



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:38 pm BST

PDB ID : 6DII
Title : Structure of Arabidopsis Fatty Acid Amide Hydrolase in Complex with methyl
linolenyl fluorophosphate
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

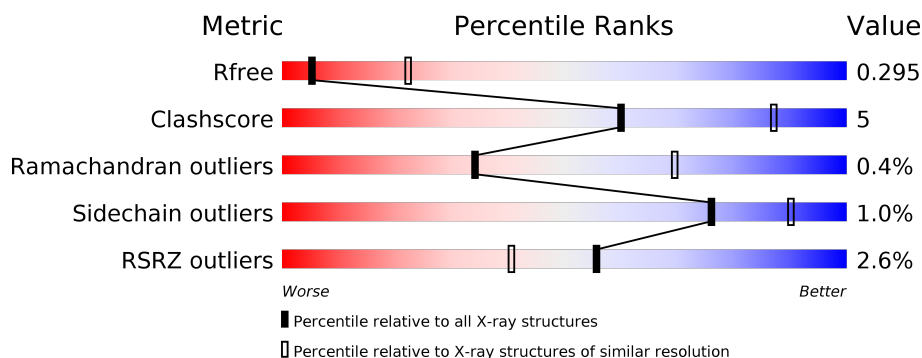
1 Overall quality at a glance

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

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Mol	Chain	Length	Quality of chain
1	G	636	<div><div><div></div><div></div><div></div></div><div>3%85%10%5%</div></div>
1	H	636	<div><div><div></div><div></div><div></div></div><div>2%84%12%•</div></div>
1	I	636	<div><div><div></div><div></div><div></div></div><div>2%82%13%5%</div></div>
1	J	636	<div><div><div></div><div></div><div></div></div><div>3%83%13%•</div></div>
1	K	636	<div><div><div></div><div></div><div></div></div><div>2%84%11%5%</div></div>
1	L	636	<div><div><div></div><div></div><div></div></div><div>2%86%11%•</div></div>

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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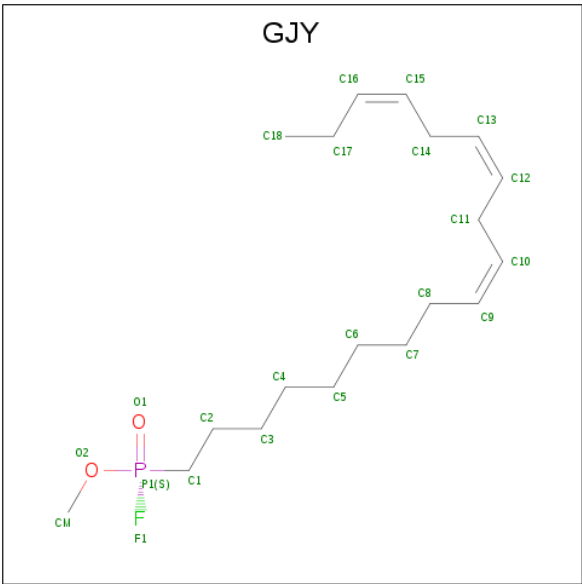
Chain	Residue	Modelled	Actual	Comment	Reference
K	617	GLN	-	expression tag	UNP Q7XJJ7
K	618	LYS	-	expression tag	UNP Q7XJJ7
K	619	LEU	-	expression tag	UNP Q7XJJ7
K	620	ILE	-	expression tag	UNP Q7XJJ7
K	621	SER	-	expression tag	UNP Q7XJJ7
K	622	GLU	-	expression tag	UNP Q7XJJ7
K	623	GLU	-	expression tag	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 (three-letter code: 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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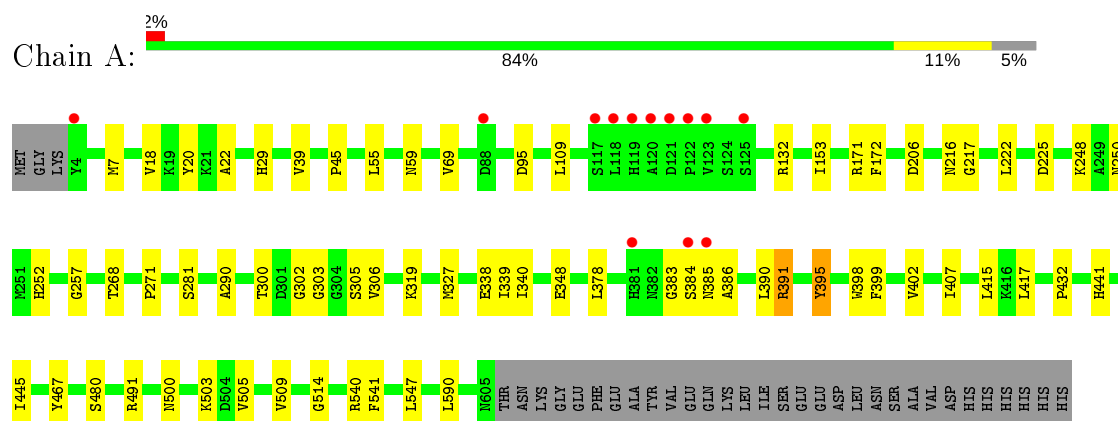
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	O	P	0	0
			22	19	2	1		
2	I	1	Total	C	O	P	0	0
			22	19	2	1		
2	J	1	Total	C	O	P	0	0
			22	19	2	1		
2	K	1	Total	C	O	P	0	0
			22	19	2	1		
2	L	1	Total	C	O	P	0	0
			22	19	2	1		

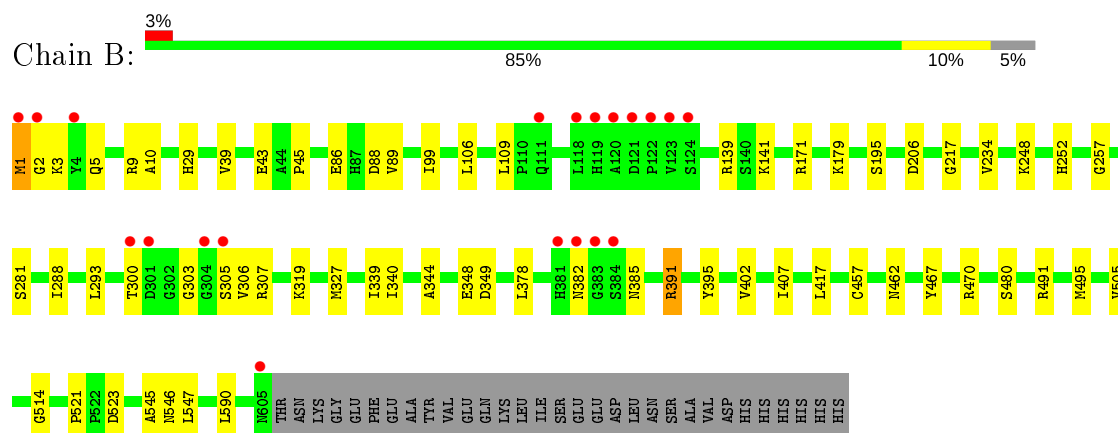
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

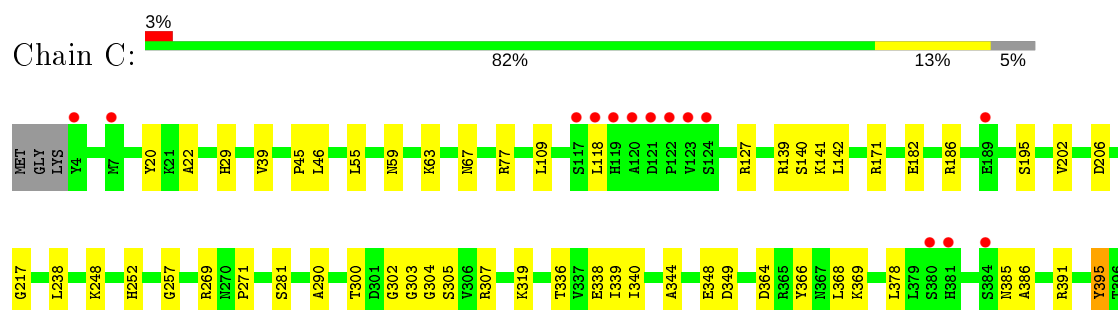
• Molecule 1: Fatty acid amide hydrolase

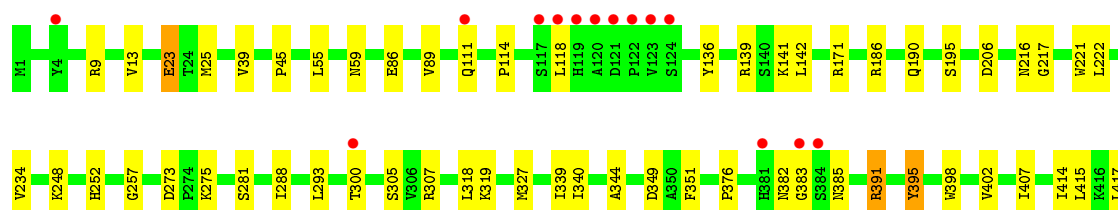
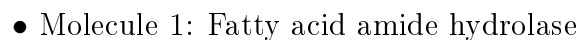
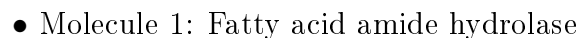
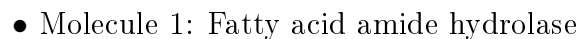


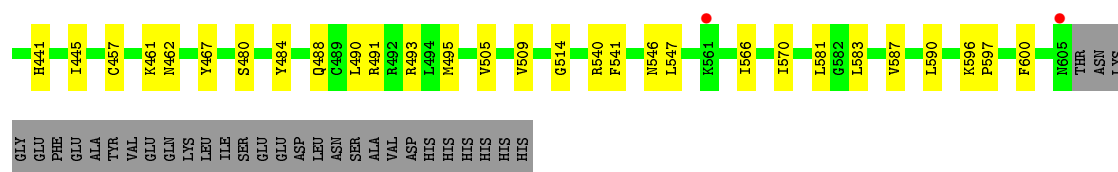
• Molecule 1: Fatty acid amide hydrolase



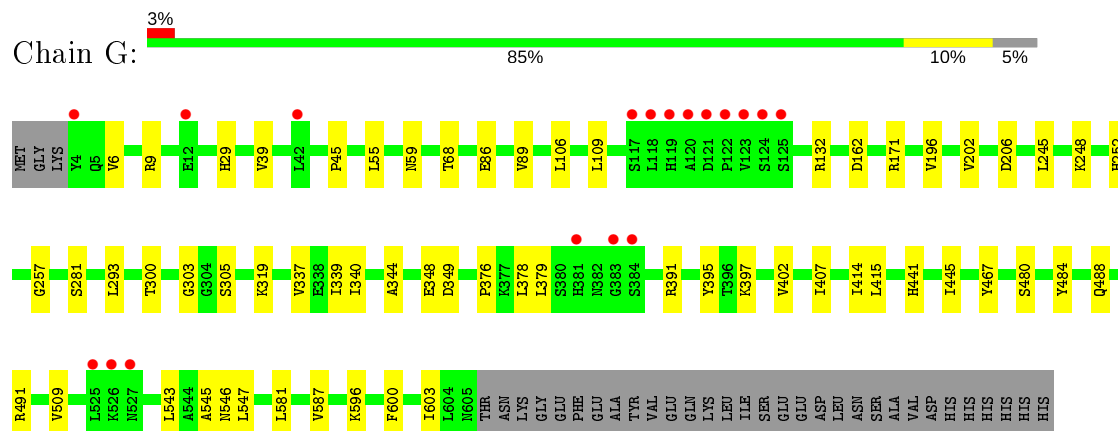
• Molecule 1: Fatty acid amide hydrolase



