Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 07:12 am GMT

PDB ID	:	2CK3
Title	:	Azide inhibited bovine F1-ATPase
Authors	:	Bowler, M.W.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	2006-04-10
Resolution	:	1.95 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 (i) 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 (i)) were used in the production of this report:

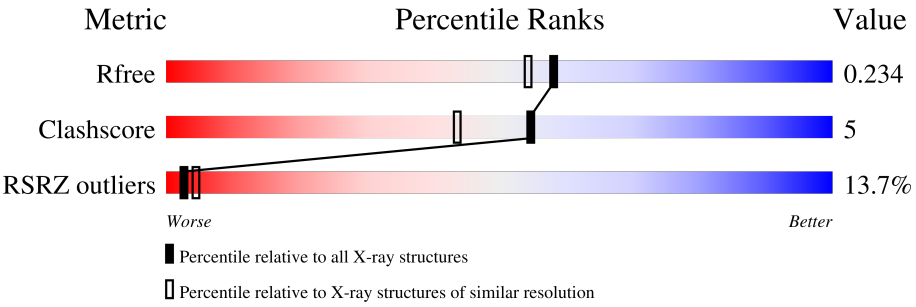
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	510	12% 85% 11% 5%
1	B	510	14% 88% 6% 6%
1	C	510	6% 86% 10% ·
2	D	482	5% 87% 10% ·
2	E	482	18% 86% 9% 5%
2	F	482	5% 90% 7% ·
3	G	272	25% 61% 6% 33%

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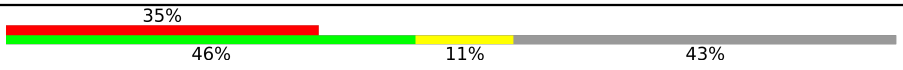
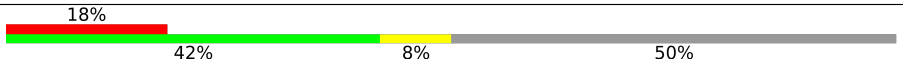
Mol	Chain	Length	Quality of chain
4	H	146	
5	I	50	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 26509 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	4	0
			3738	2359	658	709	12			
1	B	480	Total	C	N	O	S	0	1	0
			3667	2310	649	696	12			
1	C	490	Total	C	N	O	S	0	0	0
			3735	2353	659	711	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	cloning artifact	UNP P19483
B	481	GLY	SER	cloning artifact	UNP P19483
C	481	GLY	SER	cloning artifact	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	2	0
			3550	2252	602	685	11			
2	E	458	Total	C	N	O	S	0	2	0
			3486	2209	596	671	10			
2	F	466	Total	C	N	O	S	0	3	0
			3541	2248	600	682	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	182	Total	C	N	O	S	0	0	1
			1397	881	250	260	6			

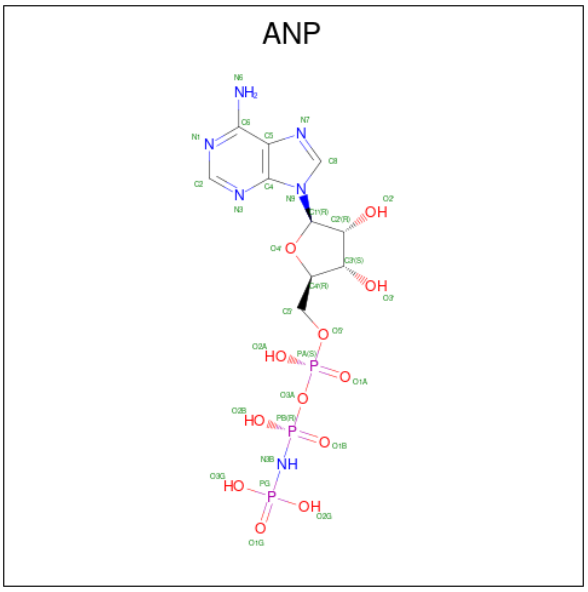
- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	83	Total	C	N	O	S	0	0	0
			620	391	102	126	1			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	25	Total	C	N	O	S	0	0	0
			203	130	38	34	1			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

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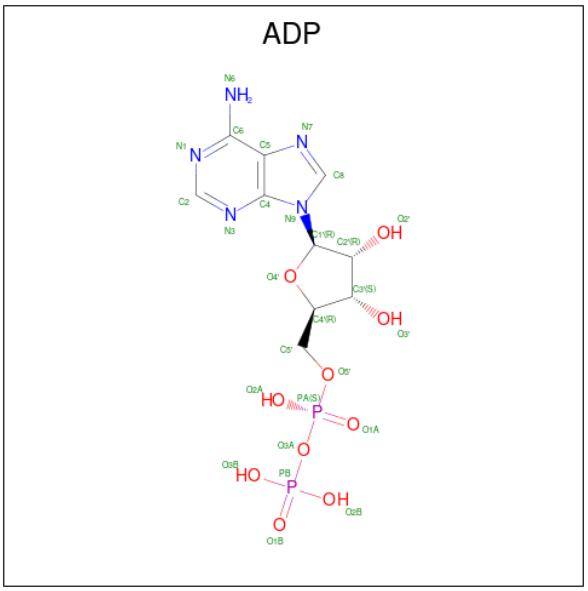
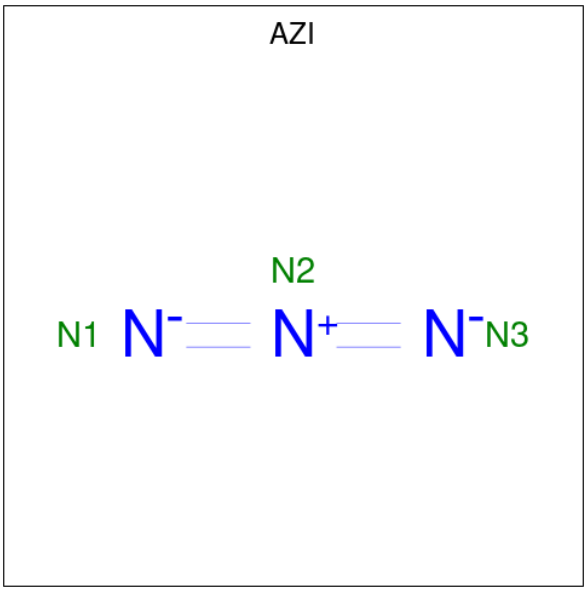
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



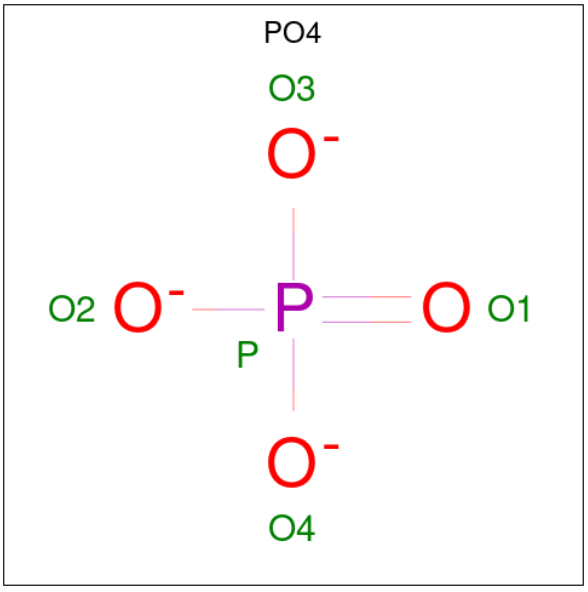
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 9 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total N 3 3	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 11 is water.

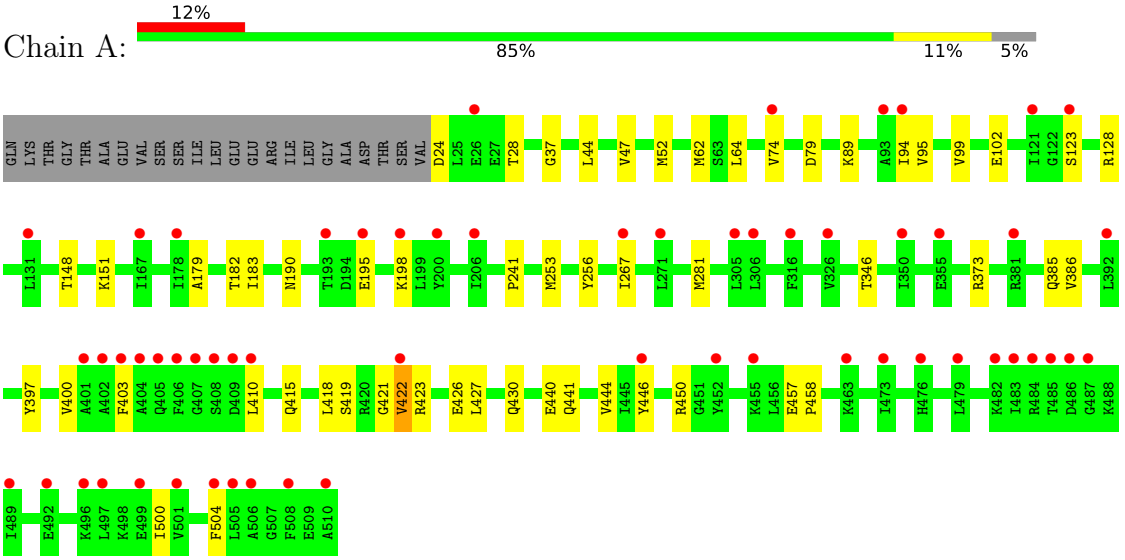
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	380	Total O 380 380	0	0
11	B	409	Total O 409 409	0	0
11	C	378	Total O 378 378	0	0
11	D	383	Total O 383 383	0	0
11	E	246	Total O 246 246	0	0
11	F	484	Total O 484 484	0	0
11	G	113	Total O 113 113	0	0
11	H	8	Total O 8 8	0	0
11	I	7	Total O 7 7	0	0

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.

