



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:59 AM BST

PDB ID : 6JWV
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS A437G with STZ-DHP
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13
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) : 2.13

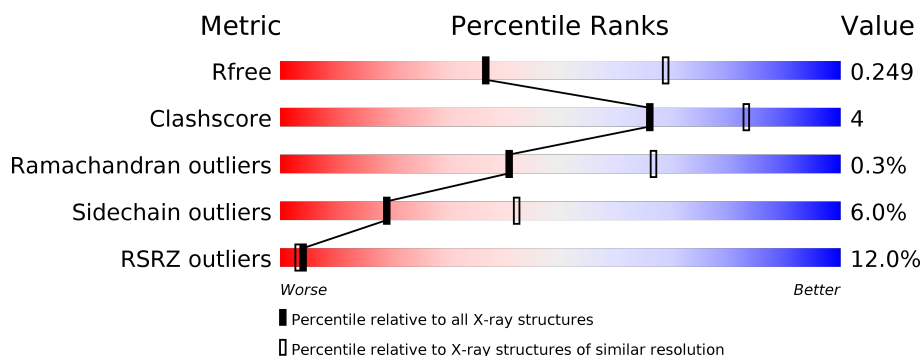
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>4%</div> <div>63%</div> <div>10%</div> <div>25%</div> </div>
1	B	728	<div> <div>14%</div> <div>63%</div> <div>10%</div> <div>26%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9403 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-dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4501	2897	741	841	22			
1	B	540	Total	C	N	O	S	0	0	0
			4454	2864	733	836	21			

There are 46 discrepancies between the modelled and reference sequences:

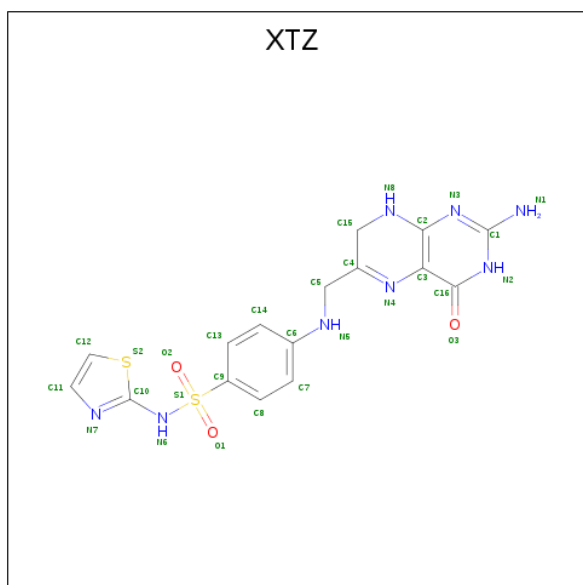
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression 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
A	728	HIS	-	expression tag	UNP Q25704
B	437	GLY	ALA	engineered mutation	UNP Q25704

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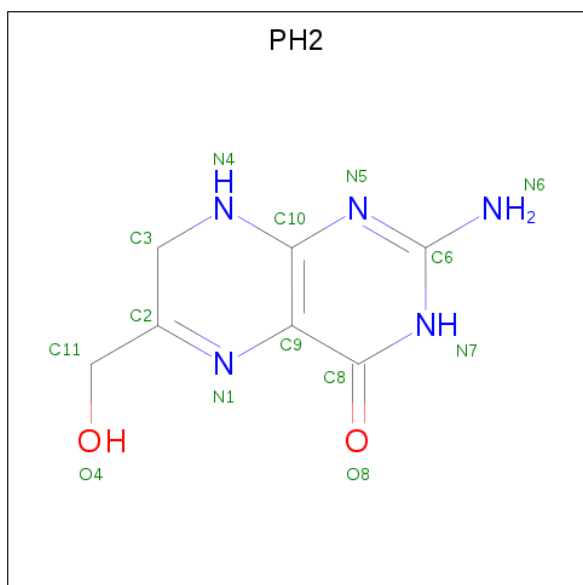
Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	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: C₁₆H₁₆N₈O₃S₂).



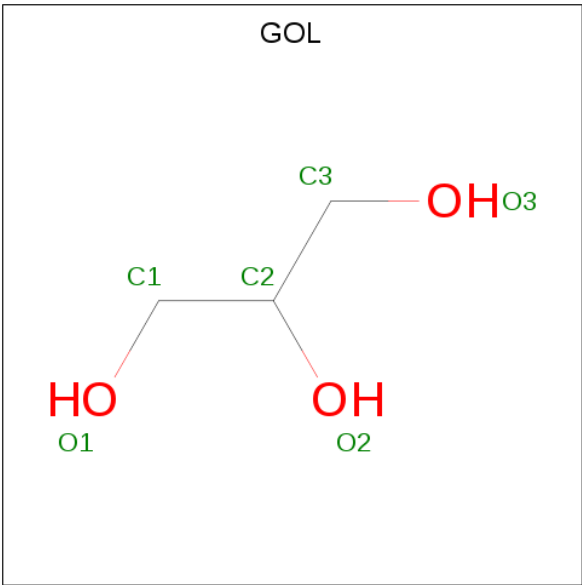
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	16	8	3	2		
2	B	1	Total	C	N	O	S	0	0
			29	16	8	3	2		

- Molecule 3 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (three-letter code: PH2) (formula: C₇H₉N₅O₂).



