Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:12 PM UTC

PDB ID	:	3CW9 / pdb_00003cw9
Title	:	4-Chlorobenzoyl-CoA Ligase/Synthetase in the Thioester-forming Conformation, bound to 4-chlorophenacyl-CoA
Authors	:	Reger, A.S.; Cao, J.; Wu, R.; Dunaway-Mariano, D.; Gulick, A.M.
Deposited on	:	2008-04-21
Resolution	:	2.00 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:

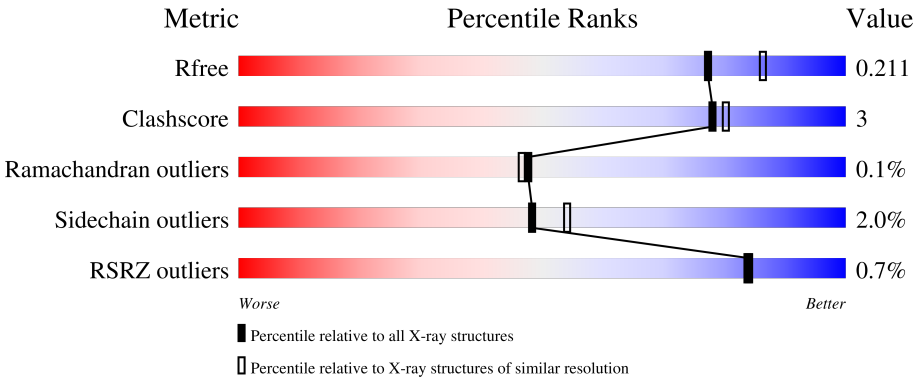
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

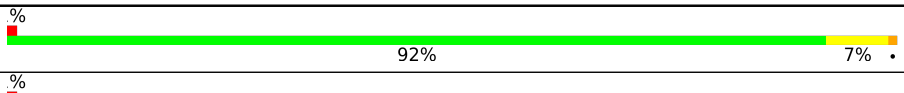
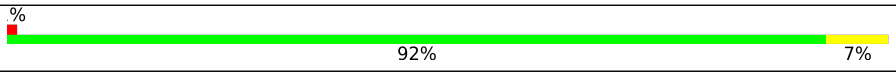
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	504	
1	B	504	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8584 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.

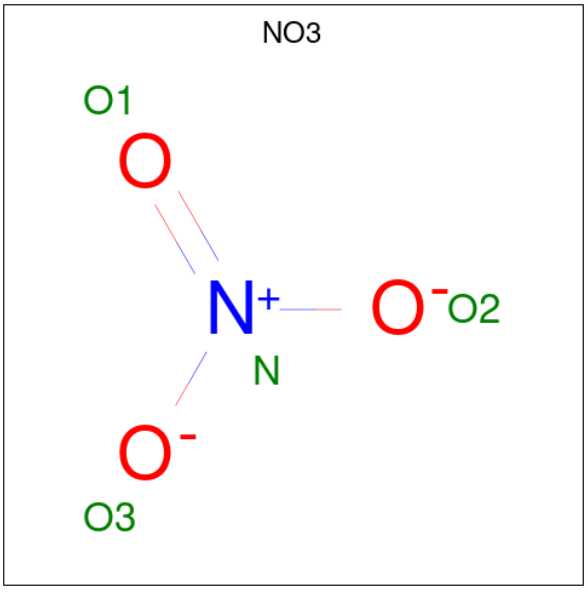
- Molecule 1 is a protein called 4-chlorobenzoyl CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3789	2394	679	703	13			
1	B	503	Total	C	N	O	S	0	0	0
			3815	2409	688	705	13			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

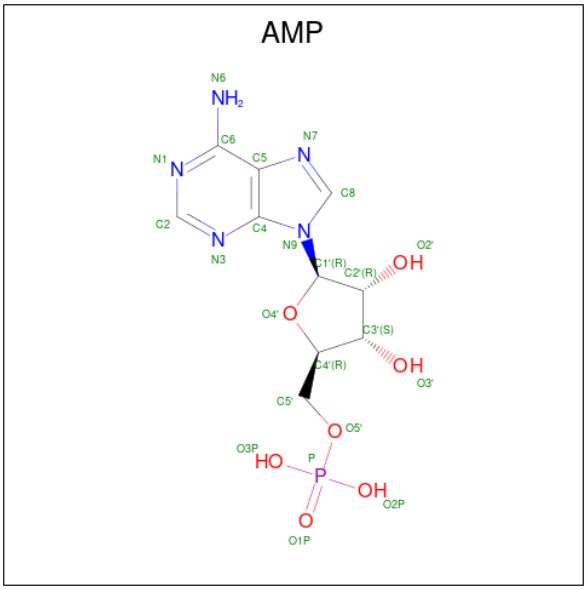
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



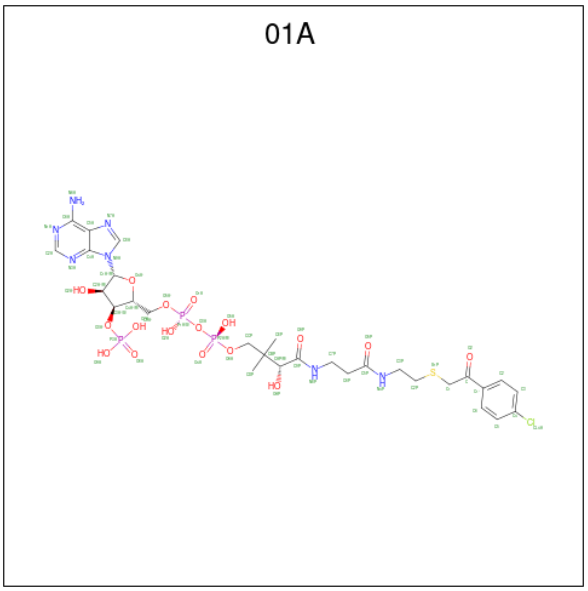
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0

