WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 27, 2024 – 10:56 PM EST

PDB ID : 1DLV

Title : BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA IN COM-
PLEX WITH COA

Authors : Modis, Y.; Wierenga, R.K.

Deposited on : 1999-12-12

Resolution : 2.29 Å(reported)

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 : 2.36

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)

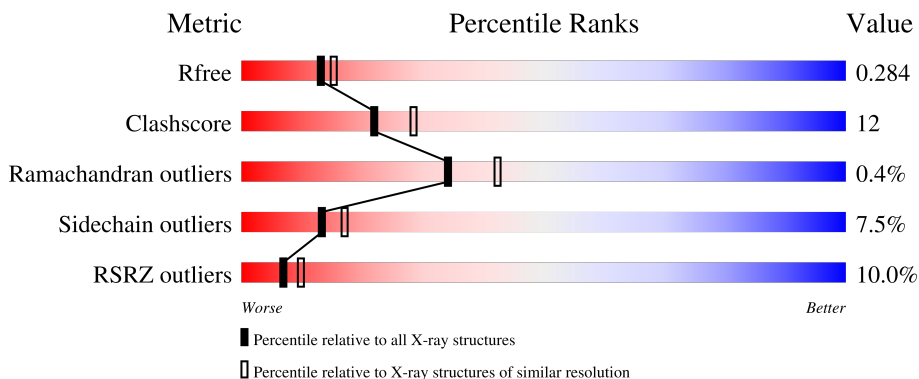Validation Pipeline (wwPDB-VP) : 2.36

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 2.29 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
Rfree		0.284
Clashscore		12
Ramachandran outliers		0.4%
Sidechain outliers		7.5%
RSRZ outliers		10.0%

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))
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 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% 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	389	.% 57% 34% 8% •
1	B	389	.% 61% 30% 7% •
1	C	389	13% 70% 24% 5%
1	D	389	25% 69% 26% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12192 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 BIOSYNTHETIC THIOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	B	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	C	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	D	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	insertion	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	11	ALA	-	insertion	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	11	ALA	-	insertion	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	11	ALA	-	insertion	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3 O⁻ — S — O⁻ O4

S

O2

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

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

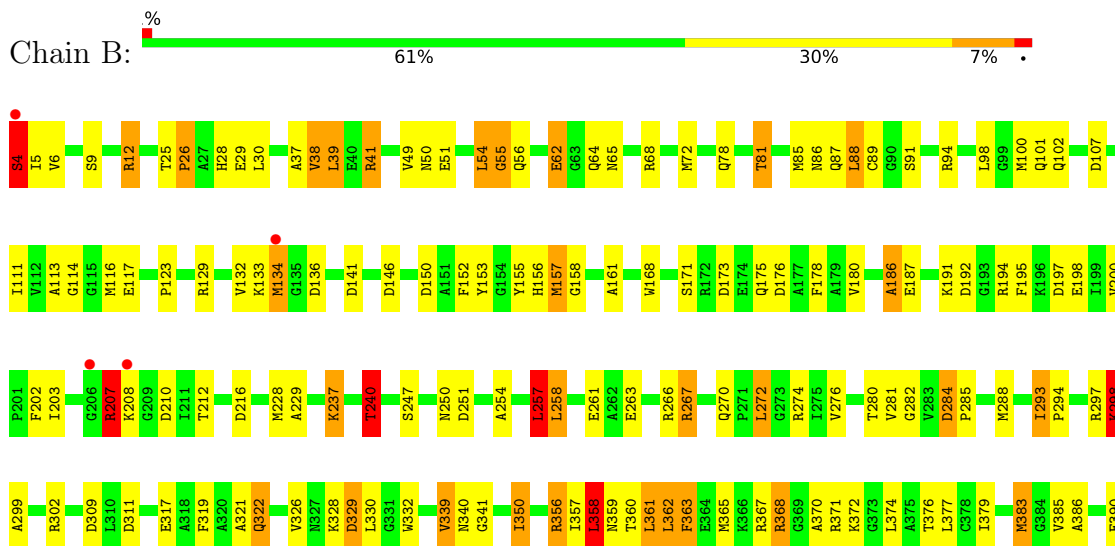| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	1	0
			287	287		
4	B	276	Total	O	3	0
			276	276		
4	C	96	Total	O	0	0
			96	96		
4	D	59	Total	O	1	0
			59	59		