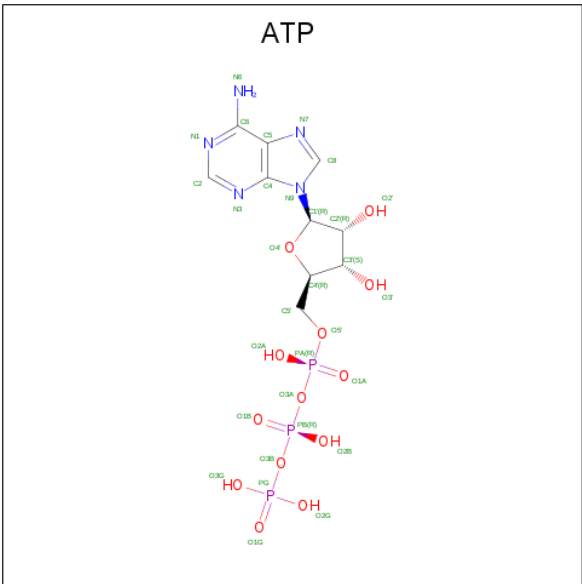
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	7	5	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- 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	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

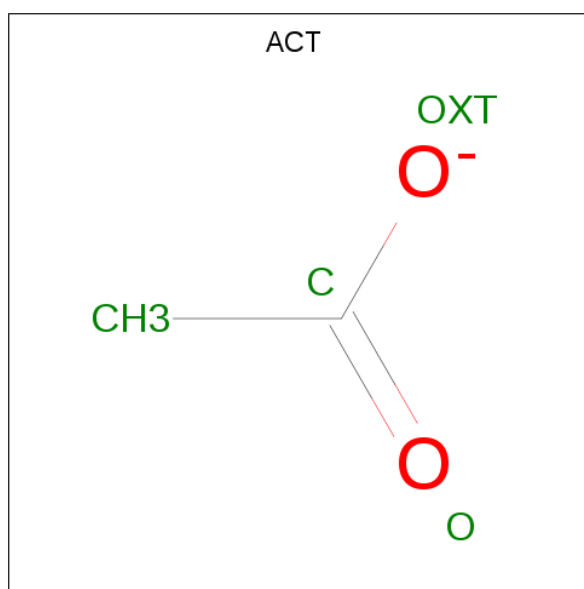
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	2	Total	Mg	0	0
			2	2		

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

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

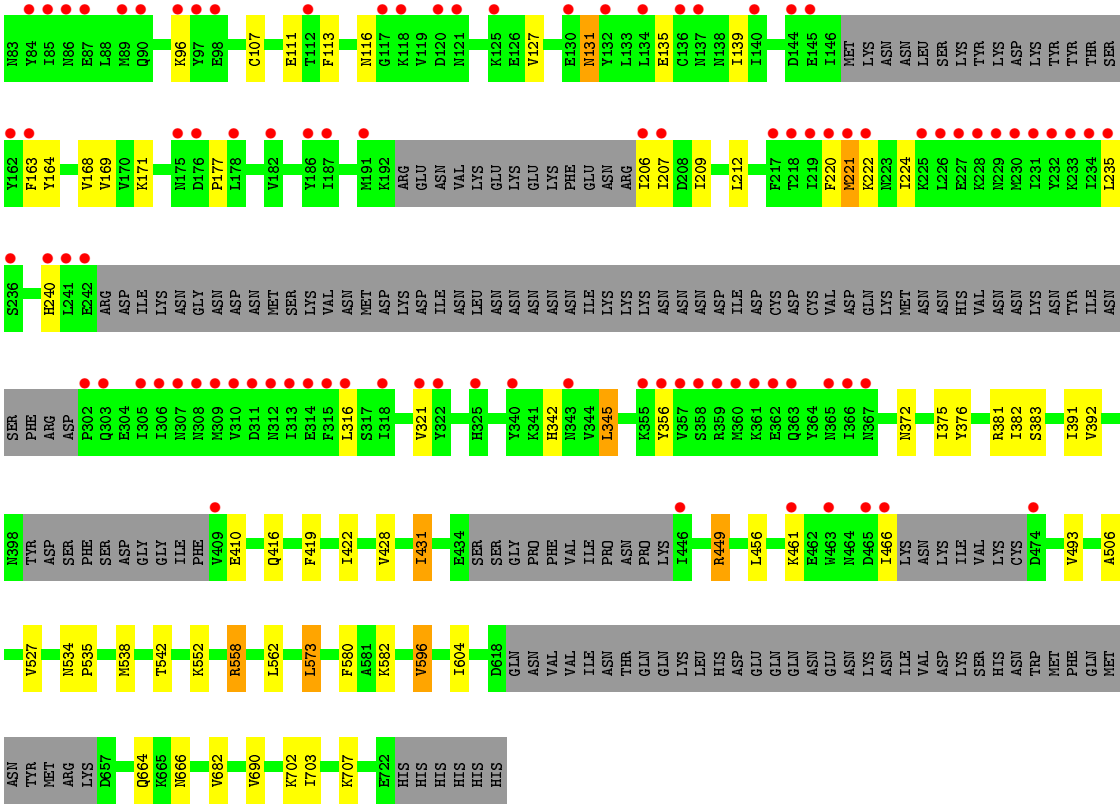
- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	210	Total 210	O 210	0	0
9	B	102	Total 102	O 102	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.89Å 136.72Å 138.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 41.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.70) 90.4 (41.88-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.14 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.206 , 0.257 0.202 , 0.249	Depositor DCC
R_{free} test set	4716 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9403	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CA, XTZ, ATP, ACT, 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	0.49	0/4568	0.70	0/6159
1	B	0.48	0/4520	0.69	0/6095
All	All	0.49	0/9088	0.70	0/12254

There are no bond length outliers.

