Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 07:29 PM JST

PDB ID	:	6JWW
Title	:	Crystal structure of Plasmodium falciparum HPPK-DHPS S436F/A437G/A613T triple mutant with STZ-DHP
Authors	:	Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on	:	2019-04-21
Resolution	:	2.75 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:

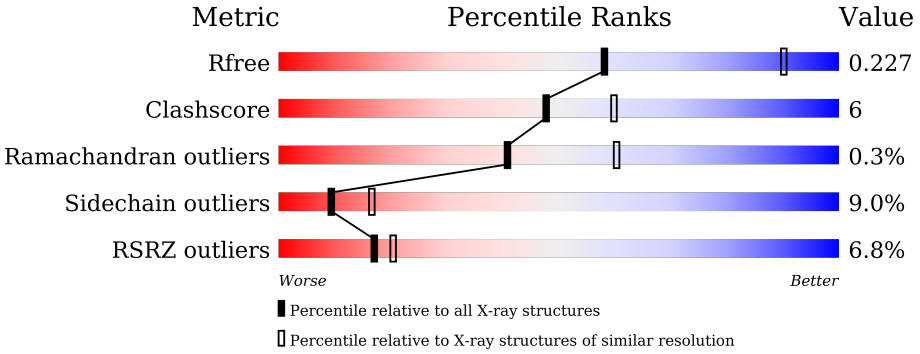
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	728	5% 59% 14% • 25%
1	B	728	6% 58% 17% • 23%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9518 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 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihyd ropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	544	4502	2902	740	838	22	0	0	0
			Total	C	N	O	S			
1	B	559	4616	2974	757	862	23	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	PHE	SER	engineered mutation	UNP Q25704
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	613	THR	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag	UNP Q25704
A	714	VAL	-	expression tag	UNP Q25704
A	715	ASP	-	expression tag	UNP Q25704
A	716	LYS	-	expression tag	UNP Q25704
A	717	LEU	-	expression tag	UNP Q25704
A	718	ALA	-	expression tag	UNP Q25704
A	719	ALA	-	expression tag	UNP Q25704
A	720	ALA	-	expression tag	UNP Q25704
A	721	LEU	-	expression tag	UNP Q25704
A	722	GLU	-	expression tag	UNP Q25704
A	723	HIS	-	expression tag	UNP Q25704
A	724	HIS	-	expression tag	UNP Q25704
A	725	HIS	-	expression tag	UNP Q25704
A	726	HIS	-	expression tag	UNP Q25704
A	727	HIS	-	expression tag	UNP Q25704

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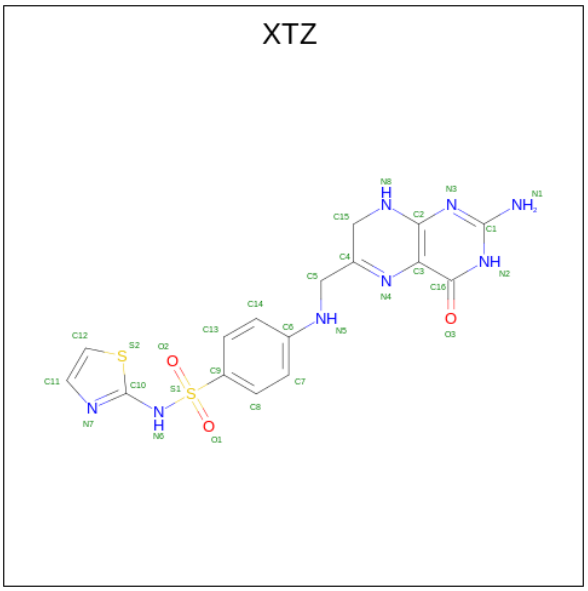
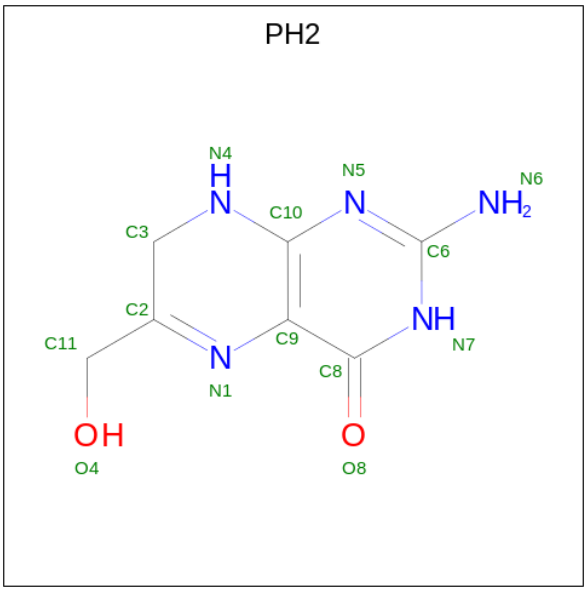
Chain	Residue	Modelled	Actual	Comment	Reference
A	728	HIS	-	expression tag	UNP Q25704
B	436	PHE	SER	engineered mutation	UNP Q25704
B	437	GLY	ALA	engineered mutation	UNP Q25704
B	613	THR	ALA	engineered mutation	UNP Q25704
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	UNP Q25704
B	714	VAL	-	expression tag	UNP Q25704
B	715	ASP	-	expression tag	UNP Q25704
B	716	LYS	-	expression tag	UNP Q25704
B	717	LEU	-	expression tag	UNP Q25704
B	718	ALA	-	expression tag	UNP Q25704
B	719	ALA	-	expression tag	UNP Q25704
B	720	ALA	-	expression tag	UNP Q25704
B	721	LEU	-	expression tag	UNP Q25704
B	722	GLU	-	expression tag	UNP Q25704
B	723	HIS	-	expression tag	UNP Q25704
B	724	HIS	-	expression tag	UNP Q25704
B	725	HIS	-	expression tag	UNP Q25704
B	726	HIS	-	expression tag	UNP Q25704
B	727	HIS	-	expression tag	UNP Q25704
B	728	HIS	-	expression tag	UNP Q25704

- Molecule 2 is 4-{[(2-amino-4-oxo-3,4,7,8-tetrahydropteridin-6-yl)methyl]amino}-N-(1,3-thiazol-2-yl)benzenesulfonamide (three-letter code: XTZ) (formula: $C_{16}H_{16}N_8O_3S_2$).



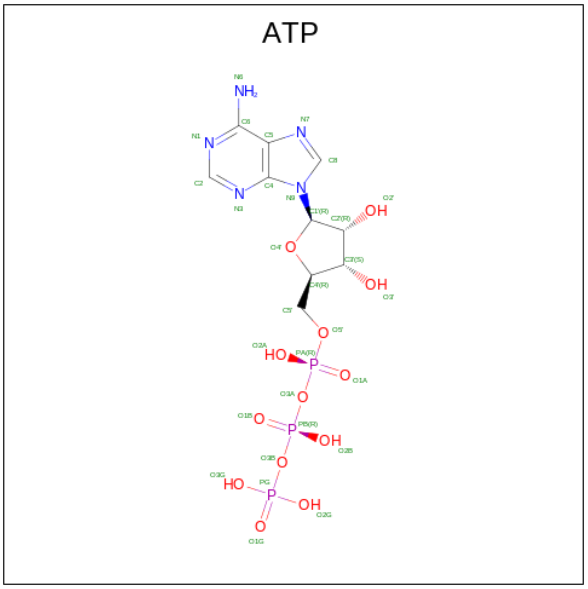
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	29	16	8	3	2	0	0
			Total	C	N	O	S		
2	B	1	29	16	8	3	2	0	0

- Molecule 3 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (three-letter code: PH2) (formula: $C_7H_9N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	7	5	2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

