Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 09:25 PM JST

PDB ID	:	6JWZ
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 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:

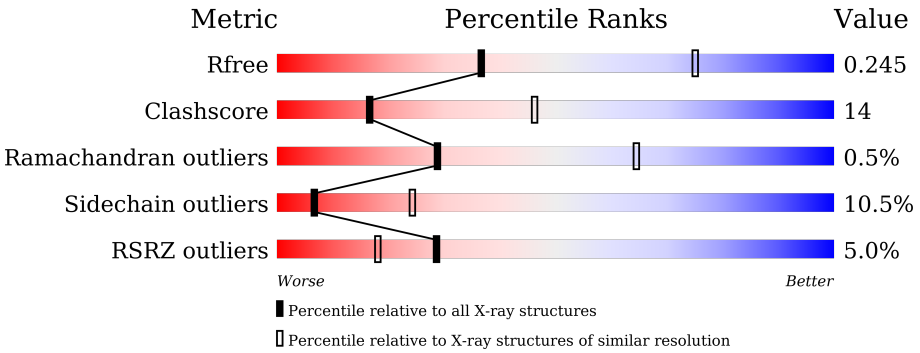
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	4% 49% 25% · 24%
1	B	728	4% 49% 25% · 22%

2 Entry composition (i)

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-dihyd ropteroate 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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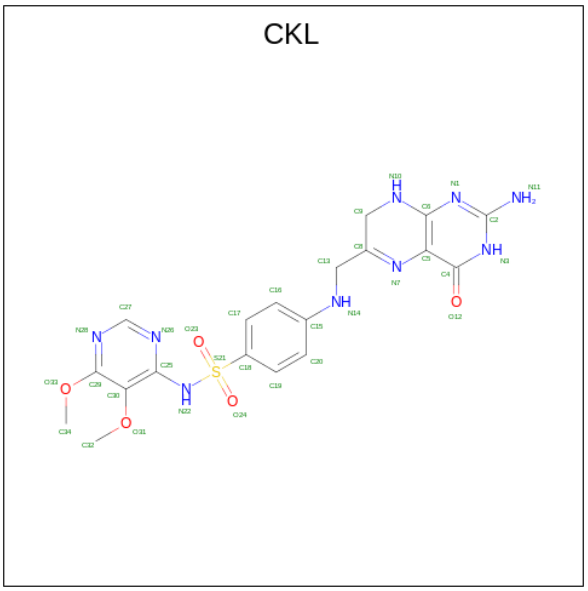
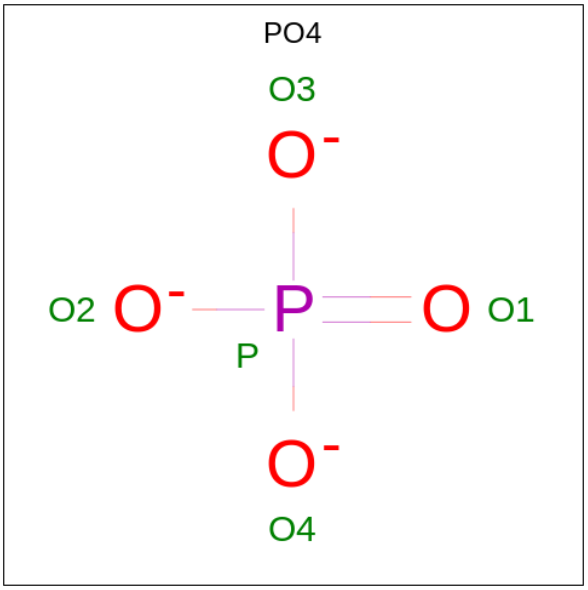
Chain	Residue	Modelled	Actual	Comment	Reference
A	728	HIS	-	expression tag	UNP Q25704
B	436	PHE	SER	engineered mutation	UNP Q25704
B	437	GLY	ALA	engineered mutation	UNP Q25704
B	613	SER	ALA	engineered mutation	UNP Q25704
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	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 (three-letter code: CKL) (formula: $C_{19}H_{21}N_9O_5S$).



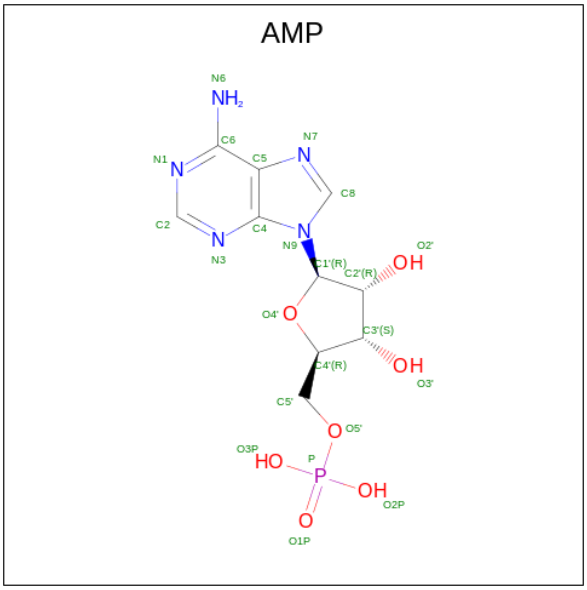
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	19	9	5	1		
2	B	1	Total	C	N	O	S	0	0
			34	19	9	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: 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 (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

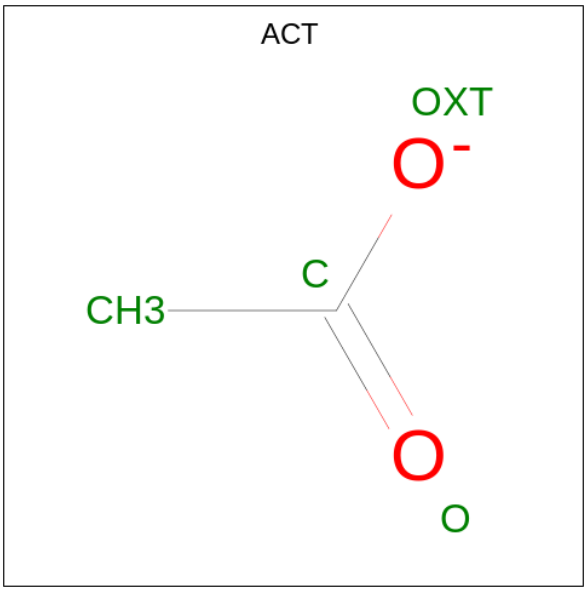
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

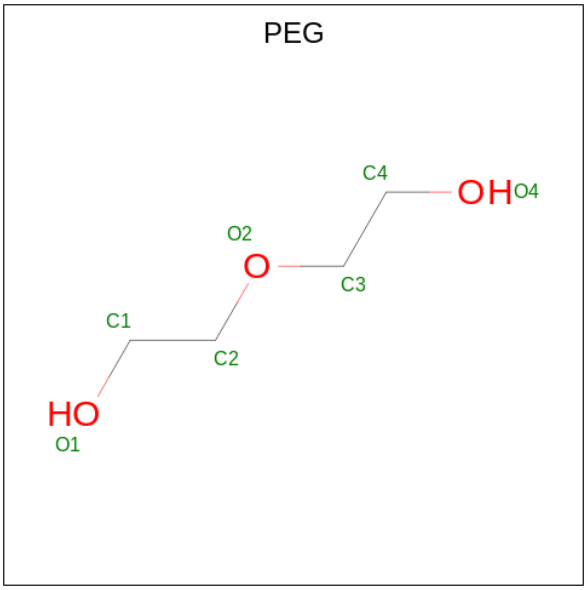
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

