



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 9BKE / pdb_00009bke
Title : STRUCTURE OF 4 - H Y D R O X Y P H E N Y L A C E T A T E 3-MONOOXYGENASE (HPAB), OXYGENASE COMPONENT FROM ES-CHERICHIA COLI MUTANT XS6 WITH AMP BOUND
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Deposited on : 2024-04-27
Resolution : 1.95 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	:	4-5-2 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

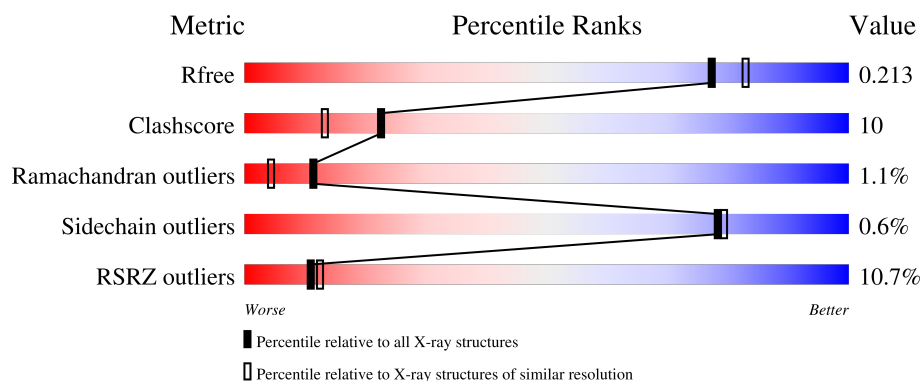
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	527	12% 80% 16% ..
1	B	527	9% 81% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16943 atoms, of which 7930 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 4-hydroxyphenylacetate 3-monooxygenase oxygenase component.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	H	N	O	S	0	0	0
			8054	2584	3963	713	768	26			
1	B	511	Total	C	H	N	O	S	0	0	0
			8015	2572	3943	708	766	26			

There are 30 discrepancies between the modelled and reference sequences:

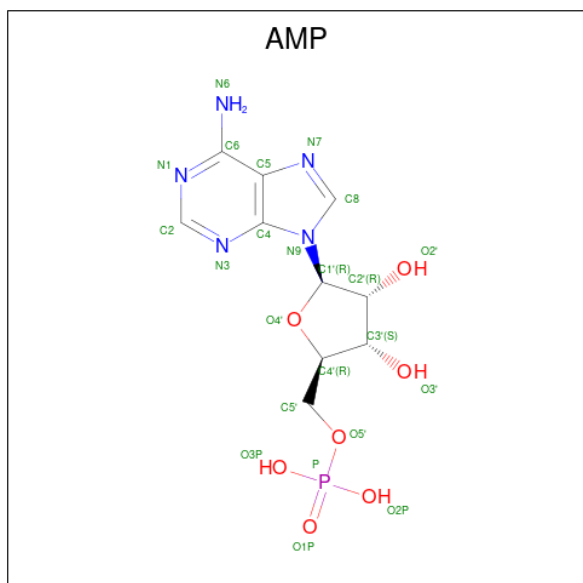
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A2G8ZEZ1
A	2	HIS	-	expression tag	UNP A0A2G8ZEZ1
A	3	HIS	-	expression tag	UNP A0A2G8ZEZ1
A	4	HIS	-	expression tag	UNP A0A2G8ZEZ1
A	5	HIS	-	expression tag	UNP A0A2G8ZEZ1
A	6	HIS	-	expression tag	UNP A0A2G8ZEZ1
A	7	HIS	-	expression tag	UNP A0A2G8ZEZ1
A	8	HIS	-	expression tag	UNP A0A2G8ZEZ1
A	215	SER	PHE	conflict	UNP A0A2G8ZEZ1
A	218	ASP	ALA	conflict	UNP A0A2G8ZEZ1
A	219	LEU	GLN	conflict	UNP A0A2G8ZEZ1
A	220	GLY	VAL	conflict	UNP A0A2G8ZEZ1
A	221	SER	MET	conflict	UNP A0A2G8ZEZ1
A	223	SER	GLU	conflict	UNP A0A2G8ZEZ1
A	224	ASP	ASN	conflict	UNP A0A2G8ZEZ1
B	1	MET	-	initiating methionine	UNP A0A2G8ZEZ1
B	2	HIS	-	expression tag	UNP A0A2G8ZEZ1
B	3	HIS	-	expression tag	UNP A0A2G8ZEZ1
B	4	HIS	-	expression tag	UNP A0A2G8ZEZ1
B	5	HIS	-	expression tag	UNP A0A2G8ZEZ1
B	6	HIS	-	expression tag	UNP A0A2G8ZEZ1
B	7	HIS	-	expression tag	UNP A0A2G8ZEZ1
B	8	HIS	-	expression tag	UNP A0A2G8ZEZ1
B	215	SER	PHE	conflict	UNP A0A2G8ZEZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	218	ASP	ALA	conflict	UNP A0A2G8ZEZ1
B	219	LEU	GLN	conflict	UNP A0A2G8ZEZ1
B	220	GLY	VAL	conflict	UNP A0A2G8ZEZ1
B	221	SER	MET	conflict	UNP A0A2G8ZEZ1
B	223	SER	GLU	conflict	UNP A0A2G8ZEZ1
B	224	ASP	ASN	conflict	UNP A0A2G8ZEZ1

