



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:12 AM BST

PDB ID : 6KCL
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS A437G/K540E with pterin and p-hydroxybenzoate
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-06-28
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

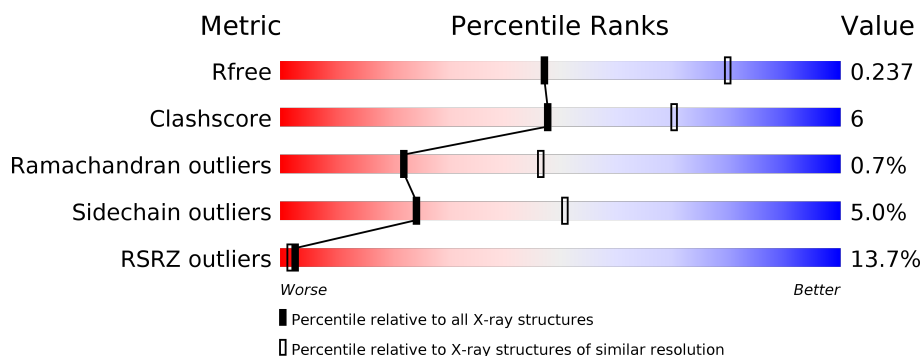
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>6%</div> <div>60% 12% 27%</div> </div>
1	B	728	<div> <div>14%</div> <div>61% 13% 25%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9225 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	533	Total	C	N	O	S	0	0	0
			4408	2839	728	819	22			
1	B	545	Total	C	N	O	S	0	0	0
			4495	2892	741	840	22			

There are 48 discrepancies between the modelled and reference sequences:

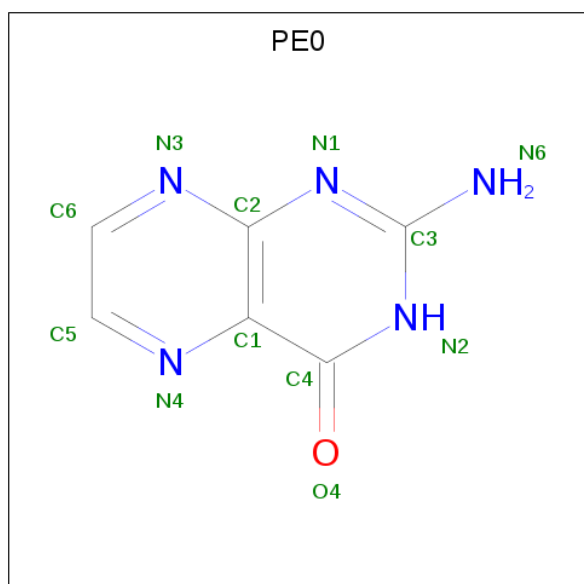
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	540	GLU	LYS	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	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

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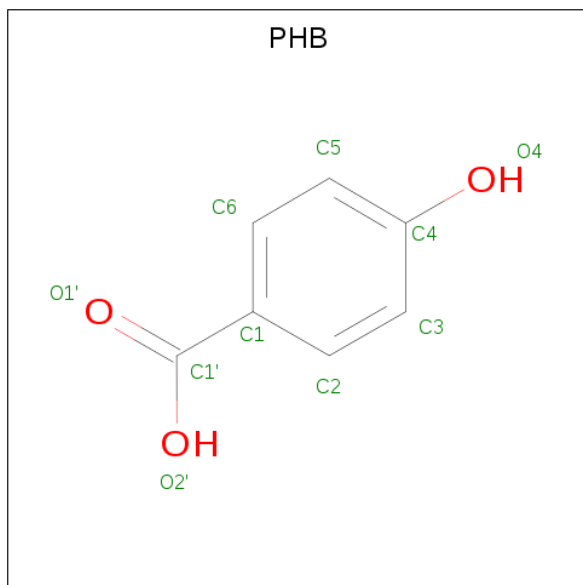
Chain	Residue	Modelled	Actual	Comment	Reference
B	437	GLY	ALA	engineered mutation	UNP Q25704
B	540	GLU	LYS	engineered mutation	UNP Q25704
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	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 PTERINE (three-letter code: PE0) (formula: C₆H₅N₅O) (labeled as "Ligand of Interest" by author).



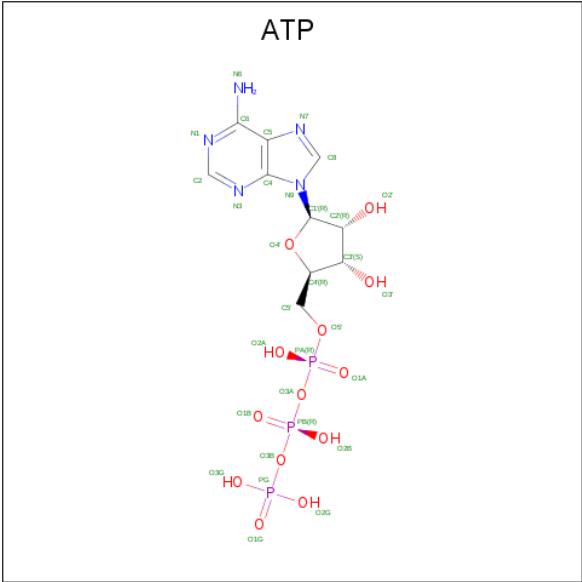
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	5	1		
2	B	1	Total	C	N	O	0	0
			12	6	5	1		

- Molecule 3 is P-HYDROXYBENZOIC ACID (three-letter code: PHB) (formula: $C_7H_6O_3$).



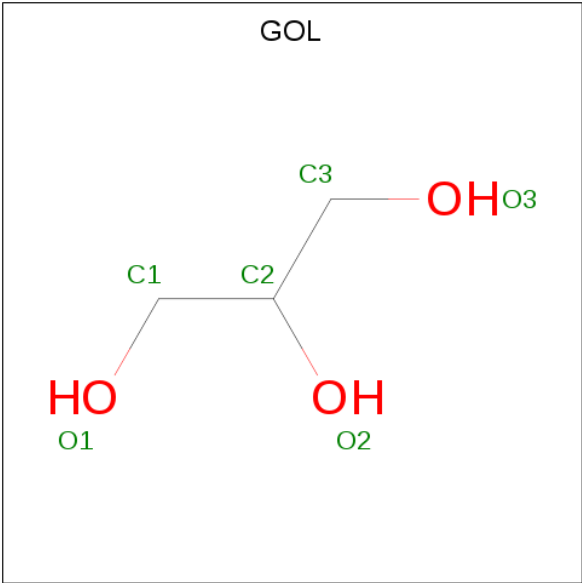
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		
3	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

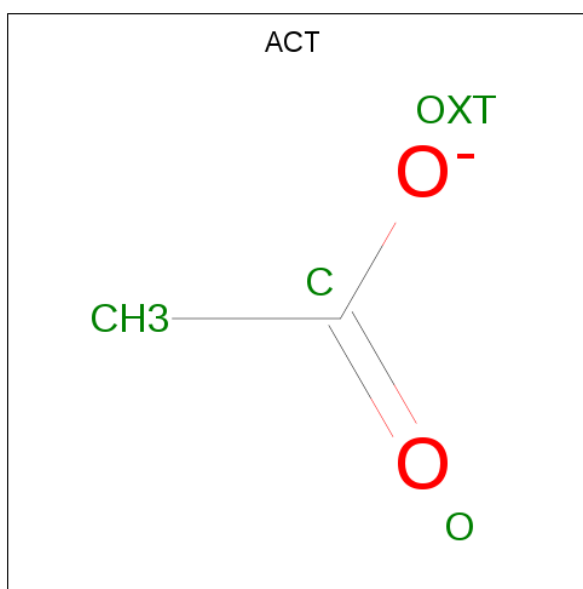
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

