



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 10:51 AM UTC

PDB ID : 6JWZ / pdb_00006jwz
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS
S436F/A437G/A613S triple mutant with SDX-DHP
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

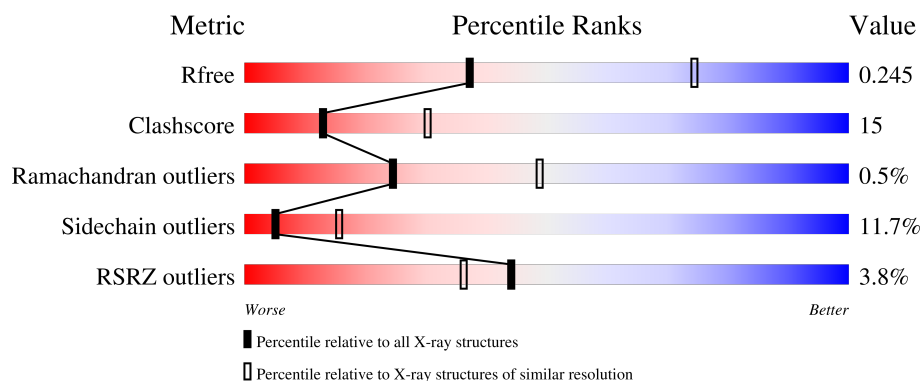
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	2% 47% 25% • 24%
1	B	728	4% 48% 26% • 22%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9505 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	550	Total	C	N	O	S	0	0	0
			4551	2925	756	847	23			
1	B	565	Total	C	N	O	S	0	0	0
			4655	2995	768	869	23			

There are 50 discrepancies between the modelled and reference sequences:

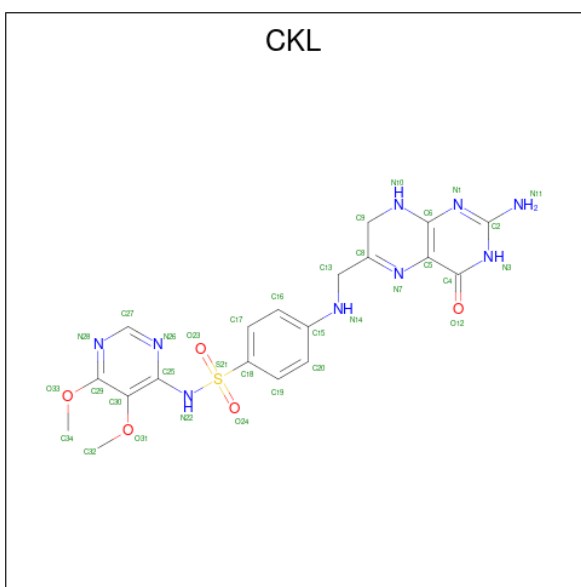
Chain	Residue	Modelled	Actual	Comment	Reference
A	436	PHE	SER	engineered mutation	UNP Q25704
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	613	SER	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710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

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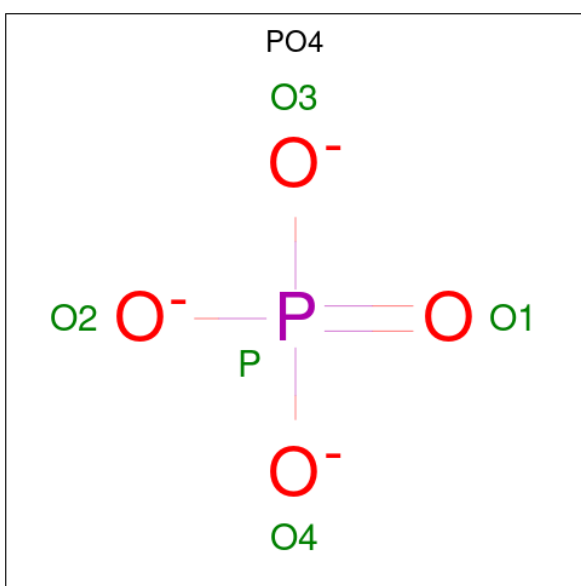
Chain	Residue	Modelled	Actual	Comment	Reference
A	728	HIS	-	expression tag	UNP Q25704
B	436	PHE	SER	engineered mutation	UNP Q25704
B	437	GLY	ALA	engineered mutation	UNP Q25704
B	613	SER	ALA	engineered mutation	UNP Q25704
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709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

- Molecule 2 is 4-[(2-azanyl-4-oxidanylidene-7,8-dihydro-3 {H}-pteridin-6-yl)methylamino]- {N}-(5,6-dimethoxypyrimidin-4-yl)benzenesulfonamide (CCD ID: CKL) (formula: C₁₉H₂₁N₉O₅S).