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



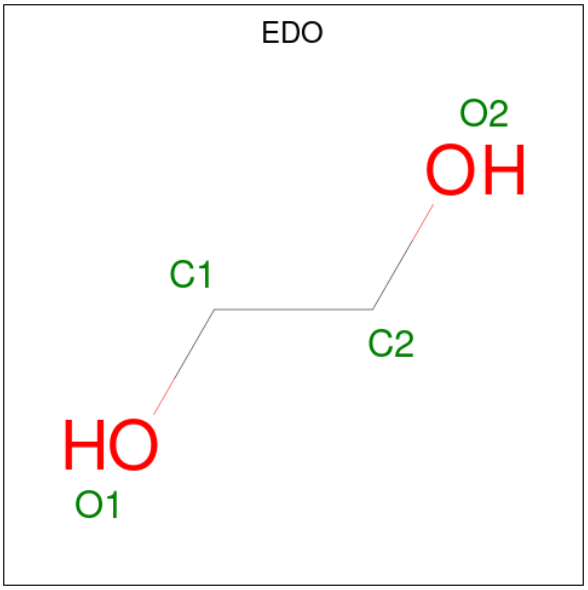
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 23 10 5 7 1	0	0
4	B	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 5 is 4-Chlorophenacyl-coenzyme A (CCD ID: 01A) (formula: $C_{29}H_{41}ClN_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	P	S	0	0
			58	29	1	7	17	3	1		
5	B	1	Total	C	Cl	N	O	P	S	0	0
			58	29	1	7	17	3	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

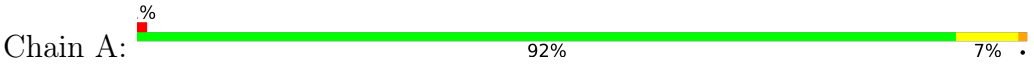
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	382	Total O 382 382	0	0
7	B	418	Total O 418 418	0	0

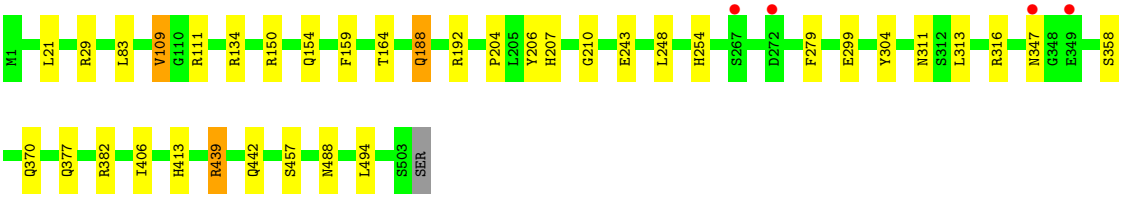
3 Residue-property plots (i)

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: 4-chlorobenzoyl CoA ligase

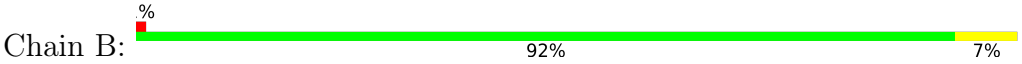
Chain A:

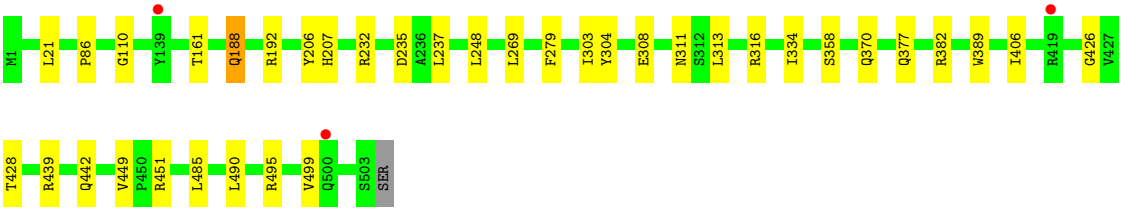




• Molecule 1: 4-chlorobenzoyl CoA ligase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.51Å 87.79Å 186.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.00 35.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (35.00-2.00) 94.6 (35.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.80 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.166 , 0.209 0.168 , 0.211	Depositor DCC
R_{free} test set	3259 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8584	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, 01A, EDO, NO3, MG

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	0.55	0/3861	0.81	2/5261 (0.0%)
1	B	0.55	0/3887	0.76	1/5291 (0.0%)
All	All	0.55	0/7748	0.78	3/10552 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	109	VAL	N-CA-C	13.68	126.38	111.88
1	A	111	ARG	N-CA-C	8.49	120.53	111.28
1	B	110	GLY	N-CA-C	6.37	121.09	112.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	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	3789	0	3810	23	0
1	B	3815	0	3868	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	8	0	0	0	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
5	A	58	0	37	3	0
5	B	58	0	37	3	0
6	A	4	0	6	0	0
7	A	382	0	0	3	0
7	B	418	0	0	2	0
All	All	8584	0	7782	44	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 3.

