



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:00 AM UTC

PDB ID : 1NDI / pdb_00001ndi
Title : Carnitine Acetyltransferase in complex with CoA
Authors : Jogl, G.; Tong, L.
Deposited on : 2002-12-09
Resolution : 2.30 Å(reported)

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

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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

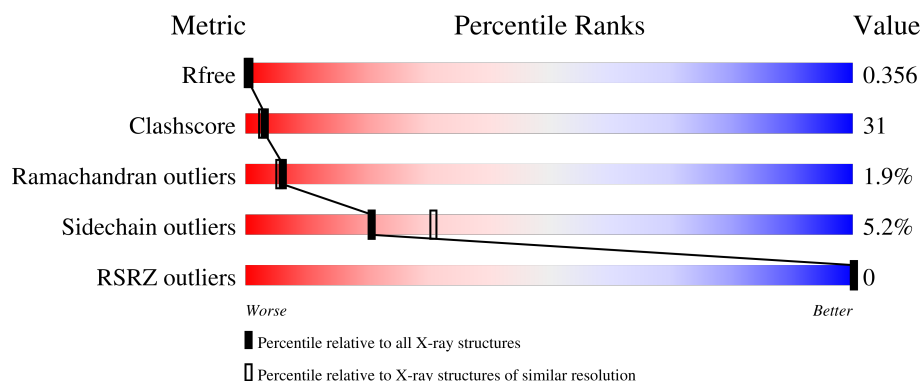
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

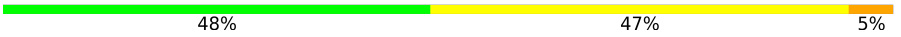
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	596	
1	B	596	

2 Entry composition [i](#)

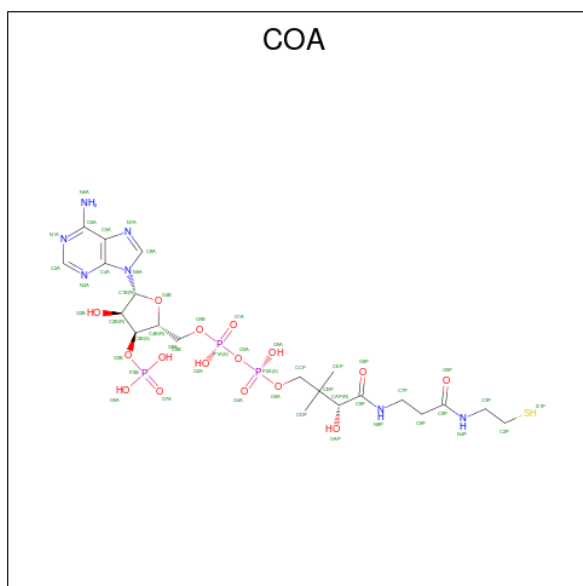
There are 3 unique types of molecules in this entry. The entry contains 10303 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carnitine Acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			
1	B	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

