wwPDB X-ray Structure Validation Summary Report (i)

Apr 30, 2024 – 06:11 pm BST

PDB ID	:	9F3Y
Title	:	CutC choline lyase in complex with difluorocholine
Authors	:	Kalnins, G.
Deposited on	:	2024-04-26
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

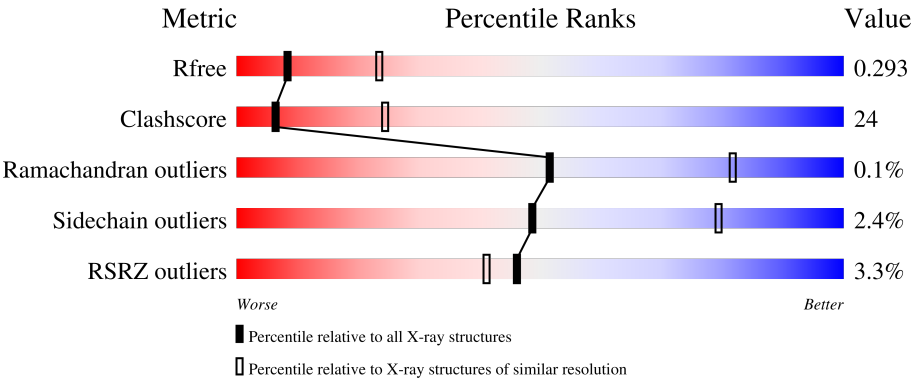
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	1150	45% 23% · 31%
1	B	1150	44% 24% · 31%
1	C	1150	39% 29% · 31%
1	D	1150	38% 30% · 31%
1	E	1150	3% 36% 32% · 31%

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Mol	Chain	Length	Quality of chain
1	F	1150	3% 36% 32% 31%
1	G	1150	6% 32% 35% 31%
1	H	1150	3% 33% 35% 31%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 50317 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 Choline trimethylamine-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	B	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	C	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	D	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	E	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	F	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	G	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	H	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A486V7R5
A	-20	GLY	-	expression tag	UNP A0A486V7R5
A	-19	SER	-	expression tag	UNP A0A486V7R5
A	-18	SER	-	expression tag	UNP A0A486V7R5
A	-17	HIS	-	expression tag	UNP A0A486V7R5
A	-16	HIS	-	expression tag	UNP A0A486V7R5
A	-15	HIS	-	expression tag	UNP A0A486V7R5
A	-14	HIS	-	expression tag	UNP A0A486V7R5
A	-13	HIS	-	expression tag	UNP A0A486V7R5
A	-12	HIS	-	expression tag	UNP A0A486V7R5
A	-11	SER	-	expression tag	UNP A0A486V7R5
A	-10	GLN	-	expression tag	UNP A0A486V7R5
A	-9	ASP	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP A0A486V7R5
A	-7	GLU	-	expression tag	UNP A0A486V7R5
A	-6	ASN	-	expression tag	UNP A0A486V7R5
A	-5	LEU	-	expression tag	UNP A0A486V7R5
A	-4	TYR	-	expression tag	UNP A0A486V7R5
A	-3	PHE	-	expression tag	UNP A0A486V7R5
A	-2	GLN	-	expression tag	UNP A0A486V7R5
A	-1	GLY	-	expression tag	UNP A0A486V7R5
A	0	SER	-	expression tag	UNP A0A486V7R5
B	-21	MET	-	initiating methionine	UNP A0A486V7R5
B	-20	GLY	-	expression tag	UNP A0A486V7R5
B	-19	SER	-	expression tag	UNP A0A486V7R5
B	-18	SER	-	expression tag	UNP A0A486V7R5
B	-17	HIS	-	expression tag	UNP A0A486V7R5
B	-16	HIS	-	expression tag	UNP A0A486V7R5
B	-15	HIS	-	expression tag	UNP A0A486V7R5
B	-14	HIS	-	expression tag	UNP A0A486V7R5
B	-13	HIS	-	expression tag	UNP A0A486V7R5
B	-12	HIS	-	expression tag	UNP A0A486V7R5
B	-11	SER	-	expression tag	UNP A0A486V7R5
B	-10	GLN	-	expression tag	UNP A0A486V7R5
B	-9	ASP	-	expression tag	UNP A0A486V7R5
B	-8	HIS	-	expression tag	UNP A0A486V7R5
B	-7	GLU	-	expression tag	UNP A0A486V7R5
B	-6	ASN	-	expression tag	UNP A0A486V7R5
B	-5	LEU	-	expression tag	UNP A0A486V7R5
B	-4	TYR	-	expression tag	UNP A0A486V7R5
B	-3	PHE	-	expression tag	UNP A0A486V7R5
B	-2	GLN	-	expression tag	UNP A0A486V7R5
B	-1	GLY	-	expression tag	UNP A0A486V7R5
B	0	SER	-	expression tag	UNP A0A486V7R5
C	-21	MET	-	initiating methionine	UNP A0A486V7R5
C	-20	GLY	-	expression tag	UNP A0A486V7R5
C	-19	SER	-	expression tag	UNP A0A486V7R5
C	-18	SER	-	expression tag	UNP A0A486V7R5
C	-17	HIS	-	expression tag	UNP A0A486V7R5
C	-16	HIS	-	expression tag	UNP A0A486V7R5
C	-15	HIS	-	expression tag	UNP A0A486V7R5
C	-14	HIS	-	expression tag	UNP A0A486V7R5
C	-13	HIS	-	expression tag	UNP A0A486V7R5
C	-12	HIS	-	expression tag	UNP A0A486V7R5
C	-11	SER	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLN	-	expression tag	UNP A0A486V7R5
C	-9	ASP	-	expression tag	UNP A0A486V7R5
C	-8	HIS	-	expression tag	UNP A0A486V7R5
C	-7	GLU	-	expression tag	UNP A0A486V7R5
C	-6	ASN	-	expression tag	UNP A0A486V7R5
C	-5	LEU	-	expression tag	UNP A0A486V7R5
C	-4	TYR	-	expression tag	UNP A0A486V7R5
C	-3	PHE	-	expression tag	UNP A0A486V7R5
C	-2	GLN	-	expression tag	UNP A0A486V7R5
C	-1	GLY	-	expression tag	UNP A0A486V7R5
C	0	SER	-	expression tag	UNP A0A486V7R5
D	-21	MET	-	initiating methionine	UNP A0A486V7R5
D	-20	GLY	-	expression tag	UNP A0A486V7R5
D	-19	SER	-	expression tag	UNP A0A486V7R5
D	-18	SER	-	expression tag	UNP A0A486V7R5
D	-17	HIS	-	expression tag	UNP A0A486V7R5
D	-16	HIS	-	expression tag	UNP A0A486V7R5
D	-15	HIS	-	expression tag	UNP A0A486V7R5
D	-14	HIS	-	expression tag	UNP A0A486V7R5
D	-13	HIS	-	expression tag	UNP A0A486V7R5
D	-12	HIS	-	expression tag	UNP A0A486V7R5
D	-11	SER	-	expression tag	UNP A0A486V7R5
D	-10	GLN	-	expression tag	UNP A0A486V7R5
D	-9	ASP	-	expression tag	UNP A0A486V7R5
D	-8	HIS	-	expression tag	UNP A0A486V7R5
D	-7	GLU	-	expression tag	UNP A0A486V7R5
D	-6	ASN	-	expression tag	UNP A0A486V7R5
D	-5	LEU	-	expression tag	UNP A0A486V7R5
D	-4	TYR	-	expression tag	UNP A0A486V7R5
D	-3	PHE	-	expression tag	UNP A0A486V7R5
D	-2	GLN	-	expression tag	UNP A0A486V7R5
D	-1	GLY	-	expression tag	UNP A0A486V7R5
D	0	SER	-	expression tag	UNP A0A486V7R5
E	-21	MET	-	initiating methionine	UNP A0A486V7R5
E	-20	GLY	-	expression tag	UNP A0A486V7R5
E	-19	SER	-	expression tag	UNP A0A486V7R5
E	-18	SER	-	expression tag	UNP A0A486V7R5
E	-17	HIS	-	expression tag	UNP A0A486V7R5
E	-16	HIS	-	expression tag	UNP A0A486V7R5
E	-15	HIS	-	expression tag	UNP A0A486V7R5
E	-14	HIS	-	expression tag	UNP A0A486V7R5
E	-13	HIS	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP A0A486V7R5
E	-11	SER	-	expression tag	UNP A0A486V7R5
E	-10	GLN	-	expression tag	UNP A0A486V7R5
E	-9	ASP	-	expression tag	UNP A0A486V7R5
E	-8	HIS	-	expression tag	UNP A0A486V7R5
E	-7	GLU	-	expression tag	UNP A0A486V7R5
E	-6	ASN	-	expression tag	UNP A0A486V7R5
E	-5	LEU	-	expression tag	UNP A0A486V7R5
E	-4	TYR	-	expression tag	UNP A0A486V7R5
E	-3	PHE	-	expression tag	UNP A0A486V7R5
E	-2	GLN	-	expression tag	UNP A0A486V7R5
E	-1	GLY	-	expression tag	UNP A0A486V7R5
E	0	SER	-	expression tag	UNP A0A486V7R5
F	-21	MET	-	initiating methionine	UNP A0A486V7R5
F	-20	GLY	-	expression tag	UNP A0A486V7R5
F	-19	SER	-	expression tag	UNP A0A486V7R5
F	-18	SER	-	expression tag	UNP A0A486V7R5
F	-17	HIS	-	expression tag	UNP A0A486V7R5
F	-16	HIS	-	expression tag	UNP A0A486V7R5
F	-15	HIS	-	expression tag	UNP A0A486V7R5
F	-14	HIS	-	expression tag	UNP A0A486V7R5
F	-13	HIS	-	expression tag	UNP A0A486V7R5
F	-12	HIS	-	expression tag	UNP A0A486V7R5
F	-11	SER	-	expression tag	UNP A0A486V7R5
F	-10	GLN	-	expression tag	UNP A0A486V7R5
F	-9	ASP	-	expression tag	UNP A0A486V7R5
F	-8	HIS	-	expression tag	UNP A0A486V7R5
F	-7	GLU	-	expression tag	UNP A0A486V7R5
F	-6	ASN	-	expression tag	UNP A0A486V7R5
F	-5	LEU	-	expression tag	UNP A0A486V7R5
F	-4	TYR	-	expression tag	UNP A0A486V7R5
F	-3	PHE	-	expression tag	UNP A0A486V7R5
F	-2	GLN	-	expression tag	UNP A0A486V7R5
F	-1	GLY	-	expression tag	UNP A0A486V7R5
F	0	SER	-	expression tag	UNP A0A486V7R5
G	-21	MET	-	initiating methionine	UNP A0A486V7R5
G	-20	GLY	-	expression tag	UNP A0A486V7R5
G	-19	SER	-	expression tag	UNP A0A486V7R5
G	-18	SER	-	expression tag	UNP A0A486V7R5
G	-17	HIS	-	expression tag	UNP A0A486V7R5
G	-16	HIS	-	expression tag	UNP A0A486V7R5
G	-15	HIS	-	expression tag	UNP A0A486V7R5

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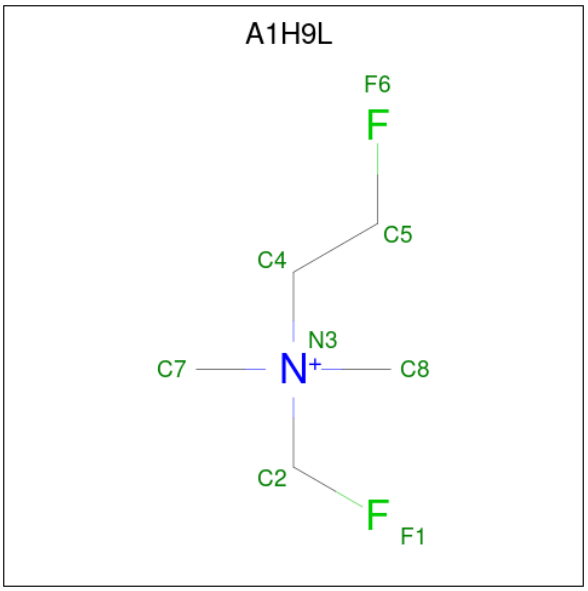
Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP A0A486V7R5
G	-13	HIS	-	expression tag	UNP A0A486V7R5
G	-12	HIS	-	expression tag	UNP A0A486V7R5
G	-11	SER	-	expression tag	UNP A0A486V7R5
G	-10	GLN	-	expression tag	UNP A0A486V7R5
G	-9	ASP	-	expression tag	UNP A0A486V7R5
G	-8	HIS	-	expression tag	UNP A0A486V7R5
G	-7	GLU	-	expression tag	UNP A0A486V7R5
G	-6	ASN	-	expression tag	UNP A0A486V7R5
G	-5	LEU	-	expression tag	UNP A0A486V7R5
G	-4	TYR	-	expression tag	UNP A0A486V7R5
G	-3	PHE	-	expression tag	UNP A0A486V7R5
G	-2	GLN	-	expression tag	UNP A0A486V7R5
G	-1	GLY	-	expression tag	UNP A0A486V7R5
G	0	SER	-	expression tag	UNP A0A486V7R5
H	-21	MET	-	initiating methionine	UNP A0A486V7R5
H	-20	GLY	-	expression tag	UNP A0A486V7R5
H	-19	SER	-	expression tag	UNP A0A486V7R5
H	-18	SER	-	expression tag	UNP A0A486V7R5
H	-17	HIS	-	expression tag	UNP A0A486V7R5
H	-16	HIS	-	expression tag	UNP A0A486V7R5
H	-15	HIS	-	expression tag	UNP A0A486V7R5
H	-14	HIS	-	expression tag	UNP A0A486V7R5
H	-13	HIS	-	expression tag	UNP A0A486V7R5
H	-12	HIS	-	expression tag	UNP A0A486V7R5
H	-11	SER	-	expression tag	UNP A0A486V7R5
H	-10	GLN	-	expression tag	UNP A0A486V7R5
H	-9	ASP	-	expression tag	UNP A0A486V7R5
H	-8	HIS	-	expression tag	UNP A0A486V7R5
H	-7	GLU	-	expression tag	UNP A0A486V7R5
H	-6	ASN	-	expression tag	UNP A0A486V7R5
H	-5	LEU	-	expression tag	UNP A0A486V7R5
H	-4	TYR	-	expression tag	UNP A0A486V7R5
H	-3	PHE	-	expression tag	UNP A0A486V7R5
H	-2	GLN	-	expression tag	UNP A0A486V7R5
H	-1	GLY	-	expression tag	UNP A0A486V7R5
H	0	SER	-	expression tag	UNP A0A486V7R5

