W O R L D W I D E
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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 02:39 pm BST

PDB ID	:	1SCU
Title	:	THE CRYSTAL STRUCTURE OF SUCCINYL-COA SYNTHETASE FROM ESCHERICHIA COLI AT 2.5 ANGSTROMS RESOLUTION
Authors	:	Wolodko, W.T.; Fraser, M.E.; James, M.N.G.; Bridger, W.A.
Deposited on	:	1993-11-18
Resolution	:	2.50 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
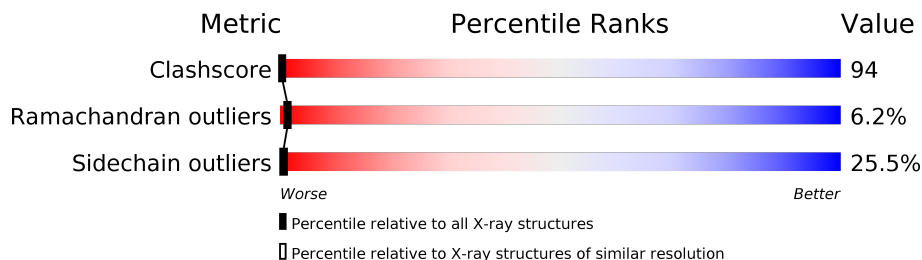with specific help available everywhere you see the (i) symbol.

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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 2.50 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	Percentile Ranks	Value
Clashscore		94
Ramachandran outliers		6.2%
Sidechain outliers		25.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	288	17% 50% 26% 7%
1	D	288	14% 51% 28% 6%
2	B	388	20% 49% 28% •
2	E	388	21% 41% 31% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10188 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 SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	0
			2083	1319	348	404	1	11			
1	D	288	Total	C	N	O	P	S	0	0	0
			2083	1319	348	404	1	11			

- Molecule 2 is a protein called SUCCINYL-COA SYNTHETASE, BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	0	0	0
			2908	1836	509	550	13			
2	E	388	Total	C	N	O	S	0	0	0
			2908	1836	509	550	13			

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
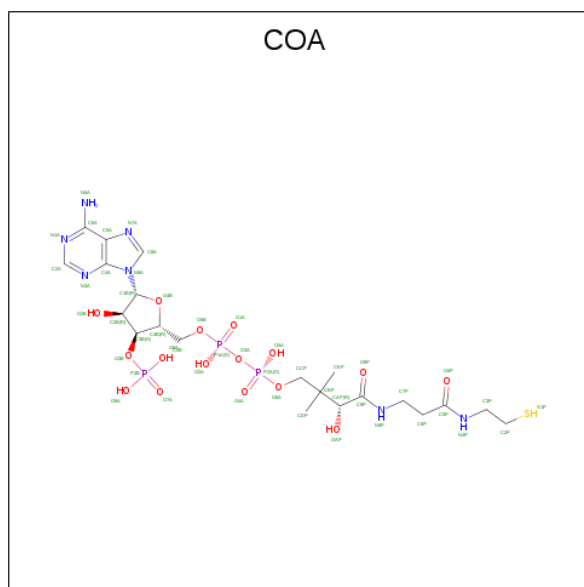
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	33	Total	O	0	0
			33	33		
4	D	25	Total	O	0	0
			25	25		
4	E	30	Total	O	0	0
			30	30		

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. 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.