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	4501	0	4589	37	0
1	B	4454	0	4538	35	0
2	A	29	0	16	2	0
2	B	29	0	16	0	0
3	A	14	0	9	0	0
4	A	6	0	8	2	0
4	B	6	0	8	0	0
5	A	31	0	12	2	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	8	0	6	0	0
8	B	8	0	6	0	0
9	A	210	0	0	3	0
9	B	102	0	0	0	0
All	All	9403	0	9208	73	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 4.

All (73) 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:B:552:LYS:HD2	1:B:596:VAL:HG13	1.58	0.84
1:B:527:VAL:HG22	1:B:573:LEU:HD12	1.63	0.80
2:A:801:XTZ:H5	4:A:803:GOL:H11	1.65	0.79
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.66	0.77
1:A:57:THR:HG21	1:A:165:ASN:OD1	1.91	0.71
2:A:801:XTZ:N7	2:A:801:XTZ:H9	2.05	0.70
1:B:375:ILE:HG21	1:B:382:ILE:HD13	1.75	0.69
1:A:396:ASN:OD1	4:A:803:GOL:H2	1.97	0.64
1:B:56:GLU:O	1:B:372:ASN:HA	1.97	0.64
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.28	0.64
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.82	0.61
1:A:63:VAL:HG11	1:A:325:HIS:HB3	1.81	0.61
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.83	0.61
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.82	0.60
1:B:221:MET:HB3	1:B:224:ILE:HD11	1.82	0.60
1:A:6:GLU:HB3	1:A:8:ILE:HG22	1.83	0.60
1:B:419:PHE:HA	1:B:422:ILE:HD12	1.83	0.59
1:A:118:LYS:HD2	1:A:118:LYS:H	1.67	0.58
1:B:392:VAL:HG22	1:B:428:VAL:HB	1.85	0.58
1:A:485:ASN:HB2	9:A:1092:HOH:O	2.05	0.57
1:A:364:TYR:HB3	1:A:366:ILE:HG12	1.88	0.56
1:A:490:LYS:HD3	1:A:516:LEU:HD22	1.87	0.55
1:B:506:ALA:HB1	1:B:558:ARG:HG2	1.88	0.55
1:B:449:ARG:HG3	1:B:449:ARG:HH11	1.71	0.54
1:B:376:TYR:O	1:B:383:SER:HB2	2.07	0.53
1:B:20:LEU:HB2	1:B:168:VAL:HG22	1.90	0.53
1:B:206:ILE:HG23	1:B:207:ILE:HG22	1.90	0.52
1:A:39:HIS:NE2	1:A:521:ASN:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PRO:HB2	1:B:316:LEU:HD11	1.92	0.52
1:B:127:VAL:HB	1:B:131:ASN:HB3	1.92	0.51
1:A:534:ASN:O	1:A:538:MET:HB2	2.10	0.51
1:A:181:LEU:HD21	5:A:804:ATP:H2'	1.92	0.50
1:A:191:MET:HE1	1:A:207:ILE:HG12	1.94	0.50
1:B:342:HIS:HB3	1:B:345:LEU:HG	1.93	0.50
1:B:431:ILE:HG21	1:B:456:LEU:HD21	1.93	0.49
1:B:375:ILE:HG12	1:B:382:ILE:HG23	1.95	0.49
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.44	0.48
1:A:592:GLN:HG2	1:B:703:ILE:O	2.14	0.47
1:A:385:LEU:HG	1:A:386:LYS:HD3	1.95	0.47
1:A:694:LYS:HE3	1:A:698:ASP:OD1	2.16	0.46
1:A:410:GLU:N	1:A:411:PRO:CD	2.78	0.46
1:A:667:ILE:HG13	1:A:689:ASP:OD2	2.16	0.46
1:A:493:VAL:HG13	1:A:519:LYS:HE3	1.97	0.46
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.98	0.46
1:B:107:CYS:SG	1:B:171:LYS:HD3	2.56	0.44
1:B:24:THR:HG23	1:B:164:TYR:HB2	1.99	0.44
1:B:391:ILE:HG21	1:B:690:VAL:HG13	1.99	0.44
1:A:428:VAL:HG22	1:A:478:ILE:HB	2.01	0.43
1:B:96:LYS:HG2	1:B:240:HIS:CD2	2.54	0.43
1:A:457:GLN:HG3	9:A:1029:HOH:O	2.19	0.43
1:A:114:LEU:HD21	1:A:337:ILE:HG22	2.01	0.42
1:A:604:ILE:HG12	1:A:682:VAL:HG11	2.01	0.42
1:A:210:ASP:HB3	1:A:320:HIS:CD2	2.54	0.42
1:A:38:LEU:HD21	1:A:168:VAL:HG11	2.01	0.42
1:A:118:LYS:CD	1:A:118:LYS:H	2.32	0.41
1:B:604:ILE:HG12	1:B:682:VAL:HG11	2.01	0.41
1:A:316:LEU:HA	5:A:804:ATP:C8	2.56	0.41
1:B:19:VAL:HG22	1:B:169:VAL:HG22	2.03	0.41
1:B:580:PHE:O	1:B:582:LYS:HD2	2.20	0.41
1:A:115:LYS:O	1:A:116:ASN:HB2	2.19	0.41
1:A:136:CYS:SG	9:A:961:HOH:O	2.62	0.41
1:B:17:ILE:HG13	1:B:113:PHE:HB2	2.03	0.41
1:B:135:GLU:O	1:B:139:ILE:HG12	2.21	0.41
1:A:324:THR:CG2	1:A:345:LEU:HD22	2.51	0.41
1:B:21:ASN:HB2	1:B:212:LEU:HD21	2.03	0.41
1:A:356:TYR:O	1:A:360:MET:HG2	2.21	0.41
1:A:341:LYS:HE2	1:A:345:LEU:O	2.21	0.40
1:A:385:LEU:O	1:A:386:LYS:HB2	2.21	0.40
1:A:38:LEU:CD2	1:A:168:VAL:HG11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:HD22	1:B:116:ASN:HA	1.64	0.40
1:B:12:GLU:O	1:B:14:LYS:HE3	2.21	0.40
1:B:37:ALA:O	1:B:41:VAL:HG23	2.22	0.40
1:B:21:ASN:O	1:B:209:ILE:HA	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	525/728 (72%)	502 (96%)	22 (4%)	1 (0%)	47	73
1	B	522/728 (72%)	496 (95%)	24 (5%)	2 (0%)	34	60
All	All	1047/1456 (72%)	998 (95%)	46 (4%)	3 (0%)	41	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	LYS
1	B	538	MET
1	A	410	GLU

