wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 07:58 PM EDT

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.

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 (1)) were used in the production of this report:

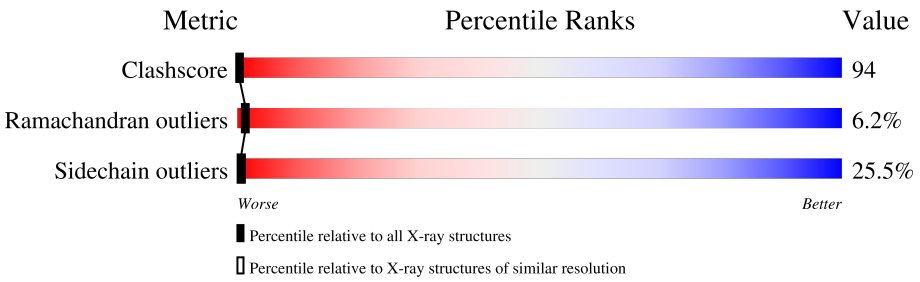
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	288	17% 50% 26% 7%
1	D	288	14% 51% 29% 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.

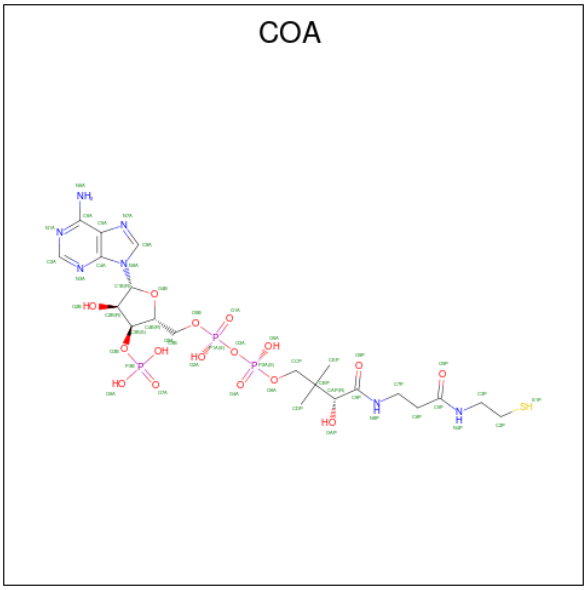
- Molecule 1 is a protein called SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT.

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

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

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

- 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
			Total	C	N	O	P	S		
3	A	1	48	21	7	16	3	1	0	0
			Total	C	N	O	P	S		
3	D	1	48	21	7	16	3	1	0	0

- Molecule 4 is water.

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

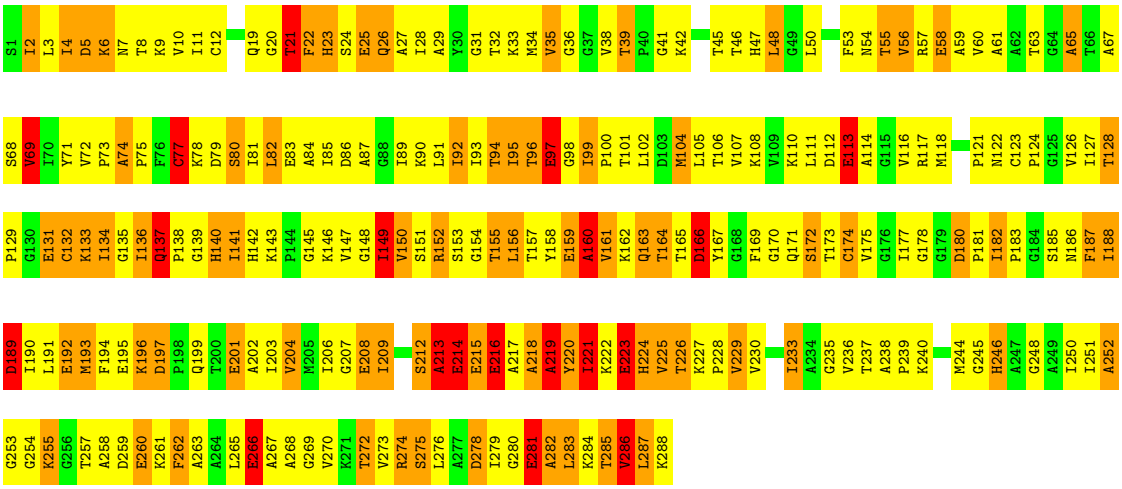
3 Residue-property plots (i)

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.