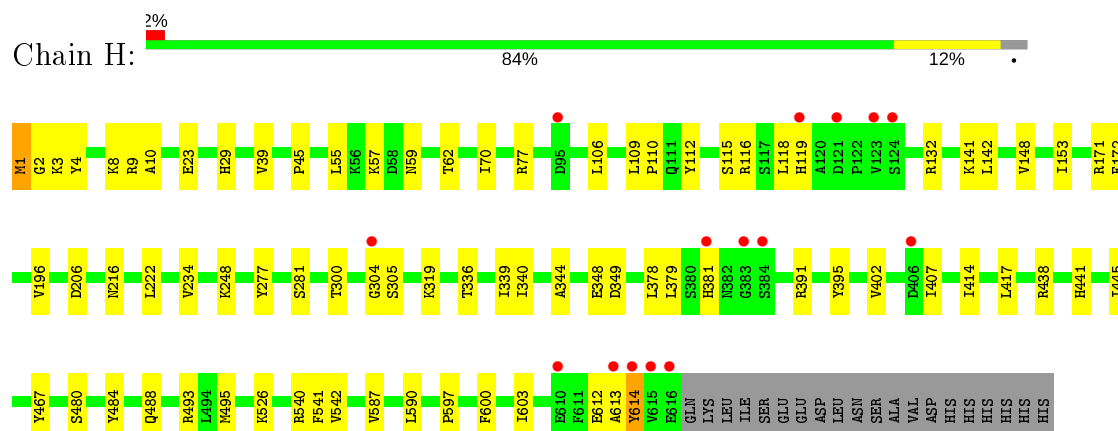




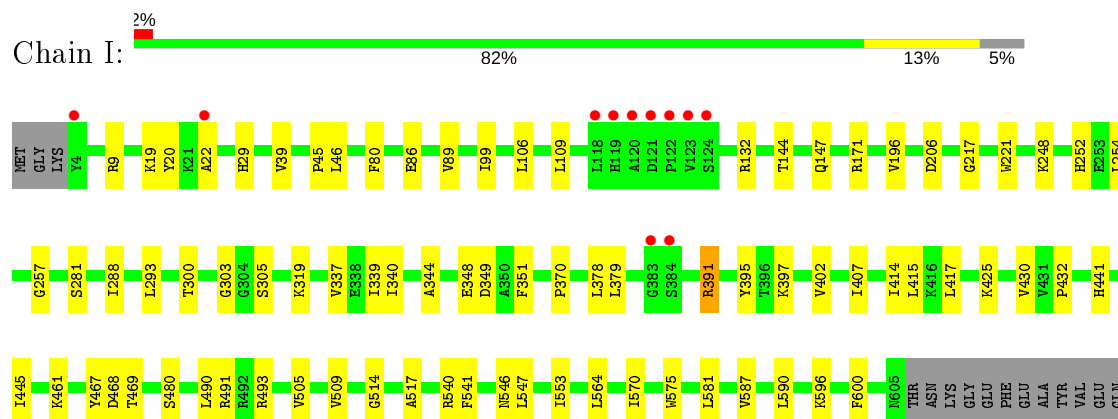
• Molecule 1: Fatty acid amide hydrolase



• Molecule 1: Fatty acid amide hydrolase



• Molecule 1: Fatty acid amide hydrolase



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 – 3.18	Depositor EDS
% Data completeness (in resolution range)	81.4 (34.61-3.20) 81.4 (34.61-3.18)	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 0.252 , 0.295	Depositor DCC
R_{free} test set	6719 reflections (5.14%)	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)	0.28 , 68.2	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/4705	0.41	0/6392
1	B	0.25	0/4726	0.41	0/6418
1	C	0.25	0/4705	0.41	0/6392
1	D	0.25	0/4726	0.42	0/6418
1	E	0.25	0/4705	0.42	0/6392
1	F	0.25	0/4726	0.42	0/6418
1	G	0.25	0/4705	0.41	0/6392
1	H	0.26	0/4818	0.42	0/6542
1	I	0.25	0/4705	0.41	0/6392
1	J	0.25	0/4818	0.42	0/6542
1	K	0.25	0/4705	0.41	0/6392
1	L	0.25	0/4818	0.41	0/6542
All	All	0.25	0/56862	0.42	0/77232

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4627	0	4654	37	0
1	C	4606	0	4626	46	0
1	D	4627	0	4654	49	0
1	E	4606	0	4626	46	0
1	F	4627	0	4654	51	0
1	G	4606	0	4626	36	0
1	H	4717	0	4733	42	0
1	I	4606	0	4626	52	0
1	J	4717	0	4733	52	0
1	K	4606	0	4626	39	0
1	L	4717	0	4733	38	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	510	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 (510) 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: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:E:381:HIS:O	1:E:382:ASN:C	2.15	0.80
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: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:J:1:MET:SD	1:J:2:GLY:N	2.69	0.66
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:N	1:J:111:GLN:OE1	2.32	0.62
1:G:206:ASP:HA	1:G:248:LYS:HE2	1.80	0.61
1:H:2:GLY:C	1:H:3:LYS:HD2	2.20	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: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: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:C:206:ASP:HA	1:C:248:LYS:HE2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:206:ASP:HA	1:D:248:LYS:HE2	1.87	0.56
1:C:480:SER:HA	1:D:480:SER:HA	1.86	0.56
1:F:402:VAL:HB	1:F:407:ILE:HD11	1.88	0.56
1:D:417:LEU:HB3	1:D:590:LEU:HD13	1.87	0.56
1:D:23:GLU:HB3	1:D:540:ARG:HH12	1.70	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: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: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
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:1:MET:H1	1:I:132:ARG:HH11	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:139:ARG:NH2	1:D:195:SER:O	2.41	0.52
1:D:1:MET:O	1:D:3:LYS:N	2.42	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:J:126:PHE:HD1	1:J:127:ARG:N	2.06	0.52
1:K:300:THR:HG22	1:K:340:ILE:HD13	1.92	0.52
1:K:9:ARG:O	1:K:493:ARG:NH2	2.37	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:206:ASP:OD2	1:E:217:GLY:N	2.43	0.52
1:E:109:LEU:HD23	1:E:378:LEU:HD12	1.91	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
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:132:ARG:NH2	1:I:348:GLU:OE2	2.41	0.51
1:I:9:ARG:O	1:I:493:ARG:NH2	2.31	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:381:HIS:C	1:E:382:ASN:O	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:480:SER:HA	1:L:480:SER:HA	1.94	0.50
1:K:8:LYS:HD3	1:K:70:ILE:HG12	1.93	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:540:ARG:HG3	1:F:541:PHE:CD2	2.48	0.49
1:F:385:ASN:HB2	1:I:19:LYS:HE2	1.95	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:252:HIS:CE1	1:C:257:GLY:HA3	2.48	0.49
1:C:55:LEU:O	1:C:59:ASN:ND2	2.38	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:302:GLY:HA3	1:D:338:GLU:HG3	1.94	0.49
1:D:129:TRP:CD2	1:D:604:LEU:HD12	2.48	0.49
1:F:86:GLU:HG3	1:F:89:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:281:SER:H	1:E:305:SER:HB3	1.79	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:I:144:THR:HG1	1:I:147:GLN:HE21	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:LYS:HE2	1:C:600:PHE:HB3	1.96	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:E:124:SER:HB3	1:E:127:ARG:HH12	1.79	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: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:D:540:ARG:HG3	1:D:541:PHE:CD2	2.50	0.47
1:G:491:ARG:HG3	1:G:547:LEU:HG	1.97	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: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: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
1:H:109:LEU:HD22	1:H:348:GLU:HG3	1.97	0.46
1:J:234:VAL:HG11	1:J:340:ILE:HG21	1.97	0.46
1:J:109:LEU:HD22	1:J:348:GLU:HG3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:171:ARG:HB2	1:C:248:LYS:HB2	1.97	0.45
1:C:39:VAL:HG21	1:C:467:TYR:HB3	1.98	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: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:L:303:GLY:N	2:L:700:GJY:O1	2.50	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: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
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:E:319:LYS:NZ	1:E:545:ALA:O	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ASP:OD1	1:G:162:ASP:N	2.48	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:55:LEU:O	1:J:59:ASN:ND2	2.45	0.44
1:J:8:LYS:HE3	1:J:68:THR:HG21	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:327:MET:HG2	1:B:340:ILE:HG12	1.99	0.43
1:B:303:GLY:N	2:B:700:GJY:O1	2.51	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: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
1:K:321:THR:OG1	1:K:577:GLU:OE2	2.24	0.43
1:L:57:LYS:HB2	1:L:57:LYS:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ARG:HD3	1:C:269:ARG:HA	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:441:HIS:CE1	1:J:543:LEU:HD22	2.54	0.42
1:J:9:ARG:HD2	1:J:9:ARG:HA	1.88	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:300:THR:O	1:G:305:SER:HB2	2.19	0.42
1:G:9:ARG:HD2	1:G:9:ARG:HA	1.67	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: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
1:H:379:LEU:O	1:H:379:LEU:HD12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:370:PRO:HB3	1:I:575:TRP:CH2	2.55	0.41
1:I:39:VAL:HG21	1:I:467:TYR:HB3	2.01	0.41
1:I:517:ALA:HB3	1:I:564:LEU:HD13	2.02	0.41
1:I:303:GLY:N	2:I:700:GJY:O1	2.53	0.41
1:E:382:ASN:O	1:E:383:GLY:C	2.58	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:HA	1:H:526:LYS:HD2	1.84	0.41
1:K:484:TYR:CZ	1:L:485:ILE:HD11	2.55	0.41
1:D:144:THR:H	1:D:147:GLN:NE2	2.19	0.41
1:C:46:LEU:HD23	1:D:46:LEU:HD23	2.03	0.41
1:E:230:LYS:HB2	1:E:230:LYS:HE3	1.88	0.41
1:G:281:SER:H	1:G:305:SER:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:484:TYR:O	1:G:488:GLN:HG2	2.20	0.41
1:G:337:VAL:HB	1:G:546:ASN:HB3	2.01	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: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: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: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:281:SER:H	1:A:305:SER:CB	2.34	0.41
1:D:307:ARG:CZ	1:D:542:VAL:HB	2.51	0.41
1:E:153:ILE:HD13	1:E:174:ALA:HB1	2.02	0.41
1:E:18:VAL:HG11	1:E:432:PRO:HA	2.03	0.41
1:J:441:HIS:O	1:J:445:ILE:HG22	2.21	0.41
1:A:153:ILE:HG12	1:A:172:PHE:HZ	1.85	0.41
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:C:563:GLY:O	1:C:595:LYS:NZ	2.46	0.40
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:H	1:E:99:ILE:HD12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:509:VAL:HG12	1:C:570:ILE:HG12	2.02	0.40
1:C:63:LYS:HD2	1:C:67:ASN:HB2	2.04	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:F:55:LEU:O	1:F:59:ASN:ND2	2.38	0.40
1:L:2:GLY:C	1:L:3:LYS:HD2	2.42	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%)	565 (94%)	32 (5%)	3 (0%)	29	67
1	B	603/636 (95%)	567 (94%)	35 (6%)	1 (0%)	47	79
1	C	600/636 (94%)	569 (95%)	30 (5%)	1 (0%)	47	79
1	D	603/636 (95%)	564 (94%)	35 (6%)	4 (1%)	22	61
1	E	600/636 (94%)	567 (94%)	29 (5%)	4 (1%)	22	61
1	F	603/636 (95%)	566 (94%)	36 (6%)	1 (0%)	47	79
1	G	600/636 (94%)	569 (95%)	29 (5%)	2 (0%)	41	74
1	H	614/636 (96%)	572 (93%)	39 (6%)	3 (0%)	29	67
1	I	600/636 (94%)	565 (94%)	34 (6%)	1 (0%)	47	79
1	J	614/636 (96%)	577 (94%)	34 (6%)	3 (0%)	29	67
1	K	600/636 (94%)	569 (95%)	28 (5%)	3 (0%)	29	67
1	L	614/636 (96%)	575 (94%)	37 (6%)	2 (0%)	41	74
All	All	7251/7632 (95%)	6825 (94%)	398 (6%)	28 (0%)	34	69

