



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 AM UTC

PDB ID : 6DII / pdb_00006dii
Title : Structure of Arabidopsis Fatty Acid Amide Hydrolase in Complex with methyl
linolenyl fluorophosphonate
Authors : Aziz, M.; Wang, X.; Tripathi, A.; Bankaitis, V.; Chapman, K.D.
Deposited on : 2018-05-23
Resolution : 3.20 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

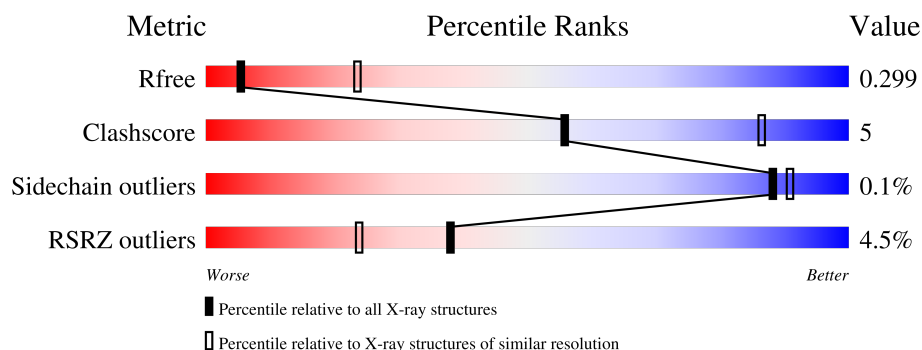
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



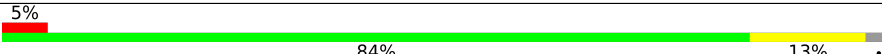
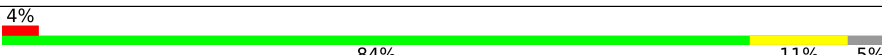
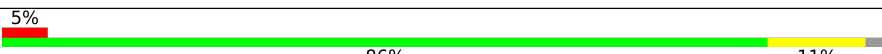
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 84% 11% 5%
1	B	636	3% 85% 10% 5%
1	C	636	3% 82% 12% 5%
1	D	636	5% 82% 13% 5%
1	E	636	4% 83% 11% 5%
1	F	636	6% 82% 14% 5%

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Mol	Chain	Length	Quality of chain
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 55932 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
			4606	2922	778	883	23			
1	B	605	Total	C	N	O	S	0	0	0
			4627	2935	782	886	24			
1	C	602	Total	C	N	O	S	0	0	0
			4606	2922	778	883	23			
1	D	605	Total	C	N	O	S	0	0	0
			4627	2935	782	886	24			
1	E	602	Total	C	N	O	S	0	0	0
			4606	2922	778	883	23			
1	F	605	Total	C	N	O	S	0	0	0
			4627	2935	782	886	24			
1	G	602	Total	C	N	O	S	0	0	0
			4606	2922	778	883	23			
1	H	616	Total	C	N	O	S	0	0	0
			4717	2992	795	906	24			
1	I	602	Total	C	N	O	S	0	0	0
			4606	2922	778	883	23			
1	J	616	Total	C	N	O	S	0	0	0
			4717	2992	795	906	24			
1	K	602	Total	C	N	O	S	0	0	0
			4606	2922	778	883	23			
1	L	616	Total	C	N	O	S	0	0	0
			4717	2992	795	906	24			

There are 348 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	612	GLU	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
B	624	ASP	-	expression tag	UNP Q7XJJ7
B	625	LEU	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
C	636	HIS	-	expression tag	UNP Q7XJJ7
D	608	LYS	-	expression tag	UNP Q7XJJ7
D	609	GLY	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	636	HIS	-	expression tag	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
J	636	HIS	-	expression tag	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

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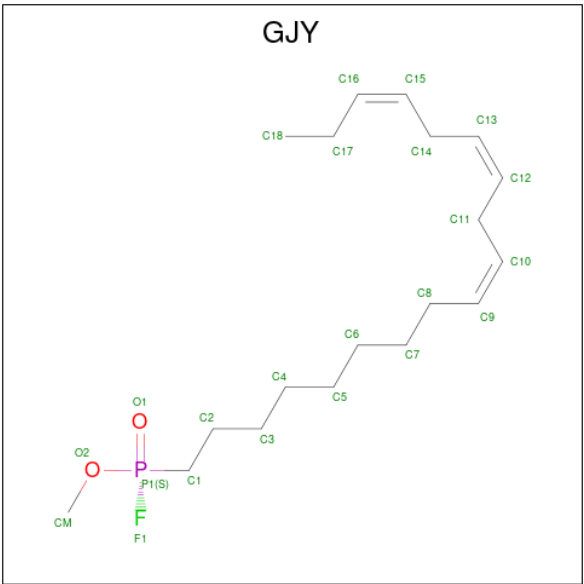
Chain	Residue	Modelled	Actual	Comment	Reference
K	617	GLN	-	expression tag	UNP Q7XJJ7
K	618	LYS	-	expression tag	UNP Q7XJJ7
K	619	LEU	-	expression tag	UNP Q7XJJ7
K	620	ILE	-	expression tag	UNP Q7XJJ7
K	621	SER	-	expression tag	UNP Q7XJJ7
K	622	GLU	-	expression tag	UNP Q7XJJ7
K	623	GLU	-	expression tag	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 methyl-9Z,12Z,15Z-octadecatrienylphosphonofluoridate (CCD ID: GJY) (formula: C₁₉H₃₄FO₂P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			22	19	2	1		
2	B	1	Total	C	O	P	0	0
			22	19	2	1		
2	C	1	Total	C	O	P	0	0
			22	19	2	1		
2	D	1	Total	C	O	P	0	0
			22	19	2	1		
2	E	1	Total	C	O	P	0	0
			22	19	2	1		
2	F	1	Total	C	O	P	0	0
			22	19	2	1		
2	G	1	Total	C	O	P	0	0
			22	19	2	1		

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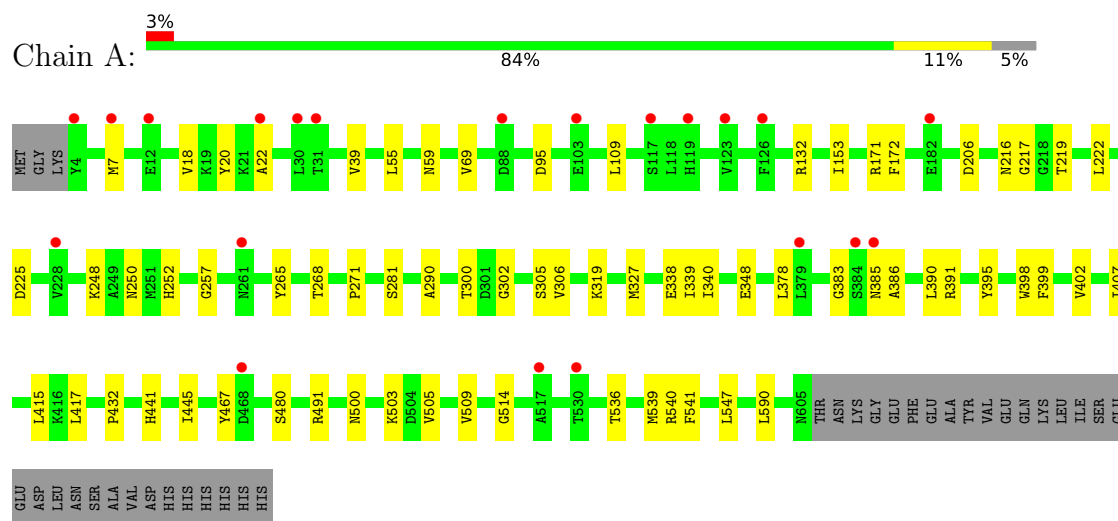
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	O	P	0	0
			22	19	2	1		
2	I	1	Total	C	O	P	0	0
			22	19	2	1		
2	J	1	Total	C	O	P	0	0
			22	19	2	1		
2	K	1	Total	C	O	P	0	0
			22	19	2	1		
2	L	1	Total	C	O	P	0	0
			22	19	2	1		

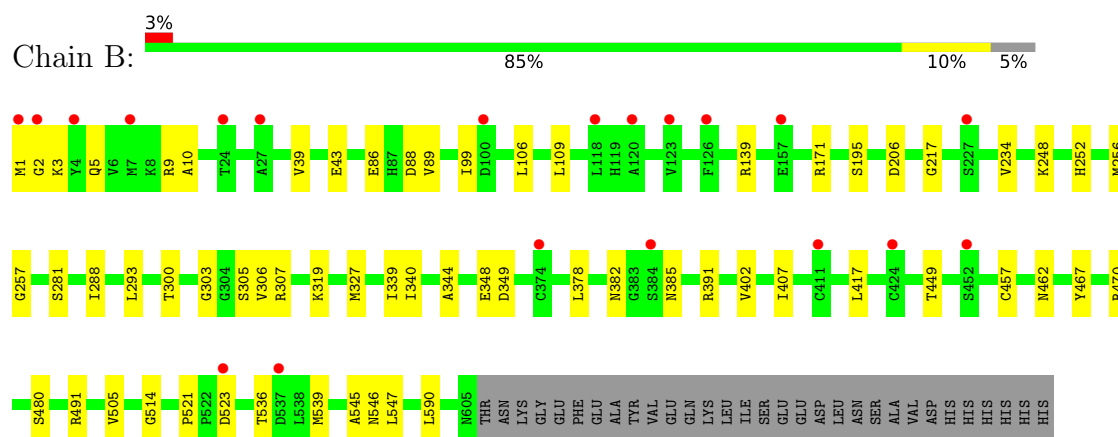
3 Residue-property plots [i](#)

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.

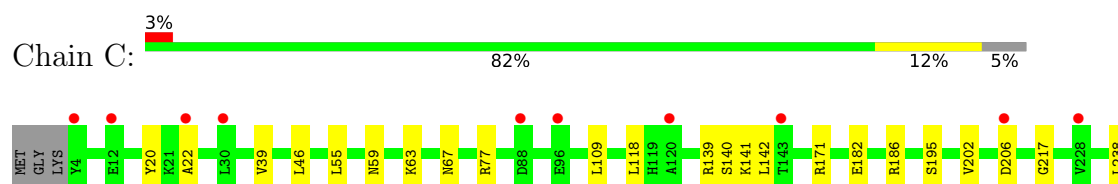
• Molecule 1: Fatty acid amide hydrolase

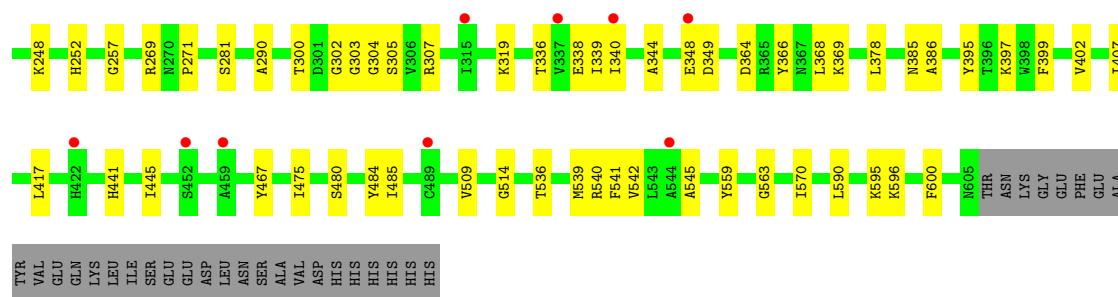


• Molecule 1: Fatty acid amide hydrolase

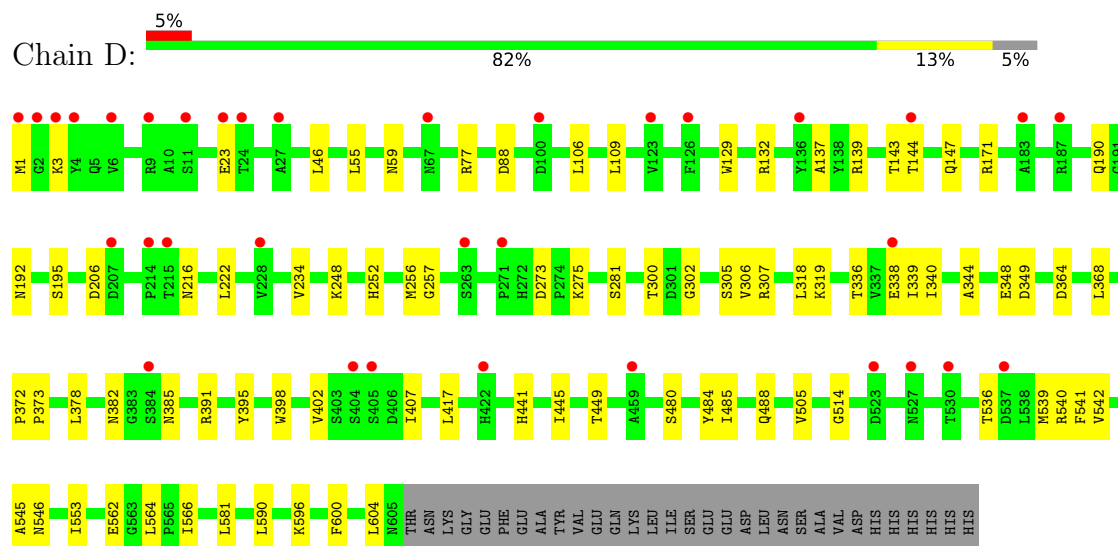


• Molecule 1: Fatty acid amide hydrolase

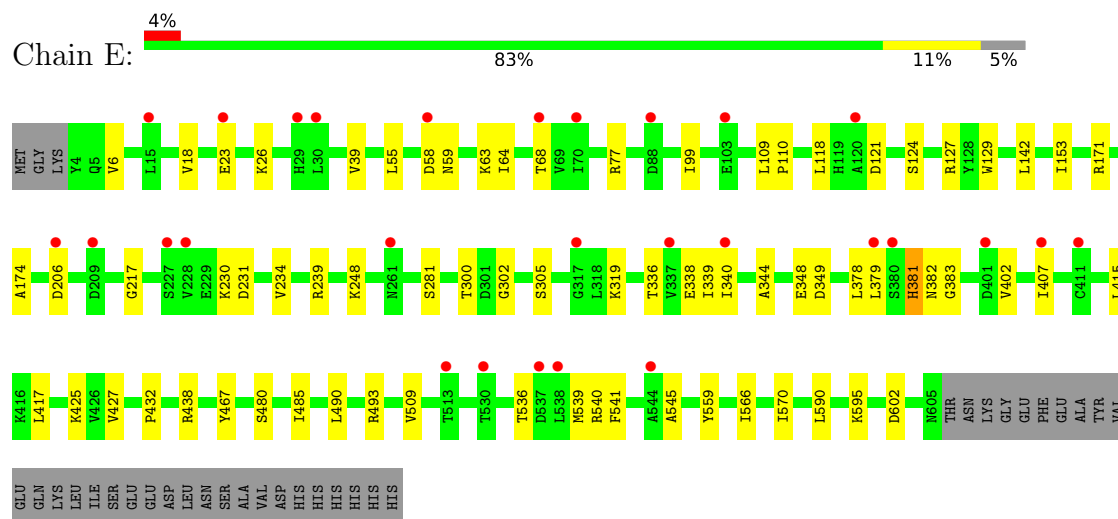




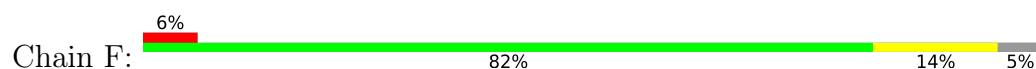
- Molecule 1: Fatty acid amide hydrolase

