



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2022 – 07:19 PM EST

PDB ID : 1IL2  
Title : Crystal Structure of the E. coli Aspartyl-tRNA Synthetase:Yeast tRNAasp:aspartyl-Adenylate Complex  
Authors : Moulinier, L.; Eiler, S.; Eriani, G.; Gangloff, J.; Thierry, J.C.; Gabriel, K.; McClain, W.H.; Moras, D.  
Deposited on : 2001-05-07  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 2.31.2  
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) : 2.31.2

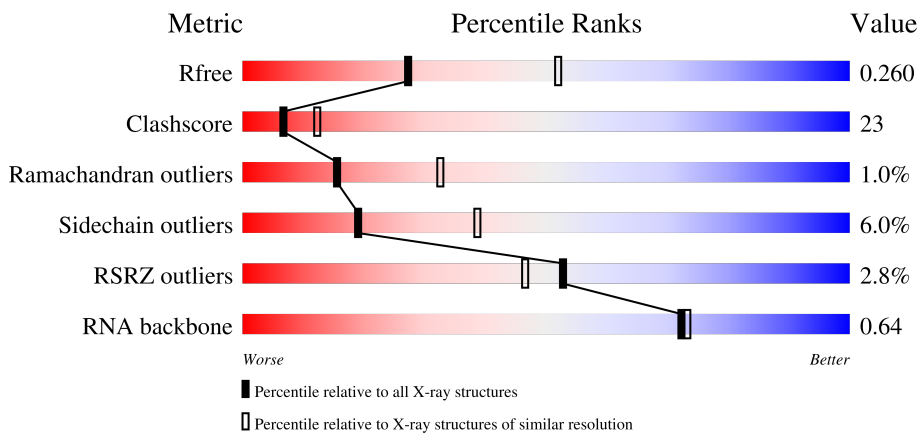
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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  $\geq 3$ , 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	C	75	
1	D	75	
2	A	590	

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Mol	Chain	Length	Quality of chain
2	B	590	

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
1	H2U	C	919	-	-	-	X
1	H2U	D	1919	-	-	-	X
3	SO4	C	701	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12753 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 RNA chain called ASPARTYL TRANSFER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	75	Total	C	N	O	P	0	0	0
			1601	715	280	531	75			
1	D	70	Total	C	N	O	P	0	0	0
			1496	668	262	496	70			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	913	PSU	U	modified residue	GB 176417
C	916	H2U	U	modified residue	GB 176417
C	919	H2U	U	modified residue	GB 176417
C	932	PSU	U	modified residue	GB 176417
C	937	1MG	G	modified residue	GB 176417
C	949	5MC	C	modified residue	GB 176417
C	954	5MU	U	modified residue	GB 176417
C	955	PSU	U	modified residue	GB 176417
D	1913	PSU	U	modified residue	GB 176417
D	1916	H2U	U	modified residue	GB 176417
D	1919	H2U	U	modified residue	GB 176417
D	1932	PSU	U	modified residue	GB 176417
D	1937	1MG	G	modified residue	GB 176417
D	1949	5MC	C	modified residue	GB 176417
D	1954	5MU	U	modified residue	GB 176417
D	1955	PSU	U	modified residue	GB 176417

- Molecule 2 is a protein called ASPARTYL-TRNA SYNTHETASE.

