wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 01:06 AM EST

PDB ID	:	1P7T
Title	:	Structure of Escherichia coli malate synthase G:pyruvate:acetyl-Coenzyme A abortive ternary complex at 1.95 angstrom resolution
Authors	:	Anstrom, D.M.; Kallio, K.; Remington, S.J.
Deposited on	:	2003-05-05
Resolution	:	1.95 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 (i)) were used in the production of this report:

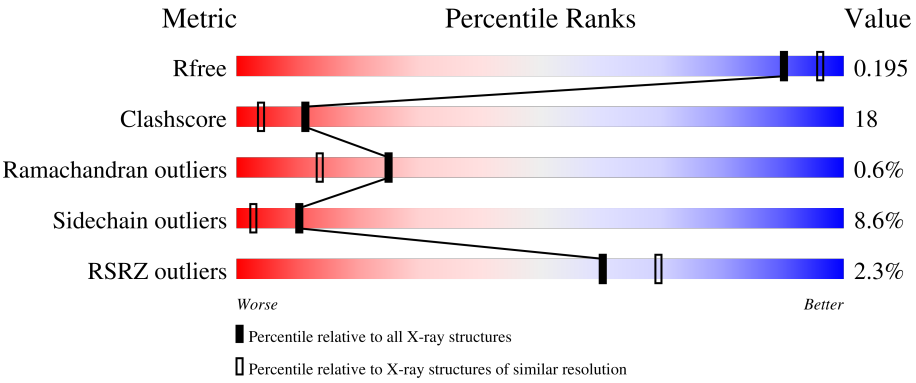
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	731	% 57% 30% 8%
2	B	731	3% 60% 29% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PYR	B	910	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11504 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 Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	706	5414	3406	956	1025	27	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	see remark 999	UNP P37330
A	2	ALA	SER	cloning artifact	UNP P37330
A	617	CSO	CYS	modified residue	UNP P37330
A	724	LEU	-	expression tag	UNP P37330
A	725	GLU	-	expression tag	UNP P37330
A	726	HIS	-	expression tag	UNP P37330
A	727	HIS	-	expression tag	UNP P37330
A	728	HIS	-	expression tag	UNP P37330
A	729	HIS	-	expression tag	UNP P37330
A	730	HIS	-	expression tag	UNP P37330
A	731	HIS	-	expression tag	UNP P37330

- Molecule 2 is a protein called Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	705	5358	3379	944	1008	27	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	see remark 999	UNP P37330
B	2	ALA	SER	cloning artifact	UNP P37330
B	617	CSO	CYS	modified residue	UNP P37330
B	688	CSO	CYS	modified residue	UNP P37330
B	724	LEU	-	expression tag	UNP P37330

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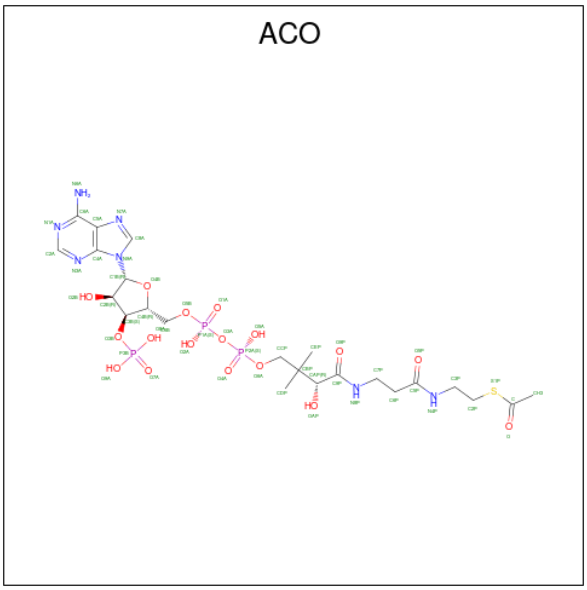
Chain	Residue	Modelled	Actual	Comment	Reference
B	725	GLU	-	expression tag	UNP P37330
B	726	HIS	-	expression tag	UNP P37330
B	727	HIS	-	expression tag	UNP P37330
B	728	HIS	-	expression tag	UNP P37330
B	729	HIS	-	expression tag	UNP P37330
B	730	HIS	-	expression tag	UNP P37330
B	731	HIS	-	expression tag	UNP P37330