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	518/696 (74%)	487 (94%)	31 (6%)	19	42
1	B	512/696 (74%)	481 (94%)	31 (6%)	18	41
All	All	1030/1392 (74%)	968 (94%)	62 (6%)	19	42

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	57	THR
1	A	64	LEU
1	A	98	GLU
1	A	118	LYS
1	A	136	CYS
1	A	144	ASP
1	A	168	VAL
1	A	192	LYS
1	A	229	ASN
1	A	303	GLN
1	A	304	GLU
1	A	314	GLU
1	A	341	LYS
1	A	347	ASN
1	A	380	ASP
1	A	381	ARG
1	A	386	LYS
1	A	417	ARG
1	A	445	LYS
1	A	449	ARG
1	A	457	GLN
1	A	460	GLN
1	A	480	SER
1	A	493	VAL
1	A	542	THR
1	A	657	ASP
1	A	664	GLN
1	A	702	LYS
1	A	706	VAL
1	A	707	LYS
1	B	9	LEU
1	B	14	LYS
1	B	21	ASN
1	B	27	ARG

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Mol	Chain	Res	Type
1	B	54	LEU
1	B	111	GLU
1	B	131	ASN
1	B	163	PHE
1	B	220	PHE
1	B	221	MET
1	B	235	LEU
1	B	321	VAL
1	B	345	LEU
1	B	356	TYR
1	B	381	ARG
1	B	410	GLU
1	B	416	GLN
1	B	431	ILE
1	B	449	ARG
1	B	461	LYS
1	B	466	ILE
1	B	493	VAL
1	B	542	THR
1	B	558	ARG
1	B	562	LEU
1	B	573	LEU
1	B	596	VAL
1	B	664	GLN
1	B	666	ASN
1	B	702	LYS
1	B	707	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	GLN
1	A	557	GLN
1	B	25	ASN
1	B	116	ASN
1	B	240	HIS
1	B	307	ASN
1	B	495	ASN

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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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$
4	GOL	A	803	-	5,5,5	0.55	0	5,5,5	0.82	0
3	PH2	A	802	6	10,15,15	1.12	1 (10%)	10,21,21	2.28	4 (40%)
4	GOL	B	802	-	5,5,5	0.40	0	5,5,5	0.42	0
8	ACT	B	805	-	1,3,3	1.42	0	0,3,3	0.00	-
5	ATP	A	804	6	26,33,33	0.91	1 (3%)	31,52,52	1.44	5 (16%)
8	ACT	A	808	-	1,3,3	1.54	0	0,3,3	0.00	-
8	ACT	B	804	-	1,3,3	1.17	0	0,3,3	0.00	-
2	XTZ	B	801	-	25,32,32	2.21	2 (8%)	27,46,46	2.35	7 (25%)
2	XTZ	A	801	-	25,32,32	2.18	2 (8%)	27,46,46	2.86	8 (29%)
8	ACT	A	807	-	1,3,3	0.49	0	0,3,3	0.00	-

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	GOL	A	803	-	-	2/4/4/4	-
3	PH2	A	802	6	-	0/0/11/11	0/2/2/2
4	GOL	B	802	-	-	0/4/4/4	-
5	ATP	A	804	6	-	4/18/38/38	0/3/3/3
2	XTZ	B	801	-	-	6/12/25/25	0/4/4/4
2	XTZ	A	801	-	-	5/12/25/25	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	XTZ	C9-S1	-9.65	1.61	1.76
2	A	801	XTZ	C9-S1	-9.64	1.61	1.76
2	A	801	XTZ	C3-C2	2.99	1.49	1.41
3	A	802	PH2	C9-C10	2.57	1.48	1.41
5	A	804	ATP	C5-C4	2.40	1.47	1.40
2	B	801	XTZ	C3-C2	2.31	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	XTZ	O2-S1-O1	-10.99	106.04	119.55
2	B	801	XTZ	O2-S1-O1	-8.11	109.58	119.55
2	A	801	XTZ	O1-S1-C9	4.71	113.78	107.97
2	A	801	XTZ	C16-N2-C1	4.64	123.30	115.93
2	B	801	XTZ	C9-S1-N6	4.35	112.30	106.83
3	A	802	PH2	C8-N7-C6	4.17	122.55	115.93
5	A	804	ATP	N3-C2-N1	-3.95	122.50	128.68
2	A	801	XTZ	C3-C16-N2	-3.81	118.22	123.43
5	A	804	ATP	PA-O3A-PB	-3.62	120.39	132.83
2	B	801	XTZ	C16-N2-C1	3.62	121.69	115.93
3	A	802	PH2	C9-C8-N7	-3.53	118.61	123.43
2	B	801	XTZ	C3-C16-N2	-3.39	118.79	123.43
2	B	801	XTZ	C16-C3-C2	3.39	116.75	114.53
3	A	802	PH2	C6-N5-C10	3.12	121.53	114.54
2	B	801	XTZ	C1-N3-C2	2.78	120.76	114.54
2	A	801	XTZ	C1-N3-C2	2.69	120.56	114.54
5	A	804	ATP	C4-C5-N7	-2.68	106.61	109.40
2	A	801	XTZ	C8-C9-S1	2.63	122.63	119.77
3	A	802	PH2	C8-C9-C10	2.21	115.97	114.53
2	B	801	XTZ	C10-N6-S1	2.21	128.18	124.16
2	A	801	XTZ	O2-S1-N6	2.20	112.25	106.73
5	A	804	ATP	C2-N1-C6	2.13	122.40	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	ATP	PB-O3B-PG	-2.03	125.86	132.83
2	A	801	XTZ	C14-C13-C9	2.02	121.54	119.45