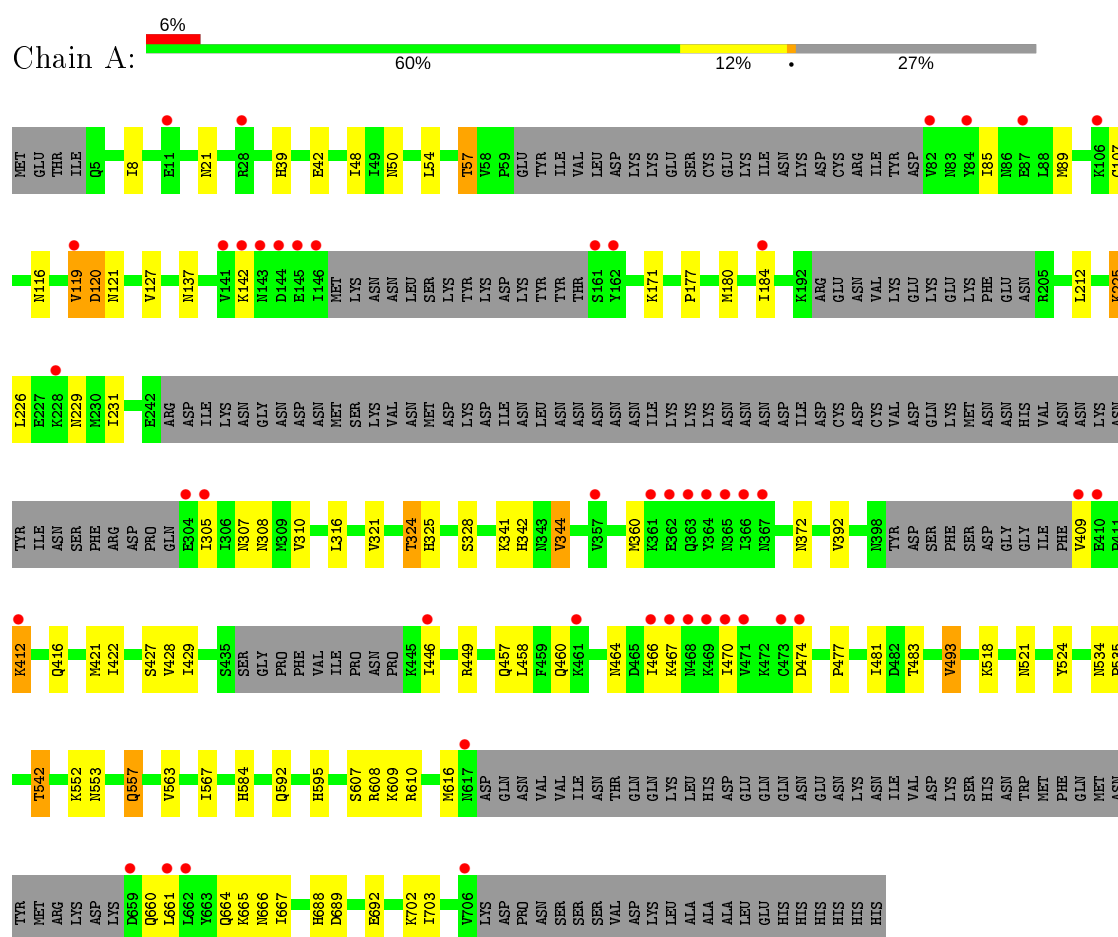
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	114	Total 114	O 114	0	0
9	B	78	Total 78	O 78	0	0

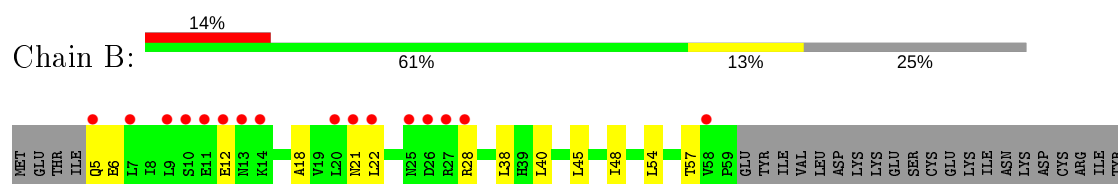
3 Residue-property plots [i](#)

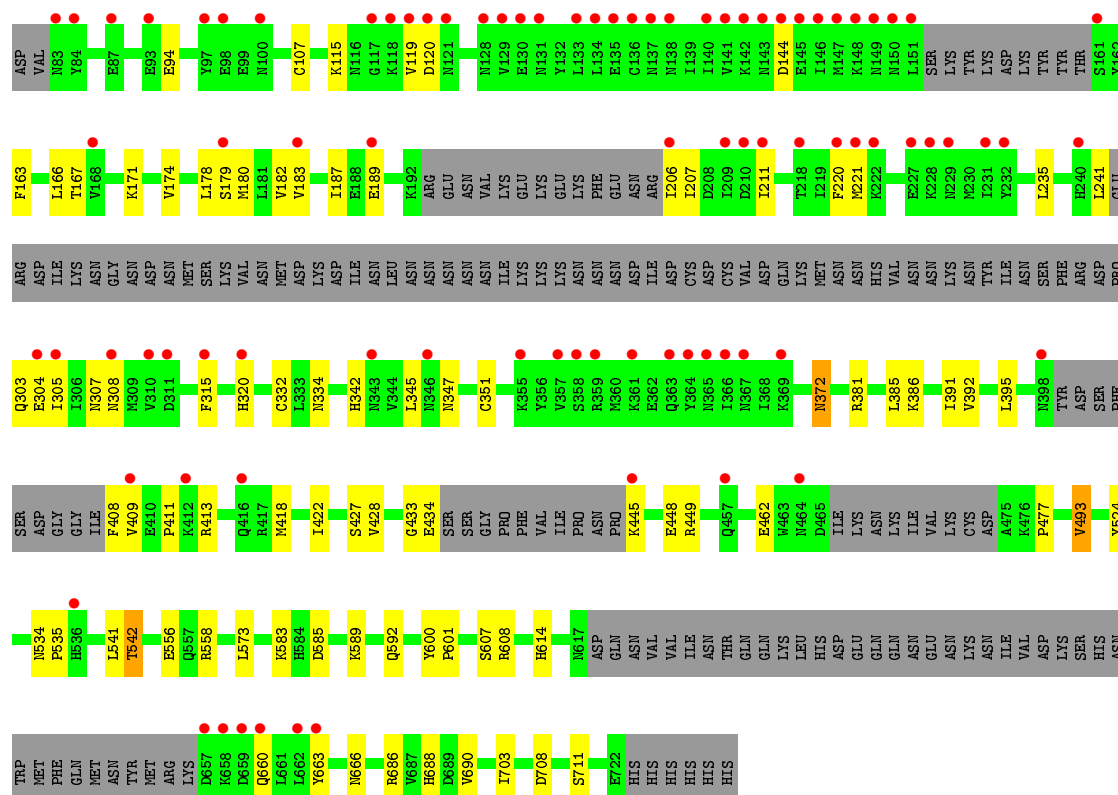
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.32Å 136.44Å 137.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.70) 98.5 (29.21-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.59 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.243 0.197 , 0.237	Depositor DCC
R_{free} test set	5154 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9225	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PHB, CA, PE0, ATP, ACT