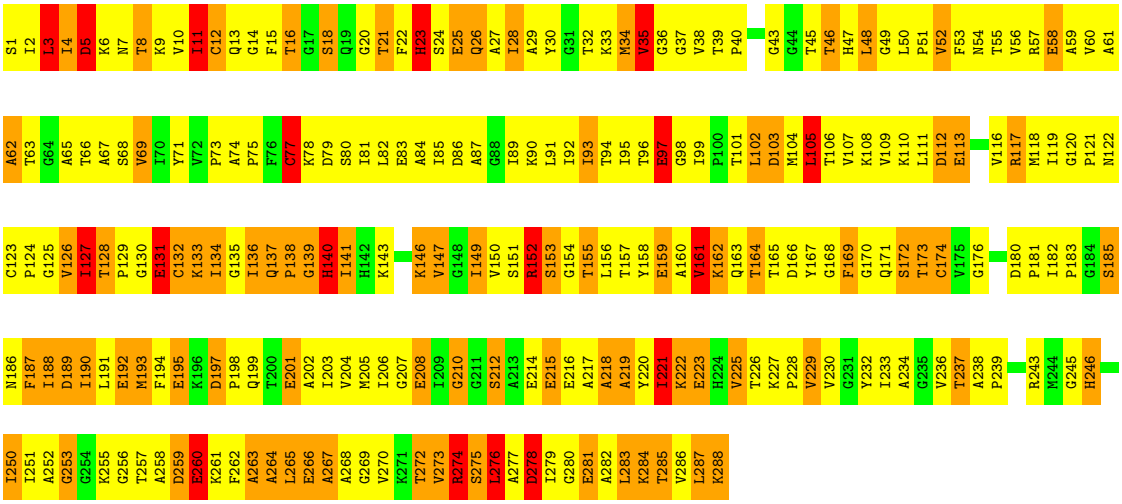
• Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT

Chain A: 17% 50% 26% 7%



• Molecule 1: SUCCINYL-COA SYNTHETASE, ALPHA SUBUNIT

Chain D: 14% 51% 29% 6%



• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT

Chain B: 20% 49% 28%

M1 N2 L3 H4 E5 Y6 Q7 F12 A13 R14 Y15 G16 L17 P18 A19 P20 V21 G22 Y23 A24 C25 T26 T27 P28 R29 E30 A31 E32 E33 A34 A35 S36 K37 I38 G41 P42 W43 V44 V45 K46 C47 Q48 V49 H50 A51 R54 G55 K56 V60 K61 V62 V63 N64 S65 K66 E67

D68 I69 R70 A71 F72 A73 E74 K79 R80 L81 V82 T83 Y84 Q85 T86 D87 A88 N89 G90 Q91 N94 Q95 I96 L97 V98 E99 T102 D103 I104 A105 K106 E107 L108 Y109 L110 G111 A112 V113 V114 D115 R116 S117 S118 R119 R120 V121 V122 F123 M124 A125 S126 T127 E128 G129 E132 I133

E134 K135 V136 A137 E138 E139 T140 P141 H142 L143 I144 H145 K146 V147 A148 L149 D150 P151 L152 T153 G154 P155 M156 P157 Y158 Q159 G160 R161 E162 L163 A164 F165 K166 L167 G168 L169 E170 G171 K172 L173 V174 Q175 Q176 F177 T178 K179 I180 F181 M182 G183 L184 A185 T186 I187 F188 L189 E190 R191 D192 L193