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

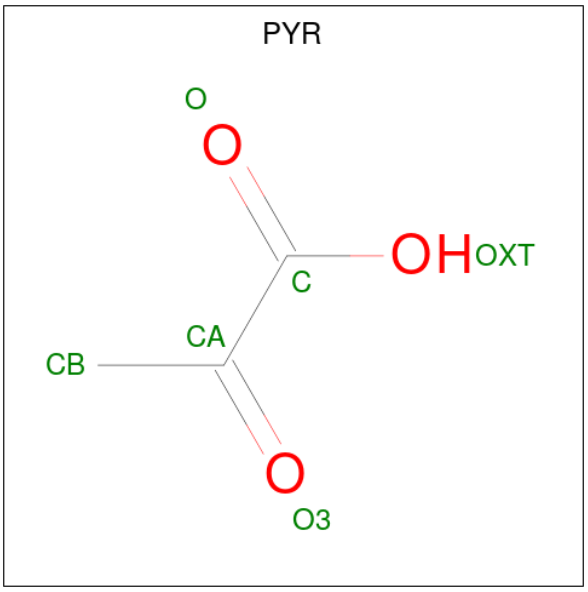
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



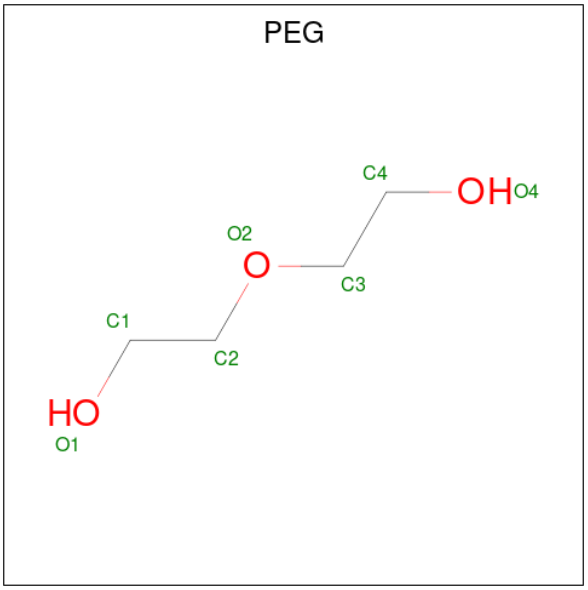
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 51 23 7 17 3 1	0	0
4	B	1	Total C N O P S 51 23 7 17 3 1	0	0

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



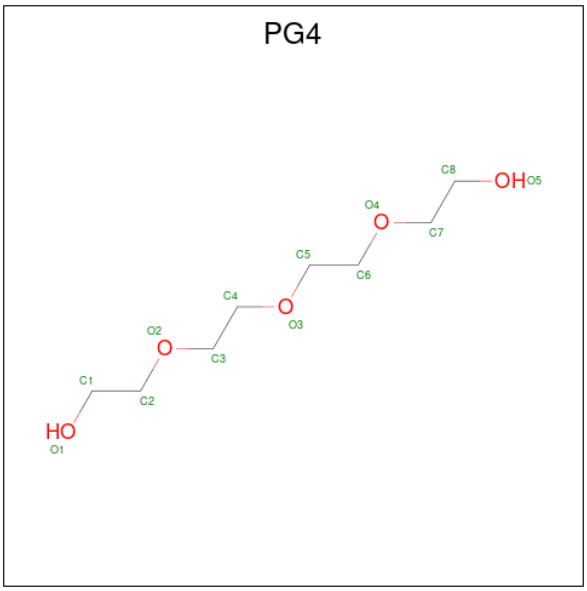
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 13 8 5	0	0
7	B	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

