Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 01:38 PM EDT

PDB ID	:	4CYJ
Title	:	Chaetomium thermophilum Pan2:Pan3 complex
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Deposited on	:	2014-04-11
Resolution	:	2.59 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:

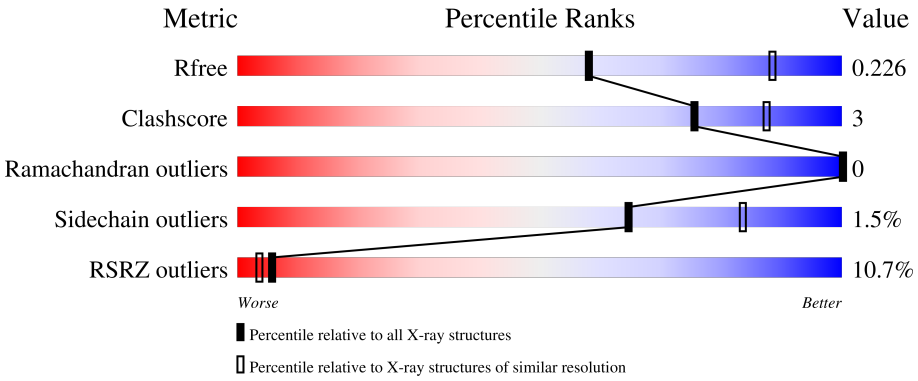
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	438	9% 85% 7% 8%
1	B	438	10% 83% 11% 6%
1	C	438	5% 88% • 8%
1	D	438	10% 87% 6% • 6%
2	E	119	20% 38% 6% 56%

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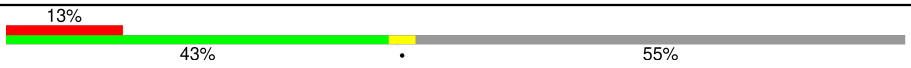
Mol	Chain	Length	Quality of chain
2	F	119	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	1000	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28335 atoms, of which 14053 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 PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3-LIKE PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	H	N	O	S	0	0	0
			6534	2074	3273	576	597	14			
1	B	412	Total	C	H	N	O	S	0	0	0
			6652	2120	3323	583	612	14			
1	C	404	Total	C	H	N	O	S	0	0	0
			6543	2075	3281	577	596	14			
1	D	411	Total	C	H	N	O	S	0	0	0
			6622	2109	3309	579	611	14			

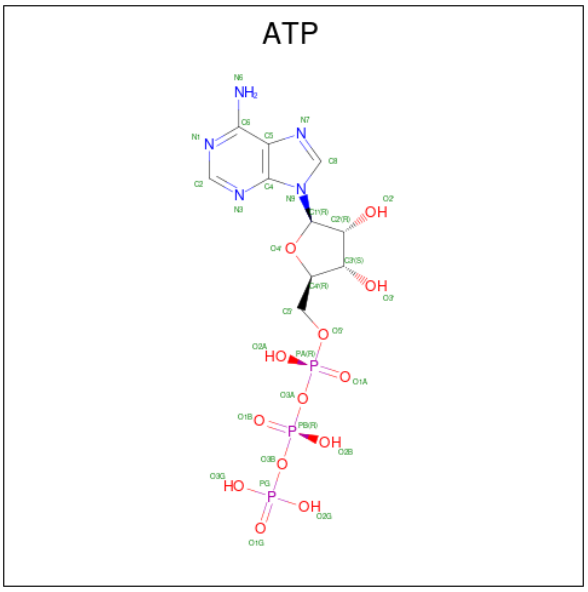
- Molecule 2 is a protein called PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	52	Total	C	H	N	O	0	0	0
			812	262	402	71	77			
2	F	54	Total	C	H	N	O	0	0	0
			850	272	421	77	80			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	340	GLY	-	expression tag	UNP G0SAK8
E	341	SER	-	expression tag	UNP G0SAK8
E	342	MET	-	expression tag	UNP G0SAK8
F	340	GLY	-	expression tag	UNP G0SAK8
F	341	SER	-	expression tag	UNP G0SAK8
F	342	MET	-	expression tag	UNP G0SAK8

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
3	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
3	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
3	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		

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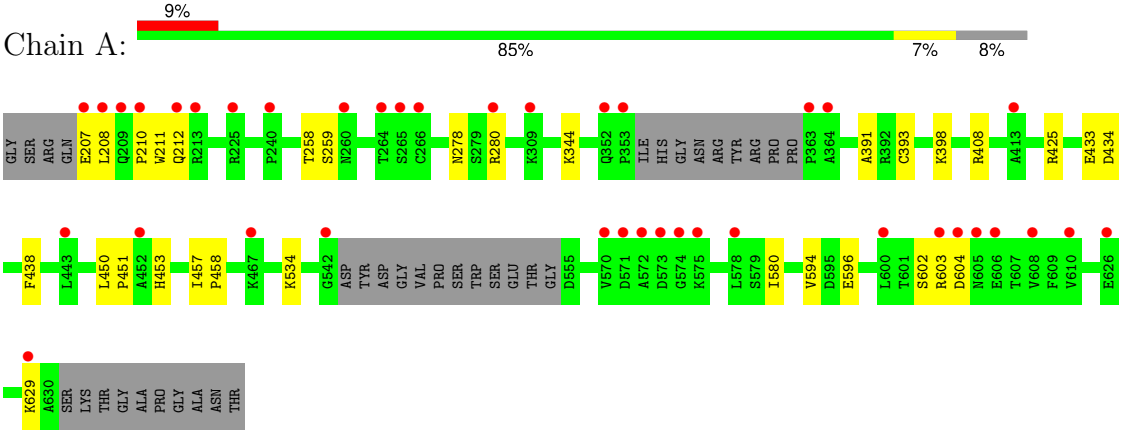
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	35	Total O 35 35	0	0
5	C	42	Total O 42 42	0	0
5	D	30	Total O 30 30	0	0
5	F	2	Total O 2 2	0	0

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.

