



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 09:44 PM JST

PDB ID : 6JWR
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS wild type with Pteroate
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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

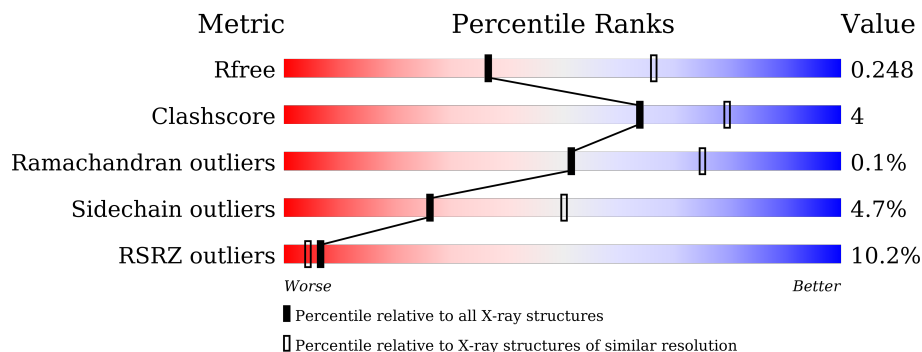
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	 5% 65% 9% 25%
1	B	728	 11% 63% 11% 25%

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 9376 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
			Total	C	N	O	S			
1	A	549	4534	2927	743	842	22	0	0	0
1	B	549	4518	2913	741	843	21	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

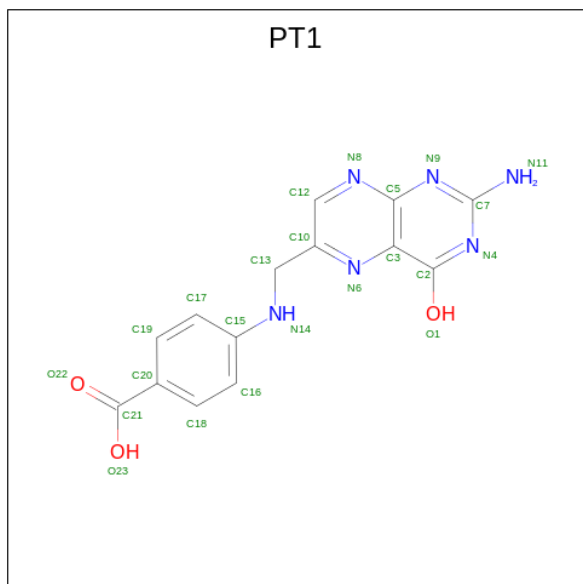
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 PTEROIC ACID (three-letter code: PT1) (formula: C₁₄H₁₂N₆O₃).



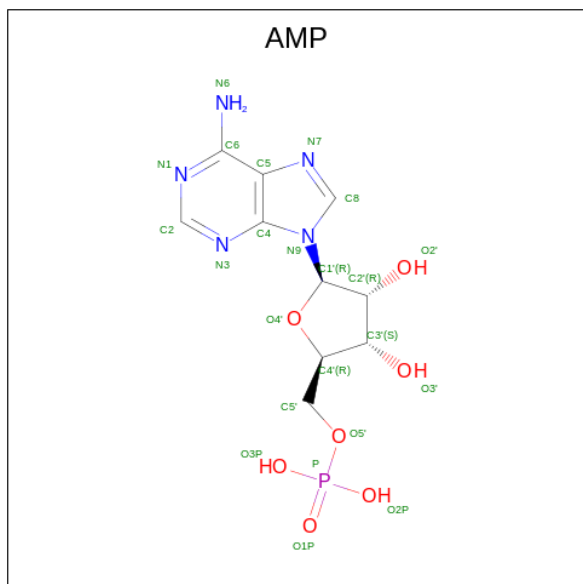
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	23	14	6	3	0	0

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).

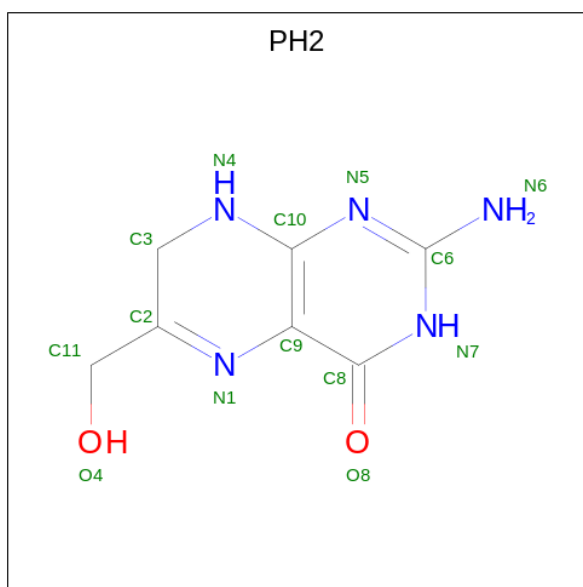


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	23	10	5	7	1	0	0
3	B	1	23	10	5	7	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (three-letter code: PH2) (formula: C₇H₉N₅O₂).

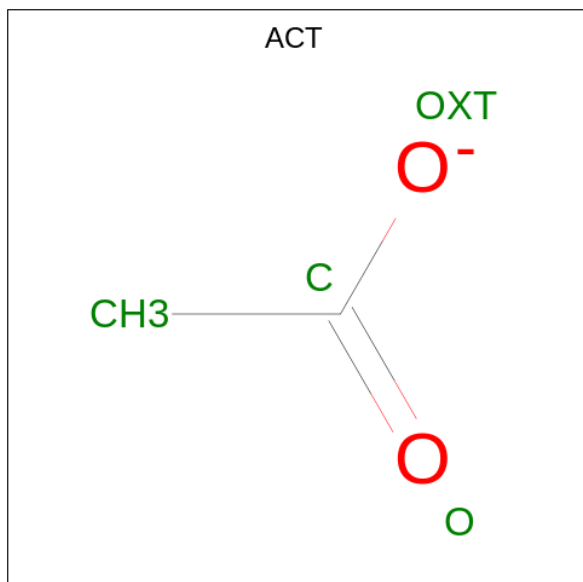


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	7	5	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