All (44) 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:150:ARG:HA	1:A:154:GLN:HE22	1.53	0.73
1:A:406:ILE:H	1:A:442:GLN:HE21	1.44	0.65
1:B:303:ILE:HG23	1:B:311:ASN:OD1	1.98	0.64
1:B:188:GLN:HE21	1:B:311:ASN:HD22	1.46	0.64
1:B:406:ILE:H	1:B:442:GLN:NE2	1.96	0.62
1:A:207:HIS:HB3	5:A:990:01A:H2PA	1.80	0.61
1:A:406:ILE:H	1:A:442:GLN:NE2	1.99	0.60
1:A:439:ARG:NH2	7:A:2574:HOH:O	2.36	0.59
1:A:316:ARG:HD3	1:B:192:ARG:NH2	2.18	0.57
1:B:428:THR:HG21	7:B:2636:HOH:O	2.04	0.57
1:A:188:GLN:HE21	1:A:311:ASN:HD22	1.51	0.57
1:A:188:GLN:HE21	1:A:311:ASN:ND2	2.03	0.56
1:B:207:HIS:HB3	5:B:991:01A:H2PA	1.89	0.55
1:B:188:GLN:HE21	1:B:311:ASN:ND2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:HIS:CB	5:A:990:01A:H2PA	2.38	0.53
1:B:377:GLN:NE2	1:B:382:ARG:HH11	2.07	0.53
1:B:207:HIS:CB	5:B:991:01A:H2PA	2.39	0.53
1:B:406:ILE:H	1:B:442:GLN:HE21	1.57	0.53
1:A:83:LEU:HD12	1:A:159:PHE:CE1	2.44	0.52
1:B:428:THR:HG22	1:B:449:VAL:O	2.12	0.50
1:A:192:ARG:NH2	1:B:316:ARG:HD3	2.27	0.49
1:A:29:ARG:HH22	1:A:243:GLU:CD	2.20	0.49
1:B:304:TYR:HB3	1:B:313:LEU:HB2	1.94	0.49
1:A:488:ASN:HB3	1:A:494:LEU:HD21	1.95	0.49
1:A:164:THR:HA	1:A:413:HIS:CD2	2.48	0.48
5:B:991:01A:H1	5:B:991:01A:H3PA	1.68	0.48
1:A:254:HIS:HE1	7:A:2211:HOH:O	1.96	0.48
1:B:232:ARG:NE	1:B:235:ASP:OD2	2.45	0.48
7:A:2334:HOH:O	1:B:358:SER:HB2	2.14	0.47
1:A:150:ARG:HA	1:A:154:GLN:NE2	2.24	0.47
1:B:86:PRO:HD2	1:B:206:TYR:CE1	2.51	0.44
1:A:299:GLU:OE2	1:A:316:ARG:HD2	2.17	0.44
1:A:204:PRO:HB3	1:A:206:TYR:CZ	2.52	0.44
1:B:237:LEU:HB3	1:B:269:LEU:HD13	1.99	0.44
1:B:334:ILE:HD12	1:B:389:TRP:CD1	2.53	0.43
1:A:188:GLN:HG2	1:A:311:ASN:HD21	1.83	0.43
1:A:304:TYR:HB3	1:A:313:LEU:HB2	2.00	0.43
1:A:377:GLN:NE2	1:A:382:ARG:HH11	2.17	0.43
5:A:990:01A:H3PA	5:A:990:01A:H1	1.77	0.42
1:B:426:GLY:H	1:B:451:ARG:CZ	2.33	0.42
1:A:204:PRO:O	1:A:210:GLY:HA3	2.19	0.41
1:B:161:THR:HG21	1:B:308:GLU:OE2	2.19	0.41
1:A:358:SER:HB2	7:B:2221:HOH:O	2.21	0.40
1:B:495:ARG:O	1:B:499:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	501/504 (99%)	490 (98%)	10 (2%)	1 (0%)	43 42
1	B	501/504 (99%)	492 (98%)	9 (2%)	0	100 100
All	All	1002/1008 (99%)	982 (98%)	19 (2%)	1 (0%)	48 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	ASN

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	391/400 (98%)	383 (98%)	8 (2%)	48 54
1	B	398/400 (100%)	390 (98%)	8 (2%)	48 54
All	All	789/800 (99%)	773 (98%)	16 (2%)	48 54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	134	ARG
1	A	188	GLN
1	A	248	LEU
1	A	279	PHE
1	A	370	GLN
1	A	439	ARG
1	A	457	SER
1	B	21	LEU
1	B	188	GLN
1	B	248	LEU
1	B	279	PHE

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Mol	Chain	Res	Type
1	B	370	GLN
1	B	439	ARG
1	B	485	LEU
1	B	490	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	154	GLN
1	A	175	GLN
1	A	188	GLN
1	A	241	GLN
1	A	254	HIS
1	A	294	GLN
1	A	311	ASN
1	A	377	GLN
1	A	442	GLN
1	A	501	GLN
1	B	54	GLN
1	B	154	GLN
1	B	175	GLN
1	B	188	GLN
1	B	295	HIS
1	B	311	ASN
1	B	367	ASN
1	B	370	GLN
1	B	377	GLN
1	B	442	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	AMP	B	999	-	25,25,25	1.50	4 (16%)	37,38,38	1.84	9 (24%)
3	NO3	B	1302	-	1,3,3	3.22	1 (100%)	0,3,3	-	-
4	AMP	A	997	-	25,25,25	1.49	5 (20%)	37,38,38	1.77	8 (21%)
5	01A	A	990	2	59,61,61	2.11	7 (11%)	85,90,90	1.93	17 (20%)
6	EDO	A	1003	-	3,3,3	0.42	0	2,2,2	0.56	0
3	NO3	A	1303	-	1,3,3	3.27	1 (100%)	0,3,3	-	-
3	NO3	B	1301	-	1,3,3	3.33	1 (100%)	0,3,3	-	-
5	01A	B	991	2	59,61,61	2.13	6 (10%)	85,90,90	1.99	17 (20%)

