



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:47 PM UTC

PDB ID : 8EY9 / pdb_00008ey9
Title : Structure of Arabidopsis fatty acid amide hydrolase mutant S305A in complex with 9-hydroxy-10,12-octadecadienoyl-ethanolamide
Authors : Aziz, M.; Wang, X.; Gaguancela, O.A.; Chapman, K.D.
Deposited on : 2022-10-26
Resolution : 3.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

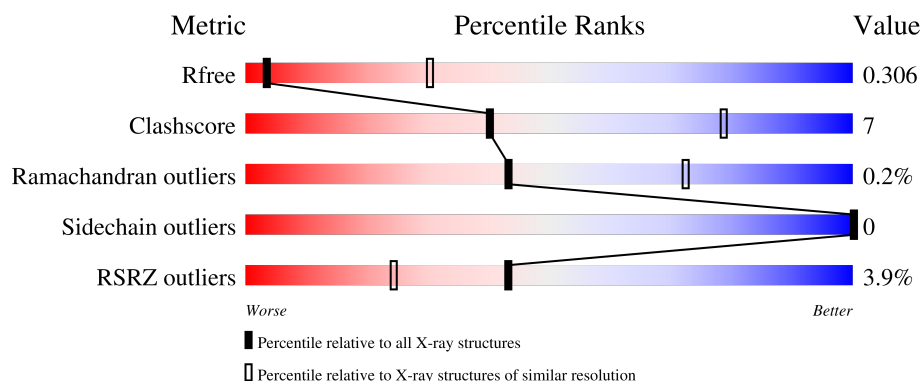
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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.



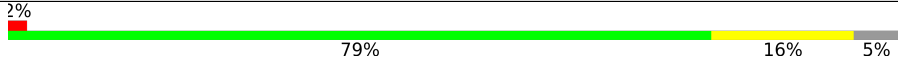
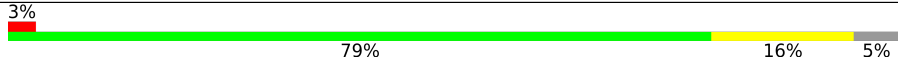
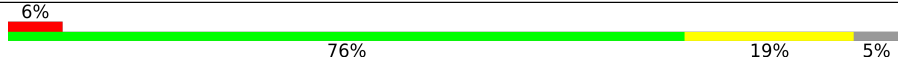
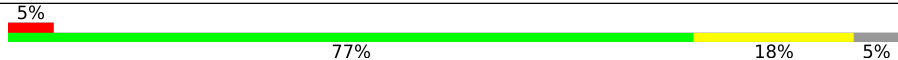
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	3% 78% 17% 5%
1	B	636	2% 81% 14% 5%
1	C	636	8% 79% 15% 5%
1	D	636	6% 78% 17% 5%
1	E	636	2% 80% 15% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	636	
1	G	636	
1	H	636	
1	I	636	
1	J	636	
1	K	636	
1	L	636	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 55530 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	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			
1	I	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	J	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	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...

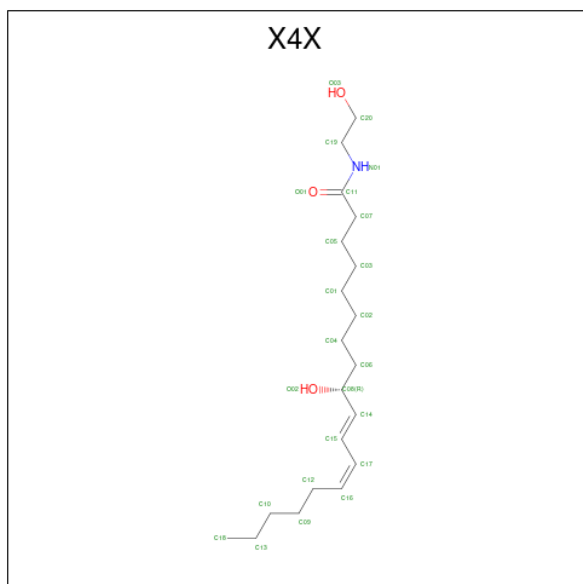
Chain	Residue	Modelled	Actual	Comment	Reference
J	636	HIS	-	expression tag	UNP Q7XJJ7
K	305	ALA	SER	engineered mutation	UNP Q7XJJ7
K	608	LYS	-	expression tag	UNP Q7XJJ7
K	609	GLY	-	expression tag	UNP Q7XJJ7
K	610	GLU	-	expression tag	UNP Q7XJJ7
K	611	PHE	-	expression tag	UNP Q7XJJ7
K	612	GLU	-	expression 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 (9R,10E,12Z)-9-hydroxy-N-(2-hydroxyethyl)octadeca-10,12-dienamide (CCD ID: X4X) (formula: C₂₀H₃₇NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	N	O	
			24	20	1	3	
						0	0

Continued on next page...

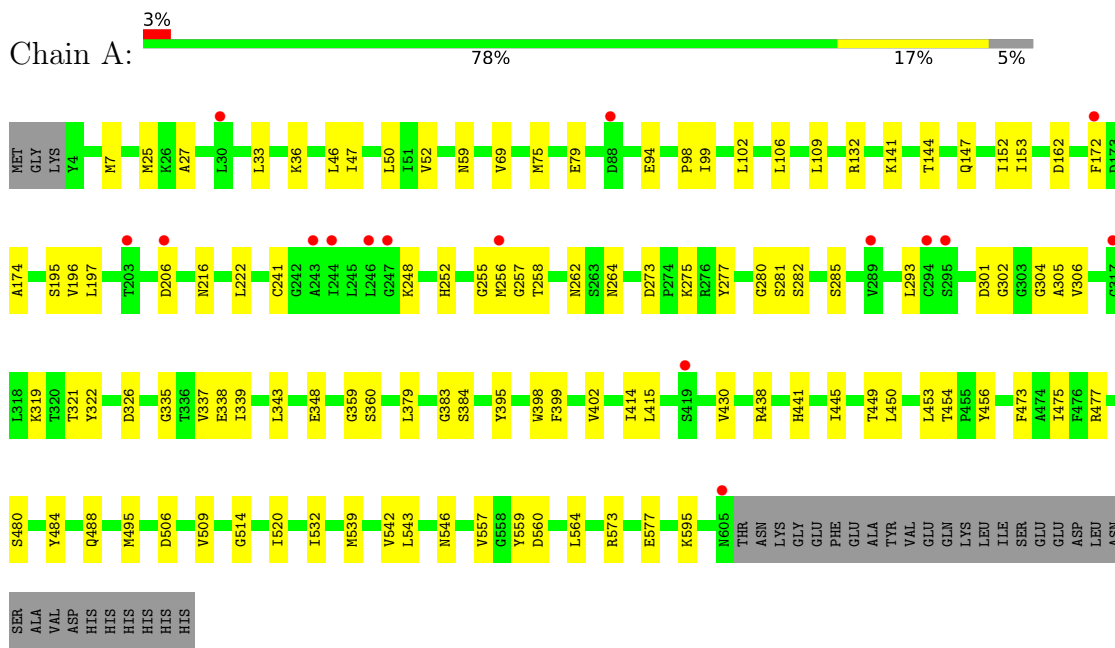
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			24	20	1	3		
2	F	1	Total	C	N	O	0	0
			24	20	1	3		
2	G	1	Total	C	N	O	0	0
			24	20	1	3		
2	H	1	Total	C	N	O	0	0
			24	20	1	3		
2	I	1	Total	C	N	O	0	0
			24	20	1	3		

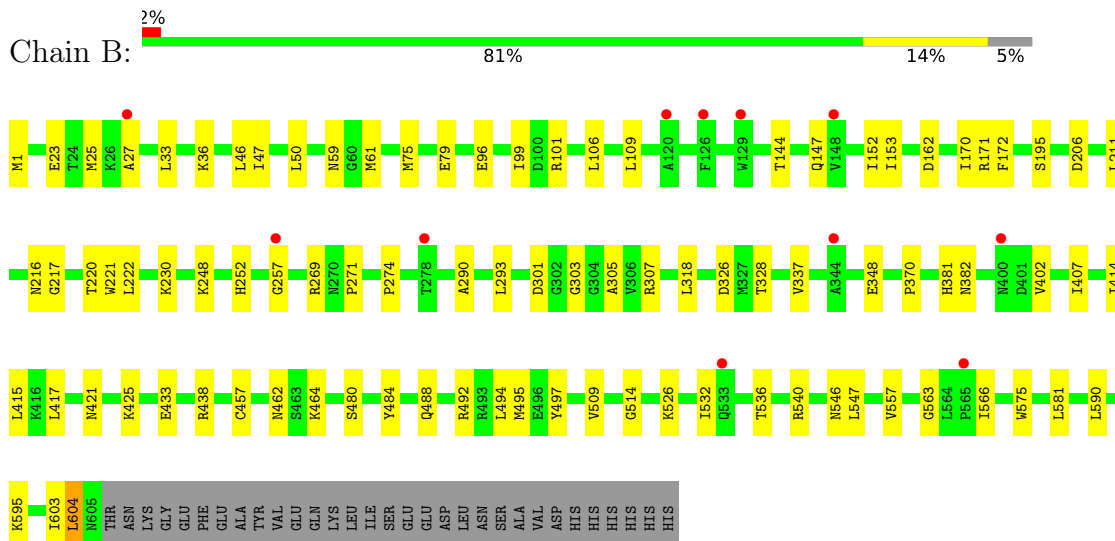
3 Residue-property plots [i](#)

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.

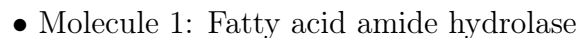
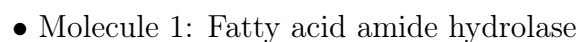
- Molecule 1: Fatty acid amide hydrolase

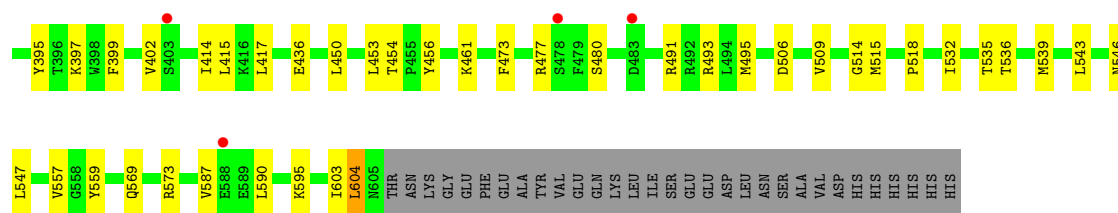


- Molecule 1: Fatty acid amide hydrolase

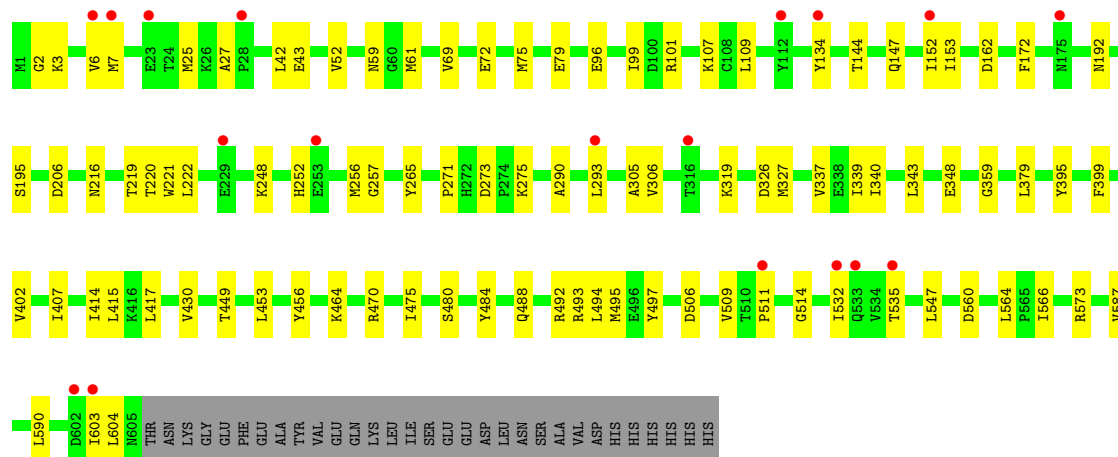
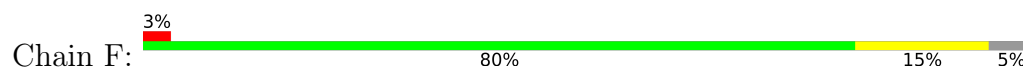


- Molecule 1: Fatty acid amide hydrolase

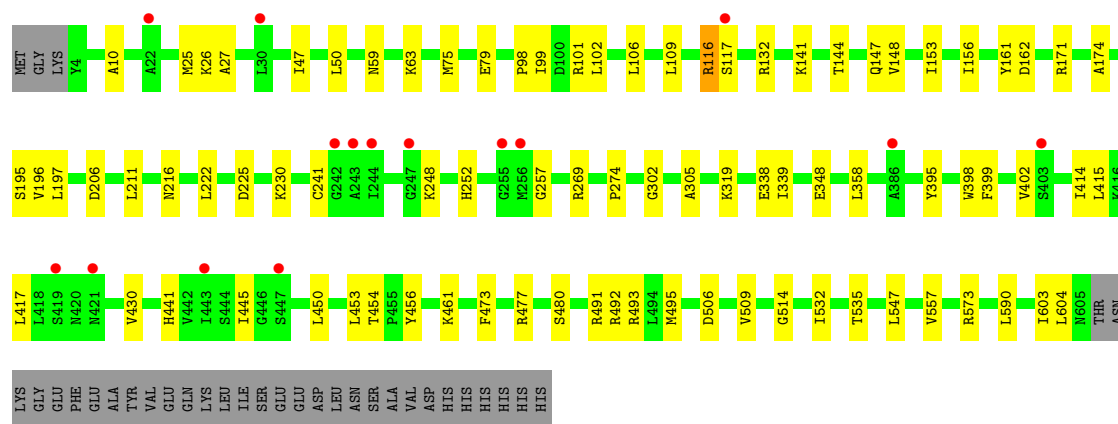
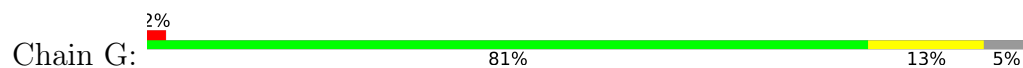




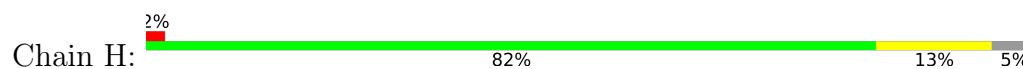
• Molecule 1: Fatty acid amide hydrolase