A194 L195 I196 E197 I198 N199 P200 L201 V202 I203 T204 K205 Q206 G207 D208 L209 I210 C211 L212 D213 G214 K215 L216 D219 A222 L223 F224 R225 Q226 P227 D228 L229 R230 E231 M232 R233 D234 Q235 S236 Q237 E238 D239 P240 R241 E242 A245 W248 E249 L250 N251 Y252 V253 A254 L255 D256 G257

N258 M262 V263 N264 G265 A266 G267 L268 A269 M270 G271 T272 M273 D274 I275 V276 K277 L278 H279 G280 G281 E282 P283 A284 N285 F286 L287 D288 V289 G292 A293 T294 K295 E296 R297 V298 T299 E300 A301 F302 K303 I304 I305 L306 S307 D308 D309 K310 V311 K312 A313 V314 L315 V316 N317 I318 F319 G320

V323 R324 C325 D326 L327 I328 A329 D330 G331 I332 I333 I333 G334 A335 V336 A337 E338 V339 G340 V341 N342 V343 P344 V345 V346 V347 R348 L349 E350 G351 N352 N353 A354 E355 L356 K359 K360 L361 A362 D363 S364 G365 L366 N367 I368 I369 A370 A371 K372 G373 L374 T375 D376 A377 A378 Q379 Q380 V381 V382

A383 A384 V385 E386 G387 K388

• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA SUBUNIT

Chain E: 21% 41% 31% 7%

M1 N2 L3 H4 E5 Y6 Q7 A8 K9 Q10 L11 F12 A13 R14 Y15 G16 L17 P18 A19 P20 C25 T26 T27 P28 R29 E30 A31 E32 E33 A34 A35 S36 K37 I38 G41 P42 W43 V44 V45 K46 V49 H50 R54 G55 K56 A57 G58 G59 V60 K61 V62 V63 N64 S65 K66 E67

D68 I69 R70 A71 F72 A73 E74 N75 W76 K79 R80 L81 V82 T83 T86 D87 A88 N89 G90 Q91 P92 V93 N94 Q95 I96 L97 V98 E99 D103 I104 A105 K106 E107 L108 Y109 L110 G111 A112 V113 V114 D115 R116 S117 S118 R119 R120 V121 V122 F123 M124 A125 S126 T127 E128 G129 G130 V131

E132 I133 E134 K135 V136 A137 E138 E139 T140 P141 H142 L143 K146 D150 P151 L152 T153 M156 P157 Y158 Q159 E162 L163 A164 L167 G168 L169 E170 L173 Q176 F177 T178 K179 I180 F181 M182 G183 L184 A185 T186 I187 F188 L189 E190 R191 D192 L195 I196 E197 I198 N199 P200

L201 V202 I203 T204 K205 Q206 G207 D208 L209 I210 C211 G214 K215 L216 G217 A218 D219 G220 N221 A222 L223 F224 R225 Q226 P227 D228 L229 R230 R233 D234 Q235 S236 Q237 E238 D239 P240 R241 E242 A243 Q244 A245 A246 Q247 W248 E249 L250 N251 Y252 V253 A254 L255 D256 G257 N258 M262 V263

N264 G265 A266 G267 L268 A269 M270 G271 T272 M273 D274 I275 V276 K277 L278 H279 G280 G281 E282 P283 A284 N285 F286 L287 D288 V289 G290 G291 G292 A293 T294 K295 E296 R297 V298 T299 E300 A301 F302 K303 I304 I305 L306 S307 D308 D309 K310 V311 K312 A313 V314 L315 V316 N317 I318 F319 G320 G321 I322 V323

R324 C325 D326 L327 I328 A329 D330 G331 I332 I333 I333 G334 A335 V336 A337 E338 V339 G340 V341 N342 V343 P344 V345 V346 V347 R348 L349 E350 G351 N352 N353 A354 E355 L356 G357 A358 K359 K360 L361 A362 D363 S364 G365 L366 N367 I368 I369 A370 A371 K372 G373 L374 T375 D376 A377 A378 Q379 Q380 V381 V382 A383

