Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:41 PM UTC

PDB ID	:	2CNQ / pdb_00002cnq
Title	:	Atomic resolution structure of SAICAR-synthase from Saccharomyces cerevisiae complexed with ADP, AICAR, succinate
Authors	:	Urusova, D.V.; Antonyuk, S.V.; Grebenko, A.I.; Levdikov, V.M.; Barynin, V.V.; Popov, A.N.; Lamzin, V.S.; Melik-Adamyan, W.R.
Deposited on	:	2006-05-23
Resolution	:	1.00 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:

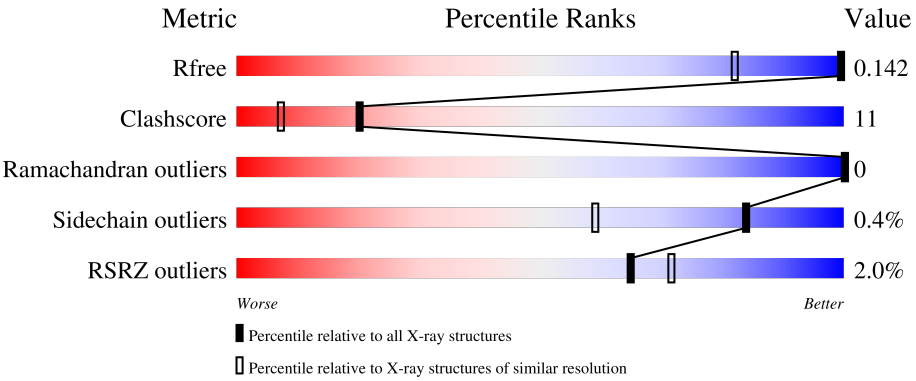
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.00 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	1358 (1.04-0.96)
Clashscore	190562	1411 (1.04-0.96)
Ramachandran outliers	187476	1347 (1.04-0.96)
Sidechain outliers	187428	1348 (1.04-0.96)
RSRZ outliers	180081	1355 (1.04-0.96)

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 <=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	306	2% 84% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AMP	A	1310[B]	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3626 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.

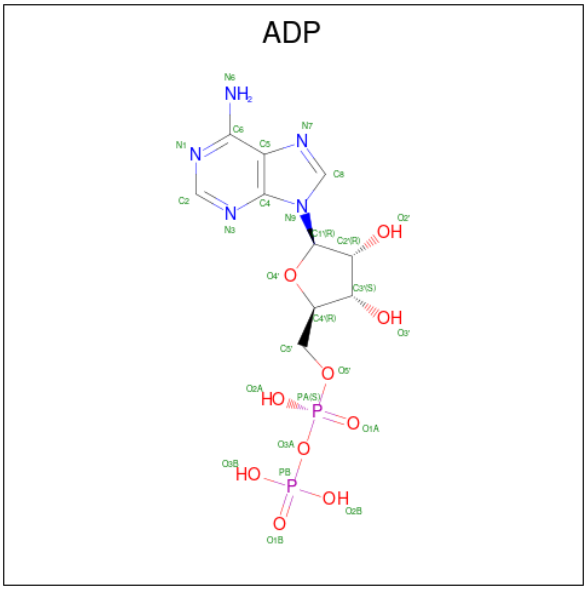
- Molecule 1 is a protein called PHOSPHORIBOSYLAMINOIMIDAZOLE-SUCCINOCARBOXAMIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	4	61	0
			2735	1768	445	519	3			

There is a discrepancy between the modelled and reference sequences:

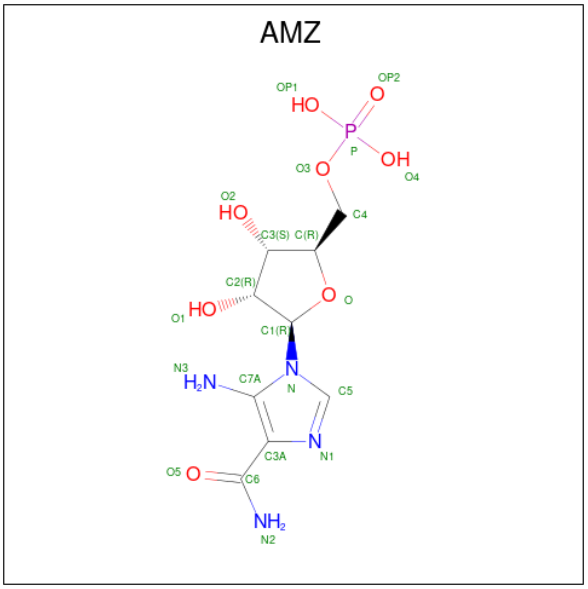
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLU	GLY	conflict	UNP P27616

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



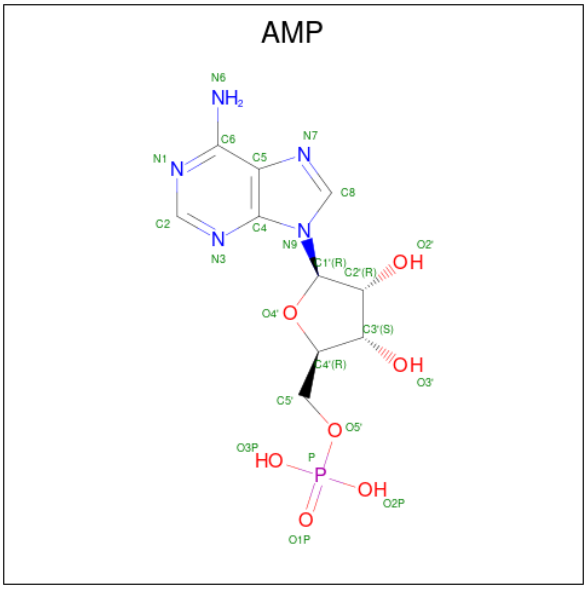
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (CCD ID: AMZ) (formula: $C_9H_{15}N_4O_8P$).



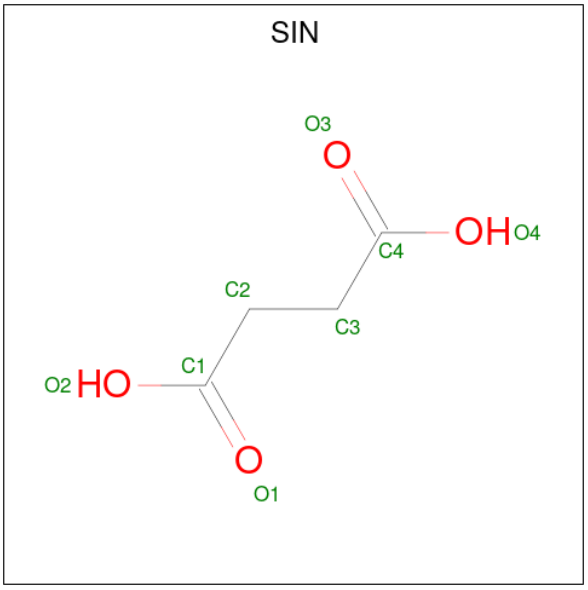
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	9	4	8	1		
3	A	1	Total	C	N	O	P	0	1
			22	9	4	8	1		

- 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	0	1
			23	10	5	7	1		

- Molecule 5 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).