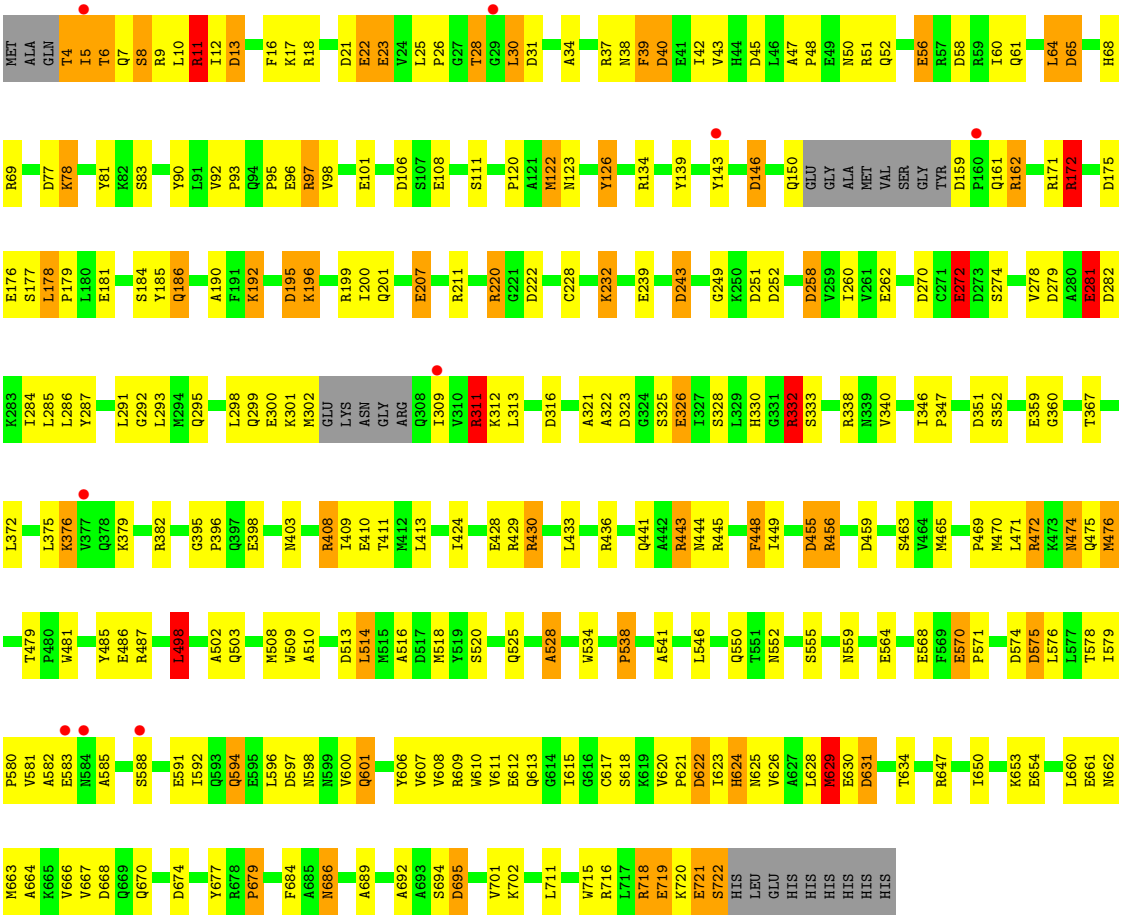
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	308	Total O 308 308	0	0
8	B	275	Total O 275 275	0	0

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 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.

