wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2020 – 11:21 AM BST

PDB ID	:	6NCF
Title	:	The structure of Stable-5-Lipoxygenase bound to AKBA
Authors	:	Newcomer, M.E.; Gilbert, N.C.; Neau, D.B.
Deposited on	:	2018-12-11
Resolution	:	2.87 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 following versions of software and data (see references (1)) were used in the production of this report:

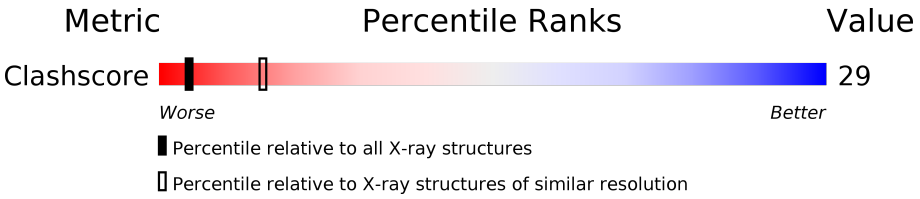
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.87 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	141614	2947 (2.90-2.86)

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 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	691	48% 49% .
1	B	691	48% 50% .
1	C	691	52% 44% .
1	D	691	53% 44% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21918 atoms, of which 47 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 Arachidonate 5-lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	0	0
			5484	3510	934	1014	26			
1	B	676	Total	C	N	O	S	0	0	0
			5490	3513	935	1016	26			
1	C	669	Total	C	N	O	S	0	0	0
			5428	3477	918	1007	26			
1	D	669	Total	C	N	O	S	0	0	0
			5428	3477	918	1007	26			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP P09917
A	-16	GLY	-	expression tag	UNP P09917
A	-15	SER	-	expression tag	UNP P09917
A	-14	SER	-	expression tag	UNP P09917
A	-13	HIS	-	expression tag	UNP P09917
A	-12	HIS	-	expression tag	UNP P09917
A	-11	HIS	-	expression tag	UNP P09917
A	-10	HIS	-	expression tag	UNP P09917
A	-9	HIS	-	expression tag	UNP P09917
A	-8	HIS	-	expression tag	UNP P09917
A	-7	SER	-	expression tag	UNP P09917
A	-6	SER	-	expression tag	UNP P09917
A	-5	GLY	-	expression tag	UNP P09917
A	-4	LEU	-	expression tag	UNP P09917
A	-3	VAL	-	expression tag	UNP P09917
A	-2	PRO	-	expression tag	UNP P09917
A	-1	ARG	-	expression tag	UNP P09917
A	0	GLY	-	expression tag	UNP P09917
A	1	SER	-	expression tag	UNP P09917
A	2	HIS	-	expression tag	UNP P09917
A	16	GLU	TRP	engineered mutation	UNP P09917

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Chain	Residue	Modelled	Actual	Comment	Reference
A	17	HIS	PHE	engineered mutation	UNP P09917
A	?	-	PRO	SEE REMARK 999	UNP P09917
A	?	-	PHE	SEE REMARK 999	UNP P09917
A	?	-	TYR	SEE REMARK 999	UNP P09917
A	43	GLY	ASN	SEE REMARK 999	UNP P09917
A	44	SER	ASP	SEE REMARK 999	UNP P09917
A	75	GLY	TRP	engineered mutation	UNP P09917
A	76	SER	LEU	engineered mutation	UNP P09917
A	240	ALA	CYS	engineered mutation	UNP P09917
A	561	ALA	CYS	engineered mutation	UNP P09917
A	653	GLU	LYS	engineered mutation	UNP P09917
A	654	ASN	LYS	engineered mutation	UNP P09917
A	655	LEU	LYS	engineered mutation	UNP P09917
B	-17	MET	-	initiating methionine	UNP P09917
B	-16	GLY	-	expression tag	UNP P09917
B	-15	SER	-	expression tag	UNP P09917
B	-14	SER	-	expression tag	UNP P09917
B	-13	HIS	-	expression tag	UNP P09917
B	-12	HIS	-	expression tag	UNP P09917
B	-11	HIS	-	expression tag	UNP P09917
B	-10	HIS	-	expression tag	UNP P09917
B	-9	HIS	-	expression tag	UNP P09917
B	-8	HIS	-	expression tag	UNP P09917
B	-7	SER	-	expression tag	UNP P09917
B	-6	SER	-	expression tag	UNP P09917
B	-5	GLY	-	expression tag	UNP P09917
B	-4	LEU	-	expression tag	UNP P09917
B	-3	VAL	-	expression tag	UNP P09917
B	-2	PRO	-	expression tag	UNP P09917
B	-1	ARG	-	expression tag	UNP P09917
B	0	GLY	-	expression tag	UNP P09917
B	1	SER	-	expression tag	UNP P09917
B	2	HIS	-	expression tag	UNP P09917
B	16	GLU	TRP	engineered mutation	UNP P09917
B	17	HIS	PHE	engineered mutation	UNP P09917
B	?	-	PRO	SEE REMARK 999	UNP P09917
B	?	-	PHE	SEE REMARK 999	UNP P09917
B	?	-	TYR	SEE REMARK 999	UNP P09917
B	43	GLY	ASN	SEE REMARK 999	UNP P09917
B	44	SER	ASP	SEE REMARK 999	UNP P09917
B	75	GLY	TRP	engineered mutation	UNP P09917
B	76	SER	LEU	engineered mutation	UNP P09917