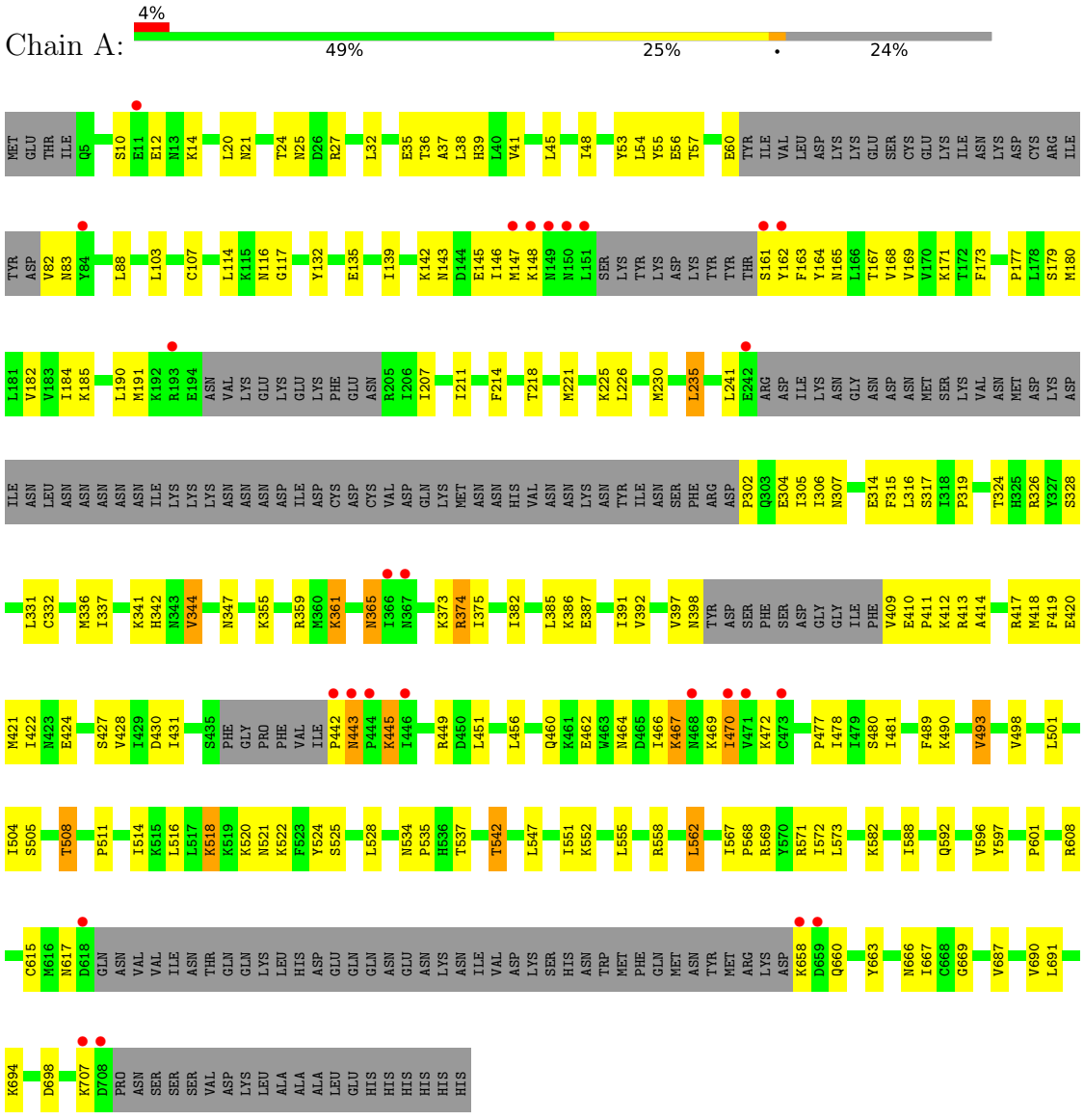
- Molecule 9 is water.

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

3 Residue-property plots (i)

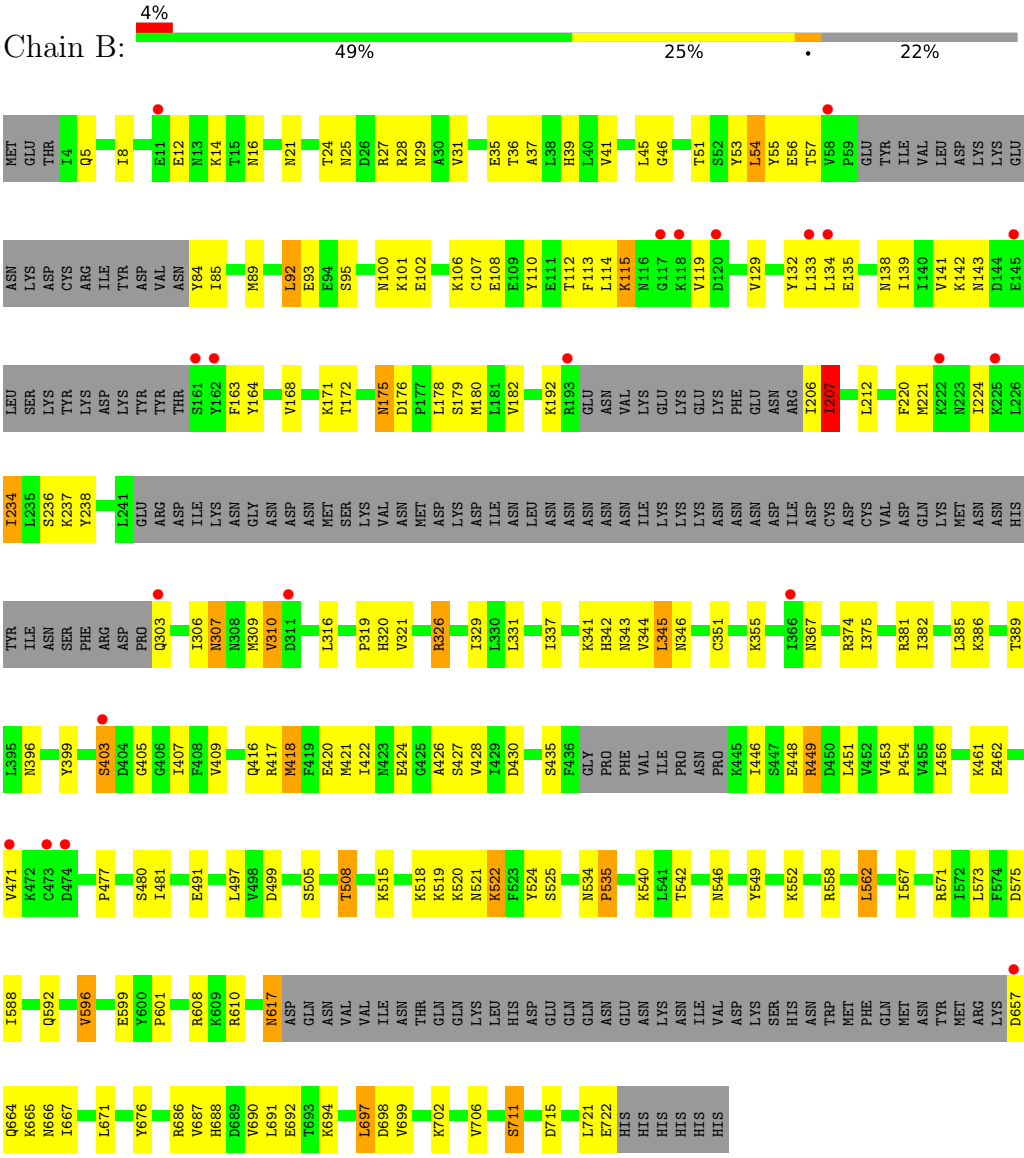
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain B:



4 Data and refinement statistics (i)

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 29.55 – 2.95	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.57-2.95) 89.4 (29.55-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (9.98%)	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)	0.31 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACT, CKL, PO4, MG, AMP, PEG

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	0.30	0/4620	0.69	0/6226
1	B	0.29	0/4727	0.68	0/6372
All	All	0.29	0/9347	0.68	0/12598

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.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	GLY	Peptide
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	117	0
1	B	4655	0	4754	154	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	268	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 14.