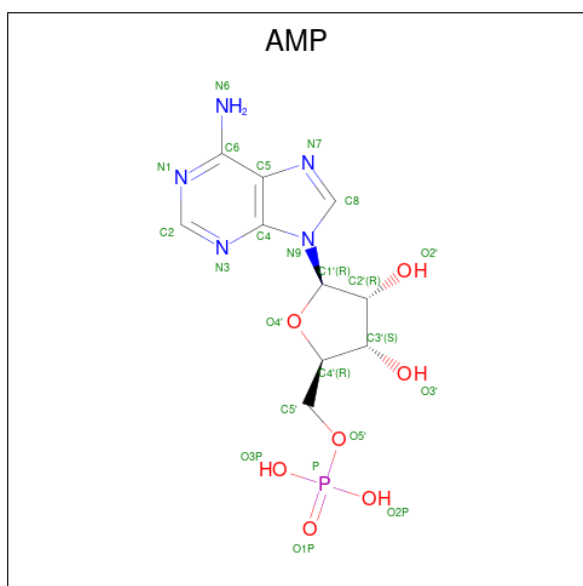
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	19	9	5	1		
2	B	1	Total	C	N	O	S	0	0
			34	19	9	5	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

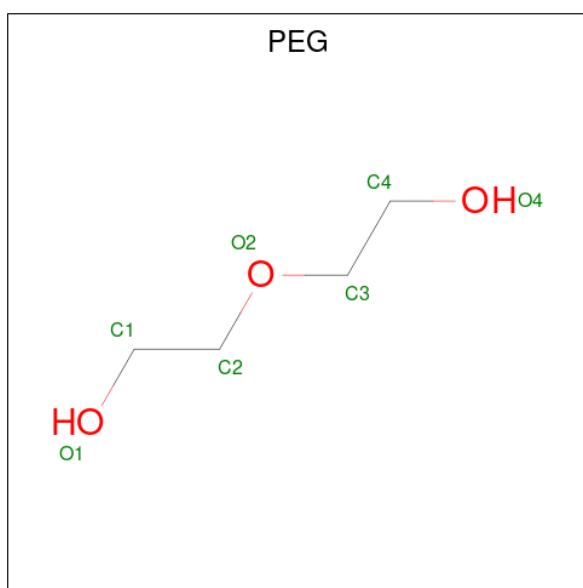
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	79	Total 79	O 79	0	0
9	B	70	Total 70	O 70	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.

- Chain A:**

Position	Conserved Residues (from top)
1	MET, ASP, LYS, THR, ILE
2	MET, ASP, LYS, THR, ILE
3	MET, ASP, LYS, THR, ILE
4	MET, ASP, LYS, THR, ILE
5	MET, ASP, LYS, THR, ILE
6	MET, ASP, LYS, THR, ILE
7	MET, ASP, LYS, THR, ILE
8	MET, ASP, LYS, THR, ILE
9	MET, ASP, LYS, THR, ILE
10	MET, ASP, LYS, THR, ILE
11	GLU
12	SER, LEU, GLN, VAL
13	SER, LEU, GLN, VAL
14	SER, LEU, GLN, VAL
15	SER, LEU, GLN, VAL
16	SER, LEU, GLN, VAL
17	SER, LEU, GLN, VAL
18	SER, LEU, GLN, VAL
19	SER, LEU, GLN, VAL
20	SER, LEU, GLN, VAL
21	SER, LEU, GLN, VAL
22	SER, LEU, GLN, VAL
23	SER, LEU, GLN, VAL
24	SER, LEU, GLN, VAL
25	SER, LEU, GLN, VAL
26	SER, LEU, GLN, VAL
27	SER, LEU, GLN, VAL
28	SER, LEU, GLN, VAL
29	SER, LEU, GLN, VAL
30	SER, LEU, GLN, VAL
31	SER, LEU, GLN, VAL
32	SER, LEU, GLN, VAL
33	SER, LEU, GLN, VAL
34	SER, LEU, GLN, VAL
35	SER, LEU, GLN, VAL
36	SER, LEU, GLN, VAL
37	SER, LEU, GLN, VAL
38	SER, LEU, GLN, VAL
39	SER, LEU, GLN, VAL
40	SER, LEU, GLN, VAL
41	SER, LEU, GLN, VAL
42	SER, LEU, GLN, VAL
43	SER, LEU, GLN, VAL
44	SER, LEU, GLN, VAL
45	SER, LEU, GLN, VAL
46	SER, LEU, GLN, VAL
47	SER, LEU, GLN, VAL
48	SER, LEU, GLN, VAL
49	SER, LEU, GLN, VAL
50	SER, LEU, GLN, VAL
51	SER, LEU, GLN, VAL
52	SER, LEU, GLN, VAL
53	SER, LEU, GLN, VAL
54	SER, LEU, GLN, VAL
55	SER, LEU, GLN, VAL
56	SER, LEU, GLN, VAL
57	SER, LEU, GLN, VAL
58	SER, LEU, GLN, VAL
59	SER, LEU, GLN, VAL
60	SER, LEU, GLN, VAL
61	SER, LEU, GLN, VAL
62	SER, LEU, GLN, VAL
63	SER, LEU, GLN, VAL
64	SER, LEU, GLN, VAL
65	SER, LEU, GLN, VAL
66	SER, LEU, GLN, VAL
67	SER, LEU, GLN, VAL
68	SER, LEU, GLN, VAL
69	SER, LEU, GLN, VAL
70	SER, LEU, GLN, VAL
71	SER, LEU, GLN, VAL
72	SER, LEU, GLN, VAL
73	SER, LEU, GLN, VAL
74	SER, LEU, GLN, VAL
75	SER, LEU, GLN, VAL
76	SER, LEU, GLN, VAL
77	SER, LEU, GLN, VAL
78	SER, LEU, GLN, VAL
79	SER, LEU, GLN, VAL
80	SER, LEU, GLN, VAL
81	SER, LEU, GLN, VAL
82	SER, LEU, GLN, VAL
83	SER, LEU, GLN, VAL
84	SER, LEU, GLN, VAL
85	SER, LEU, GLN, VAL
86	SER, LEU, GLN, VAL
87	SER, LEU, GLN, VAL
88	SER, LEU, GLN, VAL
89	SER, LEU, GLN, VAL
90	SER, LEU, GLN, VAL
91	SER, LEU, GLN, VAL
92	SER, LEU, GLN, VAL
93	SER, LEU, GLN, VAL
94	SER, LEU, GLN, VAL
95	SER, LEU, GLN, VAL
96	SER, LEU, GLN, VAL
97	SER, LEU, GLN, VAL
98	SER, LEU, GLN, VAL
99	SER, LEU, GLN, VAL
100	SER, LEU, GLN, VAL