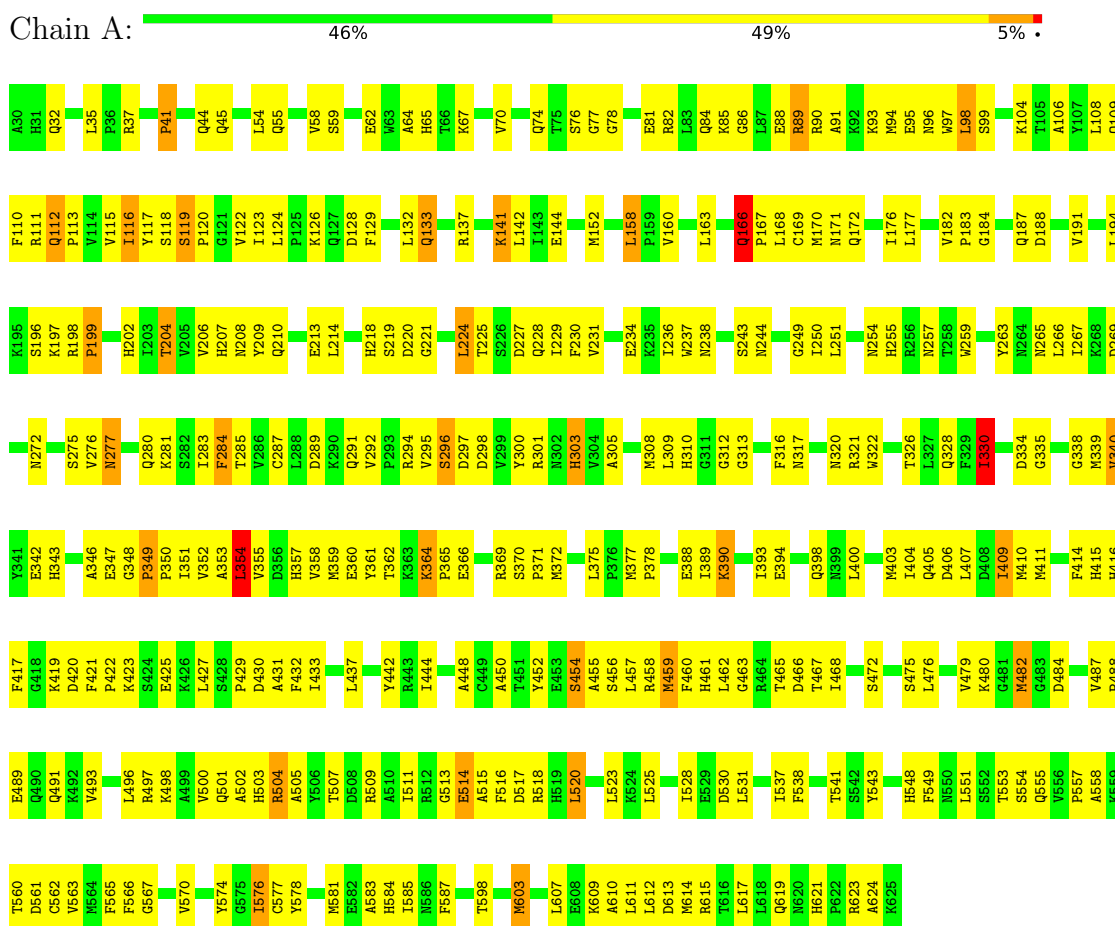
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	342	Total 342	O 342	0	0
3	B	351	Total 351	O 351	0	0

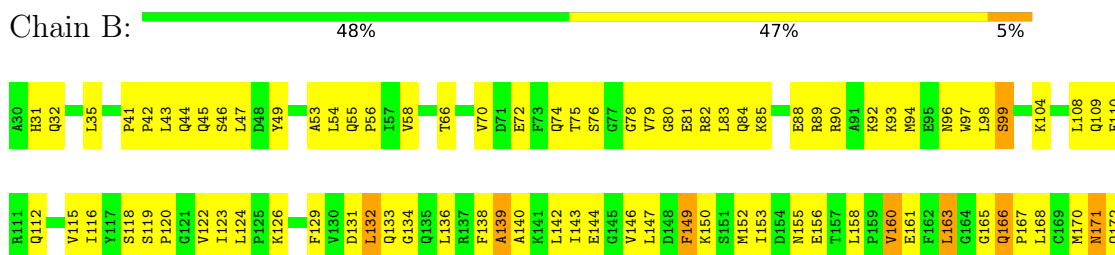
3 Residue-property plots

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: Carnitine Acetyltransferase