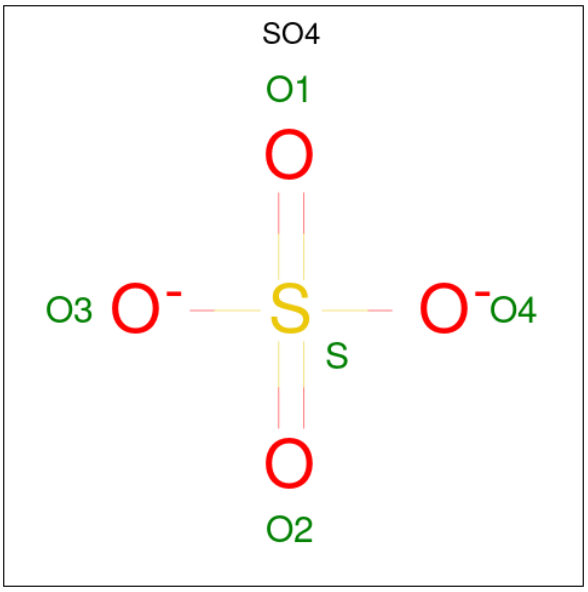


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	1

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	733	Total O 733 733	0	0

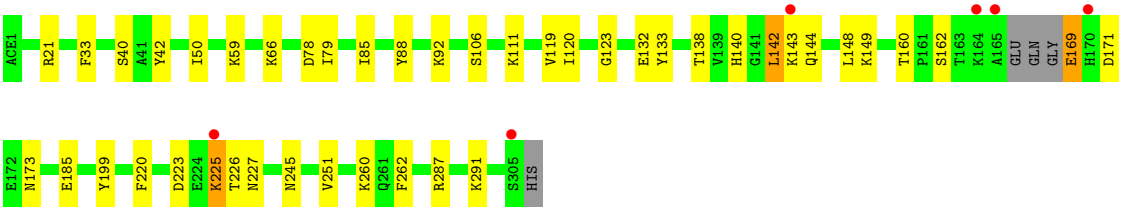
3 Residue-property plots (i)

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: PHOSPHORIBOSYLAMINOIMIDAZOLE-SUCCINOCARBOXAMIDE SYNTHASE

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.68Å 61.85Å 76.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.00 17.00 – 1.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (17.00-1.00) 96.7 (17.00-1.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 1.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.115 , 0.130 0.127 , 0.142	Depositor DCC
R_{free} test set	4546 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	8.6	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	3626	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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, SO4, ADP, SIN, AMZ, ACE, 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	1.80	2/2964 (0.1%)	0.84	3/3992 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225[A]	LYS	CE-NZ	38.67	2.65	1.49
1	A	225[B]	LYS	CE-NZ	38.67	2.65	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225[A]	LYS	CD-CE-NZ	-12.41	72.18	111.90
1	A	225[B]	LYS	CD-CE-NZ	-12.41	72.18	111.90
1	A	169	GLU	CB-CG-CD	9.57	128.87	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	LEU	Mainchain

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	2735	0	2811	60	0
2	A	54	0	24	6	0
3	A	44	0	26	0	0
4	A	23	0	12	7	0
5	A	16	0	8	6	0
6	A	1	0	0	0	0
7	A	20	0	0	0	0
8	A	733	0	0	16	0
All	All	3626	0	2881	66	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 11.

All (66) 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:287[B]:ARG:HG3	8:A:2638:HOH:O	1.28	1.27
1:A:144[B]:GLN:O	8:A:2384:HOH:O	1.53	1.27
2:A:1311:ADP:C5'	8:A:2686:HOH:O	1.79	1.26
2:A:1311:ADP:H5'2	8:A:2686:HOH:O	1.28	1.21
1:A:85[B]:ILE:CG2	4:A:1310[B]:AMP:C2	2.37	1.07
1:A:85[B]:ILE:HG21	4:A:1310[B]:AMP:C2	2.04	0.89
1:A:225[B]:LYS:HD3	1:A:225[B]:LYS:NZ	1.92	0.85
5:A:1312:SIN:O2	8:A:2703:HOH:O	1.97	0.82
1:A:85[B]:ILE:HG23	4:A:1310[B]:AMP:C2	2.13	0.82
1:A:225[A]:LYS:CD	1:A:225[A]:LYS:NZ	2.45	0.79
1:A:138[A]:THR:HG22	1:A:143[A]:LYS:HG3	1.66	0.78
1:A:85[B]:ILE:HG21	4:A:1310[B]:AMP:H2	1.49	0.75
1:A:225[A]:LYS:NZ	1:A:225[A]:LYS:HD3	2.03	0.73
1:A:149[B]:LYS:HB2	1:A:251[B]:VAL:HG12	1.72	0.70
1:A:143[B]:LYS:HE3	1:A:144[B]:GLN:O	1.92	0.68
1:A:66[B]:LYS:HE3	4:A:1310[B]:AMP:O3P	1.95	0.66
1:A:79[B]:ILE:HG23	1:A:88:TYR:CE1	2.31	0.66
1:A:66[B]:LYS:CE	4:A:1310[B]:AMP:O3P	2.47	0.63
1:A:225[B]:LYS:NZ	1:A:225[B]:LYS:CD	2.62	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225[B]:LYS:NZ	1:A:225[B]:LYS:CE	2.65	0.59
1:A:185[A]:GLU:HG2	5:A:1312:SIN:H31	1.85	0.59
1:A:119:VAL:HG11	1:A:220[B]:PHE:HE1	1.69	0.58
1:A:42:TYR:HA	2:A:1311:ADP:C8	2.39	0.57
1:A:78[B]:ASP:HB2	8:A:2252:HOH:O	2.04	0.57
1:A:119:VAL:HG11	1:A:220[B]:PHE:CE1	2.40	0.57
5:A:1313:SIN:C1	8:A:2681:HOH:O	2.52	0.57
1:A:171:ASP:OD2	2:A:1311:ADP:O3'	2.22	0.56
1:A:50:ILE:HG21	8:A:2316:HOH:O	2.06	0.56
1:A:140:HIS:CD2	8:A:2375:HOH:O	2.60	0.55
1:A:119:VAL:HG21	1:A:220[B]:PHE:HD1	1.73	0.54
1:A:223:ASP:O	1:A:227[B]:ASN:N	2.40	0.53
2:A:1311:ADP:H5'1	8:A:2686:HOH:O	1.73	0.52
1:A:132:GLU:HG2	1:A:138[B]:THR:O	2.10	0.51
1:A:42:TYR:HA	2:A:1311:ADP:N7	2.26	0.51
1:A:138[A]:THR:CG2	1:A:143[A]:LYS:HG3	2.38	0.50
1:A:133[A]:TYR:CE1	1:A:148[A]:LEU:HD12	2.47	0.49
1:A:225[A]:LYS:NZ	1:A:225[A]:LYS:HD2	2.24	0.49
1:A:92[A]:LYS:CE	8:A:2318:HOH:O	2.61	0.49
1:A:140:HIS:CD2	1:A:160:THR:HB	2.48	0.48
1:A:140:HIS:CG	1:A:160:THR:HB	2.48	0.48
1:A:138[A]:THR:HA	1:A:142:LEU:O	2.13	0.48
1:A:42:TYR:OH	5:A:1313:SIN:H31	2.14	0.48
1:A:40:SER:O	1:A:260[A]:LYS:HD3	2.15	0.47
1:A:132:GLU:CG	1:A:138[B]:THR:O	2.62	0.47
1:A:132:GLU:O	1:A:133[B]:TYR:C	2.57	0.47
1:A:85[B]:ILE:HG23	4:A:1310[B]:AMP:N3	2.30	0.47
1:A:85[B]:ILE:CD1	1:A:106:SER:HB2	2.45	0.46
1:A:226[B]:THR:HA	8:A:2529:HOH:O	2.15	0.46
1:A:42:TYR:CE1	5:A:1313:SIN:H31	2.51	0.46
1:A:92[A]:LYS:HE2	8:A:2318:HOH:O	2.16	0.46
1:A:111[A]:LYS:HG2	8:A:2347:HOH:O	2.14	0.45
1:A:133[A]:TYR:CE2	1:A:148[A]:LEU:HB2	2.52	0.44
1:A:287[B]:ARG:CG	8:A:2638:HOH:O	2.14	0.44
1:A:79[B]:ILE:HG23	1:A:88:TYR:HE1	1.82	0.43
1:A:21:ARG:HD3	1:A:33:PHE:CZ	2.54	0.43
1:A:162[B]:SER:OG	1:A:173:ASN:ND2	2.52	0.42
1:A:143[A]:LYS:HB2	1:A:143[A]:LYS:HE2	1.69	0.42
1:A:92[A]:LYS:HE3	8:A:2318:HOH:O	2.20	0.41
1:A:262:PHE:CD2	1:A:291:LYS:HE3	2.55	0.41
1:A:123:GLY:HA3	1:A:199:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ILE:HB	1:A:160:THR:O	2.21	0.41