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Chain	Residue	Modelled	Actual	Comment	Reference
B	240	ALA	CYS	engineered mutation	UNP P09917
B	561	ALA	CYS	engineered mutation	UNP P09917
B	653	GLU	LYS	engineered mutation	UNP P09917
B	654	ASN	LYS	engineered mutation	UNP P09917
B	655	LEU	LYS	engineered mutation	UNP P09917
C	-17	MET	-	initiating methionine	UNP P09917
C	-16	GLY	-	expression tag	UNP P09917
C	-15	SER	-	expression tag	UNP P09917
C	-14	SER	-	expression tag	UNP P09917
C	-13	HIS	-	expression tag	UNP P09917
C	-12	HIS	-	expression tag	UNP P09917
C	-11	HIS	-	expression tag	UNP P09917
C	-10	HIS	-	expression tag	UNP P09917
C	-9	HIS	-	expression tag	UNP P09917
C	-8	HIS	-	expression tag	UNP P09917
C	-7	SER	-	expression tag	UNP P09917
C	-6	SER	-	expression tag	UNP P09917
C	-5	GLY	-	expression tag	UNP P09917
C	-4	LEU	-	expression tag	UNP P09917
C	-3	VAL	-	expression tag	UNP P09917
C	-2	PRO	-	expression tag	UNP P09917
C	-1	ARG	-	expression tag	UNP P09917
C	0	GLY	-	expression tag	UNP P09917
C	1	SER	-	expression tag	UNP P09917
C	2	HIS	-	expression tag	UNP P09917
C	16	GLU	TRP	engineered mutation	UNP P09917
C	17	HIS	PHE	engineered mutation	UNP P09917
C	?	-	PRO	SEE REMARK 999	UNP P09917
C	?	-	PHE	SEE REMARK 999	UNP P09917
C	?	-	TYR	SEE REMARK 999	UNP P09917
C	43	GLY	ASN	SEE REMARK 999	UNP P09917
C	44	SER	ASP	SEE REMARK 999	UNP P09917
C	75	GLY	TRP	engineered mutation	UNP P09917
C	76	SER	LEU	engineered mutation	UNP P09917
C	240	ALA	CYS	engineered mutation	UNP P09917
C	561	ALA	CYS	engineered mutation	UNP P09917
C	653	GLU	LYS	engineered mutation	UNP P09917
C	654	ASN	LYS	engineered mutation	UNP P09917
C	655	LEU	LYS	engineered mutation	UNP P09917
D	-17	MET	-	initiating methionine	UNP P09917
D	-16	GLY	-	expression tag	UNP P09917
D	-15	SER	-	expression tag	UNP P09917

