wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 09:42 AM EDT

PDB ID	:	3RYO
Title	:	Crystal Structure of Enhanced Intracellular Survival (Eis) Protein from Mycobacterium tuberculosis with Acetyl CoA
Authors	:	Kim, K.H.; An, D.R.; Yoon, J.Y.; Kim, H.S.; Yoon, H.J.; Song, J.; Im, H.N.; Kim, J.; Kim, D.J.; Lee, S.J.; Kim, H.J.; Lee, J.Y.; Suh, S.W.
Deposited on	:	2011-05-11
Resolution	:	2.80 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:

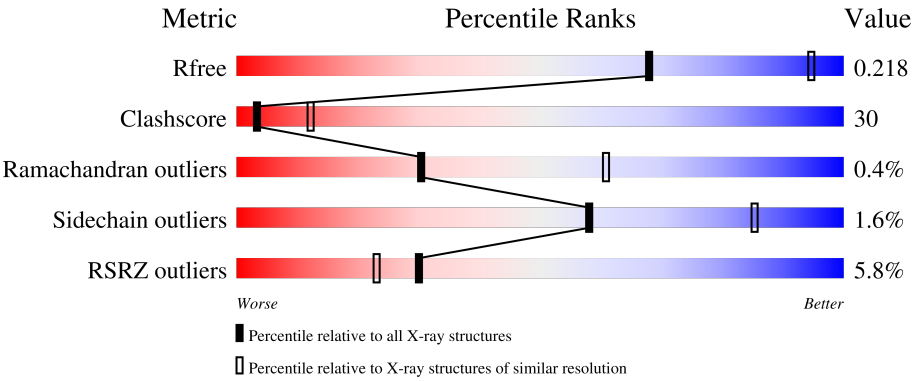
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	428	5% 60% 32% 7%
1	B	428	5% 61% 32% 7%
1	C	428	5% 60% 32% 7%
1	D	428	5% 57% 35% • 7%

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Mol	Chain	Length	Quality of chain
1	E	428	6% 57% 34% • 7%
1	F	428	6% 57% 35% • 7%
1	G	428	5% 57% 35% 7%
1	H	428	5% 56% 37% 7%
1	I	428	5% 52% 39% • 7%
1	J	428	9% 51% 40% • 7%
1	K	428	5% 62% 29% • 7%
1	L	428	3% 66% 24% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37731 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 Enhanced intracellular survival protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	B	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	C	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	D	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	E	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	F	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	G	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	H	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	I	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	J	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	K	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			
1	L	396	Total	C	N	O	S	Se	0	0	0
			3053	1921	560	560	5	7			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP P71727
A	-18	GLY	-	expression tag	UNP P71727
A	-17	SER	-	expression tag	UNP P71727
A	-16	SER	-	expression tag	UNP P71727
A	-15	HIS	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P71727
A	-13	HIS	-	expression tag	UNP P71727
A	-12	HIS	-	expression tag	UNP P71727
A	-11	HIS	-	expression tag	UNP P71727
A	-10	HIS	-	expression tag	UNP P71727
A	-9	SER	-	expression tag	UNP P71727
A	-8	SER	-	expression tag	UNP P71727
A	-7	GLY	-	expression tag	UNP P71727
A	-6	LEU	-	expression tag	UNP P71727
A	-5	VAL	-	expression tag	UNP P71727
A	-4	PRO	-	expression tag	UNP P71727
A	-3	ARG	-	expression tag	UNP P71727
A	-2	GLY	-	expression tag	UNP P71727
A	-1	SER	-	expression tag	UNP P71727
A	0	HIS	-	expression tag	UNP P71727
B	-19	MSE	-	expression tag	UNP P71727
B	-18	GLY	-	expression tag	UNP P71727
B	-17	SER	-	expression tag	UNP P71727
B	-16	SER	-	expression tag	UNP P71727
B	-15	HIS	-	expression tag	UNP P71727
B	-14	HIS	-	expression tag	UNP P71727
B	-13	HIS	-	expression tag	UNP P71727
B	-12	HIS	-	expression tag	UNP P71727
B	-11	HIS	-	expression tag	UNP P71727
B	-10	HIS	-	expression tag	UNP P71727
B	-9	SER	-	expression tag	UNP P71727
B	-8	SER	-	expression tag	UNP P71727
B	-7	GLY	-	expression tag	UNP P71727
B	-6	LEU	-	expression tag	UNP P71727
B	-5	VAL	-	expression tag	UNP P71727
B	-4	PRO	-	expression tag	UNP P71727
B	-3	ARG	-	expression tag	UNP P71727
B	-2	GLY	-	expression tag	UNP P71727
B	-1	SER	-	expression tag	UNP P71727
B	0	HIS	-	expression tag	UNP P71727
C	-19	MSE	-	expression tag	UNP P71727
C	-18	GLY	-	expression tag	UNP P71727
C	-17	SER	-	expression tag	UNP P71727
C	-16	SER	-	expression tag	UNP P71727
C	-15	HIS	-	expression tag	UNP P71727
C	-14	HIS	-	expression tag	UNP P71727
C	-13	HIS	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP P71727
C	-11	HIS	-	expression tag	UNP P71727
C	-10	HIS	-	expression tag	UNP P71727
C	-9	SER	-	expression tag	UNP P71727
C	-8	SER	-	expression tag	UNP P71727
C	-7	GLY	-	expression tag	UNP P71727
C	-6	LEU	-	expression tag	UNP P71727
C	-5	VAL	-	expression tag	UNP P71727
C	-4	PRO	-	expression tag	UNP P71727
C	-3	ARG	-	expression tag	UNP P71727
C	-2	GLY	-	expression tag	UNP P71727
C	-1	SER	-	expression tag	UNP P71727
C	0	HIS	-	expression tag	UNP P71727
D	-19	MSE	-	expression tag	UNP P71727
D	-18	GLY	-	expression tag	UNP P71727
D	-17	SER	-	expression tag	UNP P71727
D	-16	SER	-	expression tag	UNP P71727
D	-15	HIS	-	expression tag	UNP P71727
D	-14	HIS	-	expression tag	UNP P71727
D	-13	HIS	-	expression tag	UNP P71727
D	-12	HIS	-	expression tag	UNP P71727
D	-11	HIS	-	expression tag	UNP P71727
D	-10	HIS	-	expression tag	UNP P71727
D	-9	SER	-	expression tag	UNP P71727
D	-8	SER	-	expression tag	UNP P71727
D	-7	GLY	-	expression tag	UNP P71727
D	-6	LEU	-	expression tag	UNP P71727
D	-5	VAL	-	expression tag	UNP P71727
D	-4	PRO	-	expression tag	UNP P71727
D	-3	ARG	-	expression tag	UNP P71727
D	-2	GLY	-	expression tag	UNP P71727
D	-1	SER	-	expression tag	UNP P71727
D	0	HIS	-	expression tag	UNP P71727
E	-19	MSE	-	expression tag	UNP P71727
E	-18	GLY	-	expression tag	UNP P71727
E	-17	SER	-	expression tag	UNP P71727
E	-16	SER	-	expression tag	UNP P71727
E	-15	HIS	-	expression tag	UNP P71727
E	-14	HIS	-	expression tag	UNP P71727
E	-13	HIS	-	expression tag	UNP P71727
E	-12	HIS	-	expression tag	UNP P71727
E	-11	HIS	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP P71727
E	-9	SER	-	expression tag	UNP P71727
E	-8	SER	-	expression tag	UNP P71727
E	-7	GLY	-	expression tag	UNP P71727
E	-6	LEU	-	expression tag	UNP P71727
E	-5	VAL	-	expression tag	UNP P71727
E	-4	PRO	-	expression tag	UNP P71727
E	-3	ARG	-	expression tag	UNP P71727
E	-2	GLY	-	expression tag	UNP P71727
E	-1	SER	-	expression tag	UNP P71727
E	0	HIS	-	expression tag	UNP P71727
F	-19	MSE	-	expression tag	UNP P71727
F	-18	GLY	-	expression tag	UNP P71727
F	-17	SER	-	expression tag	UNP P71727
F	-16	SER	-	expression tag	UNP P71727
F	-15	HIS	-	expression tag	UNP P71727
F	-14	HIS	-	expression tag	UNP P71727
F	-13	HIS	-	expression tag	UNP P71727
F	-12	HIS	-	expression tag	UNP P71727
F	-11	HIS	-	expression tag	UNP P71727
F	-10	HIS	-	expression tag	UNP P71727
F	-9	SER	-	expression tag	UNP P71727
F	-8	SER	-	expression tag	UNP P71727
F	-7	GLY	-	expression tag	UNP P71727
F	-6	LEU	-	expression tag	UNP P71727
F	-5	VAL	-	expression tag	UNP P71727
F	-4	PRO	-	expression tag	UNP P71727
F	-3	ARG	-	expression tag	UNP P71727
F	-2	GLY	-	expression tag	UNP P71727
F	-1	SER	-	expression tag	UNP P71727
F	0	HIS	-	expression tag	UNP P71727
G	-19	MSE	-	expression tag	UNP P71727
G	-18	GLY	-	expression tag	UNP P71727
G	-17	SER	-	expression tag	UNP P71727
G	-16	SER	-	expression tag	UNP P71727
G	-15	HIS	-	expression tag	UNP P71727
G	-14	HIS	-	expression tag	UNP P71727
G	-13	HIS	-	expression tag	UNP P71727
G	-12	HIS	-	expression tag	UNP P71727
G	-11	HIS	-	expression tag	UNP P71727
G	-10	HIS	-	expression tag	UNP P71727
G	-9	SER	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP P71727
G	-7	GLY	-	expression tag	UNP P71727
G	-6	LEU	-	expression tag	UNP P71727
G	-5	VAL	-	expression tag	UNP P71727
G	-4	PRO	-	expression tag	UNP P71727
G	-3	ARG	-	expression tag	UNP P71727
G	-2	GLY	-	expression tag	UNP P71727
G	-1	SER	-	expression tag	UNP P71727
G	0	HIS	-	expression tag	UNP P71727
H	-19	MSE	-	expression tag	UNP P71727
H	-18	GLY	-	expression tag	UNP P71727
H	-17	SER	-	expression tag	UNP P71727
H	-16	SER	-	expression tag	UNP P71727
H	-15	HIS	-	expression tag	UNP P71727
H	-14	HIS	-	expression tag	UNP P71727
H	-13	HIS	-	expression tag	UNP P71727
H	-12	HIS	-	expression tag	UNP P71727
H	-11	HIS	-	expression tag	UNP P71727
H	-10	HIS	-	expression tag	UNP P71727
H	-9	SER	-	expression tag	UNP P71727
H	-8	SER	-	expression tag	UNP P71727
H	-7	GLY	-	expression tag	UNP P71727
H	-6	LEU	-	expression tag	UNP P71727
H	-5	VAL	-	expression tag	UNP P71727
H	-4	PRO	-	expression tag	UNP P71727
H	-3	ARG	-	expression tag	UNP P71727
H	-2	GLY	-	expression tag	UNP P71727
H	-1	SER	-	expression tag	UNP P71727
H	0	HIS	-	expression tag	UNP P71727
I	-19	MSE	-	expression tag	UNP P71727
I	-18	GLY	-	expression tag	UNP P71727
I	-17	SER	-	expression tag	UNP P71727
I	-16	SER	-	expression tag	UNP P71727
I	-15	HIS	-	expression tag	UNP P71727
I	-14	HIS	-	expression tag	UNP P71727
I	-13	HIS	-	expression tag	UNP P71727
I	-12	HIS	-	expression tag	UNP P71727
I	-11	HIS	-	expression tag	UNP P71727
I	-10	HIS	-	expression tag	UNP P71727
I	-9	SER	-	expression tag	UNP P71727
I	-8	SER	-	expression tag	UNP P71727
I	-7	GLY	-	expression tag	UNP P71727

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP P71727
I	-5	VAL	-	expression tag	UNP P71727
I	-4	PRO	-	expression tag	UNP P71727
I	-3	ARG	-	expression tag	UNP P71727
I	-2	GLY	-	expression tag	UNP P71727
I	-1	SER	-	expression tag	UNP P71727
I	0	HIS	-	expression tag	UNP P71727
J	-19	MSE	-	expression tag	UNP P71727
J	-18	GLY	-	expression tag	UNP P71727
J	-17	SER	-	expression tag	UNP P71727
J	-16	SER	-	expression tag	UNP P71727
J	-15	HIS	-	expression tag	UNP P71727
J	-14	HIS	-	expression tag	UNP P71727
J	-13	HIS	-	expression tag	UNP P71727
J	-12	HIS	-	expression tag	UNP P71727
J	-11	HIS	-	expression tag	UNP P71727
J	-10	HIS	-	expression tag	UNP P71727
J	-9	SER	-	expression tag	UNP P71727
J	-8	SER	-	expression tag	UNP P71727
J	-7	GLY	-	expression tag	UNP P71727
J	-6	LEU	-	expression tag	UNP P71727
J	-5	VAL	-	expression tag	UNP P71727
J	-4	PRO	-	expression tag	UNP P71727
J	-3	ARG	-	expression tag	UNP P71727
J	-2	GLY	-	expression tag	UNP P71727
J	-1	SER	-	expression tag	UNP P71727
J	0	HIS	-	expression tag	UNP P71727
K	-19	MSE	-	expression tag	UNP P71727
K	-18	GLY	-	expression tag	UNP P71727
K	-17	SER	-	expression tag	UNP P71727
K	-16	SER	-	expression tag	UNP P71727
K	-15	HIS	-	expression tag	UNP P71727
K	-14	HIS	-	expression tag	UNP P71727
K	-13	HIS	-	expression tag	UNP P71727
K	-12	HIS	-	expression tag	UNP P71727
K	-11	HIS	-	expression tag	UNP P71727
K	-10	HIS	-	expression tag	UNP P71727
K	-9	SER	-	expression tag	UNP P71727
K	-8	SER	-	expression tag	UNP P71727
K	-7	GLY	-	expression tag	UNP P71727
K	-6	LEU	-	expression tag	UNP P71727
K	-5	VAL	-	expression tag	UNP P71727

