



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 09:20 pm BST

PDB ID : 2GQ3
Title : mycobacterium tuberculosis malate synthase in complex with magnesium, malate, and coenzyme A
Authors : Anstrom, D.M.; Remington, S.J.
Deposited on : 2006-04-19
Resolution : 2.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

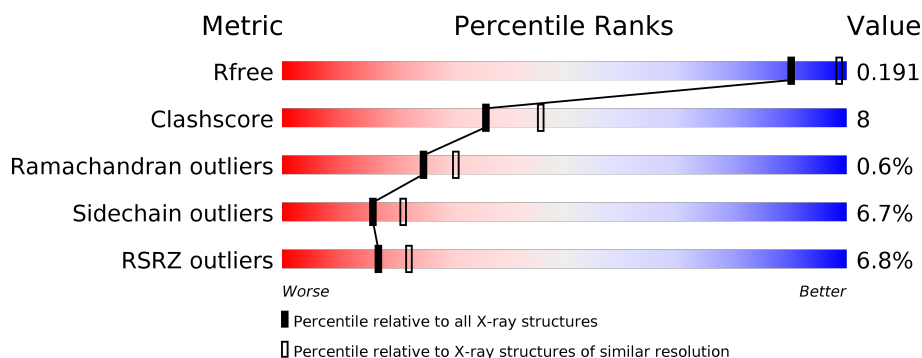
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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 $\leq 5\%$. 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	A	729	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	729	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>..</div> </div> </div>

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	MLT	A	900	X	-	-	-
3	MLT	B	901	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11633 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 G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	0	0
			5487	3444	964	1057	22			
1	B	714	Total	C	N	O	S	0	0	0
			5429	3411	953	1043	22			

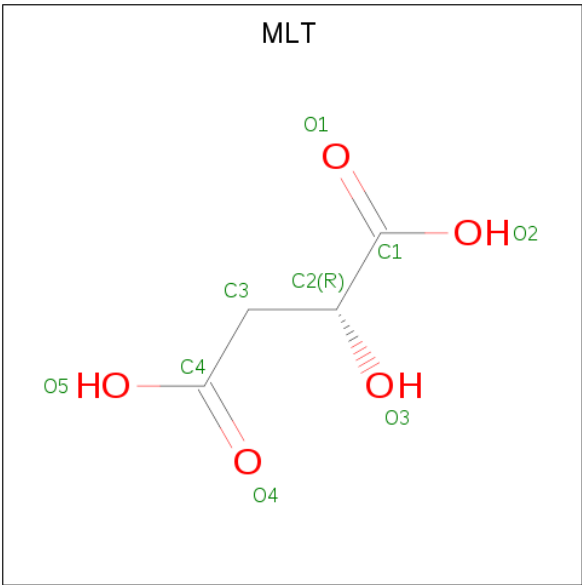
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P0A5J4
A	0	SER	-	CLONING ARTIFACT	UNP P0A5J4
B	-1	GLY	-	CLONING ARTIFACT	UNP P0A5J4
B	0	SER	-	CLONING ARTIFACT	UNP P0A5J4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

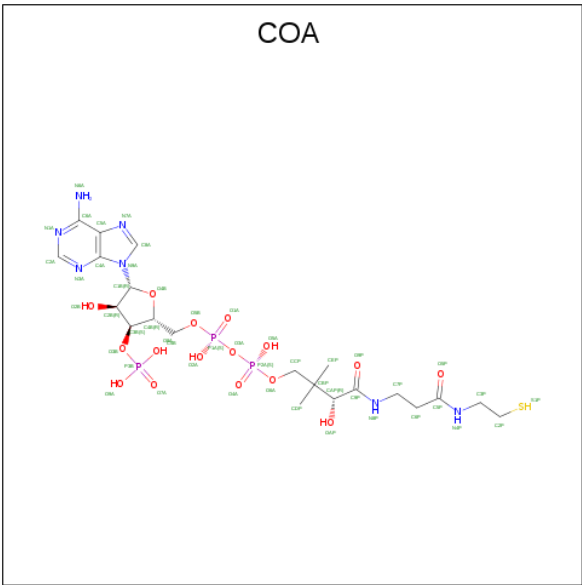
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		
3	B	1	Total	C	O	0	0
			9	4	5		