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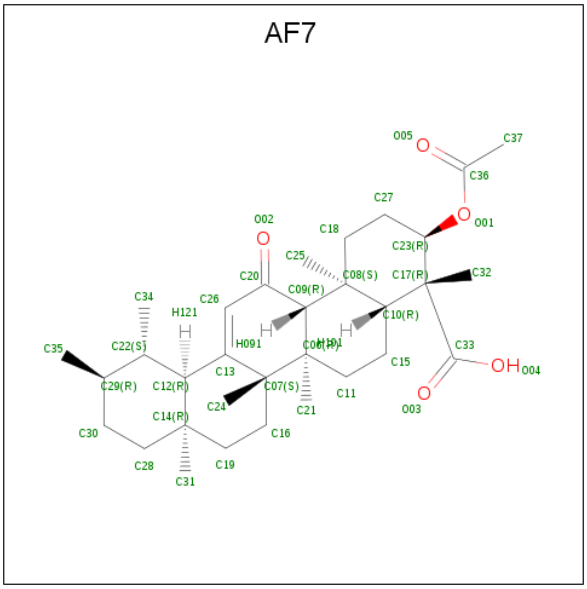
Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	SER	-	expression tag	UNP P09917
D	-13	HIS	-	expression tag	UNP P09917
D	-12	HIS	-	expression tag	UNP P09917
D	-11	HIS	-	expression tag	UNP P09917
D	-10	HIS	-	expression tag	UNP P09917
D	-9	HIS	-	expression tag	UNP P09917
D	-8	HIS	-	expression tag	UNP P09917
D	-7	SER	-	expression tag	UNP P09917
D	-6	SER	-	expression tag	UNP P09917
D	-5	GLY	-	expression tag	UNP P09917
D	-4	LEU	-	expression tag	UNP P09917
D	-3	VAL	-	expression tag	UNP P09917
D	-2	PRO	-	expression tag	UNP P09917
D	-1	ARG	-	expression tag	UNP P09917
D	0	GLY	-	expression tag	UNP P09917
D	1	SER	-	expression tag	UNP P09917
D	2	HIS	-	expression tag	UNP P09917
D	16	GLU	TRP	engineered mutation	UNP P09917
D	17	HIS	PHE	engineered mutation	UNP P09917
D	?	-	PRO	SEE REMARK 999	UNP P09917
D	?	-	PHE	SEE REMARK 999	UNP P09917
D	?	-	TYR	SEE REMARK 999	UNP P09917
D	43	GLY	ASN	SEE REMARK 999	UNP P09917
D	44	SER	ASP	SEE REMARK 999	UNP P09917
D	75	GLY	TRP	engineered mutation	UNP P09917
D	76	SER	LEU	engineered mutation	UNP P09917
D	240	ALA	CYS	engineered mutation	UNP P09917
D	561	ALA	CYS	engineered mutation	UNP P09917
D	653	GLU	LYS	engineered mutation	UNP P09917
D	654	ASN	LYS	engineered mutation	UNP P09917
D	655	LEU	LYS	engineered mutation	UNP P09917

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is (3alpha,8alpha,17alpha,18alpha)-3-(acetyloxy)-11-oxours-12-en-23-oic acid (three-letter code: AF7) (formula: $C_{32}H_{48}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	84	32	47	5	0	0