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	ATP	C5'-O5'-PA-O3A
4	A	803	GOL	C1-C2-C3-O3
2	B	801	XTZ	C7-C6-N5-C5
2	A	801	XTZ	C7-C6-N5-C5
2	B	801	XTZ	C14-C6-N5-C5
2	A	801	XTZ	C14-C6-N5-C5
4	A	803	GOL	O2-C2-C3-O3
5	A	804	ATP	C5'-O5'-PA-O1A
5	A	804	ATP	C5'-O5'-PA-O2A
2	A	801	XTZ	C13-C9-S1-O1
2	B	801	XTZ	C10-N6-S1-O1
5	A	804	ATP	O4'-C4'-C5'-O5'
2	A	801	XTZ	C8-C9-S1-O1
2	B	801	XTZ	C4-C5-N5-C6
2	A	801	XTZ	C4-C5-N5-C6
2	B	801	XTZ	C8-C9-S1-O2
2	B	801	XTZ	C13-C9-S1-O2

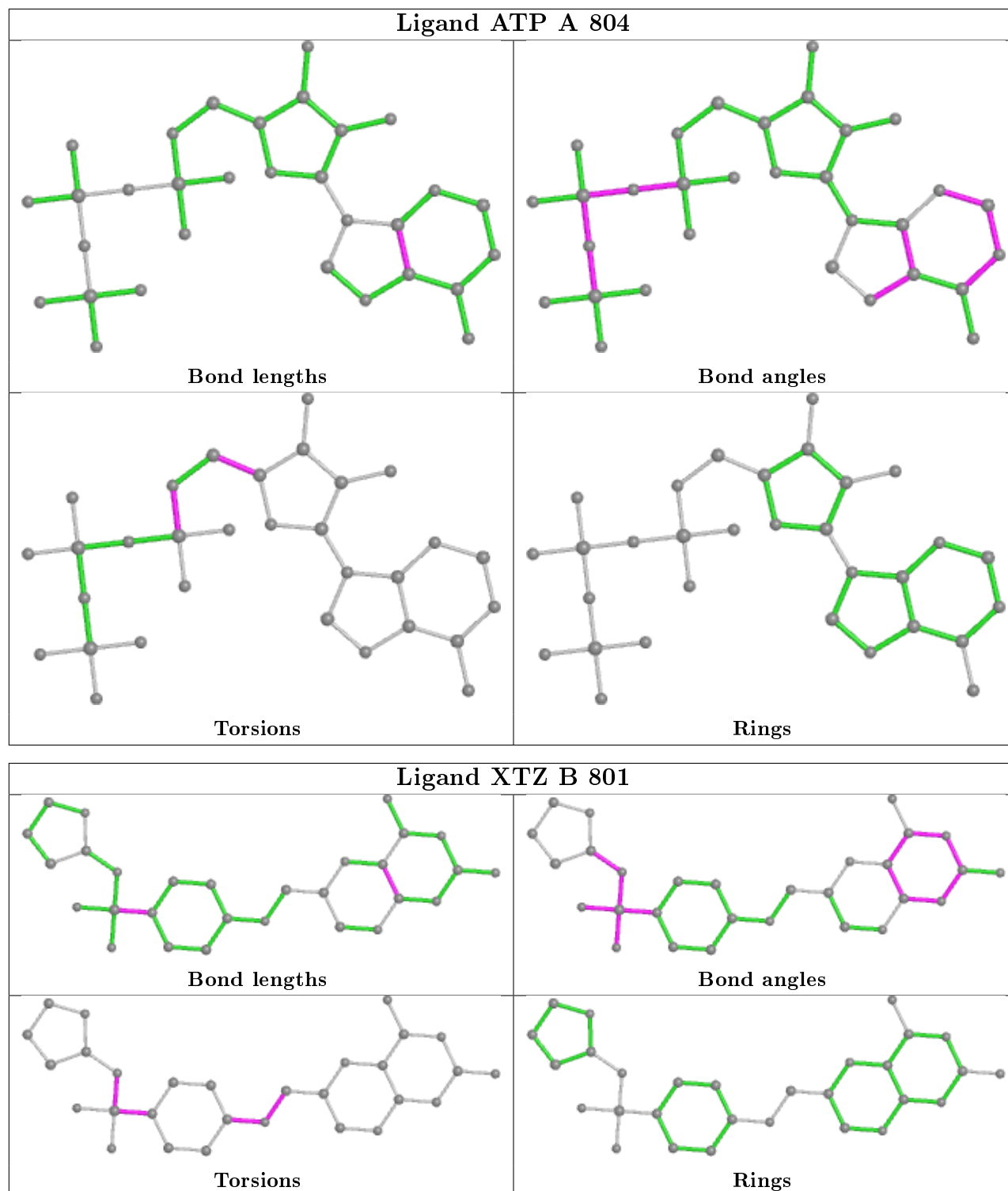
There are no ring outliers.