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	613	ALA
1	A	45	PRO
1	A	384	SER
1	C	45	PRO
1	D	2	GLY
1	D	45	PRO
1	E	45	PRO
1	E	382	ASN
1	F	45	PRO
1	G	45	PRO
1	G	379	LEU
1	H	45	PRO
1	I	45	PRO
1	J	117	SER
1	K	45	PRO
1	K	384	SER
1	L	45	PRO
1	B	45	PRO
1	E	383	GLY
1	J	45	PRO
1	K	385	ASN
1	D	11	SER
1	D	526	LYS
1	E	303	GLY
1	H	110	PRO
1	J	110	PRO
1	A	303	GLY
1	L	2	GLY

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	510/540 (94%)	507 (99%)	3 (1%)	86	94
1	B	512/540 (95%)	505 (99%)	7 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	510/540 (94%)	506 (99%)	4 (1%)	81	93
1	D	512/540 (95%)	507 (99%)	5 (1%)	76	90
1	E	510/540 (94%)	505 (99%)	5 (1%)	76	90
1	F	512/540 (95%)	506 (99%)	6 (1%)	71	88
1	G	510/540 (94%)	507 (99%)	3 (1%)	86	94
1	H	521/540 (96%)	512 (98%)	9 (2%)	60	83
1	I	510/540 (94%)	508 (100%)	2 (0%)	91	95
1	J	521/540 (96%)	514 (99%)	7 (1%)	69	87
1	K	510/540 (94%)	506 (99%)	4 (1%)	81	93
1	L	521/540 (96%)	515 (99%)	6 (1%)	71	88
All	All	6159/6480 (95%)	6098 (99%)	61 (1%)	76	90

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	391	ARG
1	A	395	TYR
1	B	1	MET
1	B	29	HIS
1	B	141	LYS
1	B	179	LYS
1	B	391	ARG
1	B	395	TYR
1	B	495	MET
1	C	29	HIS
1	C	127	ARG
1	C	391	ARG
1	C	395	TYR
1	D	29	HIS
1	D	141	LYS
1	D	391	ARG
1	D	395	TYR
1	D	495	MET
1	E	29	HIS
1	E	121	ASP
1	E	277	TYR
1	E	381	HIS

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Mol	Chain	Res	Type
1	E	391	ARG
1	F	23	GLU
1	F	111	GLN
1	F	141	LYS
1	F	391	ARG
1	F	395	TYR
1	F	495	MET
1	G	29	HIS
1	G	391	ARG
1	G	395	TYR
1	H	1	MET
1	H	4	TYR
1	H	29	HIS
1	H	141	LYS
1	H	277	TYR
1	H	391	ARG
1	H	395	TYR
1	H	495	MET
1	H	614	TYR
1	I	29	HIS
1	I	391	ARG
1	J	1	MET
1	J	29	HIS
1	J	126	PHE
1	J	179	LYS
1	J	277	TYR
1	J	395	TYR
1	J	607	ASN
1	K	29	HIS
1	K	84	GLU
1	K	391	ARG
1	K	395	TYR
1	L	4	TYR
1	L	5	GLN
1	L	29	HIS
1	L	151	ARG
1	L	379	LEU
1	L	391	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	147	GLN
1	H	5	GLN
1	I	147	GLN
1	I	382	ASN
1	K	462	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	D	700	1	18,21,22	0.33	0	15,21,24	0.36	0
2	GJY	B	700	1	18,21,22	0.33	0	15,21,24	0.37	0
2	GJY	K	700	1	18,21,22	0.34	0	15,21,24	0.35	0
2	GJY	I	700	1	18,21,22	0.34	0	15,21,24	0.34	0
2	GJY	E	700	1	18,21,22	0.34	0	15,21,24	0.38	0
2	GJY	C	700	1	18,21,22	0.34	0	15,21,24	0.35	0
2	GJY	A	700	1	18,21,22	0.33	0	15,21,24	0.35	0
2	GJY	L	700	1	18,21,22	0.33	0	15,21,24	0.32	0
2	GJY	J	700	1	18,21,22	0.34	0	15,21,24	0.37	0
2	GJY	H	700	1	18,21,22	0.35	0	15,21,24	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GJY	G	700	1	18,21,22	0.35	0	15,21,24	0.36	0
2	GJY	F	700	1	18,21,22	0.34	0	15,21,24	0.35	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	D	700	1	-	6/16/20/22	-
2	GJY	B	700	1	-	5/16/20/22	-
2	GJY	K	700	1	-	6/16/20/22	-
2	GJY	I	700	1	-	7/16/20/22	-
2	GJY	E	700	1	-	7/16/20/22	-
2	GJY	C	700	1	-	6/16/20/22	-
2	GJY	A	700	1	-	7/16/20/22	-
2	GJY	L	700	1	-	4/16/20/22	-
2	GJY	J	700	1	-	6/16/20/22	-
2	GJY	H	700	1	-	5/16/20/22	-
2	GJY	G	700	1	-	6/16/20/22	-
2	GJY	F	700	1	-	6/16/20/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	700	GJY	C1-C2-C3-C4
2	H	700	GJY	C5-C6-C7-C8
2	B	700	GJY	C4-C5-C6-C7
2	B	700	GJY	C6-C7-C8-C9
2	A	700	GJY	C1-C2-C3-C4
2	K	700	GJY	C1-C2-C3-C4
2	I	700	GJY	C1-C2-C3-C4
2	J	700	GJY	C1-C2-C3-C4
2	H	700	GJY	C1-C2-C3-C4
2	C	700	GJY	C1-C2-C3-C4

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

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

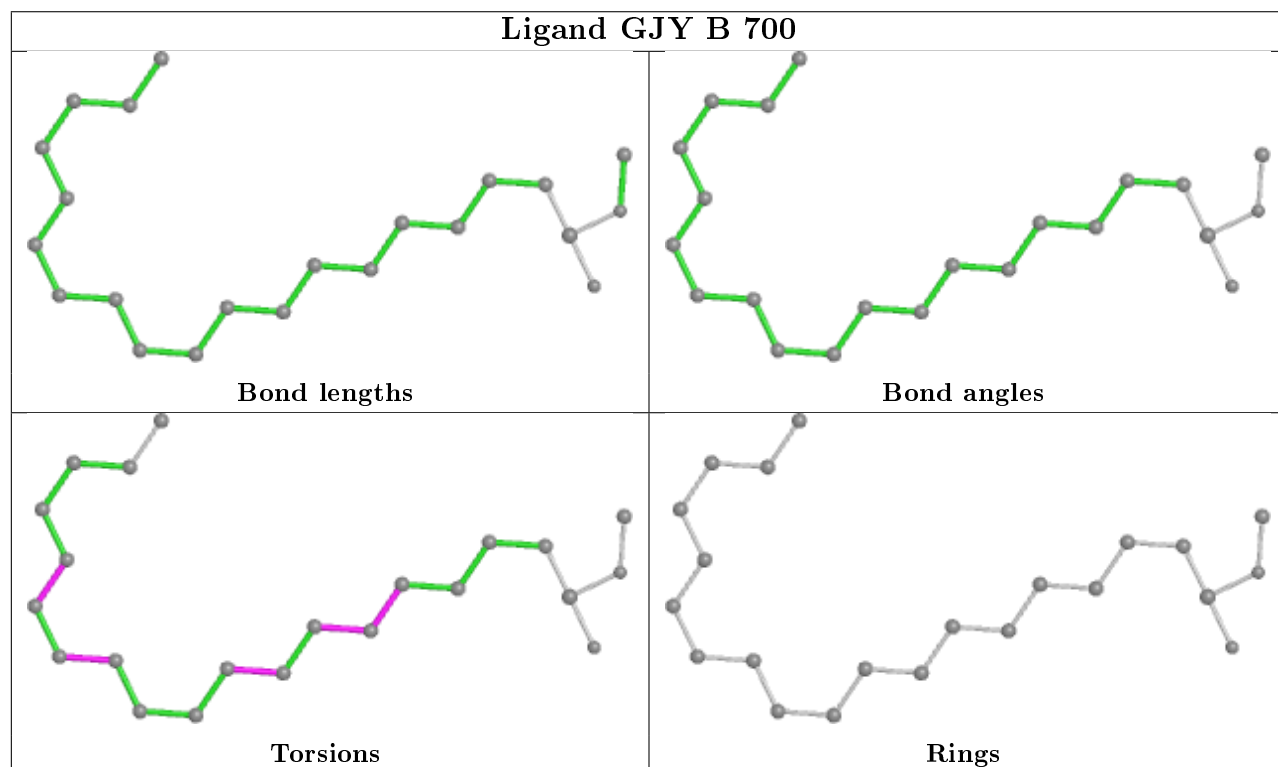
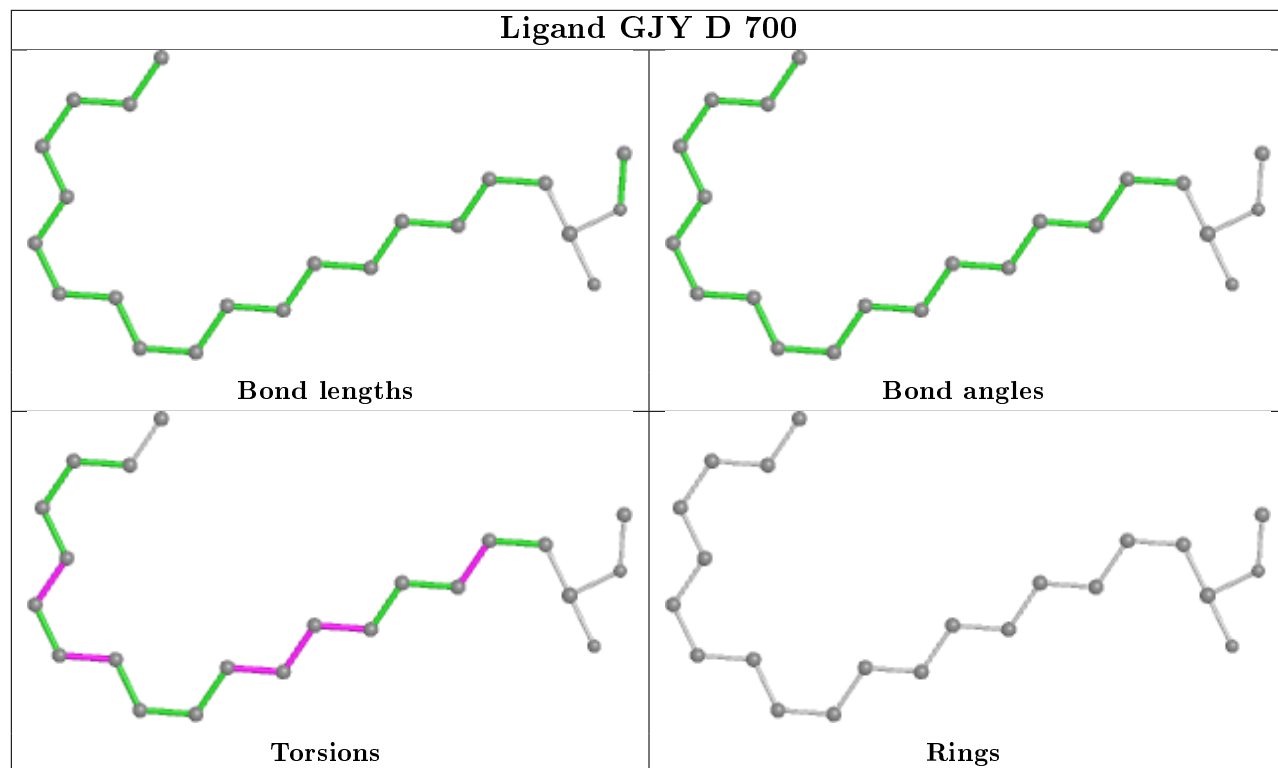
There are no ring outliers.