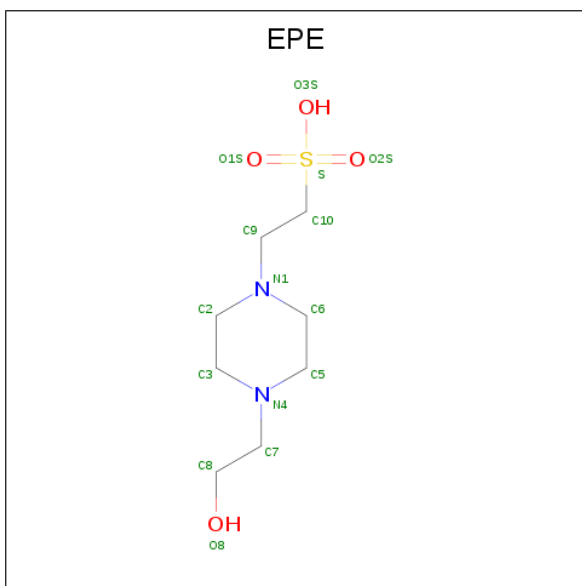
- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

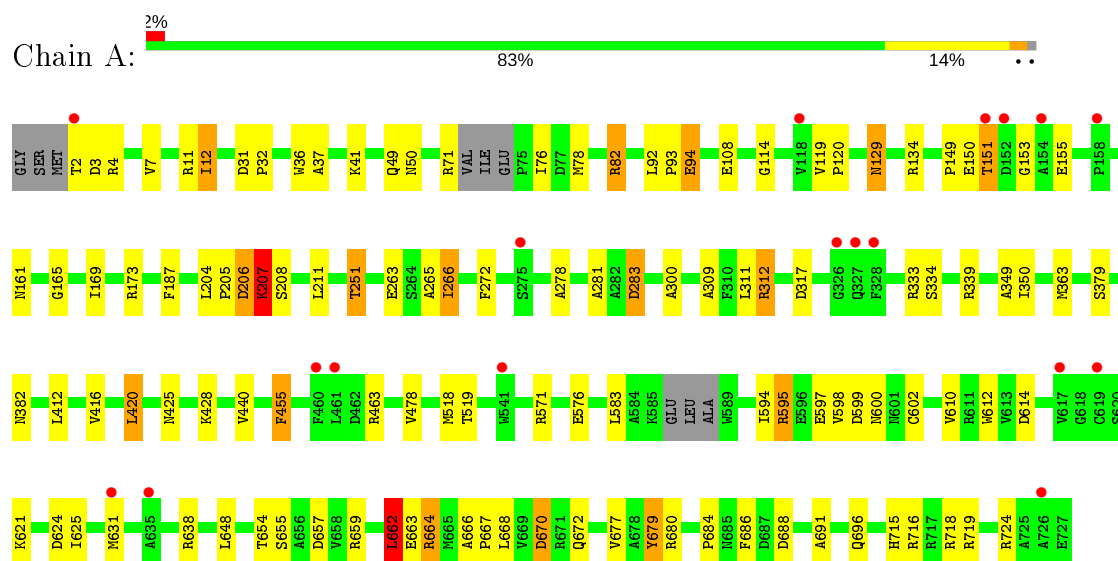
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	448	Total	O	0	0
			448	448		
6	B	169	Total	O	0	0
			169	169		