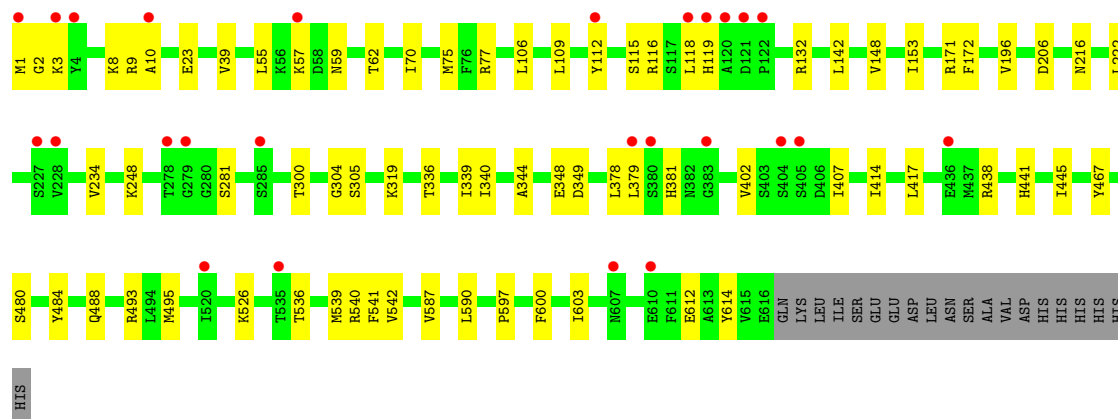


- Molecule 1: Fatty acid amide hydrolase

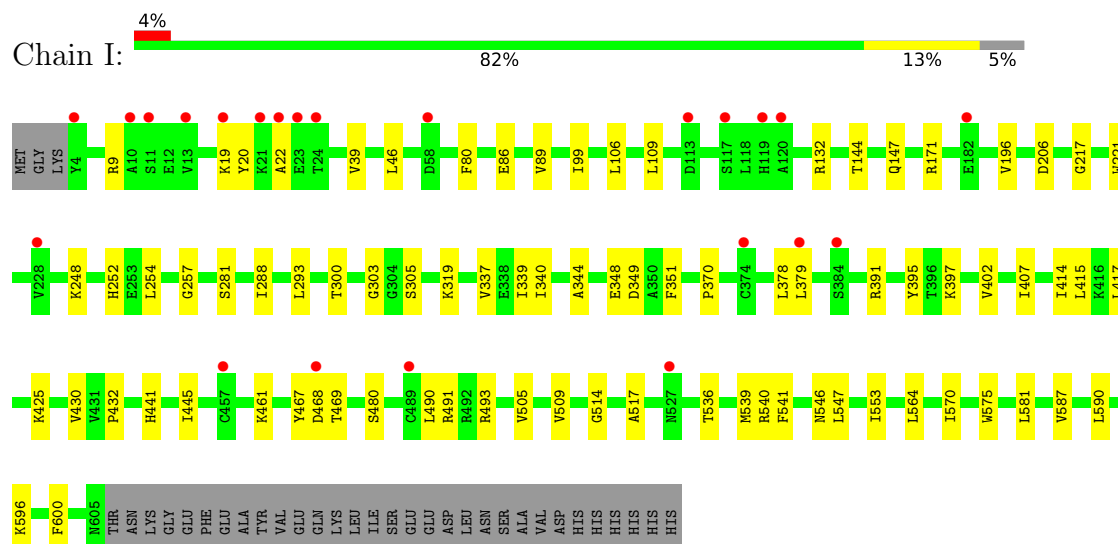


- Molecule 1: Fatty acid amide hydrolase

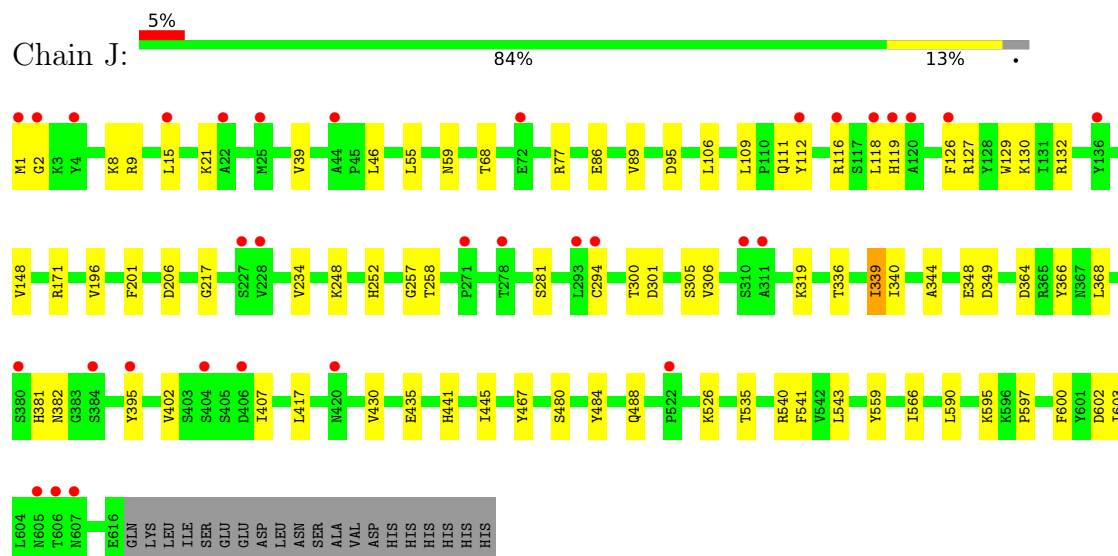




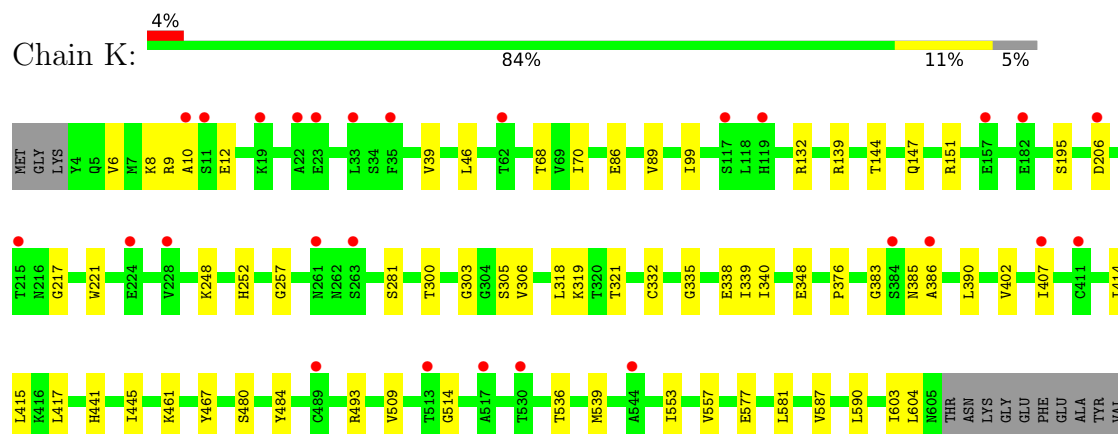
• Molecule 1: Fatty acid amide hydrolase



• Molecule 1: Fatty acid amide hydrolase

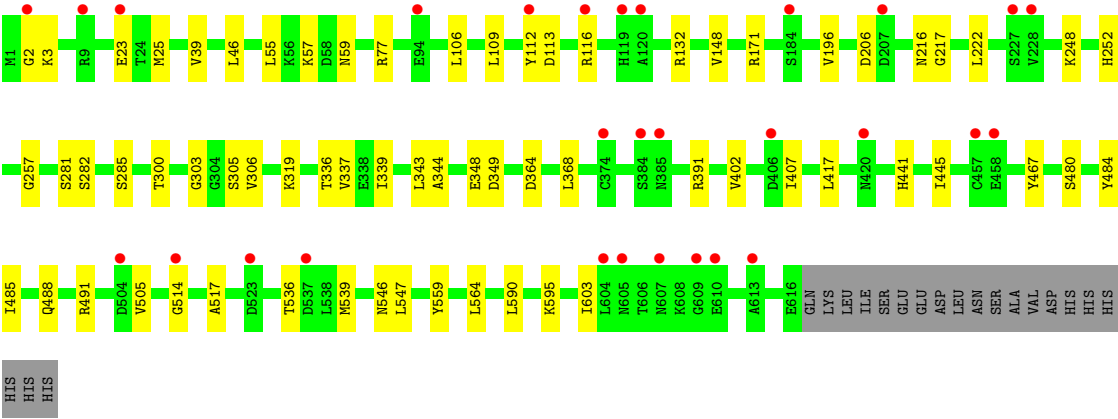
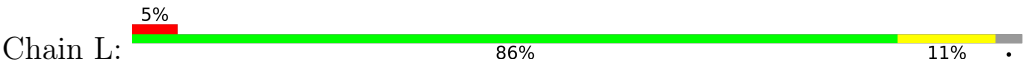


• Molecule 1: Fatty acid amide hydrolase



GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
SER
ALA
VAL
ASP
HIS
HIS
HIS
HIS
HIS

● 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	225.58Å 83.31Å 272.81Å 90.00° 110.98° 90.00°	Depositor
Resolution (Å)	34.61 – 3.20 34.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	81.4 (34.61-3.20) 82.1 (34.61-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.253 , 0.296 (Not available) , 0.299	Depositor DCC
R_{free} test set	6803 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55932	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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 64.82 % 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 7.8102e-06. 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: GJY

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	0.12	0/4705	0.26	0/6392
1	B	0.11	0/4726	0.26	0/6418
1	C	0.12	0/4705	0.26	0/6392
1	D	0.12	0/4726	0.28	0/6418
1	E	0.12	0/4705	0.29	1/6392 (0.0%)
1	F	0.13	0/4726	0.27	0/6418
1	G	0.13	0/4705	0.27	0/6392
1	H	0.14	0/4818	0.29	0/6542
1	I	0.13	0/4705	0.27	0/6392
1	J	0.14	0/4818	0.28	0/6542
1	K	0.13	0/4705	0.26	0/6392
1	L	0.13	0/4818	0.27	0/6542
All	All	0.13	0/56862	0.27	1/77232 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	381	HIS	N-CA-C	-6.31	104.32	111.07

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	4606	0	4626	42	0
1	B	4627	0	4654	39	0
1	C	4606	0	4626	48	0
1	D	4627	0	4654	52	0
1	E	4606	0	4626	47	0
1	F	4627	0	4654	53	0
1	G	4606	0	4626	38	0
1	H	4717	0	4733	44	0
1	I	4606	0	4626	53	0
1	J	4717	0	4733	52	0
1	K	4606	0	4626	41	0
1	L	4717	0	4733	39	0
2	A	22	0	0	0	0
2	B	22	0	0	1	0
2	C	22	0	0	2	0
2	D	22	0	0	0	0
2	E	22	0	0	0	0
2	F	22	0	0	0	0
2	G	22	0	0	1	0
2	H	22	0	0	0	0
2	I	22	0	0	1	0
2	J	22	0	0	0	0
2	K	22	0	0	1	0
2	L	22	0	0	1	0
All	All	55932	0	55917	530	0