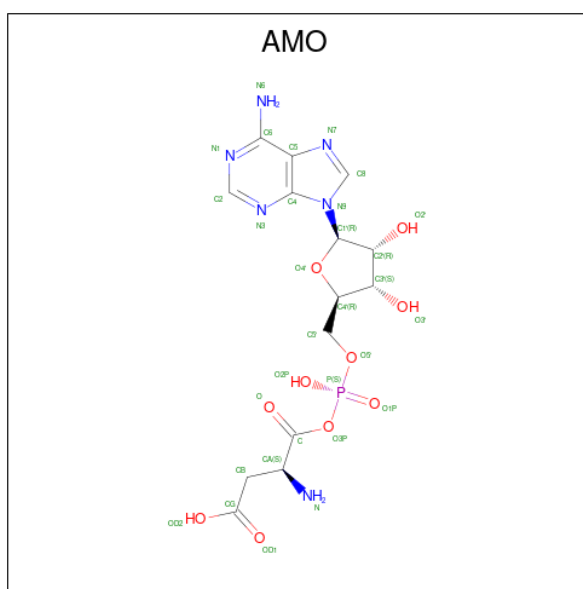
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	585	Total	C	N	O	S	0	0	0
			4591	2900	804	861	26			
2	B	585	Total	C	N	O	S	0	0	0
			4591	2900	804	861	26			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is ASPARTYL-ADENOSINE-5'-MONOPHOSPHATE (three-letter code: AMO) (formula: C<sub>14</sub>H<sub>19</sub>N<sub>6</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	14	6	10	1		
4	B	1	Total	C	N	O	P	0	0
			31	14	6	10	1		

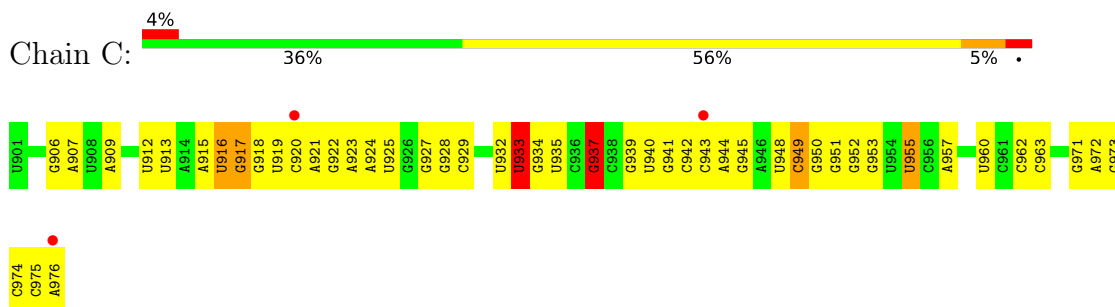
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	27	Total	O	0	0
			27	27		
5	D	33	Total	O	0	0
			33	33		
5	A	164	Total	O	0	0
			164	164		
5	B	178	Total	O	0	0
			178	178		

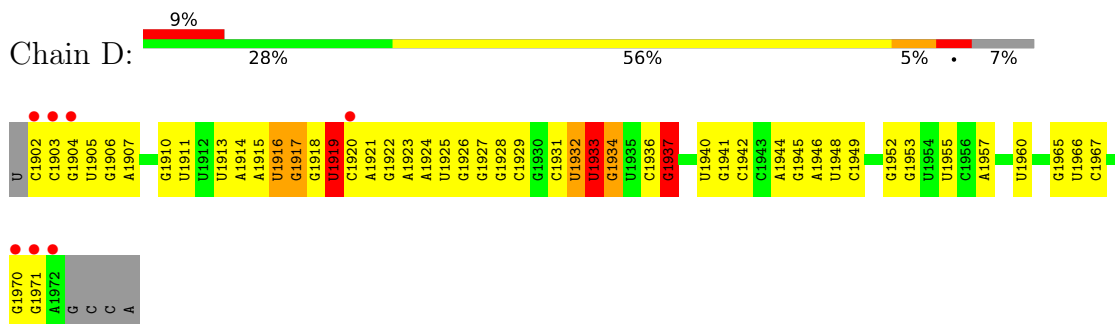
### 3 Residue-property plots [i](#)

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.