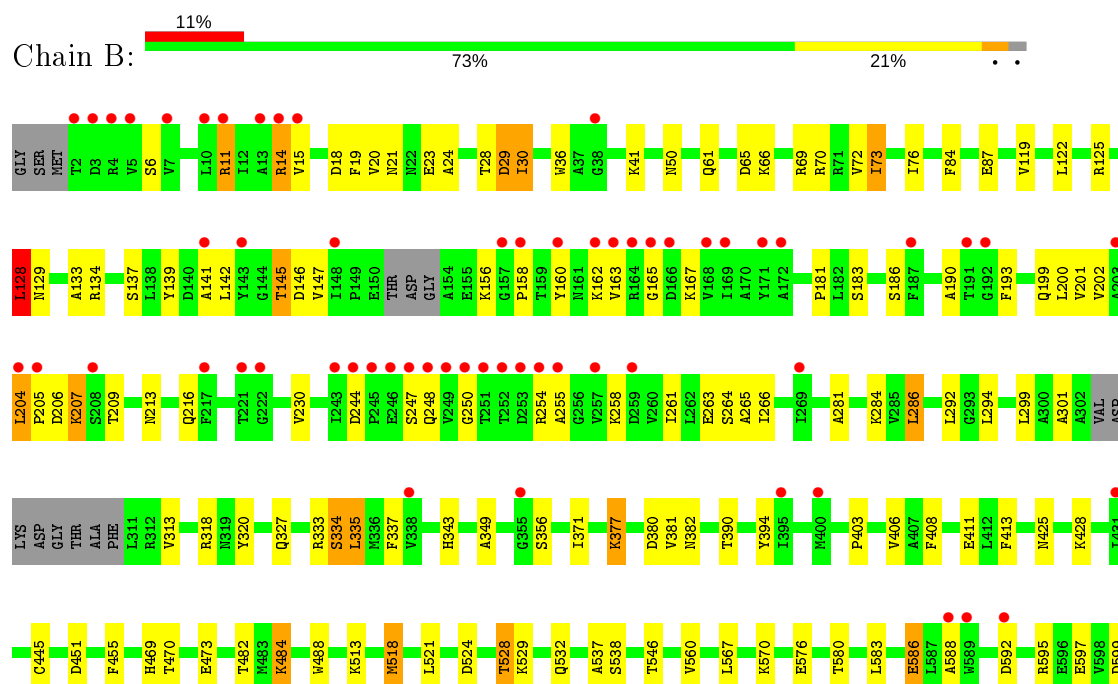
3 Residue-property plots

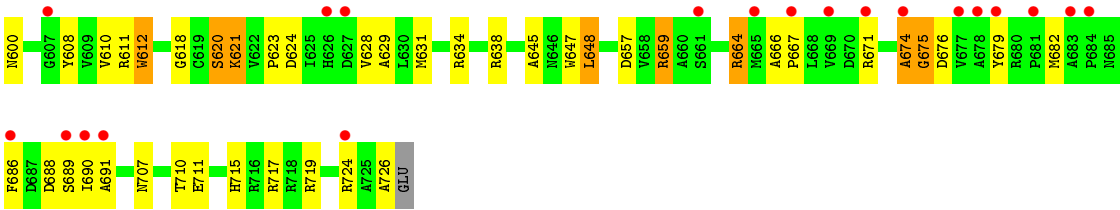
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 G



• Molecule 1: Malate synthase G





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.38 Å 120.38 Å 238.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.30 49.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.09-2.30) 99.4 (49.08-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.29 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.244 0.181 , 0.191	Depositor DCC
R_{free} test set	7746 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11633	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COA, MG, EPE, MLT

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	1.17	8/5591 (0.1%)	1.07	18/7605 (0.2%)
1	B	0.98	8/5532 (0.1%)	0.96	12/7530 (0.2%)
All	All	1.08	16/11123 (0.1%)	1.02	30/15135 (0.2%)

