



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2021 – 02:10 pm BST

PDB ID : 6Z2H
Title : Citryl-CoA lyase module of human ATP citrate lyase in complex with (3S)-citryl-CoA.
Authors : Verschueren, K.H.G.; Verstraete, K.
Deposited on : 2020-05-15
Resolution : 1.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

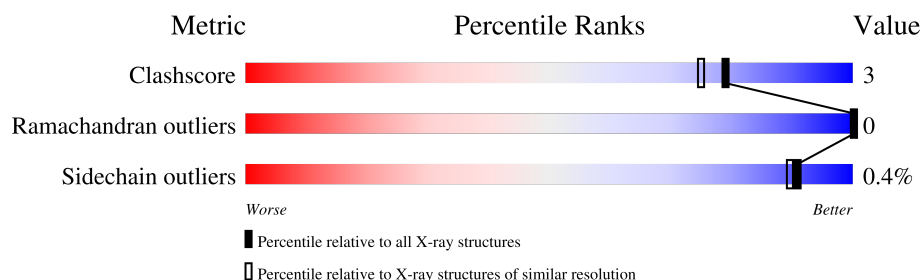
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	270	
1	B	270	
1	C	270	
1	D	270	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17370 atoms, of which 8205 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.

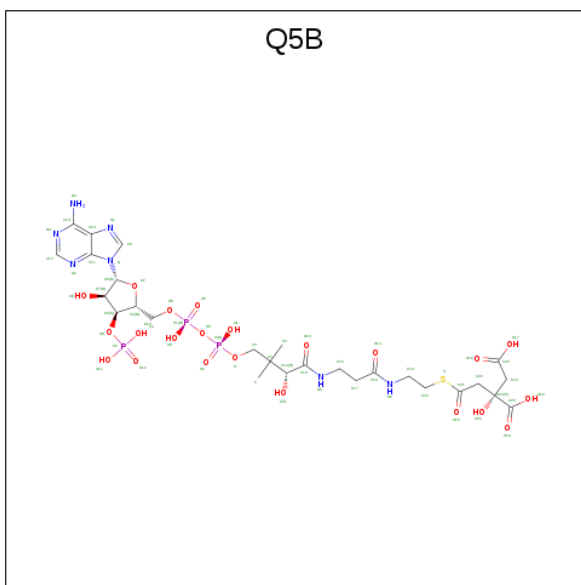
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	H	N	O	S	0	6	0
			4126	1321	2061	350	373	21			
1	B	261	Total	C	H	N	O	S	0	6	0
			4029	1298	2004	336	370	21			
1	C	263	Total	C	H	N	O	S	0	8	0
			4155	1333	2075	350	376	21			
1	D	261	Total	C	H	N	O	S	0	9	0
			4137	1327	2065	348	374	23			

There are 16 discrepancies between the modelled and reference sequences:

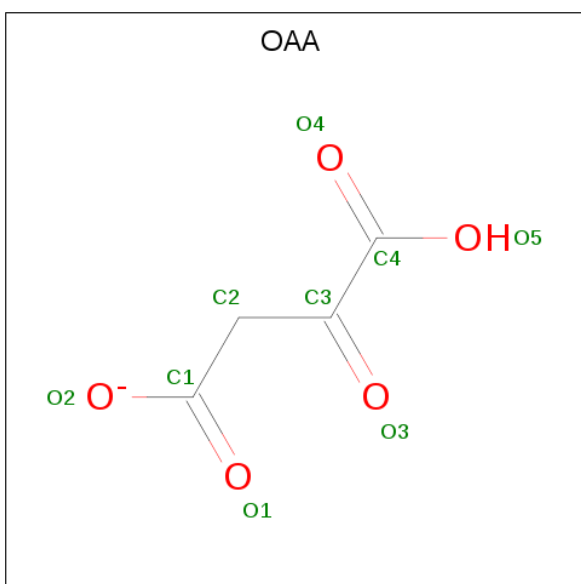
Chain	Residue	Modelled	Actual	Comment	Reference
A	832	GLY	-	expression tag	UNP P53396
A	833	SER	-	expression tag	UNP P53396
A	834	HIS	-	expression tag	UNP P53396
A	835	MET	-	expression tag	UNP P53396
B	832	GLY	-	expression tag	UNP P53396
B	833	SER	-	expression tag	UNP P53396
B	834	HIS	-	expression tag	UNP P53396
B	835	MET	-	expression tag	UNP P53396
C	832	GLY	-	expression tag	UNP P53396
C	833	SER	-	expression tag	UNP P53396
C	834	HIS	-	expression tag	UNP P53396
C	835	MET	-	expression tag	UNP P53396
D	832	GLY	-	expression tag	UNP P53396
D	833	SER	-	expression tag	UNP P53396
D	834	HIS	-	expression tag	UNP P53396
D	835	MET	-	expression tag	UNP P53396