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	359/306 (117%)	350 (98%)	9 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	325/267 (122%)	324 (100%)	1 (0%)	86 61

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	245	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	A	1310[B]	-	25,25,25	1.37	4 (16%)	37,38,38	1.92	10 (27%)
2	ADP	A	1307	6	28,29,29	1.34	5 (17%)	43,45,45	0.94	2 (4%)
3	AMZ	A	1309[A]	-	22,23,23	0.90	0	32,35,35	1.59	6 (18%)
2	ADP	A	1311	-	28,29,29	1.51	4 (14%)	43,45,45	1.95	12 (27%)
5	SIN	A	1312	-	7,7,7	1.06	0	8,8,8	1.39	1 (12%)
7	SO4	A	1317	-	4,4,4	0.27	0	6,6,6	0.55	0
3	AMZ	A	1308	-	22,23,23	0.91	1 (4%)	32,35,35	0.90	2 (6%)
7	SO4	A	1315	-	4,4,4	0.26	0	6,6,6	0.32	0
7	SO4	A	1316	-	4,4,4	0.22	0	6,6,6	0.21	0
7	SO4	A	1318[A]	-	4,4,4	0.21	0	6,6,6	0.41	0
5	SIN	A	1313	-	7,7,7	0.99	0	8,8,8	1.38	1 (12%)

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	A	1310[B]	-	-	3/10/26/26	0/3/3/3
2	ADP	A	1307	6	-	3/16/32/32	0/3/3/3
3	AMZ	A	1309[A]	-	-	3/14/30/30	0/2/2/2
2	ADP	A	1311	-	-	1/16/32/32	0/3/3/3
5	SIN	A	1312	-	-	4/5/5/5	-
3	AMZ	A	1308	-	-	0/14/30/30	0/2/2/2
5	SIN	A	1313	-	-	5/5/5/5	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1311	ADP	C5-C4	4.16	1.46	1.39
4	A	1310[B]	AMP	C5-C4	4.12	1.46	1.39
2	A	1311	ADP	C5-N7	-3.48	1.32	1.39
2	A	1311	ADP	C8-N9	-2.88	1.32	1.37
4	A	1310[B]	AMP	C4-N9	-2.83	1.31	1.37
2	A	1307	ADP	PB-O3B	-2.54	1.45	1.54
2	A	1307	ADP	C4-N9	-2.45	1.32	1.37
2	A	1307	ADP	C5-N7	-2.41	1.34	1.39
4	A	1310[B]	AMP	C5-N7	-2.28	1.34	1.39
2	A	1311	ADP	C4-N9	-2.21	1.33	1.37
4	A	1310[B]	AMP	C5-C6	2.15	1.47	1.41
2	A	1307	ADP	C8-N9	-2.14	1.33	1.37
3	A	1308	AMZ	C3A-N1	-2.08	1.34	1.39
2	A	1307	ADP	PA-O2A	-2.05	1.45	1.55