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	0.52	0/4474	0.65	1/6033 (0.0%)
1	B	0.47	0/4562	0.62	1/6151 (0.0%)
All	All	0.50	0/9036	0.64	2/12184 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	54	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	54	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	541	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4408	0	4512	56	0
1	B	4495	0	4586	57	0
2	A	12	0	5	1	0
2	B	12	0	5	0	0
3	A	10	0	4	1	0
3	B	10	0	5	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	A	6	0	8	0	0
5	B	6	0	8	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	4	0	3	0	0
8	B	4	0	3	0	0
9	A	114	0	0	6	0
9	B	78	0	0	1	0
All	All	9225	0	9163	111	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 6.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:THR:HG21	1:B:583:LYS:HE2	1.60	0.84
1:B:409:VAL:O	1:B:411:PRO:HD3	1.80	0.81
1:A:57:THR:HG22	1:A:372:ASN:OD1	1.80	0.81
1:B:422:ILE:HD11	1:B:477:PRO:HG3	1.63	0.81
1:A:57:THR:HG21	1:A:328:SER:HB3	1.67	0.75
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.58	0.75
1:A:342:HIS:HD2	1:A:344:VAL:HB	1.52	0.73
1:B:107:CYS:SG	1:B:171:LYS:NZ	2.60	0.73
1:A:595:HIS:HD2	9:A:919:HOH:O	1.72	0.72
1:B:608:ARG:HA	1:B:666:ASN:OD1	1.92	0.69
1:B:434:GLU:C	1:B:448:GLU:HG2	2.13	0.69
1:B:686:ARG:HH12	5:B:804:GOL:HO1	1.38	0.69
1:B:573:LEU:HD23	1:B:601:PRO:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:HG21	1:A:328:SER:CB	2.24	0.67
1:B:493:VAL:HG22	1:B:524:TYR:CZ	2.31	0.66
1:A:342:HIS:CD2	1:A:344:VAL:HB	2.34	0.63
1:B:189:GLU:HB3	1:B:305:ILE:HG23	1.81	0.62
1:B:422:ILE:CD1	1:B:477:PRO:HG3	2.31	0.60
1:B:342:HIS:HB3	1:B:345:LEU:HG	1.84	0.59
1:A:119:VAL:HG21	9:A:1011:HOH:O	2.04	0.58
1:A:616:MET:HE3	1:A:665:LYS:O	2.04	0.57
1:B:178:LEU:O	1:B:182:VAL:HG23	2.04	0.57
1:B:5:GLN:HG3	1:B:6:GLU:N	2.19	0.57
1:B:221:MET:O	1:B:315:PHE:HB2	2.04	0.57
1:A:553:ASN:O	1:A:557:GLN:HG2	2.04	0.57
1:A:422:ILE:HD11	1:A:477:PRO:HG3	1.88	0.56
1:A:324:THR:HG22	1:A:325:HIS:CD2	2.41	0.55
1:B:57:THR:HG22	1:B:372:ASN:OD1	2.06	0.55
1:B:686:ARG:NH1	5:B:804:GOL:O1	2.30	0.54
1:A:595:HIS:CD2	9:A:919:HOH:O	2.52	0.54
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.37	0.54
1:A:493:VAL:HG22	1:A:524:TYR:CZ	2.43	0.54
1:B:308:ASN:HD22	1:B:308:ASN:H	1.56	0.53
1:A:608:ARG:HD2	1:A:688:HIS:CD2	2.44	0.53
1:A:661:LEU:O	1:A:665:LYS:HG3	2.09	0.52
1:A:421:MET:HE3	1:A:429:ILE:HD12	1.89	0.52
1:B:167:THR:OG1	1:B:332:CYS:HB3	2.09	0.52
1:A:39:HIS:CD2	1:A:521:ASN:HA	2.44	0.52
1:A:592:GLN:HG2	1:B:703:ILE:O	2.09	0.52
1:B:206:ILE:HG23	1:B:207:ILE:HG22	1.93	0.51
1:B:45:LEU:HD22	1:B:180:MET:HG3	1.93	0.51
1:B:385:LEU:HG	1:B:386:LYS:HG2	1.93	0.50
1:B:607:SER:OG	1:B:688:HIS:HD2	1.94	0.50
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.94	0.50
1:B:189:GLU:HB3	1:B:305:ILE:CG2	2.42	0.49
1:A:85:ILE:O	1:A:89:MET:HG2	2.13	0.49
1:A:180:MET:HG2	1:A:184:ILE:HD12	1.95	0.48
1:A:422:ILE:CD1	1:A:477:PRO:HG3	2.44	0.48
1:A:703:ILE:O	1:B:592:GLN:HG2	2.13	0.48
1:B:45:LEU:HD23	1:B:174:VAL:HG21	1.95	0.48
1:A:692:GLU:OE1	1:A:692:GLU:N	2.43	0.48
1:A:231:ILE:HD12	1:A:310:VAL:HG22	1.96	0.48
1:B:372:ASN:HD22	1:B:372:ASN:N	2.11	0.48
1:A:107:CYS:SG	1:A:171:LYS:CE	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG22	1:A:428:VAL:HB	1.95	0.47
1:B:433:GLY:O	1:B:434:GLU:HB3	2.13	0.47
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.45	0.47
1:B:40:LEU:HD12	1:B:187:ILE:HG23	1.97	0.47
1:A:542:THR:HG23	1:A:542:THR:O	2.14	0.47
1:B:303:GLN:C	1:B:305:ILE:H	2.17	0.47
1:A:119:VAL:CG2	9:A:1011:HOH:O	2.63	0.47
1:B:107:CYS:SG	1:B:171:LYS:HE3	2.55	0.47
1:B:211:ILE:O	1:B:320:HIS:HB2	2.15	0.46
1:B:107:CYS:SG	1:B:171:LYS:CE	3.03	0.46
1:B:179:SER:O	1:B:183:VAL:HG23	2.15	0.46
1:B:372:ASN:N	1:B:372:ASN:ND2	2.63	0.46
1:B:395:LEU:HD22	1:B:418:MET:CG	2.46	0.46
1:A:21:ASN:HB2	1:A:212:LEU:HD11	1.98	0.46
1:A:119:VAL:HG12	1:A:120:ASP:H	1.81	0.46
1:A:42:GLU:HG2	1:A:48:ILE:HD12	1.98	0.46
1:A:116:ASN:ND2	1:A:341:LYS:O	2.49	0.45
1:B:5:GLN:CG	1:B:6:GLU:N	2.79	0.45
1:A:470:ILE:O	1:A:470:ILE:HG22	2.17	0.45
1:B:556:GLU:OE2	1:B:600:TYR:OH	2.16	0.45
1:A:667:ILE:HG12	1:A:689:ASP:OD2	2.16	0.45
1:A:610:ARG:HE	3:A:802:PHB:C1'	2.30	0.44
1:B:573:LEU:HD23	1:B:601:PRO:CB	2.46	0.44
1:B:391:ILE:HG21	1:B:690:VAL:HG13	1.99	0.44
1:A:225:LYS:HD3	1:A:225:LYS:HA	1.76	0.44
1:B:182:VAL:HG12	1:B:235:LEU:CD1	2.47	0.44
1:B:334:ASN:HB3	9:B:955:HOH:O	2.18	0.44
1:B:708:ASP:HB3	1:B:711:SER:HB3	1.98	0.44
1:B:45:LEU:CD2	1:B:180:MET:HG3	2.48	0.44
1:A:557:GLN:HG2	1:A:557:GLN:H	1.67	0.43
1:B:392:VAL:HG22	1:B:428:VAL:HB	2.00	0.43
1:A:342:HIS:HD2	1:A:344:VAL:H	1.66	0.43
1:A:50:ASN:HA	1:A:563:VAL:CG1	2.49	0.43
1:B:385:LEU:HD11	1:B:601:PRO:HA	1.99	0.43
1:A:460:GLN:O	1:A:464:ASN:ND2	2.51	0.43
1:A:607:SER:OG	1:A:688:HIS:HD2	2.02	0.43
1:B:558:ARG:HD2	1:B:558:ARG:HA	1.66	0.43
1:B:119:VAL:HG22	1:B:120:ASP:H	1.83	0.43
1:A:481:ILE:HG12	1:A:483:THR:HG22	2.01	0.43
1:B:607:SER:OG	1:B:688:HIS:CD2	2.72	0.42
1:B:18:ALA:HB1	1:B:180:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ALA:HB1	1:B:180:MET:CE	2.49	0.42
1:A:321:VAL:HG23	9:A:999:HOH:O	2.19	0.42
1:B:307:ASN:OD1	1:B:307:ASN:N	2.52	0.42
1:A:584:HIS:HD2	9:A:945:HOH:O	2.02	0.42
1:A:518:LYS:HD2	1:A:567:ILE:HD13	2.01	0.42
1:B:38:LEU:HD22	1:B:48:ILE:HD13	2.02	0.42
1:A:342:HIS:CD2	1:A:344:VAL:H	2.38	0.41
1:A:609:LYS:NZ	2:A:801:PEO:O4	2.52	0.41
1:A:137:ASN:HD22	1:A:137:ASN:N	2.17	0.41
1:A:542:THR:O	1:A:542:THR:CG2	2.68	0.41
1:B:585:ASP:OD1	1:B:614:HIS:HE1	2.03	0.41
1:B:235:LEU:HB3	1:B:241:LEU:HD11	2.03	0.41
1:A:226:LEU:O	1:A:310:VAL:HG13	2.21	0.41
1:A:702:LYS:HA	1:A:702:LYS:HD3	1.94	0.40
1:A:89:MET:HE2	1:A:521:ASN:HB2	2.02	0.40
1:A:412:LYS:HG2	1:A:458:LEU:HD21	2.04	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	517/728 (71%)	494 (96%)	19 (4%)	4 (1%)	19	43
1	B	527/728 (72%)	493 (94%)	31 (6%)	3 (1%)	25	50
All	All	1044/1456 (72%)	987 (94%)	50 (5%)	7 (1%)	22	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	LEU
1	A	446	ILE