- 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	100.20Å 136.83Å 138.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.57 – 2.95 29.57 – 2.95	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.57-2.95) 89.3 (29.57-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.194 , 0.255 0.189 , 0.245	Depositor DCC
R_{free} test set	3627 reflections (8.92%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9505	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, PO4, PEG, CKL, ACT, AMP, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/4620	1.08	4/6226 (0.1%)
1	B	0.45	0/4727	1.09	5/6372 (0.1%)
All	All	0.46	0/9347	1.08	9/12598 (0.1%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	603	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	164	TYR	CB-CA-C	5.54	119.35	110.16
1	A	172	THR	CA-CB-OG1	-5.53	101.31	109.60
1	B	508	THR	N-CA-C	-5.44	106.70	113.55

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	374	ARG	Sidechain
1	B	417	ARG	Sidechain

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	4551	0	4660	123	0
1	B	4655	0	4754	163	0
2	A	34	0	0	0	0
2	B	34	0	0	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	23	0	12	0	0
4	B	23	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
8	A	14	0	20	1	0
9	A	79	0	0	4	0
9	B	70	0	0	3	0
All	All	9505	0	9464	283	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 15.

The worst 5 of 283 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:171:LYS:HE2	1.78	1.21
1:B:107:CYS:SG	1:B:171:LYS:NZ	2.25	1.10
1:A:169:VAL:HG23	1:A:336:MET:HE3	1.29	1.08
1:A:107:CYS:SG	1:A:171:LYS:CE	2.58	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:SER:O	1:B:508:THR:HB	1.71	0.91

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%)	503 (94%)	30 (6%)	1 (0%)	43	66
1	B	551/728 (76%)	519 (94%)	28 (5%)	4 (1%)	18	40
All	All	1085/1456 (74%)	1022 (94%)	58 (5%)	5 (0%)	24	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	466	ILE
1	A	365	ASN
1	B	320	HIS
1	B	207	ILE
1	B	535	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	526/697 (76%)	470 (89%)	56 (11%)	6 19
1	B	536/697 (77%)	468 (87%)	68 (13%)	4 13
All	All	1062/1394 (76%)	938 (88%)	124 (12%)	5 16

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	ILE
1	B	520	LYS
1	B	148	LYS
1	B	518	LYS
1	B	697	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	614	HIS
1	B	617	ASN
1	B	21	ASN
1	B	16	ASN
1	B	664	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 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
2	CKL	B	801	-	34,37,37	1.99	5 (14%)	38,53,53	2.88	14 (36%)
4	AMP	A	803	5	25,25,25	1.47	4 (16%)	37,38,38	1.89	6 (16%)
3	PO4	A	802	-	4,4,4	0.28	0	6,6,6	1.36	1 (16%)
8	PEG	A	808	-	6,6,6	0.79	0	5,5,5	0.59	0
2	CKL	A	801	-	34,37,37	2.10	6 (17%)	38,53,53	2.73	11 (28%)
7	ACT	A	806	-	3,3,3	0.83	0	3,3,3	0.86	0
3	PO4	B	802	-	4,4,4	0.86	0	6,6,6	1.16	1 (16%)
8	PEG	A	807	-	6,6,6	0.60	0	5,5,5	0.42	0
7	ACT	B	806	-	3,3,3	0.82	0	3,3,3	0.82	0
4	AMP	B	803	5	25,25,25	1.43	4 (16%)	37,38,38	1.91	7 (18%)