All (268) 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:107:CYS:SG	1:A:171:LYS:CE	2.58	0.91
1:A:169:VAL:HG23	1:A:336:MET:HE3	1.52	0.91
1:B:505:SER:O	1:B:508:THR:HB	1.71	0.91
1:B:107:CYS:SG	1:B:171:LYS:CE	2.59	0.91
1:A:505:SER:O	1:A:508:THR:HB	1.73	0.87
1:A:39:HIS:CE1	1:A:521:ASN:O	2.29	0.86
1:A:169:VAL:HG23	1:A:336:MET:CE	2.06	0.85
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.41	0.85
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.58	0.84
1:B:580:PHE:O	1:B:582:LYS:HD2	1.79	0.82
1:B:608:ARG:HD2	1:B:688:HIS:ND1	1.94	0.81
1:A:588:ILE:O	1:A:592:GLN:HG3	1.81	0.81
1:B:27:ARG:HG3	1:B:164:TYR:OH	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TYR:CE1	1:B:114:LEU:HD11	2.19	0.77
1:A:20:LEU:HB2	1:A:168:VAL:HG22	1.65	0.77
1:A:608:ARG:HA	1:A:666:ASN:OD1	1.83	0.77
1:B:449:ARG:CG	1:B:449:ARG:HH11	1.98	0.76
1:B:573:LEU:HD23	1:B:601:PRO:HB2	1.67	0.76
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.68	0.75
1:B:21:ASN:HB2	1:B:212:LEU:HD21	1.69	0.73
1:B:110:TYR:HE1	1:B:114:LEU:HD11	1.52	0.73
1:A:428:VAL:HG22	1:A:478:ILE:HB	1.71	0.73
1:A:135:GLU:O	1:A:139:ILE:HG12	1.88	0.72
1:B:449:ARG:HH11	1:B:449:ARG:HG3	1.53	0.72
1:B:37:ALA:O	1:B:41:VAL:HG23	1.90	0.71
1:B:21:ASN:ND2	1:B:329:ILE:HG12	2.06	0.71
1:A:10:SER:HB3	1:A:12:GLU:HG2	1.74	0.70
1:B:422:ILE:HD13	1:B:477:PRO:HG3	1.73	0.69
1:A:39:HIS:HE1	1:A:521:ASN:O	1.73	0.69
1:B:227:GLU:HB3	1:B:230:MET:HB3	1.75	0.69
1:B:55:TYR:OH	1:B:374:ARG:NH1	2.26	0.69
1:B:89:MET:HA	1:B:92:LEU:HD21	1.76	0.68
1:B:319:PRO:HG2	1:B:344:VAL:HG11	1.75	0.67
1:A:466:ILE:HG22	1:A:466:ILE:O	1.94	0.67
1:B:45:LEU:HD22	1:B:180:MET:HG3	1.76	0.66
1:B:39:HIS:HD2	1:B:521:ASN:O	1.78	0.66
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.75	0.66
1:A:464:ASN:O	1:A:467:LYS:HB2	1.96	0.65
1:B:573:LEU:HD23	1:B:601:PRO:CB	2.28	0.64
1:A:443:ASN:HD21	1:A:445:LYS:HB2	1.64	0.63
1:B:39:HIS:CD2	1:B:521:ASN:O	2.52	0.62
1:A:660:GLN:HA	1:A:663:TYR:HD2	1.64	0.62
1:B:396:ASN:HD22	1:B:399:TYR:HB3	1.64	0.62
1:B:46:GLY:HA3	1:B:171:LYS:O	1.99	0.62
1:B:112:THR:O	1:B:115:LYS:O	2.18	0.62
1:B:519:LYS:HE2	1:B:524:TYR:HE1	1.65	0.62
1:A:466:ILE:O	1:A:466:ILE:CG2	2.47	0.61
1:A:55:TYR:OH	1:A:374:ARG:NH1	2.33	0.61
1:A:420:GLU:O	1:A:424:GLU:HG3	2.01	0.61
1:A:169:VAL:CG2	1:A:336:MET:HE3	2.29	0.61
1:B:469:LYS:H	1:B:469:LYS:HD2	1.65	0.61
1:B:422:ILE:CD1	1:B:477:PRO:HG3	2.30	0.60
1:B:449:ARG:HG3	1:B:449:ARG:NH1	2.15	0.60
1:A:55:TYR:CD2	1:A:331:LEU:HD21	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:O	1:B:207:ILE:HD13	2.02	0.60
1:B:420:GLU:HG2	1:B:424:GLU:OE2	2.02	0.60
1:A:82:VAL:HG13	1:A:83:ASN:HD22	1.67	0.60
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.83	0.60
1:A:418:MET:O	1:A:422:ILE:HG13	2.03	0.59
1:B:449:ARG:HE	1:B:491:GLU:CD	2.05	0.59
1:B:342:HIS:HD2	1:B:344:VAL:H	1.49	0.59
1:B:53:TYR:CD2	1:B:374:ARG:HD3	2.38	0.58
1:B:57:THR:HG23	1:B:163:PHE:CB	2.33	0.58
1:B:426:ALA:HB2	1:B:690:VAL:HG11	1.86	0.58
1:A:191:MET:HE3	1:A:207:ILE:HG12	1.85	0.58
1:B:449:ARG:NE	1:B:491:GLU:OE1	2.36	0.58
1:A:45:LEU:HD11	1:A:184:ILE:HG22	1.85	0.58
1:A:691:LEU:HD21	1:B:665:LYS:HG2	1.84	0.58
1:B:51:THR:HG22	1:B:168:VAL:HG12	1.86	0.57
1:A:169:VAL:CG2	1:A:336:MET:CE	2.80	0.57
1:B:396:ASN:HD22	1:B:399:TYR:CB	2.16	0.57
1:A:430:ASP:HA	1:A:480:SER:O	2.05	0.57
1:A:392:VAL:HG22	1:A:428:VAL:HB	1.87	0.57
1:A:132:TYR:CD2	1:A:344:VAL:HG21	2.40	0.57
1:A:385:LEU:HG	1:A:386:LYS:HG2	1.87	0.56
1:B:326:ARG:HH11	1:B:326:ARG:CG	2.15	0.56
1:A:180:MET:CE	1:A:211:ILE:HG12	2.35	0.56
1:A:375:ILE:HD13	1:A:382:ILE:HG23	1.86	0.56
1:A:182:VAL:HG12	1:A:235:LEU:HD13	1.88	0.56
1:B:546:ASN:ND2	1:B:549:TYR:HB2	2.21	0.55
1:B:617:ASN:H	1:B:617:ASN:ND2	2.04	0.55
1:A:169:VAL:HG23	1:A:336:MET:HE1	1.88	0.55
1:A:56:GLU:HG3	1:A:164:TYR:CE1	2.41	0.55
1:B:178:LEU:O	1:B:182:VAL:HG23	2.07	0.55
1:B:657:ASP:HA	1:B:660:GLN:CG	2.37	0.55
1:B:391:ILE:HG23	1:B:687:VAL:CG2	2.37	0.55
1:B:418:MET:O	1:B:422:ILE:HG13	2.07	0.55
1:B:175:ASN:ND2	1:B:238:TYR:OH	2.40	0.54
1:A:525:SER:OG	1:A:571:ARG:HD3	2.07	0.54
1:A:57:THR:HG23	1:A:163:PHE:HB2	1.89	0.54
1:B:57:THR:HG23	1:B:163:PHE:HB2	1.89	0.54
1:B:617:ASN:HB2	9:B:939:HOH:O	2.07	0.54
1:A:562:LEU:HB3	1:A:567:ILE:HG13	1.89	0.53
1:A:409:VAL:HG13	1:A:413:ARG:HD2	1.89	0.53
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LYS:HD2	1:B:469:LYS:N	2.24	0.53
1:B:657:ASP:HA	1:B:660:GLN:HG2	1.91	0.53
1:B:89:MET:O	1:B:92:LEU:HD11	2.09	0.53
1:B:403:SER:C	1:B:405:GLY:H	2.12	0.52
1:B:337:ILE:O	1:B:337:ILE:HG13	2.08	0.52
1:A:32:LEU:O	1:A:36:THR:OG1	2.23	0.52
1:A:60:GLU:HB3	1:A:326:ARG:HE	1.74	0.52
1:A:514:ILE:HD13	1:A:562:LEU:HD22	1.91	0.52
1:B:392:VAL:HG22	1:B:428:VAL:HB	1.91	0.52
1:B:341:LYS:NZ	1:B:345:LEU:O	2.42	0.52
1:B:671:LEU:HD11	1:B:692:GLU:HB3	1.91	0.52
1:A:319:PRO:HD3	1:A:342:HIS:NE2	2.25	0.51
1:B:519:LYS:HE2	1:B:524:TYR:CE1	2.44	0.51
1:A:302:PRO:HB2	1:A:304:GLU:OE1	2.10	0.51
1:A:534:ASN:HB2	1:A:535:PRO:HD2	1.91	0.51
1:B:57:THR:CG2	1:B:163:PHE:HB3	2.40	0.51
1:B:227:GLU:C	1:B:229:ASN:H	2.14	0.51
1:B:224:ILE:HG22	9:B:954:HOH:O	2.09	0.51
1:B:374:ARG:HD2	1:B:385:LEU:HD22	1.93	0.51
1:B:469:LYS:C	1:B:471:VAL:H	2.14	0.51
1:B:546:ASN:HD22	1:B:549:TYR:HB2	1.76	0.51
1:A:177:PRO:HG3	1:A:214:PHE:CG	2.46	0.50
1:A:374:ARG:HG3	1:A:374:ARG:HH11	1.76	0.50
1:A:421:MET:HG2	1:A:690:VAL:HG21	1.93	0.50
1:B:176:ASP:OD2	1:B:179:SER:OG	2.24	0.50
1:B:663:TYR:O	1:B:667:ILE:HG13	2.11	0.50
1:B:575:ASP:OD2	2:B:801:CKL:N3	2.45	0.50
1:A:37:ALA:O	1:A:41:VAL:HG23	2.12	0.50
1:A:53:TYR:CD2	1:A:374:ARG:HD3	2.47	0.50
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.85	0.49
1:A:573:LEU:HD23	1:A:601:PRO:HB3	1.93	0.49
1:B:132:TYR:HE2	1:B:344:VAL:HG13	1.76	0.49
1:B:227:GLU:HB3	1:B:230:MET:H	1.77	0.49
1:B:319:PRO:CD	1:B:344:VAL:HG21	2.42	0.49
1:B:453:VAL:N	1:B:454:PRO:HD2	2.27	0.49
1:B:230:MET:HG3	1:B:230:MET:O	2.11	0.49
1:A:663:TYR:O	1:A:667:ILE:HG12	2.12	0.49
1:B:525:SER:OG	1:B:571:ARG:HD3	2.12	0.49
1:A:422:ILE:HG12	1:A:477:PRO:HG3	1.95	0.49
1:B:316:LEU:HA	4:B:803:AMP:C8	2.48	0.49