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.
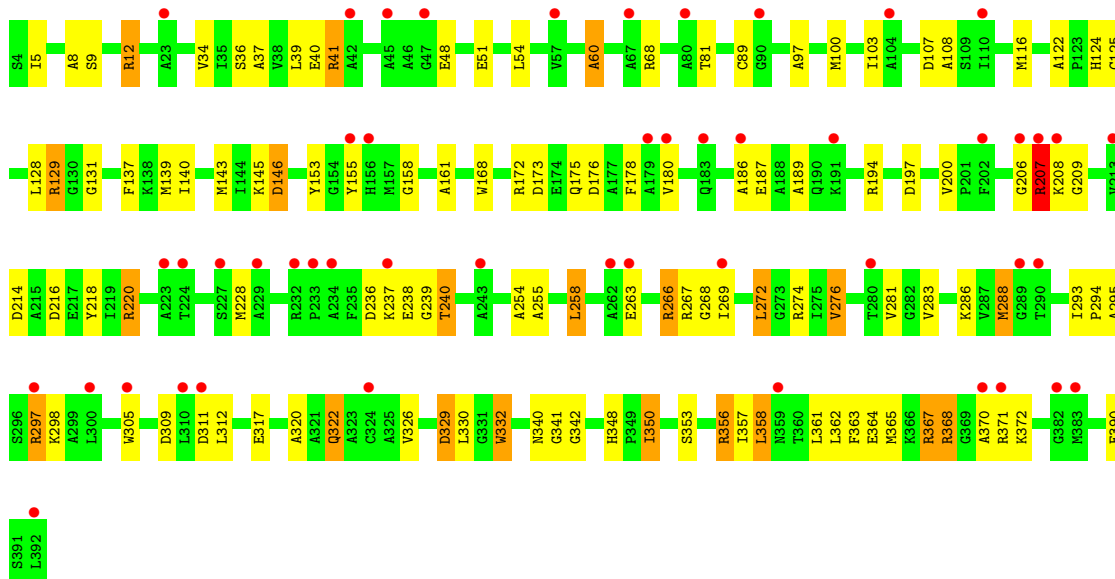
• Molecule 1: BIOSYNTHETIC THIOLASE

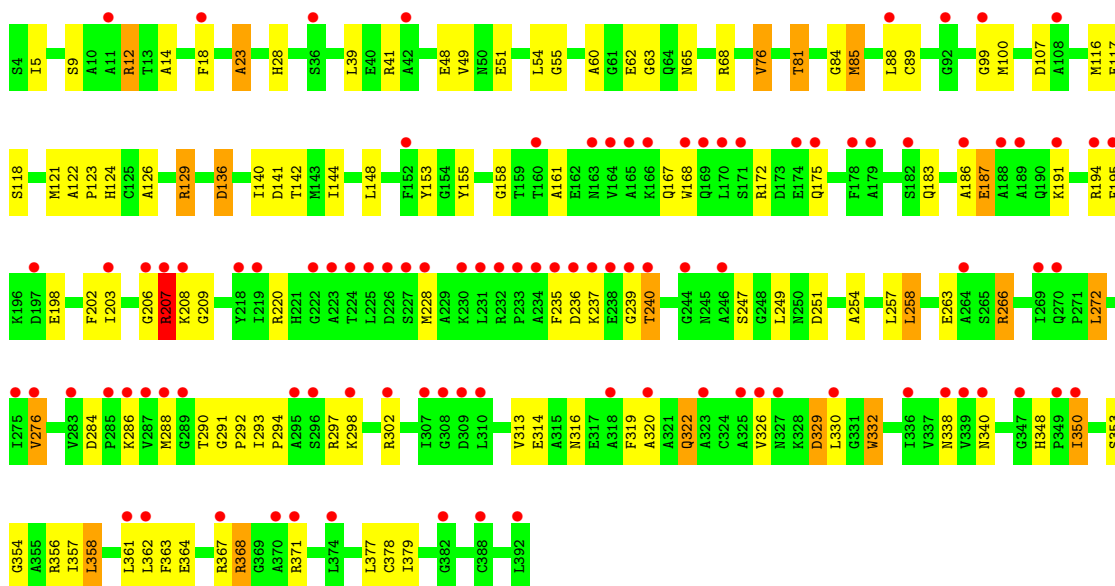

• Molecule 1: BIOSYNTHETIC THIOLASE

S391 L392

● Molecule 1: BIOSYNTHETIC THIOLASE

Chain C:

13%

70%　　　　　　　　24%　　　　5%

S4 I5 A8 S9 R12 A23 V34 I35 S36 A37 V38 L39 E40 R41 A42 A45 A46 G47 E48 E51 L54 V57 A60 A67 R68 A80 T81 C89 G90 A97 M100 I103 A104 D107 A108 S109 I110 M116 A122 P123 H124 C125

L128 R129 G130 G131 F137 K138 M139 I140 M143 I144 K145 D146 Y153 G154 Y155 H156 M157 G158 A161 W168 R172 D173 E174 Q175 D176 A177 F178 A179 V180 Q183 A186 E187 A188 A189 Q190 K191 R194 D197 V200 P201 F202 G206 R207 K208 G209 V213