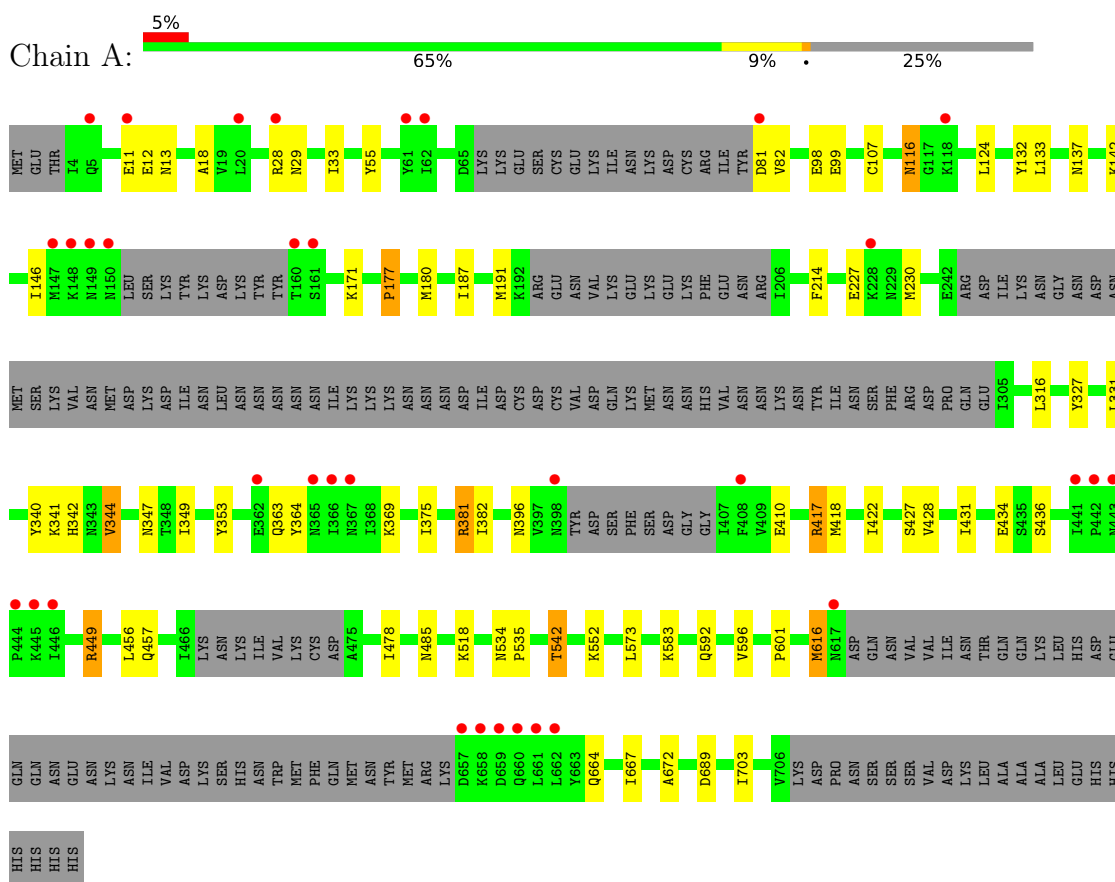
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	118	Total O 118 118	0	0
8	B	67	Total O 67 67	0	0

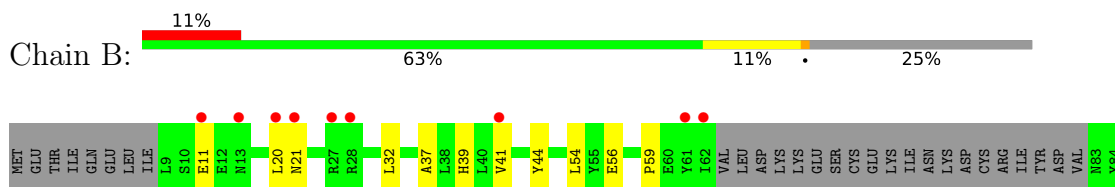
3 Residue-property plots [i](#)

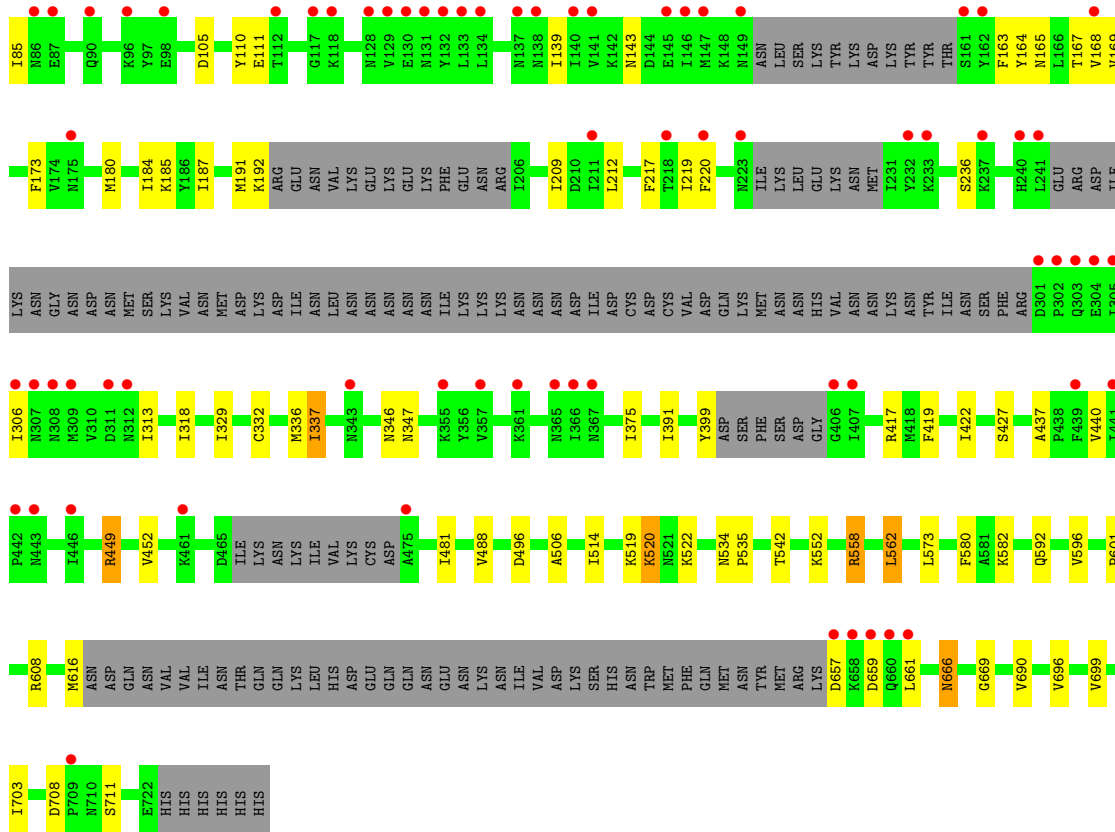
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