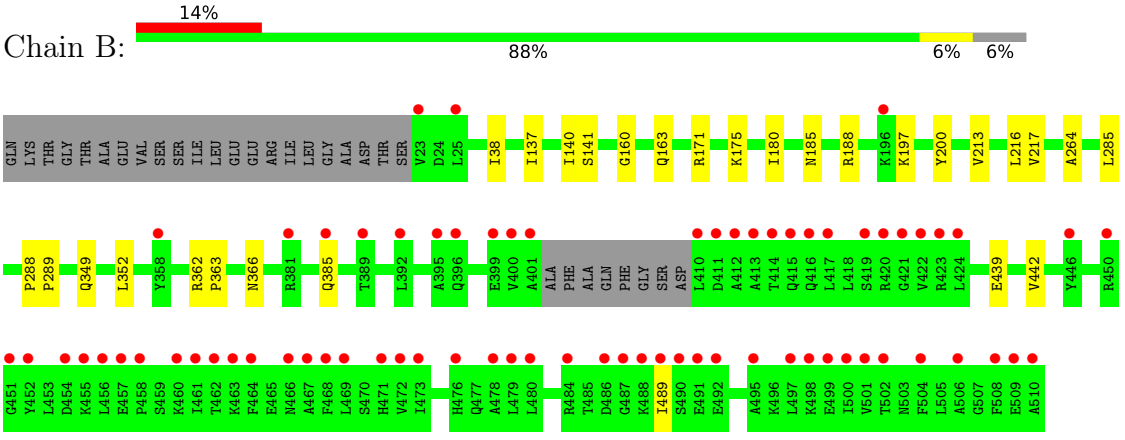
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



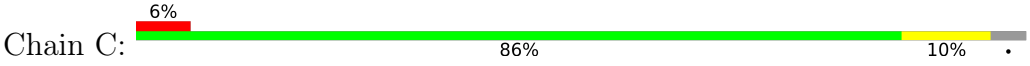
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

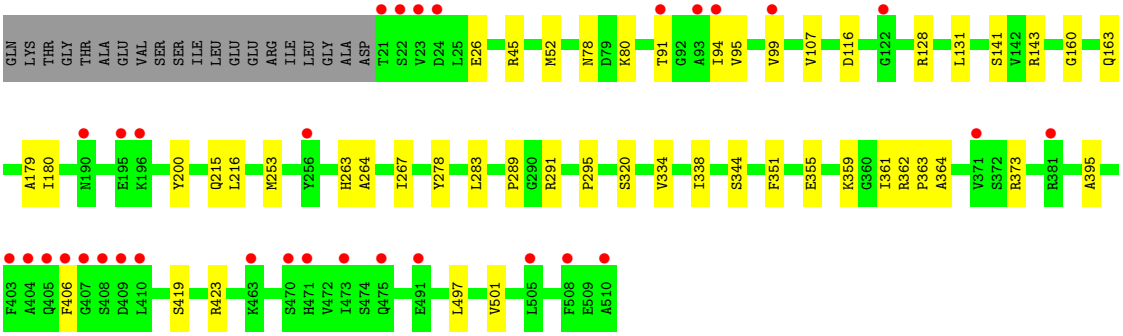
Chain B:



• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

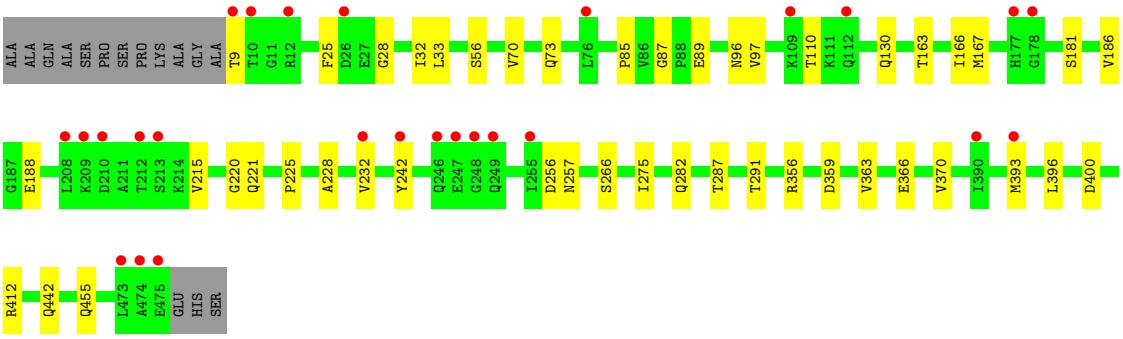
Chain C:





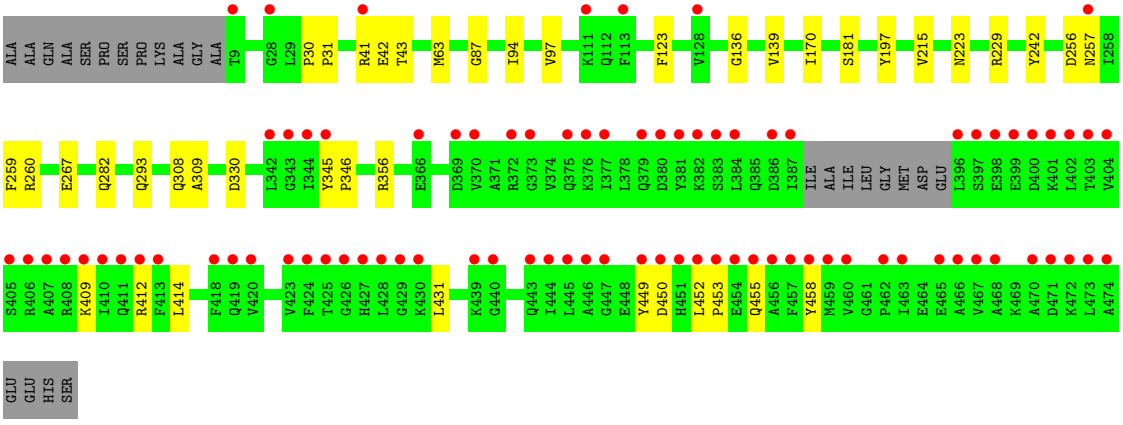
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:



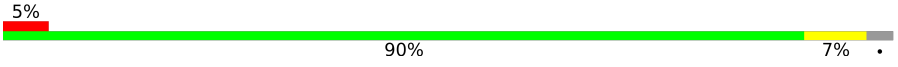
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

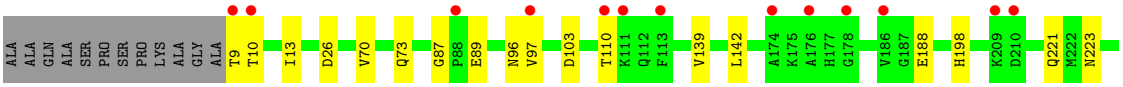
Chain E:

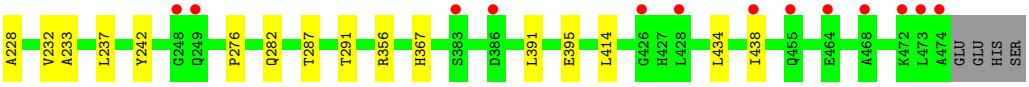


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:

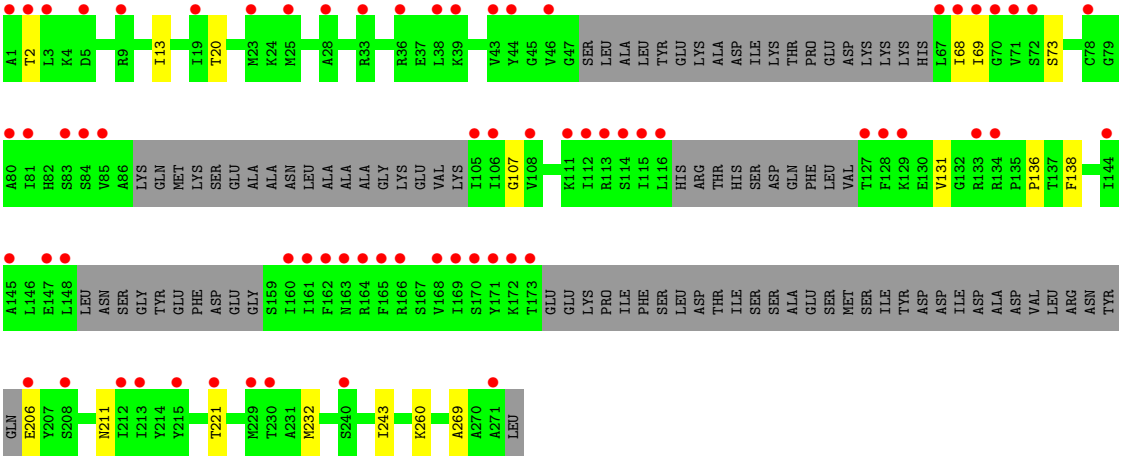






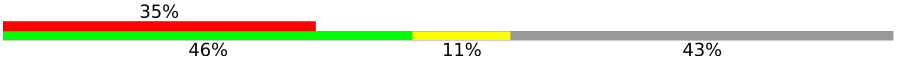
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

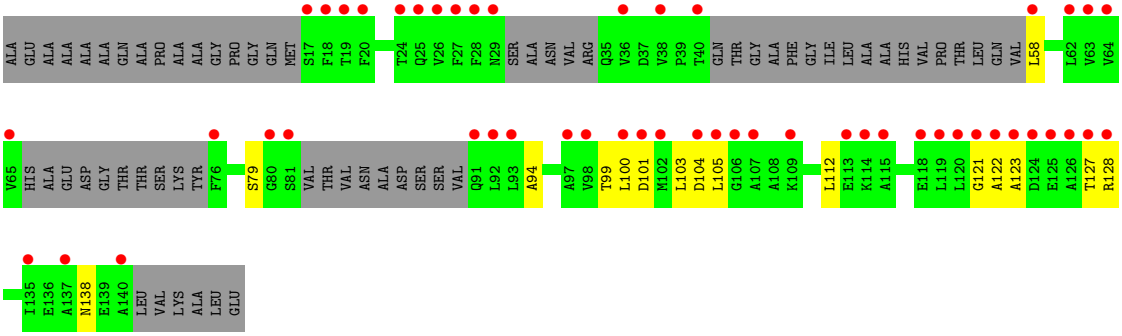
Chain G:



• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

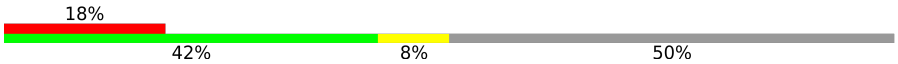
Chain H:

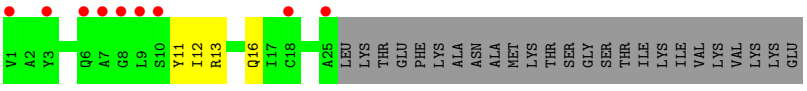




• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	261.16Å 105.22Å 122.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 43.53 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-1.95) 98.4 (43.53-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.226 0.208 , 0.234	Depositor DCC
R_{free} test set	12057 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26509	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: MG, AZI, PO4, ADP, ANP

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	0.39	2/3798 (0.1%)	0.55	0/5123
1	B	0.38	0/3718	0.52	0/5016
1	C	0.35	0/3775	0.51	0/5095
2	D	0.36	0/3611	0.55	0/4901
2	E	0.35	0/3547	0.52	0/4811
2	F	0.39	0/3607	0.54	0/4895
3	G	0.38	0/1406	0.47	0/1880
4	H	0.39	0/623	0.62	0/840
5	I	0.41	0/207	0.59	0/279
All	All	0.37	2/24292 (0.0%)	0.53	0/32840

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422[A]	VAL	CA-CB	5.47	1.66	1.54
1	A	422[B]	VAL	CA-CB	5.47	1.66	1.54

There are no bond angle outliers.

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	3738	0	3850	43	0
1	B	3667	0	3776	22	0
1	C	3735	0	3835	32	0
2	D	3550	0	3608	43	0
2	E	3486	0	3542	44	0
2	F	3541	0	3609	31	0
3	G	1397	0	1481	16	0
4	H	620	0	614	27	0
5	I	203	0	205	3	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	F	31	0	13	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	D	27	0	12	1	0
9	D	3	0	0	1	0
10	E	5	0	0	0	0
11	A	380	0	0	3	0
11	B	409	0	0	4	0
11	C	378	0	0	6	0
11	D	383	0	0	2	0
11	E	246	0	0	3	0
11	F	484	0	0	6	0
11	G	113	0	0	3	0
11	H	8	0	0	0	0
11	I	7	0	0	0	0
All	All	26509	0	24584	253	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 5.

