

Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 04:15 pm BST

PDB ID : 3CV2

Title : Atomic Resolution Structures of Escherichia coli and Bacillis anthracis Malate

Synthase A: Comparison with Isoform G and Implications for Structure Based

Drug Design

Authors: Lohman, J.R.; Remington, S.J.

Deposited on : 2008-04-17

Resolution : 1.40 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 following versions of software and data (see references (1)) 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 : 2.11

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

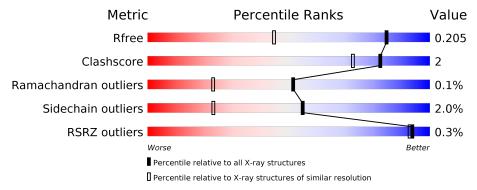
Validation Pipeline (wwPDB-VP) : 2.11

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 1.40 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 on 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	532	91%	7%				
1	В	532	92%	6%	•			



2 Entry composition (i)

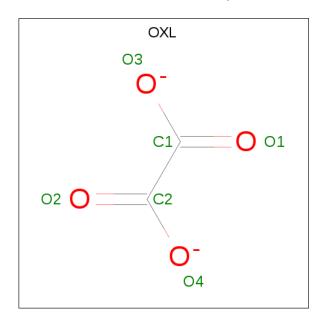
There are 5 unique types of molecules in this entry. The entry contains 9663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Malate synthase A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	524	Total 4220	C 2692	N 729	O 779	S 20	3	14	0
1	В	525	Total 4210	C 2683	N 730	O 777	S 20	0	10	0

• Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



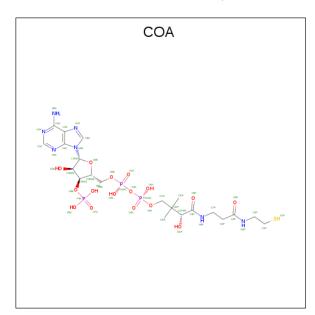
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 2 4	0	0
2	В	1	Total C O 6 2 4	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Mg 1 1	0	0
3	A	2	$\begin{array}{cc} \text{Total} & \text{Mg} \\ 2 & 2 \end{array}$	0	0

 \bullet Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
1	Λ	1	Total	С	N	О	Р	0	0	
4	4 A	1	31	10	5	13	3	0		
4	D	1	Total	С	Ν	О	Р	0	0	
4	Б	1	31	10	5	13	3	U	U	

 \bullet Molecule 5 is water.

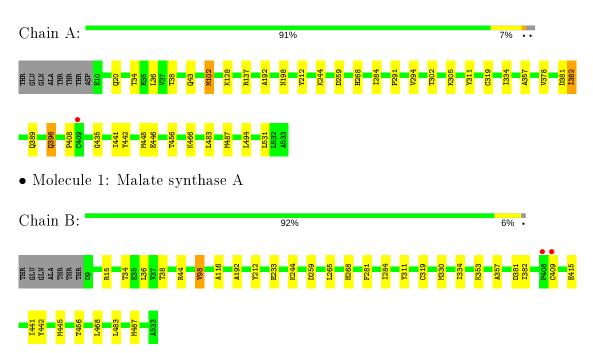
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	575	Total O 576 576	0	1
5	В	579	Total O 580 580	0	1



