



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:38 PM GMT

PDB ID : 1MT5
Title : CRYSTAL STRUCTURE OF FATTY ACID AMIDE HYDROLASE
Authors : Bracey, M.H.; Hanson, M.A.; Masuda, K.R.; Stevens, R.C.; Cravatt, B.F.
Deposited on : 2002-09-20
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

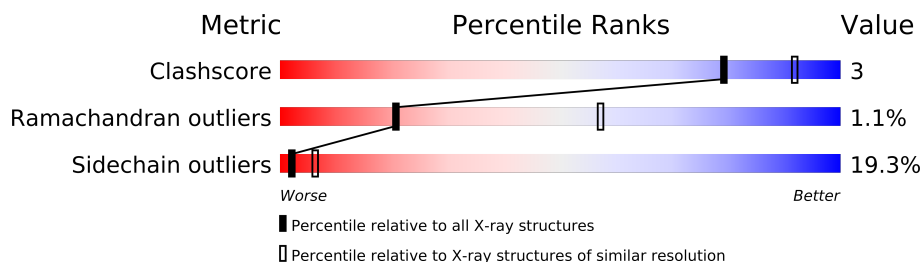
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	537	
1	B	537	
1	C	537	
1	D	537	
1	E	537	
1	F	537	
1	G	537	
1	H	537	
1	I	537	
1	J	537	
1	K	537	
1	L	537	
1	M	537	
1	N	537	
1	O	537	
1	P	537	

2 Entry composition

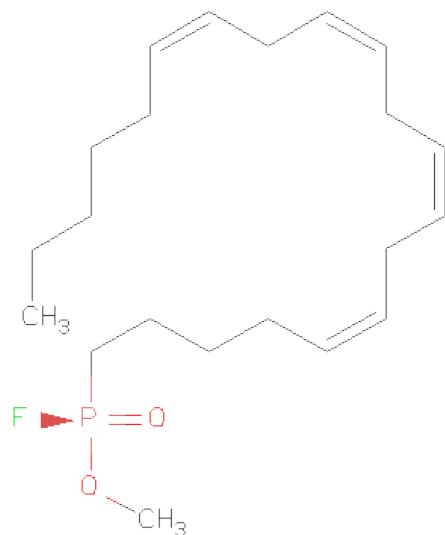
There are 2 unique types of molecules in this entry. The entry contains 64524 atoms, of which 0 are hydrogen and 0 are deuterium.

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	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	B	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	C	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	D	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	E	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	F	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	G	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	H	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	I	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	J	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	K	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	L	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	M	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	N	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	O	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	P	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			

- Molecule 2 is METHYL ARACHIDONYL FLUOROPHOSPHONATE (three-letter code: MAY) (formula: $C_{21}H_{36}FO_2P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			24	21	2	1		
2	B	1	Total	C	O	P	0	0
			24	21	2	1		
2	C	1	Total	C	O	P	0	0
			24	21	2	1		
2	D	1	Total	C	O	P	0	0
			24	21	2	1		
2	E	1	Total	C	O	P	0	0
			24	21	2	1		
2	F	1	Total	C	O	P	0	0
			24	21	2	1		
2	G	1	Total	C	O	P	0	0
			24	21	2	1		
2	H	1	Total	C	O	P	0	0
			24	21	2	1		
2	I	1	Total	C	O	P	0	0
			24	21	2	1		
2	J	1	Total	C	O	P	0	0
			24	21	2	1		
2	K	1	Total	C	O	P	0	0
			24	21	2	1		
2	L	1	Total	C	O	P	0	0
			24	21	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	O	P	0	0
			24	21	2	1		
2	N	1	Total	C	O	P	0	0
			24	21	2	1		
2	O	1	Total	C	O	P	0	0
			24	21	2	1		
2	P	1	Total	C	O	P	0	0
			24	21	2	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

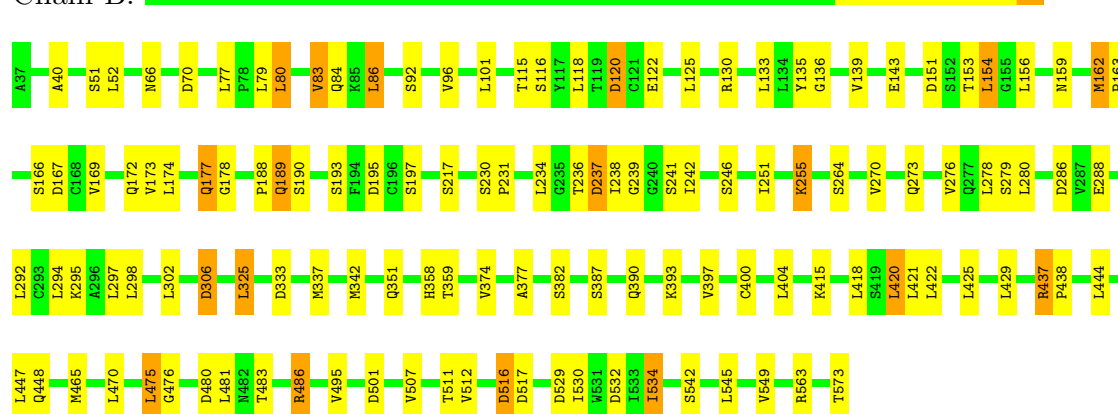
- Molecule 1: Fatty-acid amide hydrolase