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	CKL	B	801	-	-	9/18/29/29	0/4/4/4
4	AMP	A	803	5	-	1/10/26/26	0/3/3/3
8	PEG	A	808	-	-	3/4/4/4	-
2	CKL	A	801	-	-	8/18/29/29	0/4/4/4
8	PEG	A	807	-	-	2/4/4/4	-
4	AMP	B	803	5	-	8/10/26/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CKL	C18-S21	-9.68	1.61	1.76
2	B	801	CKL	C18-S21	-9.53	1.61	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	AMP	C5-C4	4.87	1.47	1.39
4	B	803	AMP	C5-C4	4.77	1.47	1.39
2	A	801	CKL	C5-C6	3.60	1.49	1.40

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CKL	O23-S21-O24	-10.91	106.27	119.52
2	A	801	CKL	C18-S21-N22	8.37	117.26	106.88
2	A	801	CKL	O23-S21-O24	-8.15	109.62	119.52
2	A	801	CKL	C34-O33-C29	6.50	123.28	117.20
4	B	803	AMP	C5-C4-N3	-5.86	118.65	126.72

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CKL	N26-C25-N22-S21
2	A	801	CKL	C30-C29-O33-C34
2	A	801	CKL	N28-C29-O33-C34
2	B	801	CKL	C30-C29-O33-C34
2	B	801	CKL	N28-C29-O33-C34

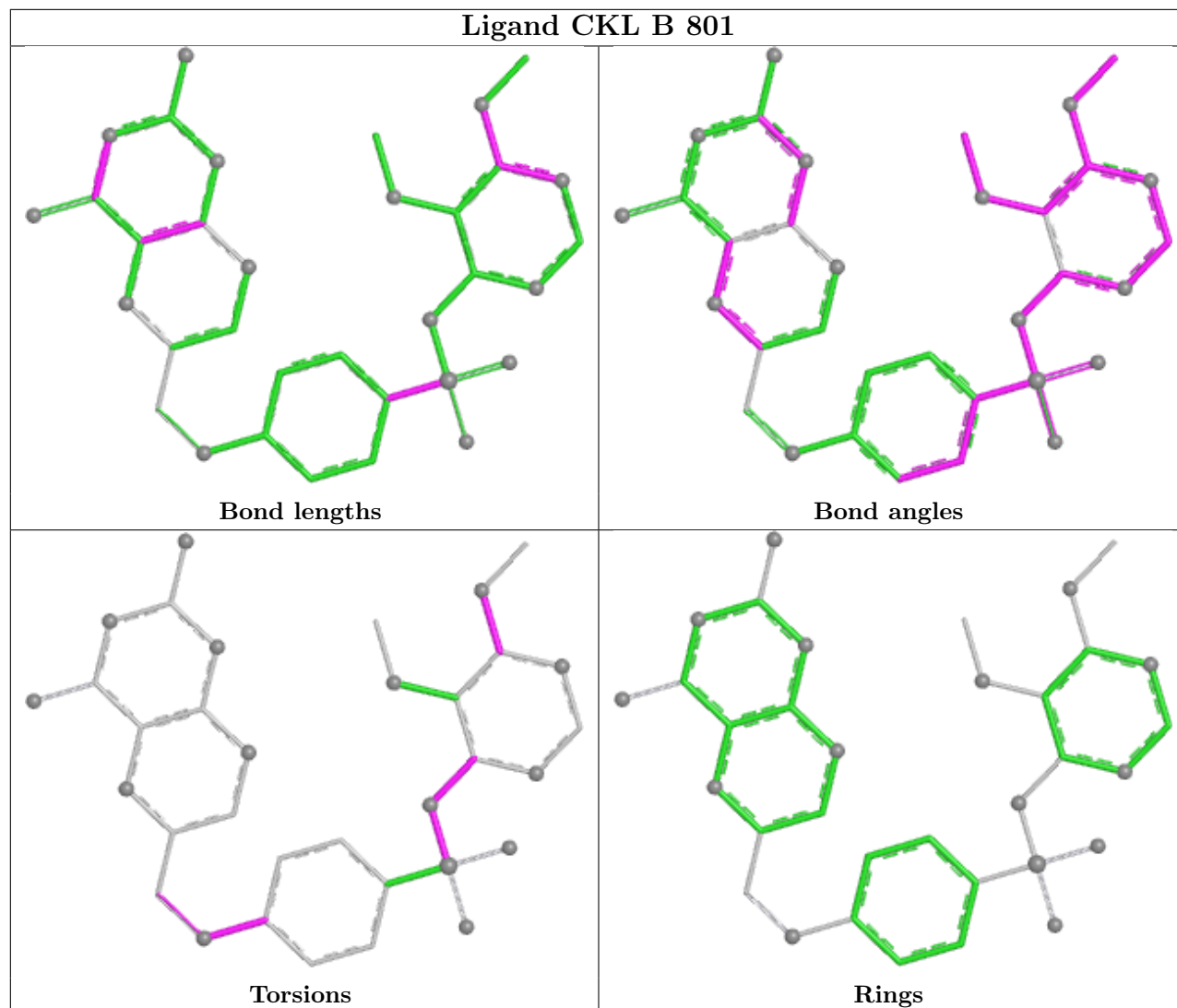
There are no ring outliers.