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Malate synthase A





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	75.20Å 71.47Å 103.26Å	Danasitan
a, b, c, α , β , γ	90.00° 90.06° 90.00°	Depositor
Resolution (Å)	25.01 - 1.40	Depositor
rtesolution (A)	24.42 - 1.40	EDS
% Data completeness	97.5 (25.01-1.40)	Depositor
(in resolution range)	97.2 (24.42-1.40)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.78 \; ({\rm at} \; 1.40 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.200	Depositor
, and the second	0.176 , 0.205	DCC
R_{free} test set	10530 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.33 \;, 31.5$	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
	0.012 for k,h,-l	
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
	0.469 for h,-k,-l	
F_o, F_c correlation	0.97	EDS
Total number of atoms	9663	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: COA, OXL, CSO, 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	Boı	nd lengths	Bond angles		
MIOI	Moi Chain		# Z > 5	RMSZ	# Z >5	
1	A	0.57	3/4346 (0.1%)	0.62	$1/5893 \ (0.0\%)$	
1	В	0.48	$1/4321 \ (0.0\%)$	0.62	$1/5858 \ (0.0\%)$	
All	All	0.53	4/8667 (0.0%)	0.62	$2/11751 \ (0.0\%)$	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	20[A]	GLN	CG-CD	14.52	1.84	1.51
1	A	20[B]	GLN	CG-CD	14.52	1.84	1.51
1	В	319	CYS	CB-SG	-8.03	1.68	1.82
1	A	319	CYS	CB-SG	-5.67	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	311	TYR	CA-CB-CG	5.35	123.57	113.40
1	В	281	PHE	CB-CG-CD2	-5.28	117.11	120.80

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	A	4220	0	4184	24	0
1	В	4210	0	4158	18	0
2	A	6	0	0	0	0
2	В	6	0	0	0	0
3	A	2	0	0	0	0
3	В	1	0	0	0	0
4	A	31	0	11	0	0
4	В	31	0	11	0	0
5	A	576	0	0	2	0
5	В	580	0	0	3	0
All	All	9663	0	8364	42	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 2.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:357:ALA:CB	1:B:382[B]:ILE:HD12	1.90	1.00
1:B:357:ALA:HB1	1:B:382[B]:ILE:HD12	1.41	0.99
1:A:382:ILE:HD11	1:A:389:GLN:NE2	1.94	0.83
1:A:396:GLN:HE21	1:A:396:GLN:H	1.27	0.81
1:B:381[B]:ASP:OD1	5:B:1194:HOH:O	1.98	0.81
1:A:381[B]:ASP:OD1	5:A:1186:HOH:O	1.97	0.81
1:A:137:ARG:HA	1:A:198:ASN:HD21	1.54	0.71
1:B:357:ALA:HB3	1:B:382[B]:ILE:HD12	1.79	0.65
1:B:284:ILE:CG2	1:B:456[A]:THR:HG22	2.30	0.61
1:B:382[B]:ILE:HD11	5:B:1200:HOH:O	2.00	0.60
1:A:284:ILE:CG2	1:A:456[A]:THR:HG22	2.32	0.59
1:B:284:ILE:HG21	1:B:456[A]:THR:HG22	1.86	0.57
1:B:334:ILE:HG12	1:B:445:MET:HG3	1.87	0.56
1:A:334:ILE:HG12	1:A:445:MET:HG3	1.87	0.56
1:A:441:ILE:HG22	1:A:442:TYR:CD2	2.43	0.54
1:A:382:ILE:HD11	1:A:389:GLN:CD	2.29	0.53
1:A:284:ILE:HG21	1:A:456[A]:THR:HG22	1.91	0.52
1:A:34:THR:O	1:A:38:THR:HG23	2.09	0.52
1:A:382:ILE:HG22	5:A:1366:HOH:O	2.08	0.52
1:B:441:ILE:HG22	1:B:442:TYR:CD2	2.45	0.52
1:B:353:LYS:NZ	5:B:1579:HOH:O	2.39	0.50
1:A:294:VAL:HG21	1:A:466:LYS:HE2	1.94	0.49
1:A:357:ALA:HB1	1:A:382:ILE:HG12	1.96	0.48
1:A:378:VAL:O	1:A:382:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	Clash overlap (Å)
1:B:34:THR:O	1:B:38:THR:HG23	2.15	0.47
1:A:128:LYS:HE3	1:A:435:GLY:O	2.15	0.46
1:B:36:LEU:HD12	1:B:192:ALA:HB2	1.97	0.45
1:B:284:ILE:HG22	1:B:456[A]:THR:HG22	1.97	0.45
1:B:483:LEU:O	1:B:487:MET:HG2	2.17	0.45
1:B:98:VAL:HG12	1:B:116:ALA:HB1	2.00	0.44
1:A:382:ILE:HD11	1:A:389:GLN:HE22	1.75	0.44
1:A:284:ILE:HG22	1:A:456[A]:THR:HG22	1.98	0.44
1:A:244:LYS:HA	1:A:268:HIS:O	2.18	0.43
1:A:36:LEU:HD12	1:A:192:ALA:HB2	2.01	0.43
1:A:483:LEU:O	1:A:487:MET:HG2	2.19	0.43
1:A:441:ILE:HD12	1:A:446:GLU:HG3	2.01	0.42
1:B:244:LYS:HA	1:B:268:HIS:O	2.19	0.42
1:A:531:LEU:HD12	1:A:531:LEU:N	2.35	0.41
1:B:415:GLU:HA	1:B:468:LEU:HD13	2.03	0.41
1:B:233:GLU:OE1	1:B:268:HIS:HE1	2.04	0.41
1:A:102:MET:HE2	1:A:102:MET:HA	2.04	0.40
1:A:302:THR:OG1	1:A:305:LYS:NZ	2.54	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	$535/532 \; (101\%)$	523 (98%)	12 (2%)	0	100	100
1	В	$532/532 \; (100\%)$	522 (98%)	9 (2%)	1 (0%)	47	21
All	All	1067/1064 (100%)	1045 (98%)	21 (2%)	1 (0%)	51	23

