wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2024 – 02:17 PM EDT

PDB ID	:	8EY1
Title	:	Structure of Arabidopsis fatty acid amide hydrolase mutant S305A in complex with N-(3-oxododecanoyl)-L-homoserine lactone
Authors	:	Aziz, M.; Wang, X.; Gaguancela, O.A.; Chapman, K.D.
Deposited on	:	2022-10-26
Resolution	:	3.20 Å(reported)

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

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

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

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

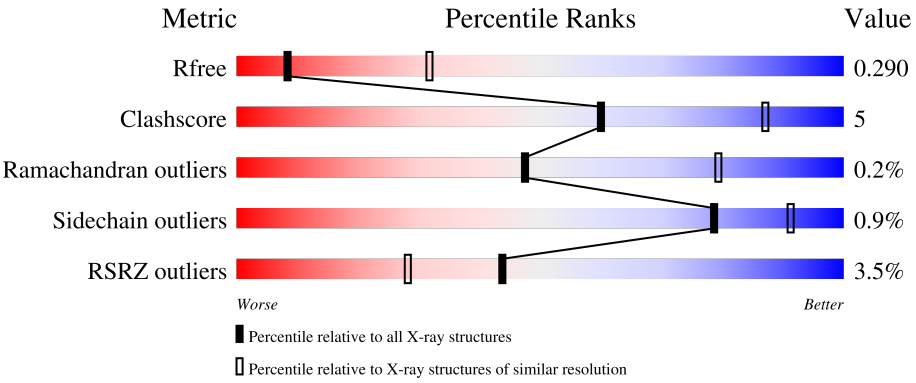
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	636	8% 81% 13% 5%
1	B	636	6% 79% 15% • 5%
1	C	636	3% 84% 10% 5%
1	D	636	2% 85% 10% 5%
1	E	636	7% 82% 13% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	636	4% 80% 15% 5%
1	G	636	2% 86% 8% 5%
1	H	636	2% 84% 13%
1	I	636	% 84% 10% 5%
1	J	636	2% 85% 11%
1	K	636	2% 87% 7% 5%
1	L	636	2% 82% 13% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OHN	F	700	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 55639 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 Fatty acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	B	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			
1	C	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	D	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			
1	E	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	F	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			
1	G	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	H	614	Total	C	N	O	S	0	0	0
			4700	2982	793	901	24			
1	I	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	J	614	Total	C	N	O	S	0	0	0
			4700	2982	793	901	24			
1	K	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	L	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	SER	engineered mutation	UNP Q7XJJ7
A	608	LYS	-	expression tag	UNP Q7XJJ7
A	609	GLY	-	expression tag	UNP Q7XJJ7
A	610	GLU	-	expression tag	UNP Q7XJJ7
A	611	PHE	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	GLU	-	expression tag	UNP Q7XJJ7
A	613	ALA	-	expression tag	UNP Q7XJJ7
A	614	TYR	-	expression tag	UNP Q7XJJ7
A	615	VAL	-	expression tag	UNP Q7XJJ7
A	616	GLU	-	expression tag	UNP Q7XJJ7
A	617	GLN	-	expression tag	UNP Q7XJJ7
A	618	LYS	-	expression tag	UNP Q7XJJ7
A	619	LEU	-	expression tag	UNP Q7XJJ7
A	620	ILE	-	expression tag	UNP Q7XJJ7
A	621	SER	-	expression tag	UNP Q7XJJ7
A	622	GLU	-	expression tag	UNP Q7XJJ7
A	623	GLU	-	expression tag	UNP Q7XJJ7
A	624	ASP	-	expression tag	UNP Q7XJJ7
A	625	LEU	-	expression tag	UNP Q7XJJ7
A	626	ASN	-	expression tag	UNP Q7XJJ7
A	627	SER	-	expression tag	UNP Q7XJJ7
A	628	ALA	-	expression tag	UNP Q7XJJ7
A	629	VAL	-	expression tag	UNP Q7XJJ7
A	630	ASP	-	expression tag	UNP Q7XJJ7
A	631	HIS	-	expression tag	UNP Q7XJJ7
A	632	HIS	-	expression tag	UNP Q7XJJ7
A	633	HIS	-	expression tag	UNP Q7XJJ7
A	634	HIS	-	expression tag	UNP Q7XJJ7
A	635	HIS	-	expression tag	UNP Q7XJJ7
A	636	HIS	-	expression tag	UNP Q7XJJ7
B	305	ALA	SER	engineered mutation	UNP Q7XJJ7
B	608	LYS	-	expression tag	UNP Q7XJJ7
B	609	GLY	-	expression tag	UNP Q7XJJ7
B	610	GLU	-	expression tag	UNP Q7XJJ7
B	611	PHE	-	expression tag	UNP Q7XJJ7
B	612	GLU	-	expression tag	UNP Q7XJJ7
B	613	ALA	-	expression tag	UNP Q7XJJ7
B	614	TYR	-	expression tag	UNP Q7XJJ7
B	615	VAL	-	expression tag	UNP Q7XJJ7
B	616	GLU	-	expression tag	UNP Q7XJJ7
B	617	GLN	-	expression tag	UNP Q7XJJ7
B	618	LYS	-	expression tag	UNP Q7XJJ7
B	619	LEU	-	expression tag	UNP Q7XJJ7
B	620	ILE	-	expression tag	UNP Q7XJJ7
B	621	SER	-	expression tag	UNP Q7XJJ7
B	622	GLU	-	expression tag	UNP Q7XJJ7
B	623	GLU	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	624	ASP	-	expression tag	UNP Q7XJJ7
B	625	LEU	-	expression tag	UNP Q7XJJ7
B	626	ASN	-	expression tag	UNP Q7XJJ7
B	627	SER	-	expression tag	UNP Q7XJJ7
B	628	ALA	-	expression tag	UNP Q7XJJ7
B	629	VAL	-	expression tag	UNP Q7XJJ7
B	630	ASP	-	expression tag	UNP Q7XJJ7
B	631	HIS	-	expression tag	UNP Q7XJJ7
B	632	HIS	-	expression tag	UNP Q7XJJ7
B	633	HIS	-	expression tag	UNP Q7XJJ7
B	634	HIS	-	expression tag	UNP Q7XJJ7
B	635	HIS	-	expression tag	UNP Q7XJJ7
B	636	HIS	-	expression tag	UNP Q7XJJ7
C	305	ALA	SER	engineered mutation	UNP Q7XJJ7
C	608	LYS	-	expression tag	UNP Q7XJJ7
C	609	GLY	-	expression tag	UNP Q7XJJ7
C	610	GLU	-	expression tag	UNP Q7XJJ7
C	611	PHE	-	expression tag	UNP Q7XJJ7
C	612	GLU	-	expression tag	UNP Q7XJJ7
C	613	ALA	-	expression tag	UNP Q7XJJ7
C	614	TYR	-	expression tag	UNP Q7XJJ7
C	615	VAL	-	expression tag	UNP Q7XJJ7
C	616	GLU	-	expression tag	UNP Q7XJJ7
C	617	GLN	-	expression tag	UNP Q7XJJ7
C	618	LYS	-	expression tag	UNP Q7XJJ7
C	619	LEU	-	expression tag	UNP Q7XJJ7
C	620	ILE	-	expression tag	UNP Q7XJJ7
C	621	SER	-	expression tag	UNP Q7XJJ7
C	622	GLU	-	expression tag	UNP Q7XJJ7
C	623	GLU	-	expression tag	UNP Q7XJJ7
C	624	ASP	-	expression tag	UNP Q7XJJ7
C	625	LEU	-	expression tag	UNP Q7XJJ7
C	626	ASN	-	expression tag	UNP Q7XJJ7
C	627	SER	-	expression tag	UNP Q7XJJ7
C	628	ALA	-	expression tag	UNP Q7XJJ7
C	629	VAL	-	expression tag	UNP Q7XJJ7
C	630	ASP	-	expression tag	UNP Q7XJJ7
C	631	HIS	-	expression tag	UNP Q7XJJ7
C	632	HIS	-	expression tag	UNP Q7XJJ7
C	633	HIS	-	expression tag	UNP Q7XJJ7
C	634	HIS	-	expression tag	UNP Q7XJJ7
C	635	HIS	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	636	HIS	-	expression tag	UNP Q7XJJ7
D	305	ALA	SER	engineered mutation	UNP Q7XJJ7
D	608	LYS	-	expression tag	UNP Q7XJJ7
D	609	GLY	-	expression tag	UNP Q7XJJ7
D	610	GLU	-	expression tag	UNP Q7XJJ7
D	611	PHE	-	expression tag	UNP Q7XJJ7
D	612	GLU	-	expression tag	UNP Q7XJJ7
D	613	ALA	-	expression tag	UNP Q7XJJ7
D	614	TYR	-	expression tag	UNP Q7XJJ7
D	615	VAL	-	expression tag	UNP Q7XJJ7
D	616	GLU	-	expression tag	UNP Q7XJJ7
D	617	GLN	-	expression tag	UNP Q7XJJ7
D	618	LYS	-	expression tag	UNP Q7XJJ7
D	619	LEU	-	expression tag	UNP Q7XJJ7
D	620	ILE	-	expression tag	UNP Q7XJJ7
D	621	SER	-	expression tag	UNP Q7XJJ7
D	622	GLU	-	expression tag	UNP Q7XJJ7
D	623	GLU	-	expression tag	UNP Q7XJJ7
D	624	ASP	-	expression tag	UNP Q7XJJ7
D	625	LEU	-	expression tag	UNP Q7XJJ7
D	626	ASN	-	expression tag	UNP Q7XJJ7
D	627	SER	-	expression tag	UNP Q7XJJ7
D	628	ALA	-	expression tag	UNP Q7XJJ7
D	629	VAL	-	expression tag	UNP Q7XJJ7
D	630	ASP	-	expression tag	UNP Q7XJJ7
D	631	HIS	-	expression tag	UNP Q7XJJ7
D	632	HIS	-	expression tag	UNP Q7XJJ7
D	633	HIS	-	expression tag	UNP Q7XJJ7
D	634	HIS	-	expression tag	UNP Q7XJJ7
D	635	HIS	-	expression tag	UNP Q7XJJ7
D	636	HIS	-	expression tag	UNP Q7XJJ7
E	305	ALA	SER	engineered mutation	UNP Q7XJJ7
E	608	LYS	-	expression tag	UNP Q7XJJ7
E	609	GLY	-	expression tag	UNP Q7XJJ7
E	610	GLU	-	expression tag	UNP Q7XJJ7
E	611	PHE	-	expression tag	UNP Q7XJJ7
E	612	GLU	-	expression tag	UNP Q7XJJ7