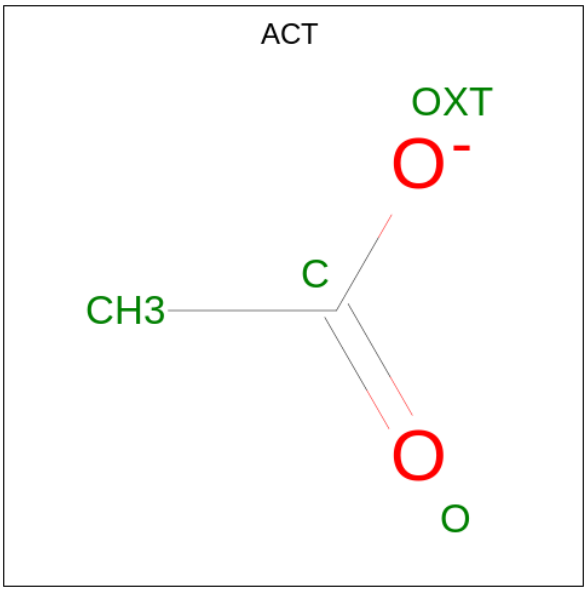


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

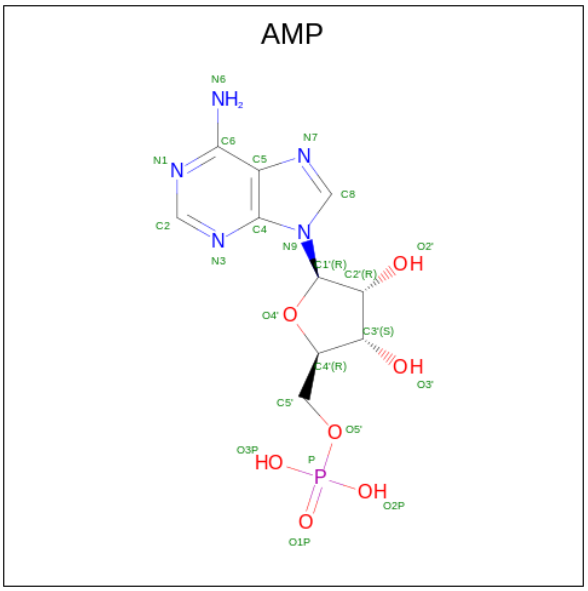


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	B	1	4	2	2	0	0
			Total	C	O		
6	B	1	4	2	2	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	B	1	1	1	0	0

- Molecule 8 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	23	10	5	7	1	0	0

- Molecule 9 is water.

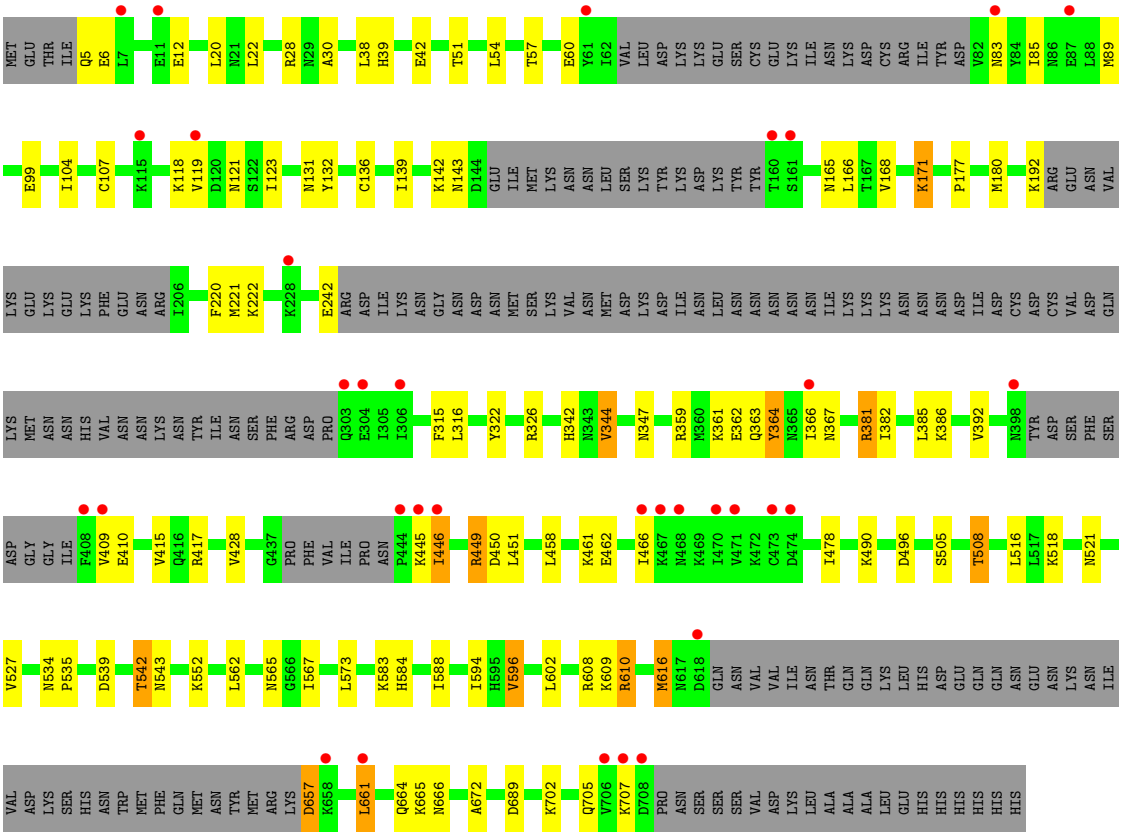
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	134	134	134	0	0
			Total	O		
9	B	120	120	120	0	0

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.

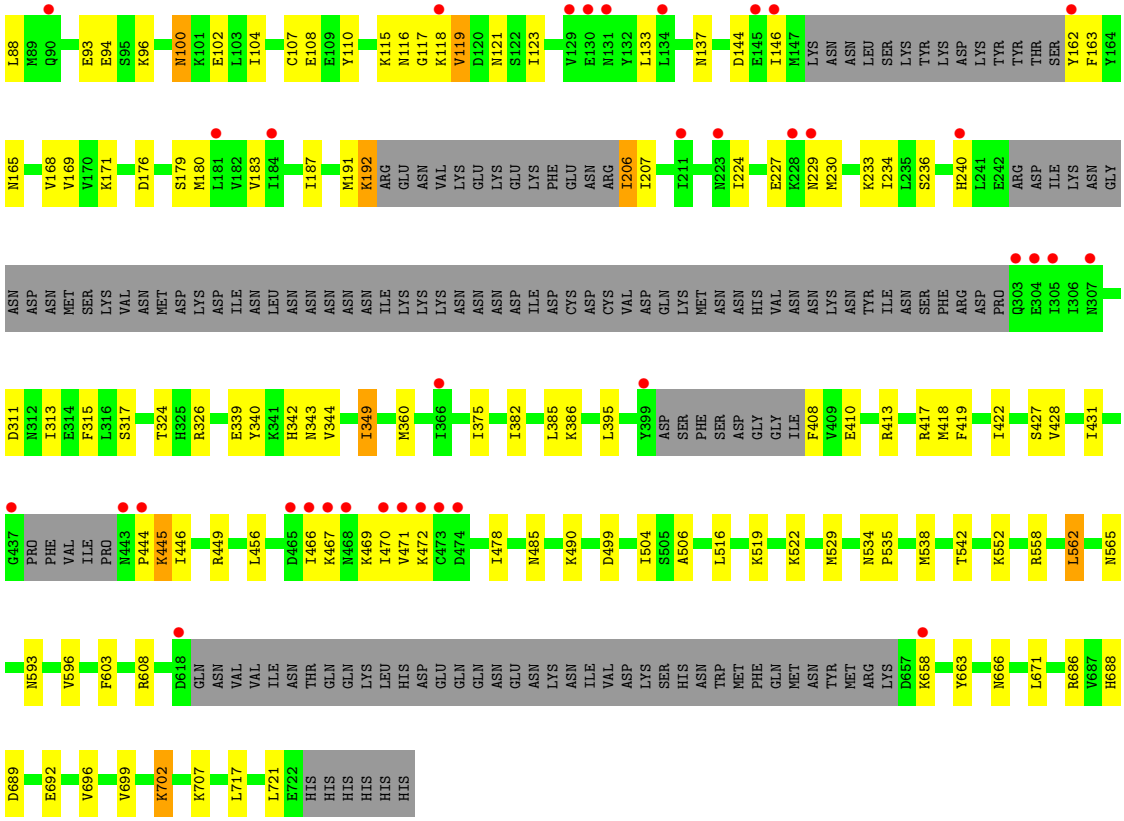
• Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase

Chain A:



• Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase

Chain B:


L88 M89 Q90 E93 E94 S95 K96 N100 K101 E102 L103 I104 C107 E108 E109 Y110 K115 N116 G117 K118 V119 D120 N121 S122 I123 V129 E130 N131 Y132 L133 L134 N137 D144 E145 I146 M147 LYS ASN ASN LEU SER LYS TYR LYS ASP LYS TYR TYR THR SER Y162 F163 Y164
N165 V168 V169 V170 K171 D176 S179 M180 L181 V182 V183 I184 I187 M191 K192 ARG GLU ASN VAL LYS GLU LYS GLU LYS PHE GLU ASN ARG I206 I207 I211 N223 I224 E227 K228 N229 M230 K233 I234 L235 S236 H240 L241 E242 ARG ASP ILE LYS ASN GLY
ASN ASP ASN MET SER LYS VAL ASN MET ASP LYS ASP ILE ASN LEU ASN ASN ASN ASN ASN ILE LYS LYS LYS LYS ASN ASN ASN ASP ILE ASP CYS ASP CYS VAL ASP GLN LYS MET ASN ASN HIS VAL ASN ASN LYS ASN TYR ILE ASN SER PHE ARG ASP PRO Q303 E304 I305 I306 N307
D311 N312 I313 E314 F315 L316 S317 T324 H325 R326 E339 Y340 K341 H342 N343 V344 I349 M360 I366 I375 I382 L385 K386 L395 Y399 ASP SER PHE SER ASP GLY GLY ILE F408 V409 E410 R413 R417 M418 F419 I422 S427 V428 I431
G437 PRO PHE VAL ILE PRO N443 P444 K445 I446 R449 L456 D465 I466 K467 N468 K469 I470 V471 K472 G473 D474 I478 N485 K490 D499 I504 S505 A506 L516 K519 K522 M529 N534 P535 M538 T542 K552 R558 L562 N565
N593 V596 F603 R608 D618 GLN ASN VAL VAL ILE ASN THR GLN GLN LYS LEU HIS ASP GLU GLN GLN ASN GLU ASN LYS ASN ILE VAL ASP LYS SER HIS ASN TRP MET PHE GLN MET ASN TYR MET ARG LYS D657 K658 Y663 N666 L671 R686 V687 H688
D689 E692 V696 V699 K702 K707 L717 L721 E722 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.63Å 136.12Å 138.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 29.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	79.4 (30.00-2.75) 79.5 (29.53-2.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.54 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.205 , 0.234 0.200 , 0.227	Depositor DCC
R_{free} test set	3999 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9518	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, XTZ, MG, ACT, CA, AMP, PH2