Chain A:



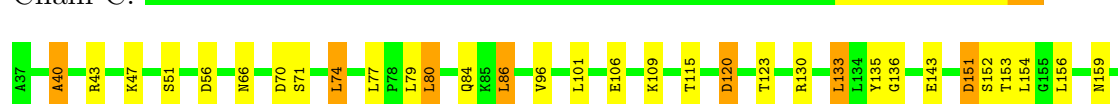
- Molecule 1: Fatty-acid amide hydrolase

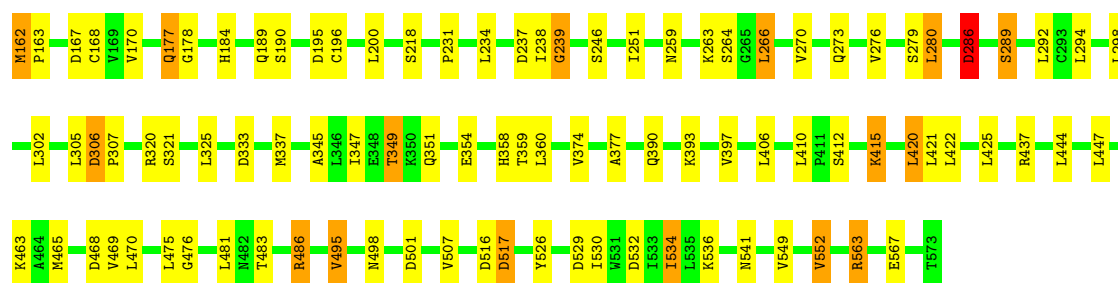
Chain B:



- Molecule 1: Fatty-acid amide hydrolase

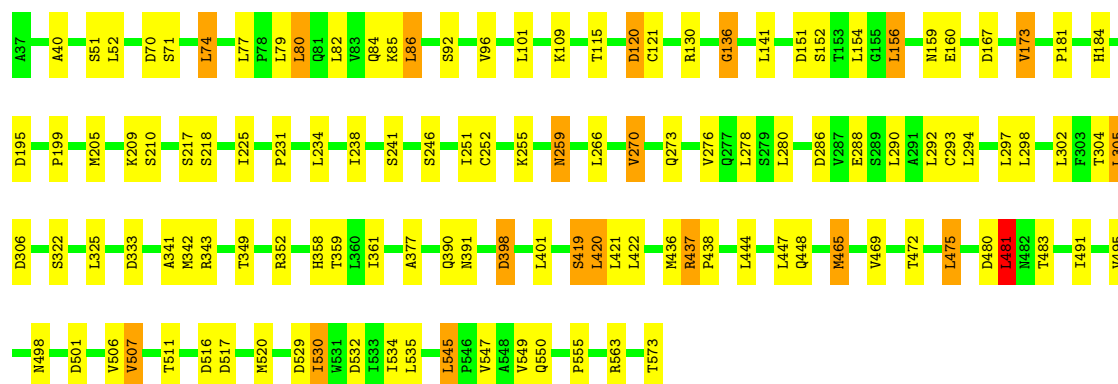
Chain C:





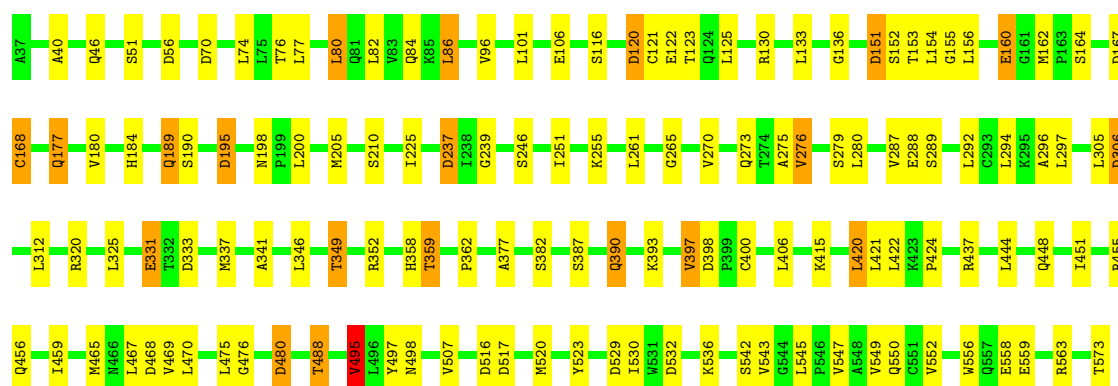
• Molecule 1: Fatty-acid amide hydrolase

