wwPDB X-ray Structure Validation Summary Report (i)

Jun 4, 2025 – 07:52 pm BST

PDB ID	:	9I35 / pdb_00009i35
Title	:	Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with octanoyl-CoA
Authors	:	Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on	:	2025-01-22
Resolution	:	2.08 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:

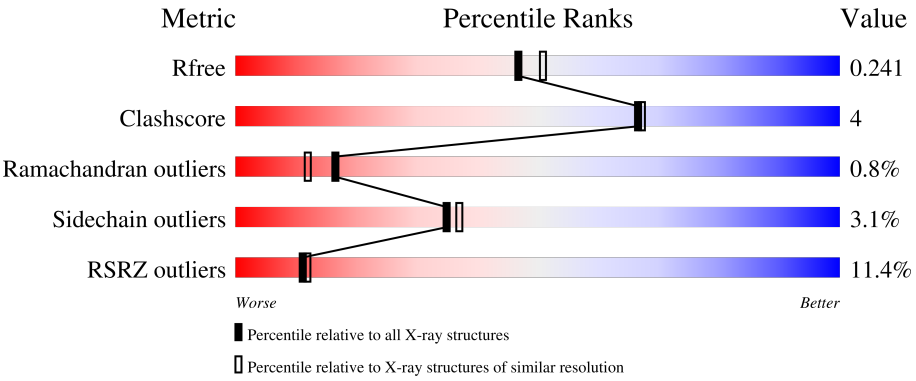
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.08 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}	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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	364	8% 85% 12%
1	B	364	12% 87% 10%
1	C	364	19% 87% 10%
1	D	364	6% 88% 9%
1	E	364	10% 86% 11%

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Mol	Chain	Length	Quality of chain
1	F	364	15% 86% 10%
1	G	364	16% 84% 12%
1	H	364	12% 86% 11%
1	I	364	4% 88% 9%
1	J	364	10% 85% 11%
1	K	364	18% 86% 11%
1	L	364	5% 88% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35020 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 Alpha-methylacyl-CoA racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	B	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	C	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	D	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	E	356	Total	C	N	O	S	0	2	0
			2698	1692	483	507	16			
1	F	359	Total	C	N	O	S	0	2	0
			2724	1708	488	512	16			
1	G	359	Total	C	N	O	S	0	3	0
			2727	1709	488	514	16			
1	H	358	Total	C	N	O	S	0	2	0
			2713	1703	486	508	16			
1	I	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	J	356	Total	C	N	O	S	0	1	0
			2695	1691	483	505	16			
1	K	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	16			
1	L	359	Total	C	N	O	S	0	2	0
			2721	1707	487	511	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	GLY	-	expression tag	UNP O06543
A	362	SER	-	expression tag	UNP O06543
A	363	GLY	-	expression tag	UNP O06543
A	364	CYS	-	expression tag	UNP O06543
B	361	GLY	-	expression tag	UNP O06543

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Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	UNP O06543
D	361	GLY	-	expression tag	UNP O06543
D	362	SER	-	expression tag	UNP O06543
D	363	GLY	-	expression tag	UNP O06543
D	364	CYS	-	expression tag	UNP O06543
E	361	GLY	-	expression tag	UNP O06543
E	362	SER	-	expression tag	UNP O06543
E	363	GLY	-	expression tag	UNP O06543
E	364	CYS	-	expression tag	UNP O06543
F	361	GLY	-	expression tag	UNP O06543
F	362	SER	-	expression tag	UNP O06543
F	363	GLY	-	expression tag	UNP O06543
F	364	CYS	-	expression tag	UNP O06543
G	361	GLY	-	expression tag	UNP O06543
G	362	SER	-	expression tag	UNP O06543
G	363	GLY	-	expression tag	UNP O06543
G	364	CYS	-	expression tag	UNP O06543
H	361	GLY	-	expression tag	UNP O06543
H	362	SER	-	expression tag	UNP O06543
H	363	GLY	-	expression tag	UNP O06543
H	364	CYS	-	expression tag	UNP O06543
I	361	GLY	-	expression tag	UNP O06543
I	362	SER	-	expression tag	UNP O06543
I	363	GLY	-	expression tag	UNP O06543
I	364	CYS	-	expression tag	UNP O06543
J	361	GLY	-	expression tag	UNP O06543
J	362	SER	-	expression tag	UNP O06543
J	363	GLY	-	expression tag	UNP O06543
J	364	CYS	-	expression tag	UNP O06543
K	361	GLY	-	expression tag	UNP O06543
K	362	SER	-	expression tag	UNP O06543
K	363	GLY	-	expression tag	UNP O06543
K	364	CYS	-	expression tag	UNP O06543
L	361	GLY	-	expression tag	UNP O06543
L	362	SER	-	expression tag	UNP O06543
L	363	GLY	-	expression tag	UNP O06543

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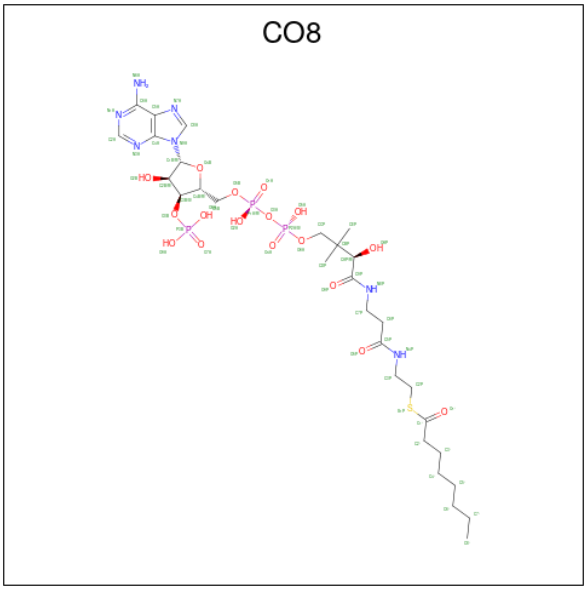
Chain	Residue	Modelled	Actual	Comment	Reference
L	364	CYS	-	expression tag	UNP O06543

- Molecule 2 is OCTANOYL-COENZYME A (CCD ID: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

- Molecule 3 is water.

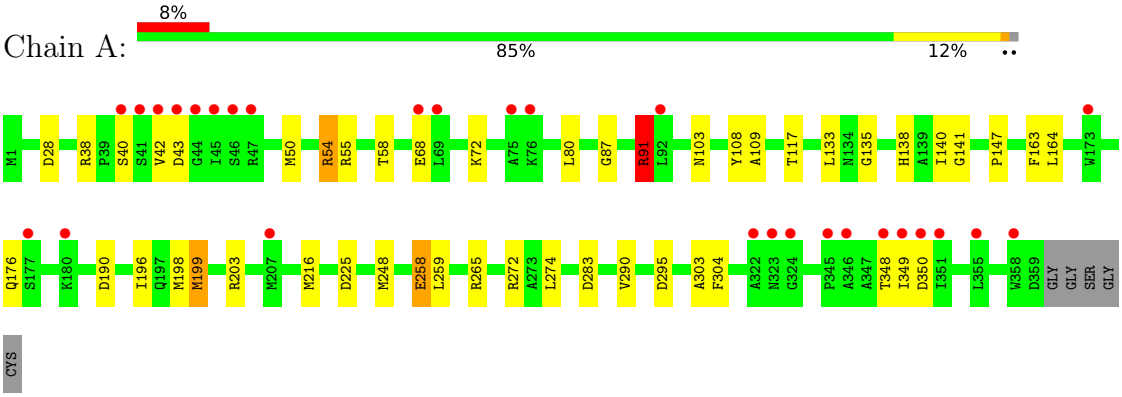
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	146	Total	O	0	0
			146	146		
3	C	147	Total	O	0	0
			147	147		
3	D	153	Total	O	0	0
			153	153		
3	E	133	Total	O	0	0
			133	133		
3	F	139	Total	O	0	0
			139	139		
3	G	128	Total	O	0	0
			128	128		
3	H	134	Total	O	0	0
			134	134		
3	I	166	Total	O	0	0
			166	166		
3	J	162	Total	O	0	0
			162	162		
3	K	151	Total	O	0	0
			151	151		
3	L	156	Total	O	0	0
			156	156		

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.

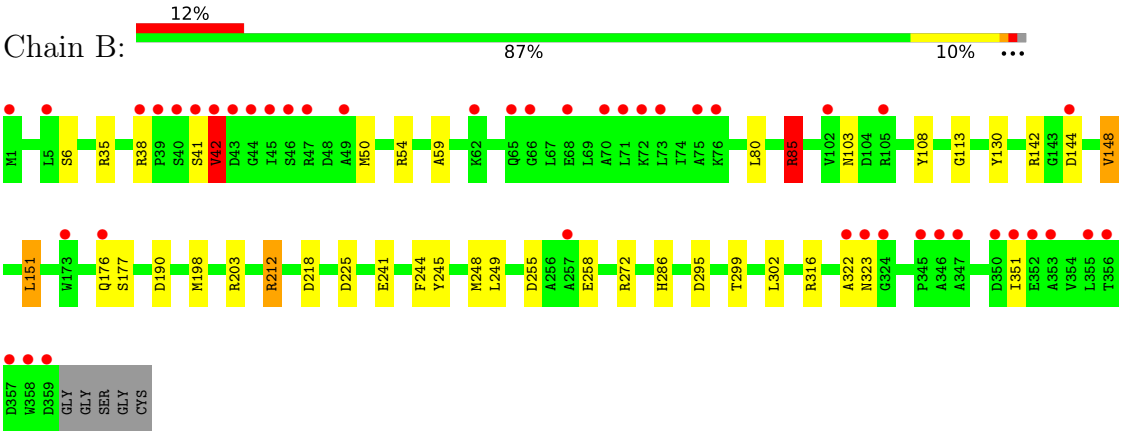
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain A:



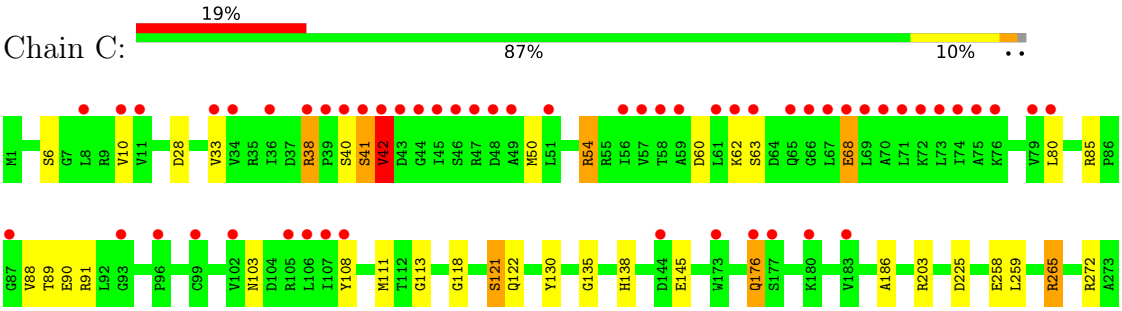
• Molecule 1: Alpha-methylacyl-CoA racemase

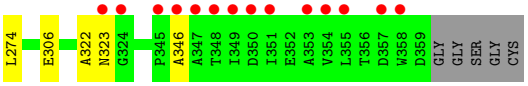
Chain B:



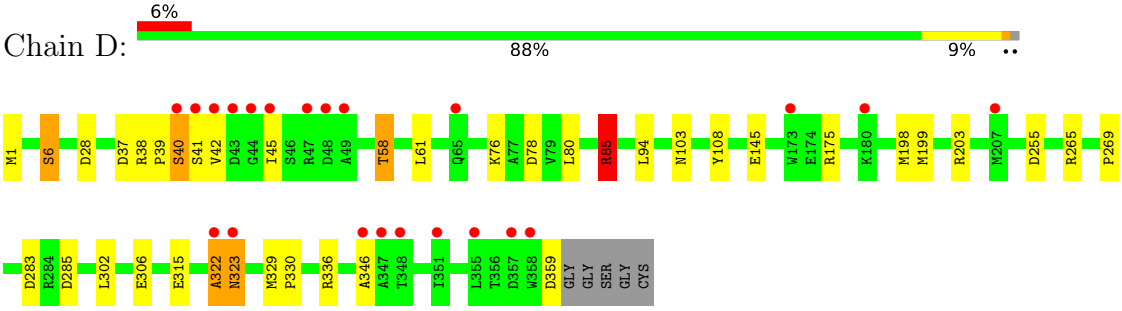
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain C:

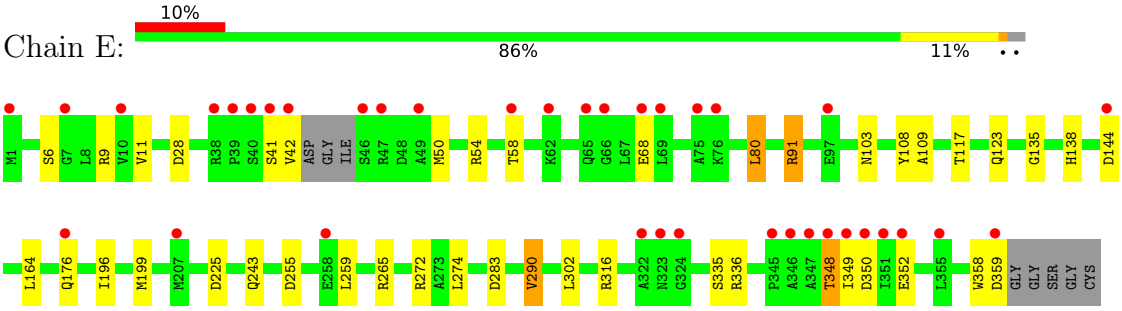




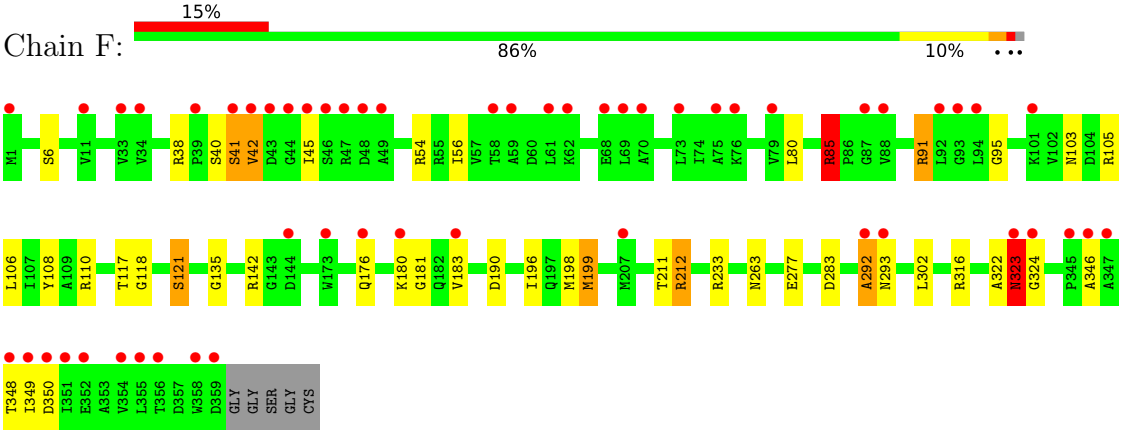
• Molecule 1: Alpha-methylacyl-CoA racemase



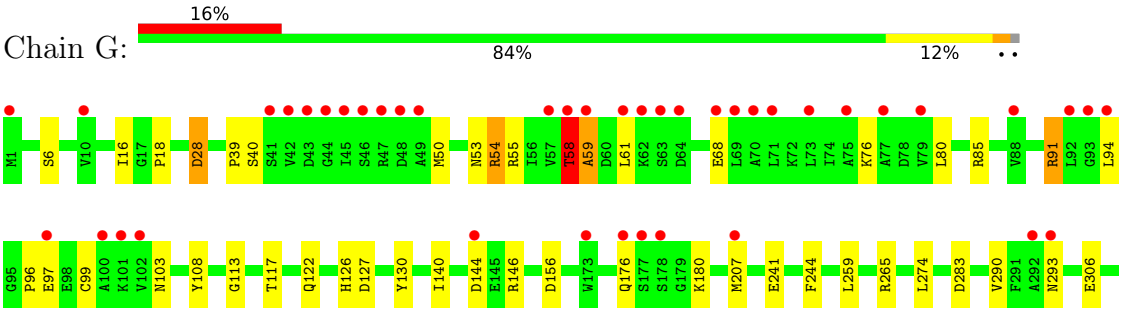
• Molecule 1: Alpha-methylacyl-CoA racemase

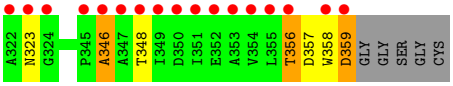


• Molecule 1: Alpha-methylacyl-CoA racemase



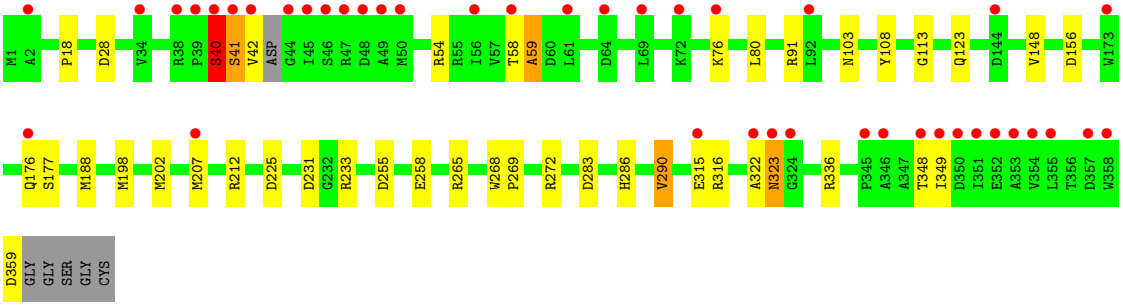
• Molecule 1: Alpha-methylacyl-CoA racemase





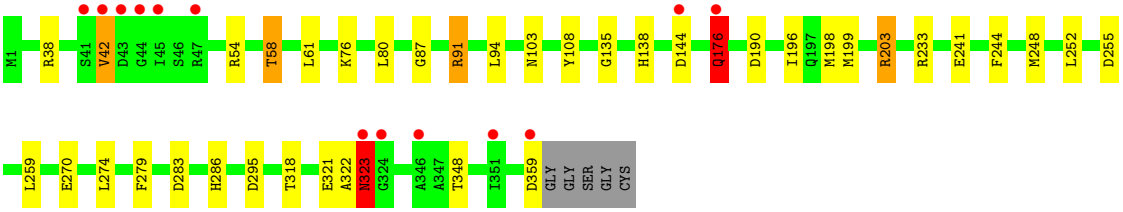
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain H:



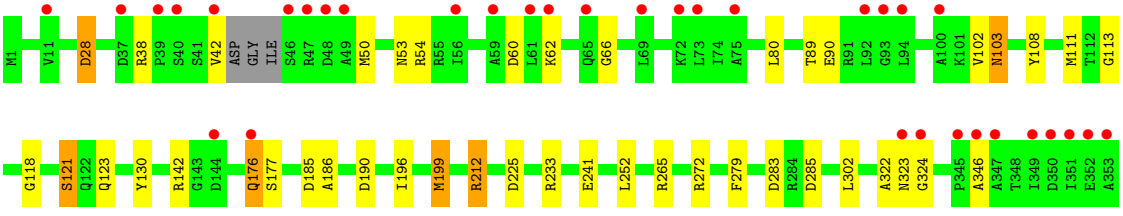
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain I:



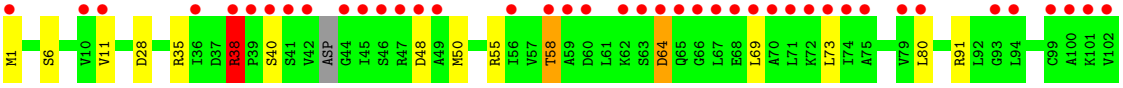
• Molecule 1: Alpha-methylacyl-CoA racemase

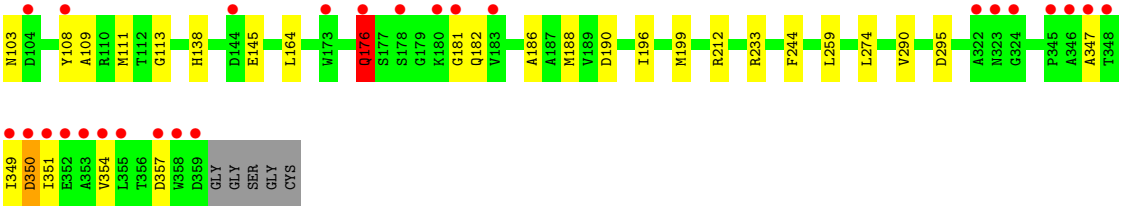
Chain J:



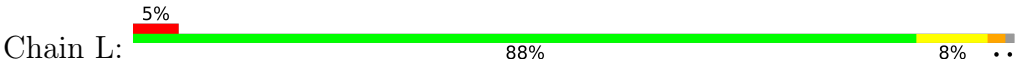
• Molecule 1: Alpha-methylacyl-CoA racemase

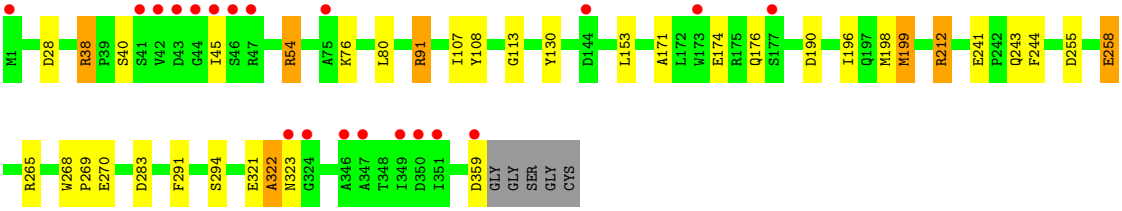
Chain K:





• Molecule 1: Alpha-methylacyl-CoA racemase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	276.31Å 276.31Å 390.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.59 – 2.08 225.59 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.59-2.08) 99.9 (225.59-2.08)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.201 , 0.233 0.212 , 0.241	Depositor DCC
R_{free} test set	22342 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.008 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	35020	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: CO8

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	0.65	0/2791	1.18	16/3797 (0.4%)
1	B	0.66	0/2782	1.16	11/3785 (0.3%)
1	C	0.64	0/2791	1.19	11/3797 (0.3%)
1	D	0.65	0/2782	1.19	12/3785 (0.3%)
1	E	0.66	0/2770	1.15	9/3767 (0.2%)
1	F	0.65	0/2791	1.16	6/3797 (0.2%)
1	G	0.65	0/2800	1.21	14/3809 (0.4%)
1	H	0.66	0/2782	1.18	10/3783 (0.3%)
1	I	0.67	0/2791	1.16	12/3797 (0.3%)
1	J	0.66	0/2761	1.19	13/3755 (0.3%)
1	K	0.66	0/2782	1.19	9/3783 (0.2%)
1	L	0.66	0/2791	1.15	8/3797 (0.2%)
All	All	0.66	0/33414	1.18	131/45452 (0.3%)

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	2
1	B	0	4
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	6
1	G	0	3
1	H	0	4
1	I	0	2
1	J	0	2
1	K	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	5
All	All	0	37

There are no bond length outliers.

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	123	GLN	CB-CA-C	10.30	126.63	109.84
1	K	58	THR	CA-CB-OG1	-10.14	94.39	109.60
1	B	203	ARG	N-CA-CB	9.26	123.87	110.16
1	D	203	ARG	CB-CA-C	-8.92	95.98	110.79
1	B	203	ARG	CB-CA-C	-8.78	95.93	110.85

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	212	ARG	Sidechain
1	B	35	ARG	Sidechain
1	B	85	ARG	Sidechain

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	2718	0	2658	21	0
1	B	2715	0	2660	23	0
1	C	2718	0	2658	23	0
1	D	2715	0	2660	19	0
1	E	2698	0	2639	22	0
1	F	2724	0	2667	27	0
1	G	2727	0	2665	31	0
1	H	2713	0	2663	21	0
1	I	2718	0	2658	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2695	0	2641	20	0
1	K	2710	0	2653	24	0
1	L	2721	0	2668	14	0
2	A	57	0	46	0	0
2	B	57	0	46	5	0
2	C	57	0	46	3	0
2	D	57	0	46	2	0
2	E	57	0	46	2	0
2	F	57	0	46	2	0
2	G	57	0	46	9	0
2	H	57	0	46	1	0
2	I	57	0	46	3	0
2	J	57	0	46	1	0
2	K	57	0	46	0	0
2	L	57	0	46	0	0
3	A	149	0	0	1	0
3	B	146	0	0	2	0
3	C	147	0	0	2	0
3	D	153	0	0	3	0
3	E	133	0	0	2	0
3	F	139	0	0	4	0
3	G	128	0	0	3	0
3	H	134	0	0	1	0
3	I	166	0	0	4	0
3	J	162	0	0	1	0
3	K	151	0	0	4	0
3	L	156	0	0	2	0
All	All	35020	0	32442	238	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 4.

