



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:47 PM UTC

PDB ID : 6JWY / pdb_00006jwy
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS A437G with SDX-DHP
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.50 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	:	4-5-2 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

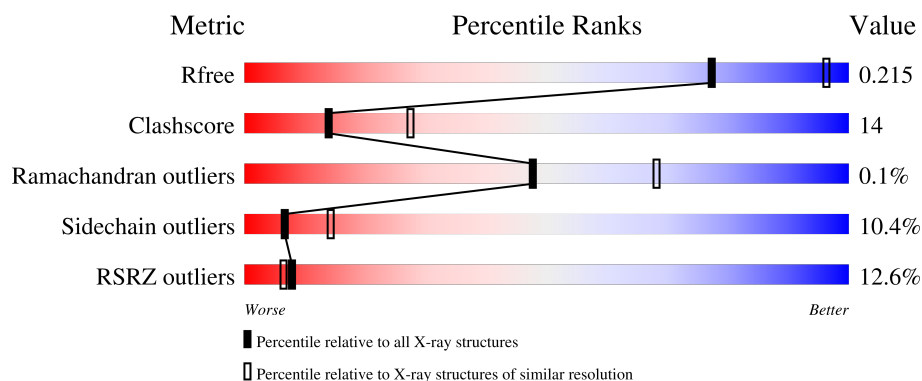
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	3% 53% 18% • 26%
1	B	728	15% 45% 24% • 27%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9241 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	538	Total	C	N	O	S	0	0	0
			4459	2873	737	826	23			
1	B	529	Total	C	N	O	S	0	0	0
			4364	2812	720	811	21			

There are 46 discrepancies between the modelled and reference sequences:

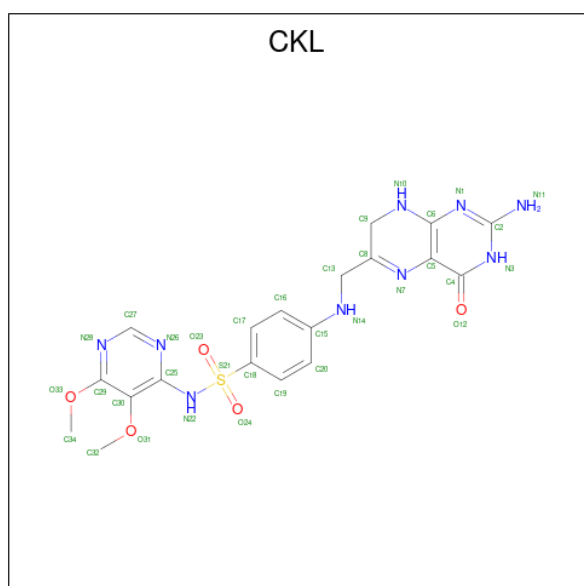
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression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

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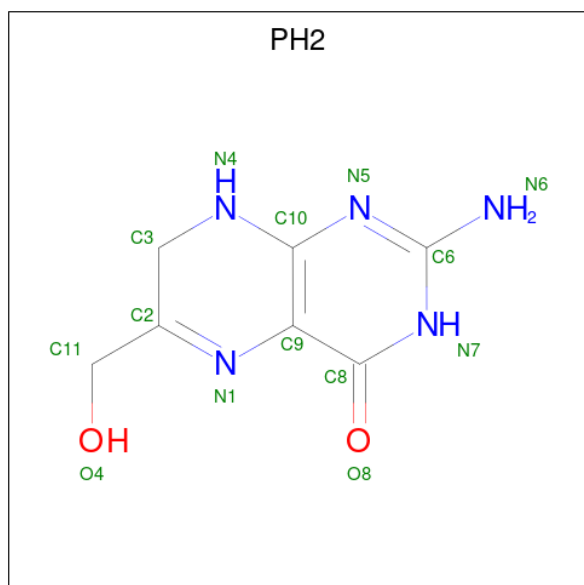
Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag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

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



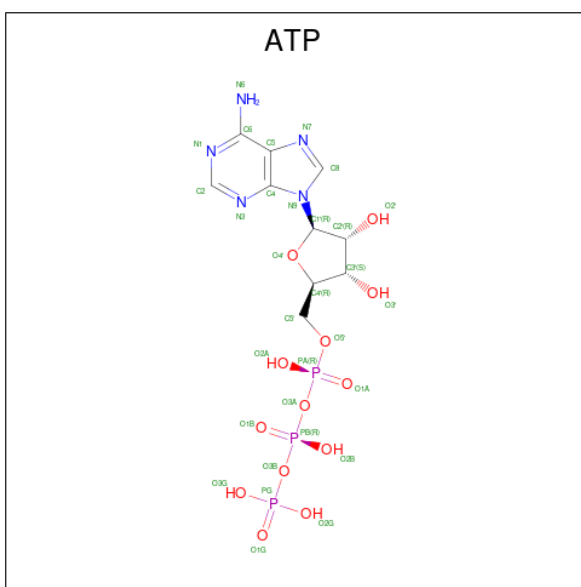
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	19	9	5	1		
2	B	1	Total	C	N	O	S	0	0
			34	19	9	5	1		

- Molecule 3 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (CCD ID: PH2) (formula: C₇H₉N₅O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
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		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

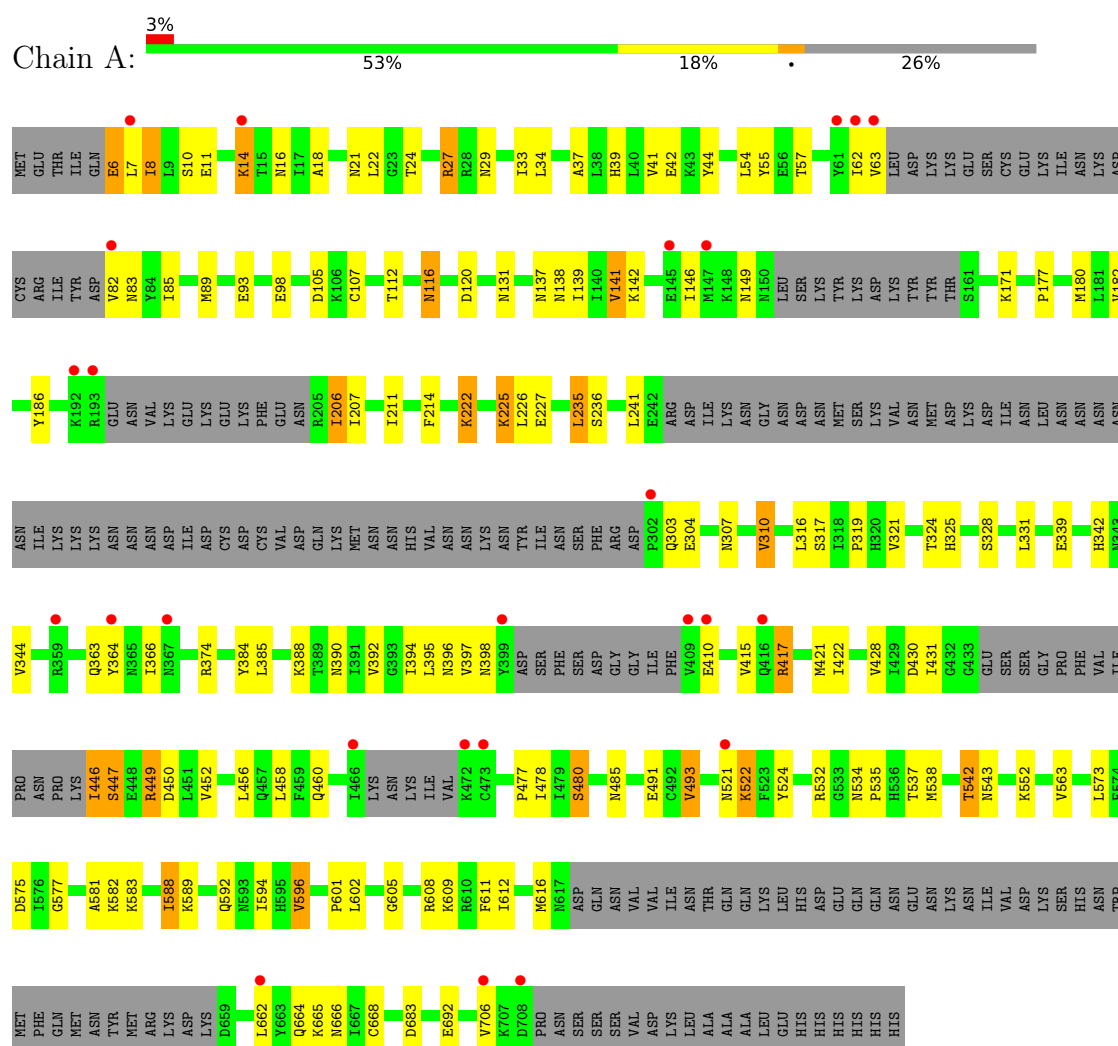
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	166	Total	O	0	0
			166	166		
8	B	84	Total	O	0	0
			84	84		