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





4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.73Å 137.01Å 138.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.5 (30.00-2.60) 91.6 (29.42-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.15 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.211 , 0.254 0.206 , 0.248	Depositor DCC
R_{free} test set	5226 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for -h,l,k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9376	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PH2, ACT, CA, 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	0.54	0/4606	0.72	0/6218
1	B	0.54	0/4592	0.72	2/6199 (0.0%)
All	All	0.54	0/9198	0.72	2/12417 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	661	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	562	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	PRO	Peptide

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	4534	0	4635	38	0
1	B	4518	0	4596	43	0
2	A	23	0	10	0	0
2	B	23	0	10	0	0
3	A	23	0	12	0	0
3	B	23	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	14	0	9	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	16	0	12	0	0
7	B	12	0	9	0	0
8	A	118	0	0	1	0
8	B	67	0	0	0	0
All	All	9376	0	9305	77	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 (77) 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:608:ARG:HA	1:B:666:ASN:ND2	2.00	0.75
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.70	0.73
1:B:514:ILE:HG12	1:B:562:LEU:HD22	1.75	0.67
1:A:573:LEU:HD23	1:A:601:PRO:HB2	1.81	0.63
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.72	0.62
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.82	0.62
1:B:217:PHE:HB3	1:B:219:ILE:HD12	1.82	0.62
1:A:107:CYS:SG	1:A:171:LYS:HE3	2.40	0.61
1:A:418:MET:O	1:A:422:ILE:HD12	2.00	0.61
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.29	0.61
1:A:449:ARG:HD3	1:A:449:ARG:C	2.20	0.61
1:B:39:HIS:CD2	1:B:520:LYS:HB3	2.38	0.58
1:B:552:LYS:HD2	1:B:596:VAL:HG13	1.85	0.58
1:B:449:ARG:HD3	1:B:449:ARG:C	2.24	0.57
1:A:133:LEU:O	1:A:137:ASN:HB2	2.03	0.57
1:B:20:LEU:HB2	1:B:168:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ALA:HB1	1:B:558:ARG:HG2	1.87	0.55
1:A:132:TYR:CD2	1:A:344:VAL:HG21	2.41	0.55
1:B:616:MET:HE1	1:B:669:GLY:HA3	1.89	0.55
1:A:107:CYS:SG	1:A:171:LYS:CE	2.95	0.54
1:B:336:MET:HB2	1:B:337:ILE:HD13	1.90	0.54
1:A:18:ALA:CB	1:A:180:MET:HE1	2.38	0.54
1:A:187:ILE:HG22	1:A:191:MET:HE2	1.89	0.54
1:A:363:GLN:HG3	1:A:364:TYR:HD1	1.72	0.53
1:B:21:ASN:HB2	1:B:212:LEU:HD21	1.90	0.52
1:B:580:PHE:O	1:B:582:LYS:HD2	2.09	0.52
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.92	0.51
1:A:29:ASN:O	1:A:33:ILE:HG12	2.11	0.51
1:B:449:ARG:HB3	1:B:488:VAL:HG22	1.93	0.50
1:A:124:LEU:HD12	1:A:177:PRO:HG2	1.93	0.50
1:B:139:ILE:O	1:B:143:ASN:HB2	2.11	0.50
1:B:616:MET:CE	1:B:669:GLY:HA3	2.41	0.50
1:A:417:ARG:O	1:A:417:ARG:HD2	2.12	0.50
1:B:573:LEU:HD23	1:B:601:PRO:HB2	1.93	0.49
1:B:37:ALA:O	1:B:41:VAL:HG23	2.12	0.49
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.95	0.49
1:B:608:ARG:HA	1:B:666:ASN:HD21	1.76	0.49
1:B:184:ILE:HG23	1:B:209:ILE:HB	1.95	0.48
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.43	0.48
1:B:44:TYR:HB2	1:B:187:ILE:HD11	1.96	0.47
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.96	0.47
1:B:419:PHE:HA	1:B:422:ILE:HD12	1.97	0.46
1:A:353:TYR:OH	1:A:369:LYS:HE3	2.15	0.46
1:B:519:LYS:O	1:B:522:LYS:N	2.49	0.46
1:B:708:ASP:HB3	1:B:711:SER:HB3	1.97	0.46
1:A:375:ILE:HG12	1:A:382:ILE:HG23	1.98	0.46
1:B:452:VAL:HG11	1:B:481:ILE:CD1	2.46	0.45
1:A:428:VAL:HG22	1:A:478:ILE:HB	1.98	0.45
1:A:592:GLN:HG2	1:B:703:ILE:O	2.16	0.45
1:B:39:HIS:NE2	1:B:520:LYS:HB3	2.30	0.45
1:B:306:ILE:HD12	1:B:306:ILE:H	1.82	0.45
1:B:437:ALA:O	1:B:440:VAL:HG22	2.17	0.45
1:B:191:MET:O	1:B:192:LYS:HB2	2.18	0.44
1:B:185:LYS:HG3	1:B:313:ILE:HG12	1.99	0.44
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.99	0.44
1:A:116:ASN:ND2	1:A:341:LYS:O	2.51	0.43
1:B:391:ILE:HG21	1:B:690:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:MET:HE1	1:B:699:VAL:CG2	2.48	0.43
1:A:485:ASN:HB3	8:A:1012:HOH:O	2.18	0.43
1:A:327:TYR:CE1	1:A:353:TYR:CE1	3.07	0.42
1:B:217:PHE:HB3	1:B:219:ILE:CD1	2.48	0.42
1:A:667:ILE:HG12	1:A:689:ASP:OD2	2.20	0.42
1:B:110:TYR:CE1	1:B:169:VAL:HG11	2.55	0.42
1:A:542:THR:HG21	1:A:583:LYS:HE2	2.02	0.42
1:A:142:LYS:HE2	1:A:146:ILE:HD11	2.02	0.42
1:A:703:ILE:O	1:B:592:GLN:HG2	2.20	0.41
1:B:56:GLU:HB2	1:B:164:TYR:CE1	2.55	0.41
1:A:28:ARG:O	1:A:381:ARG:NH2	2.54	0.41
1:A:227:GLU:HB2	1:A:230:MET:HB2	2.02	0.41
1:A:534:ASN:HB2	1:A:535:PRO:HD2	2.03	0.41
1:A:340:TYR:CE2	1:A:342:HIS:HB2	2.56	0.41
1:B:167:THR:OG1	1:B:332:CYS:HB3	2.21	0.41
1:B:21:ASN:ND2	1:B:329:ILE:HG12	2.35	0.41
1:A:55:TYR:CD2	1:A:331:LEU:HD21	2.56	0.40
1:B:180:MET:HG2	1:B:184:ILE:HD12	2.03	0.40
1:A:177:PRO:HD3	1:A:214:PHE:CD1	2.57	0.40
1:A:672:ALA:HB2	1:B:696:VAL:HA	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	533/728 (73%)	509 (96%)	24 (4%)	0	100 100
1	B	531/728 (73%)	502 (94%)	28 (5%)	1 (0%)	47 71
All	All	1064/1456 (73%)	1011 (95%)	52 (5%)	1 (0%)	51 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	520	LYS