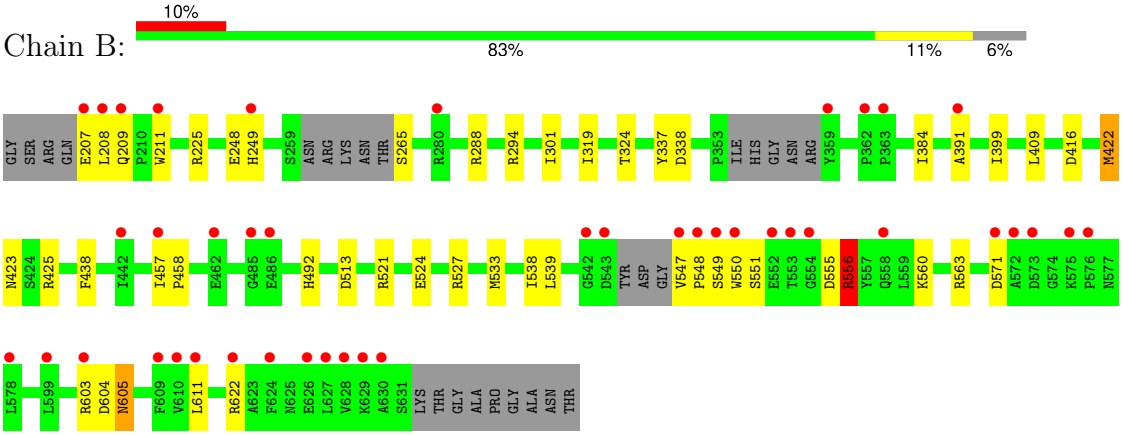
• Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3-LIKE PROTEIN

Chain A:



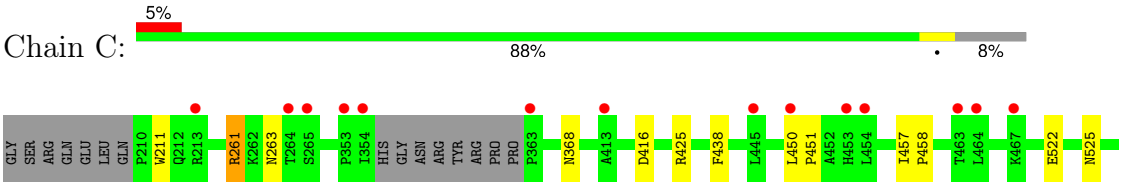
• Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3-LIKE PROTEIN

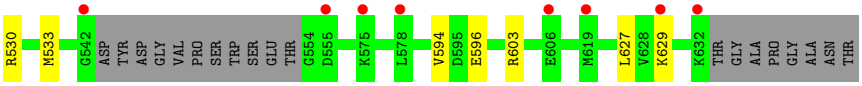
Chain B:



• Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3-LIKE PROTEIN

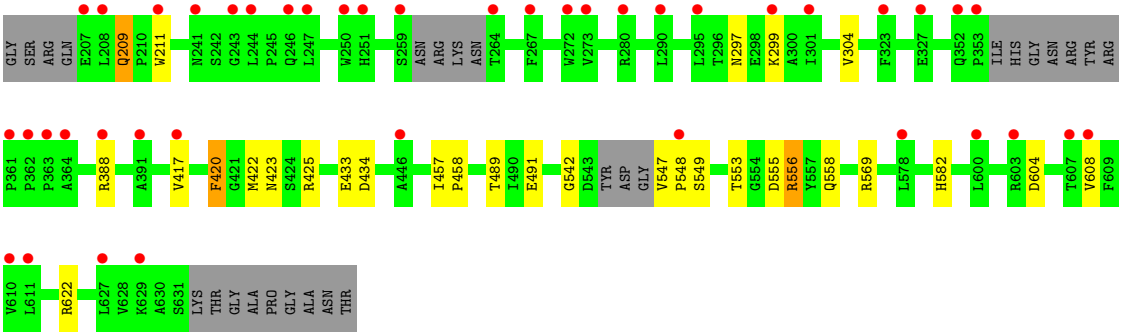
Chain C:





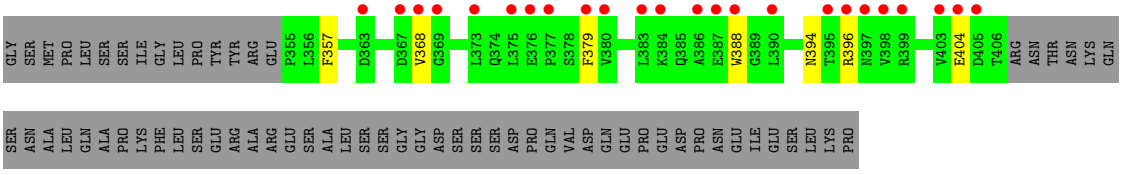
• Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3-LIKE PROTEIN

Chain D:



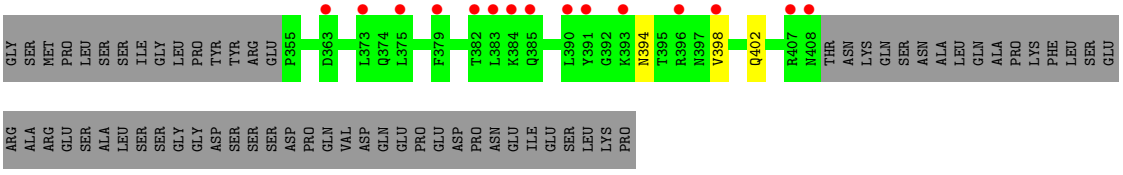
• Molecule 2: PAN2

Chain E:



• Molecule 2: PAN2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.09Å 145.36Å 101.81Å 90.00° 94.86° 90.00°	Depositor
Resolution (Å)	47.89 – 2.59 47.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.89-2.59) 99.8 (47.89-2.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.221 0.187 , 0.226	Depositor DCC
R_{free} test set	4021 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28335	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, MG

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	0.33	0/3329	0.57	0/4501
1	B	0.34	0/3402	0.59	2/4605 (0.0%)
1	C	0.35	0/3330	0.56	0/4500
1	D	0.33	0/3385	0.53	0/4582
2	E	0.29	0/421	0.51	0/575
2	F	0.31	0/440	0.56	0/600
All	All	0.33	0/14307	0.56	2/19363 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	556	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	571	ASP	CB-CG-OD2	5.17	122.95	118.30

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	3261	3273	3260	19	0
1	B	3329	3323	3310	34	2
1	C	3262	3281	3268	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3313	3309	3296	23	2
2	E	410	402	402	6	0
2	F	429	421	421	2	0
3	A	31	11	12	1	0
3	B	31	11	12	2	0
3	C	31	11	12	0	0
3	D	31	11	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	41	0	0	2	0
5	B	35	0	0	4	0
5	C	42	0	0	0	0
5	D	30	0	0	2	0
5	F	2	0	0	0	0
All	All	14282	14053	14005	88	2

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 3.