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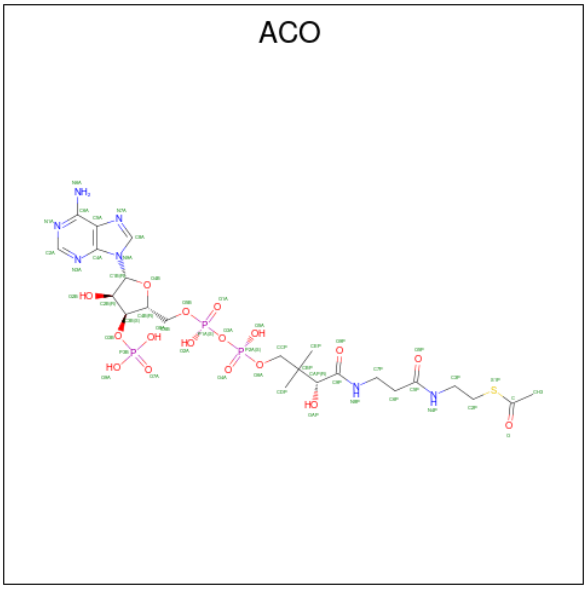
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P71727
K	-3	ARG	-	expression tag	UNP P71727
K	-2	GLY	-	expression tag	UNP P71727
K	-1	SER	-	expression tag	UNP P71727
K	0	HIS	-	expression tag	UNP P71727
L	-19	MSE	-	expression tag	UNP P71727
L	-18	GLY	-	expression tag	UNP P71727
L	-17	SER	-	expression tag	UNP P71727
L	-16	SER	-	expression tag	UNP P71727
L	-15	HIS	-	expression tag	UNP P71727
L	-14	HIS	-	expression tag	UNP P71727
L	-13	HIS	-	expression tag	UNP P71727
L	-12	HIS	-	expression tag	UNP P71727
L	-11	HIS	-	expression tag	UNP P71727
L	-10	HIS	-	expression tag	UNP P71727
L	-9	SER	-	expression tag	UNP P71727
L	-8	SER	-	expression tag	UNP P71727
L	-7	GLY	-	expression tag	UNP P71727
L	-6	LEU	-	expression tag	UNP P71727
L	-5	VAL	-	expression tag	UNP P71727
L	-4	PRO	-	expression tag	UNP P71727
L	-3	ARG	-	expression tag	UNP P71727
L	-2	GLY	-	expression tag	UNP P71727
L	-1	SER	-	expression tag	UNP P71727
L	0	HIS	-	expression tag	UNP P71727

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	74	Total	O	0	0
			74	74		
3	C	54	Total	O	0	0
			54	54		
3	D	51	Total	O	0	0
			51	51		
3	E	47	Total	O	0	0
			47	47		
3	F	48	Total	O	0	0
			48	48		
3	G	31	Total	O	0	0
			31	31		
3	H	39	Total	O	0	0
			39	39		

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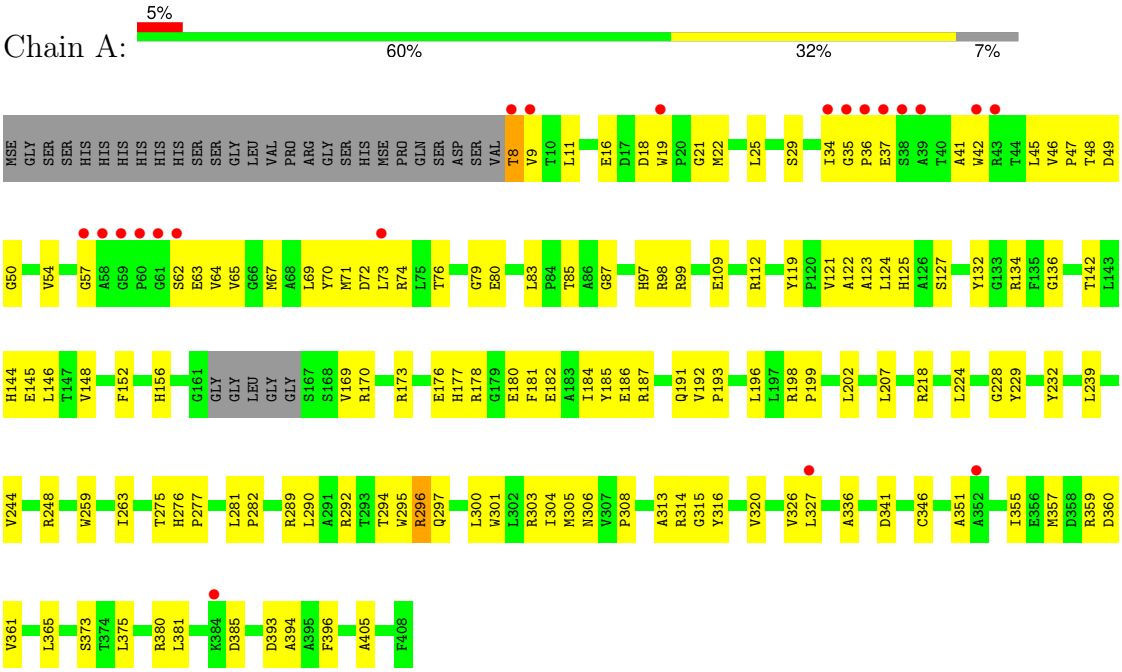
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	17	Total O 17 17	0	0
3	J	9	Total O 9 9	0	0
3	K	29	Total O 29 29	0	0
3	L	38	Total O 38 38	0	0

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: Enhanced intracellular survival protein

Chain A:



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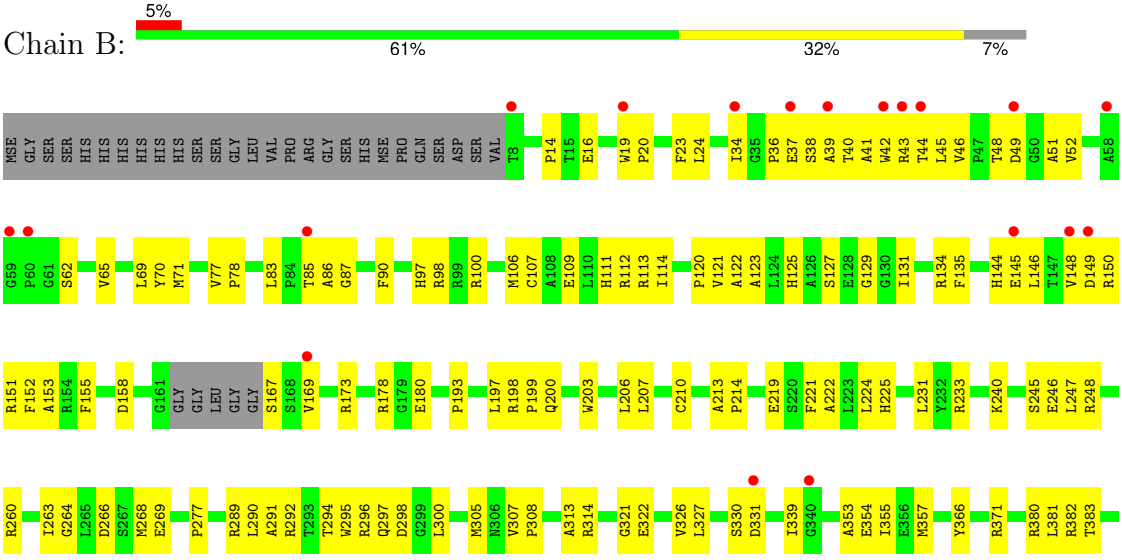
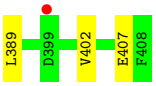
Chain B:





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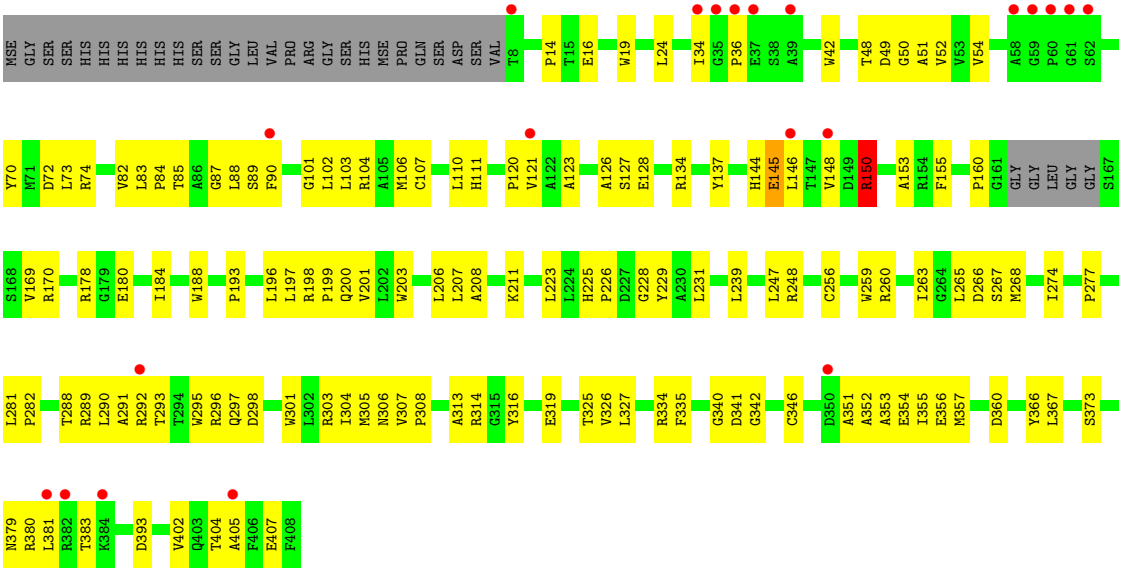
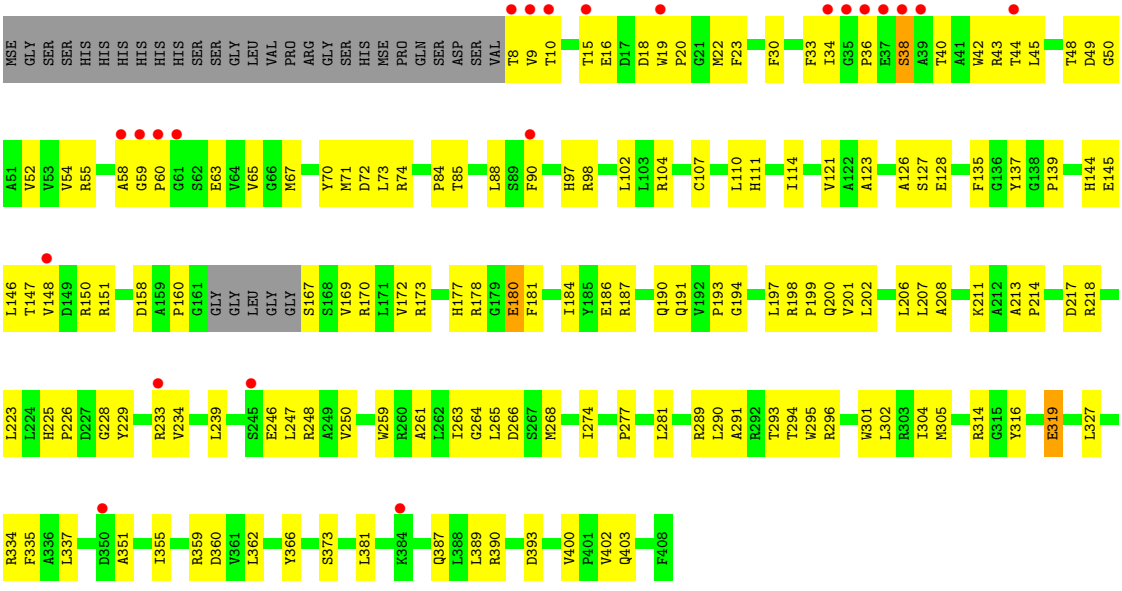
Chain C:



• Molecule 1: Enhanced intracellular survival protein

Chain D:



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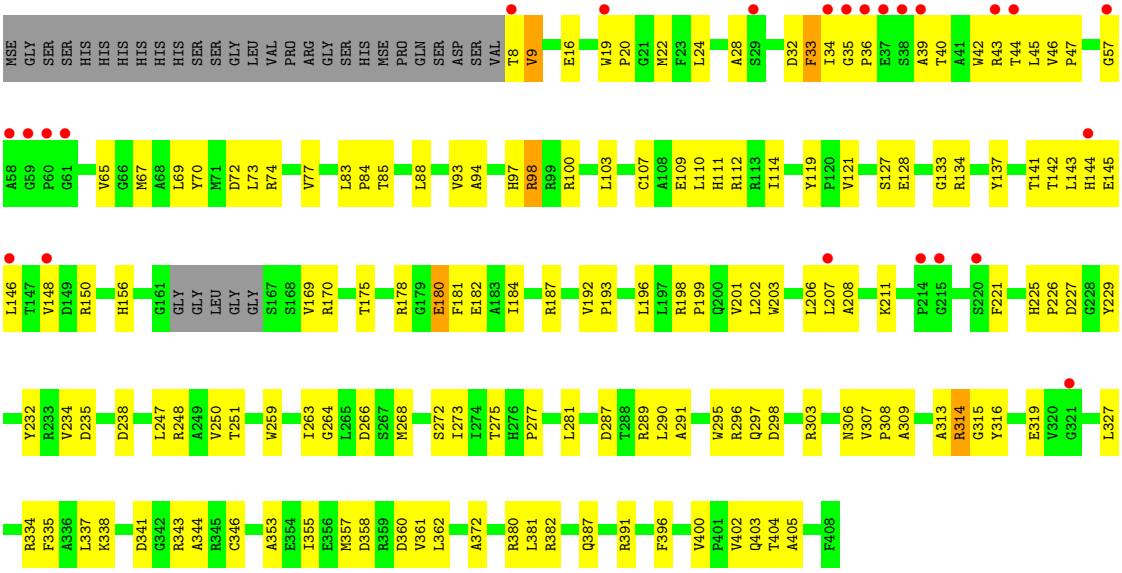
Chain E:



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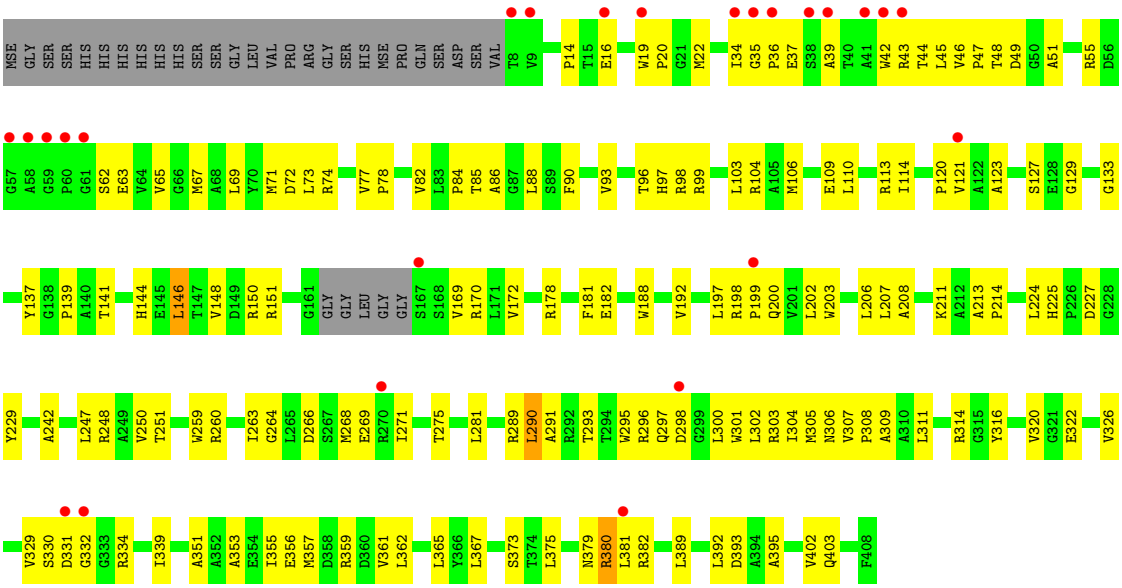
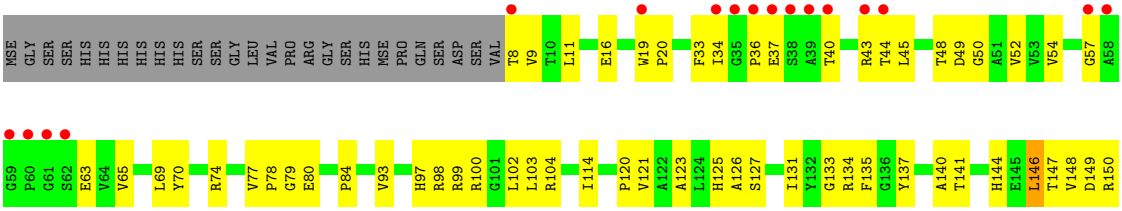
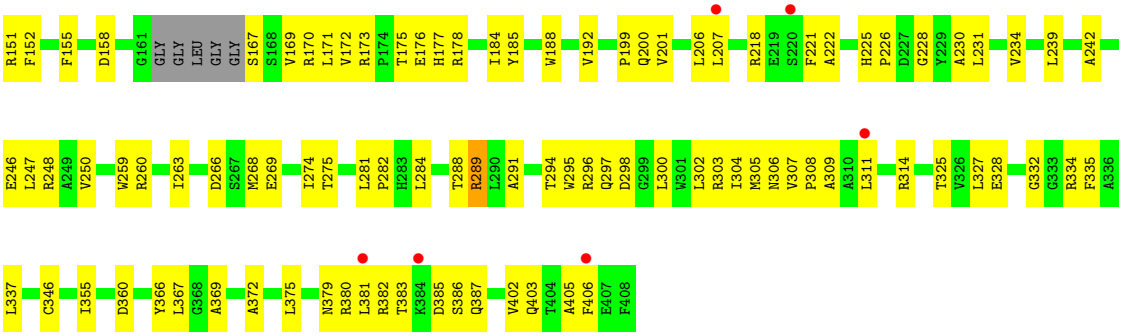
Chain F:



• Molecule 1: Enhanced intracellular survival protein

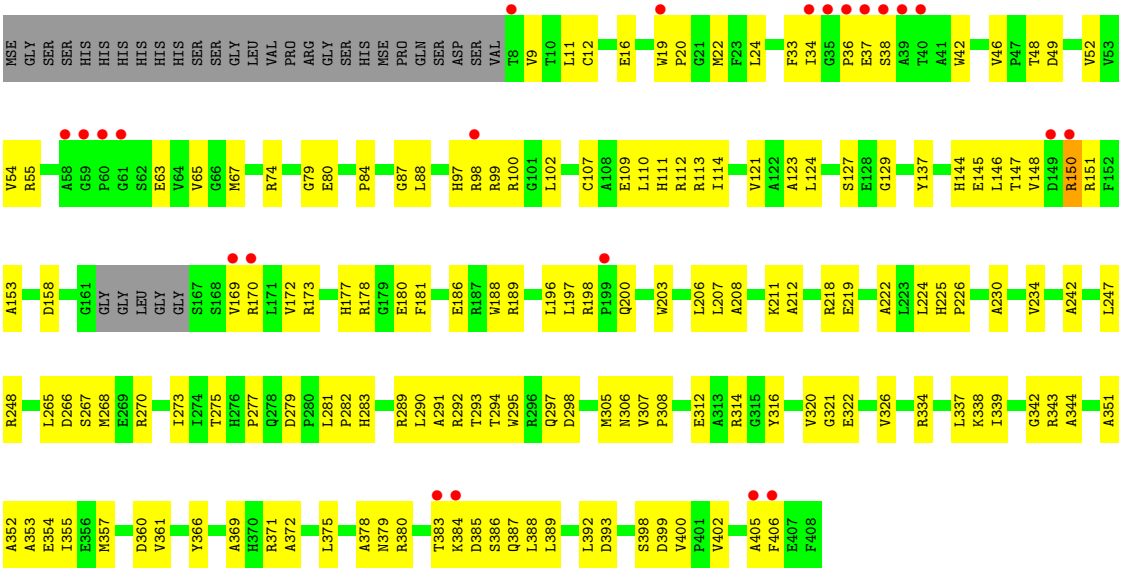
Chain G:





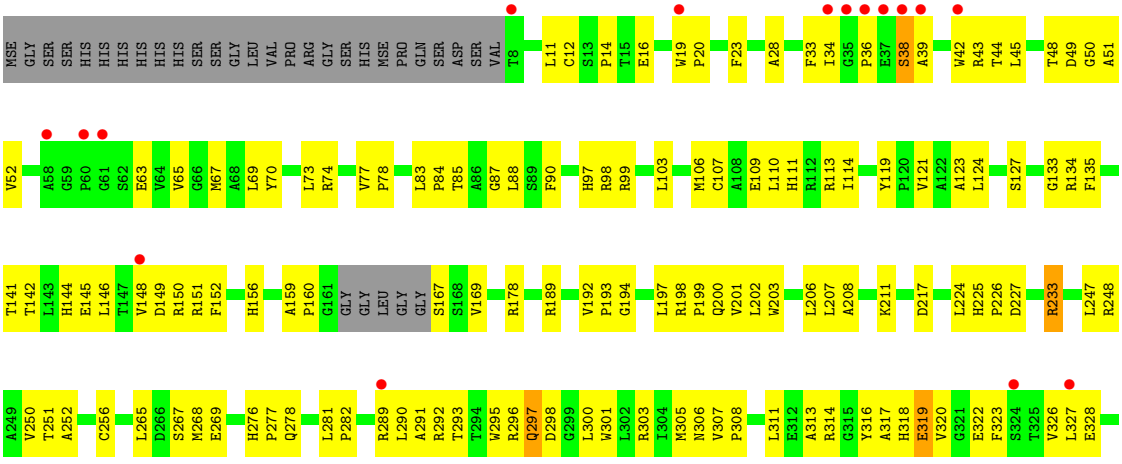
• Molecule 1: Enhanced intracellular survival protein

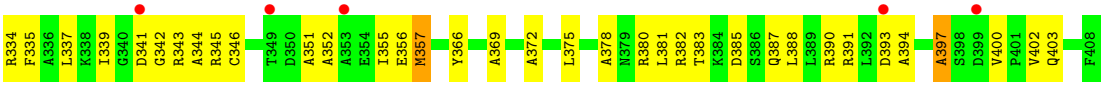
Chain H:



• Molecule 1: Enhanced intracellular survival protein

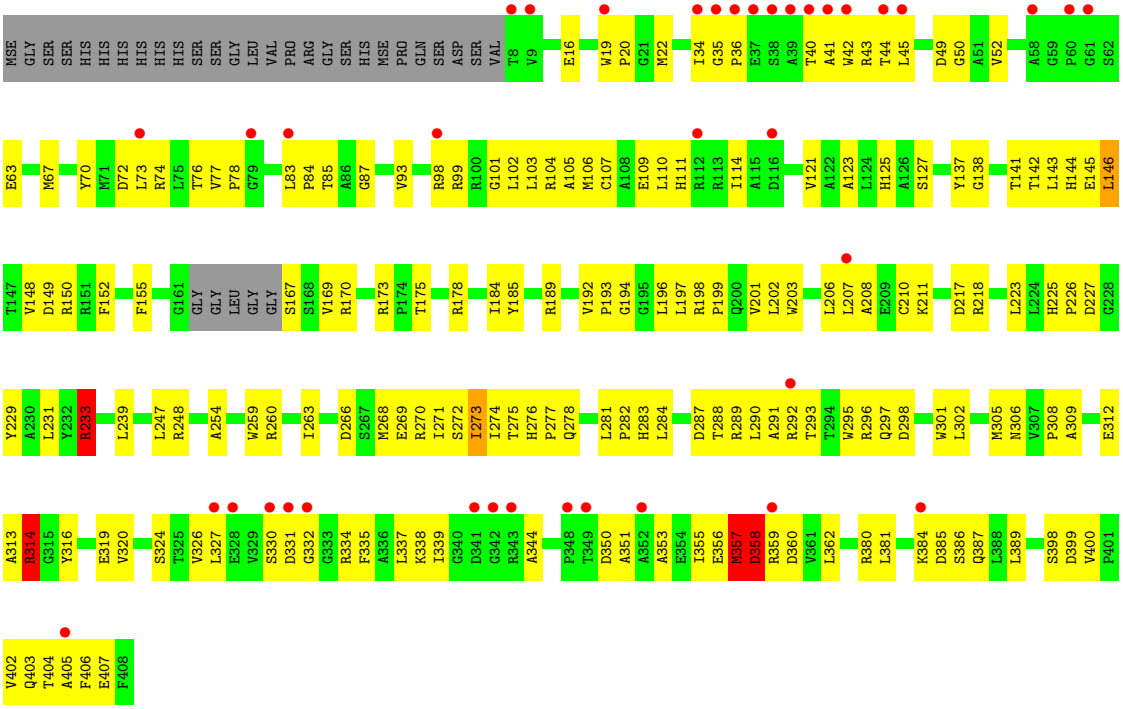
Chain I:





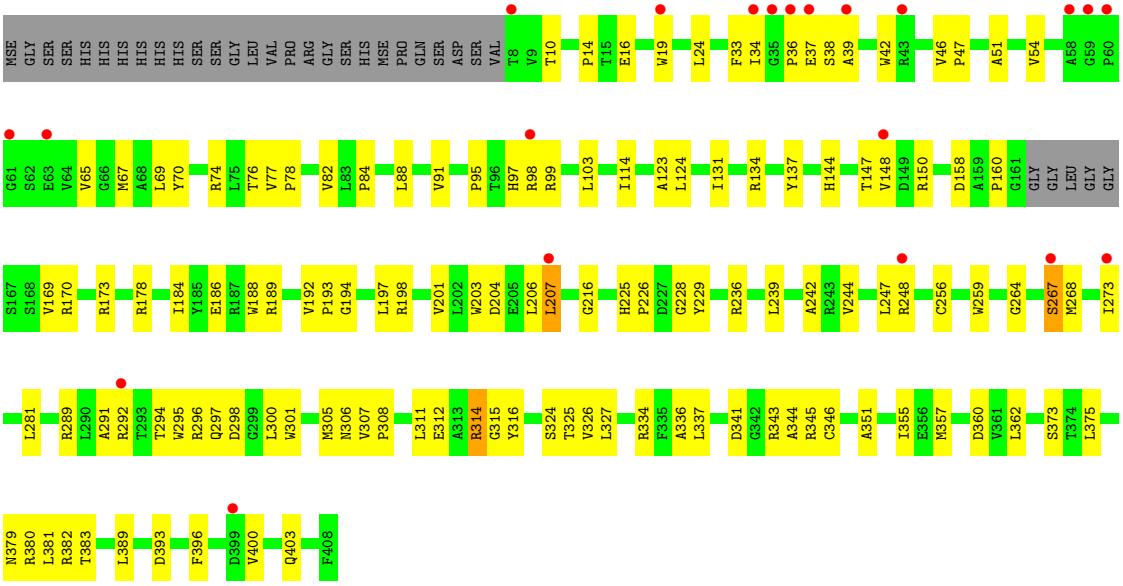
• Molecule 1: Enhanced intracellular survival protein

Chain J:



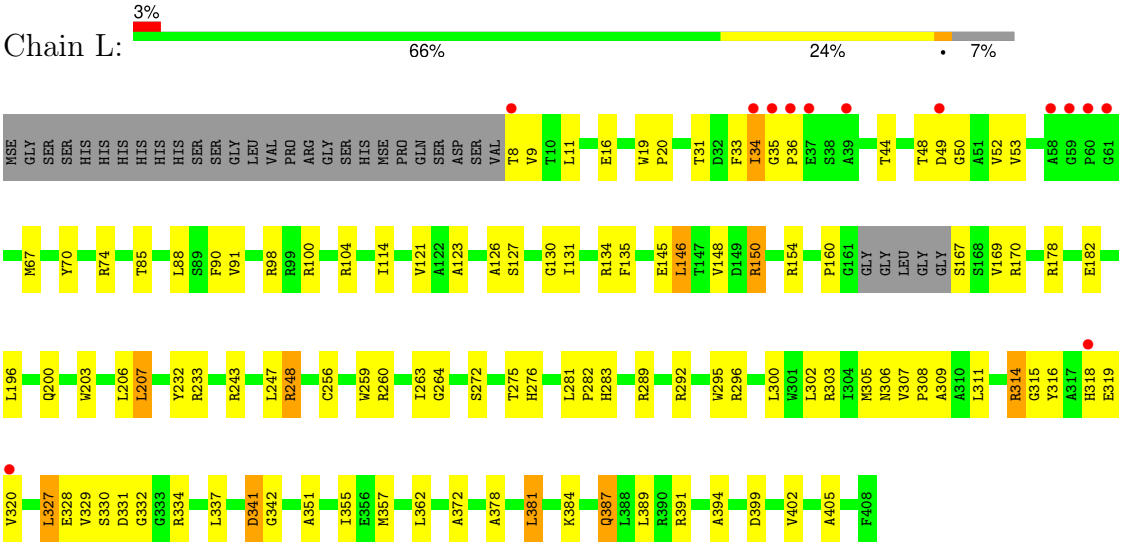
• Molecule 1: Enhanced intracellular survival protein

Chain K:



• Molecule 1: Enhanced intracellular survival protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.13Å 150.19Å 184.38Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	29.94 – 2.80 29.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.4 (29.94-2.80) 95.3 (29.94-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.87 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.192 , 0.248 0.219 , 0.218	Depositor DCC
R_{free} test set	13782 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	37731	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: ACO

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	0.44	0/3115	0.63	0/4226
1	B	0.41	0/3115	0.62	0/4226
1	C	0.41	0/3115	0.61	0/4226
1	D	0.41	0/3115	0.63	1/4226 (0.0%)
1	E	0.41	0/3115	0.62	0/4226
1	F	0.43	0/3115	0.62	1/4226 (0.0%)
1	G	0.39	0/3115	0.59	0/4226
1	H	0.39	0/3115	0.57	0/4226
1	I	0.35	0/3115	0.58	0/4226
1	J	0.37	0/3115	0.59	0/4226
1	K	0.37	0/3115	0.57	0/4226
1	L	0.41	0/3115	0.62	1/4226 (0.0%)
All	All	0.40	0/37380	0.60	3/50712 (0.0%)

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
1	C	0	1
1	F	0	1
1	J	0	2
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	88	LEU	CA-CB-CG	5.76	128.56	115.30
1	L	35	GLY	N-CA-C	5.63	127.18	113.10
1	D	337	LEU	CA-CB-CG	5.35	127.61	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ARG	Sidechain
1	C	150	ARG	Sidechain
1	F	380	ARG	Sidechain
1	J	233	ARG	Sidechain
1	J	314	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	3053	0	3020	157	0
1	B	3053	0	3020	173	0
1	C	3053	0	3020	199	0
1	D	3053	0	3020	214	0
1	E	3053	0	3020	204	2
1	F	3053	0	3020	235	0
1	G	3053	0	3020	182	0
1	H	3053	0	3020	239	0
1	I	3053	0	3020	250	0
1	J	3053	0	3020	219	1
1	K	3053	0	3020	164	1
1	L	3053	0	3018	84	2
2	A	51	0	34	6	0
2	B	51	0	33	4	0
2	C	51	0	34	12	0
2	D	51	0	33	2	0
2	E	51	0	34	8	0
2	F	51	0	33	5	0
2	G	51	0	33	6	0
2	H	51	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	51	0	34	7	0
2	J	51	0	34	3	0
2	K	51	0	34	10	0
2	L	51	0	33	5	0
3	A	46	0	0	2	0
3	B	74	0	0	6	0
3	C	54	0	0	6	0
3	D	51	0	0	5	0
3	E	47	0	0	2	0
3	F	48	0	0	2	0
3	G	31	0	0	3	0
3	H	39	0	0	4	0
3	I	17	0	0	1	0
3	J	9	0	0	6	0
3	K	29	0	0	4	0
3	L	38	0	0	3	0
All	All	37731	0	36640	2186	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 2186 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:22:MSE:HE2	1:F:42:TRP:CH2	1.32	1.64
1:C:357:MSE:HE2	1:C:381:LEU:CD1	1.21	1.57
1:F:357:MSE:HE2	1:F:381:LEU:CD1	1.27	1.57
1:D:148:VAL:CG2	1:D:291:ALA:HA	1.31	1.55
1:H:354:GLU:HA	1:H:384:LYS:NZ	1.18	1.51

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:VAL:CG1	1:L:8:THR:OG1[2_545]	1.66	0.54
1:J:49:ASP:OD1	1:K:345:ARG:NH1[2_645]	1.83	0.37
1:E:9:VAL:O	1:L:8:THR:OG1[2_545]	2.14	0.06

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	392/428 (92%)	375 (96%)	15 (4%)	2 (0%)	25	56
1	B	392/428 (92%)	373 (95%)	18 (5%)	1 (0%)	37	67
1	C	392/428 (92%)	374 (95%)	18 (5%)	0	100	100
1	D	392/428 (92%)	376 (96%)	15 (4%)	1 (0%)	37	67
1	E	392/428 (92%)	376 (96%)	16 (4%)	0	100	100
1	F	392/428 (92%)	369 (94%)	22 (6%)	1 (0%)	37	67
1	G	392/428 (92%)	379 (97%)	12 (3%)	1 (0%)	37	67
1	H	392/428 (92%)	377 (96%)	15 (4%)	0	100	100
1	I	392/428 (92%)	365 (93%)	23 (6%)	4 (1%)	13	39
1	J	392/428 (92%)	357 (91%)	31 (8%)	4 (1%)	13	39
1	K	392/428 (92%)	367 (94%)	23 (6%)	2 (0%)	25	56
1	L	392/428 (92%)	370 (94%)	21 (5%)	1 (0%)	37	67
All	All	4704/5136 (92%)	4458 (95%)	229 (5%)	17 (0%)	30	61

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	I	319	GLU
1	I	357	MSE
1	I	397	ALA
1	J	175	THR

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	311/327 (95%)	309 (99%)	2 (1%)	84 95
1	B	311/327 (95%)	310 (100%)	1 (0%)	91 97
1	C	311/327 (95%)	309 (99%)	2 (1%)	84 95
1	D	311/327 (95%)	309 (99%)	2 (1%)	84 95
1	E	311/327 (95%)	306 (98%)	5 (2%)	58 85
1	F	311/327 (95%)	308 (99%)	3 (1%)	73 91
1	G	311/327 (95%)	309 (99%)	2 (1%)	84 95
1	H	311/327 (95%)	310 (100%)	1 (0%)	91 97
1	I	311/327 (95%)	308 (99%)	3 (1%)	73 91
1	J	311/327 (95%)	304 (98%)	7 (2%)	45 78
1	K	311/327 (95%)	307 (99%)	4 (1%)	65 88
1	L	311/327 (95%)	285 (92%)	26 (8%)	9 28
All	All	3732/3924 (95%)	3674 (98%)	58 (2%)	58 85

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	150	ARG
1	L	387	GLN
1	L	52	VAL
1	L	384	LYS
1	L	314	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	318	HIS
1	K	125	HIS
1	L	318	HIS
1	F	200	GLN
1	F	125	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	ACO	C	501	-	47,53,53	1.66	9 (19%)	60,79,79	1.78	14 (23%)
2	ACO	E	501	-	47,53,53	1.69	7 (14%)	60,79,79	2.02	15 (25%)
2	ACO	L	501	-	47,53,53	1.76	8 (17%)	60,79,79	1.96	14 (23%)
2	ACO	D	501	-	47,53,53	1.65	7 (14%)	60,79,79	2.25	13 (21%)
2	ACO	J	501	-	47,53,53	1.62	7 (14%)	60,79,79	2.04	14 (23%)
2	ACO	H	501	-	47,53,53	1.67	7 (14%)	60,79,79	1.95	14 (23%)
2	ACO	K	501	-	47,53,53	1.67	7 (14%)	60,79,79	2.14	15 (25%)
2	ACO	G	501	-	47,53,53	1.72	7 (14%)	60,79,79	1.82	11 (18%)
2	ACO	A	501	-	47,53,53	1.71	7 (14%)	60,79,79	2.12	15 (25%)
2	ACO	B	501	-	47,53,53	1.76	8 (17%)	60,79,79	2.06	15 (25%)
2	ACO	I	501	-	47,53,53	1.70	8 (17%)	60,79,79	1.80	9 (15%)
2	ACO	F	501	-	47,53,53	1.77	9 (19%)	60,79,79	1.95	12 (20%)

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	ACO	C	501	-	-	15/47/67/67	0/3/3/3
2	ACO	E	501	-	-	14/47/67/67	0/3/3/3
2	ACO	L	501	-	-	9/47/67/67	0/3/3/3
2	ACO	D	501	-	-	15/47/67/67	0/3/3/3
2	ACO	J	501	-	-	18/47/67/67	0/3/3/3
2	ACO	H	501	-	-	15/47/67/67	0/3/3/3
2	ACO	K	501	-	-	16/47/67/67	0/3/3/3
2	ACO	G	501	-	-	10/47/67/67	0/3/3/3
2	ACO	A	501	-	-	11/47/67/67	0/3/3/3
2	ACO	B	501	-	-	14/47/67/67	0/3/3/3
2	ACO	I	501	-	-	14/47/67/67	0/3/3/3
2	ACO	F	501	-	-	16/47/67/67	0/3/3/3

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	ACO	C9P-N8P	5.36	1.46	1.33
2	A	501	ACO	C5P-N4P	5.27	1.45	1.33
2	L	501	ACO	C5P-N4P	5.27	1.45	1.33
2	I	501	ACO	C9P-N8P	5.13	1.45	1.33
2	F	501	ACO	C5P-N4P	5.11	1.45	1.33

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	ACO	O4B-C1B-N9A	8.14	119.54	108.75
2	D	501	ACO	O6A-CCP-CBP	7.73	122.97	110.55
2	D	501	ACO	O4B-C1B-N9A	7.59	118.81	108.75
2	K	501	ACO	O6A-CCP-CBP	7.39	122.42	110.55
2	L	501	ACO	O6A-CCP-CBP	7.18	122.09	110.55

There are no chirality outliers.