Chain D:



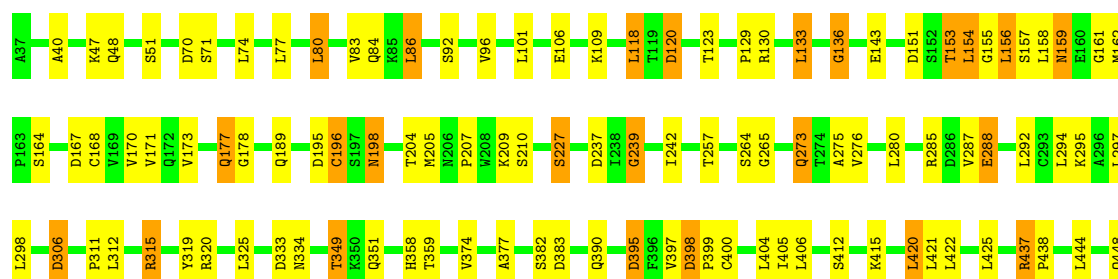
• Molecule 1: Fatty-acid amide hydrolase

Chain E:



• Molecule 1: Fatty-acid amide hydrolase

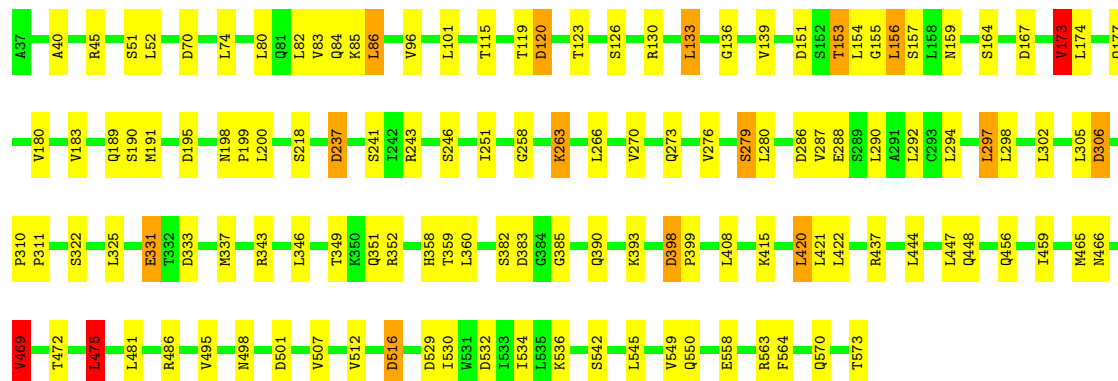
Chain F:





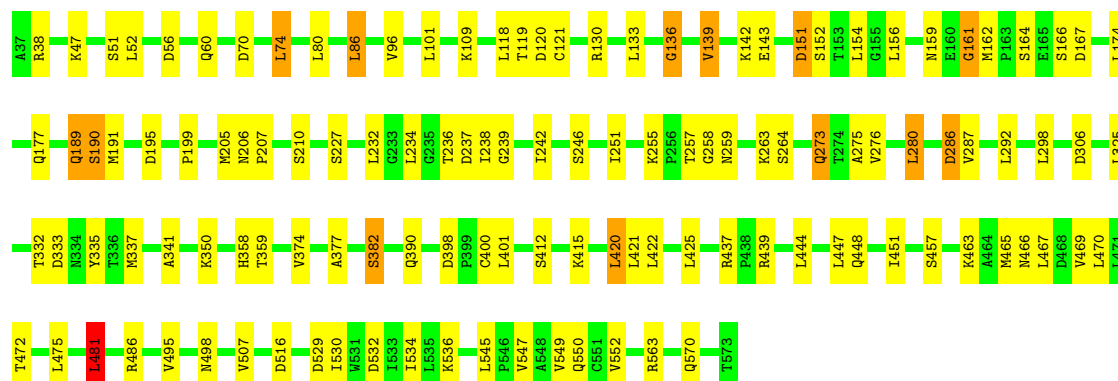
• Molecule 1: Fatty-acid amide hydrolase

Chain G:



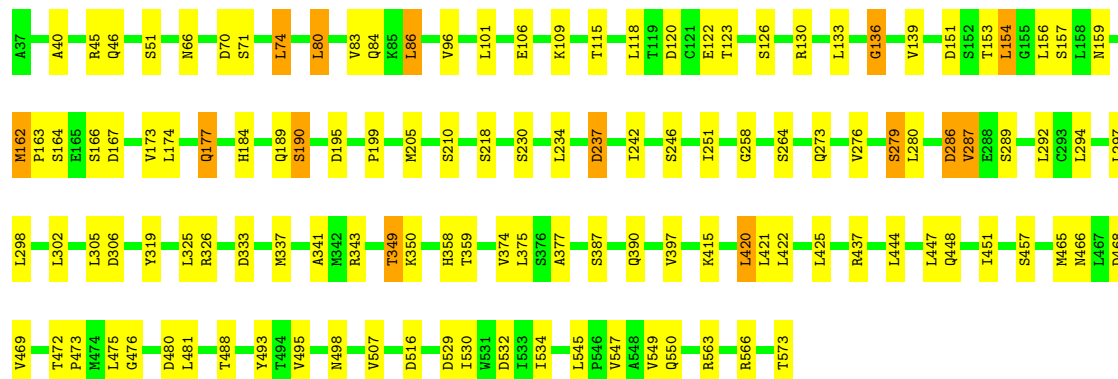
• Molecule 1: Fatty-acid amide hydrolase

Chain H:



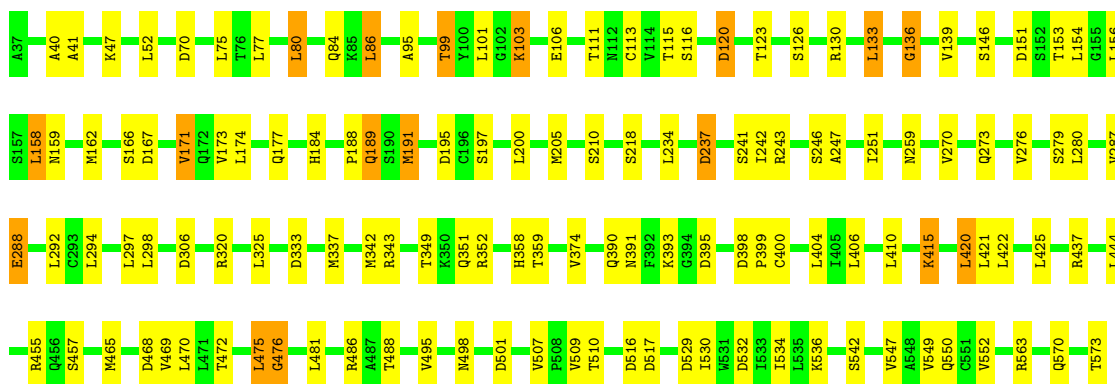
• Molecule 1: Fatty-acid amide hydrolase

Chain I:



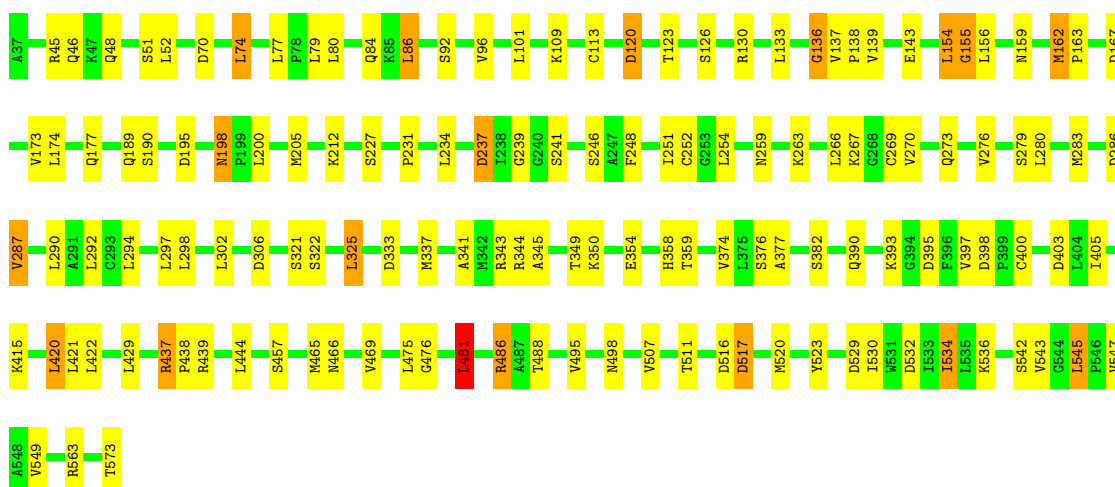
• Molecule 1: Fatty-acid amide hydrolase

Chain J:



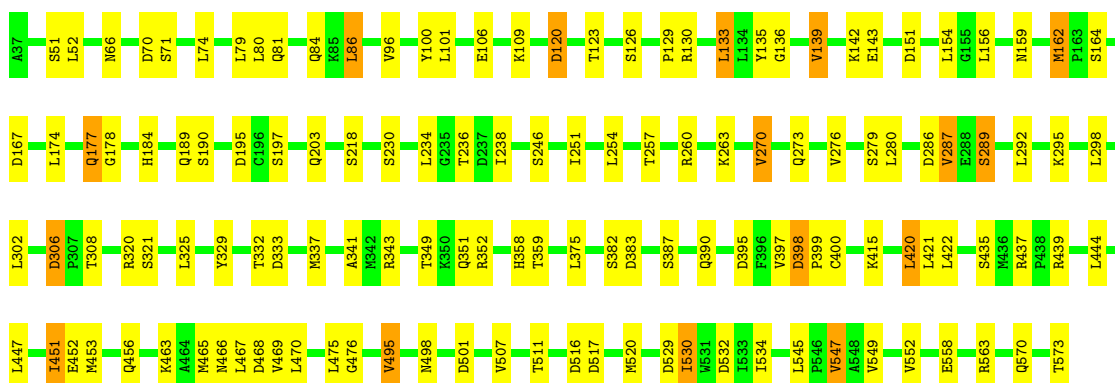
• Molecule 1: Fatty-acid amide hydrolase

Chain K:



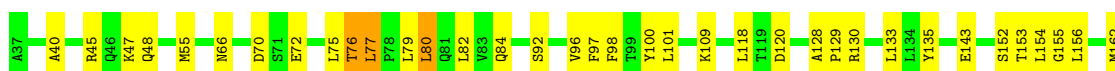
• Molecule 1: Fatty-acid amide hydrolase

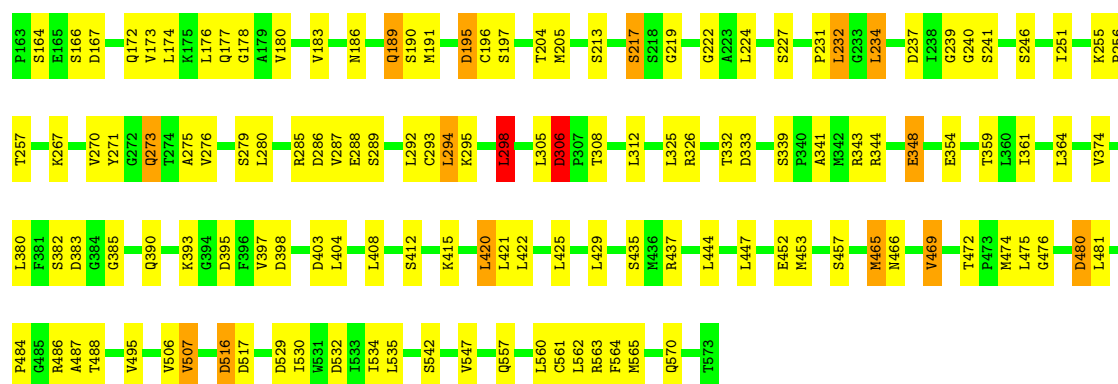
Chain L:



• Molecule 1: Fatty-acid amide hydrolase

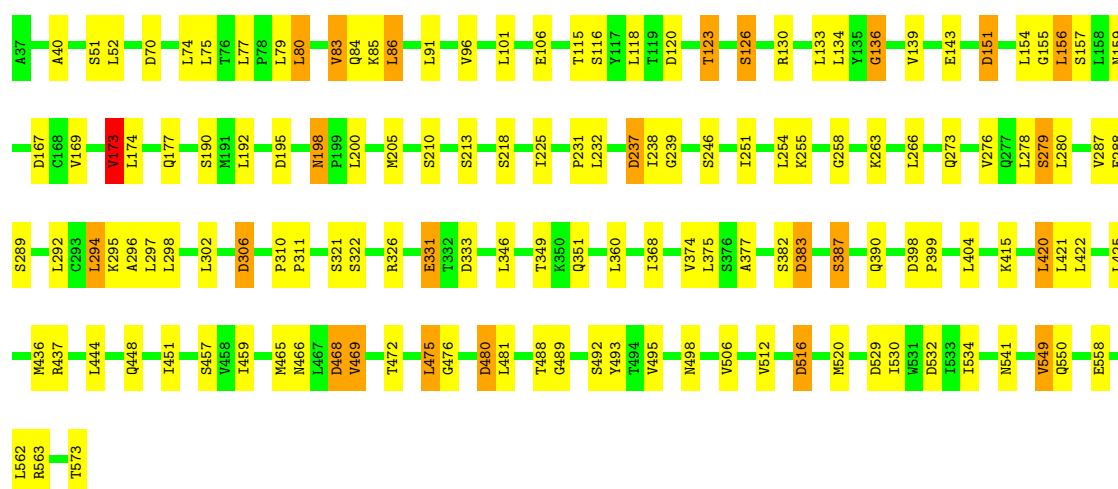
Chain M:





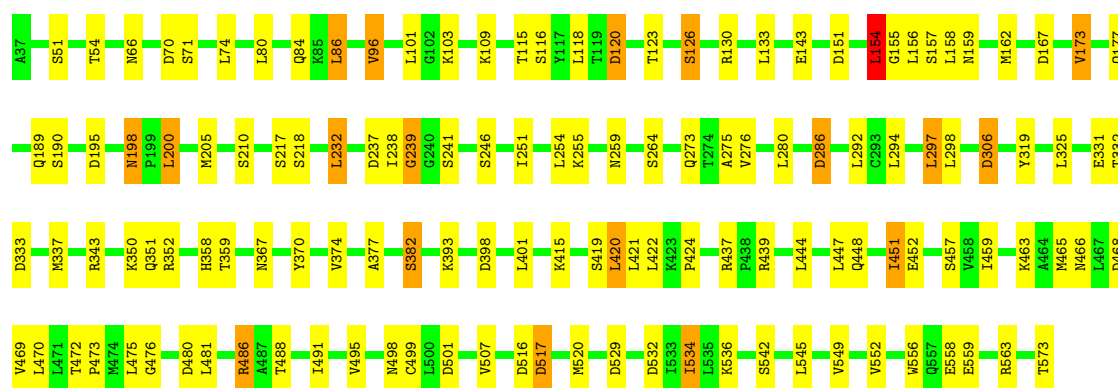
• Molecule 1: Fatty-acid amide hydrolase

Chain N:



• Molecule 1: Fatty-acid amide hydrolase

Chain O:



• Molecule 1: Fatty-acid amide hydrolase

Chain P:



V552	L444	K295	D167
E558	I451	A296	C168
E559	K463	L298	V171
R563	A464	L302	Q172
R566	A466	D306	V173
T573	A467	P307	L174
	D468	R320	Q177
	V469	S321	V183
	L470	S322	H184
	L471	L325	Q189
	T472	R326	
	P473	E331	D195
	M474	T332	P199
	L475	D333	S210
	D480	N334	
	L481	M337	S218
	R486	A341	L234
	A487	K350	D237
	T488	Q351	G240
	V495	R352	S241
	M498	H358	S246
	D501	T359	
	V507	A371	L251
	T511	V374	C252
	D516	L375	N259
	D517	S376	R260
	Y523	S382	K263
	Y526	S387	L266
	D529	Q390	C269
	I530	K393	Q273
	W531	D398	T274
	D532	L401	A275
	T533	L404	V276
	I534		
	L535		S279
	S542		L280
	L545	L420	E288
	P546	L421	S289
	V547	L425	L290
	A548		A291
	V549		L292
	Q550	R437	C293
	G553	D138	L294

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.11Å 272.02Å 147.22Å 90.00° 115.21° 90.00°	Depositor
Resolution (Å)	141.42 – 2.80	Depositor
% Data completeness (in resolution range)	71.4 (141.42-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.218 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	64524	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAY

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	0.95	2/4102 (0.0%)	0.88	16/5589 (0.3%)
1	B	0.97	2/4100 (0.0%)	0.89	14/5586 (0.3%)
1	C	0.95	2/4100 (0.0%)	0.88	16/5586 (0.3%)
1	D	0.93	2/4100 (0.0%)	0.87	17/5586 (0.3%)
1	E	1.01	3/4100 (0.1%)	0.88	16/5586 (0.3%)
1	F	0.97	3/4100 (0.1%)	0.89	16/5586 (0.3%)
1	G	0.97	2/4102 (0.0%)	0.88	16/5589 (0.3%)
1	H	0.93	0/4100	0.88	14/5586 (0.3%)
1	I	0.96	2/4102 (0.0%)	0.86	14/5589 (0.3%)
1	J	0.97	2/4100 (0.0%)	0.87	15/5586 (0.3%)
1	K	0.98	3/4100 (0.1%)	0.89	16/5586 (0.3%)
1	L	1.02	2/4102 (0.0%)	0.88	16/5589 (0.3%)
1	M	1.13	2/4102 (0.0%)	0.93	15/5589 (0.3%)
1	N	1.09	2/4100 (0.0%)	0.89	14/5586 (0.3%)
1	O	0.96	1/4102 (0.0%)	0.88	17/5589 (0.3%)
1	P	1.00	3/4100 (0.1%)	0.88	16/5586 (0.3%)
All	All	0.99	33/65612 (0.1%)	0.88	248/89394 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	4
1	F	0	6
1	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	6
1	I	0	5
1	J	0	4
1	K	0	3
1	L	0	1
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	2
All	All	0	57

