W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 09:57 PM EDT

PDB ID	:	1DM3
Title	:	ACETYLATED BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA IN COMPLEX WITH ACETYL-COA
Authors	:	Modis, Y.; Wierenga, R.K.
Deposited on	:	1999-12-13
Resolution	:	2.00 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	:	2.36.2
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)	:	2.36.2

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 2.00 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.
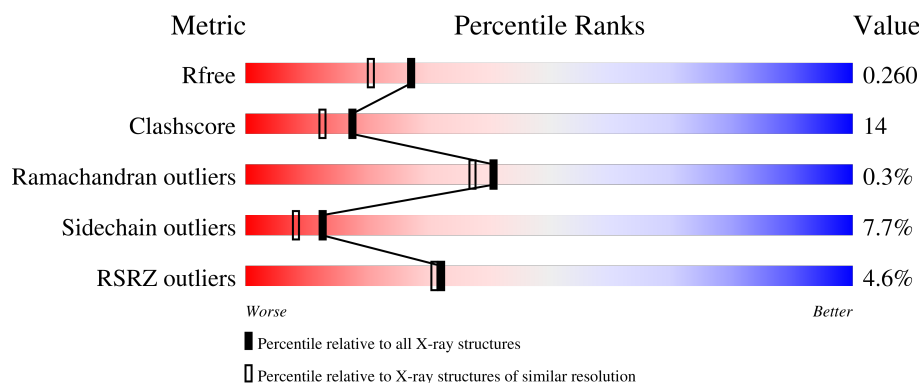
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	2% 67% 25% 6% ·
1	B	389	2% 69% 22% 7% ·
1	C	389	4% 72% 22% 5% ·
1	D	389	10% 67% 28% · ·

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
1	SCY	A	89	-	-	X	-
1	SCY	B	89	-	-	X	-
1	SCY	C	89	-	-	X	-
1	SCY	D	89	-	-	X	-
3	ACO	C	815	-	-	-	X
3	ACO	D	816	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12302 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 ACETYLATED AT CYS89.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total 2816	C 1748	N 509	O 538	S 21	0	0	0
1	B	389	Total 2816	C 1748	N 509	O 538	S 21	0	0	0
1	C	389	Total 2816	C 1748	N 509	O 538	S 21	0	0	0
1	D	389	Total 2816	C 1748	N 509	O 538	S 21	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	10	ALA	-	INSERTION	UNP P07097
D	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

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

SO4

O1

O

O3 O⁻ ─── S

S

O⁻ O4

O

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

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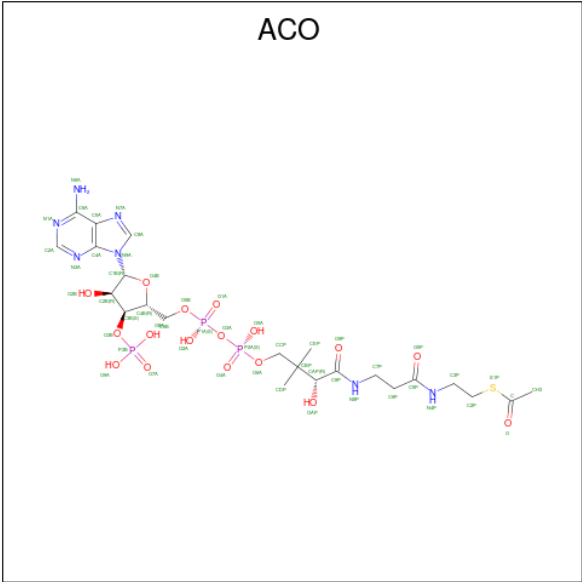
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	316	Total	O	2	0
			316	316		
4	B	300	Total	O	4	0
			300	300		
4	C	103	Total	O	1	0
			103	103		
4	D	85	Total	O	1	0
			85	85		