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

All (530) 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:E:381:HIS:O	1:E:382:ASN:C	2.15	0.84
1:E:6:VAL:HB	1:E:68:THR:HG22	1.62	0.82
1:H:1:MET:SD	1:H:2:GLY:N	2.52	0.82
1:G:319:LYS:HG2	1:G:339:ILE:HD11	1.68	0.75
1:E:110:PRO:HA	1:E:379:LEU:HD23	1.69	0.73
1:K:46:LEU:HD23	1:L:46:LEU:HD23	1.72	0.71
1:A:319:LYS:HG2	1:A:339:ILE:HD11	1.73	0.69
1:E:381:HIS:O	1:E:382:ASN:O	2.09	0.69
1:H:57:LYS:HD3	1:H:62:THR:HB	1.75	0.69
1:L:319:LYS:HG2	1:L:339:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:LYS:HG2	1:F:339:ILE:HD11	1.76	0.67
1:I:536:THR:HA	1:I:539:MET:HE2	1.76	0.66
1:C:319:LYS:HG2	1:C:339:ILE:HD11	1.76	0.66
1:I:144:THR:OG1	1:I:147:GLN:NE2	2.24	0.66
1:B:1:MET:SD	1:B:2:GLY:N	2.68	0.66
1:H:2:GLY:C	1:H:3:LYS:HD2	2.20	0.66
1:J:1:MET:SD	1:J:2:GLY:N	2.69	0.66
1:F:536:THR:HA	1:F:539:MET:HE2	1.76	0.65
1:J:597:PRO:HG2	1:J:600:PHE:HB2	1.77	0.65
1:B:319:LYS:HG2	1:B:339:ILE:HD11	1.78	0.65
1:J:319:LYS:HG2	1:J:339:ILE:HD11	1.78	0.64
1:K:332:CYS:HB2	1:K:338:GLU:HG2	1.79	0.64
1:A:417:LEU:HB3	1:A:590:LEU:HD13	1.80	0.64
1:F:23:GLU:HB3	1:F:540:ARG:HH12	1.63	0.64
1:H:597:PRO:HG2	1:H:600:PHE:HB2	1.78	0.64
1:D:88:ASP:OD2	1:D:382:ASN:ND2	2.31	0.63
1:H:9:ARG:HE	1:H:10:ALA:H	1.46	0.63
1:H:112:TYR:HA	1:H:116:ARG:NH2	2.14	0.63
1:F:186:ARG:O	1:F:190:GLN:NE2	2.30	0.63
1:L:206:ASP:HA	1:L:248:LYS:HE2	1.81	0.62
1:E:425:LYS:HE3	1:E:427:VAL:HG22	1.81	0.62
1:F:417:LEU:HB3	1:F:590:LEU:HD13	1.81	0.62
1:J:111:GLN:OE1	1:J:111:GLN:N	2.32	0.62
1:G:206:ASP:HA	1:G:248:LYS:HE2	1.80	0.61
1:A:536:THR:HA	1:A:539:MET:HE2	1.82	0.61
1:G:536:THR:HA	1:G:539:MET:HE2	1.82	0.61
1:B:9:ARG:HE	1:B:10:ALA:H	1.48	0.61
1:B:88:ASP:OD2	1:B:382:ASN:ND2	2.34	0.61
1:F:9:ARG:HG3	1:F:13:VAL:HG12	1.81	0.61
1:F:597:PRO:HG2	1:F:600:PHE:HB2	1.81	0.60
1:D:319:LYS:HG2	1:D:339:ILE:HD11	1.84	0.60
1:G:39:VAL:HG21	1:G:467:TYR:HB3	1.82	0.60
1:J:148:VAL:HG13	1:J:603:ILE:HG21	1.82	0.59
1:F:307:ARG:NH2	1:F:546:ASN:OD1	2.35	0.59
1:B:206:ASP:HA	1:B:248:LYS:HE2	1.84	0.59
1:I:319:LYS:HG2	1:I:339:ILE:HD11	1.84	0.59
1:B:536:THR:HA	1:B:539:MET:HE2	1.84	0.58
1:H:319:LYS:HG2	1:H:339:ILE:HD11	1.85	0.58
1:E:319:LYS:HG2	1:E:339:ILE:HD11	1.86	0.58
1:E:480:SER:HA	1:F:480:SER:HA	1.85	0.58
1:D:536:THR:HA	1:D:539:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ARG:HB2	1:E:248:LYS:HB2	1.86	0.58
1:G:86:GLU:HG3	1:G:89:VAL:HG21	1.86	0.58
1:C:109:LEU:HD23	1:C:378:LEU:HD12	1.86	0.58
1:H:536:THR:HA	1:H:539:MET:HE2	1.86	0.58
1:C:206:ASP:HA	1:C:248:LYS:HE2	1.85	0.57
1:K:536:THR:HA	1:K:539:MET:HE2	1.86	0.57
1:G:293:LEU:HD23	1:G:603:ILE:HD11	1.86	0.57
1:E:55:LEU:O	1:E:59:ASN:ND2	2.33	0.57
1:E:536:THR:HA	1:E:539:MET:HE2	1.87	0.57
1:L:417:LEU:HB3	1:L:590:LEU:HD13	1.87	0.56
1:K:281:SER:H	1:K:305:SER:HB3	1.70	0.56
1:A:132:ARG:NH2	1:A:348:GLU:OE2	2.38	0.56
1:G:415:LEU:HD21	1:G:509:VAL:HG21	1.87	0.56
1:C:480:SER:HA	1:D:480:SER:HA	1.86	0.56
1:D:206:ASP:HA	1:D:248:LYS:HE2	1.87	0.56
1:F:402:VAL:HB	1:F:407:ILE:HD11	1.88	0.56
1:D:23:GLU:HB3	1:D:540:ARG:HH12	1.70	0.56
1:D:417:LEU:HB3	1:D:590:LEU:HD13	1.87	0.56
1:F:39:VAL:HG21	1:F:467:TYR:HB3	1.88	0.56
1:L:281:SER:H	1:L:305:SER:HB3	1.70	0.56
1:H:1:MET:N	1:I:132:ARG:HH11	2.04	0.56
1:K:206:ASP:HA	1:K:248:LYS:HE2	1.88	0.56
1:E:381:HIS:C	1:E:382:ASN:O	2.47	0.56
1:I:109:LEU:HD23	1:I:378:LEU:HD12	1.88	0.56
1:L:39:VAL:HG21	1:L:467:TYR:HB3	1.87	0.56
1:J:281:SER:H	1:J:305:SER:HB3	1.70	0.55
1:B:206:ASP:OD2	1:B:217:GLY:N	2.39	0.55
1:I:415:LEU:HD21	1:I:509:VAL:HG21	1.88	0.55
1:A:171:ARG:HB2	1:A:248:LYS:HB2	1.88	0.55
1:D:132:ARG:NH2	1:D:348:GLU:OE2	2.39	0.55
1:E:23:GLU:OE1	1:E:438:ARG:NH2	2.39	0.55
1:G:171:ARG:HB2	1:G:248:LYS:HB2	1.88	0.55
1:J:95:ASP:OD1	1:J:95:ASP:N	2.40	0.55
1:J:206:ASP:HA	1:J:248:LYS:HE2	1.89	0.55
1:H:1:MET:H1	1:I:132:ARG:HH11	1.55	0.55
1:F:23:GLU:OE1	1:F:25:MET:N	2.36	0.54
1:H:23:GLU:OE1	1:H:438:ARG:NH1	2.40	0.54
1:L:306:VAL:HG22	1:L:343:LEU:HD11	1.88	0.54
1:A:480:SER:HA	1:B:480:SER:HA	1.90	0.54
1:B:109:LEU:HD23	1:B:378:LEU:HD12	1.88	0.54
1:L:23:GLU:OE2	1:L:25:MET:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:GLU:HG3	1:I:89:VAL:HG21	1.90	0.54
1:G:281:SER:H	1:G:305:SER:HB3	1.72	0.54
1:B:39:VAL:HG21	1:B:467:TYR:HB3	1.89	0.54
1:H:281:SER:H	1:H:305:SER:HB3	1.72	0.54
1:H:109:LEU:HD23	1:H:378:LEU:HD12	1.90	0.54
1:J:86:GLU:HG3	1:J:89:VAL:HG21	1.90	0.54
1:K:39:VAL:HG21	1:K:467:TYR:HB3	1.90	0.54
1:H:39:VAL:HG21	1:H:467:TYR:HB3	1.89	0.53
1:L:132:ARG:NH2	1:L:348:GLU:OE2	2.41	0.53
1:C:281:SER:H	1:C:305:SER:HB3	1.74	0.53
1:I:490:LEU:HD23	1:I:493:ARG:HD3	1.90	0.53
1:A:206:ASP:OD2	1:A:217:GLY:N	2.41	0.53
1:A:109:LEU:HD23	1:A:378:LEU:HD12	1.91	0.53
1:C:536:THR:HA	1:C:539:MET:HE2	1.91	0.53
1:I:468:ASP:OD1	1:I:469:THR:N	2.41	0.53
1:J:206:ASP:OD2	1:J:217:GLY:N	2.41	0.53
1:K:252:HIS:CE1	1:K:257:GLY:HA3	2.44	0.53
1:D:402:VAL:HB	1:D:407:ILE:HD11	1.90	0.53
1:B:417:LEU:HB3	1:B:590:LEU:HD13	1.90	0.52
1:D:1:MET:O	1:D:3:LYS:N	2.42	0.52
1:D:139:ARG:NH2	1:D:195:SER:O	2.41	0.52
1:F:216:ASN:HA	1:F:222:LEU:HB3	1.91	0.52
1:F:9:ARG:O	1:F:493:ARG:NH2	2.36	0.52
1:H:115:SER:HA	1:H:119:HIS:O	2.09	0.52
1:C:20:TYR:HB2	1:C:397:LYS:HE2	1.89	0.52
1:C:319:LYS:NZ	1:C:545:ALA:O	2.36	0.52
1:J:126:PHE:HD1	1:J:127:ARG:N	2.06	0.52
1:K:9:ARG:O	1:K:493:ARG:NH2	2.37	0.52
1:K:300:THR:HG22	1:K:340:ILE:HD13	1.92	0.52
1:D:364:ASP:HB3	1:D:368:LEU:HD12	1.92	0.52
1:I:80:PHE:O	1:J:366:TYR:OH	2.26	0.52
1:E:109:LEU:HD23	1:E:378:LEU:HD12	1.91	0.52
1:E:206:ASP:OD2	1:E:217:GLY:N	2.43	0.52
1:A:250:ASN:ND2	1:A:268:THR:OG1	2.39	0.52
1:E:300:THR:HG22	1:E:340:ILE:HD13	1.91	0.52
1:I:206:ASP:OD2	1:I:217:GLY:N	2.43	0.52
1:D:171:ARG:HB2	1:D:248:LYS:HB2	1.92	0.52
1:F:206:ASP:HA	1:F:248:LYS:HE2	1.92	0.51
1:G:397:LYS:H	1:G:397:LYS:HD2	1.74	0.51
1:J:106:LEU:HD23	1:J:109:LEU:HD12	1.92	0.51
1:K:319:LYS:HG2	1:K:339:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:HG23	1:B:195:SER:HB3	1.92	0.51
1:K:417:LEU:HB3	1:K:590:LEU:HD13	1.91	0.51
1:I:9:ARG:O	1:I:493:ARG:NH2	2.31	0.51
1:I:132:ARG:NH2	1:I:348:GLU:OE2	2.41	0.51
1:J:77:ARG:HG2	1:J:336:THR:HG22	1.92	0.51
1:K:86:GLU:HG3	1:K:89:VAL:HG21	1.91	0.51
1:A:281:SER:H	1:A:305:SER:HB3	1.75	0.51
1:E:26:LYS:HD2	1:E:58:ASP:OD2	2.10	0.51
1:J:39:VAL:HG21	1:J:467:TYR:HB3	1.91	0.51
1:A:206:ASP:HA	1:A:248:LYS:HE2	1.92	0.51
1:F:281:SER:H	1:F:305:SER:HB3	1.76	0.51
1:G:252:HIS:CE1	1:G:257:GLY:HA3	2.46	0.51
1:I:281:SER:H	1:I:305:SER:HB3	1.76	0.51
1:I:379:LEU:HD12	1:I:379:LEU:O	2.11	0.51
1:B:382:ASN:H	1:B:385:ASN:HD21	1.59	0.50
1:D:55:LEU:O	1:D:59:ASN:ND2	2.35	0.50
1:E:39:VAL:HG21	1:E:467:TYR:HB3	1.92	0.50
1:J:300:THR:HG22	1:J:340:ILE:HD13	1.93	0.50
1:C:206:ASP:OD2	1:C:217:GLY:N	2.44	0.50
1:B:106:LEU:HD23	1:B:109:LEU:HD12	1.93	0.50
1:C:109:LEU:HD22	1:C:348:GLU:HG3	1.94	0.50
1:G:480:SER:HA	1:H:480:SER:HA	1.94	0.50
1:B:402:VAL:HB	1:B:407:ILE:HD11	1.93	0.50
1:D:307:ARG:NH2	1:D:546:ASN:OD1	2.44	0.50
1:J:171:ARG:HB2	1:J:248:LYS:HB2	1.92	0.50
1:E:63:LYS:O	1:E:68:THR:HG23	2.12	0.50
1:K:8:LYS:HD3	1:K:70:ILE:HG12	1.93	0.50
1:K:480:SER:HA	1:L:480:SER:HA	1.94	0.50
1:D:318:LEU:HA	1:D:553:ILE:HG13	1.94	0.50
1:H:118:LEU:HD13	1:H:142:LEU:HD21	1.93	0.50
1:H:206:ASP:HA	1:H:248:LYS:HE2	1.91	0.50
1:E:109:LEU:HD22	1:E:348:GLU:HG3	1.92	0.50
1:I:480:SER:HA	1:J:480:SER:HA	1.94	0.50
1:I:254:LEU:HD12	1:I:469:THR:HG21	1.94	0.50
1:C:344:ALA:HB1	1:C:349:ASP:HB2	1.93	0.49
1:B:281:SER:H	1:B:305:SER:HB3	1.77	0.49
1:B:402:VAL:HG12	1:B:514:GLY:HA2	1.93	0.49
1:C:300:THR:HG22	1:C:340:ILE:HD13	1.94	0.49
1:J:112:TYR:HD1	1:J:116:ARG:HH21	1.59	0.49
1:K:139:ARG:NH2	1:K:195:SER:O	2.45	0.49
1:F:385:ASN:HB2	1:I:19:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:540:ARG:HG3	1:F:541:PHE:CD2	2.48	0.49
1:J:402:VAL:HB	1:J:407:ILE:HD11	1.94	0.49
1:A:216:ASN:HA	1:A:222:LEU:HB3	1.95	0.49
1:E:415:LEU:HD21	1:E:509:VAL:HG21	1.94	0.49
1:C:55:LEU:O	1:C:59:ASN:ND2	2.38	0.49
1:C:252:HIS:CE1	1:C:257:GLY:HA3	2.48	0.49
1:L:252:HIS:CE1	1:L:257:GLY:HA3	2.48	0.49
1:C:540:ARG:HG3	1:C:541:PHE:CD2	2.48	0.49
1:D:129:TRP:CD2	1:D:604:LEU:HD12	2.48	0.49
1:D:302:GLY:HA3	1:D:338:GLU:HG3	1.94	0.49
1:F:86:GLU:HG3	1:F:89:VAL:HG21	1.94	0.49
1:D:319:LYS:NZ	1:D:545:ALA:O	2.39	0.48
1:J:106:LEU:HD11	1:J:196:VAL:HB	1.95	0.48
1:D:216:ASN:HA	1:D:222:LEU:HB3	1.95	0.48
1:D:596:LYS:HE2	1:D:600:PHE:HB3	1.95	0.48
1:H:171:ARG:HB2	1:H:248:LYS:HB2	1.95	0.48
1:H:55:LEU:O	1:H:59:ASN:ND2	2.39	0.48
1:A:7:MET:SD	1:A:69:VAL:HG21	2.53	0.48
1:B:1:MET:SD	1:B:3:LYS:HG2	2.54	0.48
1:H:234:VAL:HG11	1:H:340:ILE:HG21	1.95	0.48
1:I:206:ASP:HA	1:I:248:LYS:HE2	1.95	0.48
1:I:252:HIS:CE1	1:I:257:GLY:HA3	2.49	0.48
1:K:402:VAL:HB	1:K:407:ILE:HD11	1.96	0.48
1:A:55:LEU:O	1:A:59:ASN:ND2	2.34	0.48
1:D:391:ARG:HB2	1:D:505:VAL:HA	1.94	0.48
1:G:303:GLY:N	2:G:700:GJY:O1	2.47	0.48
1:J:21:LYS:HD2	1:J:435:GLU:HG3	1.94	0.48
1:I:46:LEU:HD23	1:J:46:LEU:HD23	1.95	0.48
1:I:491:ARG:HG3	1:I:547:LEU:HG	1.96	0.48
1:K:151:ARG:NH1	1:K:603:ILE:O	2.47	0.48
1:A:39:VAL:HG21	1:A:467:TYR:HB3	1.96	0.48
1:H:344:ALA:HB1	1:H:349:ASP:HB2	1.94	0.48
1:J:129:TRP:NE1	1:J:602:ASP:OD1	2.45	0.48
1:H:106:LEU:HD11	1:H:196:VAL:HB	1.95	0.48
1:A:302:GLY:HA3	1:A:338:GLU:HG3	1.96	0.47
1:D:109:LEU:HD23	1:D:378:LEU:HD12	1.95	0.47
1:J:395:TYR:CZ	1:J:430:VAL:HG23	2.49	0.47
1:K:206:ASP:OD2	1:K:217:GLY:N	2.47	0.47
1:A:225:ASP:OD1	1:B:5:GLN:NE2	2.47	0.47
1:L:206:ASP:OD2	1:L:217:GLY:N	2.46	0.47
1:D:484:TYR:O	1:D:488:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:SER:H	1:E:305:SER:HB3	1.79	0.47
1:I:144:THR:HG1	1:I:147:GLN:HE21	1.57	0.47
1:E:129:TRP:NE1	1:E:602:ASP:OD2	2.41	0.47
1:F:206:ASP:OD2	1:F:217:GLY:N	2.47	0.47
1:F:402:VAL:HG12	1:F:514:GLY:HA2	1.96	0.47
1:I:300:THR:HG22	1:I:340:ILE:HD13	1.97	0.47
1:I:596:LYS:HE2	1:I:600:PHE:HB3	1.96	0.47
1:L:55:LEU:O	1:L:59:ASN:ND2	2.41	0.47
1:D:382:ASN:H	1:D:385:ASN:HD21	1.61	0.47
1:J:417:LEU:HB3	1:J:590:LEU:HD13	1.95	0.47
1:A:402:VAL:HB	1:A:407:ILE:HD11	1.96	0.47
1:C:118:LEU:HD13	1:C:142:LEU:HD21	1.96	0.47
1:C:596:LYS:HE2	1:C:600:PHE:HB3	1.96	0.47
1:A:395:TYR:O	1:A:399:PHE:N	2.46	0.47
1:A:415:LEU:HD21	1:A:509:VAL:HG21	1.97	0.47
1:C:366:TYR:O	1:C:369:LYS:NZ	2.37	0.47
1:C:395:TYR:O	1:C:399:PHE:N	2.46	0.47
1:D:540:ARG:HG3	1:D:541:PHE:CD2	2.50	0.47
1:E:124:SER:HB3	1:E:127:ARG:HH12	1.79	0.47
1:G:491:ARG:HG3	1:G:547:LEU:HG	1.97	0.47
1:J:118:LEU:HD23	1:J:119:HIS:HB2	1.95	0.47
1:K:144:THR:OG1	1:K:147:GLN:OE1	2.32	0.47
1:K:415:LEU:HD21	1:K:509:VAL:HG21	1.95	0.47
1:F:139:ARG:NH2	1:F:195:SER:O	2.47	0.47
1:I:109:LEU:HD22	1:I:348:GLU:HG3	1.95	0.47
1:K:303:GLY:N	2:K:700:GJY:O1	2.46	0.47
1:L:402:VAL:HB	1:L:407:ILE:HD11	1.97	0.47
1:H:75:MET:HE1	1:H:495:MET:HB2	1.97	0.47
1:H:216:ASN:HA	1:H:222:LEU:HB3	1.96	0.47
1:I:395:TYR:HE1	1:I:397:LYS:HE2	1.80	0.46
1:C:303:GLY:N	2:C:700:GJY:O1	2.49	0.46
1:C:563:GLY:O	1:C:595:LYS:NZ	2.46	0.46
1:H:132:ARG:NH2	1:H:348:GLU:OE2	2.46	0.46
1:J:252:HIS:CE1	1:J:257:GLY:HA3	2.51	0.46
1:C:271:PRO:HG2	1:C:290:ALA:HB3	1.97	0.46
1:C:484:TYR:CZ	1:D:485:ILE:HD11	2.50	0.46
1:C:140:SER:O	1:C:141:LYS:HG2	2.15	0.46
1:E:234:VAL:HG11	1:E:340:ILE:HG21	1.97	0.46
1:I:288:ILE:HG13	1:I:293:LEU:HD12	1.97	0.46
1:L:106:LEU:HD11	1:L:196:VAL:HB	1.97	0.46
1:G:132:ARG:NH2	1:G:348:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:LEU:HD22	1:H:348:GLU:HG3	1.97	0.46
1:J:109:LEU:HD22	1:J:348:GLU:HG3	1.97	0.46
1:J:234:VAL:HG11	1:J:340:ILE:HG21	1.97	0.46
1:F:234:VAL:HG11	1:F:340:ILE:HG21	1.98	0.46
1:B:86:GLU:HG3	1:B:89:VAL:HG21	1.97	0.46
1:G:55:LEU:O	1:G:59:ASN:ND2	2.46	0.46
1:E:382:ASN:O	1:E:383:GLY:C	2.58	0.46
1:F:118:LEU:HD13	1:F:142:LEU:HD21	1.97	0.46
1:A:300:THR:HG22	1:A:340:ILE:HD13	1.98	0.46
1:B:252:HIS:CE1	1:B:257:GLY:HA3	2.50	0.46
1:D:234:VAL:HG11	1:D:340:ILE:HG21	1.98	0.46
1:E:300:THR:O	1:E:305:SER:HB2	2.15	0.46
1:G:6:VAL:HB	1:G:68:THR:HG23	1.98	0.46
1:I:300:THR:O	1:I:305:SER:HB2	2.16	0.46
1:J:258:THR:H	1:J:535:THR:HG23	1.81	0.46
1:F:407:ILE:HG22	1:F:566:ILE:HG12	1.98	0.46
1:H:414:ILE:HG21	1:H:587:VAL:HG13	1.98	0.46
1:J:300:THR:O	1:J:305:SER:HB2	2.16	0.46
1:C:39:VAL:HG21	1:C:467:TYR:HB3	1.98	0.45
1:C:171:ARG:HB2	1:C:248:LYS:HB2	1.97	0.45
1:D:252:HIS:CE1	1:D:257:GLY:HA3	2.51	0.45
1:D:407:ILE:HA	1:D:566:ILE:HD13	1.98	0.45
1:G:109:LEU:HD23	1:G:378:LEU:HD12	1.97	0.45
1:K:281:SER:H	1:K:305:SER:CB	2.29	0.45
1:F:491:ARG:HG3	1:F:547:LEU:HG	1.97	0.45
1:J:540:ARG:HG3	1:J:541:PHE:CD2	2.51	0.45
1:J:559:TYR:CZ	1:J:595:LYS:HB3	2.52	0.45
1:L:303:GLY:N	2:L:700:GJY:O1	2.50	0.45
1:L:337:VAL:HB	1:L:546:ASN:HB3	1.99	0.45
1:L:364:ASP:HB3	1:L:368:LEU:HD12	1.98	0.45
1:A:252:HIS:CE1	1:A:257:GLY:HA3	2.52	0.45
1:A:271:PRO:HG2	1:A:290:ALA:HB3	1.97	0.45
1:C:364:ASP:HB3	1:C:368:LEU:HD12	1.98	0.45
1:F:509:VAL:HG12	1:F:570:ILE:HG12	1.99	0.45
1:I:171:ARG:HB2	1:I:248:LYS:HB2	1.99	0.45
1:J:130:LYS:H	1:J:130:LYS:HG2	1.61	0.45
1:A:219:THR:O	1:A:265:TYR:OH	2.24	0.45
1:D:300:THR:O	1:D:305:SER:HB2	2.16	0.45
1:E:77:ARG:HG2	1:E:336:THR:HG22	1.98	0.45
1:I:417:LEU:HB3	1:I:590:LEU:HD13	1.99	0.45
1:K:414:ILE:HG13	1:K:557:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:391:ARG:HB2	1:L:505:VAL:HA	1.99	0.45
1:C:20:TYR:CE2	1:C:22:ALA:HB2	2.52	0.45
1:C:417:LEU:HB3	1:C:590:LEU:HD13	1.99	0.45
1:D:407:ILE:HG22	1:D:566:ILE:HG12	1.99	0.45
1:F:114:PRO:HB3	1:F:136:TYR:CZ	2.52	0.45
1:F:288:ILE:HG13	1:F:293:LEU:HD12	1.98	0.45
1:E:559:TYR:CZ	1:E:595:LYS:HB3	2.52	0.45
1:B:109:LEU:HD22	1:B:348:GLU:HG3	1.99	0.45
1:E:344:ALA:HB1	1:E:349:ASP:HB2	1.99	0.45
1:F:382:ASN:ND2	1:F:383:GLY:O	2.49	0.45
1:F:414:ILE:HG21	1:F:587:VAL:HG13	1.98	0.45
1:I:402:VAL:HB	1:I:407:ILE:HD11	1.99	0.45
1:L:77:ARG:HG2	1:L:336:THR:HG22	1.99	0.45
1:B:457:CYS:HB3	1:B:462:ASN:HB2	1.99	0.45
1:B:521:PRO:HB2	1:B:523:ASP:OD1	2.17	0.45
1:G:162:ASP:OD1	1:G:162:ASP:N	2.48	0.45
1:L:2:GLY:C	1:L:3:LYS:HD2	2.42	0.45
1:L:300:THR:O	1:L:306:VAL:HG23	2.17	0.45
1:J:344:ALA:HB1	1:J:349:ASP:HB2	1.99	0.45
1:K:414:ILE:HG21	1:K:587:VAL:HG13	1.98	0.45
1:L:402:VAL:HG12	1:L:514:GLY:HA2	1.99	0.45
1:B:300:THR:O	1:B:306:VAL:HG23	2.17	0.44
1:J:8:LYS:HE3	1:J:68:THR:HG21	1.99	0.44
1:J:55:LEU:O	1:J:59:ASN:ND2	2.45	0.44
1:K:402:VAL:HG12	1:K:514:GLY:HA2	1.99	0.44
1:E:402:VAL:HB	1:E:407:ILE:HD11	1.99	0.44
1:F:351:PHE:CE1	1:F:376:PRO:HD2	2.51	0.44
1:I:20:TYR:CE2	1:I:22:ALA:HB2	2.52	0.44
1:I:441:HIS:O	1:I:445:ILE:HG22	2.17	0.44
1:B:307:ARG:NH2	1:B:546:ASN:OD1	2.51	0.44
1:D:77:ARG:HG2	1:D:336:THR:HG22	2.00	0.44
1:F:490:LEU:HD23	1:F:493:ARG:HD3	1.99	0.44
1:H:612:GLU:O	1:H:614:TYR:N	2.51	0.44
1:I:106:LEU:HD11	1:I:196:VAL:HB	1.98	0.44
1:A:327:MET:HG2	1:A:340:ILE:HG12	1.99	0.44
1:C:559:TYR:CZ	1:C:595:LYS:HB3	2.53	0.44
1:D:395:TYR:HB3	1:D:398:TRP:HB3	1.99	0.44
1:E:206:ASP:HA	1:E:248:LYS:HE2	2.00	0.44
1:I:99:ILE:H	1:I:99:ILE:HD12	1.82	0.44
1:L:216:ASN:HA	1:L:222:LEU:HB3	2.00	0.44
1:B:288:ILE:HG13	1:B:293:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:441:HIS:CE1	1:G:543:LEU:HD22	2.52	0.44
1:L:344:ALA:HB1	1:L:349:ASP:HB2	1.98	0.44
1:J:407:ILE:HA	1:J:566:ILE:HD13	2.00	0.44
1:C:485:ILE:HD11	1:D:484:TYR:CZ	2.52	0.44
1:H:540:ARG:HG3	1:H:541:PHE:CD2	2.53	0.44
1:I:337:VAL:HB	1:I:546:ASN:HB3	1.99	0.44
1:C:307:ARG:HH12	1:C:545:ALA:HB3	1.83	0.44
1:E:485:ILE:HD11	1:F:484:TYR:CZ	2.53	0.44
1:G:319:LYS:NZ	1:G:545:ALA:O	2.36	0.44
1:J:132:ARG:NH2	1:J:348:GLU:OE2	2.51	0.44
1:C:202:VAL:HG21	1:C:238:LEU:HD13	2.00	0.43
1:C:385:ASN:OD1	1:C:386:ALA:N	2.51	0.43
1:F:457:CYS:HB3	1:F:462:ASN:HB2	1.99	0.43
1:K:441:HIS:O	1:K:445:ILE:HG22	2.18	0.43
1:D:441:HIS:O	1:D:445:ILE:HG22	2.18	0.43
1:E:231:ASP:OD2	1:E:239:ARG:NE	2.44	0.43
1:F:407:ILE:HA	1:F:566:ILE:HD13	2.00	0.43
1:H:402:VAL:HB	1:H:407:ILE:HD11	1.99	0.43
1:J:300:THR:O	1:J:306:VAL:HG23	2.18	0.43
1:K:8:LYS:HE3	1:K:493:ARG:CZ	2.47	0.43
1:A:391:ARG:HB2	1:A:505:VAL:HA	2.00	0.43
1:B:303:GLY:N	2:B:700:GJY:O1	2.51	0.43
1:B:327:MET:HG2	1:B:340:ILE:HG12	1.99	0.43
1:G:344:ALA:HB1	1:G:349:ASP:HB2	2.00	0.43
1:L:517:ALA:HB3	1:L:564:LEU:HD13	1.99	0.43
1:B:139:ARG:NH2	1:B:195:SER:O	2.48	0.43
1:E:302:GLY:HA3	1:E:338:GLU:HG3	1.99	0.43
1:E:417:LEU:HB3	1:E:590:LEU:HD13	2.00	0.43
1:E:490:LEU:HD23	1:E:493:ARG:HD3	2.00	0.43
1:D:562:GLU:HG2	1:D:564:LEU:HG	2.00	0.43
1:G:109:LEU:HD22	1:G:348:GLU:HG3	2.01	0.43
1:A:300:THR:O	1:A:305:SER:HB2	2.19	0.43
1:G:300:THR:HG22	1:G:340:ILE:HD13	2.00	0.43
1:L:171:ARG:HB2	1:L:248:LYS:HB2	2.00	0.43
1:A:20:TYR:CE2	1:A:22:ALA:HB2	2.53	0.43
1:B:43:GLU:OE1	1:B:470:ARG:NH2	2.36	0.43
1:E:407:ILE:HG22	1:E:566:ILE:HG12	2.01	0.43
1:F:319:LYS:NZ	1:F:545:ALA:O	2.48	0.43
1:H:304:GLY:HA3	1:H:542:VAL:HG21	2.01	0.43
1:D:281:SER:H	1:D:305:SER:HB3	1.84	0.43
1:I:414:ILE:HG21	1:I:587:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:321:THR:OG1	1:K:577:GLU:OE2	2.24	0.43
1:L:57:LYS:HE2	1:L:57:LYS:HB2	1.86	0.43
1:F:484:TYR:O	1:F:488:GLN:HG2	2.17	0.43
1:B:391:ARG:HB2	1:B:505:VAL:HA	2.00	0.43
1:E:540:ARG:HG3	1:E:541:PHE:CD2	2.54	0.43
1:F:300:THR:O	1:F:305:SER:HB2	2.19	0.43
1:L:109:LEU:HD22	1:L:348:GLU:HG3	2.01	0.43
1:L:484:TYR:O	1:L:488:GLN:HG2	2.18	0.43
1:B:491:ARG:HG3	1:B:547:LEU:HG	2.01	0.42
1:C:300:THR:O	1:C:305:SER:HB2	2.18	0.42
1:C:402:VAL:HG12	1:C:514:GLY:HA2	2.00	0.42
1:D:190:GLN:HG3	1:D:192:ASN:OD1	2.19	0.42
1:G:402:VAL:HB	1:G:407:ILE:HD11	2.01	0.42
1:H:484:TYR:O	1:H:488:GLN:HG2	2.18	0.42
1:J:201:PHE:O	1:J:294:CYS:HB2	2.19	0.42
1:I:540:ARG:HG3	1:I:541:PHE:CD2	2.54	0.42
1:K:300:THR:O	1:K:306:VAL:HG23	2.19	0.42
1:C:269:ARG:HA	1:C:269:ARG:HD3	1.90	0.42
1:C:475:ILE:HD13	2:C:700:GJY:C17	2.49	0.42
1:E:118:LEU:HD13	1:E:142:LEU:HD21	2.02	0.42
1:J:407:ILE:HG22	1:J:566:ILE:HG12	2.01	0.42
1:A:18:VAL:HG11	1:A:432:PRO:HA	2.02	0.42
1:C:139:ARG:NH2	1:C:195:SER:O	2.52	0.42
1:J:9:ARG:HD2	1:J:9:ARG:HA	1.88	0.42
1:J:441:HIS:CE1	1:J:543:LEU:HD22	2.54	0.42
1:K:386:ALA:O	1:K:390:LEU:HG	2.20	0.42
1:A:386:ALA:O	1:A:390:LEU:HG	2.19	0.42
1:D:106:LEU:HD23	1:D:109:LEU:HD12	2.01	0.42
1:D:318:LEU:HD22	1:D:581:LEU:HD21	2.02	0.42
1:G:9:ARG:HA	1:G:9:ARG:HD2	1.67	0.42
1:G:300:THR:O	1:G:305:SER:HB2	2.19	0.42
1:G:379:LEU:C	1:G:381:HIS:H	2.27	0.42
1:K:132:ARG:NH2	1:K:348:GLU:OE2	2.50	0.42
1:K:376:PRO:HG3	1:K:581:LEU:HB2	2.02	0.42
1:A:402:VAL:HG12	1:A:514:GLY:HA2	2.00	0.42
1:B:9:ARG:NE	1:B:10:ALA:H	2.16	0.42
1:B:171:ARG:HB2	1:B:248:LYS:HB2	2.02	0.42
1:B:256:MET:HE3	1:B:449:THR:HG21	2.00	0.42
1:E:64:ILE:O	1:E:68:THR:OG1	2.37	0.42
1:F:221:TRP:CE3	1:F:461:LYS:HG2	2.55	0.42
1:F:252:HIS:CE1	1:F:257:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:379:LEU:HD12	1:H:379:LEU:O	2.19	0.42
1:J:15:LEU:HB3	1:J:430:VAL:HG11	2.02	0.42
1:L:112:TYR:HA	1:L:116:ARG:HH22	1.84	0.42
1:C:182:GLU:HB3	1:C:186:ARG:NH2	2.34	0.42
1:C:402:VAL:HB	1:C:407:ILE:HD11	2.01	0.42
1:D:137:ALA:HB1	1:D:143:THR:HG22	2.01	0.42
1:E:379:LEU:HD12	1:E:379:LEU:O	2.20	0.42
1:H:148:VAL:HG13	1:H:603:ILE:HG21	2.02	0.42
1:L:112:TYR:CG	1:L:113:ASP:N	2.87	0.42
1:A:95:ASP:OD1	1:A:95:ASP:N	2.46	0.42
1:C:441:HIS:O	1:C:445:ILE:HG22	2.20	0.42
1:D:256:MET:HE3	1:D:449:THR:HG21	2.02	0.42
1:J:301:ASP:HB3	1:J:339:ILE:HD11	2.01	0.42
1:D:273:ASP:OD1	1:D:275:LYS:HG2	2.20	0.42
1:F:171:ARG:HB2	1:F:248:LYS:HB2	2.01	0.42
1:F:273:ASP:OD1	1:F:275:LYS:HG2	2.20	0.42
1:F:395:TYR:HB3	1:F:398:TRP:HB3	2.01	0.42
1:K:6:VAL:HB	1:K:68:THR:HG23	2.02	0.42
1:K:99:ILE:HD12	1:K:99:ILE:H	1.85	0.42
1:L:148:VAL:HG13	1:L:603:ILE:HG21	2.02	0.42
1:A:540:ARG:HG3	1:A:541:PHE:CD2	2.55	0.42
1:C:304:GLY:HA3	1:C:542:VAL:HG21	2.02	0.42
1:D:402:VAL:HG12	1:D:514:GLY:HA2	2.02	0.42
1:E:509:VAL:HG12	1:E:570:ILE:HG12	2.01	0.42
1:H:417:LEU:HB3	1:H:590:LEU:HD13	2.02	0.42
1:H:441:HIS:O	1:H:445:ILE:HG22	2.19	0.42
1:I:281:SER:H	1:I:305:SER:CB	2.33	0.42
1:I:344:ALA:HB1	1:I:349:ASP:HB2	2.02	0.42
1:J:364:ASP:HB3	1:J:368:LEU:HD12	2.02	0.42
1:F:344:ALA:HB1	1:F:349:ASP:HB2	2.02	0.41
1:I:402:VAL:HG12	1:I:514:GLY:HA2	2.02	0.41
1:A:109:LEU:HD22	1:A:348:GLU:HG3	2.02	0.41
1:A:395:TYR:HB3	1:A:398:TRP:HB3	2.00	0.41
1:F:327:MET:HG2	1:F:340:ILE:HG12	2.00	0.41
1:G:106:LEU:HD11	1:G:196:VAL:HB	2.01	0.41
1:G:596:LYS:HE2	1:G:600:PHE:HB3	2.02	0.41
1:C:302:GLY:HA3	1:C:338:GLU:HG3	2.00	0.41
1:G:441:HIS:O	1:G:445:ILE:HG22	2.19	0.41
1:H:300:THR:O	1:H:305:SER:HB2	2.20	0.41
1:K:221:TRP:CE3	1:K:461:LYS:HG2	2.55	0.41
1:B:344:ALA:HB1	1:B:349:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:THR:O	1:D:306:VAL:HG23	2.20	0.41
1:H:8:LYS:NZ	1:H:70:ILE:HG12	2.35	0.41
1:H:9:ARG:O	1:H:493:ARG:NH2	2.44	0.41
1:J:381:HIS:CG	1:J:382:ASN:H	2.38	0.41
1:L:282:SER:HB3	1:L:285:SER:HB2	2.02	0.41
1:L:441:HIS:O	1:L:445:ILE:HG22	2.20	0.41
1:I:39:VAL:HG21	1:I:467:TYR:HB3	2.01	0.41
1:I:303:GLY:N	2:I:700:GJY:O1	2.53	0.41
1:I:370:PRO:HB3	1:I:575:TRP:CH2	2.55	0.41
1:I:517:ALA:HB3	1:I:564:LEU:HD13	2.02	0.41
1:E:319:LYS:NZ	1:E:545:ALA:O	2.39	0.41
1:F:596:LYS:HE2	1:F:600:PHE:HD2	1.85	0.41
1:G:202:VAL:HG23	1:G:245:LEU:HD13	2.02	0.41
1:G:491:ARG:NH1	1:G:547:LEU:O	2.53	0.41
1:H:526:LYS:HD2	1:H:526:LYS:HA	1.84	0.41
1:K:484:TYR:CZ	1:L:485:ILE:HD11	2.55	0.41
1:C:46:LEU:HD23	1:D:46:LEU:HD23	2.03	0.41
1:D:144:THR:H	1:D:147:GLN:NE2	2.19	0.41
1:E:230:LYS:HE3	1:E:230:LYS:HB2	1.88	0.41
1:G:281:SER:H	1:G:305:SER:CB	2.34	0.41
1:G:337:VAL:HB	1:G:546:ASN:HB3	2.01	0.41
1:G:484:TYR:O	1:G:488:GLN:HG2	2.20	0.41
1:H:153:ILE:HG12	1:H:172:PHE:HZ	1.86	0.41
1:K:383:GLY:O	1:K:385:ASN:N	2.53	0.41
1:G:376:PRO:HG3	1:G:581:LEU:HB2	2.03	0.41
1:I:221:TRP:CE3	1:I:461:LYS:HG2	2.56	0.41
1:I:430:VAL:O	1:I:432:PRO:HD3	2.21	0.41
1:K:604:LEU:HD23	1:K:604:LEU:HA	1.88	0.41
1:L:559:TYR:CZ	1:L:595:LYS:HB3	2.56	0.41
1:A:281:SER:H	1:A:305:SER:CB	2.34	0.41
1:B:234:VAL:HG11	1:B:340:ILE:HG21	2.03	0.41
1:C:77:ARG:HG2	1:C:336:THR:HG22	2.02	0.41
1:D:307:ARG:CZ	1:D:542:VAL:HB	2.51	0.41
1:E:18:VAL:HG11	1:E:432:PRO:HA	2.03	0.41
1:E:153:ILE:HD13	1:E:174:ALA:HB1	2.02	0.41
1:F:570:ILE:HG21	1:F:583:LEU:HD23	2.03	0.41
1:I:425:LYS:HE3	1:I:425:LYS:HB3	1.87	0.41
1:J:441:HIS:O	1:J:445:ILE:HG22	2.21	0.41
1:J:526:LYS:HA	1:J:526:LYS:HD2	1.91	0.41
1:K:318:LEU:HA	1:K:553:ILE:HG13	2.03	0.41
1:A:153:ILE:HG12	1:A:172:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:HIS:O	1:A:445:ILE:HG22	2.20	0.41
1:A:491:ARG:HG3	1:A:547:LEU:HG	2.02	0.41
1:F:318:LEU:HD22	1:F:581:LEU:HD21	2.03	0.41
1:I:553:ILE:HG22	1:I:570:ILE:HB	2.03	0.41
1:G:414:ILE:HG21	1:G:587:VAL:HG13	2.03	0.40
1:H:379:LEU:HD13	1:H:381:HIS:CE1	2.56	0.40
1:D:344:ALA:HB1	1:D:349:ASP:HB2	2.02	0.40
1:E:99:ILE:HD12	1:E:99:ILE:H	1.86	0.40
1:I:351:PHE:HD1	1:I:581:LEU:HD13	1.86	0.40
1:L:491:ARG:HG3	1:L:547:LEU:HG	2.02	0.40
1:L:536:THR:HA	1:L:539:MET:HE2	2.02	0.40
1:D:109:LEU:HD22	1:D:348:GLU:HG3	2.03	0.40
1:D:372:PRO:HA	1:D:373:PRO:HD3	1.95	0.40
1:F:391:ARG:HB2	1:F:505:VAL:HA	2.02	0.40
1:H:77:ARG:HG2	1:H:336:THR:HG22	2.04	0.40
1:I:391:ARG:HB2	1:I:505:VAL:HA	2.03	0.40
1:J:484:TYR:O	1:J:488:GLN:HG2	2.20	0.40
1:K:335:GLY:HA3	1:K:338:GLU:OE1	2.22	0.40
1:A:300:THR:O	1:A:306:VAL:HG23	2.21	0.40
1:A:383:GLY:O	1:A:385:ASN:N	2.55	0.40
1:A:500:ASN:O	1:A:503:LYS:HG2	2.21	0.40
1:B:307:ARG:HH12	1:B:545:ALA:HB3	1.86	0.40
1:C:63:LYS:HD2	1:C:67:ASN:HB2	2.04	0.40
1:C:509:VAL:HG12	1:C:570:ILE:HG12	2.02	0.40
1:F:55:LEU:O	1:F:59:ASN:ND2	2.38	0.40
1:F:415:LEU:HD21	1:F:509:VAL:HG21	2.04	0.40
1:F:441:HIS:O	1:F:445:ILE:HG22	2.21	0.40
1:K:10:ALA:C	1:K:12:GLU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	67/540 (12%)	67 (100%)	0	100	100
1	C	313/540 (58%)	313 (100%)	0	100	100
1	D	512/540 (95%)	512 (100%)	0	100	100
1	E	317/540 (59%)	316 (100%)	1 (0%)	86	88
1	G	4/540 (1%)	4 (100%)	0	100	100
1	H	225/540 (42%)	225 (100%)	0	100	100
1	I	510/540 (94%)	510 (100%)	0	100	100
1	J	521/540 (96%)	520 (100%)	1 (0%)	87	89
1	K	510/540 (94%)	510 (100%)	0	100	100
1	L	521/540 (96%)	521 (100%)	0	100	100
All	All	3500/5400 (65%)	3498 (100%)	2 (0%)	88	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	121	ASP
1	J	339	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	533	GLN
1	C	147	GLN
1	C	533	GLN
1	D	216	ASN
1	D	252	HIS
1	D	420	ASN
1	D	422	HIS
1	D	533	GLN
1	E	29	HIS
1	E	192	ASN
1	E	252	HIS
1	H	533	GLN
1	I	40	ASN