3 Residue-property plots [i](#)

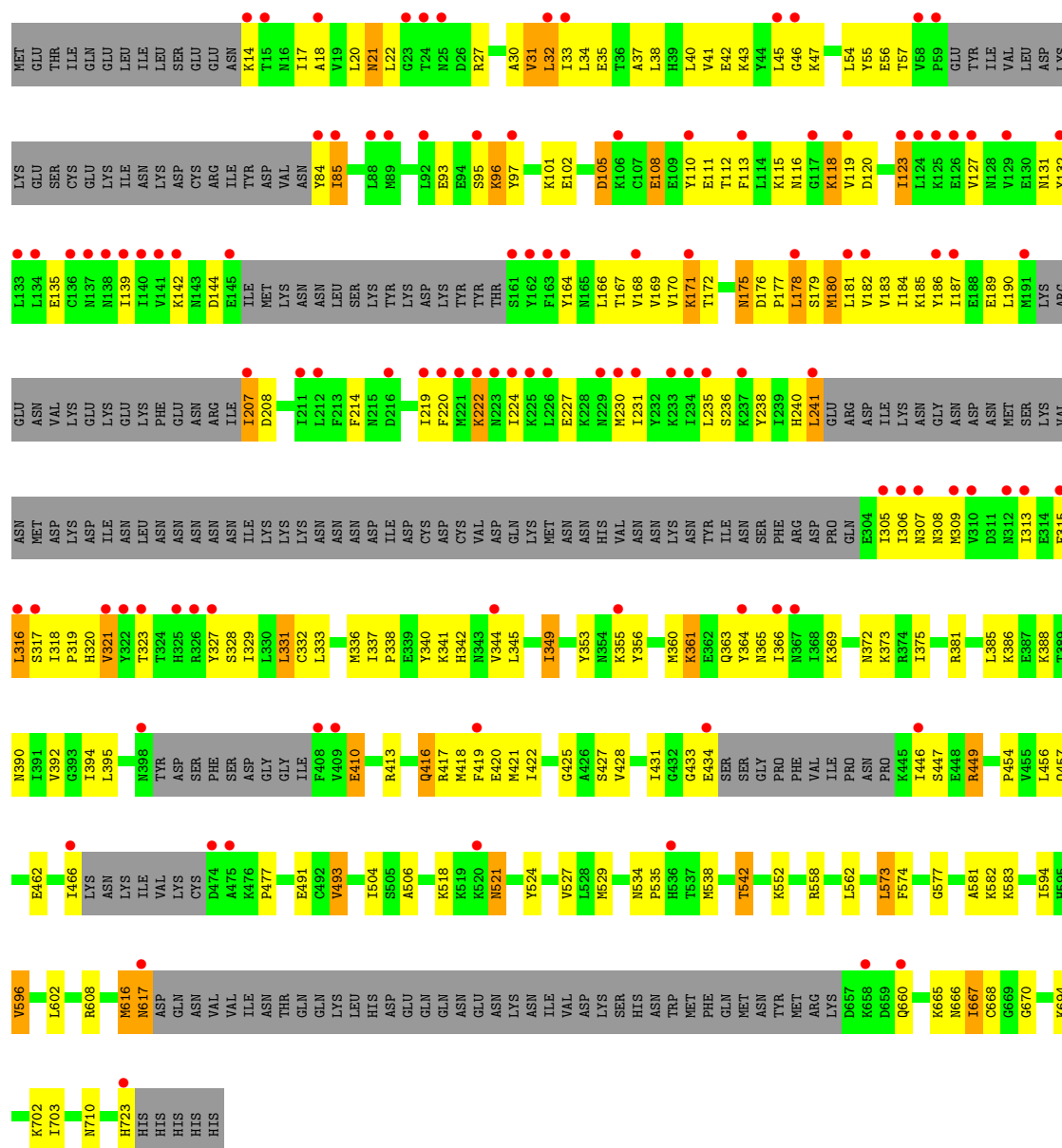
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.43Å 137.15Å 137.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.95 – 2.50 28.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	82.8 (28.95-2.50) 82.8 (28.95-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.209 , 0.221 0.200 , 0.215	Depositor DCC
R_{free} test set	2680 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9241	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, ATP, ACT, CA, CKL, PH2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/4527	1.12	4/6103 (0.1%)
1	B	0.48	0/4432	1.09	3/5977 (0.1%)
All	All	0.50	0/8959	1.10	7/12080 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	THR	CA-CB-OG1	-7.43	98.46	109.60
1	B	710	ASN	CB-CA-C	6.17	119.92	109.55
1	A	42	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	683	ASP	CB-CA-C	5.40	119.44	110.90
1	B	105	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	574	PHE	CB-CA-C	-5.20	100.75	109.48
1	A	105	ASP	CB-CA-C	-5.16	100.88	109.55

There are no chirality outliers.

There are no planarity outliers.