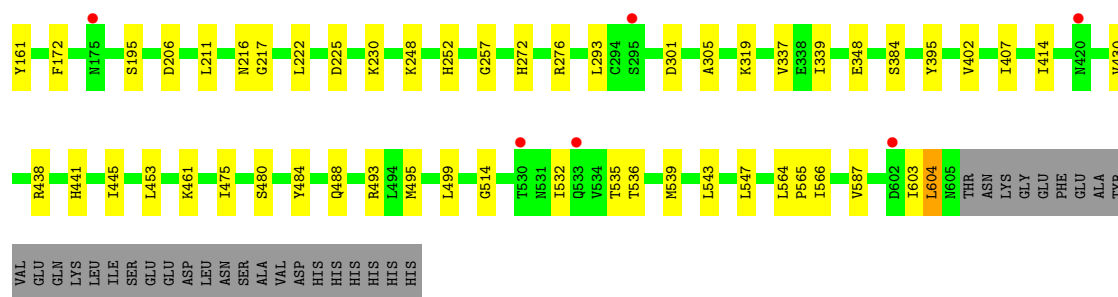


• Molecule 1: Fatty acid amide hydrolase

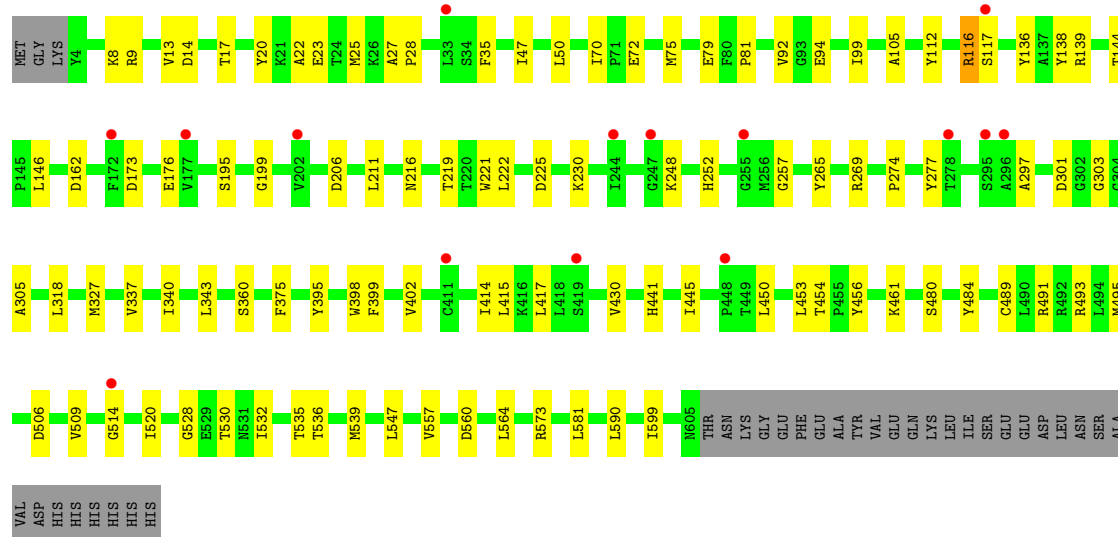
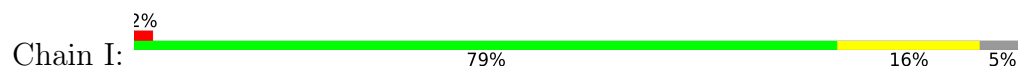


• Molecule 1: Fatty acid amide hydrolase

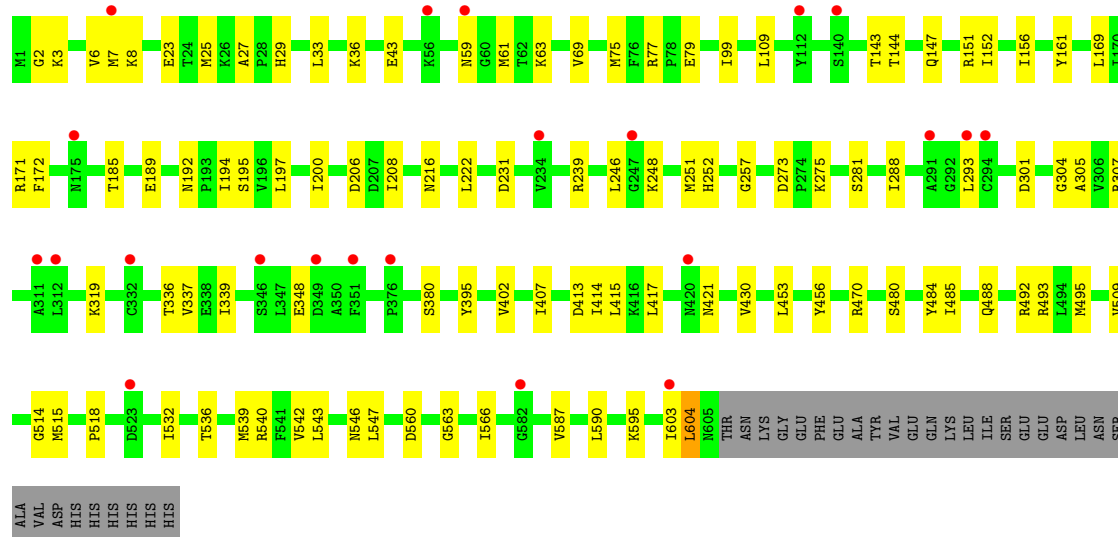
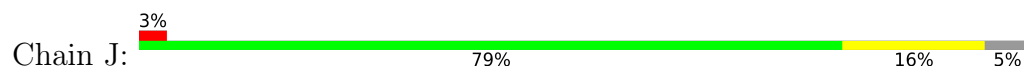




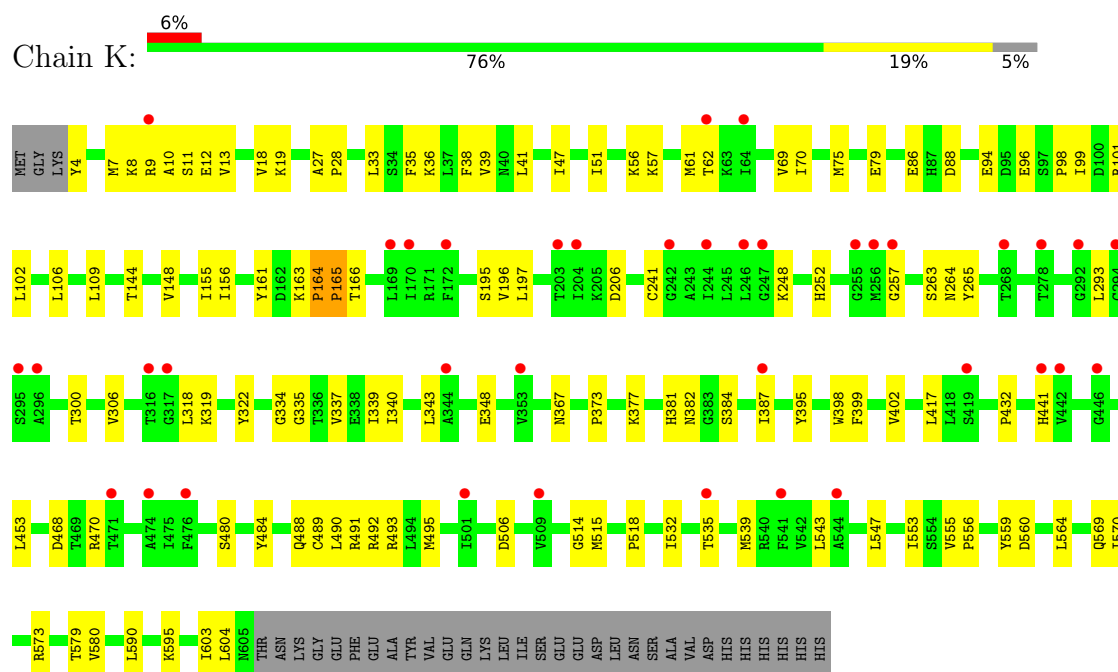
• Molecule 1: Fatty acid amide hydrolase



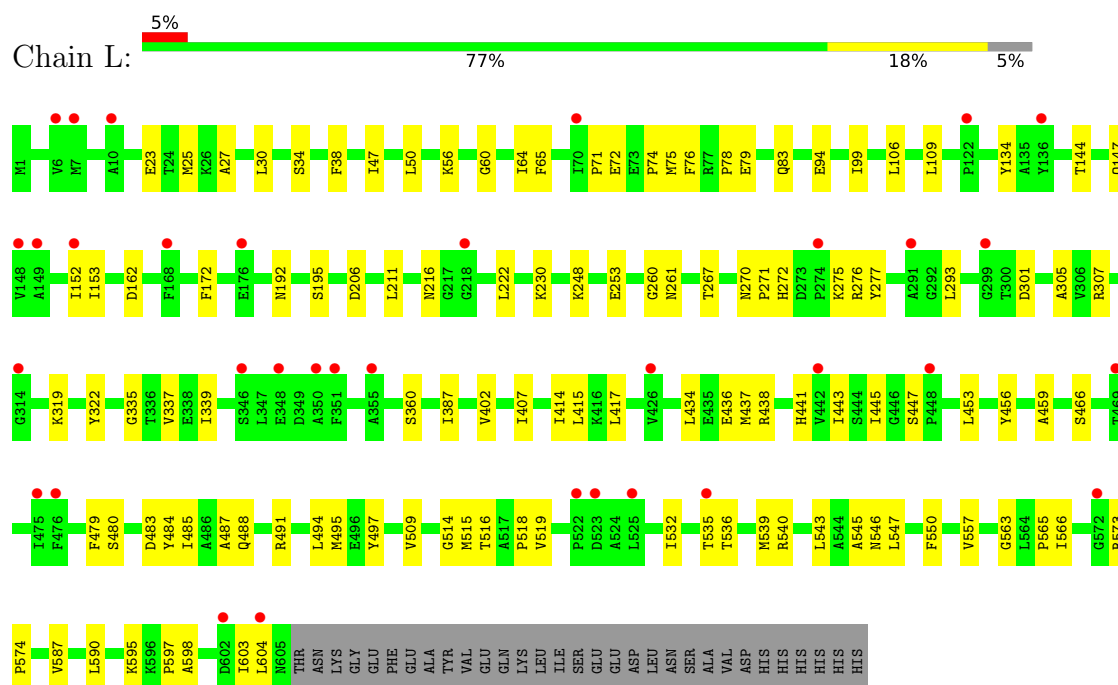
• Molecule 1: Fatty acid amide hydrolase



- Molecule 1: Fatty acid amide hydrolase



- Molecule 1: Fatty acid amide hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	222.91Å 82.91Å 271.78Å 90.00° 109.13° 90.00°	Depositor
Resolution (Å)	39.79 – 3.59 39.79 – 3.59	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.79-3.59) 96.8 (39.79-3.59)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.269 , 0.305 0.271 , 0.306	Depositor DCC
R_{free} test set	2005 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	55530	wwPDB-VP
Average B, all atoms (Å ²)	91.0	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 60.47 % 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 1.5151e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: X4X

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	0.09	0/4704	0.27	0/6391
1	B	0.08	0/4725	0.28	1/6417 (0.0%)
1	C	0.09	0/4704	0.36	5/6391 (0.1%)
1	D	0.09	0/4725	0.29	1/6417 (0.0%)
1	E	0.09	0/4704	0.37	5/6391 (0.1%)
1	F	0.09	0/4725	0.29	1/6417 (0.0%)
1	G	0.08	0/4704	0.39	5/6391 (0.1%)
1	H	0.08	0/4725	0.25	0/6417
1	I	0.10	0/4704	0.36	2/6391 (0.0%)
1	J	0.10	0/4725	0.26	0/6417
1	K	0.14	1/4704 (0.0%)	0.35	3/6391 (0.0%)
1	L	0.09	0/4725	0.28	0/6417
All	All	0.10	1/56574 (0.0%)	0.32	23/76848 (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	E	0	1
1	K	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	265	TYR	CA-CB	6.74	1.63	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	116	ARG	CB-CA-C	-19.01	81.24	111.28
1	I	116	ARG	CB-CA-C	-16.48	84.48	111.02
1	E	117	SER	N-CA-C	11.59	127.55	112.72
1	K	264	ASN	N-CA-C	11.38	123.43	111.14
1	C	603	ILE	CB-CA-C	11.34	129.89	111.29
1	C	559	TYR	CB-CA-C	10.57	132.62	112.43
1	E	116	ARG	CB-CA-C	-10.48	92.84	110.56
1	F	220	THR	CB-CA-C	9.64	126.11	109.24
1	E	117	SER	CB-CA-C	-8.15	97.01	110.37
1	B	220	THR	CB-CA-C	7.94	123.75	109.29
1	D	220	THR	CB-CA-C	7.46	122.87	109.29
1	G	116	ARG	CA-C-N	7.30	131.10	121.90
1	G	116	ARG	C-N-CA	7.30	131.10	121.90
1	K	265	TYR	CA-C-O	6.90	126.35	118.97
1	C	381	HIS	CB-CA-C	6.84	119.90	110.06
1	E	384	SER	CB-CA-C	-6.75	100.22	111.23
1	G	117	SER	CB-CA-C	-6.17	102.87	112.31
1	G	117	SER	N-CA-C	6.09	120.41	111.34
1	K	263	SER	CB-CA-C	6.06	122.22	110.46
1	C	603	ILE	CA-C-N	6.05	132.56	123.05
1	C	603	ILE	C-N-CA	6.05	132.56	123.05
1	E	220	THR	CB-CA-C	6.04	121.82	109.55
1	I	117	SER	N-CA-C	5.92	120.05	112.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	381	HIS	Peptide
1	K	164	PRO	Peptide

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	61	0
1	B	4626	0	4655	63	0
1	C	4605	0	4627	62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4626	0	4655	68	0
1	E	4605	0	4627	58	0
1	F	4626	0	4655	57	0
1	G	4605	0	4627	53	0
1	H	4626	0	4655	55	0
1	I	4605	0	4627	60	0
1	J	4626	0	4655	66	0
1	K	4605	0	4627	75	0
1	L	4626	0	4655	82	0
2	B	24	0	0	1	0
2	E	24	0	0	1	0
2	F	24	0	0	1	0
2	G	24	0	0	1	0
2	H	24	0	0	1	0
2	I	24	0	0	0	0
All	All	55530	0	55692	738	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 7.