- Molecule 2 is (3S)-citryl-Coenzyme A (three-letter code: Q5B) (formula: C₂₇H₄₂N₇O₂₂P₃S) (labeled as "Ligand of Interest" by depositor).



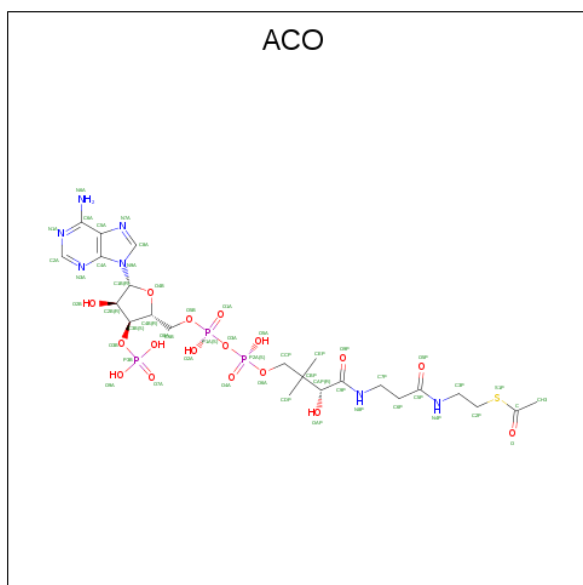
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 60	C 27	N 7	O 22	P 3	S 1	0	1
2	C	1	Total 60	C 27	N 7	O 22	P 3	S 1	0	1
2	D	1	Total 60	C 27	N 7	O 22	P 3	S 1	0	1

- Molecule 3 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 51 23 7 17 3 1	0	1
4	C	1	Total C N O P S 51 23 7 17 3 1	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	152	Total O 152 152	0	0
5	B	120	Total O 120 120	0	0
5	C	187	Total O 187 187	0	0
5	D	164	Total O 164 164	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.


Note EDS was not executed.

- Molecule 1: ATP-citrate synthase

Chain A:  93% 5% .



- Molecule 1: ATP-citrate synthase

Chain B:  91% 5% .




- Molecule 1: ATP-citrate synthase

Chain C:  94% . .



- Molecule 1: ATP-citrate synthase

Chain D:  89% 8% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.44Å 114.27Å 144.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 1.80	Depositor
% Data completeness (in resolution range)	99.7 (44.28-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.158 , 0.192	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17370	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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: Q5B, OAA, ACO

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	0.49	0/2107	0.66	0/2843
1	B	0.51	0/2069	0.63	0/2796
1	C	0.53	0/2123	0.67	0/2865
1	D	0.53	0/2113	0.64	0/2850
All	All	0.52	0/8412	0.65	0/11354

There are no bond length outliers.

There are no bond angle outliers.

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	2065	2061	2056	9	0
1	B	2025	2004	1999	12	0
1	C	2080	2075	2063	11	0
1	D	2072	2065	2071	14	0
2	A	60	0	0	1	0
2	C	60	0	0	2	0
2	D	60	0	0	1	0
3	A	9	0	2	1	0
3	C	9	0	2	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	51	0	34	1	0
4	C	51	0	34	2	0
5	A	152	0	0	0	0
5	B	120	0	0	3	0
5	C	187	0	0	2	0
5	D	164	0	0	0	0
All	All	9165	8205	8261	47	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 3.