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1311	ADP	N3-C4-N9	5.57	136.65	127.17
2	A	1311	ADP	C5-C4-N3	-5.22	119.53	126.72
4	A	1310[B]	AMP	C4-N9-C8	4.98	110.97	105.74
4	A	1310[B]	AMP	N3-C4-N9	4.39	134.63	127.17
2	A	1311	ADP	C4-N9-C8	4.20	110.15	105.74
3	A	1309[A]	AMZ	C5-N-C7A	4.13	109.80	106.62
4	A	1310[B]	AMP	C5-C4-N3	-4.13	121.03	126.72
4	A	1310[B]	AMP	N3-C2-N1	-3.76	122.89	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1309[A]	AMZ	C7A-C3A-N1	-3.57	108.56	109.91
3	A	1309[A]	AMZ	C6-C3A-C7A	-3.39	123.17	125.92
2	A	1311	ADP	N3-C2-N1	-3.31	123.58	128.58
4	A	1310[B]	AMP	C2-N3-C4	3.23	119.72	111.83
2	A	1311	ADP	O2A-PA-O3A	3.01	115.41	107.27
2	A	1311	ADP	N6-C6-N1	3.00	125.06	118.38
4	A	1310[B]	AMP	N9-C8-N7	-2.83	109.92	113.94
3	A	1309[A]	AMZ	C6-C3A-N1	2.78	128.18	123.06
2	A	1311	ADP	C2-N3-C4	2.77	118.60	111.83
5	A	1313	SIN	C3-C2-C1	-2.57	106.86	113.67
3	A	1309[A]	AMZ	N-C5-N1	-2.51	108.74	113.40
2	A	1311	ADP	C2-N1-C6	2.42	122.71	118.73
3	A	1309[A]	AMZ	C3A-C7A-N	2.41	106.74	105.75
2	A	1307	ADP	N3-C4-N9	2.32	131.12	127.17
5	A	1312	SIN	C3-C2-C1	-2.31	107.53	113.67
4	A	1310[B]	AMP	C4-C5-N7	-2.20	108.06	110.58
2	A	1311	ADP	C5-N7-C8	2.19	106.89	103.45
3	A	1308	AMZ	C5-N-C7A	2.14	108.27	106.62
2	A	1311	ADP	N9-C8-N7	-2.14	110.89	113.94
2	A	1307	ADP	C4-N9-C8	2.13	107.97	105.74
4	A	1310[B]	AMP	C6-C5-N7	2.08	136.10	132.09
4	A	1310[B]	AMP	C5-N7-C8	2.08	106.71	103.45
3	A	1308	AMZ	N-C5-N1	-2.06	109.58	113.40
2	A	1311	ADP	C4-C5-N7	-2.05	108.23	110.58
4	A	1310[B]	AMP	C2-N1-C6	2.05	122.10	118.73
2	A	1311	ADP	O3B-PB-O2B	2.00	115.30	107.80

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1311	ADP	C5'-O5'-PA-O1A
3	A	1309[A]	AMZ	C4-O3-P-OP1
3	A	1309[A]	AMZ	C4-O3-P-O4
3	A	1309[A]	AMZ	C4-O3-P-OP2
4	A	1310[B]	AMP	C5'-O5'-P-O2P
4	A	1310[B]	AMP	C5'-O5'-P-O3P
5	A	1313	SIN	C1-C2-C3-C4
2	A	1307	ADP	O4'-C4'-C5'-O5'
2	A	1307	ADP	C3'-C4'-C5'-O5'
4	A	1310[B]	AMP	C5'-O5'-P-O1P
5	A	1312	SIN	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

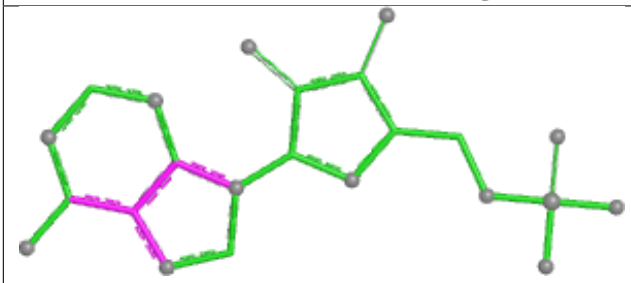
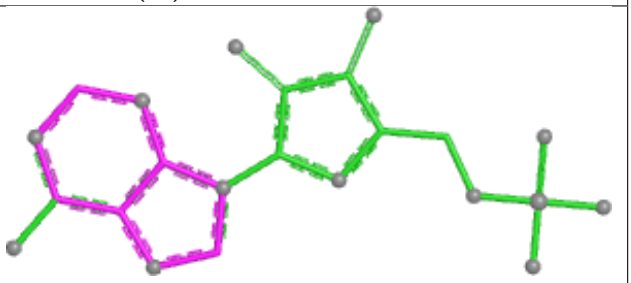
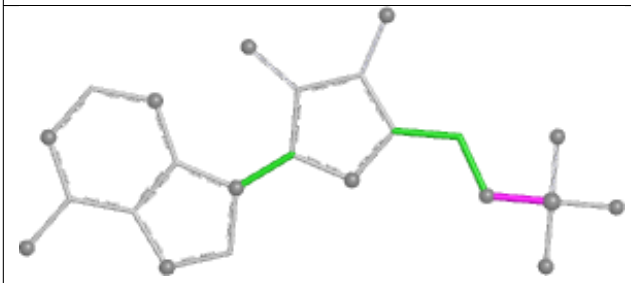
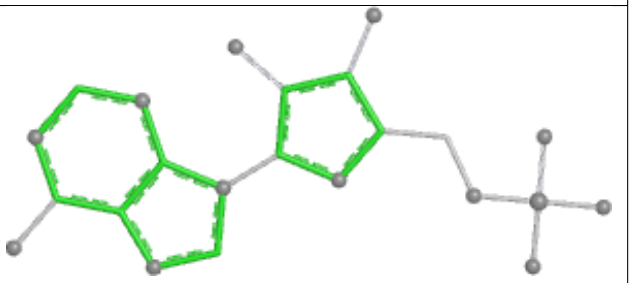
Mol	Chain	Res	Type	Atoms
2	A	1307	ADP	C4'-C5'-O5'-PA
5	A	1312	SIN	O1-C1-C2-C3
5	A	1313	SIN	C2-C3-C4-O3
5	A	1313	SIN	O2-C1-C2-C3
5	A	1313	SIN	C2-C3-C4-O4
5	A	1313	SIN	O1-C1-C2-C3
5	A	1312	SIN	C2-C3-C4-O4
5	A	1312	SIN	C2-C3-C4-O3

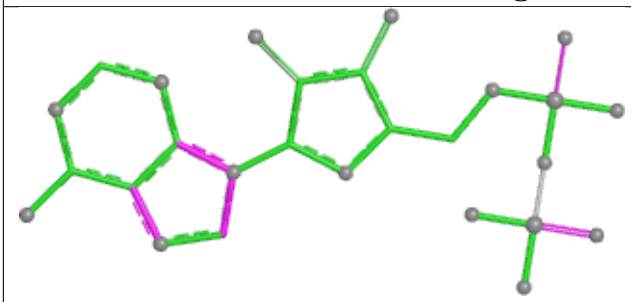
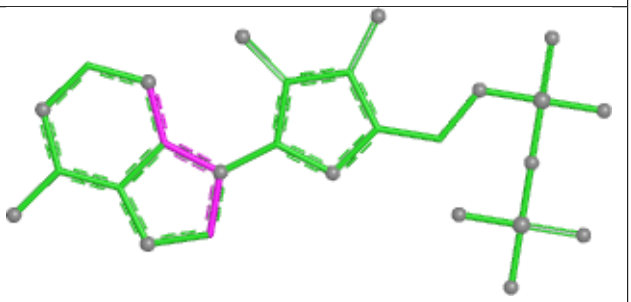
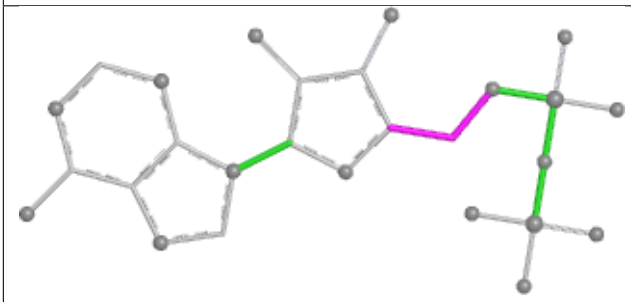
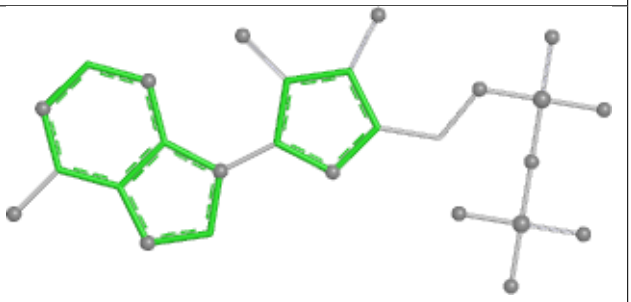
There are no ring outliers.