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	523/696 (75%)	498 (95%)	25 (5%)	25	49
1	B	519/696 (75%)	495 (95%)	24 (5%)	27	51
All	All	1042/1392 (75%)	993 (95%)	49 (5%)	26	50

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	12	GLU
1	A	13	ASN
1	A	81	ASP
1	A	82	VAL
1	A	98	GLU
1	A	99	GLU
1	A	116	ASN
1	A	177	PRO
1	A	344	VAL
1	A	347	ASN
1	A	349	ILE
1	A	381	ARG
1	A	396	ASN
1	A	410	GLU
1	A	417	ARG
1	A	427	SER
1	A	434	GLU
1	A	436	SER
1	A	449	ARG
1	A	457	GLN
1	A	518	LYS
1	A	542	THR

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Mol	Chain	Res	Type
1	A	616	MET
1	A	664	GLN
1	B	11	GLU
1	B	32	LEU
1	B	85	ILE
1	B	105	ASP
1	B	111	GLU
1	B	163	PHE
1	B	165	ASN
1	B	173	PHE
1	B	220	PHE
1	B	236	SER
1	B	318	ILE
1	B	337	ILE
1	B	346	ASN
1	B	347	ASN
1	B	399	TYR
1	B	417	ARG
1	B	427	SER
1	B	449	ARG
1	B	496	ASP
1	B	542	THR
1	B	558	ARG
1	B	657	ASP
1	B	659	ASP
1	B	666	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	116	ASN
1	A	460	GLN
1	A	553	ASN
1	A	557	GLN
1	A	617	ASN
1	B	116	ASN
1	B	143	ASN
1	B	165	ASN
1	B	343	ASN
1	B	460	GLN
1	B	557	GLN

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Mol	Chain	Res	Type
1	B	666	ASN
1	B	710	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	PT1	A	801	-	24,25,25	1.53	2 (8%)	31,35,35	1.66	5 (16%)
3	AMP	B	802	4	22,25,25	1.12	2 (9%)	25,38,38	1.46	5 (20%)
7	ACT	A	808	-	3,3,3	0.79	0	3,3,3	0.85	0
7	ACT	A	809	-	3,3,3	0.86	0	3,3,3	0.54	0
7	ACT	A	810	-	3,3,3	0.92	0	3,3,3	0.58	0
7	ACT	B	805	-	3,3,3	0.85	0	3,3,3	0.92	0
3	AMP	A	802	4	22,25,25	1.15	2 (9%)	25,38,38	1.42	4 (16%)
7	ACT	B	807	-	3,3,3	0.61	0	3,3,3	1.40	0
2	PT1	B	801	-	24,25,25	1.46	3 (12%)	31,35,35	1.99	6 (19%)
7	ACT	B	806	-	3,3,3	0.89	0	3,3,3	0.56	0
7	ACT	A	807	-	3,3,3	0.82	0	3,3,3	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PH2	A	805	4	10,15,15	1.18	1 (10%)	10,21,21	2.55	6 (60%)

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	PT1	A	801	-	-	3/9/9/9	0/3/3/3
3	AMP	B	802	4	-	3/6/26/26	0/3/3/3
3	AMP	A	802	4	-	3/6/26/26	0/3/3/3
2	PT1	B	801	-	-	2/9/9/9	0/3/3/3
5	PH2	A	805	4	-	0/0/11/11	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PT1	C3-C5	5.29	1.49	1.40
2	B	801	PT1	C3-C5	4.33	1.48	1.40
3	A	802	AMP	O4'-C1'	2.95	1.45	1.41
3	B	802	AMP	C5-C4	2.95	1.48	1.40
5	A	805	PH2	C9-C10	2.83	1.49	1.41
2	A	801	PT1	C5-N8	-2.70	1.33	1.37
3	A	802	AMP	C5-C4	2.69	1.48	1.40
2	B	801	PT1	C10-N6	2.36	1.36	1.32
2	B	801	PT1	C12-N8	2.06	1.35	1.31
3	B	802	AMP	C2-N3	2.03	1.35	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	PT1	N8-C5-N9	5.94	122.60	115.82
2	A	801	PT1	N8-C5-N9	5.83	122.47	115.82
5	A	805	PH2	C6-N7-C8	4.36	122.86	115.93
3	A	802	AMP	N3-C2-N1	-4.06	122.33	128.68
2	B	801	PT1	C7-N9-C5	3.99	119.91	115.36
2	B	801	PT1	C12-N8-C5	3.85	120.56	116.69
3	B	802	AMP	N3-C2-N1	-3.67	122.95	128.68
2	B	801	PT1	N9-C7-N4	-3.66	122.35	127.22
2	A	801	PT1	C12-N8-C5	3.56	120.27	116.69
5	A	805	PH2	C9-C8-N7	-3.45	118.72	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	PH2	C6-N5-C10	3.29	121.90	114.54
5	A	805	PH2	O4-C11-C2	3.13	115.97	111.61
3	B	802	AMP	C3'-C2'-C1'	2.76	105.14	100.98
2	A	801	PT1	C10-C13-N14	-2.61	107.30	113.07
2	B	801	PT1	C7-N4-C2	2.44	122.58	116.43
2	B	801	PT1	C10-C13-N14	-2.37	107.82	113.07
2	A	801	PT1	C7-N4-C2	2.37	122.40	116.43
5	A	805	PH2	C10-C9-C8	2.34	116.06	114.53
5	A	805	PH2	N5-C6-N7	-2.23	121.92	125.42
3	A	802	AMP	O5'-C5'-C4'	2.15	116.39	108.99
3	B	802	AMP	O3P-P-O2P	2.14	115.83	107.64
3	B	802	AMP	C2'-C3'-C4'	2.14	106.79	102.64
3	B	802	AMP	C2-N1-C6	2.13	122.40	118.75
3	A	802	AMP	O5'-P-O1P	-2.12	100.52	106.47
2	A	801	PT1	C7-N9-C5	2.11	117.77	115.36
3	A	802	AMP	C2-N1-C6	2.11	122.36	118.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