All (88) 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:D:547:VAL:N	5:D:2026:HOH:O	1.96	0.97
1:D:425:ARG:NH1	1:D:433:GLU:OE2	2.11	0.83
1:D:553:THR:O	1:D:556:ARG:NH1	2.13	0.82
1:D:297:ASN:OD1	1:D:299:LYS:N	2.18	0.75
1:D:555:ASP:OD2	1:D:622:ARG:NH1	2.20	0.74
1:B:288:ARG:NH2	3:B:900:ATP:O1A	2.26	0.69
1:A:602:SER:OG	1:A:604:ASP:O	2.09	0.68
1:B:605:ASN:O	1:B:605:ASN:ND2	2.29	0.65
1:B:555:ASP:OD2	1:B:622:ARG:NH1	2.30	0.64
1:D:423:ASN:HD21	1:D:425:ARG:HE	1.45	0.64
1:D:556:ARG:N	1:D:556:ARG:HD3	2.16	0.61
1:A:453:HIS:N	5:A:2037:HOH:O	2.33	0.61
1:C:594:VAL:HG12	1:C:596:GLU:H	1.67	0.59
1:D:209:GLN:HG2	1:D:211:TRP:CZ2	2.37	0.59
1:B:225:ARG:NH1	5:B:2001:HOH:O	2.35	0.57
1:A:207:GLU:HG3	1:A:210:PRO:HD3	1.86	0.57
1:B:547:VAL:CG2	1:B:550:TRP:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:404:GLU:OE1	2:E:404:GLU:N	2.36	0.56
1:D:608:VAL:HG13	2:F:394:ASN:HB2	1.87	0.55
1:B:209:GLN:HG2	1:B:211:TRP:CZ2	2.43	0.54
1:B:560:LYS:HD3	1:B:603:ARG:NH2	2.22	0.54
1:B:547:VAL:HG22	1:B:550:TRP:HB2	1.90	0.54
1:C:450:LEU:HG	1:C:451:PRO:HD2	1.90	0.53
1:A:594:VAL:HG12	1:A:596:GLU:H	1.74	0.52
1:B:547:VAL:HB	1:B:548:PRO:HD2	1.91	0.52
1:B:457:ILE:HB	1:B:458:PRO:HD3	1.92	0.51
1:A:425:ARG:NH1	1:A:433:GLU:OE2	2.44	0.51
1:C:603:ARG:NH2	1:D:542:GLY:O	2.44	0.50
1:D:420:PHE:C	1:D:420:PHE:CD1	2.86	0.50
1:D:548:PRO:O	1:D:549:SER:OG	2.26	0.49
1:B:492:HIS:ND1	5:B:2029:HOH:O	2.35	0.49
1:B:556:ARG:HG2	1:B:556:ARG:HH11	1.77	0.49
1:A:208:LEU:HA	1:A:211:TRP:CH2	2.48	0.49
1:D:297:ASN:OD1	1:D:299:LYS:HB3	2.13	0.49
1:D:434:ASP:OD1	5:D:2019:HOH:O	2.20	0.49
1:A:450:LEU:HG	1:A:451:PRO:HD2	1.95	0.48
1:D:489:THR:HG22	1:D:491:GLU:N	2.28	0.48
1:A:398:LYS:NZ	3:A:900:ATP:O1G	2.44	0.48
1:D:304:VAL:HG11	1:D:417:VAL:HG23	1.96	0.47
1:C:530:ARG:HA	1:C:533:MET:HE3	1.97	0.47
1:B:399:ILE:HG12	1:B:409:LEU:HD23	1.96	0.47
1:C:425:ARG:HG3	1:C:425:ARG:HH11	1.79	0.47
1:B:248:GLU:HG3	1:B:249:HIS:ND1	2.30	0.47
1:B:521:ARG:NH2	5:B:2034:HOH:O	2.38	0.47
1:B:556:ARG:N	1:B:556:ARG:HD3	2.30	0.47
1:A:208:LEU:O	1:A:212:GLN:HG2	2.14	0.46
1:C:261:ARG:HB2	1:C:261:ARG:HH11	1.81	0.46
1:B:301:ILE:CD1	1:B:324:THR:HG23	2.46	0.46
1:A:534:LYS:NZ	2:E:357:PHE:O	2.45	0.46
1:C:522:GLU:OE1	1:C:525:ASN:ND2	2.45	0.46
1:D:489:THR:HG22	1:D:491:GLU:H	1.81	0.46
1:B:211:TRP:O	2:E:368:VAL:HG22	2.15	0.46
1:D:297:ASN:OD1	1:D:297:ASN:C	2.54	0.45
1:D:457:ILE:HB	1:D:458:PRO:HD3	1.98	0.45
1:D:556:ARG:HD3	1:D:556:ARG:H	1.80	0.45
1:A:391:ALA:O	1:A:434:ASP:OD1	2.35	0.45
1:A:344:LYS:NZ	5:A:2020:HOH:O	2.37	0.44
1:B:338:ASP:OD2	5:B:2017:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:NH2	1:B:513:ASP:OD2	2.51	0.44
1:A:457:ILE:HB	1:A:458:PRO:HD3	1.99	0.44
1:C:450:LEU:HG	1:C:451:PRO:CD	2.48	0.44
1:D:547:VAL:HB	1:D:548:PRO:HD2	1.98	0.44
1:B:423:ASN:HD21	1:B:425:ARG:NH2	2.15	0.44
1:C:211:TRP:HA	1:C:368:ASN:OD1	2.18	0.44
1:B:524:GLU:OE1	1:B:527:ARG:NH1	2.51	0.44
1:B:605:ASN:HD21	2:E:394:ASN:HD22	1.66	0.43
2:E:379:PHE:CE2	2:E:396:ARG:HG3	2.53	0.43
1:A:258:THR:OG1	1:A:259:SER:N	2.51	0.43
1:B:319:ILE:CD1	1:B:337:TYR:CE1	3.01	0.43
1:B:538:ILE:HG23	1:B:550:TRP:CH2	2.53	0.43
1:D:423:ASN:OD1	1:D:425:ARG:HB2	2.18	0.43
2:F:398:VAL:HG22	2:F:402:GLN:HB3	2.01	0.43
1:A:393:CYS:SG	1:A:398:LYS:HG3	2.58	0.43
1:A:278:ASN:HD21	1:A:280:ARG:HH21	1.66	0.43
1:B:209:GLN:HG2	1:B:211:TRP:CH2	2.53	0.43
1:B:538:ILE:HG23	1:B:550:TRP:HH2	1.83	0.42
1:C:457:ILE:HB	1:C:458:PRO:HD3	2.00	0.42
1:B:265:SER:OG	3:B:900:ATP:O2G	2.38	0.42
1:B:551:SER:HB3	1:B:560:LYS:NZ	2.34	0.42
1:C:261:ARG:NH2	1:C:263:ASN:HB2	2.35	0.41
1:B:611:LEU:HD21	2:E:388:TRP:CE3	2.55	0.41
1:B:384:ILE:HD13	1:B:391:ALA:HB2	2.01	0.41
1:A:580:ILE:HD11	1:B:533:MET:HE3	2.03	0.41
1:B:604:ASP:O	1:B:605:ASN:HB3	2.21	0.41
1:D:569:ARG:HD2	1:D:582:HIS:NE2	2.35	0.41
1:B:539:LEU:HD13	1:B:563:ARG:HE	1.86	0.40
1:A:208:LEU:HA	1:A:211:TRP:CZ2	2.56	0.40
1:C:261:ARG:HD3	1:C:261:ARG:H	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:MET:CE	1:D:388:ARG:NH2[2_658]	2.05	0.15
1:B:422:MET:SD	1:D:388:ARG:NH2[2_658]	2.16	0.04