The worst 5 of 238 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:F:85:ARG:HD3	2:F:401:CO8:O1A	1.66	0.96
1:C:118:GLY:O	1:C:121:SER:OG	1.94	0.83
1:I:286:HIS:ND1	3:I:502:HOH:O	2.18	0.77
1:C:41:SER:O	1:C:42:VAL:HG23	1.85	0.76
1:D:85:ARG:HD3	2:D:401:CO8:O1A	1.85	0.75

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	359/364 (99%)	341 (95%)	16 (4%)	2 (1%)	22	18
1	B	358/364 (98%)	343 (96%)	10 (3%)	5 (1%)	9	5
1	C	359/364 (99%)	339 (94%)	18 (5%)	2 (1%)	22	18
1	D	358/364 (98%)	337 (94%)	20 (6%)	1 (0%)	37	36
1	E	354/364 (97%)	336 (95%)	15 (4%)	3 (1%)	16	12
1	F	359/364 (99%)	338 (94%)	15 (4%)	6 (2%)	7	3
1	G	360/364 (99%)	342 (95%)	15 (4%)	3 (1%)	16	12
1	H	356/364 (98%)	338 (95%)	13 (4%)	5 (1%)	9	5
1	I	359/364 (99%)	345 (96%)	11 (3%)	3 (1%)	16	12
1	J	353/364 (97%)	339 (96%)	12 (3%)	2 (1%)	22	18
1	K	356/364 (98%)	333 (94%)	21 (6%)	2 (1%)	22	18
1	L	359/364 (99%)	343 (96%)	16 (4%)	0	100	100
All	All	4290/4368 (98%)	4074 (95%)	182 (4%)	34 (1%)	16	12

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	VAL
1	F	41	SER
1	G	97	GLU
1	H	40	SER
1	H	41	SER

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	277/277 (100%)	269 (97%)	8 (3%)	37	40
1	B	276/277 (100%)	270 (98%)	6 (2%)	47	51
1	C	277/277 (100%)	267 (96%)	10 (4%)	30	31
1	D	276/277 (100%)	268 (97%)	8 (3%)	37	40
1	E	275/277 (99%)	265 (96%)	10 (4%)	30	31
1	F	277/277 (100%)	267 (96%)	10 (4%)	30	31
1	G	278/277 (100%)	268 (96%)	10 (4%)	30	31
1	H	276/277 (100%)	270 (98%)	6 (2%)	47	51
1	I	277/277 (100%)	268 (97%)	9 (3%)	34	36
1	J	274/277 (99%)	267 (97%)	7 (3%)	41	44
1	K	276/277 (100%)	269 (98%)	7 (2%)	42	46
1	L	277/277 (100%)	267 (96%)	10 (4%)	30	31
All	All	3316/3324 (100%)	3215 (97%)	101 (3%)	35	38

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	140	ILE
1	I	176	GLN
1	L	321	GLU
1	G	348	THR
1	H	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	282	HIS
1	I	122	GLN
1	L	323	ASN
1	G	286	HIS

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Mol	Chain	Res	Type
1	H	176	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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	CO8	I	401	-	51,59,59	1.61	3 (5%)	62,85,85	1.55	5 (8%)
2	CO8	K	401	-	51,59,59	1.58	3 (5%)	62,85,85	1.77	11 (17%)
2	CO8	A	401	-	51,59,59	1.52	3 (5%)	62,85,85	1.69	7 (11%)
2	CO8	G	401	-	51,59,59	1.20	2 (3%)	62,85,85	2.42	14 (22%)
2	CO8	C	401	-	51,59,59	1.48	3 (5%)	62,85,85	1.65	10 (16%)
2	CO8	L	401	-	51,59,59	1.65	3 (5%)	62,85,85	1.58	5 (8%)
2	CO8	E	401	-	51,59,59	1.54	3 (5%)	62,85,85	1.46	6 (9%)
2	CO8	F	401	-	51,59,59	1.03	3 (5%)	62,85,85	1.65	8 (12%)
2	CO8	J	401	-	51,59,59	1.03	3 (5%)	62,85,85	2.06	12 (19%)
2	CO8	D	401	-	51,59,59	1.01	4 (7%)	62,85,85	1.70	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CO8	B	401	-	51,59,59	1.70	3 (5%)	62,85,85	1.66	7 (11%)
2	CO8	H	401	-	51,59,59	1.62	3 (5%)	62,85,85	2.05	10 (16%)

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
2	CO8	I	401	-	-	7/54/74/74	0/3/3/3
2	CO8	K	401	-	-	8/54/74/74	0/3/3/3
2	CO8	A	401	-	-	9/54/74/74	0/3/3/3
2	CO8	G	401	-	-	16/54/74/74	0/3/3/3
2	CO8	C	401	-	-	13/54/74/74	0/3/3/3
2	CO8	L	401	-	-	10/54/74/74	0/3/3/3
2	CO8	E	401	-	-	12/54/74/74	0/3/3/3
2	CO8	F	401	-	-	9/54/74/74	0/3/3/3
2	CO8	J	401	-	-	18/54/74/74	0/3/3/3
2	CO8	D	401	-	-	9/54/74/74	0/3/3/3
2	CO8	B	401	-	-	12/54/74/74	0/3/3/3
2	CO8	H	401	-	-	13/54/74/74	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	CO8	C1'-S1P	9.30	1.98	1.76
2	B	401	CO8	C1'-S1P	9.08	1.98	1.76
2	I	401	CO8	C1'-S1P	9.06	1.98	1.76
2	H	401	CO8	C1'-S1P	8.86	1.97	1.76
2	E	401	CO8	C1'-S1P	8.64	1.97	1.76

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	CO8	C2P-S1P-C1'	10.36	134.11	101.87
2	J	401	CO8	C2P-S1P-C1'	10.31	133.96	101.87
2	G	401	CO8	O1'-C1'-S1P	-10.16	109.42	122.61
2	F	401	CO8	C2P-S1P-C1'	9.11	130.23	101.87
2	G	401	CO8	C7P-C6P-C5P	-8.43	98.32	112.36

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CO8	C5B-O5B-P1A-O1A
2	A	401	CO8	C5P-C6P-C7P-N8P
2	A	401	CO8	O1'-C1'-S1P-C2P
2	A	401	CO8	C2'-C1'-S1P-C2P
2	B	401	CO8	C5B-O5B-P1A-O3A

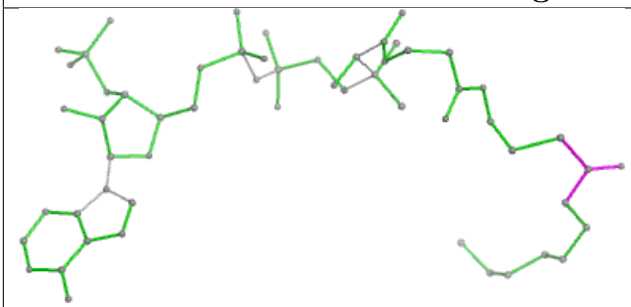
There are no ring outliers.

9 monomers are involved in 28 short contacts:

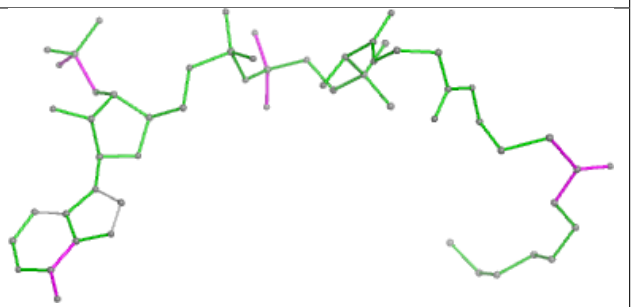
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	CO8	3	0
2	G	401	CO8	9	0
2	C	401	CO8	3	0
2	E	401	CO8	2	0
2	F	401	CO8	2	0
2	J	401	CO8	1	0
2	D	401	CO8	2	0
2	B	401	CO8	5	0
2	H	401	CO8	1	0

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.

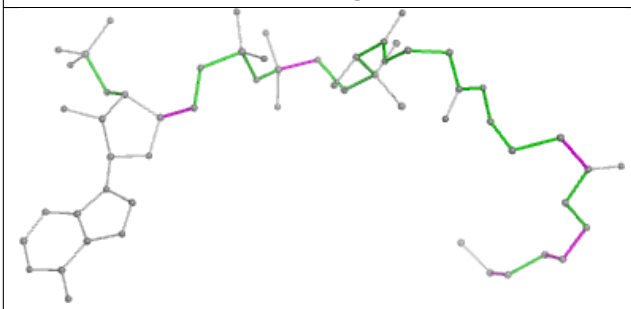
Ligand CO8 I 401



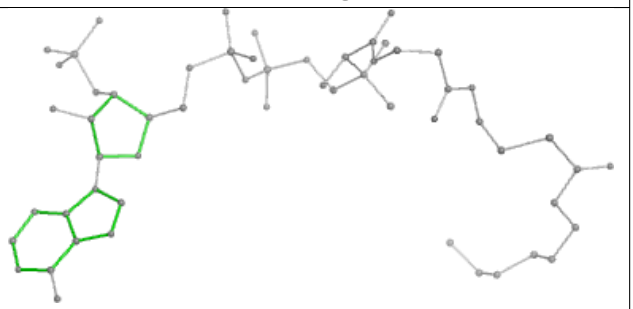
Bond lengths



Bond angles

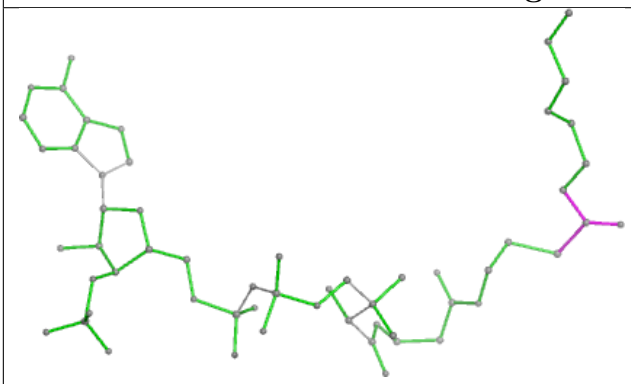


Torsions



Rings

Ligand CO8 K 401



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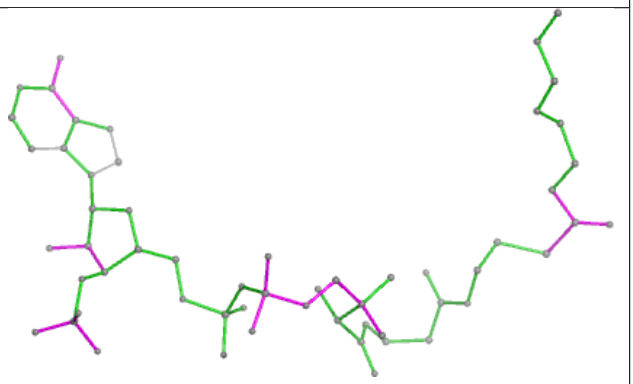
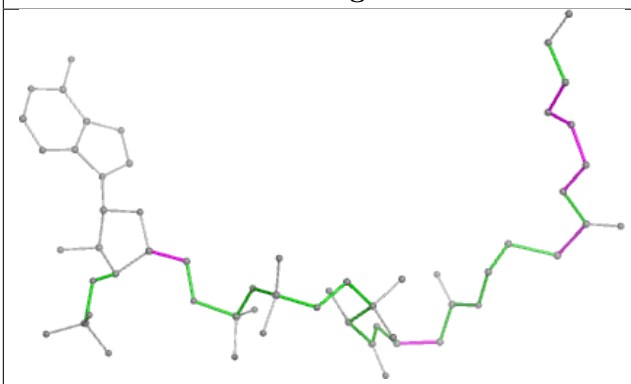