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	389	Total	O	0	0
			389	389		
3	B	415	Total	O	0	0
			415	415		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.23Å 100.23Å 336.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 1.95 39.74 – 1.95	Depositor EDS
% Data completeness (in resolution range)	76.0 (39.74-1.95) 88.4 (39.74-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.183 , 0.213 0.184 , 0.213	Depositor DCC
R_{free} test set	2000 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16943	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: AMP

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	0.56	4/4188 (0.1%)	0.76	6/5675 (0.1%)
1	B	0.57	2/4168 (0.0%)	0.74	3/5649 (0.1%)
All	All	0.57	6/8356 (0.1%)	0.75	9/11324 (0.1%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	492	MET	SD-CE	-6.18	1.64	1.79
1	A	449	MET	SD-CE	-5.82	1.65	1.79
1	A	468	TYR	CA-C	-5.55	1.45	1.52
1	B	143	GLU	CB-CG	-5.20	1.36	1.52
1	A	467	ASN	CA-C	-5.16	1.46	1.52
1	A	467	ASN	CB-CG	-5.00	1.39	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	TYR	CA-CB-CG	6.83	126.19	113.90
1	B	173	LEU	CB-CG-CD2	6.30	129.61	110.70
1	A	467	ASN	CA-C-O	-6.17	114.04	120.70
1	A	468	TYR	CA-C-N	-5.83	110.41	121.54
1	A	468	TYR	C-N-CA	-5.83	110.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	LEU	CA-CB-CG	5.66	136.10	116.30
1	A	468	TYR	N-CA-C	-5.30	99.52	110.80
1	B	278	ASN	N-CA-CB	-5.24	104.24	112.46
1	A	467	ASN	CB-CA-C	-5.04	99.75	109.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	VAL	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4091	3963	3962	88	2
1	B	4072	3943	3942	82	2
2	A	46	24	24	0	0
3	A	389	0	0	32	2
3	B	415	0	0	36	2
All	All	9013	7930	7928	169	5

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 10.