E	613	ALA	-	expression tag	UNP Q7XJJ7
E	614	TYR	-	expression tag	UNP Q7XJJ7
E	615	VAL	-	expression tag	UNP Q7XJJ7
E	616	GLU	-	expression tag	UNP Q7XJJ7
E	617	GLN	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	618	LYS	-	expression tag	UNP Q7XJJ7
E	619	LEU	-	expression tag	UNP Q7XJJ7
E	620	ILE	-	expression tag	UNP Q7XJJ7
E	621	SER	-	expression tag	UNP Q7XJJ7
E	622	GLU	-	expression tag	UNP Q7XJJ7
E	623	GLU	-	expression tag	UNP Q7XJJ7
E	624	ASP	-	expression tag	UNP Q7XJJ7
E	625	LEU	-	expression tag	UNP Q7XJJ7
E	626	ASN	-	expression tag	UNP Q7XJJ7
E	627	SER	-	expression tag	UNP Q7XJJ7
E	628	ALA	-	expression tag	UNP Q7XJJ7
E	629	VAL	-	expression tag	UNP Q7XJJ7
E	630	ASP	-	expression tag	UNP Q7XJJ7
E	631	HIS	-	expression tag	UNP Q7XJJ7
E	632	HIS	-	expression tag	UNP Q7XJJ7
E	633	HIS	-	expression tag	UNP Q7XJJ7
E	634	HIS	-	expression tag	UNP Q7XJJ7
E	635	HIS	-	expression tag	UNP Q7XJJ7
E	636	HIS	-	expression tag	UNP Q7XJJ7
F	305	ALA	SER	engineered mutation	UNP Q7XJJ7
F	608	LYS	-	expression tag	UNP Q7XJJ7
F	609	GLY	-	expression tag	UNP Q7XJJ7
F	610	GLU	-	expression tag	UNP Q7XJJ7
F	611	PHE	-	expression tag	UNP Q7XJJ7
F	612	GLU	-	expression tag	UNP Q7XJJ7
F	613	ALA	-	expression tag	UNP Q7XJJ7
F	614	TYR	-	expression tag	UNP Q7XJJ7
F	615	VAL	-	expression tag	UNP Q7XJJ7
F	616	GLU	-	expression tag	UNP Q7XJJ7
F	617	GLN	-	expression tag	UNP Q7XJJ7
F	618	LYS	-	expression tag	UNP Q7XJJ7
F	619	LEU	-	expression tag	UNP Q7XJJ7
F	620	ILE	-	expression tag	UNP Q7XJJ7
F	621	SER	-	expression tag	UNP Q7XJJ7
F	622	GLU	-	expression tag	UNP Q7XJJ7
F	623	GLU	-	expression tag	UNP Q7XJJ7
F	624	ASP	-	expression tag	UNP Q7XJJ7
F	625	LEU	-	expression tag	UNP Q7XJJ7
F	626	ASN	-	expression tag	UNP Q7XJJ7
F	627	SER	-	expression tag	UNP Q7XJJ7
F	628	ALA	-	expression tag	UNP Q7XJJ7
F	629	VAL	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	630	ASP	-	expression tag	UNP Q7XJJ7
F	631	HIS	-	expression tag	UNP Q7XJJ7
F	632	HIS	-	expression tag	UNP Q7XJJ7
F	633	HIS	-	expression tag	UNP Q7XJJ7
F	634	HIS	-	expression tag	UNP Q7XJJ7
F	635	HIS	-	expression tag	UNP Q7XJJ7
F	636	HIS	-	expression tag	UNP Q7XJJ7
G	305	ALA	SER	engineered mutation	UNP Q7XJJ7
G	608	LYS	-	expression tag	UNP Q7XJJ7
G	609	GLY	-	expression tag	UNP Q7XJJ7
G	610	GLU	-	expression tag	UNP Q7XJJ7
G	611	PHE	-	expression tag	UNP Q7XJJ7
G	612	GLU	-	expression tag	UNP Q7XJJ7
G	613	ALA	-	expression tag	UNP Q7XJJ7
G	614	TYR	-	expression tag	UNP Q7XJJ7
G	615	VAL	-	expression tag	UNP Q7XJJ7
G	616	GLU	-	expression tag	UNP Q7XJJ7
G	617	GLN	-	expression tag	UNP Q7XJJ7
G	618	LYS	-	expression tag	UNP Q7XJJ7
G	619	LEU	-	expression tag	UNP Q7XJJ7
G	620	ILE	-	expression tag	UNP Q7XJJ7
G	621	SER	-	expression tag	UNP Q7XJJ7
G	622	GLU	-	expression tag	UNP Q7XJJ7
G	623	GLU	-	expression tag	UNP Q7XJJ7
G	624	ASP	-	expression tag	UNP Q7XJJ7
G	625	LEU	-	expression tag	UNP Q7XJJ7
G	626	ASN	-	expression tag	UNP Q7XJJ7
G	627	SER	-	expression tag	UNP Q7XJJ7
G	628	ALA	-	expression tag	UNP Q7XJJ7
G	629	VAL	-	expression tag	UNP Q7XJJ7
G	630	ASP	-	expression tag	UNP Q7XJJ7
G	631	HIS	-	expression tag	UNP Q7XJJ7
G	632	HIS	-	expression tag	UNP Q7XJJ7
G	633	HIS	-	expression tag	UNP Q7XJJ7
G	634	HIS	-	expression tag	UNP Q7XJJ7
G	635	HIS	-	expression tag	UNP Q7XJJ7
G	636	HIS	-	expression tag	UNP Q7XJJ7
H	305	ALA	SER	engineered mutation	UNP Q7XJJ7
H	608	LYS	-	expression tag	UNP Q7XJJ7
H	609	GLY	-	expression tag	UNP Q7XJJ7
H	610	GLU	-	expression tag	UNP Q7XJJ7
H	611	PHE	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	612	GLU	-	expression tag	UNP Q7XJJ7
H	613	ALA	-	expression tag	UNP Q7XJJ7
H	614	TYR	-	expression tag	UNP Q7XJJ7
H	615	VAL	-	expression tag	UNP Q7XJJ7
H	616	GLU	-	expression tag	UNP Q7XJJ7
H	617	GLN	-	expression tag	UNP Q7XJJ7
H	618	LYS	-	expression tag	UNP Q7XJJ7
H	619	LEU	-	expression tag	UNP Q7XJJ7
H	620	ILE	-	expression tag	UNP Q7XJJ7
H	621	SER	-	expression tag	UNP Q7XJJ7
H	622	GLU	-	expression tag	UNP Q7XJJ7
H	623	GLU	-	expression tag	UNP Q7XJJ7
H	624	ASP	-	expression tag	UNP Q7XJJ7
H	625	LEU	-	expression tag	UNP Q7XJJ7
H	626	ASN	-	expression tag	UNP Q7XJJ7
H	627	SER	-	expression tag	UNP Q7XJJ7
H	628	ALA	-	expression tag	UNP Q7XJJ7
H	629	VAL	-	expression tag	UNP Q7XJJ7
H	630	ASP	-	expression tag	UNP Q7XJJ7
H	631	HIS	-	expression tag	UNP Q7XJJ7
H	632	HIS	-	expression tag	UNP Q7XJJ7
H	633	HIS	-	expression tag	UNP Q7XJJ7
H	634	HIS	-	expression tag	UNP Q7XJJ7
H	635	HIS	-	expression tag	UNP Q7XJJ7
H	636	HIS	-	expression tag	UNP Q7XJJ7
I	305	ALA	SER	engineered mutation	UNP Q7XJJ7
I	608	LYS	-	expression tag	UNP Q7XJJ7
I	609	GLY	-	expression tag	UNP Q7XJJ7
I	610	GLU	-	expression tag	UNP Q7XJJ7
I	611	PHE	-	expression tag	UNP Q7XJJ7
I	612	GLU	-	expression tag	UNP Q7XJJ7
I	613	ALA	-	expression tag	UNP Q7XJJ7
I	614	TYR	-	expression tag	UNP Q7XJJ7
I	615	VAL	-	expression tag	UNP Q7XJJ7
I	616	GLU	-	expression tag	UNP Q7XJJ7
I	617	GLN	-	expression tag	UNP Q7XJJ7
I	618	LYS	-	expression tag	UNP Q7XJJ7
I	619	LEU	-	expression tag	UNP Q7XJJ7
I	620	ILE	-	expression tag	UNP Q7XJJ7
I	621	SER	-	expression tag	UNP Q7XJJ7
I	622	GLU	-	expression tag	UNP Q7XJJ7
I	623	GLU	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	624	ASP	-	expression tag	UNP Q7XJJ7
I	625	LEU	-	expression tag	UNP Q7XJJ7
I	626	ASN	-	expression tag	UNP Q7XJJ7
I	627	SER	-	expression tag	UNP Q7XJJ7
I	628	ALA	-	expression tag	UNP Q7XJJ7
I	629	VAL	-	expression tag	UNP Q7XJJ7
I	630	ASP	-	expression tag	UNP Q7XJJ7
I	631	HIS	-	expression tag	UNP Q7XJJ7
I	632	HIS	-	expression tag	UNP Q7XJJ7
I	633	HIS	-	expression tag	UNP Q7XJJ7
I	634	HIS	-	expression tag	UNP Q7XJJ7
I	635	HIS	-	expression tag	UNP Q7XJJ7
I	636	HIS	-	expression tag	UNP Q7XJJ7
J	305	ALA	SER	engineered mutation	UNP Q7XJJ7
J	608	LYS	-	expression tag	UNP Q7XJJ7
J	609	GLY	-	expression tag	UNP Q7XJJ7
J	610	GLU	-	expression tag	UNP Q7XJJ7
J	611	PHE	-	expression tag	UNP Q7XJJ7
J	612	GLU	-	expression tag	UNP Q7XJJ7
J	613	ALA	-	expression tag	UNP Q7XJJ7
J	614	TYR	-	expression tag	UNP Q7XJJ7
J	615	VAL	-	expression tag	UNP Q7XJJ7
J	616	GLU	-	expression tag	UNP Q7XJJ7
J	617	GLN	-	expression tag	UNP Q7XJJ7
J	618	LYS	-	expression tag	UNP Q7XJJ7
J	619	LEU	-	expression tag	UNP Q7XJJ7
J	620	ILE	-	expression tag	UNP Q7XJJ7
J	621	SER	-	expression tag	UNP Q7XJJ7
J	622	GLU	-	expression tag	UNP Q7XJJ7
J	623	GLU	-	expression tag	UNP Q7XJJ7
J	624	ASP	-	expression tag	UNP Q7XJJ7
J	625	LEU	-	expression tag	UNP Q7XJJ7
J	626	ASN	-	expression tag	UNP Q7XJJ7
J	627	SER	-	expression tag	UNP Q7XJJ7
J	628	ALA	-	expression tag	UNP Q7XJJ7
J	629	VAL	-	expression tag	UNP Q7XJJ7
J	630	ASP	-	expression tag	UNP Q7XJJ7
J	631	HIS	-	expression tag	UNP Q7XJJ7
J	632	HIS	-	expression tag	UNP Q7XJJ7
J	633	HIS	-	expression tag	UNP Q7XJJ7
J	634	HIS	-	expression tag	UNP Q7XJJ7
J	635	HIS	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