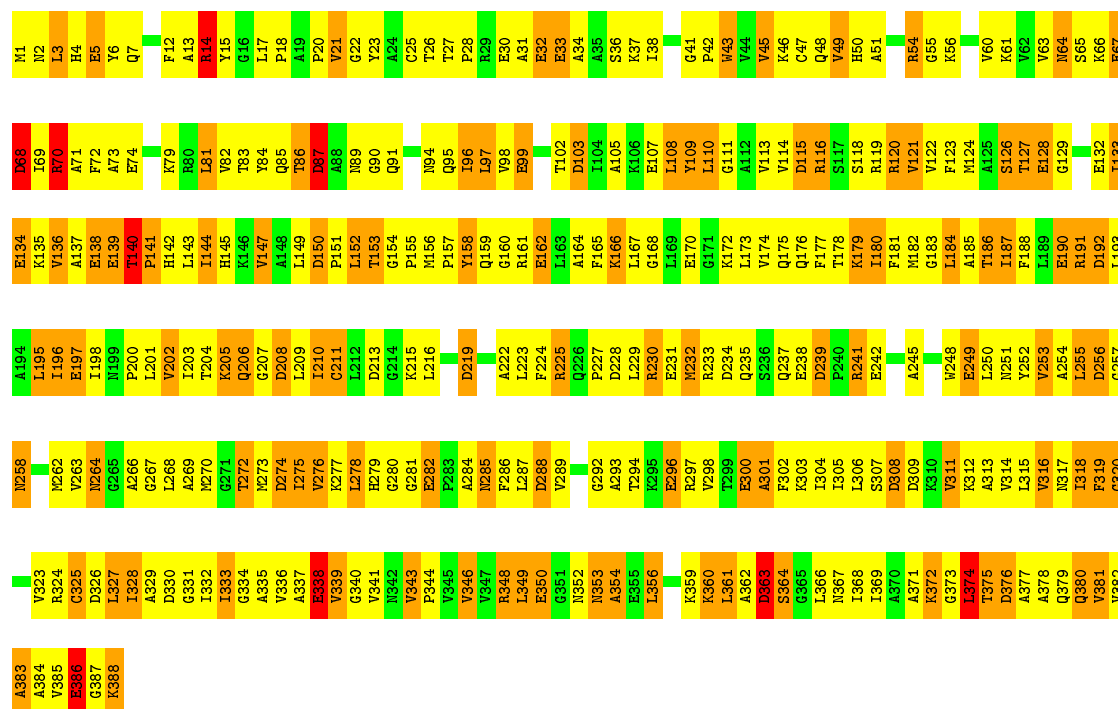- Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT
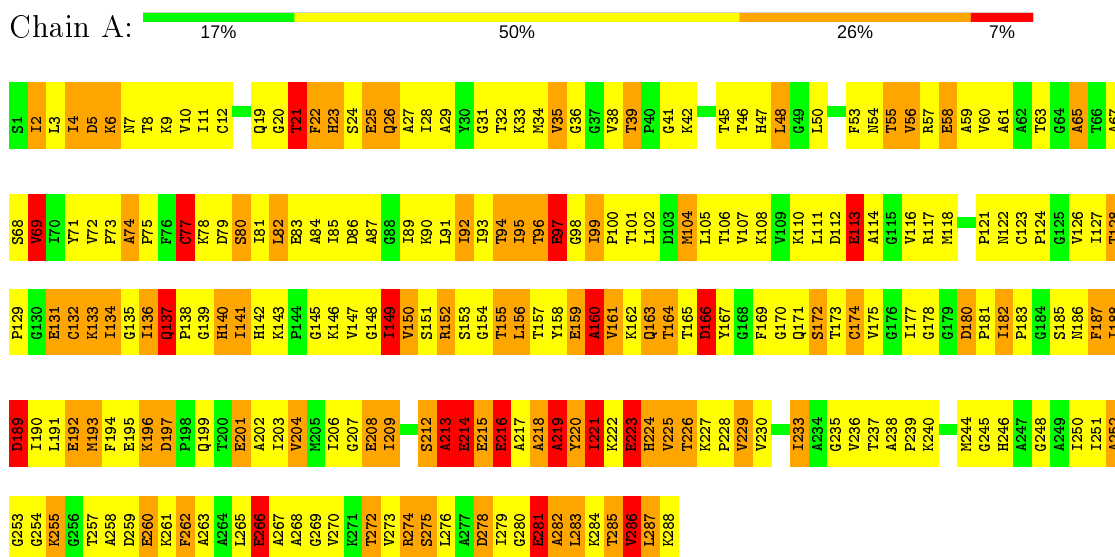
- Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT

• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT
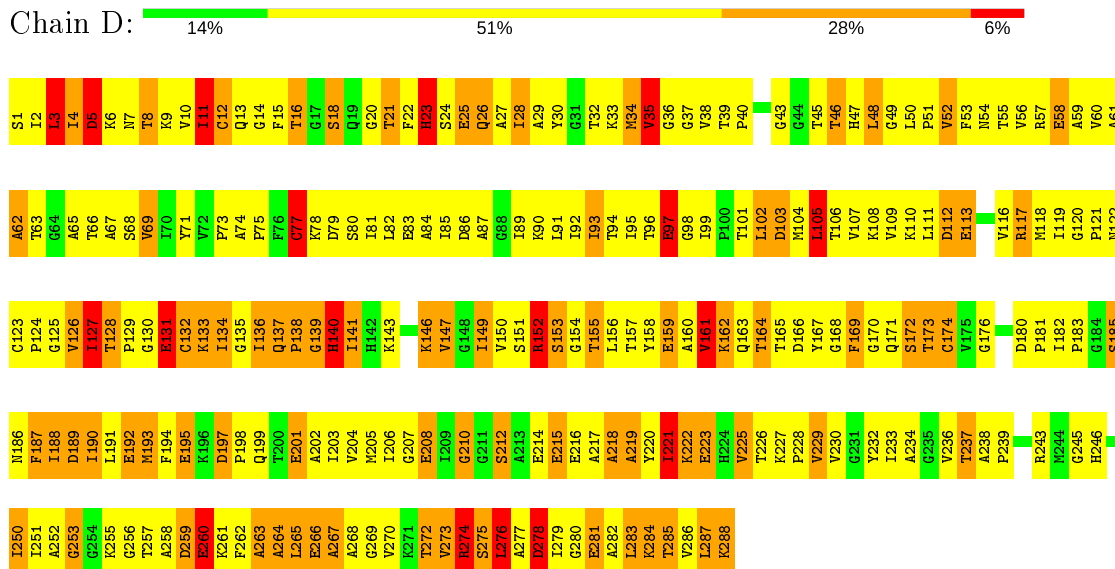
Chain B:

• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT

Chain E:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.47Å 98.47Å 400.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10188	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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:
COA, NEP

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	1.38	16/2101 (0.8%)	1.82	46/2842 (1.6%)
1	D	1.38	18/2101 (0.9%)	1.79	42/2842 (1.5%)
2	B	1.42	26/2950 (0.9%)	1.79	55/3989 (1.4%)
2	E	1.43	26/2950 (0.9%)	1.85	89/3989 (2.2%)
All	All	1.41	86/10102 (0.9%)	1.81	232/13662 (1.7%)

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	1	0
2	B	1	0
2	E	5	0
All	All	7	0

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	162	GLU	CD-OE2	10.37	1.37	1.25
2	E	350	GLU	CD-OE2	9.76	1.36	1.25
1	D	58	GLU	CD-OE2	9.60	1.36	1.25
2	E	132	GLU	CD-OE1	8.90	1.35	1.25
2	E	162	GLU	CD-OE2	8.88	1.35	1.25

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	THR	C-N-CD	-13.94	89.94	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	348	ARG	CD-NE-CZ	11.82	140.15	123.60
2	E	348	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	A	152	ARG	NE-CZ-NH2	-10.38	115.11	120.30
2	E	140	THR	C-N-CD	-9.88	98.86	120.60

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	99	ILE	CB
2	B	64	ASN	CA
2	E	64	ASN	CA
2	E	256	ASP	CA
2	E	287	LEU	CA

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	2083	0	2140	401	0
1	D	2083	0	2140	509	0
2	B	2908	0	2962	465	0
2	E	2908	0	2963	563	0
3	A	48	0	32	13	0
3	D	48	0	32	17	0
4	A	22	0	0	8	0
4	B	33	0	0	13	0
4	D	25	0	0	6	0
4	E	30	0	0	9	0
All	All	10188	0	10269	1922	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 94.