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Mol	Chain	Res	Type
1	A	119	VAL
1	B	12	GLU
1	A	142	LYS
1	B	304	GLU
1	A	466	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/696 (73%)	480 (94%)	28 (6%)	21	46
1	B	517/696 (74%)	494 (96%)	23 (4%)	28	56
All	All	1025/1392 (74%)	974 (95%)	51 (5%)	24	51

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	57	THR
1	A	120	ASP
1	A	121	ASN
1	A	127	VAL
1	A	225	LYS
1	A	229	ASN
1	A	305	ILE
1	A	307	ASN
1	A	308	ASN
1	A	324	THR
1	A	344	VAL
1	A	360	MET
1	A	409	VAL
1	A	412	LYS
1	A	416	GLN
1	A	427	SER
1	A	449	ARG

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Mol	Chain	Res	Type
1	A	457	GLN
1	A	467	LYS
1	A	474	ASP
1	A	493	VAL
1	A	542	THR
1	A	552	LYS
1	A	557	GLN
1	A	660	GLN
1	A	664	GLN
1	A	666	ASN
1	B	21	ASN
1	B	22	LEU
1	B	28	ARG
1	B	94	GLU
1	B	115	LYS
1	B	144	ASP
1	B	163	PHE
1	B	220	PHE
1	B	347	ASN
1	B	351	CYS
1	B	372	ASN
1	B	381	ARG
1	B	408	PHE
1	B	413	ARG
1	B	427	SER
1	B	445	LYS
1	B	449	ARG
1	B	462	GLU
1	B	493	VAL
1	B	542	THR
1	B	589	LYS
1	B	660	GLN
1	B	663	TYR

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

Mol	Chain	Res	Type
1	A	116	ASN
1	A	137	ASN
1	A	308	ASN
1	A	325	HIS
1	A	342	HIS

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Mol	Chain	Res	Type
1	A	390	ASN
1	A	396	ASN
1	A	584	HIS
1	A	593	ASN
1	A	595	HIS
1	A	664	GLN
1	A	688	HIS
1	B	86	ASN
1	B	150	ASN
1	B	175	ASN
1	B	308	ASN
1	B	398	ASN
1	B	614	HIS
1	B	660	GLN
1	B	688	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	A	803	6	26,33,33	0.97	1 (3%)	31,52,52	1.50	5 (16%)
4	ATP	B	803	6	26,33,33	1.03	3 (11%)	31,52,52	1.43	5 (16%)
2	PE0	A	801	-	13,13,13	1.90	3 (23%)	15,18,18	3.12	9 (60%)
3	PHB	A	802	-	8,10,10	0.61	0	10,13,13	1.27	1 (10%)
8	ACT	A	807	-	1,3,3	0.80	0	0,3,3	0.00	-
2	PE0	B	801	-	13,13,13	1.67	2 (15%)	15,18,18	3.18	9 (60%)
5	GOL	A	804	-	5,5,5	0.33	0	5,5,5	0.51	0
5	GOL	B	804	-	5,5,5	0.33	0	5,5,5	0.68	0
8	ACT	B	807	-	1,3,3	1.30	0	0,3,3	0.00	-
3	PHB	B	802	-	8,10,10	1.10	1 (12%)	10,13,13	0.93	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	A	803	6	-	5/18/38/38	0/3/3/3
4	ATP	B	803	6	-	5/18/38/38	0/3/3/3
3	PHB	A	802	-	-	0/0/4/4	0/1/1/1
2	PE0	B	801	-	-	-	0/2/2/2
5	GOL	A	804	-	-	2/4/4/4	-
5	GOL	B	804	-	-	1/4/4/4	-
2	PE0	A	801	-	-	-	0/2/2/2
3	PHB	B	802	-	-	0/0/4/4	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PE0	C4-C1	4.31	1.48	1.41
2	A	801	PE0	C1-C2	4.29	1.48	1.40
2	B	801	PE0	C4-C1	3.65	1.47	1.41
2	B	801	PE0	C1-C2	3.30	1.47	1.40
4	B	803	ATP	C5-C4	2.83	1.48	1.40
4	A	803	ATP	C5-C4	2.42	1.47	1.40
2	A	801	PE0	C1-N4	2.15	1.36	1.33
3	B	802	PHB	C1-C1'	2.10	1.49	1.47
4	B	803	ATP	O4'-C1'	2.02	1.43	1.41
4	B	803	ATP	C2-N3	2.01	1.35	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	PE0	N3-C2-N1	6.19	122.88	115.82
2	B	801	PE0	N3-C2-N1	6.06	122.74	115.82
2	B	801	PE0	C3-N1-C2	4.93	120.98	115.36
2	A	801	PE0	C3-N1-C2	4.33	120.30	115.36
2	A	801	PE0	C4-C1-C2	-4.20	117.17	119.95
2	B	801	PE0	C4-C1-C2	-4.19	117.17	119.95
2	A	801	PE0	C4-N2-C3	4.09	122.43	115.93
2	A	801	PE0	C1-C4-N2	-4.03	117.92	123.43
4	A	803	ATP	N3-C2-N1	-3.92	122.56	128.68
2	B	801	PE0	C4-C1-N4	3.77	122.93	118.24
2	A	801	PE0	C4-C1-N4	3.75	122.91	118.24
2	B	801	PE0	N1-C3-N2	-3.45	122.62	127.22
2	B	801	PE0	C1-C4-N2	-3.44	118.73	123.43
2	B	801	PE0	C4-N2-C3	3.32	121.20	115.93
4	B	803	ATP	N3-C2-N1	-3.29	123.54	128.68
2	B	801	PE0	C6-N3-C2	3.12	120.45	116.60
4	A	803	ATP	C4-C5-N7	-3.12	106.15	109.40
4	B	803	ATP	C3'-C2'-C1'	3.10	105.64	100.98
4	A	803	ATP	PB-O3B-PG	-3.04	122.40	132.83
2	A	801	PE0	N1-C3-N2	-2.87	123.40	127.22
4	A	803	ATP	PA-O3A-PB	-2.84	123.09	132.83
4	B	803	ATP	PB-O3B-PG	-2.59	123.92	132.83
4	B	803	ATP	PA-O3A-PB	-2.53	124.14	132.83
4	B	803	ATP	C4-C5-N7	-2.26	107.04	109.40
4	A	803	ATP	C2-N1-C6	2.24	122.58	118.75
2	A	801	PE0	C6-N3-C2	2.15	119.25	116.60
3	A	802	PHB	C6-C1-C2	2.11	121.79	117.59
2	B	801	PE0	C2-C1-N4	-2.10	119.89	122.32
2	A	801	PE0	C2-C1-N4	-2.07	119.92	122.32