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	469	VAL	CB-CG1	-6.53	1.39	1.52
1	A	549	VAL	CA-CB	6.08	1.67	1.54
1	A	287	VAL	CA-CB	5.88	1.67	1.54
1	D	507	VAL	CA-CB	5.77	1.66	1.54
1	F	83	VAL	CA-CB	5.72	1.66	1.54

The worst 5 of 248 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ASP	CB-CG-OD2	8.76	126.18	118.30
1	H	333	ASP	CB-CG-OD2	8.51	125.96	118.30
1	A	529	ASP	CB-CG-OD2	8.42	125.88	118.30
1	D	333	ASP	CB-CG-OD2	8.38	125.84	118.30
1	B	529	ASP	CB-CG-OD2	8.37	125.83	118.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ASP	Peptide
1	A	197	SER	Peptide
1	B	120	ASP	Peptide
1	B	40	ALA	Peptide
1	B	475	LEU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4010	0	3953	29	0
1	B	4008	0	3953	28	0
1	C	4008	0	3953	27	0
1	D	4008	0	3953	30	0
1	E	4008	0	3953	29	0
1	F	4008	0	3953	29	0
1	G	4010	0	3953	29	0
1	H	4008	0	3953	25	0
1	I	4010	0	3953	21	0
1	J	4008	0	3953	27	0
1	K	4008	0	3953	29	0
1	L	4010	0	3953	24	0
1	M	4010	0	3953	30	0
1	N	4008	0	3953	37	0
1	O	4010	0	3953	26	0
1	P	4008	0	3953	29	0
2	A	24	0	36	5	0
2	B	24	0	36	3	0
2	C	24	0	36	3	0
2	D	24	0	36	4	0
2	E	24	0	36	3	0
2	F	24	0	36	4	0
2	G	24	0	36	1	0
2	H	24	0	36	4	0
2	I	24	0	36	2	0
2	J	24	0	36	2	0
2	K	24	0	36	3	0
2	L	24	0	36	1	0
2	M	24	0	36	2	0
2	N	24	0	36	4	0
2	O	24	0	36	3	0
2	P	24	0	36	2	0
All	All	64524	0	63824	447	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 447 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:453:MET:CE	1:L:453:MET:SD	2.02	1.48
1:D:325:LEU:H	1:D:358:HIS:HD2	1.18	0.90
1:A:155:GLY:HA3	1:A:198:ASN:HD21	1.38	0.87
1:C:325:LEU:H	1:C:358:HIS:HD2	1.27	0.81
1:D:86:LEU:HG	1:D:136:GLY:HA3	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	21	57
1	B	535/537 (100%)	503 (94%)	24 (4%)	8 (2%)	15	46
1	C	535/537 (100%)	507 (95%)	23 (4%)	5 (1%)	25	63
1	D	535/537 (100%)	499 (93%)	31 (6%)	5 (1%)	25	63
1	E	535/537 (100%)	491 (92%)	36 (7%)	8 (2%)	15	46
1	F	535/537 (100%)	502 (94%)	27 (5%)	6 (1%)	21	57
1	G	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	33	72
1	H	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	21	57
1	I	535/537 (100%)	496 (93%)	37 (7%)	2 (0%)	43	80
1	J	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	33	72
1	K	535/537 (100%)	497 (93%)	32 (6%)	6 (1%)	21	57
1	L	535/537 (100%)	494 (92%)	36 (7%)	5 (1%)	25	63
1	M	535/537 (100%)	466 (87%)	57 (11%)	12 (2%)	10	32
1	N	535/537 (100%)	494 (92%)	33 (6%)	8 (2%)	15	46
1	O	535/537 (100%)	499 (93%)	30 (6%)	6 (1%)	21	57
1	P	535/537 (100%)	497 (93%)	34 (6%)	4 (1%)	30	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8560/8592 (100%)	7953 (93%)	514 (6%)	93 (1%)	21	57

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	ASP
1	A	480	ASP
1	E	189	GLN
1	E	480	ASP
1	E	488	THR