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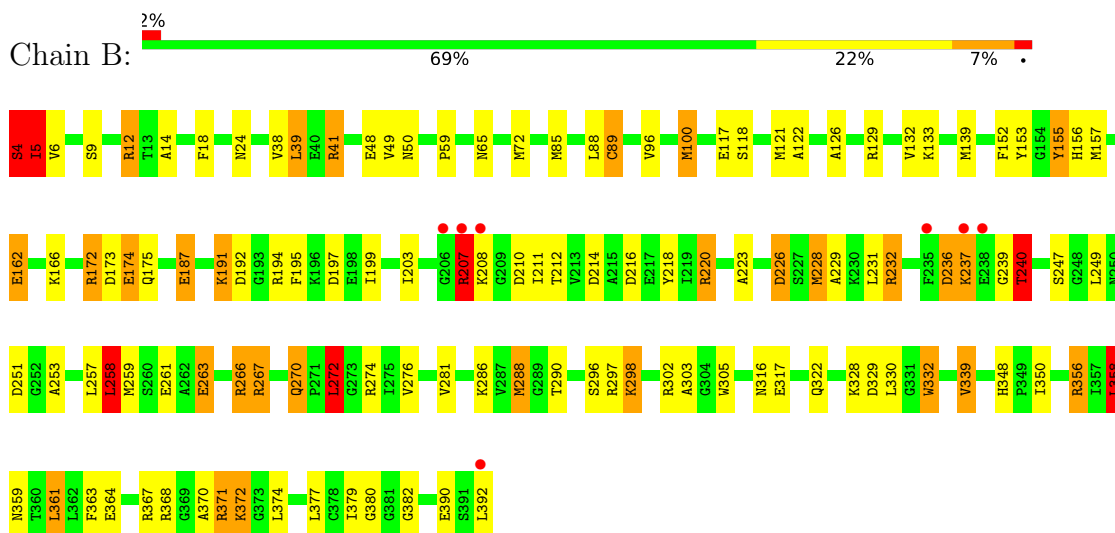 the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to 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.
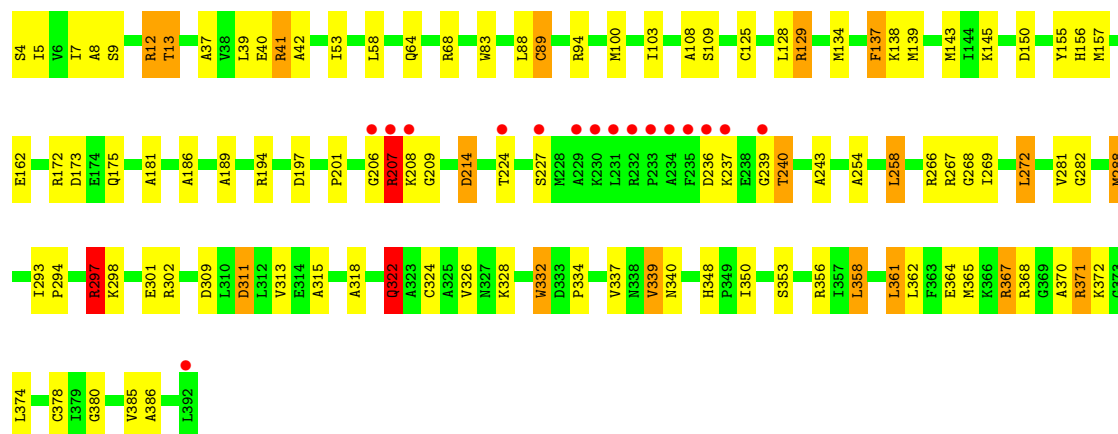
• Molecule 1: BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89

Chain A:
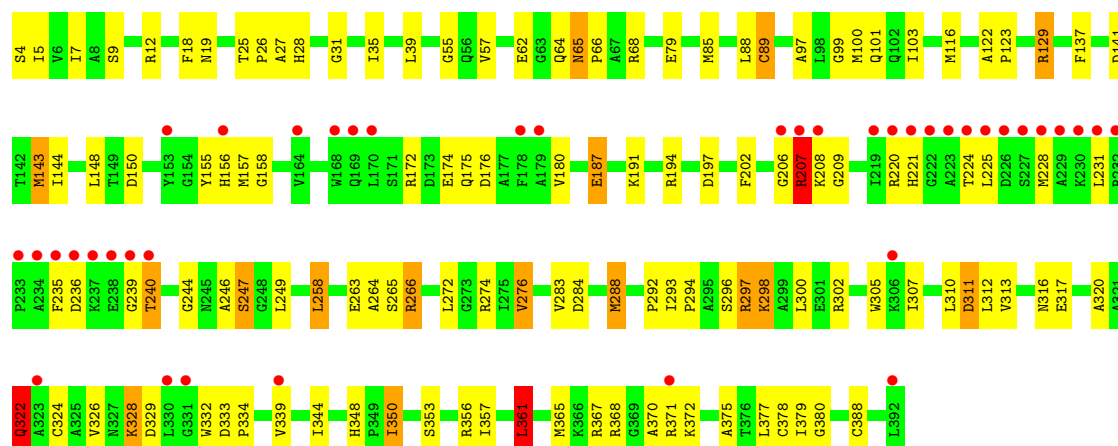

• Molecule 1: BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89

Chain B:

• Molecule 1: BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89

Chain C:

S4 I5 V6 I7 A8 S9 R12 T13 A37 V38 L39 E40 R41 A42 I53 L58 Q64 R68 W83 L88 C89 R94 M100 I103 A108 S109 C125 L128 R129 M134 F137 K138 M139 M143 I144 K145 D150 Y155 H156 M157

E162 R172 D173 E174 Q175 A181 A186 A189 R194 D197 P201 G206 R207 K208 G209 D214 T224 S227 M228 A229 K230 L231 R232 P233 A234 F235 D236 K237 E238 G239 T240 A243 A254 L258 R266 R267 G268 I269 L272 V281 G282 M288

I293 P294 R297 K298 E301 R302 D309 L310 D311 L312 V313 E314 A315 A318 Q322 A323 C324 A325 V326 N327 K328 W332 D333 P334 V337 N338 V339 N340 H348 P349 I350 S353 R356 I357 L358 L361 L362 F363 E364 M365 K366 R367 R368 G369 A370 R371 K372 G373

L374 C378 I379 G380 V385 A386 L392

• **Molecule 1:** BIOSYNTHETIC THIOLASE ACETYLATED AT CYS89

Chain D:

10%

67%   28%

S4 I5 V6 I7 A8 S9 R12 F18 N19 T25 P26 A27 H28 G31 I35 L39 G55 Q56 V57 E62 G63 Q64 N65 P66 A67 R68 E79 M85 L88 C89 A97 L98 G99 M100 Q101 Q102 I103 M116 A122 P123 R129 F137 D141

T142 M143 I144 L148 T149 D150 Y153 G154 Y155 H156 M157 G158 V164 W168 Q169 L170 S171 R172 D173 E174 Q175 D176 A177 F178 A179 V180 E187 K191 R194 D197 F202 G206 R207 K208 G209 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 L258 E263 A264 S265 R266 L272 G273 R274 I275 V276 V283 D284 M288 P292 I293 P294 A295 S296 R297 K298 A299 L300 E301 R302 W305 K306 I307 L310 D311 L312 V313 N316 E317 A320 A321

Q322 A323 C324 A325 V326 N327 K328 D329 L330 G331 W332 D333 P334 V339 I344 H348 P349 I350 S353 R356 I357 L361 M365 K366 R367 R368 G369 A370 R371 K372 A375 T376 L377 C378 I379 G380 C388 L392

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.38Å 78.85Å 149.73Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 49.82 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.00) 79.0 (49.82-1.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.256 0.223 , 0.260	Depositor DCC
R_{free} test set	7058 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.2	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, SO4, SCY

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	1.07	3/2847 (0.1%)	2.07	99/3842 (2.6%)
1	B	1.03	0/2847	2.12	107/3842 (2.8%)
1	C	0.66	0/2847	1.71	49/3842 (1.3%)
1	D	0.63	0/2847	1.56	43/3842 (1.1%)
All	All	0.87	3/11388 (0.0%)	1.88	298/15368 (1.9%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	ARG	CZ-NH2	5.30	1.40	1.33
1	A	79	GLU	CD-OE2	-5.06	1.20	1.25
1	A	79	GLU	CD-OE1	5.02	1.31	1.25

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ARG	NE-CZ-NH2	-19.89	110.36	120.30
1	C	129	ARG	NE-CZ-NH2	-18.44	111.08	120.30
1	A	228	MET	CA-CB-CG	18.43	144.63	113.30
1	B	173	ASP	CB-CG-OD2	-17.14	102.87	118.30
1	A	266	ARG	CD-NE-CZ	17.14	147.59	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	GLY	Mainchain

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	2816	0	2821	74	0
1	B	2816	0	2821	70	0
1	C	2816	0	2821	68	0
1	D	2816	0	2821	95	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	51	0	34	16	0
3	B	51	0	34	12	0
3	C	51	0	34	17	0
3	D	51	0	34	17	0
4	A	316	0	0	13	0
4	B	300	0	0	23	1
4	C	103	0	0	5	0
4	D	85	0	0	5	0
All	All	12302	0	11420	315	1

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 14.