All (738) 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:I:116:ARG:O	1:I:116:ARG:HG3	1.28	1.04
1:I:116:ARG:O	1:I:116:ARG:CG	2.02	1.04
1:E:116:ARG:O	1:E:116:ARG:HG3	1.59	1.01
1:G:116:ARG:O	1:G:116:ARG:HG3	1.74	0.85
1:B:221:TRP:O	1:B:221:TRP:CE3	2.38	0.76
1:E:319:LYS:HG2	1:E:339:ILE:HD11	1.69	0.74
1:A:282:SER:HG	1:A:285:SER:HG	1.32	0.74
1:J:208:ILE:O	1:J:248:LYS:NZ	2.18	0.74
1:H:319:LYS:HG2	1:H:339:ILE:HD11	1.71	0.72
1:G:319:LYS:HG2	1:G:339:ILE:HD11	1.71	0.71
1:B:221:TRP:O	1:B:221:TRP:HE3	1.72	0.71
1:G:75:MET:HE2	1:G:79:GLU:H	1.57	0.70
1:D:319:LYS:HG2	1:D:339:ILE:HD11	1.74	0.69
1:D:533:GLN:NE2	1:D:537:ASP:OD2	2.24	0.69
1:F:221:TRP:CD1	1:F:464:LYS:HB3	2.27	0.69
1:L:539:MET:HB3	1:L:543:LEU:HD21	1.74	0.69
1:A:319:LYS:HG2	1:A:339:ILE:HD11	1.75	0.69
1:K:9:ARG:HH11	1:K:11:SER:H	1.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:506:ASP:OD1	1:I:573:ARG:NH2	2.25	0.68
1:C:319:LYS:HG2	1:C:339:ILE:HD11	1.77	0.67
1:I:94:GLU:OE2	1:I:360:SER:OG	2.12	0.67
1:J:171:ARG:HB2	1:J:248:LYS:HB2	1.76	0.67
1:A:402:VAL:HG12	1:A:514:GLY:HA2	1.77	0.66
1:G:25:MET:SD	1:G:59:ASN:ND2	2.67	0.66
1:L:563:GLY:O	1:L:595:LYS:NZ	2.29	0.66
1:I:9:ARG:O	1:I:13:VAL:HG23	1.96	0.66
1:B:301:ASP:HA	1:B:305:ALA:HB3	1.78	0.66
1:K:319:LYS:HG2	1:K:339:ILE:HD11	1.78	0.66
1:K:441:HIS:HD2	1:K:543:LEU:HD22	1.61	0.66
1:L:99:ILE:HG23	1:L:195:SER:HB3	1.78	0.66
1:D:2:GLY:HA2	1:D:6:VAL:HG22	1.78	0.65
1:D:603:ILE:HG23	1:D:604:LEU:HG	1.78	0.65
1:E:75:MET:HE2	1:E:79:GLU:H	1.61	0.65
1:J:319:LYS:HG2	1:J:339:ILE:HD11	1.78	0.65
1:A:46:LEU:HD11	1:B:46:LEU:HD11	1.79	0.65
1:C:276:ARG:HA	1:C:520:ILE:HD13	1.79	0.65
1:H:25:MET:HG3	1:H:536:THR:HG21	1.78	0.65
1:J:75:MET:HE1	1:J:495:MET:HG2	1.79	0.64
1:L:75:MET:HE2	1:L:78:PRO:HA	1.79	0.64
1:H:603:ILE:HG22	1:H:604:LEU:HG	1.79	0.64
1:C:8:LYS:HD3	1:C:493:ARG:CZ	2.28	0.64
1:D:25:MET:HA	1:D:59:ASN:HD22	1.62	0.64
1:J:25:MET:SD	1:J:59:ASN:ND2	2.70	0.64
1:J:99:ILE:HG23	1:J:195:SER:HB3	1.80	0.64
1:J:25:MET:HG3	1:J:536:THR:HG21	1.80	0.64
1:L:277:TYR:HD2	1:L:518:PRO:HG2	1.63	0.64
1:L:402:VAL:HG12	1:L:514:GLY:HA2	1.79	0.64
1:E:491:ARG:NH1	1:E:547:LEU:O	2.31	0.63
1:C:75:MET:HE1	1:C:495:MET:HG2	1.80	0.63
1:L:415:LEU:HD21	1:L:509:VAL:HG21	1.80	0.63
1:H:402:VAL:HG12	1:H:514:GLY:HA2	1.81	0.63
1:K:75:MET:HB2	1:K:492:ARG:HB2	1.81	0.63
1:L:30:LEU:HD12	1:L:38:PHE:HB2	1.80	0.63
1:F:402:VAL:HG12	1:F:514:GLY:HA2	1.80	0.63
1:B:75:MET:HE2	1:B:79:GLU:H	1.64	0.63
1:D:99:ILE:HG23	1:D:195:SER:HB3	1.80	0.63
1:A:383:GLY:O	1:A:384:SER:HB2	1.99	0.63
1:H:206:ASP:HA	1:H:248:LYS:HE2	1.80	0.63
1:K:7:MET:HG2	1:K:69:VAL:HB	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:LYS:HG2	1:F:339:ILE:HD11	1.80	0.62
1:B:99:ILE:HG23	1:B:195:SER:HB3	1.80	0.62
1:J:144:THR:HG23	1:J:147:GLN:H	1.64	0.62
1:F:75:MET:HE2	1:F:79:GLU:H	1.65	0.62
1:D:563:GLY:O	1:D:595:LYS:NZ	2.33	0.62
1:J:603:ILE:HG22	1:J:604:LEU:HG	1.80	0.62
1:B:153:ILE:HG12	1:B:172:PHE:HZ	1.64	0.62
1:B:307:ARG:NH2	1:B:546:ASN:OD1	2.32	0.62
1:B:269:ARG:NH1	1:H:141:LYS:O	2.30	0.61
1:B:563:GLY:O	1:B:595:LYS:NZ	2.33	0.61
1:C:480:SER:HA	1:D:480:SER:HA	1.82	0.61
1:G:206:ASP:HA	1:G:248:LYS:HE2	1.81	0.61
1:C:402:VAL:HG12	1:C:514:GLY:HA2	1.82	0.61
1:G:116:ARG:O	1:G:116:ARG:CG	2.31	0.61
1:K:539:MET:HB3	1:K:543:LEU:HD21	1.83	0.60
1:J:563:GLY:O	1:J:595:LYS:NZ	2.34	0.60
1:L:153:ILE:HG12	1:L:172:PHE:HZ	1.66	0.60
1:B:152:ILE:HG23	1:B:293:LEU:HD22	1.83	0.60
1:L:25:MET:HG3	1:L:536:THR:HG21	1.83	0.60
1:F:25:MET:SD	1:F:59:ASN:ND2	2.74	0.60
1:K:99:ILE:HG23	1:K:195:SER:HB3	1.84	0.60
1:J:169:LEU:HD12	1:J:172:PHE:HD2	1.67	0.60
1:E:603:ILE:HG22	1:E:604:LEU:HG	1.84	0.60
1:I:35:PHE:HE2	1:I:528:GLY:C	2.10	0.60
1:J:23:GLU:HG3	1:J:540:ARG:HH21	1.67	0.60
1:G:506:ASP:OD1	1:G:573:ARG:NH2	2.29	0.60
1:B:221:TRP:CD1	1:B:464:LYS:HB3	2.37	0.59
1:H:216:ASN:HA	1:H:222:LEU:HB3	1.84	0.59
1:K:75:MET:HE1	1:K:495:MET:HG2	1.84	0.59
1:D:75:MET:HE2	1:D:79:GLU:H	1.67	0.59
1:L:23:GLU:HG3	1:L:540:ARG:HH21	1.67	0.59
1:K:39:VAL:HG11	1:K:470:ARG:HH21	1.68	0.59
1:B:47:ILE:HA	1:B:50:LEU:HD12	1.85	0.59
1:K:480:SER:HA	1:L:480:SER:HA	1.84	0.59
1:E:25:MET:HG3	1:E:536:THR:HG21	1.84	0.59
1:B:417:LEU:HB3	1:B:590:LEU:HD13	1.84	0.59
1:D:221:TRP:O	1:D:221:TRP:CE3	2.56	0.59
1:I:72:GLU:OE2	1:I:493:ARG:NH1	2.36	0.59
1:B:402:VAL:HG12	1:B:514:GLY:HA2	1.85	0.58
1:D:144:THR:HG23	1:D:147:GLN:H	1.68	0.58
1:B:144:THR:HG23	1:B:147:GLN:H	1.66	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ASP:OD1	1:C:573:ARG:NH2	2.32	0.58
1:H:33:LEU:HD13	1:H:33:LEU:O	2.02	0.58
1:K:4:TYR:HD2	1:L:459:ALA:HB1	1.68	0.58
1:A:506:ASP:OD1	1:A:573:ARG:NH2	2.36	0.58
1:J:402:VAL:HG12	1:J:514:GLY:HA2	1.86	0.58
1:K:441:HIS:CD2	1:K:543:LEU:HD22	2.37	0.58
1:L:271:PRO:HG2	1:L:272:HIS:HD2	1.67	0.58
1:F:2:GLY:HA2	1:F:6:VAL:HG22	1.86	0.58
1:F:206:ASP:HA	1:F:248:LYS:HE2	1.85	0.58
1:G:109:LEU:HD22	1:G:348:GLU:HG3	1.85	0.58
1:H:99:ILE:HG23	1:H:195:SER:HB3	1.85	0.58
1:L:261:ASN:ND2	1:L:277:TYR:OH	2.36	0.58
1:K:402:VAL:HG12	1:K:514:GLY:HA2	1.86	0.58
1:L:319:LYS:HG2	1:L:339:ILE:HD11	1.86	0.58
1:E:206:ASP:HA	1:E:248:LYS:HE2	1.86	0.57
1:G:603:ILE:HG22	1:G:604:LEU:N	2.19	0.57
1:K:252:HIS:NE2	1:K:468:ASP:OD2	2.35	0.57
1:L:216:ASN:HA	1:L:222:LEU:HB3	1.85	0.57
1:H:23:GLU:HA	1:H:438:ARG:HH12	1.69	0.57
1:K:28:PRO:HG2	1:K:38:PHE:HE2	1.68	0.57
1:L:491:ARG:NH1	1:L:547:LEU:O	2.37	0.57
1:A:480:SER:HA	1:B:480:SER:HA	1.86	0.57
1:E:99:ILE:HG23	1:E:195:SER:HB3	1.86	0.57
1:K:88:ASP:OD1	1:K:377:LYS:NZ	2.37	0.57
1:D:537:ASP:OD1	1:D:540:ARG:NH2	2.37	0.57
1:D:153:ILE:HG12	1:D:172:PHE:HZ	1.69	0.57
1:J:413:ASP:O	1:J:417:LEU:N	2.35	0.56
1:I:75:MET:HE1	1:I:495:MET:HG2	1.88	0.56
1:C:25:MET:SD	1:C:59:ASN:ND2	2.78	0.56
1:E:453:LEU:HD23	1:E:456:TYR:HD2	1.70	0.56
1:F:99:ILE:HG23	1:F:195:SER:HB3	1.86	0.56
1:G:453:LEU:HD23	1:G:456:TYR:HD2	1.69	0.56
1:F:109:LEU:HD22	1:F:348:GLU:HG3	1.87	0.56
1:L:83:GLN:HE22	1:L:573:ARG:HB3	1.71	0.56
1:L:443:ILE:HG13	1:L:479:PHE:CG	2.41	0.56
1:B:425:LYS:NZ	1:C:402:VAL:O	2.39	0.55
1:D:216:ASN:HA	1:D:222:LEU:HB3	1.88	0.55
1:L:414:ILE:HG13	1:L:557:VAL:HB	1.87	0.55
1:H:25:MET:HA	1:H:59:ASN:HD22	1.72	0.55
1:I:206:ASP:HA	1:I:248:LYS:HE2	1.87	0.55
1:J:206:ASP:HA	1:J:248:LYS:HE2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:417:LEU:HB3	1:L:590:LEU:HD13	1.88	0.55
1:I:225:ASP:OD2	1:I:461:LYS:NZ	2.39	0.55
1:B:603:ILE:HG22	1:B:604:LEU:HG	1.88	0.55
1:E:92:VAL:HG11	1:E:101:ARG:HG2	1.88	0.55
1:E:216:ASN:HA	1:E:222:LEU:HB3	1.88	0.55
1:E:480:SER:HA	1:F:480:SER:HA	1.88	0.55
1:F:273:ASP:OD2	1:F:275:LYS:NZ	2.38	0.55
1:L:30:LEU:HD13	1:L:34:SER:HB2	1.88	0.55
1:I:47:ILE:HA	1:I:50:LEU:HD12	1.89	0.55
1:K:70:ILE:HD12	1:K:489:CYS:HB2	1.88	0.55
1:F:216:ASN:HA	1:F:222:LEU:HB3	1.88	0.55
1:B:25:MET:SD	1:B:59:ASN:ND2	2.80	0.55
1:E:47:ILE:HA	1:E:50:LEU:HD12	1.88	0.55
1:B:414:ILE:HG13	1:B:557:VAL:HB	1.88	0.54
1:E:25:MET:SD	1:E:59:ASN:ND2	2.80	0.54
1:K:18:VAL:HG11	1:K:432:PRO:HB3	1.89	0.54
1:A:256:MET:HE3	1:A:449:THR:HG21	1.89	0.54
1:G:144:THR:HG23	1:G:147:GLN:H	1.72	0.54
1:J:156:ILE:HG23	1:J:161:TYR:HB2	1.89	0.54
1:L:206:ASP:HA	1:L:248:LYS:HE2	1.89	0.54
1:L:515:MET:HE2	1:L:518:PRO:HB3	1.89	0.54
1:D:25:MET:HG3	1:D:536:THR:HG21	1.88	0.54
1:L:441:HIS:HE2	1:L:445:ILE:HD12	1.72	0.54
1:G:75:MET:HE1	1:G:495:MET:HG2	1.90	0.54
1:H:109:LEU:HD22	1:H:348:GLU:HG3	1.90	0.54
1:L:603:ILE:HG23	1:L:604:LEU:HG	1.89	0.54
1:E:383:GLY:O	1:E:384:SER:HB2	2.08	0.54
1:K:367:ASN:ND2	1:L:79:GLU:OE1	2.38	0.54
1:E:417:LEU:HB3	1:E:590:LEU:HD13	1.90	0.54
1:G:450:LEU:O	1:G:454:THR:OG1	2.24	0.54
1:D:301:ASP:HA	1:D:305:ALA:HB3	1.90	0.54
1:D:414:ILE:HG13	1:D:557:VAL:HB	1.89	0.54
1:B:23:GLU:OE1	1:B:540:ARG:NH2	2.41	0.53
1:J:197:LEU:HA	1:J:200:ILE:HG13	1.89	0.53
1:E:8:LYS:HD3	1:E:493:ARG:CZ	2.39	0.53
1:G:395:TYR:O	1:G:399:PHE:N	2.40	0.53
1:I:269:ARG:HB3	1:I:274:PRO:HA	1.90	0.53
1:L:76:PHE:HD1	1:L:488:GLN:HG3	1.73	0.53
1:A:450:LEU:O	1:A:454:THR:OG1	2.25	0.53
1:D:417:LEU:HB3	1:D:590:LEU:HD13	1.91	0.53
1:K:506:ASP:OD1	1:K:573:ARG:NH2	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:MET:HB3	1:F:69:VAL:HB	1.90	0.53
1:B:269:ARG:HB3	1:B:274:PRO:HA	1.91	0.53
1:D:134:TYR:OH	1:D:603:ILE:HG21	2.09	0.53
1:A:75:MET:HE1	1:A:495:MET:HG2	1.91	0.53
1:D:152:ILE:HG23	1:D:293:LEU:HD22	1.91	0.53
1:I:480:SER:HA	1:J:480:SER:HA	1.91	0.53
1:K:75:MET:HE2	1:K:79:GLU:HB2	1.91	0.53
1:E:506:ASP:OD1	1:E:573:ARG:NH2	2.34	0.52
1:H:33:LEU:HD13	1:H:33:LEU:C	2.34	0.52
1:H:152:ILE:HG23	1:H:293:LEU:HD22	1.91	0.52
1:F:152:ILE:HG23	1:F:293:LEU:HD22	1.91	0.52
1:G:491:ARG:NH1	1:G:547:LEU:O	2.43	0.52
1:B:33:LEU:HA	1:B:36:LYS:HE3	1.91	0.52
1:B:206:ASP:HA	1:B:248:LYS:HE2	1.92	0.52
1:D:52:VAL:HG13	1:D:475:ILE:HG12	1.91	0.52
1:F:319:LYS:HE2	1:F:339:ILE:HG12	1.91	0.52
1:B:25:MET:HG3	1:B:536:THR:HG21	1.92	0.52
1:B:421:ASN:HA	1:C:19:LYS:HD3	1.92	0.52
1:G:414:ILE:HG13	1:G:557:VAL:HB	1.91	0.52
1:I:112:TYR:HE2	1:I:136:TYR:HB2	1.73	0.52
1:C:15:LEU:HD23	1:C:15:LEU:H	1.74	0.52
1:C:109:LEU:HD22	1:C:348:GLU:HG3	1.91	0.52
1:E:162:ASP:OD1	1:E:162:ASP:N	2.43	0.52
1:H:33:LEU:HA	1:H:36:LYS:HE3	1.92	0.52
1:K:417:LEU:HB3	1:K:590:LEU:HD13	1.92	0.52
1:L:47:ILE:HA	1:L:50:LEU:HD12	1.91	0.52
1:L:453:LEU:HD23	1:L:456:TYR:HD2	1.74	0.52
1:B:171:ARG:HB2	1:B:248:LYS:HB2	1.90	0.51
1:E:144:THR:HG23	1:E:147:GLN:H	1.76	0.51
1:K:109:LEU:HD22	1:K:348:GLU:HG3	1.92	0.51
1:A:25:MET:HE2	1:A:438:ARG:HE	1.74	0.51
1:L:270:ASN:ND2	1:L:277:TYR:O	2.43	0.51
1:A:152:ILE:HG23	1:A:293:LEU:HD22	1.91	0.51
1:C:515:MET:HE2	1:C:518:PRO:HB3	1.91	0.51
1:A:7:MET:HB3	1:A:69:VAL:HB	1.93	0.51
1:L:272:HIS:CE1	1:L:565:PRO:HG3	2.45	0.51
1:C:47:ILE:HA	1:C:50:LEU:HD12	1.93	0.51
1:D:25:MET:HE2	1:D:438:ARG:HE	1.75	0.51
1:E:109:LEU:HD22	1:E:348:GLU:HG3	1.91	0.51
1:A:206:ASP:HA	1:A:248:LYS:HE2	1.92	0.51
1:D:195:SER:OG	1:D:241:CYS:SG	2.60	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:MET:HE1	1:E:495:MET:HG2	1.93	0.51
1:G:27:ALA:HB3	1:G:532:ILE:HB	1.92	0.51
1:I:99:ILE:HG23	1:I:195:SER:HB3	1.93	0.51
1:I:560:ASP:OD1	1:I:564:LEU:N	2.43	0.51
1:B:301:ASP:OD2	1:B:307:ARG:NH2	2.41	0.51
1:G:480:SER:HA	1:H:480:SER:HA	1.93	0.51
1:I:450:LEU:O	1:I:454:THR:OG1	2.23	0.51
1:C:206:ASP:HA	1:C:248:LYS:HE2	1.92	0.50
1:D:180:GLN:HE22	1:D:245:LEU:HB2	1.75	0.50
1:D:221:TRP:O	1:D:221:TRP:HE3	1.94	0.50
1:G:26:LYS:H	1:G:59:ASN:HD21	1.57	0.50
1:J:414:ILE:HG21	1:J:587:VAL:HG13	1.93	0.50
1:K:35:PHE:HZ	1:K:468:ASP:HA	1.76	0.50
1:A:25:MET:SD	1:A:59:ASN:ND2	2.84	0.50
1:C:99:ILE:HG23	1:C:195:SER:HB3	1.92	0.50
1:C:321:THR:OG1	1:C:577:GLU:OE2	2.19	0.50
1:G:47:ILE:HA	1:G:50:LEU:HD12	1.93	0.50
1:G:102:LEU:HD11	1:G:197:LEU:HD12	1.93	0.50
1:A:109:LEU:HD22	1:A:348:GLU:HG3	1.92	0.50
1:B:75:MET:HE1	1:B:495:MET:HG2	1.93	0.50
1:E:211:LEU:HD11	1:E:230:LYS:HA	1.92	0.50
1:B:96:GLU:O	1:B:101:ARG:NH1	2.44	0.50
1:B:109:LEU:HD22	1:B:348:GLU:HG3	1.93	0.50
1:K:490:LEU:HD23	1:K:493:ARG:HD3	1.92	0.50
1:C:414:ILE:HG13	1:C:557:VAL:HB	1.92	0.50
1:F:153:ILE:HG12	1:F:172:PHE:HZ	1.76	0.50
1:H:8:LYS:NZ	1:H:68:THR:HG21	2.27	0.50
1:K:9:ARG:HD2	1:K:12:GLU:H	1.77	0.50
1:L:319:LYS:NZ	1:L:545:ALA:O	2.35	0.50
1:H:25:MET:HA	1:H:59:ASN:ND2	2.27	0.50
1:H:75:MET:HE1	1:H:495:MET:HG2	1.92	0.50
1:K:603:ILE:HG22	1:K:604:LEU:H	1.77	0.50
1:L:337:VAL:HG12	1:L:547:LEU:HA	1.93	0.50
1:H:47:ILE:HA	1:H:50:LEU:HD12	1.94	0.50
1:K:559:TYR:CZ	1:K:595:LYS:HB2	2.46	0.50
1:I:274:PRO:HG3	1:I:599:ILE:HD11	1.94	0.50
1:K:395:TYR:O	1:K:399:PHE:N	2.43	0.50
1:L:322:TYR:OH	1:L:335:GLY:O	2.24	0.50
1:F:271:PRO:HG2	1:F:290:ALA:HB3	1.94	0.50
1:G:156:ILE:HA	1:G:161:TYR:HB2	1.94	0.50
1:H:143:THR:HG21	1:H:604:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:HIS:CE1	1:I:257:GLY:HA3	2.47	0.50
1:L:319:LYS:HE2	1:L:339:ILE:HG12	1.94	0.50
1:A:47:ILE:HA	1:A:50:LEU:HD12	1.93	0.49
1:C:216:ASN:HA	1:C:222:LEU:HB3	1.93	0.49
1:D:536:THR:HA	1:D:539:MET:HE2	1.94	0.49
1:F:144:THR:HG23	1:F:147:GLN:H	1.76	0.49
1:A:258:THR:C	1:A:280:GLY:H	2.20	0.49
1:C:27:ALA:HB3	1:C:532:ILE:HB	1.94	0.49
1:F:337:VAL:HG12	1:F:547:LEU:HA	1.94	0.49
1:H:337:VAL:HG12	1:H:547:LEU:HA	1.94	0.49
1:I:402:VAL:HG12	1:I:514:GLY:HA2	1.94	0.49
1:L:441:HIS:ND1	1:L:543:LEU:HD22	2.27	0.49
1:A:106:LEU:HD11	1:A:196:VAL:HB	1.94	0.49
1:D:337:VAL:HG12	1:D:547:LEU:HA	1.94	0.49
1:F:379:LEU:HD12	1:F:379:LEU:H	1.77	0.49
1:K:47:ILE:HG22	1:K:51:ILE:HD11	1.94	0.49
1:A:395:TYR:CZ	1:A:430:VAL:HG23	2.48	0.49
1:F:417:LEU:HB3	1:F:590:LEU:HD13	1.94	0.49
1:I:417:LEU:HB3	1:I:590:LEU:HD13	1.94	0.49
1:J:109:LEU:HD22	1:J:348:GLU:HG3	1.94	0.49
1:J:380:SER:O	1:J:380:SER:OG	2.29	0.49
1:F:395:TYR:CZ	1:F:430:VAL:HG23	2.48	0.49
1:A:395:TYR:O	1:A:399:PHE:N	2.45	0.49
1:B:106:LEU:HD23	1:B:109:LEU:HD12	1.95	0.49
1:D:221:TRP:HE1	1:D:465:LEU:HD23	1.78	0.49
1:D:402:VAL:HG12	1:D:514:GLY:HA2	1.94	0.48
1:E:395:TYR:O	1:E:399:PHE:N	2.45	0.48
1:G:171:ARG:HB2	1:G:248:LYS:HB2	1.94	0.48
1:G:305:ALA:HB2	2:G:700:X4X:N01	2.27	0.48
1:H:305:ALA:HB2	2:H:700:X4X:N01	2.28	0.48
1:E:414:ILE:HG21	1:E:587:VAL:HG13	1.96	0.48
1:E:402:VAL:HG12	1:E:514:GLY:HA2	1.95	0.48
1:E:414:ILE:HG13	1:E:557:VAL:HB	1.94	0.48
1:G:211:LEU:HD11	1:G:230:LYS:HA	1.94	0.48
1:J:151:ARG:HG2	1:J:603:ILE:HG13	1.94	0.48
1:A:52:VAL:HG13	1:A:475:ILE:HG12	1.96	0.48
1:A:75:MET:HE2	1:A:79:GLU:H	1.78	0.48
1:A:216:ASN:HA	1:A:222:LEU:HB3	1.95	0.48
1:B:337:VAL:HG12	1:B:547:LEU:HA	1.95	0.48
1:B:415:LEU:HD21	1:B:509:VAL:HG21	1.95	0.48
1:G:532:ILE:HA	1:G:535:THR:OG1	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:550:PHE:CE1	1:L:574:PRO:HD3	2.49	0.48
1:C:41:LEU:HD22	1:C:47:ILE:HD11	1.96	0.48
1:C:75:MET:HB2	1:C:492:ARG:HB2	1.95	0.48
1:J:143:THR:HG21	1:J:604:LEU:HD22	1.94	0.48
1:L:271:PRO:HB2	1:L:597:PRO:HB3	1.95	0.48
1:L:436:GLU:OE1	1:L:436:GLU:N	2.43	0.48
1:J:252:HIS:CE1	1:J:257:GLY:HA3	2.49	0.48
1:K:553:ILE:O	1:K:569:GLN:HA	2.13	0.48
1:L:65:PHE:CE2	1:L:487:ALA:HB2	2.49	0.48
1:B:526:LYS:HA	1:B:526:LYS:HD2	1.71	0.48
1:G:252:HIS:CE1	1:G:257:GLY:HA3	2.48	0.48
1:I:27:ALA:HB3	1:I:532:ILE:HB	1.96	0.48
1:C:52:VAL:HG13	1:C:475:ILE:HG12	1.96	0.48
1:G:417:LEU:HB3	1:G:590:LEU:HD13	1.96	0.48
1:K:322:TYR:OH	1:K:335:GLY:O	2.26	0.48
1:K:532:ILE:HA	1:K:535:THR:OG1	2.14	0.48
1:L:443:ILE:HD11	1:L:483:ASP:HB3	1.95	0.48
1:D:106:LEU:HD23	1:D:109:LEU:HD12	1.95	0.47
1:H:10:ALA:HB2	1:H:493:ARG:CZ	2.44	0.47
1:J:25:MET:HA	1:J:59:ASN:ND2	2.29	0.47
1:J:75:MET:HE2	1:J:79:GLU:HB2	1.95	0.47
1:B:216:ASN:HA	1:B:222:LEU:HB3	1.95	0.47
1:F:43:GLU:OE2	1:F:470:ARG:NE	2.47	0.47
1:F:75:MET:HE1	1:F:495:MET:HG2	1.96	0.47
1:J:415:LEU:HD21	1:J:509:VAL:HG21	1.95	0.47
1:C:531:ASN:HB3	1:C:534:VAL:HG22	1.96	0.47
1:D:77:ARG:HG2	1:D:336:THR:HG22	1.96	0.47
1:G:162:ASP:OD1	1:G:162:ASP:N	2.47	0.47
1:G:225:ASP:OD2	1:G:461:LYS:NZ	2.39	0.47
1:H:252:HIS:CE1	1:H:257:GLY:HA3	2.49	0.47
1:I:414:ILE:HG13	1:I:557:VAL:HB	1.96	0.47
1:K:206:ASP:HA	1:K:248:LYS:HE2	1.95	0.47
1:L:270:ASN:HB2	1:L:276:ARG:O	2.14	0.47
1:D:75:MET:HE1	1:D:495:MET:HG2	1.96	0.47
1:D:109:LEU:HD22	1:D:348:GLU:HG3	1.97	0.47
1:E:271:PRO:HG2	1:E:290:ALA:HB3	1.96	0.47
1:K:560:ASP:OD1	1:K:564:LEU:N	2.46	0.47
1:L:443:ILE:O	1:L:447:SER:OG	2.31	0.47
1:A:301:ASP:HA	1:A:305:ALA:HB3	1.95	0.47
1:A:415:LEU:HD21	1:A:509:VAL:HG21	1.95	0.47
1:H:301:ASP:HA	1:H:305:ALA:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:395:TYR:O	1:I:399:PHE:N	2.43	0.47
1:I:536:THR:HA	1:I:539:MET:HE2	1.96	0.47
1:E:27:ALA:HB3	1:E:532:ILE:HB	1.96	0.47
1:I:216:ASN:HA	1:I:222:LEU:HB3	1.97	0.47
1:K:384:SER:HA	1:K:387:ILE:HB	1.96	0.47
1:A:379:LEU:HD23	1:A:379:LEU:H	1.80	0.47
1:C:211:LEU:HD11	1:C:230:LYS:HA	1.95	0.47
1:E:450:LEU:O	1:E:454:THR:OG1	2.22	0.47
1:J:152:ILE:HG23	1:J:293:LEU:HD22	1.96	0.47
1:K:155:ILE:HG21	1:K:293:LEU:HD21	1.97	0.47
1:F:3:LYS:HE3	1:I:139:ARG:HD2	1.96	0.47
1:J:77:ARG:HG2	1:J:336:THR:HG22	1.97	0.47
1:K:381:HIS:HA	1:K:382:ASN:HA	1.68	0.47
1:B:252:HIS:CE1	1:B:257:GLY:HA3	2.50	0.47
1:C:106:LEU:HD11	1:C:196:VAL:HB	1.96	0.47
1:G:415:LEU:HD21	1:G:509:VAL:HG21	1.97	0.47
1:H:75:MET:HE2	1:H:79:GLU:H	1.79	0.47
1:L:301:ASP:HA	1:L:305:ALA:HB3	1.96	0.47
1:C:337:VAL:HG12	1:C:547:LEU:HA	1.98	0.46
1:D:129:TRP:CD1	1:D:603:ILE:HG22	2.50	0.46
1:D:321:THR:OG1	1:D:577:GLU:OE2	2.19	0.46
1:E:515:MET:HE2	1:E:518:PRO:HB3	1.96	0.46