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	98	VAL

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	${f Analysed}$	Rotameric Outliers		Percentiles		
1	A	$445/447 \; (100\%)$	435 (98%)	10 (2%)	52 19		
1	В	440/447~(98%)	431 (98%)	9 (2%)	55 23		
All	All	885/894 (99%)	866 (98%)	19 (2%)	55 21		

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43[A]	GLN
1	A	43[B]	GLN
1	A	102	MET
1	A	212	TYR
1	A	259	ASP
1	A	291	PRO
1	A	382	ILE
1	A	396	GLN
1	A	408	PRO
1	A	494	LEU
1	В	15	ARG
1	В	44	ARG
1	В	212	TYR
1	В	259	ASP
1	В	265	LEU
1	В	311	TYR
1	В	330[A]	MET
1	В	330[B]	MET
1	В	409	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	39	HIS
1	A	105	ASN
1	A	198	ASN
1	A	237	ASN
1	A	263	HIS
1	A	359	ASN
1	A	389	GLN
1	A	396	GLN
1	В	237	ASN
1	В	268	HIS
1	В	436	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)

2 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	Trees	Chain	Dog	Res Link Bond lengths			В	ond ang	gles	
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	A	438	1	3,6,7	0.79	0	0,6,8	0.00	-
1	CSO	В	438	1	3,6,7	0.74	0	0,6,8	0.00	-

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	CSO	A	438	1	-	0/1/5/7	-
1	CSO	В	438	1	_	0/1/5/7	-

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	Tune	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	COA	В	1001	-	28,33,50	1.27	3 (10%)	35,52,75	1.29	2 (5%)
2	OXL	В	1000	3	0,5,5	0.00	-	0,6,6	0.00	-
2	OXL	A	1000	3	0,5,5	0.00	-	0,6,6	0.00	-
4	COA	A	1002	-	28,33,50	1.27	3 (10%)	35,52,75	1.21	2 (5%)

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	${f Res}$	Link	Chirals	${f Torsions}$	Rings
4	COA	В	1001	-	-	3/17/37/64	0/3/3/3
2	OXL	В	1000	3	-	0/0/4/4	-
2	OXL	A	1000	3	-	0/0/4/4	-
4	COA	A	1002	_	-	0/17/37/64	0/3/3/3