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Mol	Chain	Res	Type
1	I	147	GLN
1	I	216	ASN
1	I	533	GLN
1	J	462	ASN
1	J	533	GLN
1	J	605	ASN
1	K	216	ASN
1	K	422	HIS
1	K	533	GLN
1	K	605	ASN
1	L	192	ASN
1	L	216	ASN
1	L	533	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	GJY	E	700	1	18,21,22	0.34	0	16,21,24	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GJY	B	700	1	18,21,22	0.34	0	16,21,24	0.44	0
2	GJY	A	700	1	18,21,22	0.33	0	16,21,24	0.42	0
2	GJY	H	700	1	18,21,22	0.35	0	16,21,24	0.41	0
2	GJY	G	700	1	18,21,22	0.35	0	16,21,24	0.43	0
2	GJY	K	700	1	18,21,22	0.34	0	16,21,24	0.41	0
2	GJY	D	700	1	18,21,22	0.33	0	16,21,24	0.42	0
2	GJY	F	700	1	18,21,22	0.34	0	16,21,24	0.42	0
2	GJY	C	700	1	18,21,22	0.34	0	16,21,24	0.41	0
2	GJY	J	700	1	18,21,22	0.34	0	16,21,24	0.43	0
2	GJY	I	700	1	18,21,22	0.35	0	16,21,24	0.40	0
2	GJY	L	700	1	18,21,22	0.33	0	16,21,24	0.41	0