The worst 5 of 47 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:C:1049:ASP:OD1	5:C:1301:HOH:O	2.03	0.76
1:D:892[A]:MET:SD	1:D:990:LEU:HD23	2.31	0.70
1:B:991:LYS:NZ	5:B:1201:HOH:O	2.23	0.70
1:D:994[A]:VAL:HG12	1:D:1001:THR:HG21	1.78	0.66
3:C:1202[B]:OAA:C3	4:C:1203[B]:ACO:HH32	2.26	0.65

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	268/270 (99%)	261 (97%)	7 (3%)	0	100	100
1	B	265/270 (98%)	257 (97%)	8 (3%)	0	100	100
1	C	269/270 (100%)	263 (98%)	6 (2%)	0	100	100
1	D	268/270 (99%)	262 (98%)	6 (2%)	0	100	100
All	All	1070/1080 (99%)	1043 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	219/226 (97%)	219 (100%)	0	100	100
1	B	213/226 (94%)	210 (99%)	3 (1%)	67	59
1	C	220/226 (97%)	220 (100%)	0	100	100
1	D	221/226 (98%)	220 (100%)	1 (0%)	88	87
All	All	873/904 (97%)	869 (100%)	4 (0%)	91	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	913[A]	CYS
1	B	913[B]	CYS
1	B	995	ARG
1	D	1017	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	879	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	OAA	A	1202[B]	-	2,8,8	4.02	1 (50%)	2,10,10	1.87	1 (50%)
3	OAA	C	1202[B]	-	2,8,8	4.65	1 (50%)	2,10,10	1.29	0
2	Q5B	C	1201[A]	-	48,62,62	0.63	0	60,93,93	0.90	3 (5%)
2	Q5B	A	1201[A]	-	48,62,62	0.65	0	60,93,93	1.06	4 (6%)
2	Q5B	D	1201[A]	-	48,62,62	0.64	0	60,93,93	0.72	1 (1%)
4	ACO	C	1203[B]	-	45,53,53	0.86	1 (2%)	56,79,79	1.33	6 (10%)
4	ACO	A	1203[B]	-	45,53,53	0.83	1 (2%)	56,79,79	1.32	6 (10%)

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	OAA	A	1202[B]	-	-	2/2/8/8	-
3	OAA	C	1202[B]	-	-	2/2/8/8	-
2	Q5B	C	1201[A]	-	-	9/54/83/83	0/3/3/3
2	Q5B	A	1201[A]	-	-	5/54/83/83	0/3/3/3
2	Q5B	D	1201[A]	-	-	9/54/83/83	0/3/3/3
4	ACO	C	1203[B]	-	-	8/47/67/67	0/3/3/3
4	ACO	A	1203[B]	-	-	8/47/67/67	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202[B]	OAA	O3-C3	6.47	1.32	1.22
3	A	1202[B]	OAA	O3-C3	5.68	1.31	1.22
4	C	1203[B]	ACO	C5A-C4A	2.63	1.47	1.40
4	A	1203[B]	ACO	C5A-C4A	2.48	1.47	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201[A]	Q5B	C23-C22-C21	4.91	128.07	114.85
4	A	1203[B]	ACO	P2A-O3A-P1A	-4.67	116.81	132.83
4	C	1203[B]	ACO	N3A-C2A-N1A	-4.12	122.24	128.68
4	C	1203[B]	ACO	P2A-O3A-P1A	-4.05	118.92	132.83
2	C	1201[A]	Q5B	C23-C22-C21	4.05	125.77	114.85

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201[A]	Q5B	C3-O-P-O2
2	A	1201[A]	Q5B	N6-C19-C20-S
2	C	1201[A]	Q5B	C3-O-P-O2
2	C	1201[A]	Q5B	N6-C19-C20-S
2	D	1201[A]	Q5B	C3-O-P-O3