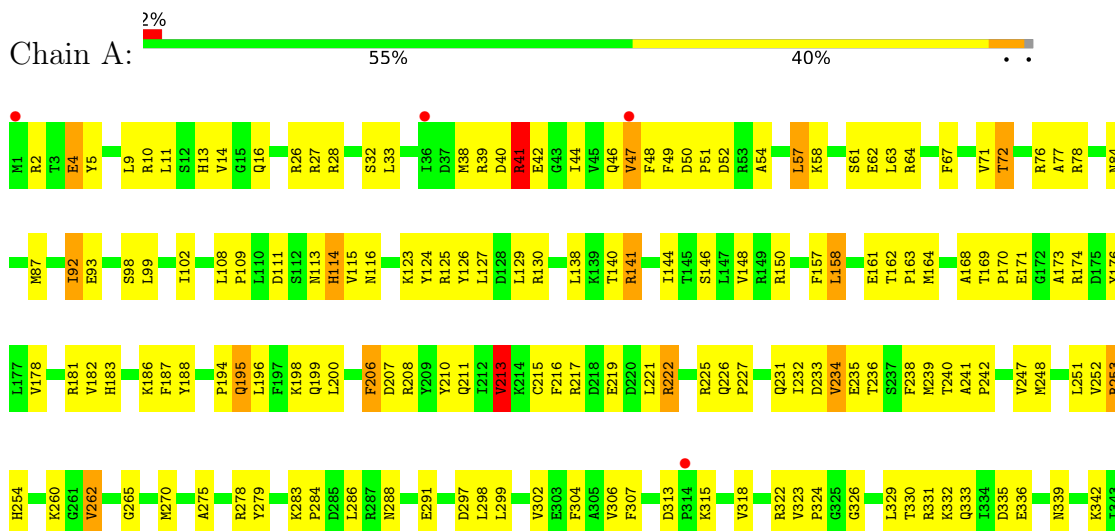
#### • Molecule 1: ASPARTYL TRANSFER RNA

