



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:03 AM BST

PDB ID : 6JWT
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS
S436F/A437G/A613T triple mutant with Pteroate
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.56 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

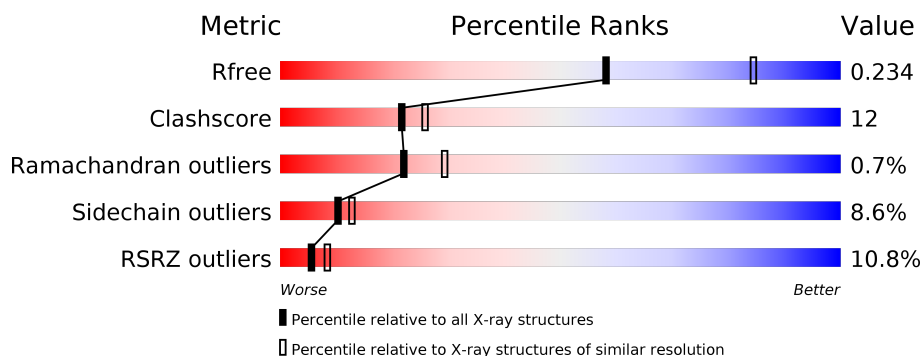
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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>9%</div> <div>53%</div> <div>20%</div> <div>•</div> <div>25%</div> </div>
1	B	728	<div> <div>8%</div> <div>58%</div> <div>17%</div> <div>•</div> <div>22%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9523 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	548	Total	C	N	O	S	0	0	0
			4534	2924	750	838	22			
1	B	571	Total	C	N	O	S	0	0	0
			4695	3026	770	876	23			

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

Continued on next page...

Continued from previous page...

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 ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).

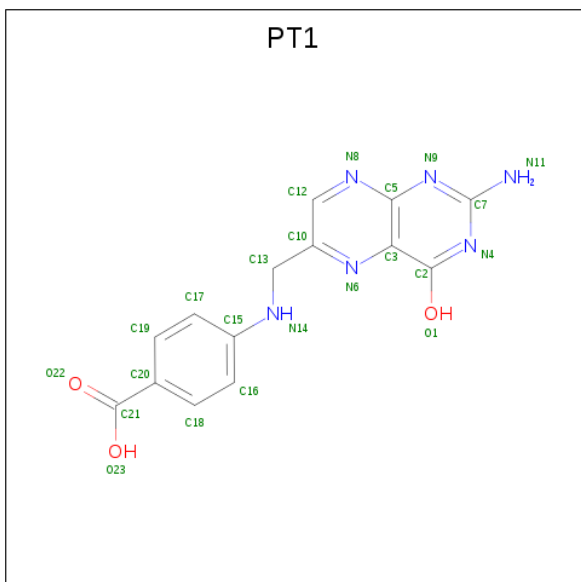


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PTEROIC ACID (three-letter code: PT1) (formula: C₁₄H₁₂N₆O₃).

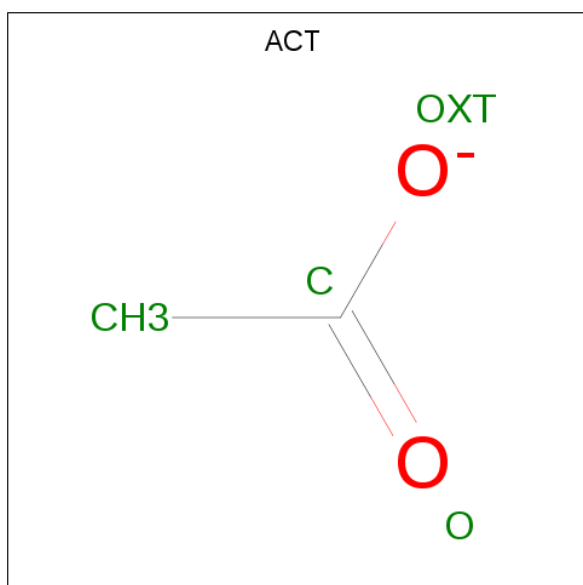


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	14	6	3		
4	B	1	Total	C	N	O	0	0
			23	14	6	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

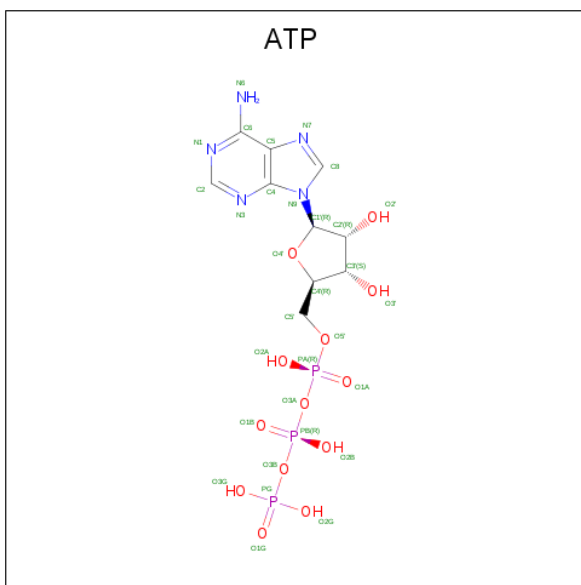
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

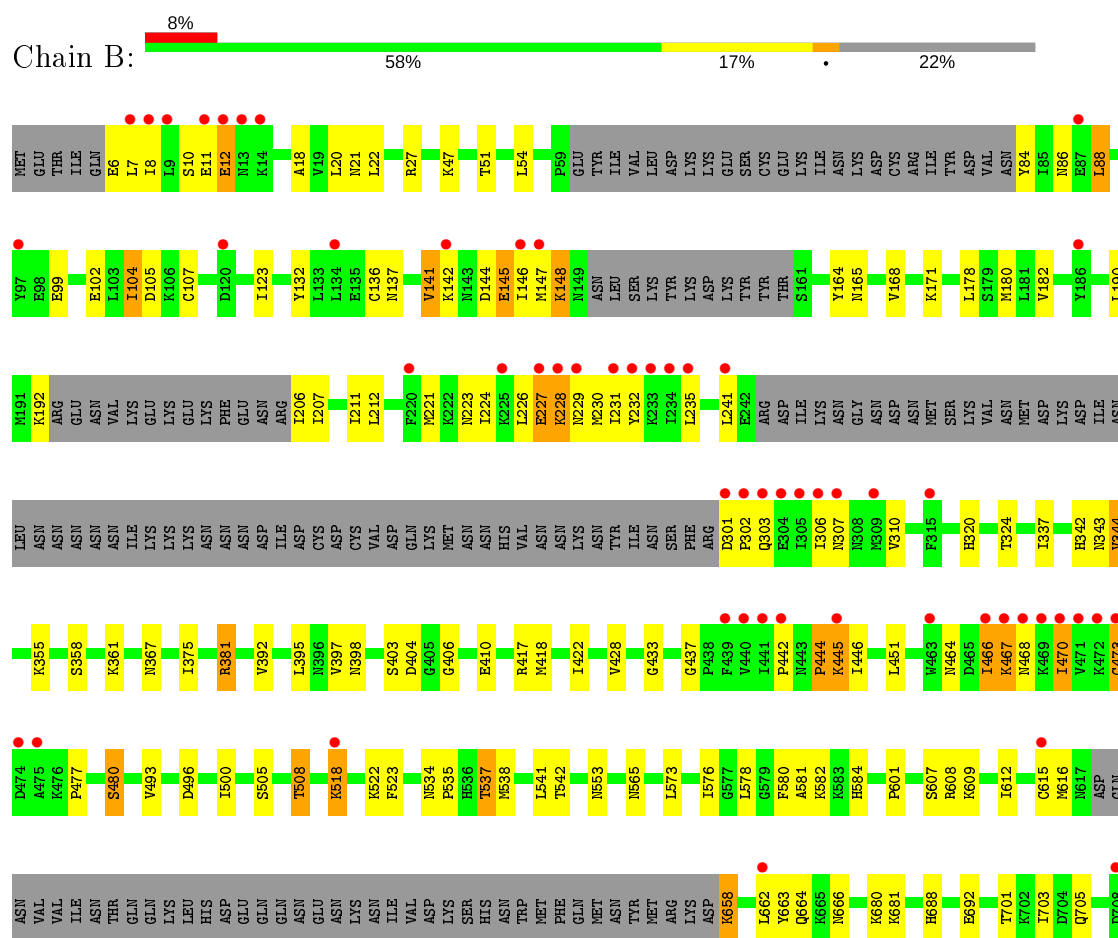
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	87	Total O 87 87	0	0
8	B	86	Total O 86 86	0	0

