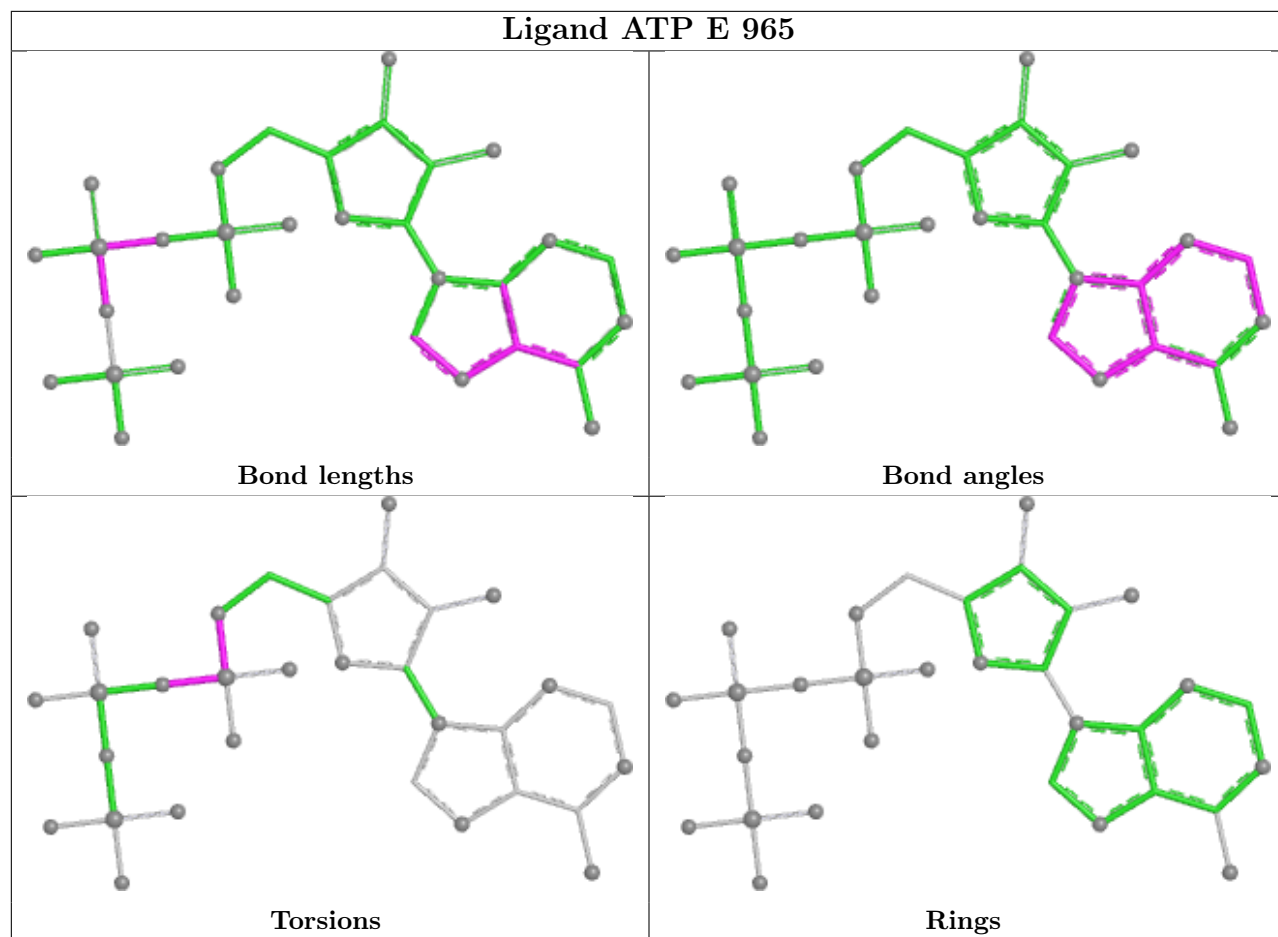


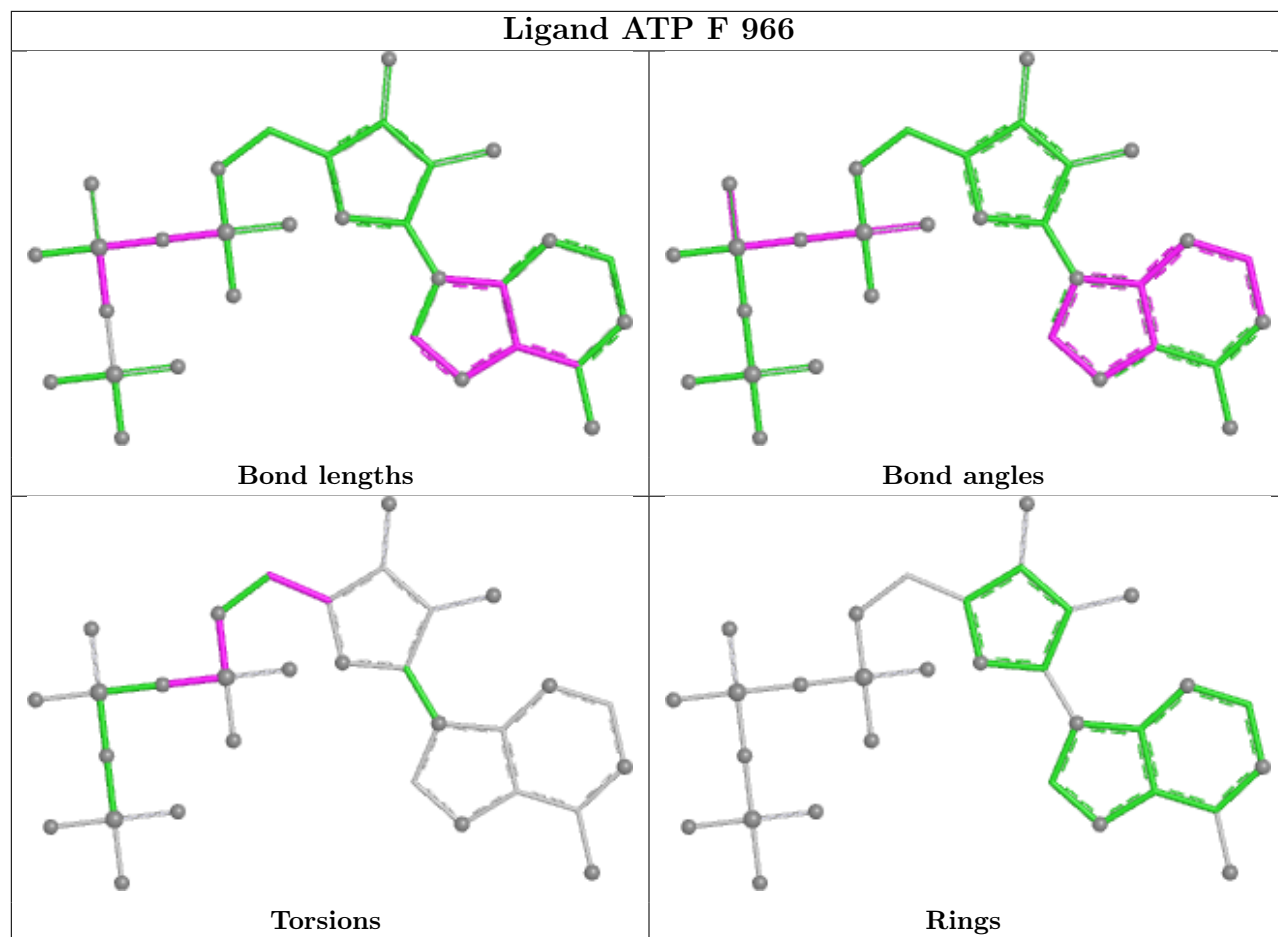


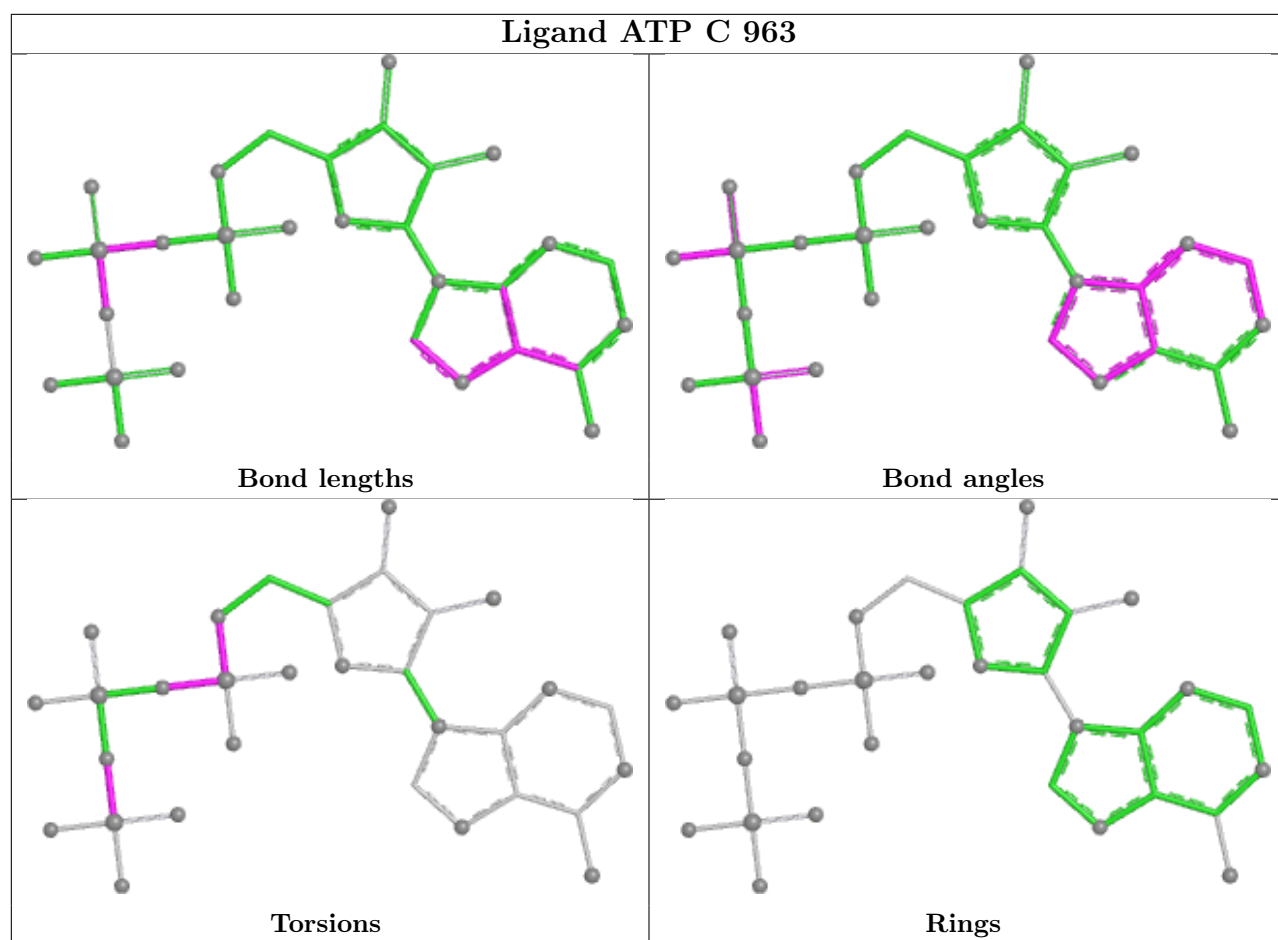
Ligand ATP A 961



Ligand ATP E 965







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	152/171 (88%)	-0.06	8 (5%) 32 34	20, 34, 69, 82	0
1	B	152/171 (88%)	0.25	12 (7%) 18 20	19, 38, 80, 92	0
1	C	152/171 (88%)	0.63	20 (13%) 7 8	22, 45, 90, 99	0
1	D	152/171 (88%)	0.50	20 (13%) 7 8	22, 40, 84, 103	0
1	E	152/171 (88%)	0.20	9 (5%) 28 30	21, 37, 74, 88	0
1	F	152/171 (88%)	0.53	21 (13%) 6 7	22, 41, 83, 99	0
All	All	912/1026 (88%)	0.34	90 (9%) 13 14	19, 39, 81, 103	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	45	LEU	6.8