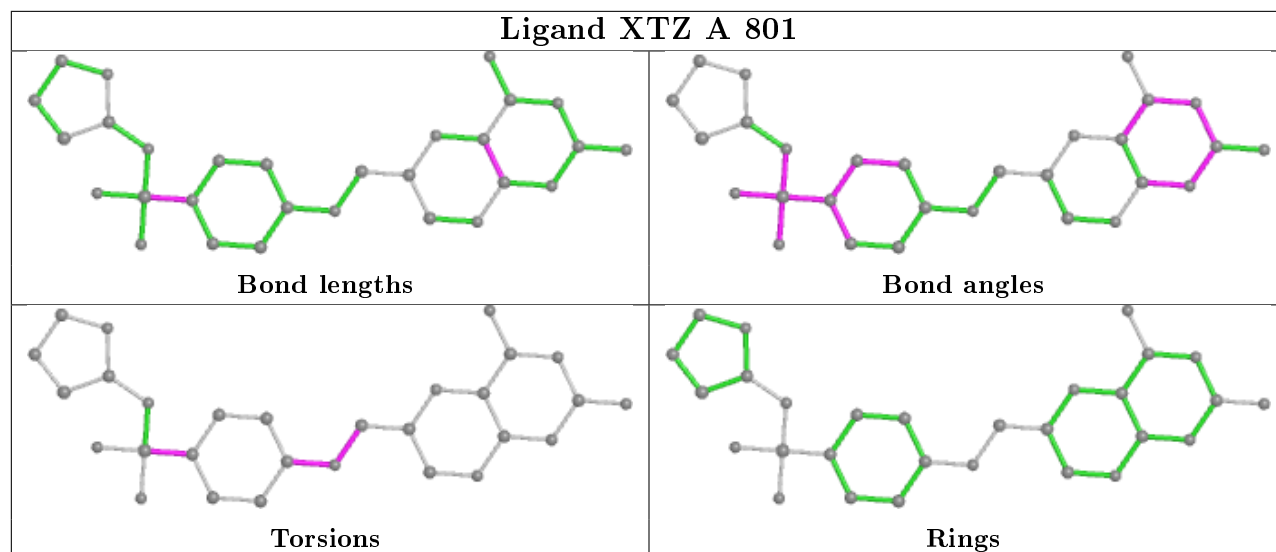
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	GOL	2	0
5	A	804	ATP	2	0
2	A	801	XTZ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/728 (74%)	-0.02	26 (4%) 30 28	7, 25, 84, 120	0
1	B	540/728 (74%)	0.80	104 (19%) 1 0	8, 58, 120, 120	0
All	All	1083/1456 (74%)	0.38	130 (12%) 4 3	7, 34, 117, 120	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	ILE	8.7
1	B	233	LYS	6.4
1	B	140	ILE	6.4
1	B	305	ILE	6.0
1	B	366	ILE	5.9
1	A	708	ASP	5.7
1	B	357	VAL	5.7
1	B	231	ILE	5.7
1	B	228	LYS	5.5
1	B	229	ASN	5.4
1	B	90	GLN	5.2
1	B	118	LYS	5.2
1	B	134	LEU	5.0
1	A	305	ILE	4.9
1	B	125	LYS	4.9
1	B	240	HIS	4.8
1	A	308	ASN	4.8
1	B	191	MET	4.7
1	B	220	PHE	4.7
1	B	311	ASP	4.7
1	B	136	CYS	4.6
1	A	304	GLU	4.6
1	A	5	GLN	4.5
1	B	316	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	221	MET	4.4
1	B	361	LYS	4.4
1	B	96	LYS	4.4
1	B	206	ILE	4.3
1	B	162	TYR	4.2
1	A	148	LYS	4.2
1	B	227	GLU	4.1
1	B	7	LEU	4.1
1	B	132	TYR	4.1
1	B	25	ASN	4.0
1	B	225	LYS	4.0
1	B	222	LYS	4.0
1	B	307	ASN	4.0
1	B	178	LEU	3.9
1	A	659	ASP	3.9
1	B	27	ARG	3.9
1	B	343	ASN	3.8
1	B	219	ILE	3.8
1	B	6	GLU	3.8
1	B	86	ASN	3.7
1	B	234	ILE	3.7
1	A	409	VAL	3.7
1	B	446	ILE	3.6
1	B	187	ILE	3.5
1	B	98	GLU	3.5
1	B	218	THR	3.5
1	B	365	ASN	3.5
1	A	303	GLN	3.4
1	B	84	TYR	3.4
1	A	149	ASN	3.4
1	B	12	GLU	3.4
1	B	359	ARG	3.4
1	B	363	GLN	3.3
1	B	207	ILE	3.3
1	A	445	LYS	3.3
1	B	309	MET	3.3
1	B	310	VAL	3.3
1	B	367	ASN	3.2
1	B	318	ILE	3.2
1	B	145	GLU	3.2
1	A	160	THR	3.2
1	A	228	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	150	ASN	3.2
1	B	144	ASP	3.1
1	A	474	ASP	3.1
1	B	232	TYR	3.0
1	B	409	VAL	3.0
1	B	137	ASN	3.0
1	B	461	LYS	3.0
1	A	466	ILE	3.0
1	B	465	ASP	2.9
1	B	226	LEU	2.9
1	B	130	GLU	2.9
1	B	87	GLU	2.9
1	B	13	ASN	2.9
1	B	362	GLU	2.8
1	B	306	ILE	2.8
1	B	315	PHE	2.8
1	A	618	ASP	2.8
1	B	121	ASN	2.7
1	B	175	ASN	2.7
1	B	325	HIS	2.7
1	B	358	SER	2.7
1	B	186	TYR	2.6
1	B	182	VAL	2.6
1	A	118	LYS	2.6
1	B	11	GLU	2.6
1	B	322	TYR	2.6
1	A	657	ASP	2.5
1	B	313	ILE	2.5
1	A	361	LYS	2.5
1	A	465	ASP	2.5
1	B	355	LYS	2.5
1	B	120	ASP	2.5
1	B	241	LEU	2.5
1	B	176	ASP	2.5
1	A	707	LYS	2.5
1	B	230	MET	2.4
1	B	303	GLN	2.4
1	B	24	THR	2.4
1	A	307	ASN	2.4
1	B	163	PHE	2.4
1	B	85	ILE	2.4
1	B	312	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	89	MET	2.4
1	B	340	TYR	2.4
1	B	112	THR	2.4
1	B	314	GLU	2.3
1	B	40	LEU	2.3
1	B	235	LEU	2.3
1	A	658	LYS	2.3
1	B	474	ASP	2.3
1	B	117	GLY	2.3
1	B	302	PRO	2.3
1	B	321	VAL	2.3
1	B	236	SER	2.3
1	A	159	TYR	2.2
1	B	217	PHE	2.2
1	B	466	ILE	2.2
1	B	97	TYR	2.2
1	A	362	GLU	2.2
1	B	308	ASN	2.2
1	B	242	GLU	2.1
1	B	360	MET	2.1
1	B	356	TYR	2.0
1	B	463	TRP	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
4	GOL	B	802	6/6	0.83	0.26	32,39,43,45	0