The worst 5 of 315 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:D:88:LEU:HB3	1:D:89:SCY:HE2	1.20	1.16
3:D:816:ACO:O5P	3:D:816:ACO:H21	1.33	1.14
1:B:288:MET:SD	3:B:814:ACO:HH33	1.89	1.13
1:B:247:SER:HB2	4:B:929:HOH:O	1.49	1.12
1:D:288:MET:SD	3:D:816:ACO:HH33	1.90	1.11

All (1) 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:B:965:HOH:O	4:B:1046:HOH:O[2_555]	2.19	0.01

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	386/389 (99%)	371 (96%)	14 (4%)	1 (0%)	41	37
1	B	386/389 (99%)	373 (97%)	12 (3%)	1 (0%)	41	37
1	C	386/389 (99%)	372 (96%)	13 (3%)	1 (0%)	41	37
1	D	386/389 (99%)	370 (96%)	14 (4%)	2 (0%)	29	23
All	All	1544/1556 (99%)	1486 (96%)	53 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

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

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	275/275 (100%)	252 (92%)	23 (8%)	11	7
1	B	275/275 (100%)	253 (92%)	22 (8%)	12	7
1	C	275/275 (100%)	253 (92%)	22 (8%)	12	7
1	D	275/275 (100%)	257 (94%)	18 (6%)	17	12
All	All	1100/1100 (100%)	1015 (92%)	85 (8%)	13	8

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	297	ARG
1	D	207	ARG
1	C	322	GLN
1	C	367	ARG
1	D	265	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	SCY	B	89	1	7,8,9	1.13	1 (14%)	3,9,11	4.45	3 (100%)
1	SCY	A	89	1	7,8,9	0.93	1 (14%)	3,9,11	2.48	3 (100%)
1	SCY	C	89	1	7,8,9	0.77	0	3,9,11	3.11	2 (66%)
1	SCY	D	89	1	7,8,9	0.70	0	3,9,11	3.85	2 (66%)

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	SCY	B	89	1	-	2/5/7/9	-
1	SCY	A	89	1	-	2/5/7/9	-
1	SCY	C	89	1	-	2/5/7/9	-
1	SCY	D	89	1	-	2/5/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	SCY	CB-CA	2.12	1.58	1.53
1	A	89	SCY	CB-SG	-2.05	1.76	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	SCY	OCD-CD-SG	-5.31	99.04	122.60
1	D	89	SCY	OCD-CD-CE	-5.26	101.48	123.07
1	B	89	SCY	CE-CD-SG	4.94	148.39	114.20
1	C	89	SCY	OCD-CD-CE	-4.71	103.73	123.07
1	D	89	SCY	OCD-CD-SG	4.07	140.69	122.60

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	89	SCY	OCD-CD-SG-CB
1	A	89	SCY	CE-CD-SG-CB
1	C	89	SCY	OCD-CD-SG-CB
1	C	89	SCY	CE-CD-SG-CB
1	D	89	SCY	OCD-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	89	SCY	8	0
1	A	89	SCY	8	0
1	C	89	SCY	11	0
1	D	89	SCY	10	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	807	-	4,4,4	0.70	0	6,6,6	0.31	0
2	SO4	B	809	-	4,4,4	0.65	0	6,6,6	0.76	0
2	SO4	A	810	-	4,4,4	0.46	0	6,6,6	0.52	0
3	ACO	A	813	-	45,53,53	2.06	9 (20%)	56,79,79	2.23	16 (28%)
3	ACO	C	815	-	45,53,53	2.03	11 (24%)	56,79,79	2.17	16 (28%)
3	ACO	D	816	-	45,53,53	1.99	9 (20%)	56,79,79	2.03	11 (19%)
2	SO4	B	812	-	4,4,4	0.83	0	6,6,6	0.99	0
3	ACO	B	814	-	45,53,53	1.93	8 (17%)	56,79,79	2.23	19 (33%)
2	SO4	A	808	-	4,4,4	0.52	0	6,6,6	0.44	0
2	SO4	A	811	-	4,4,4	0.97	0	6,6,6	0.60	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
3	ACO	C	815	-	-	10/47/67/67	0/3/3/3
3	ACO	D	816	-	-	6/47/67/67	0/3/3/3
3	ACO	A	813	-	-	12/47/67/67	0/3/3/3
3	ACO	B	814	-	-	10/47/67/67	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	813	ACO	O9P-C9P	7.37	1.38	1.23
3	C	815	ACO	O9P-C9P	6.91	1.37	1.23
3	D	816	ACO	O9P-C9P	6.79	1.36	1.23
3	B	814	ACO	O9P-C9P	6.47	1.36	1.23
3	C	815	ACO	P3B-O3B	5.00	1.68	1.59