1	C	45	LEU	6.6
1	D	38	ILE	5.8
1	B	38	ILE	4.8
1	D	158	LYS	4.8
1	F	47	THR	4.7
1	F	46	PHE	4.7
1	C	72	THR	4.6
1	B	37	PHE	4.5
1	F	48	PRO	4.4
1	F	38	ILE	4.4
1	D	48	PRO	4.2
1	F	158	LYS	4.2
1	C	38	ILE	4.2
1	D	45	LEU	4.1
1	D	46	PHE	4.1
1	F	37	PHE	4.1
1	F	71	GLU	4.1
1	B	53	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	45	LEU	4.0
1	B	45	LEU	3.9
1	C	1	MET	3.9
1	A	45	LEU	3.9
1	A	46	PHE	3.9
1	B	47	THR	3.7
1	C	123	GLU	3.6
1	D	61	GLU	3.6
1	B	155	LEU	3.3
1	F	153	HIS	3.2
1	D	156	LYS	3.1
1	A	12	ASP	3.1
1	F	123	GLU	3.1
1	F	154	ALA	3.0
1	D	37	PHE	3.0
1	D	47	THR	3.0
1	C	50	GLU	2.9
1	E	123	GLU	2.9
1	B	46	PHE	2.9
1	C	156	LYS	2.9
1	C	48	PRO	2.8
1	D	53	TYR	2.8