D214 A215 D216 E217 Y218 I219 R220 A223 T224 S227 M228 A229 R232 P233 A234 F235 D236 K237 E238 G239 T240 A243 A254 A255 L258 A262 E263 R266 R267 G268 I269 L272 G273 R274 I275 V276 T280 V281 G282 V283 K286 V287 M288 G289 T290 I293 P294 A295

S296 R297 K298 A299 L300 W305 D309 L310 D311 L312 E317 A320 A321 Q322 A323 C324 A325 V326 D329 L330 G331 W332 N340 G341 G342 H348 P349 I350 S353 R356 I357 L358 N359 T360 L361 L362 F363 E364 M365 K366 R367 R368 G369 A370 R371 K372 G382 M383 E390

S391 L392

● Molecule 1: BIOSYNTHETIC THIOLASE

Chain D:

25%

69%　　　　　　　　26%　　　　5%

S4 I5 S9 A10 A11 R12 T13 A14 F18 A23 H28 S36 L39 E40 R41 A42 E48 V49 N50 E51 L54 G55 A60 G61 E62 G63 Q64 N65 R68 V76 T81 G84 M85 L88 C89 G92 G99 M100 D107 A108 M116 E117

S118 M121 A122 P123 H124 C125 A126 R129 D136 I140 D141 T142 M143 I144 L148 F152 Y153 G154 Y155 G158 T159 T160 A161 E162 N163 V164 A165 K166 Q167 W168 Q169 L170 S171 R172 D173 E174 Q175 F178 A179 S182 Q183 A186 E187 A188 A189 Q190 K191 R194 F195

K196 D197 E198 F202 I203 G206 R207 K208 G209 Y218 I219 R220 H221 G222 A223 T224 L225 D226 S227 M228 A229 K230 L231 R232 P233 A234 F235 D236 K237 E238 G239 T240 G244 N245 A246 S247 G248 L249 N250 D251 A254 L257 L258 E263 A264 S265 R266 I269 Q270 P271 L272

I275 V276 V283 D284 P285 K286 V287 M288 G289 T290 P292 I293 P294 A295 S296 R297 K298 R302 I307 G308 D309 L310 V313 E314 A315 N316 E317 A318 F319 A320 A321 Q322 A323 C324 A325 V326 N327 K328 D329 L330 G331 W332 I336 V337 N338 V339 N340 G347 H348 P349 I350 S353

G354 A355 R356 I357 L358 L361 L362 F363 E364 R367 R368 G369 A370 R371 L374 L377 C378 I379 G382 C388 L392

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.82Å 79.30Å 149.98Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	30.00 – 2.29 29.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.29) 82.2 (29.51-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.293 0.238 , 0.284	Depositor DCC
R_{free} test set	5026 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.5	EDS
L-test for twinning[2]	$< |L| > = 0.36, < L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: SO4, 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	1.24	7/2854 (0.2%)	2.64	181/3853 (4.7%)
1	B	1.22	7/2854 (0.2%)	2.32	142/3853 (3.7%)
1	C	0.61	0/2854	1.67	46/3853 (1.2%)
1	D	0.60	0/2854	1.71	55/3853 (1.4%)
All	All	0.97	14/11416 (0.1%)	2.12	424/15412 (2.8%)

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	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	LEU	C-N	20.46	1.69	1.33
1	A	278	TRP	CZ2-CH2	-12.08	1.14	1.37
1	A	118	SER	CA-CB	11.31	1.70	1.52
1	A	278	TRP	CZ3-CH2	10.95	1.57	1.40
1	A	90	GLY	N-CA	8.92	1.59	1.46

The worst 5 of 424 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	ARG	NE-CZ-NH1	22.74	131.67	120.30
1	A	367	ARG	NE-CZ-NH1	22.35	131.47	120.30
1	A	251	ASP	CB-CG-OD1	21.21	137.39	118.30
1	C	266	ARG	NE-CZ-NH2	20.53	130.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	329	ASP	CB-CG-OD2	20.18	136.46	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ILE	Mainchain

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	2813	0	2818	68	0
1	B	2813	0	2819	72	0
1	C	2813	0	2819	64	0
1	D	2813	0	2819	70	0
2	A	15	0	0	0	0
2	B	15	0	0	1	0
3	A	48	0	32	4	0
3	B	48	0	31	2	0
3	C	48	0	31	0	0
3	D	48	0	31	2	0
4	A	287	0	0	13	2
4	B	276	0	0	17	1
4	C	96	0	0	14	0
4	D	59	0	0	10	0
All	All	12192	0	11400	269	3

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 12.

