wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 10:19 pm BST

PDB ID	:	3OPY
Title	:	Crystal structure of Pichia pastoris phosphofructokinase in the T-state
Authors	:	Strater, N.; Marek, S.; Kuettner, E.B.; Kloos, M.; Keim, A.; Bruser, A.; Kirchberger, J.; Schoneberg, T.
Deposited on	:	2010-09-02
Resolution	:	3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

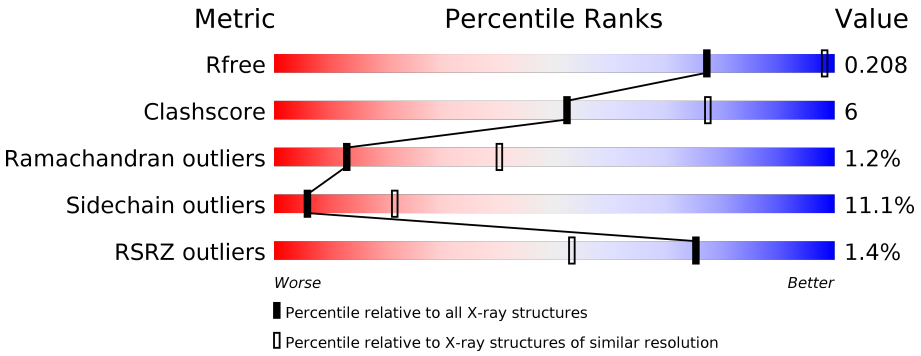
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 on 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	989	75% 18% • 5%
1	C	989	75% 17% • 5%
1	E	989	75% 17% • 5%
1	G	989	75% 17% • 5%
2	B	941	76% 16% • 6%
2	D	941	77% 16% • 6%

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Mol	Chain	Length	Quality of chain
2	F	941	3% 76% 16% 6%
2	H	941	2% 76% 16% 6%
3	I	351	65% 24% 8%
3	J	351	61% 28% 8%
3	K	351	% 67% 22% 8%
3	L	351	66% 23% 8%

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	SO4	C	991	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65025 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 6-phosphofructo-1-kinase alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	C	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	E	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	G	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			

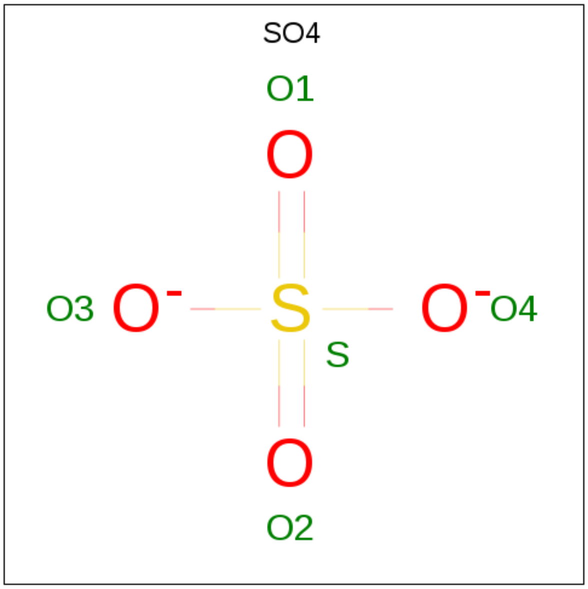
- Molecule 2 is a protein called 6-phosphofructo-1-kinase beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	D	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	F	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	H	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			

- Molecule 3 is a protein called 6-phosphofructo-1-kinase gamma-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	J	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	K	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	L	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0

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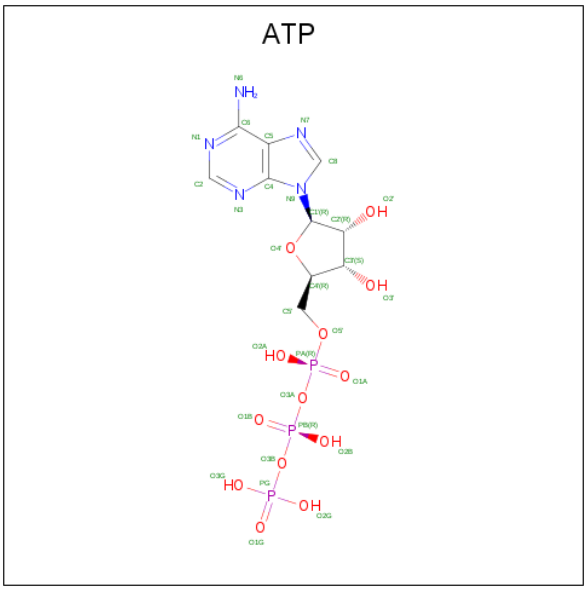
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

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



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

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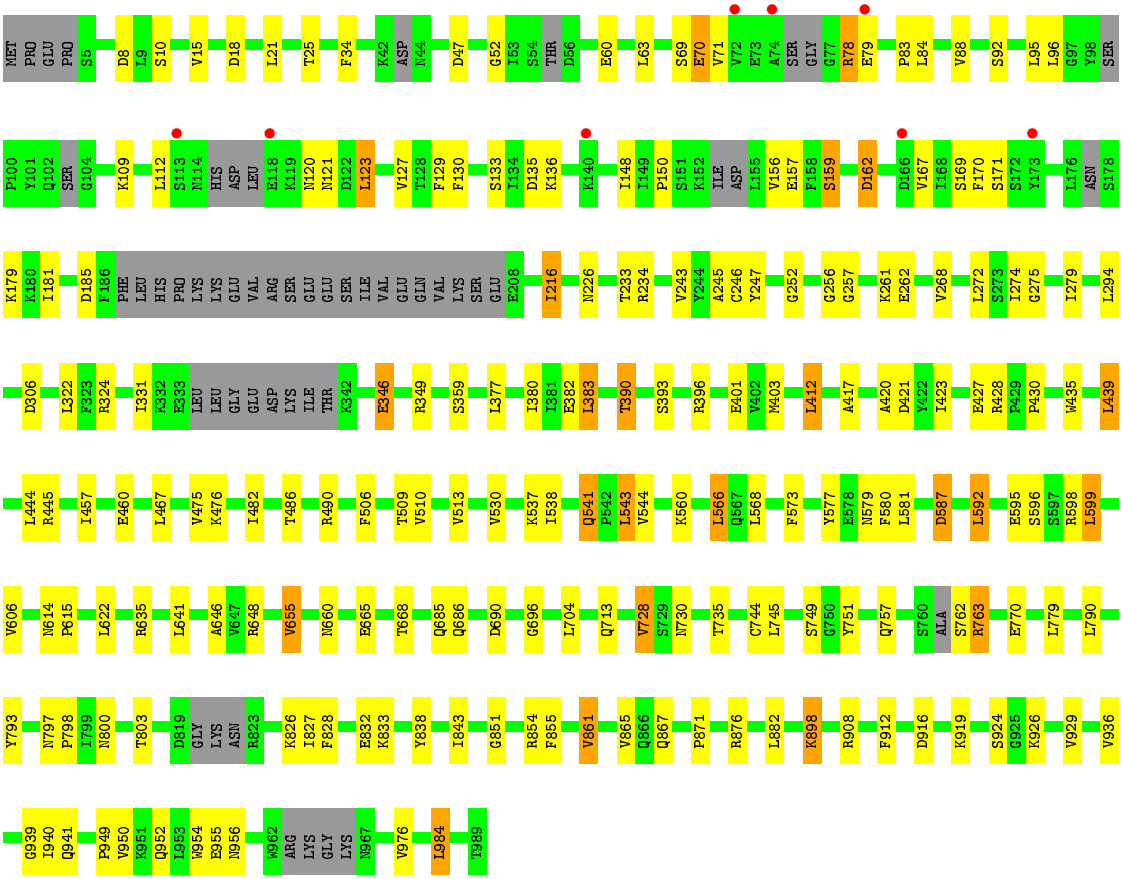
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

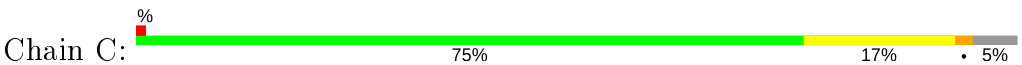
- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

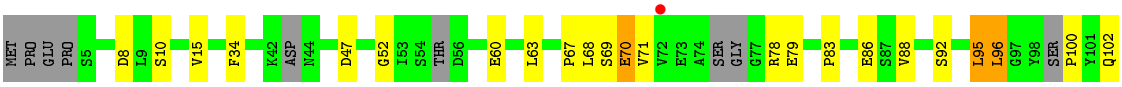
Chain A:

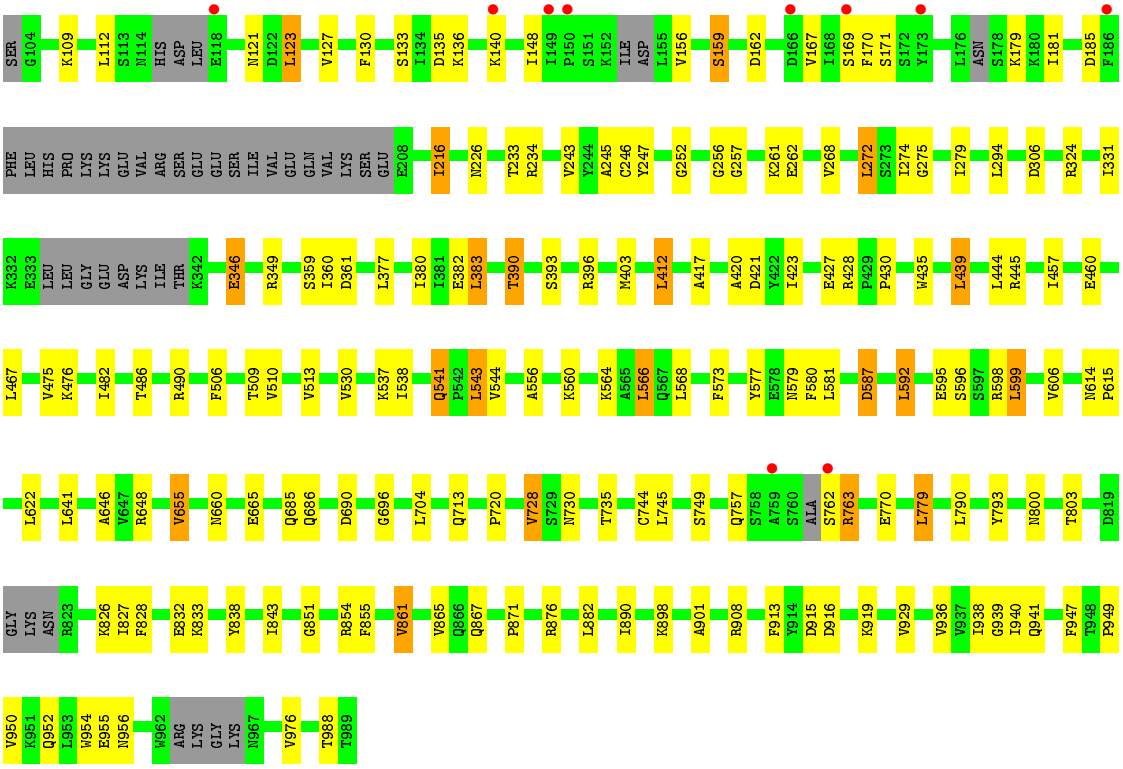


- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

Chain C:

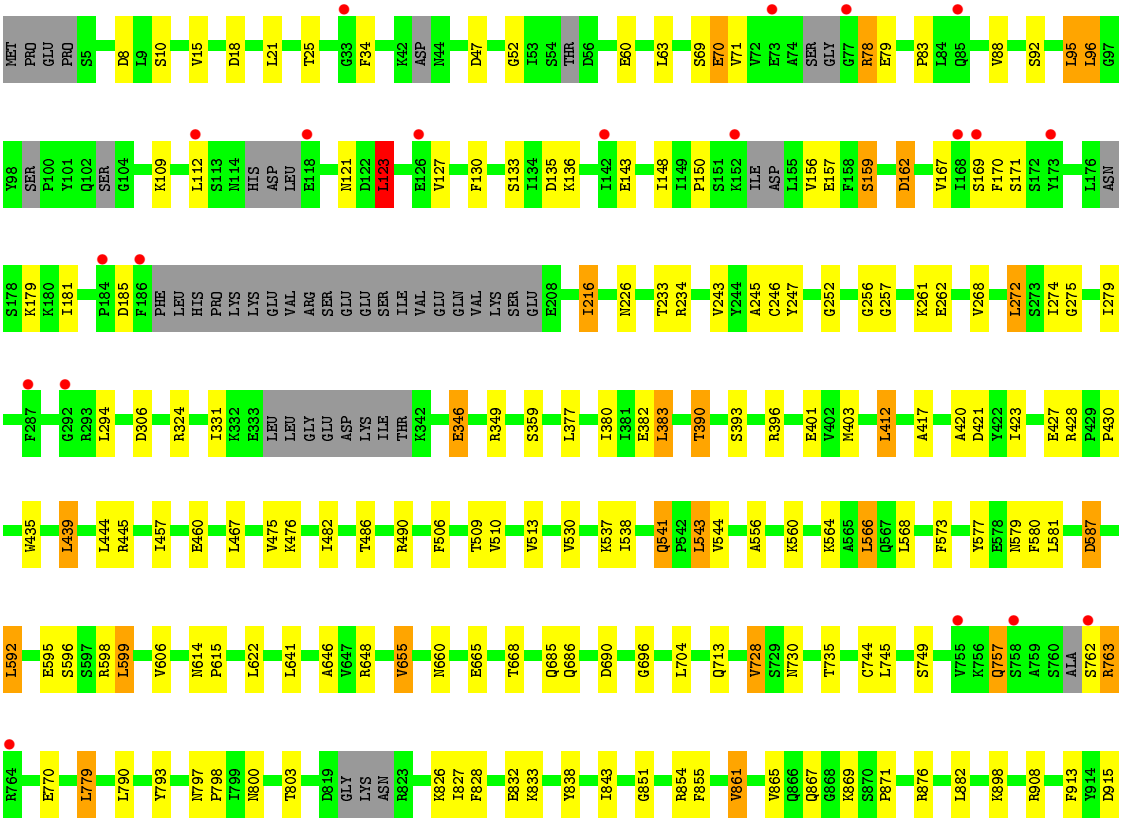


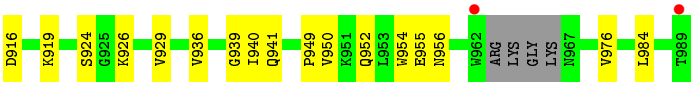




- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

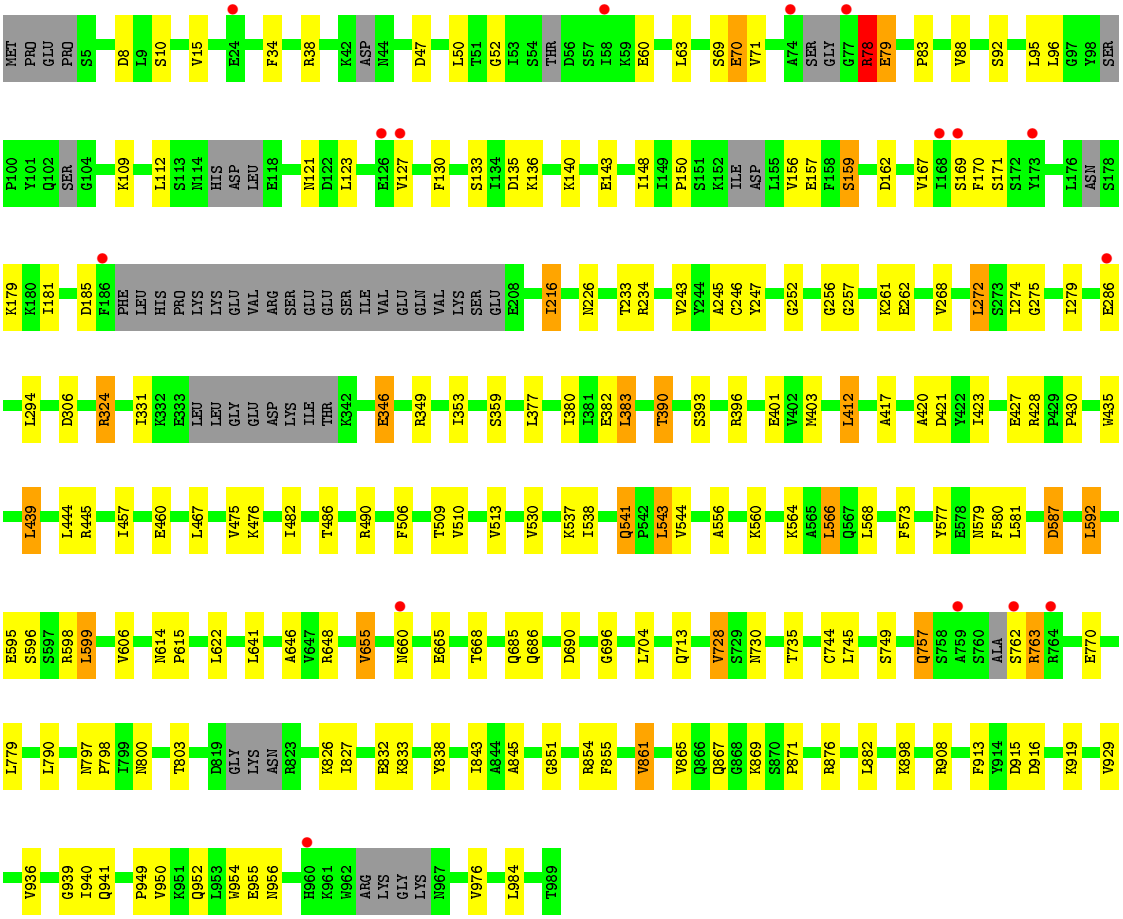
Chain E:





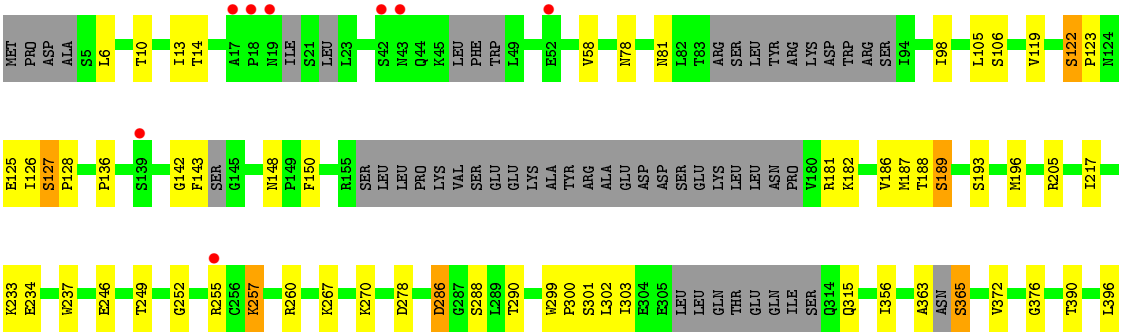
- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

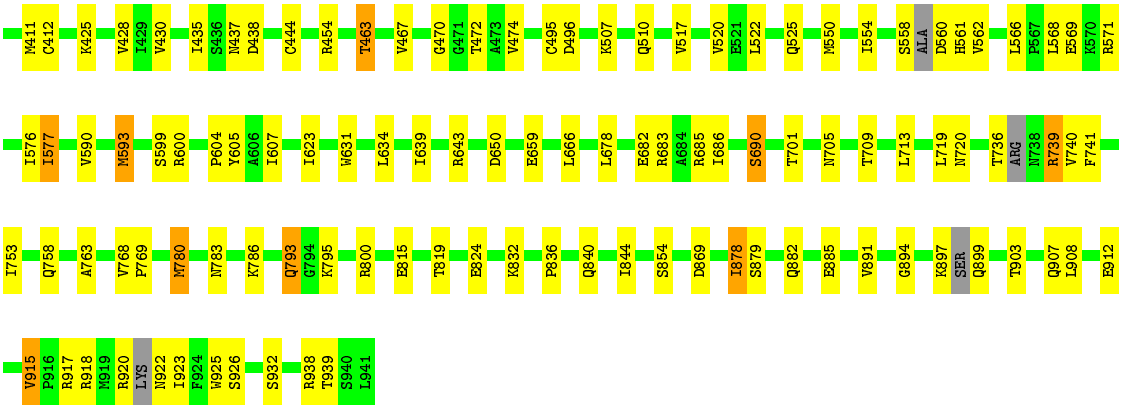
Chain G:



- Molecule 2: 6-phosphofructo-1-kinase beta-subunit

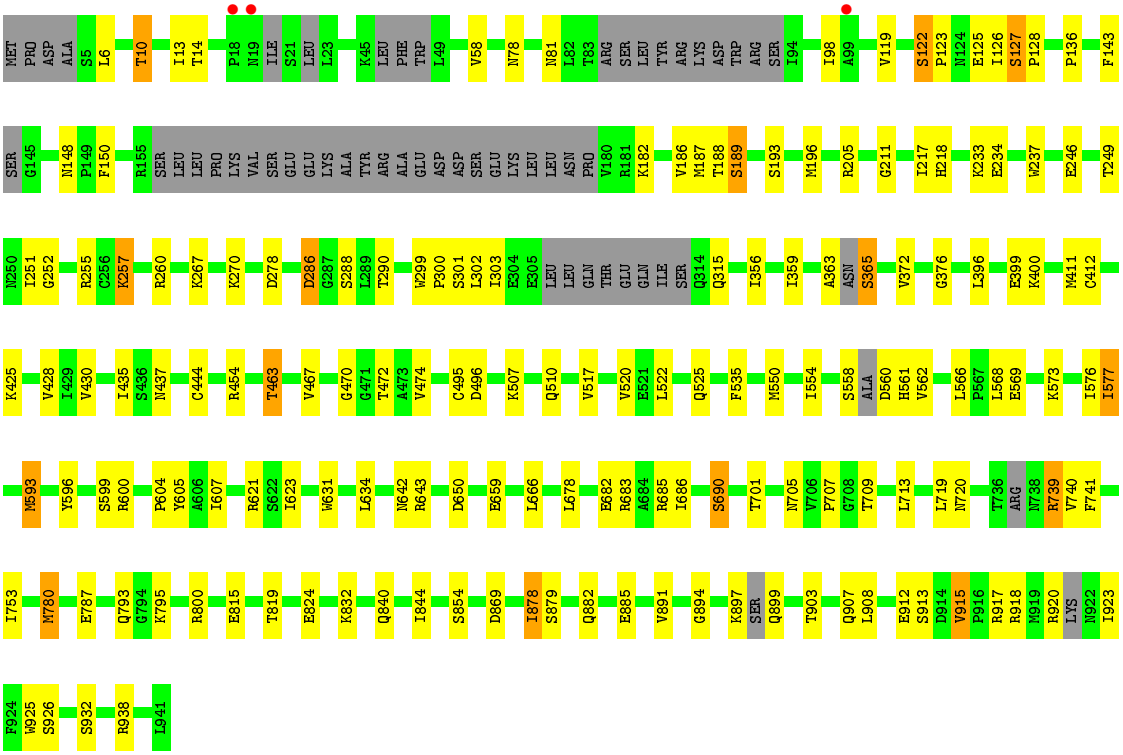
Chain B:





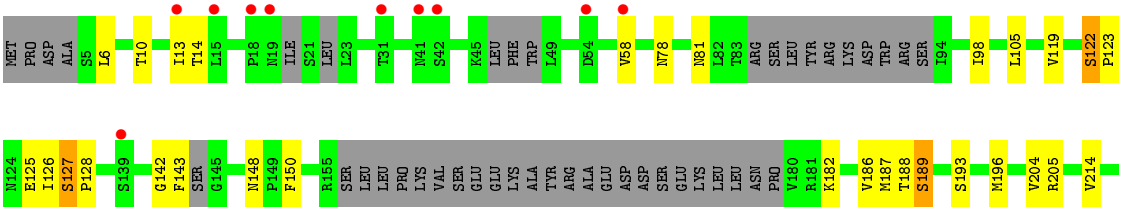
- Molecule 2: 6-phosphofructo-1-kinase beta-subunit

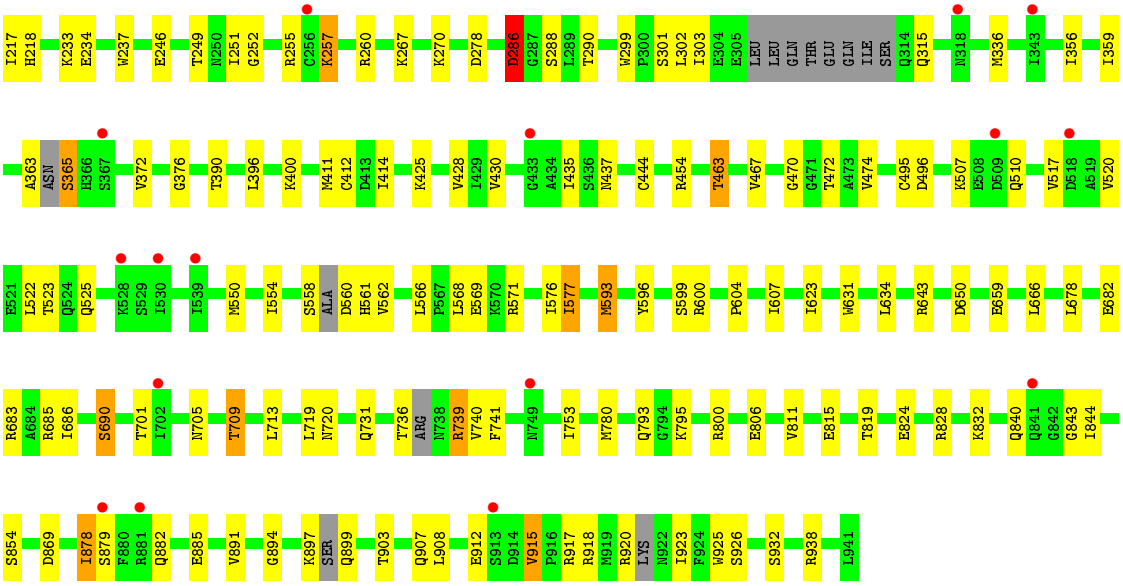
Chain D:



- Molecule 2: 6-phosphofructo-1-kinase beta-subunit

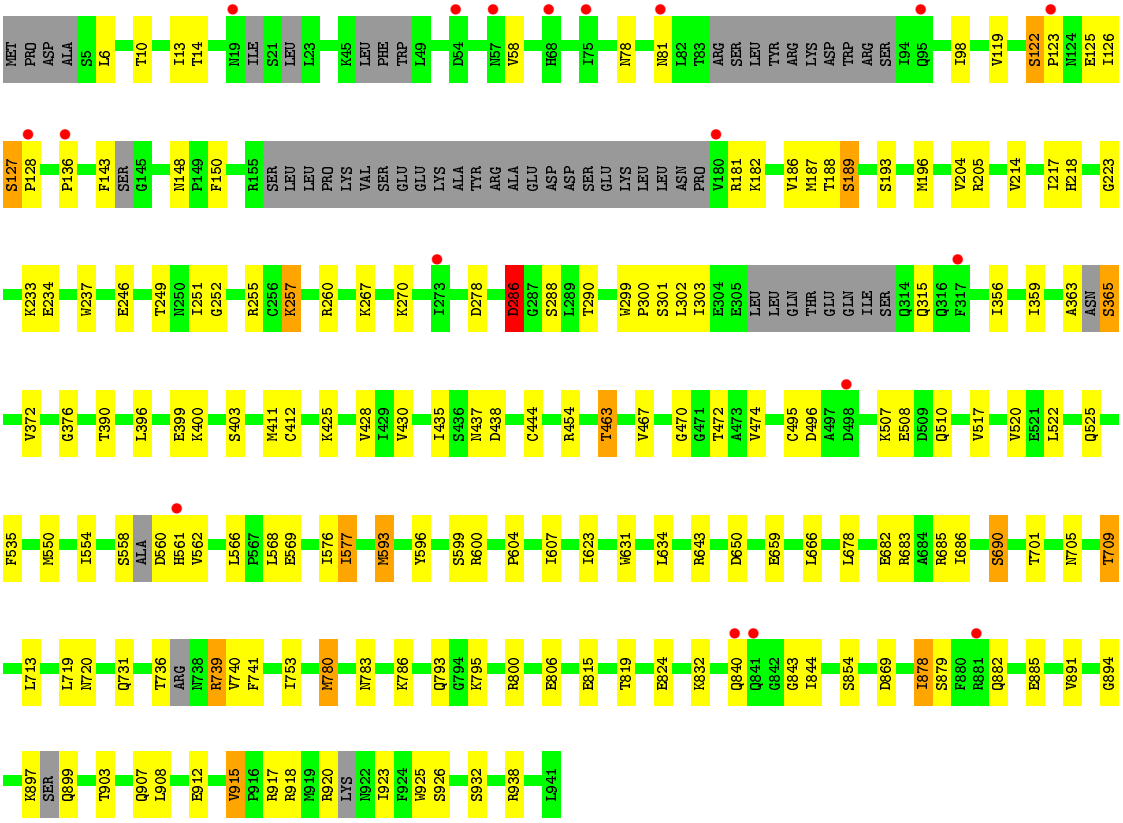
Chain F:





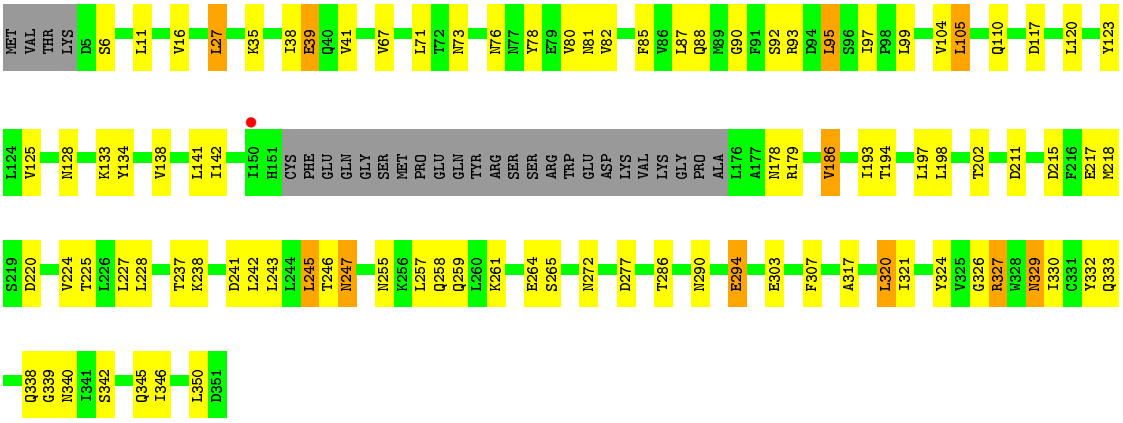
• Molecule 2: 6-phosphofructo-1-kinase beta-subunit