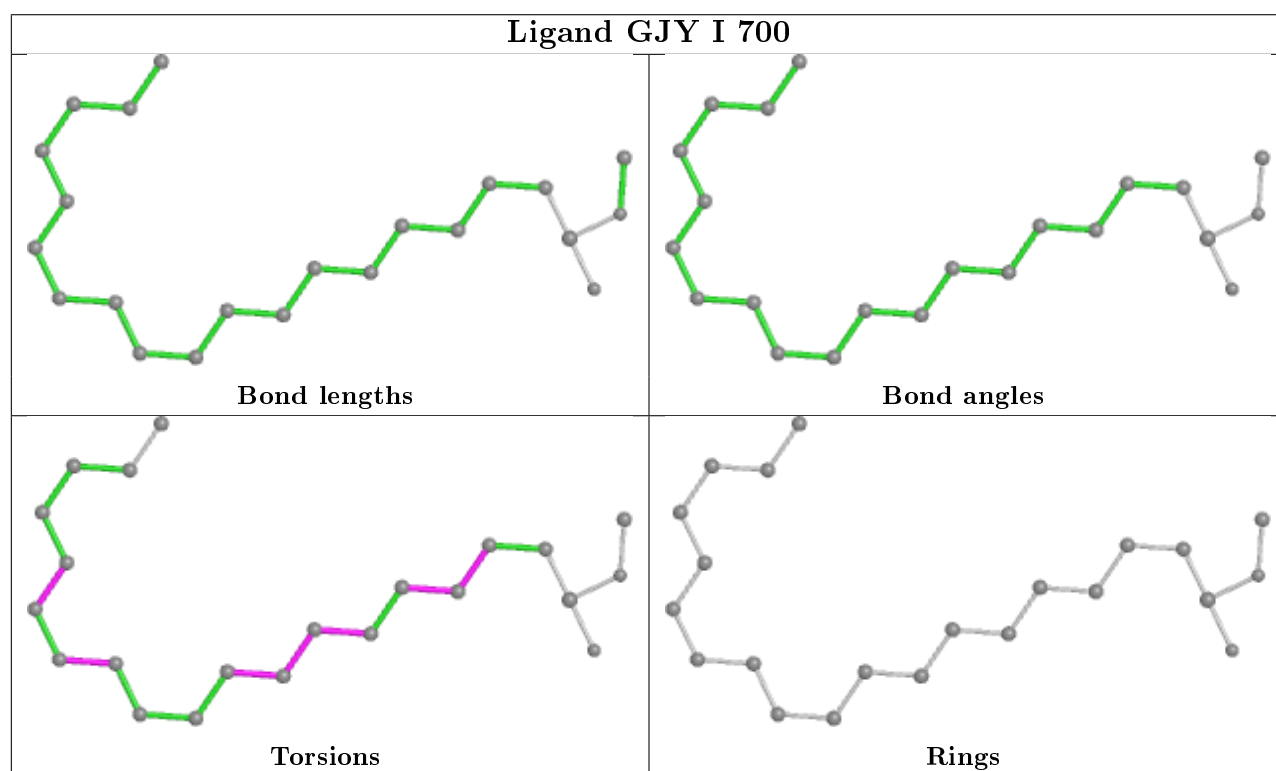
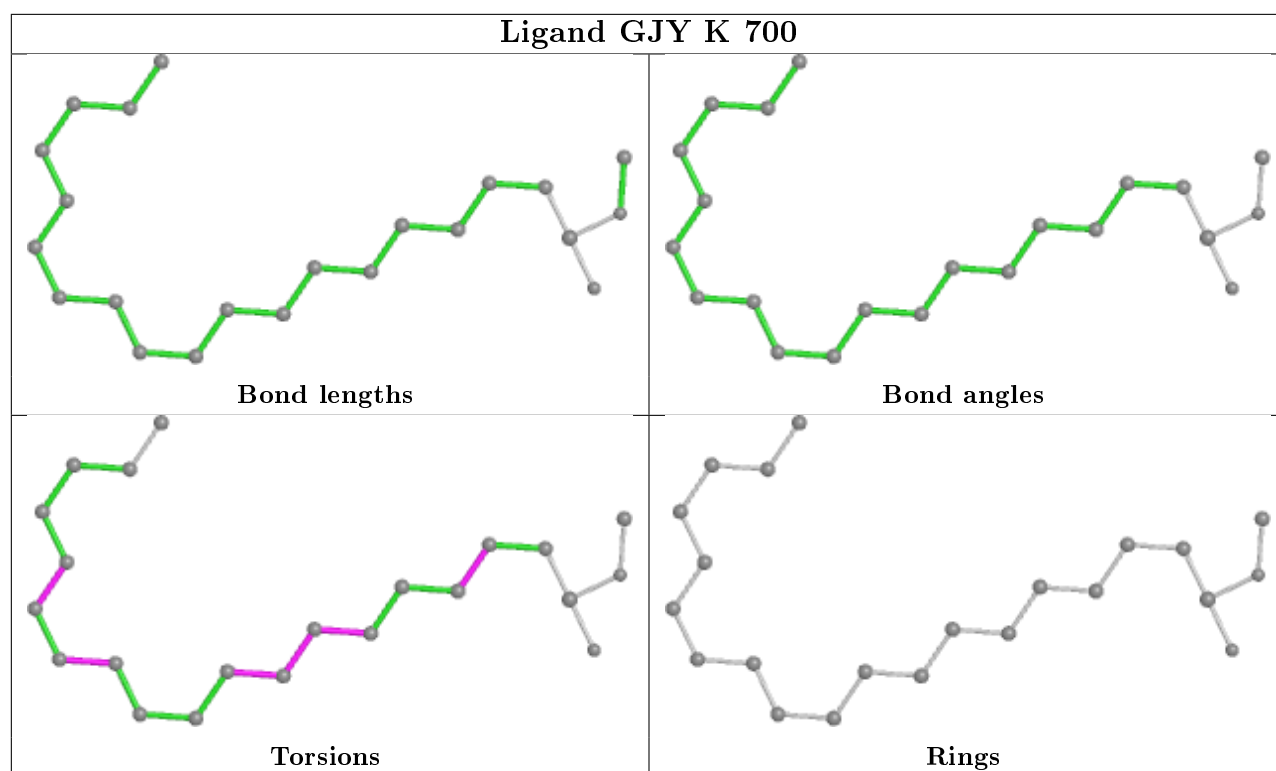
6 monomers are involved in 7 short contacts:

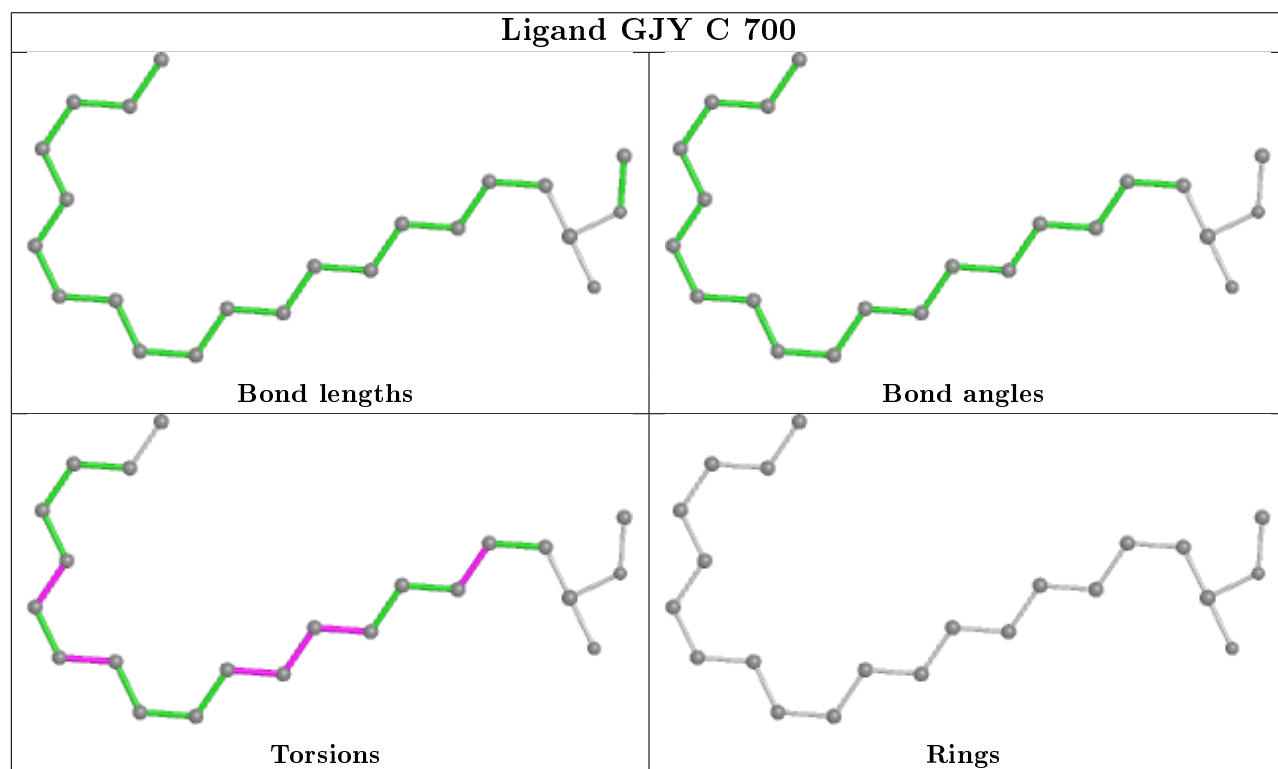
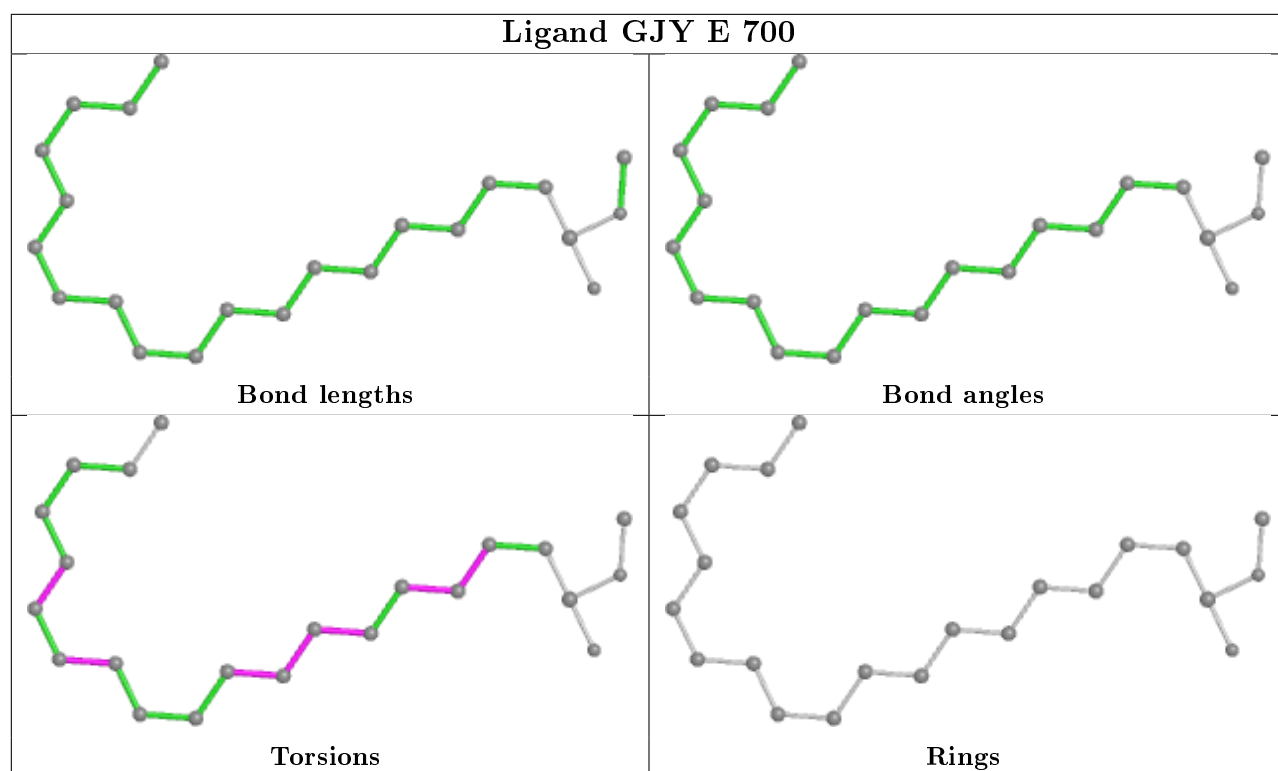
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	GJY	1	0
2	K	700	GJY	1	0
2	I	700	GJY	1	0
2	C	700	GJY	2	0
2	L	700	GJY	1	0
2	G	700	GJY	1	0