1	C	158	LYS	2.8
1	E	158	LYS	2.8
1	D	49	GLU	2.8
1	C	153	HIS	2.7
1	C	46	PHE	2.7
1	B	72	THR	2.7
1	C	71	GLU	2.7
1	D	71	GLU	2.7
1	B	48	PRO	2.7
1	F	69	MET	2.7
1	F	113	GLU	2.6
1	F	72	THR	2.6
1	A	153	HIS	2.6
1	A	123	GLU	2.6
1	E	153	HIS	2.6
1	C	47	THR	2.5
1	C	37	PHE	2.5
1	C	61	GLU	2.5
1	D	70	GLN	2.5
1	E	46	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	152	TYR	2.4
1	D	69	MET	2.4
1	F	57	GLU	2.4
1	C	53	TYR	2.4
1	D	157	GLN	2.4
1	D	153	HIS	2.3
1	F	49	GLU	2.3
1	E	38	ILE	2.3
1	B	69	MET	2.3
1	F	92	ARG	2.3
1	F	70	GLN	2.3
1	B	153	HIS	2.2
1	D	60	LYS	2.2
1	E	92	ARG	2.2
1	D	50	GLU	2.2
1	C	70	GLN	2.2
1	F	53	TYR	2.1
1	C	60	LYS	2.1
1	B	71	GLU	2.1
1	E	137	LEU	2.1
1	F	54	LEU	2.1