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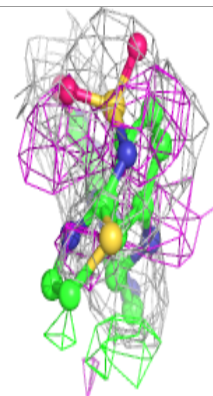
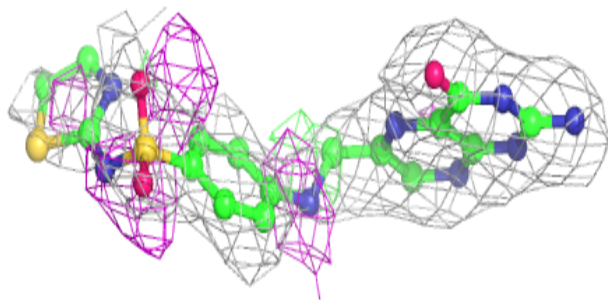
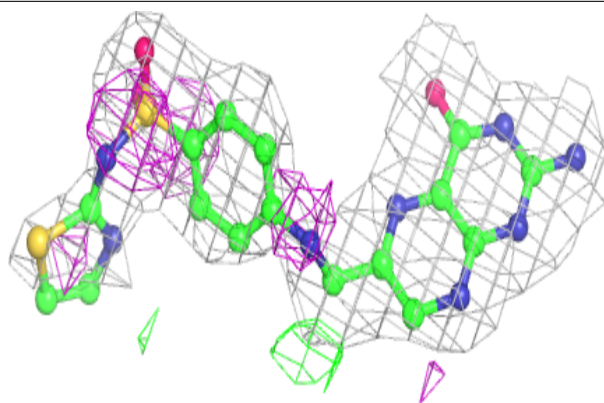
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	803	6/6	0.86	0.21	28,30,35,36	0
6	MG	B	806	1/1	0.89	0.20	74,74,74,74	0
7	CA	B	803	1/1	0.89	0.15	83,83,83,83	0
2	XTZ	A	801	29/29	0.89	0.25	14,36,100,104	0
6	MG	A	805	1/1	0.91	0.13	15,15,15,15	0
8	ACT	A	808	4/4	0.91	0.20	60,60,60,61	0
5	ATP	A	804	31/31	0.92	0.15	31,52,86,88	0
2	XTZ	B	801	29/29	0.93	0.19	13,25,48,50	0
8	ACT	B	805	4/4	0.95	0.21	37,37,38,38	0
8	ACT	A	807	4/4	0.95	0.21	26,26,26,27	0
6	MG	A	809	1/1	0.96	0.10	55,55,55,55	0
3	PH2	A	802	14/14	0.96	0.12	31,34,35,36	0
8	ACT	B	804	4/4	0.97	0.13	14,14,14,15	0
7	CA	A	806	1/1	0.98	0.10	19,19,19,19	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.