1:I:20:TYR:CZ	1:I:22:ALA:HB2	2.50	0.46
1:J:192:ASN:OD1	1:J:192:ASN:N	2.48	0.46
1:K:337:VAL:HG12	1:K:547:LEU:HA	1.95	0.46
1:L:65:PHE:HE2	1:L:487:ALA:HB2	1.80	0.46
1:A:559:TYR:CZ	1:A:595:LYS:HB2	2.50	0.46
1:C:545:ALA:HA	1:C:550:PHE:HB2	1.97	0.46
1:F:27:ALA:HB3	1:F:532:ILE:HB	1.96	0.46
1:F:252:HIS:CE1	1:F:257:GLY:HA3	2.50	0.46
1:H:144:THR:HG23	1:H:147:GLN:H	1.80	0.46
1:I:211:LEU:HD11	1:I:230:LYS:HA	1.97	0.46
1:I:415:LEU:HD21	1:I:509:VAL:HG21	1.97	0.46
1:J:337:VAL:HG12	1:J:547:LEU:HA	1.97	0.46
1:J:539:MET:O	1:J:543:LEU:HG	2.15	0.46
1:K:8:LYS:HD3	1:K:493:ARG:CZ	2.44	0.46
1:D:156:ILE:HG23	1:D:161:TYR:HB2	1.96	0.46
1:K:33:LEU:HA	1:K:36:LYS:HB2	1.98	0.46
1:L:83:GLN:NE2	1:L:573:ARG:HB3	2.30	0.46
1:F:560:ASP:OD1	1:F:564:LEU:N	2.42	0.46
1:G:395:TYR:HB3	1:G:398:TRP:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:ALA:HB3	1:H:532:ILE:HB	1.96	0.46
1:A:441:HIS:O	1:A:445:ILE:HG22	2.16	0.46
1:D:407:ILE:HA	1:D:566:ILE:HD13	1.98	0.46
1:L:484:TYR:O	1:L:488:GLN:HG2	2.16	0.46
1:C:395:TYR:O	1:C:399:PHE:N	2.48	0.46
1:C:484:TYR:CZ	1:D:485:ILE:HD11	2.50	0.46
1:H:407:ILE:HA	1:H:566:ILE:HD13	1.97	0.46
1:C:153:ILE:HG12	1:C:172:PHE:HZ	1.81	0.46
1:E:306:VAL:HG22	1:E:343:LEU:HD11	1.98	0.46
1:I:301:ASP:HA	1:I:305:ALA:HB3	1.96	0.46
1:J:8:LYS:HD3	1:J:493:ARG:CZ	2.46	0.46
1:G:402:VAL:HG12	1:G:514:GLY:HA2	1.98	0.46
1:J:216:ASN:HA	1:J:222:LEU:HB3	1.98	0.46
1:J:304:GLY:HA3	1:J:542:VAL:HG21	1.98	0.46
1:J:560:ASP:HB3	1:J:566:ILE:HD11	1.96	0.46
1:A:27:ALA:HB3	1:A:532:ILE:HB	1.97	0.46
1:H:156:ILE:HG23	1:H:161:TYR:HB2	1.98	0.46
1:I:35:PHE:CE1	1:I:530:THR:HB	2.51	0.46
1:E:559:TYR:CZ	1:E:595:LYS:HB2	2.50	0.46
1:H:153:ILE:HG12	1:H:172:PHE:HZ	1.80	0.46
1:H:414:ILE:HG21	1:H:587:VAL:HG13	1.98	0.46
1:C:302:GLY:HA3	1:C:338:GLU:HG3	1.98	0.45
1:D:23:GLU:OE1	1:D:540:ARG:NH2	2.50	0.45
1:E:45:PRO:HB2	1:E:46:LEU:HD22	1.97	0.45
1:G:603:ILE:HG22	1:G:604:LEU:H	1.80	0.45
1:H:407:ILE:HG23	1:H:566:ILE:HG23	1.97	0.45
1:I:491:ARG:NH1	1:I:547:LEU:O	2.49	0.45
1:K:41:LEU:HB3	1:K:51:ILE:HD13	1.97	0.45
1:L:276:ARG:HA	1:L:519:VAL:HA	1.99	0.45
1:A:162:ASP:OD1	1:A:162:ASP:N	2.49	0.45
1:B:407:ILE:HA	1:B:566:ILE:HD13	1.97	0.45
1:C:153:ILE:HD13	1:C:174:ALA:HB1	1.98	0.45
1:E:252:HIS:CE1	1:E:257:GLY:HA3	2.51	0.45
1:H:395:TYR:CZ	1:H:430:VAL:HG23	2.51	0.45
1:I:14:ASP:HB3	1:I:17:THR:HG22	1.97	0.45
1:L:407:ILE:HG23	1:L:566:ILE:HG23	1.98	0.45
1:C:102:LEU:HD11	1:C:197:LEU:HD12	1.98	0.45
1:D:381:HIS:HA	1:D:382:ASN:HA	1.67	0.45
1:G:216:ASN:HA	1:G:222:LEU:HB3	1.98	0.45
1:C:415:LEU:HD21	1:C:509:VAL:HG21	1.97	0.45
1:D:36:LYS:HG2	1:D:467:TYR:CZ	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:ASP:OD2	1:H:217:GLY:N	2.50	0.45
1:H:495:MET:HE2	1:H:499:LEU:HG	1.97	0.45
1:I:532:ILE:HA	1:I:535:THR:OG1	2.16	0.45
1:K:165:PRO:HD2	1:K:166:THR:H	1.81	0.45
1:F:221:TRP:CD1	1:F:464:LYS:CB	2.99	0.45
1:I:92:VAL:HG21	1:I:375:PHE:CE2	2.51	0.45
1:K:318:LEU:HA	1:K:553:ILE:HG13	1.99	0.45
1:C:559:TYR:CZ	1:C:595:LYS:HB2	2.51	0.45
1:E:536:THR:HA	1:E:539:MET:HE2	1.98	0.45
1:F:506:ASP:OD1	1:F:573:ARG:NH2	2.45	0.45
1:L:545:ALA:HA	1:L:550:PHE:HB2	1.98	0.45
1:A:560:ASP:OD1	1:A:564:LEU:N	2.47	0.45
1:C:407:ILE:HG23	1:C:566:ILE:HG23	1.99	0.45
1:I:395:TYR:CZ	1:I:430:VAL:HG23	2.52	0.45
1:K:553:ILE:HG22	1:K:570:ILE:HB	1.99	0.45
1:E:219:THR:O	1:E:265:TYR:OH	2.25	0.45
1:F:107:LYS:O	1:F:379:LEU:HD11	2.17	0.45
1:F:532:ILE:HA	1:F:535:THR:OG1	2.17	0.45
1:J:421:ASN:C	1:K:19:LYS:HD3	2.42	0.45
1:K:306:VAL:HG13	1:K:343:LEU:HG	1.99	0.45
1:L:253:GLU:OE1	1:L:466:SER:OG	2.25	0.45
1:B:381:HIS:HA	1:B:382:ASN:HA	1.58	0.45
1:C:559:TYR:O	1:C:566:ILE:HD12	2.17	0.45
1:F:414:ILE:HG21	1:F:587:VAL:HG13	1.98	0.45
1:A:153:ILE:HG12	1:A:172:PHE:HZ	1.81	0.45
1:C:25:MET:HE2	1:C:438:ARG:HE	1.82	0.45
1:G:10:ALA:HB2	1:G:493:ARG:CZ	2.47	0.45
1:J:453:LEU:HD23	1:J:456:TYR:HD2	1.81	0.45
1:L:75:MET:HG3	1:L:79:GLU:HG3	1.99	0.45
1:A:255:GLY:HA2	1:A:281:SER:OG	2.17	0.44
1:B:484:TYR:O	1:B:488:GLN:HG2	2.17	0.44
1:D:39:VAL:HG21	1:D:467:TYR:HD1	1.82	0.44
1:E:395:TYR:HE1	1:E:397:LYS:HE2	1.82	0.44
1:F:96:GLU:O	1:F:101:ARG:NH1	2.50	0.44
1:K:144:THR:O	1:K:148:VAL:HG23	2.17	0.44
1:L:307:ARG:NH2	1:L:546:ASN:OD1	2.46	0.44
1:F:219:THR:O	1:F:265:TYR:OH	2.33	0.44
1:I:70:ILE:HD12	1:I:489:CYS:HB2	1.98	0.44
1:J:43:GLU:OE2	1:J:470:ARG:NE	2.50	0.44
1:E:337:VAL:HB	1:E:546:ASN:HB3	2.00	0.44
1:K:9:ARG:NH1	1:K:11:SER:OG	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HA	1:A:36:LYS:HE3	1.99	0.44
1:C:144:THR:HG23	1:C:147:GLN:H	1.83	0.44
1:F:399:PHE:CE1	1:F:511:PRO:HD3	2.52	0.44
1:E:156:ILE:HA	1:E:161:TYR:HB2	1.98	0.44
1:E:491:ARG:HG3	1:E:547:LEU:HG	1.99	0.44
1:I:277:TYR:CZ	1:I:520:ILE:HG23	2.52	0.44
1:L:260:GLY:O	1:L:267:THR:HG23	2.18	0.44
1:C:559:TYR:CG	1:C:595:LYS:HD2	2.53	0.44
1:J:407:ILE:HA	1:J:566:ILE:HD13	1.99	0.44
1:L:56:LYS:HE3	1:L:56:LYS:HB3	1.68	0.44
1:A:337:VAL:HB	1:A:546:ASN:HB3	2.00	0.44
1:B:162:ASP:OD1	1:B:162:ASP:N	2.51	0.44
1:E:132:ARG:NH2	1:E:348:GLU:OE2	2.48	0.44
1:J:515:MET:HE2	1:J:518:PRO:HB3	1.99	0.44
1:K:96:GLU:O	1:K:101:ARG:NH1	2.50	0.44
1:L:407:ILE:HA	1:L:566:ILE:HD13	2.00	0.44
1:C:560:ASP:HB3	1:C:566:ILE:HD11	2.00	0.44
1:D:27:ALA:HB3	1:D:532:ILE:HB	2.00	0.44
1:H:211:LEU:HD11	1:H:230:LYS:HA	1.99	0.44
1:L:144:THR:HG23	1:L:147:GLN:H	1.83	0.44
1:A:322:TYR:OH	1:A:335:GLY:O	2.28	0.44
1:E:106:LEU:HD11	1:E:196:VAL:HB	2.00	0.44
1:E:225:ASP:OD2	1:E:461:LYS:NZ	2.43	0.44
1:J:27:ALA:HB3	1:J:532:ILE:HB	1.99	0.44
1:K:56:LYS:O	1:K:61:MET:N	2.51	0.44
1:C:274:PRO:HG3	1:C:599:ILE:HD11	1.99	0.43
1:F:407:ILE:HG23	1:F:566:ILE:HG23	2.00	0.43
1:J:407:ILE:HG23	1:J:566:ILE:HG23	2.00	0.43
1:J:417:LEU:HB3	1:J:590:LEU:HD13	1.98	0.43
1:E:415:LEU:HD21	1:E:509:VAL:HG21	1.99	0.43
1:G:148:VAL:HG13	1:G:603:ILE:HG21	1.99	0.43
1:H:1:MET:N	1:H:1:MET:SD	2.88	0.43
1:H:2:GLY:O	1:H:3:LYS:HD2	2.18	0.43
1:L:94:GLU:OE2	1:L:360:SER:OG	2.34	0.43
1:A:102:LEU:HD11	1:A:197:LEU:HD12	2.00	0.43
1:A:252:HIS:CE1	1:A:257:GLY:HA3	2.53	0.43
1:A:277:TYR:CD2	1:A:520:ILE:HG12	2.53	0.43
1:B:75:MET:HB2	1:B:492:ARG:HB2	1.99	0.43
1:C:322:TYR:OH	1:C:335:GLY:O	2.28	0.43
1:D:304:GLY:HA3	1:D:542:VAL:HG21	2.00	0.43
1:F:52:VAL:HG13	1:F:475:ILE:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ILE:HD13	1:G:174:ALA:HB1	1.99	0.43
1:I:138:TYR:HE2	1:I:199:GLY:HA3	1.83	0.43
1:J:7:MET:HB3	1:J:69:VAL:HB	2.00	0.43
1:D:206:ASP:HA	1:D:248:LYS:HE2	2.01	0.43
1:E:269:ARG:HB3	1:E:274:PRO:HA	2.00	0.43
1:F:134:TYR:OH	1:F:603:ILE:HG21	2.18	0.43
1:F:306:VAL:HG13	1:F:343:LEU:HG	2.00	0.43
1:L:271:PRO:O	1:L:598:ALA:N	2.51	0.43
1:A:99:ILE:HG23	1:A:195:SER:HB3	2.01	0.43
1:B:370:PRO:HB3	1:B:575:TRP:CH2	2.54	0.43
1:F:162:ASP:OD1	1:F:162:ASP:N	2.51	0.43
1:I:20:TYR:CE1	1:I:22:ALA:HB2	2.54	0.43
1:J:75:MET:HB2	1:J:492:ARG:HB2	2.01	0.43
1:A:153:ILE:HD13	1:A:174:ALA:HB1	2.01	0.43
1:C:301:ASP:HA	1:C:305:ALA:HB3	2.00	0.43
1:J:33:LEU:HA	1:J:36:LYS:HE3	2.00	0.43
1:K:28:PRO:HG2	1:K:38:PHE:CE2	2.50	0.43
1:C:106:LEU:HD23	1:C:109:LEU:HD12	2.00	0.43
1:E:64:ILE:HG21	1:E:436:GLU:HG3	2.00	0.43
1:F:72:GLU:OE1	1:F:493:ARG:NH1	2.50	0.43
1:I:337:VAL:HG12	1:I:547:LEU:HA	2.01	0.43
1:L:434:LEU:HD23	1:L:437:MET:HE3	2.00	0.43
1:C:277:TYR:N	1:C:520:ILE:HD11	2.34	0.43
1:C:560:ASP:OD1	1:C:564:LEU:N	2.47	0.43
1:D:238:LEU:HD11	1:D:298:LEU:HD21	2.01	0.43
1:E:46:LEU:HD13	1:E:46:LEU:HA	1.83	0.43
1:G:101:ARG:NH2	1:G:358:LEU:O	2.51	0.43
1:J:61:MET:HE3	1:J:61:MET:HB3	1.86	0.43
1:J:307:ARG:NH2	1:J:546:ASN:OD1	2.52	0.43
1:A:453:LEU:HD23	1:A:456:TYR:HD2	1.83	0.43
1:E:33:LEU:HD22	1:E:36:LYS:HE3	2.01	0.43
1:L:494:LEU:HA	1:L:497:TYR:HD2	1.83	0.43
1:B:170:ILE:HD11	1:B:206:ASP:CG	2.44	0.43
1:B:221:TRP:CD1	1:B:464:LYS:CB	3.02	0.43
1:D:61:MET:HE2	1:D:61:MET:HB3	1.94	0.43
1:D:277:TYR:CZ	1:D:520:ILE:HG23	2.54	0.43
1:F:42:LEU:HD23	1:F:42:LEU:HA	1.89	0.43
1:F:305:ALA:HB2	2:F:700:X4X:N01	2.34	0.43
1:I:75:MET:HE2	1:I:79:GLU:H	1.84	0.43
1:I:453:LEU:HD23	1:I:456:TYR:HD2	1.84	0.43
1:J:484:TYR:O	1:J:488:GLN:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:ALA:HB1	1:K:28:PRO:HD2	2.00	0.43
1:L:60:GLY:O	1:L:64:ILE:HD12	2.19	0.43
1:L:438:ARG:HA	1:L:543:LEU:HD12	2.01	0.43
1:A:484:TYR:O	1:A:488:GLN:HG2	2.19	0.42
1:B:407:ILE:HG23	1:B:566:ILE:HG23	2.01	0.42
1:D:2:GLY:O	1:D:3:LYS:HD2	2.19	0.42
1:H:225:ASP:OD2	1:H:461:LYS:NZ	2.45	0.42
1:B:25:MET:HA	1:B:59:ASN:HD22	1.84	0.42
1:C:88:ASP:OD2	1:C:383:GLY:HA2	2.19	0.42
1:C:277:TYR:CG	1:C:520:ILE:HD11	2.54	0.42
1:E:144:THR:HG23	1:E:147:GLN:HB2	2.00	0.42
1:G:132:ARG:NH2	1:G:348:GLU:OE2	2.40	0.42
1:G:269:ARG:HB3	1:G:274:PRO:HA	2.00	0.42
1:G:395:TYR:CZ	1:G:430:VAL:HG23	2.53	0.42
1:H:484:TYR:O	1:H:488:GLN:HG2	2.18	0.42
1:K:57:LYS:HA	1:K:62:THR:HG22	2.01	0.42
1:A:94:GLU:OE2	1:A:360:SER:OG	2.32	0.42
1:A:98:PRO:HB2	1:A:241:CYS:SG	2.60	0.42
1:D:86:GLU:OE1	1:D:579:THR:OG1	2.37	0.42
1:D:102:LEU:HD23	1:D:102:LEU:HA	1.88	0.42
1:G:302:GLY:HA3	1:G:338:GLU:HG3	2.01	0.42
1:L:27:ALA:HB3	1:L:532:ILE:HB	1.99	0.42
1:L:75:MET:HE1	1:L:495:MET:SD	2.58	0.42
1:A:321:THR:OG1	1:A:577:GLU:OE2	2.21	0.42
1:I:173:ASP:HB3	1:I:176:GLU:HB3	2.01	0.42
1:K:102:LEU:HD11	1:K:197:LEU:HD12	2.01	0.42
1:A:273:ASP:OD2	1:A:275:LYS:NZ	2.47	0.42
1:B:27:ALA:HB3	1:B:532:ILE:HB	2.00	0.42
1:D:370:PRO:HB3	1:D:575:TRP:CH2	2.54	0.42
1:F:256:MET:HE3	1:F:449:THR:HG21	2.01	0.42
1:H:384:SER:O	1:H:384:SER:OG	2.31	0.42
1:H:441:HIS:O	1:H:445:ILE:HG22	2.20	0.42
1:K:106:LEU:HD11	1:K:196:VAL:HB	2.00	0.42
1:A:132:ARG:NH2	1:A:348:GLU:OE2	2.50	0.42
1:C:453:LEU:HD23	1:C:456:TYR:HD2	1.85	0.42
1:C:485:ILE:HD11	1:D:484:TYR:CZ	2.54	0.42
1:D:75:MET:HB2	1:D:492:ARG:HB2	2.01	0.42
1:E:305:ALA:HB2	2:E:700:X4X:N01	2.34	0.42
1:E:337:VAL:HG12	1:E:547:LEU:HA	2.02	0.42
1:B:526:LYS:HD3	1:H:118:LEU:HG	2.01	0.42
1:C:10:ALA:HB2	1:C:493:ARG:CZ	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:THR:HG22	1:D:340:ILE:HG12	2.01	0.42
1:D:302:GLY:HA3	1:D:338:GLU:HG3	2.01	0.42
1:H:2:GLY:HA2	1:H:6:VAL:HG12	2.01	0.42
1:K:61:MET:HE3	1:K:61:MET:HB3	1.89	0.42
1:A:144:THR:HG23	1:A:147:GLN:HB2	2.02	0.42
1:B:305:ALA:HB2	2:B:700:X4X:N01	2.35	0.42
1:H:272:HIS:CE1	1:H:565:PRO:HG3	2.54	0.42
1:H:532:ILE:HA	1:H:535:THR:OG1	2.20	0.42
1:I:162:ASP:OD1	1:I:162:ASP:N	2.46	0.42
1:K:156:ILE:HG23	1:K:161:TYR:HB2	2.01	0.42
1:K:484:TYR:CZ	1:L:485:ILE:HD11	2.53	0.42
1:B:271:PRO:HG2	1:B:290:ALA:HB3	2.02	0.42
1:D:271:PRO:HG2	1:D:290:ALA:HB3	2.01	0.42
1:D:441:HIS:O	1:D:445:ILE:HG22	2.20	0.42
1:H:52:VAL:HG13	1:H:475:ILE:HG12	2.00	0.42
1:J:63:LYS:HE2	1:J:63:LYS:HB3	1.84	0.42
1:K:94:GLU:CG	1:K:373:PRO:HD3	2.50	0.42
1:F:415:LEU:HD21	1:F:509:VAL:HG21	2.01	0.42
1:G:26:LYS:H	1:G:59:ASN:ND2	2.17	0.42
1:G:99:ILE:HG23	1:G:195:SER:HB3	2.00	0.42
1:I:297:ALA:O	1:I:343:LEU:N	2.46	0.42
1:I:395:TYR:HB3	1:I:398:TRP:HB3	2.02	0.42
1:J:185:THR:O	1:J:189:GLU:N	2.40	0.42
1:K:10:ALA:O	1:K:13:VAL:HG12	2.19	0.42
1:L:211:LEU:HD11	1:L:230:LYS:HA	2.02	0.42
1:B:457:CYS:HB3	1:B:462:ASN:HB2	2.02	0.41
1:E:92:VAL:CG1	1:E:101:ARG:HG2	2.50	0.41
1:G:75:MET:HB2	1:G:492:ARG:HB2	2.01	0.41
1:I:105:ALA:HB2	1:I:375:PHE:CE2	2.55	0.41
1:J:301:ASP:HA	1:J:305:ALA:HB3	2.01	0.41
1:D:24:THR:HG23	1:D:438:ARG:HH22	1.85	0.41
1:F:2:GLY:O	1:F:3:LYS:HD2	2.20	0.41
1:F:75:MET:HB2	1:F:492:ARG:HB2	2.01	0.41
1:L:75:MET:CE	1:L:79:GLU:H	2.33	0.41
1:B:61:MET:HE2	1:B:61:MET:HB3	1.97	0.41
1:I:219:THR:O	1:I:265:TYR:OH	2.28	0.41
1:I:327:MET:HG2	1:I:340:ILE:HG13	2.02	0.41
1:A:338:GLU:OE2	1:A:338:GLU:N	2.53	0.41
1:F:484:TYR:O	1:F:488:GLN:HG2	2.21	0.41
1:I:441:HIS:O	1:I:445:ILE:HG22	2.20	0.41
1:K:491:ARG:NH1	1:K:547:LEU:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:532:ILE:HA	1:L:535:THR:OG1	2.21	0.41
1:B:433:GLU:OE1	1:B:497:TYR:OH	2.32	0.41
1:C:121:ASP:HB3	1:C:124:SER:OG	2.21	0.41
1:D:269:ARG:HB3	1:D:274:PRO:HA	2.01	0.41
1:E:307:ARG:NH1	1:E:569:GLN:OE1	2.51	0.41
1:E:473:PHE:O	1:E:477:ARG:HG3	2.20	0.41
1:K:163:LYS:HA	1:K:164:PRO:HD3	1.83	0.41
1:K:515:MET:HE2	1:K:518:PRO:HB3	2.02	0.41
1:L:134:TYR:OH	1:L:603:ILE:HG21	2.20	0.41
1:B:318:LEU:HD22	1:B:581:LEU:HD21	2.01	0.41
1:C:410:LYS:O	1:C:414:ILE:HG12	2.21	0.41
1:E:539:MET:O	1:E:543:LEU:HG	2.21	0.41
1:F:453:LEU:HD23	1:F:456:TYR:HD2	1.85	0.41
1:G:26:LYS:HD2	1:G:26:LYS:HA	1.69	0.41
1:G:106:LEU:HD11	1:G:196:VAL:HB	2.03	0.41
1:J:2:GLY:HA2	1:J:6:VAL:HG22	2.01	0.41
1:K:334:GLY:HA3	1:L:74:PRO:HD2	2.02	0.41
1:L:106:LEU:HD23	1:L:109:LEU:HD12	2.02	0.41
1:L:414:ILE:HG21	1:L:587:VAL:HG13	2.03	0.41
1:A:306:VAL:HG13	1:A:343:LEU:HG	2.03	0.41
1:G:473:PHE:O	1:G:477:ARG:HG3	2.21	0.41
1:I:8:LYS:HE2	1:I:70:ILE:HG22	2.03	0.41
1:J:169:LEU:HD21	1:J:288:ILE:HD12	2.03	0.41
1:A:414:ILE:HG13	1:A:557:VAL:HB	2.03	0.41
1:B:211:LEU:HD11	1:B:230:LYS:HA	2.02	0.41
1:B:326:ASP:CG	1:B:328:THR:HG1	2.29	0.41
1:D:162:ASP:OD1	1:D:162:ASP:N	2.49	0.41
1:F:327:MET:HG2	1:F:340:ILE:HG13	2.02	0.41
1:F:603:ILE:HG23	1:F:604:LEU:HD23	2.03	0.41
1:G:63:LYS:HB3	1:G:63:LYS:HE2	1.89	0.41
1:H:25:MET:HG2	1:H:438:ARG:CZ	2.51	0.41
1:K:86:GLU:OE1	1:K:579:THR:OG1	2.35	0.41
1:K:98:PRO:HB2	1:K:241:CYS:SG	2.61	0.41
1:K:484:TYR:O	1:K:488:GLN:HG2	2.21	0.41
1:L:443:ILE:HG13	1:L:479:PHE:CD2	2.55	0.41
1:C:94:GLU:OE2	1:C:360:SER:OG	2.33	0.41
1:C:326:ASP:CG	1:C:328:THR:HG1	2.27	0.41
1:D:245:LEU:HD13	1:D:245:LEU:HA	1.91	0.41
1:E:98:PRO:HA	1:E:101:ARG:HB2	2.02	0.41
1:F:326:ASP:HB2	1:F:359:GLY:O	2.20	0.41
1:G:98:PRO:HB2	1:G:241:CYS:SG	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:151:ARG:HD3	1:J:603:ILE:HA	2.01	0.41
1:J:251:MET:HB2	1:J:281:SER:O	2.21	0.41
1:J:539:MET:HA	1:J:542:VAL:HG22	2.03	0.41
1:K:94:GLU:HG3	1:K:373:PRO:HD3	2.02	0.41
1:A:539:MET:O	1:A:543:LEU:HG	2.21	0.41
1:B:494:LEU:HA	1:B:497:TYR:HD2	1.85	0.41
1:I:27:ALA:HB1	1:I:28:PRO:HD2	2.03	0.41
1:I:144:THR:HG23	1:I:146:LEU:H	1.85	0.41
1:I:318:LEU:HD22	1:I:581:LEU:HD21	2.03	0.41
1:J:2:GLY:O	1:J:3:LYS:HD2	2.21	0.41
1:K:300:THR:HG22	1:K:340:ILE:HG12	2.03	0.41
1:L:162:ASP:OD1	1:L:162:ASP:N	2.51	0.41
1:A:262:ASN:C	1:A:264:ASN:H	2.29	0.40
1:B:25:MET:HA	1:B:59:ASN:ND2	2.36	0.40
1:B:25:MET:HE2	1:B:438:ARG:HE	1.85	0.40
1:C:485:ILE:HG21	1:D:448:PRO:HA	2.04	0.40
1:F:192:ASN:O	1:F:192:ASN:ND2	2.54	0.40
1:F:494:LEU:HA	1:F:497:TYR:HD2	1.86	0.40
1:H:6:VAL:HG23	1:H:68:THR:HA	2.02	0.40
1:I:484:TYR:CZ	1:J:485:ILE:HD11	2.56	0.40
1:J:395:TYR:CZ	1:J:430:VAL:HG23	2.57	0.40
1:K:453:LEU:HD23	1:K:453:LEU:HA	1.90	0.40
1:A:144:THR:HG23	1:A:147:GLN:H	1.87	0.40
1:A:302:GLY:HA3	1:A:338:GLU:HG3	2.04	0.40
1:C:252:HIS:CE1	1:C:257:GLY:HA3	2.55	0.40
1:C:259:THR:HG23	1:C:535:THR:HG22	2.02	0.40
1:D:98:PRO:HB3	1:D:356:ALA:HA	2.03	0.40
1:G:441:HIS:O	1:G:445:ILE:HG22	2.21	0.40
1:H:41:LEU:HD22	1:H:47:ILE:HD11	2.03	0.40
1:J:29:HIS:CD2	1:J:29:HIS:C	2.99	0.40
1:L:387:ILE:H	1:L:387:ILE:HG12	1.77	0.40
1:A:326:ASP:HB2	1:A:359:GLY:O	2.22	0.40
1:B:206:ASP:OD2	1:B:217:GLY:N	2.53	0.40
1:D:382:ASN:HA	1:D:382:ASN:HD22	1.73	0.40
1:D:560:ASP:HB3	1:D:566:ILE:HD11	2.03	0.40
1:E:532:ILE:HA	1:E:535:THR:OG1	2.21	0.40
1:F:407:ILE:HA	1:F:566:ILE:HD13	2.02	0.40
1:H:453:LEU:HD23	1:H:453:LEU:HA	1.94	0.40
1:I:92:VAL:HG21	1:I:375:PHE:CD2	2.56	0.40
1:I:221:TRP:CE3	1:I:461:LYS:HD2	2.57	0.40
1:J:99:ILE:HD13	1:J:194:ILE:HG23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:LEU:HD11	1:J:246:LEU:HG	2.02	0.40
1:J:231:ASP:OD2	1:J:239:ARG:NH2	2.54	0.40
1:J:273:ASP:OD2	1:J:275:LYS:NZ	2.49	0.40
1:K:252:HIS:CE1	1:K:257:GLY:HA3	2.57	0.40
1:L:71:PRO:HG2	1:L:72:GLU:OE1	2.22	0.40
1:L:152:ILE:HG23	1:L:293:LEU:HD22	2.02	0.40
1:L:192:ASN:O	1:L:192:ASN:ND2	2.54	0.40
1:A:395:TYR:HB3	1:A:398:TRP:HB3	2.02	0.40
1:A:473:PHE:O	1:A:477:ARG:HG3	2.22	0.40
1:C:77:ARG:HG2	1:C:336:THR:HG22	2.03	0.40
1:D:131:ILE:HG23	1:D:200:ILE:HG13	2.02	0.40
1:F:61:MET:HE2	1:F:61:MET:HB3	1.92	0.40
1:G:603:ILE:CG2	1:G:604:LEU:N	2.83	0.40
1:H:276:ARG:CZ	1:H:564:LEU:HD11	2.52	0.40
1:K:570:ILE:HG22	1:K:580:VAL:HG12	2.03	0.40
1:A:304:GLY:HA3	1:A:542:VAL:HG21	2.04	0.40
1:B:1:MET:SD	1:B:1:MET:N	2.87	0.40
1:C:448:PRO:HA	1:D:485:ILE:HG21	2.03	0.40
1:H:539:MET:O	1:H:543:LEU:HG	2.21	0.40
1:I:453:LEU:HD23	1:I:453:LEU:HA	1.92	0.40
1:K:395:TYR:HB3	1:K:398:TRP:HB3	2.04	0.40
1:K:555:VAL:HG22	1:K:556:PRO:HD2	2.03	0.40
1:L:407:ILE:HD11	1:L:516:THR:HG23	2.02	0.40