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	397/438 (91%)	395 (100%)	2 (0%)	0	100	100
1	B	404/438 (92%)	401 (99%)	3 (1%)	0	100	100
1	C	398/438 (91%)	394 (99%)	4 (1%)	0	100	100
1	D	403/438 (92%)	402 (100%)	1 (0%)	0	100	100
2	E	50/119 (42%)	50 (100%)	0	0	100	100
2	F	52/119 (44%)	52 (100%)	0	0	100	100
All	All	1704/1990 (86%)	1694 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	358/385 (93%)	355 (99%)	3 (1%)	81	92
1	B	366/385 (95%)	357 (98%)	9 (2%)	47	73
1	C	358/385 (93%)	353 (99%)	5 (1%)	67	85
1	D	365/385 (95%)	359 (98%)	6 (2%)	62	82
2	E	44/103 (43%)	44 (100%)	0	100	100
2	F	46/103 (45%)	46 (100%)	0	100	100
All	All	1537/1746 (88%)	1514 (98%)	23 (2%)	65	83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	PHE
1	A	603	ARG
1	A	629	LYS
1	B	207	GLU
1	B	208	LEU
1	B	294	ARG
1	B	416	ASP
1	B	422	MET
1	B	438	PHE
1	B	549	SER
1	B	556	ARG
1	B	605	ASN
1	C	261	ARG
1	C	416	ASP
1	C	438	PHE
1	C	627	LEU
1	C	629	LYS
1	D	209	GLN
1	D	420	PHE
1	D	422	MET
1	D	556	ARG
1	D	558	GLN
1	D	604	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	HIS
1	B	605	ASN
1	C	249	HIS
1	C	349	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	ATP	A	900	4	28,33,33	0.92	1 (3%)	34,52,52	1.40	4 (11%)
3	ATP	C	900	4	28,33,33	1.03	2 (7%)	34,52,52	1.19	2 (5%)
3	ATP	D	900	4	28,33,33	1.22	3 (10%)	34,52,52	1.22	3 (8%)
3	ATP	B	900	4	28,33,33	1.18	3 (10%)	34,52,52	1.45	4 (11%)

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
3	ATP	A	900	4	-	2/18/38/38	0/3/3/3
3	ATP	C	900	4	-	3/18/38/38	0/3/3/3
3	ATP	D	900	4	-	0/18/38/38	0/3/3/3
3	ATP	B	900	4	-	2/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	900	ATP	PB-O3B	3.31	1.63	1.59
3	D	900	ATP	PA-O3A	3.02	1.62	1.59
3	B	900	ATP	PA-O3A	2.92	1.62	1.59
3	B	900	ATP	PB-O3B	2.83	1.62	1.59
3	B	900	ATP	PB-O3A	2.59	1.62	1.59
3	C	900	ATP	PB-O3B	2.58	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	900	ATP	PB-O3A	2.50	1.62	1.59
3	A	900	ATP	PB-O3B	2.10	1.61	1.59
3	C	900	ATP	C2-N3	2.03	1.35	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	900	ATP	N3-C2-N1	-4.23	122.93	128.67
3	A	900	ATP	N3-C2-N1	-4.05	123.18	128.67
3	D	900	ATP	N3-C2-N1	-4.02	123.21	128.67
3	B	900	ATP	O4'-C1'-N9	3.94	113.97	108.75
3	A	900	ATP	O4'-C1'-N9	3.82	113.81	108.75
3	C	900	ATP	N3-C2-N1	-3.56	123.84	128.67
3	C	900	ATP	N6-C6-N1	2.53	123.75	118.33
3	B	900	ATP	C1'-N9-C4	-2.49	122.26	126.64
3	D	900	ATP	O4'-C1'-N9	2.28	111.77	108.75
3	B	900	ATP	N6-C6-N1	2.20	123.03	118.33
3	D	900	ATP	N6-C6-N1	2.18	123.00	118.33
3	A	900	ATP	C4-C5-N7	-2.14	107.08	109.34
3	A	900	ATP	C1'-N9-C4	-2.03	123.07	126.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	900	ATP	C5'-O5'-PA-O1A
3	B	900	ATP	PB-O3A-PA-O2A
3	A	900	ATP	C5'-O5'-PA-O1A
3	C	900	ATP	C5'-O5'-PA-O3A
3	A	900	ATP	PA-O3A-PB-O2B
3	B	900	ATP	PB-O3A-PA-O1A
3	C	900	ATP	PG-O3B-PB-O2B

There are no ring outliers.

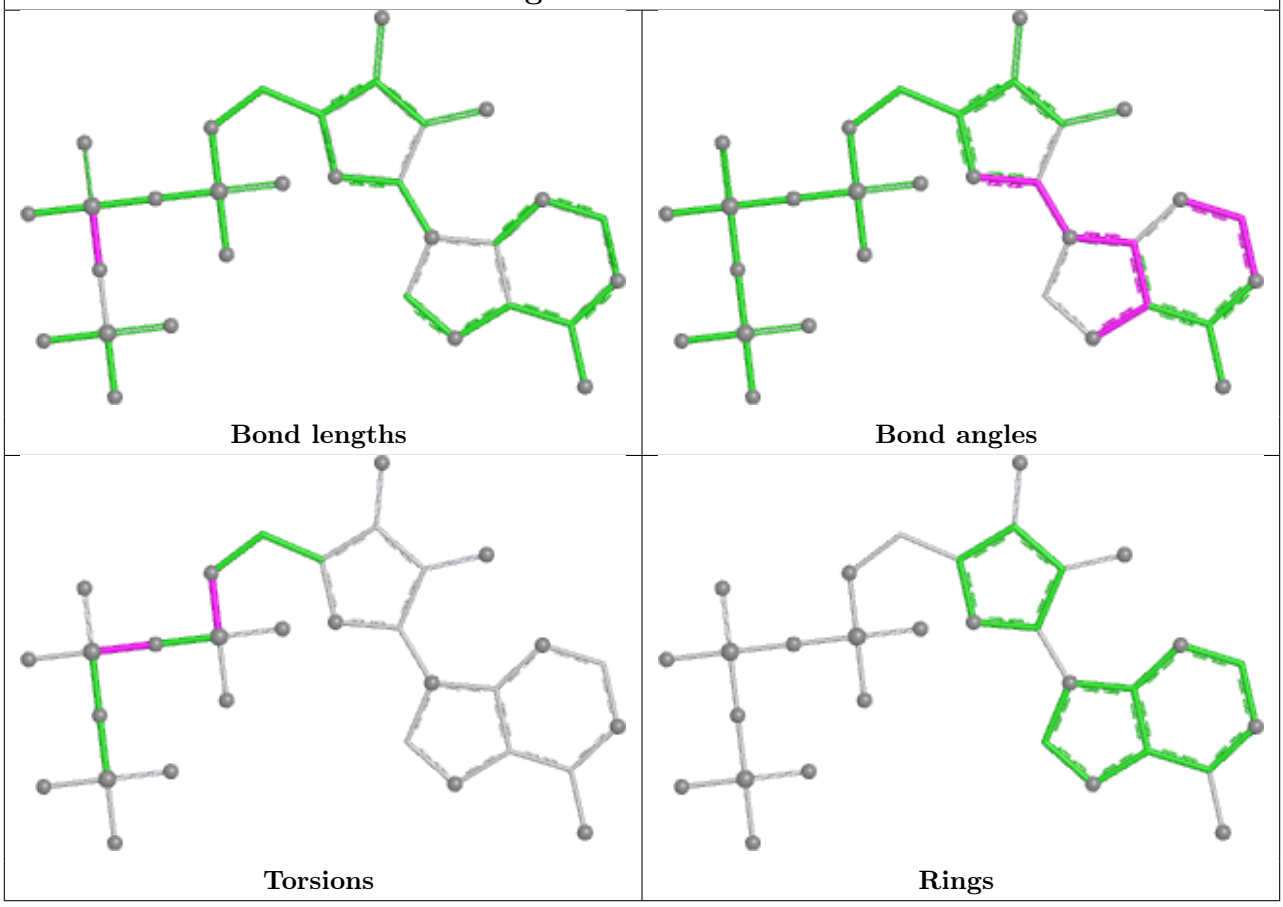
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	ATP	1	0
3	B	900	ATP	2	0