4 monomers are involved in 19 short contacts:

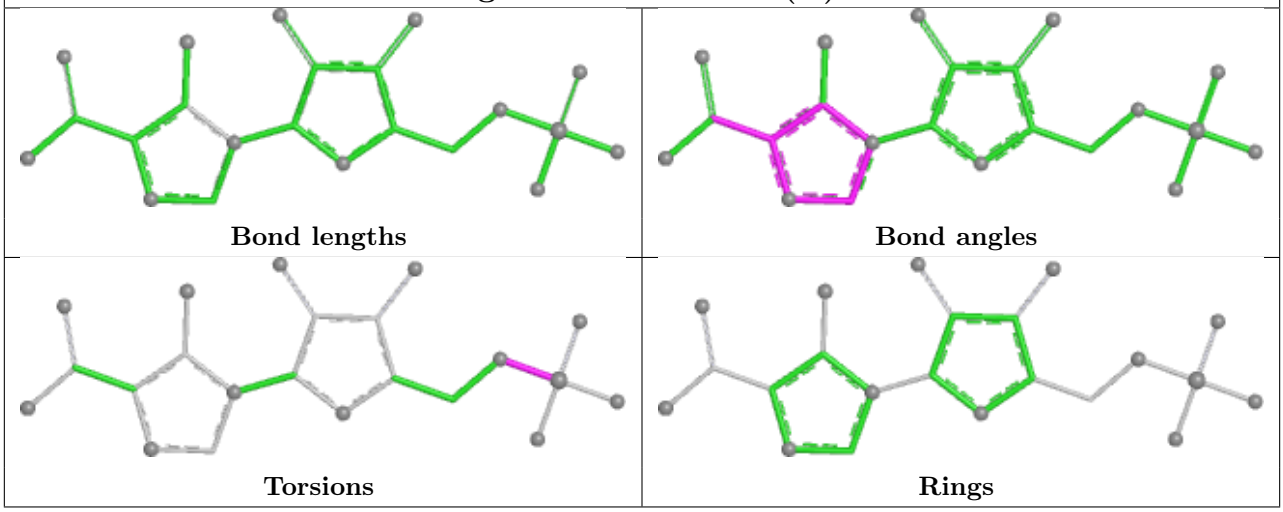
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1310[B]	AMP	7	0
2	A	1311	ADP	6	0
5	A	1312	SIN	3	0
5	A	1313	SIN	3	0

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.

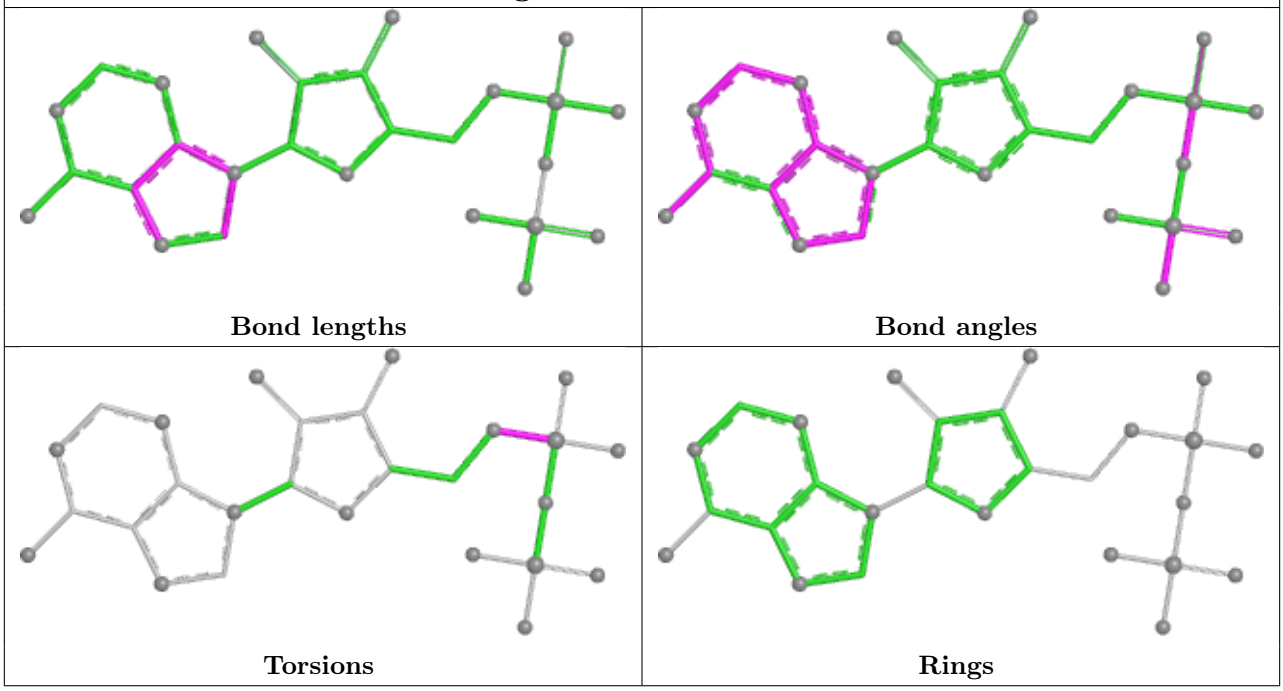
Ligand AMP A 1310 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

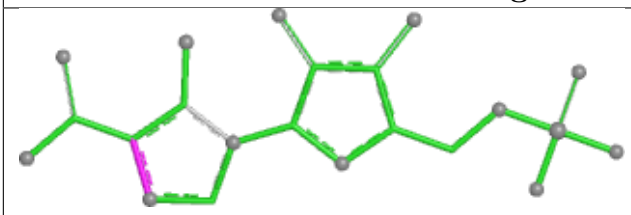
Ligand AMZ A 1309 (A)