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.

- [illegible]

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.63Å 136.60Å 138.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 2.56 47.21 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.26-2.56) 98.5 (47.21-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.196 , 0.243 0.189 , 0.234	Depositor DCC
R_{free} test set	6156 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9523	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: MG, CA, ATP, ACT, AMP, PT1

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	0.37	0/4608	0.79	2/6217 (0.0%)
1	B	0.34	0/4773	0.77	2/6442 (0.0%)
All	All	0.36	0/9381	0.78	4/12659 (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	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	663	TYR	CB-CA-C	5.64	121.68	110.40
1	A	449	ARG	CG-CD-NE	5.41	123.16	111.80
1	A	374	ARG	CG-CD-NE	-5.40	100.47	111.80
1	B	381	ARG	CG-CD-NE	5.18	122.68	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	MET	Peptide

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	4534	0	4640	116	0
1	B	4695	0	4791	106	0
2	A	23	0	12	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	10	1	0
4	B	23	0	10	1	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	A	8	0	6	0	0
6	B	8	0	6	0	0
7	B	31	0	12	2	0
8	A	87	0	0	5	0
8	B	86	0	0	5	0
All	All	9523	0	9487	224	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 12.

All (224) 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:107:CYS:SG	1:B:171:LYS:HE3	1.90	1.11
1:B:470:ILE:HG22	1:B:473:CYS:HB3	1.32	1.10
1:A:107:CYS:SG	1:A:171:LYS:CE	2.49	1.00
1:A:107:CYS:SG	1:A:171:LYS:HE3	2.07	0.94
1:B:107:CYS:SG	1:B:171:LYS:CE	2.63	0.86
1:A:584:HIS:HD2	8:A:971:HOH:O	1.59	0.85
1:B:470:ILE:HG22	1:B:473:CYS:CB	2.06	0.85
1:A:469:LYS:HG3	1:A:472:LYS:HB2	1.63	0.81
1:B:342:HIS:HD2	1:B:344:VAL:H	1.31	0.79
1:A:607:SER:OG	1:A:688:HIS:HD2	1.64	0.79
1:A:104:ILE:H	1:A:565:ASN:HD21	1.33	0.77
1:A:360:MET:CE	1:A:366:ILE:HG21	2.14	0.77
1:A:84:TYR:CE2	1:A:192:LYS:HB2	2.21	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.59	0.76
1:B:505:SER:O	1:B:508:THR:HB	1.86	0.75
1:A:136:CYS:SG	8:A:981:HOH:O	2.43	0.75
1:A:512:GLU:OE1	1:A:515:LYS:HE3	1.87	0.75
1:B:422:ILE:CD1	1:B:477:PRO:HG3	2.16	0.75
1:A:573:LEU:HD23	1:A:601:PRO:HB2	1.67	0.74
1:B:104:ILE:H	1:B:565:ASN:HD21	1.36	0.74
1:B:206:ILE:HG23	1:B:207:ILE:HG22	1.70	0.74
1:B:27:ARG:HG3	1:B:164:TYR:OH	1.88	0.73
1:B:235:LEU:HB3	1:B:241:LEU:HD11	1.71	0.73
1:B:422:ILE:HD11	1:B:477:PRO:HG3	1.70	0.72
1:A:26:ASP:OD2	1:A:29:ASN:HB2	1.90	0.71
1:B:470:ILE:CG2	1:B:473:CYS:HB3	2.18	0.70
1:A:360:MET:HE2	1:A:366:ILE:HG21	1.72	0.70
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.22	0.70
1:A:359:ARG:HH11	1:A:359:ARG:CB	2.05	0.70
1:B:105:ASP:HB2	8:B:951:HOH:O	1.92	0.68
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.24	0.68
1:B:692:GLU:N	1:B:692:GLU:OE1	2.25	0.68
1:B:580:PHE:O	1:B:582:LYS:HD2	1.94	0.67
1:A:608:ARG:HA	1:A:666:ASN:OD1	1.94	0.67
1:B:99:GLU:OE1	5:B:804:CA:CA	1.70	0.67
1:B:180:MET:CE	1:B:211:ILE:HD13	2.25	0.66
1:A:359:ARG:CG	1:A:359:ARG:HH11	2.10	0.65
1:A:398:ASN:O	1:A:409:VAL:N	2.29	0.65
7:B:801:ATP:H2'	7:B:801:ATP:N3	2.12	0.65
1:A:119:VAL:HG12	1:A:120:ASP:H	1.62	0.65
1:B:470:ILE:CG2	1:B:473:CYS:CB	2.74	0.65
1:B:51:THR:HG22	1:B:168:VAL:HG12	1.79	0.65
1:A:525:SER:OG	1:A:571:ARG:HG2	1.98	0.64
1:B:608:ARG:HA	1:B:666:ASN:OD1	1.96	0.64
1:B:144:ASP:HB2	1:B:145:GLU:OE2	1.98	0.64
1:A:534:ASN:HB2	1:A:535:PRO:HD2	1.80	0.63
1:A:18:ALA:CB	1:A:180:MET:HE1	2.28	0.63
1:A:355:LYS:O	1:A:359:ARG:HB2	1.98	0.63
1:A:692:GLU:OE1	1:A:692:GLU:N	2.22	0.63
1:B:231:ILE:HG21	1:B:306:ILE:HG23	1.81	0.62
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.81	0.62
1:B:467:LYS:CD	1:B:467:LYS:H	2.13	0.62
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.82	0.62