A384 V385 E386 G387 K388

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: NEP, 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	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(^{o})	Ideal(^{o})
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	E	270	MET
2	E	307	SER
2	E	385	VAL
2	B	262	MET
2	B	241	ARG

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

Mol	Chain	Res	Type
2	E	4	HIS
2	E	89	ASN
2	E	352	ASN
2	E	50	HIS
2	E	142	HIS

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	NEP	A	246	1	11,14,15	1.44	2 (18%)	4,20,22	2.56	2 (50%)
1	NEP	D	246	1	11,14,15	1.62	2 (18%)	4,20,22	2.38	3 (75%)

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	-4.00	1.46	1.54
1	A	246	NEP	P-O2P	-2.86	1.48	1.54
1	D	246	NEP	P-O1P	-2.44	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(^{o})	Ideal(^{o})
1	A	246	NEP	CB-CG-CD2	3.49	134.44	127.89
1	D	246	NEP	O2P-P-O3P	-2.89	107.70	113.76
1	A	246	NEP	O1P-P-O3P	-2.82	107.84	113.76
1	D	246	NEP	CB-CG-CD2	2.82	133.18	127.89
1	D	246	NEP	O1P-P-O3P	-2.20	109.14	113.76

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 monosaccharides 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	D	289	-	43,50,50	1.27	5 (11%)	56,75,75	1.17	5 (8%)
3	COA	A	289	-	43,50,50	0.95	1 (2%)	56,75,75	2.74	11 (19%)

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	D	289	-	-	16/44/64/64	0/3/3/3
3	COA	A	289	-	-	15/44/64/64	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	289	COA	P2A-O3A	3.96	1.63	1.59
3	D	289	COA	C1B-N9A	-2.88	1.42	1.49
3	D	289	COA	P1A-O3A	2.79	1.62	1.59
3	D	289	COA	C6P-C5P	2.46	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	289	COA	CCP-CBP	2.41	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	289	COA	O9A-P3B-O7A	9.85	149.20	110.83
3	A	289	COA	O3A-P1A-O1A	-9.11	83.31	110.70
3	A	289	COA	O8A-P3B-O7A	-8.99	75.80	110.83
3	A	289	COA	O2A-P1A-O3A	6.48	124.78	107.27
3	A	289	COA	C4B-O4B-C1B	-5.35	105.03	109.92

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

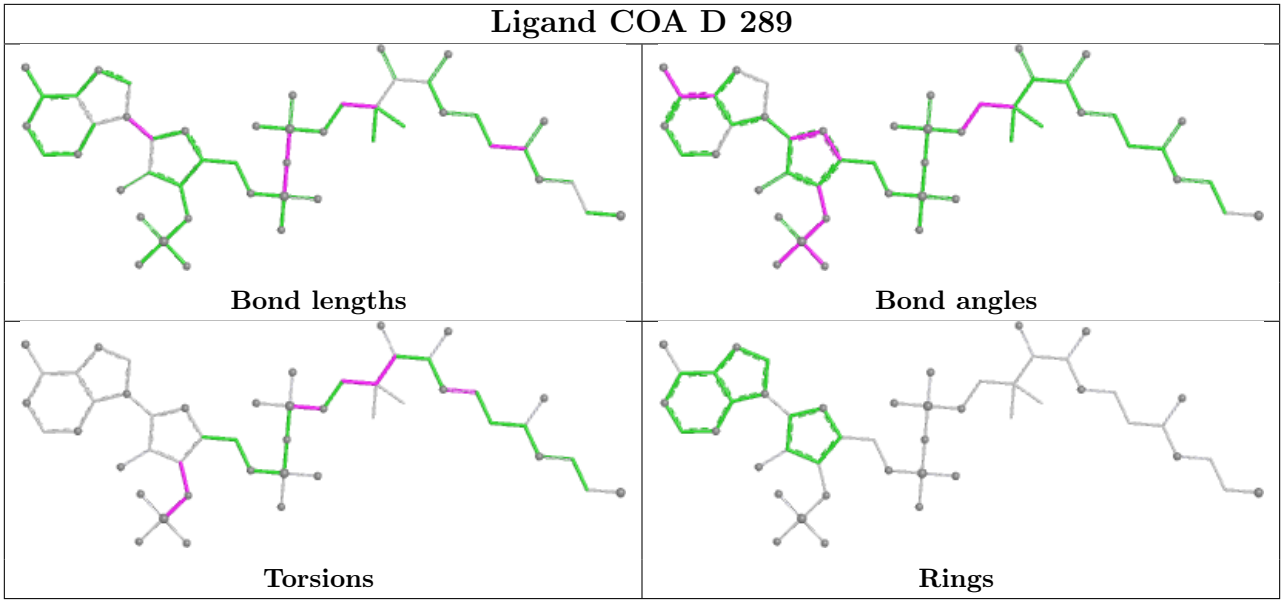
Mol	Chain	Res	Type	Atoms
3	A	289	COA	OAP-CAP-CBP-CCP
3	A	289	COA	C9P-CAP-CBP-CCP
3	A	289	COA	C9P-CAP-CBP-CDP
3	A	289	COA	OAP-CAP-CBP-CEP
3	A	289	COA	C9P-CAP-CBP-CEP