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%)	566 (94%)	33 (6%)	1 (0%)	43 72
1	B	603/636 (95%)	574 (95%)	27 (4%)	2 (0%)	36 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	600/636 (94%)	561 (94%)	38 (6%)	1 (0%)	43	72
1	D	603/636 (95%)	567 (94%)	35 (6%)	1 (0%)	43	72
1	E	600/636 (94%)	570 (95%)	29 (5%)	1 (0%)	43	72
1	F	603/636 (95%)	578 (96%)	25 (4%)	0	100	100
1	G	600/636 (94%)	564 (94%)	35 (6%)	1 (0%)	43	72
1	H	603/636 (95%)	570 (94%)	32 (5%)	1 (0%)	43	72
1	I	600/636 (94%)	562 (94%)	34 (6%)	4 (1%)	18	51
1	J	603/636 (95%)	571 (95%)	31 (5%)	1 (0%)	43	72
1	K	600/636 (94%)	565 (94%)	34 (6%)	1 (0%)	43	72
1	L	603/636 (95%)	572 (95%)	30 (5%)	1 (0%)	43	72
All	All	7218/7632 (95%)	6820 (94%)	383 (5%)	15 (0%)	43	72

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	165	PRO
1	I	23	GLU
1	I	25	MET
1	L	275	LYS
1	A	141	LYS
1	C	383	GLY
1	E	604	LEU
1	B	303	GLY
1	B	604	LEU
1	G	141	LYS
1	H	604	LEU
1	J	604	LEU
1	D	45	PRO
1	I	303	GLY
1	I	81	PRO