1:B:576:ILE:CD1	1:B:578:LEU:HG	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:SER:OG	1:A:688:HIS:CD2	2.50	0.62
1:A:466:ILE:HA	8:A:909:HOH:O	1.99	0.61
1:A:359:ARG:HH11	1:A:359:ARG:HB3	1.63	0.61
1:A:206:ILE:HG23	1:A:207:ILE:HG22	1.82	0.61
1:B:404:ASP:HB2	1:B:406:GLY:H	1.65	0.61
1:A:84:TYR:HE2	1:A:192:LYS:HB2	1.64	0.60
1:A:301:ASP:OD2	1:A:303:GLN:HB3	2.02	0.60
1:A:449:ARG:HE	1:A:491:GLU:CD	2.05	0.60
1:A:469:LYS:CG	1:A:472:LYS:HB2	2.31	0.58
1:A:18:ALA:HB1	1:A:180:MET:CE	2.33	0.58
1:A:360:MET:HE3	1:A:366:ILE:HG21	1.85	0.58
1:B:395:LEU:HD22	1:B:418:MET:HG3	1.85	0.58
1:A:360:MET:HB3	1:A:366:ILE:HG22	1.85	0.57
1:A:300:ARG:HD3	1:A:300:ARG:C	2.25	0.56
1:B:584:HIS:HD2	8:B:944:HOH:O	1.88	0.56
1:A:38:LEU:HD22	1:A:48:ILE:HD13	1.88	0.56
1:A:466:ILE:HG12	1:A:470:ILE:HD12	1.87	0.56
1:A:87:GLU:HG3	1:A:90:GLN:HG3	1.88	0.56
1:A:317:SER:O	1:A:318:ILE:HD13	2.06	0.56
1:B:180:MET:HE2	1:B:211:ILE:HD13	1.87	0.55
1:B:180:MET:HE3	1:B:211:ILE:HD13	1.87	0.55
1:B:658:LYS:HE2	1:B:658:LYS:HA	1.89	0.55
1:A:177:PRO:HG3	1:A:214:PHE:CG	2.42	0.55
1:B:397:VAL:HG12	1:B:451:LEU:HD22	1.89	0.54
1:B:467:LYS:H	1:B:467:LYS:HD3	1.71	0.54
1:B:21:ASN:HB2	1:B:212:LEU:HD11	1.88	0.54
1:A:449:ARG:CG	1:A:449:ARG:HH11	2.20	0.54
1:A:395:LEU:HD22	1:A:418:MET:HG3	1.90	0.54
1:A:145:GLU:HA	1:A:145:GLU:OE2	2.08	0.53
1:A:460:GLN:O	1:A:464:ASN:ND2	2.42	0.53
1:B:608:ARG:HD2	1:B:688:HIS:CD2	2.44	0.53
1:A:180:MET:HE2	1:A:211:ILE:HD13	1.91	0.53
1:A:184:ILE:O	1:A:188:GLU:HG3	2.09	0.52
1:B:537:THR:HG23	1:B:541:LEU:HD11	1.90	0.52
1:B:88:LEU:O	1:B:88:LEU:HD12	2.08	0.52
1:B:20:LEU:HB2	1:B:168:VAL:HG22	1.91	0.52
1:B:221:MET:HE2	1:B:224:ILE:HD11	1.90	0.52
1:A:137:ASN:O	1:A:141:VAL:HG13	2.10	0.52
1:B:142:LYS:O	1:B:146:ILE:HD13	2.09	0.52
1:A:18:ALA:CB	1:A:180:MET:CE	2.88	0.52
1:A:571:ARG:HG2	1:A:571:ARG:HH11	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLN:HE21	1:A:476:LYS:NZ	2.07	0.51
1:B:227:GLU:C	1:B:229:ASN:H	2.13	0.51
1:A:395:LEU:HD22	1:A:418:MET:CG	2.41	0.51
1:B:178:LEU:O	1:B:182:VAL:HG23	2.10	0.51
1:A:187:ILE:O	1:A:191:MET:HG3	2.11	0.51
1:B:141:VAL:O	1:B:145:GLU:OE2	2.29	0.51
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.93	0.51
1:B:105:ASP:CB	8:B:951:HOH:O	2.55	0.51
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.40	0.51
1:B:553:ASN:ND2	8:B:907:HOH:O	2.43	0.51
1:A:24:THR:HG21	1:A:30:ALA:HA	1.92	0.51
1:A:37:ALA:O	1:A:41:VAL:HG23	2.11	0.50
1:A:87:GLU:HA	1:A:90:GLN:HG3	1.94	0.50
1:B:137:ASN:O	1:B:141:VAL:CG1	2.60	0.50
1:B:534:ASN:OD1	1:B:537:THR:HB	2.11	0.50
1:A:538:MET:HE3	8:A:911:HOH:O	2.11	0.50
1:B:573:LEU:HD23	1:B:601:PRO:HB2	1.92	0.50
1:A:359:ARG:HB3	1:A:359:ARG:NH1	2.27	0.50
1:A:35:GLU:OE2	1:A:570:TYR:OH	2.22	0.49
1:A:552:LYS:HE2	1:A:556:GLU:OE2	2.12	0.49
1:A:103:LEU:HD12	1:A:511:PRO:HB2	1.94	0.49
1:A:342:HIS:HD2	1:A:344:VAL:H	1.60	0.49
1:B:227:GLU:C	1:B:229:ASN:N	2.66	0.49
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.91	0.49
1:B:107:CYS:SG	1:B:171:LYS:NZ	2.85	0.49
1:B:206:ILE:CG2	1:B:207:ILE:N	2.76	0.49
2:A:801:AMP:H2'	2:A:801:AMP:N3	2.27	0.49
1:A:410:GLU:HG2	1:A:411:PRO:HD2	1.95	0.48
1:B:392:VAL:HG22	1:B:428:VAL:HB	1.95	0.48
1:A:344:VAL:O	1:A:344:VAL:HG13	2.12	0.48
1:B:206:ILE:HG23	1:B:207:ILE:N	2.27	0.48
1:B:658:LYS:HE2	1:B:658:LYS:CA	2.42	0.48
1:A:210:ASP:HB3	1:A:320:HIS:CD2	2.48	0.48
1:B:20:LEU:HB2	1:B:168:VAL:CG2	2.43	0.48
1:A:430:ASP:OD2	1:A:686:ARG:HD2	2.14	0.48
1:A:187:ILE:HG22	1:A:191:MET:HE2	1.96	0.48
1:B:221:MET:CE	1:B:224:ILE:HD11	2.43	0.48
1:A:442:PRO:HA	8:A:965:HOH:O	2.14	0.47
1:B:145:GLU:HA	1:B:148:LYS:HB3	1.96	0.47
1:A:102:GLU:OE2	1:A:515:LYS:NZ	2.46	0.47
1:B:612:ILE:O	1:B:615:CYS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HD12	1:A:54:LEU:HD11	1.97	0.47
1:A:42:GLU:HG2	1:A:48:ILE:HG13	1.96	0.47
1:B:342:HIS:CD2	1:B:344:VAL:H	2.21	0.47
1:B:342:HIS:CD2	1:B:343:ASN:N	2.83	0.47
1:B:171:LYS:NZ	8:B:909:HOH:O	2.47	0.46