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	0.46	0/4572	0.67	0/6164
1	B	0.46	0/4688	0.69	1/6322 (0.0%)
All	All	0.46	0/9260	0.68	1/12486 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	562	LEU	CA-CB-CG	5.57	128.10	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4502	0	4599	55	0
1	B	4616	0	4709	63	0
2	A	29	0	16	1	0
2	B	29	0	16	0	0
3	A	14	0	9	2	0
4	A	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	6	0	0
6	B	8	0	6	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	23	0	12	1	0
9	A	134	0	0	2	0
9	B	120	0	0	4	0
All	All	9518	0	9385	114	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.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:171:LYS:HE3	2.01	0.99
1:A:51:THR:HG22	1:A:168:VAL:HG12	1.57	0.85
1:B:104:ILE:H	1:B:565:ASN:HD21	1.29	0.78
1:B:552:LYS:HD2	1:B:596:VAL:HG13	1.66	0.77
1:A:104:ILE:H	1:A:565:ASN:HD21	1.34	0.76
1:B:227:GLU:HB3	1:B:229:ASN:OD1	1.86	0.76
1:A:107:CYS:SG	1:A:171:LYS:CE	2.74	0.75
1:A:428:VAL:HG22	1:A:478:ILE:HB	1.68	0.75
1:B:469:LYS:HB3	1:B:472:LYS:HG2	1.69	0.75
1:A:42:GLU:HG3	1:A:99:GLU:OE2	1.85	0.74
1:A:657:ASP:O	1:A:661:LEU:HB2	1.87	0.74
1:A:608:ARG:HA	1:A:666:ASN:OD1	1.88	0.74
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.70	0.74
1:B:395:LEU:HD22	1:B:418:MET:HG3	1.70	0.72
1:A:665:LYS:HD2	9:A:941:HOH:O	1.94	0.67
1:A:364:TYR:HB3	1:A:366:ILE:HD12	1.78	0.66
1:B:191:MET:O	1:B:192:LYS:HB2	1.97	0.63
1:A:57:THR:HG21	1:A:165:ASN:OD1	1.97	0.63
1:A:527:VAL:HG22	1:A:573:LEU:HD12	1.80	0.63
1:A:542:THR:HG21	1:A:583:LYS:HE2	1.80	0.62
1:A:20:LEU:HD21	1:A:180:MET:HE1	1.83	0.61
1:A:392:VAL:HG22	1:A:428:VAL:HB	1.84	0.59
1:B:110:TYR:HE1	1:B:169:VAL:HG11	1.67	0.58
1:B:431:ILE:HG21	1:B:456:LEU:HD21	1.85	0.58
1:A:118:LYS:HG2	1:A:119:VAL:O	2.04	0.58
1:A:385:LEU:HG	1:A:386:LYS:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:CD2	1:B:418:MET:HG3	2.35	0.57
1:B:428:VAL:HG22	1:B:478:ILE:HB	1.86	0.57
1:A:505:SER:O	1:A:508:THR:HB	2.05	0.56
1:B:100:ASN:CB	1:B:102:GLU:HG2	2.35	0.56
1:B:18:ALA:HB1	1:B:180:MET:HE1	1.88	0.56
1:B:608:ARG:HG3	1:B:688:HIS:HD2	1.71	0.56
1:B:445:LYS:HG2	1:B:445:LYS:O	2.07	0.55
1:B:110:TYR:CE1	1:B:169:VAL:HG11	2.42	0.54
1:B:115:LYS:O	1:B:116:ASN:HB2	2.07	0.53
1:A:20:LEU:HD21	1:A:180:MET:CE	2.39	0.53
1:B:608:ARG:HA	1:B:666:ASN:OD1	2.08	0.53
1:A:220:PHE:HE1	1:A:222:LYS:HD3	1.74	0.53
1:A:221:MET:O	1:A:315:PHE:HB2	2.09	0.53
1:B:395:LEU:HD22	1:B:418:MET:CG	2.39	0.53
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.90	0.53
1:B:206:ILE:HG23	1:B:207:ILE:HG22	1.89	0.53
1:A:326:ARG:NH2	3:A:802:PH2:H32	2.24	0.52
1:A:342:HIS:CD2	1:A:344:VAL:H	2.28	0.52
1:B:107:CYS:SG	1:B:171:LYS:NZ	2.77	0.51
1:B:187:ILE:HG22	1:B:191:MET:HE2	1.92	0.51
1:B:121:ASN:ND2	1:B:121:ASN:H	2.09	0.51
1:B:230:MET:O	1:B:234:ILE:HG12	2.11	0.51
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.83	0.50
1:B:121:ASN:H	1:B:121:ASN:HD22	1.59	0.50
1:A:28:ARG:HH11	1:A:381:ARG:HH21	1.60	0.50
1:B:385:LEU:HG	1:B:386:LYS:HG2	1.94	0.50
1:B:60:GLU:HG3	1:B:326:ARG:HG2	1.94	0.50
1:B:179:SER:O	1:B:183:VAL:HG23	2.12	0.50
1:B:57:THR:HG23	1:B:163:PHE:HB2	1.94	0.49
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.93	0.49
1:B:593:ASN:O	1:B:596:VAL:HB	2.13	0.48
1:B:485:ASN:HB2	9:B:934:HOH:O	2.13	0.48
1:B:45:LEU:HD22	1:B:180:MET:HG3	1.95	0.48
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.44	0.48
1:B:100:ASN:HB2	1:B:102:GLU:HG2	1.95	0.48
1:B:229:ASN:OD1	1:B:230:MET:N	2.46	0.48
1:A:446:ILE:HD12	1:A:451:LEU:HG	1.94	0.48
1:B:317:SER:O	8:B:802:AMP:N6	2.42	0.48
1:B:100:ASN:HB3	1:B:102:GLU:HG2	1.96	0.47
1:A:449:ARG:HG3	1:A:450:ASP:N	2.28	0.47
1:B:419:PHE:HA	1:B:422:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:LEU:HD11	1:B:692:GLU:HB3	1.96	0.47
1:A:490:LYS:HD3	1:A:516:LEU:HD22	1.96	0.46
1:B:85:ILE:HA	1:B:88:LEU:HG	1.97	0.46
1:B:717:LEU:O	1:B:721:LEU:HG	2.15	0.46
1:B:227:GLU:HB2	1:B:230:MET:HB2	1.98	0.46
1:B:117:GLY:O	1:B:119:VAL:HG22	2.15	0.46
1:B:339:GLU:HB2	9:B:971:HOH:O	2.15	0.45
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.97	0.45
1:A:22:LEU:HD12	1:A:166:LEU:HD23	1.98	0.45
1:B:686:ARG:HB3	9:B:920:HOH:O	2.16	0.45
1:A:132:TYR:CZ	1:A:136:CYS:SG	3.11	0.44
1:A:584:HIS:CE1	1:A:610:ARG:HB3	2.52	0.44
1:B:342:HIS:HD2	1:B:344:VAL:H	1.66	0.44
1:B:96:LYS:HE3	1:B:240:HIS:HD2	1.81	0.44
1:B:224:ILE:HD12	1:B:315:PHE:HA	2.00	0.44
1:A:342:HIS:HD2	1:A:344:VAL:H	1.65	0.44
1:B:30:ALA:HB3	1:B:382:ILE:HD11	1.99	0.44
1:A:594:ILE:HD11	1:A:602:LEU:HD21	2.00	0.44
1:A:57:THR:HG23	3:A:802:PH2:HN62	1.84	0.43
1:A:22:LEU:HB2	1:A:166:LEU:HB3	2.00	0.43
1:A:30:ALA:HB3	1:A:382:ILE:HD11	2.00	0.43
1:B:123:ILE:HG21	1:B:176:ASP:HB3	2.01	0.43
1:A:609:LYS:NZ	2:A:801:XTZ:O3	2.52	0.43
1:B:229:ASN:O	1:B:233:LYS:N	2.44	0.43
1:A:518:LYS:HD2	1:A:567:ILE:HD13	2.00	0.43
1:A:89:MET:HG3	1:A:521:ASN:OD1	2.17	0.43
1:A:672:ALA:HB2	1:B:696:VAL:HA	2.00	0.43
1:A:616:MET:HE1	1:B:699:VAL:HG23	2.01	0.43
1:A:588:ILE:HD13	1:B:702:LYS:HD2	2.01	0.42
1:B:504:ILE:HA	1:B:529:MET:HB3	2.02	0.42
1:B:340:TYR:HB3	1:B:349:ILE:HD13	2.00	0.42
1:A:39:HIS:NE2	1:A:521:ASN:O	2.53	0.42
1:A:132:TYR:CD2	1:A:344:VAL:HG21	2.55	0.42
1:A:139:ILE:O	1:A:143:ASN:ND2	2.52	0.42
1:A:361:LYS:HE3	1:A:367:ASN:HA	2.01	0.42
1:B:506:ALA:HB1	1:B:558:ARG:HG3	2.01	0.42
1:B:39:HIS:CE1	1:B:519:LYS:O	2.73	0.41
1:A:322:TYR:HB3	1:A:326:ARG:HG3	2.02	0.41
1:B:490:LYS:HD3	1:B:516:LEU:HD21	2.01	0.41
1:A:38:LEU:CD2	1:A:168:VAL:HG11	2.51	0.41
1:A:616:MET:CE	1:B:699:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HB2	1:B:168:VAL:HG22	2.03	0.41
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.51	0.41
1:A:415:VAL:HG21	1:A:458:LEU:HB3	2.02	0.40
1:B:538:MET:HE3	9:B:928:HOH:O	2.21	0.40
1:A:496:ASP:HA	9:A:957:HOH:O	2.21	0.40
1:A:542:THR:O	1:A:542:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/728 (72%)	501 (95%)	25 (5%)	2 (0%)	34	53
1	B	543/728 (75%)	523 (96%)	19 (4%)	1 (0%)	47	69
All	All	1071/1456 (74%)	1024 (96%)	44 (4%)	3 (0%)	41	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	444	PRO
1	A	409	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	519/697 (74%)	476 (92%)	43 (8%)	11 20
1	B	531/697 (76%)	479 (90%)	52 (10%)	8 13
All	All	1050/1394 (75%)	955 (91%)	95 (9%)	9 16

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	12	GLU
1	A	54	LEU
1	A	60	GLU
1	A	83	ASN
1	A	85	ILE
1	A	121	ASN
1	A	123	ILE
1	A	131	ASN
1	A	142	LYS
1	A	171	LYS
1	A	192	LYS
1	A	242	GLU
1	A	344	VAL
1	A	347	ASN
1	A	359	ARG
1	A	362	GLU
1	A	363	GLN
1	A	364	TYR
1	A	381	ARG
1	A	410	GLU
1	A	417	ARG
1	A	445	LYS
1	A	446	ILE
1	A	449	ARG
1	A	461	LYS
1	A	462	GLU
1	A	466	ILE
1	A	508	THR
1	A	539	ASP
1	A	542	THR
1	A	543	ASN
1	A	562	LEU
1	A	596	VAL
1	A	610	ARG