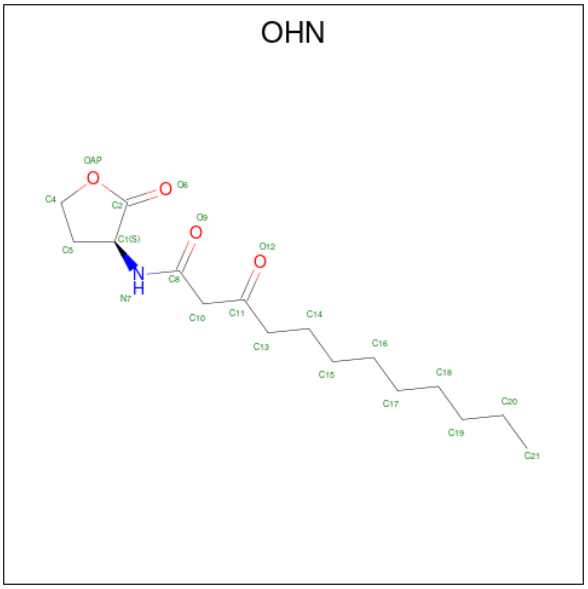
Chain	Residue	Modelled	Actual	Comment	Reference
J	636	HIS	-	expression tag	UNP Q7XJJ7
K	305	ALA	SER	engineered mutation	UNP Q7XJJ7
K	608	LYS	-	expression tag	UNP Q7XJJ7
K	609	GLY	-	expression tag	UNP Q7XJJ7
K	610	GLU	-	expression tag	UNP Q7XJJ7
K	611	PHE	-	expression tag	UNP Q7XJJ7
K	612	GLU	-	expression tag	UNP Q7XJJ7
K	613	ALA	-	expression tag	UNP Q7XJJ7
K	614	TYR	-	expression tag	UNP Q7XJJ7
K	615	VAL	-	expression tag	UNP Q7XJJ7
K	616	GLU	-	expression tag	UNP Q7XJJ7
K	617	GLN	-	expression tag	UNP Q7XJJ7
K	618	LYS	-	expression tag	UNP Q7XJJ7
K	619	LEU	-	expression tag	UNP Q7XJJ7
K	620	ILE	-	expression tag	UNP Q7XJJ7
K	621	SER	-	expression tag	UNP Q7XJJ7
K	622	GLU	-	expression tag	UNP Q7XJJ7
K	623	GLU	-	expression tag	UNP Q7XJJ7
K	624	ASP	-	expression tag	UNP Q7XJJ7
K	625	LEU	-	expression tag	UNP Q7XJJ7
K	626	ASN	-	expression tag	UNP Q7XJJ7
K	627	SER	-	expression tag	UNP Q7XJJ7
K	628	ALA	-	expression tag	UNP Q7XJJ7
K	629	VAL	-	expression tag	UNP Q7XJJ7
K	630	ASP	-	expression tag	UNP Q7XJJ7
K	631	HIS	-	expression tag	UNP Q7XJJ7
K	632	HIS	-	expression tag	UNP Q7XJJ7
K	633	HIS	-	expression tag	UNP Q7XJJ7
K	634	HIS	-	expression tag	UNP Q7XJJ7
K	635	HIS	-	expression tag	UNP Q7XJJ7
K	636	HIS	-	expression tag	UNP Q7XJJ7
L	305	ALA	SER	engineered mutation	UNP Q7XJJ7
L	608	LYS	-	expression tag	UNP Q7XJJ7
L	609	GLY	-	expression tag	UNP Q7XJJ7
L	610	GLU	-	expression tag	UNP Q7XJJ7
L	611	PHE	-	expression tag	UNP Q7XJJ7
L	612	GLU	-	expression tag	UNP Q7XJJ7
L	613	ALA	-	expression tag	UNP Q7XJJ7
L	614	TYR	-	expression tag	UNP Q7XJJ7
L	615	VAL	-	expression tag	UNP Q7XJJ7
L	616	GLU	-	expression tag	UNP Q7XJJ7
L	617	GLN	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	618	LYS	-	expression tag	UNP Q7XJJ7
L	619	LEU	-	expression tag	UNP Q7XJJ7
L	620	ILE	-	expression tag	UNP Q7XJJ7
L	621	SER	-	expression tag	UNP Q7XJJ7
L	622	GLU	-	expression tag	UNP Q7XJJ7
L	623	GLU	-	expression tag	UNP Q7XJJ7
L	624	ASP	-	expression tag	UNP Q7XJJ7
L	625	LEU	-	expression tag	UNP Q7XJJ7
L	626	ASN	-	expression tag	UNP Q7XJJ7
L	627	SER	-	expression tag	UNP Q7XJJ7
L	628	ALA	-	expression tag	UNP Q7XJJ7
L	629	VAL	-	expression tag	UNP Q7XJJ7
L	630	ASP	-	expression tag	UNP Q7XJJ7
L	631	HIS	-	expression tag	UNP Q7XJJ7
L	632	HIS	-	expression tag	UNP Q7XJJ7
L	633	HIS	-	expression tag	UNP Q7XJJ7
L	634	HIS	-	expression tag	UNP Q7XJJ7
L	635	HIS	-	expression tag	UNP Q7XJJ7
L	636	HIS	-	expression tag	UNP Q7XJJ7

- Molecule 2 is N-3-OXO-DODECANOYL-L-HOMOSERINE LACTONE (three-letter code: OHN) (formula: $C_{16}H_{27}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			21	16	1	4		

Continued on next page...

Continued from previous page...

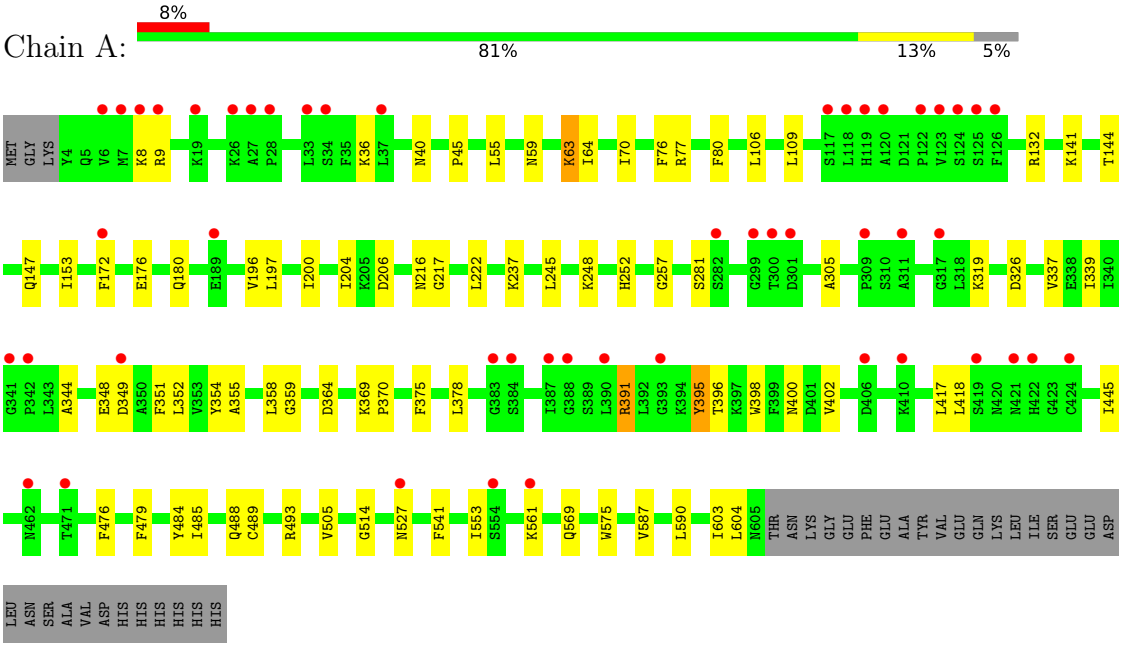
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			21	16	1	4		
2	H	1	Total	C	N	O	0	0
			21	16	1	4		
2	J	1	Total	C	N	O	0	0
			21	16	1	4		
2	L	1	Total	C	N	O	0	0
			21	16	1	4		

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.