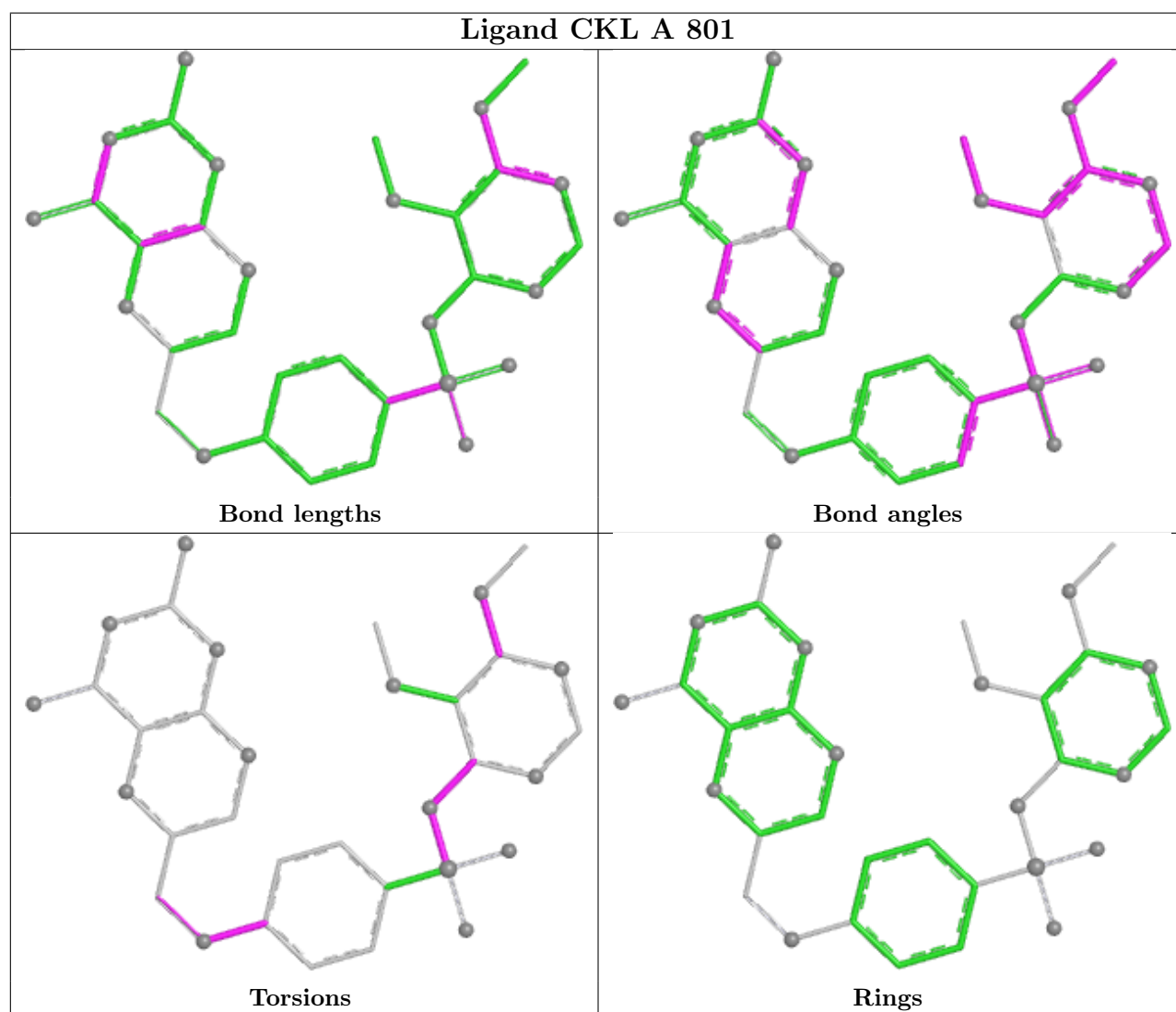
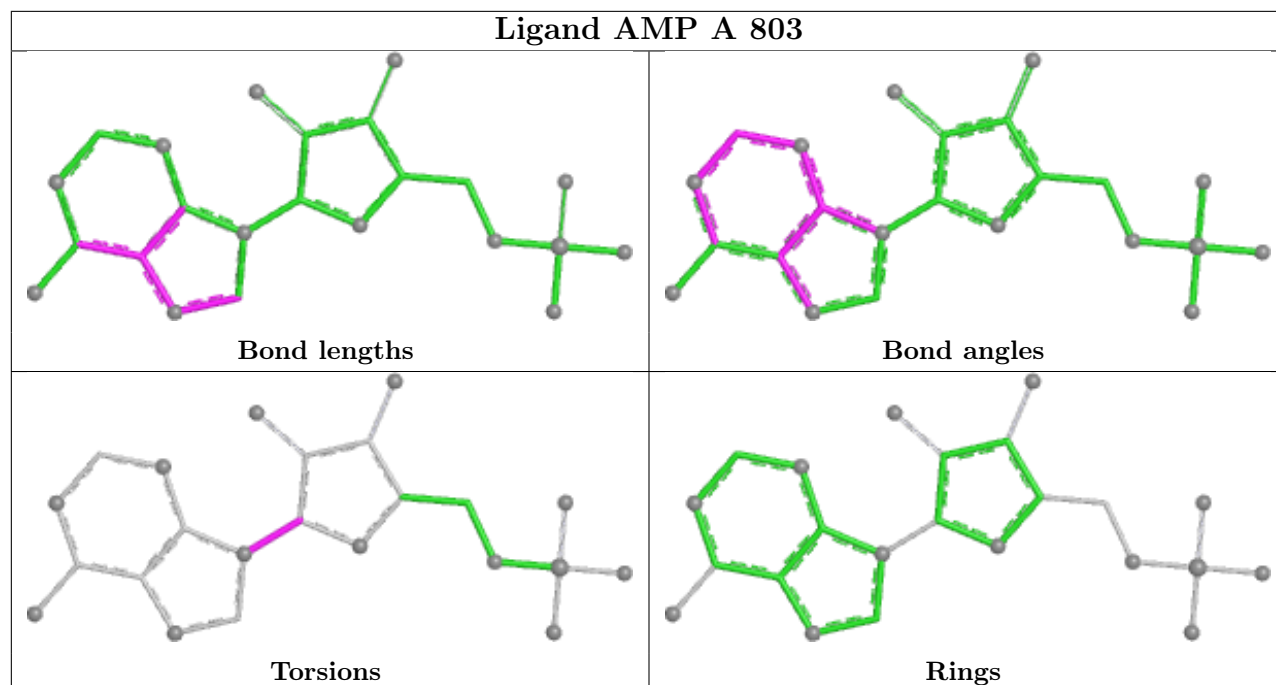
3 monomers are involved in 3 short contacts:

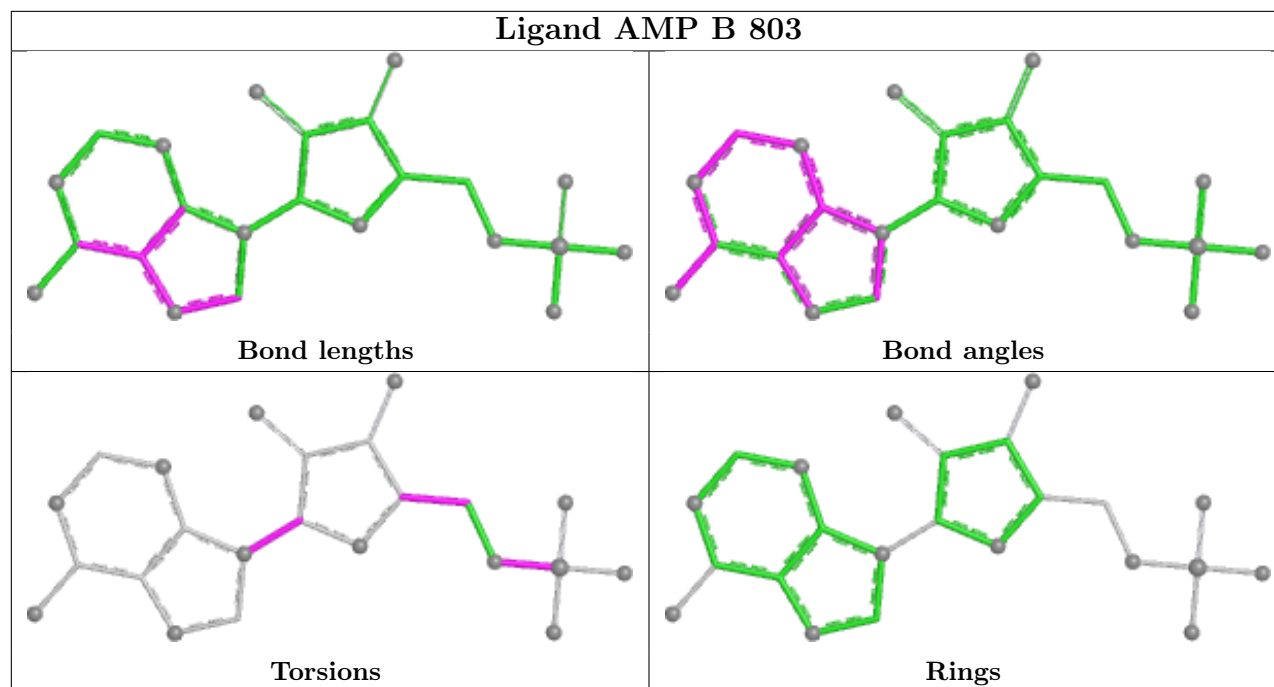
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	CKL	1	0
8	A	808	PEG	1	0
4	B	803	AMP	1	0