Chain H:



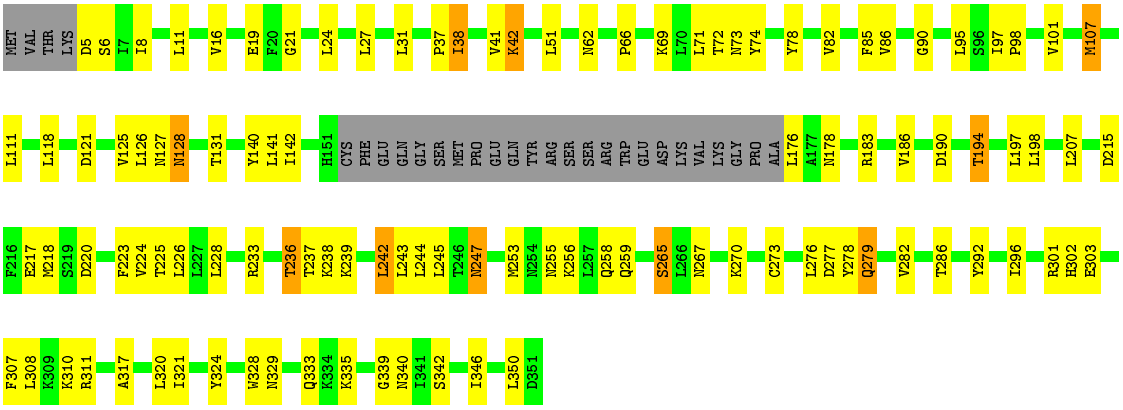
• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain I:



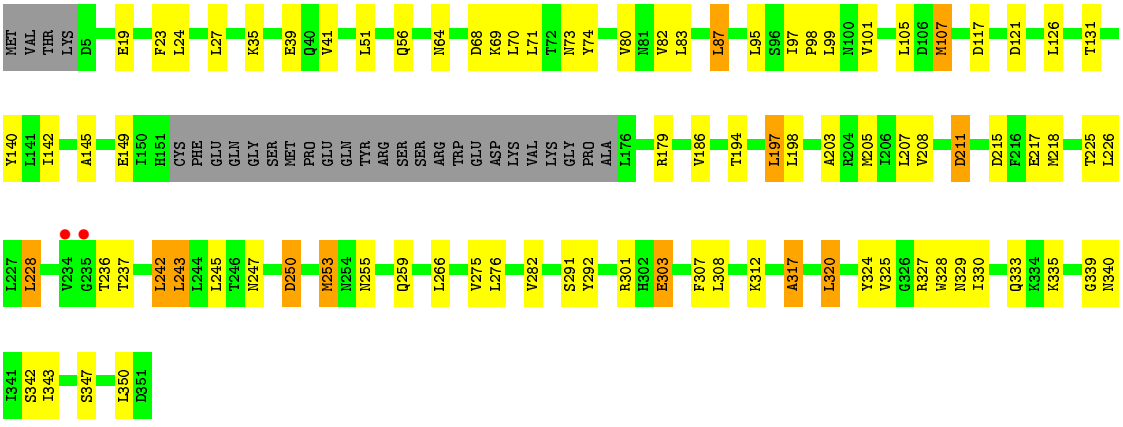
• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain J:



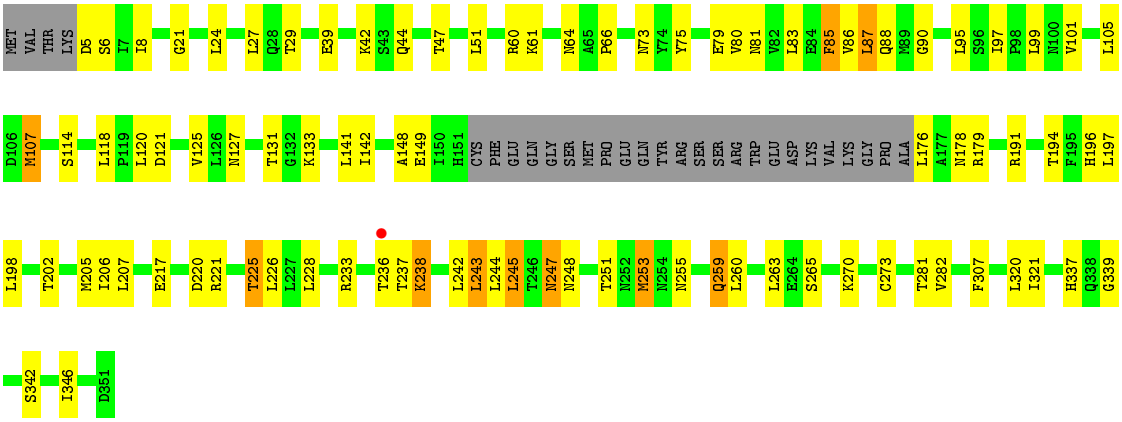
• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain K:



• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain L:


MET VAL THR LYS D5 S6 I7 I8 G21 L24 L27 Q28 T29 E39 K42 S43 Q44 T47 L51 R60 K61 N64 A65 P66 N73 Y74 Y75 E79 V80 N81 V82 L83 E84 F85 V86 L87 Q88 M89 G90 L95 S96 I97 P98 L99 N100 V101 L105
D106 M107 S114 L118 P119 L120 D121 V125 L126 N127 T131 G132 K133 L141 I142 A148 E149 I150 H151 CYS PHE GLU GLN GLY SER MET PRO GLU GLN TYR ARG SER SER ARG TRP GLU ASP LYS VAL LYS GLY PRO ALA L176 A177 N178 R179 R191 T194 F195 H196 L197
L198 T202 M205 I206 L207 E217 D220 R221 T225 L226 L227 L228 R233 T236 T237 K238 L242 L243 L244 L245 T246 N247 N248 T251 N252 M253 N254 N255 Q259 L260 L263 E264 S265 K270 C273 T281 V282 F307 L320 I321 H337 Q338 G339
S342 I346 D351

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	161.66Å 188.30Å 231.56Å 90.00° 92.85° 90.00°	Depositor
Resolution (Å)	29.80 – 3.05 29.82 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.80-3.05) 84.0 (29.82-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.06Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.200 , 0.232 0.216 , 0.208	Depositor DCC
R_{free} test set	5145 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	65025	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% 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: SO4, 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	0.49	0/7125	0.73	0/9664
1	C	0.50	0/7125	0.73	0/9664
1	E	0.46	0/7125	0.72	0/9664
1	G	0.47	0/7125	0.72	0/9664
2	B	0.51	0/6651	0.74	1/9002 (0.0%)
2	D	0.51	0/6651	0.74	1/9002 (0.0%)
2	F	0.47	0/6651	0.72	1/9002 (0.0%)
2	H	0.48	0/6651	0.73	1/9002 (0.0%)
3	I	0.61	0/2640	0.85	1/3578 (0.0%)
3	J	0.57	0/2640	0.85	0/3578
3	K	0.53	0/2640	0.80	0/3578
3	L	0.54	0/2640	0.78	0/3578
All	All	0.50	0/65664	0.75	5/88976 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	67	VAL	C-N-CA	5.33	135.04	121.70
2	F	125	GLU	C-N-CA	5.15	134.57	121.70
2	B	125	GLU	C-N-CA	5.12	134.49	121.70
2	H	125	GLU	C-N-CA	5.03	134.27	121.70
2	D	125	GLU	C-N-CA	5.02	134.26	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	915	VAL	Mainchain
2	D	915	VAL	Mainchain
1	E	123	LEU	Mainchain
2	F	915	VAL	Mainchain
2	H	915	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7008	0	6692	83	0
1	C	7008	0	6692	81	0
1	E	7008	0	6692	81	0
1	G	7008	0	6692	76	0
2	B	6546	0	6253	68	0
2	D	6546	0	6253	69	0
2	F	6546	0	6253	66	0
2	H	6546	0	6253	67	0
3	I	2590	0	2509	41	0
3	J	2590	0	2509	54	0
3	K	2590	0	2509	36	0
3	L	2590	0	2509	42	0
4	A	65	0	0	1	0
4	B	10	0	0	0	0
4	C	50	0	0	3	0
4	D	15	0	0	0	0
4	E	40	0	0	2	0
4	F	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	40	0	0	0	0
4	H	20	0	0	0	0
4	I	25	0	0	0	0
4	J	15	0	0	0	0
4	K	15	0	0	0	0
4	L	15	0	0	0	0
5	B	31	0	12	0	0
5	D	31	0	12	0	0
5	F	31	0	12	1	0
5	H	31	0	12	1	0
All	All	65025	0	61864	702	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 6.

The worst 5 of 702 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)
2:B:650:ASP:CB	2:D:148:ASN:HB2	2.01	0.90
2:F:148:ASN:HB2	2:H:650:ASP:CB	2.06	0.85
1:C:622:LEU:HD21	1:C:655:VAL:HG11	1.59	0.84
1:E:216:ILE:HG22	1:E:246:CYS:HB3	1.60	0.84
3:I:255:ASN:O	3:I:259:GLN:HG3	1.78	0.84

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	908/989 (92%)	840 (92%)	58 (6%)	10 (1%)	14	42
1	C	908/989 (92%)	841 (93%)	57 (6%)	10 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	908/989 (92%)	841 (93%)	57 (6%)	10 (1%)	14	42
1	G	908/989 (92%)	843 (93%)	55 (6%)	10 (1%)	14	42
2	B	859/941 (91%)	800 (93%)	46 (5%)	13 (2%)	10	35
2	D	859/941 (91%)	803 (94%)	45 (5%)	11 (1%)	12	38
2	F	859/941 (91%)	803 (94%)	45 (5%)	11 (1%)	12	38
2	H	859/941 (91%)	800 (93%)	46 (5%)	13 (2%)	10	35
3	I	319/351 (91%)	296 (93%)	21 (7%)	2 (1%)	25	55
3	J	319/351 (91%)	285 (89%)	29 (9%)	5 (2%)	9	33
3	K	319/351 (91%)	286 (90%)	31 (10%)	2 (1%)	25	55
3	L	319/351 (91%)	283 (89%)	33 (10%)	3 (1%)	17	47
All	All	8344/9124 (92%)	7721 (92%)	523 (6%)	100 (1%)	13	40