- Molecule 2 is difluorocholine (three-letter code: A1H9L) (formula: $C_5H_{12}F_2N$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C F N 8 5 2 1	0	0
2	B	1	Total C F N 8 5 2 1	0	0
2	C	1	Total C F N 8 5 2 1	0	0
2	D	1	Total C F N 8 5 2 1	0	0
2	E	1	Total C F N 8 5 2 1	0	0
2	F	1	Total C F N 8 5 2 1	0	0
2	G	1	Total C F N 8 5 2 1	0	0
2	H	1	Total C F N 8 5 2 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	45	Total O 45 45	0	0
3	C	40	Total O 40 40	0	0
3	D	22	Total O 22 22	0	0

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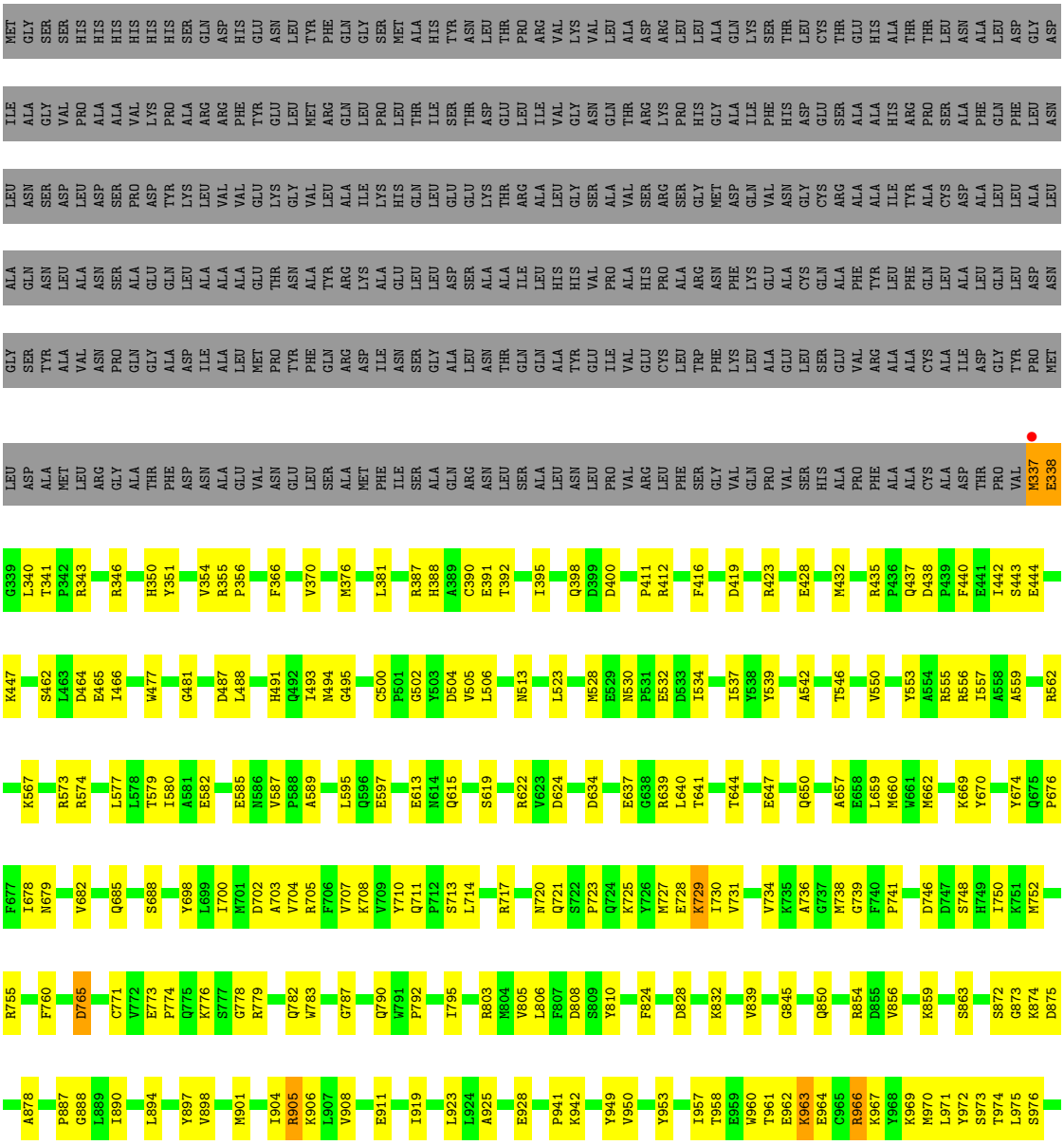
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	17	Total O 17 17	0	0
3	F	17	Total O 17 17	0	0
3	G	6	Total O 6 6	0	0
3	H	7	Total O 7 7	0	0

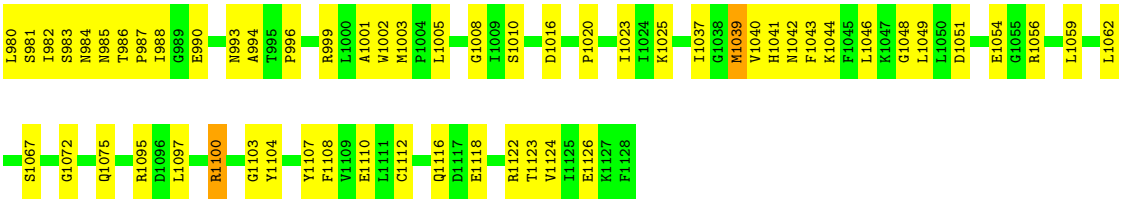
3 Residue-property plots (i)

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: Choline trimethylamine-lyase

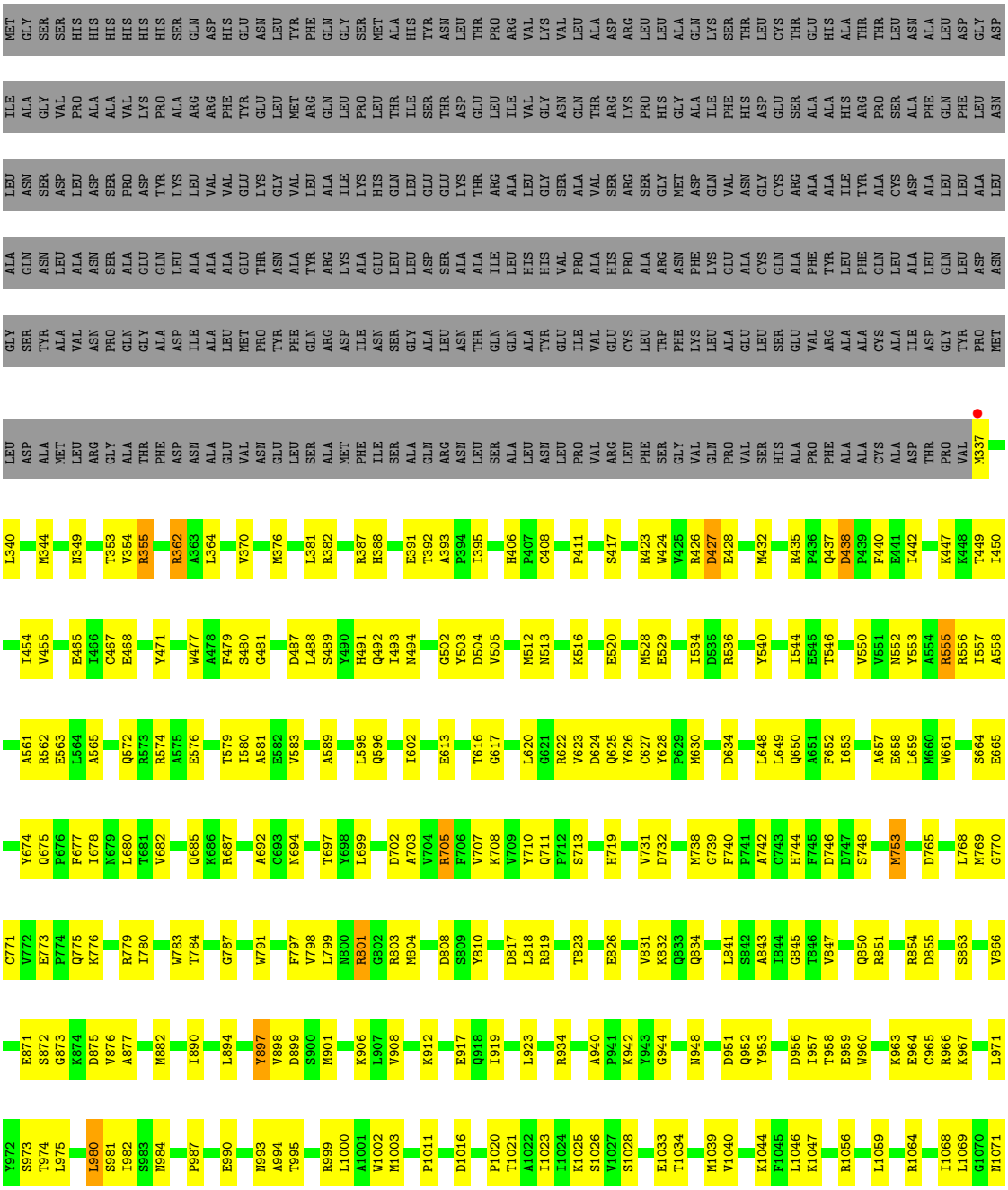
Chain A:

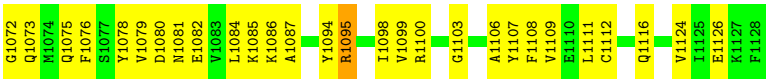




• Molecule 1: Choline trimethylamine-lyase

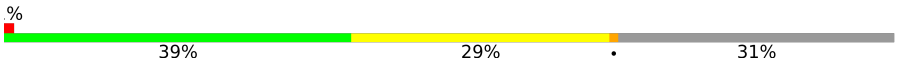
Chain B:

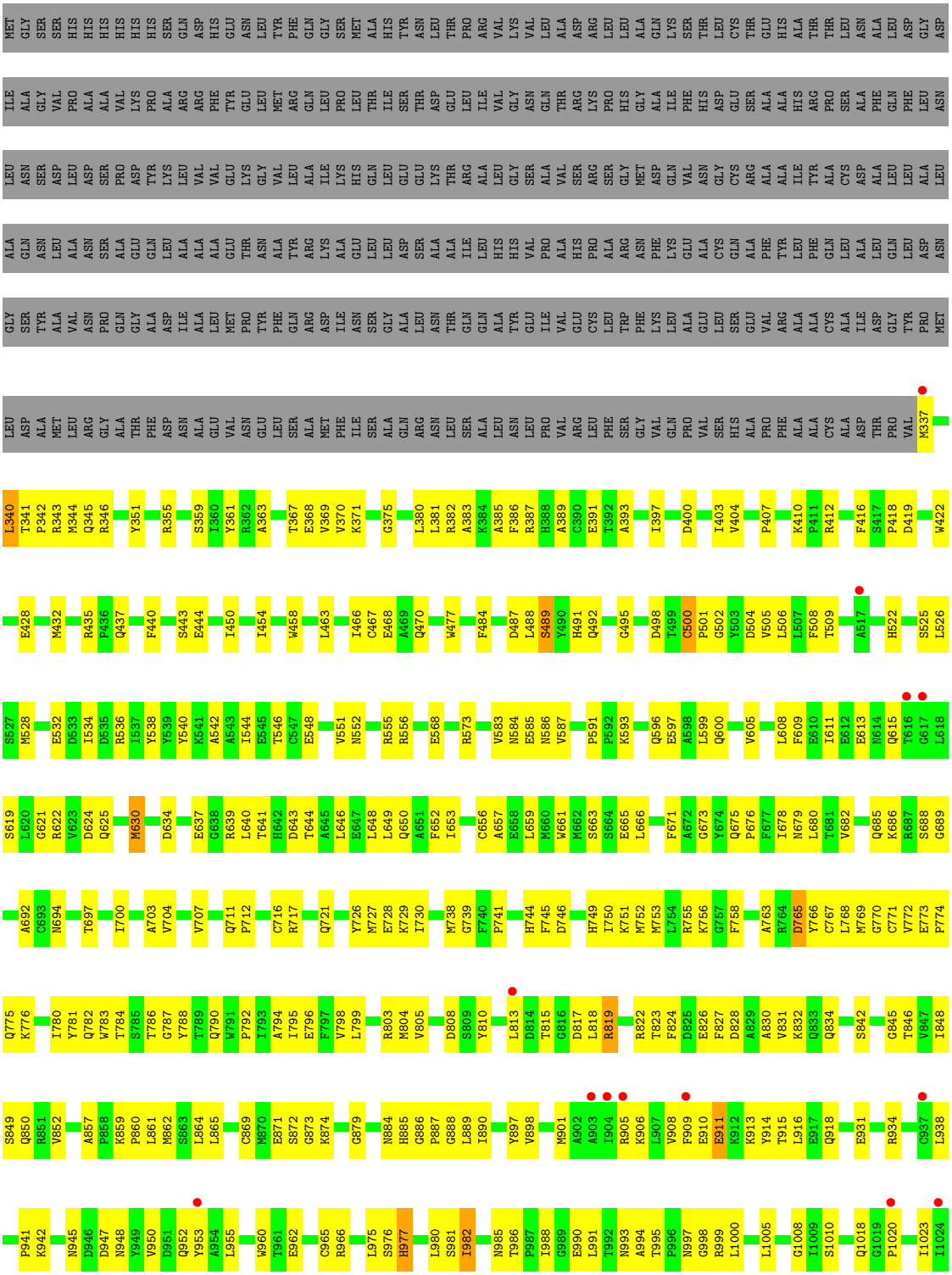


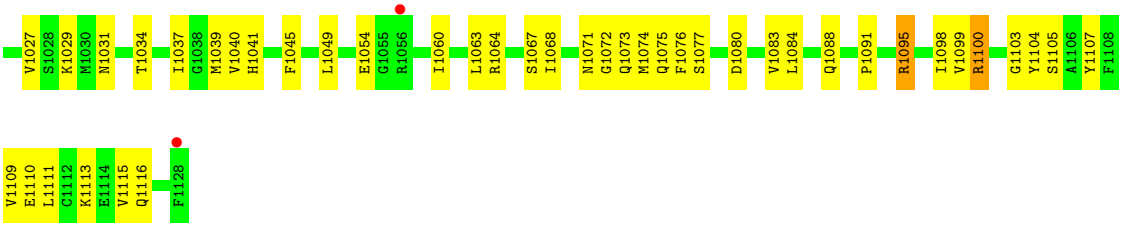


• Molecule 1: Choline trimethylamine-lyase

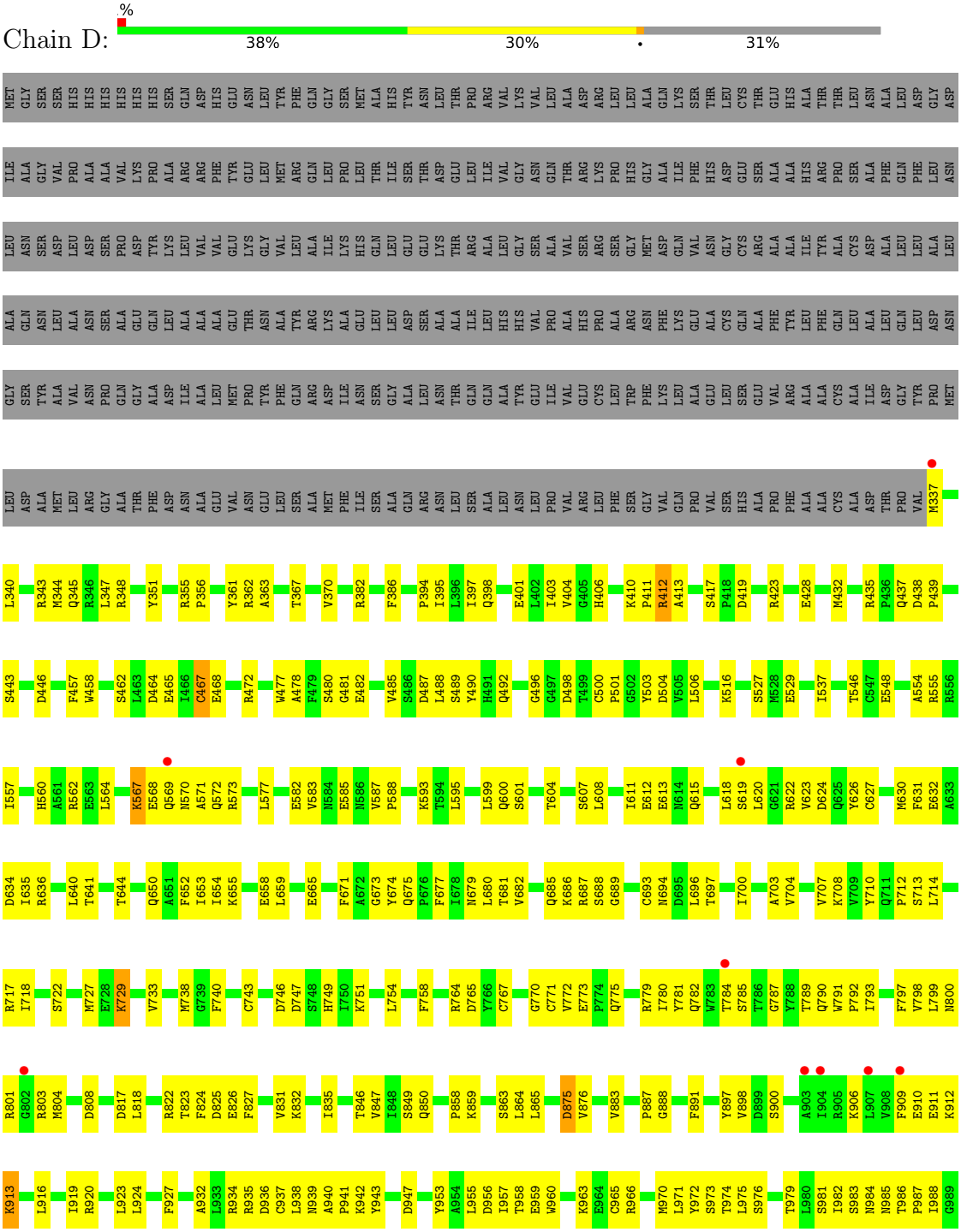
Chain C:

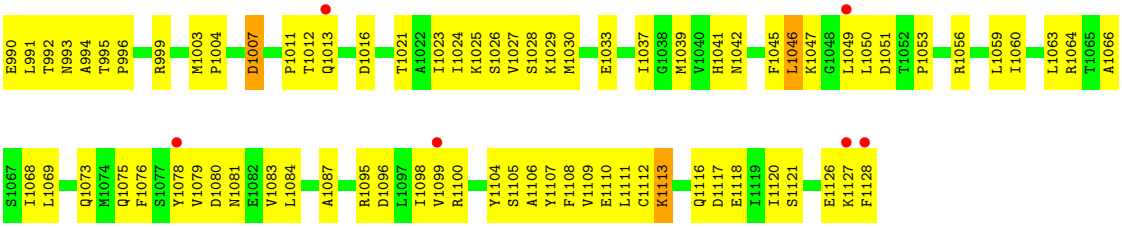






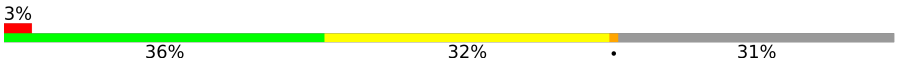
• Molecule 1: Choline trimethylamine-lyase

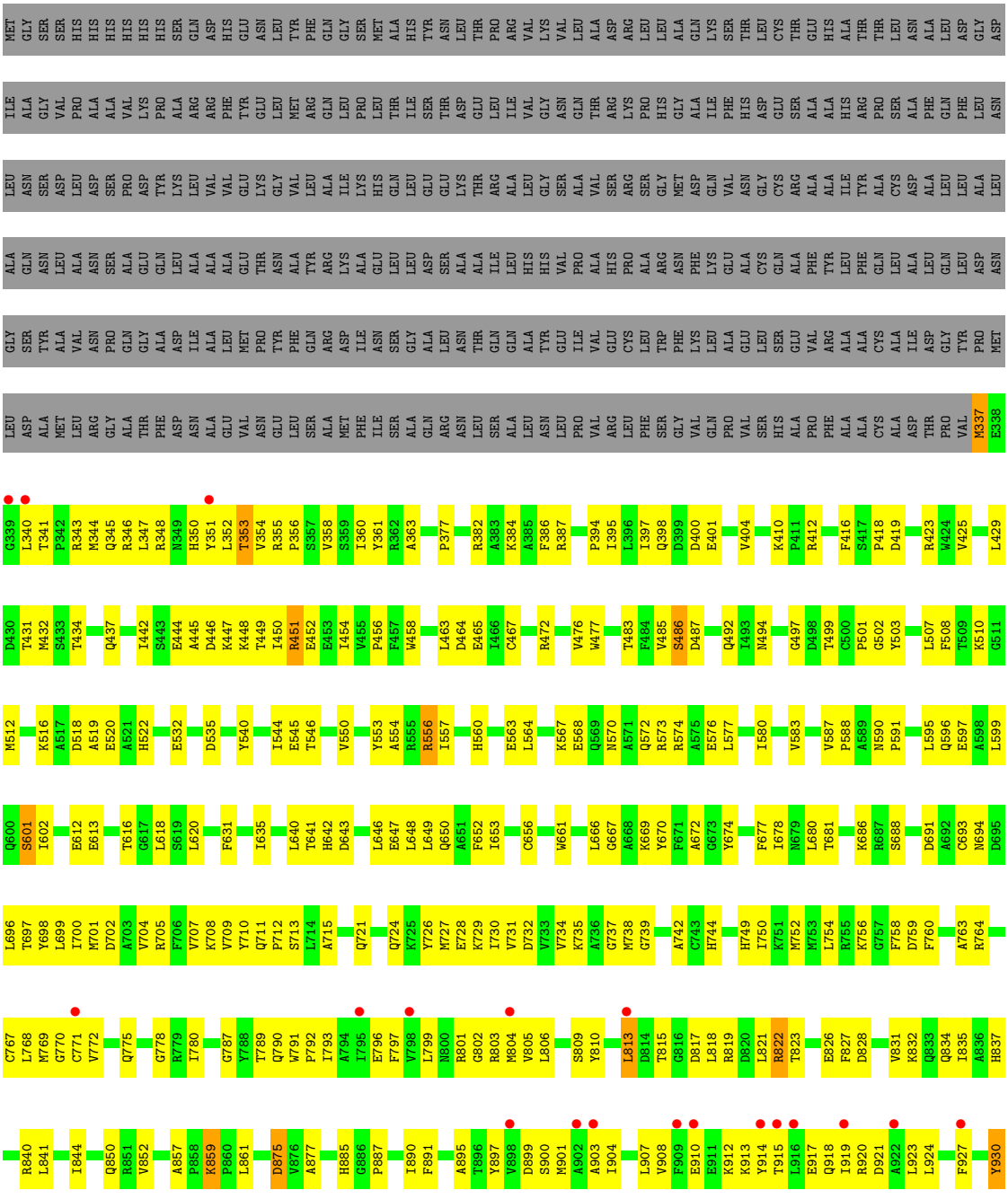


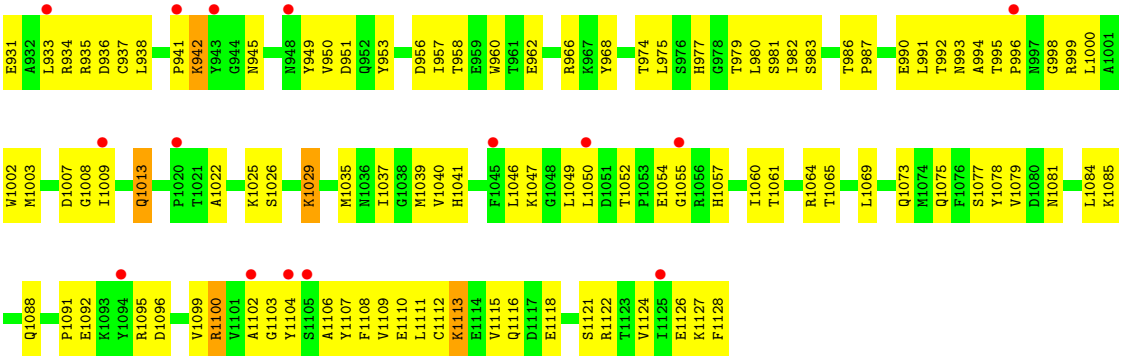


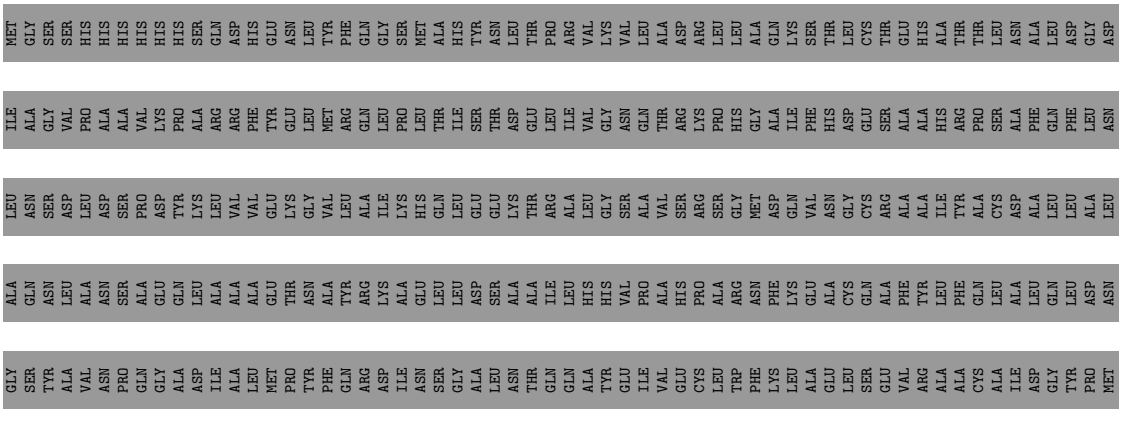
- Molecule 1: Choline trimethylamine-lyase

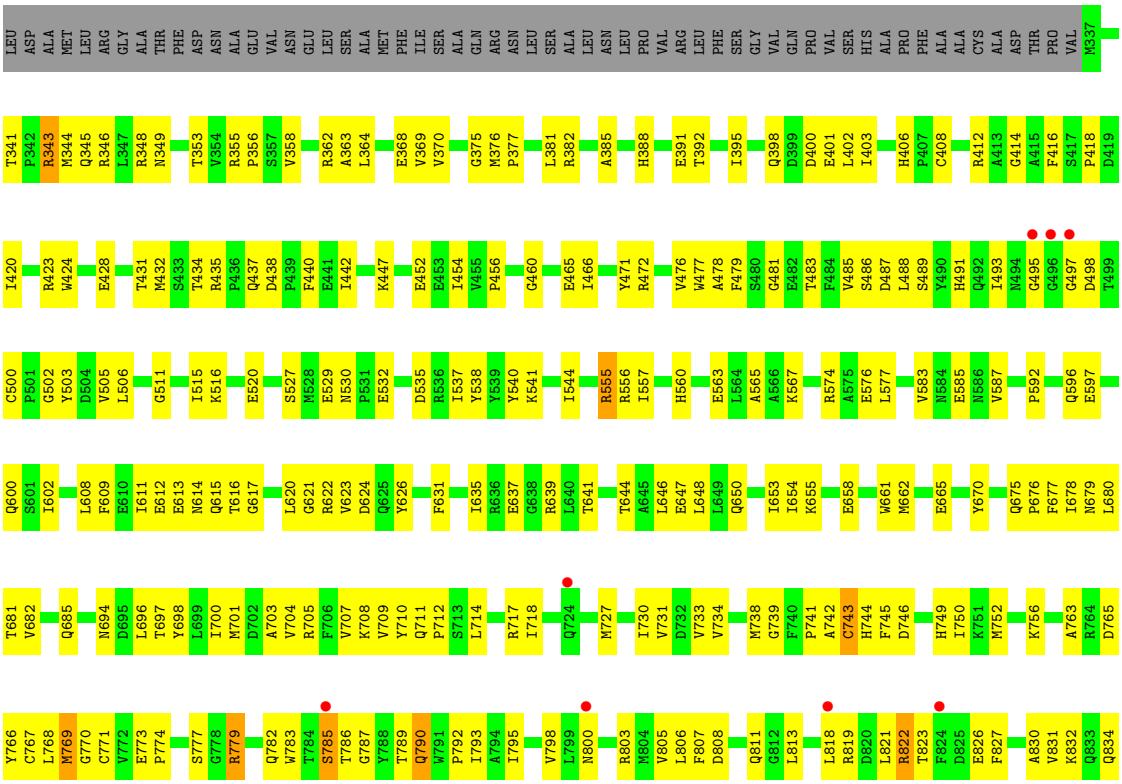
Chain E:

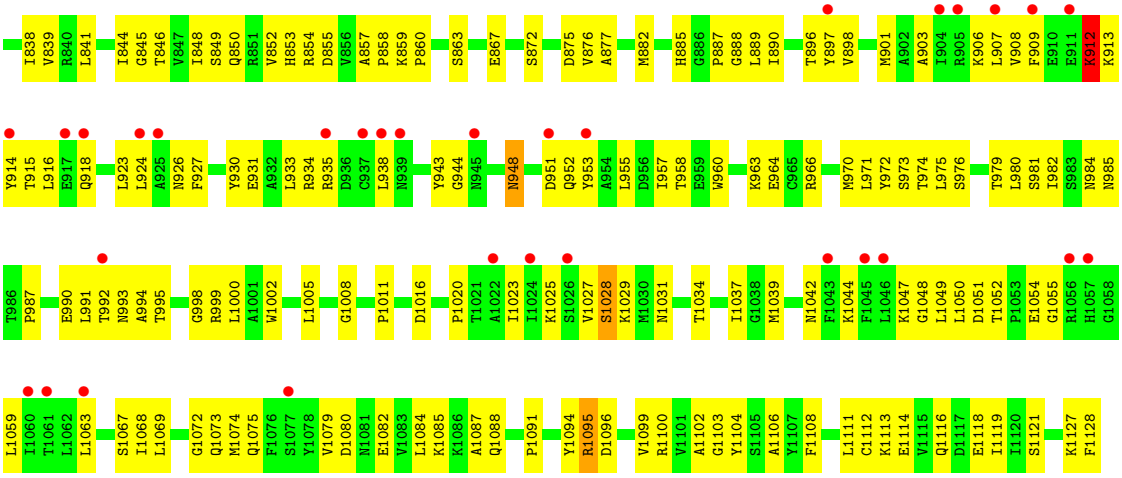






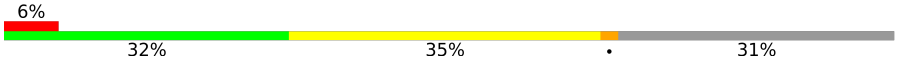


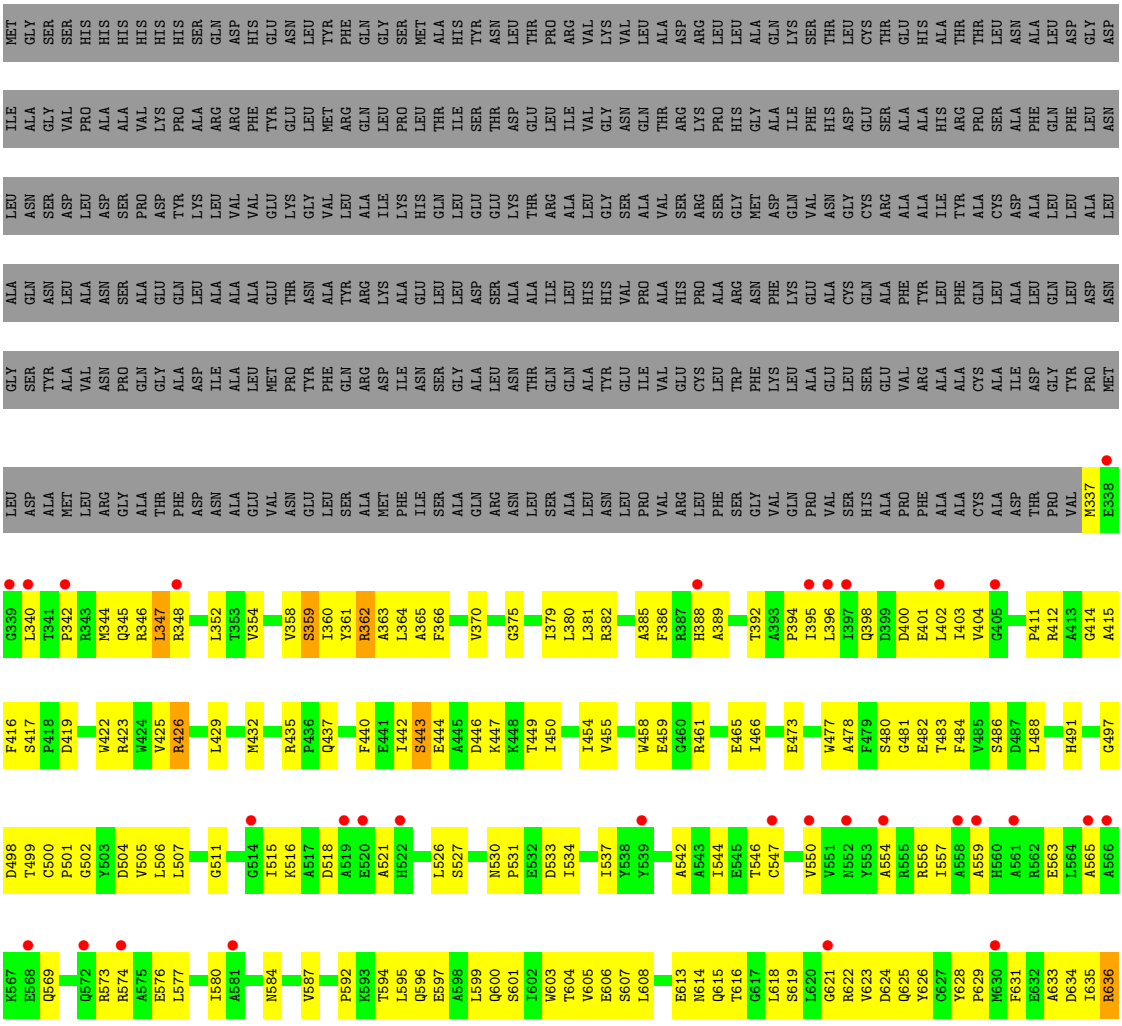


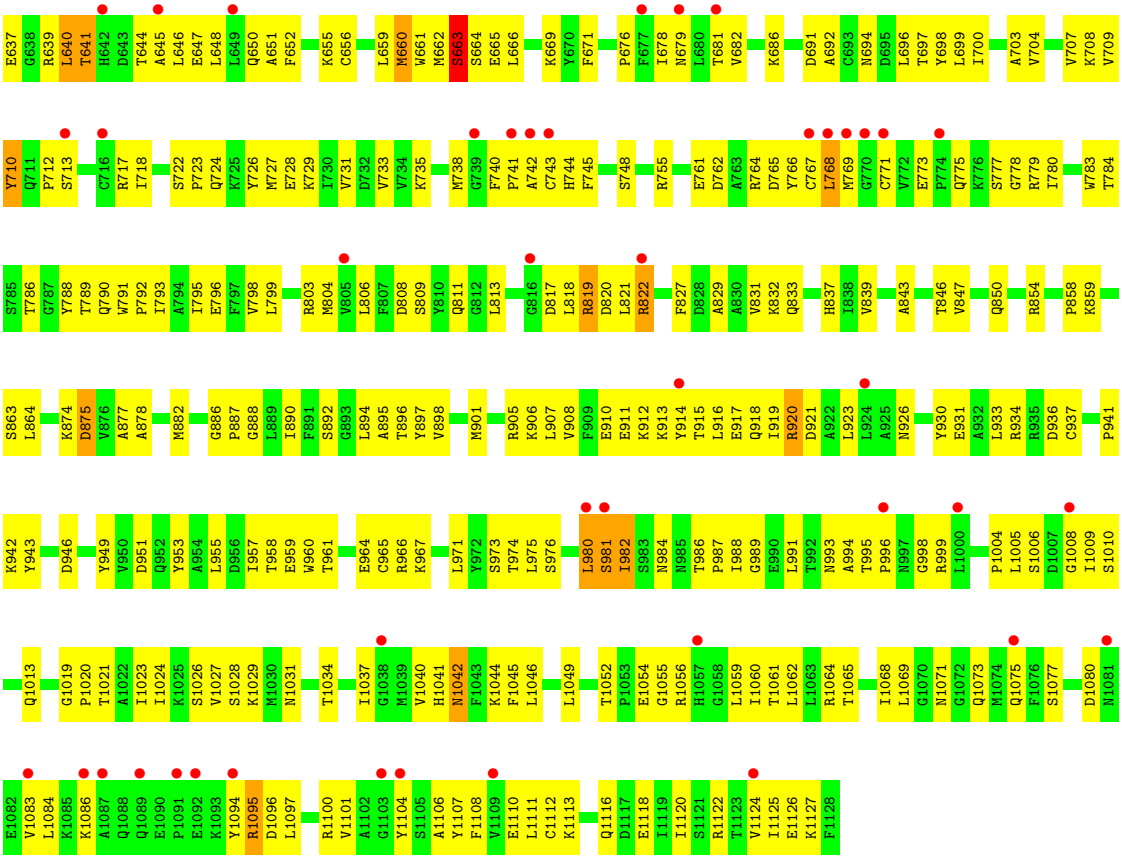


• Molecule 1: Choline trimethylamine-lyase

Chain G:

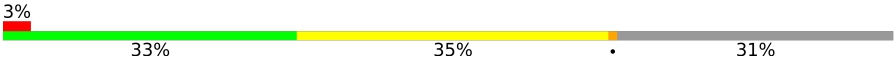


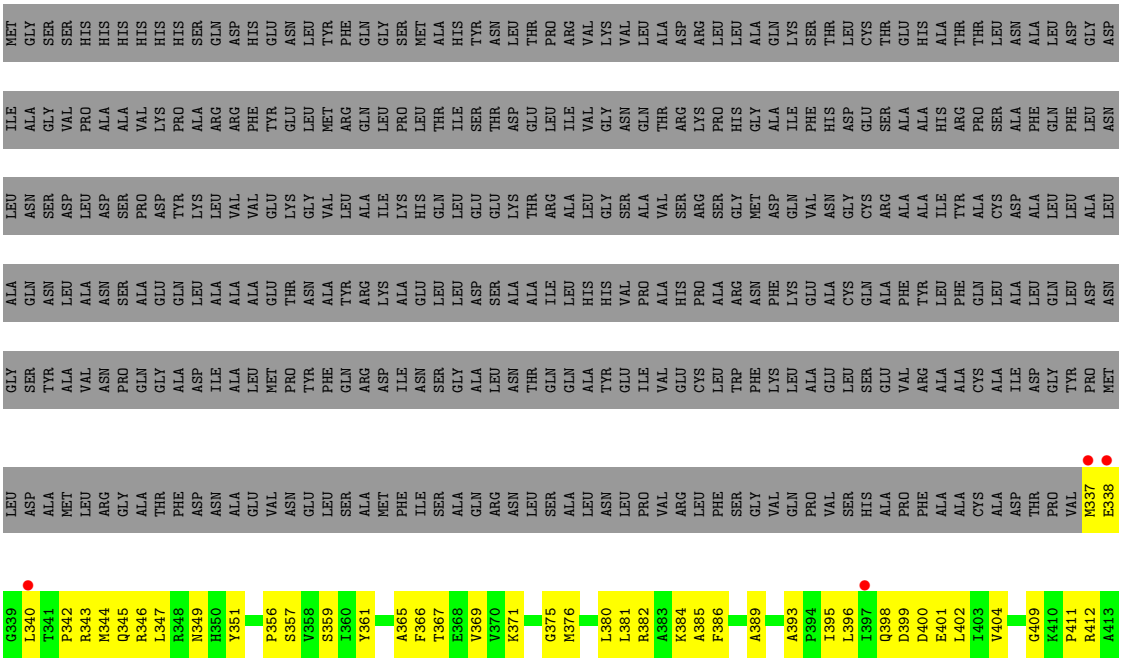


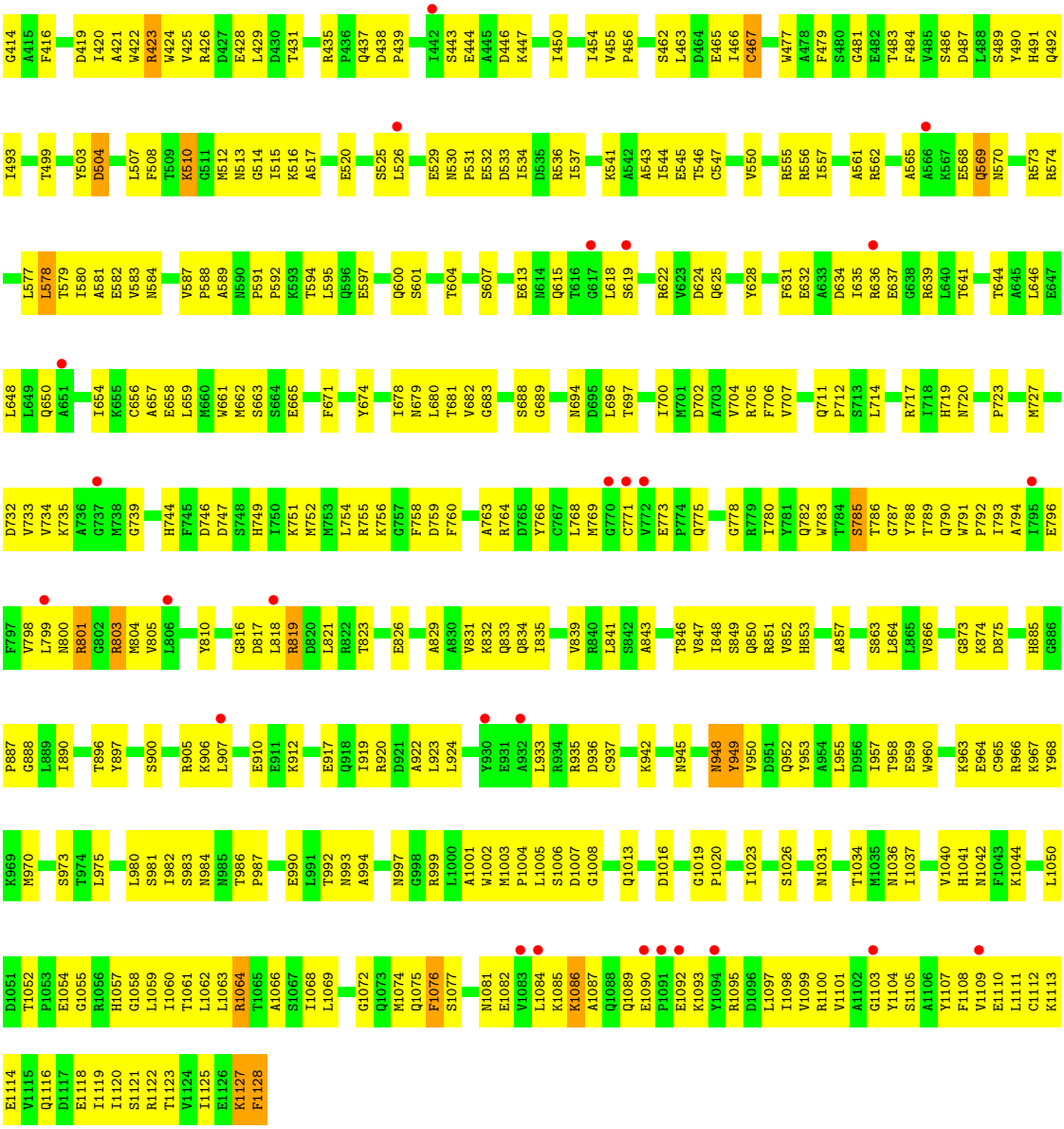


- Molecule 1: Choline trimethylamine-lyase

Chain H:






G414 A415 F416 D419 I420 A421 W422 R423 W424 V425 R426 D427 E428 L429 D430 T431 R435 P436 Q437 D438 P439 I442 S443 E444 A445 D446 K447 I450 I454 V455 P456 S462 L463 D464 E465 I466 C467 W477 A478 F479 S480 G481 E482 T483 F484 V485 S486 D487 L488 S489 Y490 H491 Q492
I493 T499 Y503 D504 L507 F508 T509 K510 G511 M512 N513 G514 I515 K516 A517 E520 S525 L526 E529 N530 P531 E532 D533 I534 D535 R536 I537 K541 A542 A543 I544 E545 T546 C547 V550 R555 R556 I557 A561 R562 A565 A566 K567 E568 Q569 N570 R573 R574
L577 L578 T579 I580 A581 E582 V583 N584 V587 P588 A589 N590 P591 P592 K593 T594 L595 Q596 E597 Q600 S601 T604 S607 E613 N614 Q615 T616 G617 L618 S619 R622 V623 D624 Q625 Y628 F631 E632 A633 D634 I635 R636 E637 G638 R639 L640 T641 T644 A645 L646 E647
L648 L649 Q650 A651 I654 K655 C656 A657 E658 L659 K660 W661 M662 S663 S664 E665 F671 Y674 I678 N679 L680 T681 V682 G683 S688 G689 N694 D695 L696 T697 I700 M701 D702 A703 V704 R705 F706 V707 Q711 P712 S713 L714 R717 I718 H719 N720 P723 M727
D732 V733 V734 K735 A736 G737 M738 G739 H744 F745 D746 D747 S748 H749 I750 K751 M752 M753 L754 R755 K756 G757 F758 D759 F760 A763 R764 D765 Y766 C767 L768 M769 G770 C771 V772 E773 P774 Q775 G778 R779 I780 Y781 Q782 W783 T784 S785 T786 G787 Y788 T789 Q790 W791 P792 I793 A794 I795 E796
F797 V798 L799 N800 R801 G802 R803 M804 V805 L806 Y810 G816 D817 L818 R819 D820 L821 R822 T823 E826 A829 A830 V831 K832 Q833 Q834 I835 V839 R840 L841 S842 A843 T846 V847 I848 S849 Q850 R851 V852 H853 A857 S863 L864 L865 V866 G873 K874 D875 H885 G886
P887 G888 L889 I890 T896 Y897 S900 R905 K906 L907 E910 E911 K912 E917 Q918 I919 R920 D921 A922 L923 L924 Y930 E931 A932 L933 R934 R935 D936 C937 K942 N945 N948 Y949 V950 D951 Q952 Y953 A954 L955 D956 I957 T958 E959 W960 K963 E964 C965 R966 K967 Y968
K969 M970 S973 T974 L975 L980 S981 I982 S983 N984 N985 T986 P987 E990 L991 T992 N993 A994 N997 G998 R999 L1000 A1001 W1002 M1003 P1004 L1005 S1006 D1007 G1008 Q1013 D1016 G1019 P1020 I1023 S1026 N1031 T1034 M1035 N1036 I1037 V1040 H1041 N1042 F1043 K1044 L1050
D1051 T1052 P1053 E1054 G1055 R1056 H1057 G1058 L1059 I1060 T1061 L1062 L1063 R1064 T1065 A1066 S1067 I1068 L1069 G1072 Q1073 M1074 Q1075 F1076 S1077 N1081 E1082 V1083 L1084 K1085 K1086 A1087 Q1088 Q1089 E1090 P1091 E1092 K1093 Y1094 R1095 D1096 L1097 I1098 V1099 R1100 V1101 A1102 G1103 Y1104 S1105 A1106 Y1107 F1108 V1109 E1110 L1111 C1112 K1113
E1114 V1115 Q1116 D1117 E1118 I1119 I1120 S1121 R1122 T1123 V1124 I1125 E1126 K1127 F1128

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	88.37Å 117.57Å 212.53Å 77.65° 85.34° 70.01°	Depositor
Resolution (Å)	44.57 – 2.90 48.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.57-2.90) 96.0 (48.73-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.220 , 0.295 0.219 , 0.293	Depositor DCC
R_{free} test set	8188 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	50317	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: A1H9L

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	0.60	0/6385	0.73	2/8640 (0.0%)
1	B	0.60	1/6385 (0.0%)	0.74	4/8640 (0.0%)
1	C	0.50	1/6385 (0.0%)	0.68	2/8640 (0.0%)
1	D	0.49	0/6385	0.68	3/8640 (0.0%)
1	E	0.47	0/6385	0.68	2/8640 (0.0%)
1	F	0.57	4/6385 (0.1%)	0.70	6/8640 (0.1%)
1	G	0.48	2/6385 (0.0%)	0.72	7/8640 (0.1%)
1	H	0.44	0/6385	0.66	1/8640 (0.0%)
All	All	0.52	8/51080 (0.0%)	0.70	27/69120 (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	B	0	1
1	E	0	3
1	F	0	1
1	G	0	6
1	H	0	5
All	All	0	16

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	356	PRO	N-CD	-15.93	1.25	1.47
1	F	912	LYS	CD-CE	10.02	1.76	1.51
1	G	822	ARG	CZ-NH1	9.73	1.45	1.33
1	F	912	LYS	CB-CG	9.32	1.77	1.52
1	G	822	ARG	CD-NE	7.39	1.59	1.46

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	822	ARG	NE-CZ-NH2	-19.50	110.55	120.30
1	G	640	LEU	CA-CB-CG	8.69	135.28	115.30
1	G	340	LEU	CB-CG-CD1	-8.53	96.50	111.00
1	B	753	MET	CG-SD-CE	-7.78	87.75	100.20
1	G	822	ARG	NH1-CZ-NH2	7.46	127.60	119.40

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	981	SER	Peptide
1	E	353	THR	Peptide
1	E	377	PRO	Peptide
1	E	640	LEU	Peptide
1	F	785	SER	Peptide

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	6254	0	6171	203	3
1	B	6254	0	6171	202	2
1	C	6254	0	6171	300	0
1	D	6254	0	6171	309	3
1	E	6254	0	6171	311	1
1	F	6254	0	6171	329	2
1	G	6254	0	6171	398	1
1	H	6254	0	6171	363	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	1	0
2	D	8	0	0	1	0
2	E	8	0	0	1	0
2	F	8	0	0	0	0
2	G	8	0	0	1	0
2	H	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	67	0	0	4	0
3	B	45	0	0	3	0
3	C	40	0	0	6	0
3	D	22	0	0	2	0
3	E	17	0	0	5	0
3	F	17	0	0	1	0
3	G	6	0	0	1	0
3	H	7	0	0	1	0
All	All	50317	0	49368	2385	6

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 24.

The worst 5 of 2385 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:912:LYS:CD	1:F:912:LYS:CE	1.76	1.63
1:F:912:LYS:CG	1:F:912:LYS:CB	1.77	1.61
1:H:568:GLU:OE1	1:H:570:ASN:N	1.72	1.20
1:A:957:ILE:HD12	1:A:958:THR:N	1.56	1.19
1:G:957:ILE:HD12	1:G:958:THR:N	1.58	1.17

The worst 5 of 6 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:A:1054:GLU:OE2	1:D:913:LYS:NZ[1_655]	1.23	0.97
1:A:1054:GLU:OE2	1:D:913:LYS:CE[1_655]	1.93	0.27
1:F:822:ARG:O	1:G:819:ARG:NH2[1_455]	2.06	0.14
1:B:808:ASP:OD1	1:F:346:ARG:NH2[1_556]	2.17	0.03
1:A:1054:GLU:OE2	1:D:913:LYS:CD[1_655]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	790/1150 (69%)	727 (92%)	63 (8%)	0	100 100
1	B	790/1150 (69%)	726 (92%)	62 (8%)	2 (0%)	41 71
1	C	790/1150 (69%)	708 (90%)	81 (10%)	1 (0%)	51 82
1	D	790/1150 (69%)	701 (89%)	89 (11%)	0	100 100
1	E	790/1150 (69%)	723 (92%)	67 (8%)	0	100 100
1	F	790/1150 (69%)	710 (90%)	79 (10%)	1 (0%)	51 82
1	G	790/1150 (69%)	711 (90%)	78 (10%)	1 (0%)	51 82
1	H	790/1150 (69%)	717 (91%)	73 (9%)	0	100 100
All	All	6320/9200 (69%)	5723 (91%)	592 (9%)	5 (0%)	51 82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	982	ILE
1	B	427	ASP
1	C	982	ILE
1	G	982	ILE
1	F	982	ILE

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	668/955 (70%)	655 (98%)	13 (2%)	57 84
1	B	668/955 (70%)	656 (98%)	12 (2%)	59 85
1	C	668/955 (70%)	651 (98%)	17 (2%)	47 78
1	D	668/955 (70%)	652 (98%)	16 (2%)	49 79
1	E	668/955 (70%)	643 (96%)	25 (4%)	34 68
1	F	668/955 (70%)	657 (98%)	11 (2%)	62 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	668/955 (70%)	651 (98%)	17 (2%)	47 78
1	H	668/955 (70%)	650 (97%)	18 (3%)	44 77
All	All	5344/7640 (70%)	5215 (98%)	129 (2%)	49 79

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	578	LEU
1	H	819	ARG
1	D	729	LYS
1	D	710	TYR
1	H	935	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	749	HIS
1	H	744	HIS
1	G	1013	GLN
1	H	373	ASN
1	H	1013	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	A1H9L	G	1201	-	5,7,7	1.78	2 (40%)	7,9,9	2.00	1 (14%)
2	A1H9L	B	1201	-	5,7,7	1.88	2 (40%)	7,9,9	2.23	1 (14%)
2	A1H9L	E	1201	-	5,7,7	1.92	1 (20%)	7,9,9	1.66	1 (14%)
2	A1H9L	D	1201	-	5,7,7	1.88	2 (40%)	7,9,9	1.96	1 (14%)
2	A1H9L	C	1201	-	5,7,7	1.90	2 (40%)	7,9,9	1.97	1 (14%)
2	A1H9L	F	1201	-	5,7,7	1.70	2 (40%)	7,9,9	1.01	1 (14%)
2	A1H9L	H	1201	-	5,7,7	1.88	3 (60%)	7,9,9	1.72	1 (14%)
2	A1H9L	A	1201	-	5,7,7	1.92	2 (40%)	7,9,9	1.79	1 (14%)

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	A1H9L	G	1201	-	-	2/4/7/7	-
2	A1H9L	B	1201	-	-	1/4/7/7	-
2	A1H9L	E	1201	-	-	1/4/7/7	-
2	A1H9L	D	1201	-	-	1/4/7/7	-
2	A1H9L	C	1201	-	-	1/4/7/7	-
2	A1H9L	F	1201	-	-	4/4/7/7	-
2	A1H9L	H	1201	-	-	1/4/7/7	-
2	A1H9L	A	1201	-	-	0/4/7/7	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	A1H9L	C4-N3	-3.21	1.45	1.52
2	E	1201	A1H9L	C4-N3	-3.19	1.45	1.52
2	D	1201	A1H9L	C4-N3	-2.91	1.46	1.52
2	A	1201	A1H9L	C4-N3	-2.90	1.46	1.52
2	B	1201	A1H9L	C4-N3	-2.64	1.46	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	A1H9L	C5-C4-N3	-5.78	105.45	115.78
2	G	1201	A1H9L	C5-C4-N3	-5.10	106.66	115.78
2	C	1201	A1H9L	C5-C4-N3	-5.09	106.68	115.78
2	D	1201	A1H9L	C5-C4-N3	-4.59	107.58	115.78
2	H	1201	A1H9L	C5-C4-N3	-4.43	107.87	115.78

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	A1H9L	N3-C4-C5-F6
2	C	1201	A1H9L	N3-C4-C5-F6
2	D	1201	A1H9L	N3-C4-C5-F6
2	E	1201	A1H9L	N3-C4-C5-F6
2	F	1201	A1H9L	N3-C4-C5-F6

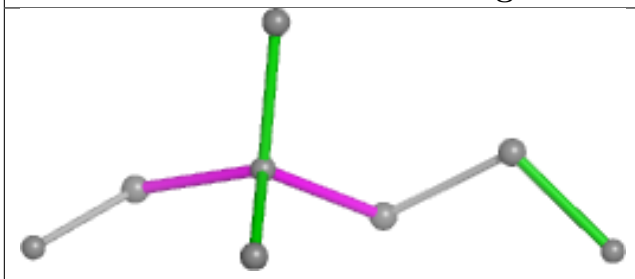
There are no ring outliers.

5 monomers are involved in 5 short contacts:

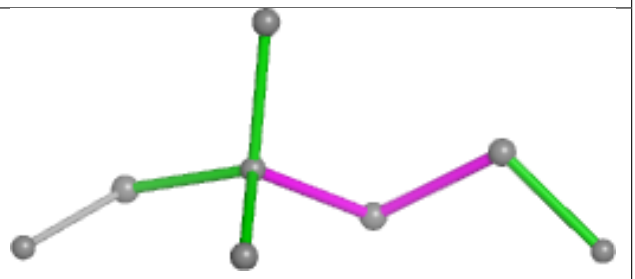
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1201	A1H9L	1	0
2	E	1201	A1H9L	1	0
2	D	1201	A1H9L	1	0
2	C	1201	A1H9L	1	0
2	H	1201	A1H9L	1	0

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.