Bond angles



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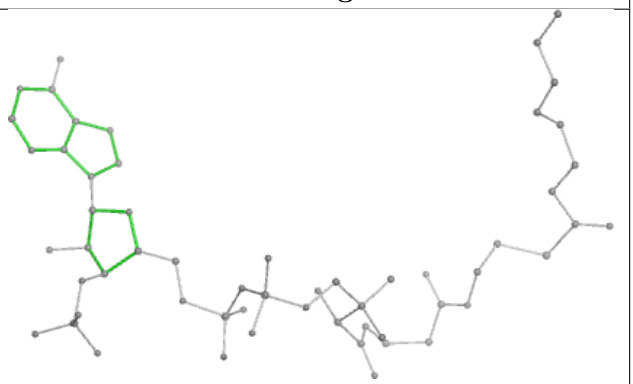
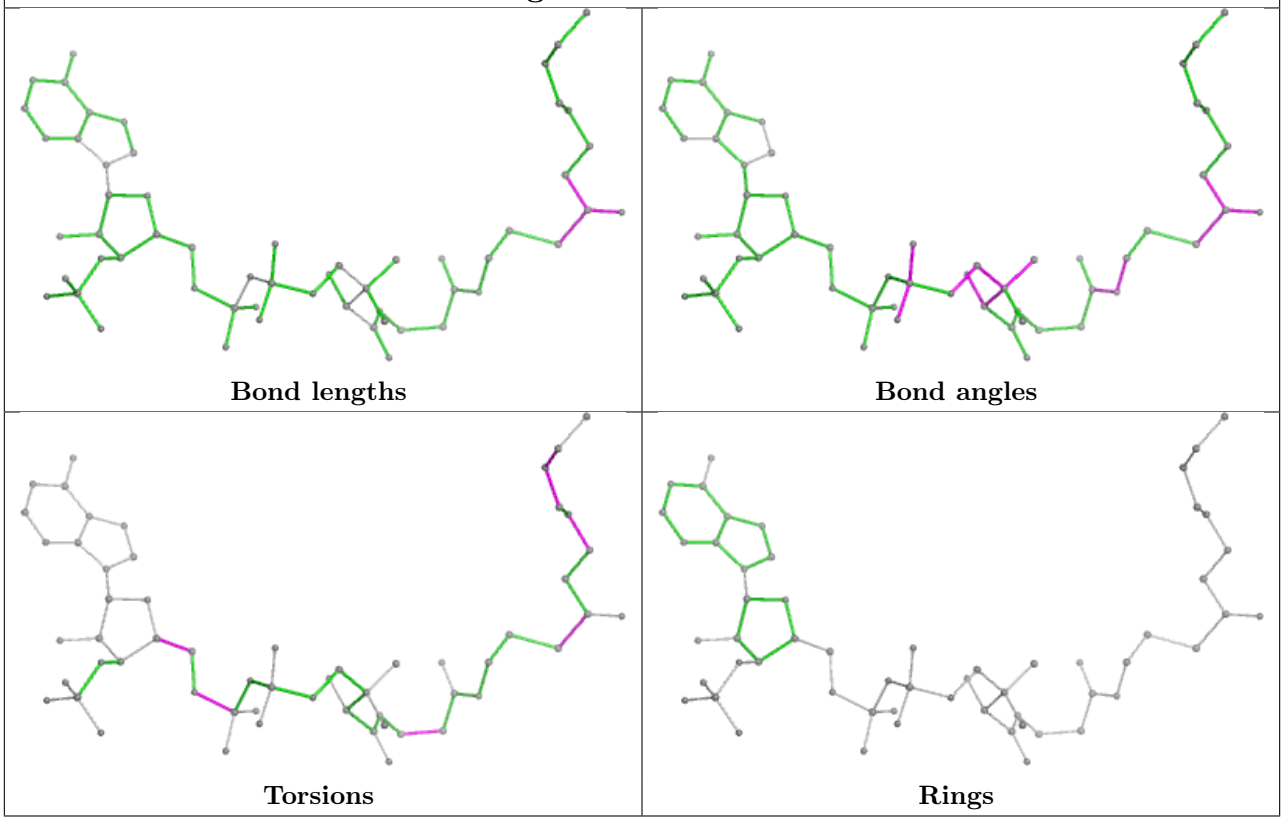


Rings

Ligand CO8 A 401



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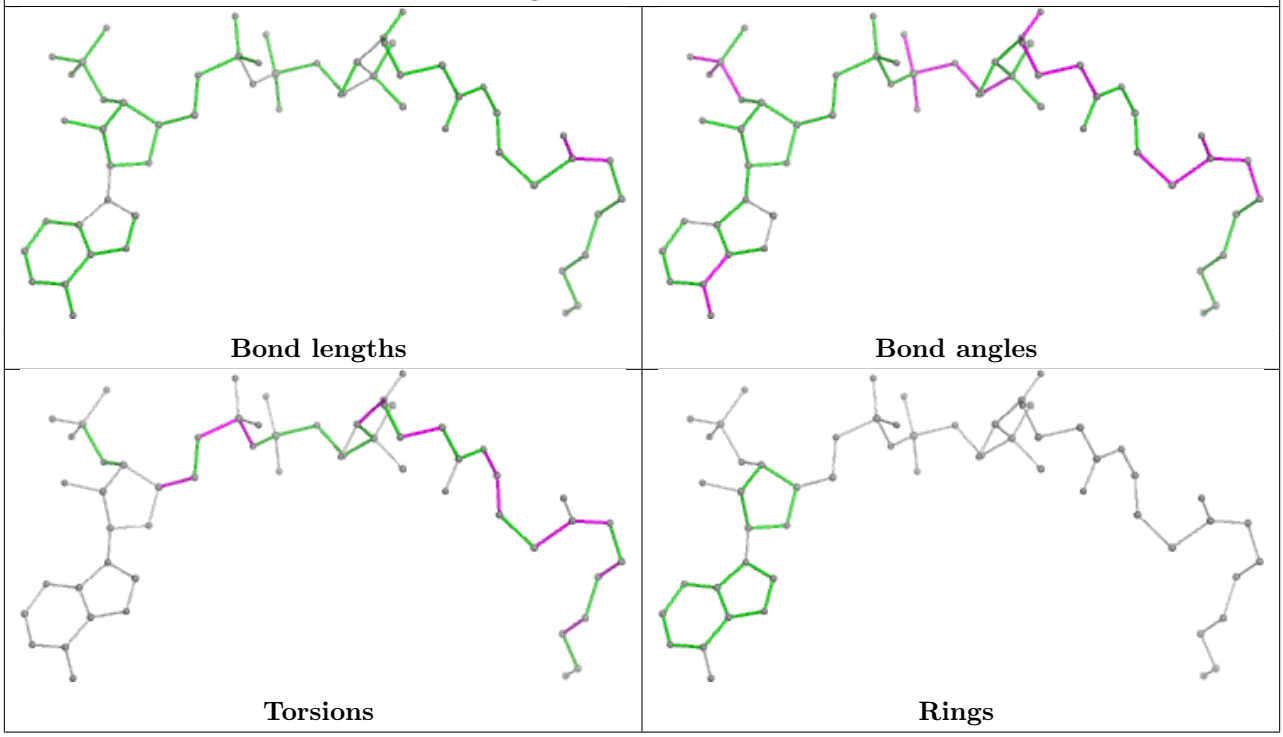

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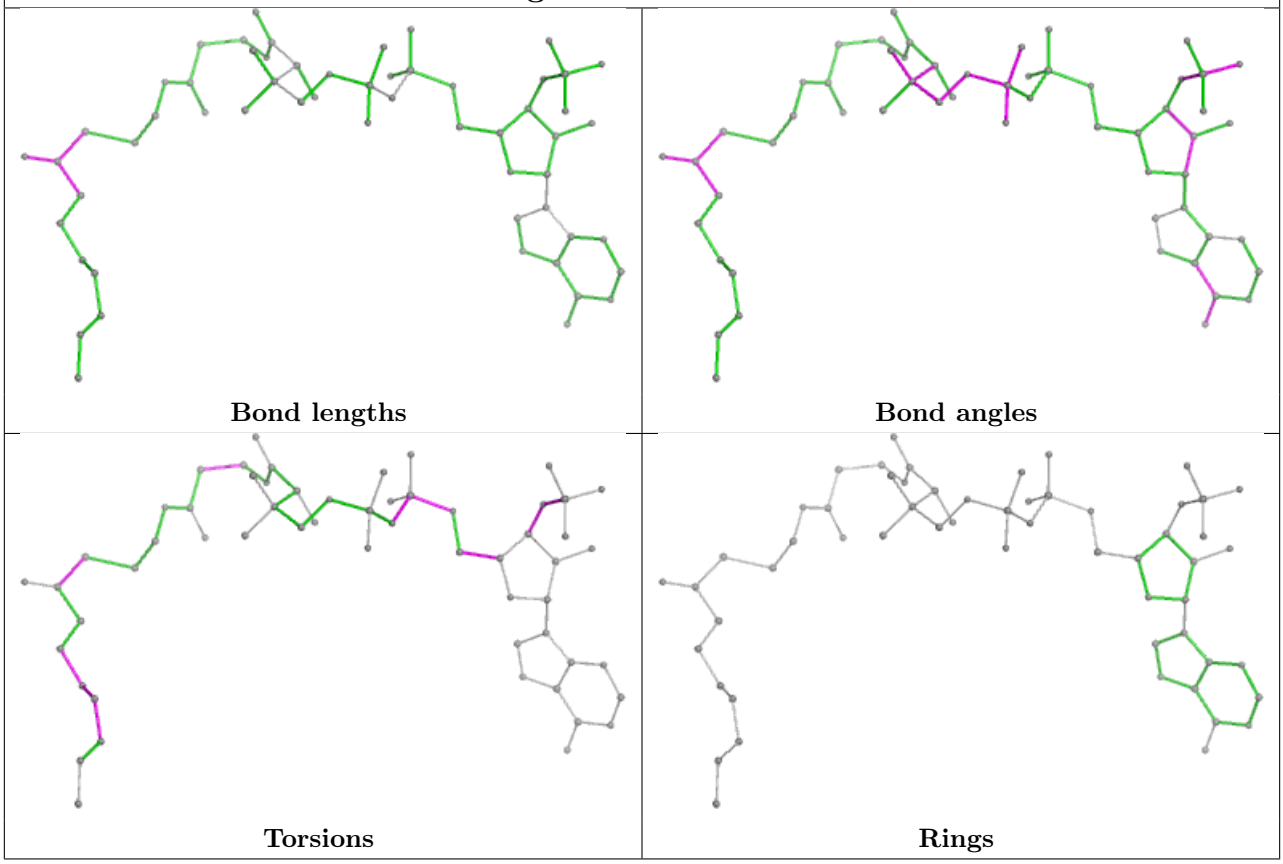
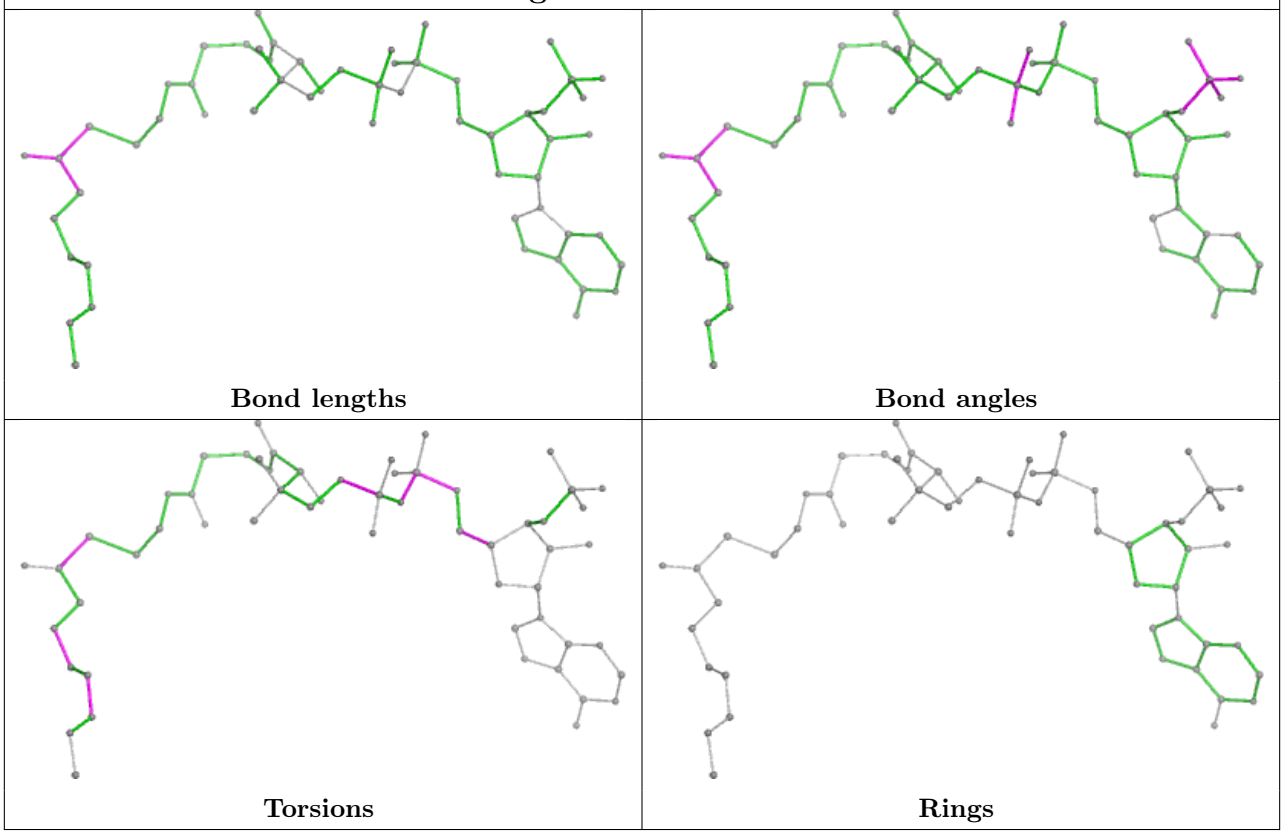