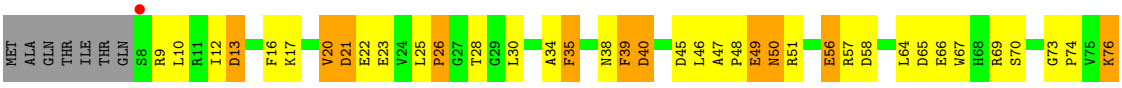
• Molecule 1: Malate synthase G

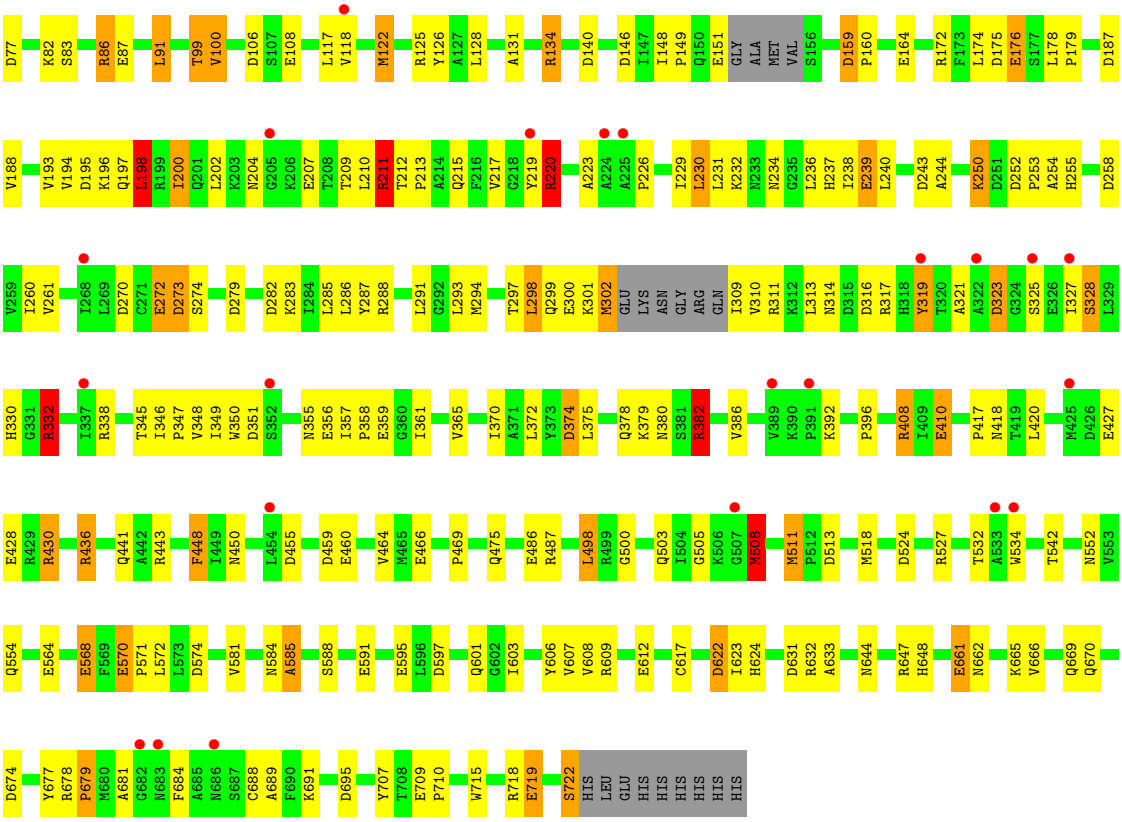
Chain A:



• Molecule 2: Malate synthase G

Chain B:




D77 K82 S83 R86 E87 L91 T99 V100 D106 S107 E108 L117 V118 M122 R125 Y126 A127 L128 A131 R134 D140 D146 I147 I148 P149 Q150 E151 GLY ALA MET VAL S156 D159 P160 E164 R172 F173 L174 D175 E176 S177 L178 P179 D187
V188 V193 V194 D195 K196 Q197 L198 R199 I200 Q201 L202 K203 N204 G205 K206 E207 T208 T209 L210 R211 T212 P213 A214 Q215 P216 V217 G218 Y219 R220 A223 A224 A225 P226 I229 L230 L231 K232 N233 N234 G235 L236 H237 I238 E239 L240 D243 A244 K250 D251 D252 P253 A254 H255 D258
V259 I260 V261 I268 L269 D270 C271 E272 D273 S274 D279 D282 K283 I284 L285 L286 Y287 R288 L291 G292 L293 M294 T297 L298 Q299 E300 K301 M302 GLU LYS ASN GLY ARG GLN I309 V310 R311 K312 L313 N314 D315 D316 R317 H318 Y319 T320 A321 A322 D323 G324 S325 E326 I327 S328 L329
H330 G331 R332 I337 R338 T345 I346 P347 V348 I349 W350 D351 S352 N355 E356 I357 P358 E359 G360 I361 V365 I370 A371 L372 Y373 D374 L375 Q378 K379 N380 S381 R382 V386 V389 K390 P391 K392 P396 R408 I409 E410 P417 N418 T419 L420 M425 D426 E427
E428 R429 R430 R436 Q441 A442 R443 F448 Y449 N450 L454 D455 D459 E460 V464 M465 E466 P469 Q475 E486 R487 L498 R499 G500 Q503 I504 G505 K506 G507 M508 M511 P512 D513 M518 D524 R527 T532 A533 W534 T542 N552 V553
Q554 E564 E568 F569 E570 P571 L572 L573 D574 V581 N584 A585 S588 E591 E595 L596 D597 Q601 G602 I603 Y606 V607 V608 R609 E612 C617 D622 I623 H624 D631 R632 A633 N644 R647 H648 E661 N662 K665 V666 Q669 Q670
D674 Y677 R678 P679 M680 A681 G682 N683 F684 A685 N686 S687 C688 A689 F690 K691 D695 Y707 T708 E709 P710 W715 R718 E719 S722 HIS LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.93Å 107.39Å 204.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 1.95 39.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.22-1.95) 90.0 (39.21-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 1.95Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.194 , 0.294 0.193 , 0.195	Depositor DCC
R_{free} test set	10721 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 102.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11504	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ACO, PYR, MG, PG4, CSO