1	C	152	TYR	2.1
1	A	138	ARG	2.1
1	F	156	LYS	2.1
1	A	49	GLU	2.0
1	D	57	GLU	2.0
1	D	123	GLU	2.0
1	A	113	GLU	2.0
1	C	58	ALA	2.0

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](#)

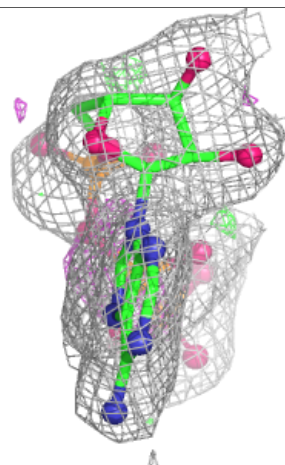
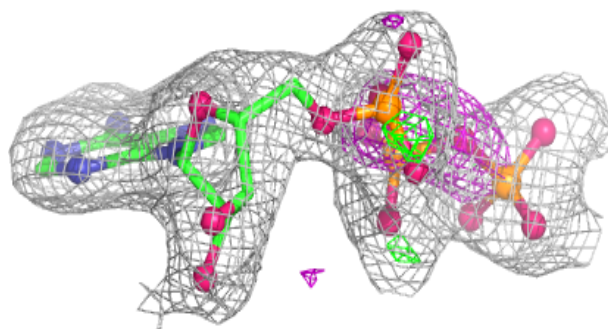
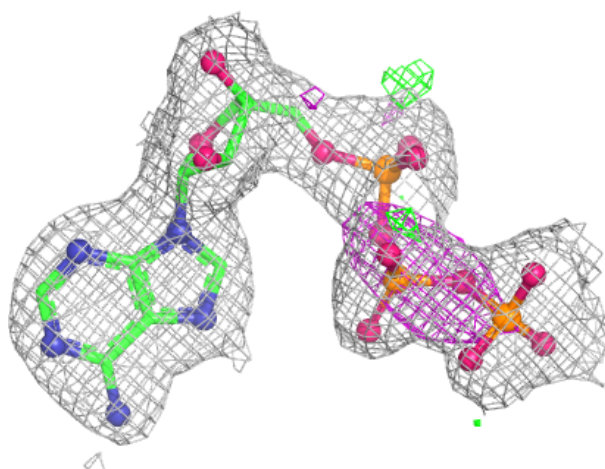
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	C	963	31/31	0.92	0.10	30,36,59,59	0
2	ATP	A	961	31/31	0.94	0.08	28,34,53,55	0
2	ATP	E	965	31/31	0.94	0.09	24,35,62,66	0
2	ATP	D	964	31/31	0.95	0.08	27,36,55,61	0
2	ATP	F	966	31/31	0.95	0.08	30,36,60,64	0
2	ATP	B	962	31/31	0.96	0.07	27,33,53,53	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.