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	4459	0	4558	102	0
1	B	4364	0	4451	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	34	0	0	2	0
2	B	34	0	0	0	0
3	A	14	0	9	0	0
4	A	31	0	12	2	0
4	B	31	0	12	3	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	8	0	6	1	0
7	B	12	0	9	0	0
8	A	166	0	0	4	0
8	B	84	0	0	3	0
All	All	9241	0	9057	260	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 (260) 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:HE3	1.78	1.22
1:B:337:ILE:HG23	1:B:340:TYR:HB2	1.38	1.04
1:A:107:CYS:SG	1:A:171:LYS:CE	2.48	1.00
1:B:527:VAL:HG22	1:B:573:LEU:HD12	1.40	0.99
1:A:616:MET:HE1	1:A:665:LYS:O	1.67	0.94
1:B:337:ILE:CG2	1:B:340:TYR:HB2	1.99	0.93
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.53	0.91
1:B:394:ILE:O	1:B:421:MET:HE1	1.72	0.90
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.37	0.89
1:A:225:LYS:HE3	1:A:225:LYS:HA	1.54	0.89
1:A:665:LYS:HE3	8:B:928:HOH:O	1.74	0.88
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.57	0.86
1:B:96:LYS:HG3	1:B:240:HIS:CD2	2.11	0.86
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.60	0.84
1:B:422:ILE:HG12	1:B:477:PRO:HG3	1.58	0.84
1:B:449:ARG:HG3	1:B:449:ARG:HH11	1.46	0.80
1:B:315:PHE:HB3	4:B:802:ATP:H1'	1.62	0.80
1:B:179:SER:O	1:B:183:VAL:HG23	1.83	0.79
1:B:608:ARG:HA	1:B:666:ASN:ND2	1.98	0.79
1:B:392:VAL:HG22	1:B:428:VAL:HB	1.65	0.77
1:B:127:VAL:HG13	1:B:131:ASN:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PHE:O	1:B:116:ASN:HB3	1.84	0.77
1:B:419:PHE:HA	1:B:422:ILE:HD12	1.66	0.76
1:B:337:ILE:CG2	1:B:340:TYR:CB	2.63	0.75
1:A:39:HIS:CE1	1:A:521:ASN:HA	2.21	0.75
1:B:42:GLU:OE2	1:B:47:LYS:HA	1.86	0.74
1:B:178:LEU:O	1:B:182:VAL:HG23	1.89	0.72
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.19	0.71
1:B:333:LEU:HD13	1:B:349:ILE:CD1	2.20	0.71
1:B:608:ARG:HA	1:B:666:ASN:HD21	1.55	0.71
1:A:18:ALA:CB	1:A:180:MET:HE1	2.22	0.70
1:B:180:MET:HG3	1:B:214:PHE:HE2	1.55	0.70
1:B:186:TYR:CE2	1:B:190:LEU:HD11	2.27	0.70
1:B:337:ILE:HG22	1:B:337:ILE:O	1.92	0.69
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.73	0.69
1:B:208:ASP:OD2	4:B:802:ATP:O1B	2.10	0.69
1:B:333:LEU:HD13	1:B:349:ILE:HD13	1.75	0.69
1:B:108:GLU:CD	1:B:108:GLU:H	1.98	0.68
1:B:187:ILE:HA	1:B:190:LEU:HD12	1.75	0.68
1:B:184:ILE:O	1:B:187:ILE:HB	1.94	0.68
1:B:668:CYS:SG	8:B:984:HOH:O	1.94	0.67
1:B:373:LYS:O	1:B:375:ILE:HD12	1.95	0.66
1:B:14:LYS:NZ	1:B:120:ASP:HB2	2.10	0.66
1:B:177:PRO:HB3	1:B:318:ILE:CD1	2.26	0.66
1:B:127:VAL:CG1	1:B:131:ASN:HB3	2.26	0.65
1:A:668:CYS:SG	8:A:1059:HOH:O	1.98	0.64
1:B:96:LYS:NZ	1:B:236:SER:O	2.28	0.64
1:B:167:THR:HG21	1:B:333:LEU:HD23	1.81	0.62
1:B:395:LEU:HD22	1:B:418:MET:HG3	1.81	0.62
1:A:27:ARG:HH11	1:A:27:ARG:CG	2.10	0.62
1:B:46:GLY:HA3	1:B:171:LYS:O	1.99	0.62
1:B:449:ARG:HH11	1:B:449:ARG:CG	2.11	0.61
1:B:45:LEU:HD22	1:B:180:MET:SD	2.40	0.61
1:B:318:ILE:HA	1:B:319:PRO:C	2.25	0.61
1:B:167:THR:OG1	1:B:332:CYS:HB3	2.00	0.60
1:B:132:TYR:OH	1:B:319:PRO:O	2.19	0.60
1:B:534:ASN:CB	1:B:535:PRO:HD2	2.31	0.60
1:B:123:ILE:O	1:B:123:ILE:HG13	2.01	0.60
1:B:113:PHE:O	1:B:116:ASN:CB	2.50	0.59
1:B:388:LYS:HE3	1:B:390:ASN:OD1	2.02	0.59
1:B:227:GLU:HB2	1:B:230:MET:HB2	1.85	0.59
1:A:177:PRO:HD3	1:A:214:PHE:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LYS:O	1:B:365:ASN:HA	2.03	0.59
1:B:493:VAL:HG22	1:B:524:TYR:CZ	2.38	0.58
1:B:577:GLY:O	1:B:582:LYS:HE2	2.03	0.58
1:B:449:ARG:HE	1:B:491:GLU:CD	2.12	0.58
1:B:17:ILE:HG21	1:B:113:PHE:CD2	2.39	0.58
1:A:37:ALA:O	1:A:41:VAL:HG23	2.04	0.57
1:B:21:ASN:C	1:B:21:ASN:HD22	2.13	0.57
1:B:527:VAL:CG2	1:B:573:LEU:HD12	2.26	0.56
1:A:396:ASN:OD1	7:A:808:ACT:H3	2.05	0.56
1:A:177:PRO:HD3	1:A:214:PHE:CE1	2.41	0.56
1:A:142:LYS:O	1:A:146:ILE:HD12	2.05	0.56
1:B:506:ALA:HB1	1:B:558:ARG:HG2	1.88	0.56
1:A:319:PRO:HD3	1:A:342:HIS:CE1	2.41	0.55
1:B:454:PRO:O	1:B:457:GLN:HB2	2.07	0.55
1:B:14:LYS:HZ3	1:B:120:ASP:HB2	1.72	0.55
1:A:89:MET:HG3	1:A:521:ASN:ND2	2.22	0.55
1:A:493:VAL:HG22	1:A:524:TYR:CZ	2.42	0.54
1:A:316:LEU:HA	4:A:803:ATP:C8	2.42	0.54
1:A:317:SER:N	4:A:803:ATP:N7	2.49	0.54
1:B:166:LEU:HG	1:B:166:LEU:O	2.06	0.54
1:B:425:GLY:HA3	1:B:694:LYS:HD3	1.89	0.54
1:A:182:VAL:HG12	1:A:235:LEU:HD13	1.89	0.54
1:B:433:GLY:O	1:B:434:GLU:HB2	2.07	0.54
1:B:227:GLU:HB2	1:B:230:MET:CB	2.38	0.54
1:A:89:MET:HE2	1:A:521:ASN:HB2	1.89	0.54
1:A:304:GLU:H	1:A:304:GLU:CD	2.16	0.53
1:B:336:MET:HE3	1:B:337:ILE:HD12	1.89	0.53
1:A:39:HIS:CE1	1:A:521:ASN:CA	2.90	0.53
1:B:20:LEU:HD21	1:B:180:MET:HE1	1.90	0.53
1:A:21:ASN:C	1:A:22:LEU:HD12	2.33	0.53
1:B:241:LEU:HD12	1:B:241:LEU:H	1.73	0.53
1:B:521:ASN:N	1:B:521:ASN:HD22	2.07	0.53
1:A:534:ASN:HB2	1:A:535:PRO:HD3	1.91	0.52
1:B:446:ILE:HG13	1:B:447:SER:H	1.74	0.52
1:B:337:ILE:CG2	1:B:337:ILE:O	2.56	0.52
1:B:31:VAL:HG12	1:B:32:LEU:N	2.24	0.52
1:B:410:GLU:HG3	1:B:410:GLU:O	2.10	0.52
1:A:449:ARG:HH11	1:A:449:ARG:CG	2.23	0.52
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.39	0.52
1:B:333:LEU:HD13	1:B:349:ILE:HD11	1.91	0.52
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HD23	1:B:431:ILE:HD12	1.92	0.51
1:B:231:ILE:O	1:B:235:LEU:HB2	2.09	0.51
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.17	0.51
1:B:449:ARG:HG3	1:B:449:ARG:NH1	2.17	0.51
1:B:167:THR:O	1:B:168:VAL:HG23	2.10	0.51
1:B:327:TYR:HB2	1:B:356:TYR:CZ	2.45	0.51
1:B:113:PHE:C	1:B:116:ASN:HB3	2.35	0.51
1:A:392:VAL:HG22	1:A:428:VAL:HB	1.93	0.51
1:B:55:TYR:CD1	1:B:331:LEU:HD21	2.46	0.51
1:A:225:LYS:HA	1:A:225:LYS:CE	2.33	0.51
1:B:85:ILE:HG13	1:B:85:ILE:O	2.11	0.50
1:B:112:THR:O	1:B:116:ASN:HA	2.11	0.50
1:A:63:VAL:HG11	1:A:325:HIS:HB3	1.92	0.50
1:B:40:LEU:HD12	1:B:187:ILE:HG23	1.92	0.50
1:B:431:ILE:HG21	1:B:456:LEU:HD21	1.92	0.50
1:A:542:THR:HG21	1:A:583:LYS:HE2	1.91	0.50
1:B:307:ASN:C	1:B:309:MET:H	2.19	0.50
1:A:395:LEU:HD23	1:A:431:ILE:HD12	1.92	0.50
1:A:449:ARG:NE	1:A:491:GLU:OE1	2.42	0.50
1:B:552:LYS:HD2	1:B:596:VAL:HG13	1.94	0.50
1:A:57:THR:HG21	1:A:328:SER:HB2	1.93	0.49
1:A:141:VAL:CG2	1:A:142:LYS:N	2.75	0.49
1:A:93:GLU:OE2	1:A:186:TYR:OH	2.25	0.49
1:A:107:CYS:SG	1:A:171:LYS:HE2	2.48	0.49
1:A:206:ILE:HG23	1:A:207:ILE:HG22	1.94	0.49
1:A:449:ARG:HH11	1:A:449:ARG:HG3	1.77	0.49
1:B:395:LEU:HD22	1:B:418:MET:CG	2.43	0.49
1:A:446:ILE:HD13	1:A:450:ASP:HB2	1.95	0.49
1:B:175:ASN:N	1:B:175:ASN:HD22	2.10	0.49
1:B:337:ILE:HG22	1:B:340:TYR:HB3	1.95	0.48
1:B:96:LYS:HG3	1:B:240:HIS:HD2	1.68	0.48
1:A:374:ARG:HD2	1:A:385:LEU:HD22	1.95	0.48
1:A:449:ARG:HE	1:A:491:GLU:CD	2.21	0.48
1:A:222:LYS:HE3	1:A:222:LYS:HB2	1.61	0.48
1:B:17:ILE:HG21	1:B:113:PHE:CG	2.48	0.48
1:B:337:ILE:HG22	1:B:340:TYR:CB	2.41	0.48
1:B:417:ARG:NH1	1:B:421:MET:HE3	2.29	0.48
1:B:111:GLU:O	1:B:115:LYS:HG2	2.14	0.48
1:A:609:LYS:NZ	2:A:801:CKL:O12	2.46	0.48
1:B:96:LYS:HB2	1:B:238:TYR:O	2.14	0.48
1:A:27:ARG:CG	1:A:27:ARG:NH1	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLU:HG2	1:B:305:ILE:HB	1.96	0.48
1:B:21:ASN:OD1	1:B:329:ILE:HG12	2.14	0.47
1:A:55:TYR:CD2	1:A:331:LEU:HD21	2.49	0.47
1:B:305:ILE:HA	1:B:308:ASN:CG	2.39	0.47
1:B:37:ALA:HB2	1:B:207:ILE:HD11	1.97	0.47
1:B:177:PRO:HB2	1:B:316:LEU:HD11	1.95	0.47
1:B:616:MET:HE1	1:B:665:LYS:O	2.14	0.47
1:A:29:ASN:O	1:A:33:ILE:HG12	2.15	0.47
1:B:27:ARG:HG2	1:B:164:TYR:OH	2.15	0.46
1:B:417:ARG:HH11	1:B:421:MET:HG3	1.79	0.46
1:B:21:ASN:HD22	1:B:22:LEU:N	2.13	0.46
1:B:27:ARG:CG	1:B:164:TYR:OH	2.63	0.46
1:A:588:ILE:CD1	1:A:611:PHE:HD1	2.29	0.46
1:B:96:LYS:HG3	1:B:240:HIS:NE2	2.28	0.46
1:A:112:THR:O	1:A:116:ASN:HA	2.16	0.46
1:A:398:ASN:HD22	1:A:398:ASN:HA	1.63	0.46
1:A:573:LEU:HD23	1:A:601:PRO:HB2	1.96	0.46
1:A:34:LEU:CD1	1:A:54:LEU:HD11	2.45	0.46
1:B:608:ARG:HH21	1:B:667:ILE:HD11	1.81	0.46
1:A:447:SER:HB2	1:A:450:ASP:OD2	2.15	0.46
1:B:56:GLU:O	1:B:372:ASN:HA	2.16	0.46
1:B:608:ARG:HH21	1:B:667:ILE:CD1	2.29	0.45
1:B:542:THR:HG21	1:B:583:LYS:HE2	1.98	0.45
1:B:186:TYR:HB2	1:B:235:LEU:HD21	1.98	0.45
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.99	0.45
1:B:95:SER:C	1:B:97:TYR:H	2.24	0.45
1:B:45:LEU:O	1:B:172:THR:HA	2.16	0.45
1:A:573:LEU:HD23	1:A:601:PRO:CB	2.46	0.45
1:B:241:LEU:H	1:B:241:LEU:CD1	2.29	0.45
1:A:363:GLN:O	1:A:363:GLN:HG2	2.16	0.45
1:B:30:ALA:O	1:B:34:LEU:HB2	2.17	0.45
1:A:236:SER:OG	1:A:241:LEU:HD12	2.17	0.45
1:B:135:GLU:OE2	1:B:222:LYS:HD2	2.18	0.44
1:B:139:ILE:HG21	1:B:315:PHE:HE2	1.82	0.44
1:A:542:THR:HG23	1:A:542:THR:O	2.17	0.44
1:A:388:LYS:HD2	1:A:390:ASN:OD1	2.18	0.44
1:B:123:ILE:HG12	1:B:176:ASP:HB3	1.99	0.44
1:A:27:ARG:CZ	1:A:384:TYR:OH	2.66	0.44
1:B:182:VAL:HG12	1:B:235:LEU:HD11	2.00	0.44
1:B:307:ASN:O	1:B:309:MET:N	2.51	0.44
1:A:588:ILE:CD1	1:A:611:PHE:CD1	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ALA:HB3	1:B:170:VAL:HB	1.98	0.44
1:B:449:ARG:CD	1:B:491:GLU:OE1	2.65	0.44
1:A:417:ARG:HD2	1:A:417:ARG:O	2.17	0.44
1:A:662:LEU:O	1:A:666:ASN:HB2	2.18	0.44
1:B:317:SER:O	4:B:802:ATP:N6	2.43	0.44
1:B:422:ILE:HG12	1:B:477:PRO:CG	2.39	0.44
1:A:430:ASP:OD1	1:A:480:SER:OG	2.36	0.43
1:A:394:ILE:O	1:A:421:MET:HE1	2.17	0.43
1:B:118:LYS:HA	1:B:118:LYS:HD2	1.70	0.43
1:A:422:ILE:HD11	1:A:477:PRO:HG3	2.00	0.43
1:A:522:LYS:HE2	8:A:974:HOH:O	2.18	0.43
1:A:575:ASP:OD2	2:A:801:CKL:N3	2.52	0.43
1:A:592:GLN:HG2	1:B:703:ILE:O	2.17	0.43
1:A:612:ILE:HG22	1:A:616:MET:HE2	2.00	0.43
1:B:182:VAL:HG12	1:B:235:LEU:CD1	2.49	0.43
1:A:449:ARG:HD2	1:A:491:GLU:OE1	2.18	0.43
1:B:96:LYS:HB2	1:B:238:TYR:C	2.44	0.43
1:B:538:MET:O	1:B:581:ALA:HA	2.18	0.43
1:A:180:MET:HE3	1:A:211:ILE:HG12	2.01	0.43
1:A:446:ILE:O	1:A:446:ILE:CG2	2.66	0.43
1:B:318:ILE:CA	1:B:319:PRO:C	2.92	0.43
1:B:333:LEU:CD1	1:B:349:ILE:HD13	2.46	0.43
1:B:337:ILE:N	1:B:338:PRO:CD	2.81	0.43
1:B:364:TYR:HB3	1:B:366:ILE:HG13	2.01	0.43
1:B:181:LEU:HD12	1:B:181:LEU:O	2.18	0.43
1:B:309:MET:O	1:B:313:ILE:HG13	2.18	0.43
1:A:485:ASN:OD1	1:A:485:ASN:C	2.62	0.43
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.87	0.42
1:B:413:ARG:O	1:B:416:GLN:N	2.52	0.42
1:B:309:MET:HB3	1:B:313:ILE:HD11	2.01	0.42
1:A:14:LYS:HD3	1:A:16:ASN:HD21	1.83	0.42
1:A:415:VAL:HG21	1:A:458:LEU:HG	2.01	0.42
1:B:333:LEU:CD1	1:B:349:ILE:CD1	2.96	0.42
1:B:504:ILE:HA	1:B:529:MET:HB3	2.01	0.42
1:A:594:ILE:CG1	1:A:602:LEU:HD21	2.50	0.42
1:B:320:HIS:ND1	1:B:321:VAL:N	2.68	0.42
1:A:39:HIS:ND1	1:A:521:ASN:HA	2.32	0.42
1:A:449:ARG:CD	1:A:491:GLU:OE1	2.68	0.42
1:A:6:GLU:C	1:A:8:ILE:H	2.28	0.41
1:A:605:GLY:O	1:A:609:LYS:NZ	2.50	0.41
1:B:185:LYS:HB2	1:B:309:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ASN:CB	1:B:535:PRO:CD	2.86	0.41
1:A:304:GLU:O	1:A:307:ASN:HB2	2.20	0.41
1:A:137:ASN:O	1:A:138:ASN:C	2.63	0.41
1:A:235:LEU:HB3	1:A:241:LEU:HD11	2.02	0.41
1:B:702:LYS:O	1:B:703:ILE:C	2.60	0.41
1:A:44:TYR:HA	8:A:961:HOH:O	2.18	0.41
1:B:385:LEU:HG	1:B:386:LYS:HG2	2.02	0.41
1:A:226:LEU:O	1:A:310:VAL:HG13	2.20	0.41
1:A:692:GLU:OE1	1:A:692:GLU:N	2.43	0.41
1:B:594:ILE:HD11	1:B:602:LEU:HD21	2.02	0.41
1:B:616:MET:O	1:B:617:ASN:C	2.64	0.41
1:A:577:GLY:O	1:A:582:LYS:HE2	2.20	0.41
1:B:35:GLU:O	1:B:38:LEU:HB2	2.20	0.41
1:B:57:THR:HG21	1:B:328:SER:CB	2.51	0.41
1:A:39:HIS:CE1	1:A:521:ASN:C	2.99	0.41
1:A:82:VAL:HG23	1:A:83:ASN:ND2	2.35	0.41
1:A:374:ARG:CD	1:A:385:LEU:HD22	2.51	0.41
1:A:428:VAL:HG22	1:A:478:ILE:HB	2.03	0.41
1:A:538:MET:O	1:A:581:ALA:HA	2.21	0.41
1:B:241:LEU:HD12	1:B:241:LEU:N	2.35	0.41
1:A:364:TYR:HB3	1:A:366:ILE:HG13	2.03	0.41
1:B:446:ILE:HD12	1:B:446:ILE:HA	1.95	0.40
1:B:342:HIS:ND1	1:B:344:VAL:HG12	2.36	0.40
1:B:419:PHE:O	1:B:420:GLU:C	2.64	0.40
1:A:532:ARG:HB2	1:A:581:ALA:CB	2.51	0.40
1:A:581:ALA:N	8:A:905:HOH:O	2.40	0.40
1:B:55:TYR:O	1:B:164:TYR:HA	2.21	0.40
1:B:110:TYR:CE1	1:B:169:VAL:HG11	2.56	0.40
1:B:353:TYR:OH	1:B:369:LYS:NZ	2.54	0.40
1:B:670:GLY:HA3	8:B:910:HOH:O	2.21	0.40
1:A:608:ARG:HA	1:A:666:ASN:OD1	2.22	0.40
1:B:37:ALA:O	1:B:41:VAL:HG23	2.21	0.40
1:B:45:LEU:CD2	1:B:180:MET:SD	3.08	0.40
1:B:542:THR:HG21	1:B:583:LYS:CE	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	520/728 (71%)	488 (94%)	31 (6%)	1 (0%)	43	63
1	B	511/728 (70%)	460 (90%)	51 (10%)	0	100	100
All	All	1031/1456 (71%)	948 (92%)	82 (8%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	513/696 (74%)	467 (91%)	46 (9%)	9	19
1	B	501/696 (72%)	442 (88%)	59 (12%)	5	11
All	All	1014/1392 (73%)	909 (90%)	105 (10%)	7	14

