



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 8EY1 / pdb_00008ey1
Title : Structure of Arabidopsis fatty acid amide hydrolase mutant S305A in complex with N-(3-oxododecanoyl)-L-homoserine lactone
Authors : Aziz, M.; Wang, X.; Gaguancela, O.A.; Chapman, K.D.
Deposited on : 2022-10-26
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

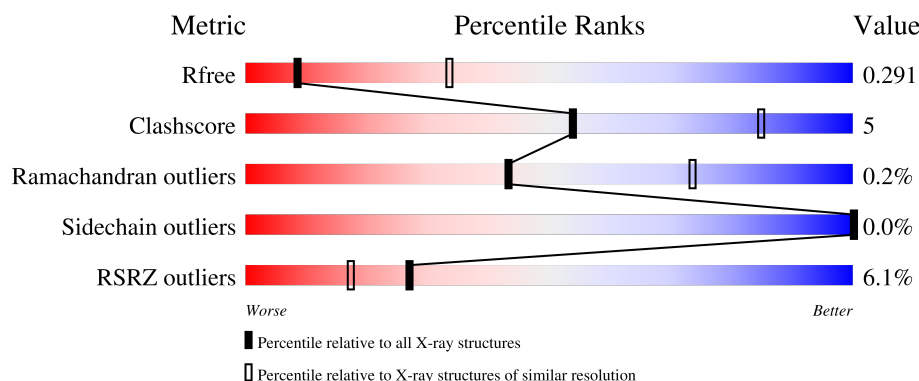
1 Overall quality at a glance

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)
Ramachandran outliers	187476	1548 (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	11% 81% 14% 5%
1	B	636	13% 80% 15% 5%
1	C	636	2% 83% 11% 5%
1	D	636	2% 86% 10% 5%
1	E	636	10% 81% 14% 5%

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Mol	Chain	Length	Quality of chain
1	F	636	14% 79% 16% 5%
1	G	636	% 86% 9% 5%
1	H	636	3% 85% 12% •
1	I	636	2% 84% 11% 5%
1	J	636	6% 84% 12% •
1	K	636	2% 87% 8% 5%
1	L	636	3% 81% 14% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 55639 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	B	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			
1	C	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	D	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			
1	E	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	F	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			
1	G	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	H	614	Total	C	N	O	S	0	0	0
			4700	2982	793	901	24			
1	I	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	J	614	Total	C	N	O	S	0	0	0
			4700	2982	793	901	24			
1	K	602	Total	C	N	O	S	0	0	0
			4605	2922	778	882	23			
1	L	605	Total	C	N	O	S	0	0	0
			4626	2935	782	885	24			