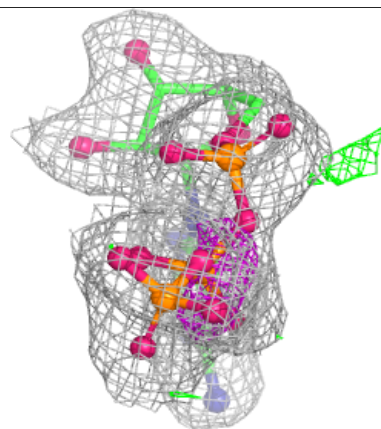
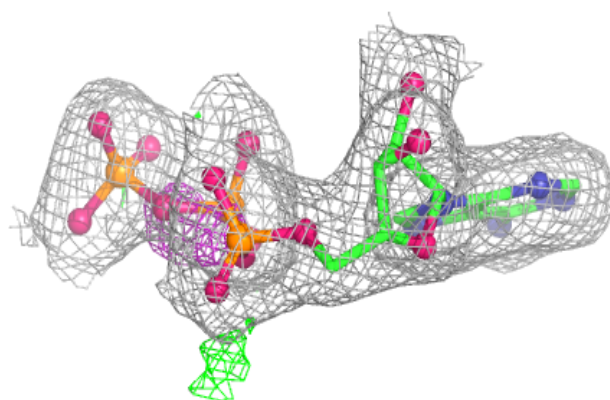
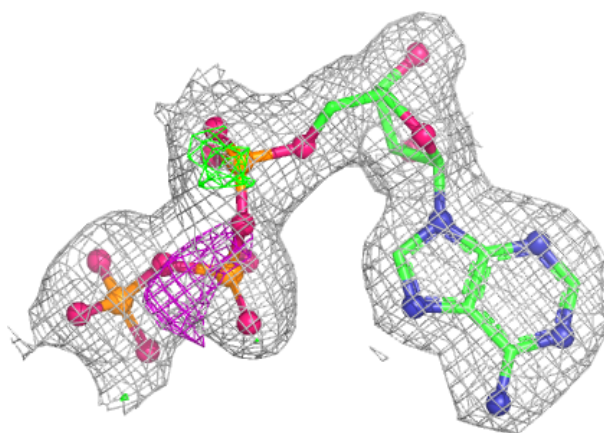
Electron density around ATP C 963:

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



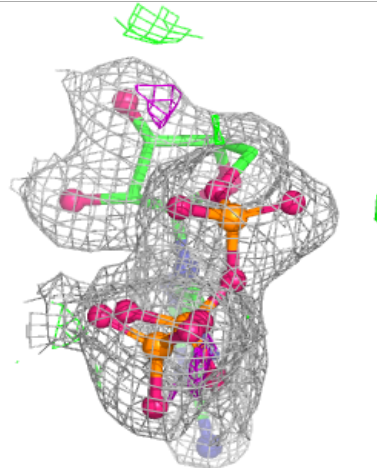
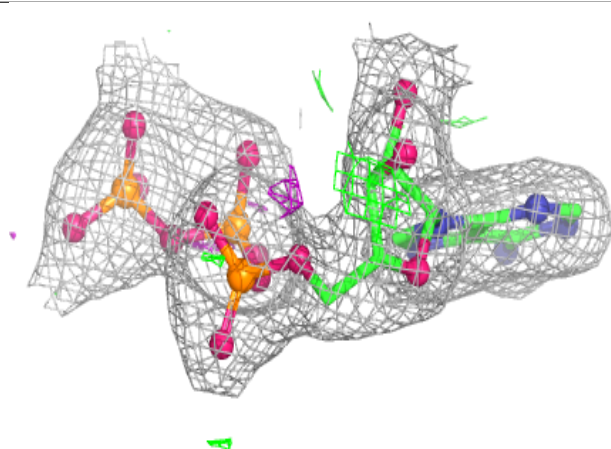
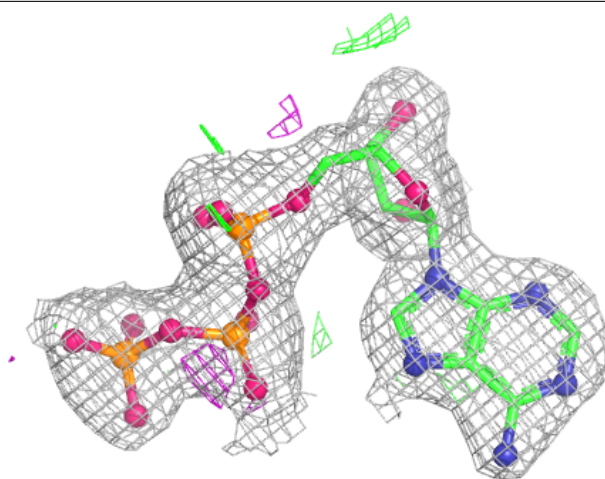
Electron density around ATP A 961:

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



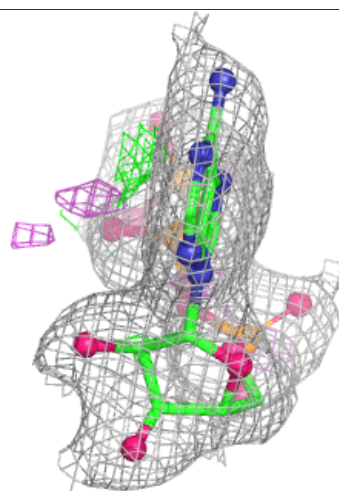
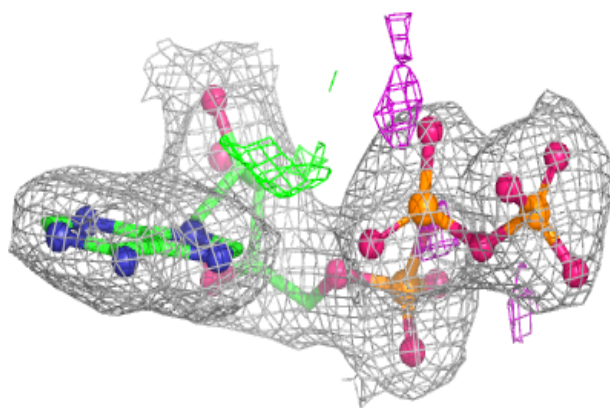
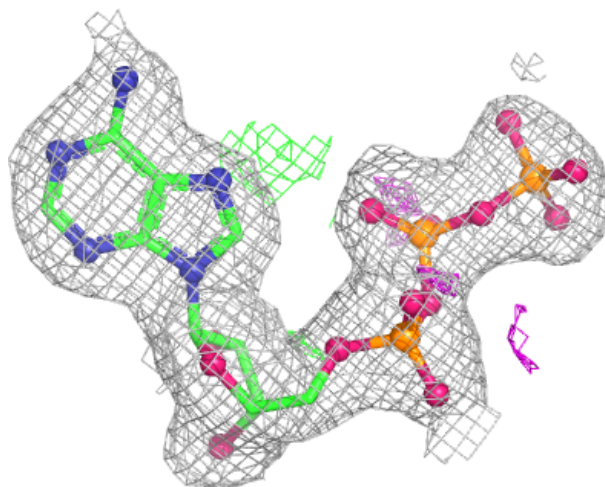
Electron density around ATP E 965:

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



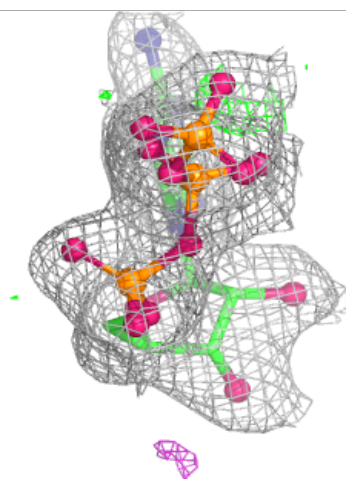
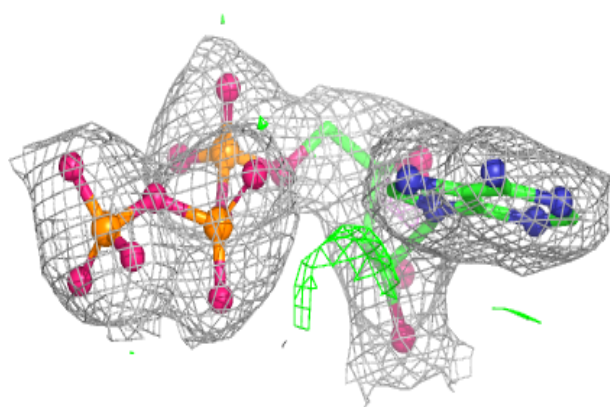
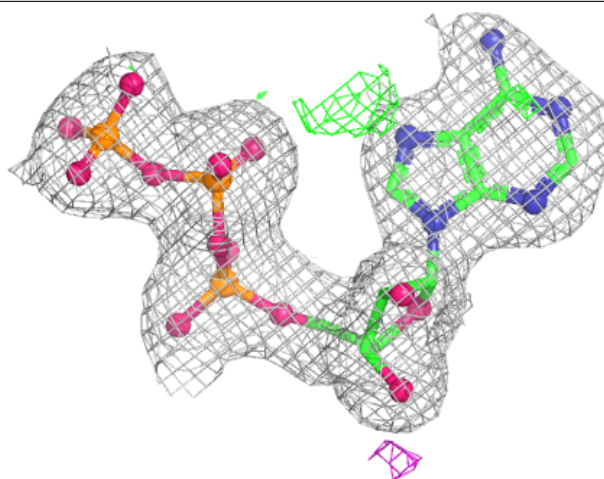
Electron density around ATP D 964:

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



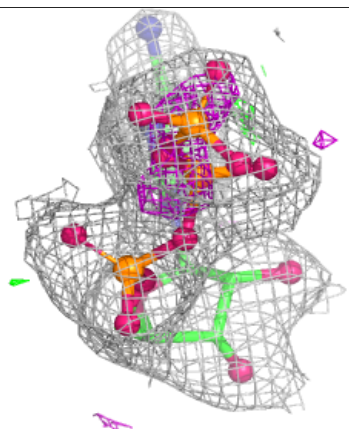
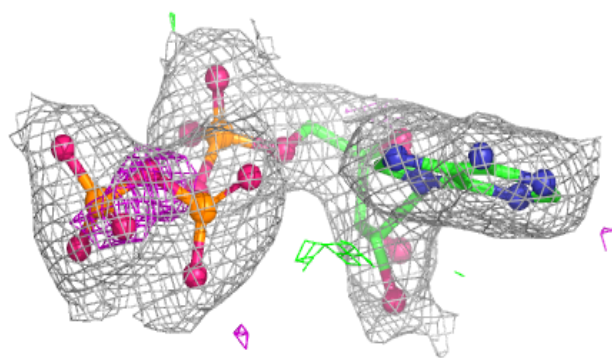
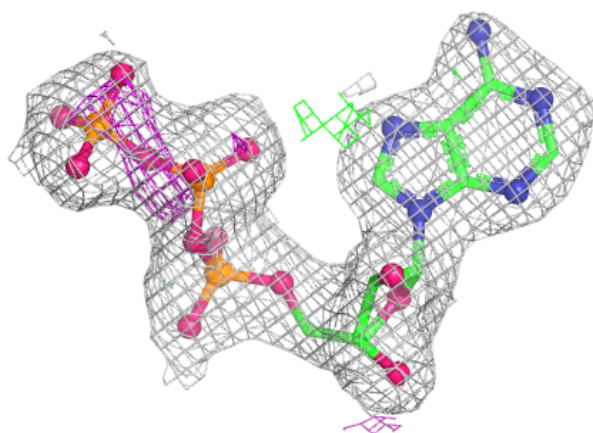
Electron density around ATP F 966:

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



Electron density around ATP B 962:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.