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	GJY	E	700	1	-	8/16/20/22	-
2	GJY	B	700	1	-	6/16/20/22	-
2	GJY	A	700	1	-	8/16/20/22	-
2	GJY	H	700	1	-	6/16/20/22	-
2	GJY	G	700	1	-	7/16/20/22	-
2	GJY	K	700	1	-	7/16/20/22	-
2	GJY	D	700	1	-	7/16/20/22	-
2	GJY	F	700	1	-	7/16/20/22	-
2	GJY	C	700	1	-	7/16/20/22	-
2	GJY	J	700	1	-	7/16/20/22	-
2	GJY	I	700	1	-	8/16/20/22	-
2	GJY	L	700	1	-	5/16/20/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	700	GJY	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	H	700	GJY	C5-C6-C7-C8
2	A	700	GJY	C1-C2-C3-C4
2	I	700	GJY	C1-C2-C3-C4
2	K	700	GJY	C1-C2-C3-C4
2	B	700	GJY	C6-C7-C8-C9
2	H	700	GJY	C1-C2-C3-C4
2	J	700	GJY	C1-C2-C3-C4
2	C	700	GJY	C1-C2-C3-C4
2	B	700	GJY	C4-C5-C6-C7
2	G	700	GJY	C1-C2-C3-C4
2	E	700	GJY	C1-C2-C3-C4
2	D	700	GJY	C1-C2-C3-C4
2	C	700	GJY	C12-C13-C14-C15
2	D	700	GJY	C10-C11-C12-C13
2	D	700	GJY	C12-C13-C14-C15
2	E	700	GJY	C12-C13-C14-C15
2	F	700	GJY	C10-C11-C12-C13
2	F	700	GJY	C12-C13-C14-C15
2	G	700	GJY	C10-C11-C12-C13
2	G	700	GJY	C12-C13-C14-C15
2	H	700	GJY	C12-C13-C14-C15
2	J	700	GJY	C10-C11-C12-C13
2	J	700	GJY	C12-C13-C14-C15
2	L	700	GJY	C12-C13-C14-C15
2	F	700	GJY	C1-C2-C3-C4
2	D	700	GJY	C4-C5-C6-C7
2	K	700	GJY	C4-C5-C6-C7
2	A	700	GJY	C4-C5-C6-C7
2	E	700	GJY	C4-C5-C6-C7
2	I	700	GJY	C4-C5-C6-C7
2	J	700	GJY	C4-C5-C6-C7
2	G	700	GJY	C4-C5-C6-C7
2	F	700	GJY	C5-C6-C7-C8
2	C	700	GJY	C4-C5-C6-C7
2	B	700	GJY	C3-C4-C5-C6
2	F	700	GJY	C4-C5-C6-C7
2	G	700	GJY	C5-C6-C7-C8
2	C	700	GJY	C5-C6-C7-C8
2	A	700	GJY	C5-C6-C7-C8
2	D	700	GJY	C6-C7-C8-C9
2	A	700	GJY	C6-C7-C8-C9
2	E	700	GJY	C6-C7-C8-C9

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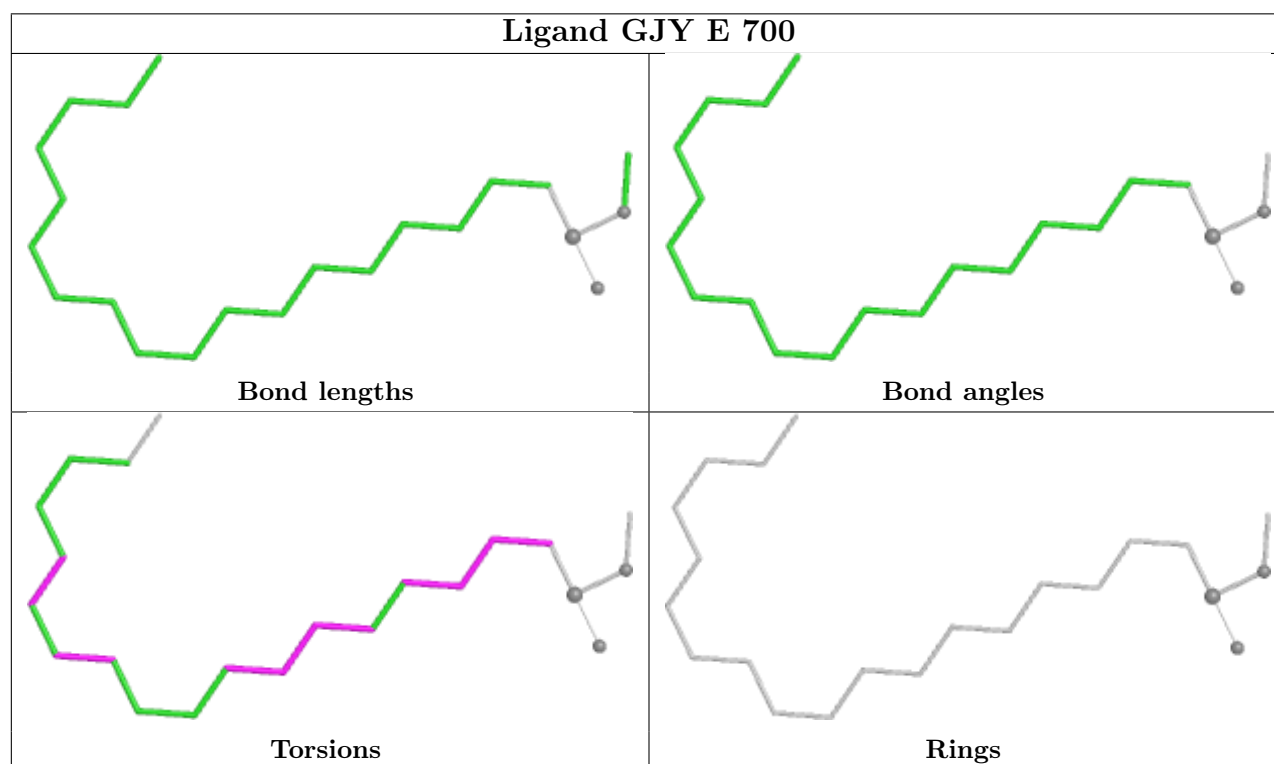
Mol	Chain	Res	Type	Atoms
2	F	700	GJY	C6-C7-C8-C9
2	K	700	GJY	C5-C6-C7-C8
2	D	700	GJY	C5-C6-C7-C8
2	K	700	GJY	C6-C7-C8-C9
2	E	700	GJY	C5-C6-C7-C8
2	J	700	GJY	C5-C6-C7-C8
2	L	700	GJY	C2-C3-C4-C5
2	A	700	GJY	P1-C1-C2-C3
2	B	700	GJY	P1-C1-C2-C3
2	C	700	GJY	P1-C1-C2-C3
2	D	700	GJY	P1-C1-C2-C3
2	E	700	GJY	P1-C1-C2-C3
2	F	700	GJY	P1-C1-C2-C3
2	G	700	GJY	P1-C1-C2-C3
2	H	700	GJY	P1-C1-C2-C3
2	I	700	GJY	P1-C1-C2-C3
2	J	700	GJY	P1-C1-C2-C3
2	L	700	GJY	P1-C1-C2-C3
2	G	700	GJY	C6-C7-C8-C9
2	I	700	GJY	C5-C6-C7-C8
2	A	700	GJY	C10-C11-C12-C13
2	A	700	GJY	C12-C13-C14-C15
2	B	700	GJY	C10-C11-C12-C13
2	B	700	GJY	C12-C13-C14-C15
2	C	700	GJY	C10-C11-C12-C13
2	E	700	GJY	C10-C11-C12-C13
2	I	700	GJY	C10-C11-C12-C13
2	I	700	GJY	C12-C13-C14-C15
2	K	700	GJY	C10-C11-C12-C13
2	K	700	GJY	C12-C13-C14-C15
2	J	700	GJY	C6-C7-C8-C9
2	C	700	GJY	C6-C7-C8-C9
2	I	700	GJY	C6-C7-C8-C9
2	H	700	GJY	C4-C5-C6-C7
2	L	700	GJY	C4-C5-C6-C7
2	H	700	GJY	C7-C8-C9-C10
2	K	700	GJY	P1-C1-C2-C3
2	E	700	GJY	C2-C3-C4-C5
2	A	700	GJY	C3-C4-C5-C6
2	I	700	GJY	C2-C3-C4-C5

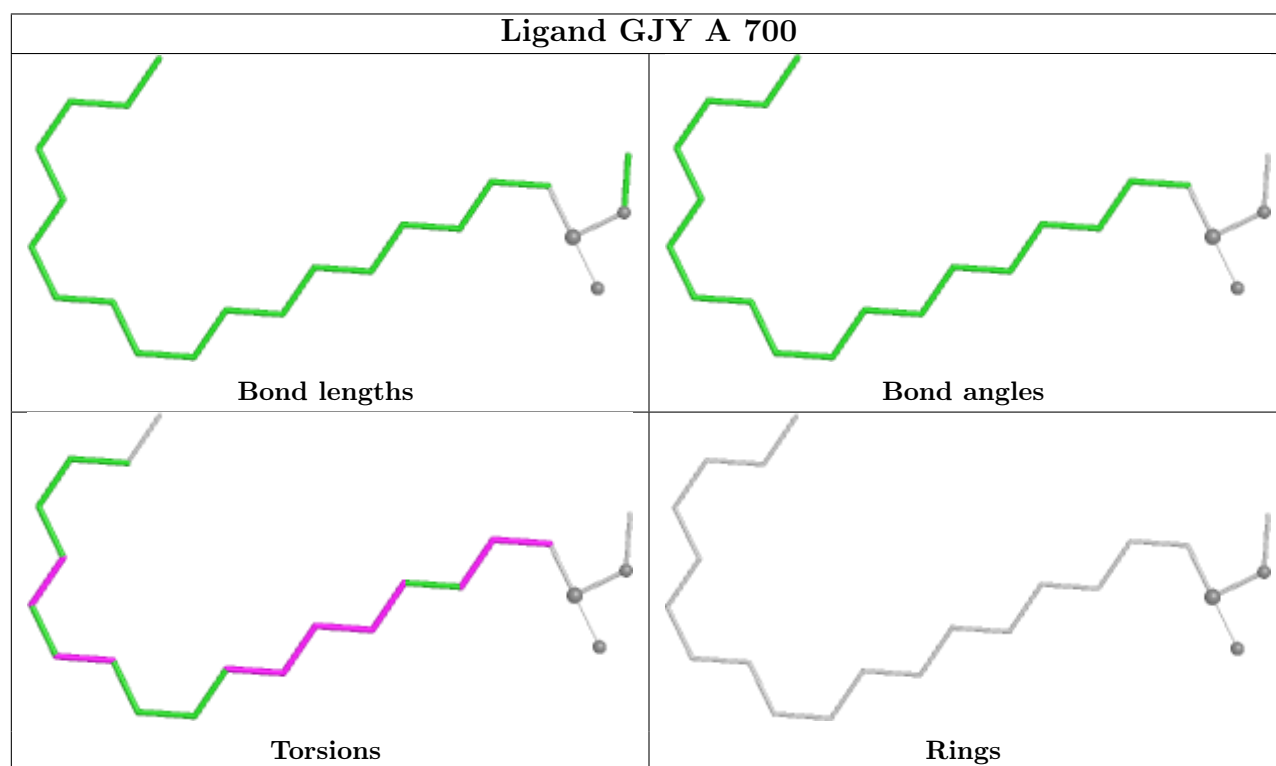
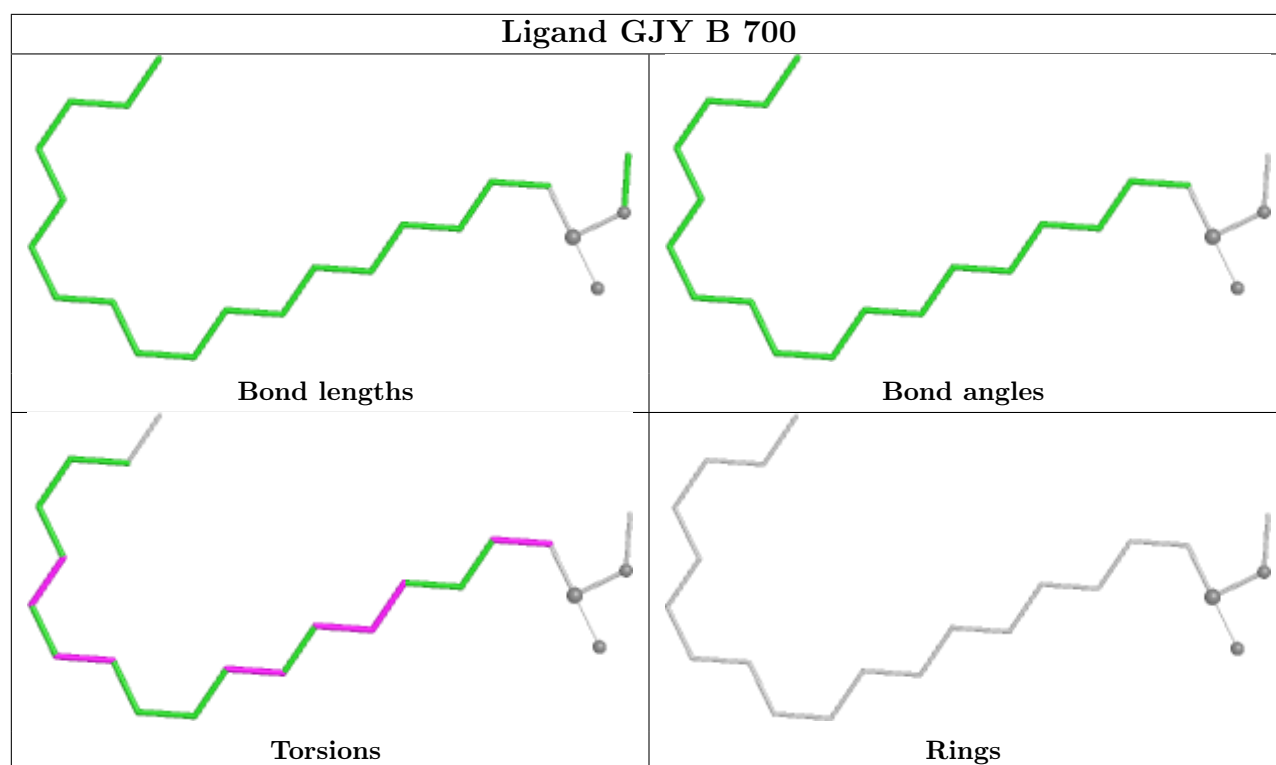
There are no ring outliers.