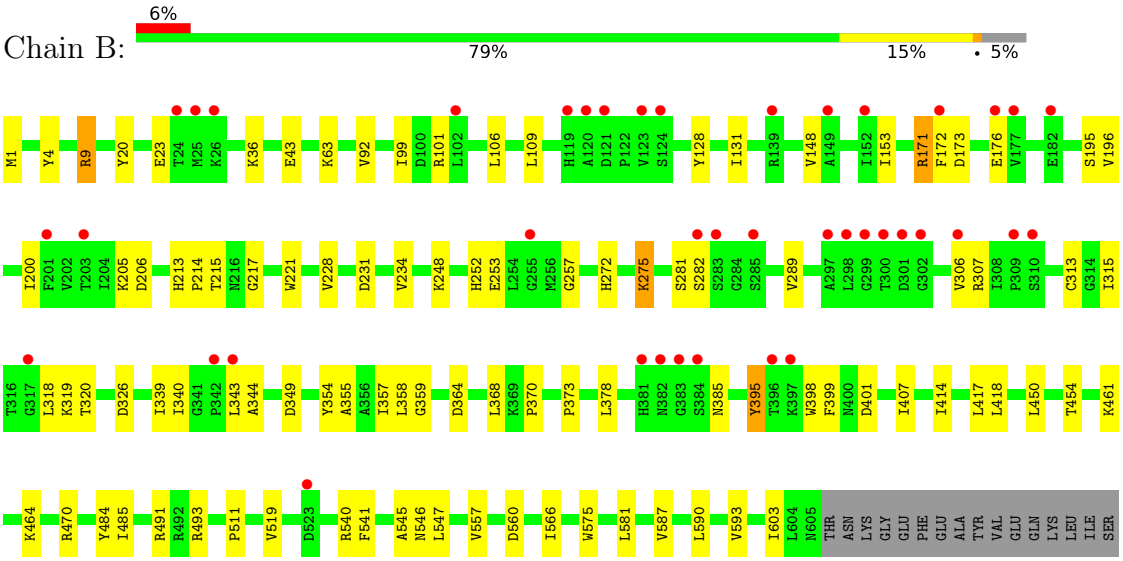
• Molecule 1: Fatty acid amide hydrolase

Chain A:



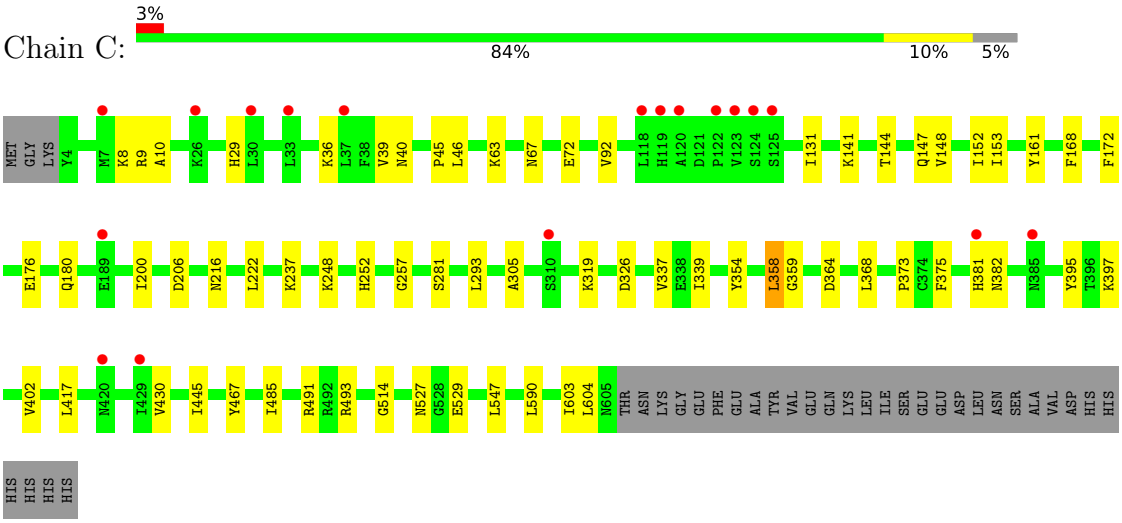
• Molecule 1: Fatty acid amide hydrolase

Chain B:



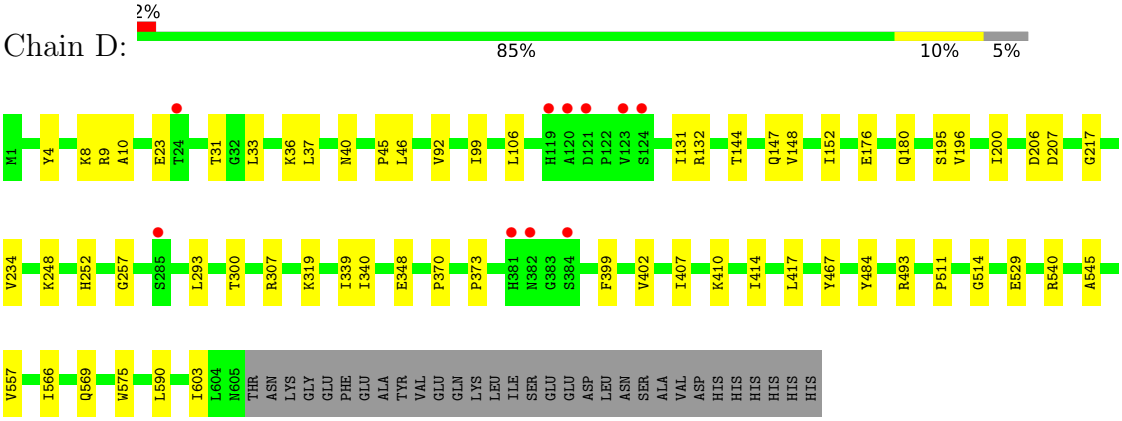
• Molecule 1: Fatty acid amide hydrolase

Chain C:



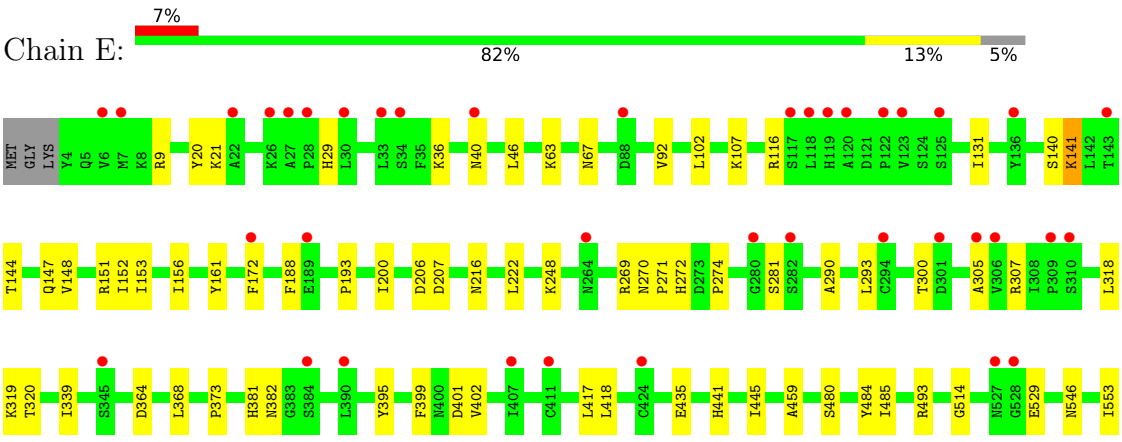
• Molecule 1: Fatty acid amide hydrolase

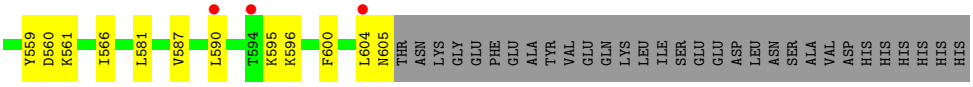
Chain D:



• Molecule 1: Fatty acid amide hydrolase

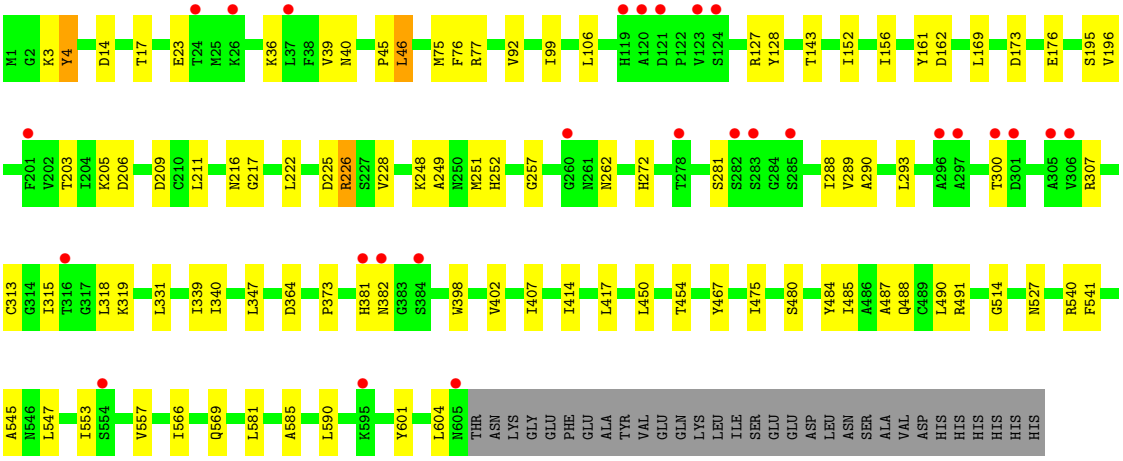
Chain E:





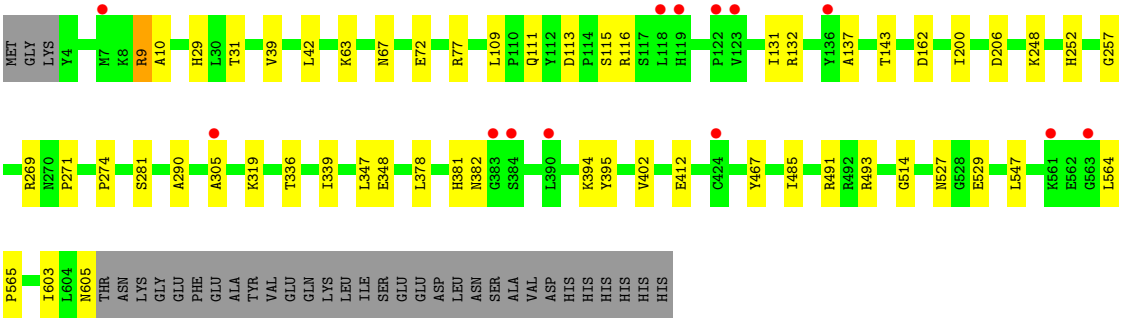
• Molecule 1: Fatty acid amide hydrolase

Chain F:



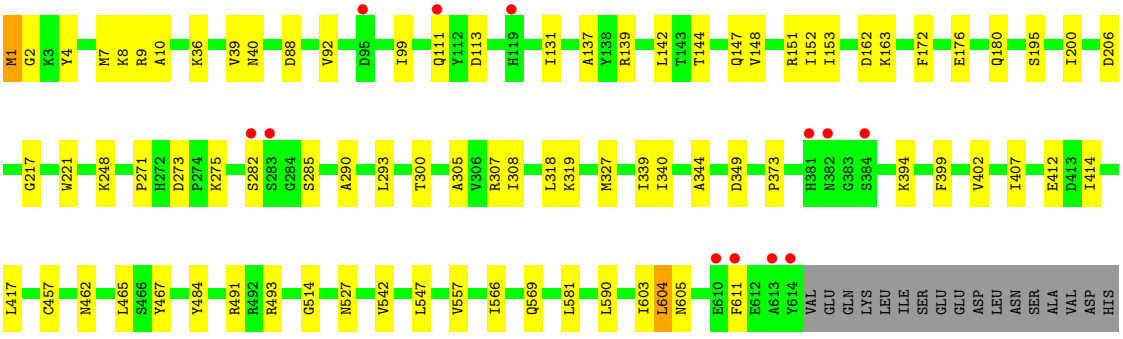
• Molecule 1: Fatty acid amide hydrolase