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Mol	Chain	Res	Type
1	A	616	MET
1	A	657	ASP
1	A	661	LEU
1	A	664	GLN
1	A	689	ASP
1	A	702	LYS
1	A	705	GLN
1	A	707	LYS
1	B	7	LEU
1	B	11	GLU
1	B	21	ASN
1	B	22	LEU
1	B	25	ASN
1	B	27	ARG
1	B	54	LEU
1	B	61	TYR
1	B	62	ILE
1	B	93	GLU
1	B	94	GLU
1	B	100	ASN
1	B	108	GLU
1	B	118	LYS
1	B	119	VAL
1	B	133	LEU
1	B	137	ASN
1	B	144	ASP
1	B	146	ILE
1	B	162	TYR
1	B	165	ASN
1	B	192	LYS
1	B	206	ILE
1	B	236	SER
1	B	311	ASP
1	B	313	ILE
1	B	324	THR
1	B	343	ASN
1	B	349	ILE
1	B	360	MET
1	B	408	PHE
1	B	410	GLU
1	B	413	ARG
1	B	417	ARG

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Mol	Chain	Res	Type
1	B	427	SER
1	B	445	LYS
1	B	446	ILE
1	B	449	ARG
1	B	466	ILE
1	B	467	LYS
1	B	470	ILE
1	B	471	VAL
1	B	499	ASP
1	B	522	LYS
1	B	542	THR
1	B	562	LEU
1	B	603	PHE
1	B	658	LYS
1	B	663	TYR
1	B	689	ASP
1	B	702	LYS
1	B	707	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	29	ASN
1	A	83	ASN
1	A	86	ASN
1	A	100	ASN
1	A	240	HIS
1	A	342	HIS
1	A	468	ASN
1	A	565	ASN
1	A	614	HIS
1	A	688	HIS
1	B	29	ASN
1	B	39	HIS
1	B	121	ASN
1	B	131	ASN
1	B	175	ASN
1	B	240	HIS
1	B	308	ASN
1	B	342	HIS
1	B	460	GLN

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Mol	Chain	Res	Type
1	B	495	ASN
1	B	565	ASN
1	B	660	GLN
1	B	688	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	ACT	B	805	-	3,3,3	0.74	0	3,3,3	0.76	0
4	ATP	A	803	5	26,33,33	0.98	1 (3%)	31,52,52	1.40	4 (12%)
6	ACT	B	804	-	3,3,3	0.74	0	3,3,3	0.74	0
2	XTZ	B	801	-	26,32,32	2.50	3 (11%)	28,46,46	2.49	7 (25%)
3	PH2	A	802	-	10,15,15	1.20	2 (20%)	10,21,21	2.57	4 (40%)
6	ACT	A	805	-	3,3,3	0.81	0	3,3,3	0.46	0
6	ACT	A	806	-	3,3,3	0.80	0	3,3,3	0.53	0
2	XTZ	A	801	-	26,32,32	2.43	4 (15%)	28,46,46	2.17	6 (21%)
8	AMP	B	802	5	22,25,25	1.04	1 (4%)	25,38,38	1.37	3 (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
4	ATP	A	803	5	-	2/18/38/38	0/3/3/3
2	XTZ	B	801	-	-	0/12/25/25	0/4/4/4
3	PH2	A	802	-	-	0/0/11/11	0/2/2/2
2	XTZ	A	801	-	-	9/12/25/25	0/4/4/4
8	AMP	B	802	5	-	2/6/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	XTZ	C9-S1	-11.28	1.59	1.76
2	A	801	XTZ	C9-S1	-10.81	1.59	1.76
2	A	801	XTZ	C3-C2	3.55	1.48	1.40
2	B	801	XTZ	C3-C2	3.24	1.48	1.40
8	B	802	AMP	C5-C4	2.68	1.48	1.40
4	A	803	ATP	C5-C4	2.63	1.47	1.40
2	A	801	XTZ	C16-N2	-2.55	1.34	1.38
2	B	801	XTZ	C10-N6	-2.54	1.35	1.40
3	A	802	PH2	C9-C10	2.36	1.48	1.41
2	A	801	XTZ	C10-N6	-2.13	1.36	1.40
3	A	802	PH2	C9-N1	-2.12	1.34	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	XTZ	O2-S1-O1	-9.76	107.55	119.55
2	A	801	XTZ	O2-S1-O1	-8.54	109.05	119.55
3	A	802	PH2	C10-C9-C8	5.01	117.81	114.53
2	B	801	XTZ	C1-N3-C2	4.79	122.07	113.43
2	A	801	XTZ	C1-N3-C2	4.12	120.87	113.43
3	A	802	PH2	C9-C8-N7	-4.10	117.83	123.43
4	A	803	ATP	N3-C2-N1	-4.07	122.32	128.68
8	B	802	AMP	N3-C2-N1	-3.53	123.17	128.68
3	A	802	PH2	C6-N7-C8	3.51	121.50	115.93
2	A	801	XTZ	O1-S1-C9	3.29	112.02	107.97
2	B	801	XTZ	O3-C16-C3	-2.88	118.96	126.60
8	B	802	AMP	C4-C5-N7	-2.77	106.51	109.40
4	A	803	ATP	PA-O3A-PB	-2.76	123.37	132.83
4	A	803	ATP	PB-O3B-PG	-2.67	123.68	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	PH2	C6-N5-C10	2.64	120.45	114.54
2	B	801	XTZ	C10-N6-S1	-2.52	119.57	124.16
2	B	801	XTZ	O2-S1-C9	2.49	111.03	107.97
2	A	801	XTZ	O3-C16-C3	-2.35	120.37	126.60
8	B	802	AMP	C3'-C2'-C1'	2.34	104.50	100.98
4	A	803	ATP	C2-N1-C6	2.31	122.70	118.75
2	B	801	XTZ	C3-N4-C4	2.30	120.80	116.24
2	A	801	XTZ	C3-N4-C4	2.21	120.62	116.24
2	A	801	XTZ	O1-S1-N6	2.10	111.99	106.73
2	B	801	XTZ	C3-C16-N2	2.04	118.38	113.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	XTZ	C10-N6-S1-C9
2	A	801	XTZ	C10-N6-S1-O2
2	A	801	XTZ	C14-C6-N5-C5
2	A	801	XTZ	C7-C6-N5-C5
2	A	801	XTZ	C8-C9-S1-O2
4	A	803	ATP	O4'-C4'-C5'-O5'
4	A	803	ATP	C3'-C4'-C5'-O5'
2	A	801	XTZ	C13-C9-S1-O2
8	B	802	AMP	O4'-C4'-C5'-O5'
2	A	801	XTZ	C4-C5-N5-C6
2	A	801	XTZ	C8-C9-S1-N6
2	A	801	XTZ	C13-C9-S1-N6
8	B	802	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