1:A:107:CYS:HG	1:A:171:LYS:HE2	1.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:O	1:A:551:ILE:HD12	2.13	0.48
1:B:113:PHE:HD2	1:B:114:LEU:HD23	1.79	0.48
1:B:552:LYS:HD2	1:B:596:VAL:HG13	1.95	0.48
1:A:180:MET:HE2	1:A:211:ILE:HG12	1.93	0.48
1:B:57:THR:HG23	1:B:163:PHE:HB3	1.96	0.48
1:A:409:VAL:HG12	1:A:414:ALA:HB2	1.95	0.47
1:B:107:CYS:SG	1:B:171:LYS:HE2	2.53	0.47
1:B:608:ARG:HA	1:B:666:ASN:OD1	2.14	0.47
1:A:41:VAL:HG13	1:A:45:LEU:HD12	1.95	0.47
1:B:129:VAL:HG13	1:B:343:ASN:HD22	1.80	0.47
1:A:462:GLU:HG3	9:A:968:HOH:O	2.13	0.47
1:B:138:ASN:HA	1:B:141:VAL:HG22	1.97	0.47
1:B:711:SER:O	1:B:715:ASP:HB2	2.15	0.47
1:A:493:VAL:HG22	1:A:524:TYR:CZ	2.50	0.47
1:A:464:ASN:HA	1:A:467:LYS:HG2	1.96	0.47
1:A:374:ARG:HD2	1:A:385:LEU:HD22	1.96	0.46
1:A:504:ILE:HG23	9:A:906:HOH:O	2.14	0.46
1:A:391:ILE:HG23	1:A:687:VAL:CG2	2.45	0.46
1:A:419:PHE:HA	1:A:422:ILE:HD12	1.97	0.46
1:A:472:LYS:HG3	1:A:472:LYS:O	2.15	0.46
1:A:114:LEU:HD21	1:A:337:ILE:HG22	1.98	0.46
1:B:319:PRO:HD3	1:B:344:VAL:HG21	1.96	0.46
1:B:694:LYS:NZ	1:B:698:ASP:OD1	2.49	0.46
1:A:410:GLU:HG2	1:A:411:PRO:HD2	1.98	0.46
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.46	0.46
1:A:568:PRO:HB2	1:A:571:ARG:HG3	1.98	0.46
1:B:25:ASN:OD1	1:B:206:ILE:HG12	2.16	0.46
1:A:694:LYS:HE2	1:A:698:ASP:OD1	2.15	0.46
1:B:307:ASN:O	1:B:310:VAL:HG23	2.15	0.46
1:B:344:VAL:HG12	1:B:345:LEU:HD23	1.98	0.45
1:B:448:GLU:HA	1:B:451:LEU:HD12	1.97	0.45
1:A:490:LYS:HD2	1:A:516:LEU:CD2	2.47	0.45
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.46	0.45
1:B:107:CYS:SG	1:B:171:LYS:HE3	2.50	0.45
1:B:374:ARG:NH2	1:B:599:GLU:OE1	2.50	0.45
1:A:142:LYS:O	1:A:146:ILE:HG13	2.16	0.45
1:A:542:THR:HG23	1:A:542:THR:O	2.17	0.45
1:B:149:ASN:O	1:B:150:ASN:C	2.54	0.45
1:A:167:THR:OG1	1:A:332:CYS:HB3	2.16	0.45
1:B:27:ARG:HA	1:B:164:TYR:CE2	2.51	0.45
1:B:31:VAL:O	1:B:35:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ILE:O	1:B:309:MET:HB2	2.16	0.45
1:B:385:LEU:HG	1:B:386:LYS:HG2	1.99	0.45
1:B:558:ARG:O	1:B:562:LEU:HD23	2.16	0.45
1:A:489:PHE:CZ	1:A:501:LEU:HB2	2.53	0.44
1:B:101:LYS:HB3	1:B:515:LYS:HG2	1.98	0.44
1:B:342:HIS:CD2	1:B:344:VAL:H	2.31	0.44
1:B:449:ARG:CD	1:B:491:GLU:OE1	2.65	0.44
1:A:235:LEU:HB3	1:A:241:LEU:HD11	1.98	0.44
1:B:389:THR:HG22	1:B:697:LEU:HD11	1.99	0.44
1:B:227:GLU:HB3	1:B:230:MET:CB	2.47	0.44
1:A:562:LEU:HB3	1:A:567:ILE:CG1	2.48	0.44
1:B:234:ILE:O	1:B:237:LYS:HB3	2.17	0.44
1:A:82:VAL:HG13	1:A:83:ASN:ND2	2.30	0.44
1:B:84:TYR:HB3	1:B:85:ILE:H	1.63	0.44
1:A:25:ASN:HB2	1:A:162:TYR:O	2.17	0.44
1:B:227:GLU:C	1:B:229:ASN:N	2.70	0.44
1:B:326:ARG:CG	1:B:326:ARG:NH1	2.76	0.44
1:A:460:GLN:O	1:A:464:ASN:ND2	2.51	0.44
1:B:392:VAL:HB	1:B:686:ARG:HA	2.00	0.44
1:B:525:SER:HA	1:B:571:ARG:HB3	2.00	0.44
1:B:36:THR:HG21	1:B:85:ILE:HG21	2.00	0.44
1:B:135:GLU:O	1:B:139:ILE:HG12	2.18	0.43
1:B:430:ASP:HA	1:B:480:SER:O	2.17	0.43
1:B:469:LYS:H	1:B:469:LYS:CD	2.29	0.43
1:A:361:LYS:O	1:A:365:ASN:HA	2.18	0.43
1:B:138:ASN:O	1:B:142:LYS:HB3	2.18	0.43
1:B:394:ILE:HD12	1:B:687:VAL:C	2.38	0.43
1:B:469:LYS:HB3	1:B:471:VAL:HG22	1.99	0.43
1:A:412:LYS:HD2	1:A:412:LYS:HA	1.85	0.43
1:B:139:ILE:O	1:B:143:ASN:HB2	2.18	0.43
1:B:12:GLU:O	1:B:12:GLU:HG3	2.19	0.43
1:B:175:ASN:ND2	1:B:175:ASN:H	2.15	0.43
1:B:522:LYS:HD3	1:B:524:TYR:CZ	2.53	0.43
1:B:456:LEU:HD13	1:B:497:LEU:HB3	2.00	0.43
8:A:808:PEG:H22	1:B:676:TYR:HE1	1.83	0.43
1:B:53:TYR:CG	1:B:374:ARG:HD3	2.53	0.43
1:B:224:ILE:HA	9:B:954:HOH:O	2.19	0.43
1:B:27:ARG:HG3	1:B:164:TYR:CZ	2.54	0.42
1:B:403:SER:C	1:B:405:GLY:N	2.71	0.42
1:B:588:ILE:O	1:B:592:GLN:HG3	2.19	0.42
1:B:608:ARG:HD2	1:B:688:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD21	1:A:180:MET:CE	2.49	0.42
1:B:221:MET:HE3	1:B:224:ILE:HG12	2.00	0.42
1:A:179:SER:O	1:A:182:VAL:HB	2.20	0.42
1:A:375:ILE:HD13	1:A:382:ILE:CG2	2.48	0.42
1:B:610:ARG:HE	1:B:610:ARG:HB3	1.73	0.42
1:A:481:ILE:HB	1:A:498:VAL:HG11	2.01	0.42
1:B:14:LYS:HG3	1:B:175:ASN:HB3	2.02	0.42
1:B:16:ASN:HB2	1:B:172:THR:CG2	2.49	0.42
1:A:53:TYR:CG	1:A:374:ARG:HD3	2.55	0.42
1:A:525:SER:HA	1:A:571:ARG:HB3	2.00	0.42
1:A:35:GLU:HA	1:A:38:LEU:HB2	2.01	0.42
1:A:88:LEU:HD11	1:A:190:LEU:HD22	2.01	0.42
1:A:307:ASN:ND2	9:A:909:HOH:O	2.53	0.42
1:A:397:VAL:HG12	1:A:451:LEU:HB3	2.02	0.42
1:A:221:MET:O	1:A:315:PHE:HB2	2.19	0.42
1:B:326:ARG:HG3	1:B:326:ARG:NH1	2.19	0.42
1:A:518:LYS:HE3	9:A:967:HOH:O	2.20	0.42
1:A:669:GLY:CA	1:B:699:VAL:HG21	2.49	0.41
1:B:24:THR:OG1	1:B:25:ASN:N	2.52	0.41
1:A:470:ILE:H	1:A:470:ILE:HG13	1.66	0.41
1:A:569:ARG:HA	1:A:572:ILE:HD12	2.02	0.41
1:B:55:TYR:CD2	1:B:331:LEU:HD21	2.55	0.41
1:A:169:VAL:CG2	1:A:336:MET:HE1	2.50	0.41
1:A:596:VAL:HG12	1:A:597:TYR:CD2	2.56	0.41
1:B:21:ASN:HD21	1:B:329:ILE:HG12	1.84	0.41
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.85	0.41
1:B:102:GLU:O	1:B:102:GLU:HG3	2.20	0.41
1:B:375:ILE:HG21	1:B:382:ILE:HG12	2.02	0.41
1:B:469:LYS:C	1:B:471:VAL:N	2.74	0.41
1:B:562:LEU:HD13	1:B:567:ILE:HG13	2.02	0.41
1:A:24:THR:HG23	1:A:164:TYR:HB2	2.03	0.41
1:A:373:LYS:HE2	1:A:387:GLU:OE2	2.21	0.41
1:A:489:PHE:CE1	1:A:501:LEU:HB2	2.56	0.41
1:A:542:THR:O	1:A:542:THR:CG2	2.69	0.41
1:B:394:ILE:HD13	1:B:688:HIS:NE2	2.36	0.41
1:B:396:ASN:ND2	1:B:399:TYR:H	2.19	0.41
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.84	0.41
1:A:57:THR:OG1	1:A:328:SER:HB3	2.22	0.40
1:A:143:ASN:O	1:A:147:MET:HG2	2.21	0.40
1:A:615:CYS:HB3	1:B:702:LYS:HG3	2.03	0.40
1:B:56:GLU:HB2	1:B:164:TYR:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:HIS:CD2	1:B:344:VAL:HB	2.56	0.40
1:B:178:LEU:HD22	1:B:221:MET:CE	2.52	0.40
1:B:391:ILE:HG21	1:B:690:VAL:HG13	2.04	0.40
1:B:461:LYS:HG3	1:B:462:GLU:N	2.36	0.40
1:A:38:LEU:HD22	1:A:48:ILE:HD13	2.02	0.40
1:A:528:LEU:HD13	1:A:558:ARG:HB3	2.03	0.40
1:B:108:GLU:OE1	1:B:108:GLU:HA	2.22	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%)	503 (94%)	30 (6%)	1 (0%)	47 79
1	B	551/728 (76%)	519 (94%)	28 (5%)	4 (1%)	22 56
All	All	1085/1456 (74%)	1022 (94%)	58 (5%)	5 (0%)	29 64