Ligand CO8 L 401



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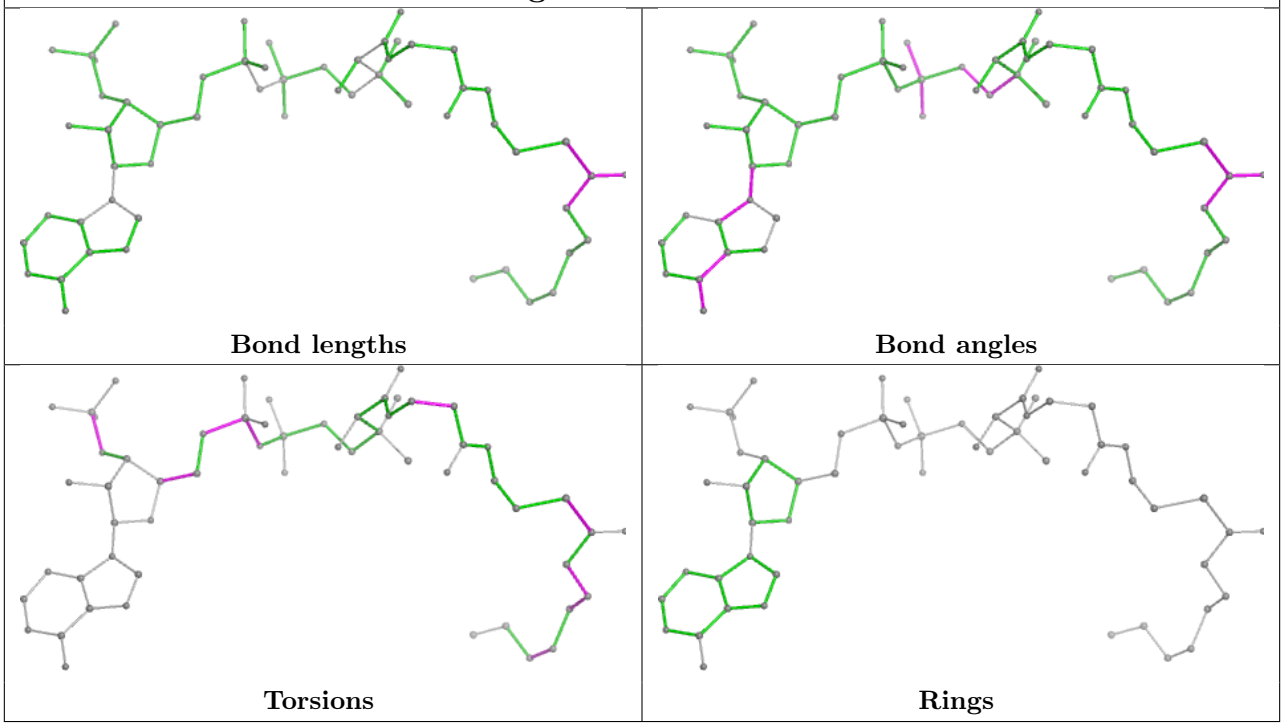
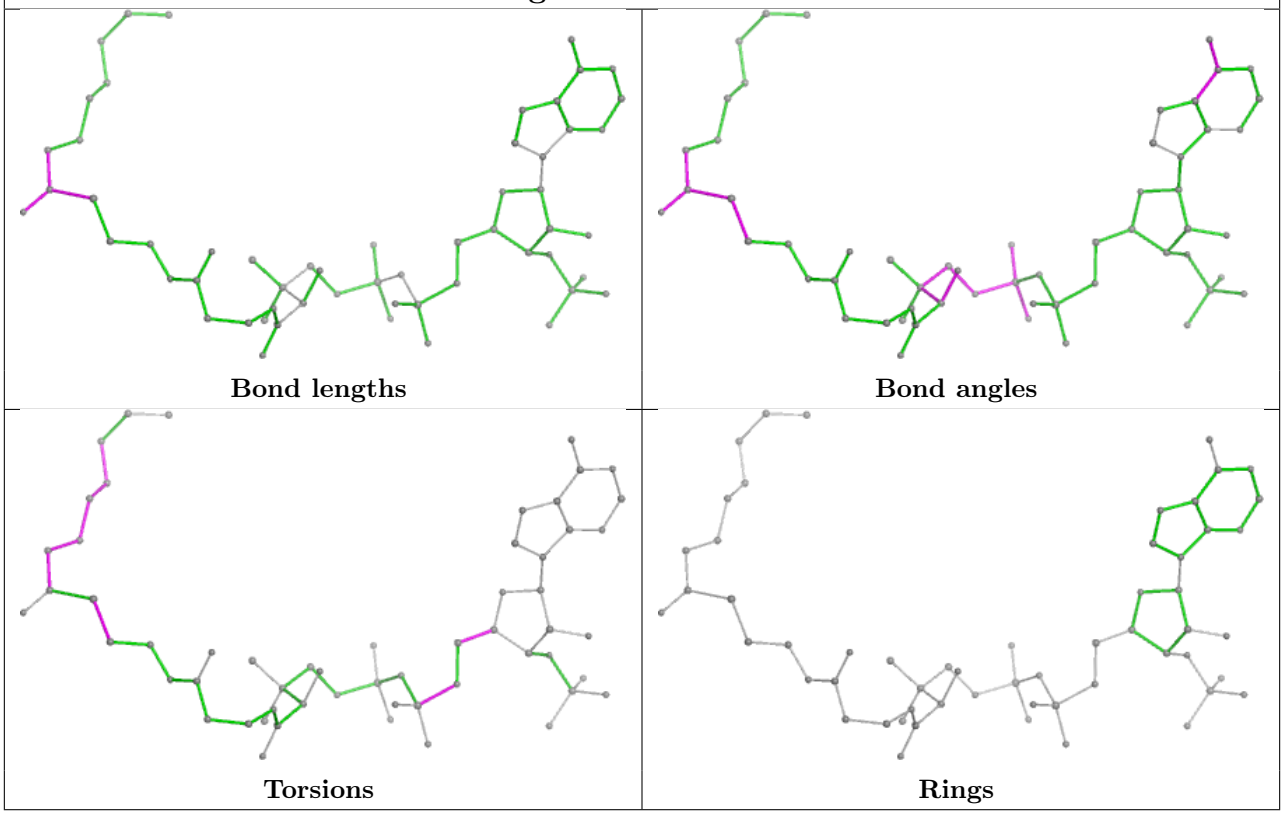
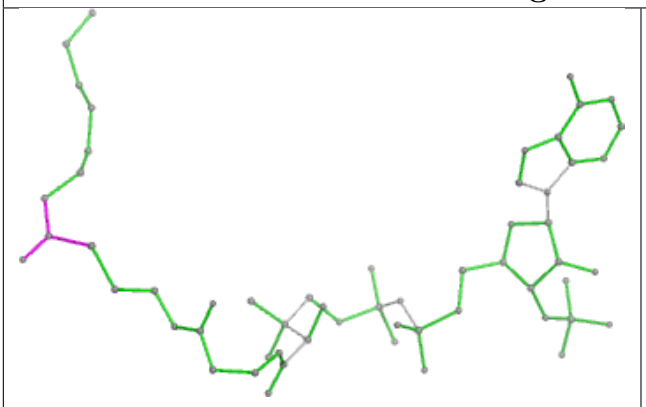


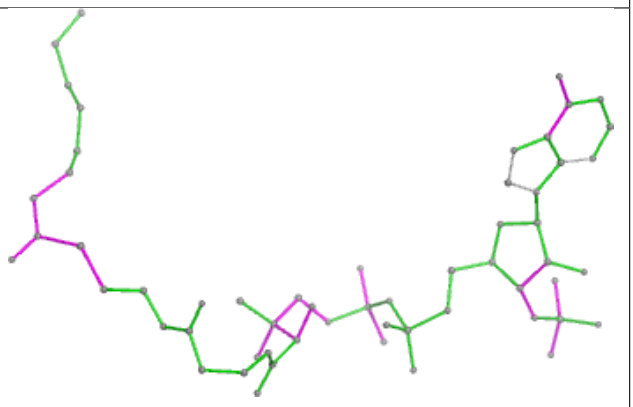
Ligand CO8 F 401



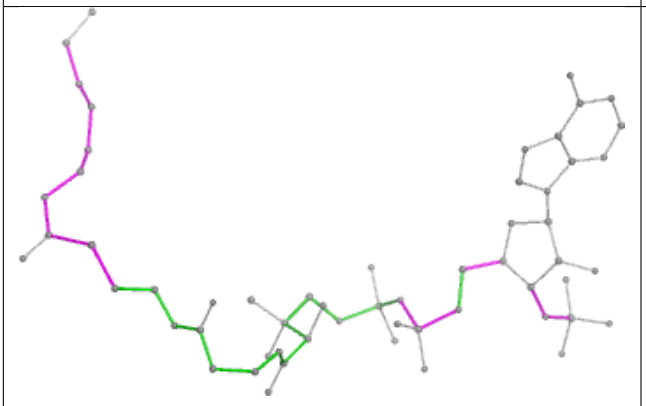
Ligand CO8 J 401



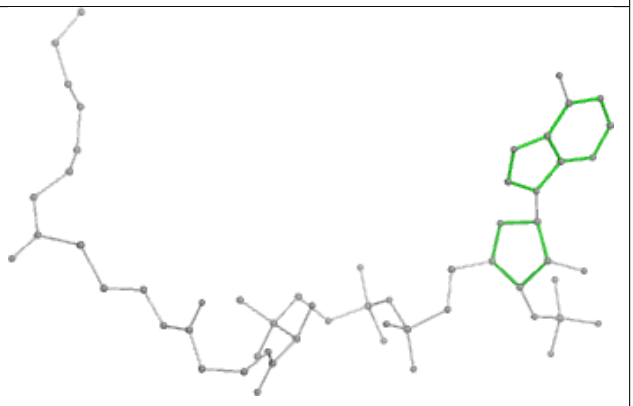
Bond lengths



Bond angles

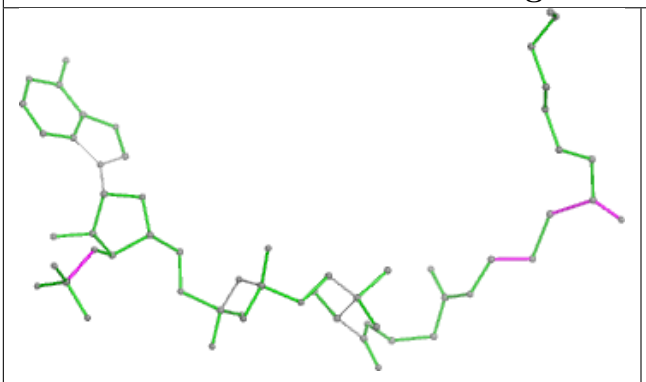


Torsions



Rings

Ligand CO8 D 401



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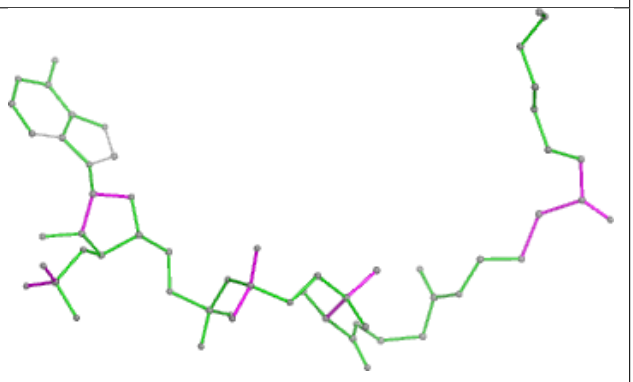
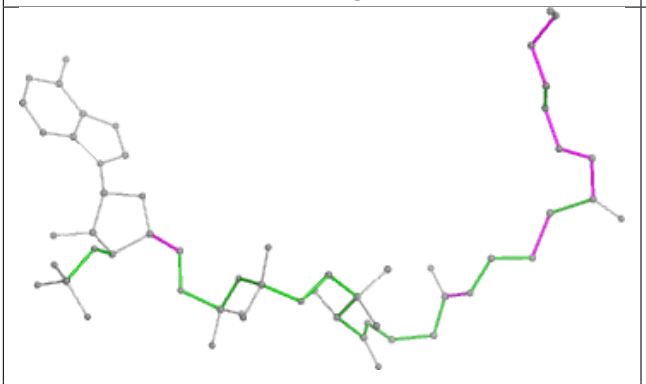