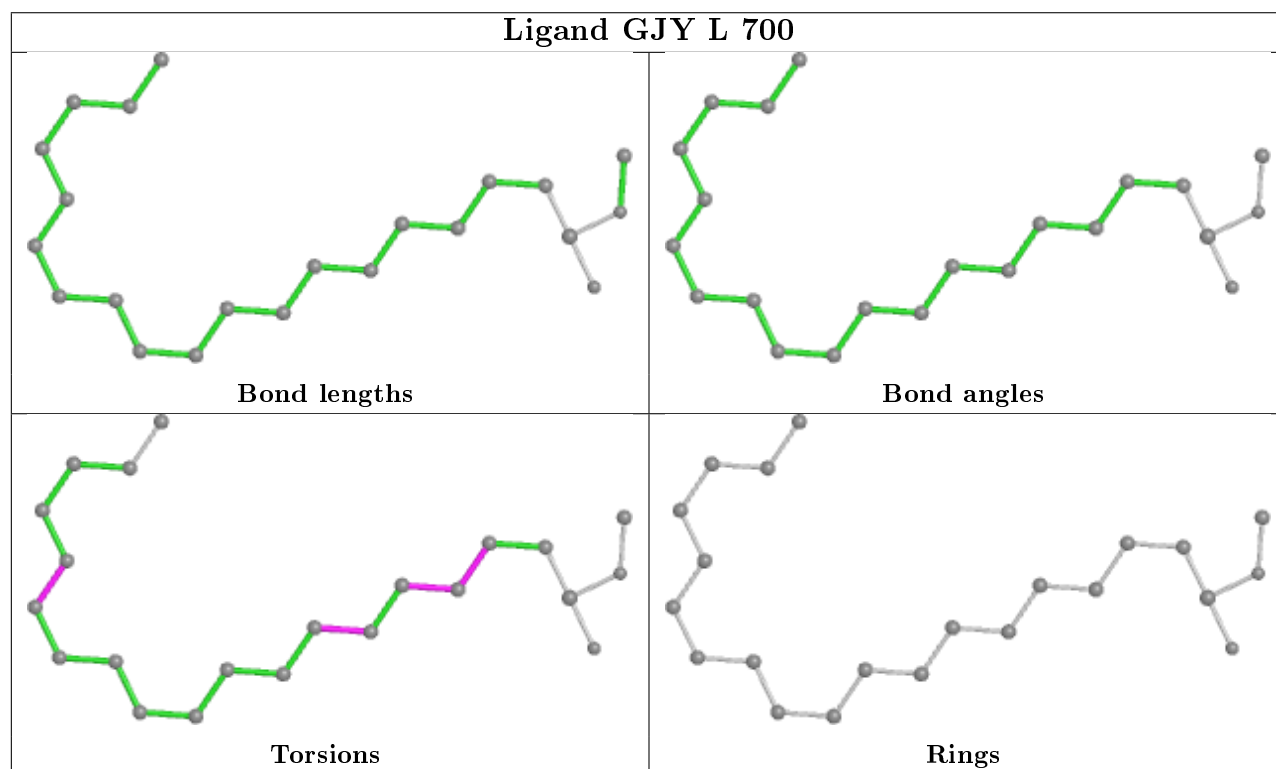
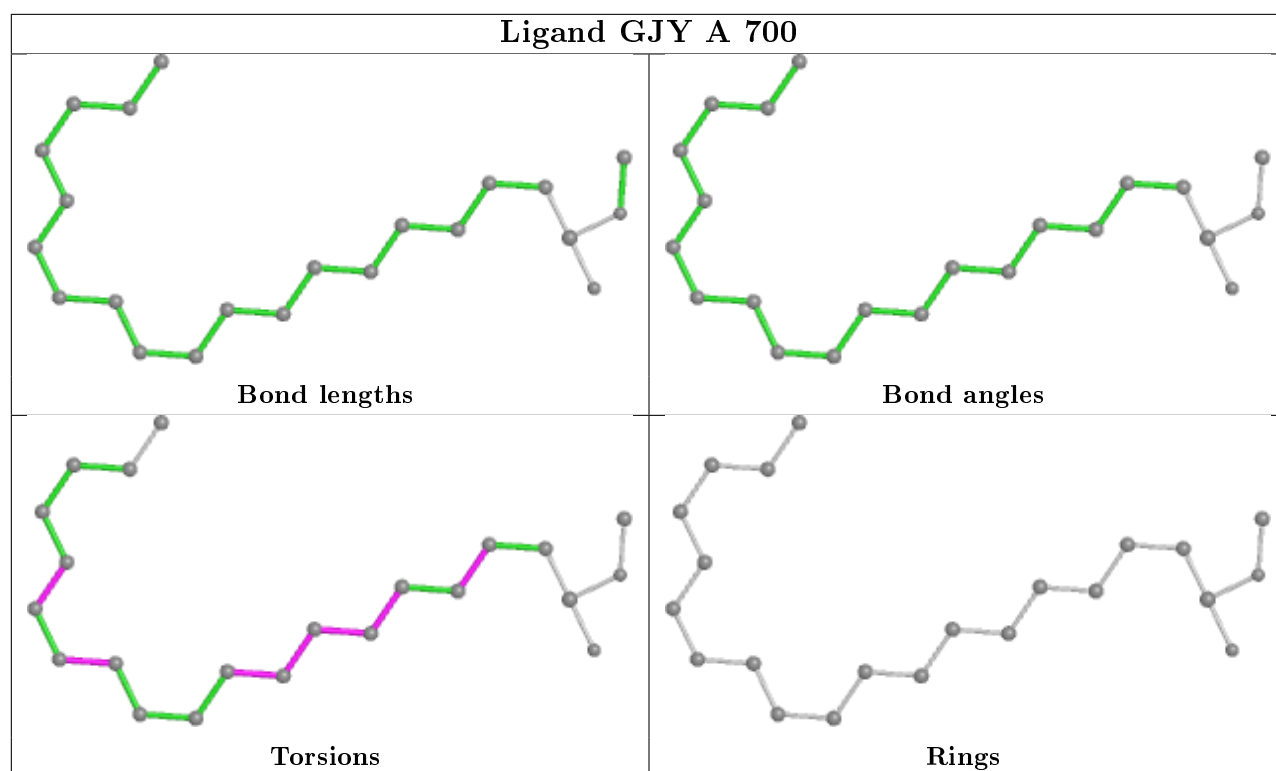
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

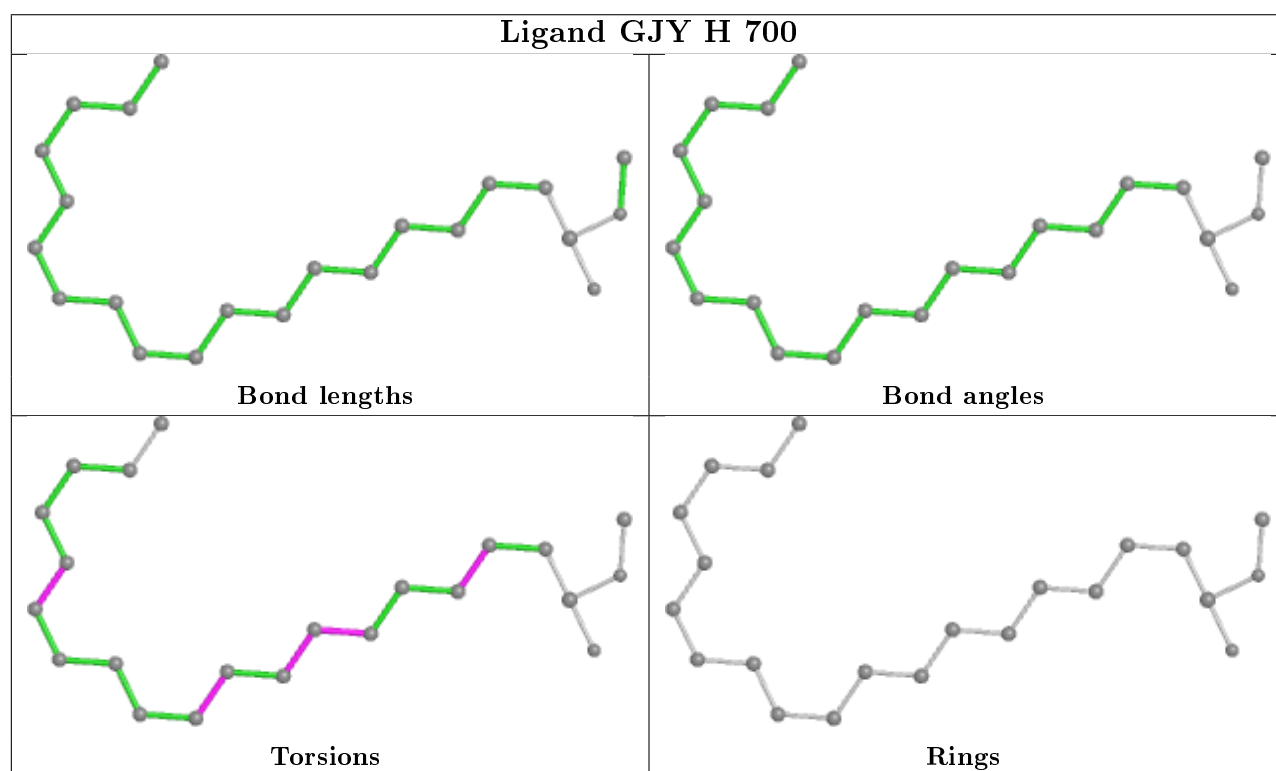
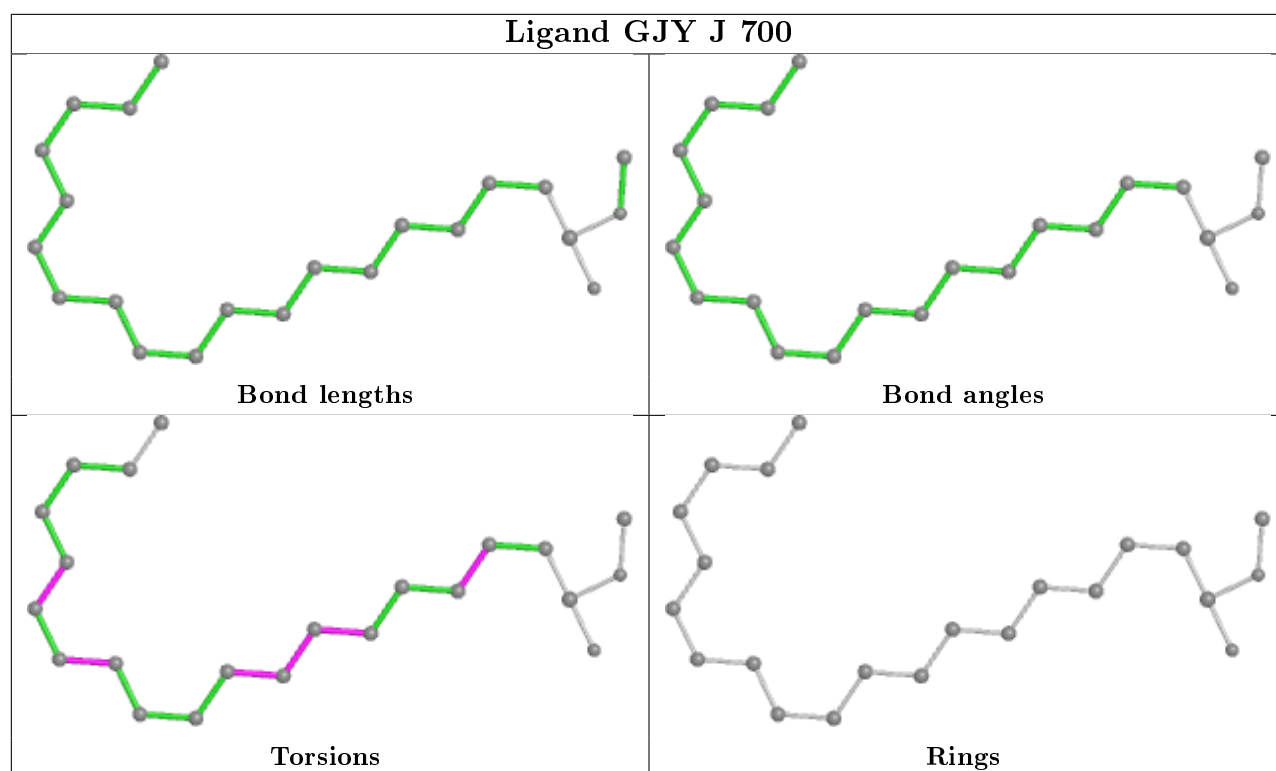
equivalents in the CSD to analyse the geometry.