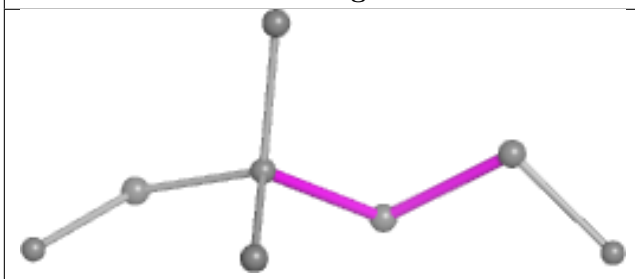
Ligand A1H9L G 1201



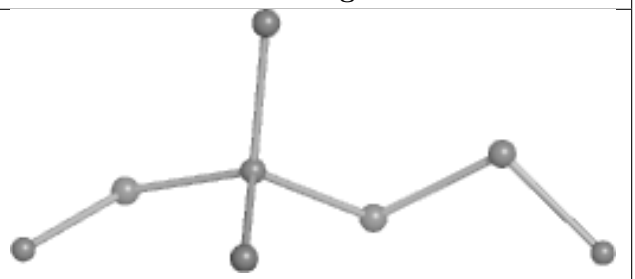
Bond lengths



Bond angles

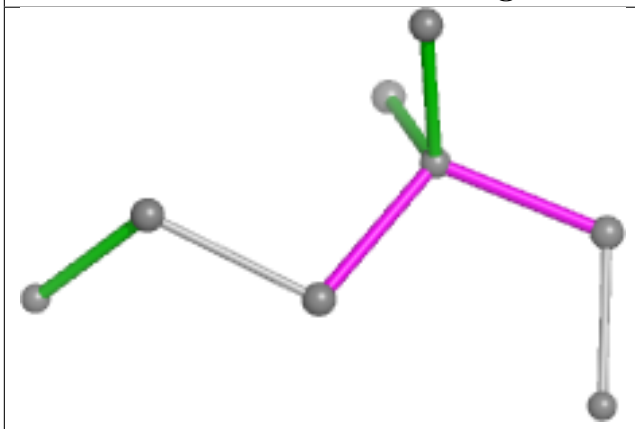


Torsions

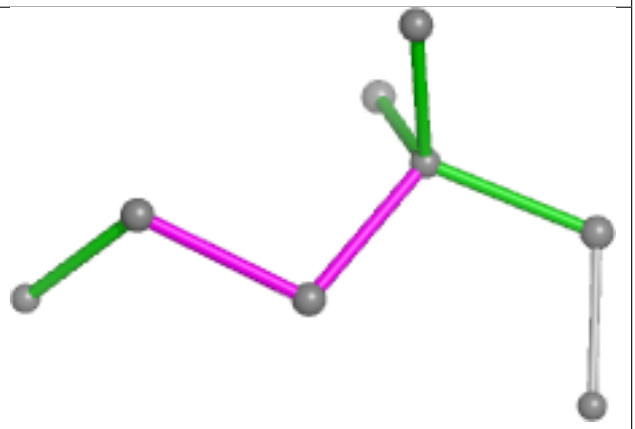


Rings

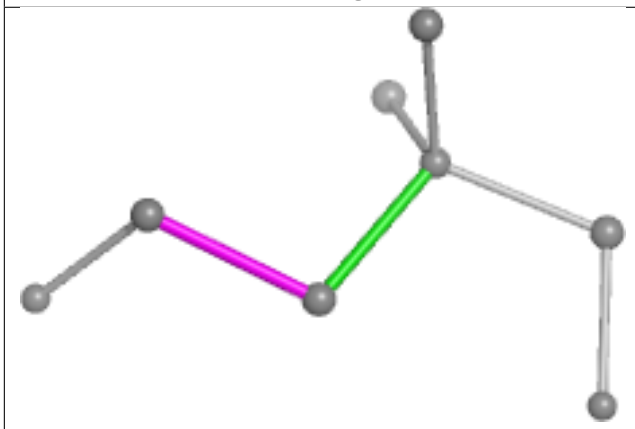
Ligand A1H9L B 1201



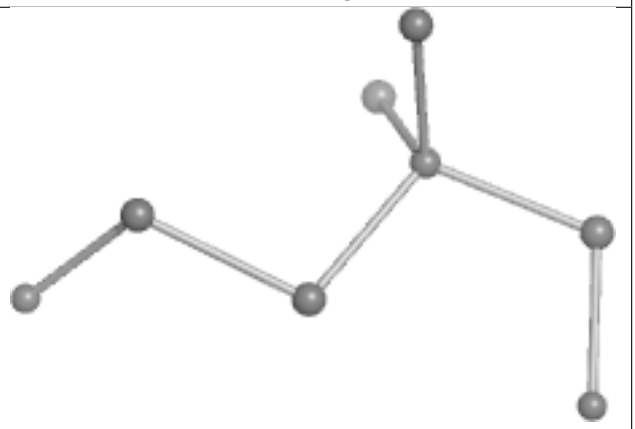
Bond lengths



Bond angles

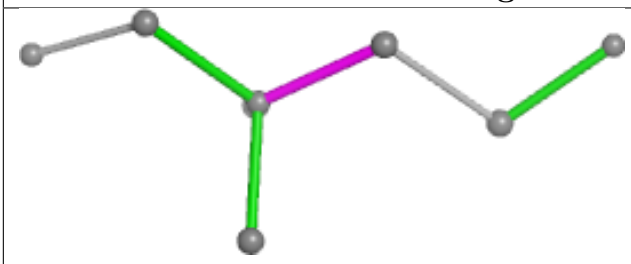


Torsions

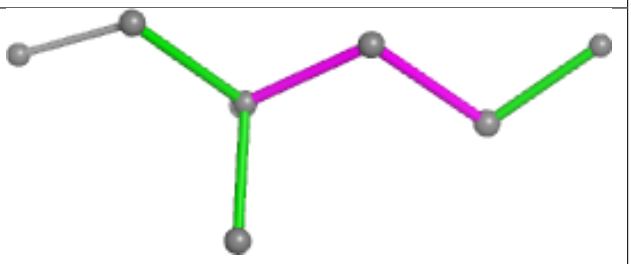


Rings

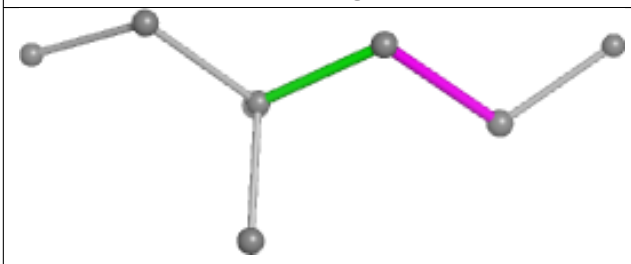
Ligand A1H9L E 1201



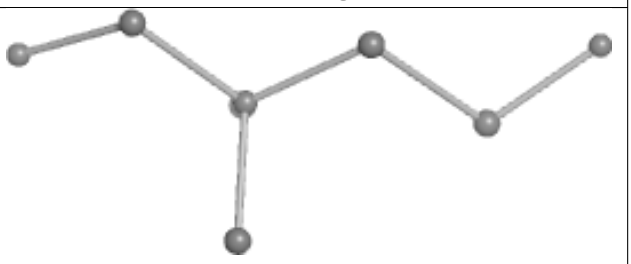
Bond lengths



Bond angles

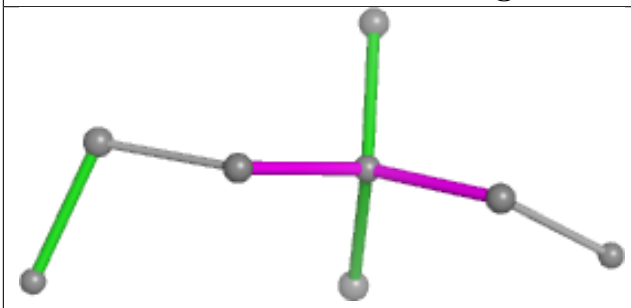


Torsions

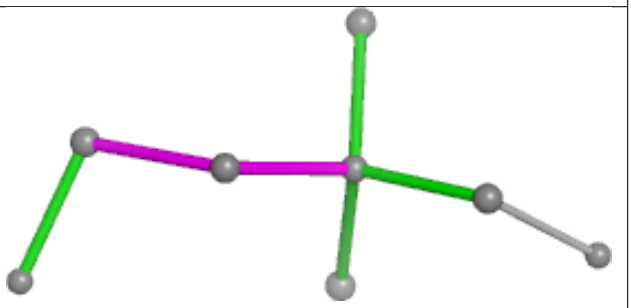


Rings

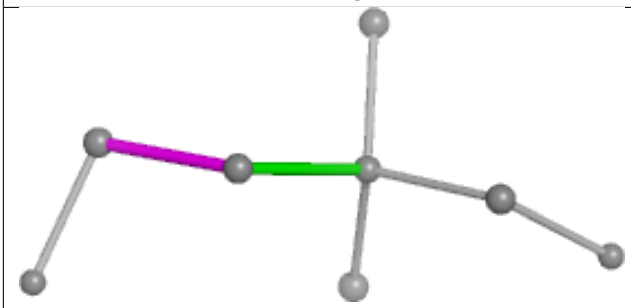
Ligand A1H9L D 1201



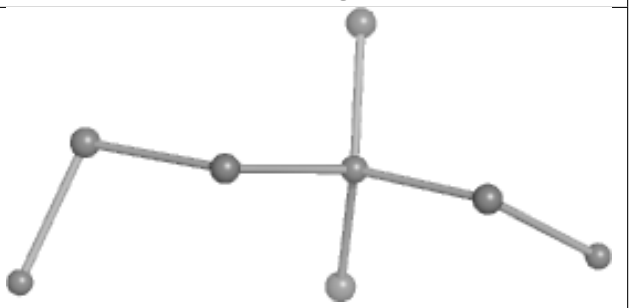
Bond lengths



Bond angles

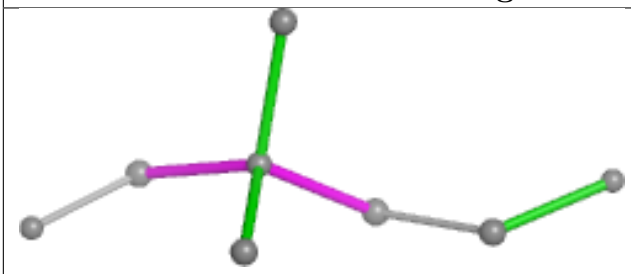


Torsions



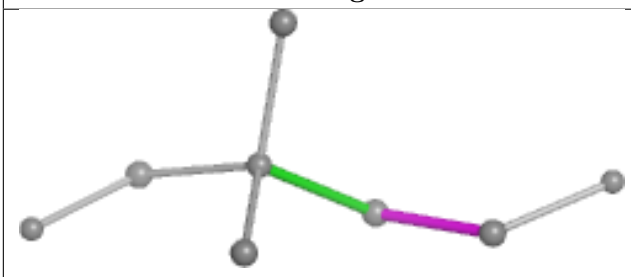
Rings

Ligand A1H9L C 1201

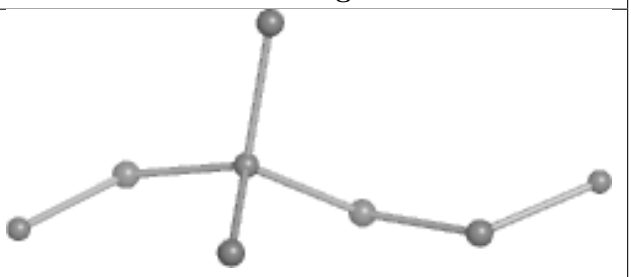


Bond lengths

Bond angles

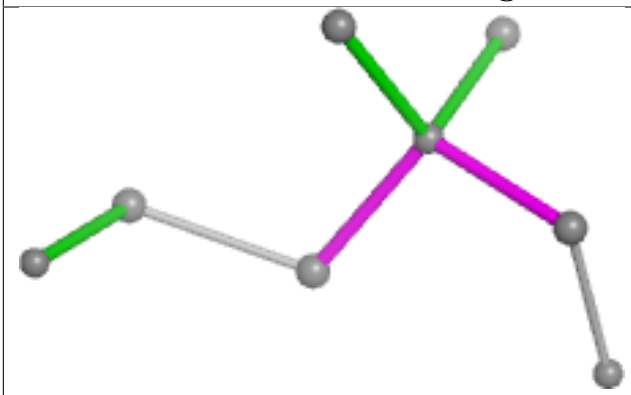


Torsions

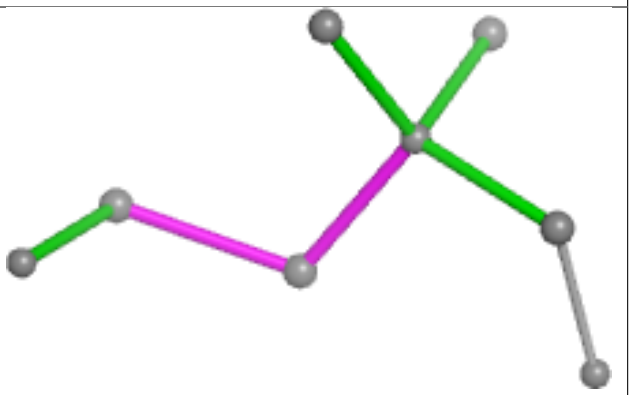


Rings

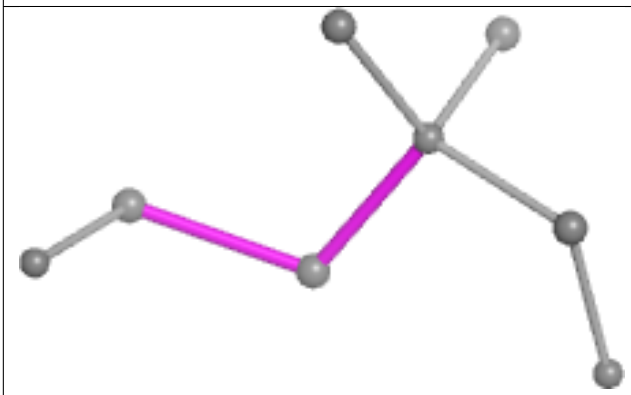
Ligand A1H9L F 1201



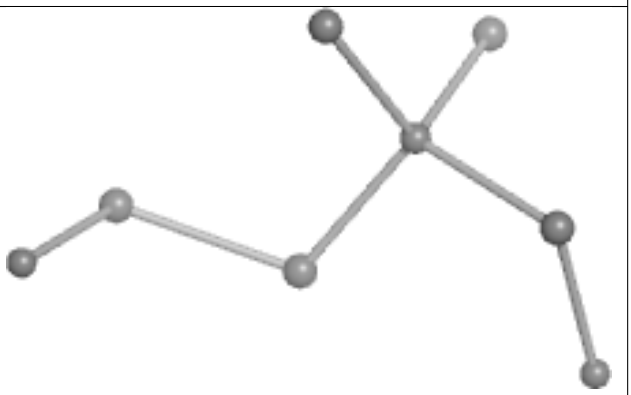
Bond lengths



Bond angles

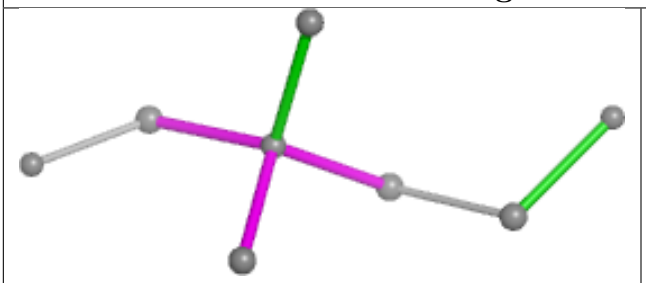


Torsions



Rings

Ligand A1H9L H 1201



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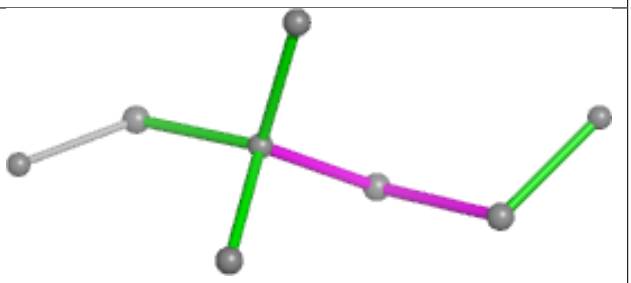
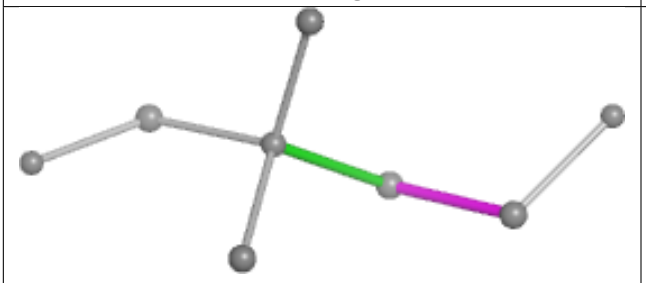