1:A:449:ARG:NE	1:A:491:GLU:OE1	2.44	0.46
1:A:609:LYS:NZ	4:A:804:PT1:O1	2.49	0.46
1:B:107:CYS:HG	1:B:171:LYS:CE	2.29	0.46
1:A:41:VAL:HG13	1:A:45:LEU:HD12	1.97	0.46
1:B:18:ALA:CB	1:B:180:MET:HE1	2.46	0.46
1:A:18:ALA:HB2	1:A:180:MET:HE1	1.97	0.46
1:B:47:LYS:NZ	1:B:104:ILE:HD13	2.31	0.46
1:B:6:GLU:HA	1:B:6:GLU:OE1	2.16	0.46
1:A:359:ARG:HH11	1:A:359:ARG:HG2	1.80	0.46
1:B:21:ASN:C	1:B:22:LEU:HD12	2.35	0.46
1:A:18:ALA:HB1	1:A:180:MET:HE3	1.98	0.46
1:B:480:SER:HB2	1:B:500:ILE:HB	1.99	0.45
1:A:130:GLU:HA	1:A:133:LEU:HD12	1.98	0.45
1:A:229:ASN:O	1:A:233:LYS:HB2	2.16	0.45
1:B:537:THR:CG2	1:B:541:LEU:HD11	2.47	0.45
1:A:344:VAL:CG1	1:A:344:VAL:O	2.64	0.45
1:A:592:GLN:HG2	1:B:703:ILE:O	2.17	0.45
1:B:10:SER:O	1:B:12:GLU:N	2.46	0.45
1:A:410:GLU:O	1:A:411:PRO:C	2.54	0.44
1:A:542:THR:HG21	1:A:583:LYS:HE2	1.98	0.44
1:B:398:ASN:HB2	1:B:433:GLY:O	2.17	0.44
1:A:87:GLU:HA	1:A:90:GLN:CG	2.46	0.44
1:B:576:ILE:HD11	1:B:578:LEU:HG	1.97	0.44
1:B:231:ILE:HG22	1:B:232:TYR:N	2.31	0.44
1:B:658:LYS:N	1:B:658:LYS:CD	2.81	0.44
1:A:31:VAL:O	1:A:35:GLU:HB2	2.17	0.44
1:B:609:LYS:NZ	4:B:803:PT1:O1	2.51	0.44
1:A:139:ILE:HG13	1:A:220:PHE:HZ	1.82	0.44
1:B:607:SER:OG	1:B:688:HIS:HD2	2.01	0.44
1:A:187:ILE:HG22	1:A:191:MET:CE	2.47	0.44
1:A:449:ARG:HH11	1:A:449:ARG:HG3	1.83	0.43
1:B:10:SER:C	1:B:12:GLU:H	2.19	0.43
1:A:39:HIS:CE1	1:A:521:ASN:HA	2.53	0.43
1:B:132:TYR:CZ	1:B:136:CYS:SG	3.10	0.43
1:B:466:ILE:O	1:B:466:ILE:HG23	2.18	0.43
1:B:680:LYS:O	1:B:681:LYS:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:CD2	1:B:418:MET:HG3	2.47	0.43
1:B:137:ASN:O	1:B:141:VAL:HG12	2.17	0.43
1:A:180:MET:HE1	1:A:214:PHE:CD2	2.54	0.43
1:A:230:MET:O	1:A:234:ILE:HD12	2.18	0.43
1:B:518:LYS:HG3	1:B:523:PHE:CE1	2.54	0.43
1:A:107:CYS:SG	1:A:171:LYS:HE2	2.52	0.43
1:B:302:PRO:O	1:B:306:ILE:HG13	2.18	0.43
1:B:361:LYS:HD3	1:B:367:ASN:ND2	2.33	0.43
1:B:437:GLY:O	1:B:535:PRO:HB3	2.18	0.43
1:A:460:GLN:NE2	1:A:476:LYS:NZ	2.67	0.43
1:A:14:LYS:NZ	1:A:16:ASN:HD21	2.17	0.42
1:A:103:LEU:HA	1:A:565:ASN:ND2	2.34	0.42
1:A:368:ILE:HG13	1:A:372:ASN:ND2	2.35	0.42
1:B:47:LYS:HZ2	1:B:104:ILE:HD13	1.84	0.42
1:B:211:ILE:O	1:B:320:HIS:HB2	2.20	0.42
1:A:493:VAL:HG13	1:A:519:LYS:HE2	2.00	0.42
1:A:96:LYS:HE3	1:A:240:HIS:CE1	2.54	0.42
1:A:409:VAL:CG1	1:A:414:ALA:HB2	2.50	0.42
1:B:342:HIS:CD2	1:B:344:VAL:HB	2.55	0.42
1:B:518:LYS:NZ	1:B:565:ASN:O	2.51	0.42
7:B:801:ATP:H3'	7:B:801:ATP:O3A	2.20	0.42
1:B:137:ASN:O	1:B:141:VAL:HG13	2.20	0.42
1:B:658:LYS:HD2	1:B:658:LYS:N	2.35	0.42
1:A:38:LEU:HD22	1:A:48:ILE:CD1	2.49	0.42
1:B:228:LYS:HG3	1:B:228:LYS:H	1.62	0.41
1:B:381:ARG:HD2	1:B:381:ARG:HA	1.81	0.41
1:B:701:THR:O	1:B:705:GLN:HG2	2.20	0.41
1:A:177:PRO:HB2	1:A:316:LEU:HD21	2.01	0.41
1:A:392:VAL:CG2	1:A:684:LEU:HD23	2.51	0.41
1:B:464:ASN:C	1:B:466:ILE:H	2.22	0.41
1:A:460:GLN:HE21	1:A:476:LYS:HZ1	1.67	0.41
1:B:470:ILE:CG2	1:B:473:CYS:HB2	2.48	0.41
1:B:705:GLN:HA	1:B:705:GLN:NE2	2.36	0.41
1:A:364:TYR:HB3	1:A:366:ILE:HD13	2.02	0.41
1:A:392:VAL:HG22	1:A:428:VAL:HB	2.01	0.41
1:B:444:PRO:HB2	1:B:445:LYS:H	1.67	0.41
1:B:538:MET:O	1:B:581:ALA:HA	2.21	0.41
1:A:20:LEU:HB2	1:A:168:VAL:HG22	2.02	0.41
1:A:230:MET:HG3	1:A:234:ILE:HD12	2.03	0.41
1:B:307:ASN:O	1:B:310:VAL:HG23	2.21	0.41
1:A:96:LYS:HD2	1:A:236:SER:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:O	1:A:424:GLU:HG3	2.20	0.40
1:A:90:GLN:H	1:A:90:GLN:HG2	1.60	0.40
1:A:22:LEU:HB3	1:A:34:LEU:HD22	2.03	0.40
1:A:87:GLU:CG	1:A:90:GLN:HG3	2.52	0.40
1:B:301:ASP:OD1	1:B:303:GLN:HB3	2.21	0.40
1:B:6:GLU:HB3	1:B:8:ILE:HB	2.03	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	534/728 (73%)	508 (95%)	24 (4%)	2 (0%)	34	45
1	B	559/728 (77%)	524 (94%)	29 (5%)	6 (1%)	14	19
All	All	1093/1456 (75%)	1032 (94%)	53 (5%)	8 (1%)	22	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	444	PRO
1	A	465	ASP
1	B	11	GLU
1	B	12	GLU
1	A	367	ASN
1	B	228	LYS
1	B	442	PRO
1	B	470	ILE