All (253) 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)
4:H:122:ALA:HA	4:H:123:ALA:CB	1.74	1.18
3:G:68:ILE:HB	3:G:69:ILE:HA	1.30	1.13
2:D:89:GLU:HG3	2:D:110:THR:HB	1.29	1.09
2:E:256:ASP:HA	2:E:257[B]:ASN:HB3	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:104:ASP:HA	4:H:105:LEU:HB2	1.31	1.09
2:D:228:ALA:O	2:D:232[A]:VAL:HG13	1.52	1.09
4:H:121:GLY:HA3	4:H:122:ALA:HB3	1.40	1.03
4:H:122:ALA:HA	4:H:123:ALA:HB2	1.38	1.01
4:H:99:THR:HA	4:H:100:LEU:HB2	1.46	0.95
2:D:97:VAL:HA	2:D:232[B]:VAL:HG23	1.49	0.94
2:F:282:GLN:H	2:F:282:GLN:HE21	1.06	0.93
2:E:282:GLN:H	2:E:282:GLN:HE21	1.14	0.91
4:H:104:ASP:CA	4:H:105:LEU:HB2	2.01	0.91
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.53	0.90
3:G:20:THR:HG22	3:G:232:MET:HE3	1.53	0.90
2:D:282:GLN:H	2:D:282:GLN:HE21	0.94	0.89
1:A:74[B]:VAL:CG1	1:A:241:PRO:HG3	2.02	0.89
2:E:63:MET:SD	11:E:2044:HOH:O	2.30	0.88
4:H:122:ALA:HA	4:H:123:ALA:HB3	1.56	0.83
4:H:104:ASP:HA	4:H:105:LEU:CB	2.07	0.83
1:A:79:ASP:HB3	11:A:2059:HOH:O	1.80	0.82
4:H:122:ALA:CA	4:H:123:ALA:CB	2.58	0.81
4:H:122:ALA:CA	4:H:123:ALA:HB2	2.10	0.81
1:B:197:LYS:HG3	11:B:2225:HOH:O	1.81	0.80
2:F:97[B]:VAL:HG23	11:F:2278:HOH:O	1.79	0.80
1:A:74[B]:VAL:HG12	1:A:241:PRO:HG3	1.60	0.79
1:A:151:LYS:H	1:A:430:GLN:HE22	1.30	0.79
2:E:257[B]:ASN:HB2	2:E:309:ALA:O	1.83	0.78
1:C:291:ARG:HD2	11:C:2226:HOH:O	1.85	0.77
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.32	0.77
1:A:195:GLU:HA	1:A:198[B]:LYS:HD3	1.66	0.76
2:F:97[A]:VAL:HG12	2:F:232:VAL:HB	1.66	0.76
4:H:99:THR:CA	4:H:100:LEU:HB2	2.16	0.75
2:E:256:ASP:OD1	2:E:257[B]:ASN:ND2	2.19	0.75
2:D:282:GLN:H	2:D:282:GLN:NE2	1.78	0.75
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.71	0.73
2:D:85:PRO:HB3	2:D:110:THR:HG21	1.69	0.73
2:D:97:VAL:HA	2:D:232[B]:VAL:CG2	2.19	0.72
3:G:2:THR:HB	11:G:2006:HOH:O	1.89	0.72
2:E:256:ASP:HA	2:E:257[B]:ASN:CB	2.07	0.72
2:D:282:GLN:HE21	2:D:282:GLN:N	1.79	0.71
2:F:223:ASN:HD22	2:F:223:ASN:H	1.36	0.70
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.74	0.70
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.72	0.70
1:A:418:LEU:O	1:A:422[B]:VAL:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41[B]:ARG:HG2	2:E:42:GLU:N	2.05	0.69
1:B:171:ARG:HD3	11:E:2224:HOH:O	1.94	0.68
2:D:97:VAL:CA	2:D:232[B]:VAL:HG23	2.23	0.67
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.77	0.66
2:F:97[A]:VAL:CG1	2:F:232:VAL:HB	2.25	0.66
2:D:89:GLU:CG	2:D:110:THR:HB	2.19	0.66
1:A:37:GLY:HA2	11:A:2059:HOH:O	1.96	0.65
2:D:89:GLU:HG3	2:D:110:THR:CB	2.17	0.65
4:H:121:GLY:HA3	4:H:122:ALA:CB	2.18	0.65
4:H:127:THR:N	4:H:128:ARG:HB2	2.12	0.64
1:A:102:GLU:HG3	1:A:123:SER:HA	1.80	0.64
1:A:419:SER:O	1:A:423:ARG:HD3	1.99	0.63
3:G:68:ILE:CB	3:G:69:ILE:HA	2.12	0.63
2:D:96:ASN:C	2:D:96:ASN:HD22	2.02	0.63
4:H:127:THR:H	4:H:128:ARG:HB2	1.64	0.62
4:H:127:THR:H	4:H:128:ARG:CB	2.13	0.62
1:C:160:GLY:H	1:C:163:GLN:NE2	1.98	0.61
2:F:97[A]:VAL:HG12	2:F:232:VAL:CB	2.31	0.60
1:C:128:ARG:HD2	1:C:131:LEU:HG	1.83	0.60
4:H:103:LEU:HB3	4:H:105:LEU:HD13	1.83	0.60
2:F:96:ASN:C	2:F:96:ASN:HD22	2.05	0.60
1:A:74[B]:VAL:HG12	1:A:241:PRO:CG	2.30	0.59
2:F:282:GLN:HE21	2:F:282:GLN:N	1.88	0.59
4:H:99:THR:HB	4:H:101:ASP:H	1.68	0.59
2:E:257[A]:ASN:OD1	2:E:260:ARG:HG3	2.03	0.58
3:G:260:LYS:HD2	11:G:2048:HOH:O	2.02	0.58
4:H:99:THR:HA	4:H:100:LEU:CB	2.26	0.58
2:D:85:PRO:HB3	2:D:110:THR:CG2	2.32	0.58
1:A:190:ASN:HA	1:A:198[A]:LYS:HG2	1.86	0.57
1:B:38:ILE:HD12	1:B:285:LEU:HD21	1.86	0.57
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.86	0.57
2:D:188:GLU:O	2:D:221:GLN:HB3	2.02	0.57
1:B:137:ILE:HG13	2:F:103:ASP:HA	1.86	0.57
1:B:366:ASN:ND2	11:B:2359:HOH:O	2.32	0.57
1:C:78:ASN:ND2	11:C:2058:HOH:O	2.35	0.57
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.86	0.57
4:H:127:THR:CA	4:H:128:ARG:HB2	2.34	0.57
2:E:63:MET:HE3	2:E:97:VAL:HG21	1.87	0.57
2:D:186:VAL:HG13	2:D:232[A]:VAL:CG2	2.35	0.56
1:B:160:GLY:H	1:B:163:GLN:NE2	2.03	0.56
2:E:412:ARG:HG2	2:E:458:TYR:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.41	0.56
2:F:282:GLN:H	2:F:282:GLN:NE2	1.90	0.56
1:A:440:GLU:O	1:A:444:VAL:HG12	2.05	0.56
4:H:58:LEU:N	5:I:11:TYR:HH	2.04	0.55
2:D:366:GLU:O	2:D:370:VAL:HG23	2.06	0.55
1:B:175:LYS:HG2	1:B:352:LEU:HD12	1.89	0.55
1:C:344:SER:HA	9:D:1092:AZI:N3	2.22	0.55
1:A:410:LEU:HD12	1:A:415:GLN:HG3	1.89	0.55
1:B:160:GLY:H	1:B:163:GLN:HE21	1.55	0.55
1:B:385:GLN:HE22	1:B:489:ILE:HB	1.71	0.54
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.89	0.54
2:F:223:ASN:HD22	2:F:223:ASN:N	2.02	0.54
1:A:44:LEU:O	1:A:47:VAL:HG22	2.07	0.54
4:H:127:THR:HB	4:H:128:ARG:HB2	1.88	0.54
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.89	0.53
1:B:439:GLU:O	1:B:442:VAL:HG12	2.08	0.53
1:A:427:LEU:HD22	1:A:444:VAL:HG23	1.91	0.53
2:F:188:GLU:O	2:F:221:GLN:HB3	2.09	0.52
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.90	0.52
2:E:223:ASN:HD22	2:E:223:ASN:H	1.56	0.52
1:C:215:GLN:HB3	2:F:356:ARG:HH22	1.75	0.52
2:D:220:GLY:HA3	2:D:232[A]:VAL:HG11	1.92	0.52
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.91	0.52
1:C:497:LEU:O	1:C:501:VAL:HG22	2.09	0.52
3:G:73:SER:HA	3:G:131:VAL:HG23	1.92	0.52
1:C:94:ILE:HG22	1:C:95:VAL:H	1.75	0.52
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.37	0.51
2:E:41[B]:ARG:HD3	2:E:43:THR:O	2.08	0.51
2:E:223:ASN:HD22	2:E:223:ASN:N	2.09	0.51
1:C:355:GLU:HG2	1:C:359:LYS:HE2	1.93	0.51
2:E:452:LEU:HB3	2:E:453:PRO:HD2	1.94	0.50
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.46	0.50
2:D:221:GLN:HE21	2:D:221:GLN:HA	1.75	0.50
2:E:229:ARG:HH22	2:E:267:GLU:CD	2.13	0.50
4:H:99:THR:HB	4:H:101:ASP:N	2.26	0.50
2:E:41[B]:ARG:CG	2:E:42:GLU:N	2.70	0.50
1:A:148:THR:HA	1:A:182:THR:HG23	1.94	0.50
1:C:338:ILE:HD12	11:C:2266:HOH:O	2.11	0.50
1:C:160:GLY:H	1:C:163:GLN:HE21	1.60	0.50
2:E:345:TYR:HA	2:E:346:PRO:C	2.30	0.50
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:257[B]:ASN:HB3	2:E:309:ALA:HB3	1.94	0.50
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.74	0.49
1:A:183:ILE:HD11	1:A:267:ILE:HD13	1.93	0.49
5:I:13:ARG:HH11	5:I:16:GLN:NE2	2.11	0.49
2:F:287:THR:O	2:F:291:THR:HG23	2.13	0.49
1:A:74[A]:VAL:HG22	1:A:241:PRO:HG3	1.93	0.49
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.48	0.49
4:H:127:THR:CB	4:H:128:ARG:HB2	2.43	0.49
3:G:13:ILE:HG22	3:G:243:ILE:HG13	1.95	0.48
1:C:355:GLU:HB2	11:C:2274:HOH:O	2.14	0.48
1:A:74[A]:VAL:HG21	1:A:281:MET:HG2	1.96	0.48
2:E:257[B]:ASN:ND2	11:E:2167:HOH:O	2.45	0.48
1:B:217:VAL:HG11	2:E:123:PHE:HZ	1.78	0.48
2:E:449:TYR:HD2	2:E:452:LEU:HD12	1.78	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.79	0.48
3:G:260:LYS:HG3	11:G:2100:HOH:O	2.13	0.48
1:A:446:TYR:CE1	1:A:450:ARG:HD2	2.48	0.48
2:F:97[B]:VAL:HG22	2:F:232:VAL:HB	1.95	0.48
2:E:257[A]:ASN:OD1	2:E:259:PHE:HB3	2.13	0.47
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.50	0.47
1:C:141:SER:HB2	1:C:143:ARG:HH21	1.79	0.47
1:B:288:PRO:HB3	2:F:276:PRO:HG3	1.96	0.47
2:F:139:VAL:HG22	11:F:2444:HOH:O	2.14	0.47
1:B:140:ILE:HG13	11:F:2264:HOH:O	2.15	0.47
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.50	0.47
2:E:257[A]:ASN:OD1	2:E:260:ARG:N	2.47	0.47
1:C:78:ASN:HD22	1:C:80:LYS:H	1.63	0.46
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.50	0.46
2:F:26:ASP:HB2	11:F:2003:HOH:O	2.15	0.46
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.45	0.46
1:A:419:SER:O	1:A:422[B]:VAL:HG13	2.16	0.46
1:C:395:ALA:HB2	11:C:2302:HOH:O	2.15	0.46
1:C:362:ARG:HA	1:C:363:PRO:C	2.36	0.46
2:D:130:GLN:HE22	2:D:356:ARG:HD2	1.81	0.46
2:D:287:THR:O	2:D:291:THR:HG23	2.16	0.46
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.96	0.46
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.80	0.46
4:H:121:GLY:CA	4:H:122:ALA:HB3	2.29	0.46
1:A:198[B]:LYS:HB2	11:A:2216:HOH:O	2.15	0.46
1:A:446:TYR:HE1	1:A:450:ARG:HD2	1.80	0.46
1:B:213:VAL:O	1:B:217:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:69:ILE:HG23	3:G:107:GLY:H	1.81	0.46
4:H:122:ALA:N	4:H:123:ALA:HB2	2.31	0.45
1:A:385:GLN:HG3	1:A:386:VAL:HG13	1.97	0.45
2:E:330:ASP:HA	2:E:356:ARG:HD2	1.97	0.45
2:F:391:LEU:HB3	2:F:395:GLU:HG3	1.99	0.45
2:D:370:VAL:HG21	2:D:442:GLN:HG3	1.99	0.45
1:A:500:ILE:O	1:A:504:PHE:HB2	2.17	0.45
3:G:206:GLU:O	5:I:12:ILE:HD11	2.16	0.45
1:A:457:GLU:HA	1:A:458:PRO:HD2	1.75	0.45
1:A:62:MET:CE	1:A:64:LEU:HD21	2.47	0.45
1:A:99:VAL:HG13	1:A:256:TYR:HB2	1.99	0.45
2:D:225:PRO:HB2	11:D:2042:HOH:O	2.16	0.45
1:C:107:VAL:HB	1:C:116:ASP:HB3	1.99	0.45
2:D:167:MET:HE1	11:D:2170:HOH:O	2.17	0.45
1:A:151:LYS:H	1:A:430:GLN:NE2	2.07	0.45
2:E:256:ASP:CA	2:E:257[B]:ASN:CB	2.89	0.45
4:H:112:LEU:HG	4:H:138:ASN:HB3	1.99	0.45
2:D:97:VAL:HG13	2:D:232[B]:VAL:HG23	1.99	0.44
3:G:68:ILE:HB	3:G:69:ILE:CA	2.23	0.44
2:D:25:PHE:O	2:D:56:SER:HB3	2.18	0.44
1:A:400:VAL:HG13	1:A:403:PHE:CE1	2.52	0.44
1:A:441:GLN:O	1:A:444:VAL:HG13	2.17	0.44
1:B:362:ARG:HA	1:B:363:PRO:C	2.37	0.44
2:E:412:ARG:HH11	2:E:455:GLN:HE22	1.64	0.44
1:B:141:SER:HB3	11:F:2259:HOH:O	2.17	0.44
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.33	0.44
2:F:139:VAL:HG13	2:F:414:LEU:HB3	2.00	0.44
1:A:346:THR:O	1:A:373:ARG:NH2	2.51	0.44
1:A:99:VAL:HG22	1:A:253:MET:HA	1.99	0.44
2:E:181:SER:HB2	2:E:215:VAL:HG13	1.99	0.44
2:D:96:ASN:C	2:D:96:ASN:ND2	2.71	0.43
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.43
2:E:63:MET:HE3	2:E:97:VAL:CG2	2.48	0.43
1:C:362:ARG:NH1	11:C:2278:HOH:O	2.50	0.43
2:D:9:THR:HG21	2:D:28:GLY:HA3	2.00	0.43
1:C:179:ALA:HB1	1:C:267:ILE:HD13	2.00	0.43
2:F:142:LEU:HD12	2:F:438:ILE:HD13	2.01	0.43
1:B:289:PRO:HD3	11:B:2292:HOH:O	2.18	0.43
2:F:70:VAL:H	2:F:73:GLN:HE21	1.68	0.42
3:G:68:ILE:HB	3:G:69:ILE:HD13	2.00	0.42
2:D:97:VAL:HG22	2:D:232[A]:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:SER:O	1:C:423:ARG:HD2	2.20	0.42
2:D:359:ASP:O	2:D:363:VAL:HG22	2.20	0.42
3:G:138:PHE:HE1	3:G:211:ASN:HD22	1.68	0.42
1:C:99:VAL:HG22	1:C:253:MET:HA	2.02	0.42
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.02	0.42
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.92	0.42
1:B:349:GLN:NE2	11:B:2348:HOH:O	2.35	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB3	2.02	0.42
2:F:198:HIS:HD2	11:F:2134:HOH:O	2.01	0.42
2:D:412:ARG:HE	2:D:455:GLN:NE2	2.18	0.41
4:H:79:SER:O	4:H:94:ALA:HA	2.20	0.41
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.55	0.41
1:A:24:ASP:O	1:A:28:THR:OG1	2.37	0.41
2:E:257[B]:ASN:CB	2:E:309:ALA:HB3	2.50	0.41
1:B:200:TYR:O	1:B:264:ALA:HA	2.21	0.41
1:C:361:ILE:O	1:C:364:ALA:HA	2.20	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.81	0.41
1:A:28:THR:HG22	1:A:89:LYS:HG2	2.02	0.41
1:C:406:PHE:CE1	2:D:393:MET:HB2	2.55	0.41
2:D:188:GLU:H	2:D:221:GLN:NE2	2.19	0.41
2:D:163:THR:O	2:D:166:ILE:HG22	2.20	0.41
2:F:97[B]:VAL:HG21	2:F:228:ALA:HB1	2.03	0.41
1:C:52:MET:O	1:C:91:THR:HB	2.21	0.41
2:D:73:GLN:HE21	2:D:73:GLN:HB2	1.71	0.41
2:E:30:PRO:HA	2:E:31:PRO:HD2	1.96	0.41
2:E:282:GLN:H	2:E:282:GLN:NE2	1.96	0.41
2:F:9:THR:HB	2:F:10:THR:H	1.62	0.41
2:E:139:VAL:HG12	2:E:414:LEU:HD22	2.01	0.41
2:F:13:ILE:HD12	2:F:73:GLN:HB3	2.02	0.41
2:F:367:HIS:CE1	2:F:434:LEU:HD11	2.56	0.41
1:C:263:HIS:HD2	1:C:320:SER:OG	2.04	0.40
2:D:32:ILE:O	2:D:33:LEU:HB2	2.21	0.40
2:E:257[A]:ASN:ND2	2:E:259:PHE:H	2.19	0.40
2:F:233:ALA:O	2:F:237:LEU:HD13	2.21	0.40
1:A:74[B]:VAL:HG11	1:A:241:PRO:HG3	1.97	0.40
2:D:275[B]:ILE:HG22	3:G:269:ALA:HA	2.04	0.40
1:C:200:TYR:O	1:C:264:ALA:HA	2.20	0.40
2:D:70:VAL:H	2:D:73:GLN:HE21	1.70	0.40
3:G:136:PRO:CD	3:G:221:THR:HG21	2.49	0.40
1:C:373:ARG:HA	8:D:600:ADP:O3'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	ANP	F	600	7	29,33,33	1.81	8 (27%)	31,52,52	1.96	5 (16%)
8	ADP	D	600	7	24,29,29	1.01	2 (8%)	29,45,45	1.16	2 (6%)
9	AZI	D	1092	-	0,2,2	-	-	0,1,1	-	-
6	ANP	A	600	7	29,33,33	1.80	9 (31%)	31,52,52	1.94	5 (16%)
6	ANP	C	600	7	29,33,33	1.74	6 (20%)	31,52,52	2.01	7 (22%)
10	PO4	E	602	-	4,4,4	0.90	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ANP	B	600	7	29,33,33	1.78	6 (20%)	31,52,52	1.78	4 (12%)