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	LEU
1	A	8	ILE
1	A	10	SER
1	A	11	GLU

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Mol	Chain	Res	Type
1	A	14	LYS
1	A	27	ARG
1	A	62	ILE
1	A	85	ILE
1	A	98	GLU
1	A	116	ASN
1	A	131	ASN
1	A	139	ILE
1	A	141	VAL
1	A	149	ASN
1	A	206	ILE
1	A	222	LYS
1	A	225	LYS
1	A	227	GLU
1	A	235	LEU
1	A	303	GLN
1	A	310	VAL
1	A	321	VAL
1	A	324	THR
1	A	339	GLU
1	A	344	VAL
1	A	397	VAL
1	A	410	GLU
1	A	417	ARG
1	A	446	ILE
1	A	447	SER
1	A	449	ARG
1	A	452	VAL
1	A	460	GLN
1	A	480	SER
1	A	493	VAL
1	A	522	LYS
1	A	537	THR
1	A	542	THR
1	A	543	ASN
1	A	563	VAL
1	A	588	ILE
1	A	589	LYS
1	A	596	VAL
1	A	664	GLN
1	A	706	VAL
1	B	21	ASN

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Mol	Chain	Res	Type
1	B	31	VAL
1	B	32	LEU
1	B	33	ILE
1	B	43	LYS
1	B	84	TYR
1	B	85	ILE
1	B	93	GLU
1	B	96	LYS
1	B	101	LYS
1	B	102	GLU
1	B	105	ASP
1	B	108	GLU
1	B	118	LYS
1	B	119	VAL
1	B	123	ILE
1	B	142	LYS
1	B	144	ASP
1	B	171	LYS
1	B	175	ASN
1	B	178	LEU
1	B	180	MET
1	B	207	ILE
1	B	219	ILE
1	B	220	PHE
1	B	222	LYS
1	B	224	ILE
1	B	241	LEU
1	B	306	ILE
1	B	316	LEU
1	B	321	VAL
1	B	323	THR
1	B	331	LEU
1	B	341	LYS
1	B	345	LEU
1	B	349	ILE
1	B	355	LYS
1	B	360	MET
1	B	361	LYS
1	B	363	GLN
1	B	381	ARG
1	B	410	GLU
1	B	416	GLN

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Mol	Chain	Res	Type
1	B	427	SER
1	B	449	ARG
1	B	462	GLU
1	B	466	ILE
1	B	493	VAL
1	B	518	LYS
1	B	521	ASN
1	B	542	THR
1	B	562	LEU
1	B	573	LEU
1	B	596	VAL
1	B	616	MET
1	B	617	ASN
1	B	660	GLN
1	B	667	ILE
1	B	723	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	83	ASN
1	A	240	HIS
1	A	308	ASN
1	A	343	ASN
1	A	365	ASN
1	A	398	ASN
1	A	521	ASN
1	A	614	HIS
1	A	617	ASN
1	A	664	GLN
1	B	21	ASN
1	B	90	GLN
1	B	91	ASN
1	B	165	ASN
1	B	175	ASN
1	B	215	ASN
1	B	223	ASN
1	B	308	ASN
1	B	521	ASN
1	B	660	GLN
1	B	666	ASN