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

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	550/728 (75%)	-0.23	13 (2%) 59 51	12, 36, 104, 120	0
1	B	565/728 (77%)	0.12	29 (5%) 33 28	11, 51, 110, 120	0
All	All	1115/1456 (76%)	-0.05	42 (3%) 44 36	11, 43, 109, 120	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	4.2
1	A	302	PRO	4.0
1	A	151	LEU	3.9
1	B	663	TYR	3.7
1	B	226	LEU	3.7

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

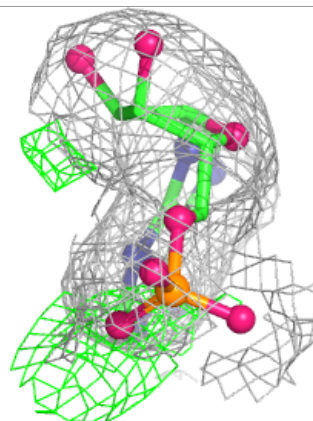
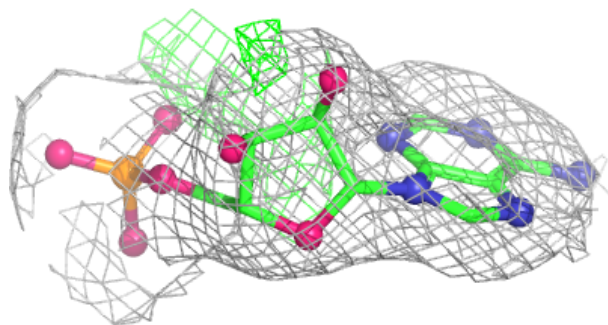
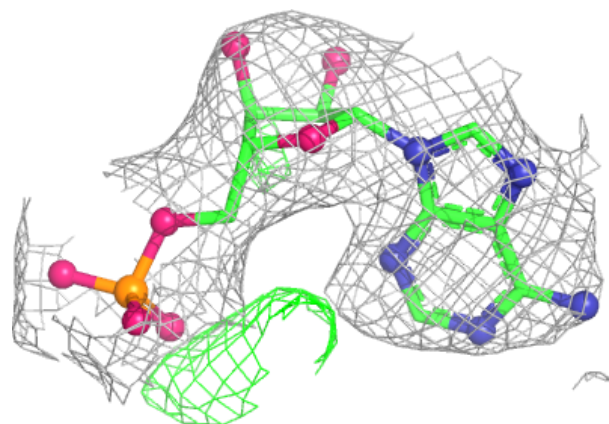
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	PEG	A	807	7/7	0.75	0.30	65,67,75,76	0
8	PEG	A	808	7/7	0.81	0.22	46,53,60,63	0
3	PO4	B	802	5/5	0.86	0.20	70,77,79,80	0
3	PO4	A	802	5/5	0.88	0.13	44,52,56,58	0
4	AMP	A	803	23/23	0.88	0.10	45,54,81,81	0
4	AMP	B	803	23/23	0.90	0.10	75,83,120,120	0
2	CKL	A	801	34/34	0.92	0.13	13,29,102,107	0
7	ACT	A	806	4/4	0.92	0.13	31,31,33,36	0
5	MG	B	804	1/1	0.95	0.07	65,65,65,65	0
2	CKL	B	801	34/34	0.95	0.10	14,32,108,110	0
5	MG	A	804	1/1	0.96	0.09	28,28,28,28	0
7	ACT	B	806	4/4	0.97	0.06	14,14,14,14	0
6	CA	A	805	1/1	0.99	0.02	37,37,37,37	0
6	CA	B	805	1/1	0.99	0.03	63,63,63,63	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.