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
6	ANP	F	600	7	-	3/14/38/38	0/3/3/3
8	ADP	D	600	7	-	2/12/32/32	0/3/3/3
6	ANP	A	600	7	-	3/14/38/38	0/3/3/3
6	ANP	C	600	7	-	3/14/38/38	0/3/3/3
6	ANP	B	600	7	-	2/14/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	ANP	PB-N3B	4.27	1.74	1.63
6	B	600	ANP	PG-N3B	4.20	1.74	1.63
6	F	600	ANP	PB-N3B	4.18	1.74	1.63
6	C	600	ANP	PG-N3B	4.17	1.74	1.63
6	A	600	ANP	PB-N3B	4.17	1.74	1.63
6	A	600	ANP	PG-N3B	4.08	1.74	1.63
6	F	600	ANP	PG-N3B	4.05	1.73	1.63
6	C	600	ANP	PB-N3B	3.99	1.73	1.63
6	F	600	ANP	PG-O1G	3.68	1.52	1.46
6	A	600	ANP	PG-O1G	3.44	1.51	1.46
6	F	600	ANP	PB-O1B	3.22	1.51	1.46
6	B	600	ANP	PB-O1B	3.18	1.51	1.46
6	B	600	ANP	PG-O1G	3.05	1.51	1.46
6	C	600	ANP	PG-O1G	3.05	1.51	1.46
6	C	600	ANP	PB-O1B	3.01	1.50	1.46
6	A	600	ANP	PB-O1B	2.75	1.50	1.46
6	B	600	ANP	C5-C4	2.61	1.47	1.40
6	A	600	ANP	C5-C4	2.60	1.47	1.40
6	F	600	ANP	C5-C4	2.54	1.47	1.40
8	D	600	ADP	C5-C4	2.54	1.47	1.40
6	C	600	ANP	C5-C4	2.49	1.47	1.40
6	A	600	ANP	PB-O2B	-2.29	1.50	1.56
6	A	600	ANP	PG-O2G	-2.26	1.50	1.56
6	C	600	ANP	PB-O2B	-2.19	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	ANP	PG-O2G	-2.13	1.51	1.56
8	D	600	ADP	C2-N3	2.06	1.35	1.32
6	B	600	ANP	PB-O2B	-2.04	1.51	1.56
6	A	600	ANP	PG-O3G	-2.03	1.51	1.56
6	A	600	ANP	C2-N3	2.03	1.35	1.32
6	F	600	ANP	PG-O3G	-2.02	1.51	1.56
6	F	600	ANP	PB-O2B	-2.01	1.51	1.56