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	AMP	B	999	-	-	4/10/26/26	0/3/3/3
5	01A	A	990	2	-	7/56/72/72	0/4/4/4
4	AMP	A	997	-	-	0/10/26/26	0/3/3/3
6	EDO	A	1003	-	-	0/1/1/1	-
5	01A	B	991	2	-	9/56/72/72	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	991	01A	C1-C	-12.37	1.33	1.51
5	A	990	01A	C1-C	-12.05	1.34	1.51
5	B	991	01A	C1-S1P	-5.91	1.66	1.81
5	A	990	01A	C1-S1P	-5.91	1.66	1.81
5	A	990	01A	O9P-C9P	5.23	1.33	1.23
5	B	991	01A	O9P-C9P	4.96	1.32	1.23
4	B	999	AMP	C5-C4	4.89	1.47	1.39
4	A	997	AMP	C5-C4	4.73	1.47	1.39
3	B	1301	NO3	O1-N	3.33	1.40	1.24
3	A	1303	NO3	O1-N	3.27	1.40	1.24
3	B	1302	NO3	O1-N	3.22	1.40	1.24
4	B	999	AMP	C5-C6	2.79	1.48	1.41
5	A	990	01A	C9P-N8P	-2.67	1.27	1.33
4	A	997	AMP	C5-C6	2.64	1.48	1.41
5	A	990	01A	P1A-O3A	2.62	1.62	1.59
5	B	991	01A	C9P-N8P	-2.60	1.27	1.33
5	A	990	01A	P2A-O3A	2.56	1.62	1.59
5	B	991	01A	P1A-O3A	2.50	1.62	1.59
4	B	999	AMP	C8-N7	2.42	1.36	1.31
4	A	997	AMP	C8-N7	2.41	1.36	1.31
5	B	991	01A	C8A-N7A	2.14	1.35	1.31
4	A	997	AMP	C5-N7	-2.07	1.35	1.39
5	A	990	01A	C4-CL4A	2.07	1.79	1.74
4	B	999	AMP	C5-N7	-2.02	1.35	1.39
4	A	997	AMP	C4-N9	-2.02	1.33	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	990	01A	C1-C-C1'	8.11	127.24	117.99
5	B	991	01A	C1-C-C1'	7.54	126.59	117.99
5	B	991	01A	C-C1-S1P	6.00	130.87	111.38
5	A	990	01A	C-C1-S1P	5.73	129.96	111.38
5	B	991	01A	N3A-C2A-N1A	-5.44	120.35	128.58
4	A	997	AMP	C5-C4-N3	-5.40	119.28	126.72
4	B	999	AMP	C5-C4-N3	-5.33	119.37	126.72
5	A	990	01A	N3A-C2A-N1A	-5.12	120.84	128.58
5	B	991	01A	C5A-C4A-N3A	-4.83	120.07	126.72
5	A	990	01A	C5A-C4A-N3A	-4.82	120.08	126.72
5	B	991	01A	O2-C-C1	-4.42	113.52	120.41
4	B	999	AMP	N3-C4-N9	4.37	134.61	127.17
4	A	997	AMP	N3-C4-N9	4.11	134.16	127.17
5	A	990	01A	C3P-N4P-C5P	4.01	130.29	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	999	AMP	N3-C2-N1	-3.75	122.90	128.58
4	B	999	AMP	C2-N3-C4	3.68	120.82	111.83
4	A	997	AMP	C2-N3-C4	3.63	120.70	111.83
5	B	991	01A	N9A-C8A-N7A	-3.54	108.91	113.94
5	A	990	01A	C2A-N3A-C4A	3.54	120.47	111.83
5	B	991	01A	C2A-N3A-C4A	3.52	120.44	111.83
5	A	990	01A	O2-C-C1	-3.48	114.98	120.41
4	A	997	AMP	N3-C2-N1	-3.48	123.31	128.58
5	B	991	01A	N3A-C4A-N9A	3.34	132.84	127.17
5	A	990	01A	N9A-C8A-N7A	-3.32	109.23	113.94
4	A	997	AMP	C4-C5-N7	-3.24	106.88	110.58
5	B	991	01A	C2P-S1P-C1	-3.15	96.52	101.72
5	A	990	01A	N3A-C4A-N9A	3.09	132.42	127.17
5	B	991	01A	CDP-CBP-CAP	3.09	114.04	108.77
4	B	999	AMP	C4-C5-N7	-3.05	107.10	110.58
5	B	991	01A	C3P-N4P-C5P	3.01	128.42	122.82
5	B	991	01A	C4A-N9A-C8A	2.94	108.82	105.74
4	B	999	AMP	C4-N9-C8	2.71	108.58	105.74
5	A	990	01A	C4A-C5A-N7A	-2.55	107.67	110.58
5	B	991	01A	C2P-C3P-N4P	-2.45	107.31	112.41
5	A	990	01A	C4A-N9A-C8A	2.45	108.31	105.74
5	A	990	01A	C5A-N7A-C8A	2.45	107.29	103.45
5	B	991	01A	C5A-N7A-C8A	2.43	107.27	103.45
5	B	991	01A	C7P-N8P-C9P	2.34	126.75	122.55
5	B	991	01A	C4A-C5A-N7A	-2.34	107.90	110.58
5	B	991	01A	CEP-CBP-CCP	2.22	111.88	108.22
5	A	990	01A	CAP-C9P-N8P	2.21	120.67	116.48
5	A	990	01A	O2-C-C1'	-2.21	117.78	120.73
4	A	997	AMP	C6-C5-N7	2.21	136.34	132.09
5	A	990	01A	C7P-C6P-C5P	-2.20	108.73	112.39
4	A	997	AMP	C4-N9-C8	2.18	108.03	105.74
4	B	999	AMP	C2-N1-C6	2.11	122.20	118.73
4	B	999	AMP	C5-N7-C8	2.11	106.76	103.45
5	A	990	01A	C6P-C7P-N8P	-2.09	107.55	112.00
5	A	990	01A	C2P-S1P-C1	-2.08	98.30	101.72
4	A	997	AMP	C2-N1-C6	2.07	122.13	118.73
4	B	999	AMP	C6-C5-N7	2.05	136.05	132.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	999	AMP	C5'-O5'-P-O3P
5	A	990	01A	C-C1-S1P-C2P
5	A	990	01A	O2-C-C1-S1P
5	A	990	01A	C1'-C-C1-S1P
5	A	990	01A	C1-C-C1'-C6
5	A	990	01A	C1-C-C1'-C2
5	B	991	01A	C-C1-S1P-C2P
5	B	991	01A	O2-C-C1-S1P
5	B	991	01A	C1'-C-C1-S1P
5	B	991	01A	C1-C-C1'-C6
5	B	991	01A	C1-C-C1'-C2
5	A	990	01A	O2-C-C1'-C2
5	A	990	01A	O2-C-C1'-C6
5	B	991	01A	O2-C-C1'-C6
5	B	991	01A	O2-C-C1'-C2
4	B	999	AMP	C5'-O5'-P-O1P
5	B	991	01A	O4A'-C4A'-C5A'-O5A'
4	B	999	AMP	C5'-O5'-P-O2P
5	B	991	01A	C3A'-C4A'-C5A'-O5A'
4	B	999	AMP	C3'-C4'-C5'-O5'

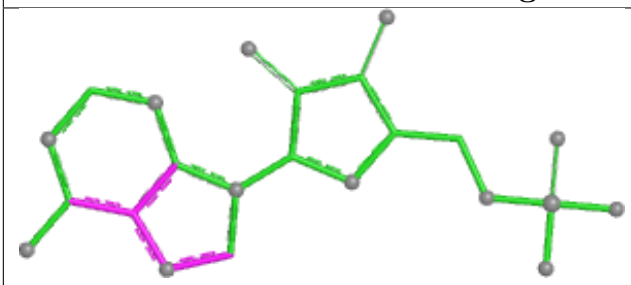
There are no ring outliers.