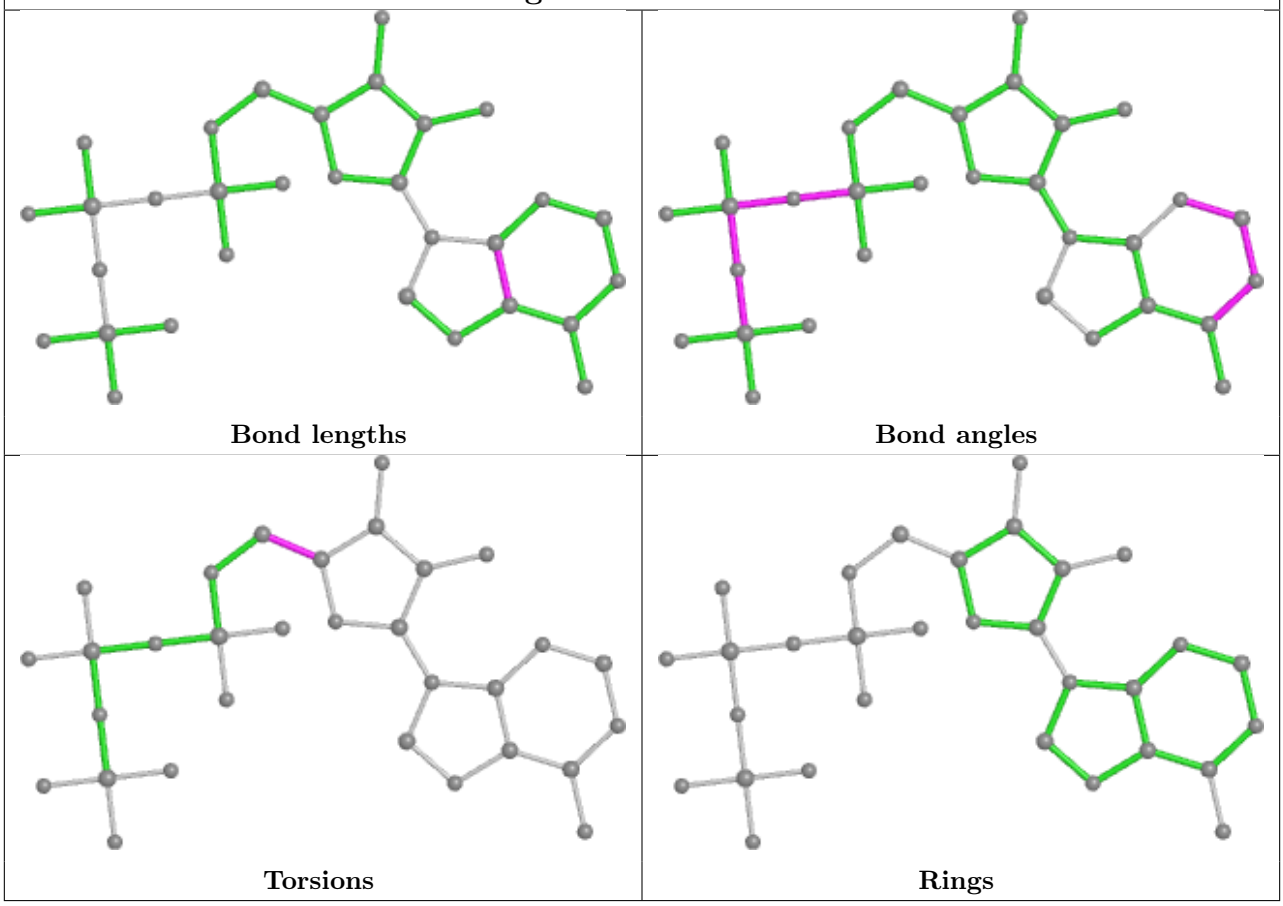
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PH2	2	0
2	A	801	XTZ	1	0
8	B	802	AMP	1	0

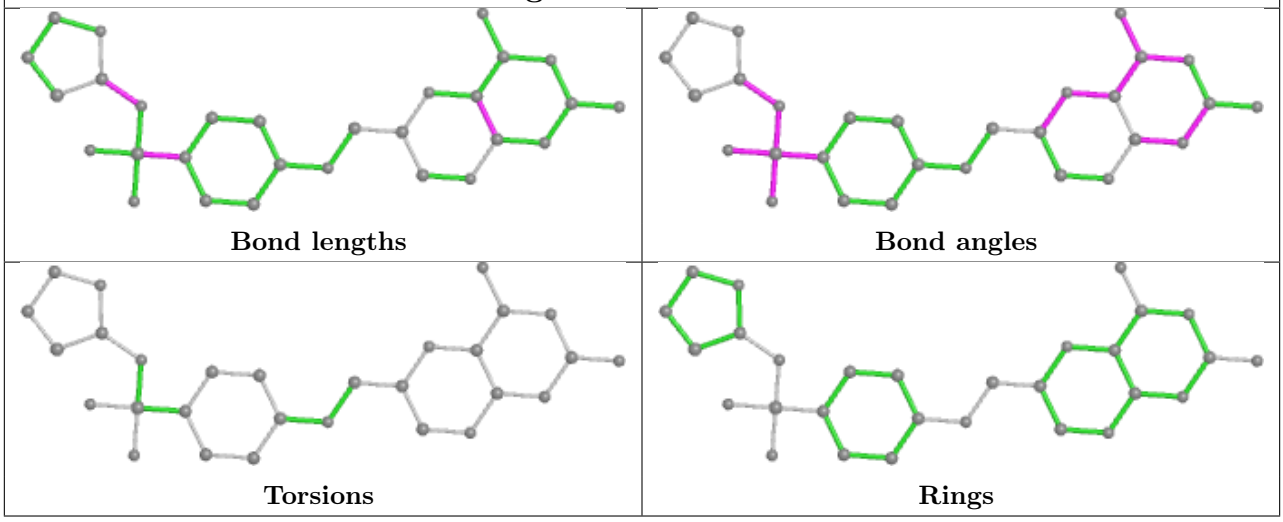
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

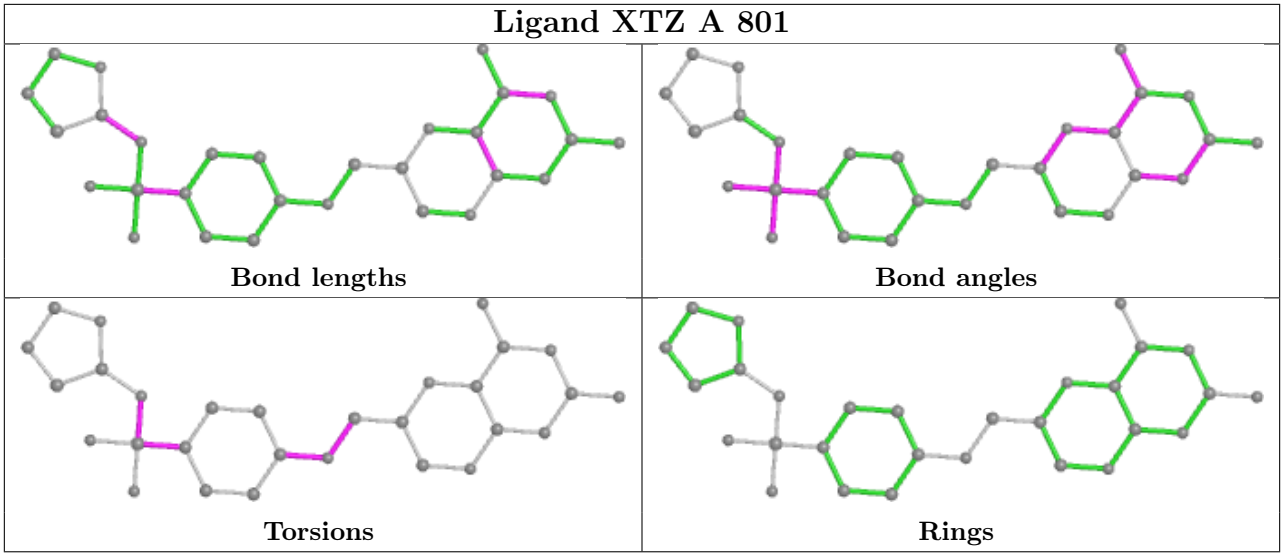
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