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	SER	engineered mutation	UNP Q7XJJ7
A	608	LYS	-	expression tag	UNP Q7XJJ7
A	609	GLY	-	expression tag	UNP Q7XJJ7
A	610	GLU	-	expression tag	UNP Q7XJJ7
A	611	PHE	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	612	GLU	-	expression tag	UNP Q7XJJ7
A	613	ALA	-	expression tag	UNP Q7XJJ7
A	614	TYR	-	expression tag	UNP Q7XJJ7
A	615	VAL	-	expression tag	UNP Q7XJJ7
A	616	GLU	-	expression tag	UNP Q7XJJ7
A	617	GLN	-	expression tag	UNP Q7XJJ7
A	618	LYS	-	expression tag	UNP Q7XJJ7
A	619	LEU	-	expression tag	UNP Q7XJJ7
A	620	ILE	-	expression tag	UNP Q7XJJ7
A	621	SER	-	expression tag	UNP Q7XJJ7
A	622	GLU	-	expression tag	UNP Q7XJJ7
A	623	GLU	-	expression tag	UNP Q7XJJ7
A	624	ASP	-	expression tag	UNP Q7XJJ7
A	625	LEU	-	expression tag	UNP Q7XJJ7
A	626	ASN	-	expression tag	UNP Q7XJJ7
A	627	SER	-	expression tag	UNP Q7XJJ7
A	628	ALA	-	expression tag	UNP Q7XJJ7
A	629	VAL	-	expression tag	UNP Q7XJJ7
A	630	ASP	-	expression tag	UNP Q7XJJ7
A	631	HIS	-	expression tag	UNP Q7XJJ7
A	632	HIS	-	expression tag	UNP Q7XJJ7
A	633	HIS	-	expression tag	UNP Q7XJJ7
A	634	HIS	-	expression tag	UNP Q7XJJ7
A	635	HIS	-	expression tag	UNP Q7XJJ7
A	636	HIS	-	expression tag	UNP Q7XJJ7
B	305	ALA	SER	engineered mutation	UNP Q7XJJ7
B	608	LYS	-	expression tag	UNP Q7XJJ7
B	609	GLY	-	expression tag	UNP Q7XJJ7
B	610	GLU	-	expression tag	UNP Q7XJJ7
B	611	PHE	-	expression tag	UNP Q7XJJ7
B	612	GLU	-	expression tag	UNP Q7XJJ7
B	613	ALA	-	expression tag	UNP Q7XJJ7
B	614	TYR	-	expression tag	UNP Q7XJJ7
B	615	VAL	-	expression tag	UNP Q7XJJ7
B	616	GLU	-	expression tag	UNP Q7XJJ7
B	617	GLN	-	expression tag	UNP Q7XJJ7
B	618	LYS	-	expression tag	UNP Q7XJJ7
B	619	LEU	-	expression tag	UNP Q7XJJ7
B	620	ILE	-	expression tag	UNP Q7XJJ7
B	621	SER	-	expression tag	UNP Q7XJJ7
B	622	GLU	-	expression tag	UNP Q7XJJ7
B	623	GLU	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	624	ASP	-	expression tag	UNP Q7XJJ7
B	625	LEU	-	expression tag	UNP Q7XJJ7
B	626	ASN	-	expression tag	UNP Q7XJJ7
B	627	SER	-	expression tag	UNP Q7XJJ7
B	628	ALA	-	expression tag	UNP Q7XJJ7
B	629	VAL	-	expression tag	UNP Q7XJJ7
B	630	ASP	-	expression tag	UNP Q7XJJ7
B	631	HIS	-	expression tag	UNP Q7XJJ7
B	632	HIS	-	expression tag	UNP Q7XJJ7
B	633	HIS	-	expression tag	UNP Q7XJJ7
B	634	HIS	-	expression tag	UNP Q7XJJ7
B	635	HIS	-	expression tag	UNP Q7XJJ7
B	636	HIS	-	expression tag	UNP Q7XJJ7
C	305	ALA	SER	engineered mutation	UNP Q7XJJ7
C	608	LYS	-	expression tag	UNP Q7XJJ7
C	609	GLY	-	expression tag	UNP Q7XJJ7
C	610	GLU	-	expression tag	UNP Q7XJJ7
C	611	PHE	-	expression tag	UNP Q7XJJ7
C	612	GLU	-	expression tag	UNP Q7XJJ7
C	613	ALA	-	expression tag	UNP Q7XJJ7
C	614	TYR	-	expression tag	UNP Q7XJJ7
C	615	VAL	-	expression tag	UNP Q7XJJ7
C	616	GLU	-	expression tag	UNP Q7XJJ7
C	617	GLN	-	expression tag	UNP Q7XJJ7
C	618	LYS	-	expression tag	UNP Q7XJJ7
C	619	LEU	-	expression tag	UNP Q7XJJ7
C	620	ILE	-	expression tag	UNP Q7XJJ7
C	621	SER	-	expression tag	UNP Q7XJJ7
C	622	GLU	-	expression tag	UNP Q7XJJ7
C	623	GLU	-	expression tag	UNP Q7XJJ7
C	624	ASP	-	expression tag	UNP Q7XJJ7
C	625	LEU	-	expression tag	UNP Q7XJJ7
C	626	ASN	-	expression tag	UNP Q7XJJ7
C	627	SER	-	expression tag	UNP Q7XJJ7
C	628	ALA	-	expression tag	UNP Q7XJJ7
C	629	VAL	-	expression tag	UNP Q7XJJ7
C	630	ASP	-	expression tag	UNP Q7XJJ7
C	631	HIS	-	expression tag	UNP Q7XJJ7
C	632	HIS	-	expression tag	UNP Q7XJJ7
C	633	HIS	-	expression tag	UNP Q7XJJ7
C	634	HIS	-	expression tag	UNP Q7XJJ7
C	635	HIS	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	636	HIS	-	expression tag	UNP Q7XJJ7
D	305	ALA	SER	engineered mutation	UNP Q7XJJ7
D	608	LYS	-	expression tag	UNP Q7XJJ7
D	609	GLY	-	expression tag	UNP Q7XJJ7
D	610	GLU	-	expression tag	UNP Q7XJJ7
D	611	PHE	-	expression tag	UNP Q7XJJ7
D	612	GLU	-	expression tag	UNP Q7XJJ7
D	613	ALA	-	expression tag	UNP Q7XJJ7
D	614	TYR	-	expression tag	UNP Q7XJJ7
D	615	VAL	-	expression tag	UNP Q7XJJ7
D	616	GLU	-	expression tag	UNP Q7XJJ7
D	617	GLN	-	expression tag	UNP Q7XJJ7
D	618	LYS	-	expression tag	UNP Q7XJJ7
D	619	LEU	-	expression tag	UNP Q7XJJ7
D	620	ILE	-	expression tag	UNP Q7XJJ7
D	621	SER	-	expression tag	UNP Q7XJJ7
D	622	GLU	-	expression tag	UNP Q7XJJ7
D	623	GLU	-	expression tag	UNP Q7XJJ7
D	624	ASP	-	expression tag	UNP Q7XJJ7
D	625	LEU	-	expression tag	UNP Q7XJJ7
D	626	ASN	-	expression tag	UNP Q7XJJ7
D	627	SER	-	expression tag	UNP Q7XJJ7
D	628	ALA	-	expression tag	UNP Q7XJJ7
D	629	VAL	-	expression tag	UNP Q7XJJ7
D	630	ASP	-	expression tag	UNP Q7XJJ7
D	631	HIS	-	expression tag	UNP Q7XJJ7
D	632	HIS	-	expression tag	UNP Q7XJJ7
D	633	HIS	-	expression tag	UNP Q7XJJ7
D	634	HIS	-	expression tag	UNP Q7XJJ7
D	635	HIS	-	expression tag	UNP Q7XJJ7
D	636	HIS	-	expression tag	UNP Q7XJJ7
E	305	ALA	SER	engineered mutation	UNP Q7XJJ7
E	608	LYS	-	expression tag	UNP Q7XJJ7
E	609	GLY	-	expression tag	UNP Q7XJJ7
E	610	GLU	-	expression tag	UNP Q7XJJ7
E	611	PHE	-	expression tag	UNP Q7XJJ7
E	612	GLU	-	expression tag	UNP Q7XJJ7
E	613	ALA	-	expression tag	UNP Q7XJJ7
E	614	TYR	-	expression tag	UNP Q7XJJ7
E	615	VAL	-	expression tag	UNP Q7XJJ7
E	616	GLU	-	expression tag	UNP Q7XJJ7
E	617	GLN	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	618	LYS	-	expression tag	UNP Q7XJJ7
E	619	LEU	-	expression tag	UNP Q7XJJ7
E	620	ILE	-	expression tag	UNP Q7XJJ7
E	621	SER	-	expression tag	UNP Q7XJJ7
E	622	GLU	-	expression tag	UNP Q7XJJ7
E	623	GLU	-	expression tag	UNP Q7XJJ7
E	624	ASP	-	expression tag	UNP Q7XJJ7
E	625	LEU	-	expression tag	UNP Q7XJJ7
E	626	ASN	-	expression tag	UNP Q7XJJ7
E	627	SER	-	expression tag	UNP Q7XJJ7
E	628	ALA	-	expression tag	UNP Q7XJJ7
E	629	VAL	-	expression tag	UNP Q7XJJ7
E	630	ASP	-	expression tag	UNP Q7XJJ7
E	631	HIS	-	expression tag	UNP Q7XJJ7
E	632	HIS	-	expression tag	UNP Q7XJJ7
E	633	HIS	-	expression tag	UNP Q7XJJ7
E	634	HIS	-	expression tag	UNP Q7XJJ7
E	635	HIS	-	expression tag	UNP Q7XJJ7