All (6) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
4	В	1001	COA	C2A-N3A	3.73	1.38	1.32
4	A	1002	COA	P2A-O4A	3.56	1.62	1.50
4	A	1002	COA	C2A-N3A	3.49	1.37	1.32
4	В	1001	COA	P2A-O4A	3.42	1.61	1.50
4	В	1001	COA	C2A-N1A	2.46	1.38	1.33
4	A	1002	COA	C2A-N1A	2.35	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
4	В	1001	COA	N3A-C2A-N1A	-5.02	120.83	128.68
4	A	1002	COA	N3A-C2A-N1A	-4.67	121.38	128.68
4	В	1001	COA	P1A-O3A-P2A	-2.93	122.79	132.83
4	A	1002	COA	P1A-O3A-P2A	-2.49	124.27	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

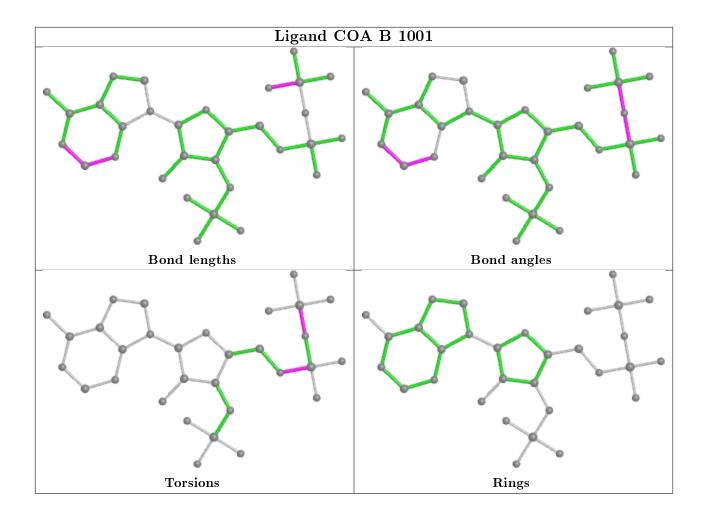
Mol	Chain	Res	Type	Atoms
4	В	1001	COA	P1A-O3A-P2A-O5A
4	В	1001	COA	P1A-O3A-P2A-O6A
4	В	1001	COA	C5B-O5B-P1A-O1A

There are no ring outliers.

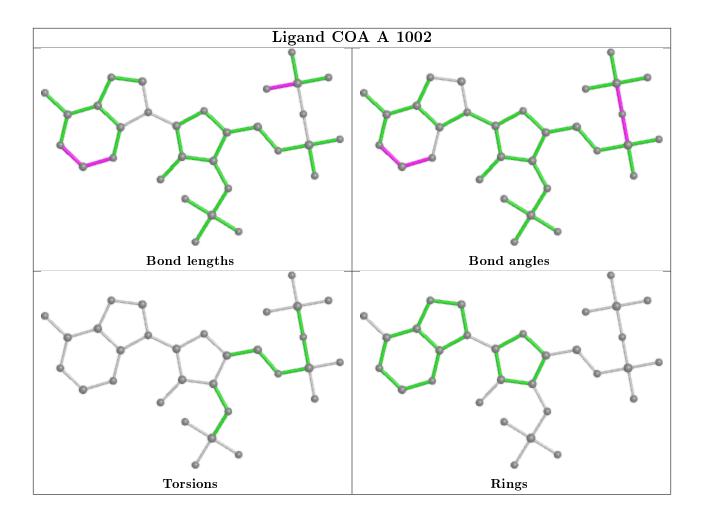
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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)

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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	523/532~(98%)	-0.54	1 (0%) 95 93	11, 18, 31, 35	12 (2%)
1	В	524/532~(98%)	-0.54	2 (0%) 92 91	11, 18, 30, 39	13 (2%)
All	All	1047/1064 (98%)	-0.54	3 (0%) 94 93	11, 18, 31, 39	25 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	CYS	6.8
1	В	409	CYS	4.5
1	В	408	PRO	3.7

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^{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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
1	CSO	Α	438	7/8	0.95	0.07	15,19,20,21	1
1	CSO	В	438	7/8	0.96	0.07	16,19,19,20	1

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.