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Mol	Chain	Res	Type
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 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	$\# Z > 2$
4	ATP	B	802	5	32,33,33	0.83	2 (6%)	48,52,52	0.64	1 (2%)
7	ACT	A	808	-	3,3,3	1.22	0	3,3,3	0.69	0
2	CKL	A	801	-	34,37,37	2.04	3 (8%)	38,53,53	2.94	13 (34%)
4	ATP	A	803	5	32,33,33	0.57	0	48,52,52	0.63	0
7	ACT	B	805	-	3,3,3	0.97	0	3,3,3	0.77	0
3	PH2	A	802	-	12,15,15	0.71	1 (8%)	11,21,21	1.45	1 (9%)
7	ACT	B	806	-	3,3,3	1.23	0	3,3,3	0.63	0
7	ACT	A	807	-	3,3,3	0.88	0	3,3,3	0.84	0
2	CKL	B	801	-	34,37,37	1.93	2 (5%)	38,53,53	3.00	18 (47%)
7	ACT	B	804	-	3,3,3	1.08	0	3,3,3	0.90	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
4	ATP	B	802	5	-	4/22/38/38	0/3/3/3
2	CKL	A	801	-	-	6/18/29/29	0/4/4/4
4	ATP	A	803	5	-	5/22/38/38	0/3/3/3
3	PH2	A	802	-	-	0/0/11/11	0/2/2/2
2	CKL	B	801	-	-	3/18/29/29	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CKL	C18-S21	-9.81	1.61	1.76
2	B	801	CKL	C18-S21	-9.52	1.61	1.76
2	A	801	CKL	C5-C6	3.11	1.47	1.40
4	B	802	ATP	PA-O3A	2.91	1.62	1.59
2	B	801	CKL	C5-C6	2.12	1.45	1.40
2	A	801	CKL	O33-C29	2.09	1.38	1.35
4	B	802	ATP	PB-O3A	2.00	1.61	1.59
3	A	802	PH2	C9-N1	2.00	1.41	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CKL	O23-S21-O24	-11.57	105.47	119.52
2	A	801	CKL	O23-S21-O24	-11.14	105.99	119.52
2	A	801	CKL	O23-S21-C18	5.97	115.51	107.98
2	A	801	CKL	N26-C27-N28	-5.33	120.51	128.58
2	B	801	CKL	N26-C27-N28	-5.13	120.81	128.58
2	A	801	CKL	C34-O33-C29	5.06	121.93	117.20
2	B	801	CKL	O24-S21-C18	4.99	114.28	107.98
2	B	801	CKL	C2-N1-C6	4.93	122.07	113.36
2	A	801	CKL	O24-S21-N22	4.46	117.61	106.74
2	B	801	CKL	C18-S21-N22	4.26	112.16	106.88
2	A	801	CKL	C2-N1-C6	3.77	120.02	113.36
2	B	801	CKL	O12-C4-C5	-3.75	116.62	126.53
3	A	802	PH2	C6-N5-C10	3.58	119.68	113.36
2	A	801	CKL	C18-S21-N22	-3.35	102.72	106.88
2	A	801	CKL	C30-C29-N28	-3.21	119.04	122.75
2	B	801	CKL	C34-O33-C29	3.12	120.12	117.20
2	B	801	CKL	C5-C4-N3	2.93	120.71	113.25
2	B	801	CKL	C30-C29-N28	-2.88	119.41	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CKL	C20-C19-C18	2.87	122.23	119.44
2	A	801	CKL	C27-N28-C29	2.82	121.44	115.63
2	A	801	CKL	C13-N14-C15	2.81	127.85	122.42
2	A	801	CKL	C5-C4-N3	2.76	120.27	113.25
2	B	801	CKL	C2-N3-C4	-2.71	120.20	125.11
2	A	801	CKL	O12-C4-C5	-2.63	119.59	126.53
2	B	801	CKL	C17-C18-S21	2.53	122.54	119.76
2	B	801	CKL	C27-N28-C29	2.53	120.84	115.63
2	B	801	CKL	O33-C29-C30	2.30	121.04	116.94
2	B	801	CKL	C5-N7-C8	2.30	120.81	116.24
2	B	801	CKL	O24-S21-N22	2.27	112.27	106.74
2	B	801	CKL	N22-C25-N26	2.22	122.64	118.40
2	B	801	CKL	C25-N22-S21	2.20	128.35	124.44
2	A	801	CKL	C32-O31-C30	2.18	120.67	114.74
4	B	802	ATP	C2'-C1'-N9	2.08	118.47	113.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

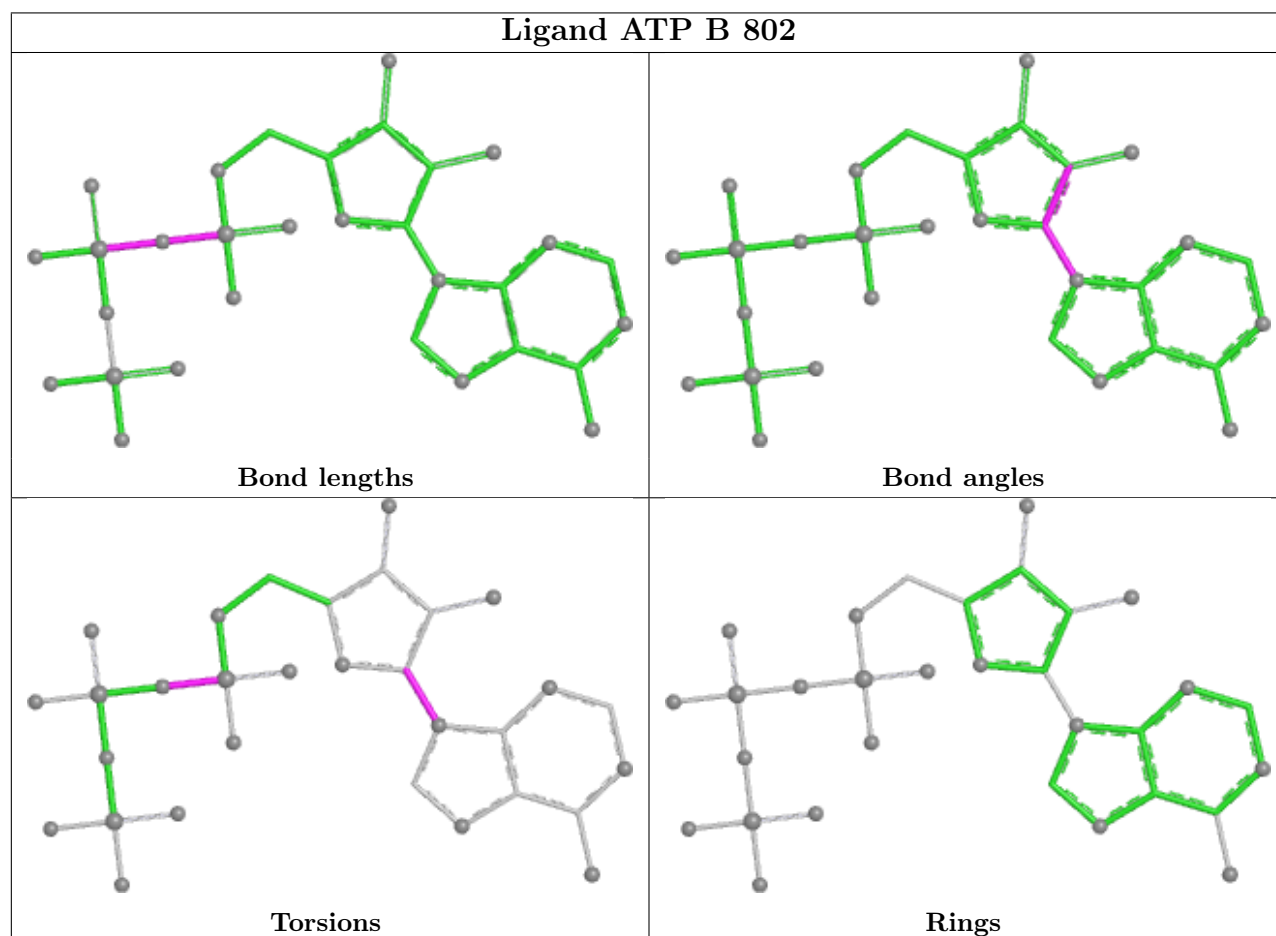
Mol	Chain	Res	Type	Atoms
2	A	801	CKL	C25-N22-S21-O23
2	B	801	CKL	C30-C29-O33-C34
2	B	801	CKL	N28-C29-O33-C34
4	B	802	ATP	PB-O3A-PA-O5'
2	A	801	CKL	N28-C29-O33-C34
2	A	801	CKL	C30-C29-O33-C34
2	A	801	CKL	C25-N22-S21-O24
2	A	801	CKL	C25-N22-S21-C18
4	A	803	ATP	PB-O3A-PA-O1A
2	B	801	CKL	C8-C13-N14-C15
4	A	803	ATP	PA-O3A-PB-O1B
4	A	803	ATP	O4'-C4'-C5'-O5'
4	B	802	ATP	O4'-C1'-N9-C8
4	B	802	ATP	C2'-C1'-N9-C8
4	A	803	ATP	PA-O3A-PB-O2B
4	B	802	ATP	C2'-C1'-N9-C4
2	A	801	CKL	C8-C13-N14-C15
4	A	803	ATP	PB-O3A-PA-O2A

There are no ring outliers.