E	636	HIS	-	expression tag	UNP Q7XJJ7
F	305	ALA	SER	engineered mutation	UNP Q7XJJ7
F	608	LYS	-	expression tag	UNP Q7XJJ7
F	609	GLY	-	expression tag	UNP Q7XJJ7
F	610	GLU	-	expression tag	UNP Q7XJJ7
F	611	PHE	-	expression tag	UNP Q7XJJ7
F	612	GLU	-	expression tag	UNP Q7XJJ7
F	613	ALA	-	expression tag	UNP Q7XJJ7
F	614	TYR	-	expression tag	UNP Q7XJJ7
F	615	VAL	-	expression tag	UNP Q7XJJ7
F	616	GLU	-	expression tag	UNP Q7XJJ7
F	617	GLN	-	expression tag	UNP Q7XJJ7
F	618	LYS	-	expression tag	UNP Q7XJJ7
F	619	LEU	-	expression tag	UNP Q7XJJ7
F	620	ILE	-	expression tag	UNP Q7XJJ7
F	621	SER	-	expression tag	UNP Q7XJJ7
F	622	GLU	-	expression tag	UNP Q7XJJ7
F	623	GLU	-	expression tag	UNP Q7XJJ7
F	624	ASP	-	expression tag	UNP Q7XJJ7
F	625	LEU	-	expression tag	UNP Q7XJJ7
F	626	ASN	-	expression tag	UNP Q7XJJ7
F	627	SER	-	expression tag	UNP Q7XJJ7
F	628	ALA	-	expression tag	UNP Q7XJJ7
F	629	VAL	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	630	ASP	-	expression tag	UNP Q7XJJ7
F	631	HIS	-	expression tag	UNP Q7XJJ7
F	632	HIS	-	expression tag	UNP Q7XJJ7
F	633	HIS	-	expression tag	UNP Q7XJJ7
F	634	HIS	-	expression tag	UNP Q7XJJ7
F	635	HIS	-	expression tag	UNP Q7XJJ7
F	636	HIS	-	expression tag	UNP Q7XJJ7
G	305	ALA	SER	engineered mutation	UNP Q7XJJ7
G	608	LYS	-	expression tag	UNP Q7XJJ7
G	609	GLY	-	expression tag	UNP Q7XJJ7
G	610	GLU	-	expression tag	UNP Q7XJJ7
G	611	PHE	-	expression tag	UNP Q7XJJ7
G	612	GLU	-	expression tag	UNP Q7XJJ7
G	613	ALA	-	expression tag	UNP Q7XJJ7
G	614	TYR	-	expression tag	UNP Q7XJJ7
G	615	VAL	-	expression tag	UNP Q7XJJ7
G	616	GLU	-	expression tag	UNP Q7XJJ7
G	617	GLN	-	expression tag	UNP Q7XJJ7
G	618	LYS	-	expression tag	UNP Q7XJJ7
G	619	LEU	-	expression tag	UNP Q7XJJ7
G	620	ILE	-	expression tag	UNP Q7XJJ7
G	621	SER	-	expression tag	UNP Q7XJJ7
G	622	GLU	-	expression tag	UNP Q7XJJ7
G	623	GLU	-	expression tag	UNP Q7XJJ7
G	624	ASP	-	expression tag	UNP Q7XJJ7
G	625	LEU	-	expression tag	UNP Q7XJJ7
G	626	ASN	-	expression tag	UNP Q7XJJ7
G	627	SER	-	expression tag	UNP Q7XJJ7
G	628	ALA	-	expression tag	UNP Q7XJJ7
G	629	VAL	-	expression tag	UNP Q7XJJ7
G	630	ASP	-	expression tag	UNP Q7XJJ7
G	631	HIS	-	expression tag	UNP Q7XJJ7
G	632	HIS	-	expression tag	UNP Q7XJJ7
G	633	HIS	-	expression tag	UNP Q7XJJ7
G	634	HIS	-	expression tag	UNP Q7XJJ7
G	635	HIS	-	expression tag	UNP Q7XJJ7
G	636	HIS	-	expression tag	UNP Q7XJJ7
H	305	ALA	SER	engineered mutation	UNP Q7XJJ7
H	608	LYS	-	expression tag	UNP Q7XJJ7
H	609	GLY	-	expression tag	UNP Q7XJJ7
H	610	GLU	-	expression tag	UNP Q7XJJ7
H	611	PHE	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	612	GLU	-	expression tag	UNP Q7XJJ7
H	613	ALA	-	expression tag	UNP Q7XJJ7
H	614	TYR	-	expression tag	UNP Q7XJJ7
H	615	VAL	-	expression tag	UNP Q7XJJ7
H	616	GLU	-	expression tag	UNP Q7XJJ7
H	617	GLN	-	expression tag	UNP Q7XJJ7
H	618	LYS	-	expression tag	UNP Q7XJJ7
H	619	LEU	-	expression tag	UNP Q7XJJ7
H	620	ILE	-	expression tag	UNP Q7XJJ7
H	621	SER	-	expression tag	UNP Q7XJJ7
H	622	GLU	-	expression tag	UNP Q7XJJ7
H	623	GLU	-	expression tag	UNP Q7XJJ7
H	624	ASP	-	expression tag	UNP Q7XJJ7
H	625	LEU	-	expression tag	UNP Q7XJJ7
H	626	ASN	-	expression tag	UNP Q7XJJ7
H	627	SER	-	expression tag	UNP Q7XJJ7
H	628	ALA	-	expression tag	UNP Q7XJJ7
H	629	VAL	-	expression tag	UNP Q7XJJ7
H	630	ASP	-	expression tag	UNP Q7XJJ7
H	631	HIS	-	expression tag	UNP Q7XJJ7
H	632	HIS	-	expression tag	UNP Q7XJJ7
H	633	HIS	-	expression tag	UNP Q7XJJ7
H	634	HIS	-	expression tag	UNP Q7XJJ7
H	635	HIS	-	expression tag	UNP Q7XJJ7
H	636	HIS	-	expression tag	UNP Q7XJJ7
I	305	ALA	SER	engineered mutation	UNP Q7XJJ7
I	608	LYS	-	expression tag	UNP Q7XJJ7
I	609	GLY	-	expression tag	UNP Q7XJJ7
I	610	GLU	-	expression tag	UNP Q7XJJ7
I	611	PHE	-	expression tag	UNP Q7XJJ7
I	612	GLU	-	expression tag	UNP Q7XJJ7
I	613	ALA	-	expression tag	UNP Q7XJJ7
I	614	TYR	-	expression tag	UNP Q7XJJ7
I	615	VAL	-	expression tag	UNP Q7XJJ7
I	616	GLU	-	expression tag	UNP Q7XJJ7
I	617	GLN	-	expression tag	UNP Q7XJJ7
I	618	LYS	-	expression tag	UNP Q7XJJ7
I	619	LEU	-	expression tag	UNP Q7XJJ7
I	620	ILE	-	expression tag	UNP Q7XJJ7
I	621	SER	-	expression tag	UNP Q7XJJ7
I	622	GLU	-	expression tag	UNP Q7XJJ7
I	623	GLU	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	624	ASP	-	expression tag	UNP Q7XJJ7
I	625	LEU	-	expression tag	UNP Q7XJJ7
I	626	ASN	-	expression tag	UNP Q7XJJ7
I	627	SER	-	expression tag	UNP Q7XJJ7
I	628	ALA	-	expression tag	UNP Q7XJJ7
I	629	VAL	-	expression tag	UNP Q7XJJ7
I	630	ASP	-	expression tag	UNP Q7XJJ7
I	631	HIS	-	expression tag	UNP Q7XJJ7
I	632	HIS	-	expression tag	UNP Q7XJJ7
I	633	HIS	-	expression tag	UNP Q7XJJ7
I	634	HIS	-	expression tag	UNP Q7XJJ7
I	635	HIS	-	expression tag	UNP Q7XJJ7
I	636	HIS	-	expression tag	UNP Q7XJJ7
J	305	ALA	SER	engineered mutation	UNP Q7XJJ7
J	608	LYS	-	expression tag	UNP Q7XJJ7
J	609	GLY	-	expression tag	UNP Q7XJJ7
J	610	GLU	-	expression tag	UNP Q7XJJ7
J	611	PHE	-	expression tag	UNP Q7XJJ7
J	612	GLU	-	expression tag	UNP Q7XJJ7
J	613	ALA	-	expression tag	UNP Q7XJJ7
J	614	TYR	-	expression tag	UNP Q7XJJ7
J	615	VAL	-	expression tag	UNP Q7XJJ7
J	616	GLU	-	expression tag	UNP Q7XJJ7
J	617	GLN	-	expression tag	UNP Q7XJJ7
J	618	LYS	-	expression tag	UNP Q7XJJ7
J	619	LEU	-	expression tag	UNP Q7XJJ7
J	620	ILE	-	expression tag	UNP Q7XJJ7
J	621	SER	-	expression tag	UNP Q7XJJ7
J	622	GLU	-	expression tag	UNP Q7XJJ7
J	623	GLU	-	expression tag	UNP Q7XJJ7
J	624	ASP	-	expression tag	UNP Q7XJJ7
J	625	LEU	-	expression tag	UNP Q7XJJ7
J	626	ASN	-	expression tag	UNP Q7XJJ7
J	627	SER	-	expression tag	UNP Q7XJJ7
J	628	ALA	-	expression tag	UNP Q7XJJ7
J	629	VAL	-	expression tag	UNP Q7XJJ7
J	630	ASP	-	expression tag	UNP Q7XJJ7
J	631	HIS	-	expression tag	UNP Q7XJJ7
J	632	HIS	-	expression tag	UNP Q7XJJ7
J	633	HIS	-	expression tag	UNP Q7XJJ7
J	634	HIS	-	expression tag	UNP Q7XJJ7
J	635	HIS	-	expression tag	UNP Q7XJJ7