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	600	ANP	O1G-PG-N3B	-7.75	100.36	111.77
6	C	600	ANP	O1G-PG-N3B	-7.67	100.47	111.77
6	A	600	ANP	O1G-PG-N3B	-7.49	100.75	111.77
6	B	600	ANP	O1G-PG-N3B	-6.10	102.79	111.77
6	B	600	ANP	O2B-PB-O1B	3.73	117.74	109.92
6	A	600	ANP	O2B-PB-O1B	3.63	117.53	109.92
6	C	600	ANP	O2B-PB-O1B	3.60	117.46	109.92
6	C	600	ANP	N3-C2-N1	-3.55	123.12	128.68
6	F	600	ANP	N3-C2-N1	-3.37	123.41	128.68
6	A	600	ANP	N3-C2-N1	-3.35	123.44	128.68
6	B	600	ANP	N3-C2-N1	-3.33	123.47	128.68
8	D	600	ADP	N3-C2-N1	-3.27	123.57	128.68
6	F	600	ANP	O2B-PB-O1B	3.17	116.56	109.92
6	C	600	ANP	C4-C5-N7	-2.84	106.44	109.40
6	B	600	ANP	C4-C5-N7	-2.79	106.49	109.40
6	A	600	ANP	C4-C5-N7	-2.74	106.55	109.40
6	C	600	ANP	O2G-PG-O3G	2.72	114.87	107.64
6	F	600	ANP	O2G-PG-O3G	2.59	114.53	107.64
8	D	600	ADP	C4-C5-N7	-2.45	106.84	109.40
6	F	600	ANP	C4-C5-N7	-2.43	106.87	109.40
6	C	600	ANP	PB-O3A-PA	-2.17	124.96	132.62
6	A	600	ANP	O2G-PG-O3G	2.16	113.39	107.64
6	C	600	ANP	C2-N1-C6	2.01	122.20	118.75

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
6	B	600	ANP	PG-N3B-PB-O3A
6	C	600	ANP	PB-N3B-PG-O1G
6	C	600	ANP	PG-N3B-PB-O1B
6	F	600	ANP	PG-N3B-PB-O1B
6	F	600	ANP	PA-O3A-PB-O1B
6	F	600	ANP	PA-O3A-PB-O2B
8	D	600	ADP	PA-O3A-PB-O2B
8	D	600	ADP	PA-O3A-PB-O3B
6	A	600	ANP	PG-N3B-PB-O3A
6	C	600	ANP	PG-N3B-PB-O3A

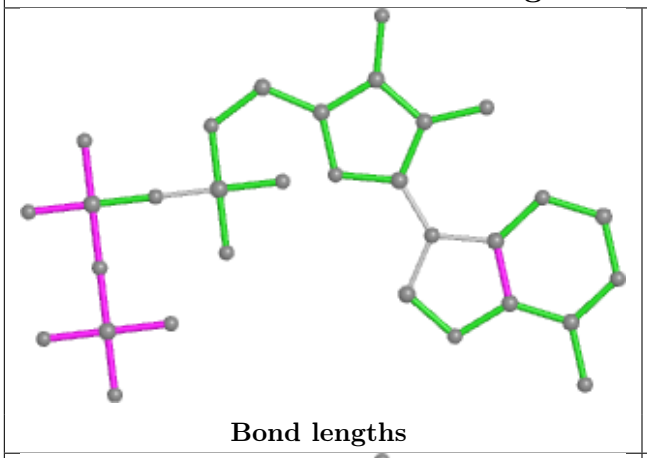
There are no ring outliers.

2 monomers are involved in 2 short contacts:

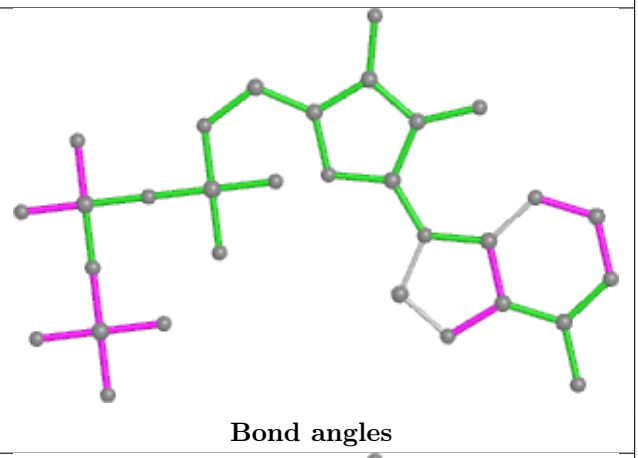
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	600	ADP	1	0
9	D	1092	AZI	1	0

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 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.