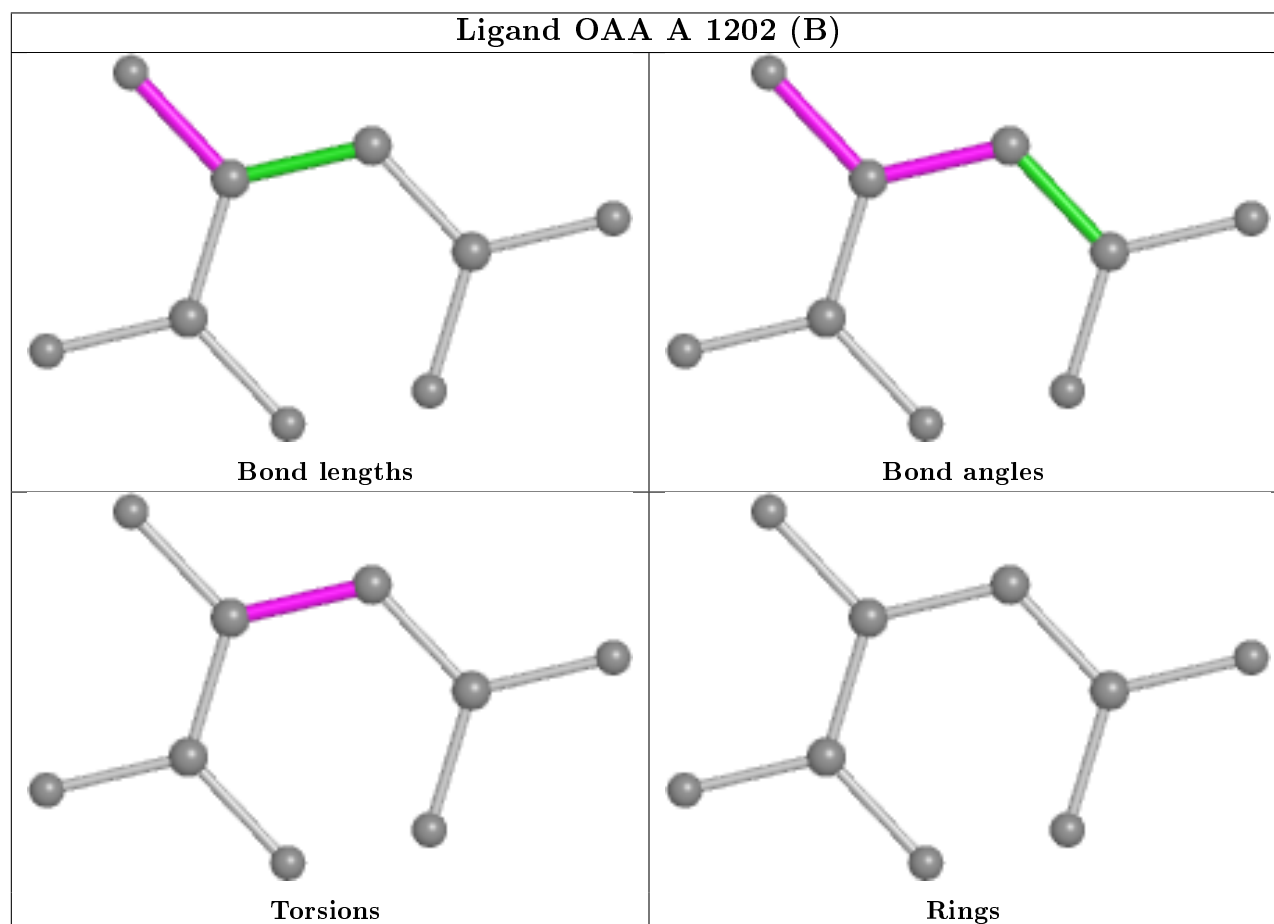
There are no ring outliers.