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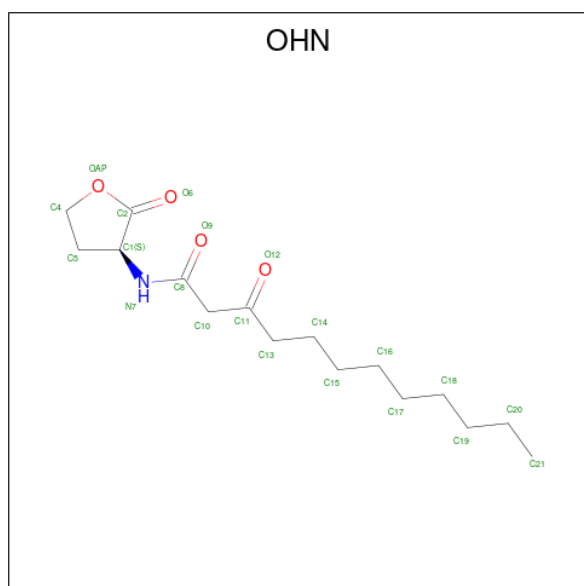
Chain	Residue	Modelled	Actual	Comment	Reference
J	636	HIS	-	expression tag	UNP Q7XJJ7
K	305	ALA	SER	engineered mutation	UNP Q7XJJ7
K	608	LYS	-	expression tag	UNP Q7XJJ7
K	609	GLY	-	expression tag	UNP Q7XJJ7
K	610	GLU	-	expression tag	UNP Q7XJJ7
K	611	PHE	-	expression tag	UNP Q7XJJ7
K	612	GLU	-	expression tag	UNP Q7XJJ7
K	613	ALA	-	expression tag	UNP Q7XJJ7
K	614	TYR	-	expression tag	UNP Q7XJJ7
K	615	VAL	-	expression tag	UNP Q7XJJ7
K	616	GLU	-	expression tag	UNP Q7XJJ7
K	617	GLN	-	expression tag	UNP Q7XJJ7
K	618	LYS	-	expression tag	UNP Q7XJJ7
K	619	LEU	-	expression tag	UNP Q7XJJ7
K	620	ILE	-	expression tag	UNP Q7XJJ7
K	621	SER	-	expression tag	UNP Q7XJJ7
K	622	GLU	-	expression tag	UNP Q7XJJ7
K	623	GLU	-	expression tag	UNP Q7XJJ7
K	624	ASP	-	expression tag	UNP Q7XJJ7
K	625	LEU	-	expression tag	UNP Q7XJJ7
K	626	ASN	-	expression tag	UNP Q7XJJ7
K	627	SER	-	expression tag	UNP Q7XJJ7
K	628	ALA	-	expression tag	UNP Q7XJJ7
K	629	VAL	-	expression tag	UNP Q7XJJ7
K	630	ASP	-	expression tag	UNP Q7XJJ7
K	631	HIS	-	expression tag	UNP Q7XJJ7
K	632	HIS	-	expression tag	UNP Q7XJJ7
K	633	HIS	-	expression tag	UNP Q7XJJ7
K	634	HIS	-	expression tag	UNP Q7XJJ7
K	635	HIS	-	expression tag	UNP Q7XJJ7
K	636	HIS	-	expression tag	UNP Q7XJJ7
L	305	ALA	SER	engineered mutation	UNP Q7XJJ7
L	608	LYS	-	expression tag	UNP Q7XJJ7
L	609	GLY	-	expression tag	UNP Q7XJJ7
L	610	GLU	-	expression tag	UNP Q7XJJ7
L	611	PHE	-	expression tag	UNP Q7XJJ7
L	612	GLU	-	expression tag	UNP Q7XJJ7
L	613	ALA	-	expression tag	UNP Q7XJJ7
L	614	TYR	-	expression tag	UNP Q7XJJ7
L	615	VAL	-	expression tag	UNP Q7XJJ7
L	616	GLU	-	expression tag	UNP Q7XJJ7
L	617	GLN	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
L	618	LYS	-	expression tag	UNP Q7XJJ7
L	619	LEU	-	expression tag	UNP Q7XJJ7
L	620	ILE	-	expression tag	UNP Q7XJJ7
L	621	SER	-	expression tag	UNP Q7XJJ7
L	622	GLU	-	expression tag	UNP Q7XJJ7
L	623	GLU	-	expression tag	UNP Q7XJJ7
L	624	ASP	-	expression tag	UNP Q7XJJ7
L	625	LEU	-	expression tag	UNP Q7XJJ7
L	626	ASN	-	expression tag	UNP Q7XJJ7
L	627	SER	-	expression tag	UNP Q7XJJ7
L	628	ALA	-	expression tag	UNP Q7XJJ7
L	629	VAL	-	expression tag	UNP Q7XJJ7
L	630	ASP	-	expression tag	UNP Q7XJJ7
L	631	HIS	-	expression tag	UNP Q7XJJ7
L	632	HIS	-	expression tag	UNP Q7XJJ7
L	633	HIS	-	expression tag	UNP Q7XJJ7
L	634	HIS	-	expression tag	UNP Q7XJJ7
L	635	HIS	-	expression tag	UNP Q7XJJ7
L	636	HIS	-	expression tag	UNP Q7XJJ7