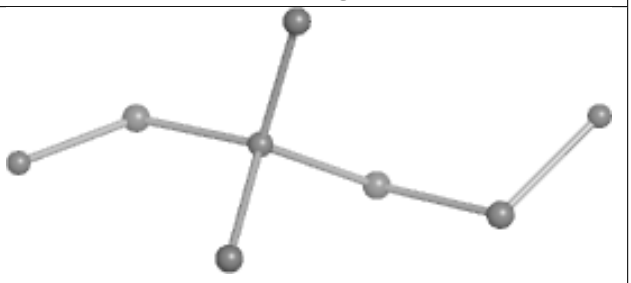


Bond angles

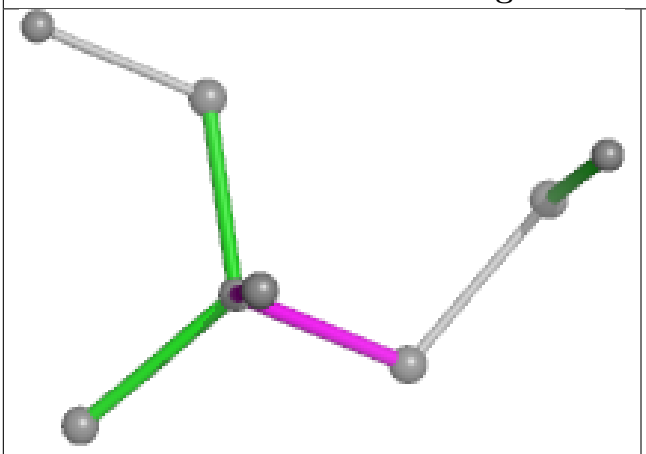


Torsions

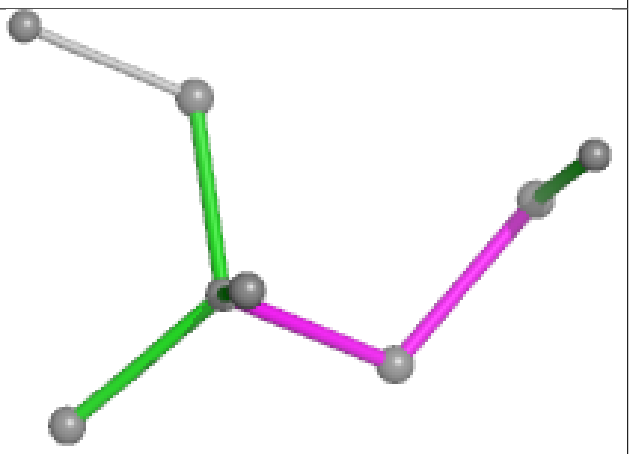


Rings

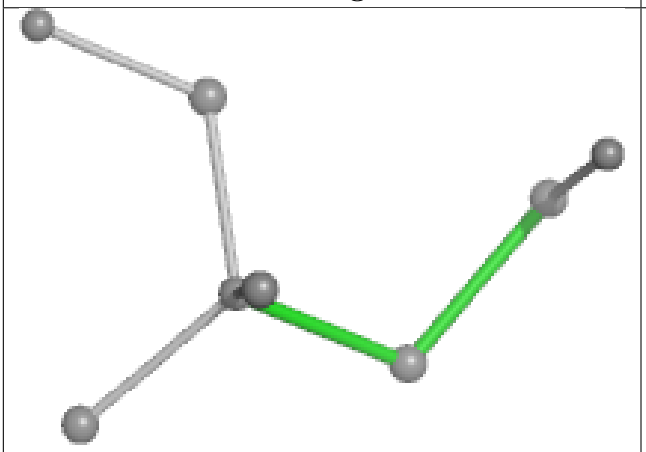
Ligand A1H9L A 1201



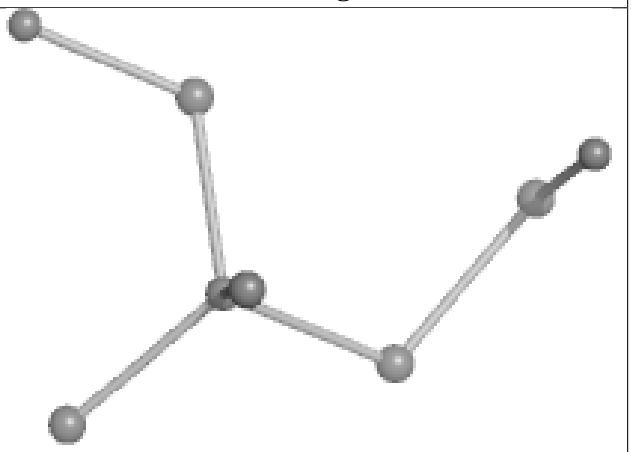
Bond lengths



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	792/1150 (68%)	-0.55	1 (0%) 95 96	15, 28, 50, 86	0
1	B	792/1150 (68%)	-0.51	1 (0%) 95 96	14, 29, 46, 67	0
1	C	792/1150 (68%)	-0.03	15 (1%) 66 65	28, 51, 70, 112	0
1	D	792/1150 (68%)	0.04	15 (1%) 66 65	24, 59, 81, 102	0
1	E	792/1150 (68%)	0.21	34 (4%) 35 31	26, 65, 102, 121	0
1	F	792/1150 (68%)	0.11	39 (4%) 29 26	28, 54, 77, 95	0
1	G	792/1150 (68%)	0.53	74 (9%) 8 6	40, 72, 101, 113	0
1	H	792/1150 (68%)	0.25	30 (3%) 40 36	39, 71, 96, 121	0
All	All	6336/9200 (68%)	0.01	209 (3%) 46 41	14, 54, 90, 121	0

The worst 5 of 209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	916	LEU	5.6
1	G	771	CYS	5.4
1	H	1091	PRO	5.0
1	E	909	PHE	5.0
1	E	919	ILE	4.9

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

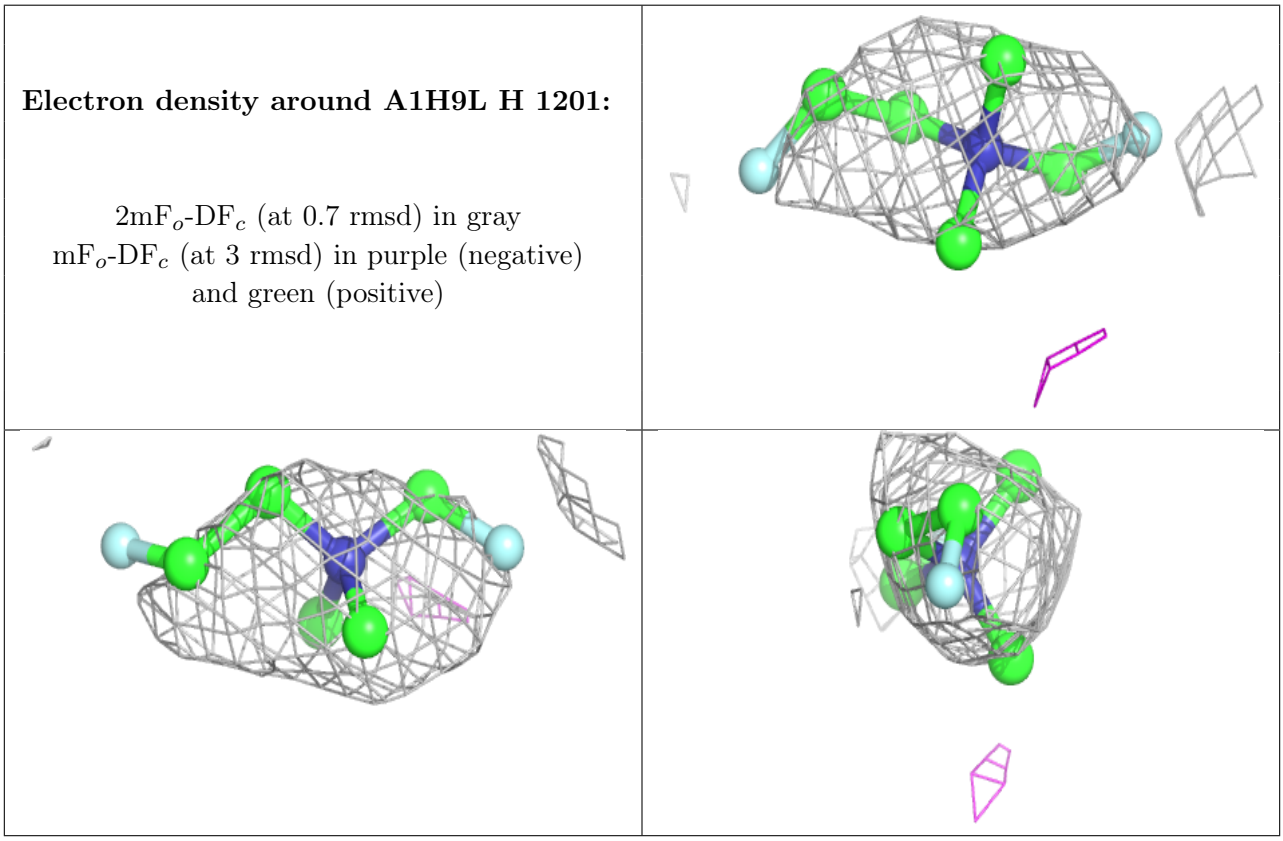
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A1H9L	H	1201	8/8	0.83	0.37	70,75,81,86	0
2	A1H9L	G	1201	8/8	0.86	0.31	62,71,75,75	0
2	A1H9L	D	1201	8/8	0.92	0.29	48,54,58,64	0
2	A1H9L	C	1201	8/8	0.93	0.31	40,43,51,64	0
2	A1H9L	E	1201	8/8	0.94	0.32	48,55,57,58	0
2	A1H9L	B	1201	8/8	0.96	0.17	20,23,27,30	0
2	A1H9L	F	1201	8/8	0.96	0.23	55,57,60,62	0
2	A1H9L	A	1201	8/8	0.97	0.18	18,25,29,41	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.