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	1.31	28/5509 (0.5%)	1.63	103/7485 (1.4%)
2	B	1.28	28/5447 (0.5%)	1.60	93/7407 (1.3%)
All	All	1.29	56/10956 (0.5%)	1.62	196/14892 (1.3%)

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	GLU	CD-OE2	10.15	1.36	1.25
2	B	207	GLU	CD-OE2	9.06	1.35	1.25
1	A	108	GLU	CD-OE2	8.95	1.35	1.25
2	B	164	GLU	CD-OE2	8.52	1.35	1.25
2	B	87	GLU	CD-OE2	8.48	1.34	1.25

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	436	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	A	316	ASP	CB-CG-OD2	-11.49	107.96	118.30
1	A	436	ARG	NE-CZ-NH1	11.41	126.01	120.30
2	B	382	ARG	NE-CZ-NH2	-11.23	114.69	120.30
2	B	678	ARG	NE-CZ-NH2	-11.20	114.70	120.30

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	5414	0	5271	191	0
2	B	5358	0	5172	186	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	51	0	34	9	0
4	B	51	0	34	11	0
5	A	6	0	0	3	0
5	B	6	0	0	4	0
6	A	7	0	10	1	0
7	B	26	0	36	8	0
8	A	308	0	0	9	0
8	B	275	0	0	9	0
All	All	11504	0	10557	383	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 18.

The worst 5 of 383 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:A:476:MET:HE1	1:A:481:TRP:HE1	1.15	1.10
1:A:476:MET:HE3	1:A:479:THR:HG21	1.32	1.10
2:B:86:ARG:HH11	2:B:86:ARG:HB2	1.21	1.05
2:B:86:ARG:HB2	2:B:86:ARG:NH1	1.81	0.95
1:A:470:MET:HE1	1:A:581:VAL:HG12	1.46	0.94

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	699/731 (96%)	666 (95%)	30 (4%)	3 (0%)	34 22
2	B	697/731 (95%)	665 (95%)	27 (4%)	5 (1%)	22 11
All	All	1396/1462 (96%)	1331 (95%)	57 (4%)	8 (1%)	25 14

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	ARG
1	A	28	THR
2	B	585	ALA
2	B	26	PRO
1	A	585	ALA

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	555/606 (92%)	501 (90%)	54 (10%)	8 2
2	B	538/605 (89%)	498 (93%)	40 (7%)	13 4
All	All	1093/1211 (90%)	999 (91%)	94 (9%)	10 3

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	LEU
2	B	220	ARG
2	B	76	LYS
2	B	176	GLU
2	B	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	683	ASN

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Mol	Chain	Res	Type
2	B	197	GLN
2	B	683	ASN
2	B	299	GLN
2	B	38	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 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	CSO	A	617	1	3,6,7	1.22	0	0,6,8	-	-
2	CSO	B	617	2	3,6,7	0.63	0	0,6,8	-	-
2	CSO	B	688	2	3,6,7	2.28	1 (33%)	0,6,8	-	-

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	CSO	A	617	1	-	0/1/5/7	-
2	CSO	B	617	2	-	0/1/5/7	-
2	CSO	B	688	2	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	688	CSO	CB-CA	3.75	1.62	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	617	CSO	2	0
2	B	617	CSO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
7	PG4	B	1003	-	12,12,12	0.59	0	11,11,11	0.48	0
4	ACO	A	800	-	45,53,53	1.08	1 (2%)	56,79,79	1.22	5 (8%)
6	PEG	A	1001	-	6,6,6	0.79	0	5,5,5	0.34	0
5	PYR	B	910	3	5,5,5	1.35	1 (20%)	3,6,6	1.98	1 (33%)
4	ACO	B	900	-	45,53,53	1.19	5 (11%)	56,79,79	1.26	5 (8%)
5	PYR	A	810	3	5,5,5	1.76	2 (40%)	3,6,6	1.71	1 (33%)
7	PG4	B	1002	-	12,12,12	1.16	1 (8%)	11,11,11	0.56	0