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	646	ALA
2	B	127	SER
2	B	150	PHE
2	B	303	ILE
1	C	646	ALA

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	725/835 (87%)	648 (89%)	77 (11%)	6	23
1	C	725/835 (87%)	650 (90%)	75 (10%)	7	24
1	E	725/835 (87%)	648 (89%)	77 (11%)	6	23
1	G	725/835 (87%)	646 (89%)	79 (11%)	6	22
2	B	670/799 (84%)	600 (90%)	70 (10%)	7	24
2	D	670/799 (84%)	602 (90%)	68 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	670/799 (84%)	600 (90%)	70 (10%)	7 24
2	H	670/799 (84%)	598 (89%)	72 (11%)	6 23
3	I	282/322 (88%)	242 (86%)	40 (14%)	3 13
3	J	282/322 (88%)	239 (85%)	43 (15%)	3 10
3	K	282/322 (88%)	245 (87%)	37 (13%)	4 15
3	L	282/322 (88%)	248 (88%)	34 (12%)	5 17
All	All	6708/7824 (86%)	5966 (89%)	742 (11%)	6 21

5 of 742 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	596	SER
2	F	719	LEU
3	K	197	LEU
1	E	745	LEU
2	F	233	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	81	ASN
1	G	85	GLN
3	L	81	ASN
2	F	148	ASN
2	F	705	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

69 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	$\#\|Z\| > 2$
4	SO4	I	354	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	G	995	-	4,4,4	0.14	0	6,6,6	0.27	0
4	SO4	E	995	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	H	945	-	4,4,4	0.28	0	6,6,6	0.37	0
4	SO4	C	994	-	4,4,4	0.41	0	6,6,6	0.28	0
4	SO4	A	1001	-	4,4,4	0.52	0	6,6,6	0.23	0
4	SO4	D	944	-	4,4,4	0.28	0	6,6,6	0.41	0
4	SO4	C	997	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	E	990	-	4,4,4	0.26	0	6,6,6	0.11	0
4	SO4	C	993	-	4,4,4	0.15	0	6,6,6	0.48	0
4	SO4	A	1000	-	4,4,4	0.25	0	6,6,6	0.23	0
4	SO4	I	355	-	4,4,4	0.31	0	6,6,6	0.16	0
4	SO4	F	945	-	4,4,4	0.21	0	6,6,6	0.23	0
4	SO4	I	356	-	4,4,4	0.25	0	6,6,6	0.15	0
4	SO4	J	352	-	4,4,4	0.24	0	6,6,6	0.24	0
4	SO4	A	991	-	4,4,4	0.95	0	6,6,6	0.26	0
4	SO4	E	994	-	4,4,4	0.32	0	6,6,6	0.13	0
4	SO4	I	353	-	4,4,4	0.25	0	6,6,6	0.32	0
4	SO4	G	994	-	4,4,4	0.31	0	6,6,6	0.24	0
4	SO4	F	943	-	4,4,4	0.39	0	6,6,6	0.31	0
4	SO4	H	944	-	4,4,4	0.19	0	6,6,6	0.34	0
4	SO4	B	943	-	4,4,4	0.55	0	6,6,6	0.28	0
4	SO4	L	353	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	L	354	-	4,4,4	0.16	0	6,6,6	0.14	0
4	SO4	E	992	-	4,4,4	0.25	0	6,6,6	0.25	0
4	SO4	E	996	-	4,4,4	0.16	0	6,6,6	0.15	0
5	ATP	F	942	-	26,33,33	1.47	3 (11%)	31,52,52	1.26	2 (6%)
4	SO4	K	352	-	4,4,4	0.27	0	6,6,6	0.35	0
4	SO4	E	991	-	4,4,4	0.76	0	6,6,6	0.24	0
4	SO4	L	352	-	4,4,4	0.08	0	6,6,6	0.10	0
5	ATP	B	942	-	26,33,33	1.42	5 (19%)	31,52,52	1.31	4 (12%)
4	SO4	G	992	-	4,4,4	0.48	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	990	-	4,4,4	0.63	0	6,6,6	0.30	0
5	ATP	D	942	-	26,33,33	1.48	6 (23%)	31,52,52	1.52	7 (22%)
4	SO4	H	946	-	4,4,4	0.22	0	6,6,6	0.23	0
4	SO4	A	999	-	4,4,4	0.74	0	6,6,6	0.20	0
4	SO4	C	991	-	4,4,4	0.60	0	6,6,6	0.23	0
4	SO4	A	997	-	4,4,4	0.24	0	6,6,6	0.24	0
4	SO4	C	990	-	4,4,4	0.81	0	6,6,6	0.38	0
4	SO4	D	943	-	4,4,4	0.87	0	6,6,6	0.39	0
4	SO4	E	997	-	4,4,4	0.19	0	6,6,6	0.20	0
4	SO4	G	996	-	4,4,4	0.19	0	6,6,6	0.10	0
4	SO4	A	994	-	4,4,4	0.21	0	6,6,6	0.38	0
4	SO4	A	996	-	4,4,4	0.48	0	6,6,6	0.30	0
4	SO4	I	352	-	4,4,4	0.58	0	6,6,6	0.50	0
4	SO4	H	943	-	4,4,4	0.18	0	6,6,6	0.33	0
4	SO4	A	992	-	4,4,4	0.29	0	6,6,6	0.19	0
4	SO4	G	991	-	4,4,4	0.44	0	6,6,6	0.50	0
4	SO4	E	993	-	4,4,4	0.21	0	6,6,6	0.40	0
4	SO4	A	995	-	4,4,4	0.52	0	6,6,6	0.23	0
4	SO4	J	354	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	D	945	-	4,4,4	0.19	0	6,6,6	0.40	0
4	SO4	C	996	-	4,4,4	0.55	0	6,6,6	0.46	0
4	SO4	J	353	-	4,4,4	0.29	0	6,6,6	0.20	0
5	ATP	H	942	-	26,33,33	1.42	3 (11%)	31,52,52	1.42	6 (19%)
4	SO4	G	990	-	4,4,4	0.43	0	6,6,6	0.39	0
4	SO4	C	999	-	4,4,4	0.21	0	6,6,6	0.07	0
4	SO4	K	354	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	A	998	-	4,4,4	0.62	0	6,6,6	0.35	0
4	SO4	G	993	-	4,4,4	0.29	0	6,6,6	0.31	0
4	SO4	F	944	-	4,4,4	0.38	0	6,6,6	0.24	0
4	SO4	A	993	-	4,4,4	0.22	0	6,6,6	0.21	0
4	SO4	B	944	-	4,4,4	0.53	0	6,6,6	0.56	0
4	SO4	G	997	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	C	998	-	4,4,4	0.20	0	6,6,6	0.20	0
4	SO4	C	992	-	4,4,4	1.18	0	6,6,6	0.24	0
4	SO4	K	353	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	C	995	-	4,4,4	0.30	0	6,6,6	0.18	0
4	SO4	A	1002	-	4,4,4	0.24	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	H	942	-	-	1/18/38/38	0/3/3/3
5	ATP	B	942	-	-	1/18/38/38	0/3/3/3
5	ATP	D	942	-	-	1/18/38/38	0/3/3/3
5	ATP	F	942	-	-	4/18/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	942	ATP	O4'-C1'	4.38	1.47	1.41
5	D	942	ATP	O2'-C2'	4.24	1.53	1.43
5	F	942	ATP	C2-N3	3.33	1.37	1.32
5	H	942	ATP	C4-N3	3.31	1.40	1.35
5	F	942	ATP	C2-N1	2.82	1.39	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	942	ATP	O2G-PG-O3B	3.71	117.06	104.64
5	B	942	ATP	O2'-C2'-C1'	3.42	123.48	110.85
5	D	942	ATP	PA-O3A-PB	-3.34	121.37	132.83
5	H	942	ATP	C5-C6-N6	3.31	125.38	120.35
5	H	942	ATP	O2G-PG-O3B	3.14	115.18	104.64

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	942	ATP	PB-O3A-PA-O5'
5	H	942	ATP	PB-O3A-PA-O5'
5	F	942	ATP	C5'-O5'-PA-O1A
5	F	942	ATP	O4'-C4'-C5'-O5'
5	D	942	ATP	PG-O3B-PB-O2B

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	990	SO4	1	0
5	F	942	ATP	1	0
4	E	991	SO4	1	0
4	C	991	SO4	2	0
4	C	996	SO4	1	0