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	509/539 (94%)	509 (100%)	0	100	100
1	B	511/539 (95%)	511 (100%)	0	100	100
1	C	509/539 (94%)	509 (100%)	0	100	100
1	D	511/539 (95%)	511 (100%)	0	100	100
1	E	509/539 (94%)	509 (100%)	0	100	100
1	F	511/539 (95%)	511 (100%)	0	100	100
1	G	509/539 (94%)	509 (100%)	0	100	100
1	H	511/539 (95%)	511 (100%)	0	100	100
1	I	509/539 (94%)	509 (100%)	0	100	100
1	J	511/539 (95%)	511 (100%)	0	100	100
1	K	509/539 (94%)	509 (100%)	0	100	100
1	L	511/539 (95%)	511 (100%)	0	100	100
All	All	6120/6468 (95%)	6120 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	83	GLN
1	A	223	HIS
1	A	381	HIS
1	A	531	ASN
1	A	605	ASN
1	B	192	ASN
1	C	83	GLN
1	C	192	ASN
1	C	531	ASN
1	D	40	ASN
1	D	180	GLN
1	D	192	ASN
1	D	382	ASN
1	D	462	ASN
1	D	533	GLN
1	D	605	ASN
1	E	29	HIS
1	E	180	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	59	ASN
1	F	67	ASN
1	F	531	ASN
1	G	40	ASN
1	G	59	ASN
1	G	180	GLN
1	G	223	HIS
1	G	381	HIS
1	G	531	ASN
1	G	605	ASN
1	H	40	ASN
1	H	59	ASN
1	H	192	ASN
1	H	223	HIS
1	I	29	HIS
1	I	180	GLN
1	I	462	ASN
1	I	531	ASN
1	J	40	ASN
1	J	59	ASN
1	J	531	ASN
1	J	605	ASN
1	K	29	HIS
1	K	261	ASN
1	K	262	ASN
1	K	382	ASN
1	K	531	ASN
1	L	40	ASN
1	L	261	ASN
1	L	272	HIS
1	L	462	ASN
1	L	605	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	X4X	I	700	-	23,23,23	1.44	3 (13%)	24,24,24	1.03	2 (8%)
2	X4X	H	700	-	23,23,23	1.44	3 (13%)	24,24,24	1.10	3 (12%)
2	X4X	E	700	-	23,23,23	1.45	3 (13%)	24,24,24	1.11	3 (12%)
2	X4X	B	700	-	23,23,23	1.46	3 (13%)	24,24,24	1.11	3 (12%)
2	X4X	G	700	-	23,23,23	1.45	3 (13%)	24,24,24	1.05	3 (12%)
2	X4X	F	700	-	23,23,23	1.45	3 (13%)	24,24,24	1.16	3 (12%)