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
7	PG4	B	1003	-	-	4/10/10/10	-
4	ACO	A	800	-	-	12/47/67/67	0/3/3/3
6	PEG	A	1001	-	-	2/4/4/4	-
5	PYR	B	910	3	-	0/4/4/4	-
4	ACO	B	900	-	-	13/47/67/67	0/3/3/3
5	PYR	A	810	3	-	0/4/4/4	-
7	PG4	B	1002	-	-	6/10/10/10	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	ACO	P3B-O3B	-4.03	1.51	1.59
4	B	900	ACO	C6P-C5P	2.90	1.56	1.51
5	A	810	PYR	O-C	2.65	1.29	1.22
5	A	810	PYR	CB-CA	-2.54	1.45	1.50
4	B	900	ACO	P1A-O5B	-2.34	1.49	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	900	ACO	C1B-N9A-C4A	-5.08	117.72	126.64
4	A	800	ACO	C6P-C5P-N4P	-3.39	110.72	116.42
4	A	800	ACO	C1B-N9A-C4A	-3.07	121.25	126.64
5	A	810	PYR	OXT-C-CA	2.96	122.06	113.97
5	B	910	PYR	OXT-C-CA	2.93	121.99	113.97

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	ACO	C5B-O5B-P1A-O1A
4	A	800	ACO	C5B-O5B-P1A-O3A
4	A	800	ACO	P1A-O3A-P2A-O6A
4	A	800	ACO	CAP-CBP-CCP-O6A
4	A	800	ACO	S1P-C2P-C3P-N4P

There are no ring outliers.

7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1003	PG4	3	0

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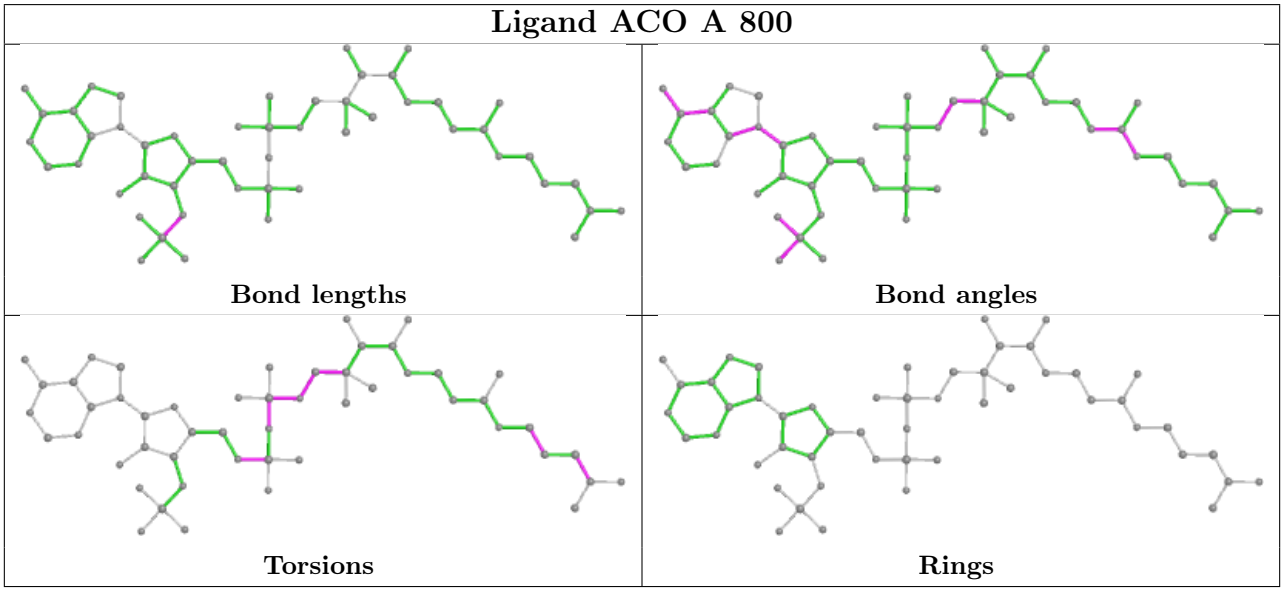
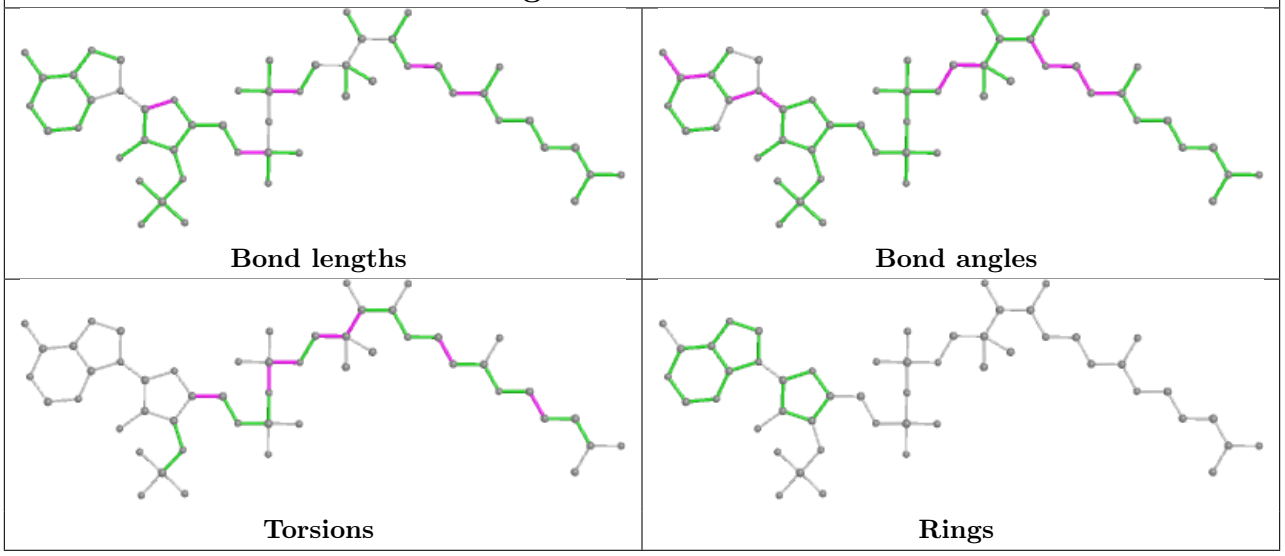
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	ACO	9	0
6	A	1001	PEG	1	0
5	B	910	PYR	4	0
4	B	900	ACO	11	0
5	A	810	PYR	3	0
7	B	1002	PG4	5	0