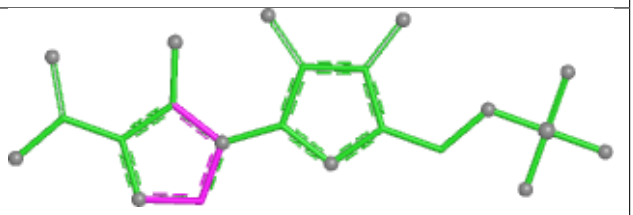
Ligand ADP A 1311



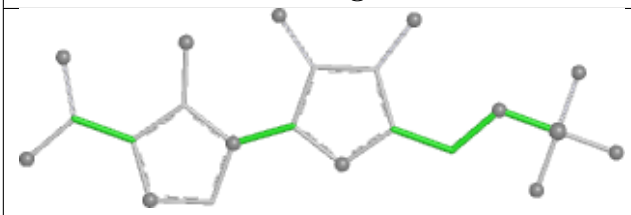
Ligand AMZ A 1308



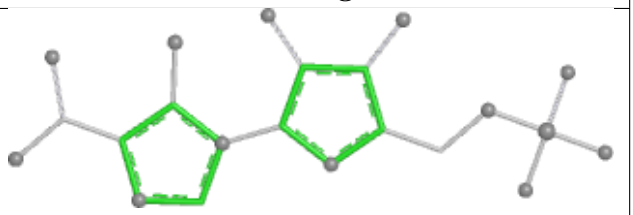
Bond lengths



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	301/306 (98%)	-0.25	6 (1%)	65 71	3, 8, 13, 23	66 (21%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225[A]	LYS	4.1
1	A	165	ALA	2.9
1	A	305[A]	SER	2.9
1	A	164	LYS	2.4
1	A	143[A]	LYS	2.2
1	A	170	HIS	2.0

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
5	SIN	A	1312	8/8	0.54	0.23	22,24,25,25	8

Continued on next page...

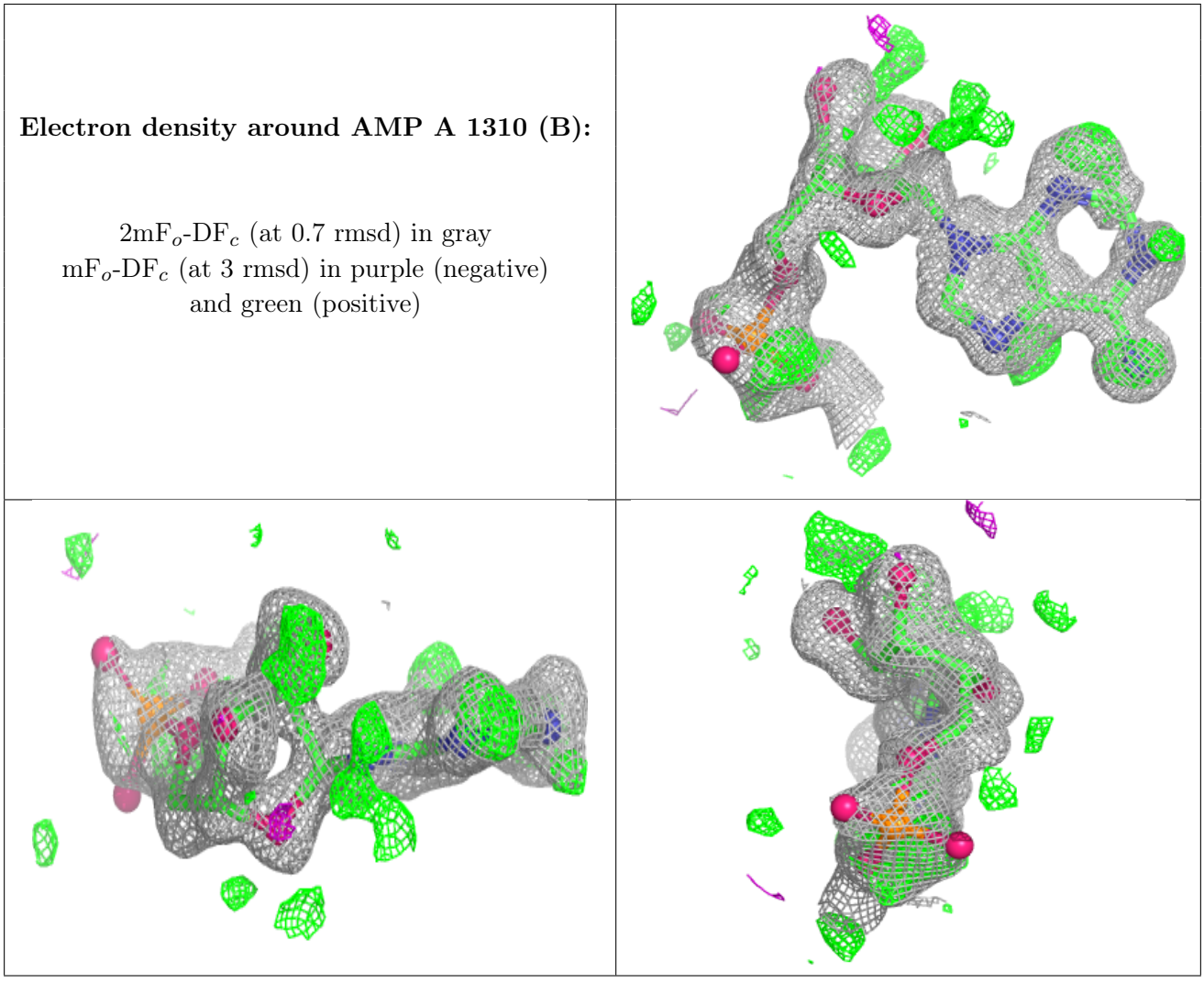
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SIN	A	1313	8/8	0.76	0.20	9,16,17,19	8
4	AMP	A	1310[B]	23/23	0.78	0.14	9,11,22,23	23
7	SO4	A	1316	5/5	0.88	0.10	21,22,22,22	5
7	SO4	A	1318[A]	5/5	0.89	0.17	10,10,13,13	5
3	AMZ	A	1309[A]	22/22	0.92	0.10	5,13,23,23	22
7	SO4	A	1317	5/5	0.92	0.10	12,12,14,15	5
2	ADP	A	1311	27/27	0.92	0.13	6,14,16,17	27
7	SO4	A	1315	5/5	0.95	0.10	14,14,17,17	5
2	ADP	A	1307	27/27	0.99	0.04	6,6,9,11	0
3	AMZ	A	1308	22/22	0.99	0.03	6,7,9,12	0
6	MG	A	1314	1/1	1.00	0.07	7,7,7,7	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.