All (169) 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:411:LEU:N	3:B:603:HOH:O	1.79	1.12
1:A:411:LEU:N	3:A:701:HOH:O	1.82	1.09
1:B:505:GLN:OE1	3:B:601:HOH:O	1.70	1.09
1:B:109:GLU:OE2	3:B:602:HOH:O	1.75	1.02
1:A:467:ASN:O	1:A:468:TYR:HB2	1.61	1.01
1:A:409:ILE:HA	3:A:712:HOH:O	1.61	0.98
1:A:401:GLU:O	1:A:405:THR:HG22	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:OE2	3:A:703:HOH:O	1.88	0.91
1:A:43:VAL:O	3:A:702:HOH:O	1.86	0.91
1:B:147:ARG:NH1	3:B:605:HOH:O	2.01	0.91
1:A:468:TYR:O	1:A:470:GLY:N	2.06	0.88
1:A:200:VAL:O	3:A:704:HOH:O	1.96	0.83
1:A:386:ARG:NH2	1:A:478:GLN:OE1	2.10	0.82
1:A:343:GLN:OE1	3:A:706:HOH:O	1.97	0.81
1:A:180:ASP:O	3:A:705:HOH:O	1.96	0.81
1:A:8:HIS:O	3:A:707:HOH:O	2.01	0.79
1:A:439:HIS:ND1	3:A:713:HOH:O	2.15	0.79
1:A:164:ILE:HG12	3:A:739:HOH:O	1.84	0.77
1:A:411:LEU:CA	3:A:701:HOH:O	2.26	0.76
1:B:335:GLY:O	3:B:607:HOH:O	2.03	0.76
1:B:9:LYS:N	3:B:618:HOH:O	2.18	0.74
1:B:411:LEU:CA	3:B:603:HOH:O	2.29	0.73
1:B:224:ASP:N	3:B:604:HOH:O	1.97	0.73
1:B:504:ASP:OD2	3:B:608:HOH:O	2.05	0.73
1:A:468:TYR:C	1:A:470:GLY:H	1.97	0.72
1:B:468:TYR:O	1:B:469:SER:HB3	1.87	0.72
1:A:188:GLU:OE2	3:A:708:HOH:O	2.07	0.72
1:A:468:TYR:OH	3:A:709:HOH:O	2.08	0.71
1:B:215:SER:OG	3:B:610:HOH:O	2.09	0.70
1:A:165:VAL:N	3:A:704:HOH:O	2.03	0.70
1:A:215:SER:OG	3:A:710:HOH:O	2.10	0.69
1:B:410:TYR:CD1	3:B:603:HOH:O	2.45	0.69
1:A:409:ILE:O	3:A:712:HOH:O	2.12	0.67
1:B:438:ASP:OD1	3:B:611:HOH:O	2.11	0.66
1:A:411:LEU:HA	3:A:701:HOH:O	1.89	0.66
1:B:215:SER:N	3:B:610:HOH:O	2.28	0.65
1:B:401:GLU:OE2	3:B:612:HOH:O	2.14	0.65
1:B:278:ASN:OD1	3:B:613:HOH:O	2.15	0.65
1:A:406:SER:O	1:A:409:ILE:HG22	1.97	0.64
1:B:84:GLY:N	3:B:617:HOH:O	2.17	0.64
1:A:162:HIS:O	1:A:162:HIS:HD2	1.80	0.64
1:A:401:GLU:OE2	3:A:714:HOH:O	2.15	0.64
1:A:468:TYR:O	1:A:469:SER:HB3	1.98	0.63
1:B:223:SER:HB3	3:B:604:HOH:O	1.98	0.63
1:B:183:ILE:HD12	1:B:276:MET:CE	2.29	0.63
1:B:468:TYR:O	1:B:469:SER:CB	2.47	0.63
1:B:411:LEU:HA	3:B:603:HOH:O	1.94	0.63
1:B:184:LYS:HE3	1:B:186:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:O	1:B:181:VAL:HG22	2.00	0.62
1:A:162:HIS:O	1:A:162:HIS:CD2	2.52	0.62
1:B:386:ARG:HD3	1:B:469:SER:OG	1.99	0.61
1:B:277:ASP:OD1	1:B:278:ASN:ND2	2.34	0.60
1:A:164:ILE:HA	3:A:739:HOH:O	2.01	0.60
1:A:468:TYR:O	3:A:715:HOH:O	2.16	0.59
1:A:391:MET:HE3	3:B:1011:HOH:O	2.03	0.58
1:B:162:HIS:ND1	1:B:164:ILE:HD12	2.17	0.58
1:B:215:SER:CA	3:B:610:HOH:O	2.50	0.58
1:B:404:VAL:O	1:B:404:VAL:HG12	2.03	0.58