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	523/697 (75%)	479 (92%)	44 (8%)	11	13
1	B	541/697 (78%)	494 (91%)	47 (9%)	10	12
All	All	1064/1394 (76%)	973 (91%)	91 (9%)	10	13

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	27	ARG
1	A	58	VAL
1	A	82	VAL
1	A	85	ILE
1	A	90	GLN
1	A	104	ILE
1	A	123	ILE
1	A	129	VAL
1	A	145	GLU
1	A	163	PHE
1	A	165	ASN
1	A	207	ILE
1	A	218	THR
1	A	222	LYS
1	A	226	LEU
1	A	300	ARG
1	A	301	ASP
1	A	324	THR
1	A	344	VAL
1	A	346	ASN
1	A	347	ASN
1	A	349	ILE
1	A	350	ARG
1	A	359	ARG
1	A	409	VAL
1	A	413	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	417	ARG
1	A	445	LYS
1	A	446	ILE
1	A	449	ARG
1	A	457	GLN
1	A	466	ILE
1	A	493	VAL
1	A	518	LYS
1	A	542	THR
1	A	543	ASN
1	A	562	LEU
1	A	617	ASN
1	A	657	ASP
1	A	660	GLN
1	A	661	LEU
1	A	702	LYS
1	A	706	VAL
1	B	7	LEU
1	B	84	TYR
1	B	86	ASN
1	B	88	LEU
1	B	102	GLU
1	B	104	ILE
1	B	123	ILE
1	B	141	VAL
1	B	145	GLU
1	B	147	MET
1	B	148	LYS
1	B	165	ASN
1	B	190	LEU
1	B	192	LYS
1	B	223	ASN
1	B	226	LEU
1	B	227	GLU
1	B	230	MET
1	B	324	THR
1	B	337	ILE
1	B	344	VAL
1	B	355	LYS
1	B	358	SER
1	B	403	SER
1	B	410	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	417	ARG
1	B	445	LYS
1	B	446	ILE
1	B	466	ILE
1	B	467	LYS
1	B	468	ASN
1	B	473	CYS
1	B	480	SER
1	B	493	VAL
1	B	496	ASP
1	B	508	THR
1	B	518	LYS
1	B	522	LYS
1	B	537	THR
1	B	542	THR
1	B	616	MET
1	B	658	LYS
1	B	662	LEU
1	B	664	GLN
1	B	710	ASN
1	B	711	SER
1	B	722	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	29	ASN
1	A	39	HIS
1	A	100	ASN
1	A	165	ASN
1	A	342	HIS
1	A	460	GLN
1	A	565	ASN
1	A	584	HIS
1	A	593	ASN
1	A	688	HIS
1	B	21	ASN
1	B	100	ASN
1	B	116	ASN
1	B	137	ASN
1	B	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	342	HIS
1	B	363	GLN
1	B	367	ASN
1	B	390	ASN
1	B	553	ASN
1	B	565	ASN
1	B	584	HIS
1	B	617	ASN
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, 5 are monoatomic - leaving 8 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	$\# Z > 2$
2	AMP	A	801	3	22,25,25	0.63	0	25,38,38	0.79	1 (4%)
7	ATP	B	801	3	26,33,33	0.62	0	31,52,52	1.08	2 (6%)
6	ACT	B	805	-	1,3,3	1.38	0	0,3,3	0.00	-
6	ACT	A	807	-	1,3,3	6.65	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PT1	A	804	-	22,25,25	1.48	3 (13%)	28,35,35	2.19	9 (32%)
6	ACT	B	806	-	1,3,3	5.74	1 (100%)	0,3,3	0.00	-
6	ACT	A	806	-	1,3,3	5.17	1 (100%)	0,3,3	0.00	-
4	PT1	B	803	-	22,25,25	1.82	6 (27%)	28,35,35	2.78	11 (39%)

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
2	AMP	A	801	3	-	1/6/26/26	0/3/3/3
4	PT1	B	803	-	-	3/5/9/9	0/3/3/3
7	ATP	B	801	3	-	3/18/38/38	0/3/3/3
4	PT1	A	804	-	-	3/5/9/9	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	807	ACT	CH3-C	6.65	1.57	1.48
6	B	806	ACT	CH3-C	5.74	1.56	1.48
6	A	806	ACT	CH3-C	5.17	1.55	1.48
4	B	803	PT1	C20-C21	4.69	1.52	1.47
4	A	804	PT1	C3-C5	3.87	1.47	1.40
4	B	803	PT1	C10-N6	3.35	1.38	1.32
4	A	804	PT1	C20-C21	3.19	1.50	1.47
4	B	803	PT1	C18-C16	3.17	1.44	1.38
4	B	803	PT1	C3-C5	2.27	1.44	1.40
4	A	804	PT1	C10-N6	2.06	1.36	1.32
4	B	803	PT1	C5-N8	2.06	1.39	1.37
4	B	803	PT1	C7-N11	2.04	1.38	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	PT1	N8-C5-N9	7.39	124.25	115.82
4	A	804	PT1	N8-C5-N9	7.06	123.88	115.82
4	B	803	PT1	C7-N9-C5	7.02	123.38	115.36
4	B	803	PT1	C12-N8-C5	5.00	121.72	116.69
4	A	804	PT1	C7-N9-C5	4.76	120.79	115.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	PT1	N9-C7-N4	-4.10	121.76	127.22
4	B	803	PT1	C5-C3-N6	-3.98	117.61	122.41
4	B	803	PT1	C10-C12-N8	-3.91	119.29	123.13
4	B	803	PT1	C3-C5-N9	-3.03	116.79	121.71
4	A	804	PT1	N9-C7-N4	-2.88	123.38	127.22
7	B	801	ATP	C3'-C2'-C1'	2.72	105.07	100.98
4	A	804	PT1	C19-C20-C21	-2.67	116.78	120.37
4	B	803	PT1	C10-C13-N14	-2.58	107.37	113.07
4	B	803	PT1	N11-C7-N4	2.33	120.88	117.25
4	A	804	PT1	C10-C13-N14	-2.32	107.94	113.07
4	A	804	PT1	C3-C5-N9	-2.26	118.05	121.71
4	A	804	PT1	O1-C2-C3	-2.25	115.47	119.67
4	A	804	PT1	C12-N8-C5	2.24	118.95	116.69
4	A	804	PT1	O1-C2-N4	2.23	123.33	117.44
4	B	803	PT1	C10-N6-C3	2.15	121.52	118.04
4	B	803	PT1	C13-C10-N6	2.13	120.44	116.66
2	A	801	AMP	C5-C6-N6	2.13	123.59	120.35
7	B	801	ATP	PA-O3A-PB	-2.06	125.74	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	801	ATP	PB-O3B-PG-O3G
4	B	803	PT1	C10-C13-N14-C15
4	A	804	PT1	C10-C13-N14-C15
4	A	804	PT1	C16-C15-N14-C13
4	A	804	PT1	C17-C15-N14-C13
4	B	803	PT1	C17-C15-N14-C13
4	B	803	PT1	C16-C15-N14-C13
2	A	801	AMP	C4'-C5'-O5'-P
7	B	801	ATP	C4'-C5'-O5'-PA
7	B	801	ATP	PB-O3B-PG-O2G

There are no ring outliers.