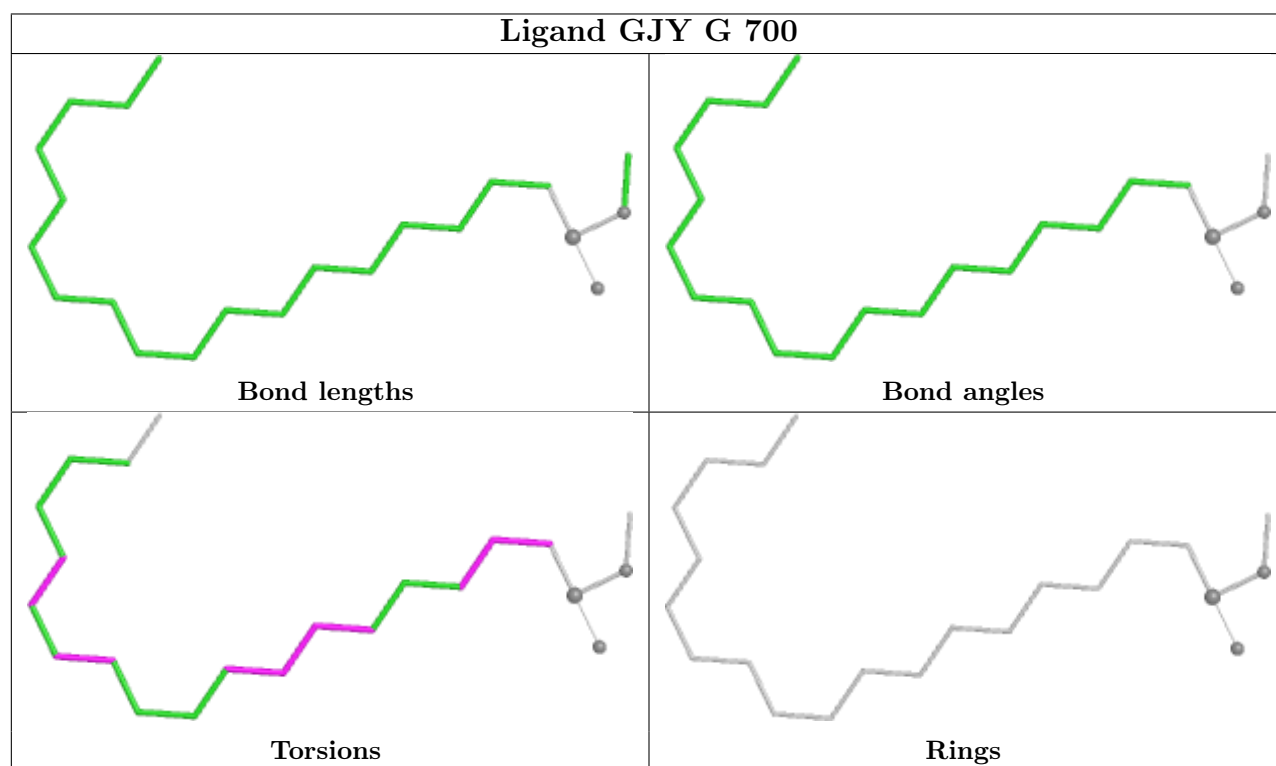
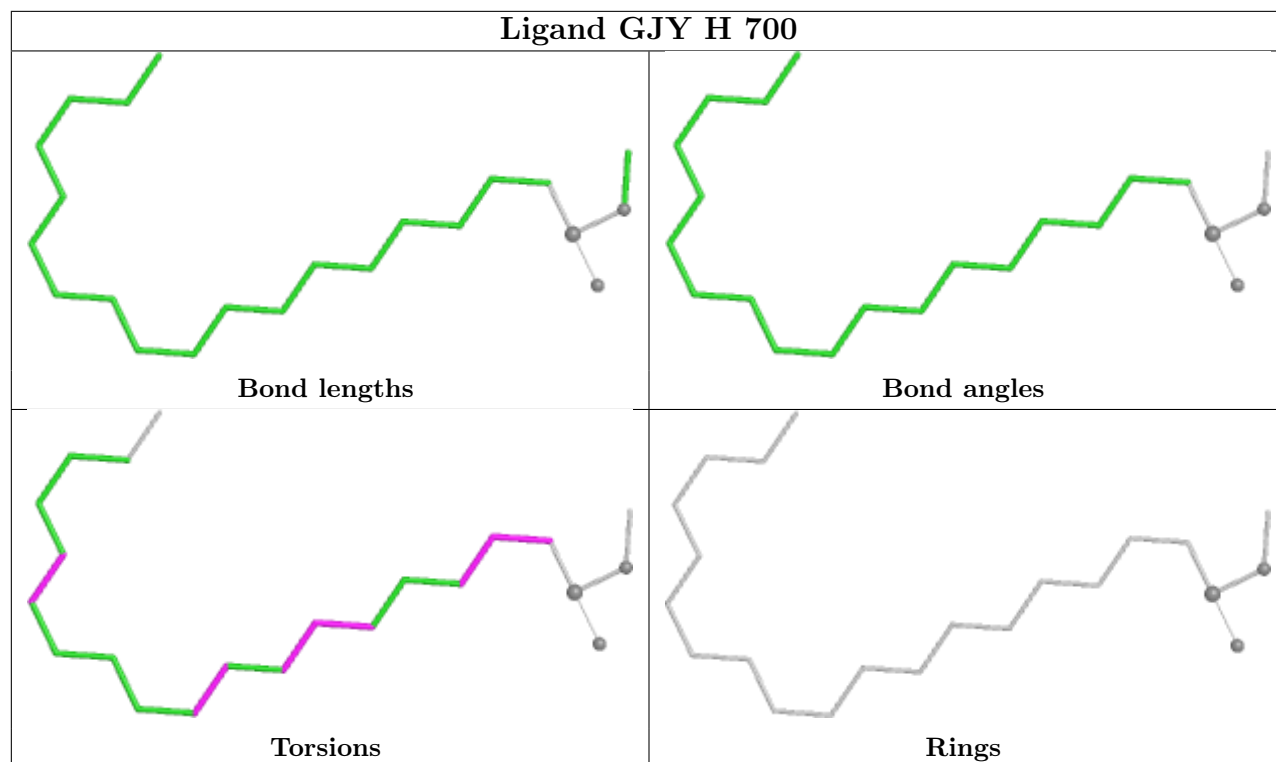
6 monomers are involved in 7 short contacts:

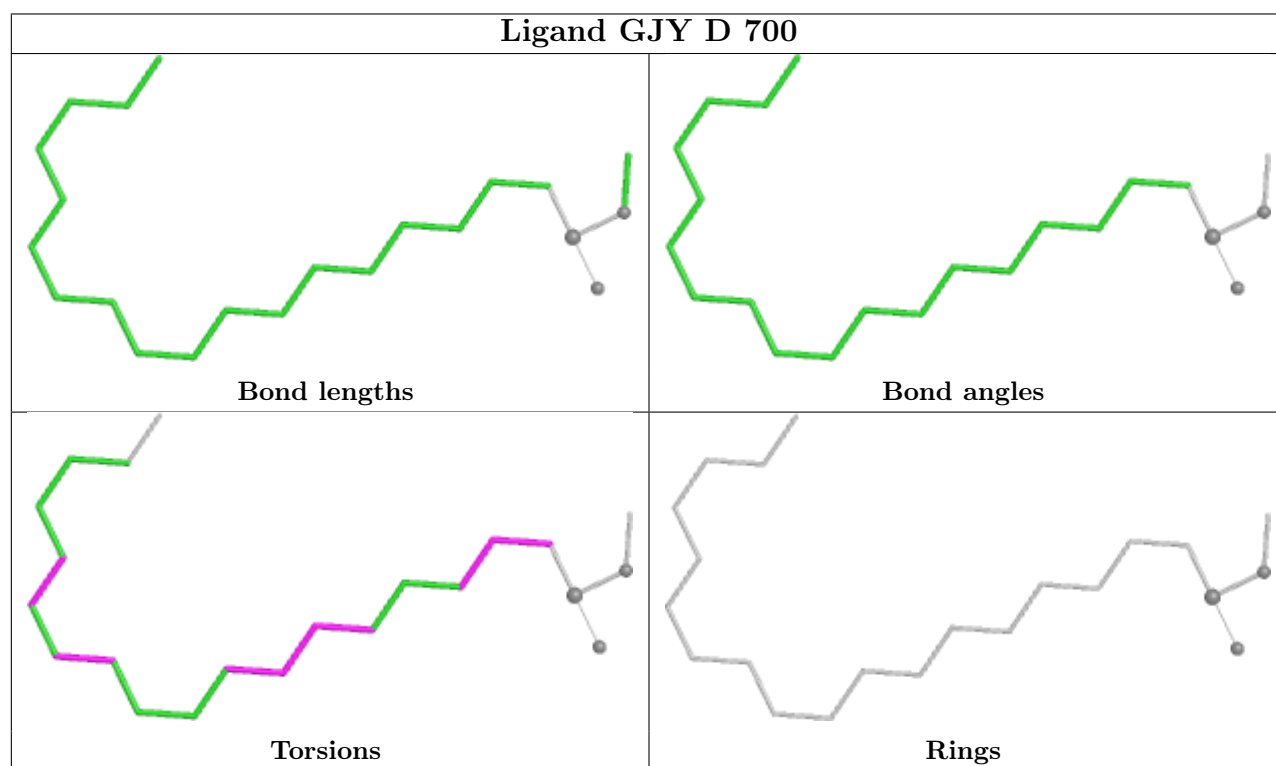
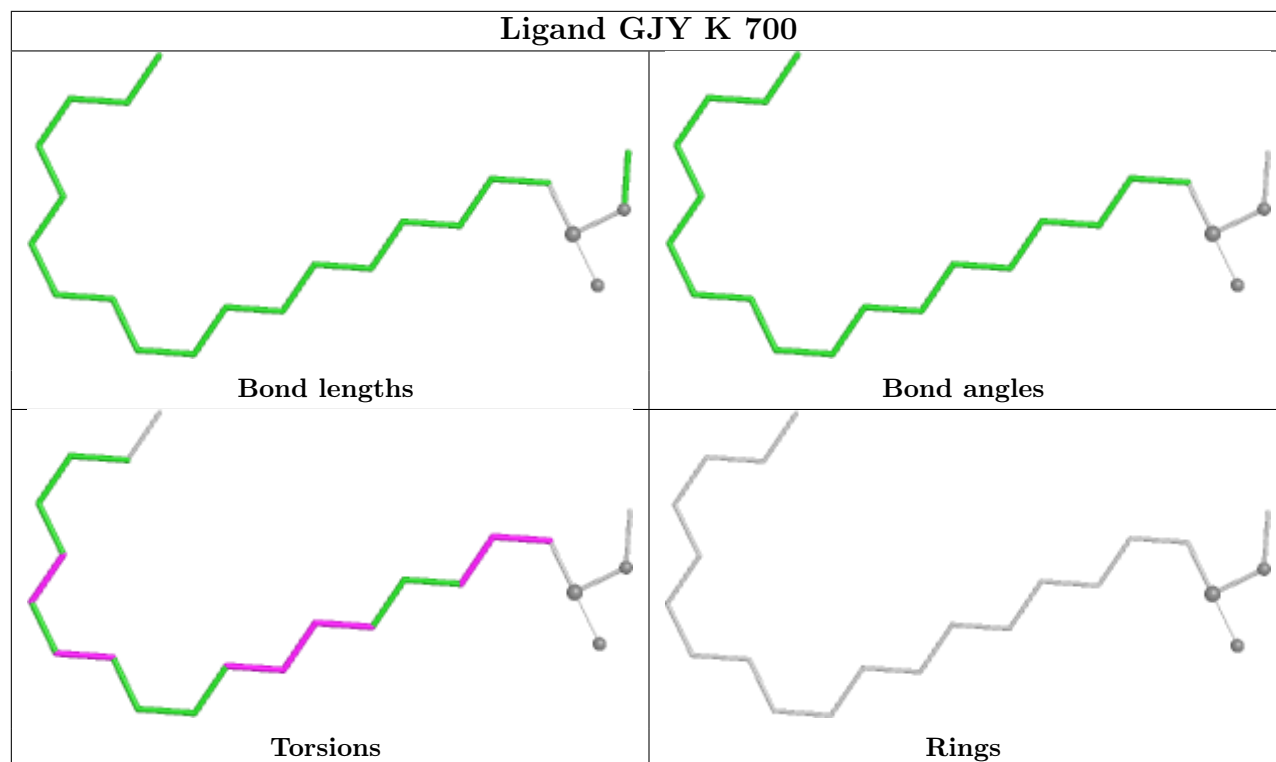
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	GJY	1	0
2	G	700	GJY	1	0
2	K	700	GJY	1	0
2	C	700	GJY	2	0
2	I	700	GJY	1	0
2	L	700	GJY	1	0

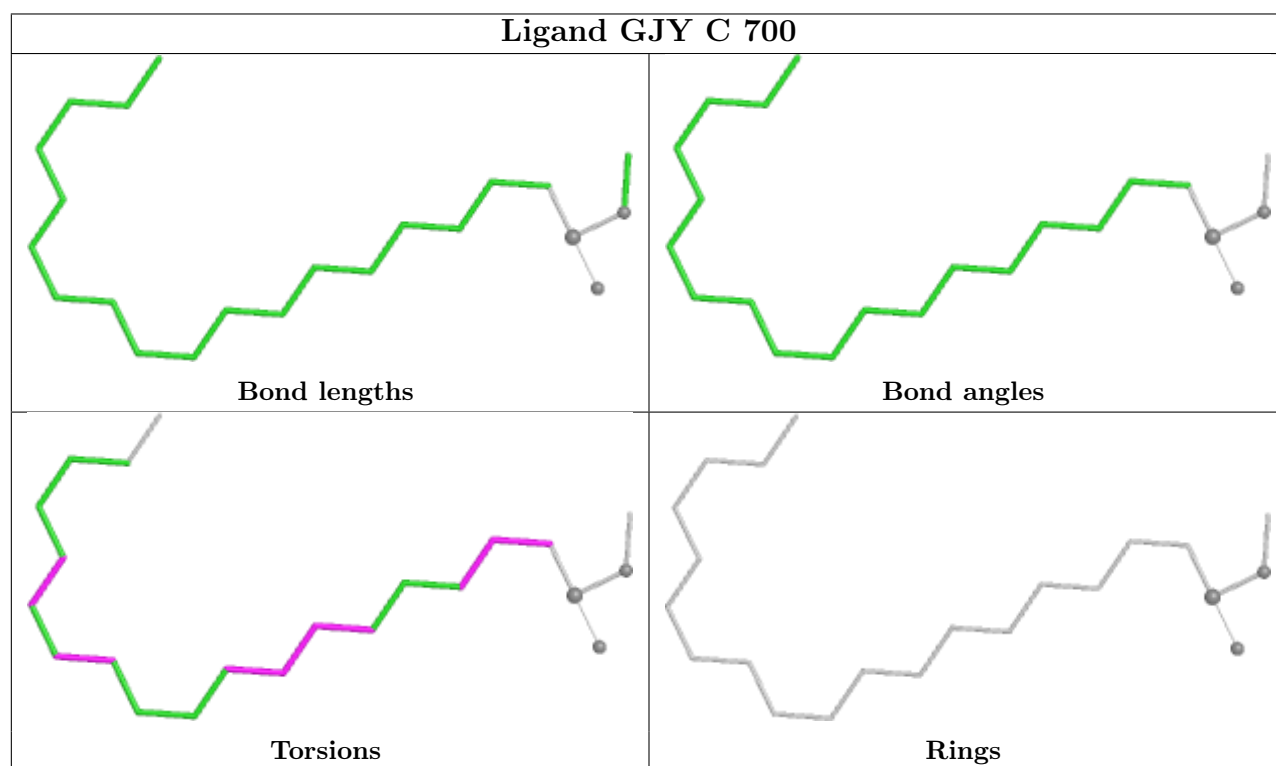
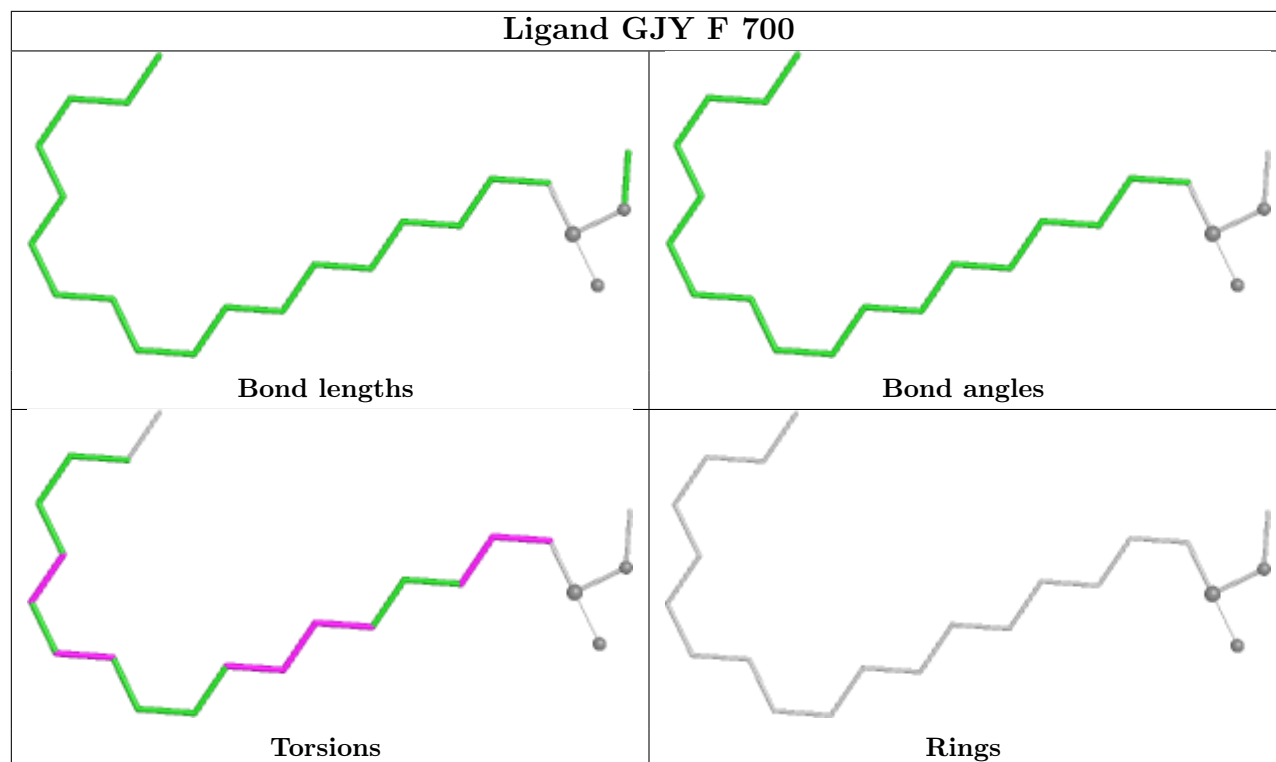
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