1:A:215:SER:CA	3:A:710:HOH:O	2.52	0.57
1:A:523:ASP:O	1:A:527:LYS:HG2	2.04	0.57
1:B:214:GLY:O	3:B:615:HOH:O	2.17	0.57
1:B:278:ASN:CB	3:B:613:HOH:O	2.53	0.56
1:B:61:GLN:HG3	3:B:637:HOH:O	2.04	0.56
1:B:194:ILE:HA	1:B:279:VAL:O	2.06	0.55
1:A:391:MET:SD	3:B:1011:HOH:O	2.58	0.55
1:B:164:ILE:HG22	1:B:164:ILE:O	2.05	0.55
1:B:173:LEU:HD22	1:B:177:LYS:HE3	1.89	0.55
1:B:61:GLN:CG	3:B:637:HOH:O	2.55	0.54
1:B:277:ASP:O	1:B:278:ASN:HB2	2.07	0.54
1:B:225:PRO:HD3	3:B:604:HOH:O	2.06	0.54
1:B:176:ASP:O	1:B:177:LYS:CB	2.56	0.54
1:A:164:ILE:HG22	1:A:164:ILE:O	2.08	0.54
1:A:184:LYS:HE2	3:A:705:HOH:O	2.08	0.53
1:B:169:ILE:CD1	1:B:181:VAL:HG21	2.39	0.53
1:A:391:MET:CE	3:B:1011:HOH:O	2.56	0.53
1:A:124:TYR:OH	1:A:162:HIS:HE1	1.92	0.53
1:A:464:TYR:O	1:A:468:TYR:CD2	2.63	0.52
1:A:120:ARG:NH2	1:A:162:HIS:NE2	2.57	0.52
1:A:468:TYR:C	1:A:470:GLY:N	2.56	0.51
1:A:164:ILE:HG23	3:A:739:HOH:O	2.11	0.51
1:A:26:TYR:CZ	1:A:30:LEU:HD11	2.46	0.51
1:A:405:THR:OG1	1:A:406:SER:N	2.44	0.50
1:A:215:SER:N	3:A:710:HOH:O	2.45	0.50
1:B:68:LYS:NZ	3:B:634:HOH:O	2.44	0.50
1:A:183:ILE:HD12	1:A:276:MET:CE	2.42	0.50
1:B:183:ILE:HD12	1:B:276:MET:HE3	1.94	0.50
1:B:410:TYR:O	1:B:411:LEU:C	2.54	0.50
1:A:9:LYS:HE3	1:A:12:ASP:OD2	2.12	0.49
1:B:308:TYR:N	1:B:309:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HD2	1:A:301:GLU:OE2	2.13	0.49
1:A:498:ARG:HD2	3:A:726:HOH:O	2.11	0.49
1:B:187:LYS:HD3	1:B:189:THR:HG22	1.95	0.48
1:B:309:PRO:HB2	1:B:382:LEU:HD22	1.96	0.48
1:A:261:TYR:HB3	1:A:264:SER:HB2	1.96	0.48
1:B:84:GLY:CA	3:B:617:HOH:O	2.61	0.48
1:B:164:ILE:O	1:B:164:ILE:CG2	2.61	0.47
1:A:518:ASP:OD2	3:A:718:HOH:O	2.20	0.47
1:B:278:ASN:HB3	3:B:613:HOH:O	2.13	0.47
1:A:162:HIS:CD2	1:A:162:HIS:C	2.91	0.47
1:A:165:VAL:HB	3:A:704:HOH:O	2.14	0.47
1:B:43:VAL:HG13	1:B:49:HIS:CD2	2.50	0.47
1:B:518:ASP:OD2	3:B:620:HOH:O	2.21	0.47
1:B:278:ASN:CG	3:B:613:HOH:O	2.57	0.47
1:B:162:HIS:ND1	1:B:164:ILE:CD1	2.78	0.46
1:A:309:PRO:HB2	1:A:382:LEU:HD22	1.97	0.46
1:B:225:PRO:HB2	1:B:290:ARG:HB3	1.98	0.46
1:B:468:TYR:CD1	1:B:468:TYR:C	2.92	0.46
1:B:230:MET:HE1	1:B:298:TRP:CD2	2.51	0.46
1:A:176:ASP:O	1:A:177:LYS:CB	2.63	0.46
1:A:174:PRO:HD2	1:A:177:LYS:CE	2.47	0.45
1:A:338:GLU:O	3:A:719:HOH:O	2.21	0.45
1:B:308:TYR:CD1	1:B:308:TYR:C	2.95	0.45
1:A:231:PHE:CZ	1:A:276:MET:HE1	2.52	0.45
1:A:409:ILE:HG23	1:A:410:TYR:N	2.31	0.45
1:A:410:TYR:O	1:A:411:LEU:C	2.60	0.45
1:B:156:THR:OG1	1:B:158:LEU:HG	2.16	0.45
1:B:169:ILE:HD11	1:B:182:TYR:CE2	2.52	0.45