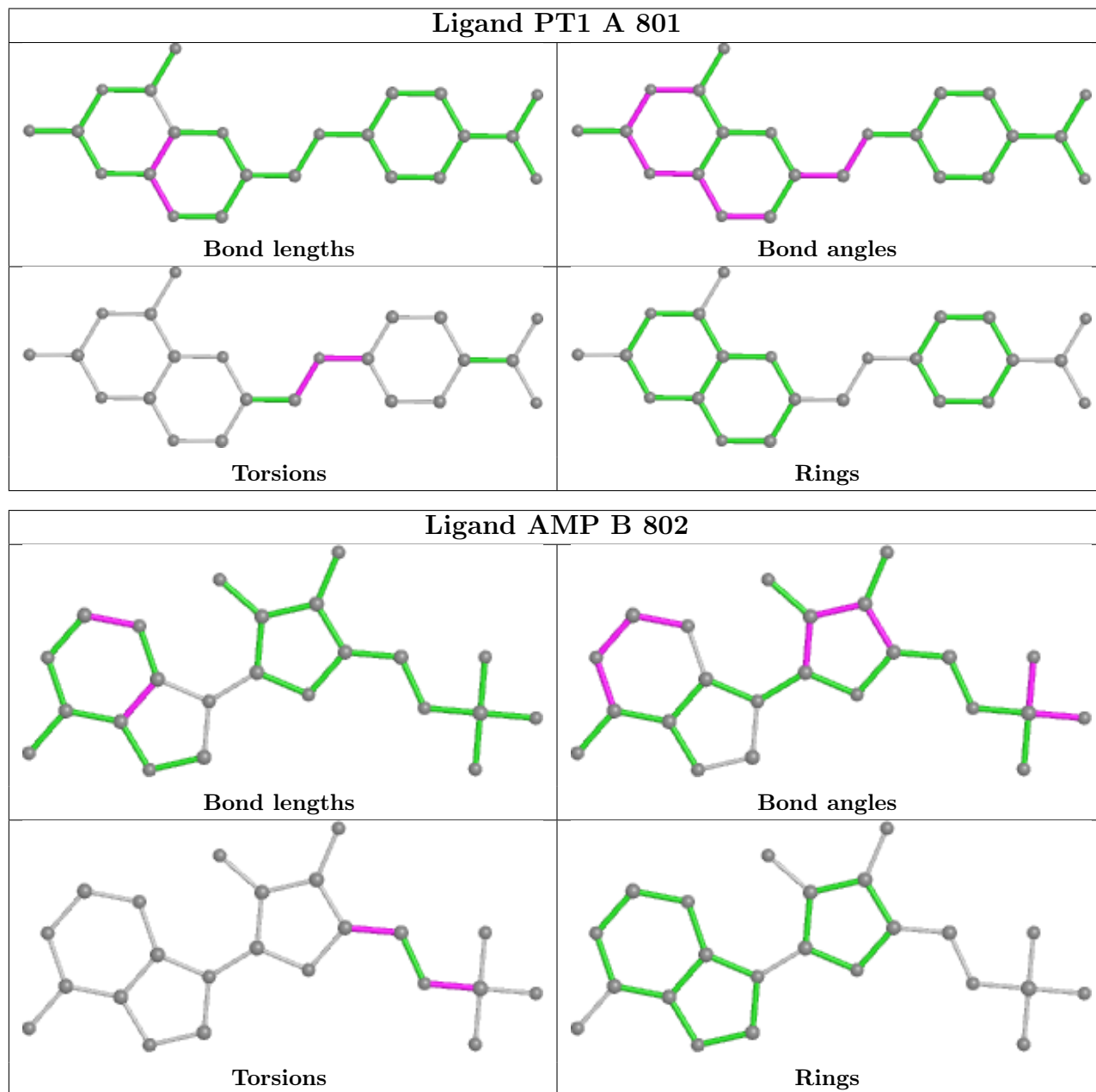
Mol	Chain	Res	Type	Atoms
2	A	801	PT1	C10-C13-N14-C15
3	A	802	AMP	O4'-C4'-C5'-O5'
3	A	802	AMP	C3'-C4'-C5'-O5'
3	B	802	AMP	C5'-O5'-P-O1P
3	A	802	AMP	C4'-C5'-O5'-P
2	B	801	PT1	C10-C13-N14-C15
2	A	801	PT1	C17-C15-N14-C13
2	B	801	PT1	C16-C15-N14-C13
3	B	802	AMP	C5'-O5'-P-O2P
3	B	802	AMP	O4'-C4'-C5'-O5'
2	A	801	PT1	C16-C15-N14-C13