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
3	D	816	ACO	C2P-C3P-N4P	-6.90	97.92	112.42
3	A	813	ACO	C2P-C3P-N4P	-6.24	99.31	112.42
3	A	813	ACO	C6P-C5P-N4P	5.62	125.88	116.42
3	C	815	ACO	C2P-C3P-N4P	-5.49	100.88	112.42
3	B	814	ACO	O5P-C5P-C6P	-5.48	111.99	122.02

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	813	ACO	C5B-O5B-P1A-O1A
3	A	813	ACO	C5B-O5B-P1A-O2A
3	A	813	ACO	CAP-C9P-N8P-C7P
3	A	813	ACO	C5P-C6P-C7P-N8P
3	A	813	ACO	C2P-C3P-N4P-C5P

There are no ring outliers.

4 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	813	ACO	16	0
3	C	815	ACO	17	0
3	D	816	ACO	17	0
3	B	814	ACO	12	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 A 813

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO C 815

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO D 816

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO B 814

Bond lengths

Bond angles

Torsions

Rings
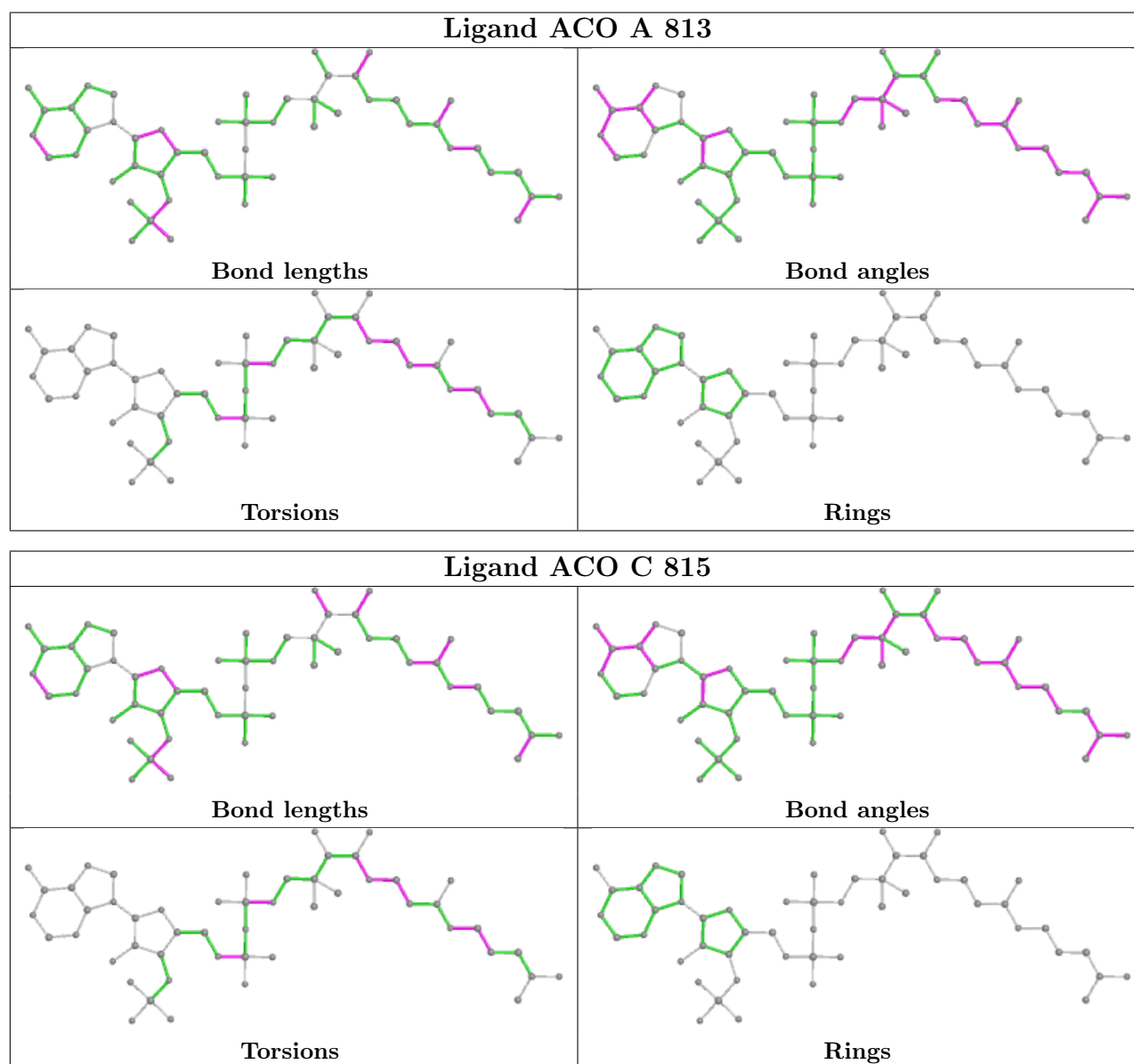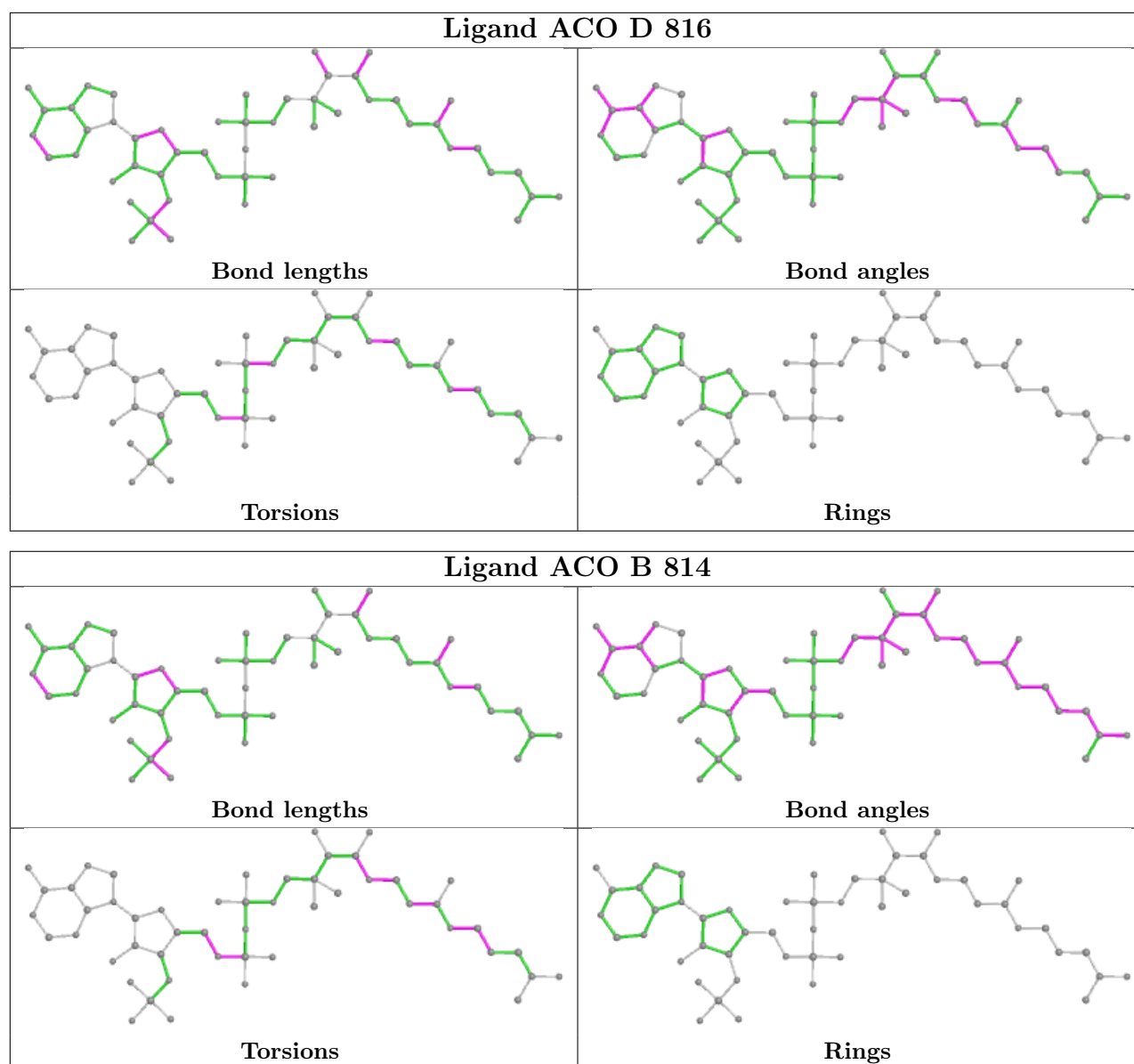
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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(Å^2)	Q<0.9
1	A	388/389 (99%)	-0.57	8 (2%)	63	62	11, 18, 40, 81	0
1	B	388/389 (99%)	-0.54	7 (1%)	68	66	11, 18, 40, 88	0
1	C	388/389 (99%)	0.10	16 (4%)	37	36	22, 36, 64, 110	0
1	D	388/389 (99%)	0.55	40 (10%)	6	6	23, 41, 99, 127	0
All	All	1552/1556 (99%)	-0.12	71 (4%)	32	31	11, 31, 67, 127	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	LYS	6.6
1	D	230	LYS	6.5
1	C	237	LYS	6.2
1	D	226	ASP	5.9
1	D	235	PHE	5.8