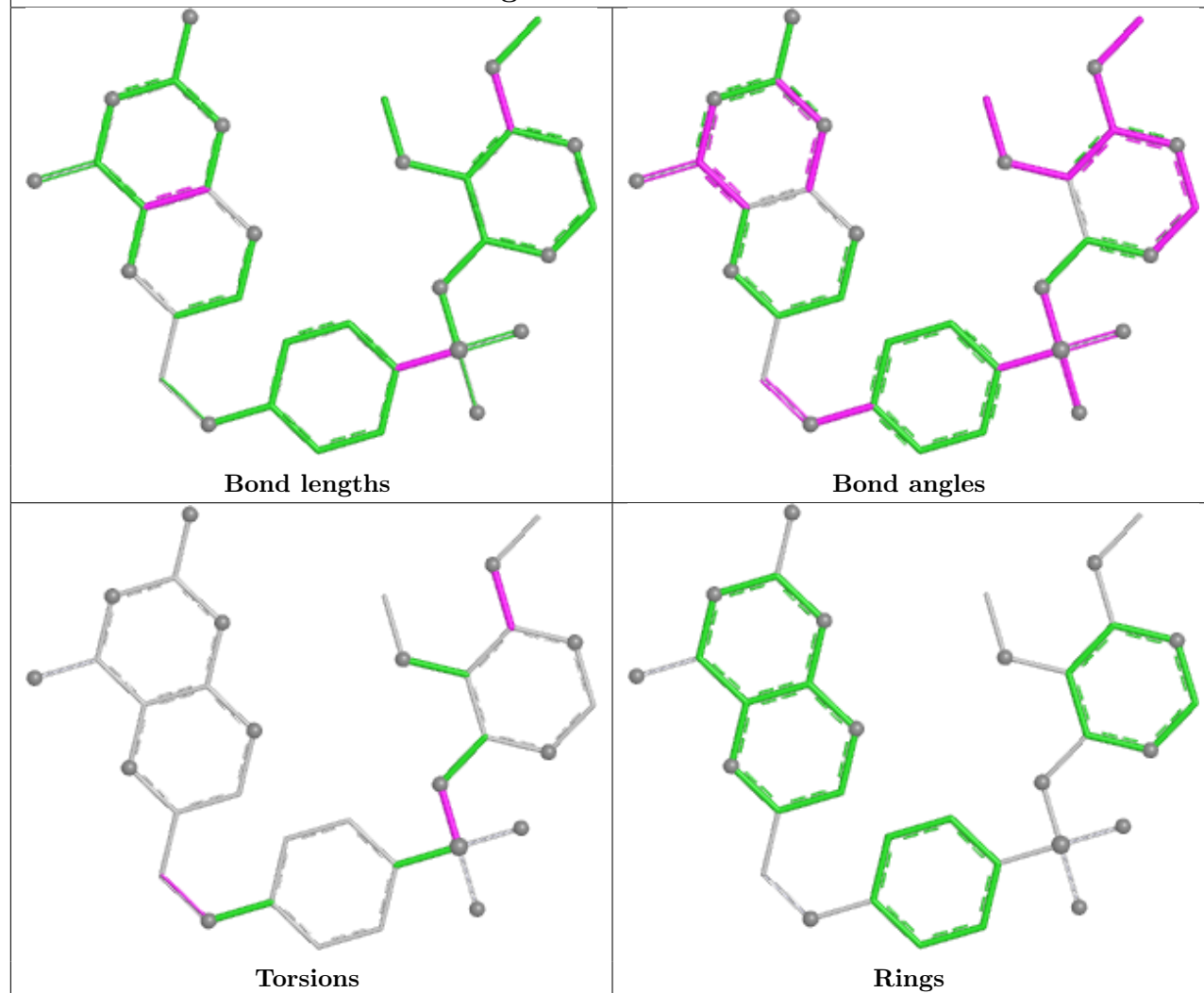
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	ATP	3	0
7	A	808	ACT	1	0
2	A	801	CKL	2	0
4	A	803	ATP	2	0

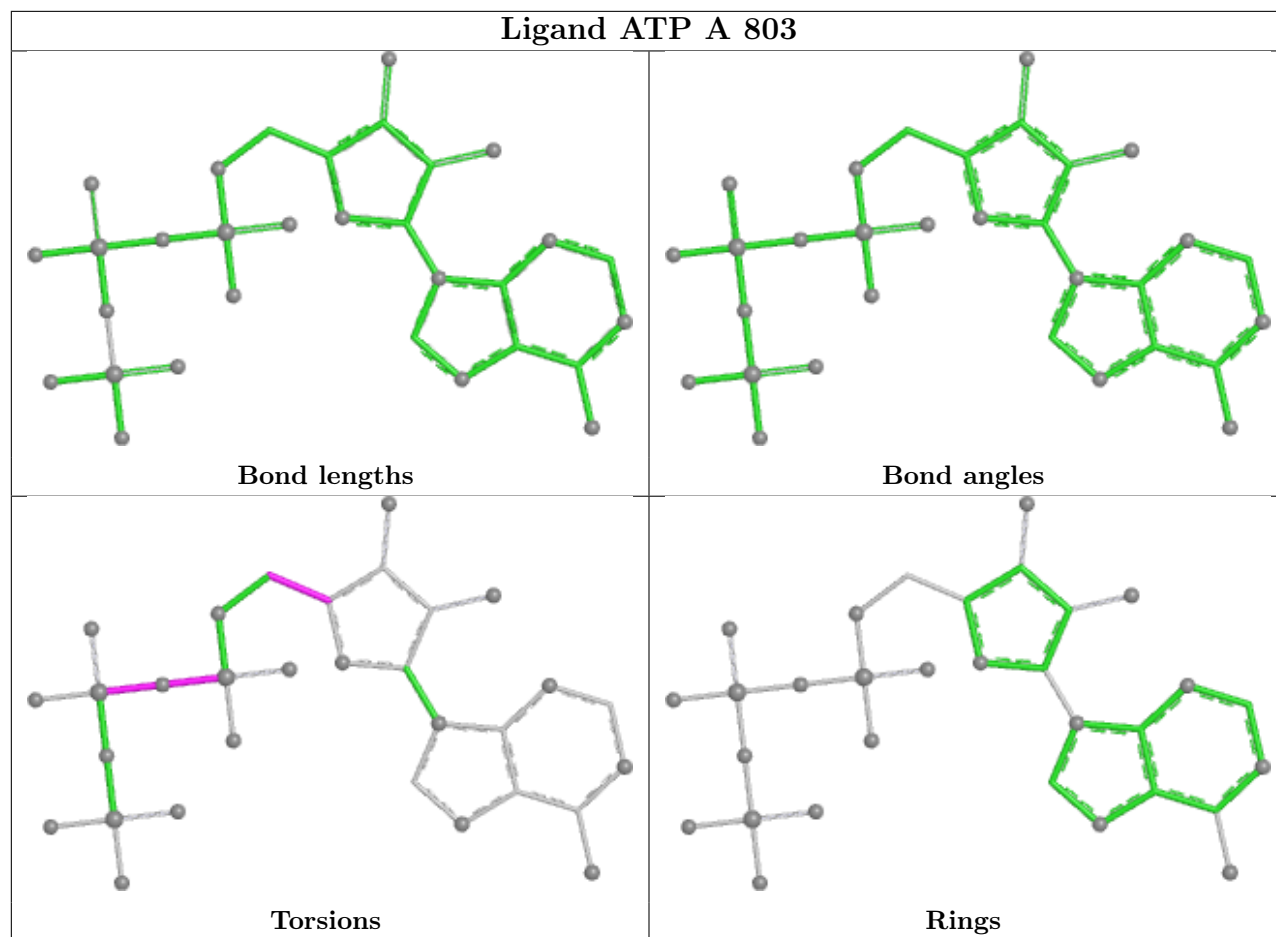
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