The worst 5 of 1922 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)
2:E:343:VAL:CG1	2:E:344:PRO:HD2	1.16	1.62
1:A:104:MET:HA	1:A:104:MET:CE	1.33	1.51
1:D:2:ILE:HD11	1:D:193:MET:CB	1.35	1.49
2:E:343:VAL:HG13	2:E:344:PRO:CD	1.40	1.49
1:A:4:ILE:HD11	1:A:132:CYS:SG	1.50	1.48

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	285/288 (99%)	209 (73%)	52 (18%)	24 (8%)	1	1
1	D	285/288 (99%)	207 (73%)	53 (19%)	25 (9%)	1	0
2	B	386/388 (100%)	315 (82%)	59 (15%)	12 (3%)	4	5
2	E	386/388 (100%)	307 (80%)	57 (15%)	22 (6%)	1	1
All	All	1342/1352 (99%)	1038 (77%)	221 (16%)	83 (6%)	1	1

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	164	THR
1	A	213	ALA
1	A	219	ALA
1	A	221	ILE

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	217/217 (100%)	169 (78%)	48 (22%)	1	1
1	D	217/217 (100%)	159 (73%)	58 (27%)	0	0
2	B	298/298 (100%)	221 (74%)	77 (26%)	0	1
2	E	298/298 (100%)	218 (73%)	80 (27%)	0	0
All	All	1030/1030 (100%)	767 (74%)	263 (26%)	0	1

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	367	ASN
1	D	131	GLU
2	E	325	CYS
2	B	381	VAL
1	D	28	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	367	ASN
2	E	4	HIS
2	E	352	ASN
2	B	380	GLN
1	D	137	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	NEP	A	246	1	10,14,15	1.51	2 (20%)	5,20,22	2.50	3 (60%)
1	NEP	D	246	1	10,14,15	1.70	2 (20%)	5,20,22	1.96	2 (40%)

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	NEP	A	246	1	-	0/5/12/14	0/1/1/1
1	NEP	D	246	1	-	3/5/12/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	NEP	P-O2P	-4.09	1.46	1.54
1	A	246	NEP	P-O2P	-2.93	1.48	1.54
1	D	246	NEP	P-O1P	-2.51	1.49	1.54
1	A	246	NEP	CD2-CG	2.30	1.39	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	NEP	CB-CG-CD2	3.15	134.44	127.95
1	A	246	NEP	CB-CA-C	-3.02	105.81	111.47
1	D	246	NEP	O2P-P-O3P	-2.66	107.70	113.44
1	A	246	NEP	O1P-P-O3P	-2.59	107.84	113.44
1	D	246	NEP	CB-CG-CD2	2.54	133.18	127.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	246	NEP	O-C-CA-CB
1	D	246	NEP	CA-CB-CG-ND1
1	D	246	NEP	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	246	NEP	4	0
1	D	246	NEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	#$|Z| > 2$
3	COA	A	289	-	41,50,50	0.94	1 (2%)	52,75,75	2.30	9 (17%)
3	COA	D	289	-	41,50,50	0.91	1 (2%)	52,75,75	1.26	5 (9%)

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	COA	A	289	-	-	15/44/64/64	0/3/3/3
3	COA	D	289	-	-	17/44/64/64	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	289	COA	C6P-C5P	2.59	1.56	1.51
3	A	289	COA	C4A-N3A	-2.26	1.32	1.35

The worst 5 of 14 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	289	COA	O9A-P3B-O7A	9.84	149.20	110.68
3	A	289	COA	O8A-P3B-O7A	-8.91	75.80	110.68
3	D	289	COA	P2A-O3A-P1A	-4.92	115.93	132.83
3	A	289	COA	C7P-N8P-C9P	-4.59	114.41	122.59
3	A	289	COA	O4B-C1B-C2B	-3.73	101.47	106.93