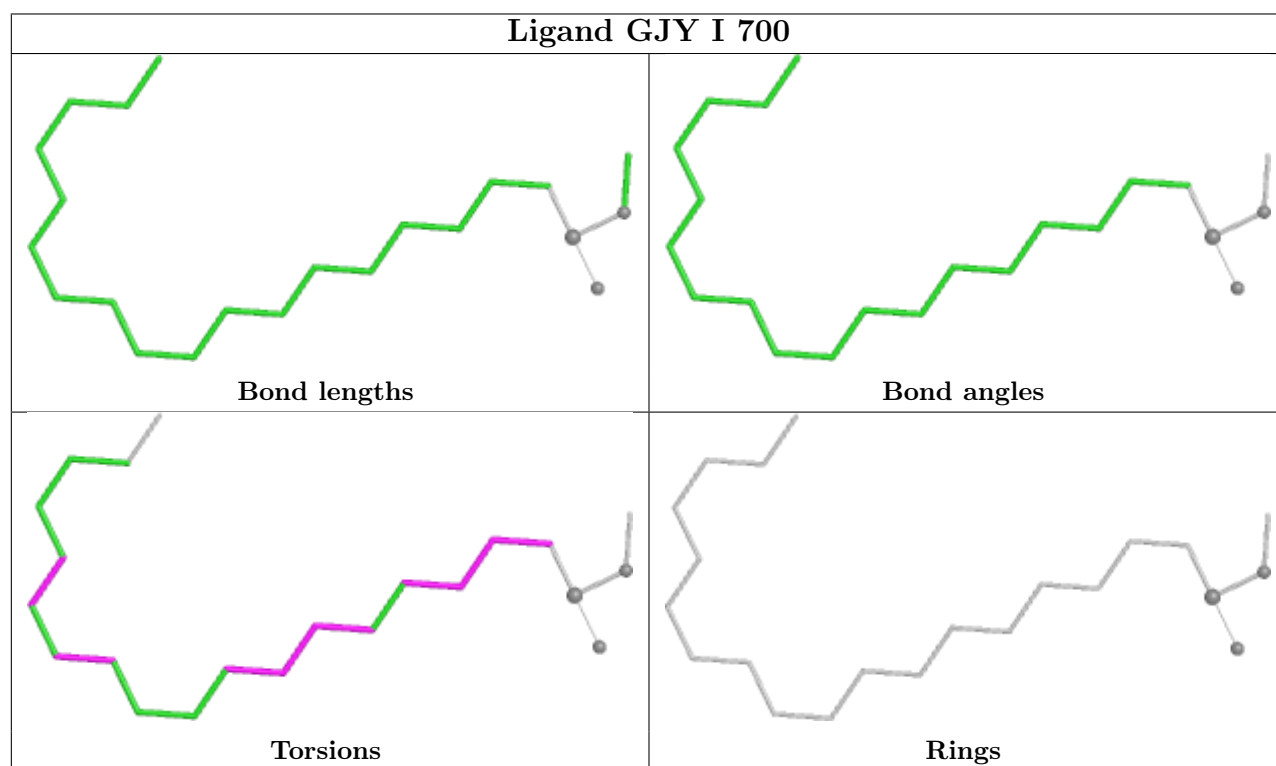
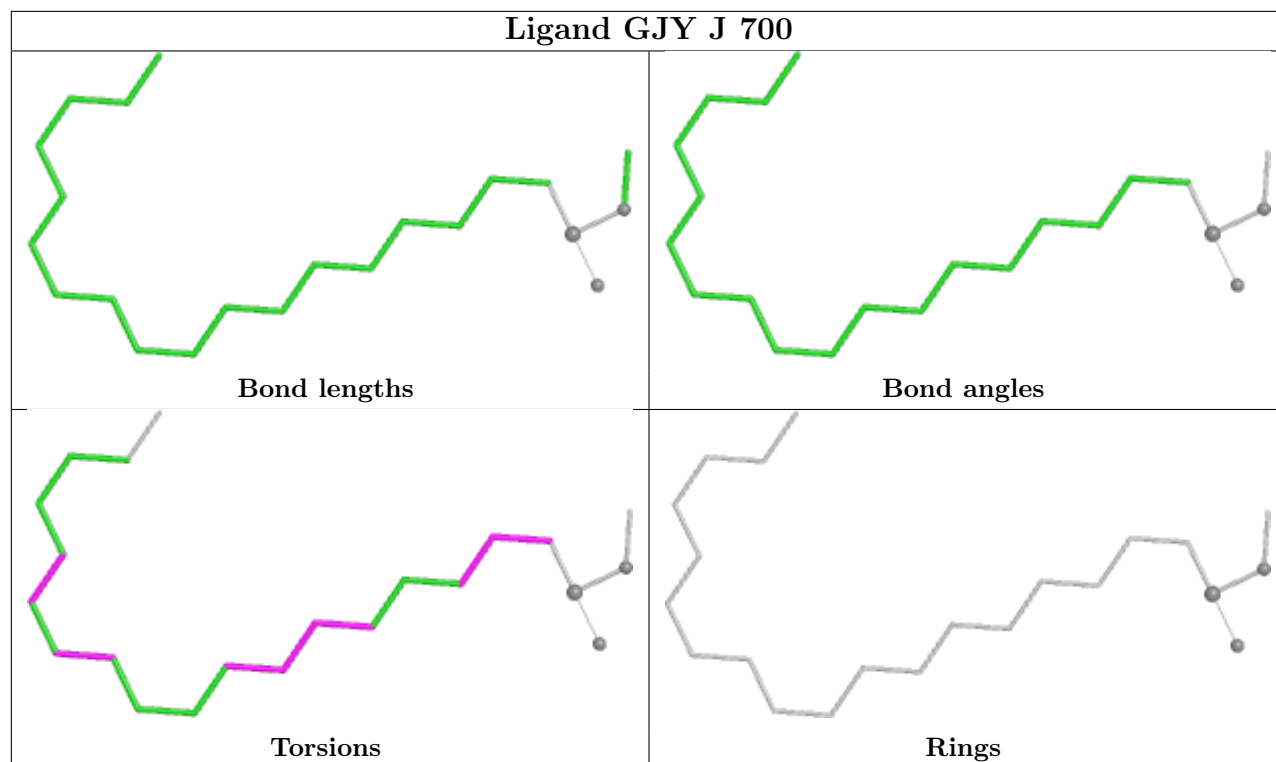


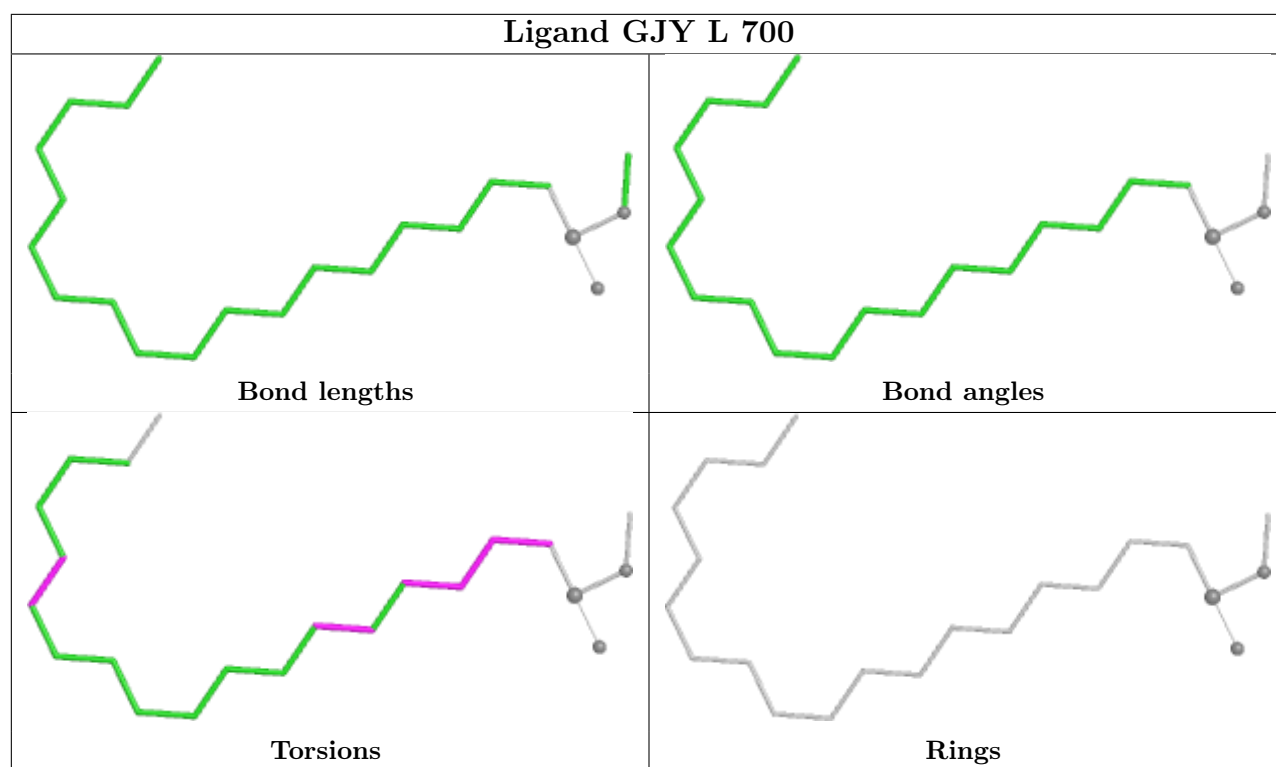












5.7 Other polymers [i](#)

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%)	0.44	21 (3%)	47	29	32, 70, 127, 291	0
1	B	605/636 (95%)	0.46	20 (3%)	49	30	32, 73, 142, 299	0
1	C	602/636 (94%)	0.50	19 (3%)	50	31	34, 69, 132, 292	0
1	D	605/636 (95%)	0.63	34 (5%)	30	19	36, 76, 141, 325	0
1	E	602/636 (94%)	0.67	28 (4%)	36	23	29, 74, 137, 286	0
1	F	605/636 (95%)	0.68	39 (6%)	25	16	31, 69, 136, 290	0
1	G	602/636 (94%)	0.52	26 (4%)	40	24	30, 66, 125, 293	0
1	H	616/636 (96%)	0.52	26 (4%)	40	25	32, 68, 143, 279	0
1	I	602/636 (94%)	0.44	23 (3%)	44	27	30, 61, 123, 272	0
1	J	616/636 (96%)	0.54	33 (5%)	31	20	31, 62, 137, 255	0
1	K	602/636 (94%)	0.52	27 (4%)	38	24	24, 63, 125, 269	0
1	L	616/636 (96%)	0.51	29 (4%)	36	23	25, 64, 133, 284	0
All	All	7275/7632 (95%)	0.53	325 (4%)	38	24	24, 68, 136, 325	0

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	22	ALA	8.3
1	K	22	ALA	7.5
1	D	2	GLY	5.8
1	G	22	ALA	5.7
1	B	384	SER	5.2
1	A	22	ALA	4.7
1	B	1	MET	4.7
1	K	411	CYS	4.4
1	E	103	GLU	4.4
1	F	4	TYR	4.1
1	I	23	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	30	LEU	4.0
1	H	3	LYS	4.0
1	G	103	GLU	3.9
1	E	340	ILE	3.9
1	J	607	ASN	3.9
1	F	9	ARG	3.8
1	F	27	ALA	3.8
1	D	384	SER	3.8
1	A	261	ASN	3.8
1	H	404	SER	3.7
1	I	228	VAL	3.7
1	A	7	MET	3.6
1	K	228	VAL	3.4
1	K	117	SER	3.4
1	G	35	PHE	3.4
1	D	523	ASP	3.4
1	A	103	GLU	3.3
1	E	530	THR	3.3
1	H	607	ASN	3.3
1	B	157	GLU	3.3
1	H	118	LEU	3.3
1	A	379	LEU	3.2
1	G	411	CYS	3.2
1	A	12	GLU	3.2
1	B	100	ASP	3.2
1	J	404	SER	3.2
1	E	261	ASN	3.2
1	D	1	MET	3.1
1	B	537	ASP	3.1
1	E	88	ASP	3.1
1	K	489	CYS	3.1
1	E	228	VAL	3.1
1	G	6	VAL	3.1
1	A	385	ASN	3.1
1	D	214	PRO	3.1
1	K	386	ALA	3.1
1	F	383	GLY	3.1
1	G	384	SER	3.1
1	K	11	SER	3.1
1	J	126	PHE	3.1
1	F	591	ALA	3.1
1	H	1	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	523	ASP	3.0
1	J	22	ALA	3.0
1	L	457	CYS	3.0
1	F	457	CYS	3.0
1	K	513	THR	3.0
1	F	10	ALA	2.9
1	H	10	ALA	2.9
1	A	384	SER	2.9
1	L	384	SER	2.9
1	J	120	ALA	2.9
1	L	184	SER	2.9
1	B	374	CYS	2.9
1	C	22	ALA	2.9
1	E	411	CYS	2.9
1	J	44	ALA	2.9
1	B	2	GLY	2.9
1	A	30	LEU	2.9
1	G	117	SER	2.9
1	D	338	GLU	2.9
1	K	530	THR	2.8
1	G	228	VAL	2.8
1	J	2	GLY	2.8
1	E	380	SER	2.8
1	J	384	SER	2.8
1	E	513	THR	2.8
1	L	607	ASN	2.8
1	G	88	ASP	2.8
1	C	143	THR	2.8
1	F	338	GLU	2.8
1	I	182	GLU	2.8
1	D	126	PHE	2.8
1	I	468	ASP	2.7
1	L	604	LEU	2.7
1	B	227	SER	2.7
1	F	337	VAL	2.7
1	A	530	THR	2.7
1	L	116	ARG	2.7
1	F	67	ASN	2.7
1	A	228	VAL	2.7
1	D	27	ALA	2.7
1	D	459	ALA	2.7
1	H	228	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	119	HIS	2.7
1	G	374	CYS	2.7
1	H	383	GLY	2.7
1	E	68	THR	2.7
1	F	314	GLY	2.6
1	E	379	LEU	2.6
1	E	544	ALA	2.6
1	K	33	LEU	2.6
1	A	88	ASP	2.6
1	J	406	ASP	2.6
1	B	4	TYR	2.6
1	J	1	MET	2.6
1	L	94	GLU	2.6
1	H	4	TYR	2.6
1	D	537	ASP	2.6
1	G	385	ASN	2.6
1	K	182	GLU	2.6
1	F	234	VAL	2.6
1	G	509	VAL	2.6
1	L	120	ALA	2.6
1	D	527	ASN	2.6
1	B	27	ALA	2.6
1	J	294	CYS	2.5
1	J	310	SER	2.5
1	F	599	ILE	2.5
1	A	126	PHE	2.5
1	L	227	SER	2.5
1	L	9	ARG	2.5
1	E	206	ASP	2.5
1	G	261	ASN	2.5
1	F	263	SER	2.5
1	I	58	ASP	2.5
1	B	118	LEU	2.5
1	J	4	TYR	2.5
1	F	341	GLY	2.5
1	F	228	VAL	2.5
1	H	380	SER	2.5
1	F	24	THR	2.5
1	H	57	LYS	2.5
1	F	118	LEU	2.5
1	K	119	HIS	2.5
1	G	363	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	11	SER	2.4
1	L	374	CYS	2.4
1	E	209	ASP	2.4
1	E	401	ASP	2.4
1	L	406	ASP	2.4
1	I	117	SER	2.4
1	H	535	THR	2.4
1	J	420	ASN	2.4
1	F	537	ASP	2.4
1	L	523	ASP	2.4
1	L	228	VAL	2.4
1	H	120	ALA	2.4
1	J	25	MET	2.4
1	K	157	GLU	2.4
1	H	405	SER	2.4
1	G	530	THR	2.4
1	G	594	THR	2.4
1	L	514	GLY	2.4
1	E	538	LEU	2.4
1	H	379	LEU	2.4
1	I	379	LEU	2.4
1	C	489	CYS	2.4
1	B	24	THR	2.4
1	F	511	PRO	2.4
1	I	10	ALA	2.4
1	D	530	THR	2.3
1	I	374	CYS	2.4
1	L	119	HIS	2.3
1	F	483	ASP	2.3
1	F	5	GLN	2.3
1	F	111	GLN	2.3
1	J	293	LEU	2.3
1	K	35	PHE	2.3
1	H	436	GLU	2.3
1	L	2	GLY	2.3
1	D	422	HIS	2.3
1	H	119	HIS	2.3
1	J	15	LEU	2.3
1	C	228	VAL	2.3
1	J	116	ARG	2.3
1	E	407	ILE	2.3
1	C	544	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	384	SER	2.3
1	I	4	TYR	2.3
1	B	126	PHE	2.3
1	F	72	GLU	2.3
1	D	215	THR	2.3
1	H	285	SER	2.3
1	C	30	LEU	2.3
1	J	118	LEU	2.3
1	B	424	CYS	2.3
1	G	605	ASN	2.3
1	L	385	ASN	2.3
1	L	605	ASN	2.3
1	L	537	ASP	2.3
1	D	228	VAL	2.3
1	E	23	GLU	2.3
1	F	6	VAL	2.3
1	K	224	GLU	2.3
1	F	2	GLY	2.3
1	H	227	SER	2.3
1	I	11	SER	2.3
1	J	227	SER	2.3
1	G	540	ARG	2.3
1	H	610	GLU	2.2
1	K	407	ILE	2.2
1	K	62	THR	2.2
1	D	405	SER	2.2
1	J	112	TYR	2.2
1	D	123	VAL	2.2
1	J	228	VAL	2.2
1	C	206	ASP	2.2
1	K	206	ASP	2.2
1	L	207	ASP	2.2
1	G	603	ILE	2.2
1	D	183	ALA	2.2
1	L	609	GLY	2.2
1	F	143	THR	2.2
1	H	278	THR	2.2
1	J	278	THR	2.2
1	C	452	SER	2.2
1	I	384	SER	2.2
1	J	380	SER	2.2
1	B	411	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	15	LEU	2.2
1	E	58	ASP	2.2
1	G	349	ASP	2.2
1	G	379	LEU	2.2
1	H	121	ASP	2.2
1	H	122	PRO	2.2
1	J	271	PRO	2.2
1	K	517	ALA	2.2
1	D	3	LYS	2.2
1	I	19	LYS	2.2
1	A	119	HIS	2.2
1	J	119	HIS	2.2
1	J	395	TYR	2.2
1	C	337	VAL	2.2
1	F	380	SER	2.2
1	F	404	SER	2.2
1	G	282	SER	2.2
1	L	23	GLU	2.2
1	F	279	GLY	2.2
1	F	522	PRO	2.2
1	G	522	PRO	2.2
1	I	120	ALA	2.2
1	I	489	CYS	2.2
1	I	21	LYS	2.2
1	D	9	ARG	2.2
1	D	6	VAL	2.2
1	D	136	TYR	2.2
1	L	112	TYR	2.2
1	A	117	SER	2.2
1	C	459	ALA	2.2
1	F	459	ALA	2.2
1	K	10	ALA	2.2
1	D	271	PRO	2.2
1	G	116	ARG	2.2
1	A	468	ASP	2.2
1	D	100	ASP	2.2
1	L	504	ASP	2.2
1	D	144	THR	2.1
1	A	4	TYR	2.1
1	C	4	TYR	2.1
1	D	263	SER	2.1
1	D	404	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	227	SER	2.1
1	F	452	SER	2.1
1	K	23	GLU	2.1
1	L	610	GLU	2.1
1	D	67	ASN	2.1
1	I	527	ASN	2.1
1	D	207	ASP	2.1
1	I	457	CYS	2.1
1	J	606	THR	2.1
1	K	215	THR	2.1
1	K	19	LYS	2.1
1	C	96	GLU	2.1
1	F	227	SER	2.1
1	K	263	SER	2.1
1	E	537	ASP	2.1
1	I	13	VAL	2.1
1	E	29	HIS	2.1
1	F	3	LYS	2.1
1	I	24	THR	2.1
1	C	120	ALA	2.1
1	J	311	ALA	2.1
1	C	12	GLU	2.1
1	B	452	SER	2.1
1	F	400	ASN	2.1
1	L	420	ASN	2.1
1	C	340	ILE	2.1
1	C	422	HIS	2.1
1	D	4	TYR	2.1
1	D	24	THR	2.1
1	E	120	ALA	2.1
1	G	27	ALA	2.1
1	K	544	ALA	2.1
1	C	348	GLU	2.1
1	J	522	PRO	2.1
1	B	120	ALA	2.1
1	J	72	GLU	2.1
1	L	458	GLU	2.1
1	A	123	VAL	2.0
1	H	520	ILE	2.0
1	B	7	MET	2.0
1	I	113	ASP	2.0
1	J	136	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	317	GLY	2.0
1	H	279	GLY	2.0
1	D	23	GLU	2.0
1	B	123	VAL	2.0
1	D	187	ARG	2.0
1	G	227	SER	2.0
1	J	605	ASN	2.0
1	K	261	ASN	2.0
1	A	31	THR	2.0
1	A	517	ALA	2.0
1	L	613	ALA	2.0
1	H	112	TYR	2.0
1	B	523	ASP	2.0
1	C	88	ASP	2.0
1	F	121	ASP	2.0
1	A	182	GLU	2.0
1	E	337	VAL	2.0
1	C	315	ILE	2.0
1	E	70	ILE	2.0
1	F	99	ILE	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	GJY	E	700	22/23	0.87	0.17	53,71,77,82	0
2	GJY	H	700	22/23	0.88	0.13	52,57,63,83	0
2	GJY	I	700	22/23	0.88	0.17	52,71,77,81	0