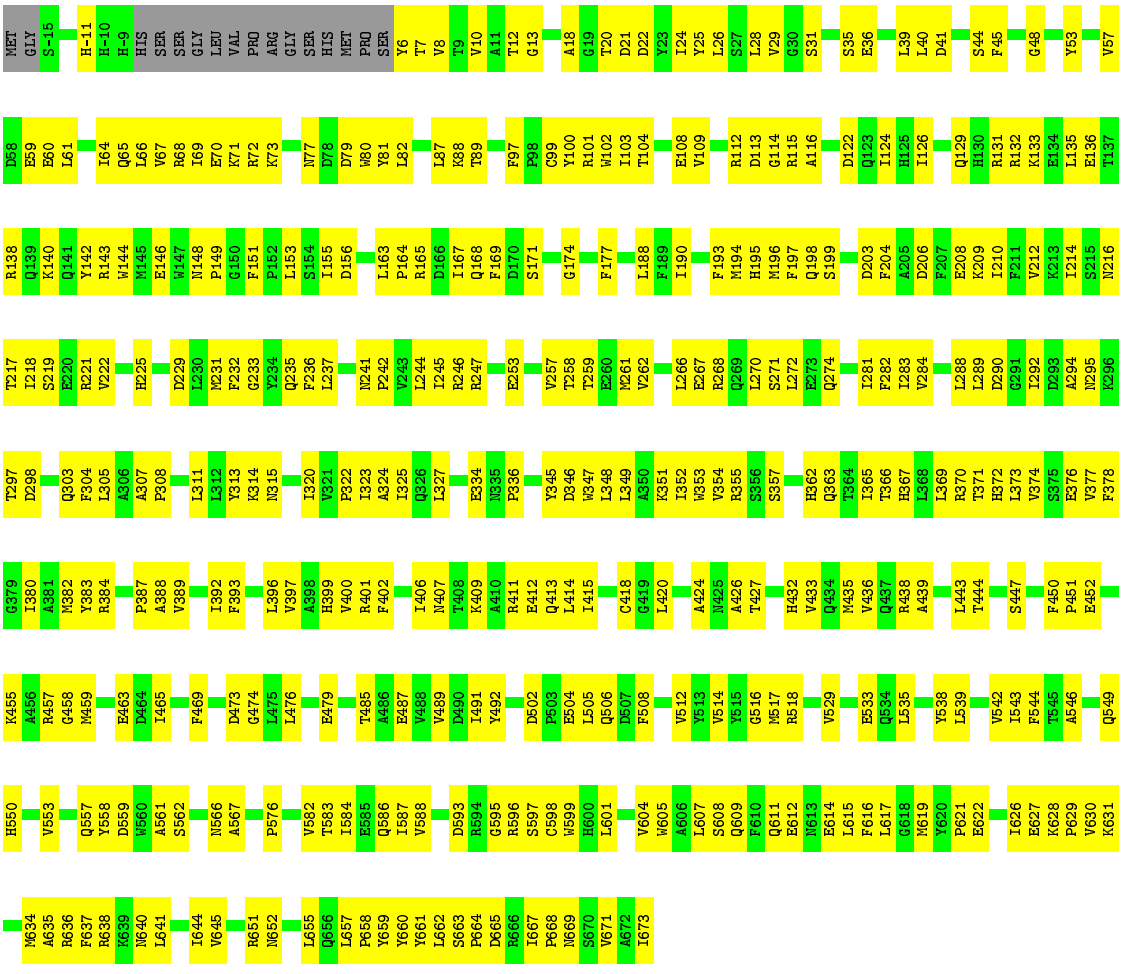
3 Residue-property plots (i)

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. 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. 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 failed to run properly.

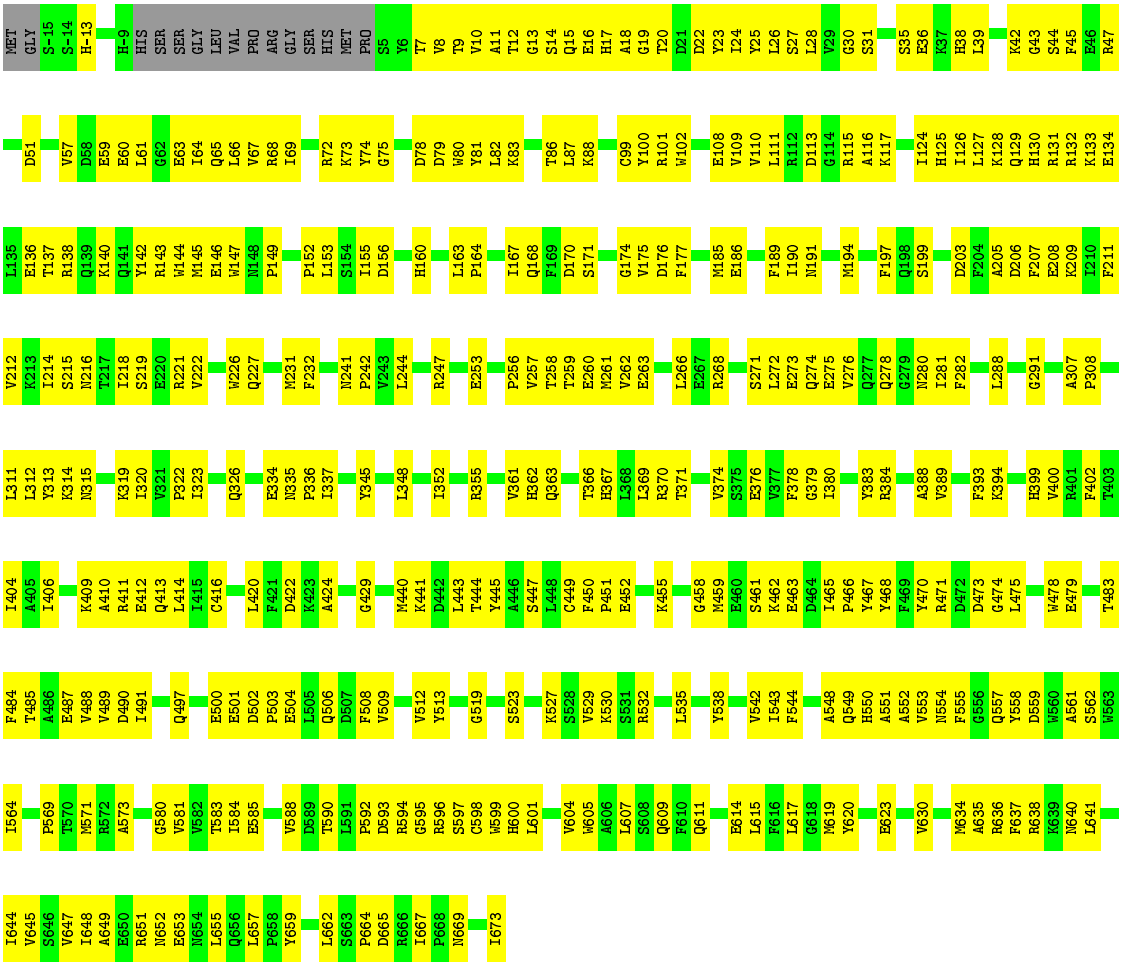
- Molecule 1: Arachidonate 5-lipoxygenase