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	526/697 (76%)	477 (91%)	49 (9%)	9 30
1	B	536/697 (77%)	473 (88%)	63 (12%)	5 20
All	All	1062/1394 (76%)	950 (90%)	112 (10%)	7 24

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	21	ASN
1	A	27	ARG
1	A	54	LEU
1	A	116	ASN
1	A	145	GLU
1	A	148	LYS
1	A	161	SER
1	A	165	ASN
1	A	173	PHE
1	A	185	LYS
1	A	218	THR
1	A	225	LYS
1	A	226	LEU
1	A	230	MET
1	A	235	LEU
1	A	305	ILE
1	A	306	ILE
1	A	314	GLU
1	A	317	SER
1	A	324	THR
1	A	341	LYS
1	A	344	VAL
1	A	347	ASN
1	A	355	LYS
1	A	359	ARG
1	A	361	LYS
1	A	398	ASN
1	A	417	ARG
1	A	427	SER
1	A	442	PRO
1	A	443	ASN
1	A	445	LYS

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Mol	Chain	Res	Type
1	A	449	ARG
1	A	467	LYS
1	A	469	LYS
1	A	470	ILE
1	A	493	VAL
1	A	508	THR
1	A	518	LYS
1	A	520	LYS
1	A	522	LYS
1	A	537	THR
1	A	542	THR
1	A	562	LEU
1	A	582	LYS
1	A	617	ASN
1	A	658	LYS
1	A	707	LYS
1	B	5	GLN
1	B	8	ILE
1	B	28	ARG
1	B	29	ASN
1	B	54	LEU
1	B	92	LEU
1	B	93	GLU
1	B	95	SER
1	B	100	ASN
1	B	106	LYS
1	B	115	LYS
1	B	119	VAL
1	B	133	LEU
1	B	134	LEU
1	B	148	LYS
1	B	175	ASN
1	B	192	LYS
1	B	207	ILE
1	B	220	PHE
1	B	230	MET
1	B	234	ILE
1	B	236	SER
1	B	303	GLN
1	B	307	ASN
1	B	310	VAL
1	B	321	VAL

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Mol	Chain	Res	Type
1	B	326	ARG
1	B	345	LEU
1	B	346	ASN
1	B	351	CYS
1	B	355	LYS
1	B	367	ASN
1	B	381	ARG
1	B	403	SER
1	B	407	ILE
1	B	409	VAL
1	B	416	GLN
1	B	418	MET
1	B	421	MET
1	B	427	SER
1	B	435	SER
1	B	446	ILE
1	B	449	ARG
1	B	466	ILE
1	B	481	ILE
1	B	499	ASP
1	B	508	THR
1	B	518	LYS
1	B	520	LYS
1	B	522	LYS
1	B	540	LYS
1	B	542	THR
1	B	562	LEU
1	B	596	VAL
1	B	617	ASN
1	B	658	LYS
1	B	664	GLN
1	B	691	LEU
1	B	697	LEU
1	B	706	VAL
1	B	711	SER
1	B	721	LEU
1	B	722	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS

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Mol	Chain	Res	Type
1	A	83	ASN
1	A	443	ASN
1	A	614	HIS
1	B	21	ASN
1	B	29	ASN
1	B	39	HIS
1	B	100	ASN
1	B	116	ASN
1	B	137	ASN
1	B	165	ASN
1	B	175	ASN
1	B	223	ASN
1	B	307	ASN
1	B	342	HIS
1	B	346	ASN
1	B	396	ASN
1	B	546	ASN
1	B	617	ASN
1	B	710	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 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	$\#\|Z\| > 2$
8	PEG	A	807	-	6,6,6	0.59	0	5,5,5	0.43	0
4	AMP	B	803	5	22,25,25	0.99	1 (4%)	25,38,38	1.30	3 (12%)
2	CKL	A	801	-	32,37,37	2.14	6 (18%)	37,53,53	2.67	10 (27%)
7	ACT	A	806	-	3,3,3	0.78	0	3,3,3	0.86	0
8	PEG	A	808	-	6,6,6	0.78	0	5,5,5	0.59	0
2	CKL	B	801	-	32,37,37	2.03	5 (15%)	37,53,53	2.85	13 (35%)
3	PO4	A	802	-	4,4,4	0.26	0	6,6,6	1.31	1 (16%)
3	PO4	B	802	-	4,4,4	0.81	0	6,6,6	1.11	1 (16%)
4	AMP	A	803	5	22,25,25	1.04	2 (9%)	25,38,38	1.38	2 (8%)
7	ACT	B	806	-	3,3,3	0.77	0	3,3,3	0.82	0

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
8	PEG	A	807	-	-	1/4/4/4	-
4	AMP	B	803	5	-	5/6/26/26	0/3/3/3
2	CKL	A	801	-	-	8/18/29/29	0/4/4/4
8	PEG	A	808	-	-	3/4/4/4	-
2	CKL	B	801	-	-	9/18/29/29	0/4/4/4
4	AMP	A	803	5	-	1/6/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CKL	C18-S21	-9.66	1.61	1.76
2	B	801	CKL	C18-S21	-9.51	1.61	1.76
2	A	801	CKL	C5-C6	3.60	1.49	1.40
2	B	801	CKL	C5-C6	3.19	1.48	1.40
2	A	801	CKL	O33-C29	2.87	1.39	1.35
2	A	801	CKL	C4-N3	-2.72	1.33	1.38
4	A	803	AMP	O4'-C1'	2.71	1.44	1.41
4	A	803	AMP	C5-C4	2.59	1.47	1.40
4	B	803	AMP	C5-C4	2.52	1.47	1.40
2	B	801	CKL	C29-N28	2.34	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CKL	C29-N28	2.33	1.36	1.32
2	B	801	CKL	C4-N3	-2.22	1.34	1.38
2	B	801	CKL	O33-C29	2.21	1.38	1.35
2	A	801	CKL	O24-S21	2.10	1.45	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	CKL	O23-S21-O24	-10.80	106.27	119.55
2	A	801	CKL	C18-S21-N22	8.29	117.26	106.83
2	A	801	CKL	O23-S21-O24	-8.07	109.62	119.55
2	A	801	CKL	C34-O33-C29	6.13	123.28	117.21
2	A	801	CKL	N26-C27-N28	-5.09	120.64	128.60
2	B	801	CKL	N26-C27-N28	-5.08	120.65	128.60
2	B	801	CKL	O23-S21-C18	4.58	113.61	107.97
2	B	801	CKL	C18-S21-N22	-4.55	101.11	106.83
2	B	801	CKL	O24-S21-C18	4.55	113.57	107.97
2	B	801	CKL	C2-N1-C6	4.38	121.33	113.43
4	A	803	AMP	N3-C2-N1	-4.03	122.38	128.68
2	A	801	CKL	C2-N1-C6	3.51	119.76	113.43
2	A	801	CKL	C27-N28-C29	3.36	121.51	115.88
4	B	803	AMP	N3-C2-N1	-3.32	123.48	128.68
2	B	801	CKL	C34-O33-C29	3.23	120.41	117.21
2	B	801	CKL	C27-N28-C29	3.04	120.96	115.88
2	B	801	CKL	C16-C17-C18	2.68	122.22	119.45
3	A	802	PO4	O4-P-O2	2.41	115.70	107.97
2	A	801	CKL	C17-C18-S21	2.37	122.35	119.77
4	A	803	AMP	C2-N1-C6	2.36	122.79	118.75
2	B	801	CKL	C5-N7-C8	2.28	120.76	116.24
2	A	801	CKL	O33-C29-C30	2.24	121.30	116.95
2	A	801	CKL	C5-N7-C8	2.19	120.60	116.24
2	B	801	CKL	O33-C29-C30	2.18	121.18	116.95
2	A	801	CKL	C32-O31-C30	2.18	120.75	114.78
2	B	801	CKL	N22-C25-N26	2.17	122.83	118.66
4	B	803	AMP	N6-C6-N1	2.15	123.04	118.57
4	B	803	AMP	C3'-C2'-C1'	2.08	104.12	100.98
3	B	802	PO4	O3-P-O2	2.08	114.65	107.97
2	B	801	CKL	C32-O31-C30	2.06	120.42	114.78

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CKL	C30-C29-O33-C34
2	A	801	CKL	N28-C29-O33-C34
2	B	801	CKL	C25-N22-S21-O24
2	B	801	CKL	C30-C29-O33-C34
2	B	801	CKL	N28-C29-O33-C34
4	B	803	AMP	C5'-O5'-P-O1P
4	B	803	AMP	C5'-O5'-P-O2P
4	B	803	AMP	C5'-O5'-P-O3P
4	B	803	AMP	C3'-C4'-C5'-O5'
4	B	803	AMP	O4'-C4'-C5'-O5'
8	A	808	PEG	O2-C3-C4-O4
2	A	801	CKL	N26-C25-N22-S21
2	B	801	CKL	C25-N22-S21-O23
2	B	801	CKL	C25-N22-S21-C18
8	A	807	PEG	O2-C3-C4-O4
2	A	801	CKL	C8-C13-N14-C15
8	A	808	PEG	C1-C2-O2-C3
2	A	801	CKL	C16-C15-N14-C13
2	A	801	CKL	C20-C15-N14-C13
2	A	801	CKL	C25-N22-S21-O23
2	A	801	CKL	C30-C25-N22-S21
2	B	801	CKL	C30-C25-N22-S21
8	A	808	PEG	C4-C3-O2-C2
2	B	801	CKL	N26-C25-N22-S21
2	B	801	CKL	C8-C13-N14-C15
4	A	803	AMP	O4'-C4'-C5'-O5'
2	B	801	CKL	C16-C15-N14-C13

There are no ring outliers.