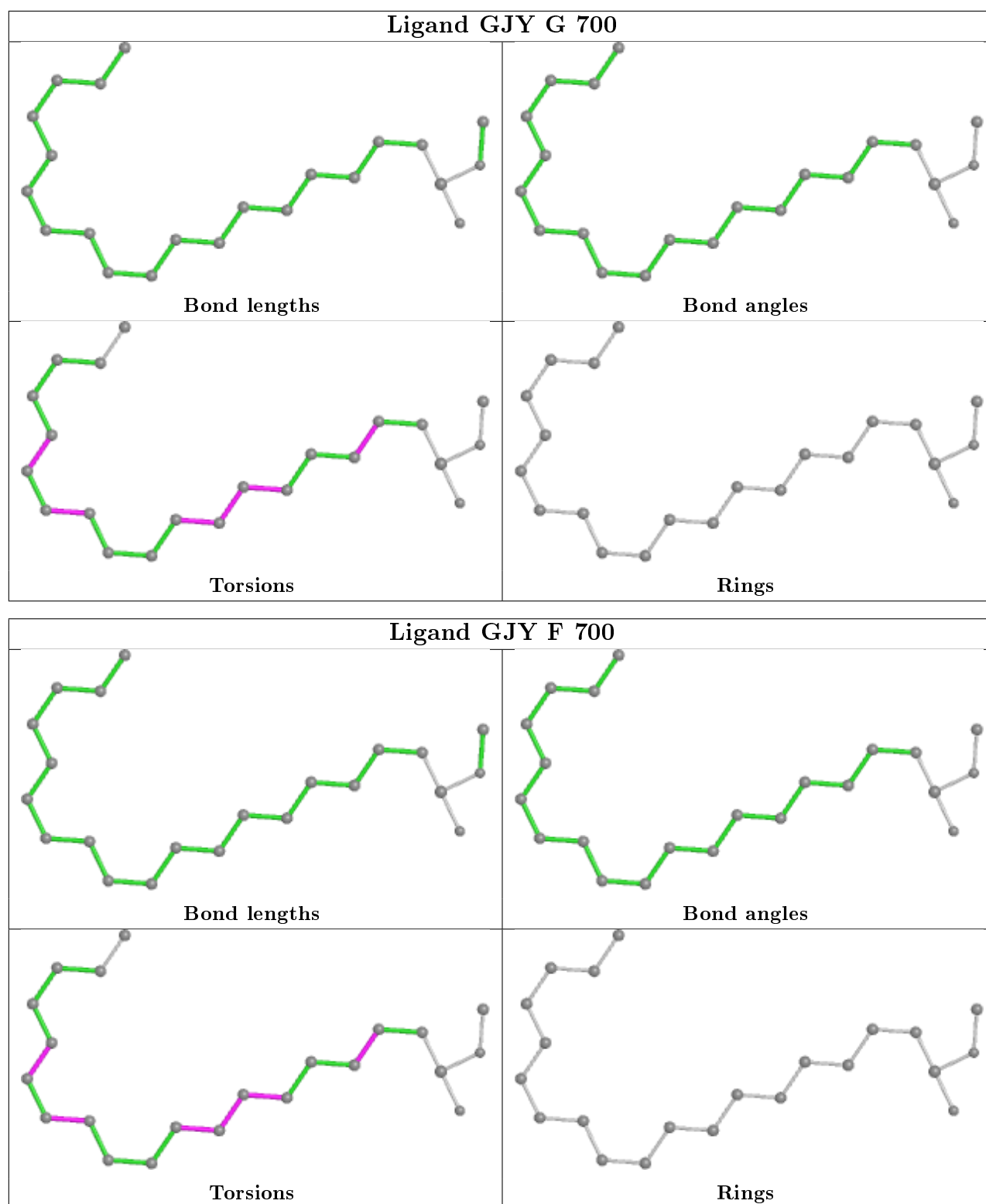












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.16	13 (2%)	62	48	32, 70, 127, 291	0
1	B	605/636 (95%)	-0.10	20 (3%)	46	30	32, 73, 142, 299	0
1	C	602/636 (94%)	-0.14	16 (2%)	54	39	34, 69, 132, 292	0
1	D	605/636 (95%)	-0.01	18 (2%)	50	34	36, 76, 141, 325	0
1	E	602/636 (94%)	-0.06	17 (2%)	53	37	29, 74, 137, 286	0
1	F	605/636 (95%)	-0.07	16 (2%)	56	40	31, 69, 136, 290	0
1	G	602/636 (94%)	-0.15	18 (2%)	50	34	30, 66, 125, 293	0
1	H	616/636 (96%)	-0.11	15 (2%)	59	44	32, 68, 143, 279	0
1	I	602/636 (94%)	-0.20	11 (1%)	68	55	30, 61, 123, 272	0
1	J	616/636 (96%)	-0.15	18 (2%)	51	36	31, 62, 137, 255	0
1	K	602/636 (94%)	-0.21	13 (2%)	62	48	24, 63, 125, 269	0
1	L	616/636 (96%)	-0.16	12 (1%)	66	53	25, 64, 133, 284	0
All	All	7275/7632 (95%)	-0.13	187 (2%)	56	40	24, 68, 136, 325	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	119	HIS	10.1
1	F	119	HIS	9.9
1	B	119	HIS	9.6
1	G	119	HIS	9.3
1	H	119	HIS	8.0
1	F	384	SER	7.5
1	C	123	VAL	7.5
1	F	121	ASP	7.4
1	I	119	HIS	7.2
1	B	121	ASP	6.8
1	B	120	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	121	ASP	6.4
1	D	123	VAL	6.2
1	L	119	HIS	6.2
1	D	384	SER	6.1
1	G	384	SER	6.1
1	B	123	VAL	6.1
1	G	122	PRO	6.0
1	J	119	HIS	5.9
1	F	123	VAL	5.9
1	C	122	PRO	5.8
1	E	118	LEU	5.6
1	A	119	HIS	5.3
1	J	382	ASN	5.3
1	K	122	PRO	5.3
1	C	119	HIS	5.2
1	A	118	LEU	5.2
1	D	124	SER	5.1
1	K	119	HIS	5.1
1	B	384	SER	5.1
1	F	120	ALA	5.0
1	E	119	HIS	4.9
1	A	123	VAL	4.9
1	E	122	PRO	4.8
1	E	123	VAL	4.8
1	C	118	LEU	4.8
1	C	121	ASP	4.7
1	D	122	PRO	4.7
1	G	123	VAL	4.5
1	D	382	ASN	4.5
1	I	122	PRO	4.5
1	I	118	LEU	4.5
1	B	122	PRO	4.3
1	I	123	VAL	4.2
1	C	120	ALA	4.2
1	K	123	VAL	4.2
1	B	124	SER	4.1
1	D	2	GLY	4.0
1	B	381	HIS	4.0
1	H	381	HIS	3.9
1	D	383	GLY	3.9
1	E	125	SER	3.9
1	H	383	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	118	LEU	3.8
1	H	610	GLU	3.8
1	H	384	SER	3.8
1	L	384	SER	3.8
1	G	121	ASP	3.8
1	F	122	PRO	3.7
1	A	385	ASN	3.7
1	A	122	PRO	3.7
1	G	381	HIS	3.7
1	F	124	SER	3.6
1	K	121	ASP	3.6
1	A	120	ALA	3.6
1	F	4	TYR	3.6
1	K	4	TYR	3.6
1	H	614	TYR	3.5
1	E	121	ASP	3.4
1	B	382	ASN	3.4
1	D	300	THR	3.4
1	A	381	HIS	3.4
1	A	121	ASP	3.4
1	H	615	VAL	3.3
1	C	384	SER	3.3
1	J	406	ASP	3.3
1	A	384	SER	3.3
1	H	123	VAL	3.3
1	F	118	LEU	3.2
1	H	121	ASP	3.2
1	J	384	SER	3.2
1	D	120	ALA	3.2
1	G	118	LEU	3.2
1	L	123	VAL	3.1
1	D	381	HIS	3.1
1	F	111	GLN	3.1
1	C	380	SER	3.1
1	F	605	ASN	3.1
1	A	117	SER	3.0
1	F	381	HIS	3.0
1	K	384	SER	3.0
1	I	22	ALA	2.9
1	C	4	TYR	2.9
1	A	4	TYR	2.9
1	G	4	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	616	GLU	2.9
1	I	121	ASP	2.9
1	J	614	TYR	2.9
1	L	120	ALA	2.8
1	F	300	THR	2.8
1	H	95	ASP	2.8
1	B	2	GLY	2.8
1	B	1	MET	2.8
1	H	406	ASP	2.8
1	E	4	TYR	2.8
1	G	383	GLY	2.8
1	L	383	GLY	2.8
1	D	111	GLN	2.8
1	E	30	LEU	2.8
1	C	124	SER	2.7
1	H	616	GLU	2.7
1	A	125	SER	2.7
1	C	117	SER	2.7
1	G	526	LYS	2.7
1	B	301	ASP	2.7
1	C	7	MET	2.6
1	E	382	ASN	2.6
1	F	117	SER	2.6
1	D	118	LEU	2.6
1	L	300	THR	2.6
1	C	424	CYS	2.6
1	K	22	ALA	2.6
1	D	301	ASP	2.6
1	I	124	SER	2.6
1	I	384	SER	2.6
1	F	383	GLY	2.5
1	I	120	ALA	2.5
1	B	4	TYR	2.5
1	H	613	ALA	2.5
1	J	123	VAL	2.5
1	G	124	SER	2.5
1	A	88	ASP	2.4
1	J	613	ALA	2.4
1	K	118	LEU	2.4
1	H	304	GLY	2.4
1	C	381	HIS	2.4
1	E	117	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	527	ASN	2.4
1	E	88	ASP	2.3
1	L	614	TYR	2.3
1	K	562	GLU	2.3
1	J	615	VAL	2.3
1	I	4	TYR	2.3
1	E	381	HIS	2.3
1	F	561	LYS	2.3
1	G	527	ASN	2.3
1	J	304	GLY	2.3
1	K	12	GLU	2.3
1	E	384	SER	2.3
1	E	120	ALA	2.3
1	E	527	ASN	2.3
1	L	305	SER	2.2
1	B	305	SER	2.2
1	B	300	THR	2.2
1	J	121	ASP	2.2
1	G	117	SER	2.2
1	H	124	SER	2.2
1	J	4	TYR	2.2
1	J	120	ALA	2.2
1	K	120	ALA	2.2
1	G	525	LEU	2.2
1	L	615	VAL	2.2
1	E	526	LYS	2.2
1	J	383	GLY	2.2
1	J	229	GLU	2.2
1	B	111	GLN	2.2
1	D	404	SER	2.2
1	G	120	ALA	2.2
1	J	404	SER	2.1
1	K	117	SER	2.1
1	D	406	ASP	2.1
1	L	613	ALA	2.1
1	I	383	GLY	2.1
1	J	379	LEU	2.1
1	B	605	ASN	2.1
1	G	42	LEU	2.1
1	L	381	HIS	2.1
1	L	406	ASP	2.1
1	J	381	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	189	GLU	2.1
1	C	526	LYS	2.0
1	G	125	SER	2.0
1	B	383	GLY	2.0
1	G	12	GLU	2.0
1	B	304	GLY	2.0
1	E	182	GLU	2.0
1	D	305	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