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	2
1	B	0	4
All	All	0	6

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	ARG	CZ-NH2	14.31	1.51	1.33
1	B	686	PHE	CG-CD1	6.75	1.48	1.38
1	B	14	ARG	NE-CZ	6.36	1.41	1.33
1	B	686	PHE	CE2-CZ	6.33	1.49	1.37
1	A	478	VAL	CB-CG1	6.24	1.66	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	ARG	NE-CZ-NH1	14.83	127.71	120.30
1	A	638	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	B	14	ARG	NE-CZ-NH1	-12.57	114.02	120.30
1	A	312	ARG	NE-CZ-NH2	-10.37	115.12	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	ARG	NE-CZ-NH1	9.59	125.09	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	THR	Peptide
1	A	206	ASP	Peptide
1	B	183	SER	Peptide
1	B	586	GLU	Peptide
1	B	674	ALA	Peptide

5.2 Too-close contacts

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	5487	0	5407	78	0
1	B	5429	0	5345	100	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	3	0	0
3	B	9	0	3	0	0
4	A	48	0	31	20	0
5	A	15	0	17	1	0
5	B	15	0	17	1	0
6	A	448	0	0	1	0
6	B	169	0	0	2	0
All	All	11633	0	10823	175	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 8.

The worst 5 of 175 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:206:ASP:HB2	1:A:207:LYS:HB2	1.33	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:HH21	1:B:11:ARG:HG2	1.13	1.06
1:A:631:MET:SD	4:A:800:COA:H62	2.04	0.97
1:B:204:LEU:HB3	1:B:205:PRO:HD2	1.55	0.88
1:A:206:ASP:HB2	1:A:207:LYS:CB	2.04	0.86

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	714/729 (98%)	701 (98%)	12 (2%)	1 (0%)	51	64
1	B	708/729 (97%)	670 (95%)	31 (4%)	7 (1%)	15	17
All	All	1422/1458 (98%)	1371 (96%)	43 (3%)	8 (1%)	25	31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	B	586	GLU
1	B	588	ALA
1	B	207	LYS
1	B	29	ASP

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	575/586 (98%)	545 (95%)	30 (5%)	23	32
1	B	567/586 (97%)	521 (92%)	46 (8%)	11	15
All	All	1142/1172 (97%)	1066 (93%)	76 (7%)	16	21

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	50	ASN
1	B	129	ASN
1	B	631	MET
1	B	70	ARG
1	B	76	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
1	B	21	ASN
1	B	532	GLN
1	A	340	ASN
1	B	495	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
3	MLT	B	901	2	2,8,8	0.70	0	3,10,10	4.15	2 (66%)
5	EPE	B	6000	-	15,15,15	0.76	1 (6%)	18,20,20	2.47	7 (38%)
5	EPE	A	5000	-	15,15,15	1.34	2 (13%)	18,20,20	2.27	8 (44%)
4	COA	A	800	-	41,50,50	1.82	2 (4%)	52,75,75	2.18	14 (26%)
3	MLT	A	900	2	2,8,8	0.98	0	3,10,10	5.30	3 (100%)

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
3	MLT	B	901	2	1/1/3/3	2/2/8/8	-
5	EPE	B	6000	-	-	3/9/19/19	0/1/1/1
5	EPE	A	5000	-	-	2/9/19/19	0/1/1/1
4	COA	A	800	-	-	16/44/64/64	0/3/3/3
3	MLT	A	900	2	1/1/3/3	2/2/8/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	COA	O9P-C9P	9.89	1.43	1.23
5	A	5000	EPE	C10-S	3.55	1.82	1.77
4	A	800	COA	C2A-N3A	3.38	1.37	1.32
5	A	5000	EPE	O1S-S	2.61	1.52	1.45
5	B	6000	EPE	C10-S	2.19	1.80	1.77

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	COA	C7P-N8P-C9P	8.53	137.81	122.59
3	A	900	MLT	C3-C2-C1	-8.28	100.56	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	6000	EPE	O1S-S-C10	7.11	115.48	106.92
3	B	901	MLT	C3-C2-C1	-6.34	103.02	111.10
4	A	800	COA	N3A-C2A-N1A	-5.50	120.08	128.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	901	MLT	C2
3	A	900	MLT	C2

5 of 25 torsion outliers are listed below:

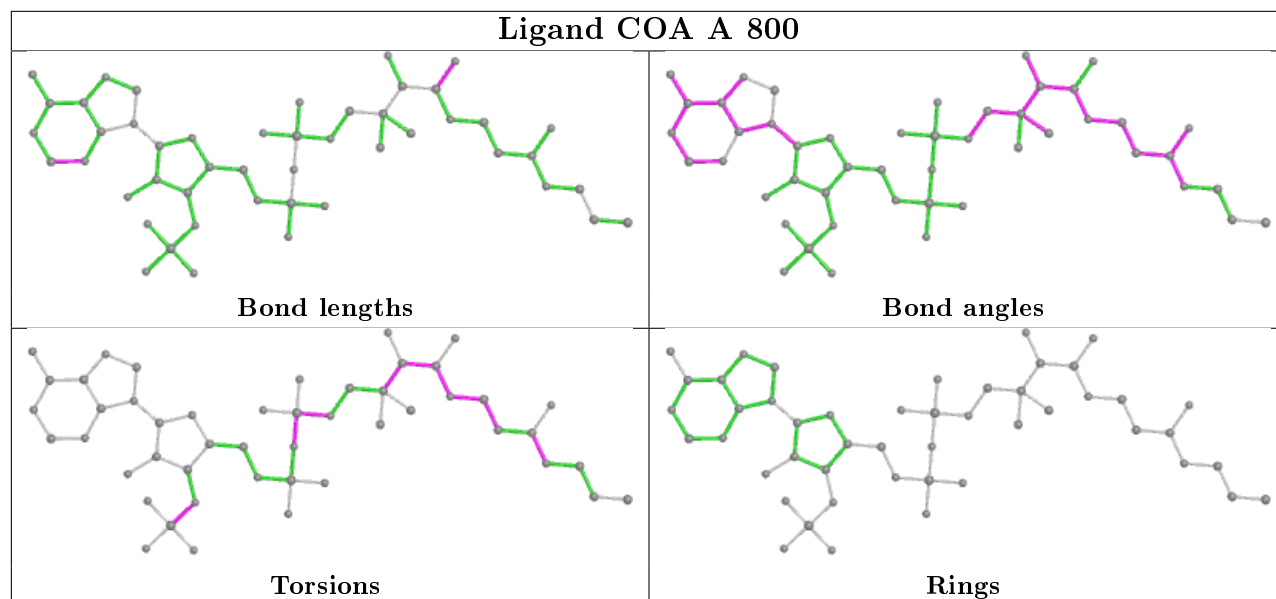
Mol	Chain	Res	Type	Atoms
5	B	6000	EPE	S-C10-C9-N1
3	B	901	MLT	O3-C2-C3-C4
4	A	800	COA	P1A-O3A-P2A-O6A
4	A	800	COA	CCP-O6A-P2A-O4A
4	A	800	COA	CCP-O6A-P2A-O5A

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	6000	EPE	1	0
5	A	5000	EPE	1	0
4	A	800	COA	20	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, 95th 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	720/729 (98%)	0.19	18 (2%) 57 64	31, 38, 52, 75	1 (0%)
1	B	714/729 (97%)	0.57	80 (11%) 5 7	28, 39, 50, 64	0
All	All	1434/1458 (98%)	0.38	98 (6%) 17 22	28, 38, 50, 75	1 (0%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	PRO	6.4
1	B	247	SER	5.1
1	B	204	LEU	4.9
1	B	251	THR	4.6
1	B	245	PRO	4.4