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	X4X	I	700	-	-	9/23/23/23	-
2	X4X	H	700	-	-	9/23/23/23	-
2	X4X	E	700	-	-	12/23/23/23	-
2	X4X	B	700	-	-	13/23/23/23	-
2	X4X	G	700	-	-	9/23/23/23	-
2	X4X	F	700	-	-	13/23/23/23	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	X4X	C11-N01	5.21	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	700	X4X	C11-N01	5.20	1.45	1.33
2	B	700	X4X	C11-N01	5.19	1.45	1.33
2	G	700	X4X	C11-N01	5.18	1.45	1.33
2	F	700	X4X	C11-N01	5.17	1.45	1.33
2	I	700	X4X	C11-N01	5.16	1.45	1.33
2	G	700	X4X	C17-C15	2.87	1.53	1.44
2	B	700	X4X	C17-C15	2.82	1.53	1.44
2	F	700	X4X	C17-C15	2.82	1.53	1.44
2	H	700	X4X	C17-C15	2.81	1.53	1.44
2	E	700	X4X	C17-C15	2.80	1.53	1.44
2	I	700	X4X	C17-C15	2.79	1.53	1.44
2	B	700	X4X	O01-C11	-2.31	1.18	1.23
2	F	700	X4X	O01-C11	-2.25	1.18	1.23
2	G	700	X4X	O01-C11	-2.22	1.18	1.23
2	I	700	X4X	O01-C11	-2.22	1.18	1.23
2	E	700	X4X	O01-C11	-2.21	1.18	1.23
2	H	700	X4X	O01-C11	-2.15	1.19	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	700	X4X	O03-C20-C19	2.52	120.77	111.50
2	F	700	X4X	C07-C11-N01	2.50	120.91	116.34
2	F	700	X4X	C08-C14-C15	-2.49	119.32	124.78
2	B	700	X4X	C07-C11-N01	2.49	120.89	116.34
2	F	700	X4X	O03-C20-C19	2.41	120.34	111.50
2	G	700	X4X	O03-C20-C19	2.40	120.32	111.50
2	E	700	X4X	O03-C20-C19	2.39	120.29	111.50
2	H	700	X4X	C07-C11-N01	2.38	120.69	116.34
2	E	700	X4X	C07-C11-N01	2.36	120.64	116.34
2	B	700	X4X	O03-C20-C19	2.35	120.14	111.50
2	E	700	X4X	C08-C14-C15	-2.29	119.77	124.78
2	I	700	X4X	O03-C20-C19	2.21	119.61	111.50
2	B	700	X4X	C08-C14-C15	-2.17	120.02	124.78
2	G	700	X4X	C08-C14-C15	-2.15	120.07	124.78
2	G	700	X4X	C07-C11-N01	2.08	120.13	116.34
2	H	700	X4X	C08-C14-C15	-2.06	120.27	124.78
2	I	700	X4X	C19-N01-C11	-2.04	119.02	122.82

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	700	X4X	O02-C08-C14-C15
2	B	700	X4X	N01-C19-C20-O03
2	F	700	X4X	C04-C06-C08-C14
2	F	700	X4X	C04-C06-C08-O02
2	B	700	X4X	C07-C11-N01-C19
2	E	700	X4X	C07-C11-N01-C19
2	F	700	X4X	C07-C11-N01-C19
2	G	700	X4X	C07-C11-N01-C19
2	H	700	X4X	C07-C11-N01-C19
2	I	700	X4X	C07-C11-N01-C19
2	B	700	X4X	O01-C11-N01-C19
2	E	700	X4X	O01-C11-N01-C19
2	F	700	X4X	O01-C11-N01-C19
2	G	700	X4X	O01-C11-N01-C19
2	H	700	X4X	O01-C11-N01-C19
2	I	700	X4X	O01-C11-N01-C19
2	H	700	X4X	C01-C03-C05-C07
2	I	700	X4X	C12-C09-C10-C13
2	H	700	X4X	C14-C15-C17-C16
2	I	700	X4X	C01-C03-C05-C07
2	G	700	X4X	C02-C01-C03-C05
2	I	700	X4X	C02-C01-C03-C05
2	B	700	X4X	C03-C05-C07-C11
2	E	700	X4X	C03-C05-C07-C11
2	F	700	X4X	C03-C05-C07-C11
2	H	700	X4X	C02-C01-C03-C05
2	E	700	X4X	C01-C03-C05-C07
2	B	700	X4X	C01-C03-C05-C07
2	G	700	X4X	C09-C10-C13-C18
2	E	700	X4X	C09-C10-C13-C18
2	B	700	X4X	C10-C09-C12-C16
2	F	700	X4X	C01-C03-C05-C07
2	B	700	X4X	C09-C10-C13-C18
2	H	700	X4X	C09-C10-C13-C18
2	F	700	X4X	C09-C10-C13-C18
2	F	700	X4X	C10-C09-C12-C16
2	H	700	X4X	C10-C09-C12-C16
2	I	700	X4X	C09-C10-C13-C18
2	E	700	X4X	O02-C08-C14-C15
2	E	700	X4X	C02-C01-C03-C05
2	G	700	X4X	C10-C09-C12-C16
2	B	700	X4X	C06-C08-C14-C15
2	E	700	X4X	C06-C08-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	700	X4X	C02-C01-C03-C05
2	E	700	X4X	C10-C09-C12-C16
2	F	700	X4X	C02-C01-C03-C05
2	I	700	X4X	C10-C09-C12-C16
2	G	700	X4X	C03-C01-C02-C04
2	G	700	X4X	C12-C09-C10-C13
2	F	700	X4X	N01-C19-C20-O03
2	H	700	X4X	C03-C01-C02-C04
2	E	700	X4X	C12-C09-C10-C13
2	I	700	X4X	C03-C01-C02-C04
2	F	700	X4X	C12-C09-C10-C13
2	F	700	X4X	O02-C08-C14-C15
2	B	700	X4X	C12-C09-C10-C13
2	H	700	X4X	C12-C09-C10-C13
2	G	700	X4X	C03-C05-C07-C11
2	G	700	X4X	O02-C08-C14-C15
2	F	700	X4X	C06-C08-C14-C15
2	I	700	X4X	C09-C12-C16-C17
2	B	700	X4X	C04-C06-C08-C14
2	B	700	X4X	C04-C06-C08-O02
2	E	700	X4X	C04-C06-C08-C14
2	E	700	X4X	C04-C06-C08-O02

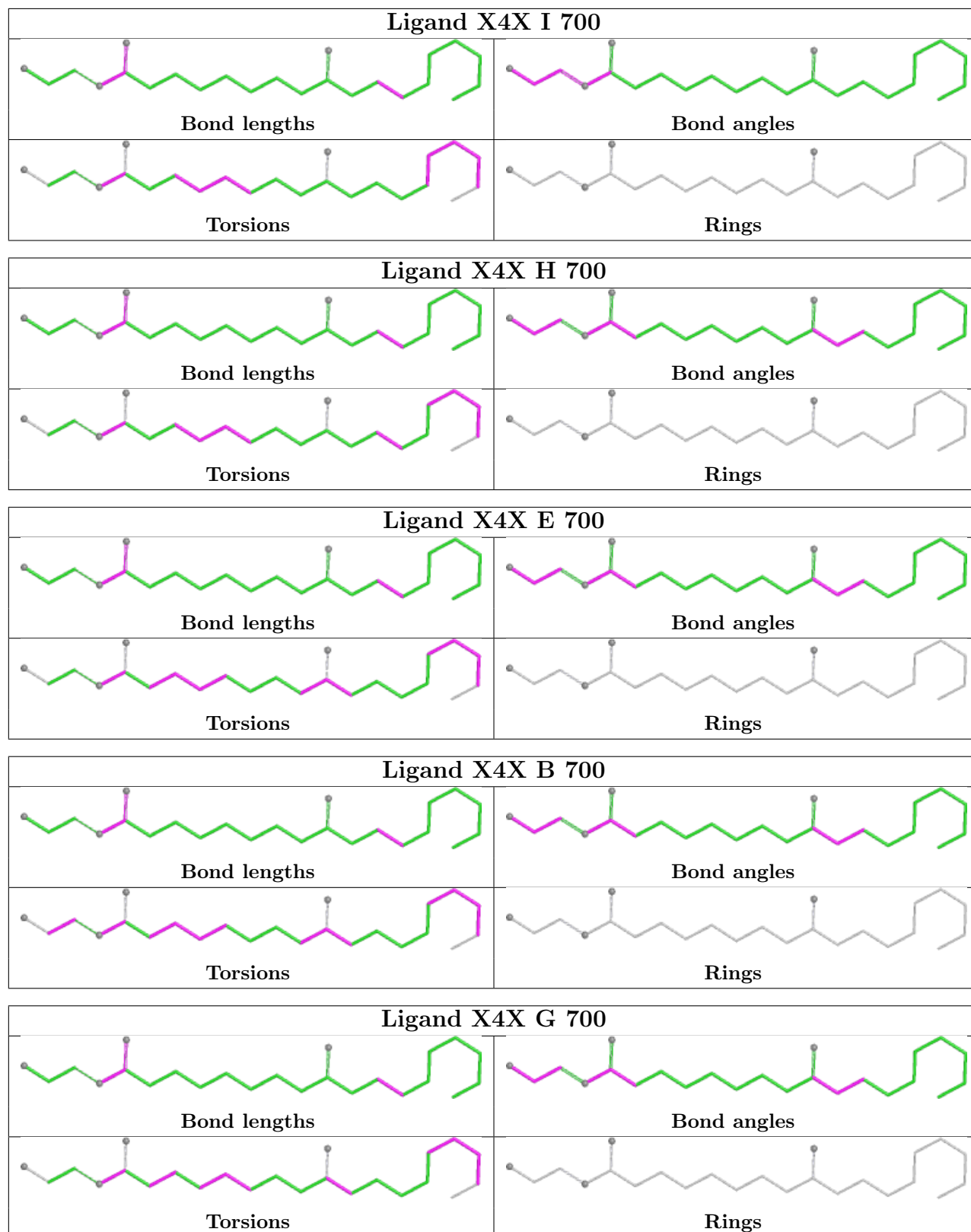
There are no ring outliers.