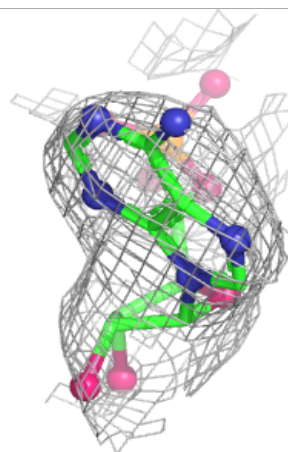
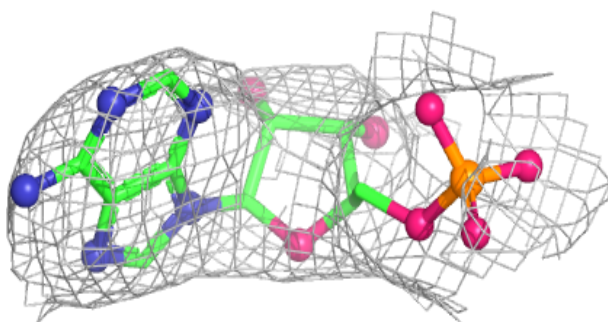
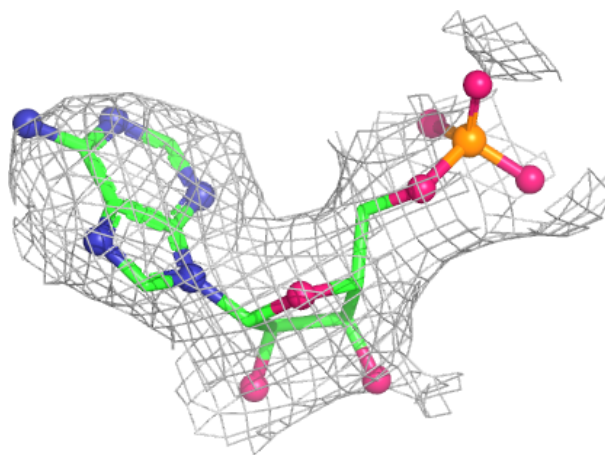
Electron density around AMP A 803:

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



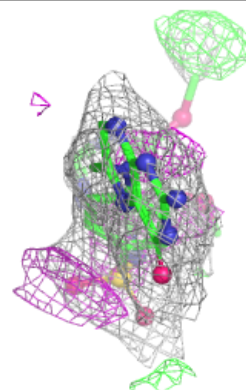
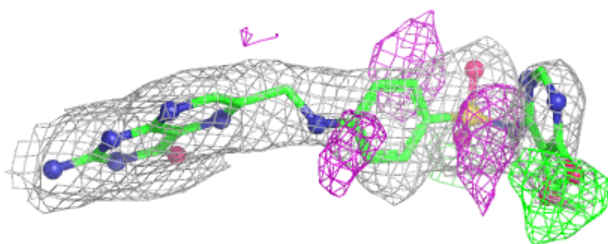
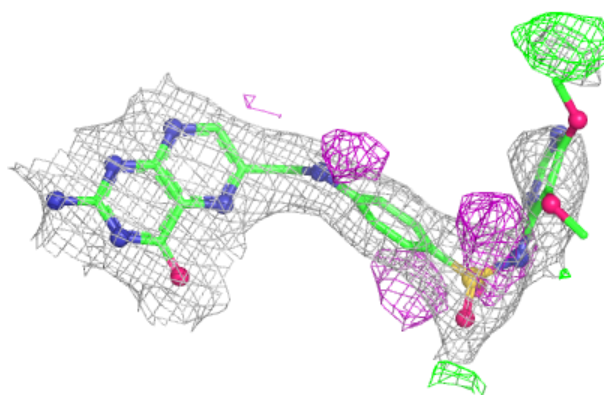
Electron density around AMP B 803:

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

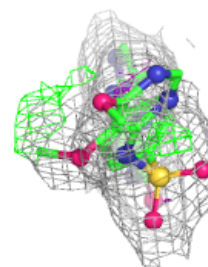
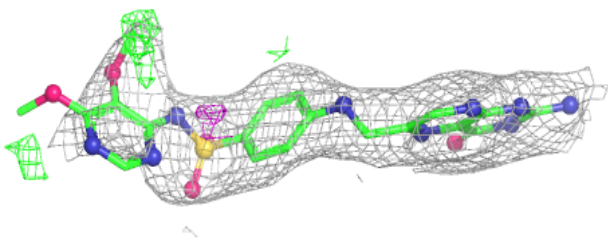
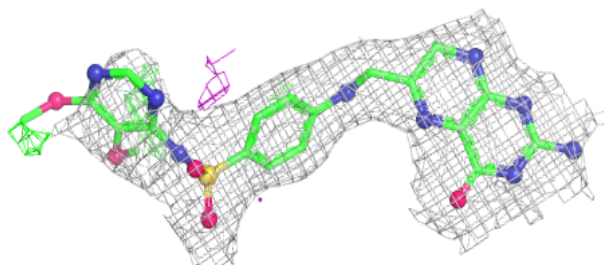


Electron density around CKL A 801:

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

**Electron density around CKL 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.