Chain A:



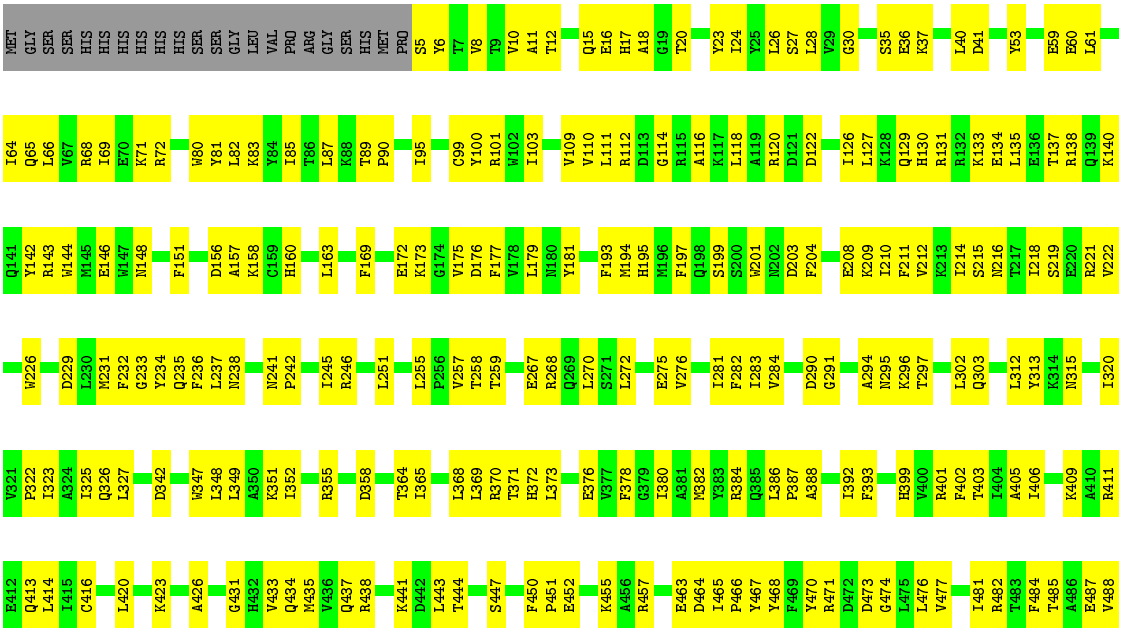
- Molecule 1: Arachidonate 5-lipoxygenase

Chain B:



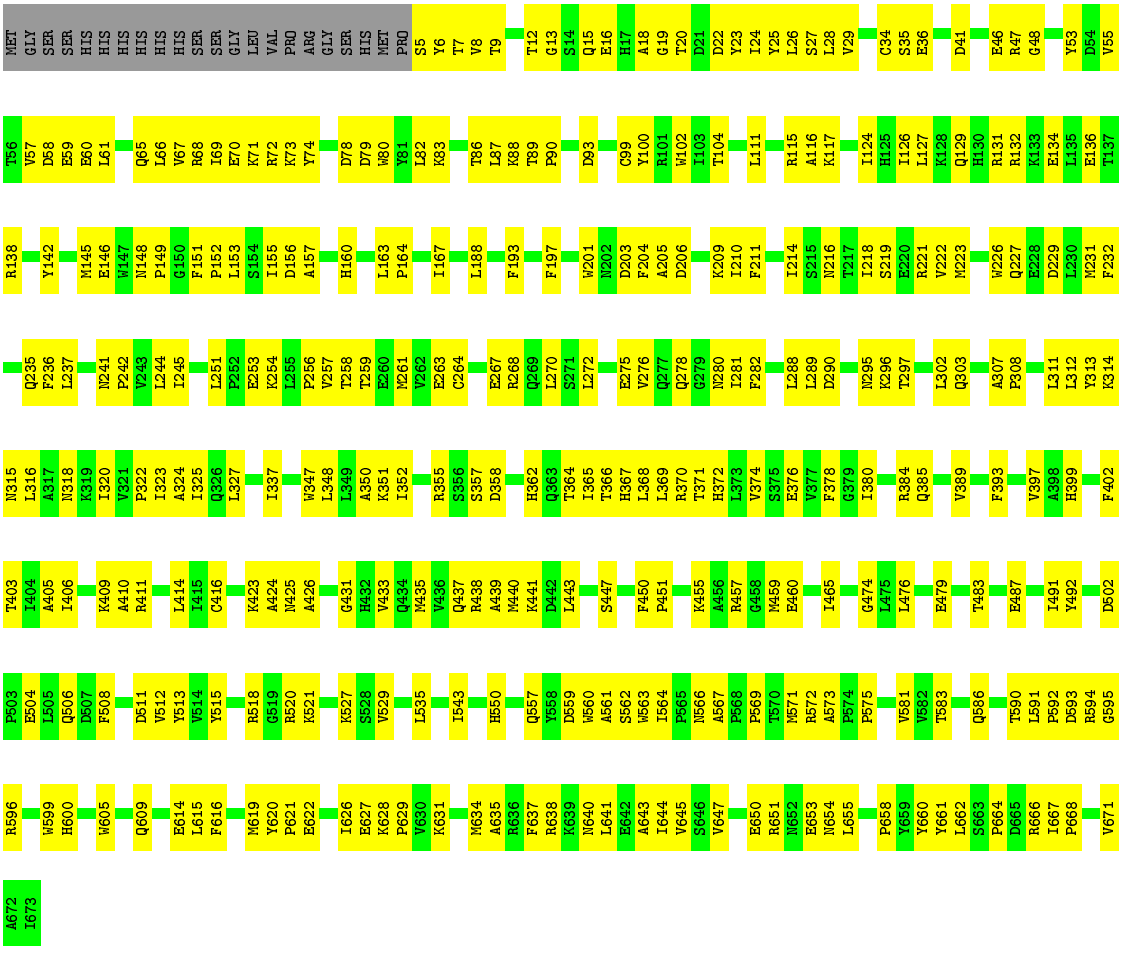
• Molecule 1: Arachidonate 5-lipoxygenase

Chain C:



- Molecule 1: Arachidonate 5-lipoxygenase

Chain D:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.87Å 203.72Å 110.44Å 90.00° 109.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.87	Depositor
% Data completeness (in resolution range)	95.2 (50.00-2.87)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.12rc2_2821	Depositor
R, R_{free}	0.275 , 0.297	Depositor
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.034	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.110 for h,-k,-h-l	Depositor
Outliers	3 of 69332 reflections (0.004%)	Xtriage
Total number of atoms	21918	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 71.77 % 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 2.4806e-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: AF7, FE2

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	0.31	0/5625	0.50	0/7631
1	B	0.30	0/5631	0.49	0/7639
1	C	0.31	0/5565	0.50	0/7551
1	D	0.30	0/5565	0.50	0/7551
All	All	0.30	0/22386	0.50	0/30372

There are no bond length outliers.