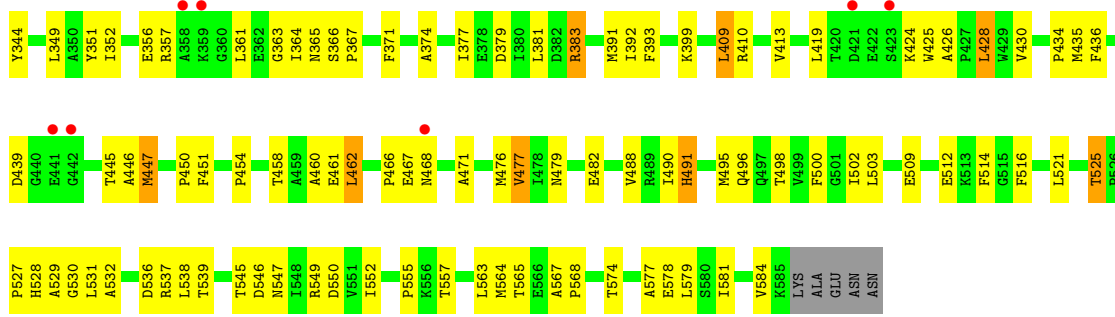


#### • Molecule 1: ASPARTYL TRANSFER RNA

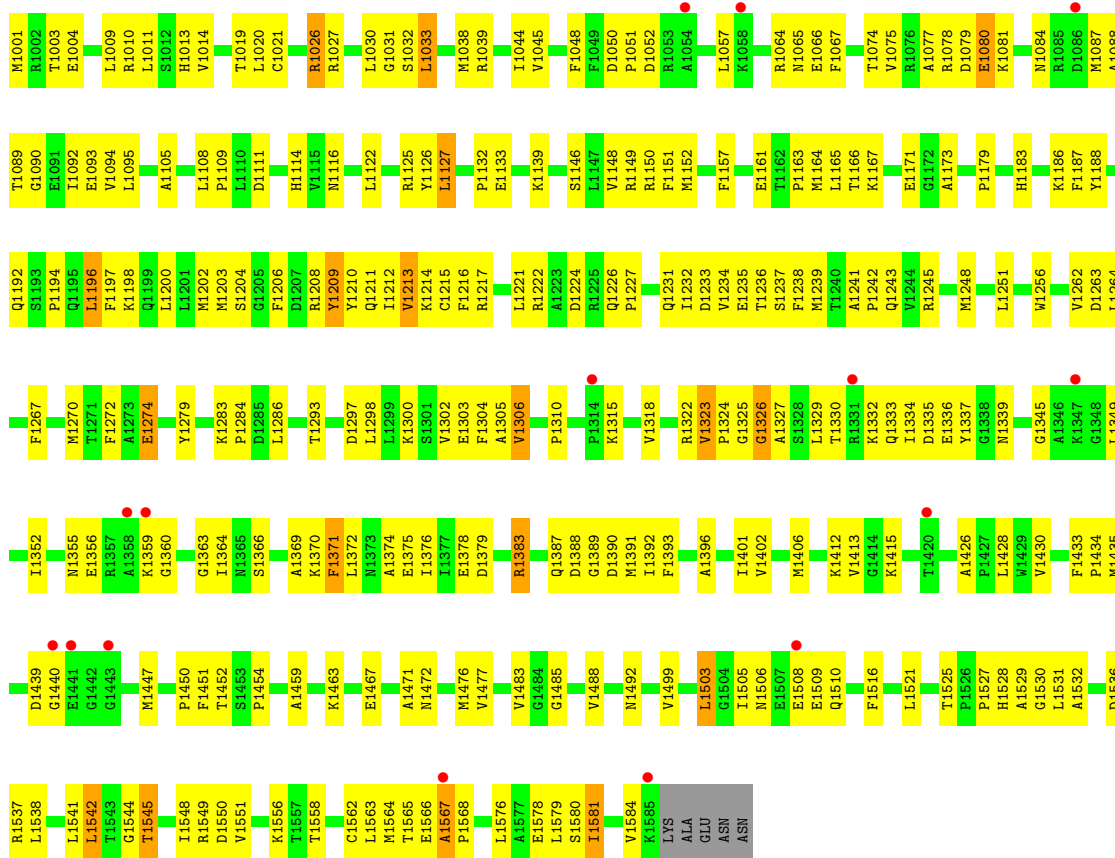


#### • Molecule 2: ASPARTYL-TRNA SYNTHETASE





● Molecule 2: ASPARTYL-TRNA SYNTHETASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.80Å 222.80Å 80.80Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	11.50 – 2.60 24.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.1 (11.50-2.60) 84.7 (24.27-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	3.70	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.50Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.204 , 0.257 0.208 , 0.260	Depositor DCC
$R_{free}$ test set	3668 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5MC, 5MU, SO4, AMO, 1MG, H2U, PSU

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	C	0.42	0/1604	0.71	1/2500 (0.0%)
1	D	0.41	1/1487 (0.1%)	0.68	1/2318 (0.0%)
2	A	0.40	0/4677	0.72	3/6320 (0.0%)
2	B	0.39	0/4677	0.72	1/6320 (0.0%)
All	All	0.40	1/12445 (0.0%)	0.71	6/17458 (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	C	0	2
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1902	C	P-O5'	5.67	1.65	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1902	C	O5'-P-OP2	-6.61	99.75	105.70
2	B	1232	ILE	N-CA-C	-6.43	93.65	111.00
2	A	213	VAL	CB-CA-C	-6.02	99.96	111.40
2	A	206	PHE	N-CA-C	-6.01	94.78	111.00
2	A	232	ILE	N-CA-C	-5.72	95.55	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	918	G	Sidechain
1	C	933	U	Sidechain
1	D	1933	U	Sidechain

## 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	C	1601	0	811	54	0
1	D	1496	0	757	32	0
2	A	4591	0	4590	246	0
2	B	4591	0	4587	246	0
3	B	5	0	0	0	0
3	C	5	0	0	2	0
4	A	31	0	17	1	0
4	B	31	0	17	1	0
5	A	164	0	0	11	0
5	B	178	0	0	8	0
5	C	27	0	0	2	0
5	D	33	0	0	0	0
All	All	12753	0	10779	537	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 23.