Chain G:



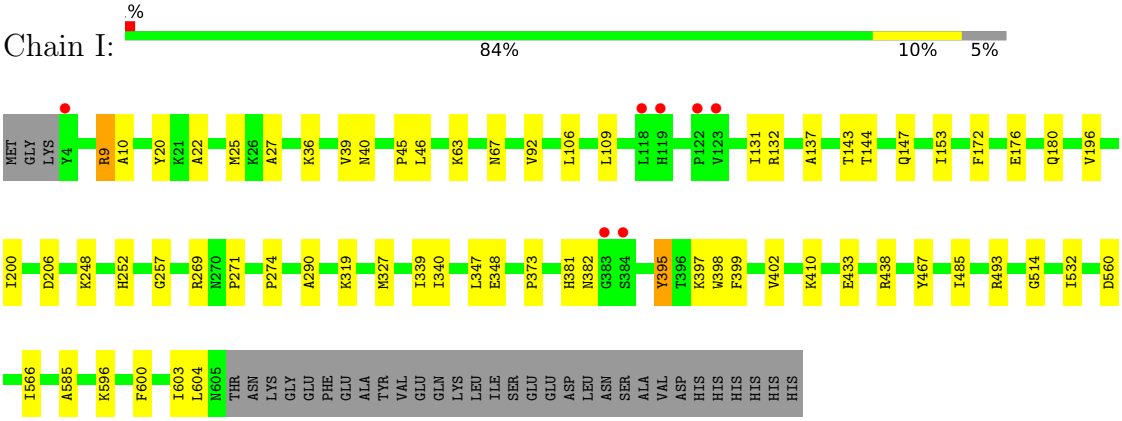
• Molecule 1: Fatty acid amide hydrolase

Chain H:



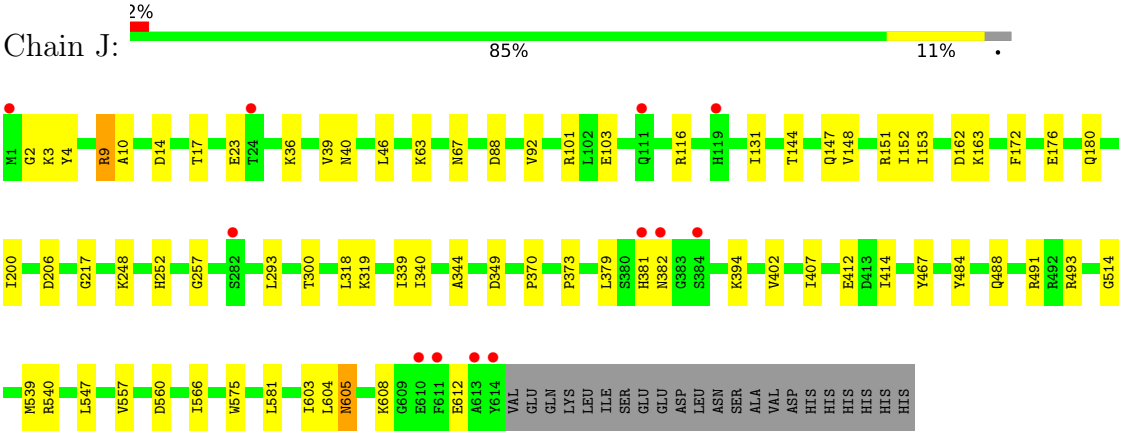
• Molecule 1: Fatty acid amide hydrolase

Chain I:



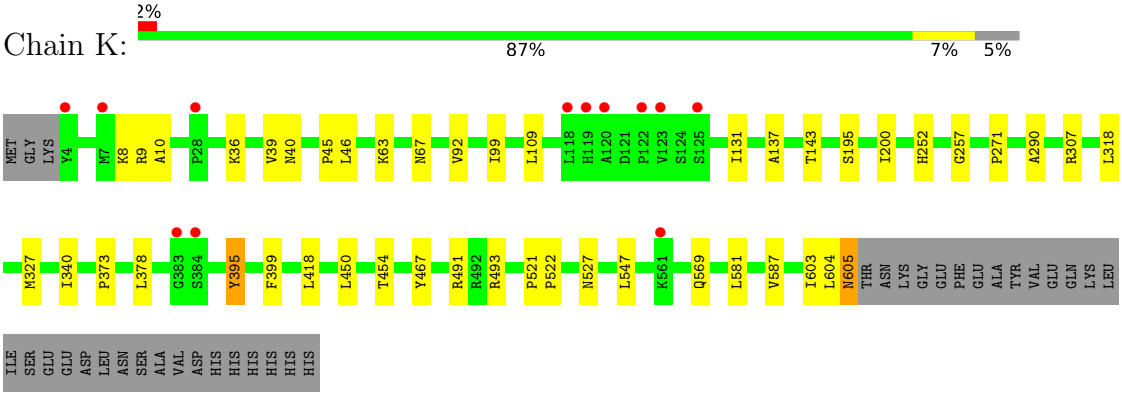
• Molecule 1: Fatty acid amide hydrolase

Chain J:



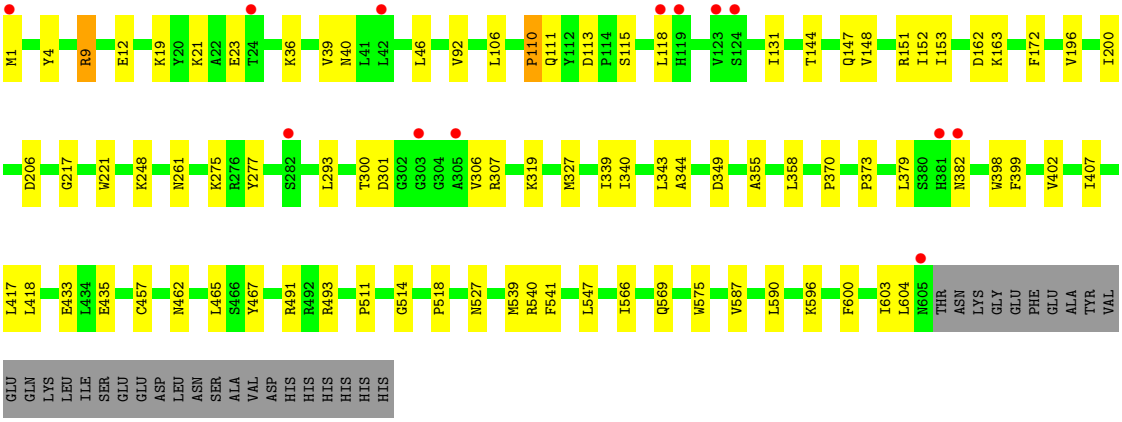
• Molecule 1: Fatty acid amide hydrolase

Chain K:



• Molecule 1: Fatty acid amide hydrolase

Chain L:


M1 Y4 R9 E12 K19 Y20 K21 A22 E23 T24 K36 V39 N40 L41 L42 L46 V92 L106 P110 Q111 Y112 D113 P114 S115 L118 H119 V123 S124 I131 T144 Q147 V148 R151 I152 I153 D162 K163 F172 V196 I200
D206 G217 W221 K248 N261 K275 R276 Y277 S282 L293 T300 D301 G302 G303 G304 A305 V306 R307 K319 M327 I339 I340 L343 A344 D349 A355 L358 P370 P373 L379 S380 H381 N382 W398 F399 V402 I407
L417 L418 E433 L434 E435 C457 N462 L465 S466 Y467 R491 R492 R493 P511 G514 P518 N527 M539 R540 F541 L547 I566 Q569 W575 V587 L590 K596 F600 I603 L604 N605 THR ASN LYS GLY GLU PHE GLU ALA TYR VAL
GLU GLN LYS LEU ILE SER GLU GLU ASP LEU ASN SER ALA VAL ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	225.54Å 83.75Å 270.94Å 90.00° 109.57° 90.00°	Depositor
Resolution (Å)	39.82 – 3.20 39.82 – 3.20	Depositor EDS
% Data completeness (in resolution range)	88.9 (39.82-3.20) 88.9 (39.82-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.259 , 0.290 0.260 , 0.290	Depositor DCC
R_{free} test set	1980 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å^2)	75.3	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	55639	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0747e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: OHN

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	0.24	0/4704	0.40	0/6391
1	B	0.24	0/4725	0.40	0/6417
1	C	0.24	0/4704	0.40	0/6391
1	D	0.24	0/4725	0.41	0/6417
1	E	0.24	0/4704	0.40	0/6391
1	F	0.24	0/4725	0.41	0/6417
1	G	0.24	0/4704	0.41	0/6391
1	H	0.24	0/4801	0.40	0/6519
1	I	0.24	0/4704	0.41	0/6391
1	J	0.25	0/4801	0.44	2/6519 (0.0%)
1	K	0.24	0/4704	0.40	0/6391
1	L	0.24	0/4725	0.40	0/6417
All	All	0.24	0/56726	0.41	2/77052 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	605	ASN	CB-CA-C	7.11	124.61	110.40
1	J	605	ASN	N-CA-C	-6.42	93.68	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4605	0	4627	51	0
1	B	4626	0	4655	63	0
1	C	4605	0	4627	36	0
1	D	4626	0	4655	34	0
1	E	4605	0	4627	47	0
1	F	4626	0	4655	60	0
1	G	4605	0	4627	31	0
1	H	4700	0	4719	47	0
1	I	4605	0	4627	37	0
1	J	4700	0	4719	43	0
1	K	4605	0	4627	24	0
1	L	4626	0	4655	49	0
2	D	21	0	27	1	0
2	F	21	0	27	2	0
2	H	21	0	27	2	0
2	J	21	0	27	2	0
2	L	21	0	27	3	0
All	All	55639	0	55955	513	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 513 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)
2:H:700:OHN:C2	2:H:700:OHN:OAP	1.68	1.18
2:J:700:OHN:C2	2:J:700:OHN:OAP	1.68	1.15
2:L:700:OHN:OAP	2:L:700:OHN:C2	1.68	1.14
2:F:700:OHN:OAP	2:F:700:OHN:C2	1.68	1.12
2:D:700:OHN:OAP	2:D:700:OHN:C2	1.68	1.11