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 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 ACO B 900



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

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, 95^{th} 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	705/731 (96%)	-0.08	9 (1%)	77	83	14, 26, 53, 100	0
2	B	703/731 (96%)	0.08	23 (3%)	46	56	14, 27, 58, 99	0
All	All	1408/1462 (96%)	-0.00	32 (2%)	60	69	14, 26, 56, 100	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	682	GLY	6.3
1	A	309	ILE	4.2
2	B	683	ASN	3.8
1	A	584	ASN	2.9
2	B	352	SER	2.9

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

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, 95^{th} 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	CSO	B	688	7/8	0.95	0.12	22,24,45,47	0
1	CSO	A	617	7/8	0.96	0.10	23,26,45,85	0
2	CSO	B	617	7/8	0.98	0.07	16,24,30,35	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

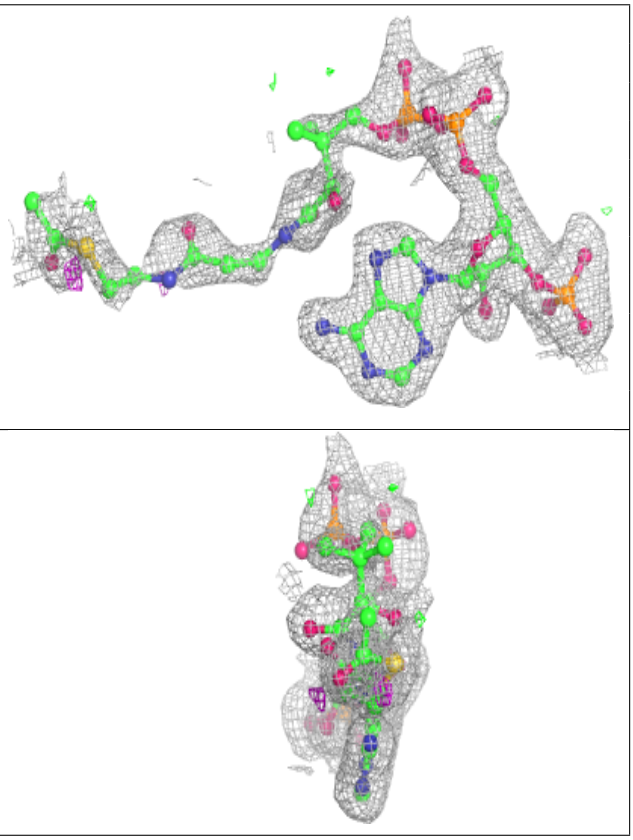
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	PG4	B	1003	13/13	0.83	0.17	44,56,68,68	0
7	PG4	B	1002	13/13	0.84	0.19	29,40,64,66	0
6	PEG	A	1001	7/7	0.85	0.20	43,44,47,48	0
4	ACO	B	900	51/51	0.92	0.15	23,53,98,100	0
4	ACO	A	800	51/51	0.92	0.14	17,50,91,96	0
3	MG	A	1000	1/1	0.98	0.09	16,16,16,16	0
5	PYR	A	810	6/6	0.98	0.14	13,20,21,44	0
5	PYR	B	910	6/6	0.98	0.19	20,23,32,32	0
3	MG	B	1001	1/1	0.99	0.11	17,17,17,17	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.