- Molecule 2 is N-3-OXO-DODECANOYL-L-HOMOSERINE LACTONE (CCD ID: OHN) (formula: C₁₆H₂₇NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			21	16	1	4		

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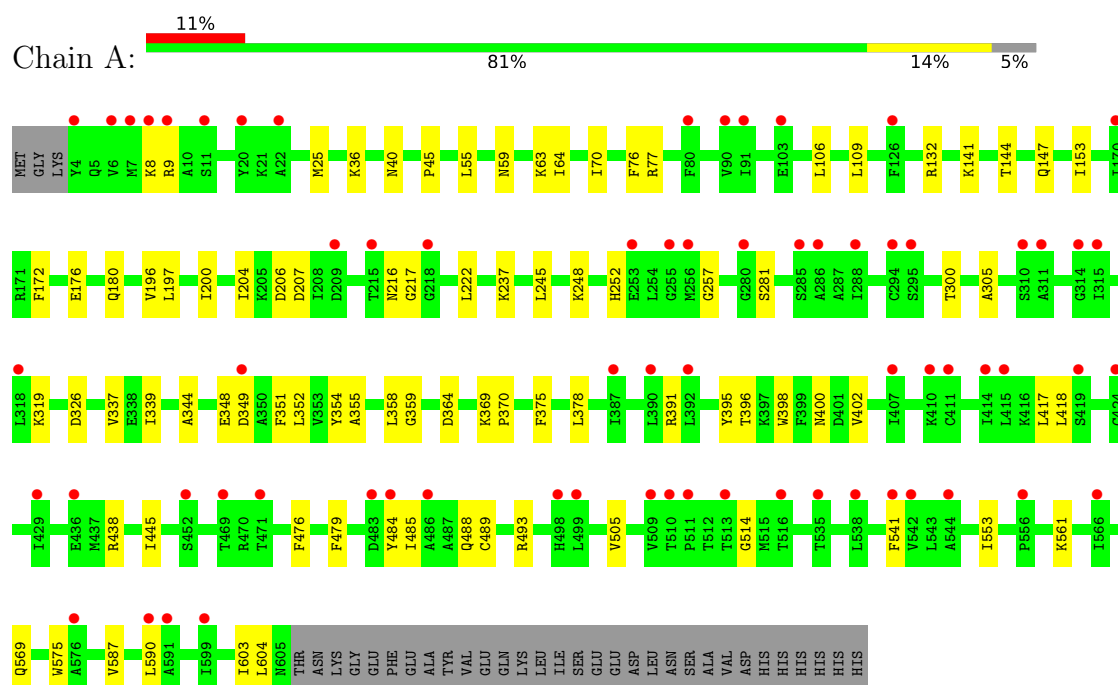
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			21	16	1	4		
2	H	1	Total	C	N	O	0	0
			21	16	1	4		
2	J	1	Total	C	N	O	0	0
			21	16	1	4		
2	L	1	Total	C	N	O	0	0
			21	16	1	4		