1:B:363:MET:HE2	1:B:382:LEU:HD23	1.98	0.45
1:A:59:VAL:O	1:A:62:LEU:HB2	2.17	0.44
1:A:214:GLY:C	3:A:710:HOH:O	2.60	0.44
1:B:164:ILE:HG12	3:B:615:HOH:O	2.17	0.44
1:A:124:TYR:HB3	3:A:727:HOH:O	2.17	0.44
1:B:9:LYS:N	1:B:10:PRO:HD2	2.32	0.44
1:B:431:VAL:HG12	1:B:431:VAL:O	2.17	0.44
1:A:49:HIS:ND1	1:A:50:PRO:HD2	2.33	0.44
1:B:49:HIS:ND1	1:B:50:PRO:HD2	2.33	0.44
1:A:231:PHE:HZ	1:A:276:MET:HE1	1.83	0.44
1:B:404:VAL:O	1:B:405:THR:C	2.61	0.44
1:A:308:TYR:N	1:A:309:PRO:CD	2.80	0.44
1:B:225:PRO:HG2	1:B:290:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:VAL:HG12	1:A:431:VAL:O	2.18	0.43
1:B:299:THR:OG1	3:B:619:HOH:O	2.18	0.43
1:A:404:VAL:CG2	1:A:408:LEU:HD11	2.48	0.43
1:B:333:CYS:HB3	1:B:437:MET:SD	2.58	0.43
1:A:260:ASP:HA	1:A:447:LYS:HD3	2.01	0.43
1:B:164:ILE:HA	3:B:615:HOH:O	2.17	0.43
1:A:162:HIS:HB2	1:A:164:ILE:HD11	2.01	0.43
1:A:308:TYR:CD1	1:A:308:TYR:C	2.96	0.43
1:A:196:SER:HG	1:A:278:ASN:H	1.66	0.43
1:A:35:GLU:CD	1:A:241:LYS:HG2	2.44	0.42
1:B:435:ASN:OD1	1:B:435:ASN:N	2.52	0.42
1:B:498:ARG:NH2	3:B:606:HOH:O	2.03	0.42
1:A:104:ARG:HG2	1:A:314:VAL:HG21	2.02	0.42
1:A:404:VAL:HG23	1:A:408:LEU:HG	2.02	0.42
1:A:183:ILE:HD12	1:A:276:MET:HE3	2.00	0.42
1:A:435:ASN:HB3	3:A:922:HOH:O	2.20	0.42
1:B:261:TYR:HB3	1:B:264:SER:HB2	2.01	0.42
1:B:420:ASN:OD1	1:B:420:ASN:C	2.62	0.42
1:A:174:PRO:HD2	1:A:177:LYS:HE2	2.02	0.42
1:A:234:PRO:HG2	1:A:237:ALA:HB2	2.02	0.42
1:B:35:GLU:HG3	1:B:42:ARG:CZ	2.50	0.42
1:A:194:ILE:HA	1:A:279:VAL:O	2.19	0.42
1:B:125:LYS:NZ	1:B:162:HIS:HB3	2.35	0.42
1:A:50:PRO:HB2	1:A:250:MET:HG3	2.02	0.42
1:B:59:VAL:O	1:B:62:LEU:HB2	2.20	0.42
1:B:88:HIS:HB3	1:B:91:PHE:CD1	2.54	0.42
1:B:366:GLU:HB2	1:B:378:ASP:HB2	2.02	0.41
1:B:297:ARG:NH1	1:B:301:GLU:OE1	2.53	0.41
1:A:133:GLY:HA3	1:A:150:TYR:CG	2.55	0.41
1:B:14:ARG:CZ	1:B:156:THR:HG22	2.49	0.41
1:A:156:THR:OG1	1:A:158:LEU:HG	2.21	0.41
1:A:519:ILE:HG21	1:B:50:PRO:HB3	2.03	0.41
1:A:438:ASP:OD1	1:A:440:VAL:HB	2.21	0.41
1:B:333:CYS:HB2	1:B:442:ARG:HG3	2.03	0.41
1:A:11:GLU:OE2	1:A:152:ARG:NE	2.46	0.40
1:A:120:ARG:HA	1:A:120:ARG:HD2	1.88	0.40
1:A:306:ARG:HB3	3:A:731:HOH:O	2.20	0.40
1:B:44:LYS:HD3	1:B:44:LYS:HA	1.88	0.40
1:A:366:GLU:HB2	1:A:378:ASP:HB2	2.04	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:O	1:B:187:LYS:NZ[1_655]	1.87	0.33
1:A:278:ASN:O	1:B:187:LYS:HZ2[1_655]	1.29	0.31
3:A:1038:HOH:O	3:B:854:HOH:O[7_555]	1.98	0.22
3:B:948:HOH:O	3:B:948:HOH:O[5_755]	2.09	0.11
3:A:823:HOH:O	3:A:921:HOH:O[7_555]	2.18	0.02