• Molecule 1: Carnitine Acetyltransferase



E582	K492	H415	E342	D269	Y173
T585	V493	H416	H343	K270	Y174
N586	E494	F417	A344	N271	Q175
F587	L495	L496	A345	V272	I176
S588	L496	D420	A346	L177	L177
V589	V500	P422	E347	S178	S178
			G348		
			P349		
Y592	A505	E425	P350	I279	G184
N593	Y506	Y506	I351	Q280	P185
S594	T507	P429	V352	K281	K186
C595	D508	D430	A353	S282	Q187
A596	R509	A431	L354	I283	D188
E597	A510	F432	V355	F284	
T598	I511	I433	D356	T285	K195
N599	R512	A440	H357	V286	S196
A600	G513		V358	C287	
A601	E514	I444	E360	R294	H202
R602	A515	Y445	Y361	V295	I203
	F516			S296	T204
E608	D517	T451	K364	D297	V206
K609	R518	Y452		D298	H207
		E453	L367	V299	N208
L612	K524	S454	V368	Y300	Y209
D613	A527	A455	R369	H303	Q210
L617	I528	S456	S370	V304	F211
L618	L457	R458	P371	A305	F212
Q619	M534	M459	M372	G306	E213
				Q307	T225
P622	M539	F460	M377	M308	S226
K625	D540	H461	P378	L309	D227
	T541	L462	K379	H310	Q228
		G463	K380	G311	I229
	M547	R464	L381	G312	F230
H548	F549	T465	R382	K315	V231
F549	N550	D466	F383		Q232
N550	L551	T467	N384		L233
S552	T553	I468	I385	G319	E234
		S470	T396	N320	K235
		A471	E394	R321	I236
		S472		W322	W237
				F323	
				D324	S240
V563	V563	L476	Q398	K325	L241
N564	F565	A477	N399	L326	Q242
F565		F478	L400	L327	S243
		V479	S401	Q328	N244
P568		K480	I402	F329	K245
V569		G481	M403	I330	F246
V570		M482	I404		P247
		G483	Q405		
Y574	G575	D484	D406	E333	
I576	S485	S485	L407	D334	T252
C577	T486	D486	D408	G335	
Y578	V487	P488	I409	S336	W259
N579	E489	E489	M410	C337	
P580	Q490	Q490	M411	G338	Y263
M581	Q491	Q491	L412	M339	I267
			T413	V340	
			F414	Y341	K268

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.26Å 92.05Å 122.90Å 90.00° 128.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.3 (30.00-2.30) 76.6 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.363 0.271 , 0.356	Depositor DCC
R_{free} test set	4090 reflections (7.24%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10303	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

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	0.57	1/4872 (0.0%)	1.01	19/6600 (0.3%)
1	B	0.61	1/4872 (0.0%)	1.00	19/6600 (0.3%)
All	All	0.59	2/9744 (0.0%)	1.01	38/13200 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	ILE	CA-CB	7.25	1.65	1.54
1	A	41	PRO	CA-C	5.83	1.55	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	N-CA-C	-7.87	104.28	114.04
1	B	353	ALA	N-CA-C	-7.37	104.09	113.23
1	A	119	SER	CA-C-N	6.84	127.09	119.90
1	A	119	SER	C-N-CA	6.84	127.09	119.90
1	B	364	LYS	CA-C-N	6.27	126.29	119.89

There are no chirality outliers.

There are no planarity outliers.

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	4757	0	4733	293	0
1	B	4757	0	4733	299	0
2	A	48	0	32	5	0
2	B	48	0	32	7	0
3	A	342	0	0	31	0
3	B	351	0	0	53	0
All	All	10303	0	9530	595	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 31.

The worst 5 of 595 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:B:410:MET:HG2	1:B:601:ALA:HA	1.36	1.05
1:B:585:ILE:HG22	3:B:6421:HOH:O	1.60	1.02
1:A:90:ARG:HD3	1:A:97:TRP:HB2	1.44	0.98
1:A:32:GLN:HE22	1:A:170:MET:H	1.15	0.93
1:A:310:HIS:HD2	1:A:312:GLY:H	1.15	0.90

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	594/596 (100%)	501 (84%)	81 (14%)	12 (2%)	6 5
1	B	594/596 (100%)	532 (90%)	52 (9%)	10 (2%)	7 7
All	All	1188/1192 (100%)	1033 (87%)	133 (11%)	22 (2%)	6 5

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	SER
1	B	515	ALA
1	B	485	SER
1	B	622	PRO
1	A	172	GLN

5.3.2 Protein sidechains ⓘ

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	524/524 (100%)	492 (94%)	32 (6%)	17	24
1	B	524/524 (100%)	501 (96%)	23 (4%)	25	38
All	All	1048/1048 (100%)	993 (95%)	55 (5%)	21	31

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	GLU
1	B	163	LEU
1	B	625	LYS
1	B	470	SER
1	A	517	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	ASN
1	B	135	GLN
1	B	619	GLN
1	A	586	ASN
1	B	84	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	COA	B	6170	-	47,50,50	1.55	6 (12%)	69,75,75	1.52	10 (14%)
2	COA	A	5170	-	47,50,50	1.40	6 (12%)	69,75,75	1.53	10 (14%)