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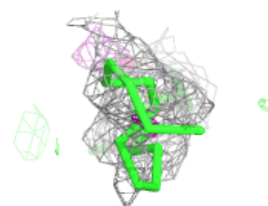
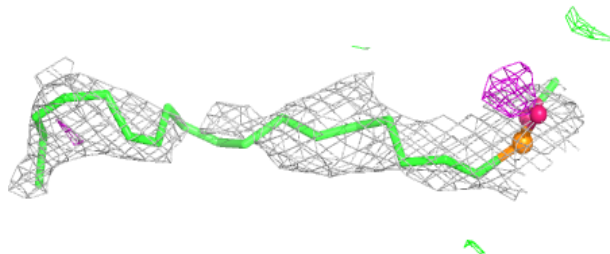
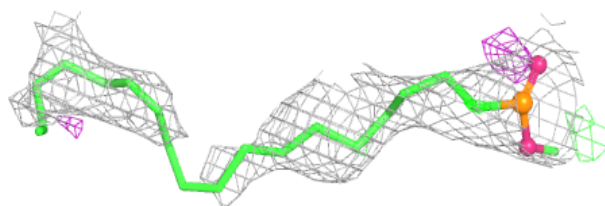
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GJY	K	700	22/23	0.88	0.17	46,65,70,75	0
2	GJY	D	700	22/23	0.89	0.16	56,75,81,85	0
2	GJY	C	700	22/23	0.89	0.15	50,68,74,79	0
2	GJY	G	700	22/23	0.89	0.16	52,70,76,81	0
2	GJY	J	700	22/23	0.90	0.14	37,56,62,66	0
2	GJY	F	700	22/23	0.90	0.14	53,71,77,82	0
2	GJY	B	700	22/23	0.91	0.13	55,73,78,82	0
2	GJY	L	700	22/23	0.92	0.12	54,73,79,83	0
2	GJY	A	700	22/23	0.93	0.12	54,73,79,83	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.

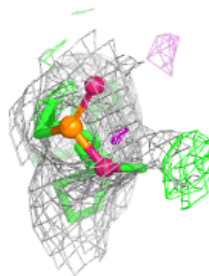
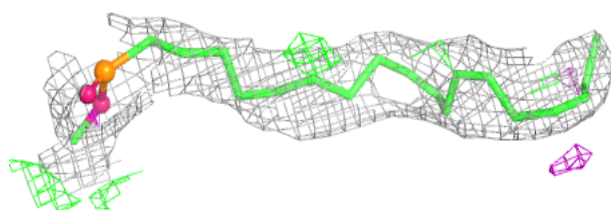
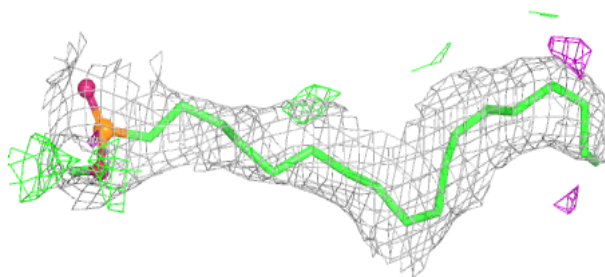
Electron density around GJY E 700:

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

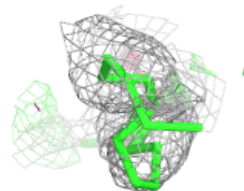
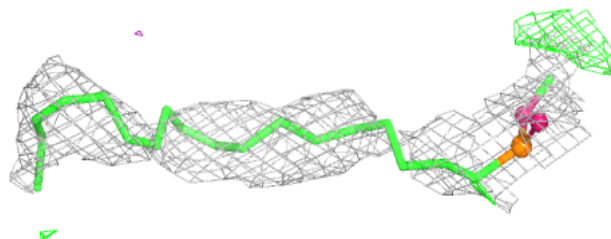
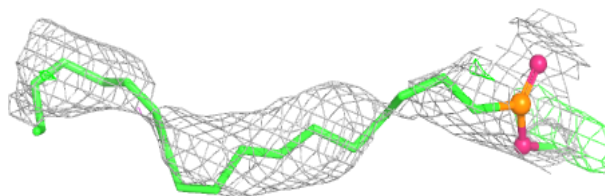


Electron density around GJY H 700:

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and green (positive)

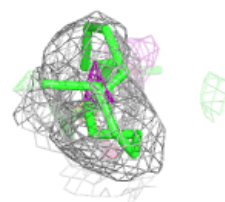
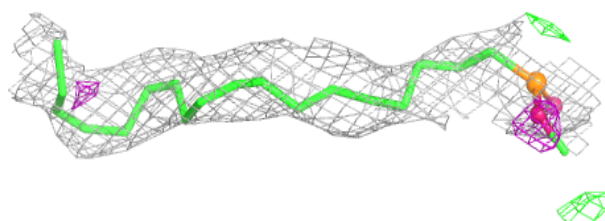
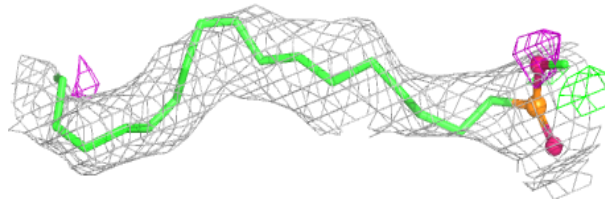
**Electron density around GJY I 700:**

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and green (positive)

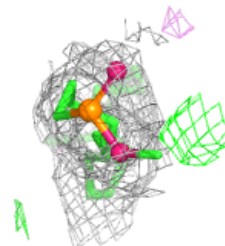
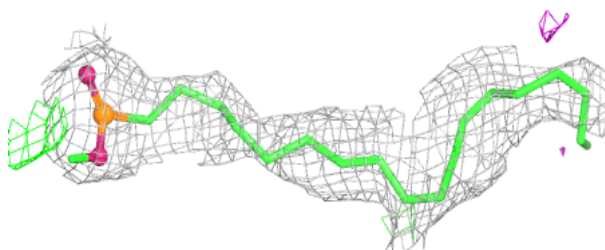


Electron density around GJY K 700:

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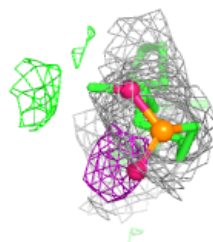
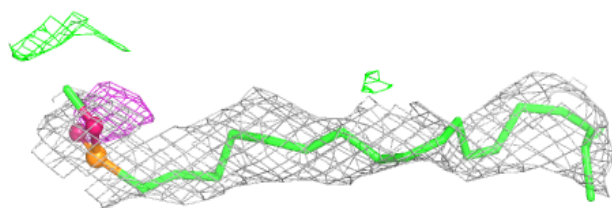
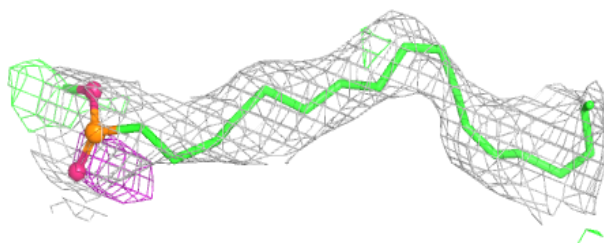
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

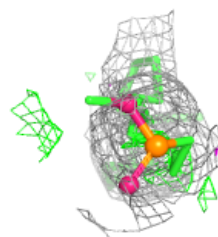
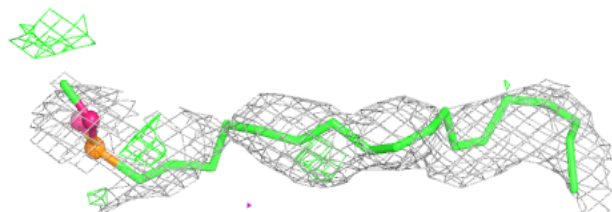
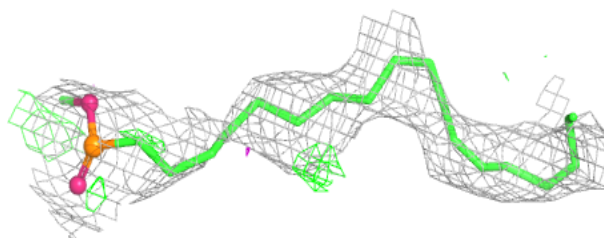


Electron density around GJY C 700:

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and green (positive)

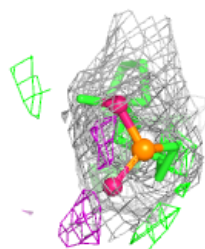
**Electron density around GJY G 700:**

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and green (positive)

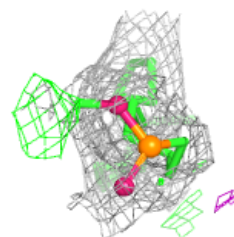
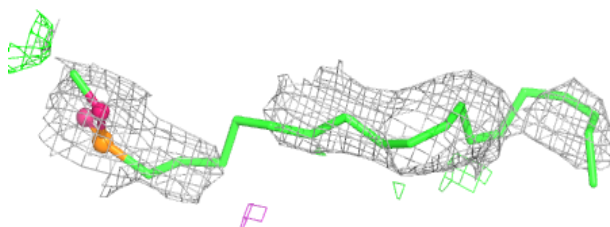
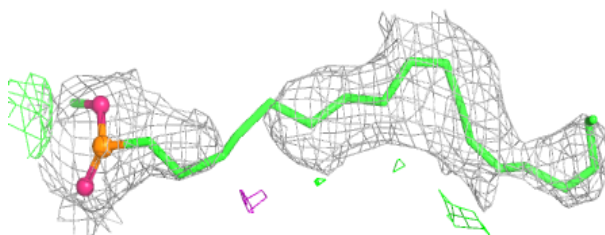


Electron density around GJY J 700:

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and green (positive)

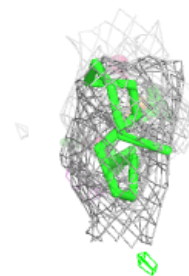
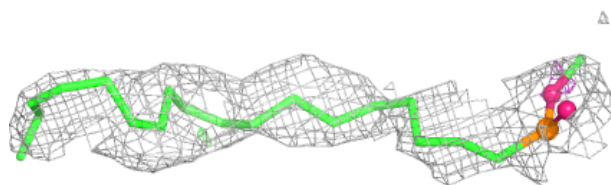
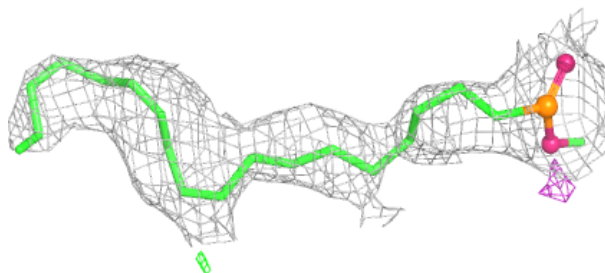
**Electron density around GJY F 700:**

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and green (positive)

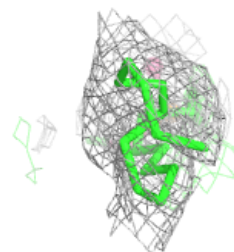
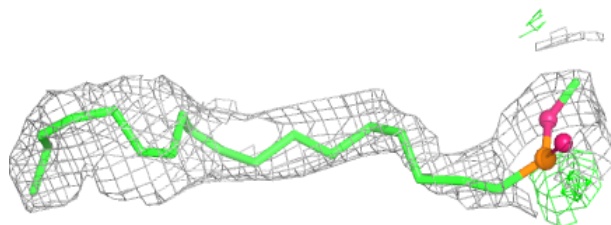
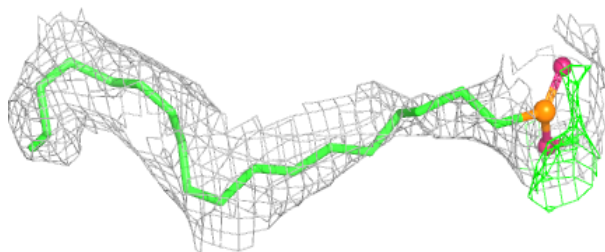


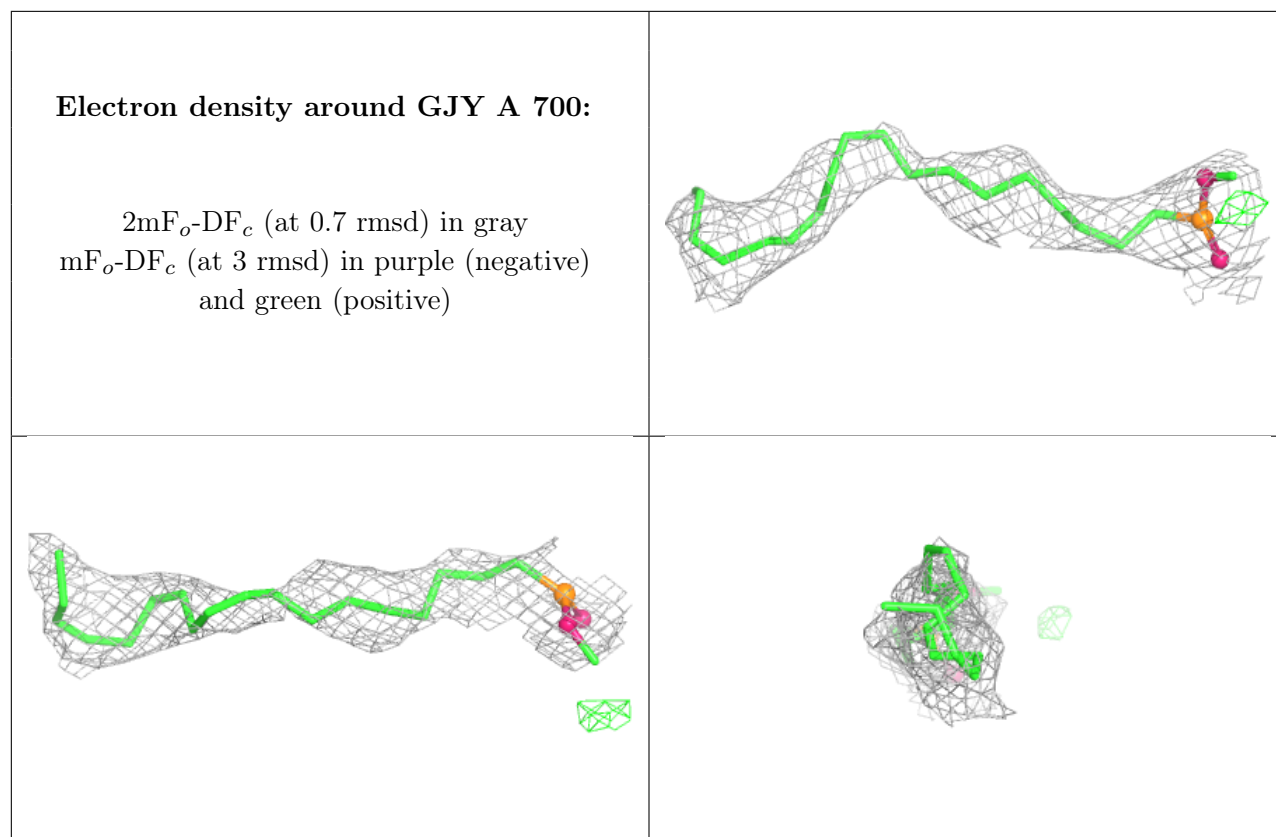
Electron density around GJY B 700:

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and green (positive)

**Electron density around GJY L 700:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.