The worst 5 of 537 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)
2:A:236:THR:HB	2:A:239:MET:HE3	1.38	1.02
2:A:545:THR:HG22	2:A:547:ASN:H	1.23	0.99
2:B:1009:LEU:HA	2:B:1013:HIS:HD2	1.27	0.99
2:A:161:GLU:HA	2:A:211:GLN:NE2	1.80	0.96
2:A:547:ASN:OD1	2:A:549:ARG:HG2	1.66	0.95

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	
2	A	583/590 (99%)	539 (92%)	40 (7%)	4 (1%)	22	43
2	B	583/590 (99%)	520 (89%)	55 (9%)	8 (1%)	11	22
All	All	1166/1180 (99%)	1059 (91%)	95 (8%)	12 (1%)	15	32

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	41	ARG
2	A	115	VAL
2	B	1305	ALA
2	B	1326	GLY
2	B	1567	ALA

### 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	
2	A	486/490 (99%)	453 (93%)	33 (7%)	16	32
2	B	486/490 (99%)	461 (95%)	25 (5%)	24	46
All	All	972/980 (99%)	914 (94%)	58 (6%)	19	39

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	491	HIS
2	B	1545	THR
2	B	1033	LEU
2	B	1542	LEU
2	B	1274	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1116	ASN
2	B	1497	GLN
2	B	1199	GLN
2	A	491	HIS
2	B	1114	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	6 (8%)	0
1	D	69/75 (92%)	6 (8%)	1 (1%)
All	All	143/150 (95%)	12 (8%)	1 (0%)

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	917	G
1	C	919	H2U
1	C	933	U
1	C	934	G
1	C	937	1MG

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	1933	U

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

16 non-standard protein/DNA/RNA residues 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
1	H2U	C	916	1	18,21,22	0.86	1 (5%)	21,30,33	0.64	0
1	5MU	D	1954	1	19,22,23	0.34	0	28,32,35	0.53	0
1	PSU	D	1913	1	18,21,22	1.82	1 (5%)	22,30,33	0.83	1 (4%)
1	5MU	C	954	1	19,22,23	0.28	0	28,32,35	0.37	0
1	H2U	D	1916	1	18,21,22	0.67	1 (5%)	21,30,33	0.73	1 (4%)
1	PSU	D	1932	1	18,21,22	1.78	1 (5%)	22,30,33	0.76	1 (4%)
1	PSU	D	1955	1	18,21,22	1.82	1 (5%)	22,30,33	0.64	0
1	PSU	C	932	1	18,21,22	1.80	1 (5%)	22,30,33	0.76	1 (4%)
1	PSU	C	913	1	18,21,22	1.77	1 (5%)	22,30,33	0.82	0
1	5MC	D	1949	1	18,22,23	0.34	0	26,32,35	0.87	2 (7%)
1	H2U	D	1919	1	18,21,22	0.69	1 (5%)	21,30,33	0.74	0
1	1MG	D	1937	1	18,26,27	0.96	1 (5%)	19,39,42	1.47	3 (15%)
1	1MG	C	937	1	18,26,27	0.97	1 (5%)	19,39,42	1.41	3 (15%)
1	H2U	C	919	1	18,21,22	0.60	0	21,30,33	0.73	0
1	PSU	C	955	1	18,21,22	1.75	1 (5%)	22,30,33	0.70	1 (4%)
1	5MC	C	949	1	18,22,23	0.32	0	26,32,35	0.88	2 (7%)

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
1	H2U	C	916	1	-	0/7/38/39	0/2/2/2
1	5MU	D	1954	1	-	0/7/25/26	0/2/2/2
1	PSU	D	1913	1	-	3/7/25/26	0/2/2/2
1	5MU	C	954	1	-	0/7/25/26	0/2/2/2
1	H2U	D	1916	1	-	0/7/38/39	0/2/2/2
1	PSU	D	1932	1	-	1/7/25/26	0/2/2/2
1	PSU	D	1955	1	-	0/7/25/26	0/2/2/2
1	PSU	C	932	1	-	1/7/25/26	0/2/2/2
1	PSU	C	913	1	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	D	1949	1	-	0/7/25/26	0/2/2/2
1	H2U	D	1919	1	-	4/7/38/39	0/2/2/2
1	1MG	D	1937	1	-	1/3/25/26	0/3/3/3
1	1MG	C	937	1	-	0/3/25/26	0/3/3/3
1	H2U	C	919	1	-	0/7/38/39	0/2/2/2
1	PSU	C	955	1	-	1/7/25/26	0/2/2/2
1	5MC	C	949	1	-	2/7/25/26	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1913	PSU	C6-N1	-7.20	1.24	1.36
1	D	1932	PSU	C6-N1	-7.19	1.24	1.36
1	D	1955	PSU	C6-N1	-7.10	1.24	1.36
1	C	913	PSU	C6-N1	-7.10	1.24	1.36
1	C	955	PSU	C6-N1	-7.05	1.24	1.36