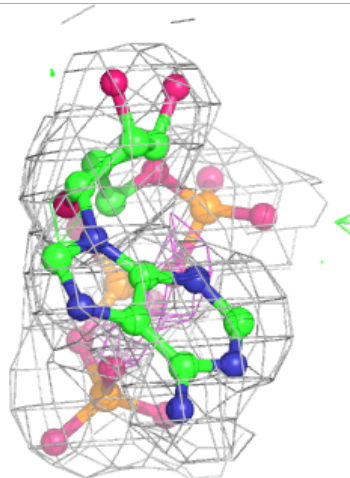
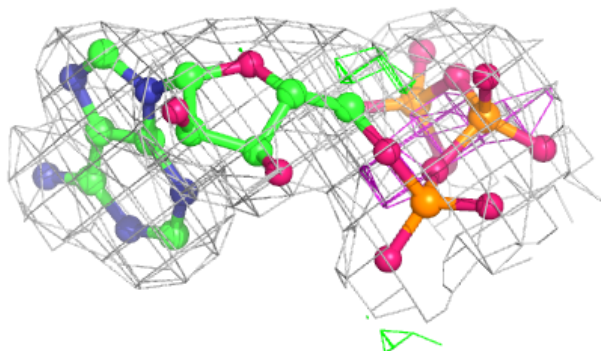
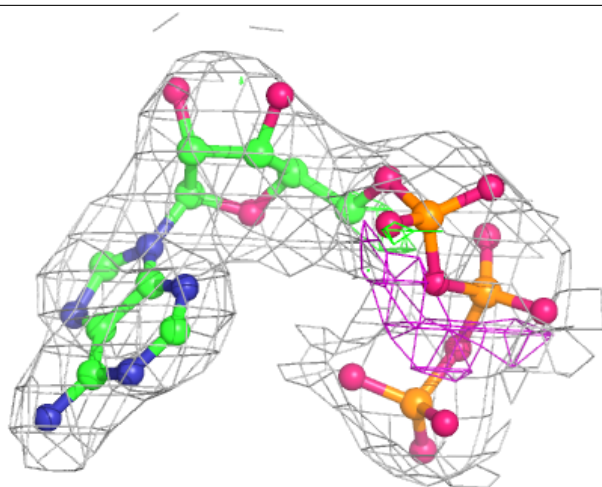
Electron density around XTZ A 801:

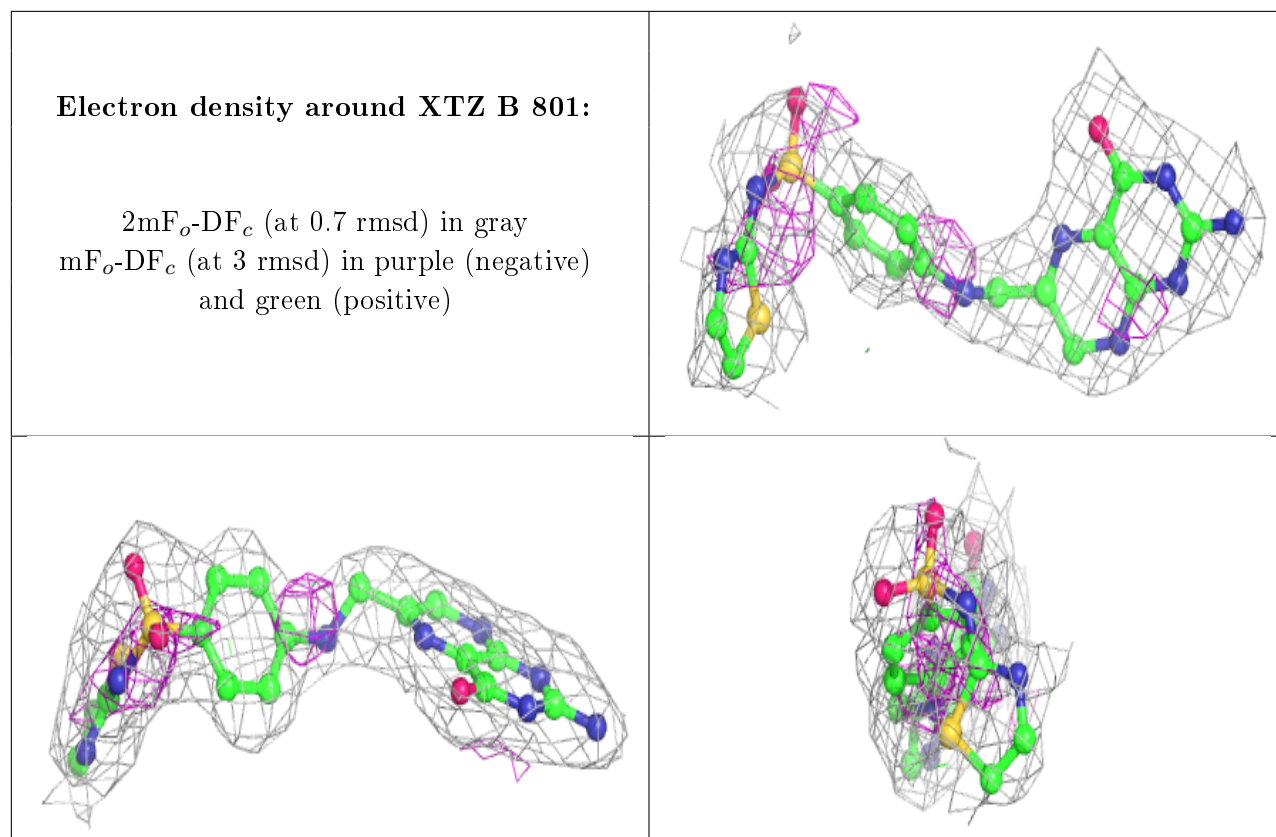
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 804:

$2mF_o-DF_c$ (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.