There are no bond angle outliers.

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	5484	0	5357	349	0
1	B	5490	0	5362	335	0
1	C	5428	0	5315	291	0
1	D	5428	0	5315	280	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	37	47	0	11	0
All	All	21871	47	21349	1236	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 29.

The worst 5 of 1236 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:A:65:GLN:HE22	1:A:124:ILE:HD11	1.14	1.13
1:B:262:VAL:HG11	1:B:323:ILE:HD12	1.25	1.10
1:B:424:ALA:HA	1:B:596:ARG:HG3	1.35	1.09
1:A:615:LEU:HA	1:A:619:MET:HE2	1.37	1.06
1:A:262:VAL:HG11	1:A:323:ILE:HD12	1.38	1.04

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
3	AF7	B	702	1	39,41,41	2.30	14 (35%)	62,70,70	2.84	31 (50%)

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
3	AF7	B	702	1	-	2/4/106/106	0/5/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	AF7	C17-C33	6.51	1.61	1.50
3	B	702	AF7	C07-C13	4.45	1.61	1.53
3	B	702	AF7	C26-C20	4.13	1.54	1.46
3	B	702	AF7	C17-C10	3.94	1.66	1.56
3	B	702	AF7	C27-C23	3.60	1.59	1.51

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	AF7	C24-C07-C13	7.62	114.89	106.95
3	B	702	AF7	C24-C07-C06	-6.97	105.81	112.33
3	B	702	AF7	C06-C09-C08	-6.58	113.30	118.10
3	B	702	AF7	C09-C08-C10	6.47	114.02	106.47
3	B	702	AF7	C18-C08-C09	5.30	113.94	108.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

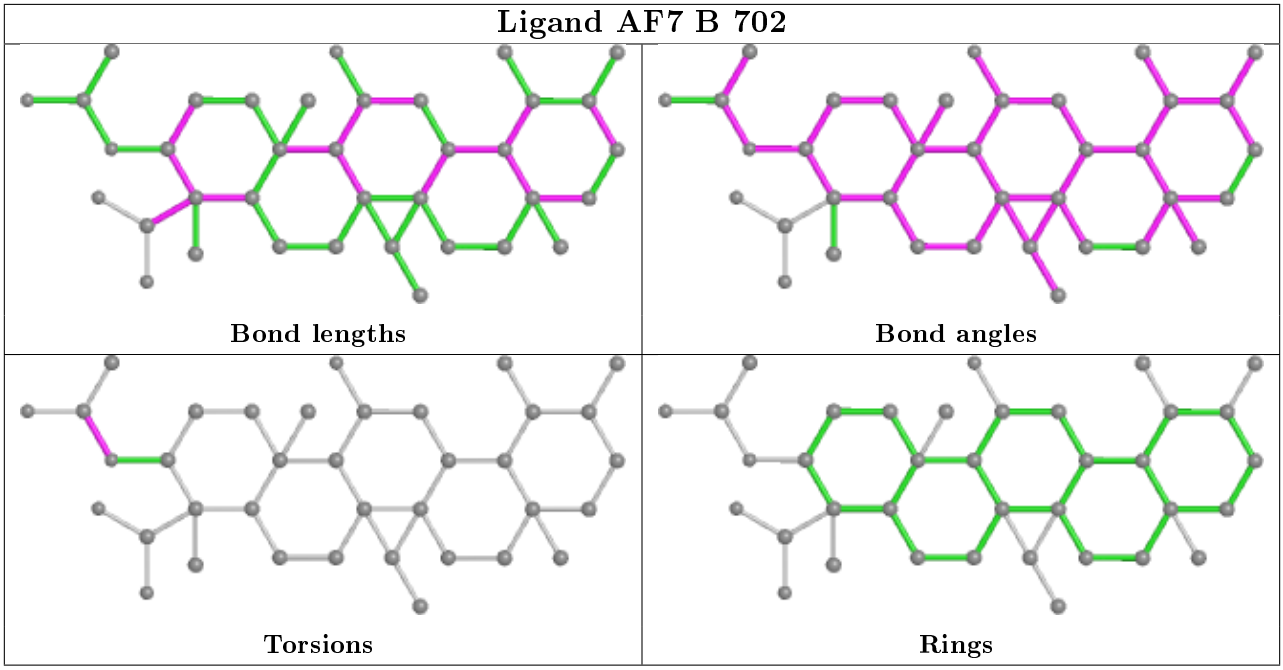
Mol	Chain	Res	Type	Atoms
3	B	702	AF7	C37-C36-O01-C23
3	B	702	AF7	O05-C36-O01-C23

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	AF7	11	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.