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1937	1MG	C2-N1-C6	4.56	124.65	120.95
1	C	937	1MG	C2-N1-C6	4.44	124.55	120.95
1	D	1949	5MC	C5-C6-N1	-3.27	119.97	123.34
1	D	1937	1MG	CM1-N1-C2	-2.97	117.64	120.72
1	C	949	5MC	C5-C6-N1	-2.95	120.30	123.34

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	1919	H2U	O4'-C1'-N1-C2
1	D	1919	H2U	O4'-C1'-N1-C6
1	D	1913	PSU	O4'-C4'-C5'-O5'
1	D	1919	H2U	C2'-C1'-N1-C6
1	D	1919	H2U	C2'-C1'-N1-C2

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	916	H2U	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	1916	H2U	1	0
1	D	1932	PSU	1	0
1	D	1919	H2U	1	0
1	D	1937	1MG	1	0
1	C	937	1MG	1	0
1	C	955	PSU	1	0
1	C	949	5MC	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	SO4	C	701	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	B	1701	-	4,4,4	0.23	0	6,6,6	0.10	0
4	AMO	B	1831	-	28,33,33	0.81	1 (3%)	31,49,49	1.33	2 (6%)
4	AMO	A	831	-	28,33,33	0.84	1 (3%)	31,49,49	1.58	3 (9%)

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	AMO	B	1831	-	-	1/17/39/39	0/3/3/3
4	AMO	A	831	-	-	1/17/39/39	0/3/3/3

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	831	AMO	P-O3P	2.57	1.65	1.60
4	B	1831	AMO	P-O3P	2.08	1.64	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	831	AMO	O3P-P-O5'	7.13	123.74	102.92
4	B	1831	AMO	O3P-P-O5'	5.61	119.31	102.92
4	A	831	AMO	C5-C6-N6	2.41	124.01	120.35
4	B	1831	AMO	C5-C6-N6	2.32	123.88	120.35
4	A	831	AMO	O2P-P-O3P	-2.19	96.98	104.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