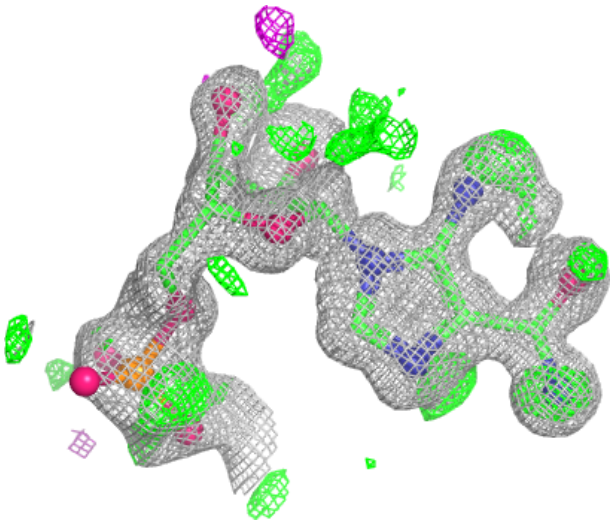
Electron density around AMP A 1310 (B):

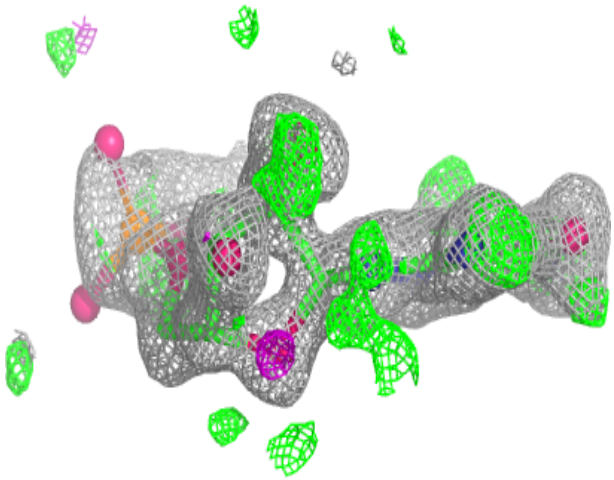
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

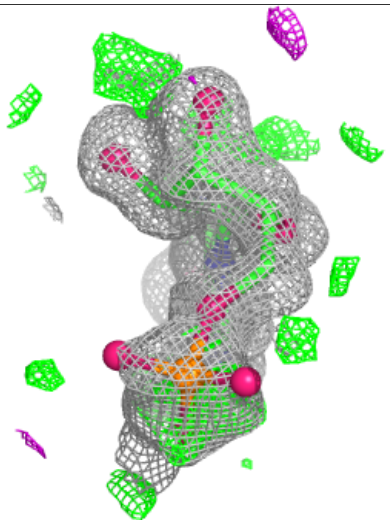


Electron density around AMZ A 1309 (A):

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

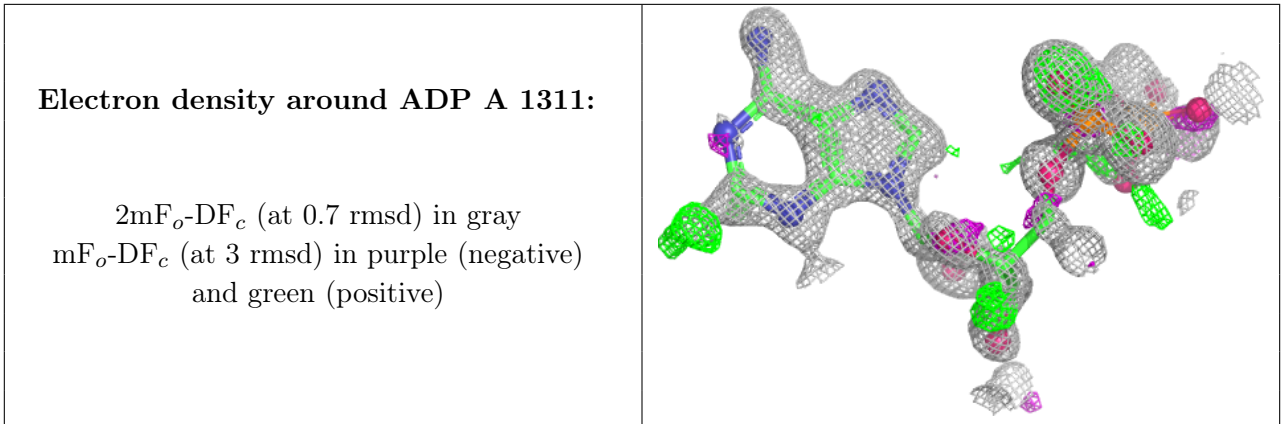


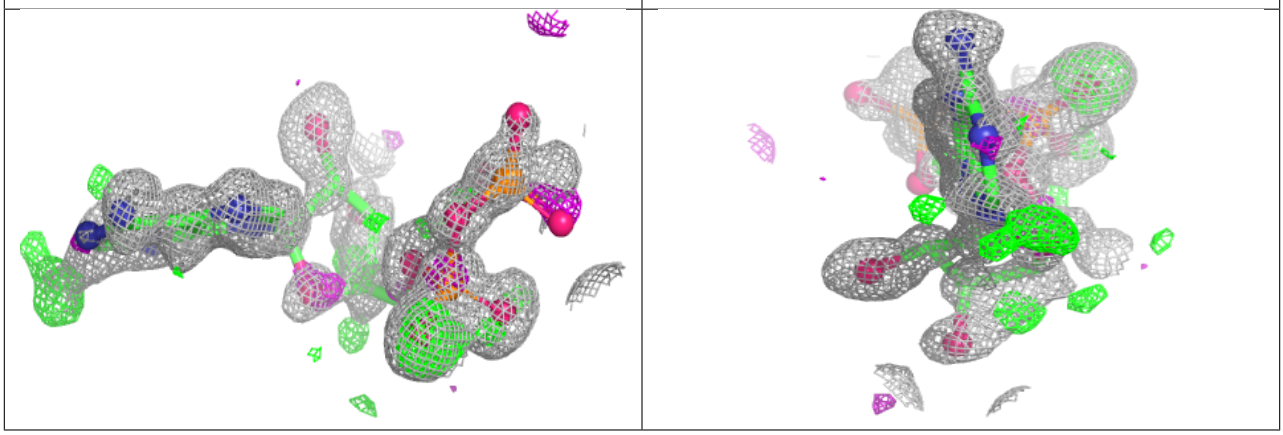




Electron density around ADP A 1311:

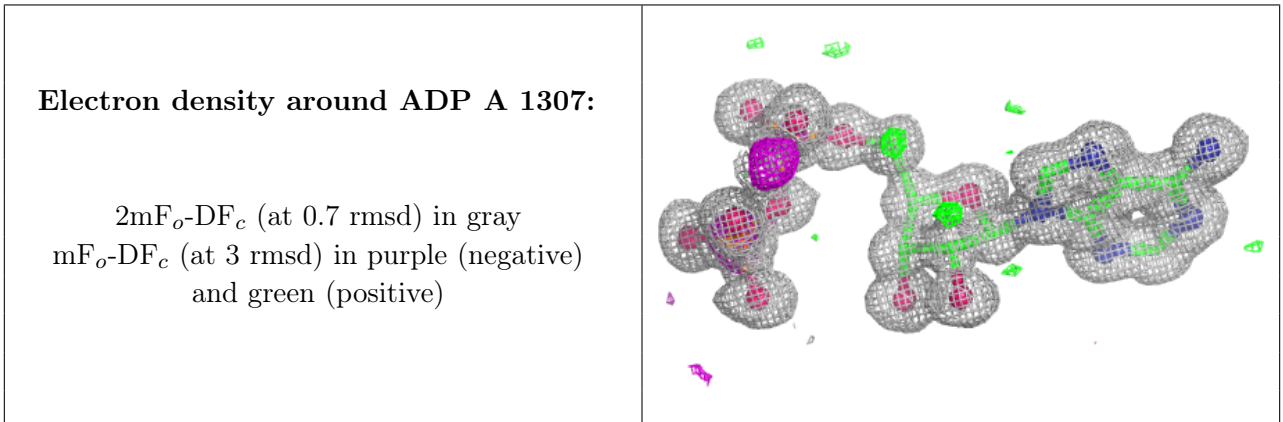
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

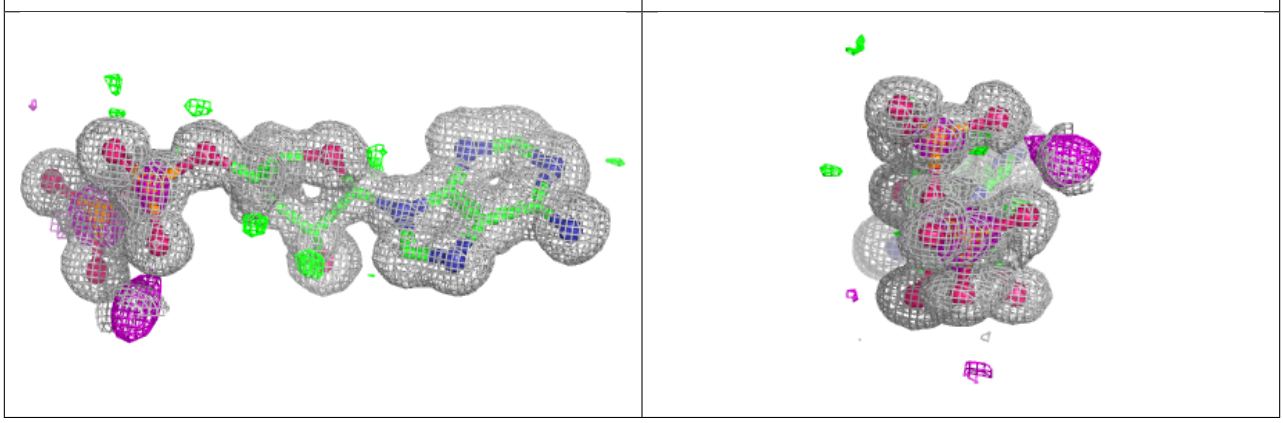




Electron density around ADP A 1307:

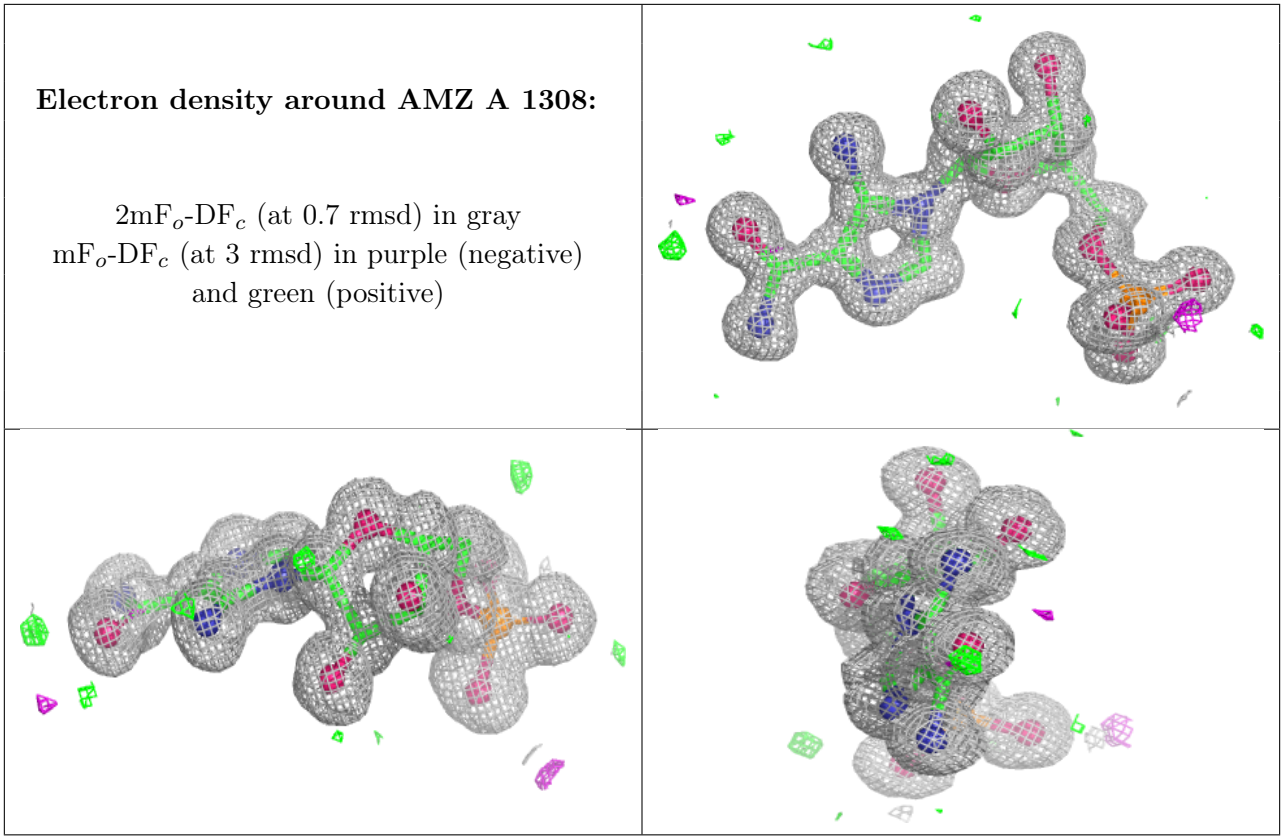
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around AMZ A 1308:

$2mF_o$-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.