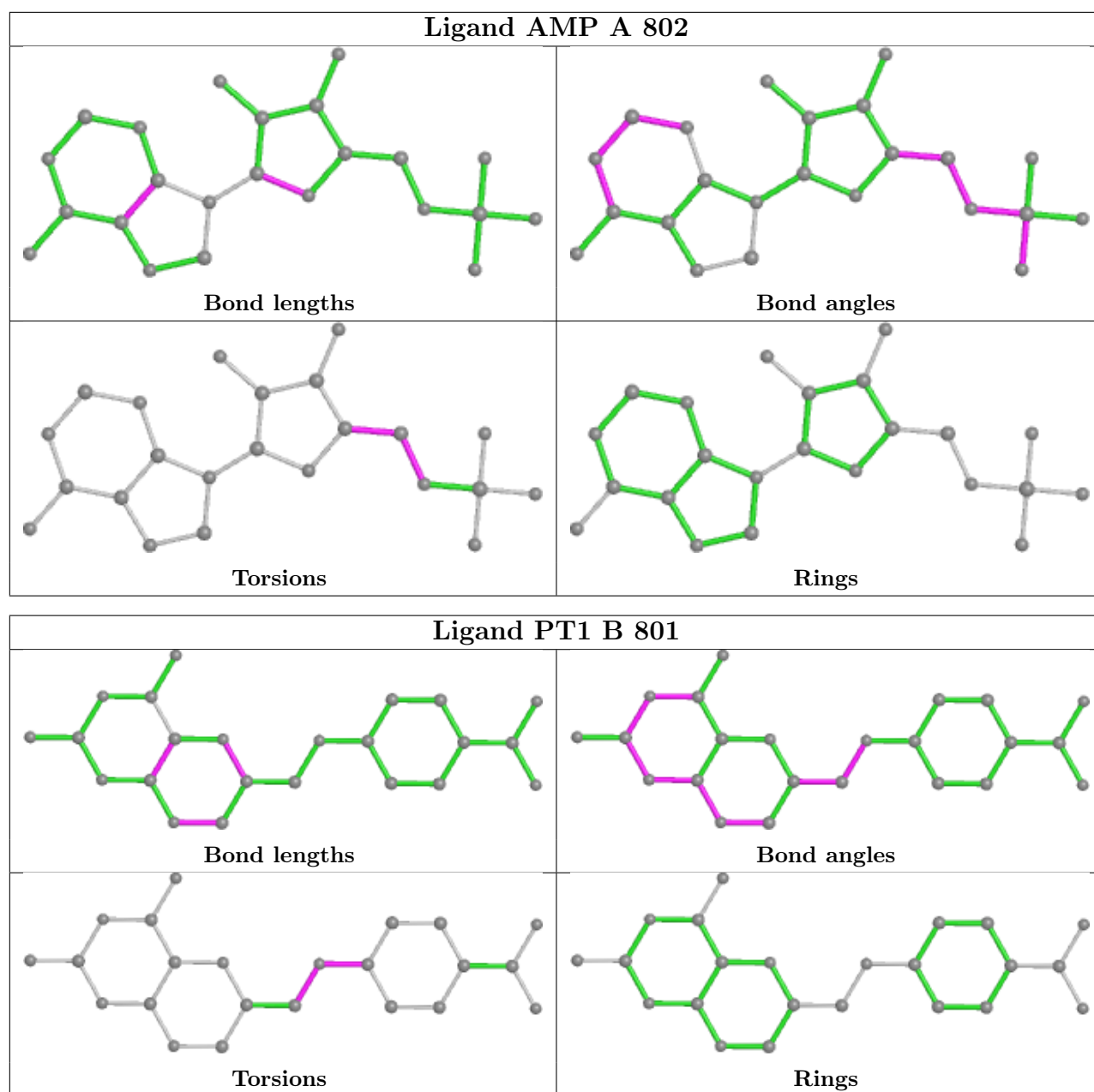
There are no ring outliers.

No monomer is involved in short contacts.

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	549/728 (75%)	-0.02	34 (6%) 20 15	15, 34, 91, 120	0
1	B	549/728 (75%)	0.53	78 (14%) 2 1	15, 60, 117, 120	0
All	All	1098/1456 (75%)	0.26	112 (10%) 6 4	15, 43, 113, 120	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	ASN	7.0
1	B	134	LEU	6.9
1	B	118	LYS	6.4
1	B	305	ILE	6.1
1	B	441	ILE	5.2
1	B	147	MET	5.2
1	A	11	GLU	5.1
1	B	366	ILE	5.0
1	B	146	ILE	4.6
1	A	659	ASP	4.6
1	B	367	ASN	4.5
1	A	662	LEU	4.5
1	B	131	ASN	4.4
1	B	90	GLN	4.4
1	B	303	GLN	4.3
1	B	439	PHE	4.3
1	B	301	ASP	4.3
1	B	96	LYS	4.2
1	B	129	VAL	4.2
1	B	240	HIS	4.1
1	B	133	LEU	4.1
1	A	443	ASN	4.1
1	B	241	LEU	4.0
1	B	442	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	160	THR	4.0
1	B	130	GLU	4.0
1	B	232	TYR	3.9
1	A	118	LYS	3.9
1	B	660	GLN	3.8
1	A	661	LEU	3.7
1	B	62	ILE	3.7
1	B	312	ASN	3.7
1	B	233	LYS	3.6
1	B	13	ASN	3.6
1	B	657	ASP	3.6
1	B	138	ASN	3.5
1	B	140	ILE	3.5
1	A	657	ASP	3.4
1	B	141	VAL	3.4
1	B	357	VAL	3.4
1	A	617	ASN	3.3
1	B	86	ASN	3.3
1	B	658	LYS	3.2
1	B	406	GLY	3.2
1	A	147	MET	3.2
1	A	366	ILE	3.2
1	B	709	PRO	3.2
1	B	137	ASN	3.2
1	B	302	PRO	3.1
1	B	98	GLU	3.1
1	A	445	LYS	3.1
1	B	20	LEU	3.1
1	A	441	ILE	3.1
1	A	5	GLN	3.0
1	A	62	ILE	3.0
1	A	81	ASP	3.0
1	B	661	LEU	3.0
1	A	660	GLN	3.0
1	B	306	ILE	2.9
1	B	27	ARG	2.9
1	A	149	ASN	2.8
1	B	443	ASN	2.8
1	B	162	TYR	2.7
1	B	61	TYR	2.7
1	B	145	GLU	2.7
1	B	311	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	444	PRO	2.6
1	B	149	ASN	2.6
1	B	161	SER	2.6
1	B	87	GLU	2.6
1	B	308	ASN	2.6
1	A	28	ARG	2.6
1	B	28	ARG	2.5
1	A	367	ASN	2.5
1	A	658	LYS	2.5
1	A	362	GLU	2.5
1	B	211	ILE	2.5
1	A	446	ILE	2.5
1	B	446	ILE	2.4
1	B	365	ASN	2.4
1	B	132	TYR	2.4
1	B	220	PHE	2.4
1	A	442	PRO	2.3
1	B	175	ASN	2.3
1	A	161	SER	2.3
1	B	475	ALA	2.3
1	A	408	PHE	2.3
1	A	148	LYS	2.2
1	B	117	GLY	2.2
1	B	112	THR	2.2
1	B	659	ASP	2.2
1	A	365	ASN	2.2
1	B	223	ASN	2.2
1	B	355	LYS	2.2
1	A	228	LYS	2.2
1	B	309	MET	2.2
1	B	461	LYS	2.2
1	B	168	VAL	2.2
1	B	237	LYS	2.1
1	B	218	THR	2.1
1	A	398	ASN	2.1
1	B	21	ASN	2.1
1	A	20	LEU	2.1
1	A	150	ASN	2.1
1	B	343	ASN	2.1
1	B	361	LYS	2.1
1	B	41	VAL	2.1
1	B	11	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	407	ILE	2.0
1	B	128	ASN	2.0
1	B	304	GLU	2.0
1	A	61	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.