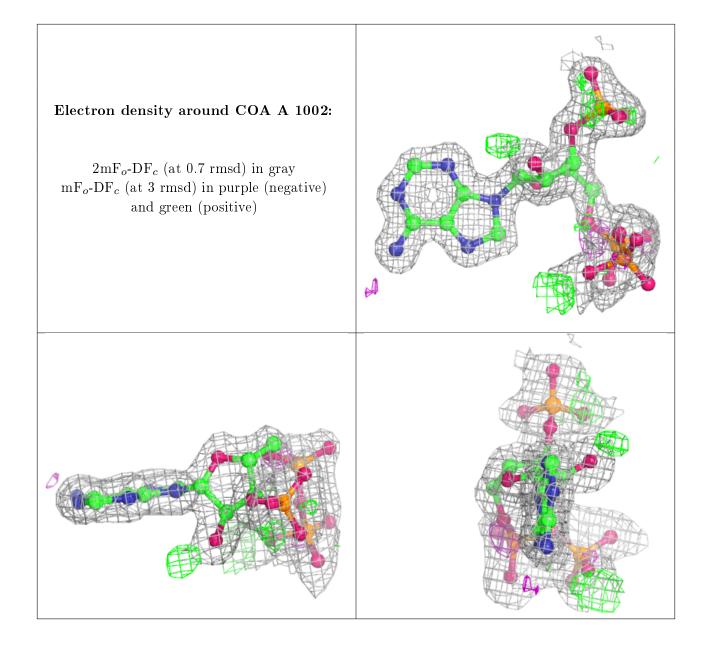
6.4 Ligands (i)

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^{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.

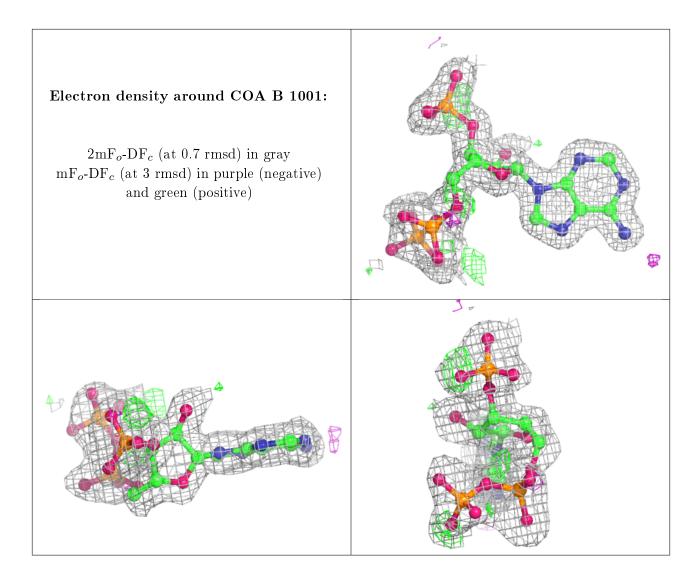
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
4	COA	A	1002	31/48	0.92	0.09	13,23,44,45	31
4	COA	В	1001	31/48	0.93	0.09	15,23,43,44	31
3	MG	A	1001	1/1	0.97	0.15	33,33,33,33	0
2	OXL	В	1000	6/6	0.98	0.06	12,12,16,20	0
2	OXL	A	1000	6/6	0.99	0.04	11,13,15,19	0
3	MG	A	1	1/1	0.99	0.06	12,12,12,12	0
3	MG	В	1	1/1	1.00	0.05	11,11,11,11	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.









6.5 Other polymers (i)

There are no such residues in this entry.