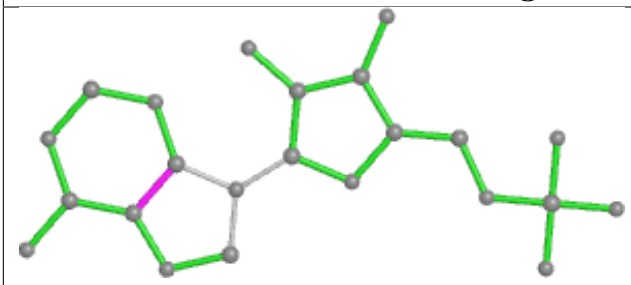
3 monomers are involved in 3 short contacts:

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

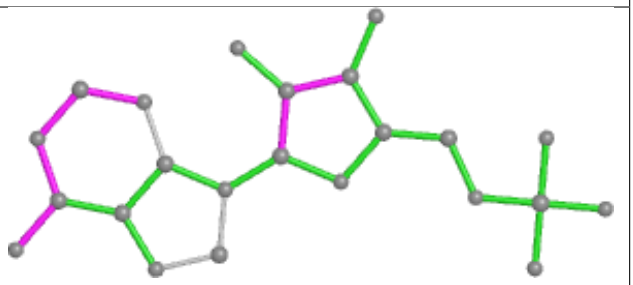
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