## 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, 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
1	SCY	C	89	9/10	0.73	0.25	29,37,57,59	0
1	SCY	D	89	9/10	0.85	0.22	33,37,55,57	0
1	SCY	A	89	9/10	0.91	0.14	13,14,28,33	0
1	SCY	B	89	9/10	0.91	0.13	13,16,29,34	0

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	ACO	D	816	51/51	0.35	0.61	83,97,100,101	0
3	ACO	C	815	51/51	0.40	0.58	72,86,90,91	0
3	ACO	A	813	51/51	0.63	0.31	43,60,75,77	0
3	ACO	B	814	51/51	0.65	0.34	43,59,75,76	0
2	SO4	B	812	5/5	0.83	0.19	40,40,44,44	0
2	SO4	A	811	5/5	0.85	0.20	52,53,53,56	0
2	SO4	B	807	5/5	0.95	0.17	51,52,54,54	0
2	SO4	A	808	5/5	0.96	0.14	51,52,53,54	0
2	SO4	B	809	5/5	0.97	0.12	44,46,47,48	0
2	SO4	A	810	5/5	0.98	0.14	44,46,47,48	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Electron density around ACO D 816:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
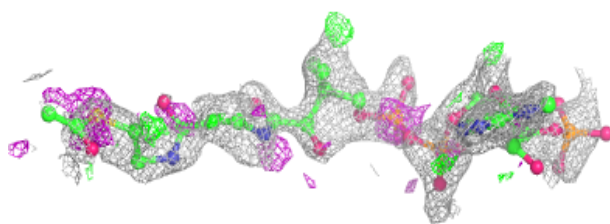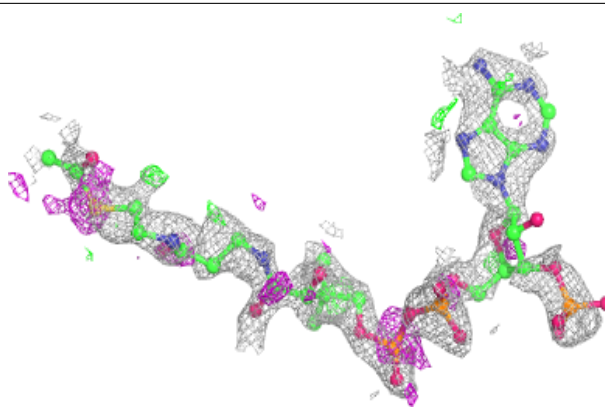and green (positive)
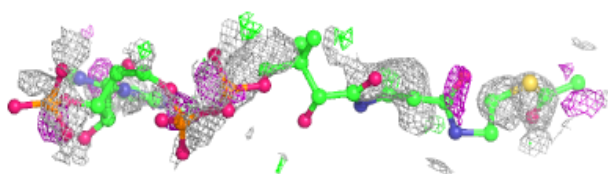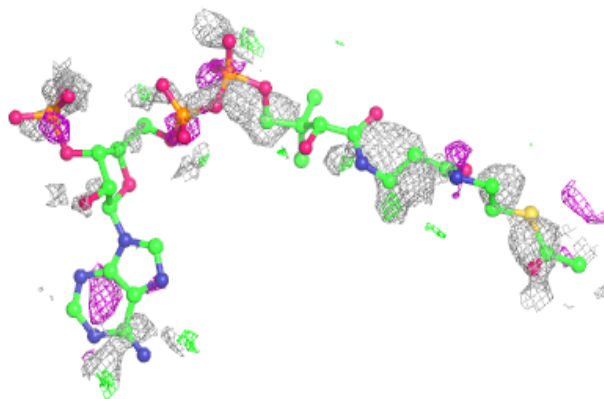
Electron density around ACO C 815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
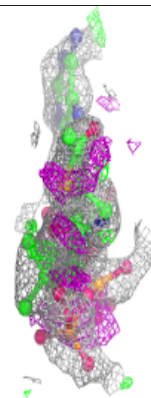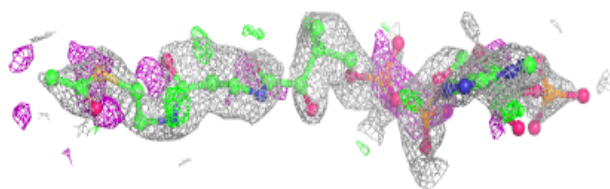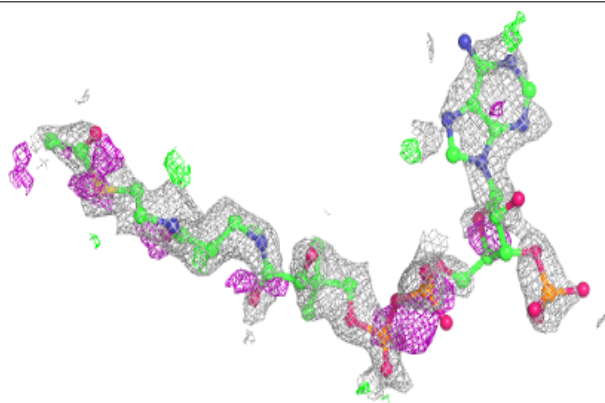mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
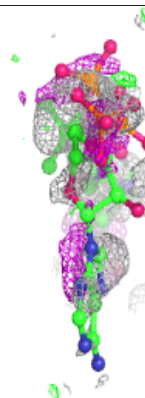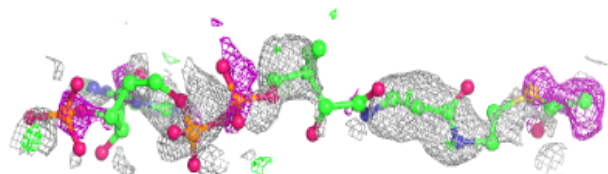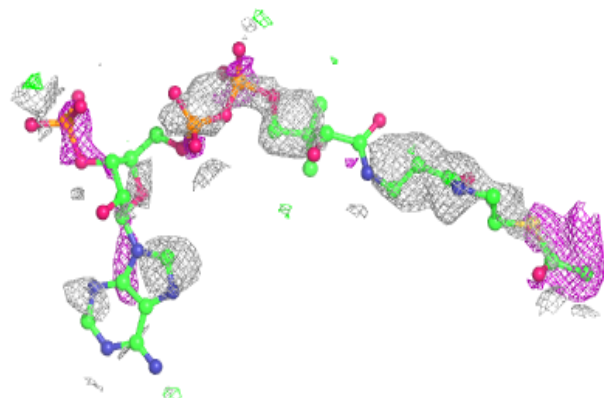
Electron density around ACO A 813:

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

Electron density around ACO B 814:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.