

Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 06:54 AM EST

PDB ID	:	1C0K
Title	:	CRYSTAL STRUCTURE ANALYSIS OF D-AMINO ACID OXIDASE IN
		COMPLEX WITH L-LACTATE
Authors	:	Umhau, S.; Molla, G.; Diederichs, K.; Pilone, M.S.; Ghisla, S.; Welte, W.;
		Pollegioni, L.
Deposited on		
Resolution	:	1.46 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 (i) 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 (i)) were used in the production of this report:

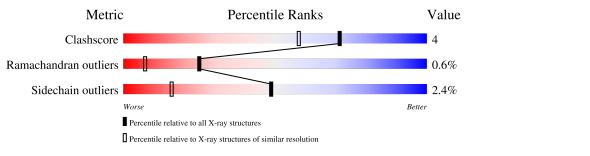
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.46 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)

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%

Mol	Chain	Length	Quality of chain		
1	А	363	90%	9%	•

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
3	LAC	А	1364	Х	-	-	-



$1\mathrm{C0K}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3482 atoms, of which 1 is hydrogen 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.

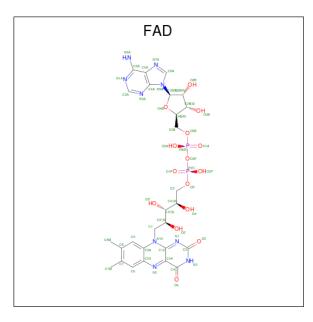
• Molecule 1 is a protein called PROTEIN (D-AMINO ACID OXIDASE).

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	363	Total 2799	C 1763	N 500	O 525	S 11	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	999	LEU	-	cloning artifact	UNP P80324
А	1000	MET	-	cloning artifact	UNP P80324

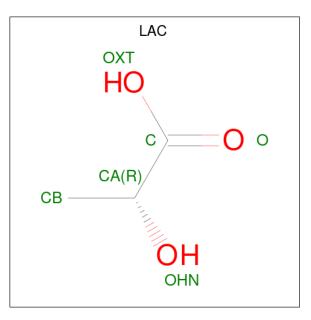
• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
2	А	1	Total 54	С 27	Н 1	N 9		Р 2	0	0



• Molecule 3 is LACTIC ACID (three-letter code: LAC) (formula: C₃H₆O₃).



Μ	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
e j	}	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is water.

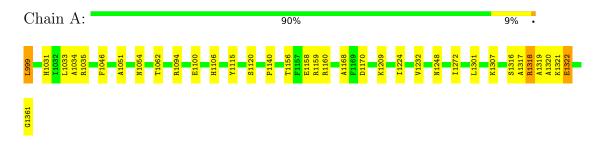
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	623	Total O 623 623	0	0



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. 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. 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: PROTEIN (D-AMINO ACID OXIDASE)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants	120.67Å 120.67Å 136.37Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 - 1.46	Depositor
Resolution (A)	42.54 - 1.47	EDS
% Data completeness	99.1 (100.00-1.46)	Depositor
(in resolution range)	98.3 (42.54 - 1.47)	EDS
R _{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.86 (at 1.47 \text{\AA})$	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
II, II, <i>free</i>	0.137 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	13.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 78.9	EDS
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3482	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage'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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, LAC

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).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	5.05	2/2881~(0.1%)	0.86	3/3915~(0.1%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	1361	GLY	C-OXT	270.41	6.37	1.23
1	А	1318	ARG	NE-CZ	7.44	1.42	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	1062	THR	C-N-CA	5.57	135.62	121.70
1	А	1035	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	А	1320	ALA	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

There are no planarity outliers.

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	А	2799	0	2778	19	0
2	А	53	1	28	1	0
3	А	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashe
4	А	623	0	0	6	0
All	All	3481	1	2806	20	0

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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 4.