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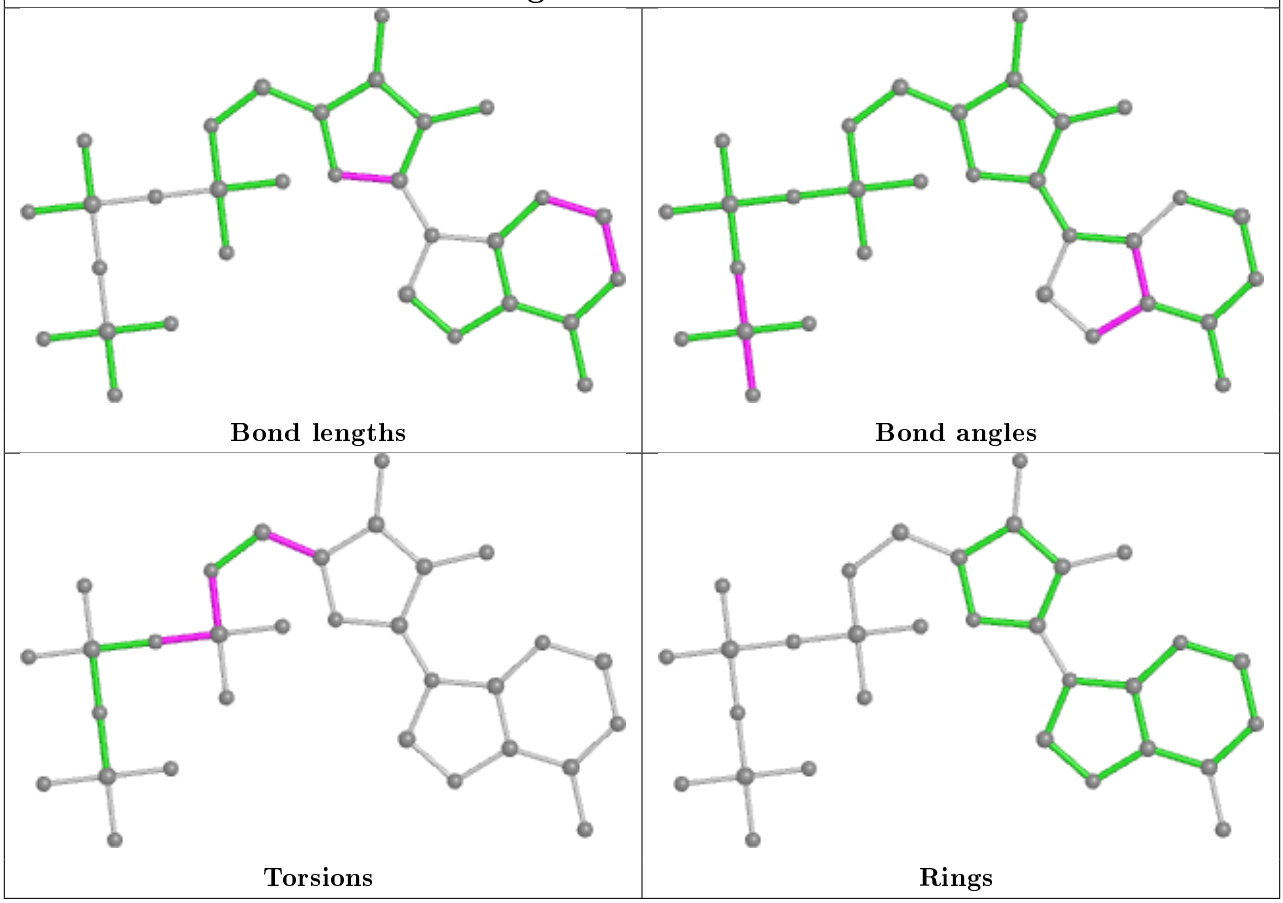
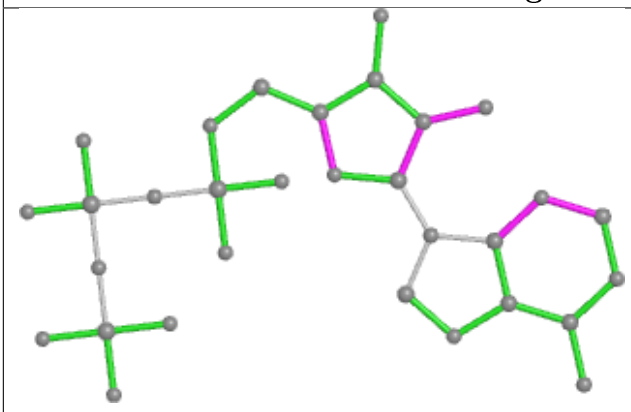
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	942	ATP	1	0
4	A	993	SO4	1	0

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.