4 monomers are involved in 5 short contacts:

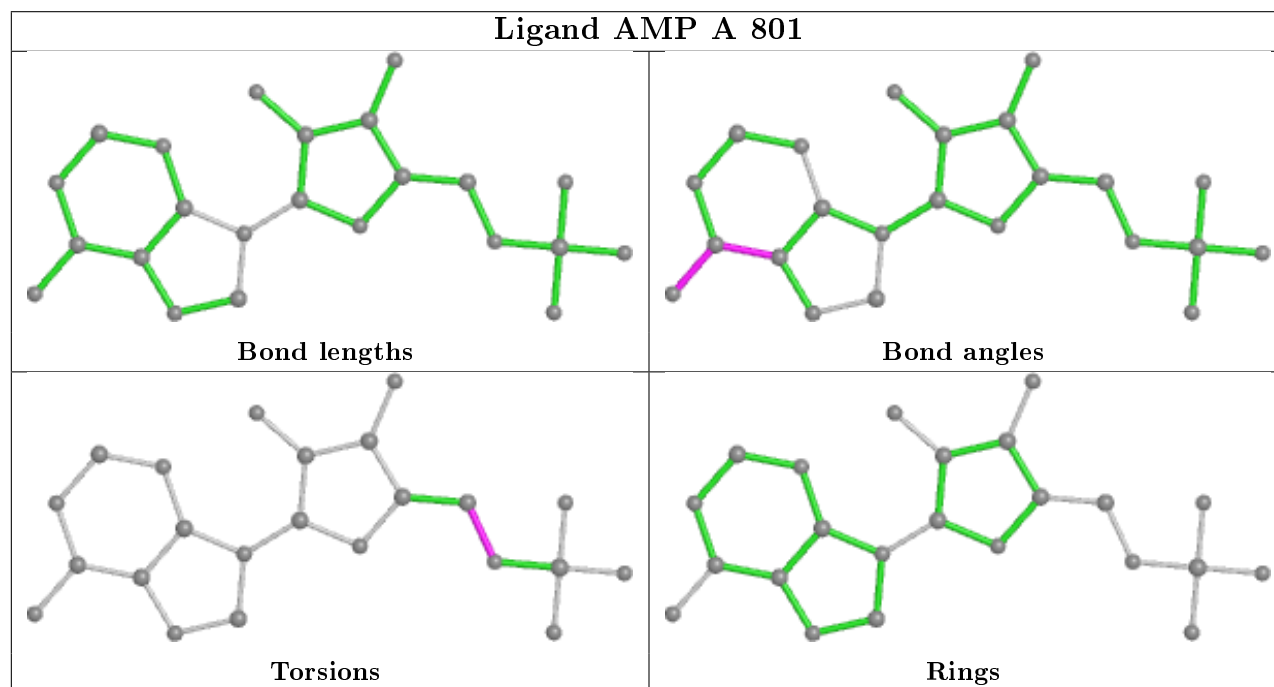
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	AMP	1	0
7	B	801	ATP	2	0
4	A	804	PT1	1	0

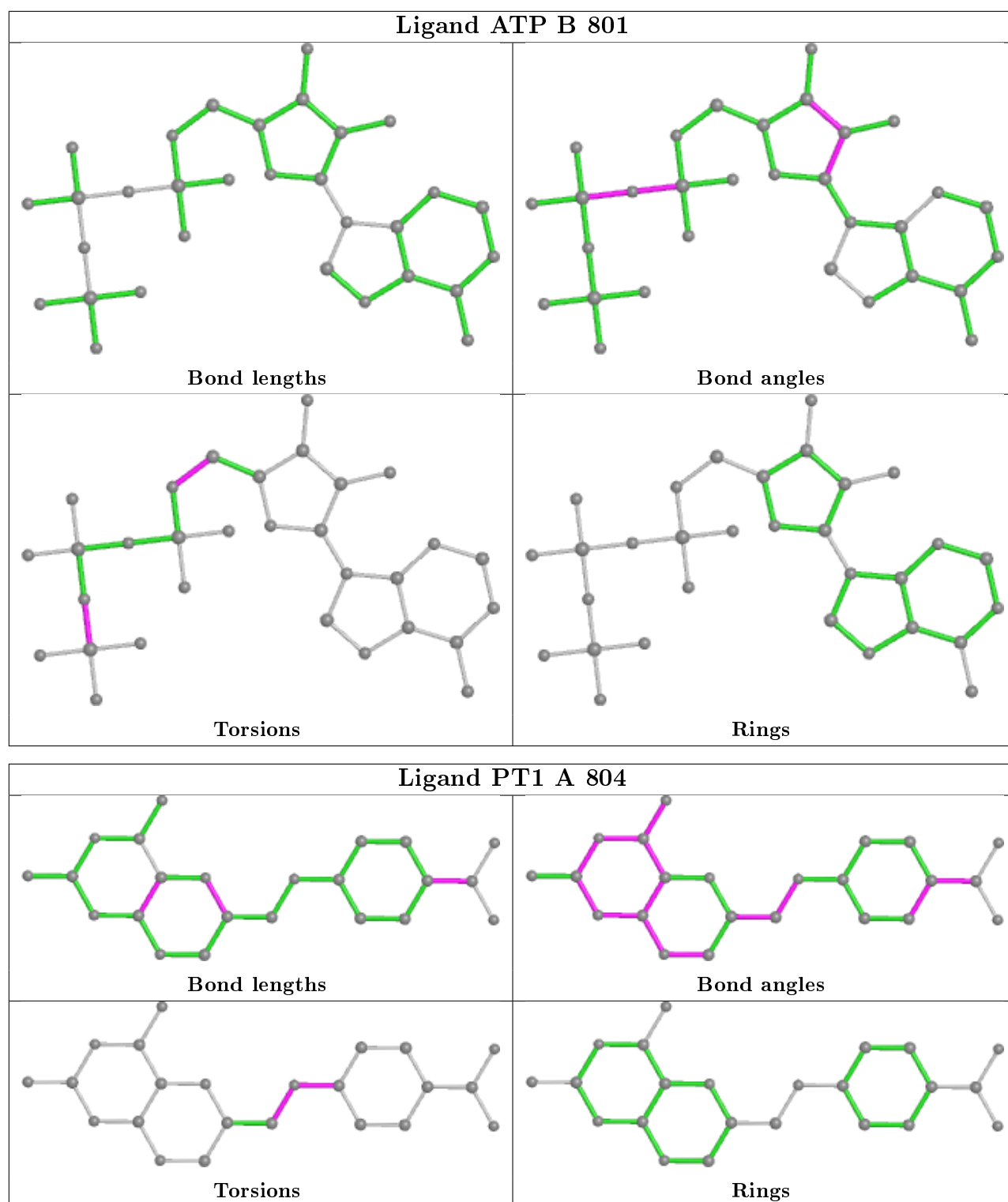
Continued on next page...