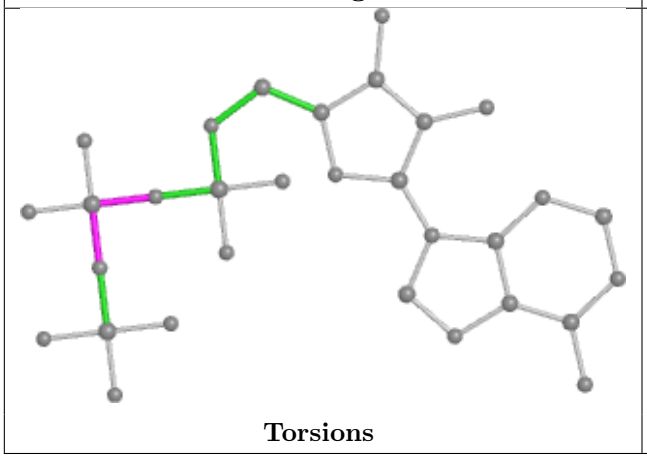
Ligand ANP F 600



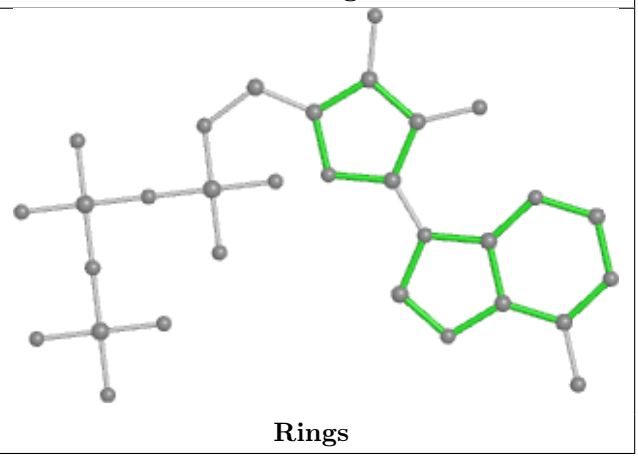
Bond lengths



Bond angles

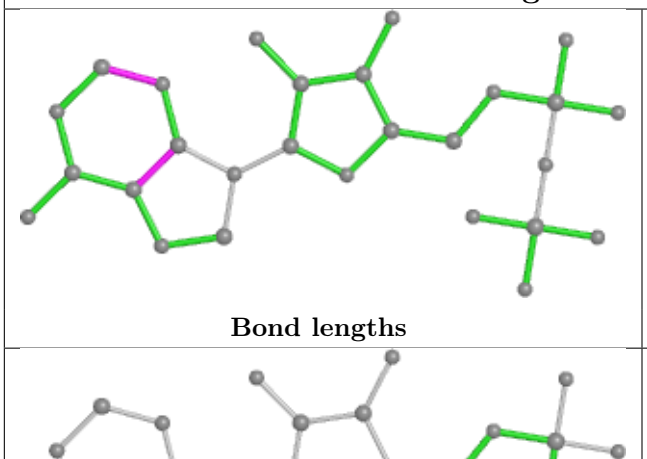


Torsions

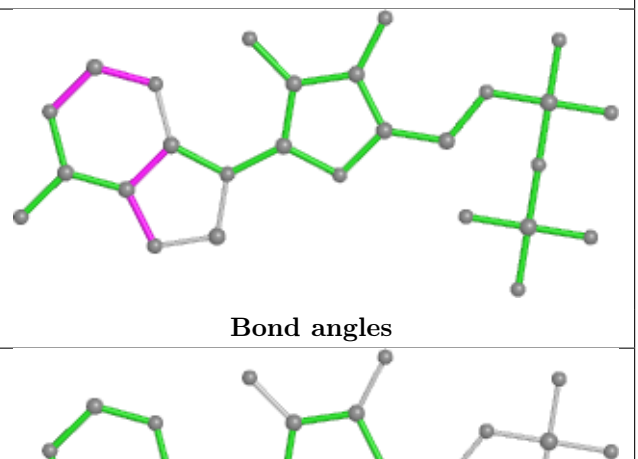


Rings

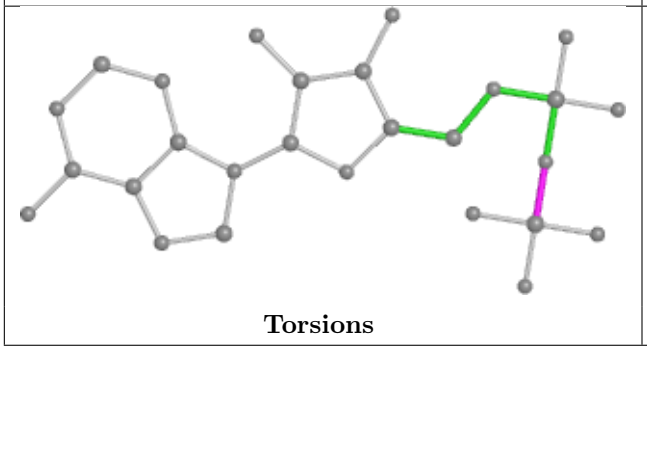
Ligand ADP D 600



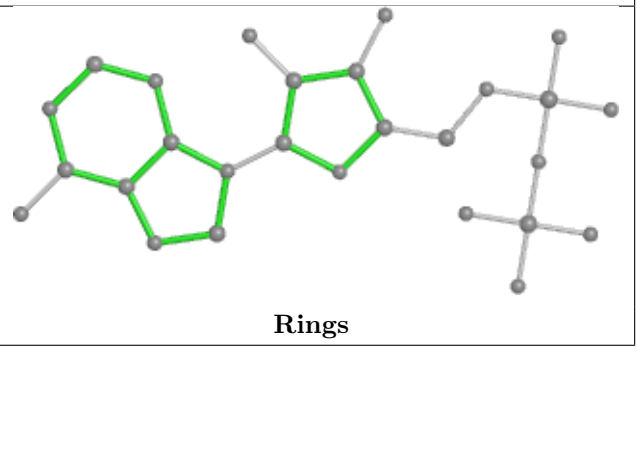
Bond lengths



Bond angles

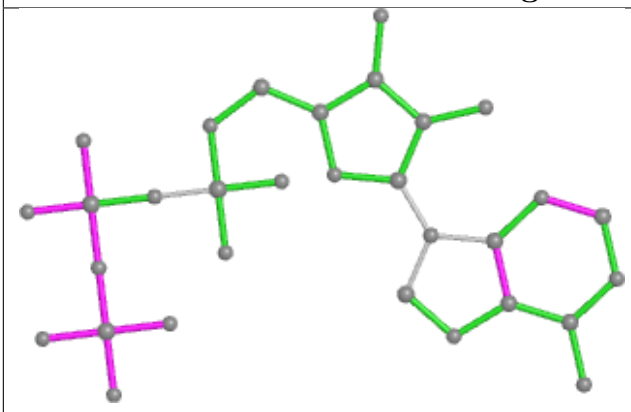


Torsions

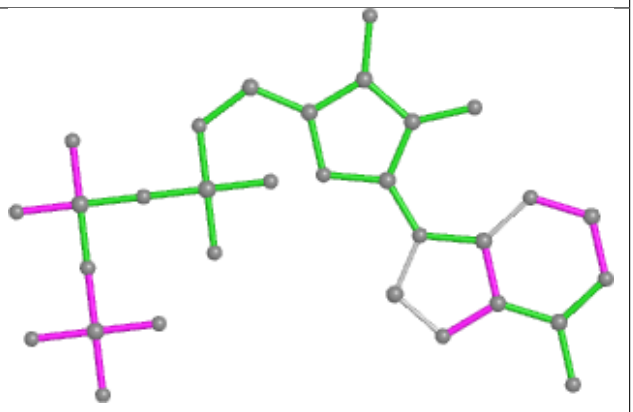


Rings

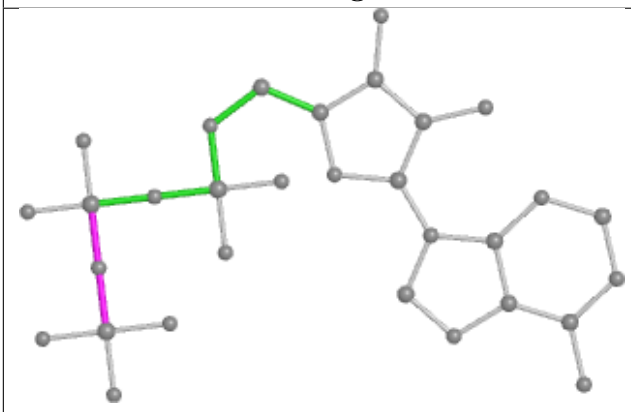
Ligand ANP A 600



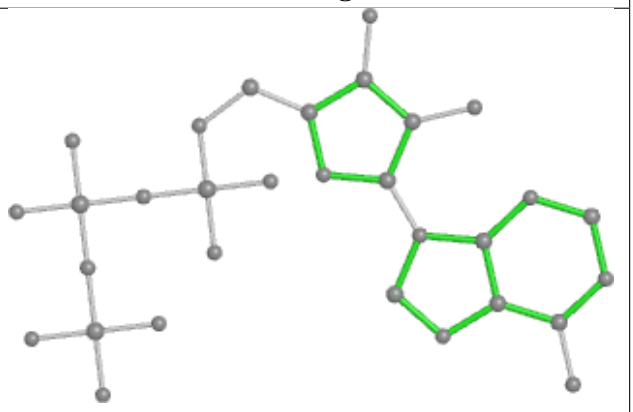
Bond lengths



Bond angles

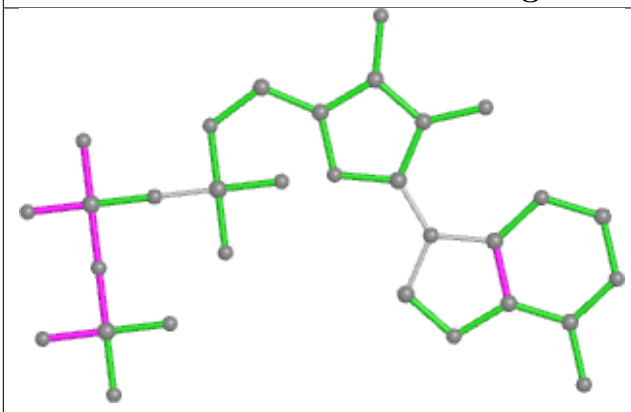


Torsions

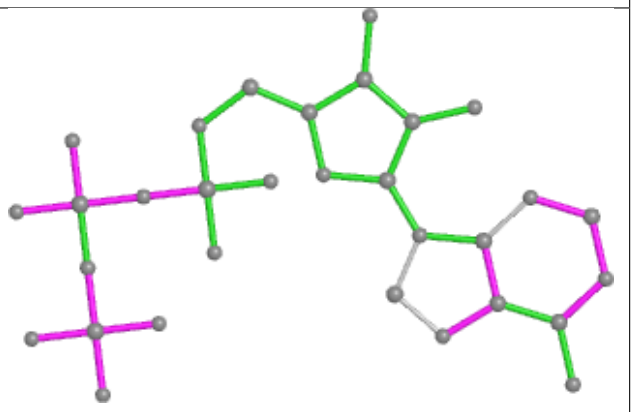


Rings

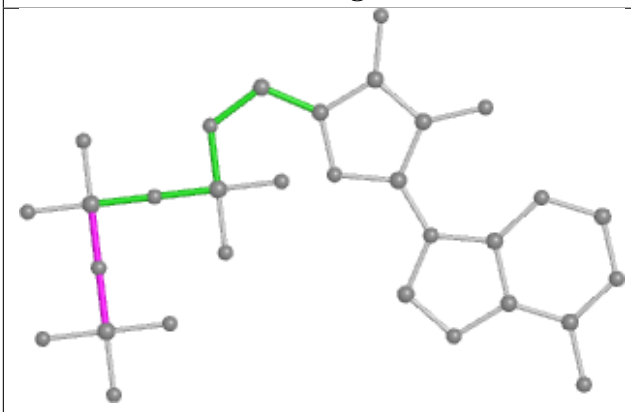
Ligand ANP C 600



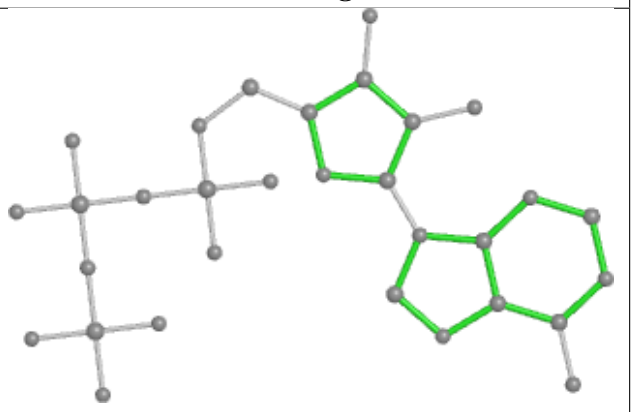
Bond lengths



Bond angles

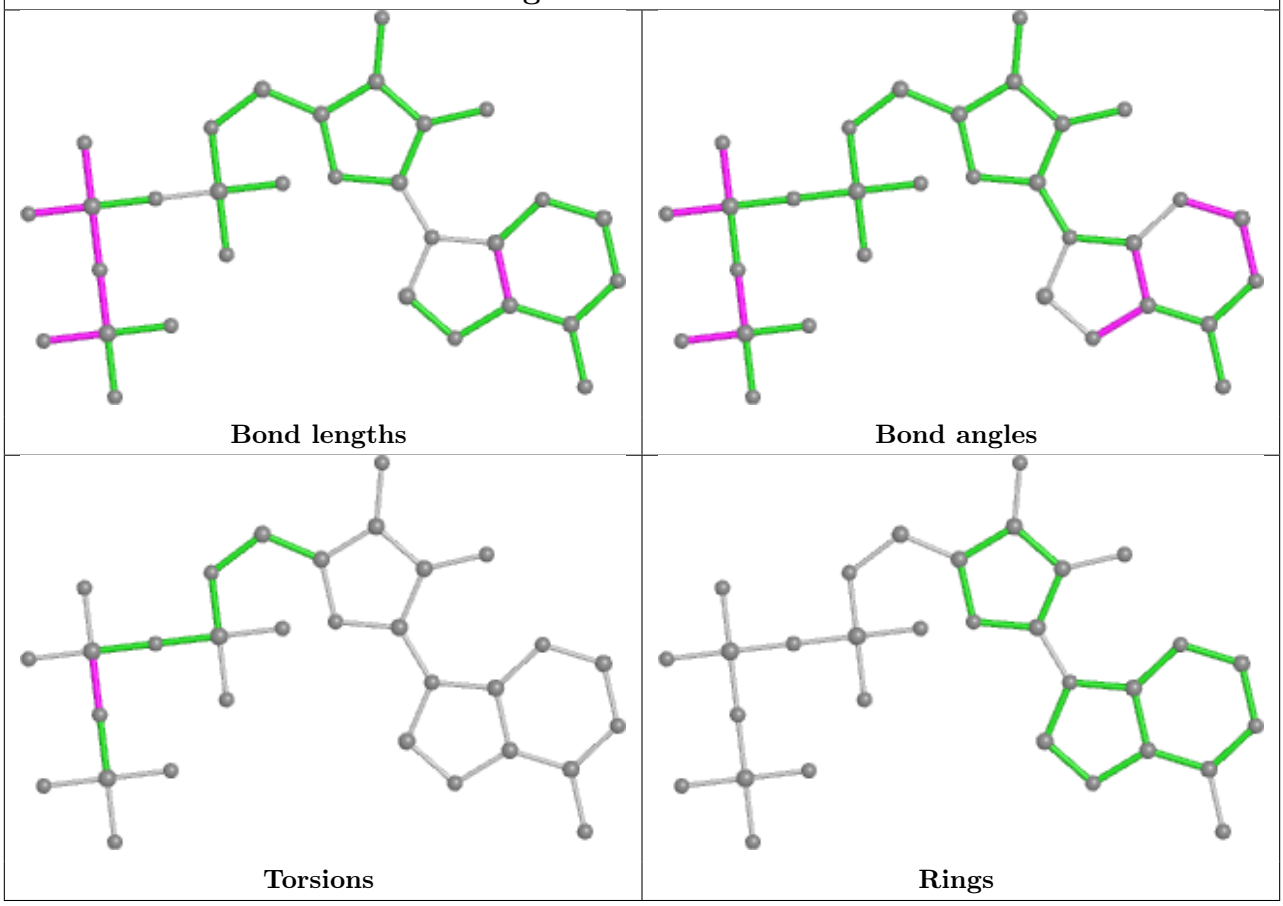


Torsions



Rings

Ligand ANP B 600



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	487/510 (95%)	0.84	59 (12%) 4 7	12, 21, 45, 63	0
1	B	480/510 (94%)	0.83	72 (15%) 2 3	10, 20, 57, 82	0
1	C	490/510 (96%)	0.63	32 (6%) 18 27	12, 21, 38, 75	0
2	D	467/482 (96%)	0.55	26 (5%) 24 33	12, 19, 41, 67	0
2	E	458/482 (95%)	1.06	86 (18%) 1 1	12, 24, 64, 77	0
2	F	466/482 (96%)	0.45	26 (5%) 24 33	13, 19, 41, 62	0
3	G	182/272 (66%)	1.90	69 (37%) 0 0	10, 29, 48, 58	0
4	H	83/146 (56%)	2.75	51 (61%) 0 0	5, 26, 44, 49	0
5	I	25/50 (50%)	2.29	9 (36%) 0 0	8, 17, 43, 46	0
All	All	3138/3444 (91%)	0.86	430 (13%) 3 4	5, 21, 50, 82	0

All (430) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	THR	12.0
3	G	106	ILE	11.7
1	B	510	ALA	10.7
4	H	105	LEU	10.0
2	E	470	ALA	9.7
1	C	406	PHE	9.5
1	C	407	GLY	9.2
4	H	100	LEU	9.2
2	E	384	LEU	8.2
1	C	22	SER	8.1
1	B	401	ALA	8.1
1	B	413	ALA	8.1
2	E	387	ILE	8.1
2	F	473	LEU	8.0
3	G	160	ILE	7.8