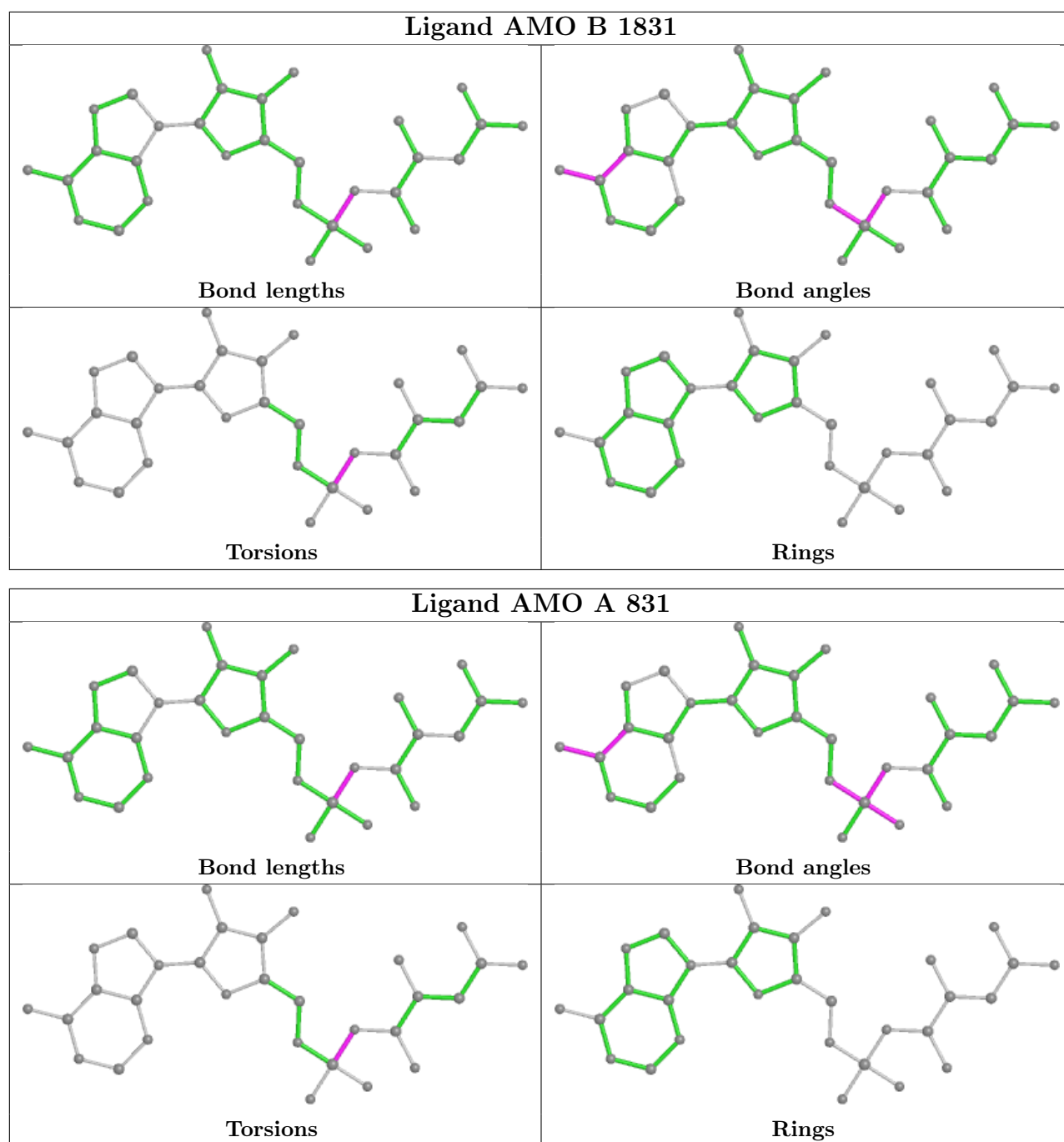
Mol	Chain	Res	Type	Atoms
4	A	831	AMO	C-O3P-P-O5'
4	B	1831	AMO	C-O3P-P-O5'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	SO4	2	0
4	B	1831	AMO	1	0
4	A	831	AMO	1	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.



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	67/75 (89%)	0.15	3 (4%) 33 26	36, 59, 80, 99	0
1	D	62/75 (82%)	0.21	7 (11%) 5 3	39, 54, 94, 101	0
2	A	585/590 (99%)	-0.21	11 (1%) 66 62	18, 37, 66, 86	0
2	B	585/590 (99%)	-0.16	15 (2%) 56 50	20, 40, 67, 92	0
All	All	1299/1330 (97%)	-0.15	36 (2%) 53 46	18, 41, 70, 101	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1920	C	6.9
1	D	1972	A	5.8
1	C	976	A	4.5
1	C	920	C	4.3
1	D	1902	C	4.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H2U	D	1919	20/21	0.72	0.52	92,101,101,101	0
1	H2U	C	919	20/21	0.78	0.40	99,101,101,101	0
1	5MU	C	954	21/22	0.84	0.24	38,70,83,85	0
1	PSU	C	955	20/21	0.85	0.24	64,76,87,89	0
1	1MG	D	1937	24/25	0.85	0.28	58,72,100,101	0
1	5MC	C	949	21/22	0.87	0.22	50,68,87,89	0
1	1MG	C	937	24/25	0.88	0.26	57,66,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	C	932	20/21	0.90	0.16	50,70,76,81	0
1	PSU	D	1932	20/21	0.94	0.16	55,63,66,70	0
1	PSU	C	913	20/21	0.94	0.16	44,52,60,60	0
1	PSU	D	1955	20/21	0.94	0.14	37,49,56,57	0
1	PSU	D	1913	20/21	0.95	0.15	43,56,63,64	0
1	5MC	D	1949	21/22	0.95	0.18	46,51,54,57	0
1	5MU	D	1954	21/22	0.95	0.14	29,45,51,52	0
1	H2U	D	1916	20/21	0.95	0.22	59,65,69,71	0
1	H2U	C	916	20/21	0.96	0.19	63,67,72,73	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