Bond angles



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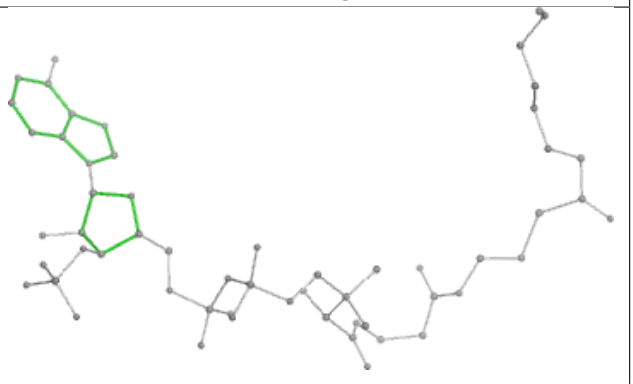
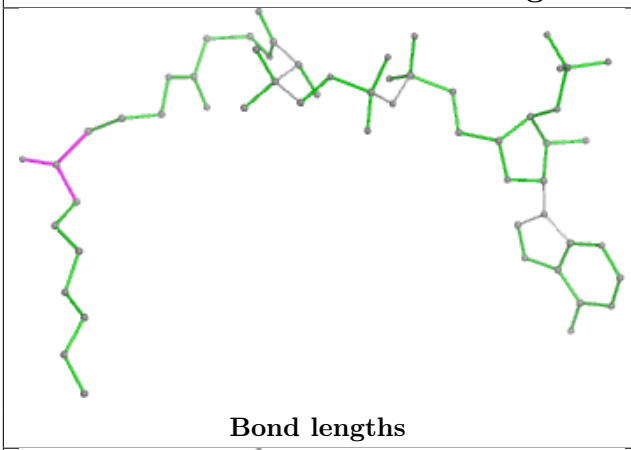
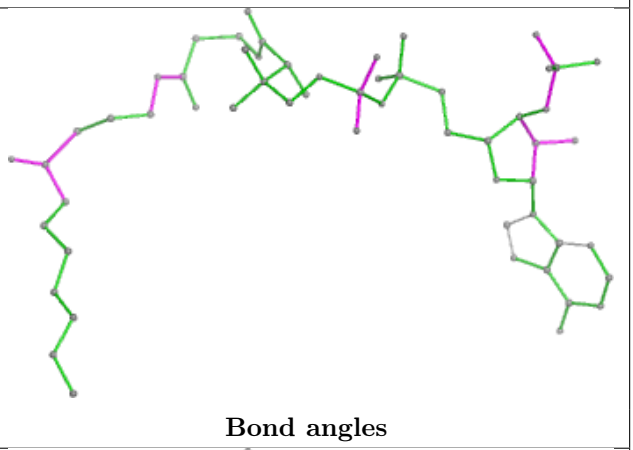


Rings

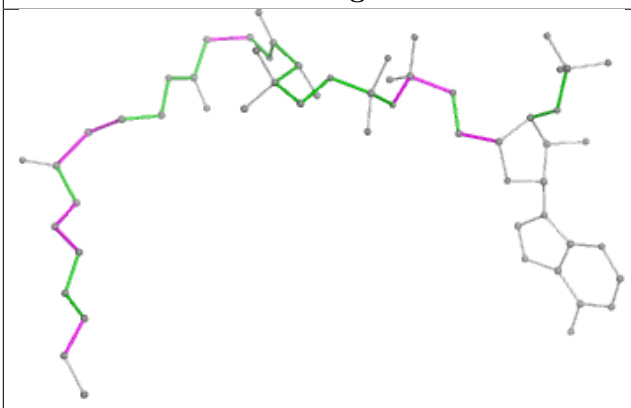
Ligand CO8 B 401



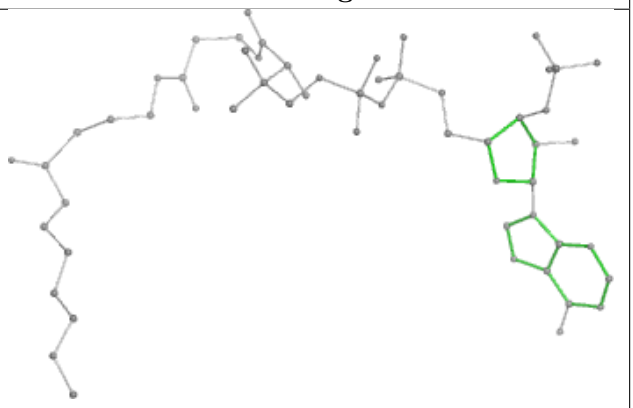
Bond lengths



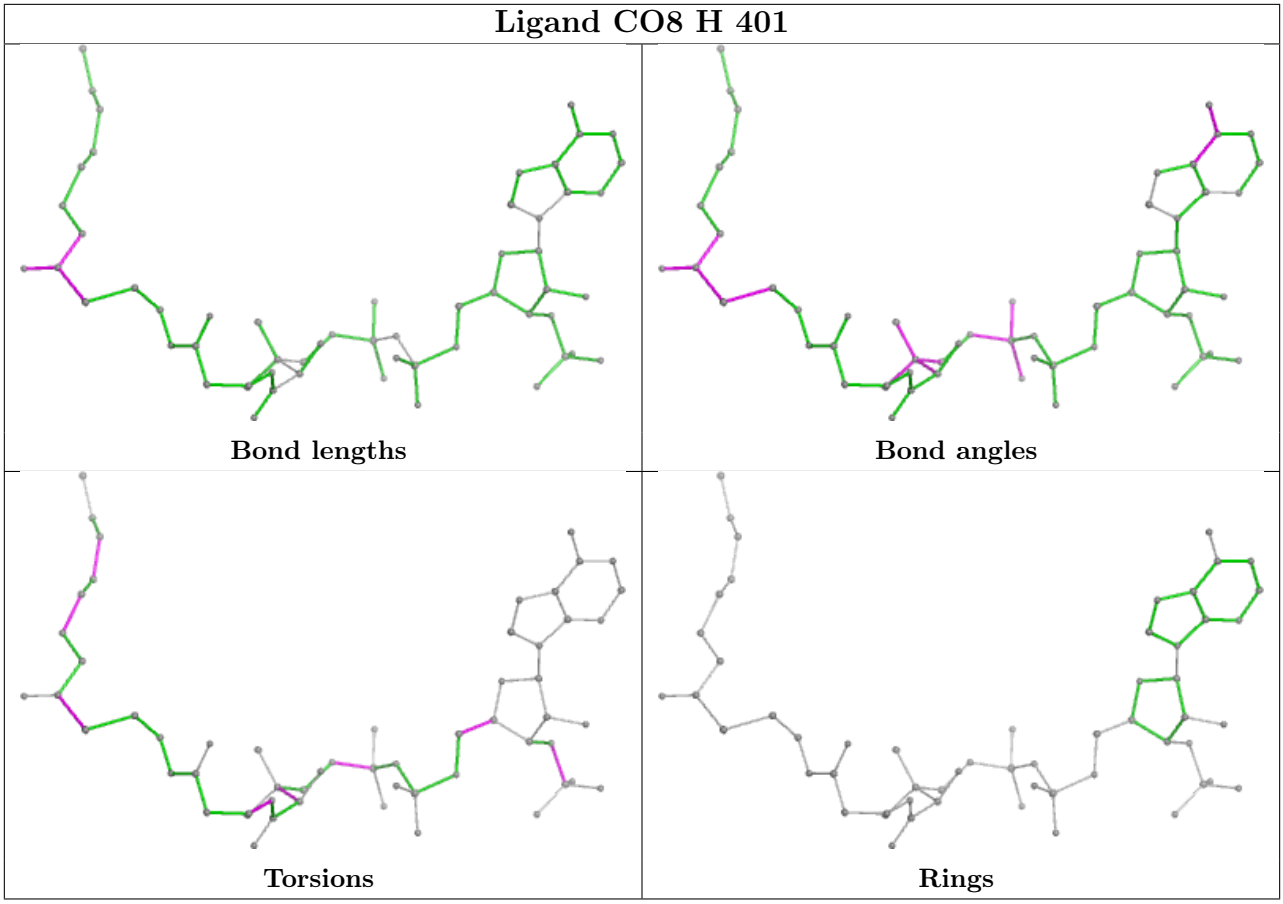
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	359/364 (98%)	0.46	28 (7%) 20 22	21, 35, 71, 106	2 (0%)
1	B	359/364 (98%)	0.56	44 (12%) 9 10	21, 36, 76, 116	1 (0%)
1	C	359/364 (98%)	0.70	69 (19%) 4 4	21, 35, 75, 114	2 (0%)
1	D	359/364 (98%)	0.35	22 (6%) 28 30	21, 34, 69, 115	1 (0%)
1	E	356/364 (97%)	0.47	37 (10%) 13 14	21, 35, 73, 101	2 (0%)
1	F	359/364 (98%)	0.64	54 (15%) 6 7	14, 36, 75, 111	2 (0%)
1	G	359/364 (98%)	0.70	59 (16%) 5 6	15, 37, 75, 113	3 (0%)
1	H	358/364 (98%)	0.51	42 (11%) 10 11	18, 36, 82, 113	2 (0%)
1	I	359/364 (98%)	0.19	13 (3%) 46 48	20, 32, 62, 98	2 (0%)
1	J	356/364 (97%)	0.40	37 (10%) 13 14	21, 33, 69, 103	1 (0%)
1	K	358/364 (98%)	0.70	67 (18%) 4 4	20, 34, 77, 113	2 (0%)
1	L	359/364 (98%)	0.29	20 (5%) 31 33	16, 34, 64, 106	2 (0%)
All	All	4300/4368 (98%)	0.50	492 (11%) 11 12	14, 35, 73, 116	22 (0%)

The worst 5 of 492 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	346	ALA	8.7
1	E	346	ALA	7.2
1	E	42	VAL	6.6
1	K	42	VAL	6.6
1	D	42	VAL	6.4

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

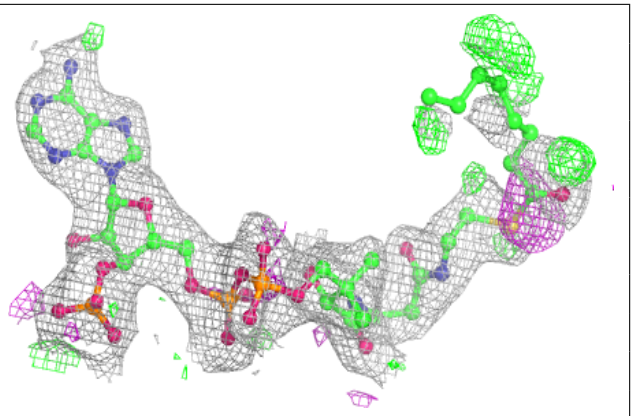
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

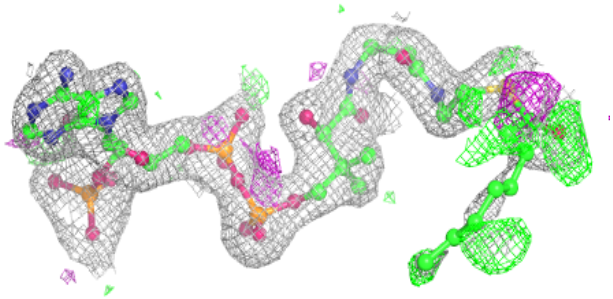
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO8	E	401	57/57	0.92	0.14	28,45,101,103	0
2	CO8	F	401	57/57	0.92	0.14	25,44,89,96	0
2	CO8	H	401	57/57	0.92	0.15	31,45,96,106	0
2	CO8	J	401	57/57	0.92	0.14	26,43,77,95	0
2	CO8	B	401	57/57	0.93	0.14	24,44,81,91	0
2	CO8	G	401	57/57	0.93	0.14	24,42,73,79	0
2	CO8	C	401	57/57	0.93	0.14	26,44,88,97	0
2	CO8	A	401	57/57	0.93	0.13	24,41,81,85	0
2	CO8	K	401	57/57	0.94	0.13	25,44,83,93	0
2	CO8	L	401	57/57	0.95	0.12	21,31,82,93	0
2	CO8	I	401	57/57	0.96	0.10	21,32,76,81	0
2	CO8	D	401	57/57	0.96	0.11	20,31,90,97	0

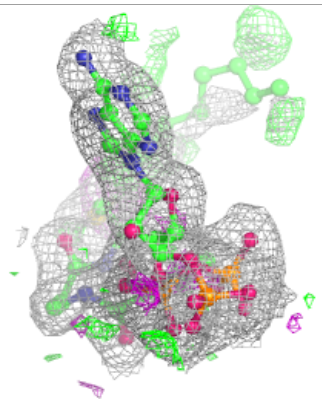
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CO8 E 401:

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

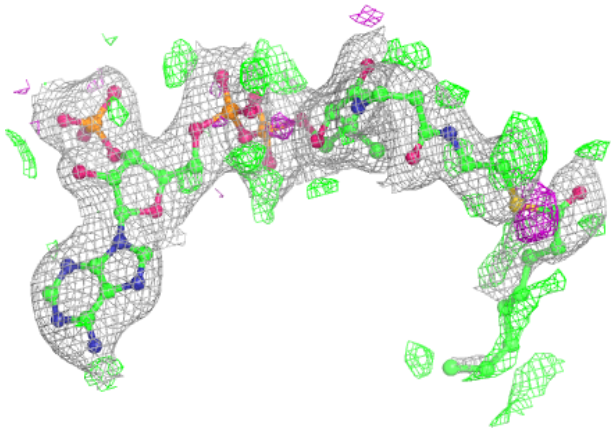


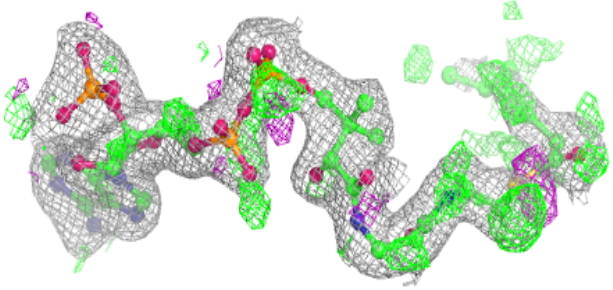


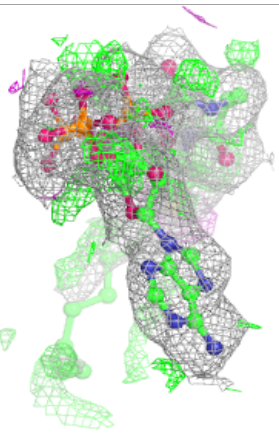


Electron density around CO8 F 401:

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

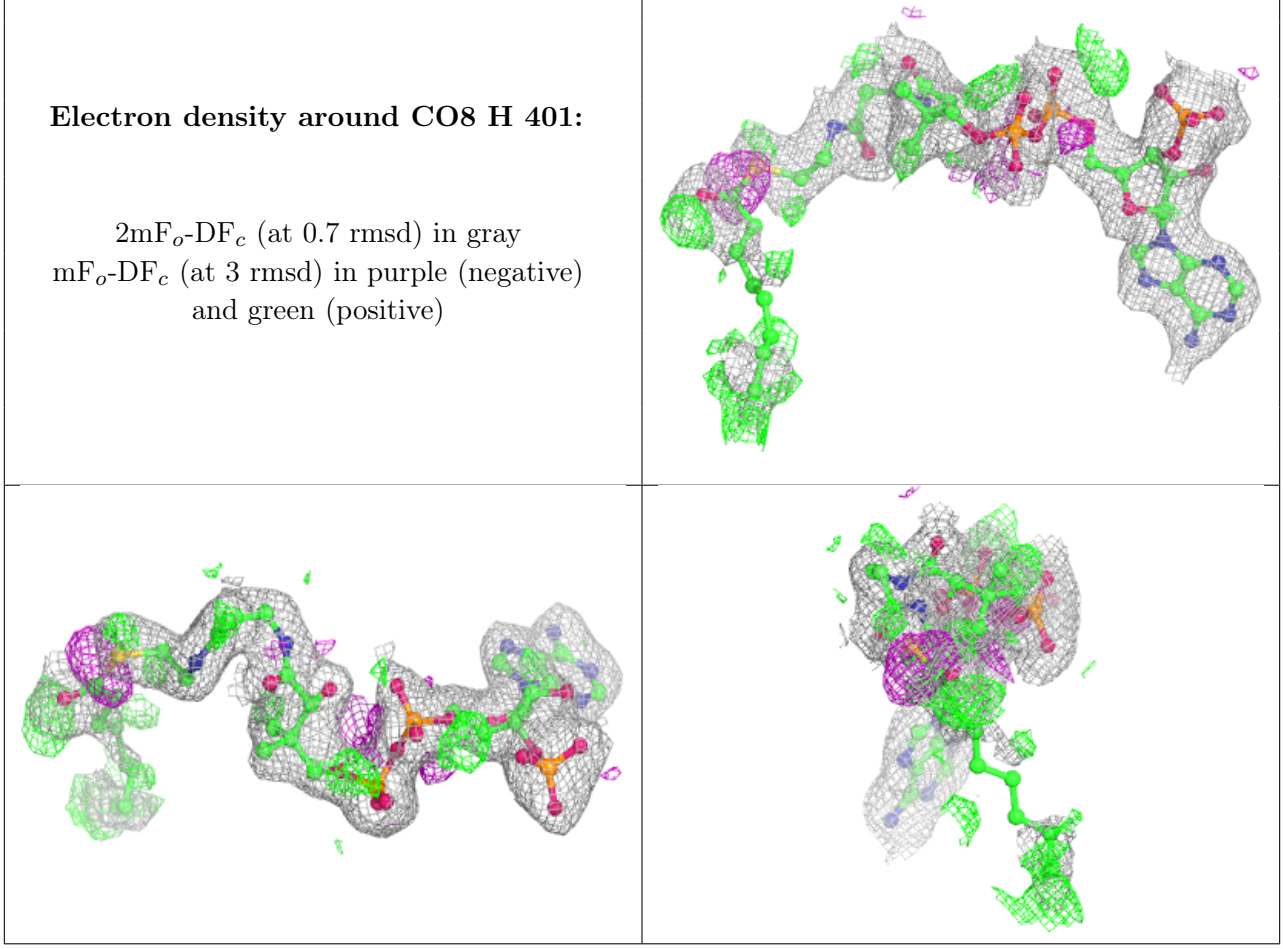






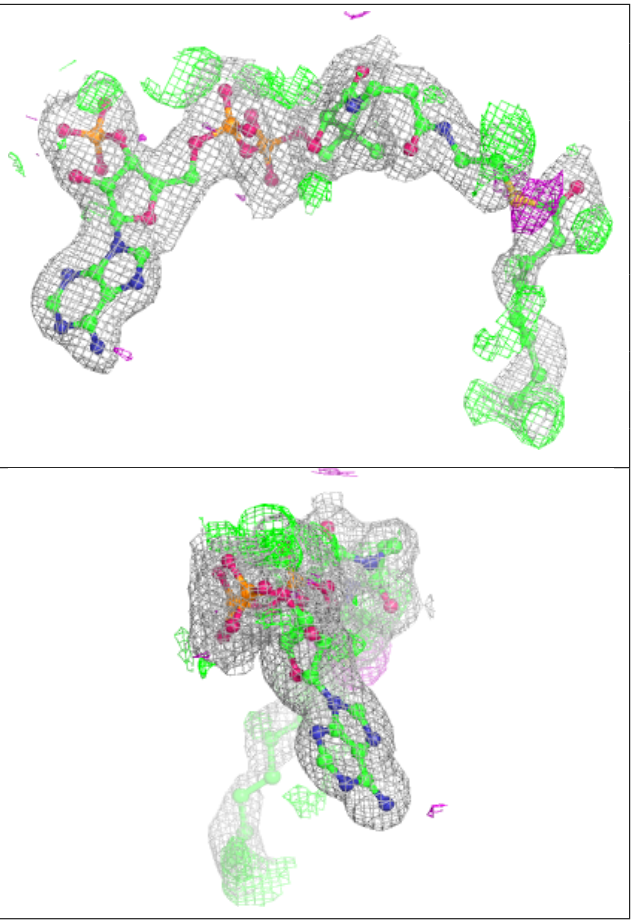
Electron density around CO8 H 401:

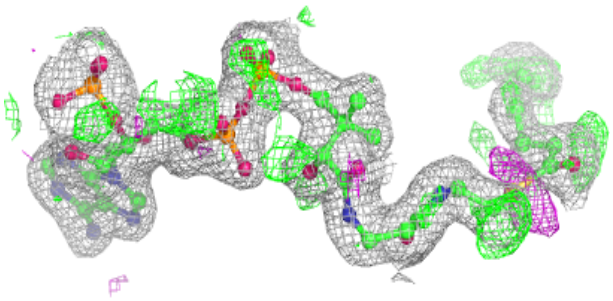
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CO8 J 401:

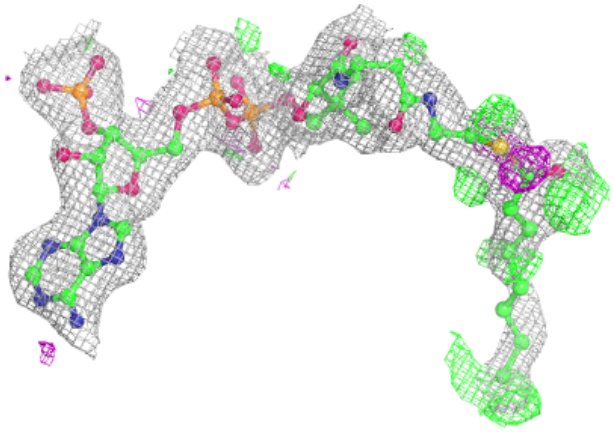
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

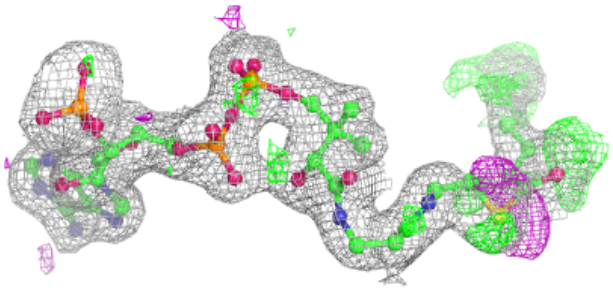


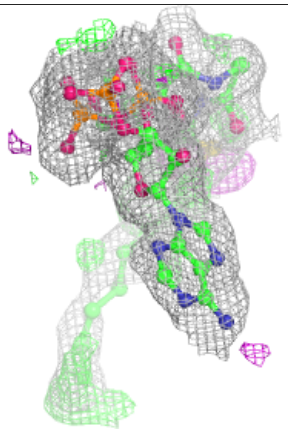


Electron density around CO8 B 401:

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

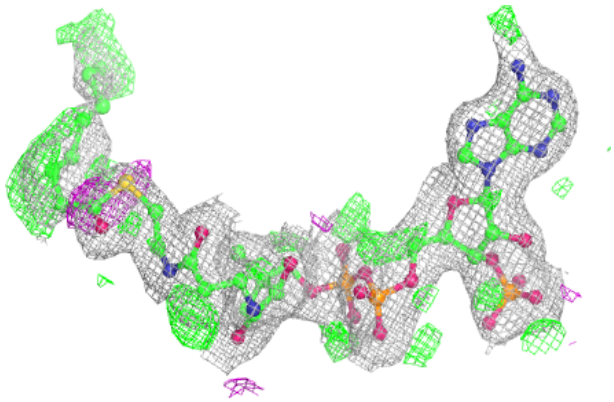


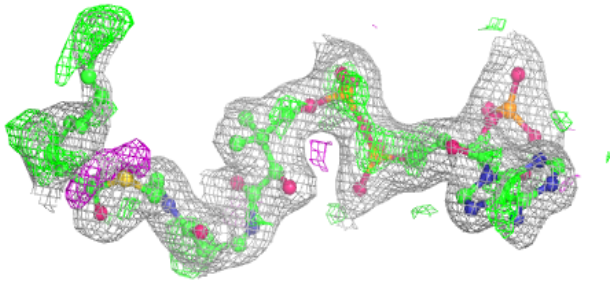


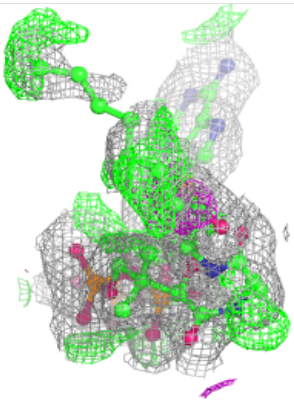


Electron density around CO8 G 401:

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

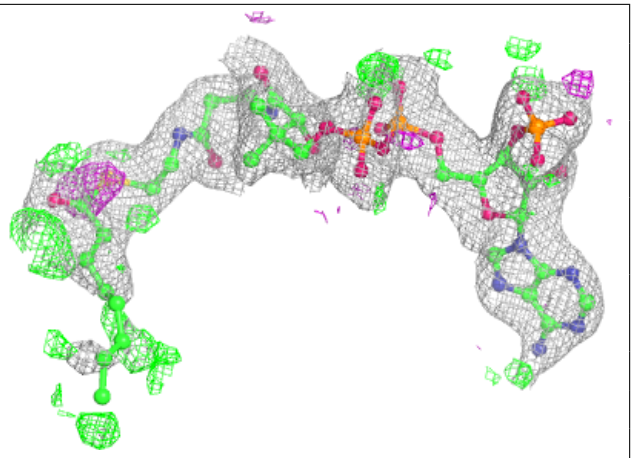


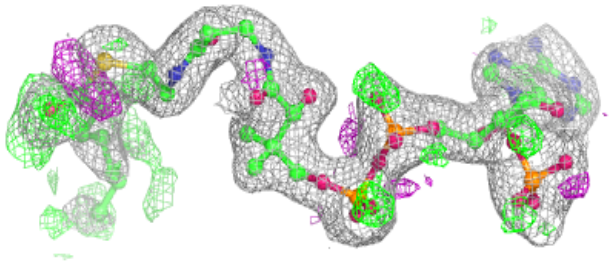


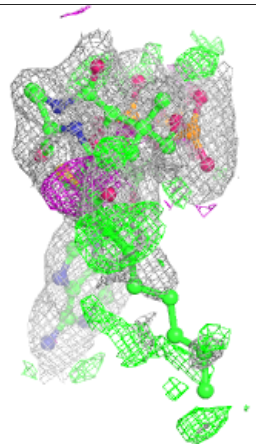


Electron density around CO8 C 401:

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

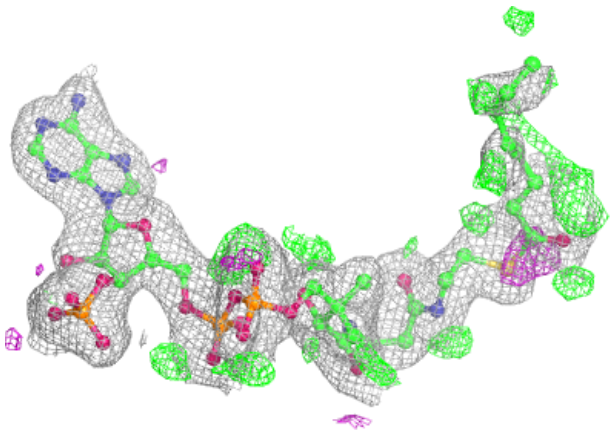


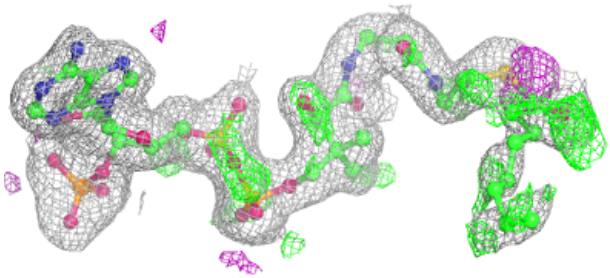


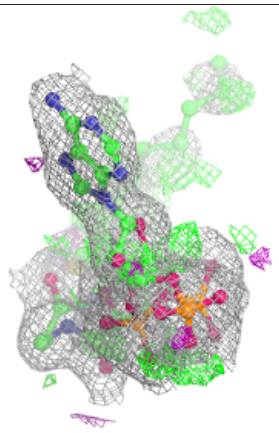


Electron density around CO8 A 401:

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

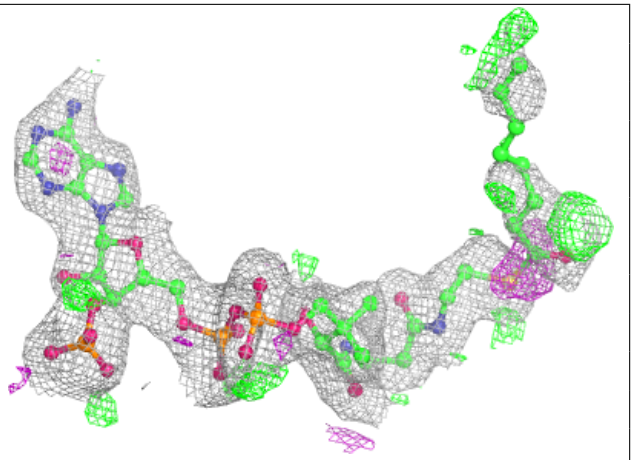


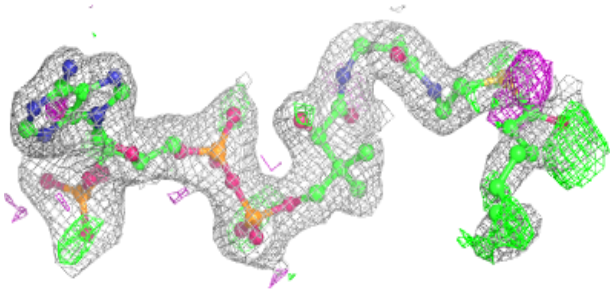


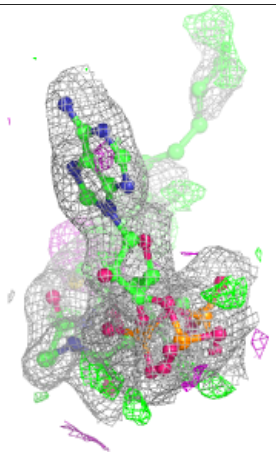


Electron density around CO8 K 401:

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

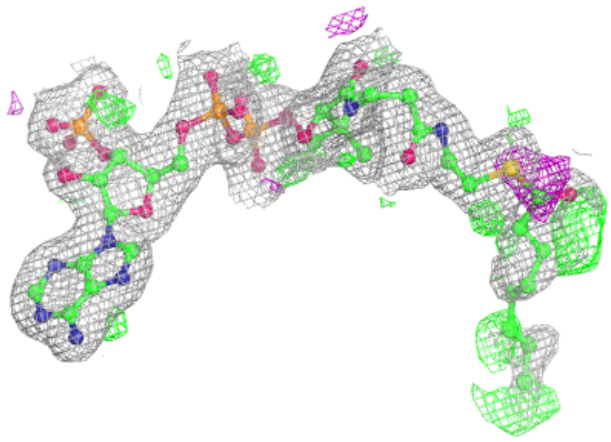


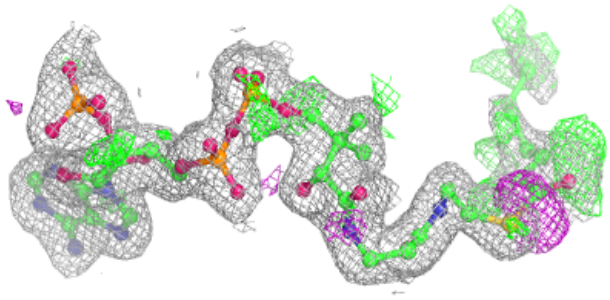


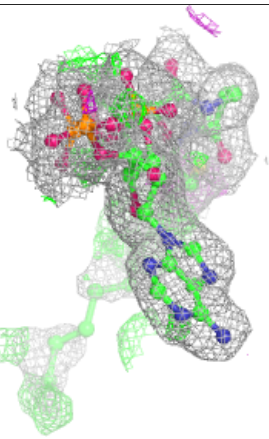


Electron density around CO8 L 401:

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

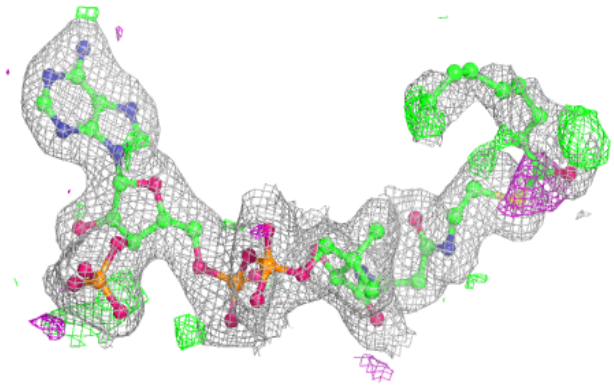


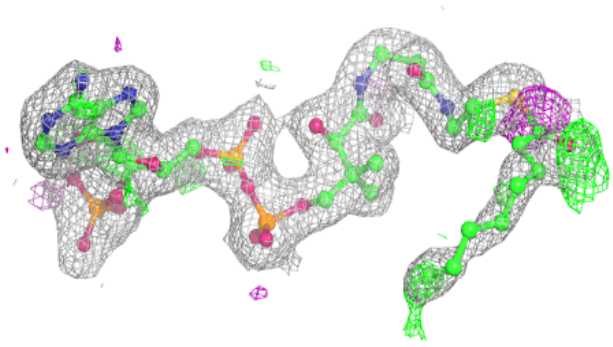


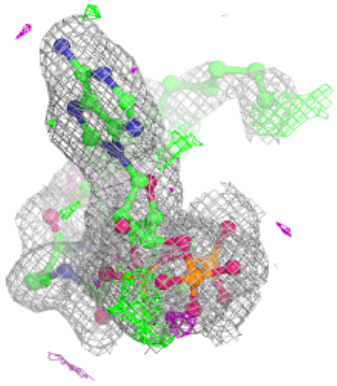


Electron density around CO8 I 401:

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

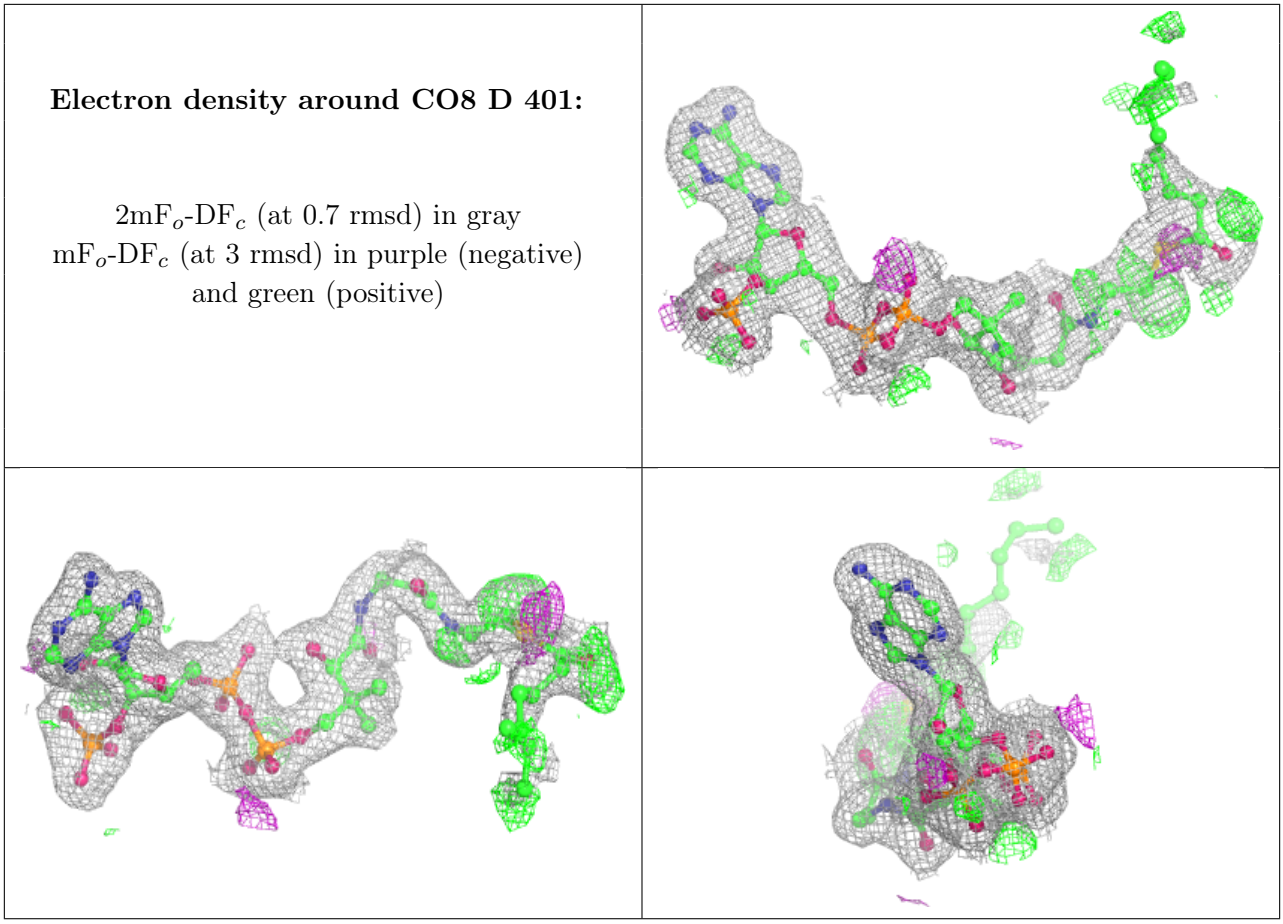






Electron density around CO8 D 401:

$2mF_o$-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.