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	509/527 (97%)	487 (96%)	16 (3%)	6 (1%)	10	4
1	B	507/527 (96%)	487 (96%)	15 (3%)	5 (1%)	12	5
All	All	1016/1054 (96%)	974 (96%)	31 (3%)	11 (1%)	11	4

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	LEU
1	A	468	TYR
1	B	405	THR
1	B	411	LEU
1	A	177	LYS
1	A	9	LYS
1	B	177	LYS
1	A	201	VAL
1	A	224	ASP
1	B	201	VAL
1	B	224	ASP

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	432/443 (98%)	430 (100%)	2 (0%)	81	82
1	B	430/443 (97%)	427 (99%)	3 (1%)	76	76
All	All	862/886 (97%)	857 (99%)	5 (1%)	78	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	TRP
1	A	229	LEU
1	B	110	TRP
1	B	333	CYS
1	B	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	61	GLN
1	A	144	GLN
1	A	162	HIS
1	A	505	GLN
1	B	144	GLN
1	B	343	GLN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AMP	A	601	-	25,25,25	1.40	5 (20%)	37,38,38	1.93	11 (29%)
2	AMP	A	602	-	25,25,25	1.51	4 (16%)	37,38,38	1.95	9 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	A	601	-	-	0/10/26/26	0/3/3/3
2	AMP	A	602	-	-	0/10/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	AMP	C5-C4	5.17	1.48	1.39
2	A	601	AMP	C5-C4	4.52	1.47	1.39
2	A	602	AMP	C8-N7	3.29	1.38	1.31
2	A	601	AMP	C8-N7	2.78	1.37	1.31
2	A	602	AMP	C5-C6	2.57	1.48	1.41
2	A	601	AMP	C5-C6	2.49	1.47	1.41
2	A	601	AMP	C5-N7	-2.42	1.34	1.39
2	A	602	AMP	C5-N7	-2.31	1.34	1.39
2	A	601	AMP	C4-N9	-2.01	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	AMP	C5-C4-N3	-6.22	118.16	126.72
2	A	601	AMP	C5-C4-N3	-5.25	119.49	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AMP	N3-C2-N1	-4.56	121.67	128.58
2	A	602	AMP	N3-C2-N1	-4.24	122.17	128.58
2	A	602	AMP	N3-C4-N9	4.16	134.24	127.17
2	A	602	AMP	C2-N3-C4	4.11	121.86	111.83
2	A	601	AMP	C2-N3-C4	3.97	121.52	111.83
2	A	601	AMP	N3-C4-N9	3.94	133.87	127.17
2	A	602	AMP	C4-C5-N7	-3.67	106.39	110.58
2	A	601	AMP	C4-C5-N7	-3.35	106.75	110.58
2	A	601	AMP	C4-N9-C8	2.70	108.57	105.74
2	A	602	AMP	C5-N7-C8	2.68	107.67	103.45
2	A	601	AMP	C5-N7-C8	2.66	107.64	103.45
2	A	601	AMP	N9-C8-N7	-2.50	110.40	113.94
2	A	601	AMP	C2-N1-C6	2.48	122.80	118.73
2	A	601	AMP	C6-C5-N7	2.42	136.75	132.09
2	A	602	AMP	C2-N1-C6	2.22	122.38	118.73
2	A	602	AMP	C6-C5-N7	2.15	136.23	132.09
2	A	601	AMP	O3P-P-O2P	2.09	115.63	107.80
2	A	602	AMP	O3P-P-O2P	2.04	115.46	107.80