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	ATP	C5'-O5'-PA-O1A
4	A	803	ATP	C5'-O5'-PA-O2A
4	A	803	ATP	C3'-C4'-C5'-O5'
4	B	803	ATP	C5'-O5'-PA-O1A
4	B	803	ATP	C5'-O5'-PA-O2A
4	B	803	ATP	C3'-C4'-C5'-O5'
4	A	803	ATP	O4'-C4'-C5'-O5'

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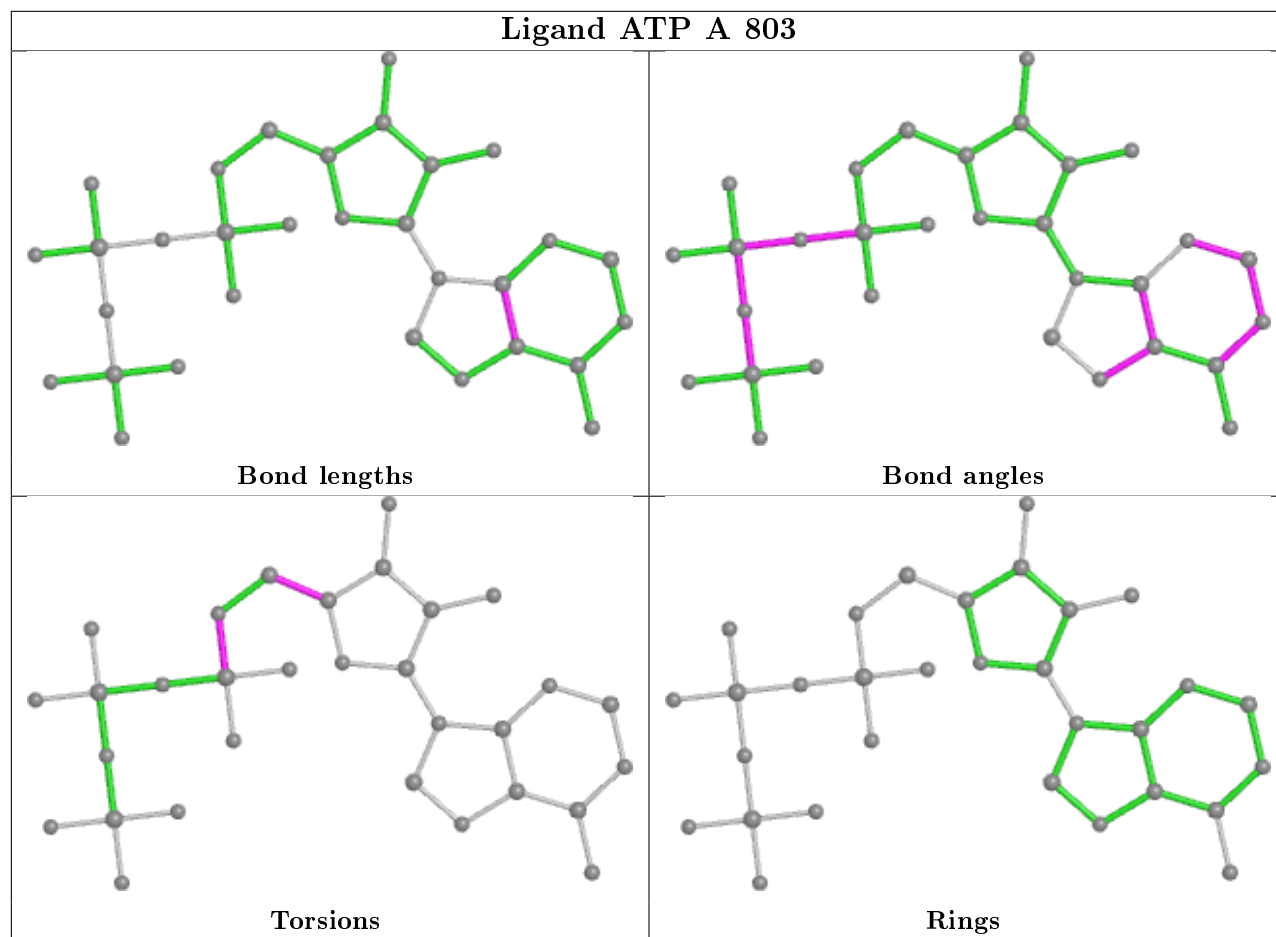
Mol	Chain	Res	Type	Atoms
4	B	803	ATP	O4'-C4'-C5'-O5'
5	A	804	GOL	O2-C2-C3-O3
4	B	803	ATP	C5'-O5'-PA-O3A
5	B	804	GOL	O1-C1-C2-O2
4	A	803	ATP	C5'-O5'-PA-O3A
5	A	804	GOL	C1-C2-C3-O3

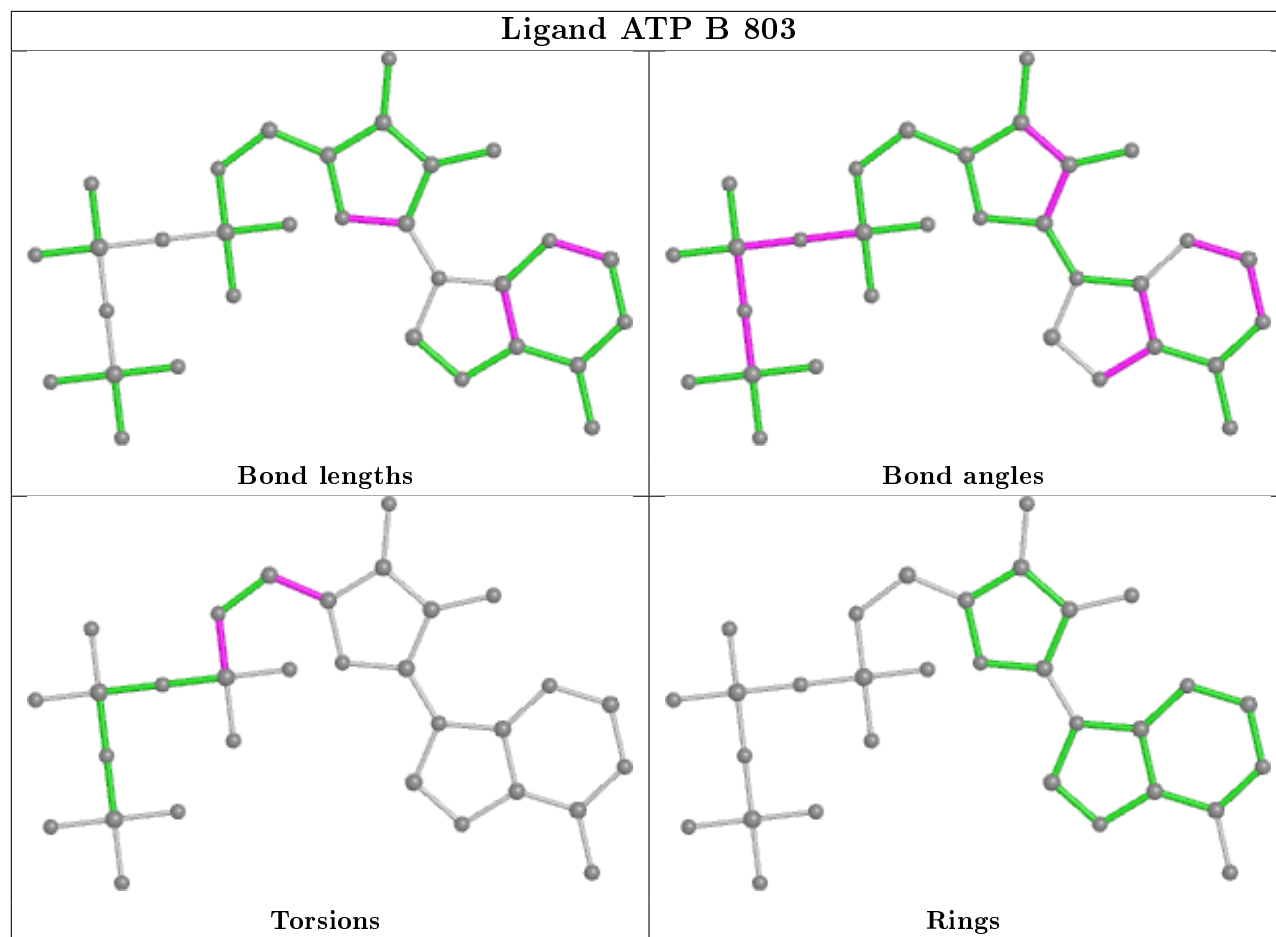
There are no ring outliers.