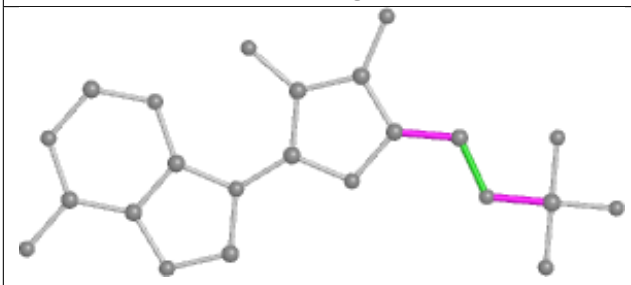
Ligand AMP B 803



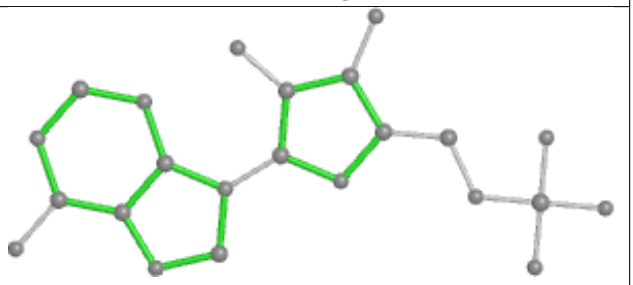
Bond lengths



Bond angles

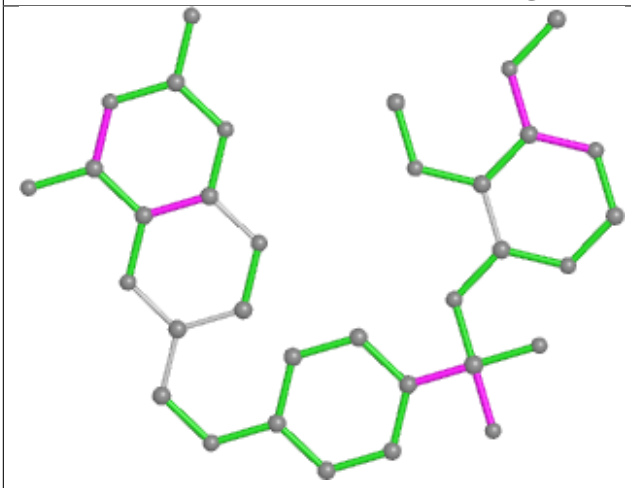


Torsions

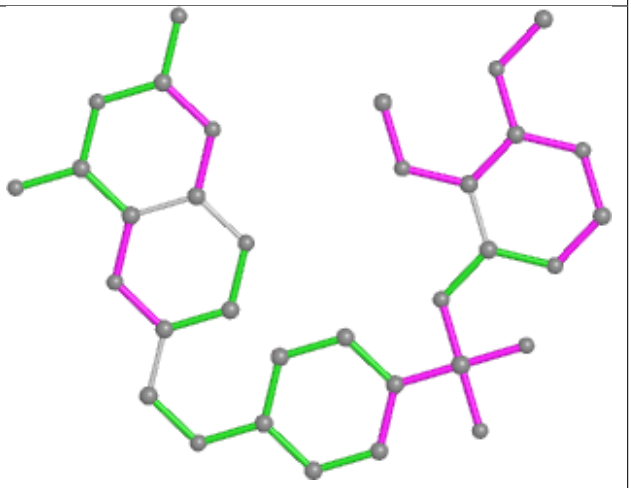


Rings

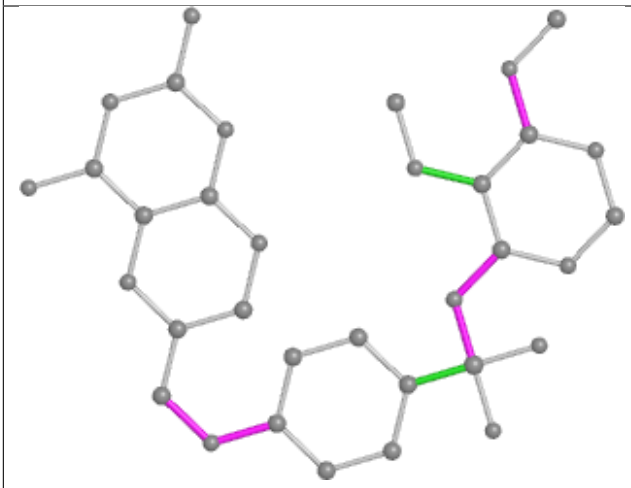
Ligand CKL A 801



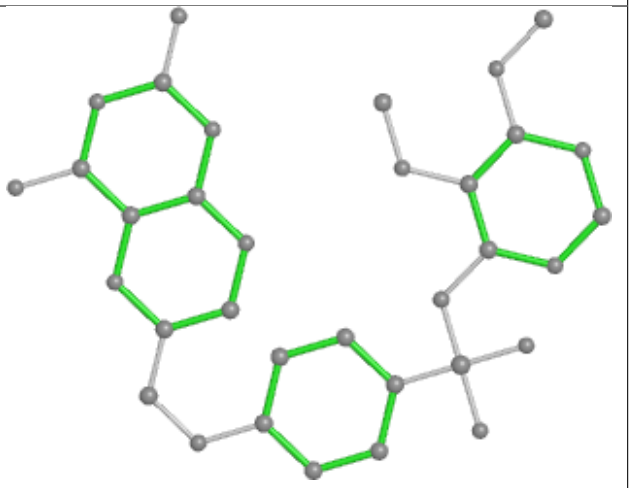
Bond lengths



Bond angles

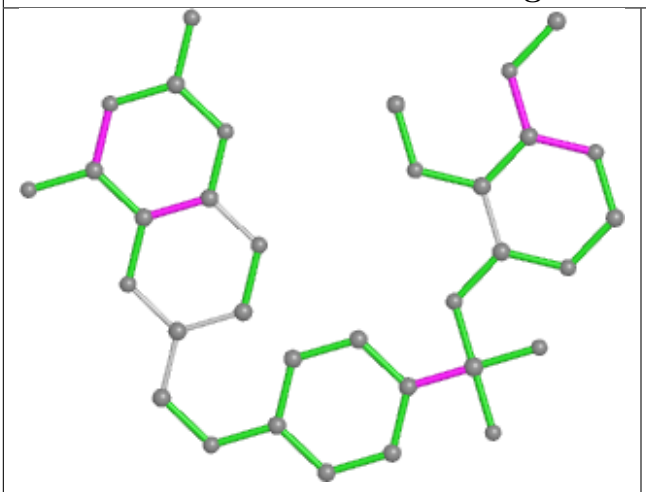


Torsions

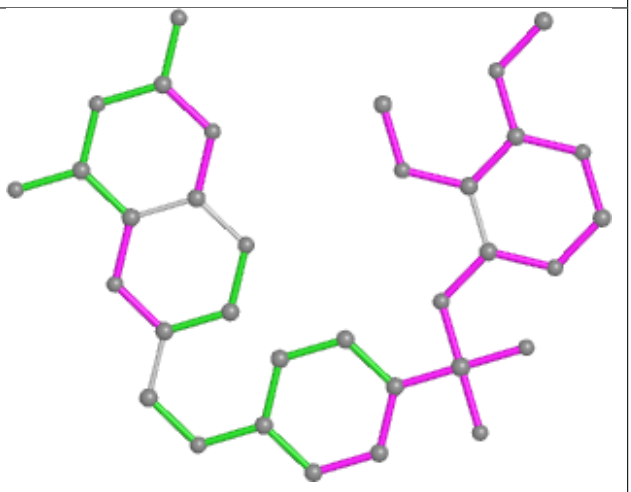


Rings

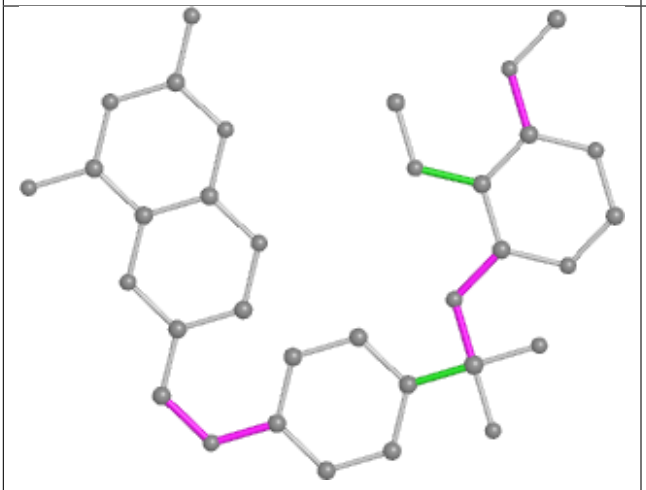
Ligand CKL B 801



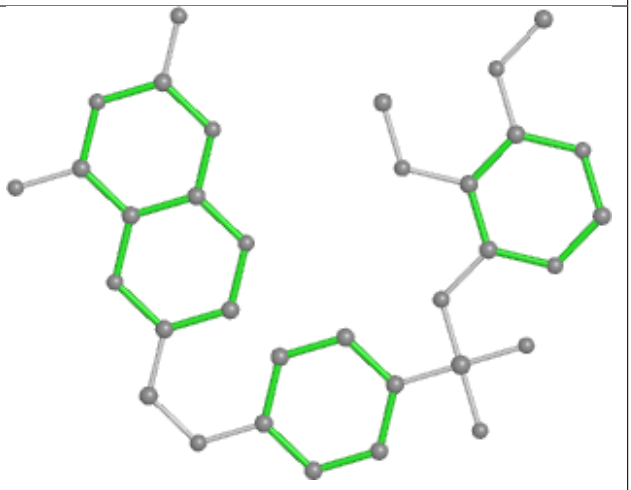
Bond lengths



Bond angles

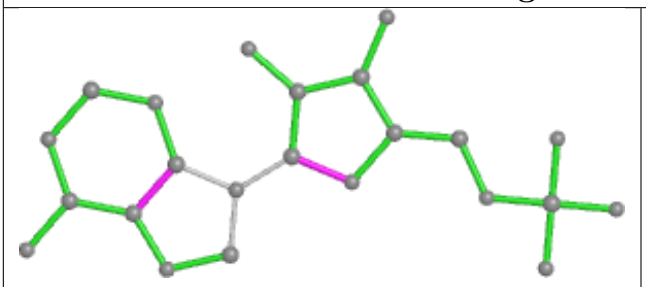


Torsions

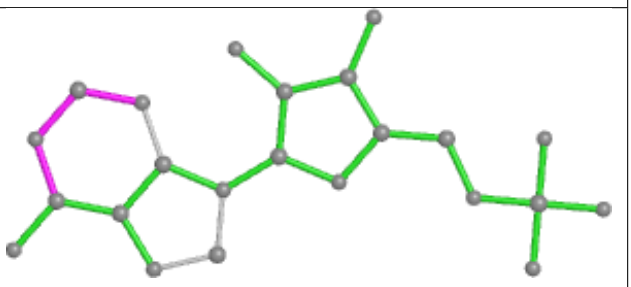


Rings

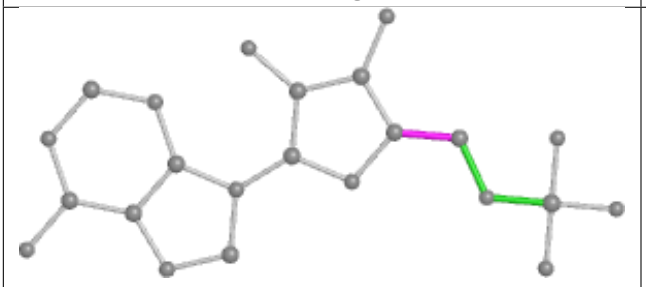
Ligand AMP A 803



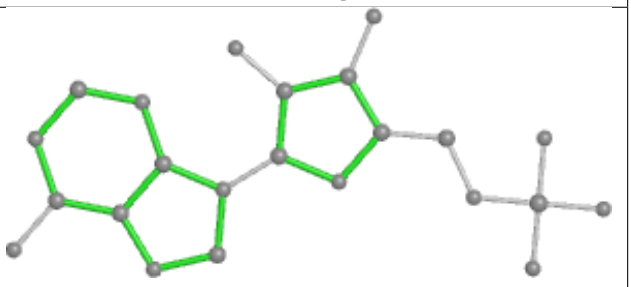
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	-0.12	26 (4%)	31	20	12, 36, 104, 120	0
1	B	565/728 (77%)	0.07	30 (5%)	26	16	11, 51, 110, 120	0
All	All	1115/1456 (76%)	-0.03	56 (5%)	28	18	11, 43, 109, 120	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	ASN	6.5
1	A	470	ILE	6.5
1	A	468	ASN	6.1
1	B	473	CYS	4.5
1	B	134	LEU	4.4
1	B	468	ASN	4.3
1	A	11	GLU	4.3
1	A	442	PRO	4.0
1	A	708	ASP	3.9
1	B	303	GLN	3.9
1	B	118	LYS	3.8
1	A	444	PRO	3.6
1	B	150	ASN	3.6
1	B	162	TYR	3.5
1	A	151	LEU	3.5
1	A	150	ASN	3.4
1	B	146	ILE	3.4
1	B	470	ILE	3.3
1	B	471	VAL	3.3
1	A	473	CYS	3.2
1	B	161	SER	3.2
1	A	161	SER	3.1
1	B	474	ASP	3.1
1	B	133	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	193	ARG	3.0
1	A	446	ILE	2.9
1	A	658	LYS	2.9
1	A	366	ILE	2.9
1	A	149	ASN	2.9
1	A	147	MET	2.8
1	A	367	ASN	2.8
1	A	618	ASP	2.8
1	B	117	GLY	2.7
1	A	707	LYS	2.7
1	B	149	ASN	2.5
1	B	222	LYS	2.5
1	A	242	GLU	2.5
1	B	225	LYS	2.5
1	B	467	LYS	2.5
1	B	120	ASP	2.5
1	A	193	ARG	2.4
1	A	162	TYR	2.4
1	B	58	VAL	2.4
1	A	471	VAL	2.4
1	A	148	LYS	2.4
1	B	145	GLU	2.4
1	B	147	MET	2.4
1	B	311	ASP	2.4
1	B	366	ILE	2.4
1	A	84	TYR	2.3
1	B	466	ILE	2.3
1	A	659	ASP	2.2
1	B	403	SER	2.2
1	B	657	ASP	2.1
1	B	11	GLU	2.1
1	B	658	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

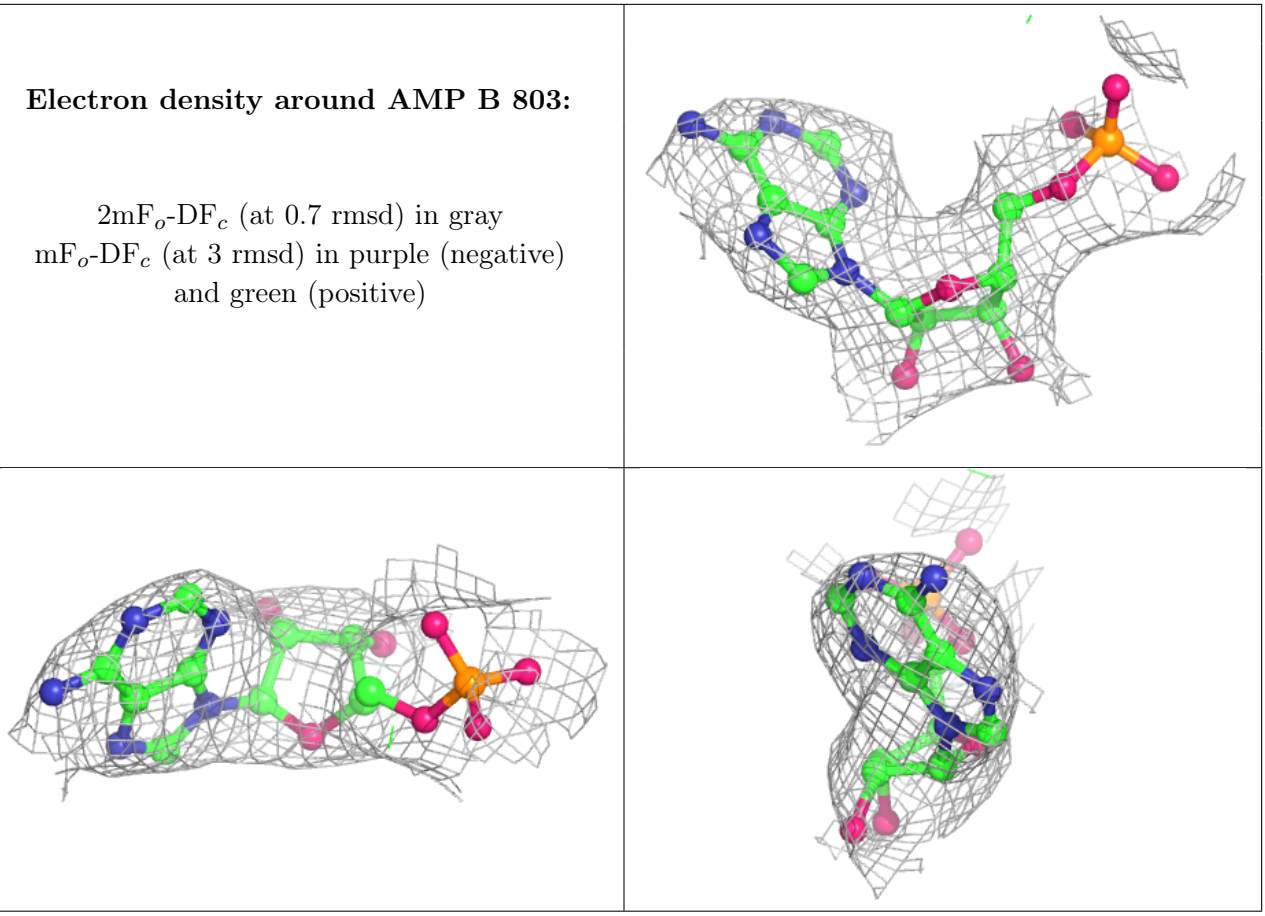
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	MG	B	804	1/1	0.59	0.20	65,65,65,65	0
8	PEG	A	807	7/7	0.86	0.19	65,67,75,76	0
4	AMP	B	803	23/23	0.88	0.22	75,83,120,120	0
8	PEG	A	808	7/7	0.88	0.21	46,53,60,63	0
2	CKL	A	801	34/34	0.90	0.24	13,29,102,107	0
3	PO4	B	802	5/5	0.92	0.20	70,77,79,80	0
2	CKL	B	801	34/34	0.94	0.18	14,32,108,110	0
4	AMP	A	803	23/23	0.94	0.18	45,54,81,81	0
3	PO4	A	802	5/5	0.95	0.16	44,52,56,58	0
7	ACT	B	806	4/4	0.96	0.14	14,14,14,14	0
5	MG	A	804	1/1	0.96	0.26	28,28,28,28	0
7	ACT	A	806	4/4	0.96	0.26	31,31,33,36	0
6	CA	A	805	1/1	0.97	0.12	37,37,37,37	0
6	CA	B	805	1/1	0.99	0.06	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.