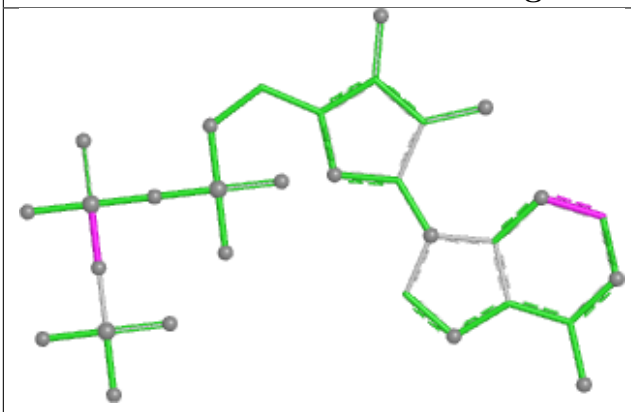
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

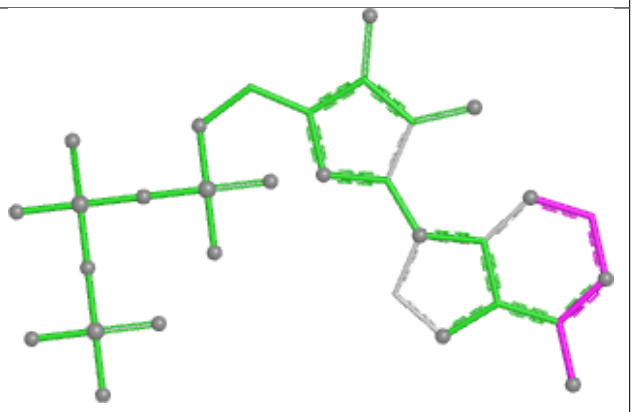
Ligand ATP A 900



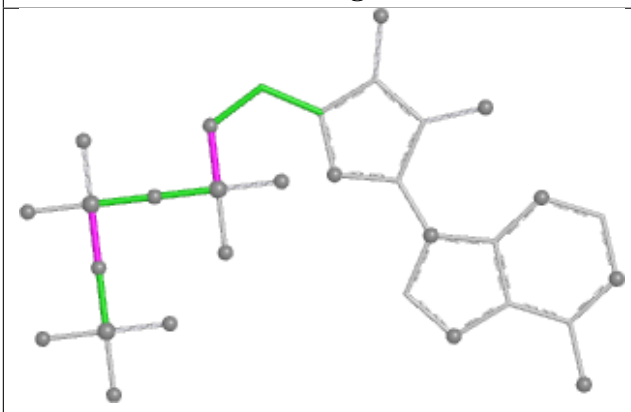
Ligand ATP C 900



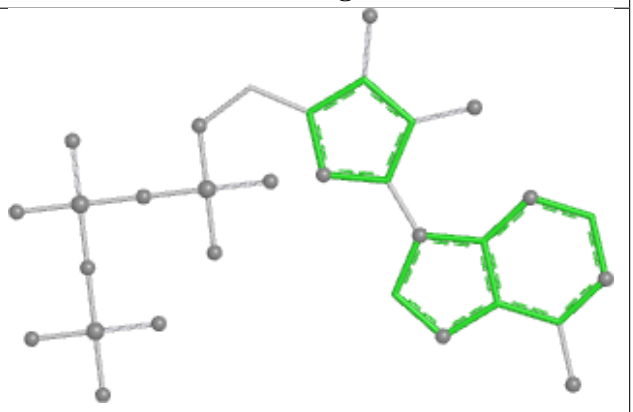
Bond lengths



Bond angles

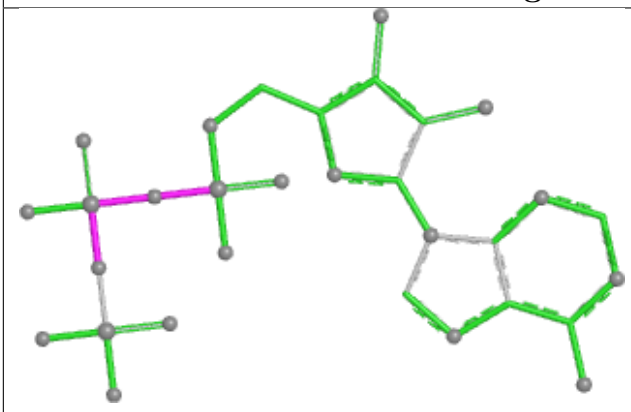


Torsions

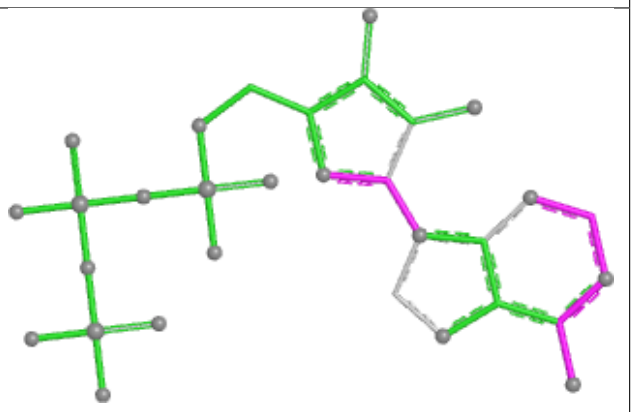


Rings

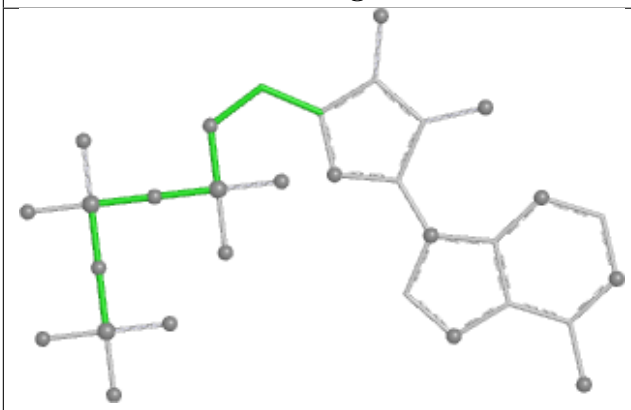
Ligand ATP D 900



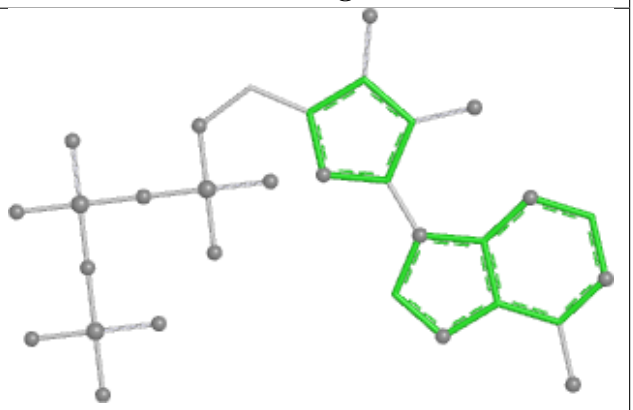
Bond lengths



Bond angles

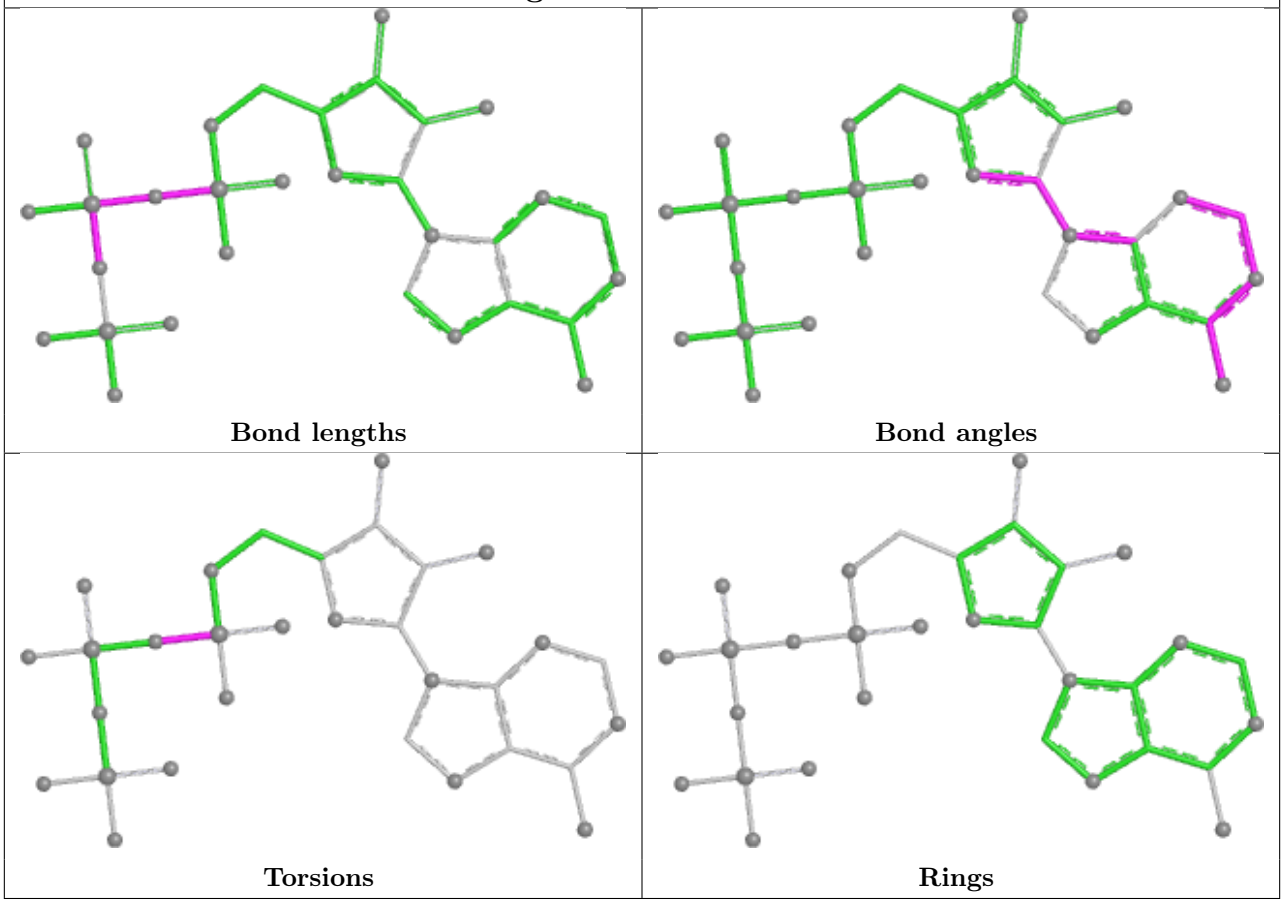


Torsions



Rings

Ligand ATP B 900



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, 95^{th} 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	403/438 (92%)	0.81	39 (9%) 7 5	33, 58, 121, 157	0
1	B	412/438 (94%)	0.76	43 (10%) 6 4	33, 62, 116, 140	0
1	C	404/438 (92%)	0.68	22 (5%) 25 20	35, 56, 109, 125	0
1	D	411/438 (93%)	0.88	42 (10%) 6 4	34, 65, 112, 138	0
2	E	52/119 (43%)	1.91	24 (46%) 0 0	67, 105, 128, 137	0
2	F	54/119 (45%)	1.34	15 (27%) 0 0	50, 92, 122, 127	0
All	All	1736/1990 (87%)	0.83	185 (10%) 6 3	33, 62, 118, 157	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	361	PRO	10.2
1	D	362	PRO	9.1
1	C	354	ILE	8.9
1	B	629	LYS	7.6
1	D	363	PRO	6.4
2	E	396	ARG	6.0
1	B	547	VAL	5.9
2	E	375	LEU	5.8
1	B	359	TYR	5.7
1	A	208	LEU	5.5
2	E	398	VAL	5.2
2	F	398	VAL	5.0
1	C	353	PRO	4.9
1	B	578	LEU	4.8
2	E	403	VAL	4.8
1	C	464	LEU	4.7
2	F	390	LEU	4.6
1	B	548	PRO	4.5