All (20) 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:1033:LEU:HD11	1:A:1170[B]:ASP:OD2	1.85	0.76
1:A:1317:ALA:O	1:A:1318:ARG:HG3	1.87	0.75
1:A:1301:LEU:O	1:A:1322:GLU:HA	1.88	0.72
1:A:1272:ILE:HG12	4:A:3230:HOH:O	1.91	0.71
1:A:1321:LYS:O	1:A:1322:GLU:HB2	2.00	0.60
1:A:1209:LYS:HE2	4:A:3245:HOH:O	2.04	0.57
1:A:1100:GLU:OE1	1:A:1106:HIS:HE1	1.88	0.56
1:A:1317:ALA:HB3	4:A:3428:HOH:O	2.06	0.56
1:A:1140:PRO:HG3	4:A:3179:HOH:O	2.07	0.53
1:A:1031:HIS:HD2	1:A:1156:THR:OG1	1.93	0.52
1:A:1031:HIS:HE1	1:A:1158:GLU:OE1	1.94	0.50
1:A:1106:HIS:HD2	1:A:1115:TYR:OH	1.95	0.50
1:A:1307:LYS:HG3	1:A:1307:LYS:O	2.09	0.49
1:A:1168:ALA:O	1:A:1170[B]:ASP:OD1	2.30	0.49
1:A:1224:ILE:HG23	1:A:1232[B]:VAL:HG11	1.97	0.46
1:A:1034:ALA:O	1:A:1159:ARG:HA	2.17	0.45
1:A:999:LEU:N	4:A:3593:HOH:O	2.50	0.45
1:A:1160:ARG:NH1	1:A:1170[B]:ASP:OD2	2.50	0.45
1:A:1051:ALA:HA	2:A:1363:FAD:C5X	2.49	0.42

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	А	365/363~(101%)	350~(96%)	13 (4%)	2~(0%)	29 9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1322	GLU
1	А	1319	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	299/295~(101%)	292~(98%)	7 (2%)	50 17

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	999	LEU
1	А	1046	PHE
1	А	1054	ASN
1	А	1094	ARG
1	А	1120	SER
1	А	1248	ASN
1	А	1316	SER

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

Mol	Chain	Res	Type
1	А	1004	GLN
1	А	1031	HIS
1	А	1054	ASN
1	А	1106	HIS
1	А	1167	GLN
1	А	1177	ASN
1	А	1248	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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).

Mal	Mol Type Chain Res Li		Link	Bond lengths			Bond angles			
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	FAD	А	1363	-	$53,\!58,\!58$	2.74	20 (37%)	68,89,89	<mark>3.53</mark>	30 (44%)
3	LAC	А	1364	-	$5,\!5,\!5$	2.94	1 (20%)	4,6,6	2.91	2 (50%)

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	FAD	А	1363	-	-	1/30/50/50	0/6/6/6
3	LAC	А	1364	-	1/1/2/2	2/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	1363	FAD	O4-C4	6.29	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1363	FAD	C6-C5X	6.27	1.49	1.40
2	A	1363	FAD	C2B-C3B	-5.93	1.37	1.53
3	A	1364	LAC	O-C	5.76	1.39	1.22
2	A	1363	FAD	O3'-C3'	-5.40	1.30	1.43
2	A	1363	FAD	C9A-N10	5.25	1.50	1.41
2	А	1363	FAD	C9A-C5X	-5.14	1.32	1.41
2	А	1363	FAD	C2A-N3A	4.96	1.40	1.32
2	А	1363	FAD	C2'-C3'	-4.88	1.44	1.53
2	А	1363	FAD	O2'-C2'	4.49	1.52	1.43
2	А	1363	FAD	C1'-N10	-3.89	1.38	1.48
2	А	1363	FAD	C2A-N1A	3.28	1.40	1.33
2	А	1363	FAD	C4X-N5	3.14	1.36	1.30
2	А	1363	FAD	C3B-C4B	3.12	1.61	1.53
2	А	1363	FAD	C4A-N3A	2.95	1.39	1.35
2	А	1363	FAD	O2B-C2B	-2.86	1.36	1.43
2	А	1363	FAD	O4B-C1B	2.55	1.44	1.41
2	А	1363	FAD	C8M-C8	2.45	1.55	1.51
2	А	1363	FAD	C10-N1	2.42	1.38	1.33
2	А	1363	FAD	P-O2P	-2.24	1.44	1.55
2	А	1363	FAD	C5A-C4A	-2.18	1.35	1.40