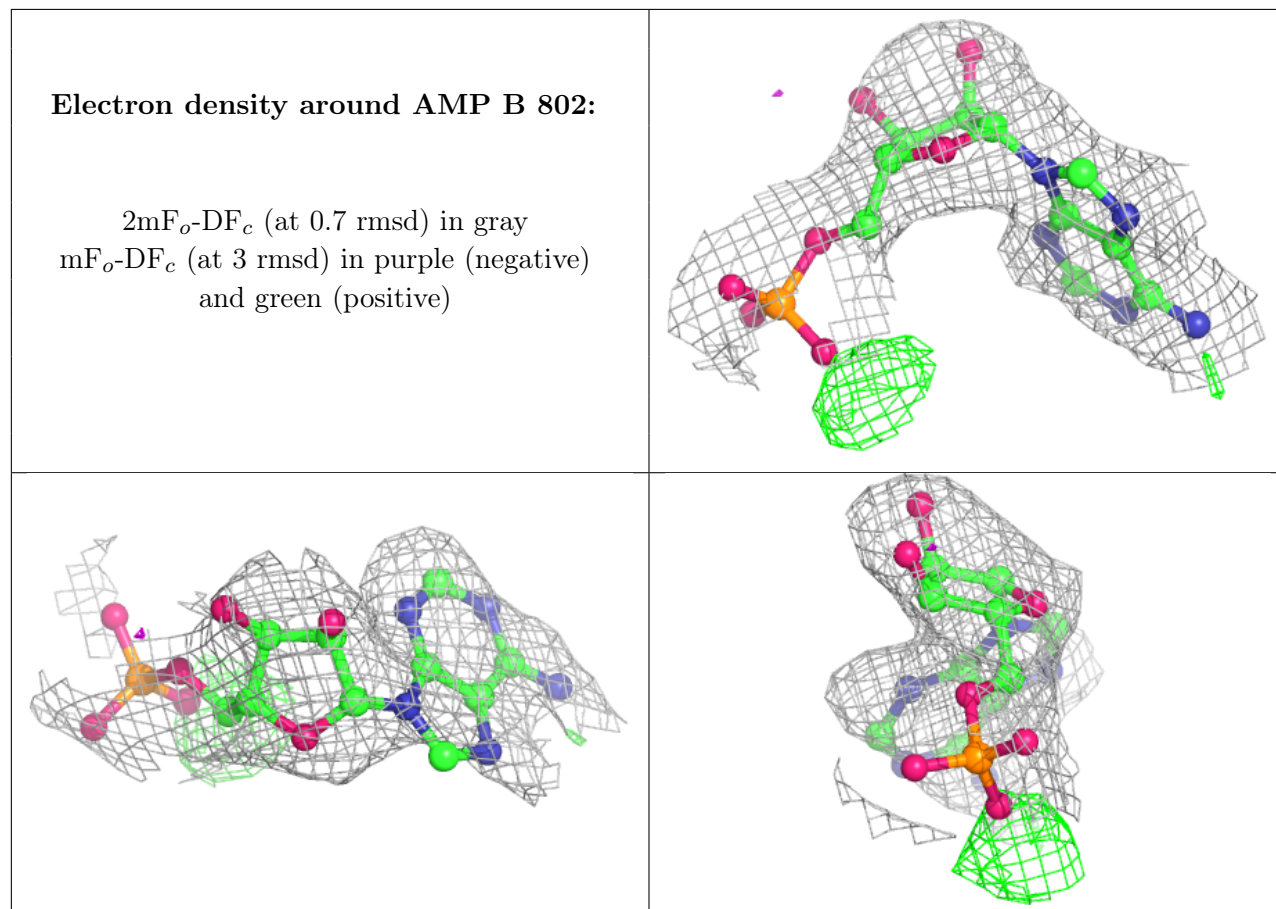
6.4 Ligands [i](#)

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
4	MG	B	803	1/1	0.46	0.29	70,70,70,70	0
3	AMP	B	802	23/23	0.73	0.22	85,95,107,111	0
6	CA	B	804	1/1	0.91	0.09	70,70,70,70	0
7	ACT	B	807	4/4	0.91	0.23	37,41,42,46	0
3	AMP	A	802	23/23	0.93	0.14	35,42,57,65	0
5	PH2	A	805	14/14	0.93	0.16	43,50,54,56	0
7	ACT	A	807	4/4	0.94	0.16	40,40,40,44	0
7	ACT	A	810	4/4	0.95	0.24	47,50,54,54	0
7	ACT	A	809	4/4	0.95	0.17	50,51,52,57	0
2	PT1	B	801	23/23	0.96	0.14	18,19,21,21	0
2	PT1	A	801	23/23	0.96	0.16	14,16,23,24	0
4	MG	A	803	1/1	0.97	0.13	23,23,23,23	0
6	CA	A	806	1/1	0.97	0.16	40,40,40,40	0
7	ACT	B	805	4/4	0.97	0.14	16,17,18,18	0
7	ACT	A	808	4/4	0.97	0.14	28,28,29,30	0
7	ACT	B	806	4/4	0.98	0.18	37,37,38,38	0
4	MG	A	804	1/1	0.98	0.26	31,31,31,31	0