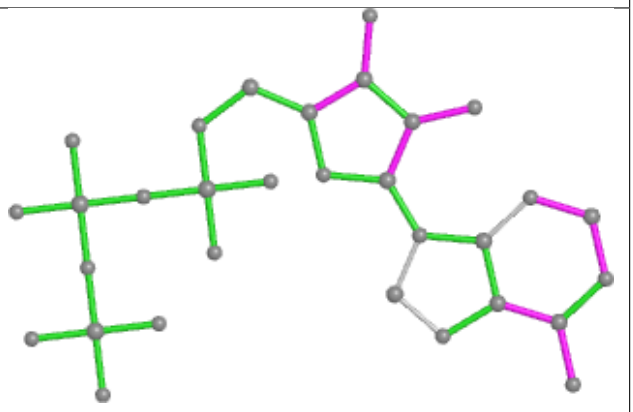
Ligand ATP F 942



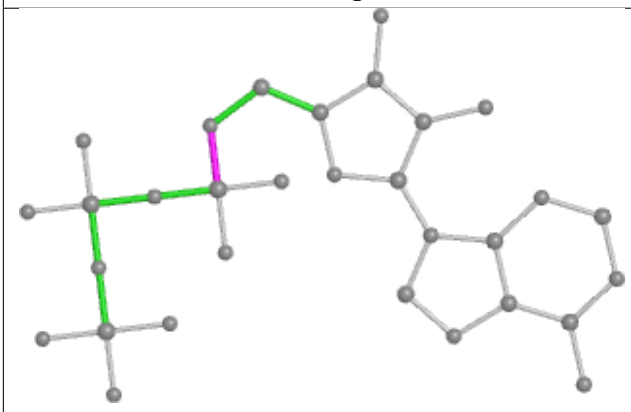
Ligand ATP B 942



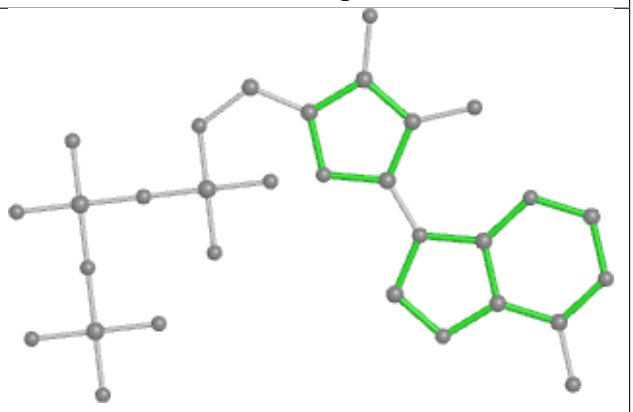
Bond lengths



Bond angles

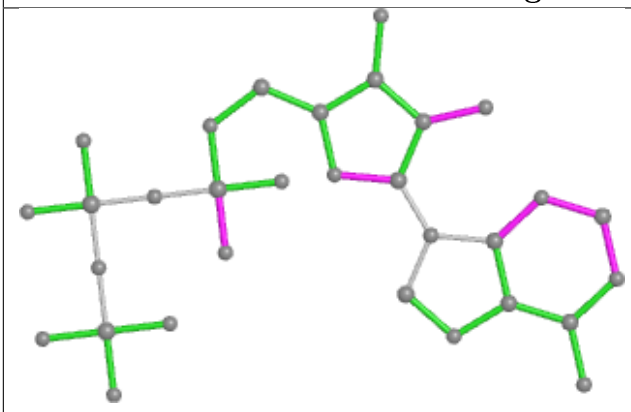


Torsions

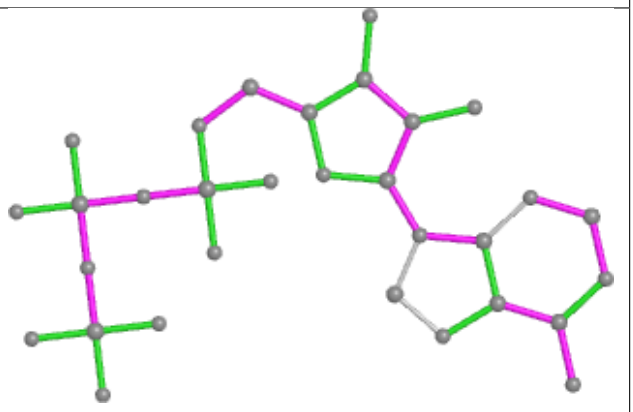


Rings

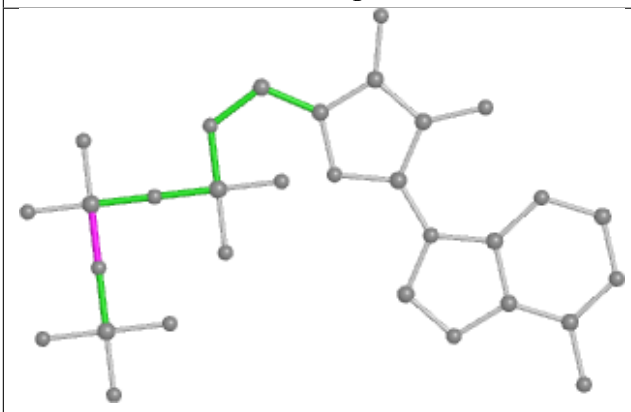
Ligand ATP D 942



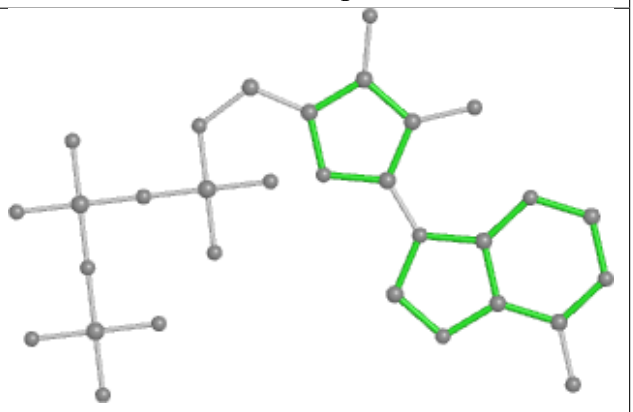
Bond lengths



Bond angles

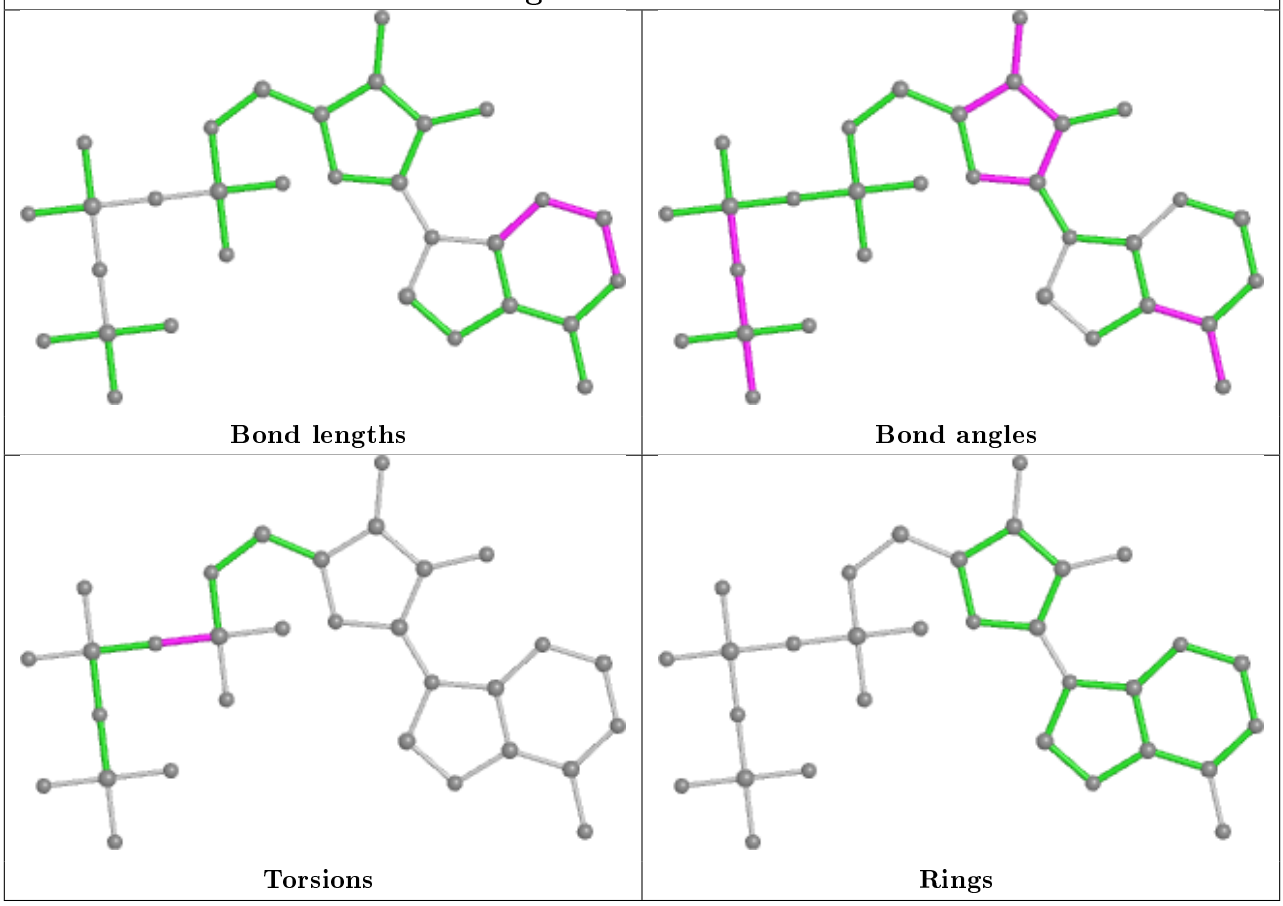


Torsions



Rings

Ligand ATP H 942



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	936/989 (94%)	-0.10	8 (0%) 84 66	19, 52, 102, 146	0
1	C	936/989 (94%)	-0.07	11 (1%) 79 58	21, 53, 107, 163	0
1	E	936/989 (94%)	0.13	22 (2%) 59 34	31, 75, 120, 163	0
1	G	936/989 (94%)	0.06	16 (1%) 70 46	31, 70, 114, 160	0
2	B	884/941 (93%)	-0.09	8 (0%) 84 66	20, 52, 109, 163	0
2	D	884/941 (93%)	-0.08	3 (0%) 94 85	20, 51, 113, 186	0
2	F	884/941 (93%)	0.19	26 (2%) 51 26	43, 83, 126, 191	0
2	H	884/941 (93%)	0.11	18 (2%) 65 41	38, 72, 133, 184	0
3	I	323/351 (92%)	-0.30	1 (0%) 94 85	22, 47, 84, 106	0
3	J	323/351 (92%)	-0.31	0 100 100	17, 47, 84, 113	0
3	K	323/351 (92%)	-0.17	2 (0%) 89 76	38, 66, 96, 121	0
3	L	323/351 (92%)	-0.07	1 (0%) 94 85	47, 72, 104, 125	0
All	All	8572/9124 (93%)	-0.02	116 (1%) 75 53	17, 64, 116, 191	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	173	TYR	7.5
1	E	77	GLY	7.1
1	C	173	TYR	6.6
1	E	989	THR	6.3
1	E	764	ARG	5.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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	SO4	I	354	5/5	0.76	0.28	160,164,165,166	0
4	SO4	C	999	5/5	0.76	0.25	147,152,152,153	0
4	SO4	C	998	5/5	0.80	0.18	119,123,124,125	0
4	SO4	J	354	5/5	0.83	0.16	140,144,145,145	0
4	SO4	L	354	5/5	0.84	0.21	129,133,134,135	0
4	SO4	L	352	5/5	0.85	0.15	122,127,128,128	0
4	SO4	I	355	5/5	0.85	0.24	131,135,136,137	0
4	SO4	I	356	5/5	0.85	0.17	125,129,130,130	0
4	SO4	G	997	5/5	0.85	0.17	135,139,139,140	0
4	SO4	K	354	5/5	0.85	0.16	136,141,141,142	0
4	SO4	E	996	5/5	0.86	0.18	123,127,128,129	0
4	SO4	L	353	5/5	0.88	0.21	165,169,170,170	0
4	SO4	A	995	5/5	0.88	0.16	116,120,121,122	0
4	SO4	A	1000	5/5	0.88	0.13	105,109,110,110	0
4	SO4	C	997	5/5	0.89	0.18	113,117,118,118	0
4	SO4	E	990	5/5	0.89	0.21	110,114,115,115	0
4	SO4	F	945	5/5	0.89	0.17	113,118,118,119	0
4	SO4	A	1002	5/5	0.89	0.16	131,136,136,137	0
4	SO4	H	946	5/5	0.90	0.18	116,120,121,121	0
4	SO4	A	998	5/5	0.90	0.22	84,87,89,90	0
4	SO4	E	997	5/5	0.90	0.21	124,128,129,129	0
4	SO4	E	994	5/5	0.90	0.17	118,122,123,124	0
4	SO4	J	352	5/5	0.90	0.19	104,108,109,109	0
4	SO4	K	352	5/5	0.91	0.18	88,92,93,94	0
5	ATP	H	942	31/31	0.92	0.17	69,70,102,104	0
4	SO4	A	1001	5/5	0.92	0.15	90,94,95,96	0
4	SO4	G	996	5/5	0.92	0.11	133,137,138,139	0
4	SO4	G	993	5/5	0.93	0.17	97,101,102,103	0
4	SO4	D	944	5/5	0.94	0.14	79,83,83,85	0
4	SO4	H	944	5/5	0.94	0.16	94,99,99,100	0
4	SO4	A	997	5/5	0.95	0.17	102,106,107,108	0
4	SO4	K	353	5/5	0.95	0.17	95,100,100,100	0

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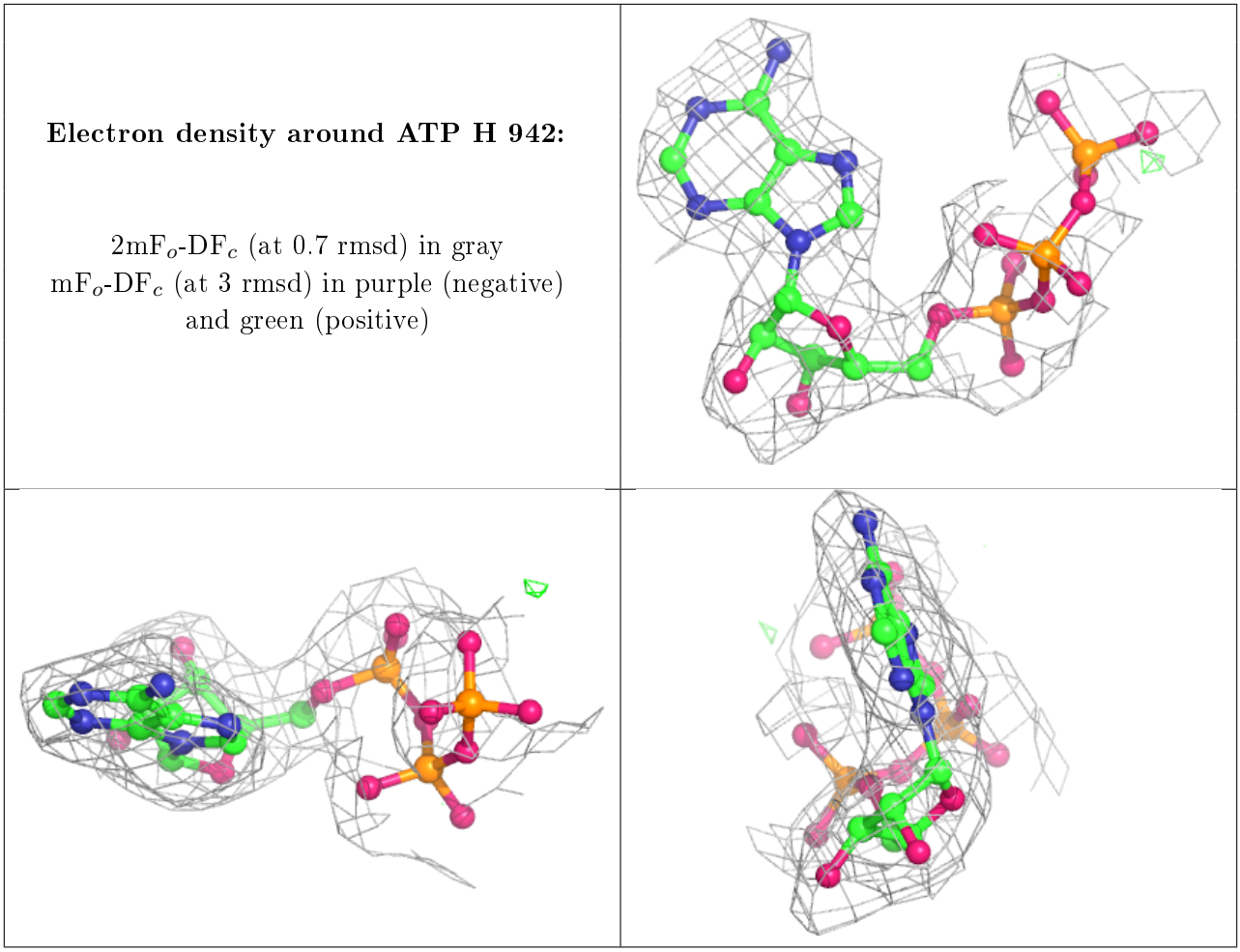
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ATP	F	942	31/31	0.95	0.17	83,87,104,105	0
4	SO4	E	995	5/5	0.96	0.14	95,99,100,100	0
4	SO4	I	353	5/5	0.96	0.22	91,95,97,97	0
4	SO4	E	992	5/5	0.96	0.16	94,99,100,100	0
4	SO4	J	353	5/5	0.96	0.17	83,87,88,88	0
4	SO4	C	992	5/5	0.96	0.17	61,65,65,66	0
4	SO4	I	352	5/5	0.96	0.19	66,69,71,71	0
4	SO4	E	991	5/5	0.96	0.15	66,70,72,72	0
4	SO4	G	995	5/5	0.97	0.16	96,101,101,102	0
4	SO4	G	994	5/5	0.97	0.17	86,89,92,92	0
4	SO4	A	992	5/5	0.97	0.15	76,80,80,82	0
5	ATP	D	942	31/31	0.97	0.16	38,42,53,56	0
4	SO4	E	993	5/5	0.97	0.16	93,97,99,99	0
4	SO4	C	994	5/5	0.97	0.17	87,91,92,92	0
4	SO4	A	994	5/5	0.97	0.19	61,65,66,68	0
4	SO4	C	995	5/5	0.97	0.17	85,89,90,90	0
4	SO4	G	990	5/5	0.97	0.20	63,66,69,70	0
5	ATP	B	942	31/31	0.98	0.18	34,36,55,57	0
4	SO4	G	992	5/5	0.98	0.15	79,83,84,85	0
4	SO4	A	990	5/5	0.98	0.14	70,74,75,76	0
4	SO4	F	944	5/5	0.98	0.18	79,84,84,85	0
4	SO4	A	996	5/5	0.98	0.19	45,48,50,53	0
4	SO4	H	943	5/5	0.98	0.20	69,73,74,75	0
4	SO4	A	993	5/5	0.98	0.14	82,87,88,88	0
4	SO4	F	943	5/5	0.98	0.18	68,73,74,74	0
4	SO4	G	991	5/5	0.98	0.18	55,58,60,61	0
4	SO4	A	991	5/5	0.98	0.15	57,61,62,64	0
4	SO4	C	990	5/5	0.98	0.19	43,45,48,50	0
4	SO4	C	996	5/5	0.98	0.21	46,49,51,53	0
4	SO4	C	993	5/5	0.98	0.17	57,60,61,64	0
4	SO4	B	944	5/5	0.99	0.21	36,40,41,42	0
4	SO4	C	991	5/5	0.99	0.17	58,61,63,65	0
4	SO4	B	943	5/5	0.99	0.21	45,49,50,50	0
4	SO4	D	945	5/5	0.99	0.19	49,53,55,55	0
4	SO4	H	945	5/5	0.99	0.17	59,64,65,66	0
4	SO4	D	943	5/5	0.99	0.22	33,36,38,40	0
4	SO4	A	999	5/5	0.99	0.19	46,50,51,52	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.