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	COA	B	6170	-	-	11/48/64/64	0/3/3/3
2	COA	A	5170	-	-	4/48/64/64	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6170	COA	P2A-O3A	5.06	1.65	1.59
2	B	6170	COA	P1A-O3A	4.75	1.64	1.59
2	B	6170	COA	P3B-O7A	3.83	1.62	1.50
2	A	5170	COA	P3B-O7A	3.74	1.62	1.50
2	A	5170	COA	P1A-O3A	3.63	1.63	1.59

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6170	COA	N3A-C2A-N1A	-5.31	120.55	128.58
2	A	5170	COA	N3A-C2A-N1A	-5.30	120.56	128.58
2	A	5170	COA	C5A-C4A-N3A	-4.94	119.91	126.72
2	B	6170	COA	C5A-C4A-N3A	-4.91	119.95	126.72
2	A	5170	COA	C2A-N3A-C4A	3.73	120.95	111.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

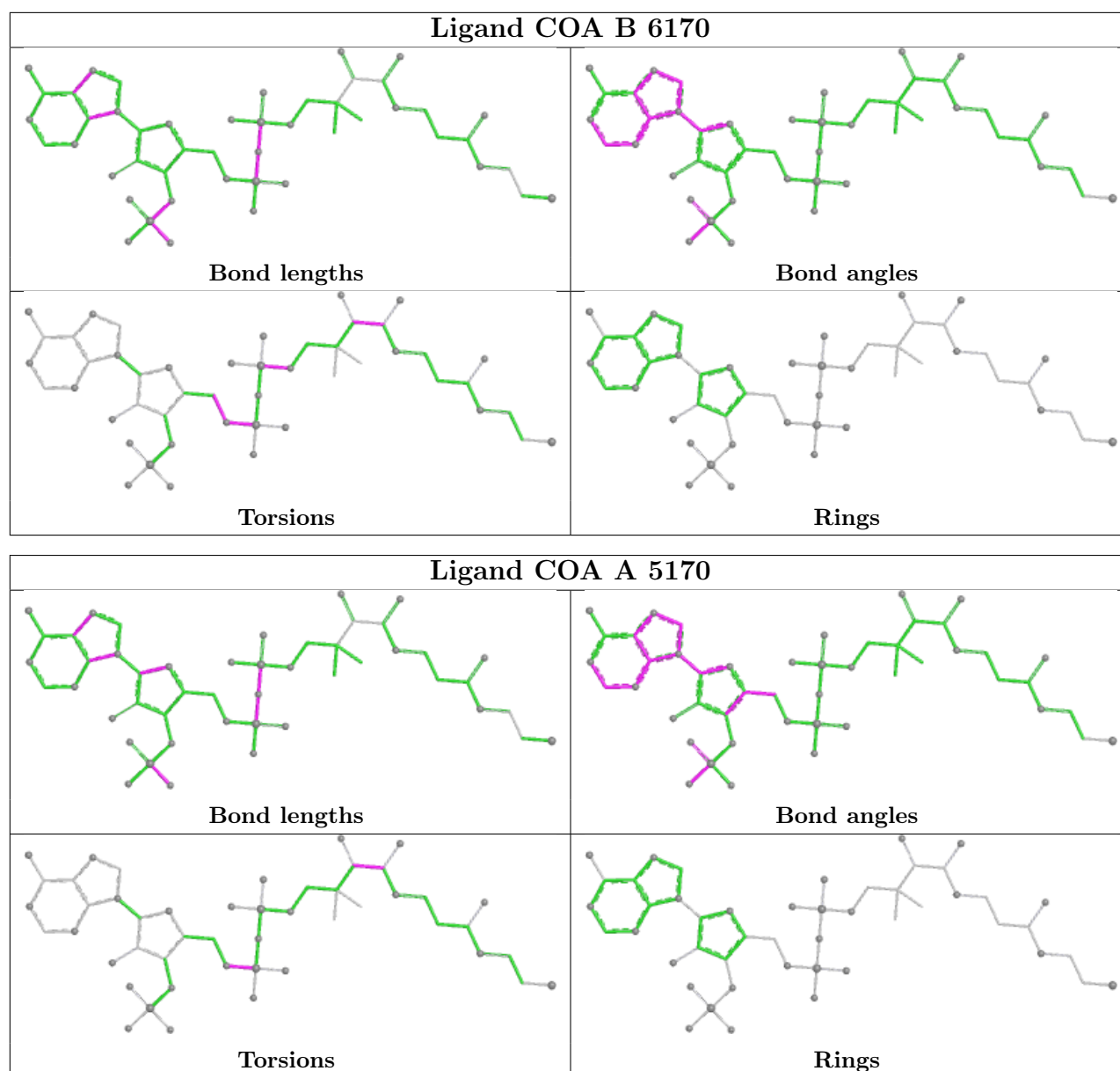
Mol	Chain	Res	Type	Atoms
2	A	5170	COA	C5B-O5B-P1A-O2A
2	B	6170	COA	C5B-O5B-P1A-O2A
2	B	6170	COA	CCP-O6A-P2A-O3A
2	B	6170	COA	CCP-O6A-P2A-O4A
2	B	6170	COA	CCP-O6A-P2A-O5A