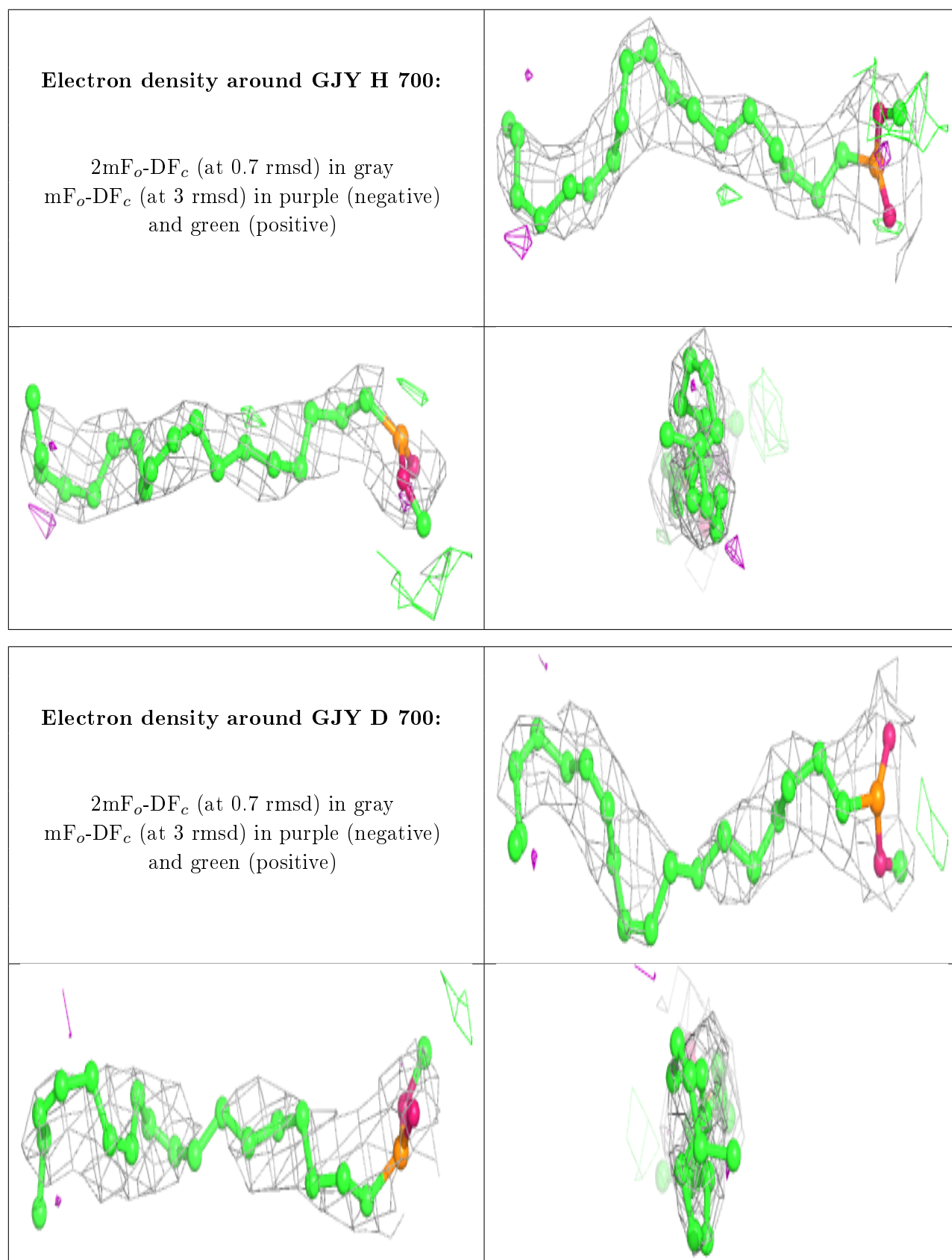
6.4 Ligands ⓘ

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	H	700	22/23	0.86	0.29	52,57,63,83	0
2	GJY	D	700	22/23	0.87	0.34	56,75,81,85	0
2	GJY	G	700	22/23	0.87	0.34	52,70,76,81	0
2	GJY	E	700	22/23	0.88	0.32	53,71,77,82	0
2	GJY	L	700	22/23	0.88	0.31	54,73,79,83	0
2	GJY	B	700	22/23	0.88	0.32	55,73,78,82	0
2	GJY	I	700	22/23	0.88	0.32	52,71,77,81	0
2	GJY	K	700	22/23	0.89	0.31	46,65,70,75	0
2	GJY	F	700	22/23	0.89	0.29	53,71,77,82	0
2	GJY	J	700	22/23	0.91	0.25	37,56,62,66	0
2	GJY	A	700	22/23	0.91	0.28	54,73,79,83	0
2	GJY	C	700	22/23	0.92	0.25	50,68,74,79	0

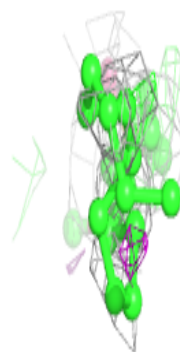
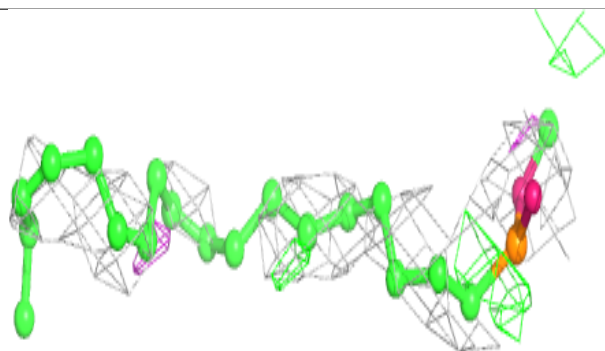
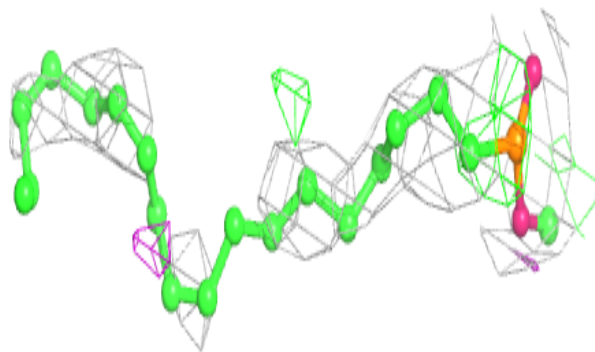
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

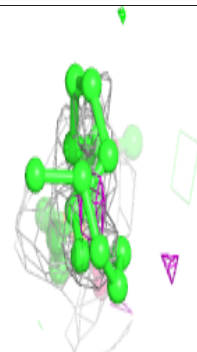
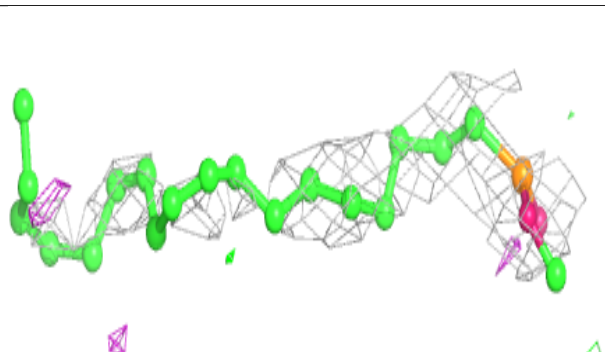
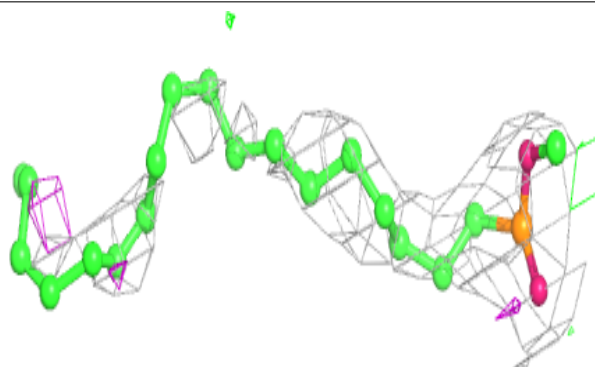


Electron density around GJY G 700:

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

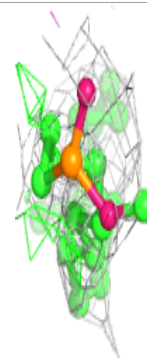
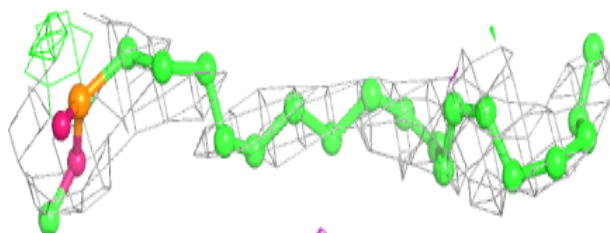
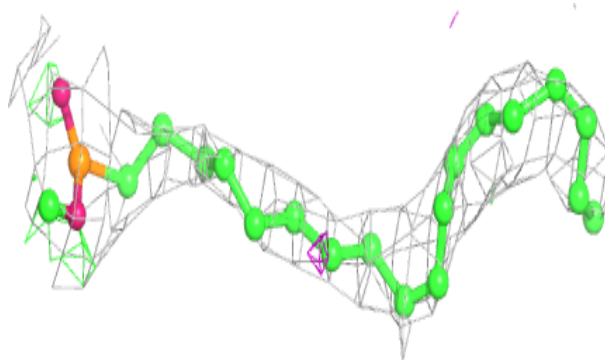
**Electron density around GJY E 700:**