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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

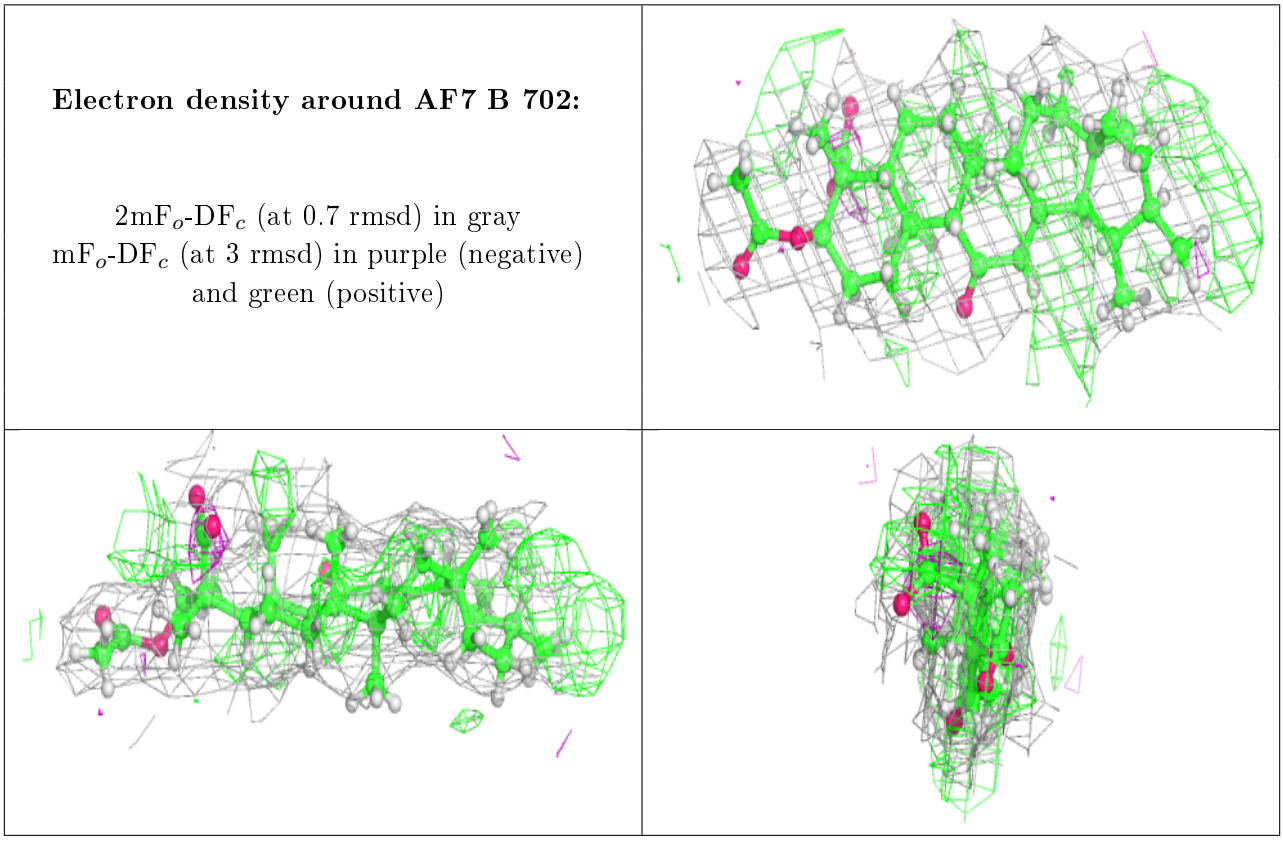
6.4 Ligands

EDS failed to run properly - this section is therefore empty.

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 AF7 B 702:

$2mF_o$-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)

EDS failed to run properly - this section is therefore empty.