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6170	COA	7	0
2	A	5170	COA	5	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	596/596 (100%)	-1.13	0 100 100	13, 47, 89, 134	0
1	B	596/596 (100%)	-1.19	0 100 100	14, 42, 72, 99	0
All	All	1192/1192 (100%)	-1.16	0 100 100	13, 44, 85, 134	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

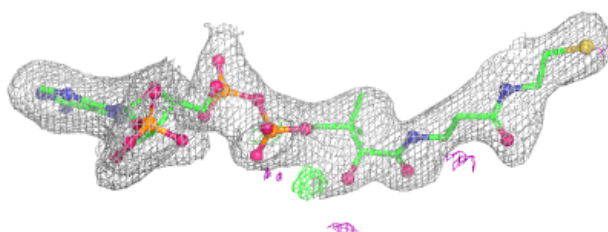
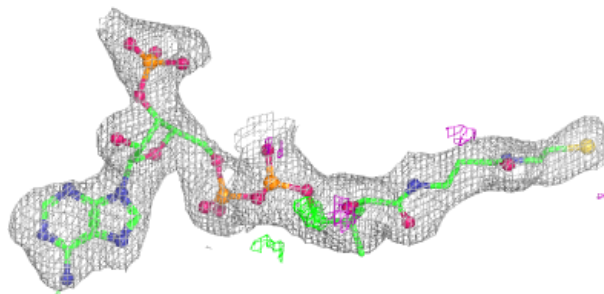
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	A	5170	48/48	0.99	0.04	39,54,60,62	0
2	COA	B	6170	48/48	0.99	0.04	36,53,64,65	0

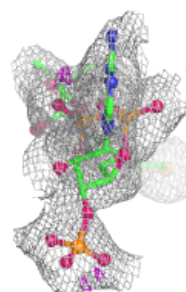
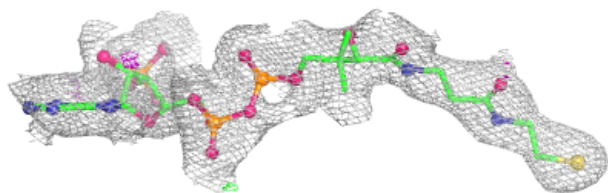
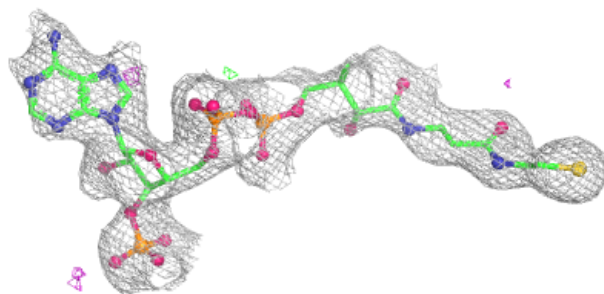
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA A 5170:

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

**Electron density around COA B 6170:**

$2mF_o-DF_c$ (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.