5 of 167 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ACO	O4B-C4B-C5B-O5B
2	A	501	ACO	C5B-O5B-P1A-O2A
2	A	501	ACO	C5B-O5B-P1A-O3A
2	A	501	ACO	CDP-CBP-CCP-O6A
2	A	501	ACO	CEP-CBP-CCP-O6A

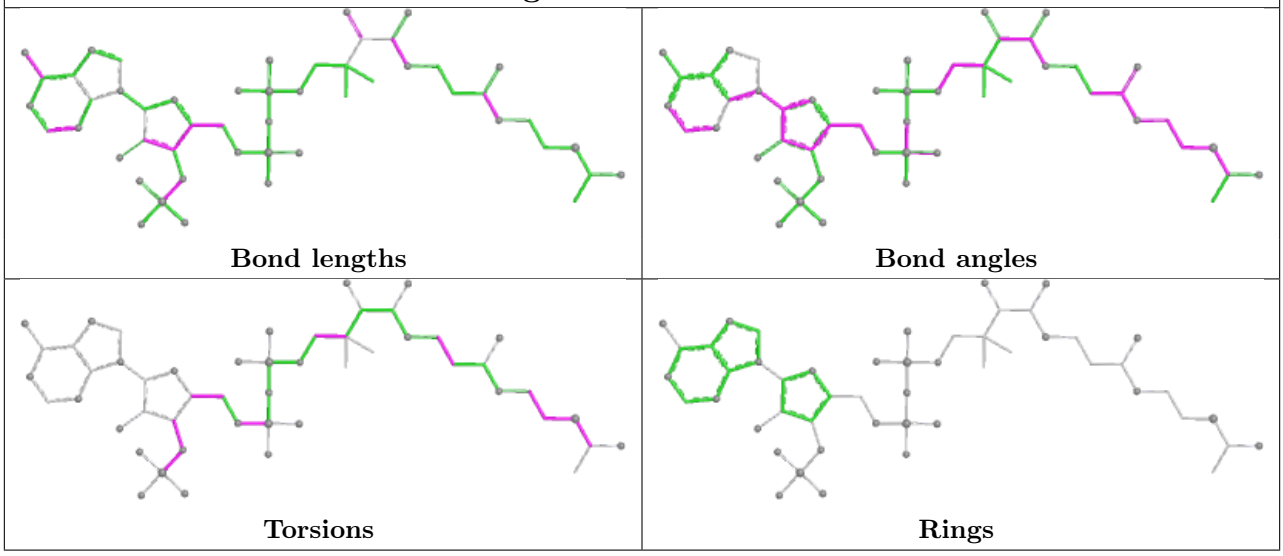
There are no ring outliers.

12 monomers are involved in 70 short contacts:

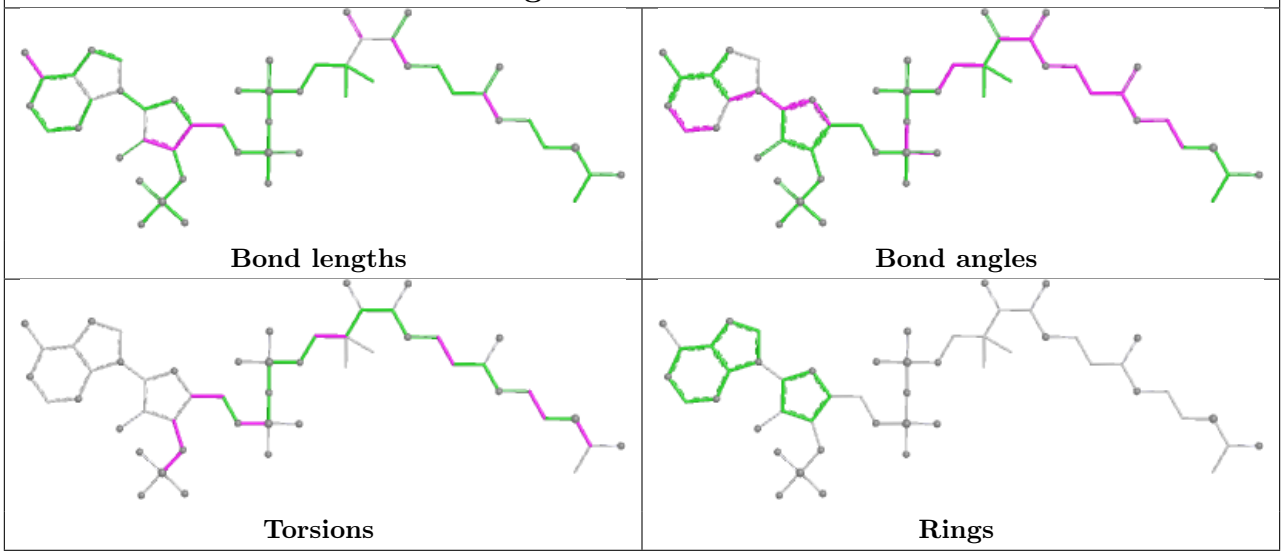
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	ACO	12	0
2	E	501	ACO	8	0
2	L	501	ACO	5	0
2	D	501	ACO	2	0
2	J	501	ACO	3	0
2	H	501	ACO	2	0
2	K	501	ACO	10	0
2	G	501	ACO	6	0
2	A	501	ACO	6	0
2	B	501	ACO	4	0
2	I	501	ACO	7	0
2	F	501	ACO	5	0

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.