7 monomers are involved in 7 short contacts:

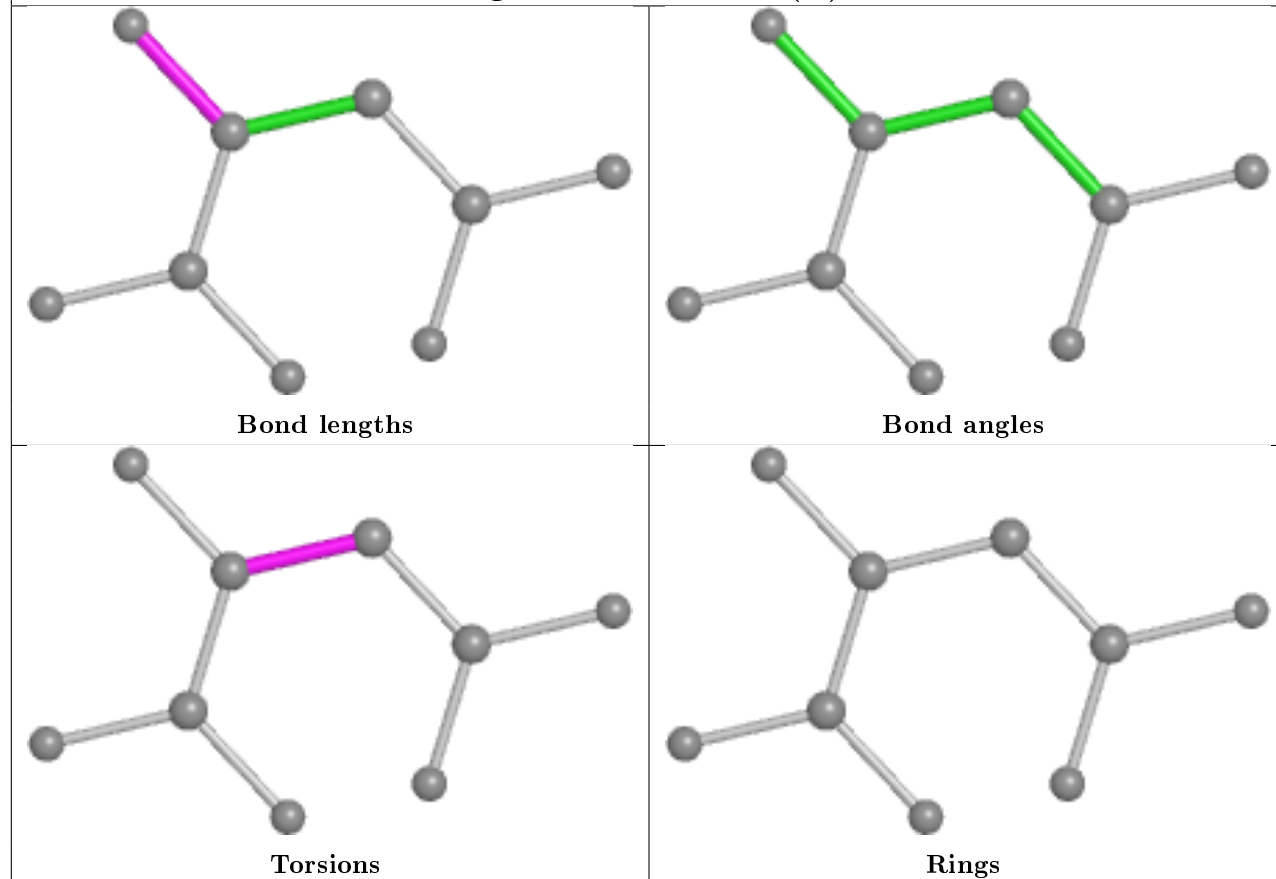
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202[B]	OAA	1	0
3	C	1202[B]	OAA	2	0
2	C	1201[A]	Q5B	2	0
2	A	1201[A]	Q5B	1	0
2	D	1201[A]	Q5B	1	0
4	C	1203[B]	ACO	2	0
4	A	1203[B]	ACO	1	0