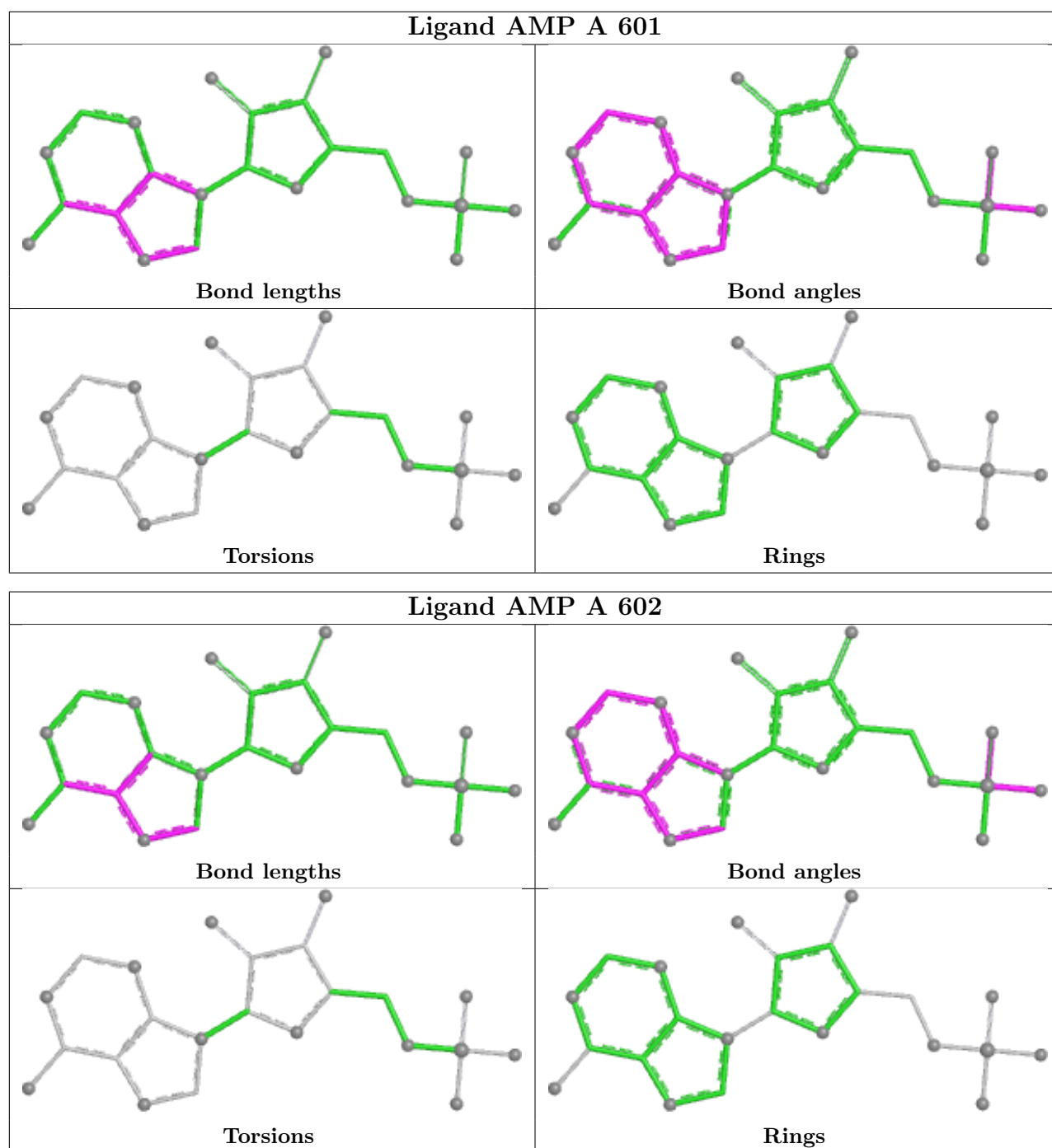
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	513/527 (97%)	0.58	61 (11%)	9 10	7, 26, 66, 134	0
1	B	511/527 (96%)	0.38	49 (9%)	13 15	7, 23, 59, 145	0
All	All	1024/1054 (97%)	0.48	110 (10%)	11 12	7, 25, 62, 145	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	ILE	11.0
1	B	409	ILE	9.3
1	B	169	ILE	9.0
1	A	468	TYR	8.3
1	B	175	THR	7.7
1	A	410	TYR	7.6
1	B	178	VAL	7.5
1	B	164	ILE	7.3
1	B	174	PRO	7.2
1	B	468	TYR	7.0
1	A	164	ILE	6.8
1	B	173	LEU	6.8
1	A	175	THR	6.8
1	A	181	VAL	6.8
1	B	410	TYR	6.5
1	B	168	PRO	6.3
1	A	173	LEU	6.1
1	A	174	PRO	5.9
1	A	8	HIS	5.8
1	A	177	LYS	5.7
1	A	178	VAL	5.6
1	A	169	ILE	5.0
1	B	179	LYS	4.9
1	B	184	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	176	ASP	4.7
1	A	434	SER	4.7
1	B	177	LYS	4.6
1	A	168	PRO	4.4
1	B	172	HIS	4.3
1	A	190	ASP	4.2
1	A	215	SER	4.2
1	B	171	ARG	4.2
1	A	162	HIS	4.0
1	B	181	VAL	3.9
1	B	436	GLY	3.9
1	A	184	LYS	3.9
1	A	179	LYS	3.9
1	A	171	ARG	3.8
1	B	278	ASN	3.7
1	B	170	ASP	3.7
1	A	525	LEU	3.6
1	A	289	TYR	3.6
1	A	227	PHE	3.5
1	A	435	ASN	3.4
1	B	176	ASP	3.4
1	B	292	PHE	3.3
1	B	434	SER	3.3
1	A	405	THR	3.3
1	A	182	TYR	3.2
1	A	223	SER	3.2
1	A	172	HIS	3.2
1	B	435	ASN	3.1
1	B	215	SER	3.1
1	A	185	LEU	3.1
1	A	170	ASP	3.0
1	B	405	THR	3.0
1	A	183	ILE	2.9
1	B	194	ILE	2.9
1	B	469	SER	2.9
1	A	436	GLY	2.8
1	A	180	ASP	2.8
1	A	527	LYS	2.8
1	A	238	ASP	2.8
1	A	33	GLY	2.7
1	A	469	SER	2.7
1	A	292	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	333	CYS	2.7
1	A	224	ASP	2.7
1	A	299	THR	2.6
1	B	185	LEU	2.6
1	A	194	ILE	2.6
1	A	523	ASP	2.6
1	B	180	ASP	2.6
1	B	200	VAL	2.6
1	B	167	PRO	2.5
1	B	182	TYR	2.5
1	B	429	LYS	2.5
1	B	432	ARG	2.5
1	A	430	TYR	2.5
1	B	430	TYR	2.5
1	B	526	LEU	2.5
1	A	42	ARG	2.5
1	A	277	ASP	2.5
1	B	517	ASP	2.5
1	A	515	ASN	2.4
1	B	339	PHE	2.4
1	B	423	ILE	2.4
1	A	44	LYS	2.4
1	B	192	GLY	2.4
1	A	37	TYR	2.3
1	B	227	PHE	2.3
1	A	338	GLU	2.3
1	B	422	GLN	2.3
1	B	524	LYS	2.3
1	A	201	VAL	2.3
1	A	226	ASP	2.3
1	A	467	ASN	2.3
1	B	187	LYS	2.3
1	A	518	ASP	2.2
1	A	278	ASN	2.2
1	A	300	MET	2.2
1	B	418	LEU	2.2
1	B	190	ASP	2.2
1	A	167	PRO	2.2
1	A	189	THR	2.1
1	A	192	GLY	2.1
1	B	276	MET	2.1
1	A	191	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	300	MET	2.0
1	A	225	PRO	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](#)