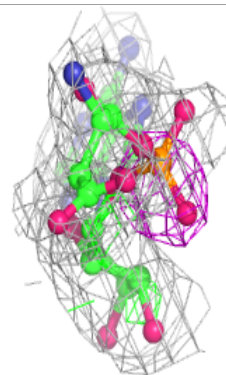
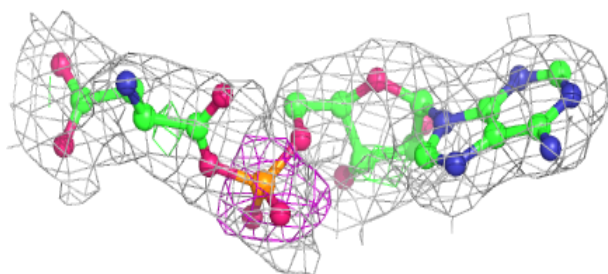
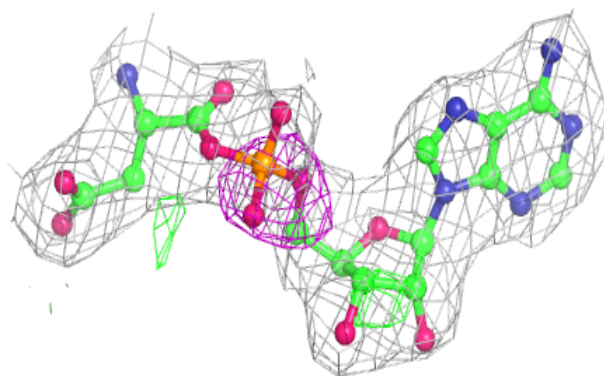
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	AMO	B	1831	31/31	0.91	0.20	23,36,65,75	0
4	AMO	A	831	31/31	0.94	0.16	16,33,64,72	0
3	SO4	C	701	5/5	0.94	0.22	97,97,100,101	0
3	SO4	B	1701	5/5	0.96	0.15	64,68,72,72	0

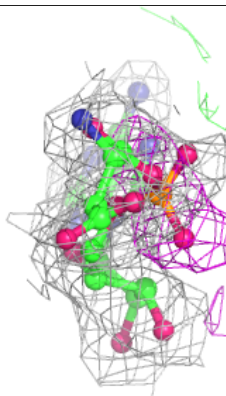
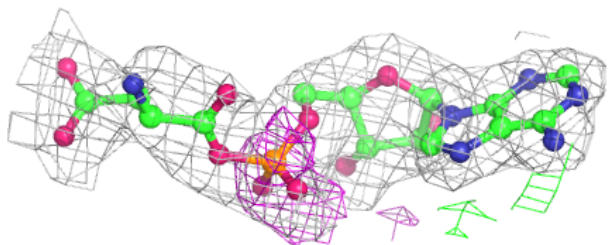
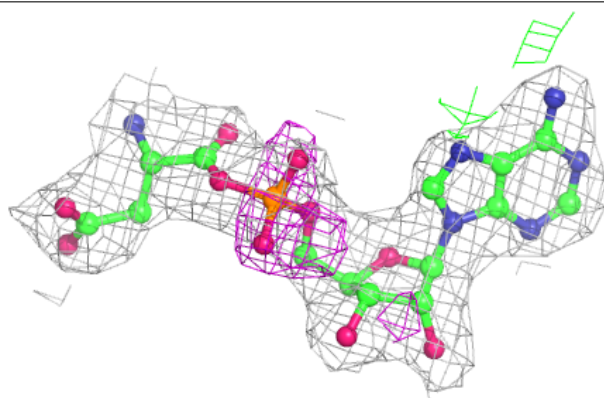
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AMO B 1831:**

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

**Electron density around AMO A 831:**

$2mF_o-DF_c$  (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.