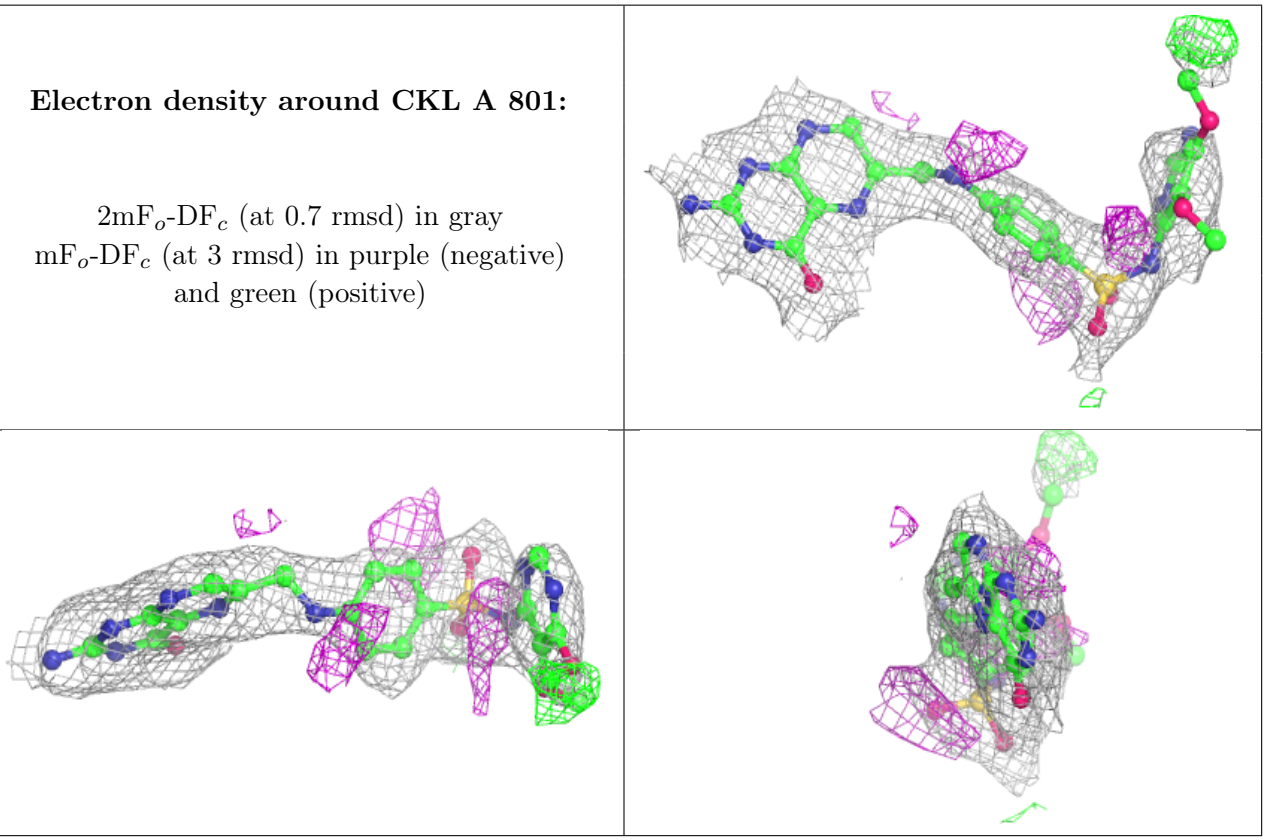
Electron density around AMP B 803:

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



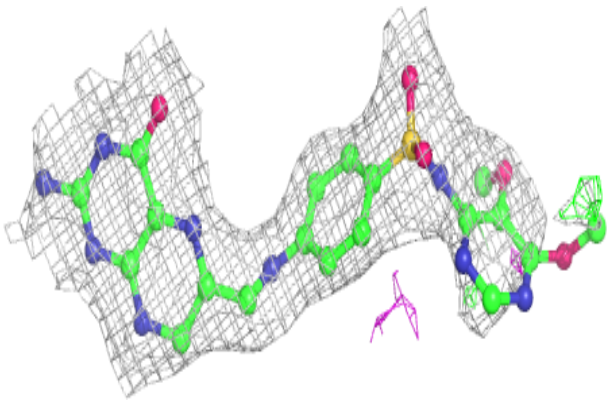
Electron density around CKL A 801:

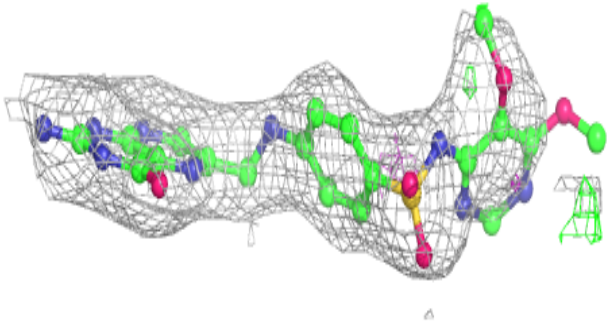
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

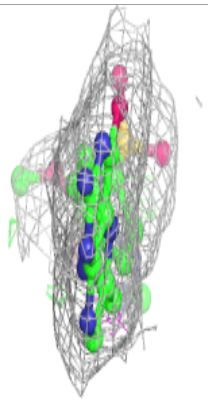


Electron density around CKL B 801:

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

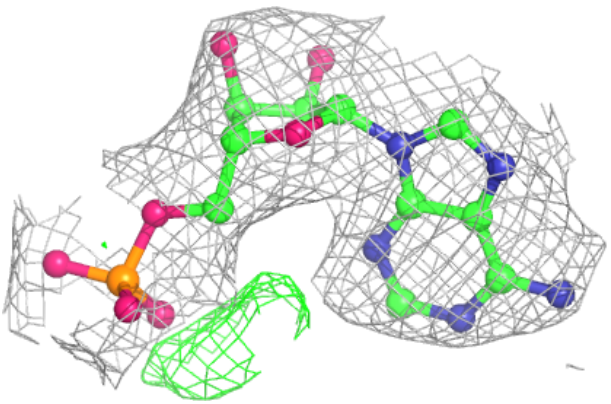


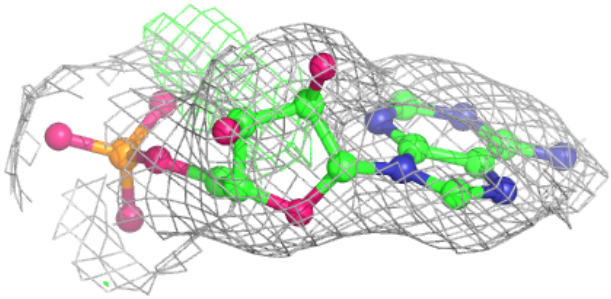


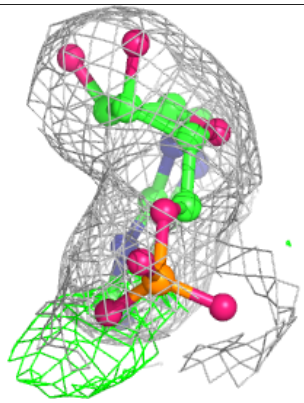


Electron density around AMP A 803:

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







6.5 Other polymers (i)

There are no such residues in this entry.