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

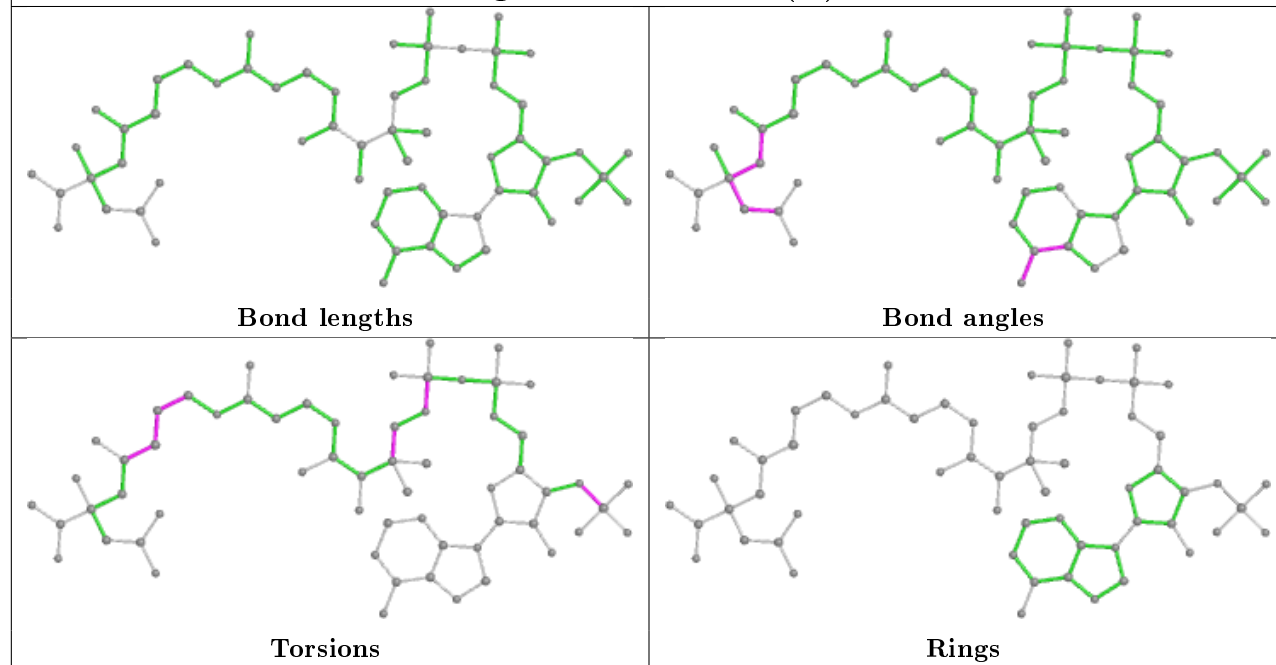
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