2 monomers are involved in 6 short contacts:

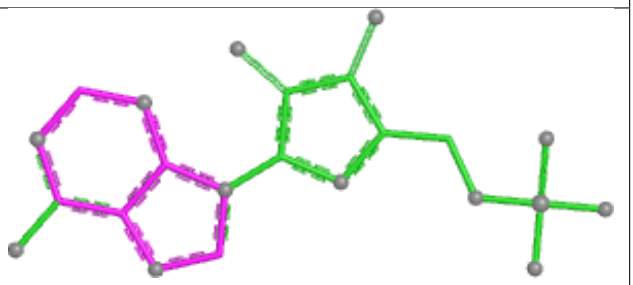
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	990	01A	3	0
5	B	991	01A	3	0

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

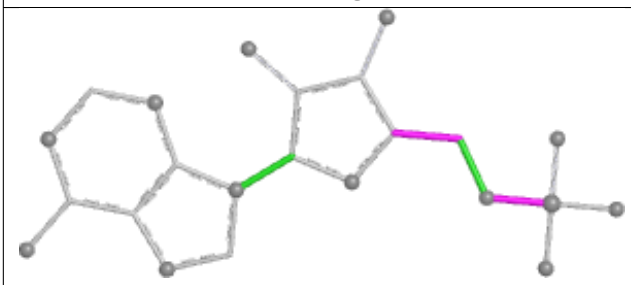
Ligand AMP B 999



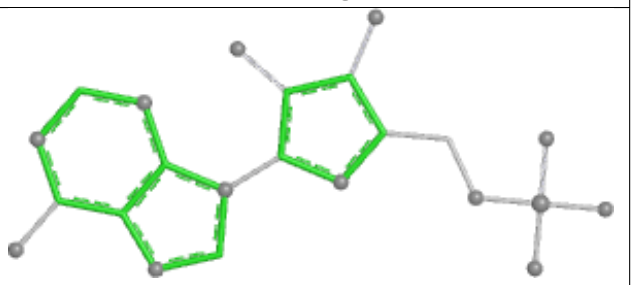
Bond lengths



Bond angles

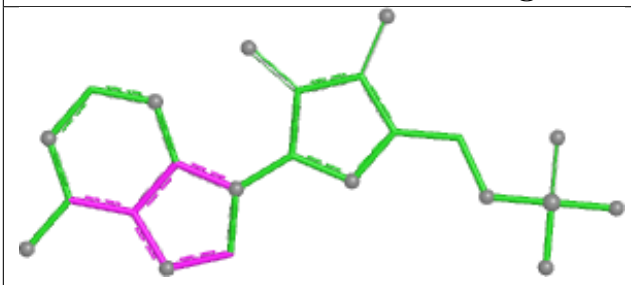


Torsions

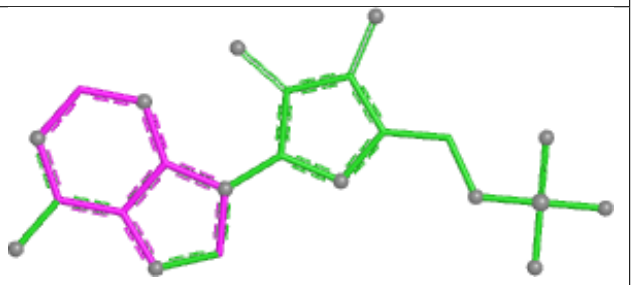


Rings

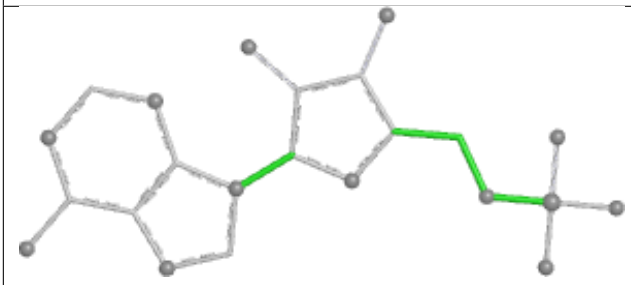
Ligand AMP A 997



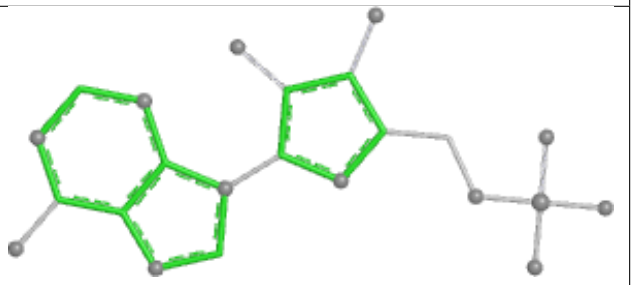