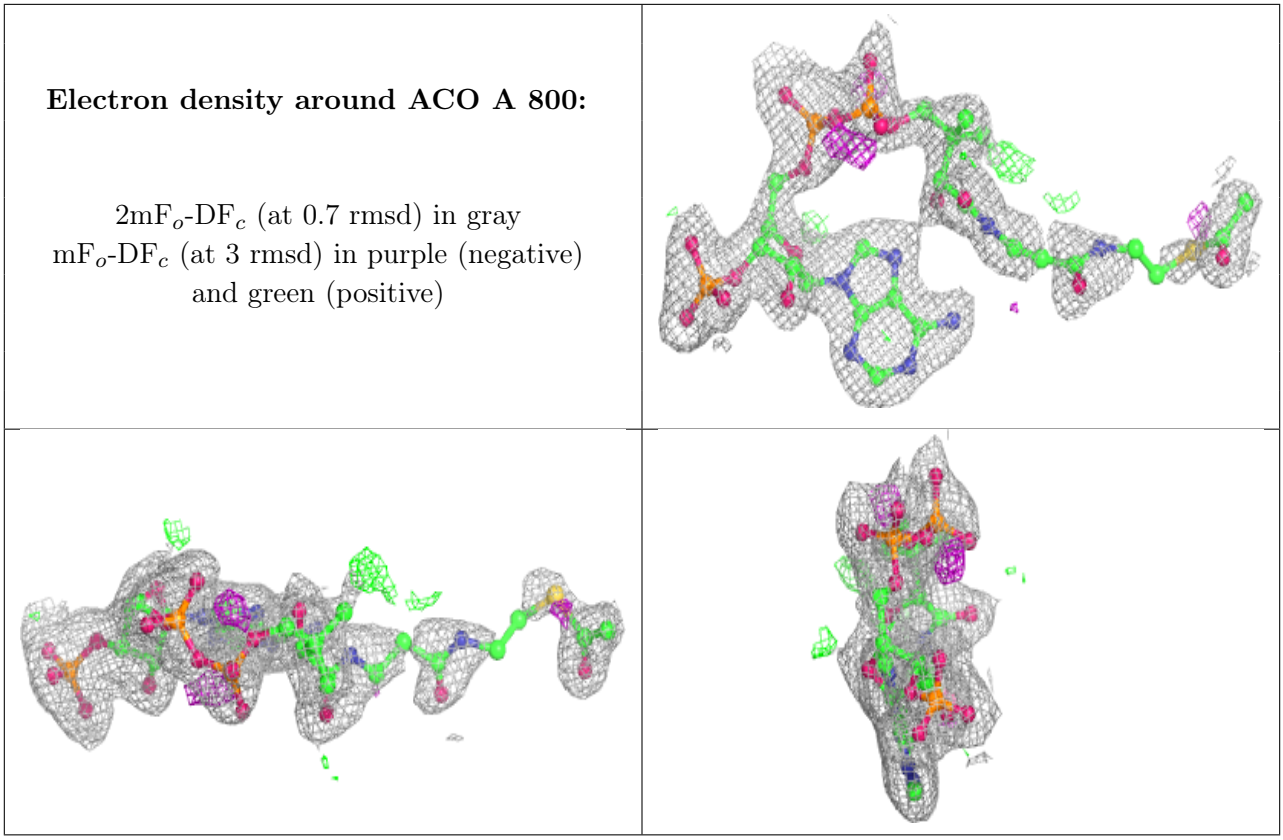
Electron density around ACO B 900:

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



Electron density around ACO A 800:

$2mF_o$-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.