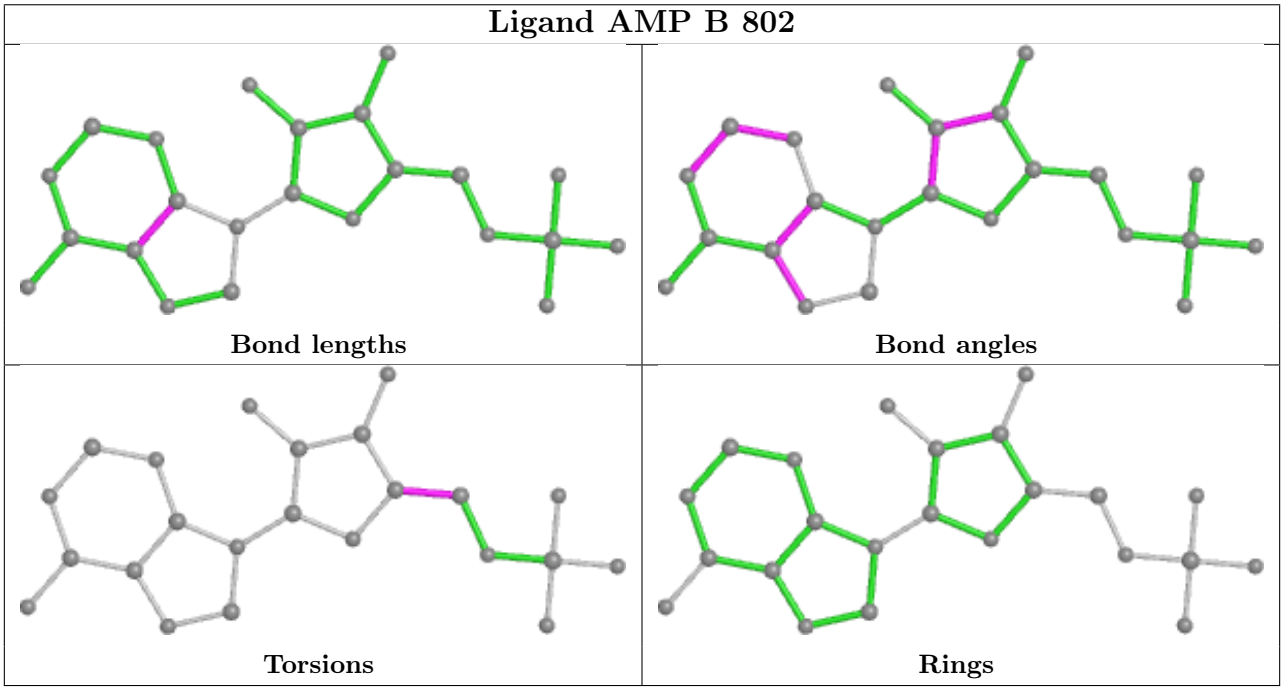
Ligand ATP A 803



Ligand XTZ B 801







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	544/728 (74%)	-0.01	33 (6%)	21	26	9, 27, 75, 120	0
1	B	559/728 (76%)	0.23	42 (7%)	14	17	10, 39, 95, 120	0
All	All	1103/1456 (75%)	0.11	75 (6%)	17	20	9, 32, 86, 120	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	ILE	7.8
1	B	473	CYS	7.3
1	B	471	VAL	7.0
1	A	471	VAL	6.5
1	A	468	ASN	6.0
1	A	473	CYS	5.8
1	B	468	ASN	5.4
1	B	466	ILE	4.8
1	A	467	LYS	4.7
1	B	467	LYS	4.6
1	B	87	GLU	4.5
1	A	160	THR	4.3
1	A	470	ILE	4.3
1	B	618	ASP	4.1
1	A	708	ASP	4.1
1	A	303	GLN	4.1
1	B	146	ILE	4.1
1	A	161	SER	3.9
1	B	84	TYR	3.9
1	A	408	PHE	3.8
1	B	304	GLU	3.6
1	A	366	ILE	3.6
1	B	145	GLU	3.6
1	A	409	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	131	ASN	3.3
1	B	437	GLY	3.3
1	A	61	TYR	3.2
1	B	223	ASN	3.2
1	A	445	LYS	3.0
1	B	474	ASP	3.0
1	A	119	VAL	3.0
1	B	444	PRO	3.0
1	A	304	GLU	2.9
1	B	228	LYS	2.9
1	B	240	HIS	2.8
1	A	466	ILE	2.8
1	B	12	GLU	2.8
1	B	399	TYR	2.8
1	A	618	ASP	2.7
1	A	474	ASP	2.7
1	B	27	ARG	2.7
1	B	211	ILE	2.7
1	A	11	GLU	2.6
1	B	184	ILE	2.6
1	A	658	LYS	2.6
1	B	307	ASN	2.5
1	B	11	GLU	2.5
1	B	134	LEU	2.5
1	A	83	ASN	2.5
1	B	465	ASP	2.4
1	A	707	LYS	2.4
1	B	90	GLN	2.4
1	A	87	GLU	2.4
1	B	118	LYS	2.3
1	B	28	ARG	2.3
1	B	129	VAL	2.3
1	A	446	ILE	2.3
1	B	472	LYS	2.2
1	A	444	PRO	2.2
1	A	661	LEU	2.2
1	B	130	GLU	2.2
1	B	303	GLN	2.2
1	A	306	ILE	2.1
1	B	162	TYR	2.1
1	B	443	ASN	2.1
1	A	706	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	2.1
1	A	228	LYS	2.0
1	B	181	LEU	2.0
1	B	658	LYS	2.0
1	B	305	ILE	2.0
1	B	366	ILE	2.0
1	B	229	ASN	2.0
1	A	398	ASN	2.0
1	A	115	LYS	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)

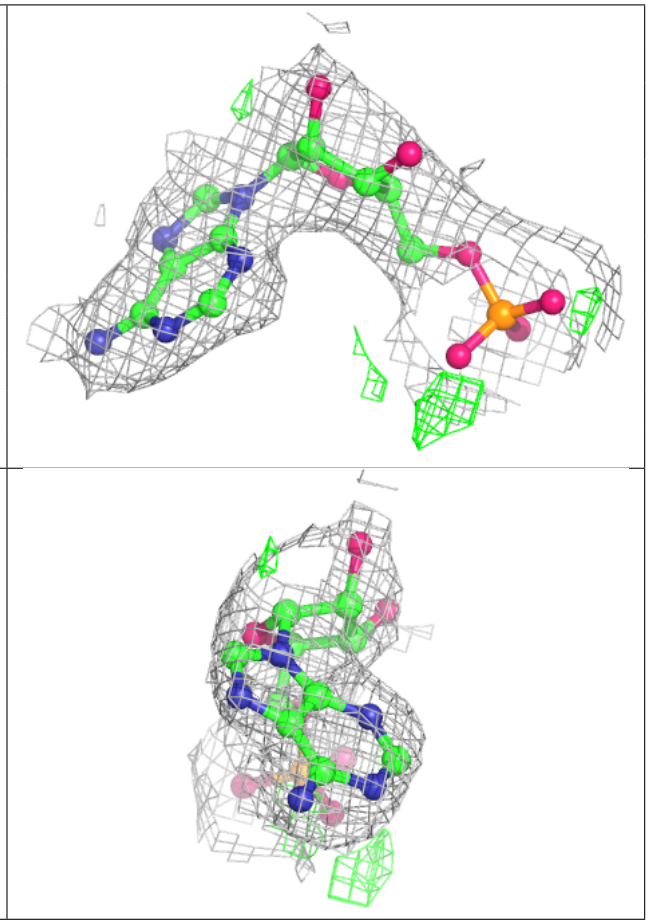
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	B	806	1/1	0.82	0.08	50,50,50,50	0
8	AMP	B	802	23/23	0.86	0.23	60,69,85,88	0
2	XTZ	A	801	29/29	0.88	0.24	14,24,55,59	0
5	MG	B	803	1/1	0.89	0.32	51,51,51,51	0
4	ATP	A	803	31/31	0.90	0.17	38,56,84,88	0
6	ACT	A	805	4/4	0.91	0.29	35,37,37,39	0
3	PH2	A	802	14/14	0.93	0.16	28,29,30,30	0
7	CA	A	807	1/1	0.94	0.10	32,32,32,32	0
6	ACT	B	805	4/4	0.95	0.17	36,36,37,38	0
2	XTZ	B	801	29/29	0.95	0.15	14,20,42,47	0
5	MG	A	804	1/1	0.97	0.16	17,17,17,17	0
6	ACT	A	806	4/4	0.97	0.17	30,30,31,31	0
6	ACT	B	804	4/4	0.98	0.13	19,19,19,20	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.