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

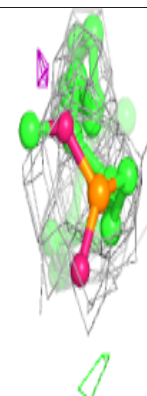
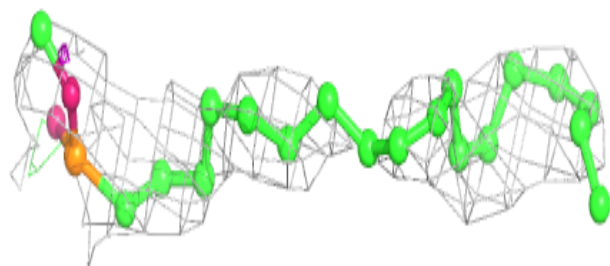
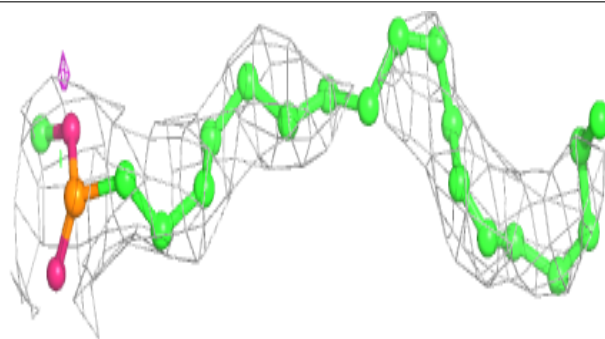


Electron density around GJY L 700:

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

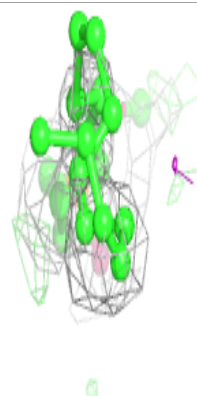
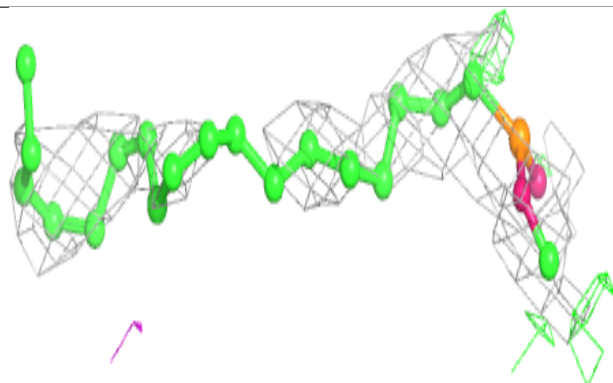
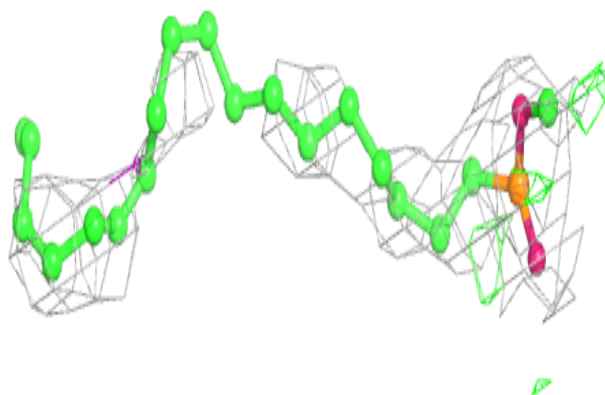
**Electron density around GJY B 700:**

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

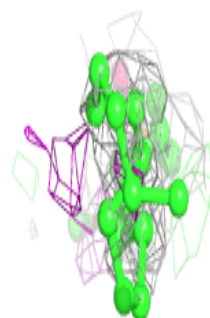
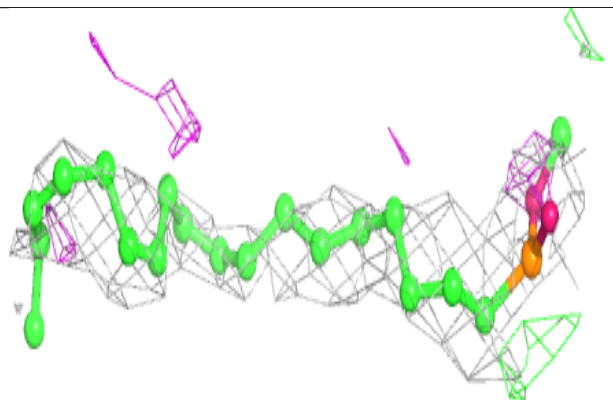
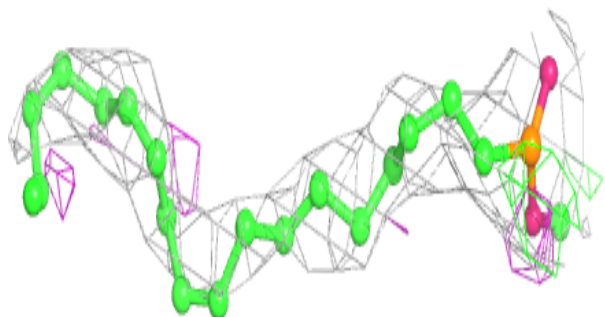


Electron density around GJY I 700:

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

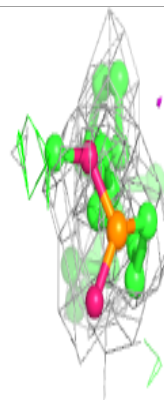
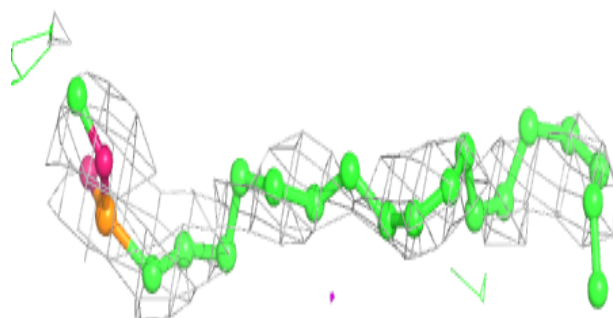
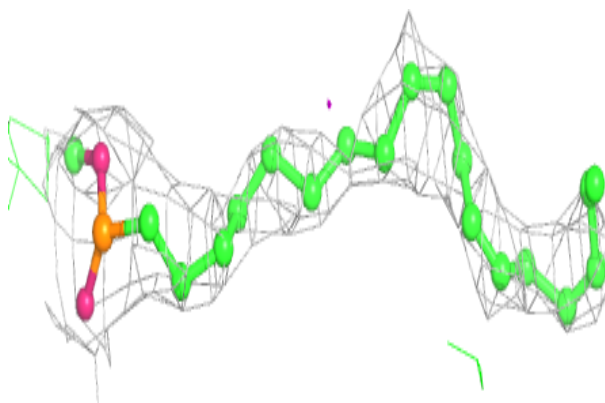
**Electron density around GJY K 700:**

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

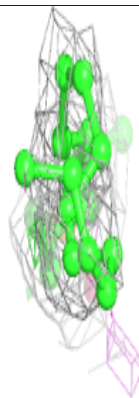
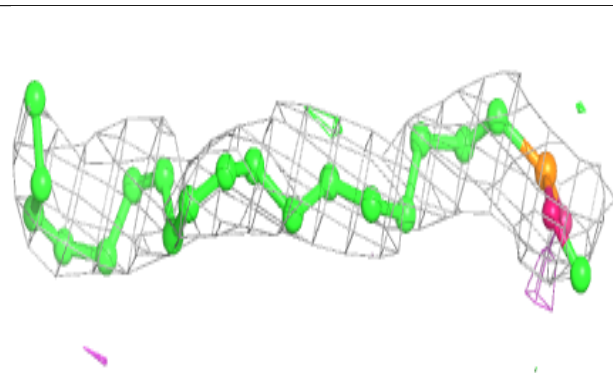
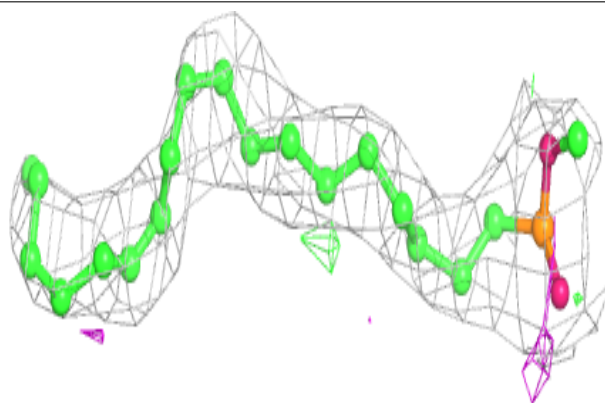


Electron density around GJY F 700:

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

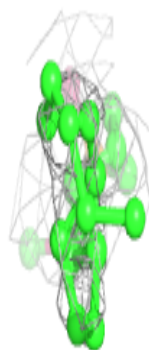
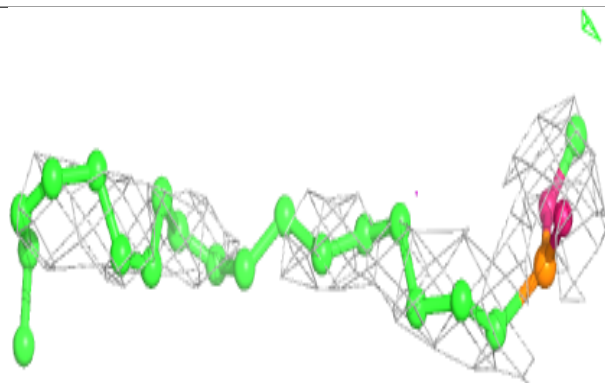
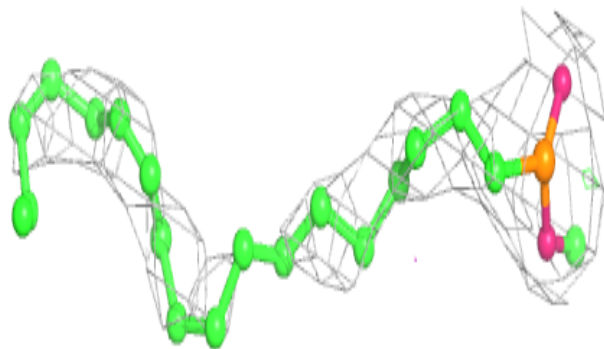
**Electron density around GJY J 700:**

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

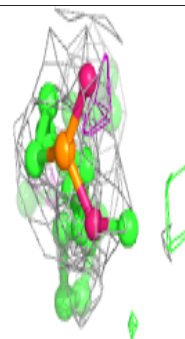
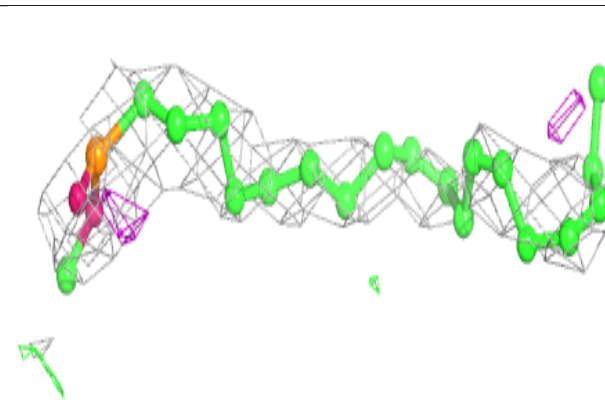
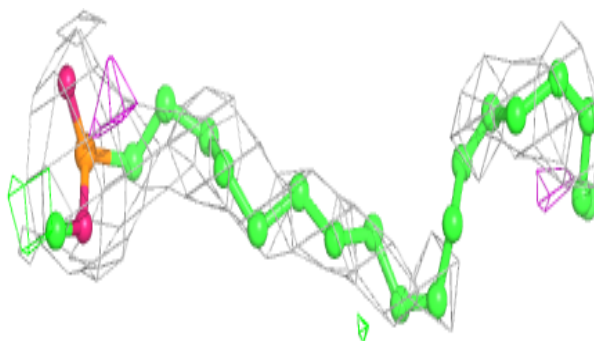


Electron density around GJY A 700:

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

**Electron density around GJY C 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

There are no such residues in this entry.