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

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

6.3 Carbohydrates [i](#)

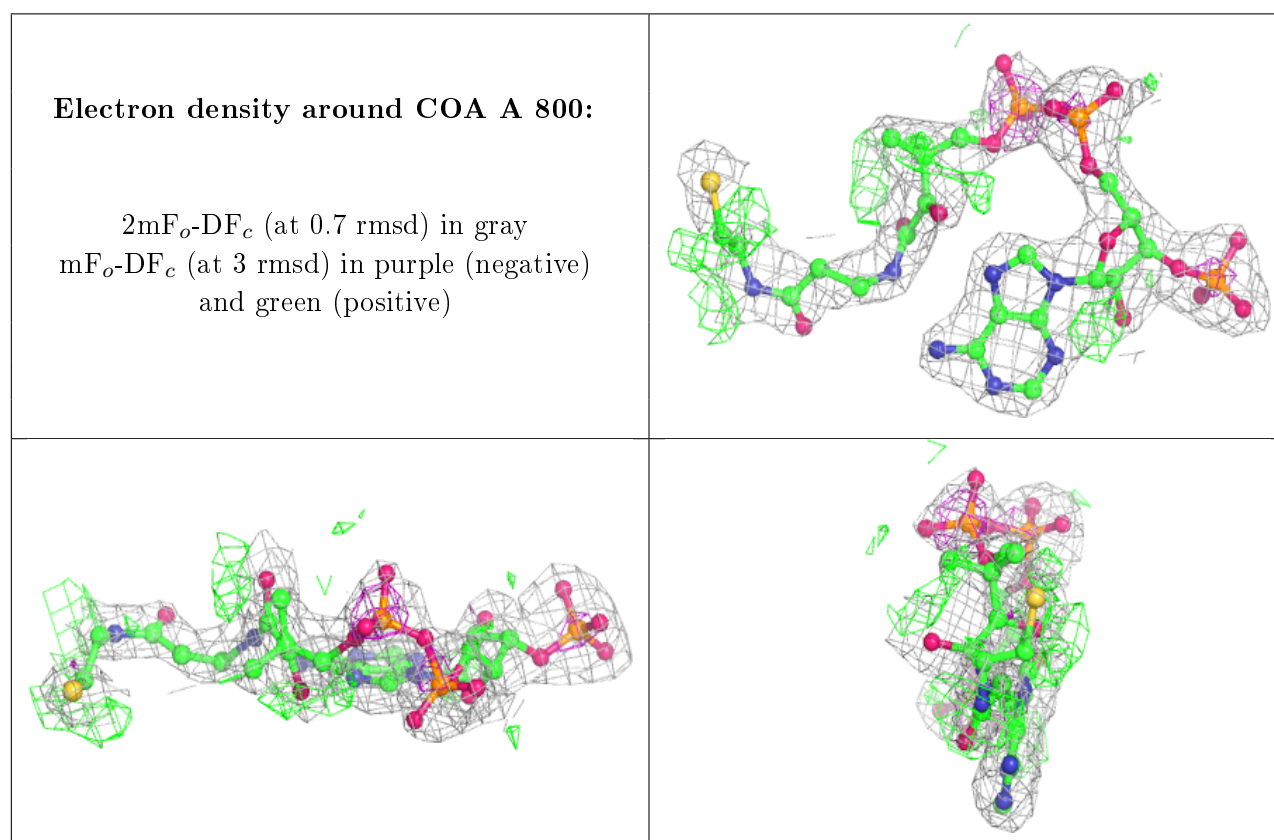
There are no carbohydrates in this entry.

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, 95th 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(\AA^2)	Q<0.9
4	COA	A	800	48/48	0.90	0.20	23,41,52,56	48
2	MG	B	1003	1/1	0.93	0.29	76,76,76,76	0
5	EPE	A	5000	15/15	0.93	0.13	52,55,61,62	0
5	EPE	B	6000	15/15	0.94	0.24	80,93,97,97	0
3	MLT	B	901	9/9	0.95	0.08	29,37,49,53	0
2	MG	A	1002	1/1	0.95	0.24	40,40,40,40	0
3	MLT	A	900	9/9	0.97	0.12	19,23,43,49	0
2	MG	B	1001	1/1	0.97	0.04	37,37,37,37	0
2	MG	A	1000	1/1	0.98	0.08	24,24,24,24	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 ⓘ

There are no such residues in this entry.