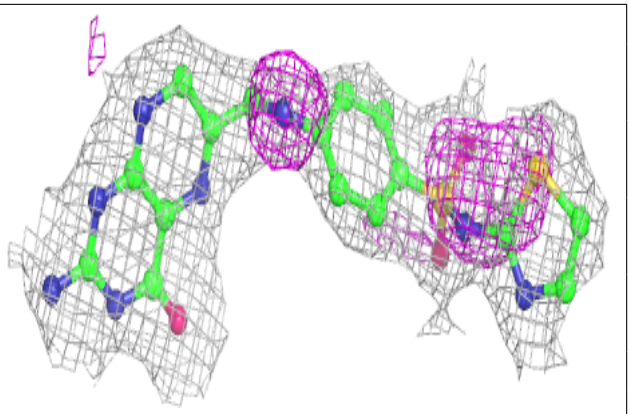
Electron density around AMP B 802:

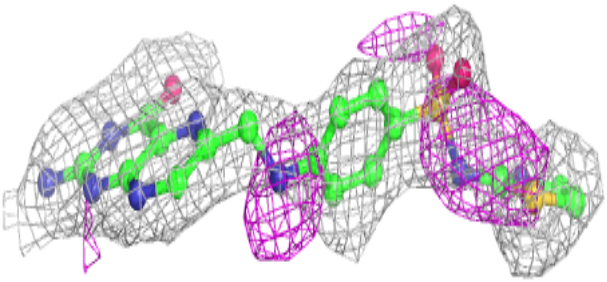
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

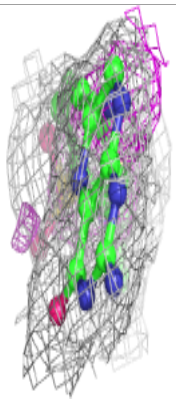


Electron density around XTZ A 801:

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

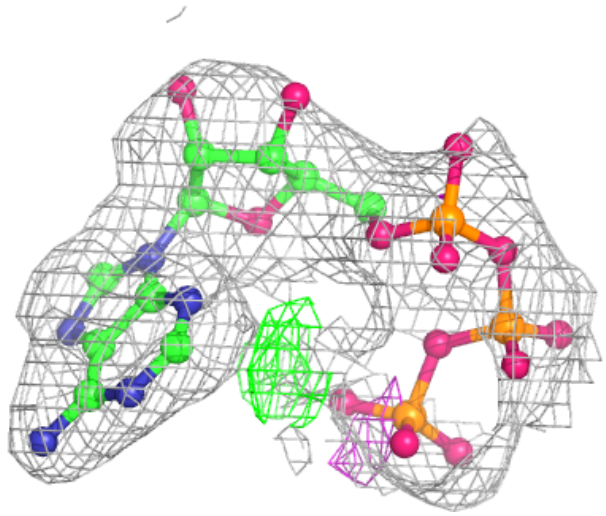


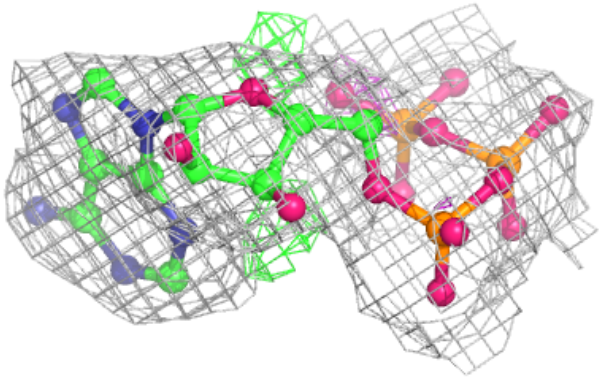


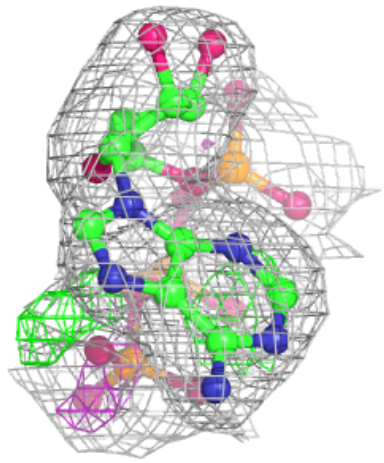


Electron density around ATP A 803:

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

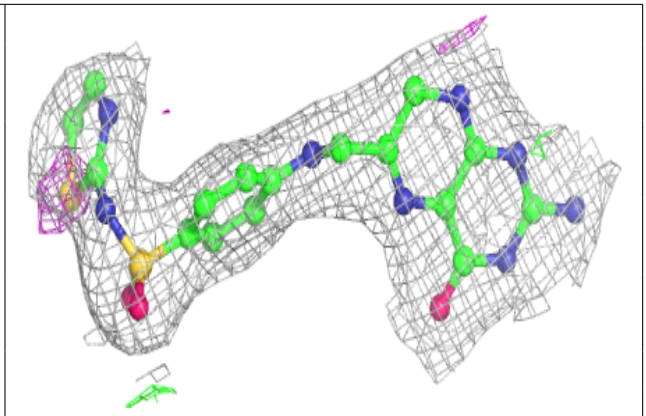


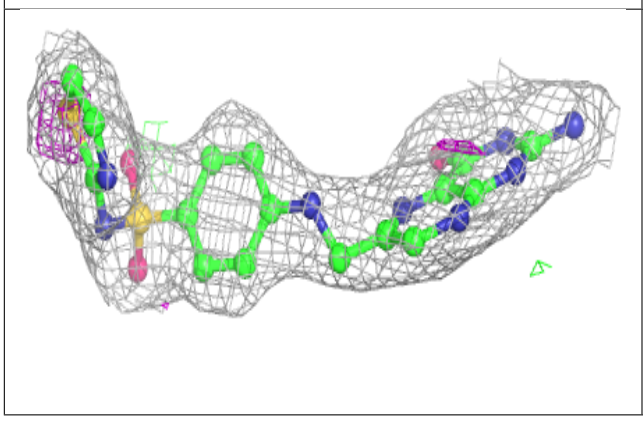


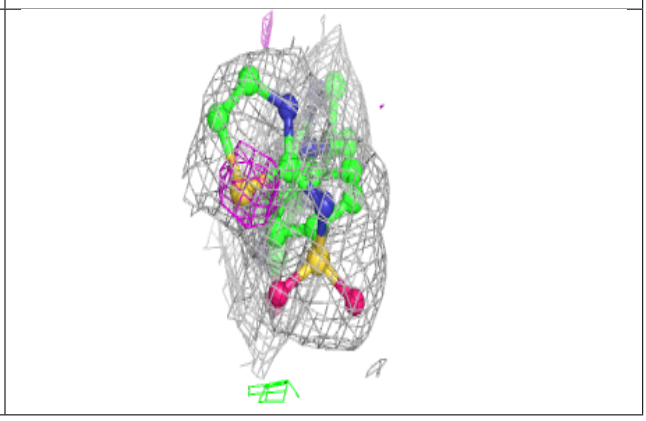


Electron density around XTZ B 801:

$2mF_o$-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.