The worst 5 of 269 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:54:LEU:C	1:B:55:GLY:N	1.69	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.25	1.00
1:B:258:LEU:HG	4:B:5222:HOH:O	1.65	0.97
1:A:175:GLN:HE22	1:A:240:THR:CG2	1.79	0.95
1:B:356:ARG:C	1:B:356:ARG:HD2	1.92	0.89

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:5238:HOH:O	4:A:5280:HOH:O[2_645]	1.94	0.26
4:A:5078:HOH:O	4:A:5084:HOH:O[2_655]	2.13	0.07
4:B:5202:HOH:O	4:B:5234:HOH:O[2_555]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	387/389 (100%)	369 (95%)	17 (4%)	1 (0%)	41	50
1	B	387/389 (100%)	376 (97%)	10 (3%)	1 (0%)	41	50
1	C	387/389 (100%)	365 (94%)	21 (5%)	1 (0%)	41	50
1	D	387/389 (100%)	370 (96%)	14 (4%)	3 (1%)	19	23
All	All	1548/1556 (100%)	1480 (96%)	62 (4%)	6 (0%)	34	42

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE
1	B	350	ILE
1	D	23	ALA
1	D	65	ASN

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	276/276 (100%)	250 (91%)	26 (9%)	8	10
1	B	276/276 (100%)	255 (92%)	21 (8%)	13	16
1	C	276/276 (100%)	258 (94%)	18 (6%)	17	23
1	D	276/276 (100%)	258 (94%)	18 (6%)	17	23
All	All	1104/1104 (100%)	1021 (92%)	83 (8%)	13	17

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	298	LYS
1	D	257	LEU
1	C	332	TRP
1	D	39	LEU
1	D	288	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	316	ASN
1	D	175	GLN
1	C	78	GLN
1	B	184	ASN
1	C	175	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)

10 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	SO4	A	5002	-	4,4,4	0.64	0	6,6,6	0.35	0
2	SO4	A	5005	-	4,4,4	0.81	0	6,6,6	0.69	0
2	SO4	B	5006	-	4,4,4	0.54	0	6,6,6	0.66	0
3	COA	A	1001	-	41,50,50	2.21	12 (29%)	52,75,75	3.04	21 (40%)
3	COA	B	2001	-	41,50,50	1.96	13 (31%)	52,75,75	2.45	14 (26%)
2	SO4	B	5001	-	4,4,4	0.81	0	6,6,6	0.46	0
3	COA	C	3001	-	41,50,50	2.00	11 (26%)	52,75,75	1.97	12 (23%)
2	SO4	A	5004	-	4,4,4	0.77	0	6,6,6	0.76	0
2	SO4	B	5003	-	4,4,4	0.75	0	6,6,6	0.28	0
3	COA	D	4001	-	41,50,50	2.00	11 (26%)	52,75,75	2.05	13 (25%)

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	4001	-	-	12/44/64/64	0/3/3/3
3	COA	C	3001	-	-	11/44/64/64	0/3/3/3
3	COA	A	1001	-	-	6/44/64/64	0/3/3/3
3	COA	B	2001	-	-	7/44/64/64	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	COA	O9P-C9P	6.88	1.37	1.23
3	C	3001	COA	O9P-C9P	6.25	1.35	1.23
3	A	1001	COA	P3B-O3B	6.25	1.71	1.59
3	D	4001	COA	O9P-C9P	6.24	1.35	1.23
3	B	2001	COA	O9P-C9P	5.89	1.35	1.23

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2001	COA	C7P-C6P-C5P	10.49	129.83	112.36
3	A	1001	COA	C2P-C3P-N4P	-9.68	90.19	112.31
3	C	3001	COA	C7P-N8P-C9P	7.96	136.78	122.59
3	D	4001	COA	C7P-N8P-C9P	7.49	135.95	122.59
3	A	1001	COA	C6P-C7P-N8P	7.24	126.51	111.90

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	COA	C5B-O5B-P1A-O1A
3	A	1001	COA	C5B-O5B-P1A-O2A
3	B	2001	COA	C5B-O5B-P1A-O1A
3	B	2001	COA	C5B-O5B-P1A-O2A
3	C	3001	COA	C5B-O5B-P1A-O1A

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	COA	4	0
3	B	2001	COA	2	0
2	B	5001	SO4	1	0
3	D	4001	COA	2	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 1001	
Bond lengths	Bond angles
Torsions	Rings