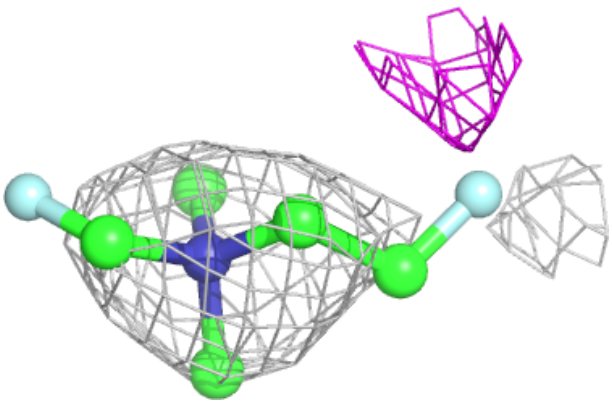
Electron density around A1H9L H 1201:

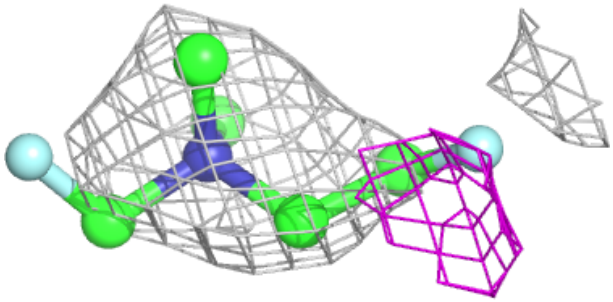
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

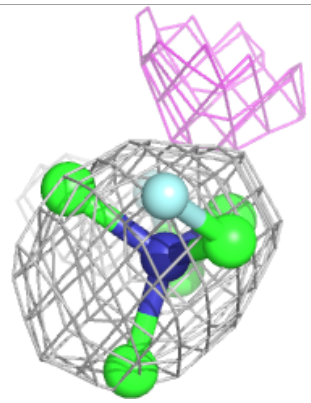


Electron density around A1H9L G 1201:

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

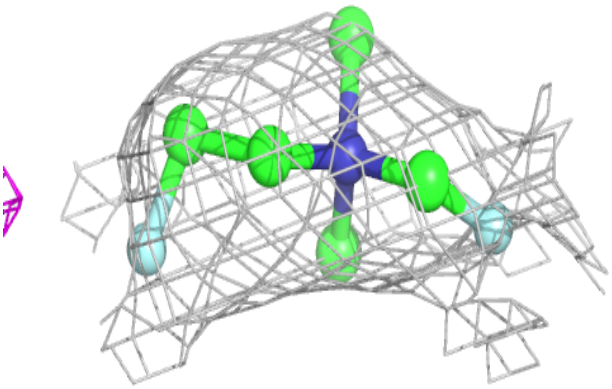


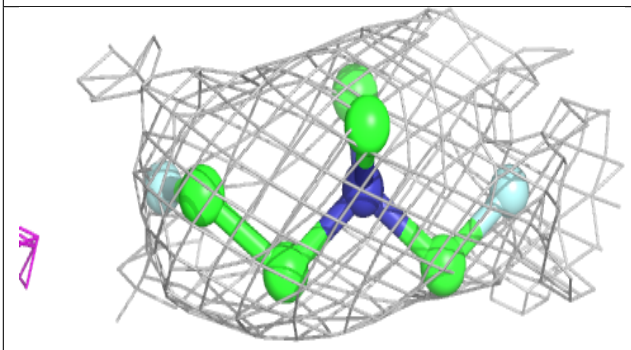


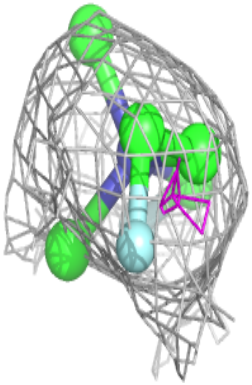


Electron density around A1H9L D 1201:

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

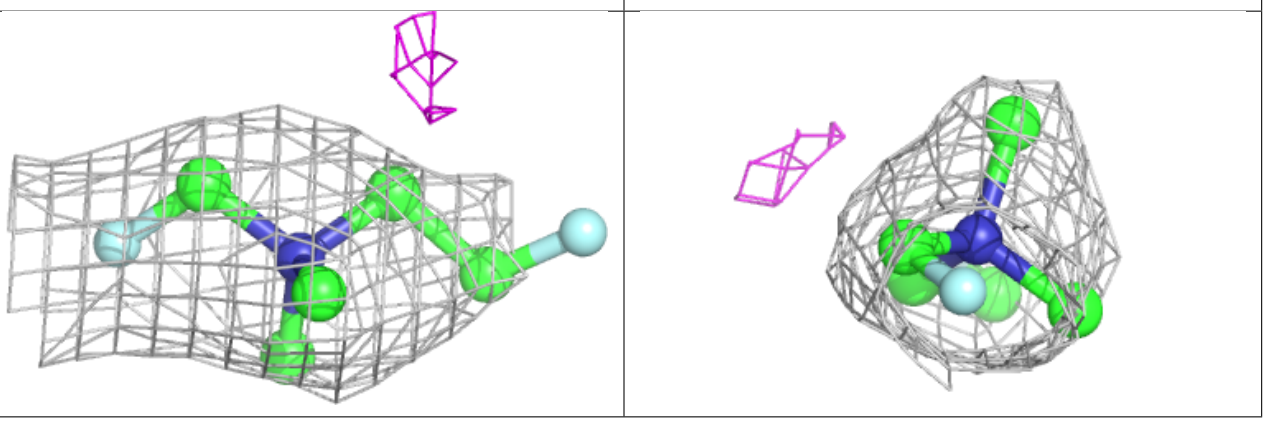






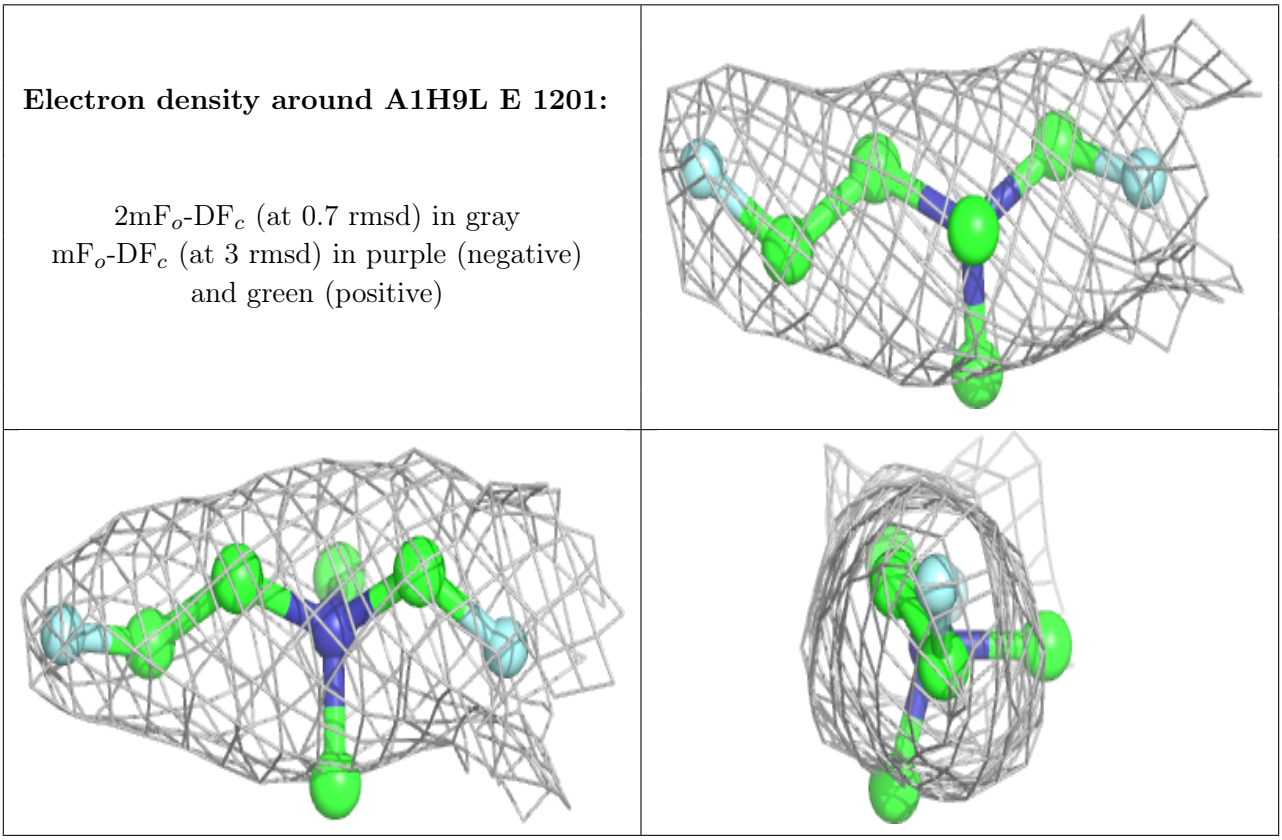
Electron density around A1H9L C 1201:

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



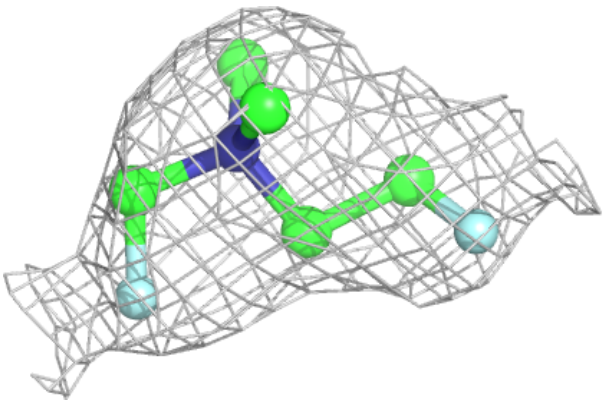
Electron density around A1H9L E 1201:

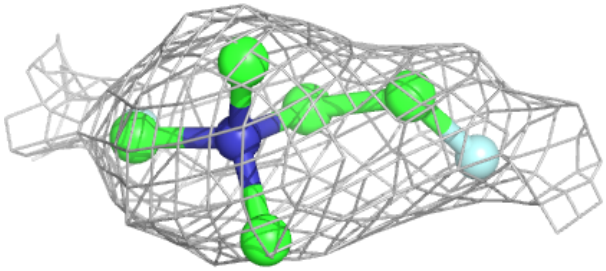
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

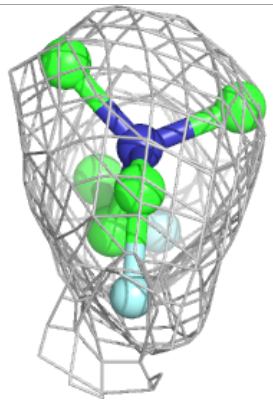


Electron density around A1H9L B 1201:

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

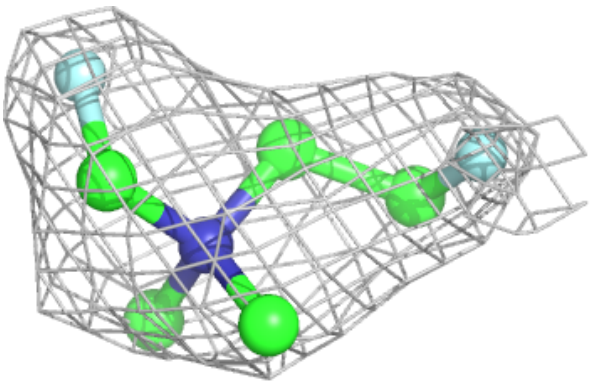


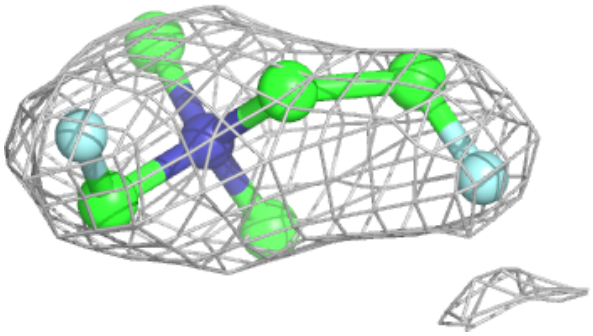


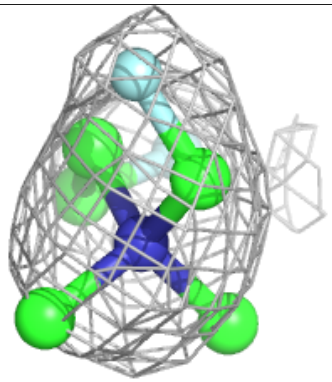


Electron density around A1H9L F 1201:

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

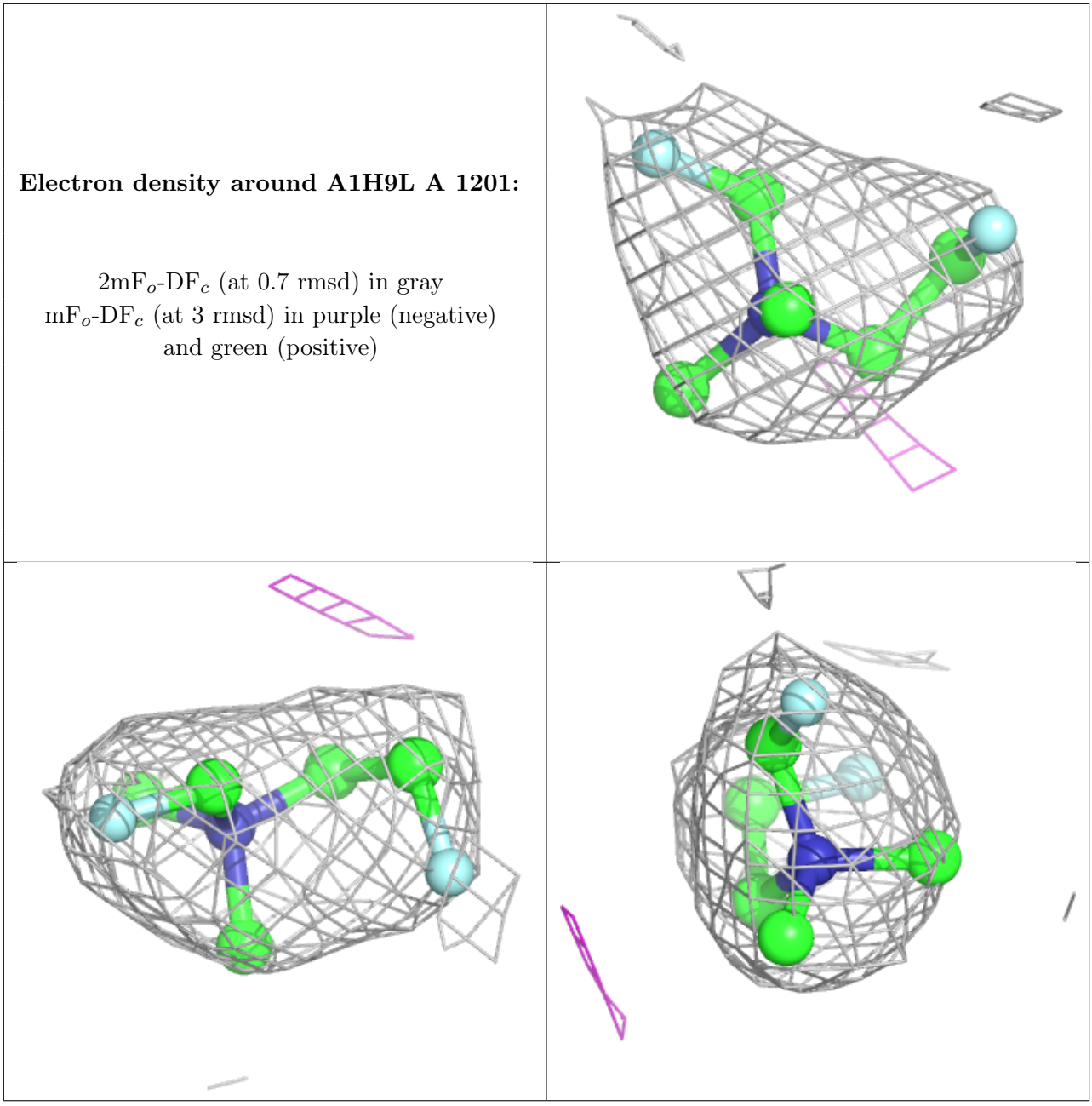






Electron density around A1H9L A 1201:

$2mF_o$-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

There are no such residues in this entry.