3 monomers are involved in 4 short contacts:

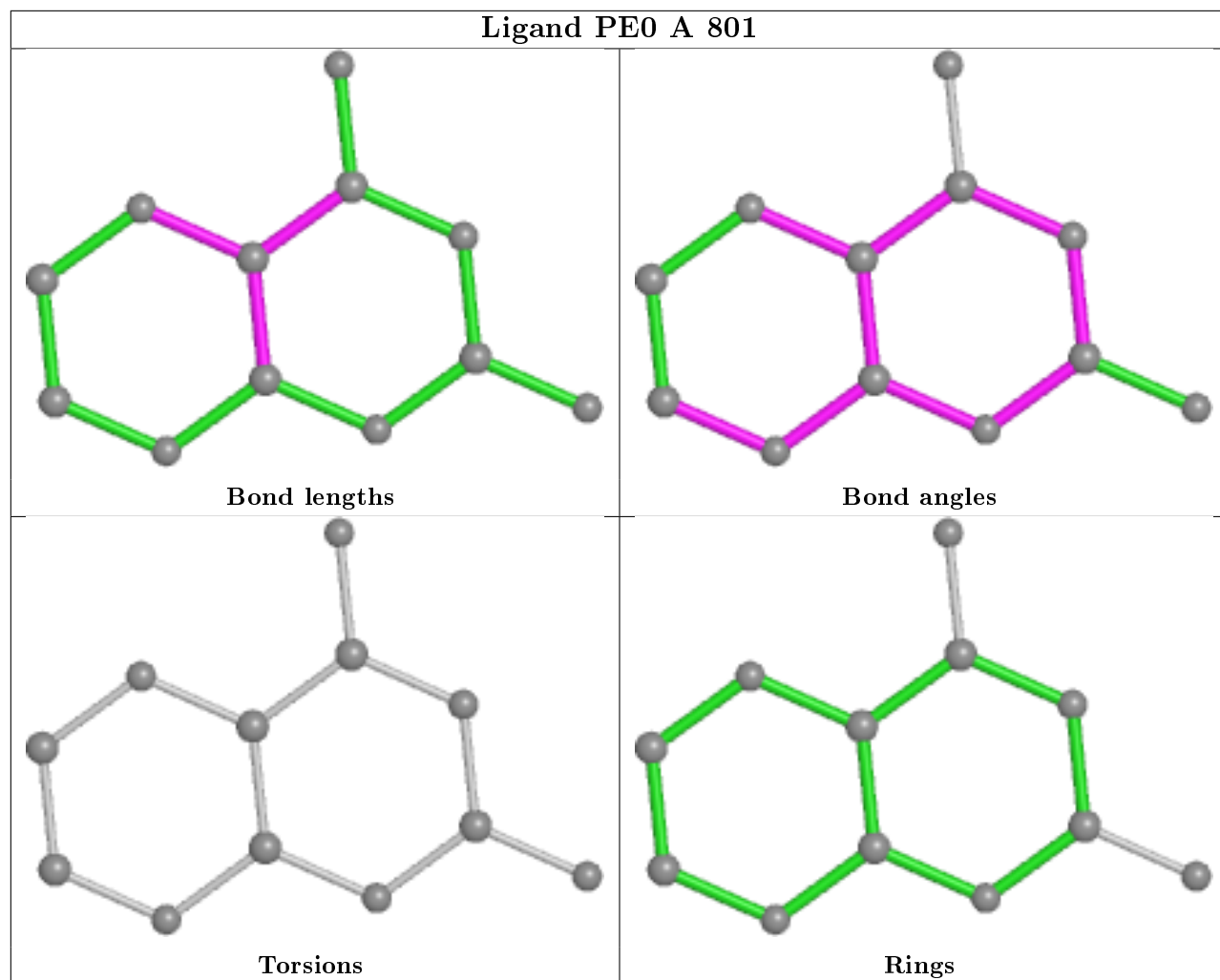
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PE0	1	0
3	A	802	PHB	1	0
5	B	804	GOL	2	0

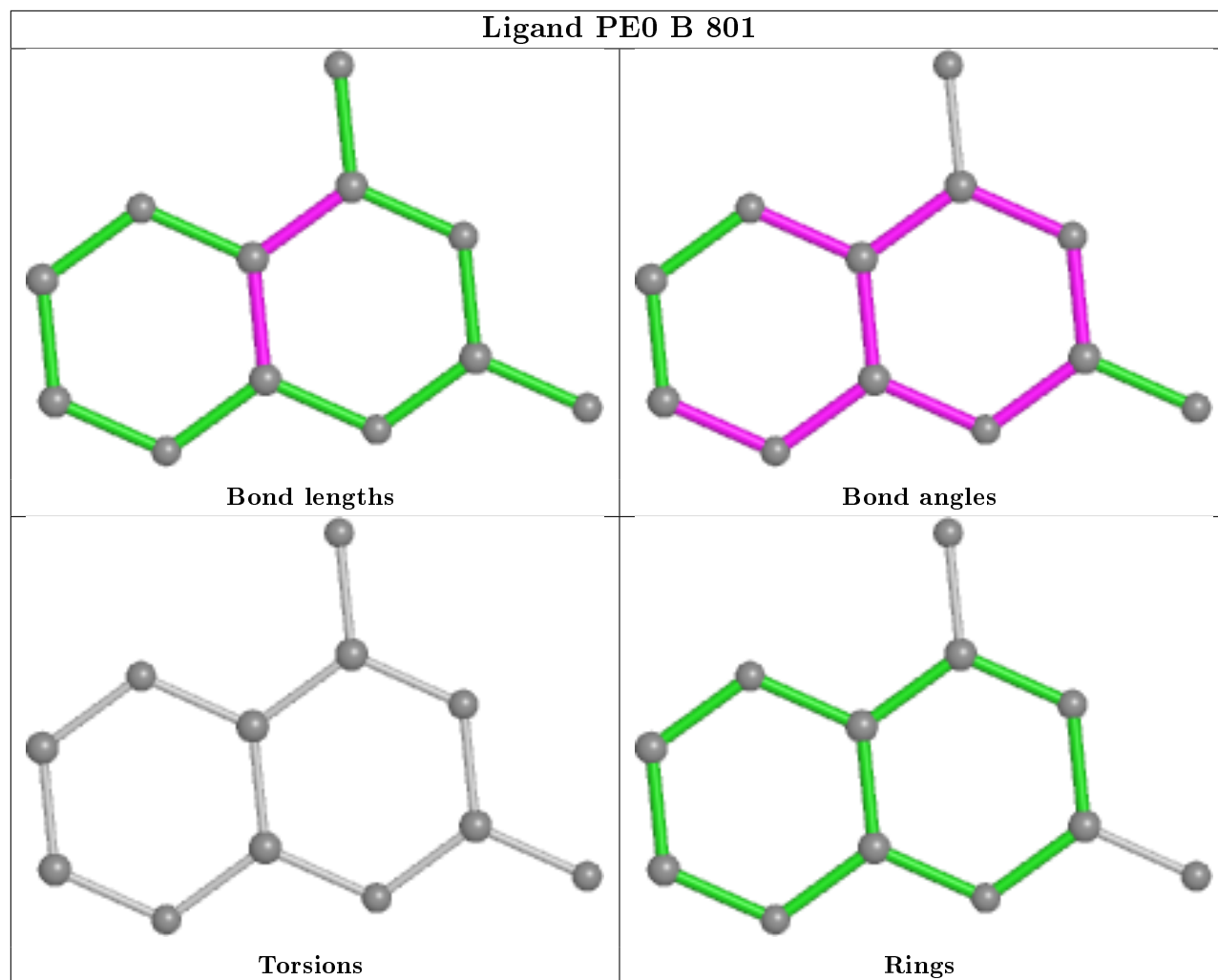
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 PE0 A 801