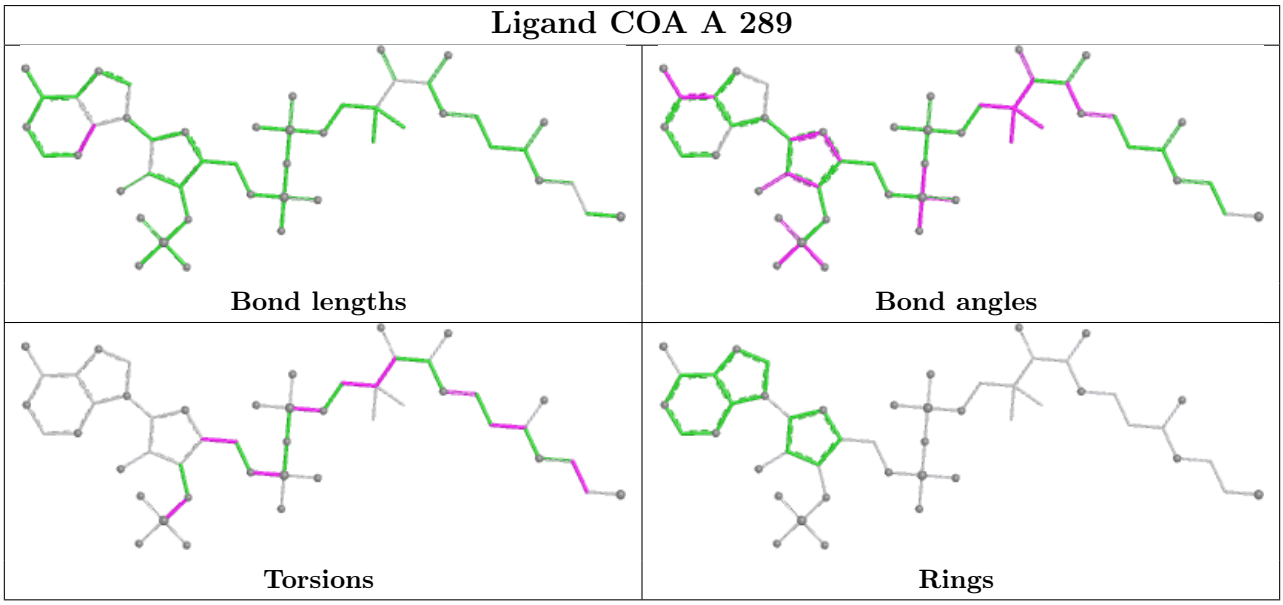
There are no ring outliers.

2 monomers are involved in 30 short contacts:

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





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.