5.3.2 Protein sidechains ⓘ

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	426/455 (94%)	354 (83%)	72 (17%)	3	9
1	B	425/455 (93%)	351 (83%)	74 (17%)	3	8
1	C	425/455 (93%)	341 (80%)	84 (20%)	2	6
1	D	425/455 (93%)	354 (83%)	71 (17%)	3	9
1	E	425/455 (93%)	345 (81%)	80 (19%)	2	7
1	F	425/455 (93%)	339 (80%)	86 (20%)	2	5
1	G	426/455 (94%)	345 (81%)	81 (19%)	2	6
1	H	425/455 (93%)	350 (82%)	75 (18%)	3	8
1	I	426/455 (94%)	344 (81%)	82 (19%)	2	6
1	J	425/455 (93%)	344 (81%)	81 (19%)	2	6
1	K	425/455 (93%)	341 (80%)	84 (20%)	2	6
1	L	426/455 (94%)	338 (79%)	88 (21%)	2	5
1	M	426/455 (94%)	323 (76%)	103 (24%)	1	3
1	N	425/455 (93%)	345 (81%)	80 (19%)	2	7
1	O	426/455 (94%)	340 (80%)	86 (20%)	2	5
1	P	425/455 (93%)	339 (80%)	86 (20%)	2	5
All	All	6806/7280 (94%)	5493 (81%)	1313 (19%)	2	6

5 of 1313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	390	GLN
1	J	210	SER
1	O	481	LEU
1	H	469	VAL
1	I	292	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	189	GLN
1	I	498	ASN
1	O	498	ASN
1	H	259	ASN
1	H	498	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	MAY	A	600	1	22,23,24	9.50	1 (4%)	20,23,26	0.91	2 (10%)
2	MAY	B	600	1	22,23,24	8.92	1 (4%)	20,23,26	0.85	2 (10%)
2	MAY	C	600	1	22,23,24	4.57	1 (4%)	20,23,26	0.90	2 (10%)
2	MAY	D	600	1	22,23,24	2.97	1 (4%)	20,23,26	0.96	2 (10%)
2	MAY	E	600	1	22,23,24	6.62	1 (4%)	20,23,26	0.90	1 (5%)
2	MAY	F	600	1	22,23,24	4.53	1 (4%)	20,23,26	0.79	1 (5%)
2	MAY	G	600	1	22,23,24	7.43	1 (4%)	20,23,26	0.96	2 (10%)
2	MAY	H	600	1	22,23,24	10.45	1 (4%)	20,23,26	0.90	1 (5%)
2	MAY	I	600	1	22,23,24	4.95	1 (4%)	20,23,26	0.85	1 (5%)
2	MAY	J	600	1	22,23,24	5.30	1 (4%)	20,23,26	0.81	1 (5%)
2	MAY	K	600	1	22,23,24	5.60	1 (4%)	20,23,26	0.88	2 (10%)
2	MAY	L	600	1	22,23,24	5.05	1 (4%)	20,23,26	0.98	2 (10%)
2	MAY	M	600	1	22,23,24	6.09	1 (4%)	20,23,26	0.90	2 (10%)
2	MAY	N	600	1	22,23,24	6.30	1 (4%)	20,23,26	0.91	1 (5%)
2	MAY	O	600	1	22,23,24	4.28	1 (4%)	20,23,26	0.86	2 (10%)
2	MAY	P	600	1	22,23,24	6.35	1 (4%)	20,23,26	0.84	2 (10%)

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	MAY	A	600	1	-	0/18/22/24	0/0/0/0
2	MAY	B	600	1	-	0/18/22/24	0/0/0/0
2	MAY	C	600	1	-	0/18/22/24	0/0/0/0
2	MAY	D	600	1	-	0/18/22/24	0/0/0/0
2	MAY	E	600	1	-	0/18/22/24	0/0/0/0
2	MAY	F	600	1	-	0/18/22/24	0/0/0/0
2	MAY	G	600	1	-	0/18/22/24	0/0/0/0
2	MAY	H	600	1	-	0/18/22/24	0/0/0/0
2	MAY	I	600	1	-	0/18/22/24	0/0/0/0
2	MAY	J	600	1	-	0/18/22/24	0/0/0/0
2	MAY	K	600	1	-	0/18/22/24	0/0/0/0
2	MAY	L	600	1	-	0/18/22/24	0/0/0/0
2	MAY	M	600	1	-	0/18/22/24	0/0/0/0
2	MAY	N	600	1	-	0/18/22/24	0/0/0/0
2	MAY	O	600	1	-	0/18/22/24	0/0/0/0
2	MAY	P	600	1	-	0/18/22/24	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	600	MAY	P1-C1	-48.94	1.78	1.84
2	A	600	MAY	P1-C1	-44.53	1.79	1.84
2	B	600	MAY	P1-C1	-41.76	1.79	1.84
2	G	600	MAY	P1-C1	-34.80	1.80	1.84
2	E	600	MAY	P1-C1	-30.98	1.80	1.84

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	MAY	C3-C2-C1	-2.58	107.04	114.14
2	N	600	MAY	P1-O2-CM	2.56	123.34	117.35
2	D	600	MAY	C3-C2-C1	-2.51	107.22	114.14
2	E	600	MAY	C3-C2-C1	-2.45	107.41	114.14
2	L	600	MAY	C3-C2-C1	-2.42	107.47	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.