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	533/728 (73%)	0.12	45 (8%) 11 9	11, 30, 91, 120	0
1	B	545/728 (74%)	0.71	103 (18%) 1 0	12, 57, 119, 120	0
All	All	1078/1456 (74%)	0.42	148 (13%) 3 2	11, 40, 116, 120	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	MET	7.4
1	A	471	VAL	6.7
1	B	151	LEU	6.6
1	B	145	GLU	6.4
1	B	305	ILE	5.9
1	B	367	ASN	5.3
1	B	364	TYR	5.3
1	B	13	ASN	5.2
1	B	138	ASN	5.1
1	B	229	ASN	4.9
1	B	148	LYS	4.9
1	B	366	ILE	4.8
1	B	150	ASN	4.7
1	A	468	ASN	4.7
1	B	134	LEU	4.7
1	A	361	LYS	4.6
1	A	146	ILE	4.6
1	B	11	GLU	4.5
1	B	149	ASN	4.4
1	B	129	VAL	4.4
1	B	137	ASN	4.4
1	B	135	GLU	4.4
1	B	130	GLU	4.4
1	B	228	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	660	GLN	4.3
1	B	222	LYS	4.3
1	B	118	LYS	4.3
1	B	365	ASN	4.3
1	A	470	ILE	4.2
1	B	304	GLU	4.1
1	B	358	SER	4.0
1	B	22	LEU	3.8
1	B	409	VAL	3.8
1	B	27	ARG	3.8
1	B	28	ARG	3.8
1	A	466	ILE	3.8
1	B	161	SER	3.7
1	A	142	LYS	3.7
1	B	220	PHE	3.6
1	B	657	ASP	3.5
1	B	146	ILE	3.5
1	B	7	LEU	3.5
1	B	12	GLU	3.4
1	B	131	ASN	3.4
1	B	58	VAL	3.4
1	A	162	TYR	3.3
1	B	659	ASP	3.3
1	A	659	ASP	3.3
1	B	361	LYS	3.3
1	B	9	LEU	3.2
1	B	97	TYR	3.2
1	B	98	GLU	3.1
1	A	706	VAL	3.1
1	A	473	CYS	3.1
1	B	231	ILE	3.1
1	B	141	VAL	3.1
1	B	20	LEU	3.1
1	A	363	GLN	3.1
1	B	120	ASP	3.0
1	A	161	SER	3.0
1	B	142	LYS	3.0
1	B	144	ASP	3.0
1	A	143	ASN	3.0
1	B	359	ARG	2.9
1	B	315	PHE	2.9
1	B	206	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	227	GLU	2.9
1	A	474	ASP	2.9
1	A	365	ASN	2.9
1	B	119	VAL	2.8
1	A	84	TYR	2.8
1	A	145	GLU	2.8
1	B	84	TYR	2.8
1	A	28	ARG	2.8
1	A	367	ASN	2.8
1	B	14	LYS	2.7
1	A	305	ILE	2.7
1	A	661	LEU	2.7
1	A	410	GLU	2.7
1	B	140	ILE	2.7
1	B	100	ASN	2.7
1	B	464	ASN	2.7
1	B	369	LYS	2.7
1	A	446	ILE	2.7
1	A	362	GLU	2.6
1	B	87	GLU	2.6
1	B	211	ILE	2.6
1	B	346	ASN	2.6
1	B	363	GLN	2.6
1	B	209	ILE	2.6
1	B	121	ASN	2.6
1	A	87	GLU	2.6
1	A	304	GLU	2.6
1	A	366	ILE	2.6
1	B	218	THR	2.6
1	B	398	ASN	2.6
1	A	82	VAL	2.6
1	B	83	ASN	2.6
1	A	144	ASP	2.6
1	A	106	LYS	2.5
1	A	364	TYR	2.5
1	B	133	LEU	2.5
1	B	25	ASN	2.5
1	B	10	SER	2.5
1	A	141	VAL	2.5
1	B	662	LEU	2.5
1	A	617	ASN	2.4
1	B	232	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	536	HIS	2.4
1	B	457	GLN	2.4
1	B	5	GLN	2.3
1	B	357	VAL	2.3
1	B	355	LYS	2.3
1	B	128	ASN	2.3
1	B	189	GLU	2.3
1	B	136	CYS	2.3
1	A	184	ILE	2.3
1	B	21	ASN	2.2
1	B	343	ASN	2.2
1	A	461	LYS	2.2
1	B	221	MET	2.2
1	B	320	HIS	2.2
1	A	412	LYS	2.2
1	A	119	VAL	2.2
1	A	357	VAL	2.2
1	B	310	VAL	2.2
1	B	240	HIS	2.2
1	B	168	VAL	2.2
1	B	26	ASP	2.2
1	B	179	SER	2.1
1	B	93	GLU	2.1
1	B	311	ASP	2.1
1	A	409	VAL	2.1
1	B	210	ASP	2.1
1	B	183	VAL	2.1
1	B	143	ASN	2.1
1	B	117	GLY	2.1
1	A	11	GLU	2.1
1	B	416	GLN	2.1
1	A	467	LYS	2.1
1	A	228	LYS	2.1
1	B	412	LYS	2.1
1	B	658	LYS	2.0
1	B	663	TYR	2.0
1	A	469	LYS	2.0
1	B	308	ASN	2.0
1	A	662	LEU	2.0
1	B	445	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](#)