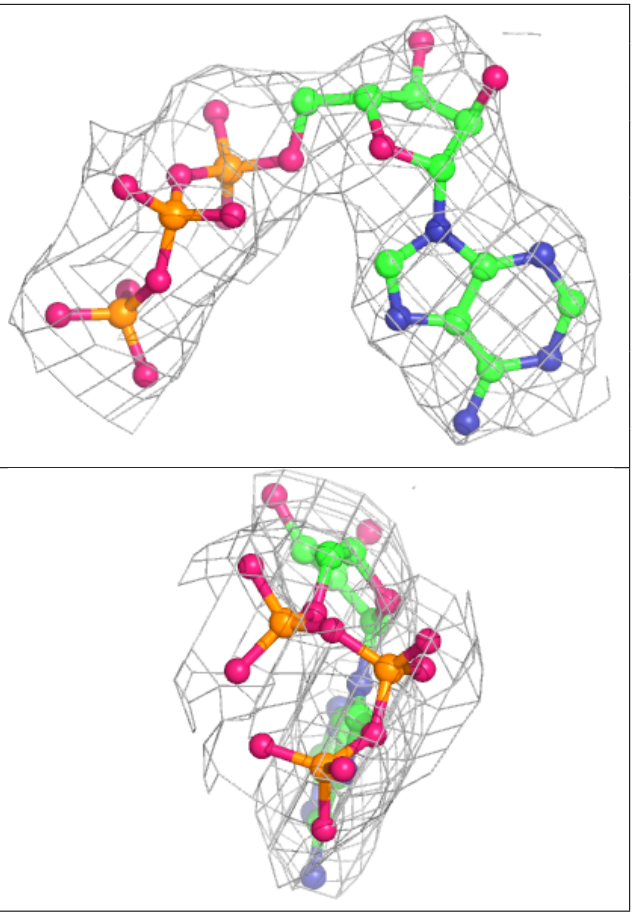
Electron density around ATP H 942:

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



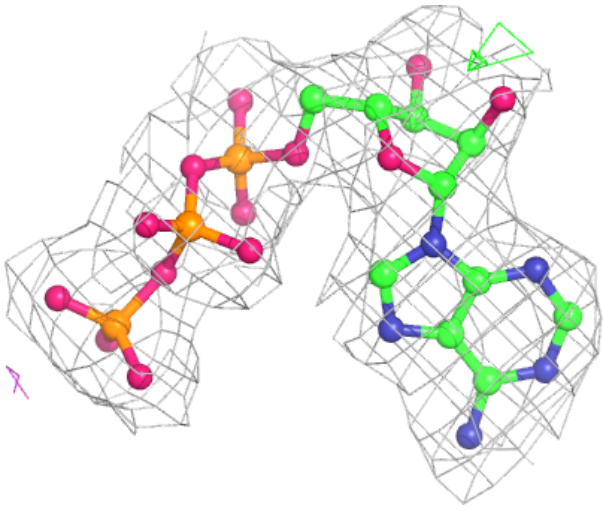
Electron density around ATP F 942:

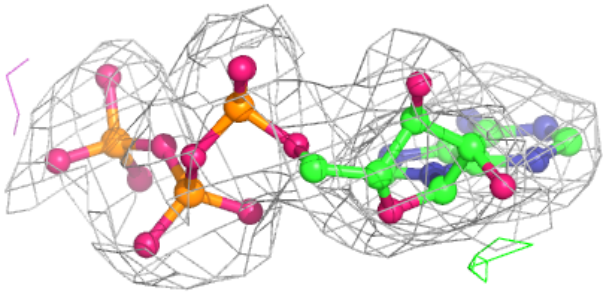
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

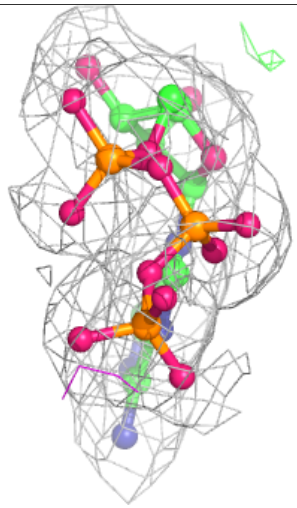


Electron density around ATP D 942:

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

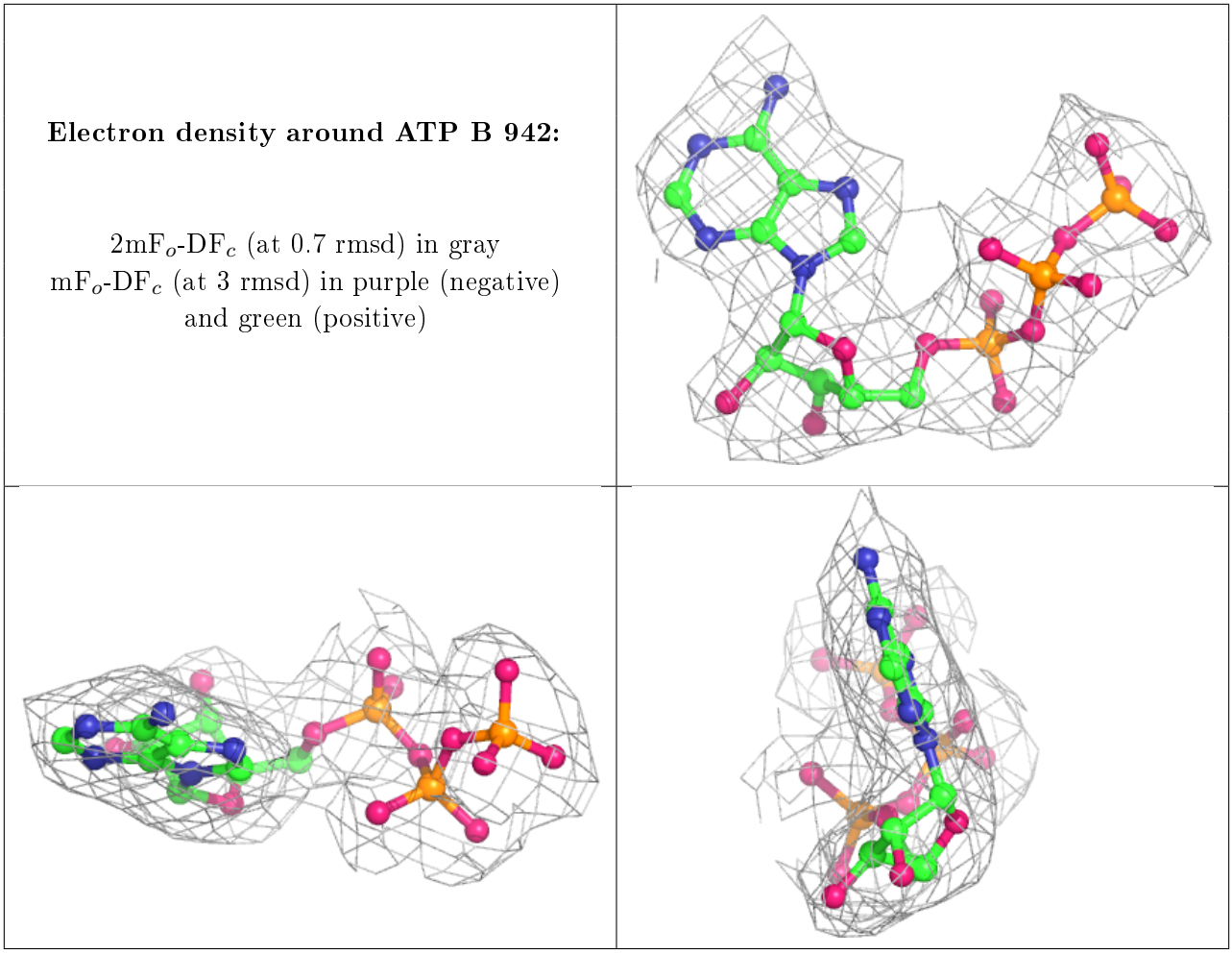






Electron density around ATP B 942:

$2mF_o$-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.