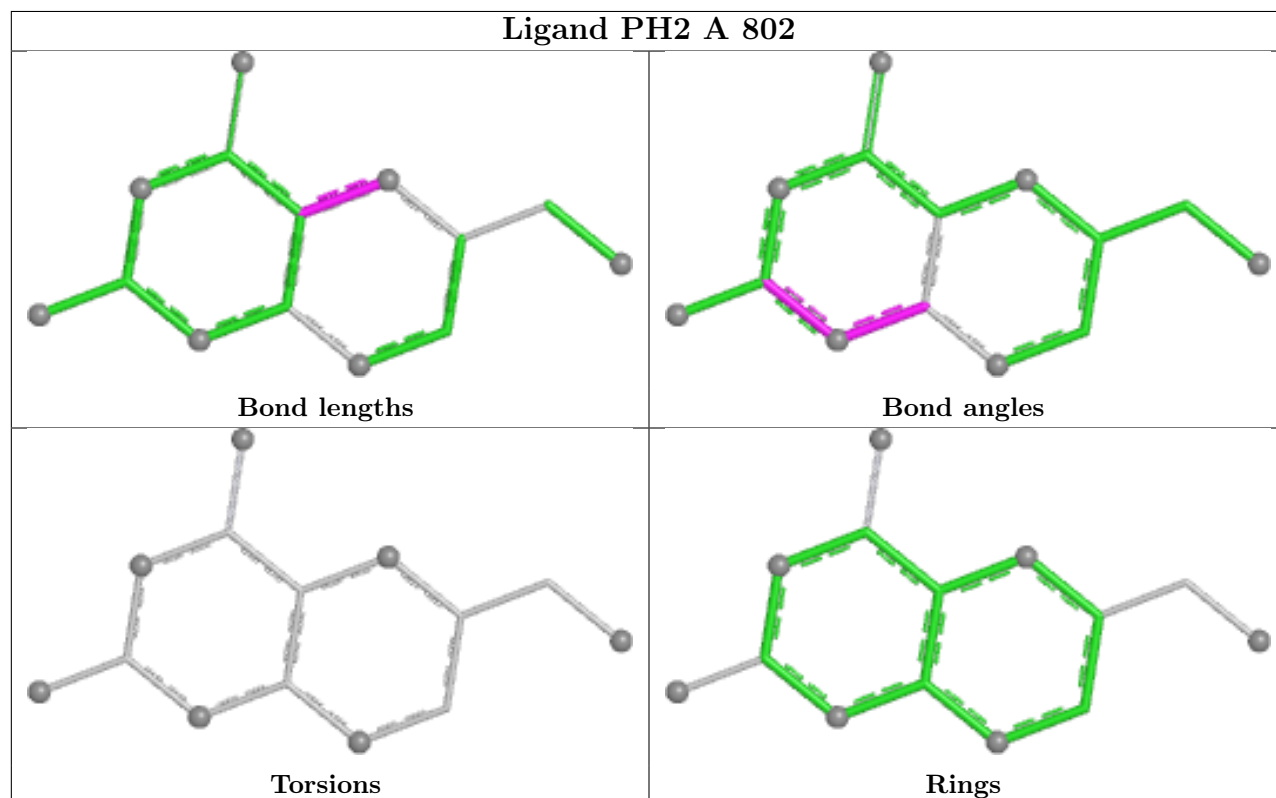
Ligand CKL A 801

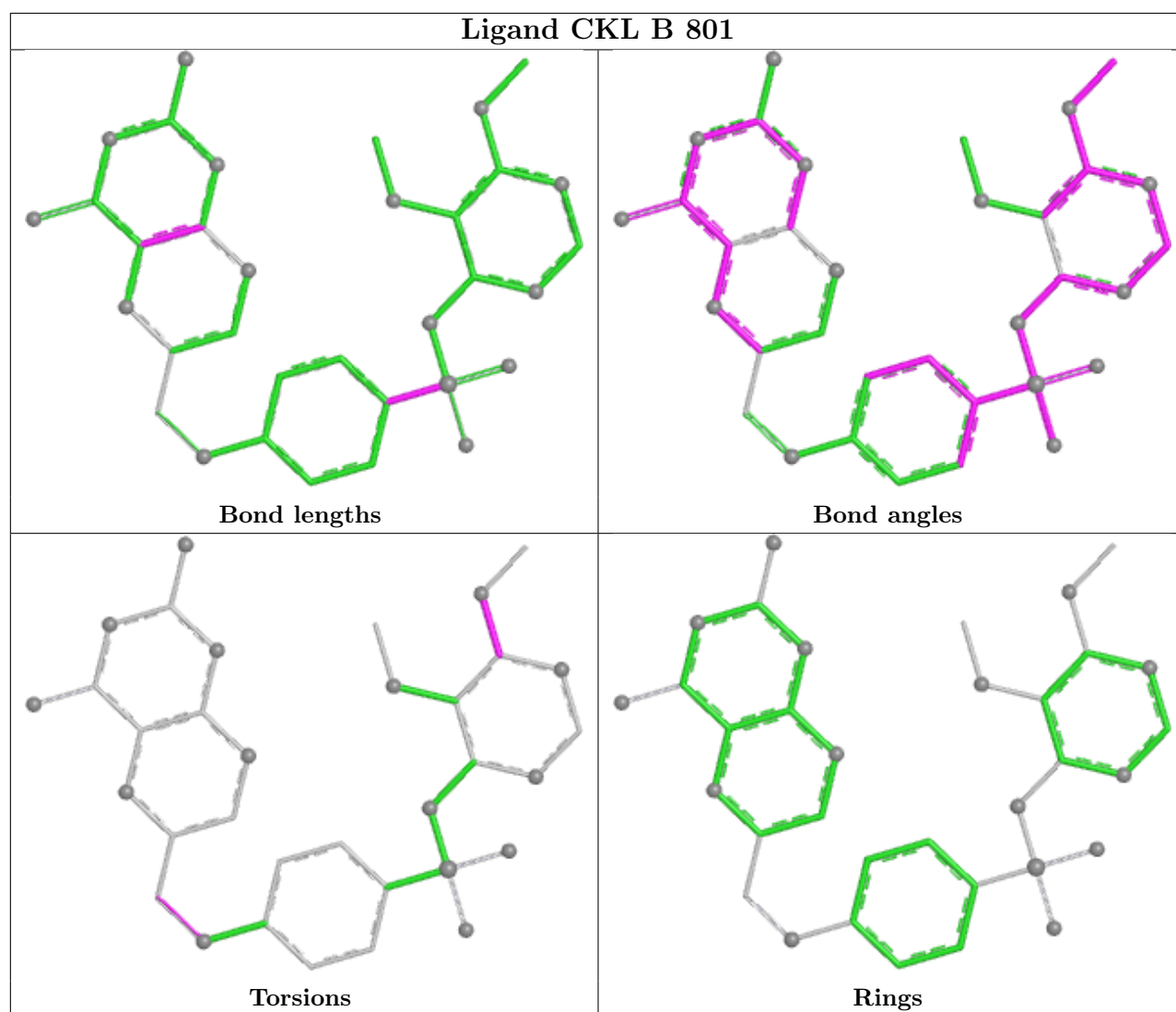


Ligand ATP A 803



Ligand PH2 A 802





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	538/728 (73%)	-0.10	25 (4%) 37 33	10, 31, 93, 120	0
1	B	529/728 (72%)	0.82	109 (20%) 2 2	12, 61, 119, 120	0
All	All	1067/1456 (73%)	0.35	134 (12%) 8 6	10, 41, 114, 120	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	6.3
1	B	306	ILE	6.3
1	B	231	ILE	6.1
1	A	62	ILE	5.9
1	A	472	LYS	5.6
1	B	163	PHE	5.5
1	A	302	PRO	5.5
1	A	409	VAL	5.2
1	B	226	LEU	5.0
1	B	139	ILE	4.7
1	A	7	LEU	4.7
1	B	466	ILE	4.6
1	B	408	PHE	4.5
1	B	235	LEU	4.5
1	B	129	VAL	4.3
1	A	399	TYR	4.3
1	B	162	TYR	4.2
1	B	409	VAL	4.2
1	B	141	VAL	4.1
1	B	309	MET	4.0
1	B	326	ARG	3.9
1	B	224	ILE	3.8
1	B	315	PHE	3.7
1	B	119	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	191	MET	3.6
1	B	234	ILE	3.6
1	B	88	LEU	3.5
1	B	84	TYR	3.5
1	B	136	CYS	3.4
1	A	63	VAL	3.4
1	B	212	LEU	3.4
1	B	133	LEU	3.4
1	B	446	ILE	3.4
1	B	126	GLU	3.3
1	B	305	ILE	3.3
1	B	59	PRO	3.3
1	B	344	VAL	3.3
1	B	222	LYS	3.2
1	B	207	ILE	3.2
1	A	61	TYR	3.2
1	B	310	VAL	3.2
1	A	662	LEU	3.2
1	B	125	LYS	3.2
1	B	322	TYR	3.2
1	A	147	MET	3.1
1	B	32	LEU	3.1
1	B	85	ILE	3.1
1	B	220	PHE	3.0
1	B	219	ILE	3.0
1	B	658	LYS	3.0
1	B	140	ILE	3.0
1	B	221	MET	2.9
1	B	134	LEU	2.9
1	A	410	GLU	2.9
1	B	178	LEU	2.9
1	B	520	LYS	2.8
1	B	89	MET	2.8
1	B	142	LYS	2.8
1	B	225	LYS	2.8
1	B	97	TYR	2.8
1	B	25	ASN	2.8
1	B	307	ASN	2.8
1	B	92	LEU	2.8
1	B	23	GLY	2.7
1	B	14	LYS	2.7
1	B	475	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	123	ILE	2.7
1	B	137	ASN	2.7
1	B	164	TYR	2.7
1	B	367	ASN	2.6
1	A	706	VAL	2.6
1	B	127	VAL	2.6
1	B	316	LEU	2.6
1	B	325	HIS	2.6
1	B	241	LEU	2.6
1	B	18	ALA	2.6
1	B	161	SER	2.6
1	B	317	SER	2.6
1	B	364	TYR	2.6
1	B	474	ASP	2.5
1	B	229	ASN	2.5
1	B	366	ILE	2.5
1	B	124	LEU	2.5
1	B	617	ASN	2.5
1	B	95	SER	2.5
1	B	434	GLU	2.5
1	B	237	LYS	2.4
1	A	359	ARG	2.4
1	B	117	GLY	2.4
1	B	313	ILE	2.4
1	A	466	ILE	2.4
1	B	168	VAL	2.4
1	A	14	LYS	2.4
1	B	110	TYR	2.3
1	B	321	VAL	2.3
1	A	521	ASN	2.3
1	A	145	GLU	2.3
1	B	233	LYS	2.3
1	B	58	VAL	2.3
1	B	138	ASN	2.3
1	B	106	LYS	2.3
1	B	223	ASN	2.3
1	B	398	ASN	2.3
1	A	193	ARG	2.3
1	B	186	TYR	2.3
1	B	145	GLU	2.2
1	A	367	ASN	2.2
1	B	312	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	416	GLN	2.2
1	B	46	GLY	2.2
1	B	24	THR	2.2
1	B	230	MET	2.2
1	B	113	PHE	2.2
1	B	419	PHE	2.2
1	B	182	VAL	2.2
1	B	660	GLN	2.2
1	A	364	TYR	2.1
1	B	132	TYR	2.1
1	B	33	ILE	2.1
1	B	187	ILE	2.1
1	A	708	ASP	2.1
1	B	15	THR	2.1
1	B	211	ILE	2.1
1	B	216	ASP	2.1
1	B	536	HIS	2.1
1	B	723	HIS	2.1
1	B	323	THR	2.1
1	A	192	LYS	2.1
1	A	473	CYS	2.1
1	B	45	LEU	2.0
1	B	171	LYS	2.0
1	B	355	LYS	2.0
1	B	181	LEU	2.0
1	B	327	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