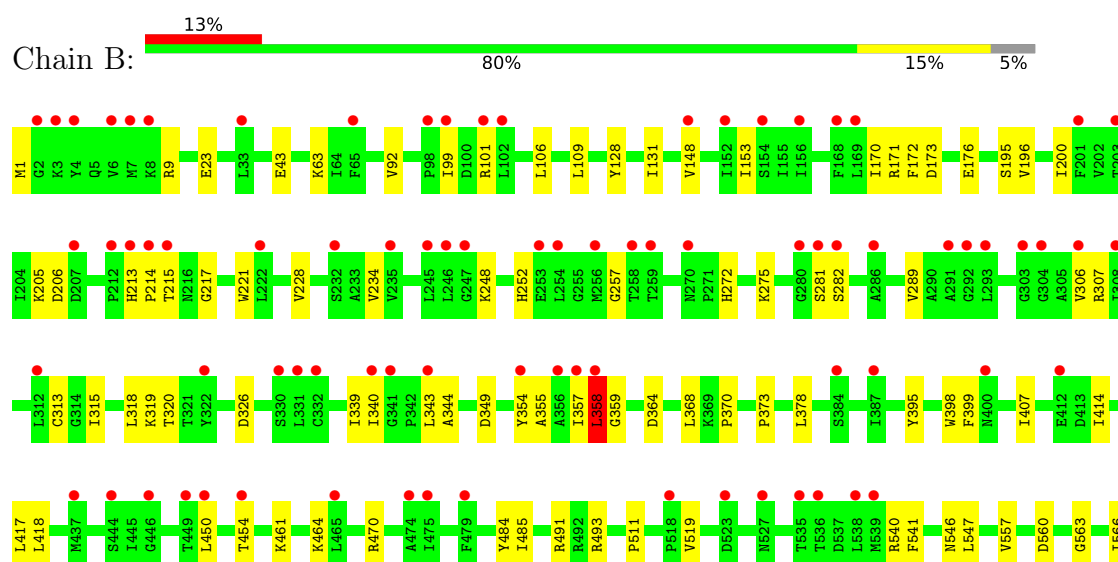
3 Residue-property plots [i](#)

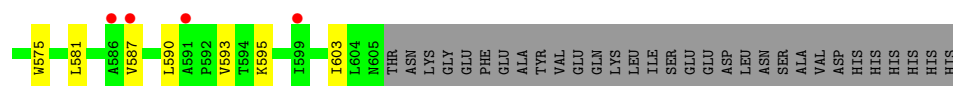
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fatty acid amide hydrolase