Bond lengths



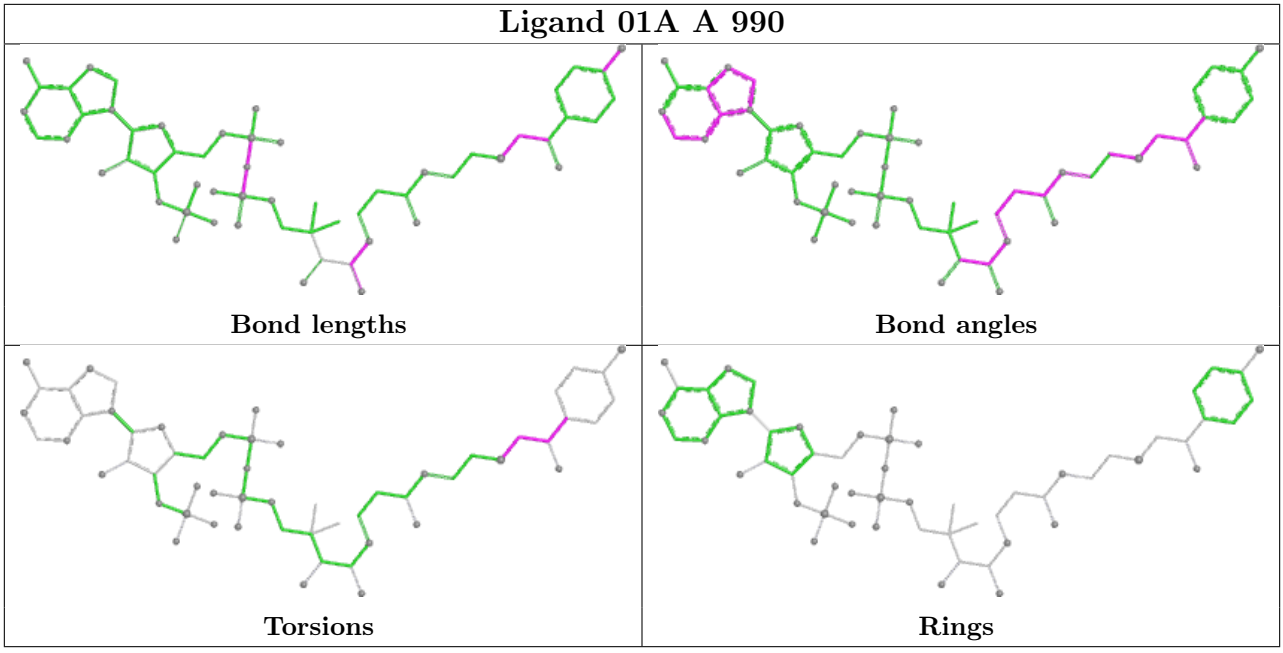
Bond angles

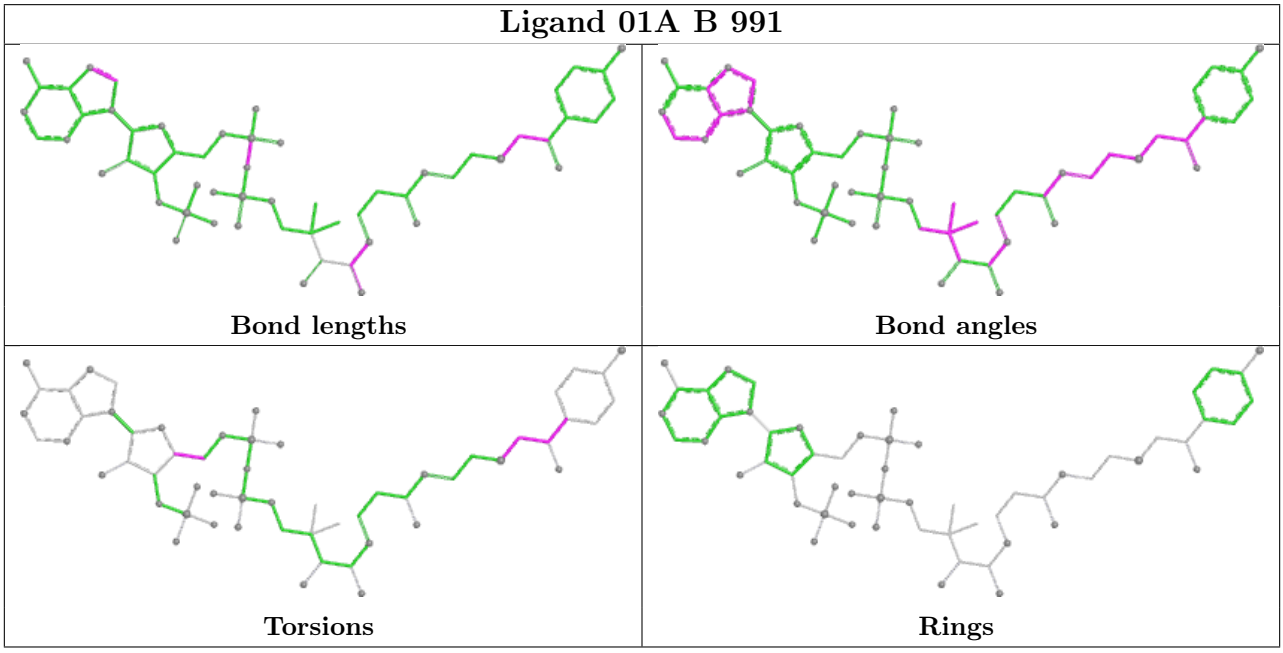


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	503/504 (99%)	-0.31	4 (0%)	82	82	12, 17, 28, 35	0
1	B	503/504 (99%)	-0.38	3 (0%)	85	85	11, 16, 25, 42	0
All	All	1006/1008 (99%)	-0.34	7 (0%)	84	84	11, 17, 27, 42	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	ASN	2.7
1	A	349	GLU	2.4
1	A	272	ASP	2.4
1	B	139	TYR	2.3
1	B	419	ARG	2.1
1	B	500	GLN	2.1
1	A	267	SER	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