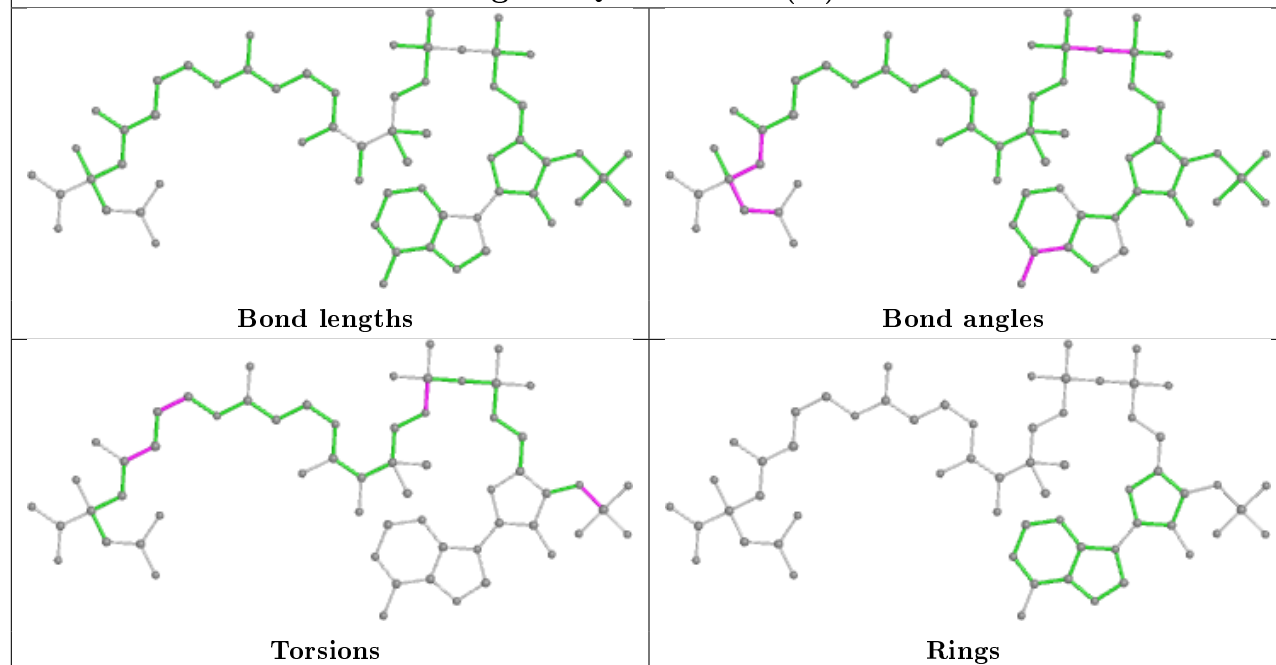
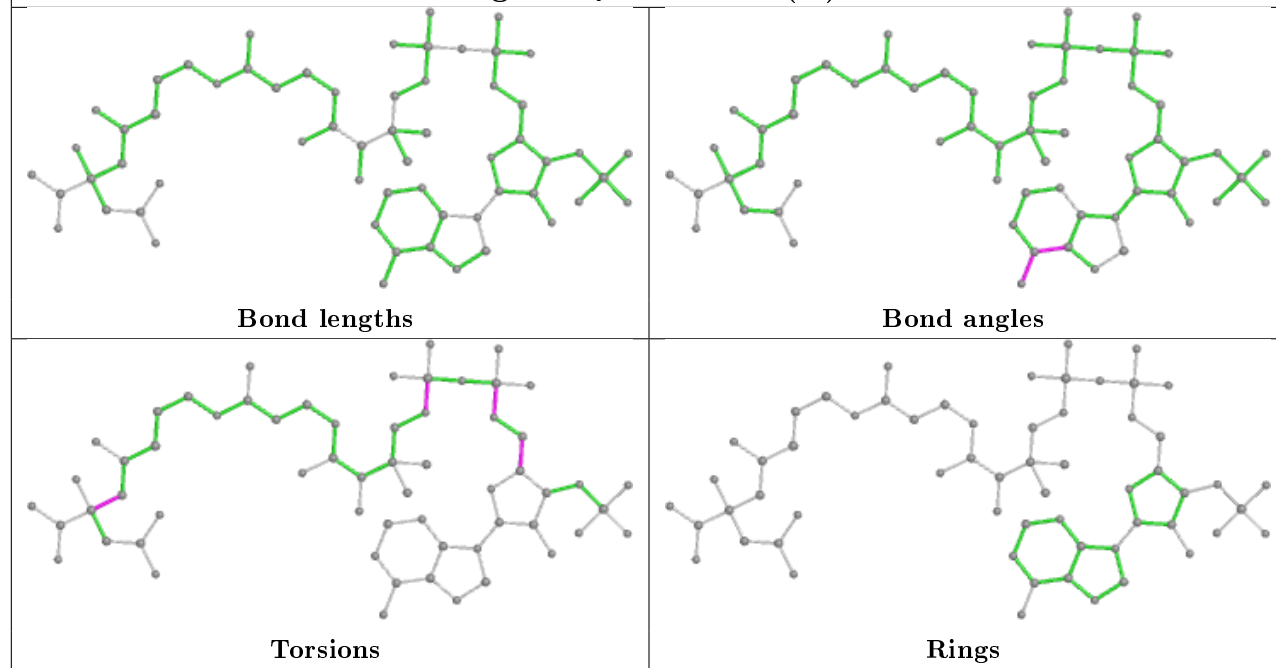