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All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1363	FAD	C9A-C5X-N5	9.78	133.06	122.43
2	А	1363	FAD	C6-C7-C8	-9.30	106.34	119.67
2	А	1363	FAD	C9-C8-C7	8.97	132.53	119.67
2	А	1363	FAD	C6-C5X-C9A	-7.77	107.95	118.94
2	А	1363	FAD	C9-C9A-N10	-7.13	112.19	121.84
2	А	1363	FAD	O4B-C1B-C2B	-6.74	97.07	106.93
2	А	1363	FAD	C9-C9A-C5X	6.51	132.42	120.11
2	А	1363	FAD	C4X-C10-N10	6.14	125.46	116.48
2	А	1363	FAD	O3'-C3'-C2'	5.22	121.43	108.81
2	А	1363	FAD	C8M-C8-C7	-5.20	110.07	120.74
2	А	1363	FAD	C9A-C9-C8	-5.13	108.97	119.30
2	А	1363	FAD	O2-C2-N1	5.09	130.26	121.83
3	А	1364	LAC	CB-CA-C	5.01	121.98	110.63
2	А	1363	FAD	C5X-C6-C7	4.82	129.56	120.71
2	А	1363	FAD	C5X-N5-C4X	-4.48	110.63	118.07
2	А	1363	FAD	C7M-C7-C8	4.17	129.29	120.74
2	А	1363	FAD	C9A-N10-C10	-4.09	114.40	120.77
2	А	1363	FAD	C5X-C9A-N10	-3.67	114.17	117.95

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1363	FAD	C2B-C3B-C4B	-3.55	95.74	102.64
2	А	1363	FAD	C3B-C2B-C1B	3.17	105.75	100.98
2	А	1363	FAD	C4A-C5A-N7A	-3.13	106.14	109.40
2	А	1363	FAD	C1'-N10-C9A	3.05	125.59	120.51
2	А	1363	FAD	O5B-C5B-C4B	-3.00	98.67	108.99
2	А	1363	FAD	C4-C4X-C10	2.86	121.60	116.79
2	А	1363	FAD	N3-C2-N1	-2.73	114.03	119.38
2	А	1363	FAD	C10-N1-C2	2.70	122.31	116.90
2	А	1363	FAD	O2B-C2B-C1B	-2.69	100.94	110.85
2	А	1363	FAD	O3B-C3B-C2B	2.68	120.50	111.82
2	А	1363	FAD	C7M-C7-C6	2.62	124.33	119.49
2	А	1363	FAD	O3'-C3'-C4'	-2.45	102.90	108.81
3	А	1364	LAC	OXT-C-O	2.37	129.47	124.09
2	А	1363	FAD	C4X-C10-N1	-2.27	119.46	124.73

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All (1) chirality outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atom
3	А	1364	LAC	CA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1364	LAC	OXT-C-CA-CB
3	А	1364	LAC	O-C-CA-CB
2	А	1363	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

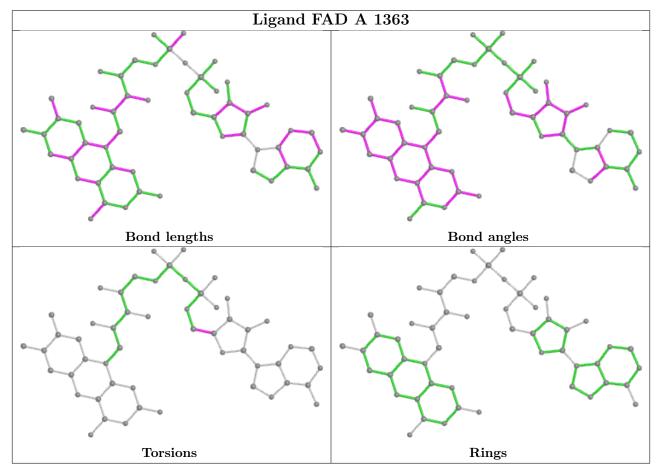
1 monomer is involved in 1 short contact:

Mo	1 (Chain	Res	Type	Clashes	Symm-Clashes
2		А	1363	FAD	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 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.



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

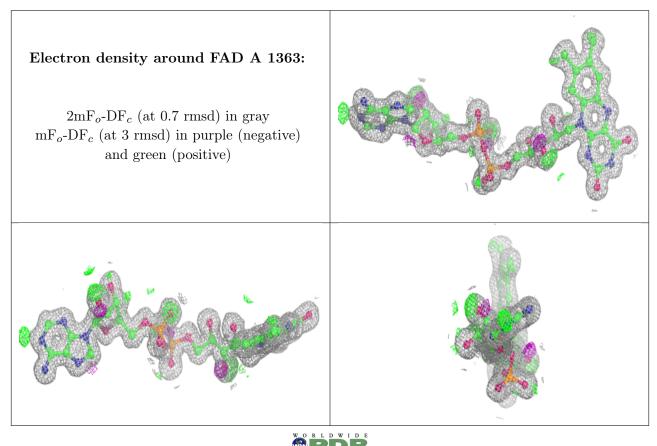
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