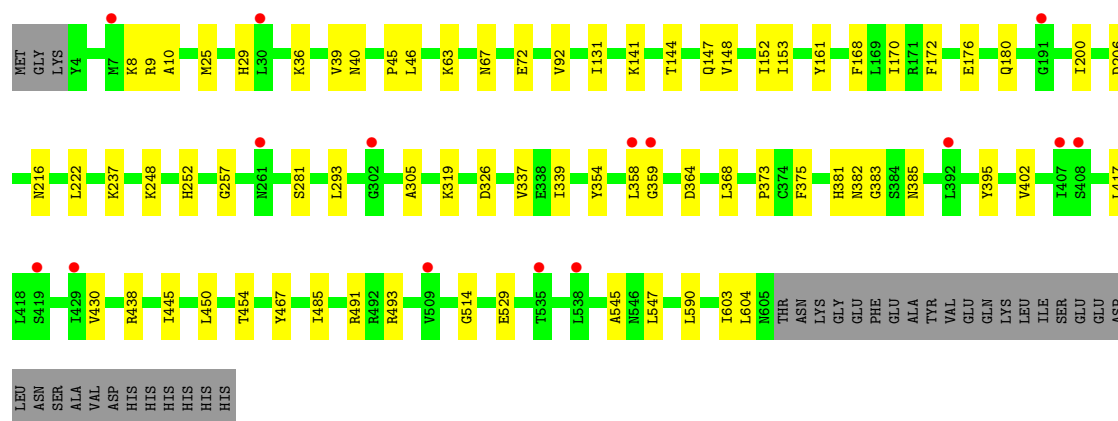
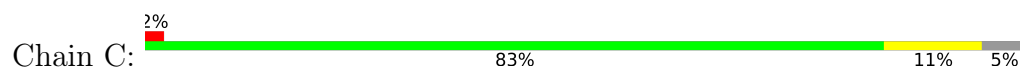


• Molecule 1: Fatty acid amide hydrolase

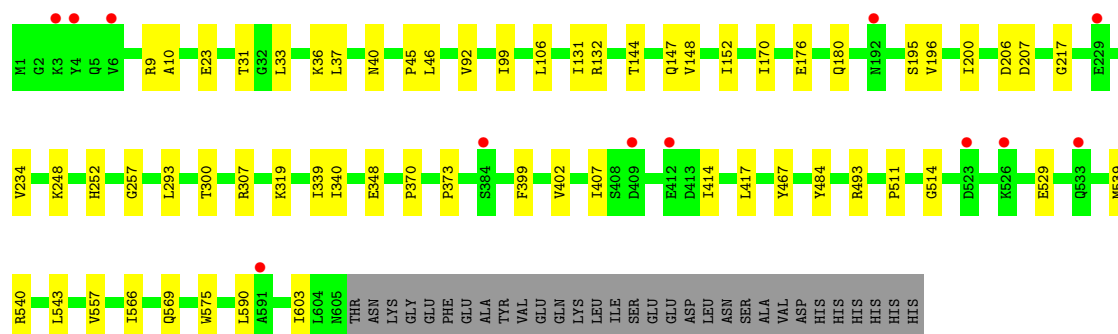
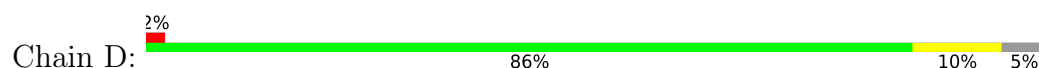




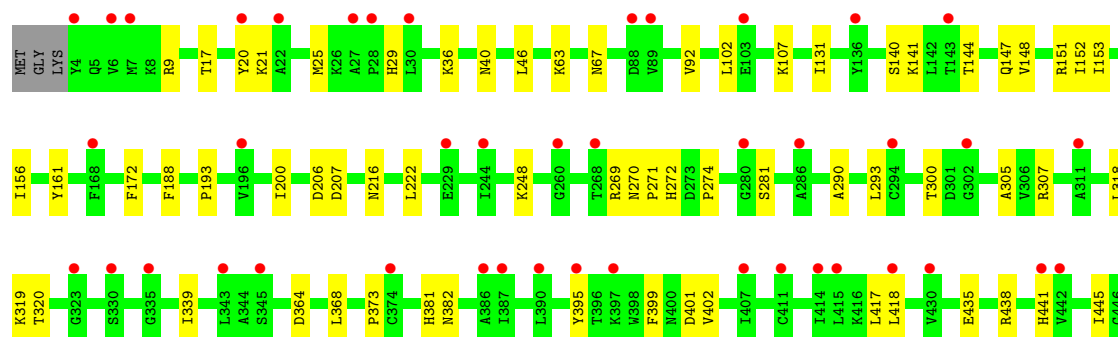
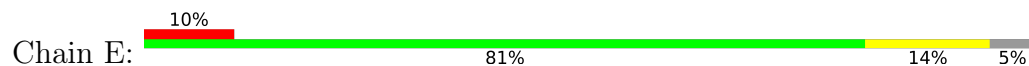
● Molecule 1: Fatty acid amide hydrolase