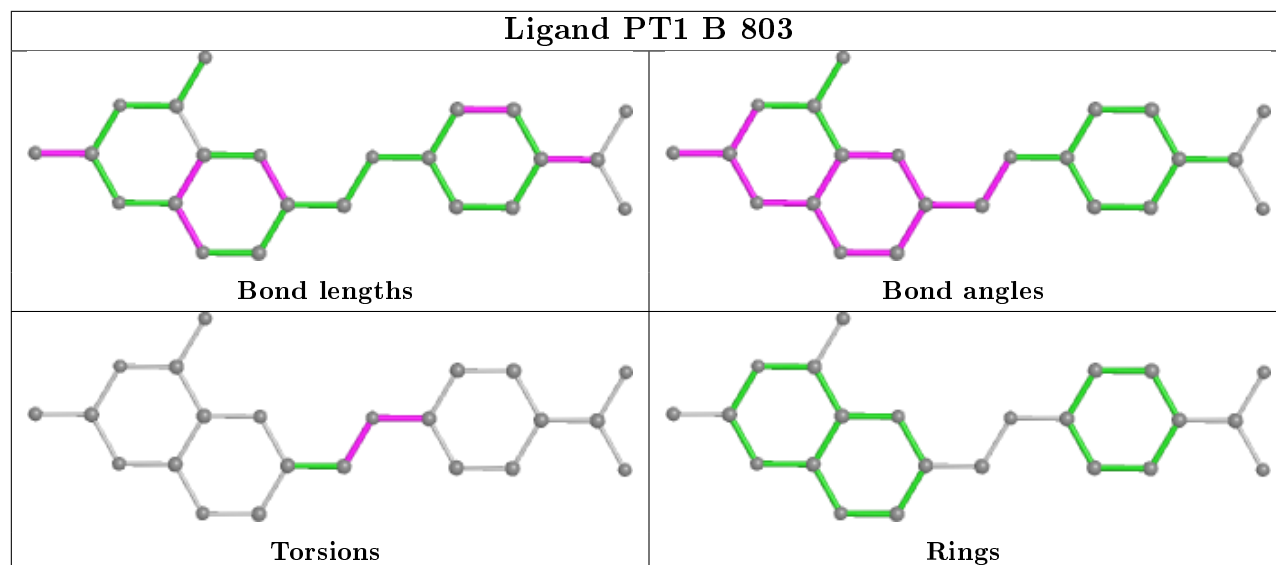
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	PT1	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 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	548/728 (75%)	0.75	65 (11%) 4 6	24, 53, 118, 120	0
1	B	571/728 (78%)	0.52	56 (9%) 7 10	25, 56, 118, 120	0
All	All	1119/1456 (76%)	0.64	121 (10%) 5 8	24, 55, 118, 120	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	PRO	9.4
1	A	467	LYS	9.0
1	A	470	ILE	8.8
1	B	441	ILE	8.7
1	A	471	VAL	8.7
1	B	473	CYS	8.6
1	A	473	CYS	7.5
1	A	444	PRO	7.4
1	A	439	PHE	6.9
1	A	708	ASP	6.5
1	A	310	VAL	6.5
1	A	440	VAL	6.5
1	A	305	ILE	6.5
1	A	84	TYR	6.5
1	A	302	PRO	6.3
1	A	468	ASN	6.0
1	B	468	ASN	5.9
1	A	304	GLU	5.9
1	A	658	LYS	5.6
1	B	442	PRO	5.5
1	B	472	LYS	5.4
1	B	301	ASP	5.4
1	A	469	LYS	5.4
1	A	443	ASN	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	470	ILE	5.3
1	A	228	LYS	5.2
1	B	302	PRO	5.2
1	B	231	ILE	5.2
1	B	471	VAL	5.1
1	A	300	ARG	5.1
1	A	307	ASN	4.9
1	B	440	VAL	4.7
1	B	11	GLU	4.6
1	A	243	ARG	4.6
1	B	147	MET	4.5
1	B	467	LYS	4.5
1	A	445	LYS	4.5
1	A	303	GLN	4.4
1	B	304	GLU	4.4
1	B	474	ASP	4.4
1	A	441	ILE	4.4
1	A	232	TYR	4.3
1	A	367	ASN	4.3
1	A	186	TYR	4.2
1	B	303	GLN	4.1
1	A	472	LYS	4.1
1	B	305	ILE	4.1
1	A	229	ASN	4.1
1	B	307	ASN	4.0
1	A	299	PHE	3.9
1	A	301	ASP	3.9
1	A	365	ASN	3.8
1	B	220	PHE	3.8
1	B	710	ASN	3.8
1	A	123	ILE	3.8
1	A	58	VAL	3.8
1	A	162	TYR	3.8
1	A	466	ILE	3.7
1	B	229	ASN	3.7
1	A	142	LYS	3.7
1	A	364	TYR	3.7
1	A	308	ASN	3.7
1	A	366	ILE	3.6
1	B	439	PHE	3.6
1	B	235	LEU	3.5
1	A	446	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	306	ILE	3.3
1	B	469	LYS	3.3
1	A	206	ILE	3.3
1	A	306	ILE	3.3
1	A	11	GLU	3.2
1	B	12	GLU	3.2
1	A	161	SER	3.2
1	B	445	LYS	3.2
1	B	708	ASP	3.2
1	B	146	ILE	3.2
1	A	220	PHE	3.1
1	B	232	TYR	3.1
1	B	466	ILE	3.0
1	B	241	LEU	2.9
1	A	311	ASP	2.9
1	B	7	LEU	2.9
1	B	228	LYS	2.9
1	A	357	VAL	2.9
1	B	615	CYS	2.9
1	B	475	ALA	2.8
1	B	134	LEU	2.8
1	B	227	GLU	2.7
1	A	474	ASP	2.7
1	B	225	LYS	2.6
1	A	227	GLU	2.5
1	A	87	GLU	2.5
1	B	87	GLU	2.5
1	A	659	ASP	2.5
1	B	14	LYS	2.5
1	A	125	LYS	2.5
1	A	128	ASN	2.5
1	B	13	ASN	2.5
1	B	8	ILE	2.5
1	B	315	PHE	2.4
1	B	309	MET	2.4
1	A	309	MET	2.3
1	A	120	ASP	2.3
1	B	186	TYR	2.3
1	A	141	VAL	2.3
1	B	120	ASP	2.2
1	A	475	ALA	2.2
1	B	463	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	9	LEU	2.2
1	B	662	LEU	2.2
1	B	234	ILE	2.2
1	A	706	VAL	2.2
1	A	117	GLY	2.2
1	A	28	ARG	2.1
1	A	127	VAL	2.1
1	A	361	LYS	2.1
1	B	518	LYS	2.1
1	B	233	LYS	2.1
1	A	131	ASN	2.0
1	B	142	LYS	2.0
1	B	97	TYR	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
3	MG	A	803	1/1	0.83	0.15	67,67,67,67	0
6	ACT	A	807	4/4	0.85	0.21	48,50,50,62	0
7	ATP	B	801	31/31	0.90	0.13	53,84,120,120	0
6	ACT	B	806	4/4	0.91	0.17	49,51,65,67	0
3	MG	A	802	1/1	0.91	0.08	50,50,50,50	0
2	AMP	A	801	23/23	0.93	0.14	51,83,120,120	0
5	CA	B	804	1/1	0.95	0.25	80,80,80,80	0
5	CA	A	805	1/1	0.96	0.20	63,63,63,63	0
6	ACT	B	805	4/4	0.96	0.15	28,31,33,34	0
6	ACT	A	806	4/4	0.97	0.12	33,43,44,45	0

Continued on next page...

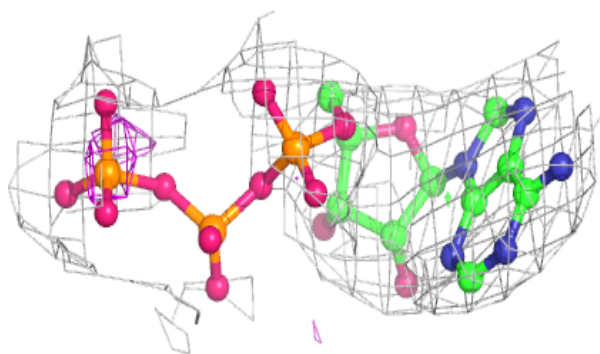
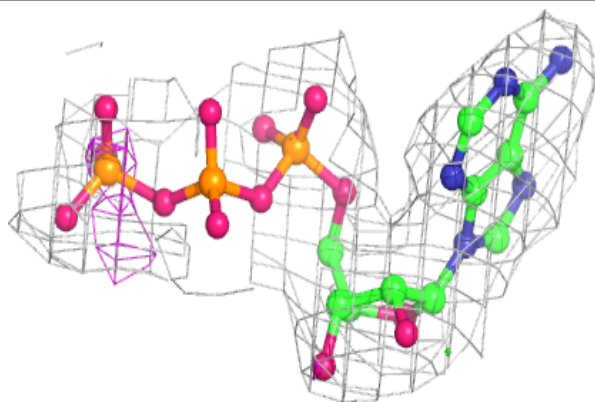
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PT1	A	804	23/23	0.97	0.14	21,25,31,36	0
3	MG	B	802	1/1	0.97	0.10	44,44,44,44	0
4	PT1	B	803	23/23	0.98	0.14	22,26,31,37	0