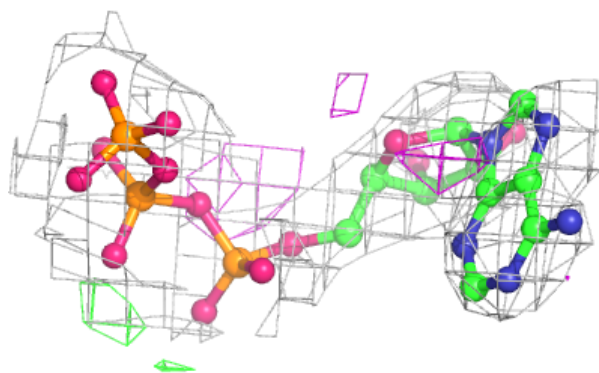
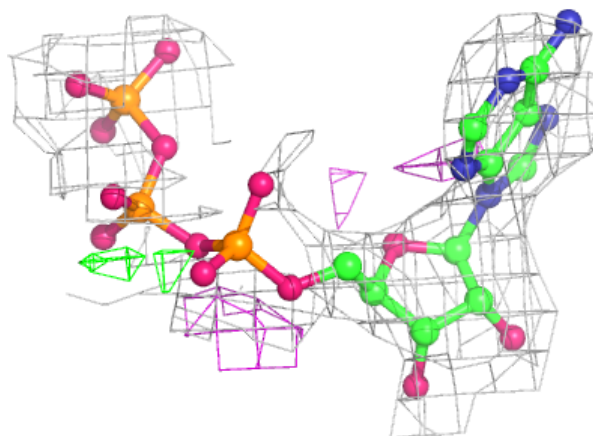
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ATP	B	803	31/31	0.83	0.18	93,97,112,114	0
6	MG	B	805	1/1	0.85	0.16	52,52,52,52	0
6	MG	A	805	1/1	0.91	0.10	24,24,24,24	0
4	ATP	A	803	31/31	0.92	0.13	38,49,92,96	0
7	CA	B	806	1/1	0.93	0.05	63,63,63,63	0
5	GOL	B	804	6/6	0.94	0.16	30,35,37,37	0
3	PHB	A	802	10/10	0.96	0.16	24,26,27,30	0
5	GOL	A	804	6/6	0.97	0.13	29,31,34,36	0
3	PHB	B	802	10/10	0.97	0.15	23,24,26,28	0
8	ACT	A	807	4/4	0.98	0.15	22,22,23,25	0
2	PE0	B	801	12/12	0.98	0.18	19,19,21,21	0
2	PE0	A	801	12/12	0.99	0.15	13,13,13,13	0
8	ACT	B	807	4/4	0.99	0.11	18,18,19,20	0
7	CA	A	806	1/1	0.99	0.12	23,23,23,23	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.

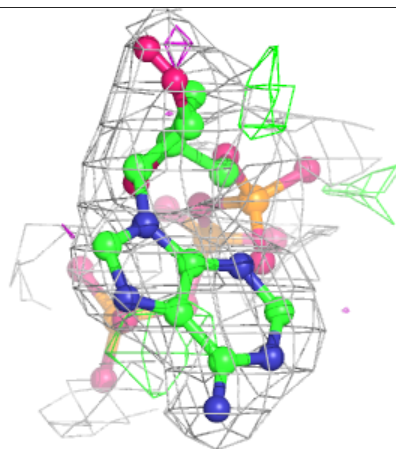
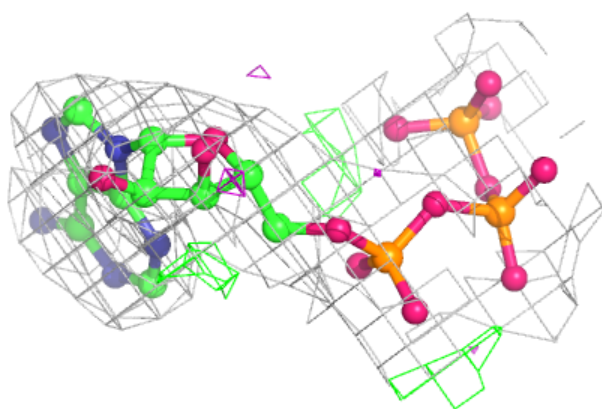
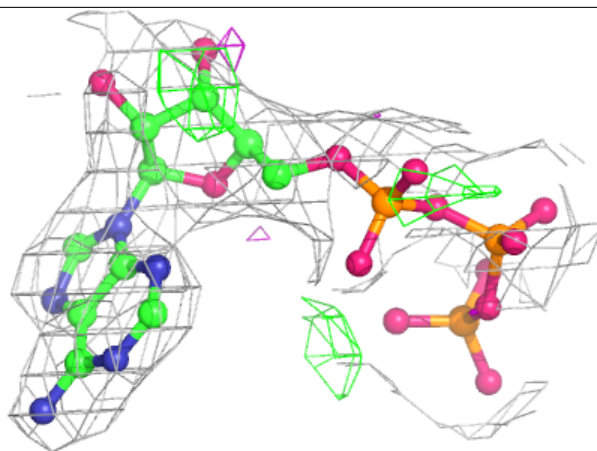
Electron density around ATP B 803:

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



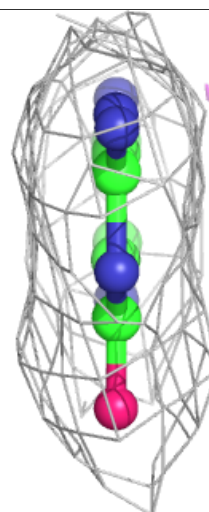
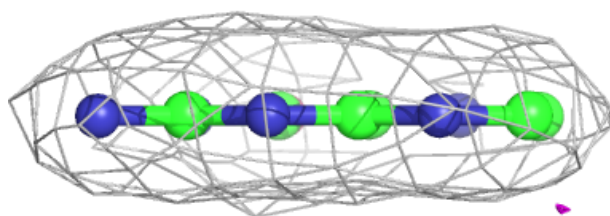
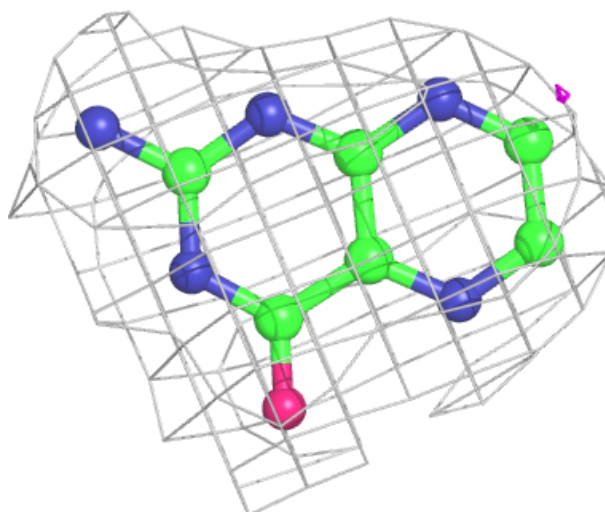
Electron density around ATP A 803:

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



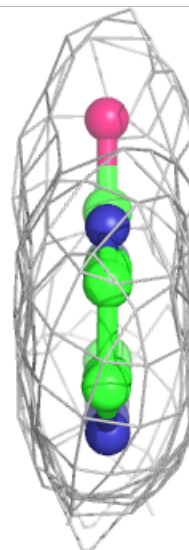
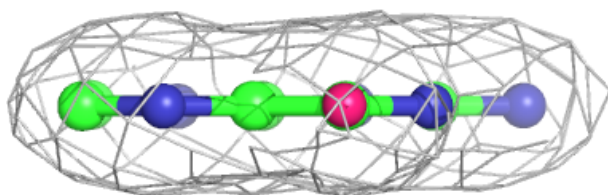
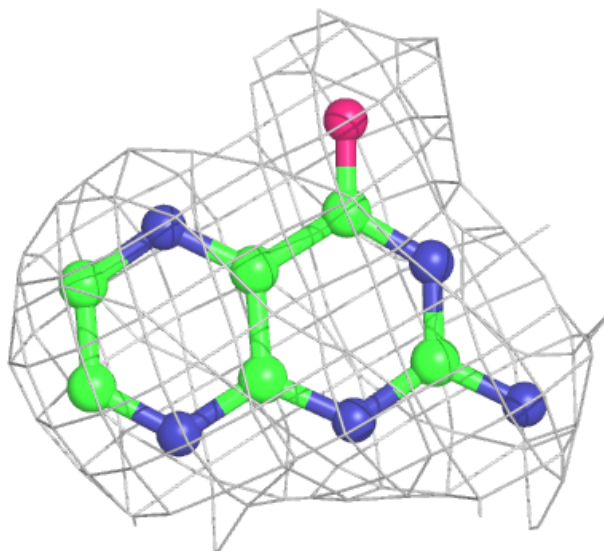
Electron density around PE0 B 801:

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



Electron density around PE0 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.