1	B	208	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	213	ARG	4.3
1	D	301	ILE	4.2
1	C	363	PRO	4.1
1	D	280	ARG	4.0
1	A	353	PRO	3.9
1	B	552	GLU	3.9
2	E	379	PHE	3.9
1	B	572	ALA	3.9
1	C	632	LYS	3.9
1	D	247	LEU	3.8
1	D	353	PRO	3.8
2	F	391	TYR	3.8
1	A	352	GLN	3.8
1	D	610	VAL	3.7
1	D	250	TRP	3.7
2	F	382	THR	3.7
1	A	209	GLN	3.7
1	D	244	LEU	3.7
1	A	608	VAL	3.7
2	E	397	ASN	3.6
2	E	404	GLU	3.6
1	B	630	ALA	3.6
1	B	628	VAL	3.6
2	F	408	ASN	3.6
1	D	259	SER	3.6
1	B	575	LYS	3.6
2	E	384	LYS	3.4
1	B	599	LEU	3.4
1	B	543	ASP	3.4
1	D	243	GLY	3.4
1	B	609	PHE	3.3
1	A	363	PRO	3.3
1	B	571	ASP	3.3
1	B	610	VAL	3.3
1	B	209	GLN	3.3
1	B	542	GLY	3.3
1	B	573	ASP	3.2
1	C	542	GLY	3.2
1	B	211	TRP	3.2
1	A	225	ARG	3.2
1	A	210	PRO	3.2
1	D	241	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	E	376	GLU	3.2
2	E	390	LEU	3.2
1	A	571	ASP	3.1
1	A	213	ARG	3.1
1	A	266	CYS	3.1
1	D	603	ARG	3.1
1	D	290	LEU	3.0
2	E	388	TRP	3.0
1	A	626	GLU	3.0
1	A	604	ASP	3.0
1	B	362	PRO	2.9
2	F	379	PHE	2.9
1	A	574	GLY	2.9
1	A	212	GLN	2.9
2	E	380	VAL	2.9
1	A	606	GLU	2.9
1	A	603	ARG	2.8
1	A	572	ALA	2.8
1	B	576	PRO	2.8
1	C	413	ALA	2.8
2	F	363	ASP	2.8
1	D	246	GLN	2.8
1	B	442	ILE	2.8
1	D	295	LEU	2.8
1	B	626	GLU	2.7
2	E	383	LEU	2.7
2	E	395	THR	2.7
2	E	405	ASP	2.7
2	F	384	LYS	2.7
1	B	363	PRO	2.7
1	C	629	LYS	2.7
1	A	207	GLU	2.7
1	C	453	HIS	2.6
1	A	573	ASP	2.6
1	A	575	LYS	2.6
1	D	629	LYS	2.6
1	D	548	PRO	2.6
2	E	377	PRO	2.6
2	F	375	LEU	2.6
1	D	578	LEU	2.6
2	E	387	GLU	2.6
1	D	208	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	452	ALA	2.5