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

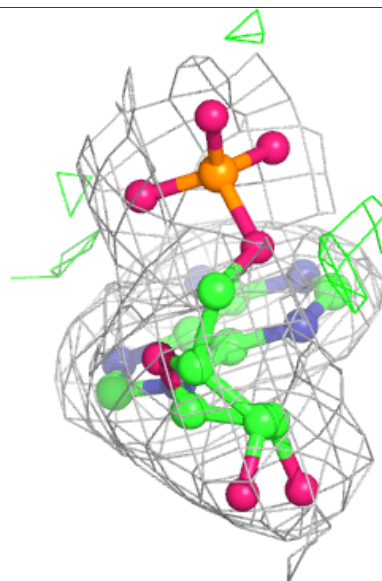
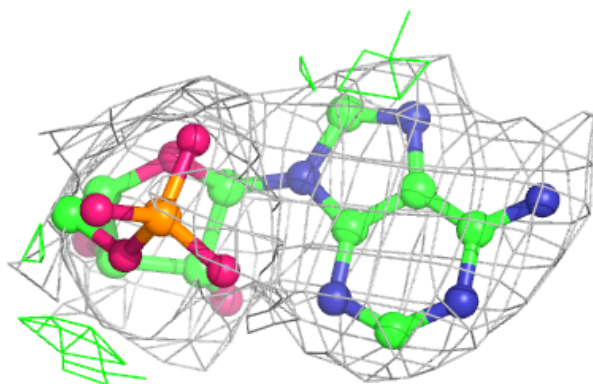
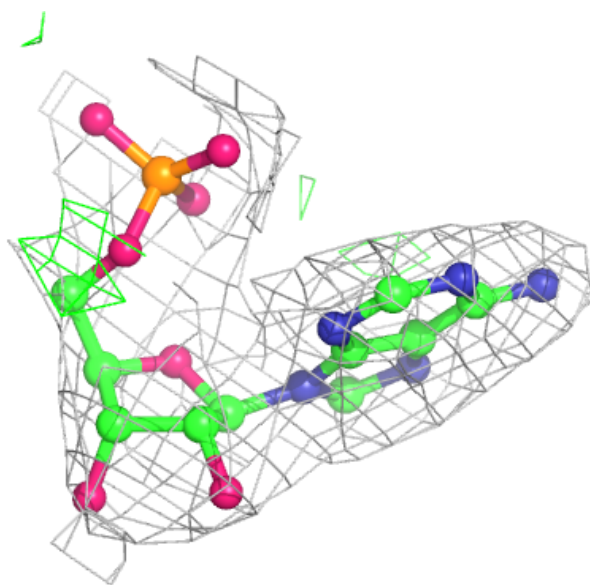
Electron density around ATP B 801:

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



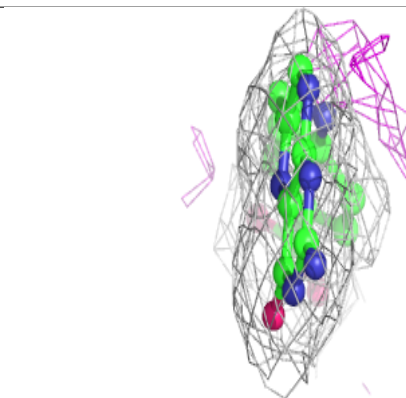
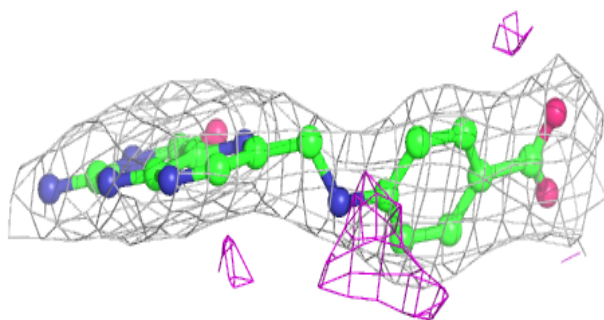
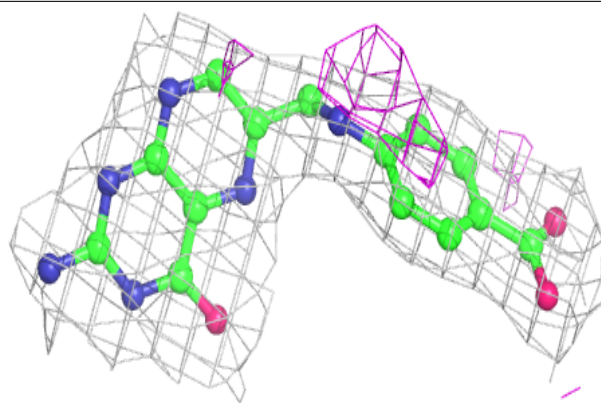
Electron density around AMP A 801:

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

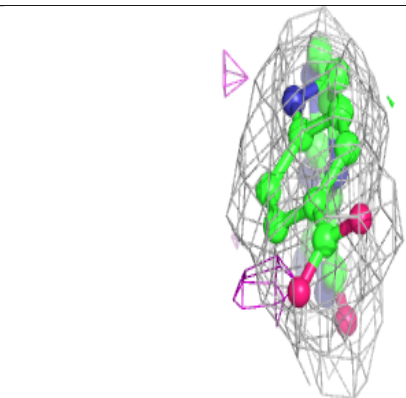
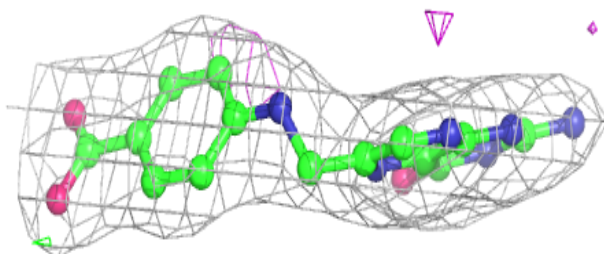
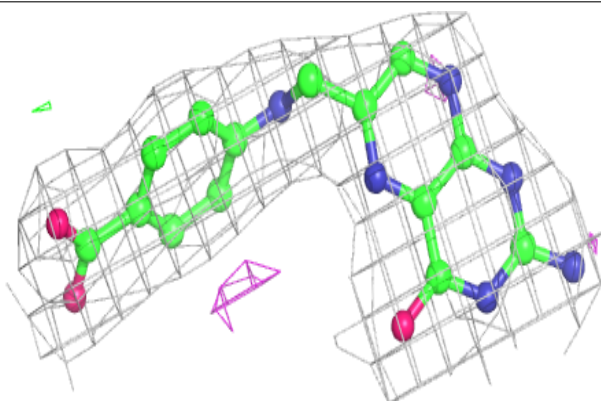


Electron density around PT1 A 804:

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

**Electron density around PT1 B 803:**

$2mF_o-DF_c$ (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.