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	600/636 (94%)	569 (95%)	29 (5%)	2 (0%)	41 74
1	B	603/636 (95%)	571 (95%)	32 (5%)	0	100 100
1	C	600/636 (94%)	574 (96%)	24 (4%)	2 (0%)	41 74
1	D	603/636 (95%)	576 (96%)	26 (4%)	1 (0%)	47 79
1	E	600/636 (94%)	572 (95%)	28 (5%)	0	100 100
1	F	603/636 (95%)	575 (95%)	27 (4%)	1 (0%)	47 79
1	G	600/636 (94%)	574 (96%)	25 (4%)	1 (0%)	47 79
1	H	612/636 (96%)	581 (95%)	29 (5%)	2 (0%)	41 74
1	I	600/636 (94%)	573 (96%)	26 (4%)	1 (0%)	47 79
1	J	612/636 (96%)	589 (96%)	23 (4%)	0	100 100
1	K	600/636 (94%)	576 (96%)	23 (4%)	1 (0%)	47 79
1	L	603/636 (95%)	568 (94%)	34 (6%)	1 (0%)	47 79
All	All	7236/7632 (95%)	6898 (95%)	326 (4%)	12 (0%)	47 79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	C	45	PRO
1	D	45	PRO
1	F	45	PRO
1	H	605	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	509/539 (94%)	504 (99%)	5 (1%)	76 90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	511/539 (95%)	502 (98%)	9 (2%)	59 82
1	C	509/539 (94%)	506 (99%)	3 (1%)	86 94
1	D	511/539 (95%)	508 (99%)	3 (1%)	86 94
1	E	509/539 (94%)	506 (99%)	3 (1%)	86 94
1	F	511/539 (95%)	505 (99%)	6 (1%)	71 88
1	G	509/539 (94%)	505 (99%)	4 (1%)	81 93
1	H	518/539 (96%)	510 (98%)	8 (2%)	65 85
1	I	509/539 (94%)	506 (99%)	3 (1%)	86 94
1	J	518/539 (96%)	513 (99%)	5 (1%)	76 90
1	K	509/539 (94%)	506 (99%)	3 (1%)	86 94
1	L	511/539 (95%)	506 (99%)	5 (1%)	76 90
All	All	6134/6468 (95%)	6077 (99%)	57 (1%)	78 91

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	527	ASN
1	L	382	ASN
1	H	88	ASP
1	L	275	LYS
1	K	395	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	180	GLN
1	J	67	ASN
1	F	213	HIS
1	L	40	ASN
1	I	40	ASN

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)

5 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	OHN	D	700	-	21,21,21	4.71	6 (28%)	20,25,25	3.55	7 (35%)
2	OHN	J	700	-	21,21,21	4.68	7 (33%)	20,25,25	3.68	7 (35%)
2	OHN	H	700	-	21,21,21	4.68	7 (33%)	20,25,25	3.49	7 (35%)
2	OHN	L	700	-	21,21,21	4.70	7 (33%)	20,25,25	3.47	7 (35%)
2	OHN	F	700	-	21,21,21	4.71	7 (33%)	20,25,25	3.43	8 (40%)

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	OHN	D	700	-	-	5/17/27/27	0/1/1/1
2	OHN	J	700	-	-	8/17/27/27	0/1/1/1
2	OHN	H	700	-	-	8/17/27/27	0/1/1/1
2	OHN	L	700	-	-	7/17/27/27	0/1/1/1
2	OHN	F	700	-	-	8/17/27/27	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	OHN	OAP-C2	15.17	1.68	1.35
2	H	700	OHN	OAP-C2	15.14	1.68	1.35
2	L	700	OHN	OAP-C2	15.10	1.68	1.35
2	J	700	OHN	OAP-C2	15.04	1.68	1.35
2	F	700	OHN	OAP-C2	15.01	1.68	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	700	OHN	OAP-C2-O6	-11.62	109.37	121.42
2	D	700	OHN	OAP-C2-O6	-11.04	109.98	121.42
2	L	700	OHN	OAP-C2-O6	-10.76	110.26	121.42
2	H	700	OHN	OAP-C2-O6	-10.68	110.35	121.42
2	F	700	OHN	OAP-C2-O6	-10.39	110.64	121.42

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	700	OHN	C2-C1-N7-C8
2	F	700	OHN	C11-C10-C8-O9
2	F	700	OHN	C11-C10-C8-N7
2	H	700	OHN	C11-C10-C8-O9
2	H	700	OHN	C11-C10-C8-N7

There are no ring outliers.

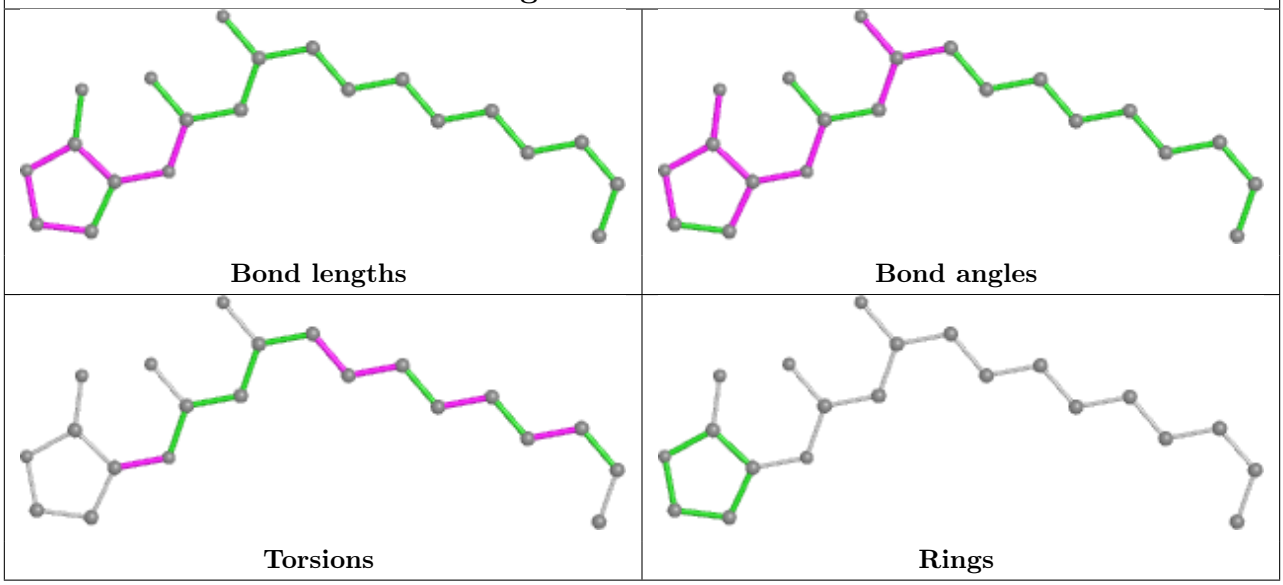
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	700	OHN	1	0
2	J	700	OHN	2	0
2	H	700	OHN	2	0
2	L	700	OHN	3	0
2	F	700	OHN	2	0

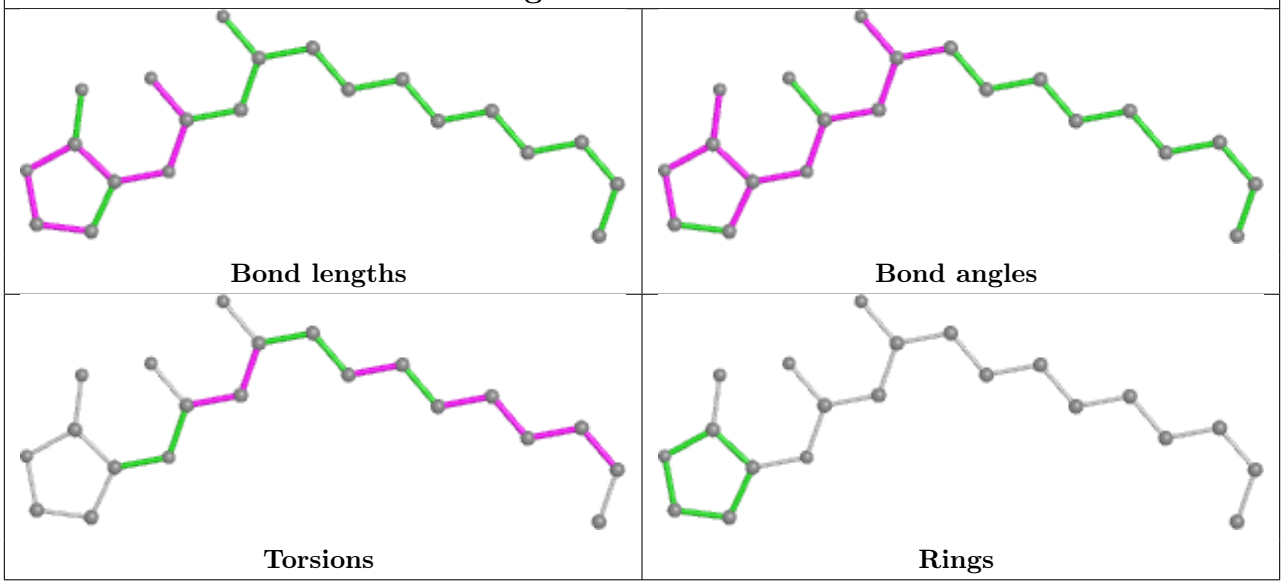
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