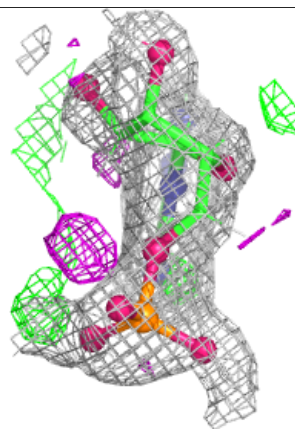
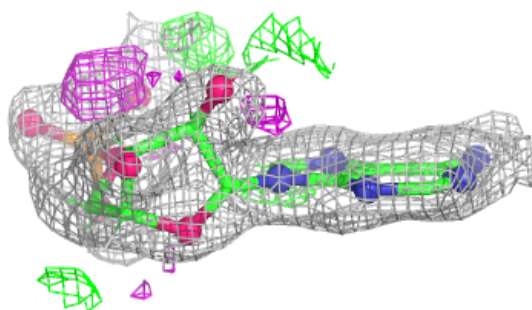
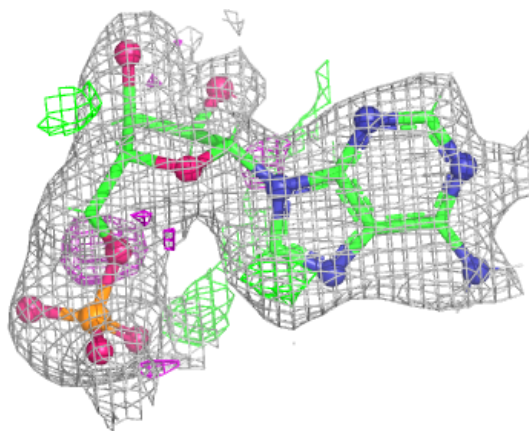
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
2	AMP	A	601	23/23	0.81	0.20	43,67,88,93	0
2	AMP	A	602	23/23	0.86	0.16	27,49,68,70	0

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

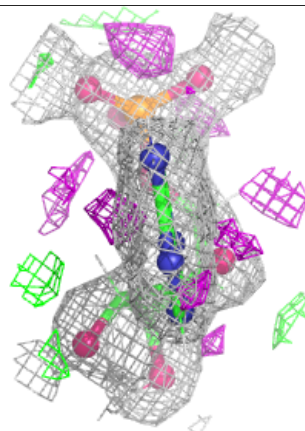
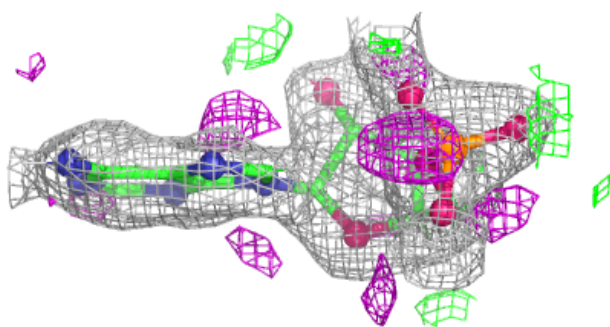
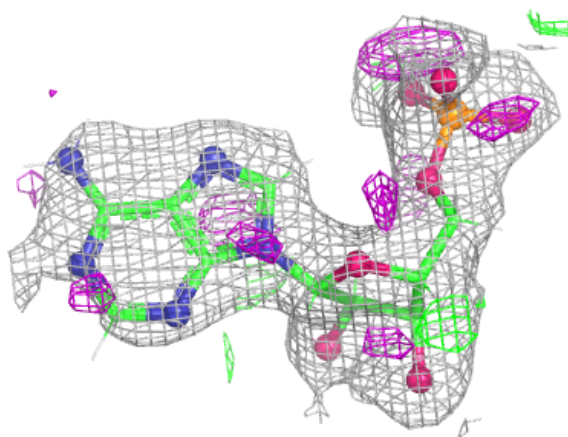
Electron density around AMP A 601:

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



Electron density around AMP A 602:

$2mF_o-DF_c$ (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.