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Mol	Chain	Res	Type	RSRZ
2	E	400	ASP	7.8
2	E	407	ALA	7.7
5	I	9	LEU	7.7
3	G	212	ILE	7.6
2	E	424	PHE	7.6
2	E	423	VAL	7.6
2	E	457	PHE	7.3
1	A	195	GLU	7.3
2	E	428	LEU	7.2
1	B	508	PHE	7.2
2	E	427	HIS	7.1
3	G	85	VAL	7.1
2	E	446	ALA	7.1
1	B	410	LEU	7.1
2	E	402	LEU	7.0
2	F	9	THR	6.7
2	E	377	ILE	6.7
2	D	9	THR	6.6
1	C	23	VAL	6.6
2	D	248	GLY	6.5
1	B	495	ALA	6.4
3	G	43	VAL	6.4
2	E	345	TYR	6.3
5	I	8	GLY	6.3
1	B	412	ALA	6.3
2	E	467	VAL	6.2
5	I	7	ALA	6.2
2	E	449	TYR	6.1
2	E	468	ALA	6.1
4	H	65	VAL	6.1
4	H	27	PHE	6.1
5	I	6	GLN	5.9
3	G	105	ILE	5.9
2	E	456	ALA	5.9
3	G	70	GLY	5.8
4	H	92	LEU	5.8
3	G	69	ILE	5.8
1	B	456	LEU	5.8
1	B	417	LEU	5.7
1	B	451	GLY	5.7
2	E	460	VAL	5.7
2	E	401	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
2	E	474	ALA	5.6
2	E	445	LEU	5.5
2	F	474	ALA	5.5
2	E	398	GLU	5.5
3	G	116	LEU	5.5
1	B	419	SER	5.4
2	E	453	PRO	5.4
3	G	112	ILE	5.4
2	E	452	LEU	5.4
4	H	62	LEU	5.4
2	E	473	LEU	5.3
1	C	94	ILE	5.3
1	B	416	GLN	5.3
4	H	28	PHE	5.3
1	B	455	LYS	5.3
3	G	148	LEU	5.3
2	E	451	HIS	5.3
2	F	178	GLY	5.2
3	G	71	VAL	5.2
2	E	458	TYR	5.2
2	E	383	SER	5.1
1	C	409	ASP	5.1
1	B	468	PHE	5.1
4	H	18	PHE	5.1
1	B	506	ALA	5.1
2	E	41[A]	ARG	5.0
1	B	464	PHE	5.0
4	H	101	ASP	5.0
1	A	446	TYR	5.0
1	A	483	ILE	5.0
1	A	510	ALA	4.8
1	B	504	PHE	4.8
4	H	107	ALA	4.8
1	B	411	ASP	4.8
1	A	404	ALA	4.7
1	B	414	THR	4.7
1	A	406	PHE	4.7
1	B	400	VAL	4.7
3	G	114	SER	4.7
2	E	379	GLN	4.7
2	F	10	THR	4.7
1	C	93	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
3	G	215	TYR	4.6
3	G	46	VAL	4.5
2	E	472	LYS	4.5
5	I	1	VAL	4.5
3	G	25	MET	4.5
1	A	489	ILE	4.5
2	F	472	LYS	4.4
3	G	128	PHE	4.4
2	E	454	GLU	4.4
4	H	123	ALA	4.4
2	E	471	ASP	4.4
3	G	169	ILE	4.3
4	H	120	LEU	4.3
1	B	479	LEU	4.2
2	E	462	PRO	4.2
1	A	501	VAL	4.2
1	B	392	LEU	4.2
3	G	115	ILE	4.2
4	H	125	GLU	4.2
2	D	473	LEU	4.2
4	H	20	PHE	4.2
1	B	23	VAL	4.2
2	E	425	THR	4.2
3	G	168	VAL	4.2
2	F	248	GLY	4.1
4	H	119	LEU	4.1
1	A	422[A]	VAL	4.1
1	B	499	GLU	4.1
1	B	469	LEU	4.1
2	E	257[A]	ASN	4.1
1	A	407	GLY	4.0
1	B	476	HIS	4.0
1	A	408	SER	4.0
2	D	232[A]	VAL	4.0
2	E	386	ASP	4.0
4	H	104	ASP	4.0
3	G	161	ILE	3.9
4	H	126	ALA	3.9
4	H	91	GLN	3.9
1	C	405	GLN	3.9
1	A	497	LEU	3.9
3	G	80	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
4	H	58	LEU	3.8
4	H	122	ALA	3.8
2	E	439	LYS	3.8
4	H	24	THR	3.8
4	H	26	VAL	3.8
1	A	402	ALA	3.7
3	G	3	LEU	3.7
3	G	172	LYS	3.7
1	A	485	THR	3.7
2	E	410	ILE	3.7
1	A	499	GLU	3.7
2	E	342	LEU	3.7
2	D	246	GLN	3.7
2	E	406	ARG	3.6
1	B	492	GLU	3.6
2	E	404	VAL	3.6
4	H	38	VAL	3.6
3	G	165	PHE	3.6
4	H	118	GLU	3.6
3	G	145	ALA	3.6
3	G	81	ILE	3.5
4	H	121	GLY	3.5
3	G	127	THR	3.5
1	A	381	ARG	3.5
2	D	475	GLU	3.5
1	A	409	ASP	3.5
1	A	121	ILE	3.5
4	H	19	THR	3.5
2	E	381	TYR	3.5
3	G	67	LEU	3.5
4	H	102	MET	3.5
2	E	405	SER	3.5
2	E	409	LYS	3.4
1	B	458	PRO	3.4
2	F	210	ASP	3.4
1	A	405	GLN	3.4
1	B	488	LYS	3.4
4	H	64	VAL	3.4
1	B	509	GLU	3.4
1	C	475	GLN	3.4
2	E	399	GLU	3.4
1	A	504	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	473	ILE	3.3
2	E	370	VAL	3.3
5	I	25	ALA	3.3
2	E	397	SER	3.3
1	C	508	PHE	3.3
1	B	415	GLN	3.3
4	H	29	ASN	3.3
1	A	401	ALA	3.3
1	B	463	LYS	3.3
3	G	113	ARG	3.3
3	G	147	GLU	3.3
1	B	395	ALA	3.3
1	B	399	GLU	3.3
1	B	457	GLU	3.3
2	E	373	GLY	3.2
1	B	491	GLU	3.2
2	E	447	GLY	3.2
2	E	375	GLN	3.2
3	G	171	TYR	3.2
1	B	454	ASP	3.1
3	G	129	LYS	3.1
3	G	33	ARG	3.1
2	E	403	THR	3.1
1	B	467	ALA	3.1
1	B	486	ASP	3.1
2	E	413	PHE	3.1
2	E	396	LEU	3.1
1	B	423	ARG	3.1
1	B	450	ARG	3.1
3	G	2	THR	3.1
2	D	249	GLN	3.1
3	G	68	ILE	3.1
2	F	428	LEU	3.1
2	E	412	ARG	3.1
1	B	446	TYR	3.1
5	I	10	SER	3.0
3	G	39	LYS	3.0
2	E	455	GLN	3.0
2	F	468	ALA	3.0
1	A	508	PHE	3.0
1	B	500	ILE	3.0
1	A	484	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	170	SER	3.0
3	G	208	SER	3.0
3	G	221	THR	3.0
3	G	163	ASN	3.0
2	F	426	GLY	3.0
1	C	195	GLU	3.0
2	E	466	ALA	3.0
1	A	476	HIS	3.0
4	H	93	LEU	3.0
2	D	26	ASP	3.0
4	H	124	ASP	3.0
1	A	123	SER	3.0
2	D	177	HIS	3.0
2	D	474	ALA	3.0
3	G	133	ARG	2.9
4	H	128	ARG	2.9
3	G	173	THR	2.9
2	D	76	LEU	2.9
2	D	209	LYS	2.9
3	G	162	PHE	2.9
1	B	358	TYR	2.9
3	G	144	ILE	2.9
1	B	420	ARG	2.9
1	A	410	LEU	2.9
2	E	426	GLY	2.9
4	H	97	ALA	2.9
1	A	305	LEU	2.9
1	A	496	LYS	2.9
2	F	174	ALA	2.9
3	G	271	ALA	2.9
1	B	490	SER	2.8
2	D	242	TYR	2.8
1	C	99	VAL	2.8
3	G	36	ARG	2.8
1	A	479	LEU	2.8
2	F	111	LYS	2.8
1	A	267	ILE	2.8
3	G	83	SER	2.8
4	H	76	PHE	2.8
1	B	466	ASN	2.8
2	E	9	THR	2.8
1	C	408	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	93	ALA	2.8
1	B	396	GLN	2.8
4	H	98	VAL	2.8
2	E	430	LYS	2.8
4	H	113	GLU	2.8
2	F	383[A]	SER	2.8
1	A	74[A]	VAL	2.8
1	B	472	VAL	2.8
1	C	24	ASP	2.7
2	E	344	ILE	2.7
3	G	19	ILE	2.7
2	D	393	MET	2.7
2	E	459	MET	2.7
2	E	111	LYS	2.7
2	E	382	LYS	2.7
1	B	422	VAL	2.7
4	H	114	LYS	2.7
1	B	489	ILE	2.7
2	E	443	GLN	2.7
3	G	1	ALA	2.7
1	A	455	LYS	2.7
4	H	36	VAL	2.7
1	B	461	ILE	2.7
2	D	212	THR	2.7
1	A	316	PHE	2.7
2	E	420	VAL	2.7
1	B	421	GLY	2.7
2	E	429	GLY	2.7
2	F	209	LYS	2.7
3	G	72	SER	2.7
2	D	210	ASP	2.7
3	G	5	ASP	2.7
3	G	78	CYS	2.7
3	G	111	LYS	2.6
3	G	28	ALA	2.6
1	A	94	ILE	2.6
1	A	403	PHE	2.6
1	A	506	ALA	2.6
1	C	122	GLY	2.6
2	E	411	GLN	2.6
1	A	355[A]	GLU	2.6
3	G	108	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	256	TYR	2.6
2	E	444	ILE	2.6
5	I	18	CYS	2.6
4	H	127	THR	2.6
1	A	487	GLY	2.6
4	H	106	GLY	2.6
1	C	463	LYS	2.6
2	E	465	GLU	2.6
1	B	498	LYS	2.5
1	A	473	ILE	2.5
2	F	438	ILE	2.5
2	E	376	LYS	2.5
4	H	17	SER	2.5
1	C	190	ASN	2.5
4	H	80	GLY	2.5
3	G	9	ARG	2.5
1	C	403	PHE	2.5
1	A	306	LEU	2.5
2	F	249	GLN	2.5
1	B	484	ARG	2.5
1	A	482	LYS	2.5
2	E	128	VAL	2.5
1	A	505	LEU	2.5
2	E	343	GLY	2.4
2	E	463	ILE	2.4
2	D	10	THR	2.4
1	A	131	LEU	2.4
1	B	480	LEU	2.4
4	H	109	LYS	2.4
1	B	501	VAL	2.4
1	C	471	HIS	2.4
1	B	460	LYS	2.4
1	A	206	ILE	2.4
1	C	371	VAL	2.4
2	D	178	GLY	2.4
1	C	473	ILE	2.4
1	B	452	TYR	2.3
1	A	492	GLU	2.3
2	E	113	PHE	2.3
3	G	206	GLU	2.3
1	B	196	LYS	2.3
3	G	240	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	366	GLU	2.3
1	B	497	LEU	2.3
1	A	167	ILE	2.3
1	A	178	ILE	2.3
2	F	186	VAL	2.3
3	G	166	ARG	2.3
1	C	470	SER	2.3
3	G	84	SER	2.3
3	G	23	MET	2.2
2	F	88	PRO	2.2
2	F	110	THR	2.2
4	H	63	VAL	2.2
1	A	350	ILE	2.2
1	B	381	ARG	2.2
2	E	380	ASP	2.2
1	A	452	TYR	2.2
3	G	44	TYR	2.2
1	C	196	LYS	2.2
2	D	109	LYS	2.2
2	F	113	PHE	2.2
4	H	137	ALA	2.2
1	A	326	VAL	2.2
2	E	28	GLY	2.2
2	E	408	ARG	2.2
1	A	193	THR	2.2
1	B	462	THR	2.2
1	B	471	HIS	2.2
2	E	440	GLY	2.2
1	C	505	LEU	2.2
2	D	12	ARG	2.2
2	D	247	GLU	2.2
4	H	115	ALA	2.2
1	A	486	ASP	2.2
4	H	81	SER	2.2
1	C	510	ALA	2.2
2	E	419	GLN	2.2
1	B	389	THR	2.1
1	C	91	THR	2.1
2	F	464	GLU	2.1
3	G	134	ARG	2.1
3	G	164	ARG	2.1
1	A	463	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	176	ALA	2.1
2	D	390	ILE	2.1
3	G	213	ILE	2.1
1	A	392	LEU	2.1
4	H	140	ALA	2.1
2	E	372	ARG	2.1
2	E	450	ASP	2.1
2	F	455	GLN	2.1
1	C	491	GLU	2.1
3	G	229	MET	2.1
4	H	135	ILE	2.1
2	F	97[A]	VAL	2.1
1	B	478	ALA	2.1
1	C	410	LEU	2.1
3	G	38	LEU	2.1
1	B	502	THR	2.0
4	H	40	THR	2.0
1	A	200	TYR	2.0
2	F	386	ASP	2.0
5	I	3	TYR	2.0
2	D	213	SER	2.0
2	E	418	PHE	2.0
1	A	198[A]	LYS	2.0
1	C	404	ALA	2.0
1	B	25	LEU	2.0
2	D	208	LEU	2.0
2	D	255	ILE	2.0
1	A	26	GLU	2.0
1	B	385	GLN	2.0
4	H	25	GLN	2.0
1	B	487	GLY	2.0
2	D	112	GLN	2.0
2	E	369	ASP	2.0
1	A	271	LEU	2.0
1	B	424	LEU	2.0
3	G	230	THR	2.0
1	C	381	ARG	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)