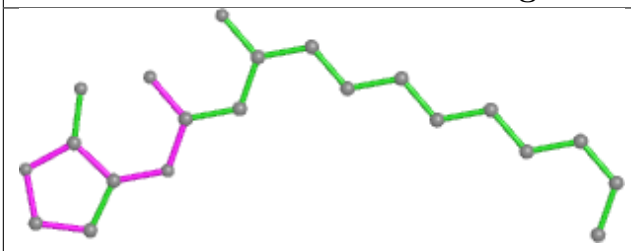
Ligand OHN D 700



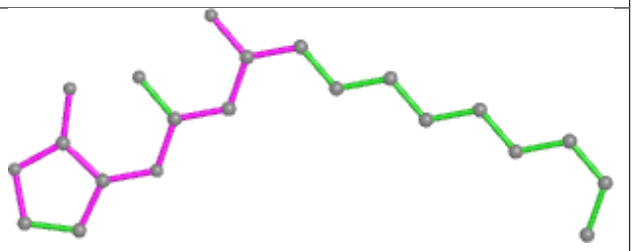
Ligand OHN J 700



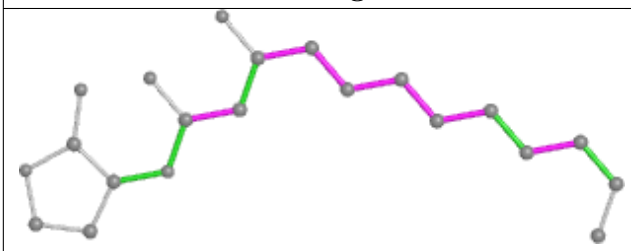
Ligand OHN H 700



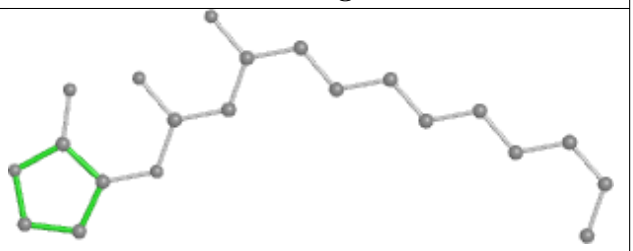
Bond lengths



Bond angles

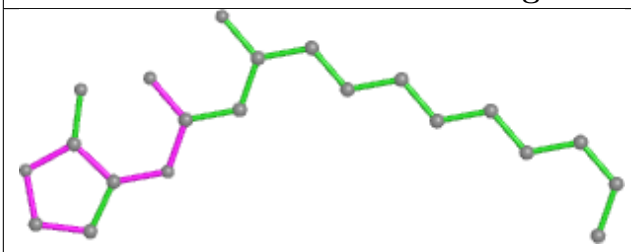


Torsions

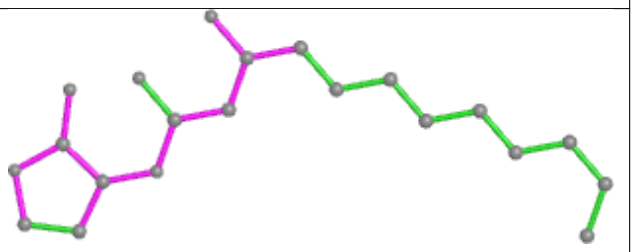


Rings

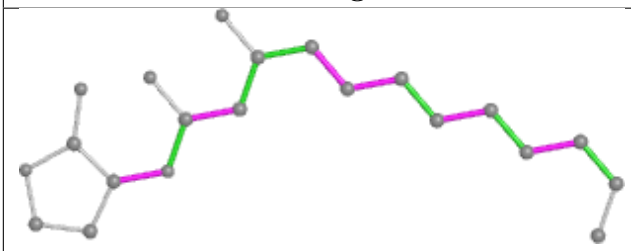
Ligand OHN L 700



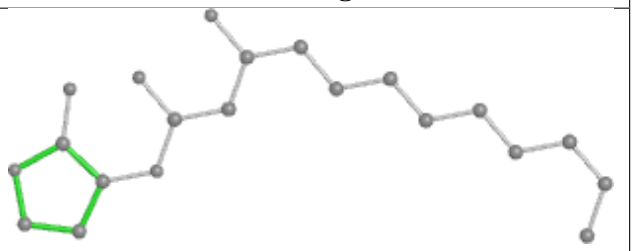
Bond lengths



Bond angles

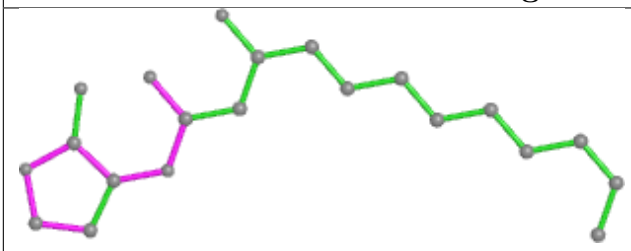


Torsions

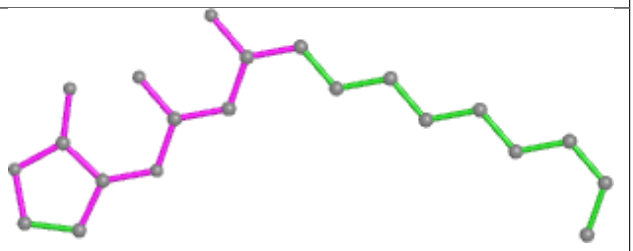


Rings

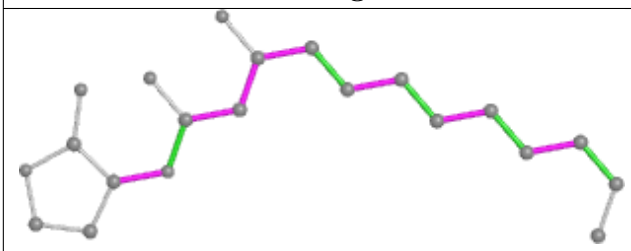
Ligand OHN F 700



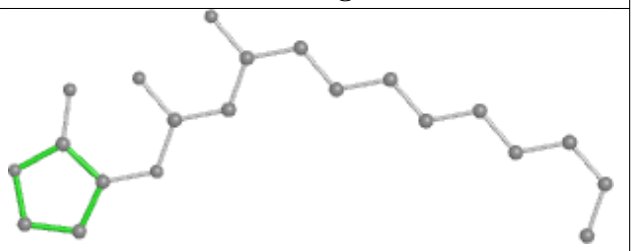
Bond lengths



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	602/636 (94%)	0.44	49 (8%)	12	6	79, 111, 146, 213	0
1	B	605/636 (95%)	0.47	41 (6%)	17	10	77, 113, 145, 230	0
1	C	602/636 (94%)	0.05	18 (2%)	50	34	53, 80, 117, 218	0
1	D	605/636 (95%)	-0.16	10 (1%)	70	57	42, 61, 93, 192	0
1	E	602/636 (94%)	0.40	42 (6%)	16	9	74, 107, 142, 217	0
1	F	605/636 (95%)	0.38	27 (4%)	33	21	69, 101, 130, 224	0
1	G	602/636 (94%)	-0.10	13 (2%)	62	48	49, 76, 106, 187	0
1	H	614/636 (96%)	-0.09	12 (1%)	65	51	48, 69, 107, 243	0
1	I	602/636 (94%)	-0.20	7 (1%)	79	67	38, 57, 86, 175	0
1	J	614/636 (96%)	-0.09	12 (1%)	65	51	40, 56, 88, 199	0
1	K	602/636 (94%)	-0.11	12 (1%)	65	51	49, 73, 104, 188	0
1	L	605/636 (95%)	-0.06	13 (2%)	63	49	48, 76, 104, 172	0
All	All	7260/7632 (95%)	0.08	256 (3%)	44	28	38, 80, 134, 243	0

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	383	GLY	7.2
1	J	119	HIS	6.7
1	A	28	PRO	6.4
1	B	24	THR	6.2
1	F	382	ASN	6.2

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)

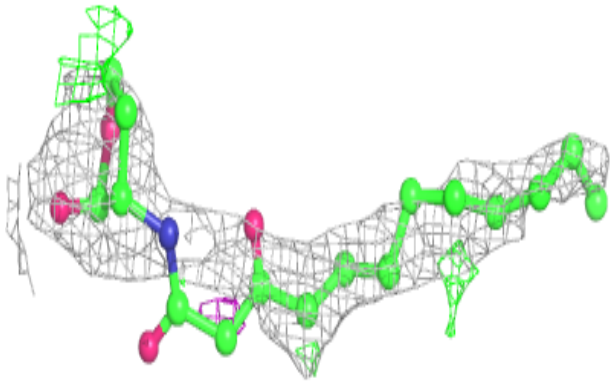
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

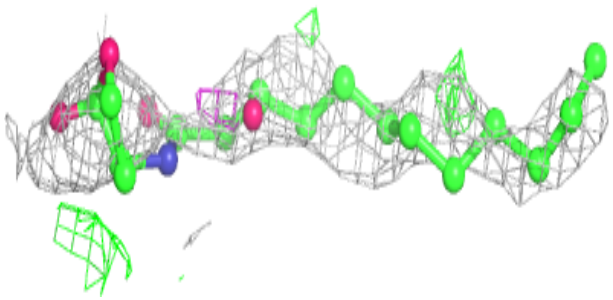
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OHN	F	700	21/21	0.76	0.42	90,97,102,106	0
2	OHN	D	700	21/21	0.82	0.31	58,66,71,74	0
2	OHN	H	700	21/21	0.83	0.35	63,70,75,78	0
2	OHN	L	700	21/21	0.83	0.31	67,75,79,83	0
2	OHN	J	700	21/21	0.88	0.27	43,51,56,59	0

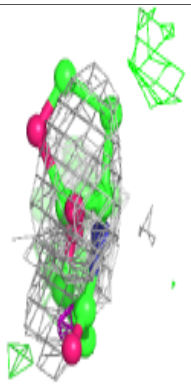
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OHN F 700:

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

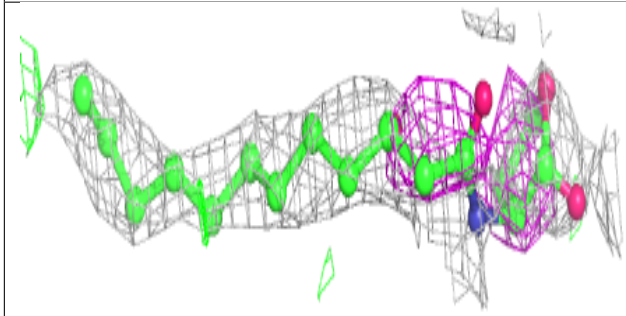


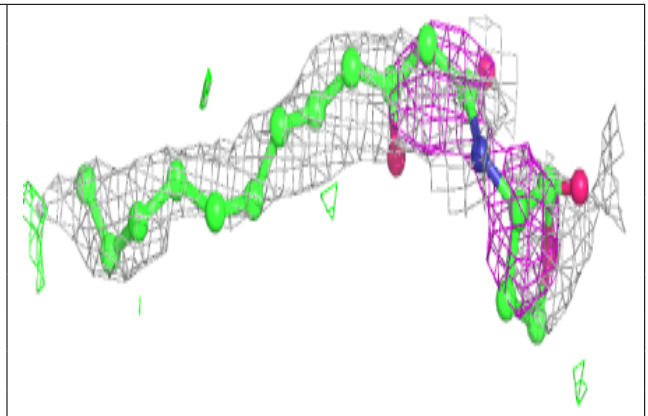


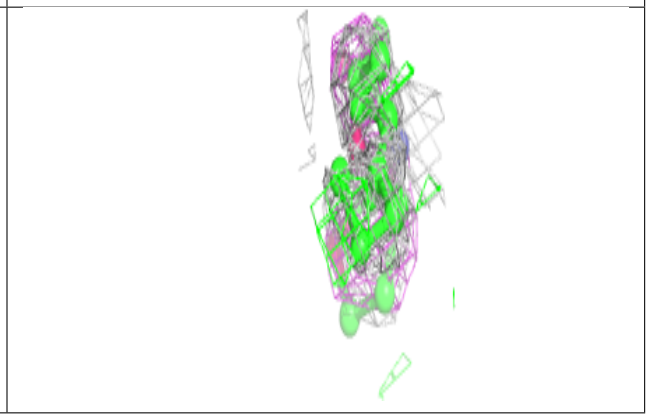


Electron density around OHN D 700:

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

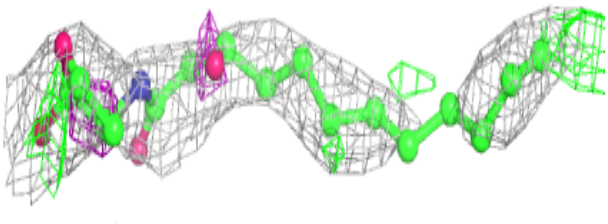


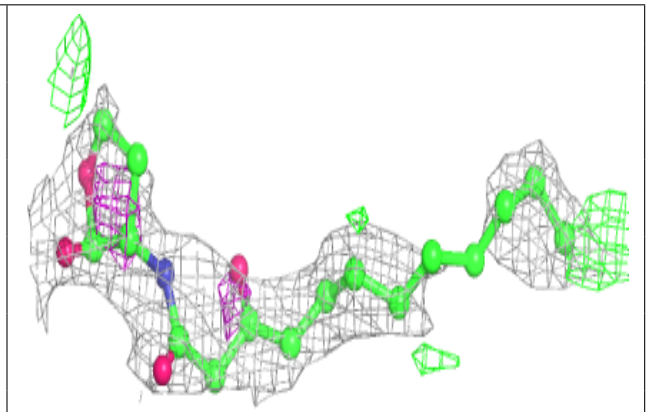


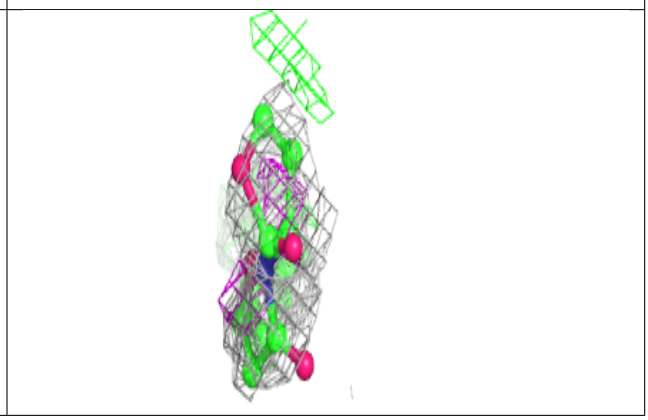


Electron density around OHN H 700:

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

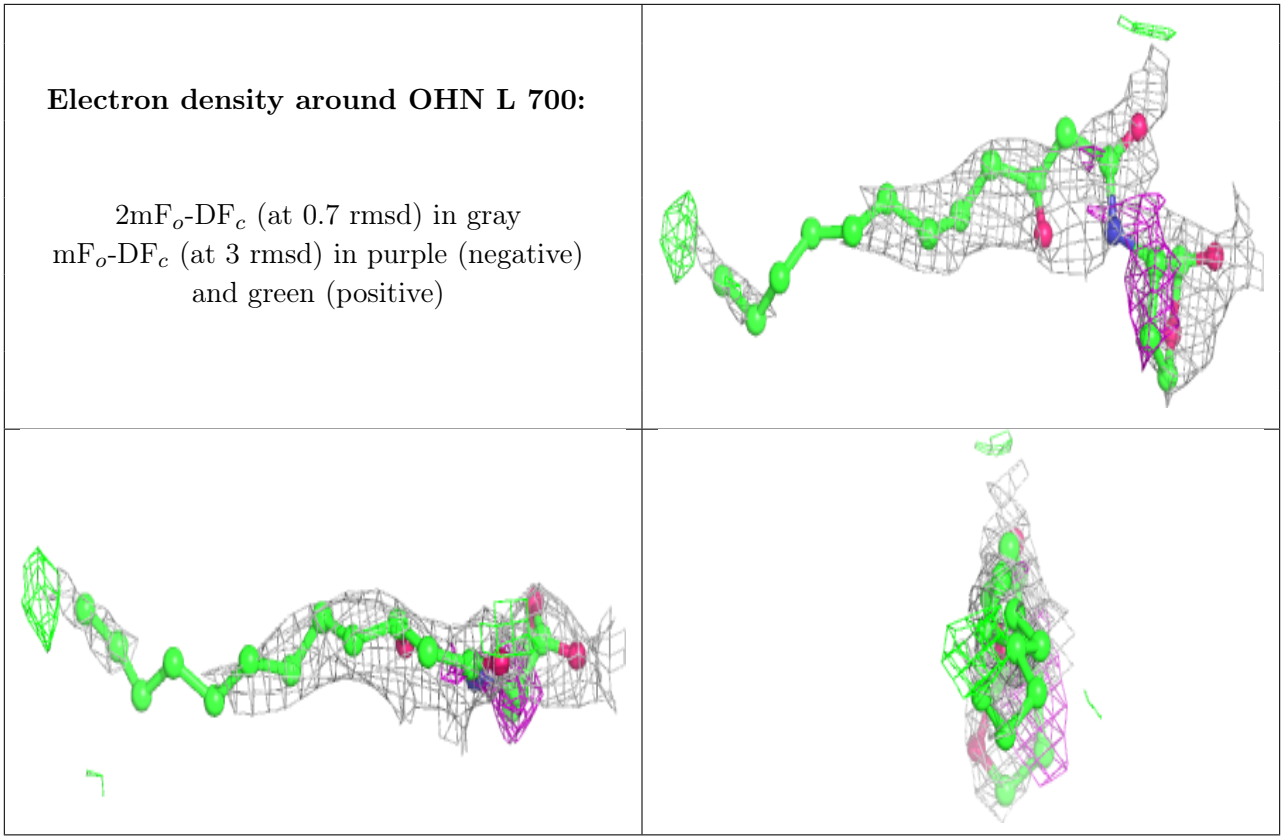






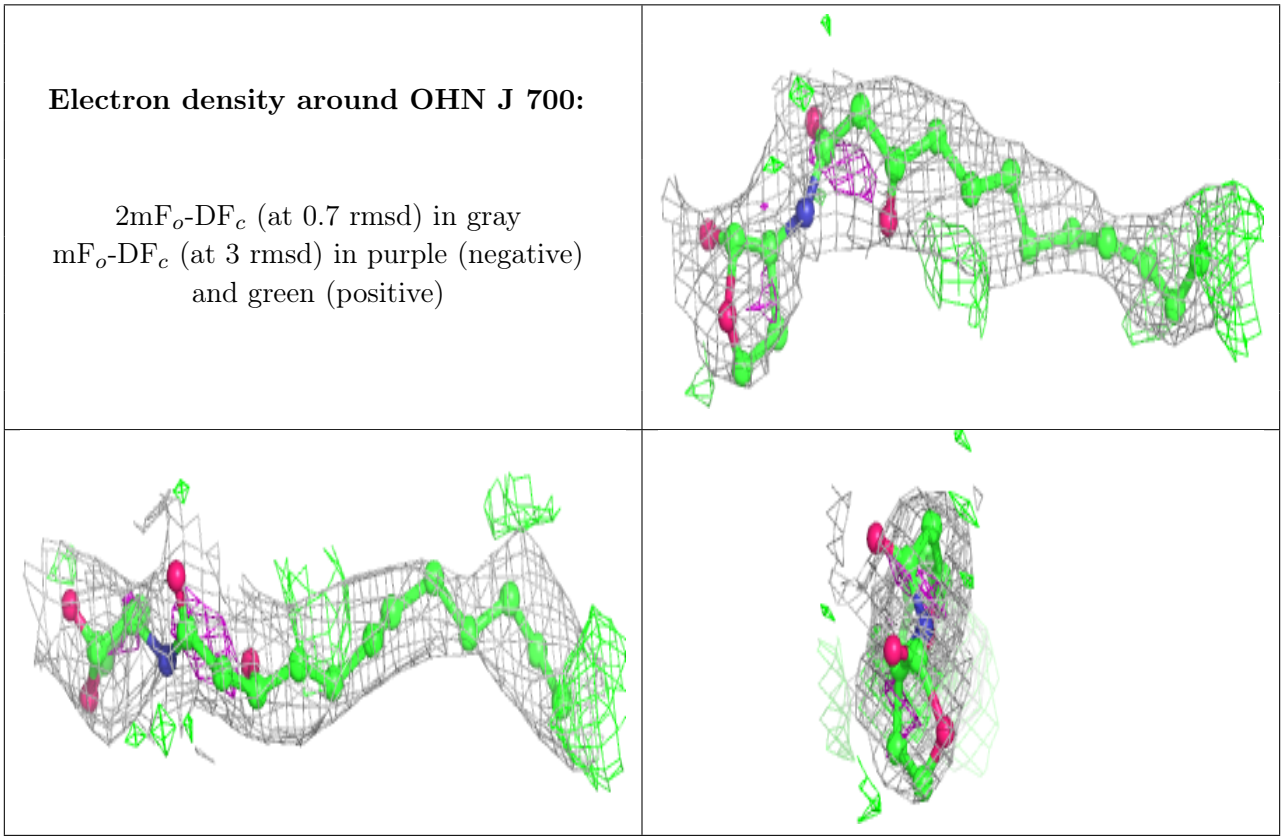
Electron density around OHN L 700:

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



Electron density around OHN J 700:

$2mF_o$-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.