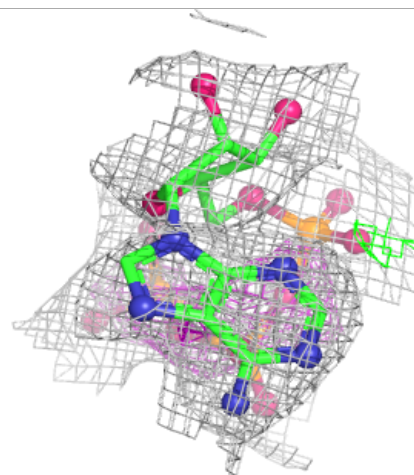
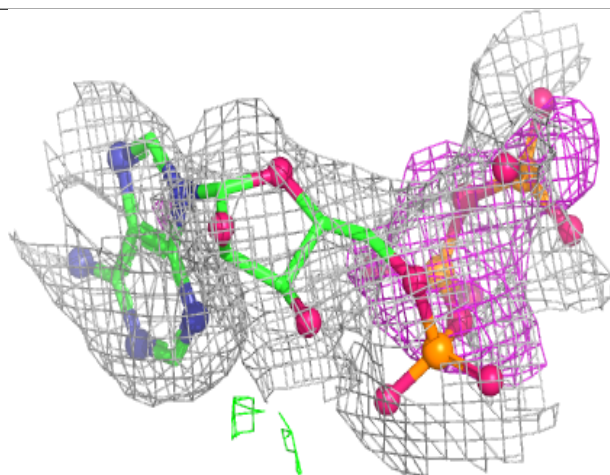
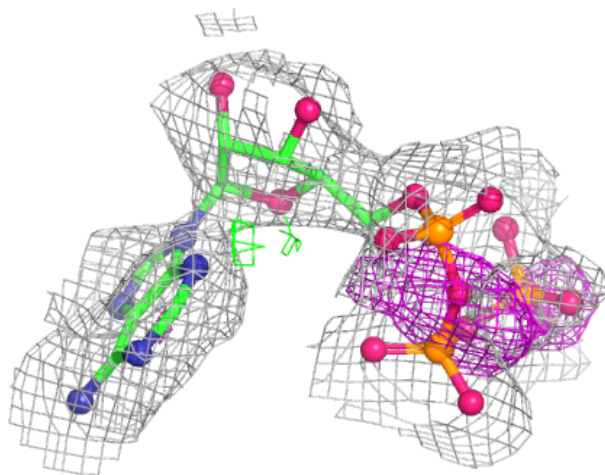
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	ATP	B	802	31/31	0.59	0.17	87,116,120,120	0
3	PH2	A	802	14/14	0.87	0.12	57,62,77,82	0
5	MG	A	804	1/1	0.88	0.13	79,79,79,79	0
4	ATP	A	803	31/31	0.89	0.11	30,60,120,120	0
7	ACT	B	805	4/4	0.92	0.10	31,35,36,38	0
7	ACT	B	806	4/4	0.92	0.16	40,41,43,47	0
7	ACT	A	808	4/4	0.93	0.10	31,31,35,37	0
2	CKL	A	801	34/34	0.96	0.10	9,26,96,104	0
2	CKL	B	801	34/34	0.96	0.09	12,26,97,104	0
7	ACT	A	807	4/4	0.96	0.08	27,29,29,29	0
5	MG	B	803	1/1	0.97	0.07	80,80,80,80	0
6	CA	A	806	1/1	0.98	0.03	25,25,25,25	0
7	ACT	B	804	4/4	0.98	0.07	19,20,20,20	0
5	MG	A	805	1/1	0.99	0.02	27,27,27,27	0

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

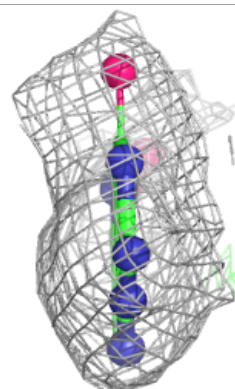
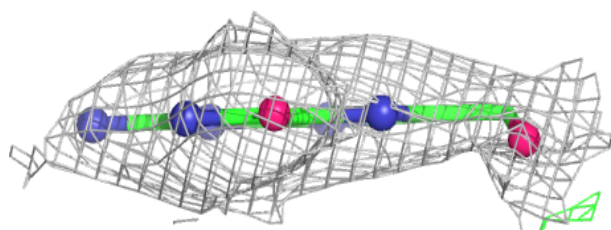
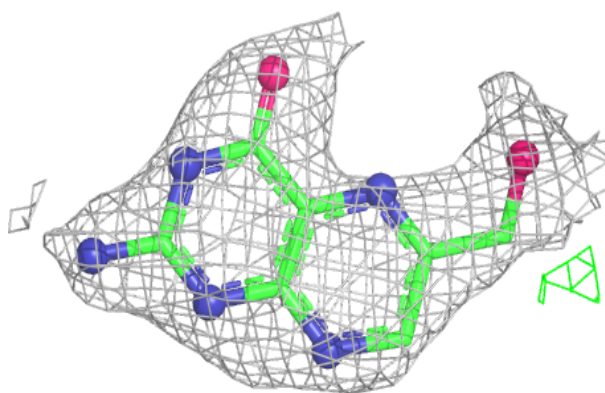
Electron density around ATP B 802:

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



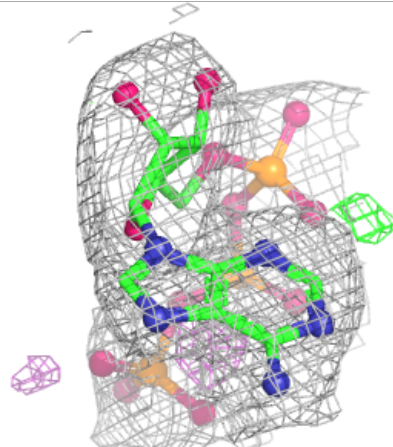
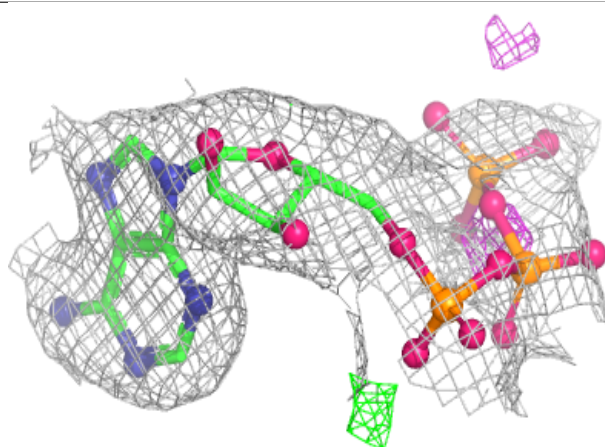
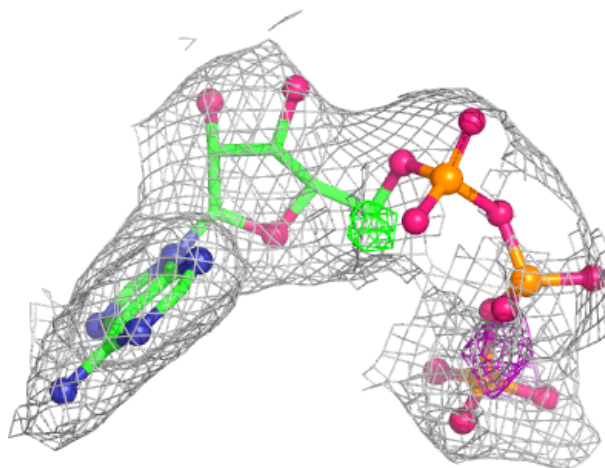
Electron density around PH2 A 802:

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



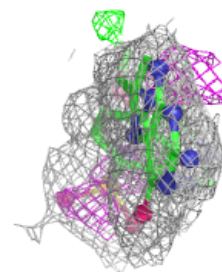
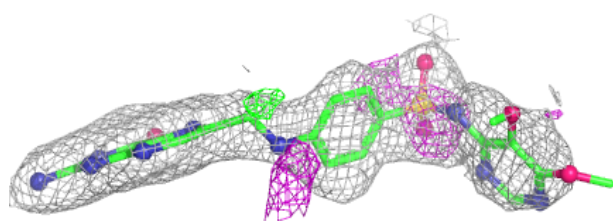
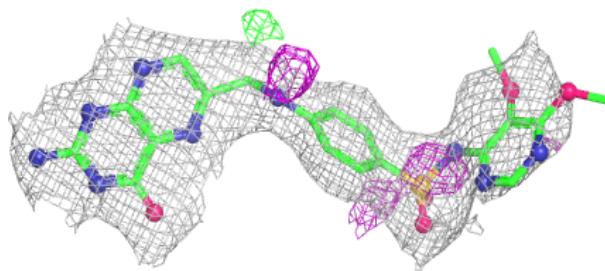
Electron density around ATP A 803:

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

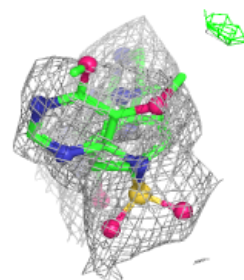
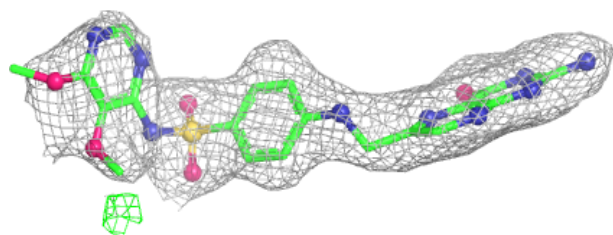
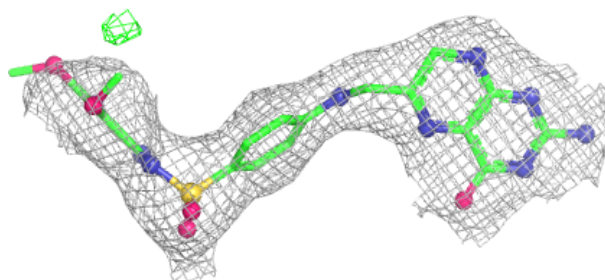


Electron density around CKL A 801:

$2mF_o-DF_c$ (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.