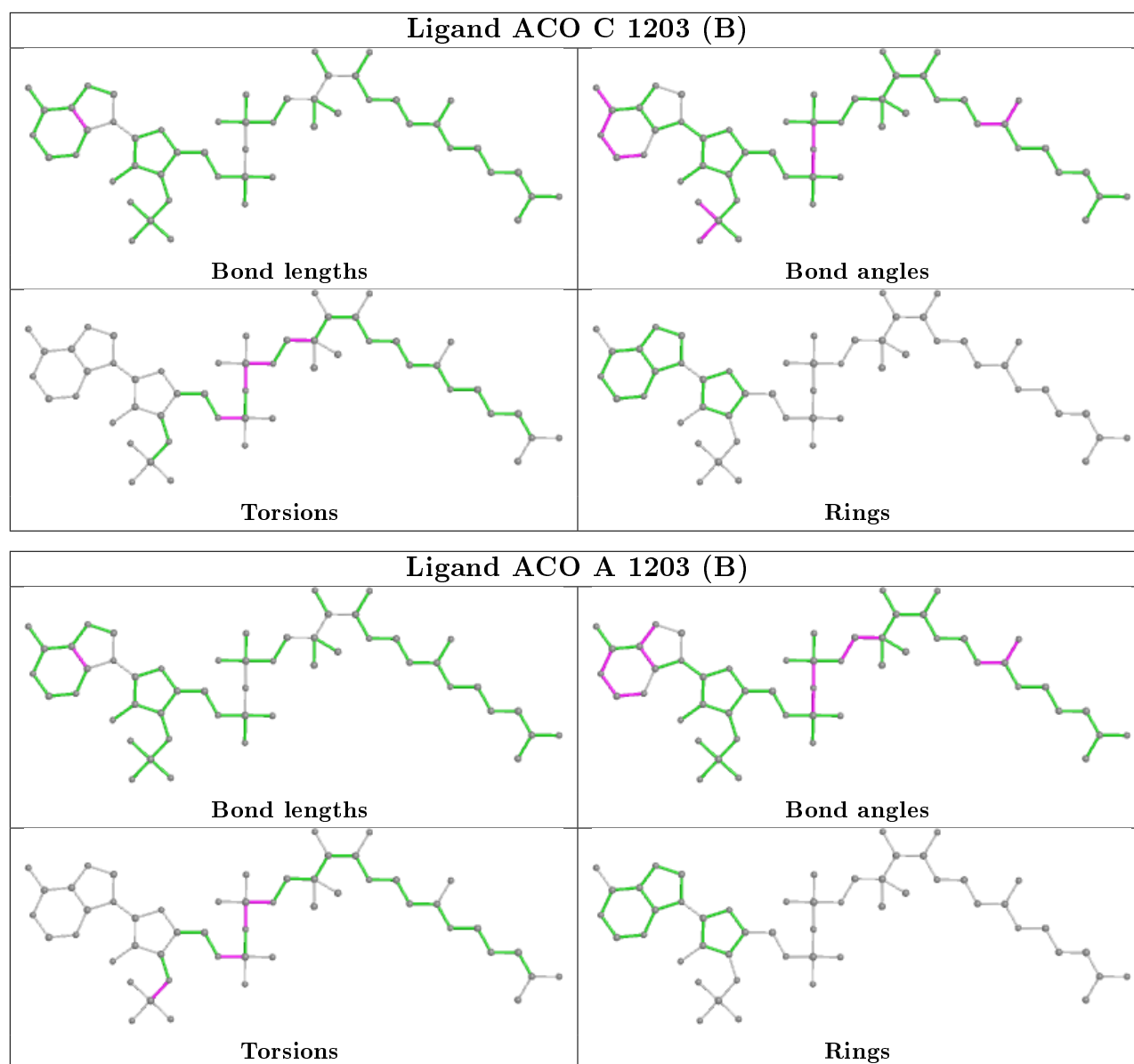
Ligand OAA C 1202 (B)



Ligand Q5B C 1201 (A)



Ligand Q5B A 1201 (A)**Ligand Q5B D 1201 (A)**



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.