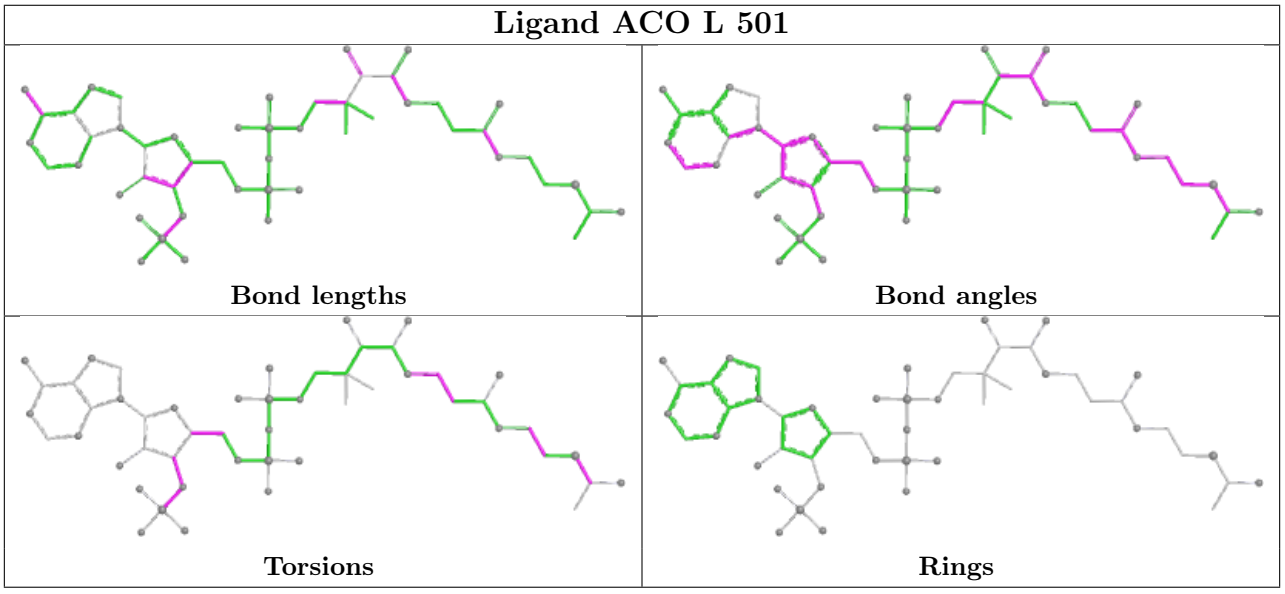
Ligand ACO C 501



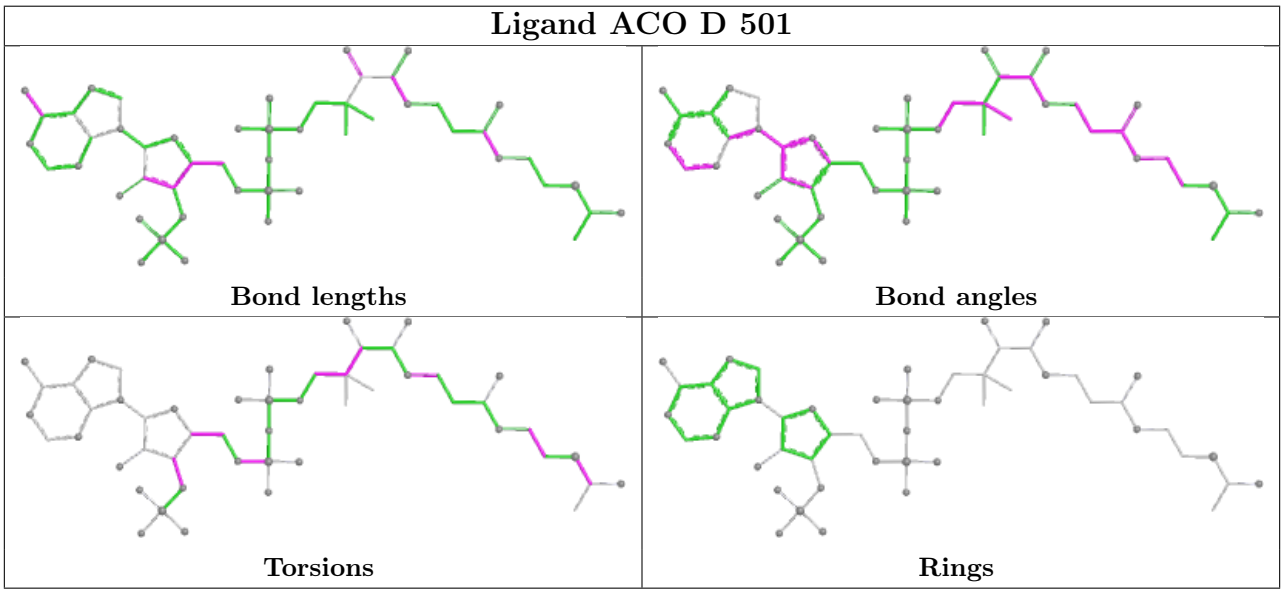
Ligand ACO E 501



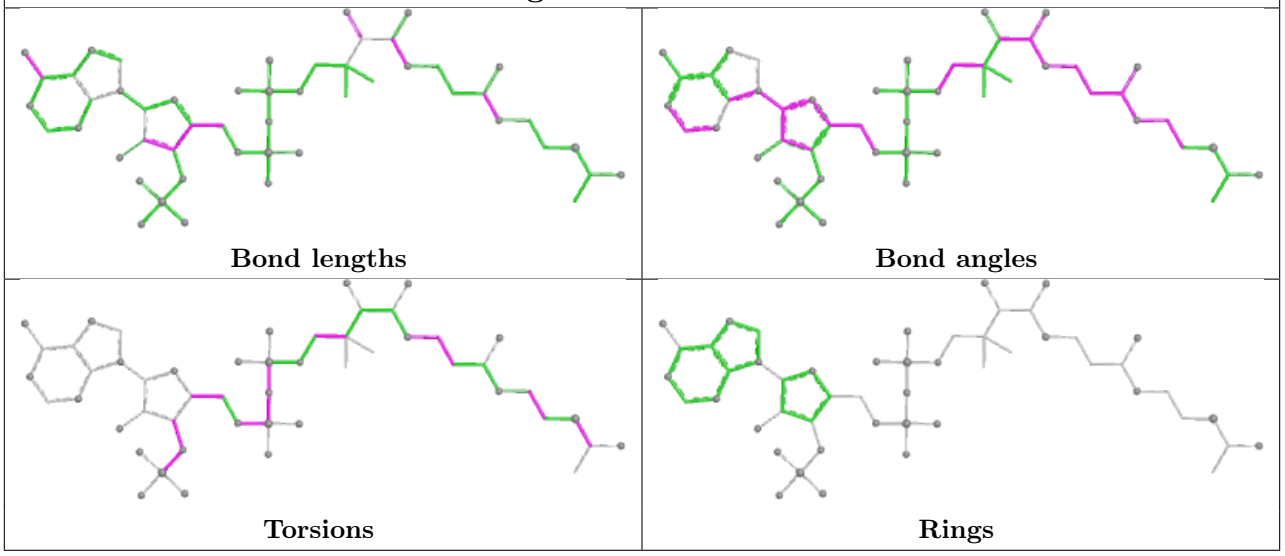
Ligand ACO L 501



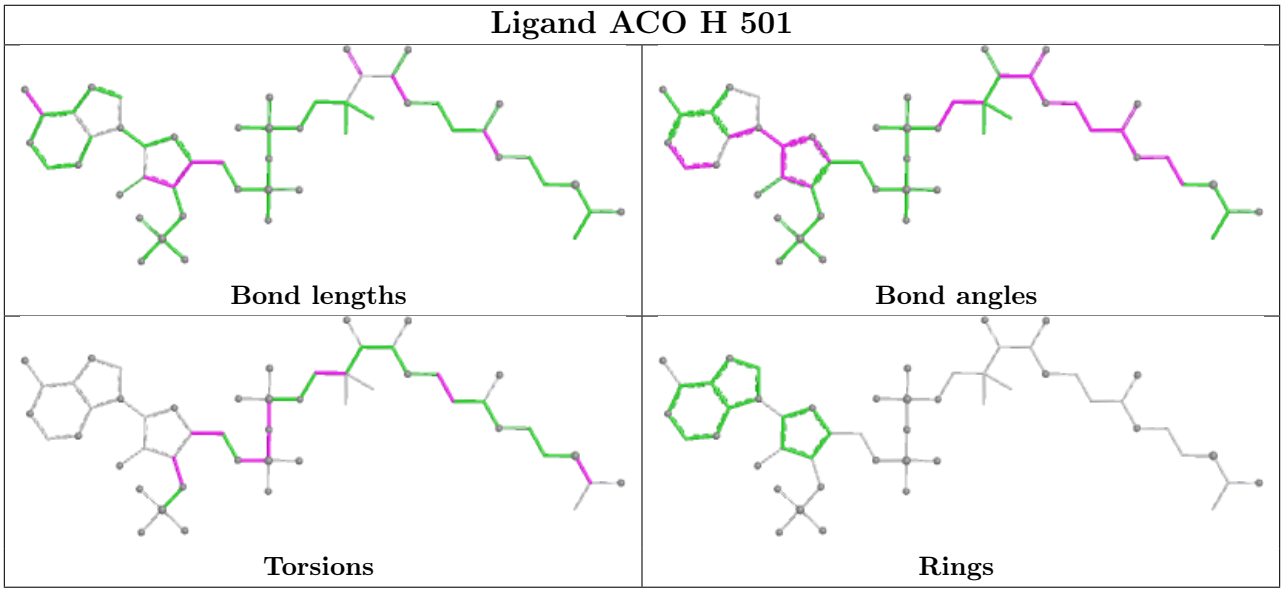
Ligand ACO D 501



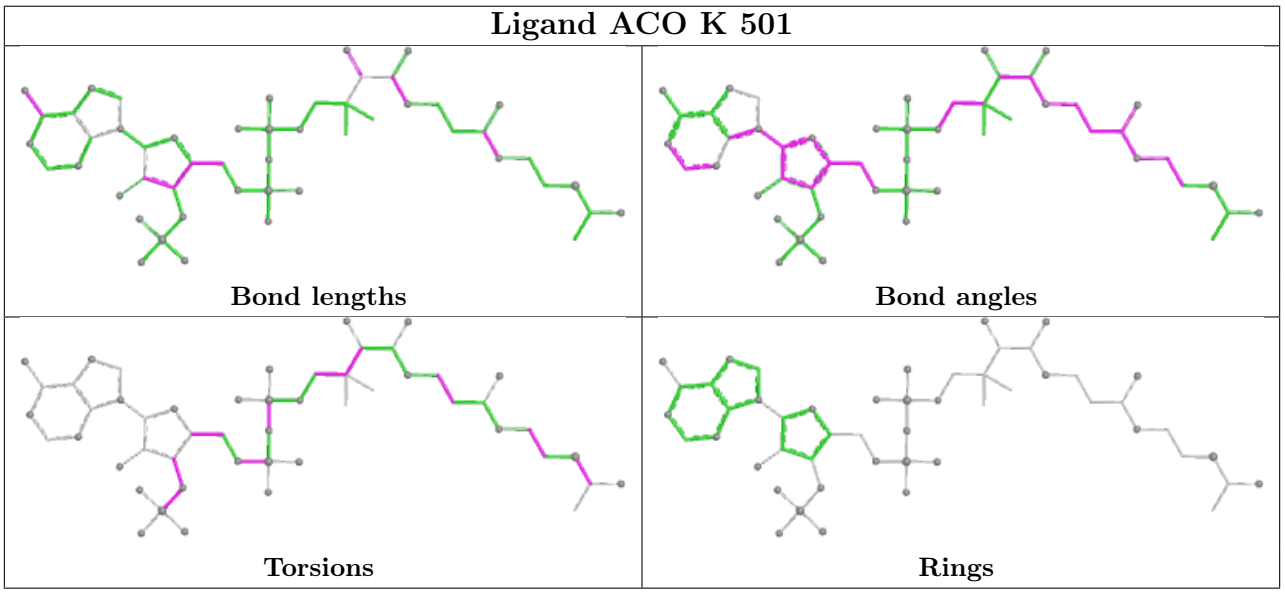
Ligand ACO J 501



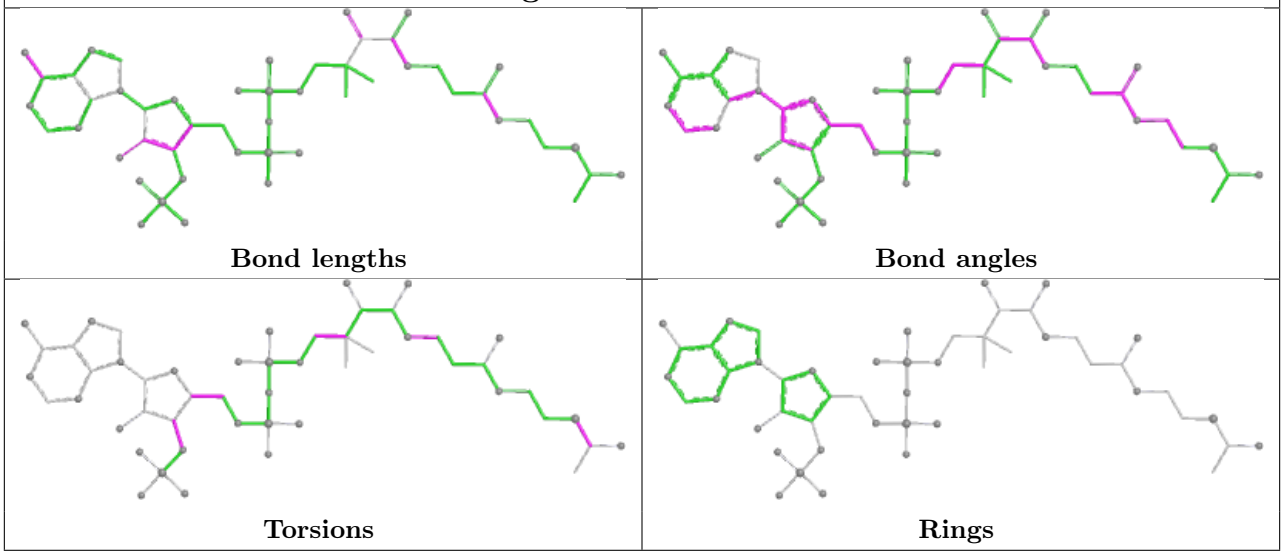
Ligand ACO H 501



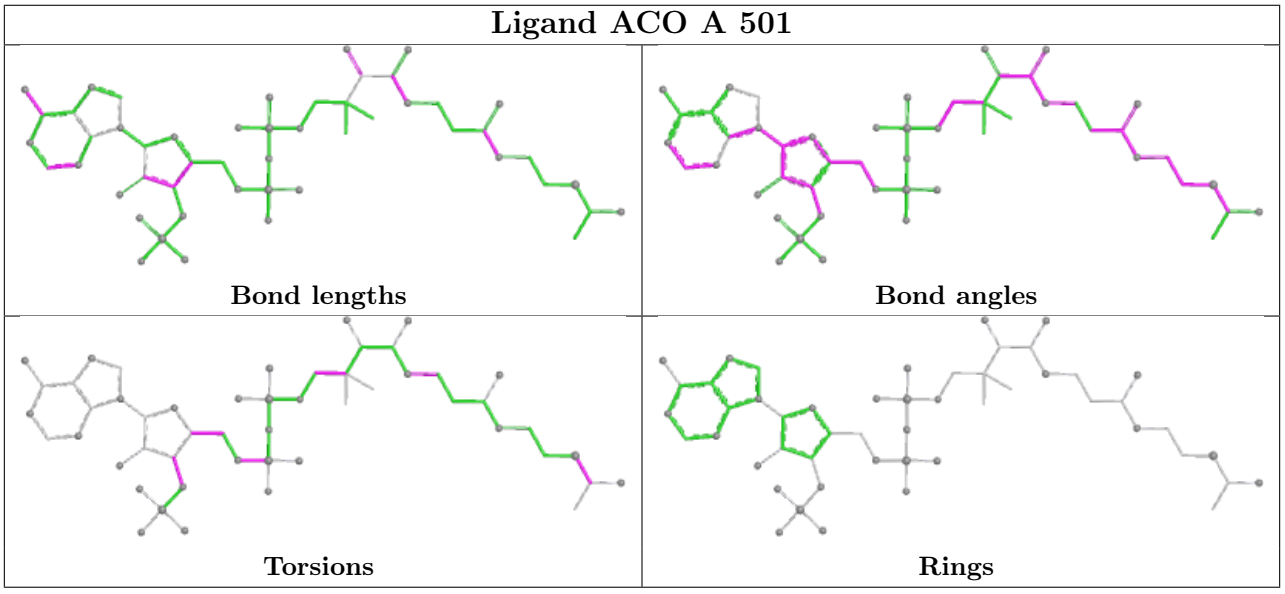
Ligand ACO K 501



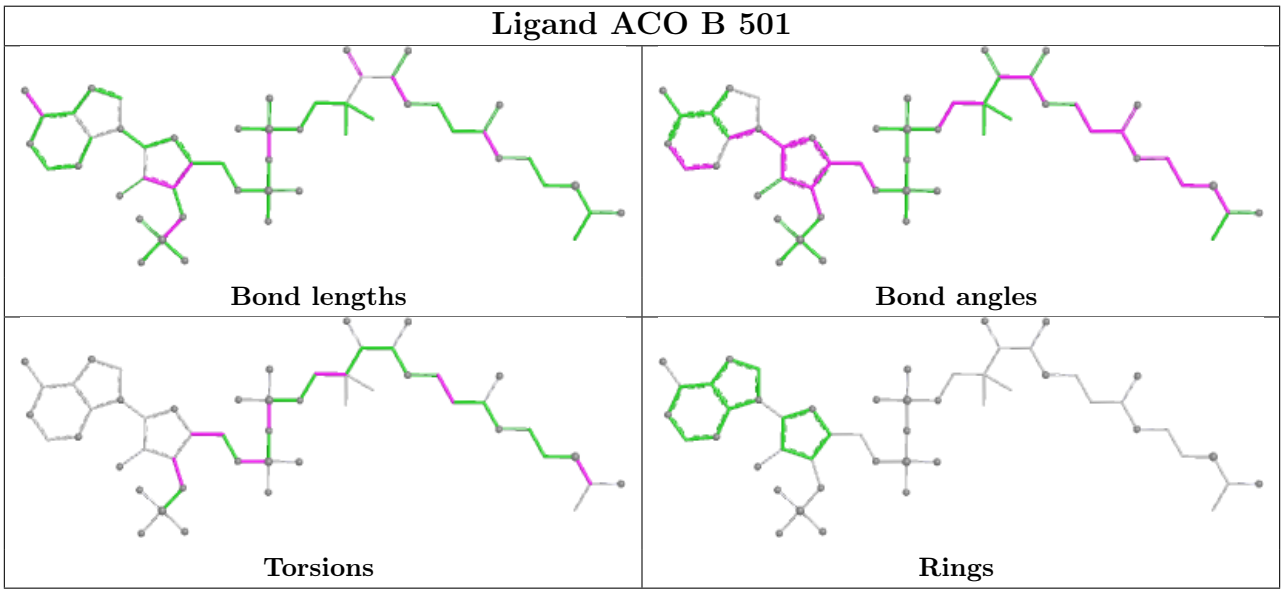
Ligand ACO G 501



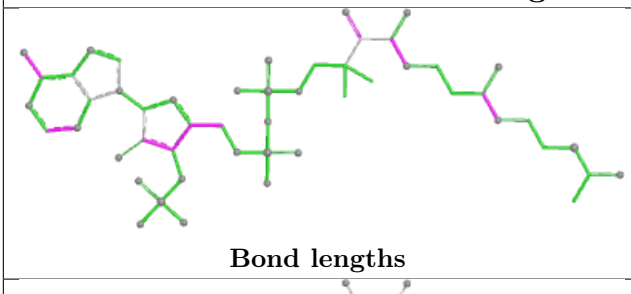
Ligand ACO A 501



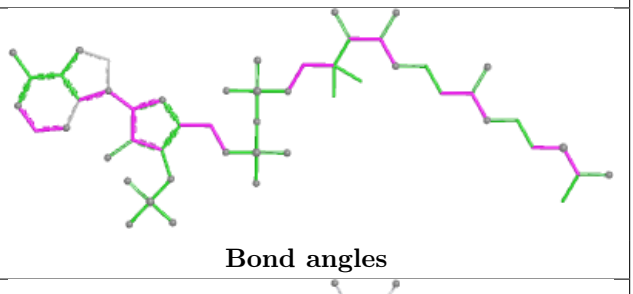
Ligand ACO B 501



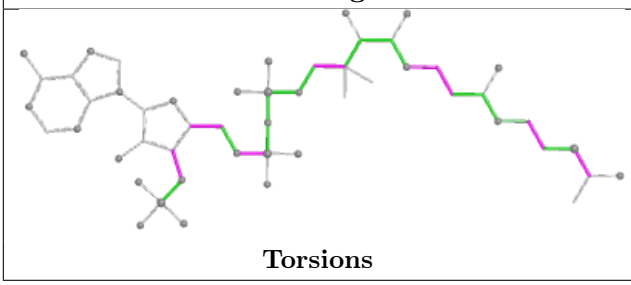
Ligand ACO I 501



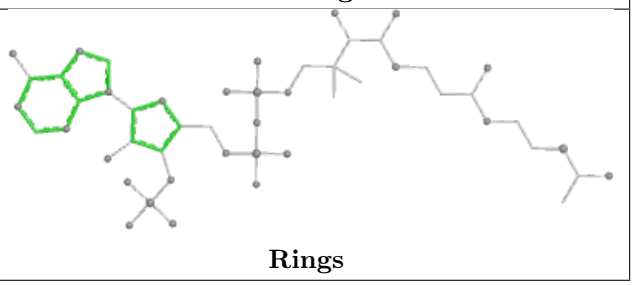
Bond lengths



Bond angles

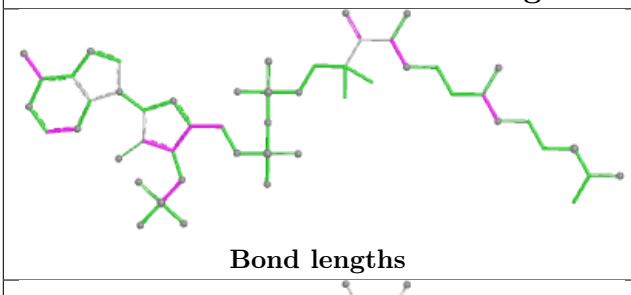


Torsions

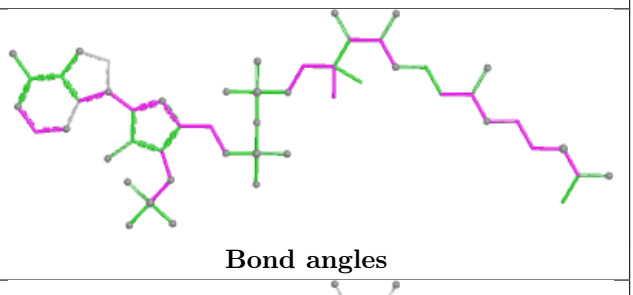


Rings

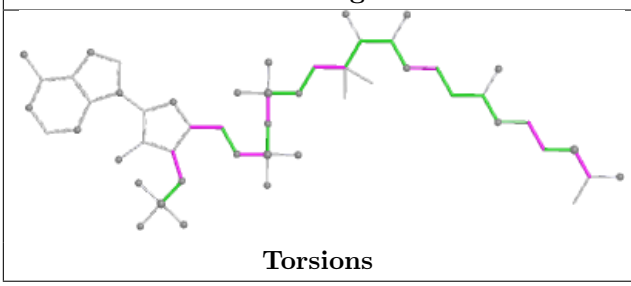
Ligand ACO F 501



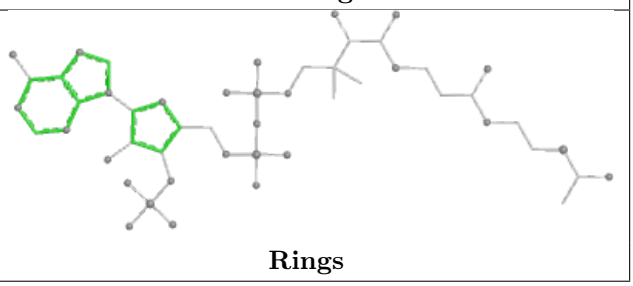
Bond lengths



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, 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	389/428 (90%)	-0.17	21 (5%)	32	25	16, 28, 63, 139	0
1	B	389/428 (90%)	-0.16	20 (5%)	34	27	18, 27, 65, 161	0
1	C	389/428 (90%)	-0.07	21 (5%)	32	25	21, 30, 66, 152	0
1	D	389/428 (90%)	-0.03	22 (5%)	30	24	18, 29, 65, 144	0
1	E	389/428 (90%)	0.01	24 (6%)	28	21	17, 30, 66, 158	0
1	F	389/428 (90%)	0.00	25 (6%)	27	20	20, 30, 72, 125	0
1	G	389/428 (90%)	0.07	23 (5%)	29	22	22, 35, 67, 162	0
1	H	389/428 (90%)	0.07	23 (5%)	29	22	23, 36, 72, 165	0
1	I	389/428 (90%)	0.38	21 (5%)	32	25	24, 47, 78, 163	0
1	J	389/428 (90%)	0.62	39 (10%)	14	11	24, 51, 81, 166	0
1	K	389/428 (90%)	0.17	21 (5%)	32	25	24, 43, 78, 157	0
1	L	389/428 (90%)	-0.14	13 (3%)	49	41	23, 35, 69, 160	0