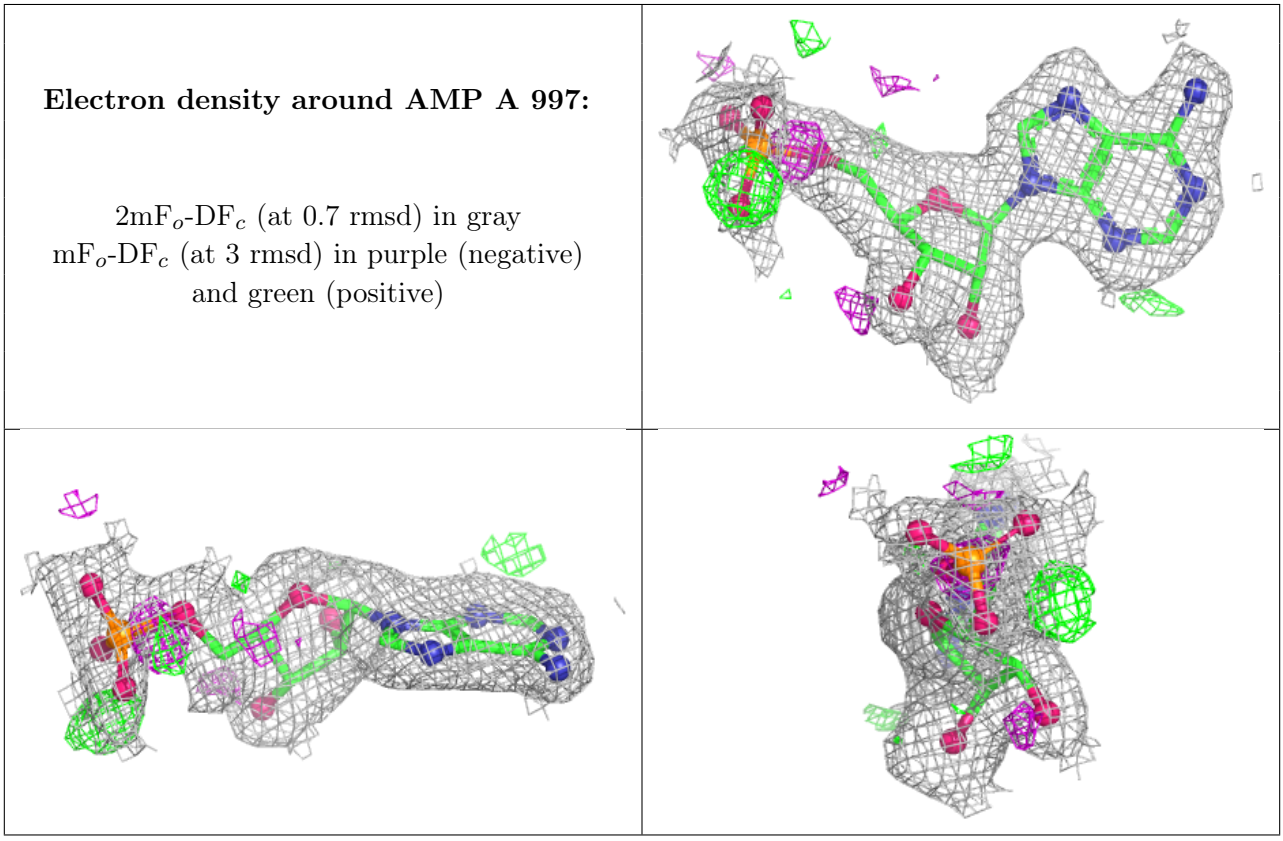
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	1002	1/1	0.80	0.20	54,54,54,54	0
3	NO3	B	1301	4/4	0.81	0.16	46,47,47,47	0
6	EDO	A	1003	4/4	0.81	0.11	28,28,30,30	0
3	NO3	A	1303	4/4	0.86	0.17	35,37,37,37	0
2	MG	A	1001	1/1	0.88	0.10	44,44,44,44	0
4	AMP	A	997	23/23	0.93	0.07	12,14,20,21	4
4	AMP	B	999	23/23	0.93	0.07	12,13,25,25	4
3	NO3	B	1302	4/4	0.93	0.14	25,25,26,26	0
5	01A	B	991	58/58	0.94	0.08	14,20,33,33	0
5	01A	A	990	58/58	0.95	0.07	15,20,30,31	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.

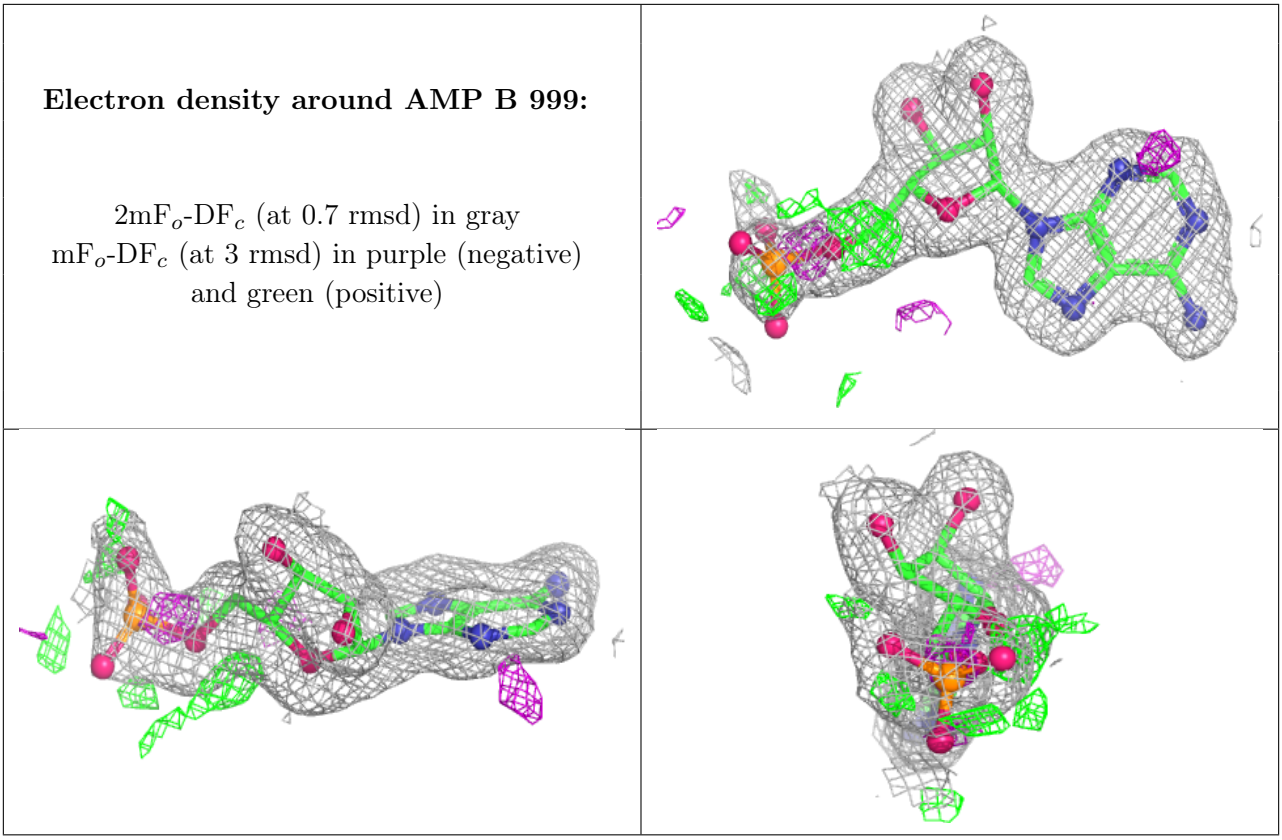
Electron density around AMP A 997:

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



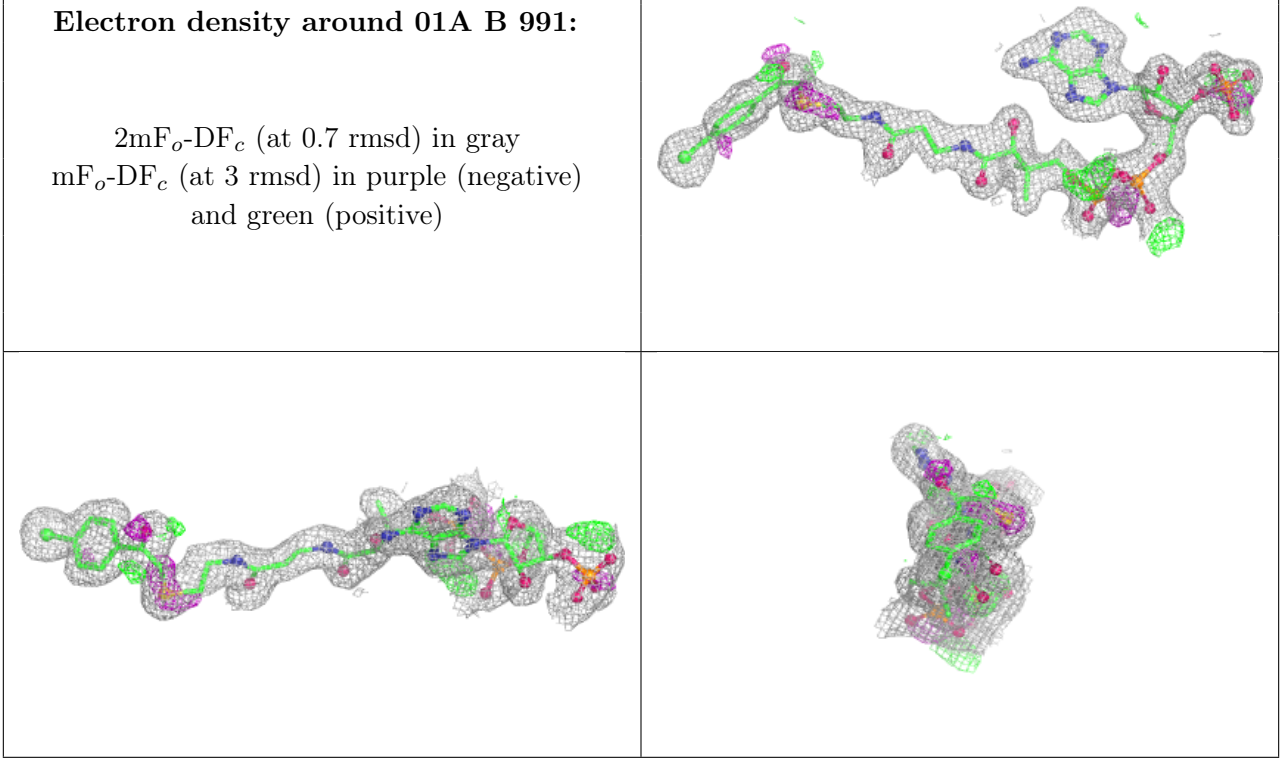
Electron density around AMP B 999:

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



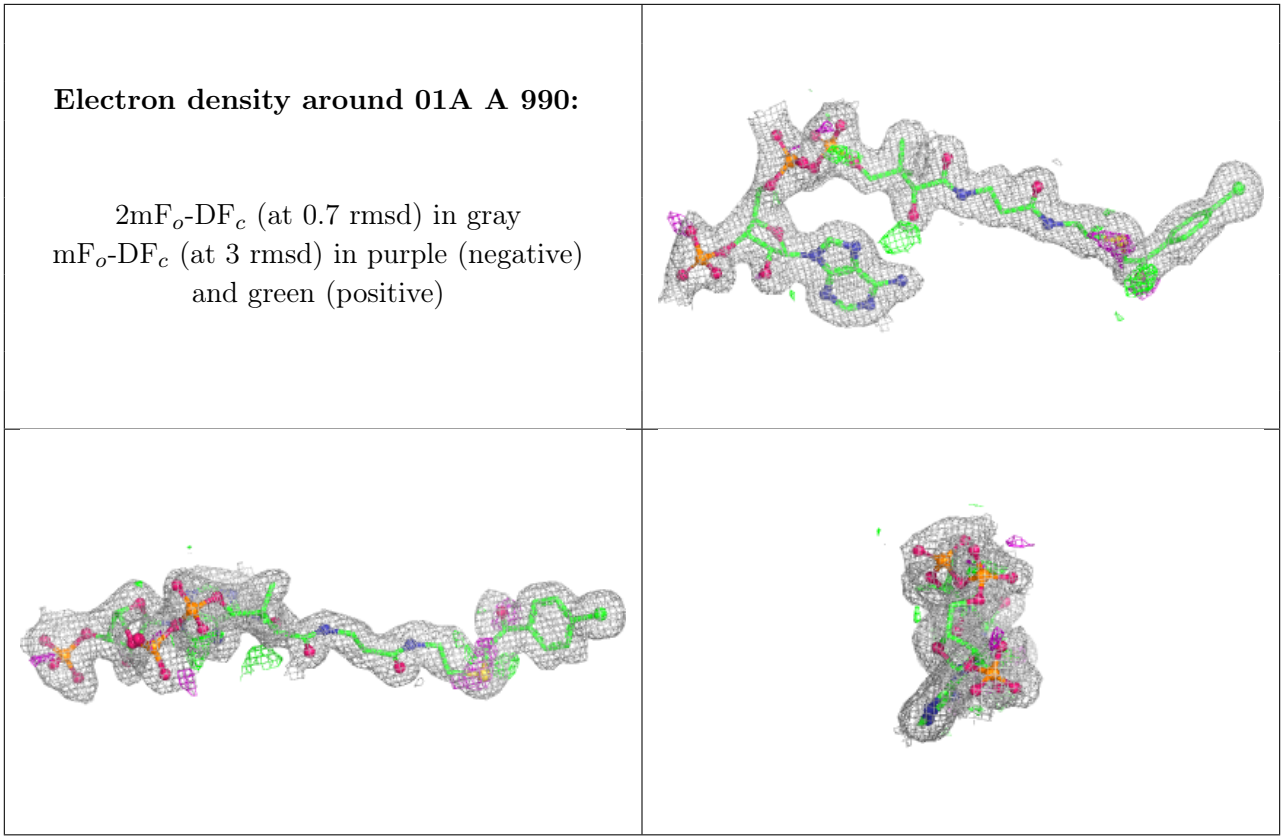
Electron density around 01A B 991:

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



Electron density around 01A A 990:

$2mF_o$-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.