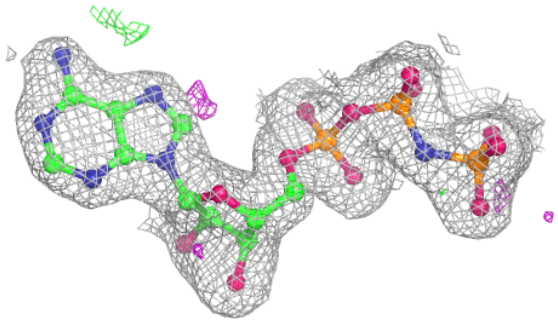
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

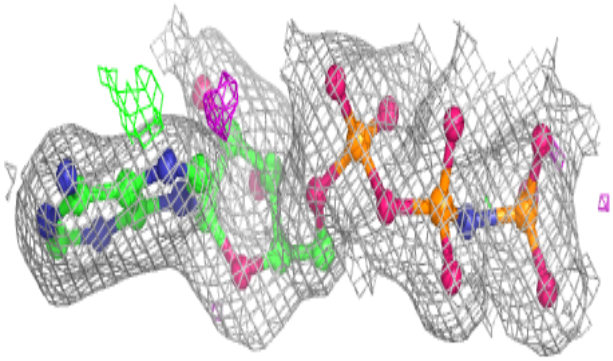
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	PO4	E	602	5/5	0.88	0.17	68,69,72,72	0
9	AZI	D	1092	3/3	0.92	0.16	17,17,19,25	0
7	MG	A	601	1/1	0.96	0.10	14,14,14,14	0
7	MG	B	601	1/1	0.96	0.09	19,19,19,19	0
6	ANP	B	600	31/31	0.97	0.10	13,19,27,32	0
6	ANP	C	600	31/31	0.98	0.11	12,16,19,19	0
7	MG	C	601	1/1	0.98	0.11	17,17,17,17	0
7	MG	D	601	1/1	0.98	0.07	16,16,16,16	0
7	MG	F	601	1/1	0.98	0.13	13,13,13,13	0
8	ADP	D	600	27/27	0.98	0.13	10,17,21,22	0
6	ANP	F	600	31/31	0.98	0.12	12,16,20,22	0
6	ANP	A	600	31/31	0.98	0.14	11,15,20,23	0

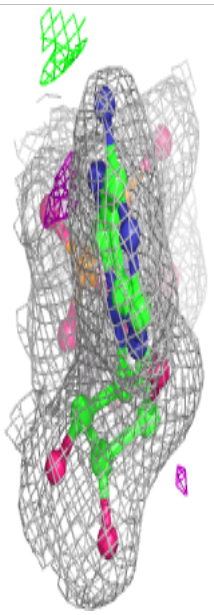
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 600:

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

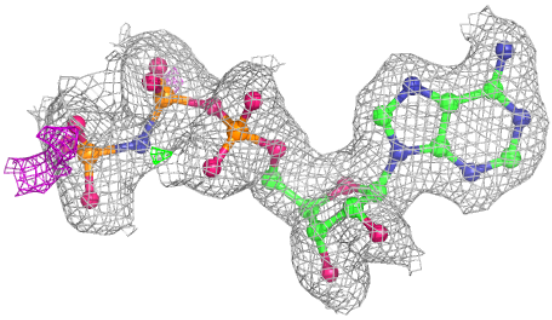


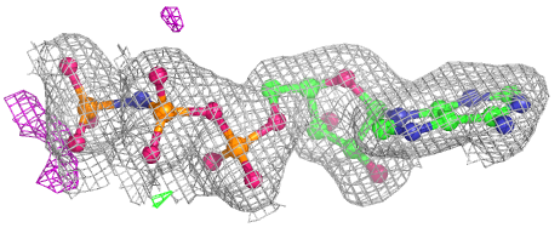


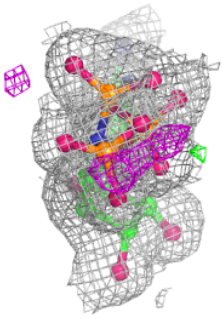


Electron density around ANP C 600:

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

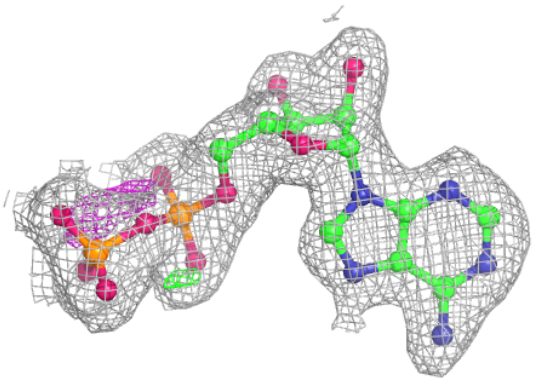


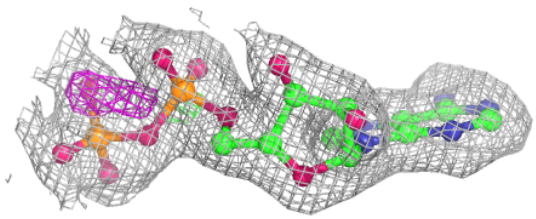


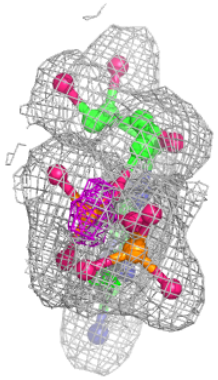


Electron density around ADP D 600:

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

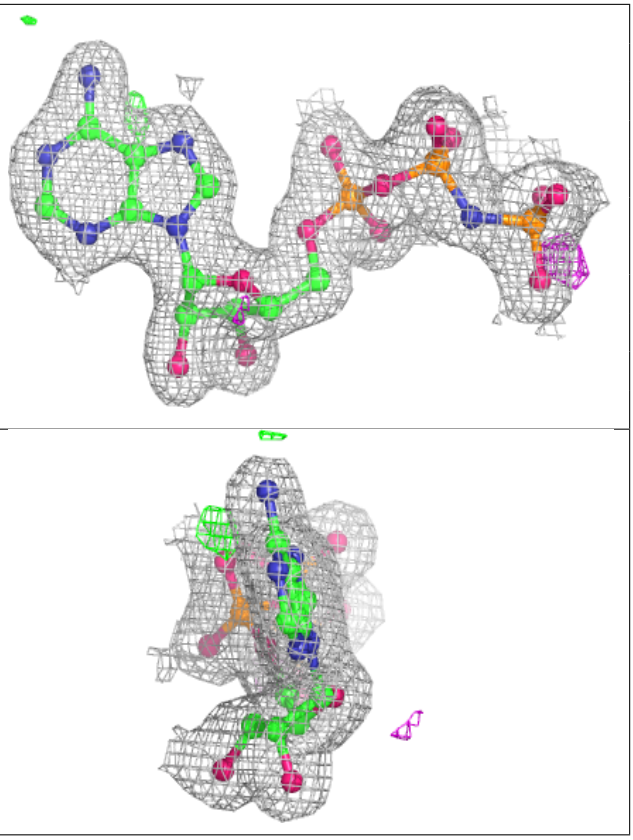


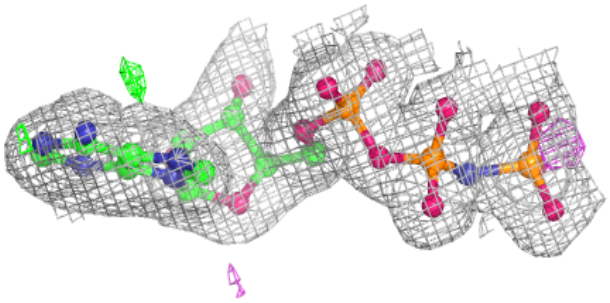




Electron density around ANP F 600:

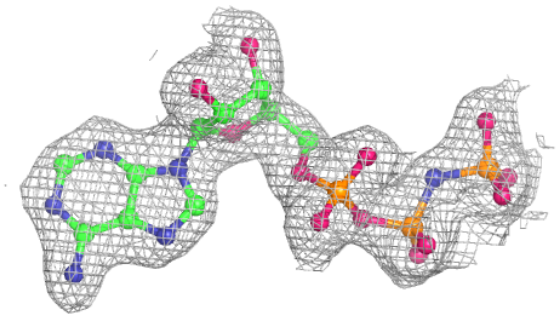
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

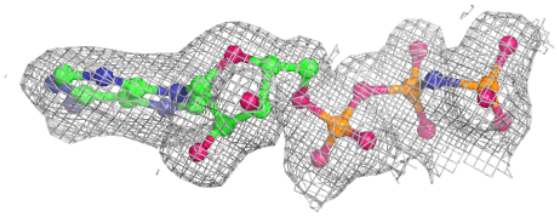


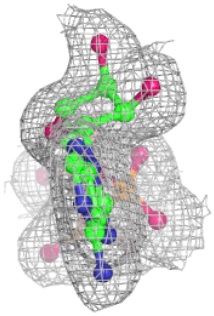


Electron density around ANP A 600:

$2mF_o$-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.