1	A	578	LEU	2.5
1	D	323	PHE	2.5
1	B	280	ARG	2.5
2	F	407	ARG	2.5
1	D	267	PHE	2.5
1	A	600	LEU	2.5
1	D	388	ARG	2.5
1	D	446	ALA	2.5
1	D	207	GLU	2.5
1	B	549	SER	2.5
1	B	624	PHE	2.5
1	A	413	ALA	2.5
1	B	462	GLU	2.5
1	A	280	ARG	2.4
2	E	399	ARG	2.4
1	C	606	GLU	2.4
2	E	368	VAL	2.4
1	C	575	LYS	2.4
1	B	622	ARG	2.4
1	B	457	ILE	2.4
1	B	485	GLY	2.4
2	E	386	ALA	2.4
1	C	619	MET	2.4
2	F	396	ARG	2.4
2	F	383	LEU	2.4
2	E	369	GLY	2.4
1	B	249	HIS	2.4
1	C	454	LEU	2.4
1	A	570	VAL	2.3
1	C	467	LYS	2.3
1	C	463	THR	2.3
1	B	603	ARG	2.3
1	B	550	TRP	2.3
1	D	299	LYS	2.3
1	D	352	GLN	2.3
1	A	240	PRO	2.3
1	A	542	GLY	2.3
1	B	486	GLU	2.3
1	B	627	LEU	2.2
1	C	265	SER	2.2
1	C	264	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	393	LYS	2.2
1	A	443	LEU	2.2
1	B	391	ALA	2.2
1	C	450	LEU	2.2
1	C	578	LEU	2.2
1	D	611	LEU	2.2
2	E	373	LEU	2.2
1	B	554	GLY	2.2
1	A	467	LYS	2.2
1	D	607	THR	2.2
1	D	608	VAL	2.2
1	A	264	THR	2.2
1	C	555	ASP	2.2
1	D	391	ALA	2.2
1	D	264	THR	2.2
1	B	611	LEU	2.2
1	C	445	LEU	2.2
1	D	272	TRP	2.1
2	E	363	ASP	2.1
1	D	327	GLU	2.1
1	B	558	GLN	2.1
1	B	207	GLU	2.1
1	D	211	TRP	2.1
1	D	364	ALA	2.1
2	F	373	LEU	2.1
1	A	605	ASN	2.1
1	A	364	ALA	2.1
2	E	367	ASP	2.1
1	D	600	LEU	2.1
2	F	385	GLN	2.1
1	B	553	THR	2.1
1	D	273	VAL	2.1
1	D	627	LEU	2.1
1	A	309	LYS	2.1
1	D	417	VAL	2.0
1	A	265	SER	2.0
1	A	629	LYS	2.0
1	D	251	HIS	2.0
1	A	260	ASN	2.0
1	A	610	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

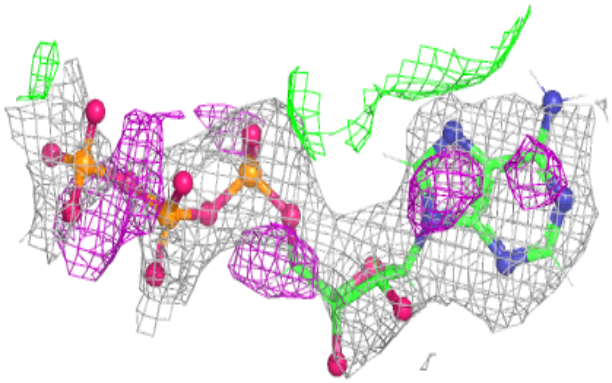
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