There are no chirality outliers.
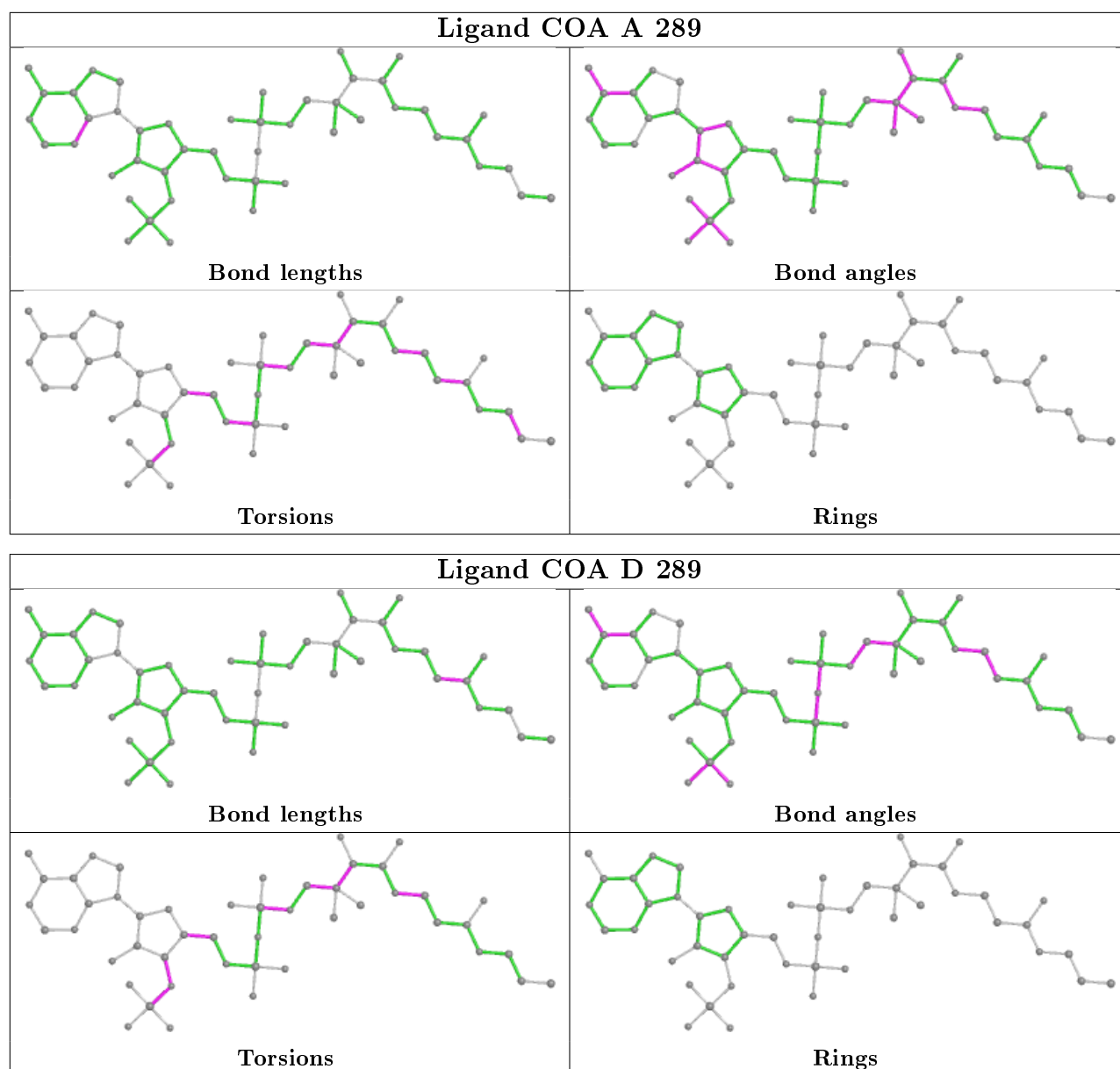
5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	289	COA	C3B-O3B-P3B-O7A
3	A	289	COA	OAP-CAP-CBP-CCP
3	A	289	COA	C9P-CAP-CBP-CCP
3	A	289	COA	C9P-CAP-CBP-CDP
3	A	289	COA	OAP-CAP-CBP-CEP

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	289	COA	13	0
3	D	289	COA	17	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.

Ligand COA A 289

Bond lengths

Bond angles

Torsions

Rings

Ligand COA D 289

Bond lengths

Bond angles

Torsions

Rings

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.