All	All	4668/5136 (90%)	0.06	273 (5%)	30	23	16, 35, 74, 166	0

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	42	TRP	14.0
1	E	60	PRO	8.4
1	A	60	PRO	7.5
1	A	8	THR	7.4
1	B	42	TRP	7.0

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)

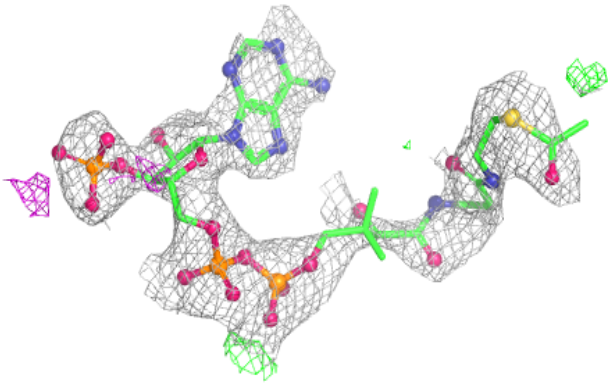
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

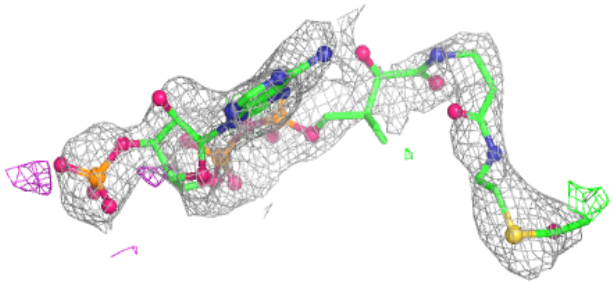
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACO	J	501	51/51	0.79	0.15	54,68,82,89	0
2	ACO	I	501	51/51	0.80	0.13	44,63,78,97	0
2	ACO	E	501	51/51	0.81	0.14	38,57,82,89	0
2	ACO	H	501	51/51	0.82	0.13	41,57,73,81	0
2	ACO	D	501	51/51	0.86	0.12	34,51,70,81	0
2	ACO	K	501	51/51	0.86	0.11	45,56,70,77	0
2	ACO	F	501	51/51	0.87	0.11	34,48,66,73	0
2	ACO	C	501	51/51	0.88	0.11	33,50,71,83	0
2	ACO	A	501	51/51	0.88	0.11	30,46,67,81	0
2	ACO	B	501	51/51	0.91	0.10	29,42,54,61	0
2	ACO	G	501	51/51	0.92	0.09	28,40,60,73	0
2	ACO	L	501	51/51	0.92	0.10	26,38,61,72	0

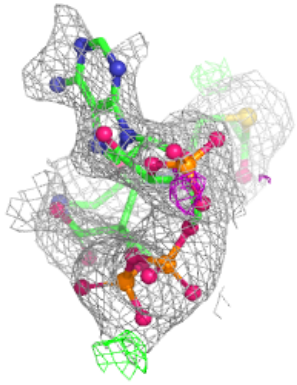
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO J 501:

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

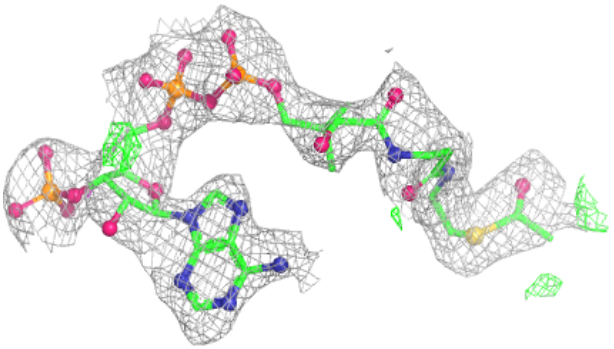


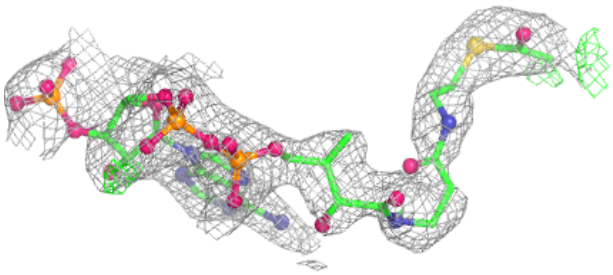


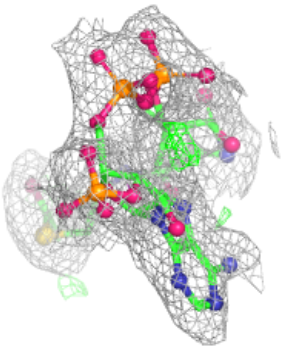


Electron density around ACO I 501:

$2mF_o$-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 E 501:

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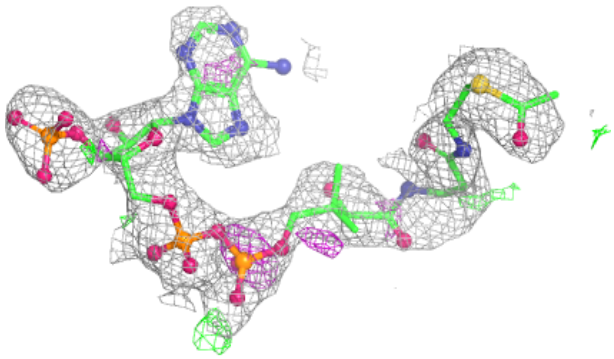
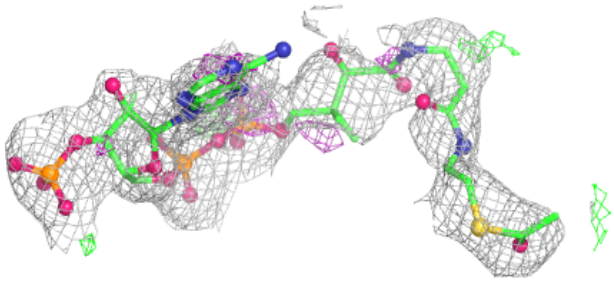
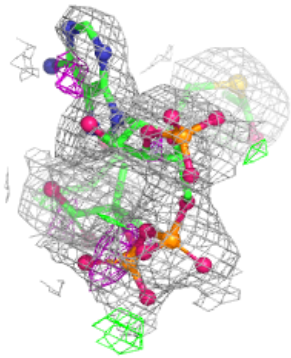
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

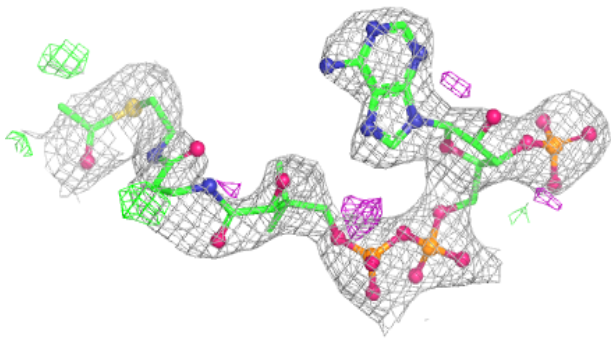


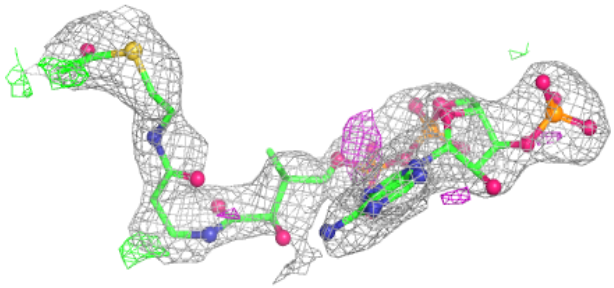


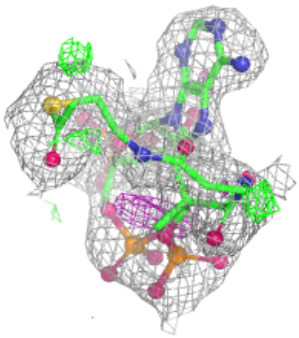


Electron density around ACO H 501:

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

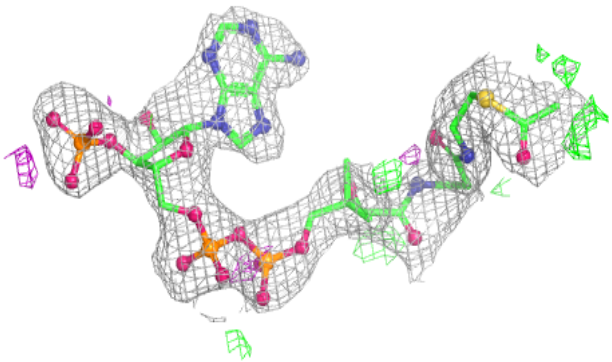


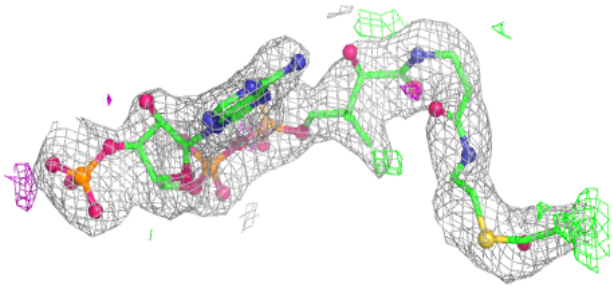


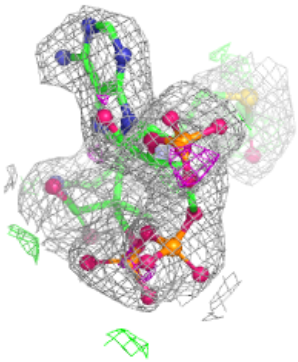


Electron density around ACO D 501:

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

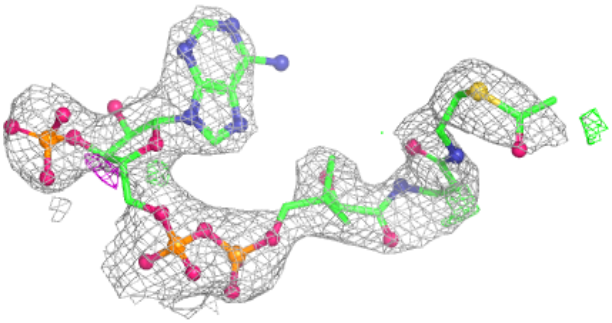


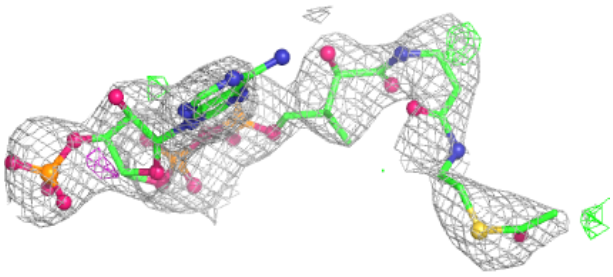


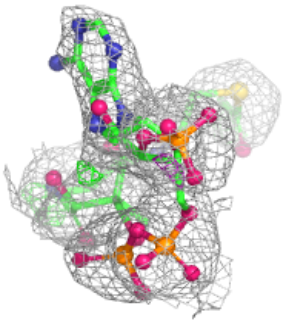


Electron density around ACO K 501:

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

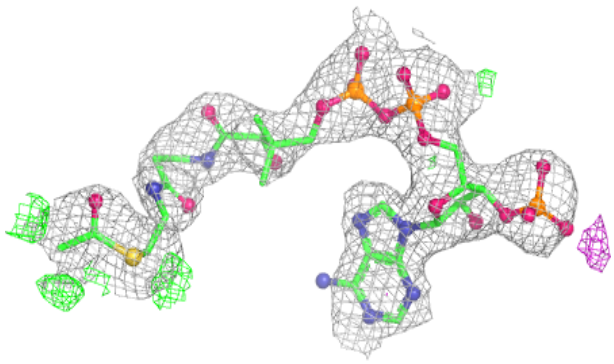


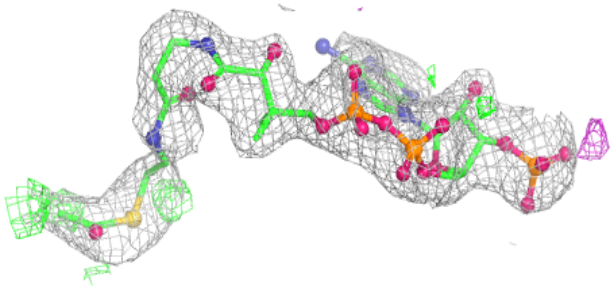


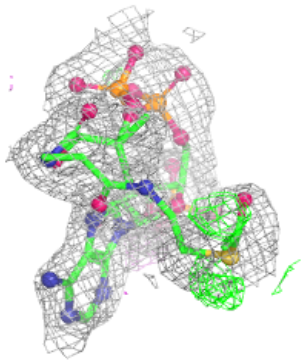


Electron density around ACO F 501:

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

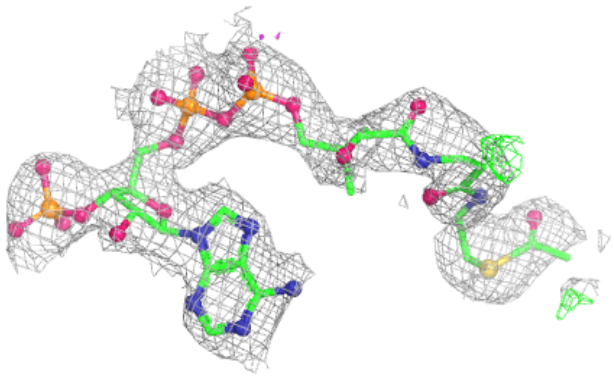


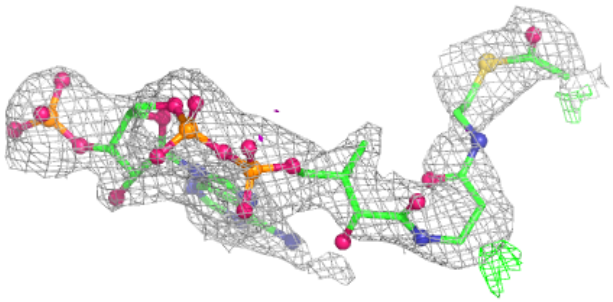


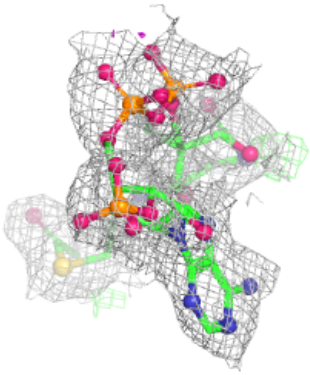


Electron density around ACO C 501:

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

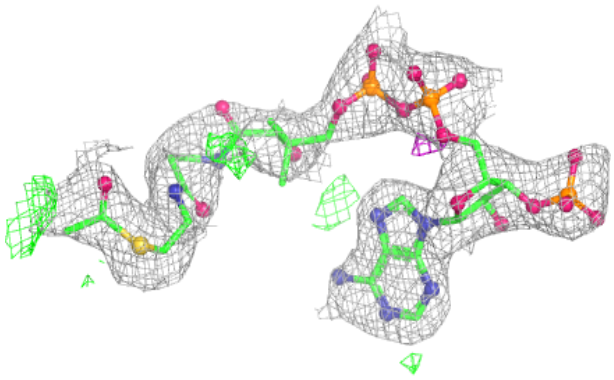


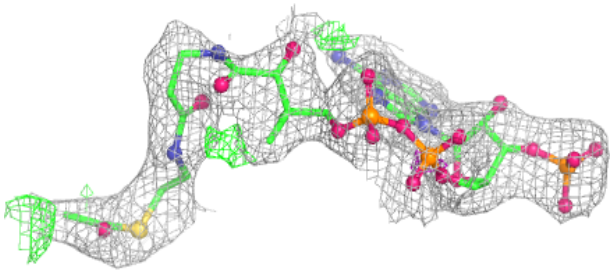




Electron density around ACO A 501:

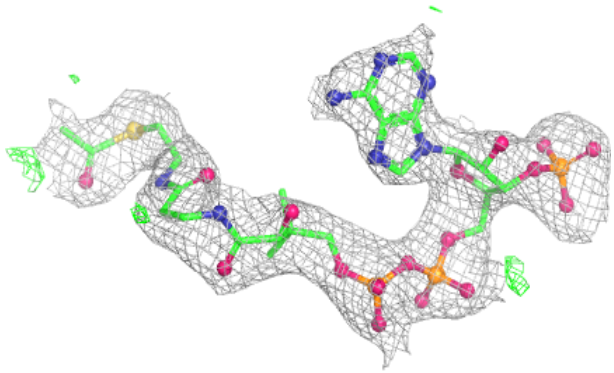
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

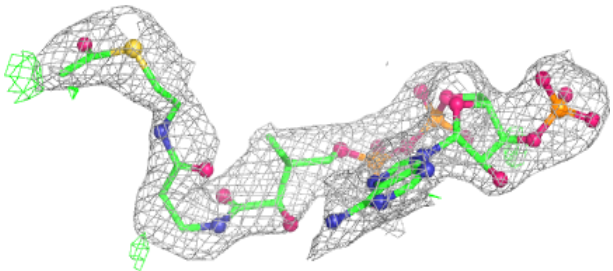


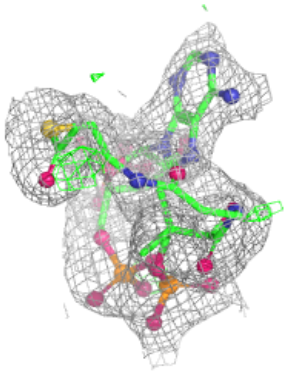


Electron density around ACO B 501:

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

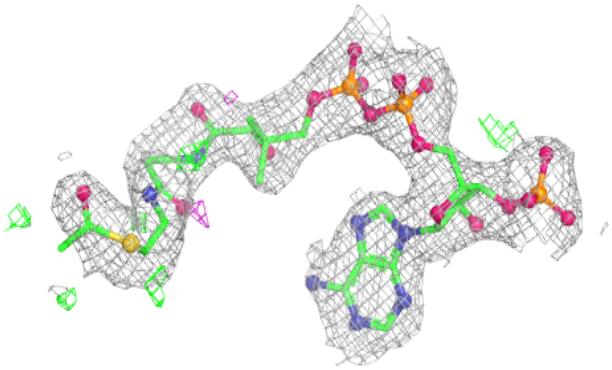


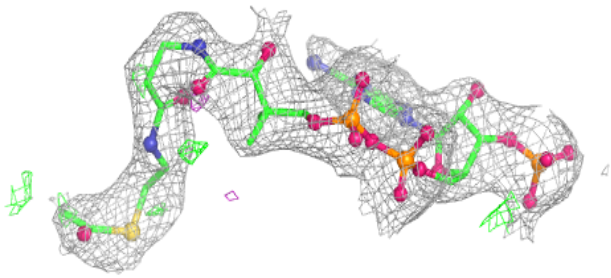


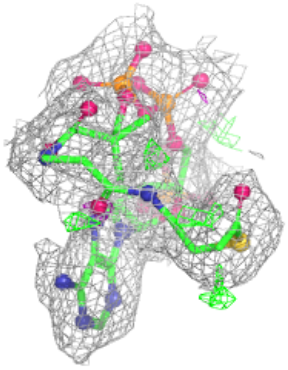


Electron density around ACO G 501:

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

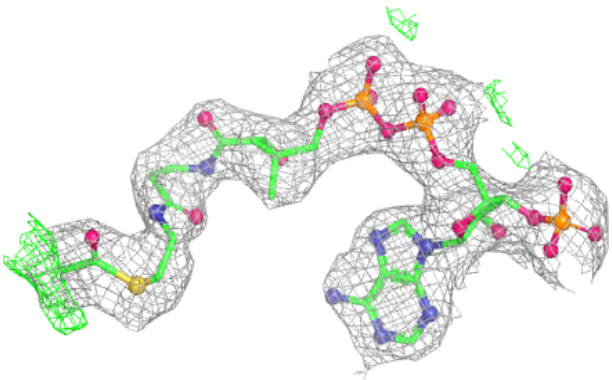


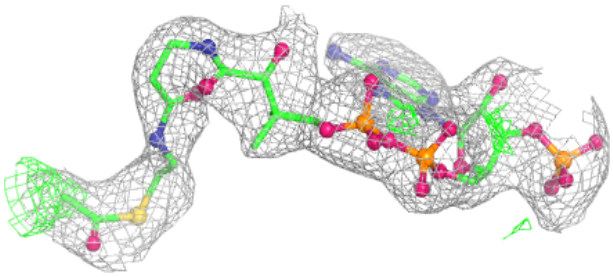


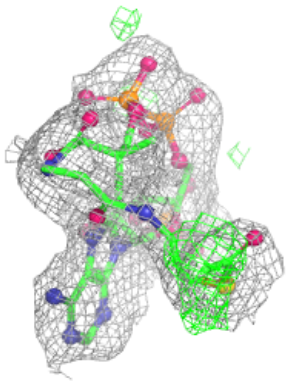


Electron density around ACO L 501:

$2mF_o$-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.