Ligand COA B 2001	
Bond lengths	Bond angles
Torsions	Rings

Ligand COA C 3001

Bond lengths

Bond angles

Torsions

Rings

Ligand COA D 4001

Bond lengths

Bond angles

Torsions

Rings
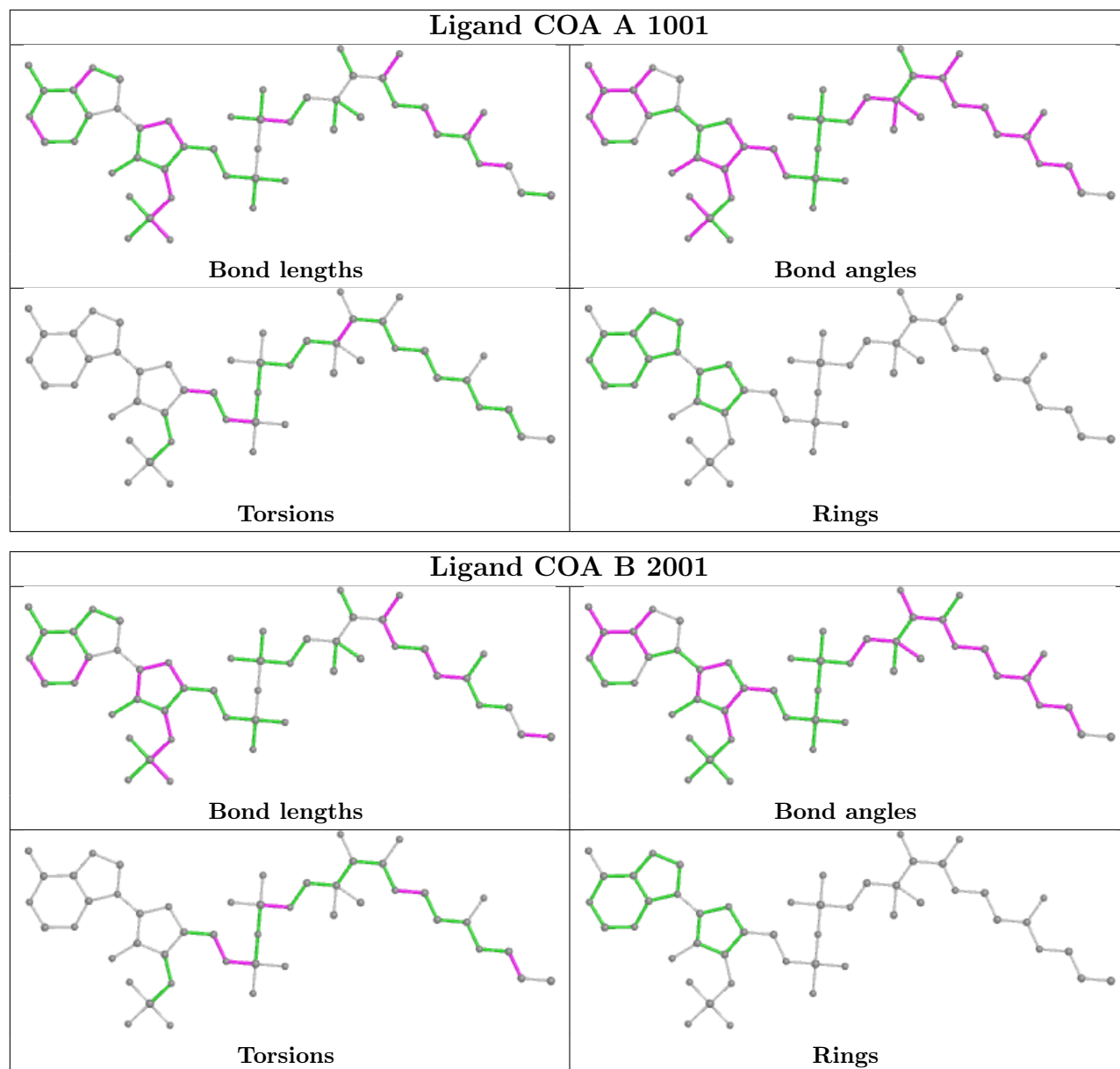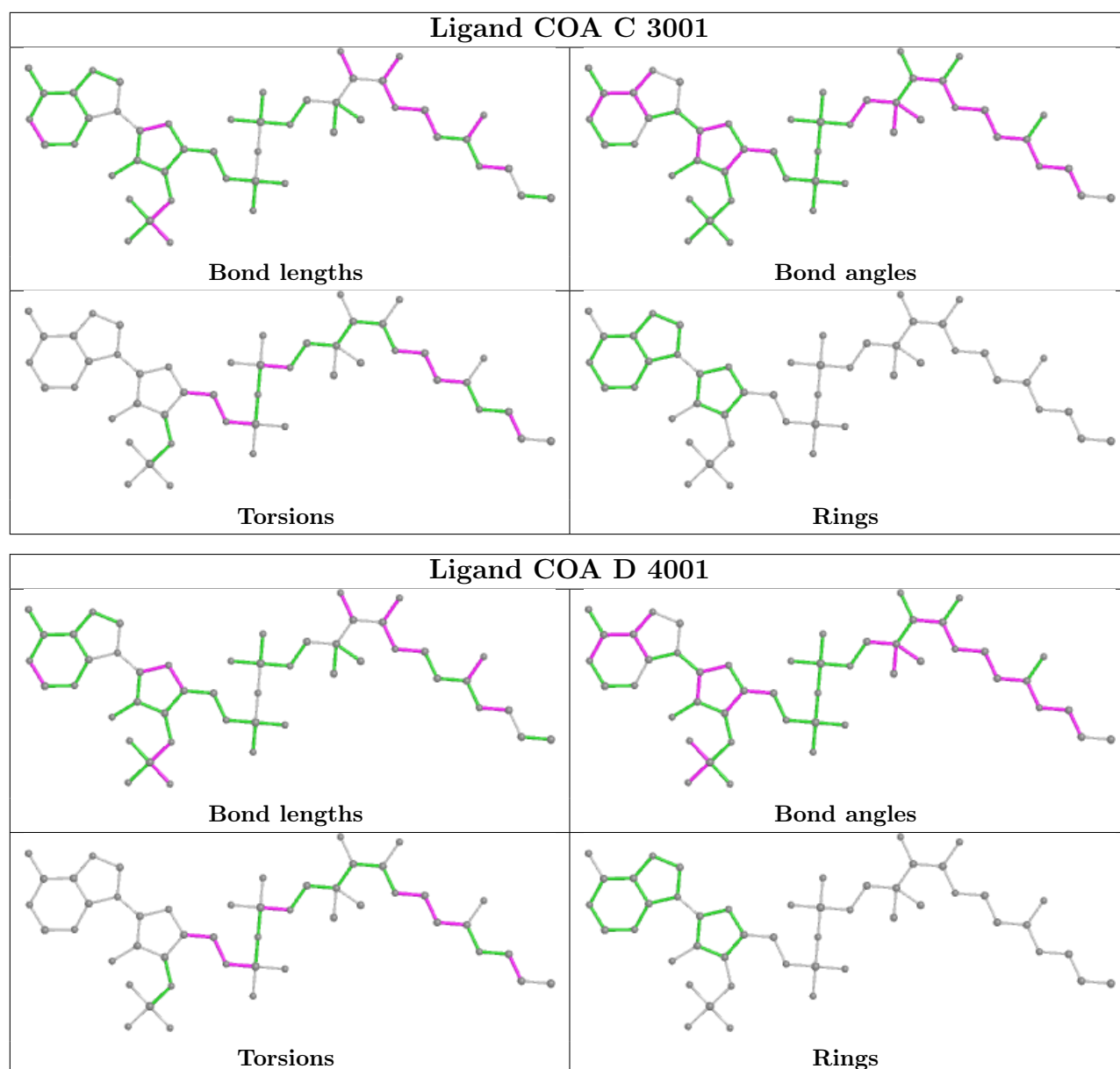
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	54:LEU	C	55:GLY	N	1.69