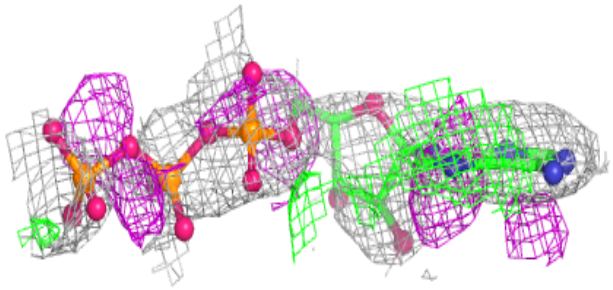
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	1000	1/1	0.54	0.33	75,75,75,75	0
4	MG	B	1000	1/1	0.71	0.29	87,87,87,87	0
4	MG	A	1000	1/1	0.73	0.42	71,71,71,71	0
3	ATP	B	900	31/31	0.79	0.31	51,100,164,182	0
3	ATP	D	900	31/31	0.88	0.20	57,80,119,174	0
3	ATP	C	900	31/31	0.95	0.23	40,63,125,132	0
3	ATP	A	900	31/31	0.96	0.18	34,55,116,144	0
4	MG	D	1000	1/1	0.96	0.06	76,76,76,76	0

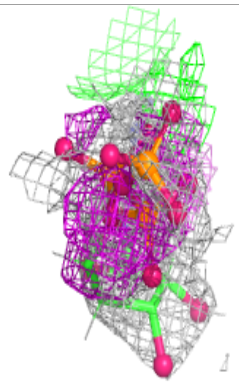
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 900:

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

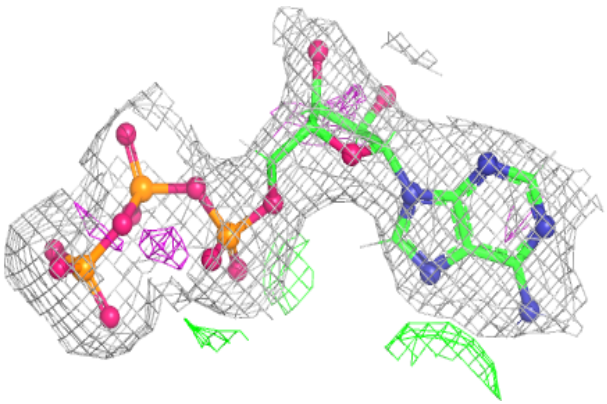


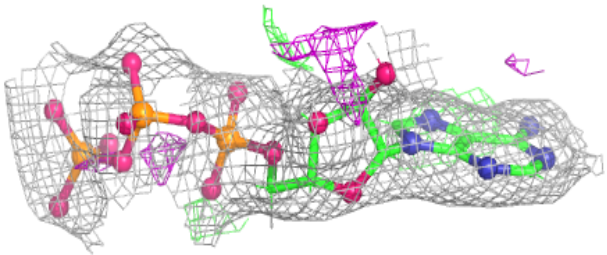


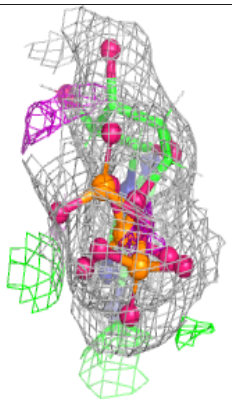


Electron density around ATP D 900:

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

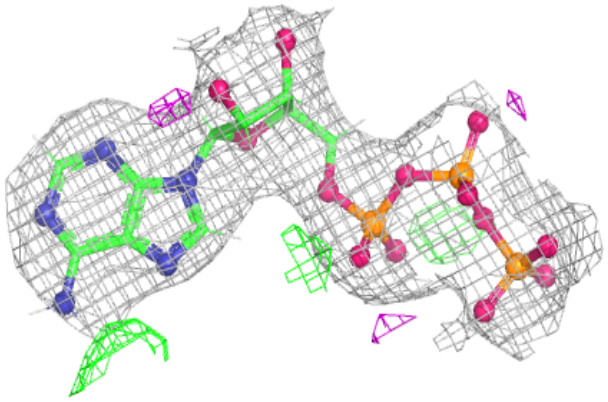


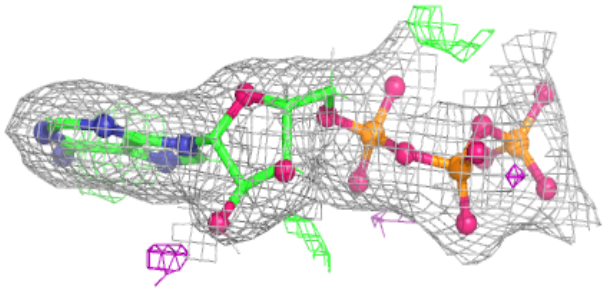


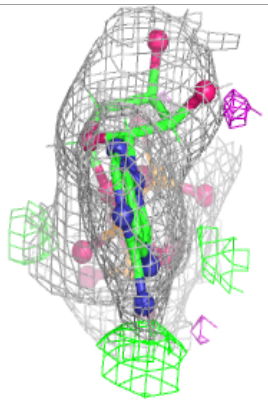


Electron density around ATP C 900:

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

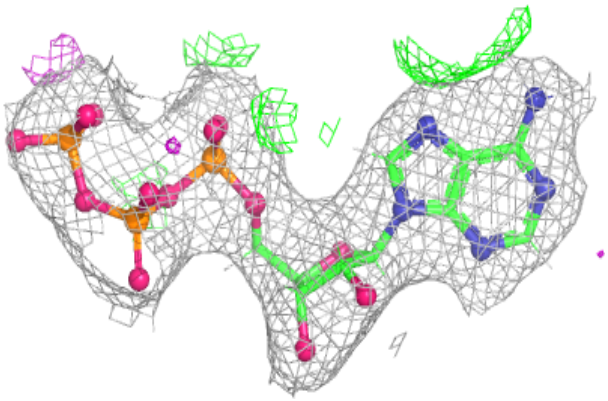


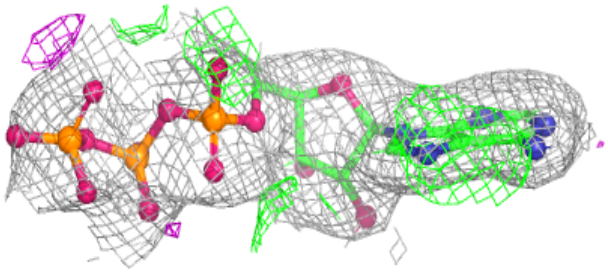


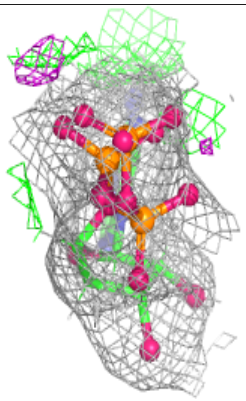


Electron density around ATP A 900:

$2mF_o$-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.