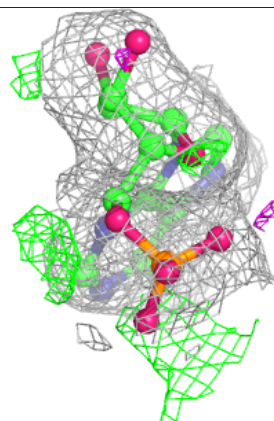
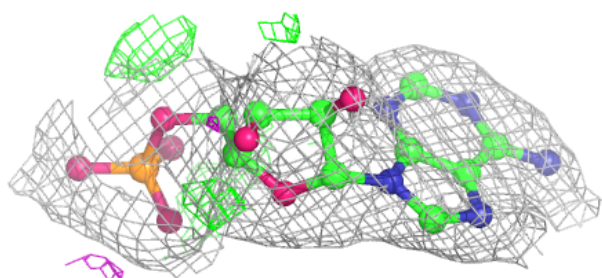
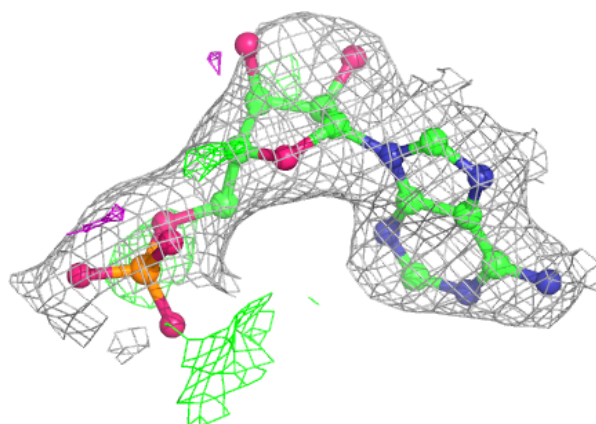
The following is a graphical depiction of the model fit to experimental electron density of all

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.

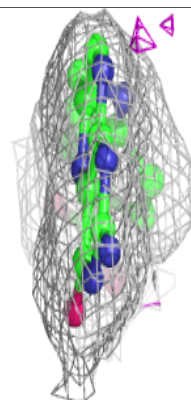
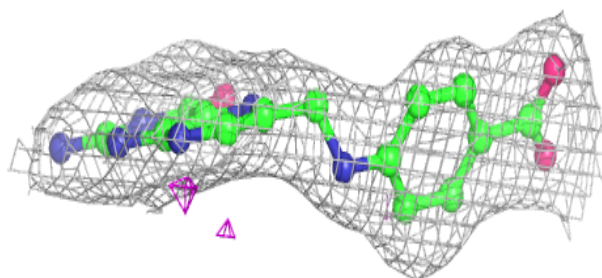
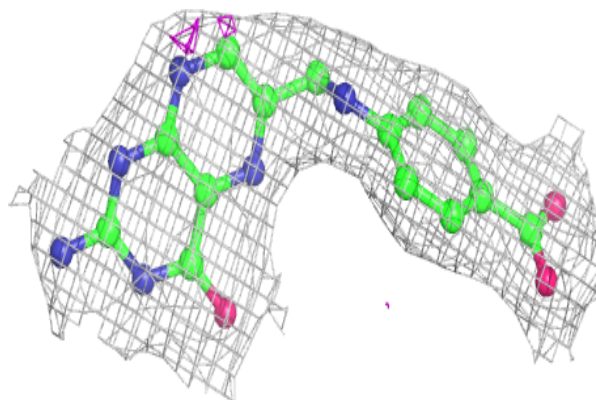


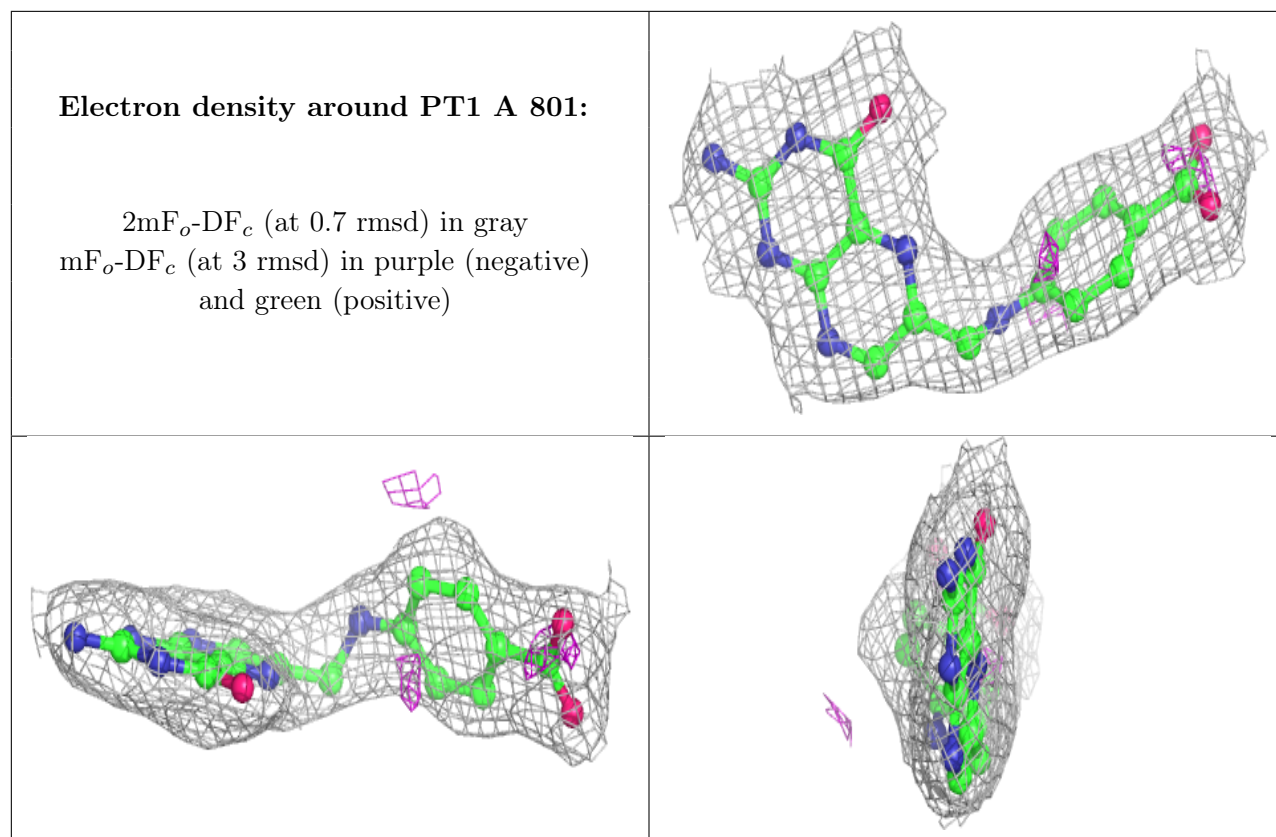
Electron density around AMP A 802:

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

**Electron density around PT1 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.