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	389/389 (100%)	-0.21	4 (1%)	82	86	8, 17, 38, 83	0
1	B	389/389 (100%)	-0.15	5 (1%)	77	81	7, 18, 41, 95	0
1	C	389/389 (100%)	0.78	49 (12%)	3	5	16, 42, 74, 116	0
1	D	389/389 (100%)	1.29	98 (25%)	0	0	19, 48, 102, 127	0
All	All	1556/1556 (100%)	0.43	156 (10%)	7	10	7, 35, 75, 127	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	MET	8.0
1	D	307	ILE	7.0
1	D	330	LEU	6.7
1	D	164	VAL	6.1
1	D	169	GLN	5.9

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	COA	D	4001	48/48	0.69	0.28	79,112,123,124	0
3	COA	C	3001	48/48	0.80	0.20	56,78,93,95	0
2	SO4	A	5005	5/5	0.86	0.20	48,50,51,54	0
2	SO4	B	5001	5/5	0.90	0.14	56,56,58,58	0
3	COA	B	2001	48/48	0.93	0.13	15,29,52,57	0
2	SO4	B	5006	5/5	0.93	0.16	39,41,43,43	0
3	COA	A	1001	48/48	0.93	0.13	12,29,45,47	0
2	SO4	A	5002	5/5	0.95	0.13	58,60,61,62	0
2	SO4	A	5004	5/5	0.96	0.10	47,49,51,54	0
2	SO4	B	5003	5/5	0.97	0.13	50,52,54,57	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 D 4001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
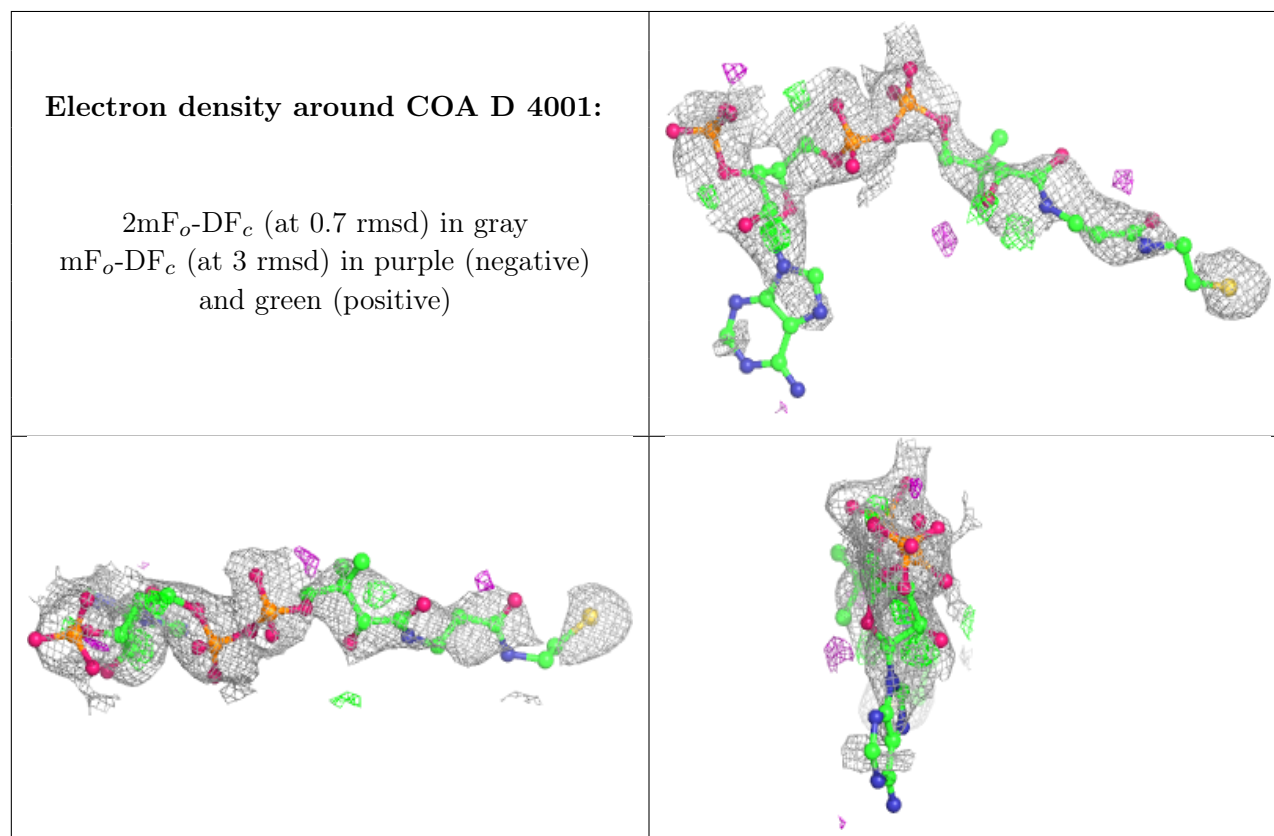
Electron density around COA C 3001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
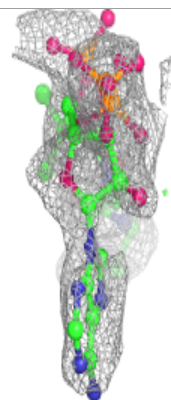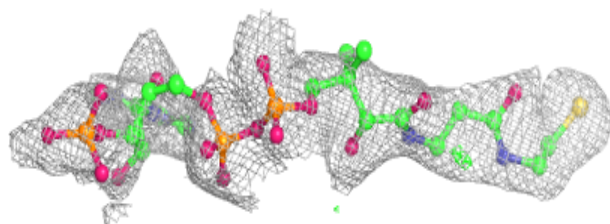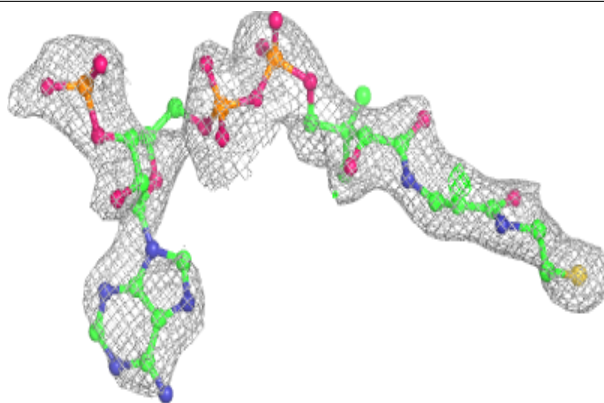
Electron density around COA B 2001:

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

Electron density around COA A 1001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
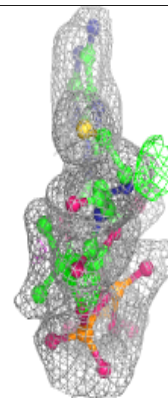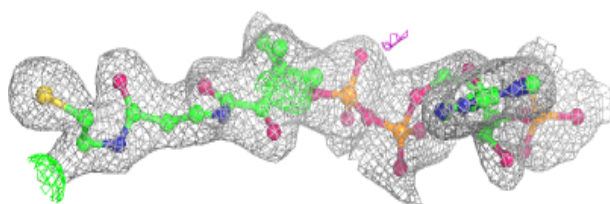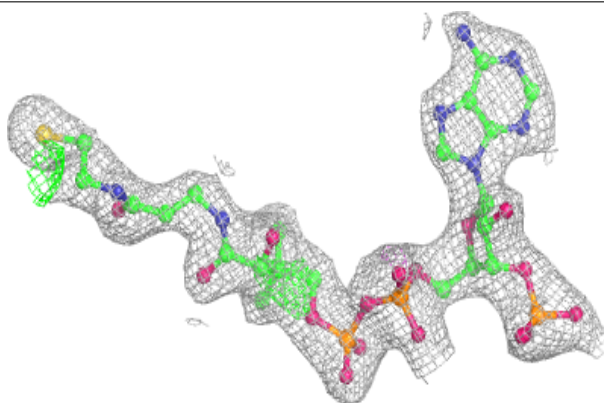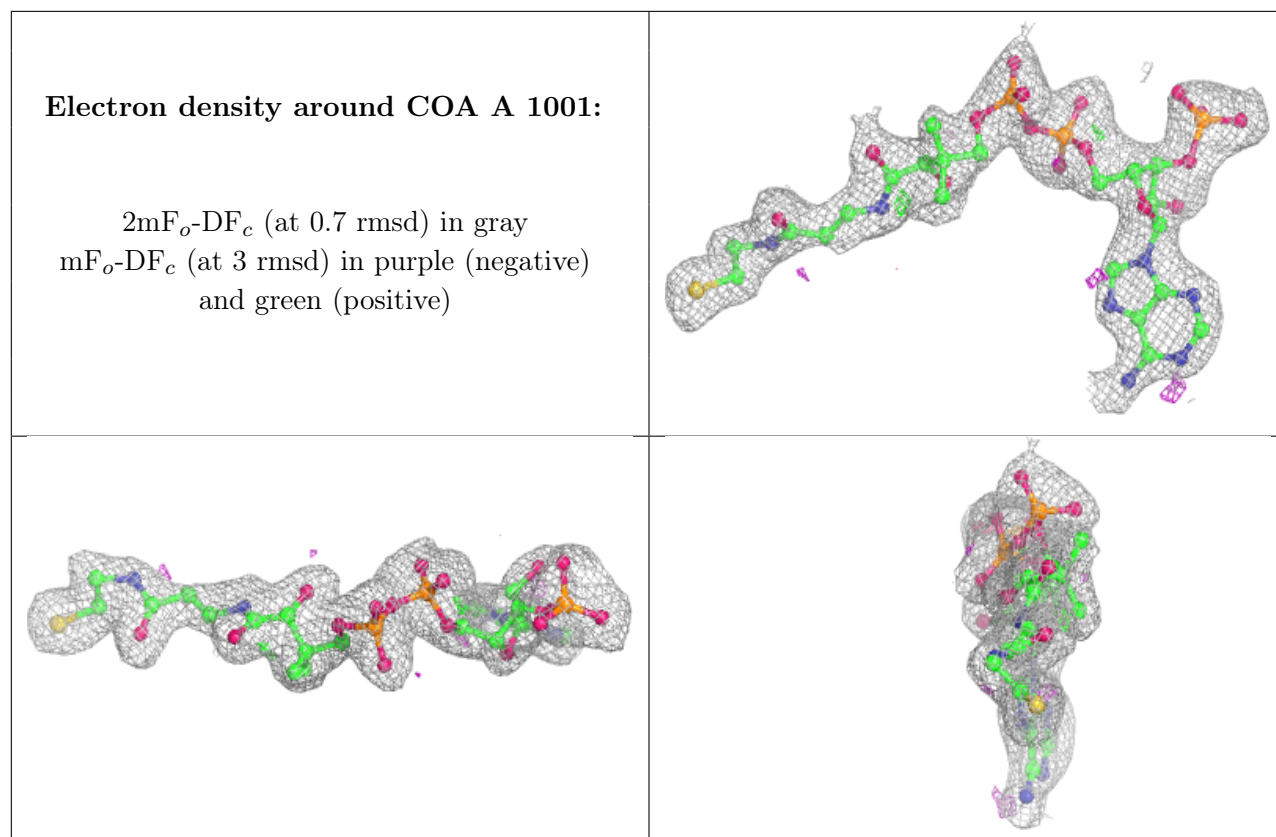
6.5 Other polymers (i)

There are no such residues in this entry.