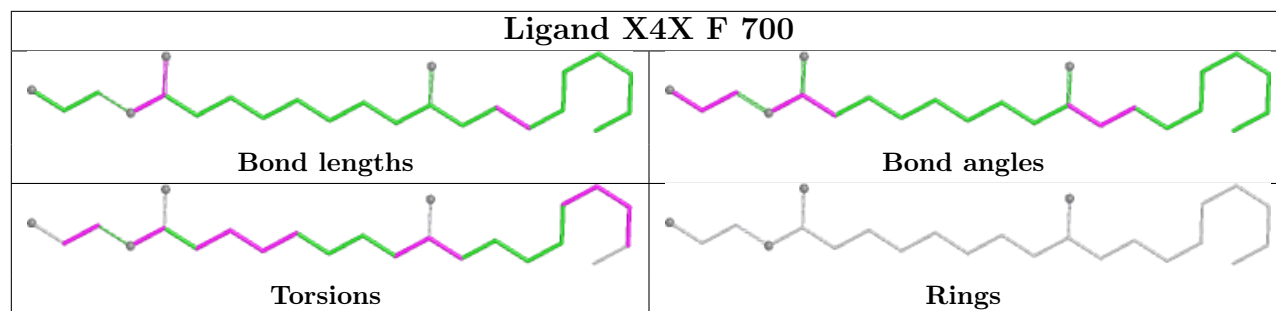
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	700	X4X	1	0
2	E	700	X4X	1	0
2	B	700	X4X	1	0
2	G	700	X4X	1	0
2	F	700	X4X	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 than 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 [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, 95th 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%)	0.34	16 (2%)	56	32	63, 86, 116, 251	0
1	B	605/636 (95%)	0.26	11 (1%)	67	40	58, 76, 113, 262	0
1	C	602/636 (94%)	0.91	50 (8%)	17	12	73, 101, 130, 250	0
1	D	605/636 (95%)	0.70	39 (6%)	25	16	64, 94, 129, 275	0
1	E	602/636 (94%)	0.30	12 (1%)	65	38	54, 71, 100, 231	0
1	F	605/636 (95%)	0.32	18 (2%)	52	30	54, 73, 102, 210	0
1	G	602/636 (94%)	0.22	15 (2%)	58	34	44, 60, 89, 219	0
1	H	605/636 (95%)	0.32	13 (2%)	63	37	49, 66, 92, 184	0
1	I	602/636 (94%)	0.33	15 (2%)	58	34	56, 78, 109, 224	0
1	J	605/636 (95%)	0.38	22 (3%)	46	26	63, 98, 139, 253	0
1	K	602/636 (94%)	0.70	38 (6%)	26	16	74, 110, 146, 252	0
1	L	605/636 (95%)	0.75	34 (5%)	30	18	85, 137, 175, 305	0
All	All	7242/7632 (94%)	0.46	283 (3%)	43	24	44, 85, 147, 305	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	247	GLY	9.1
1	A	247	GLY	8.8
1	K	203	THR	6.9
1	L	149	ALA	6.5
1	C	22	ALA	5.9
1	K	246	LEU	5.3
1	J	294	CYS	5.2
1	K	295	SER	5.0
1	I	247	GLY	4.6
1	K	244	ILE	4.5
1	K	256	MET	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	411	CYS	4.4
1	K	294	CYS	4.4
1	D	148	VAL	4.4
1	D	126	PHE	4.2
1	C	294	CYS	4.2
1	C	469	THR	4.1
1	C	247	GLY	4.1
1	B	129	TRP	4.0
1	L	535	THR	4.0
1	H	533	GLN	4.0
1	H	420	ASN	3.9
1	L	350	ALA	3.8
1	A	295	SER	3.8
1	G	386	ALA	3.8
1	C	598	ALA	3.7
1	K	169	LEU	3.7
1	E	22	ALA	3.7
1	J	56	LYS	3.7
1	C	442	VAL	3.4
1	H	530	THR	3.4
1	C	554	SER	3.4
1	G	256	MET	3.4
1	H	136	TYR	3.4
1	D	149	ALA	3.4
1	I	244	ILE	3.3
1	C	296	ALA	3.3
1	D	196	VAL	3.3
1	I	295	SER	3.3
1	I	177	VAL	3.3
1	K	353	VAL	3.3
1	C	538	LEU	3.3
1	C	6	VAL	3.3
1	D	603	ILE	3.3
1	L	291	ALA	3.3
1	J	420	ASN	3.3
1	C	393	GLY	3.3
1	A	256	MET	3.2
1	H	175	ASN	3.2
1	E	255	GLY	3.2
1	K	442	VAL	3.2
1	L	469	THR	3.2
1	C	253	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	134	TYR	3.2
1	C	588	GLU	3.1
1	L	6	VAL	3.1
1	I	255	GLY	3.1
1	K	62	THR	3.1
1	C	544	ALA	3.1
1	D	234	VAL	3.1
1	D	523	ASP	3.1
1	C	507	VAL	3.1
1	D	291	ALA	3.1
1	L	148	VAL	3.1
1	L	523	ASP	3.1
1	D	152	ILE	3.0
1	G	247	GLY	3.0
1	J	351	PHE	3.0
1	C	297	ALA	3.0
1	A	203	THR	3.0
1	C	196	VAL	3.0
1	C	254	LEU	3.0
1	A	246	LEU	3.0
1	J	291	ALA	3.0
1	F	134	TYR	3.0
1	A	294	CYS	3.0
1	C	255	GLY	3.0
1	E	172	PHE	2.9
1	D	486	ALA	2.9
1	F	602	ASP	2.9
1	D	247	GLY	2.9
1	J	523	ASP	2.9
1	K	446	GLY	2.9
1	J	59	ASN	2.9
1	L	348	GLU	2.9
1	C	29	HIS	2.8
1	I	419	SER	2.8
1	C	446	GLY	2.8
1	C	386	ALA	2.8
1	C	504	ASP	2.8
1	B	344	ALA	2.8
1	H	23	GLU	2.8
1	K	544	ALA	2.8
1	F	28	PRO	2.8
1	D	212	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	533	GLN	2.8
1	C	517	ALA	2.8
1	G	243	ALA	2.8
1	C	246	LEU	2.7
1	G	244	ILE	2.7
1	K	172	PHE	2.7
1	K	344	ALA	2.7
1	E	6	VAL	2.7
1	C	590	LEU	2.7
1	D	538	LEU	2.7
1	A	289	VAL	2.7
1	D	246	LEU	2.7
1	C	398	TRP	2.7
1	F	603	ILE	2.7
1	J	112	TYR	2.7
1	D	292	GLY	2.6
1	C	256	MET	2.6
1	K	242	GLY	2.6
1	K	474	ALA	2.6
1	C	509	VAL	2.6
1	K	501	ILE	2.6
1	L	152	ILE	2.6
1	G	255	GLY	2.6
1	I	514	GLY	2.6
1	H	7	MET	2.6
1	L	218	GLY	2.6
1	L	602	ASP	2.6
1	D	340	ILE	2.6
1	D	475	ILE	2.6
1	B	120	ALA	2.6
1	C	453	LEU	2.6
1	D	417	LEU	2.6
1	L	7	MET	2.6
1	L	604	LEU	2.6
1	K	476	PHE	2.6
1	D	479	PHE	2.6
1	D	442	VAL	2.5
1	C	441	HIS	2.5
1	D	129	TRP	2.5
1	A	206	ASP	2.5
1	E	483	ASP	2.5
1	C	172	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	572	GLY	2.5
1	K	9	ARG	2.5
1	H	112	TYR	2.5
1	C	23	GLU	2.5
1	A	244	ILE	2.5
1	G	421	ASN	2.5
1	E	403	SER	2.5
1	G	419	SER	2.5
1	H	119	HIS	2.4
1	K	541	PHE	2.4
1	L	274	PRO	2.4
1	C	404	SER	2.4
1	L	426	VAL	2.4
1	B	126	PHE	2.4
1	D	445	ILE	2.4
1	E	23	GLU	2.4
1	J	293	LEU	2.4
1	L	314	GLY	2.4
1	C	244	ILE	2.4
1	D	178	ILE	2.4
1	D	245	LEU	2.4
1	I	296	ALA	2.4
1	E	247	GLY	2.4
1	L	122	PRO	2.4
1	L	442	VAL	2.4
1	A	30	LEU	2.4
1	B	27	ALA	2.4
1	C	353	VAL	2.4
1	F	293	LEU	2.4
1	L	346	SER	2.3
1	I	33	LEU	2.3
1	A	88	ASP	2.3
1	J	349	ASP	2.3
1	D	337	VAL	2.3
1	K	278	THR	2.3
1	L	355	ALA	2.3
1	K	387	ILE	2.3
1	G	117	SER	2.3
1	J	376	PRO	2.3
1	K	419	SER	2.3
1	D	509	VAL	2.3
1	I	202	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	351	PHE	2.3
1	C	466	SER	2.3
1	D	346	SER	2.3
1	E	478	SER	2.3
1	C	359	GLY	2.3
1	F	316	THR	2.3
1	C	407	ILE	2.3
1	K	170	ILE	2.3
1	H	120	ALA	2.3
1	L	136	TYR	2.3
1	G	403	SER	2.3
1	A	317	GLY	2.3
1	D	280	GLY	2.3
1	H	602	ASP	2.3
1	C	566	ILE	2.2
1	D	168	PHE	2.2
1	I	411	CYS	2.2
1	B	257	GLY	2.2
1	J	247	GLY	2.2
1	J	175	ASN	2.2
1	F	7	MET	2.2
1	B	148	VAL	2.2
1	K	509	VAL	2.2
1	A	243	ALA	2.2
1	G	22	ALA	2.2
1	D	447	SER	2.2
1	J	346	SER	2.2
1	L	525	LEU	2.2
1	F	535	THR	2.2
1	K	268	THR	2.2
1	L	475	ILE	2.2
1	H	3	LYS	2.2
1	D	27	ALA	2.2
1	J	7	MET	2.2
1	D	232	SER	2.2
1	J	140	SER	2.2
1	G	242	GLY	2.2
1	K	317	GLY	2.2
1	G	443	ILE	2.2
1	K	204	ILE	2.2
1	K	535	THR	2.2
1	H	295	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	312	LEU	2.2
1	J	603	ILE	2.2
1	K	64	ILE	2.2
1	K	257	GLY	2.2
1	L	168	PHE	2.2
1	B	400	ASN	2.2
1	C	576	ALA	2.1
1	C	533	GLN	2.1
1	J	332	CYS	2.1
1	A	172	PHE	2.1
1	D	215	THR	2.1
1	K	316	THR	2.1
1	C	30	LEU	2.1
1	L	10	ALA	2.1
1	A	419	SER	2.1
1	K	441	HIS	2.1
1	I	278	THR	2.1
1	L	70	ILE	2.1
1	D	177	VAL	2.1
1	C	284	GLY	2.1
1	C	229	GLU	2.1
1	C	392	LEU	2.1
1	C	435	GLU	2.1
1	F	229	GLU	2.1
1	L	176	GLU	2.1
1	J	311	ALA	2.1
1	F	152	ILE	2.1
1	B	533	GLN	2.1
1	D	498	HIS	2.1
1	C	314	GLY	2.1
1	E	169	LEU	2.1
1	G	30	LEU	2.1
1	I	448	PRO	2.1
1	L	448	PRO	2.1
1	B	278	THR	2.1
1	E	588	GLU	2.1
1	K	471	THR	2.1
1	D	532	ILE	2.1
1	I	117	SER	2.1
1	J	582	GLY	2.1
1	K	292	GLY	2.1
1	J	234	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	299	GLY	2.0
1	F	511	PRO	2.0
1	D	602	ASP	2.0
1	K	296	ALA	2.0
1	A	605	ASN	2.0
1	F	112	TYR	2.0
1	L	522	PRO	2.0
1	F	23	GLU	2.0
1	C	295	SER	2.0
1	I	172	PHE	2.0
1	L	476	PHE	2.0
1	F	175	ASN	2.0
1	K	255	GLY	2.0
1	B	565	PRO	2.0
1	F	532	ILE	2.0
1	D	343	LEU	2.0
1	F	253	GLU	2.0
1	G	447	SER	2.0
1	E	202	VAL	2.0
1	F	6	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	X4X	B	700	24/24	0.85	0.21	74,74,74,74	0
2	X4X	F	700	24/24	0.85	0.21	72,72,72,72	0
2	X4X	I	700	24/24	0.86	0.19	78,78,78,78	0

Continued on next page...

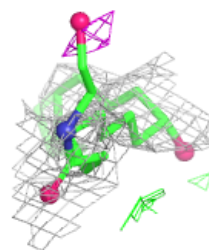
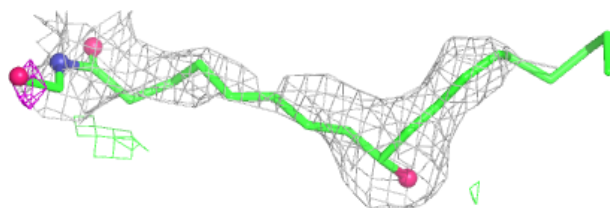
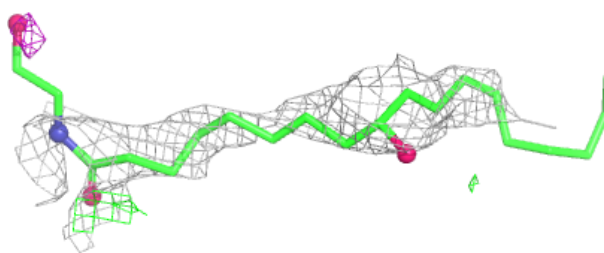
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	X4X	H	700	24/24	0.88	0.17	60,60,60,60	0
2	X4X	G	700	24/24	0.88	0.18	60,60,60,60	0
2	X4X	E	700	24/24	0.89	0.16	68,68,68,68	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.

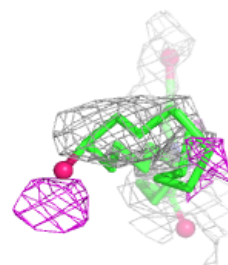
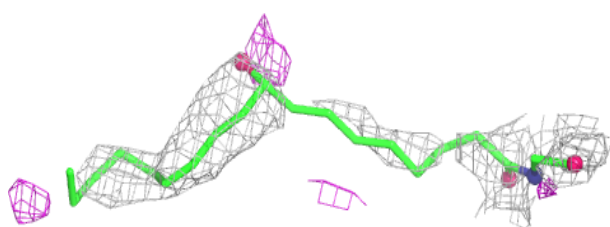
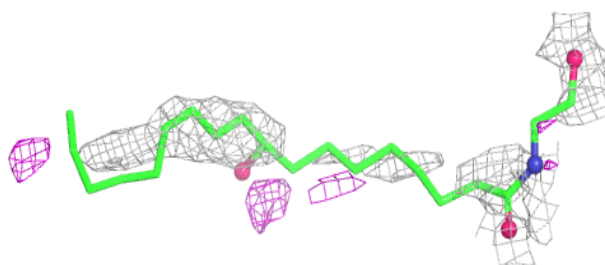
Electron density around X4X B 700:

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

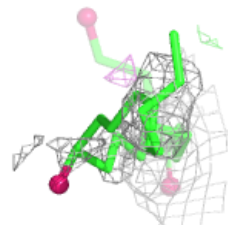
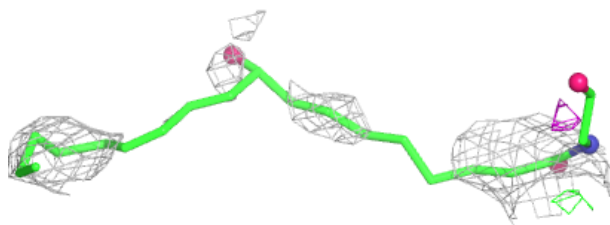
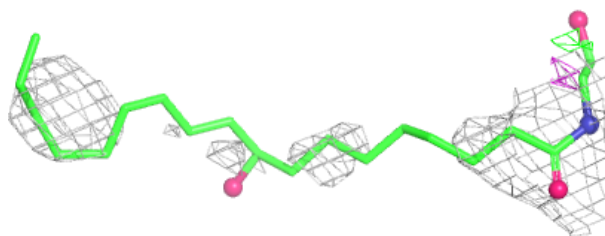


Electron density around X4X F 700:

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

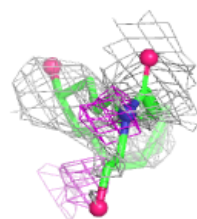
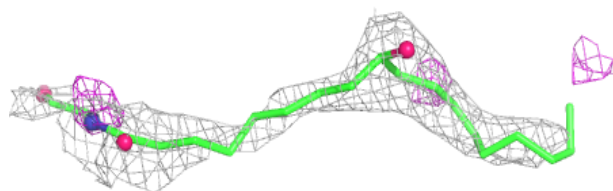
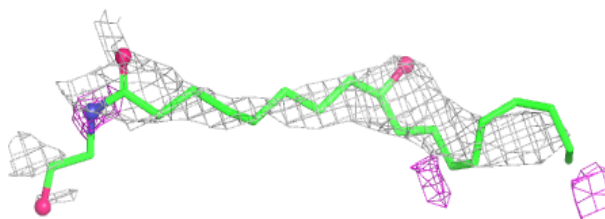
**Electron density around X4X I 700:**

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

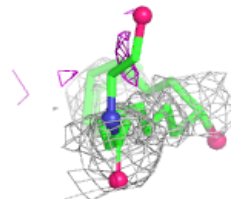
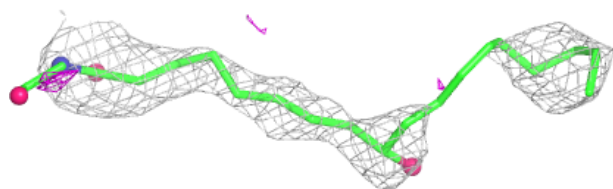
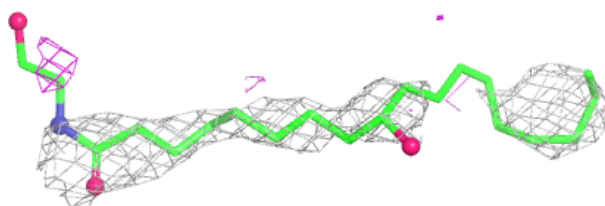


Electron density around X4X H 700:

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

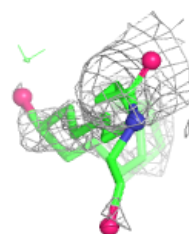
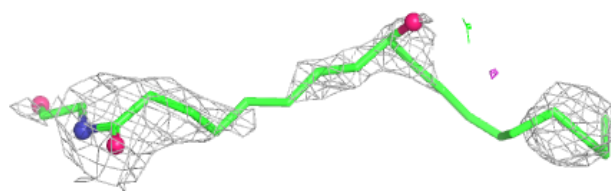
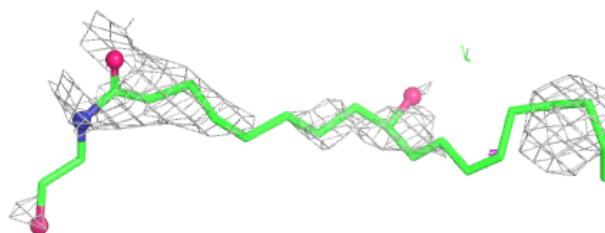
**Electron density around X4X G 700:**

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



Electron density around X4X E 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.