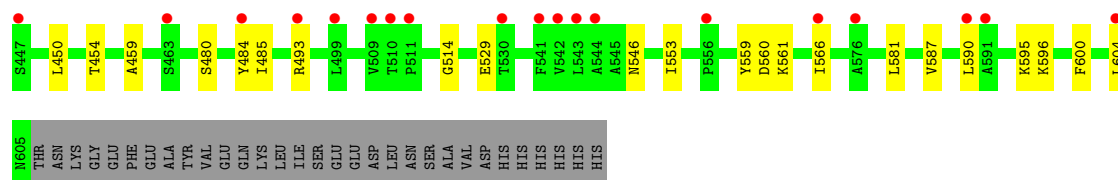


● Molecule 1: Fatty acid amide hydrolase



● Molecule 1: Fatty acid amide hydrolase

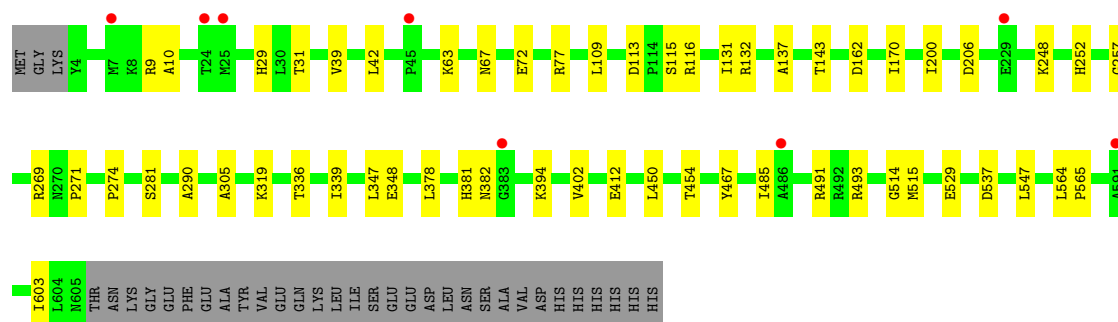
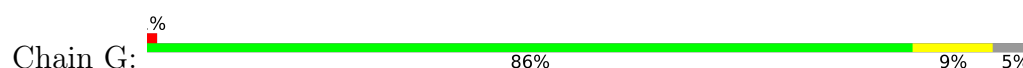




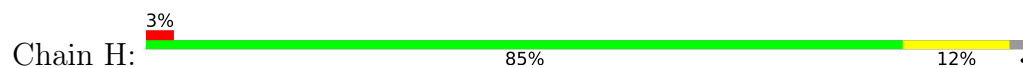
• Molecule 1: Fatty acid amide hydrolase

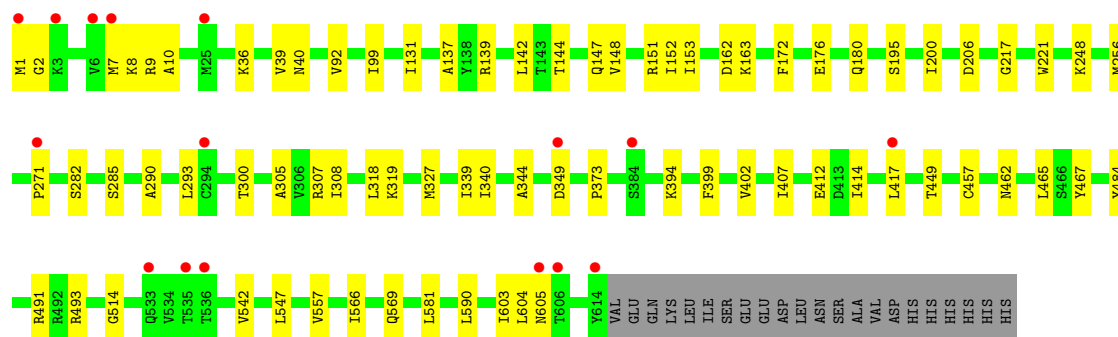


• Molecule 1: Fatty acid amide hydrolase

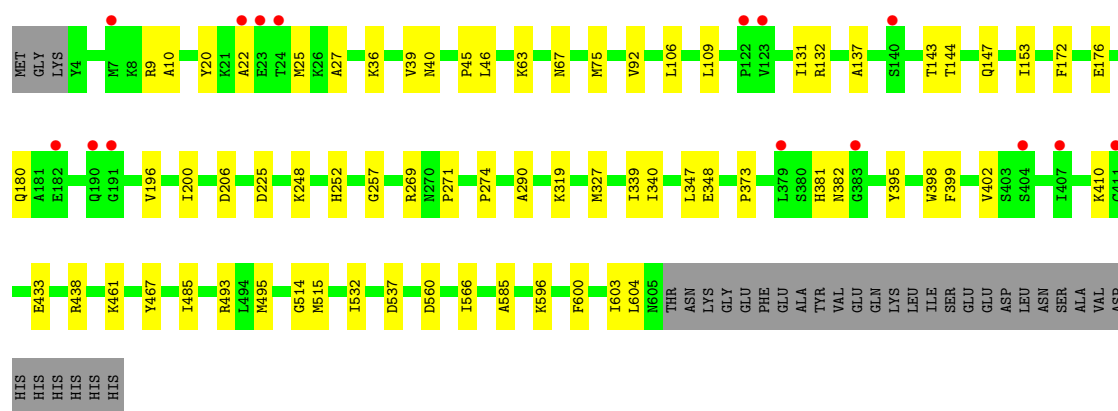
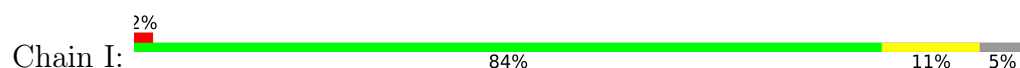


• Molecule 1: Fatty acid amide hydrolase

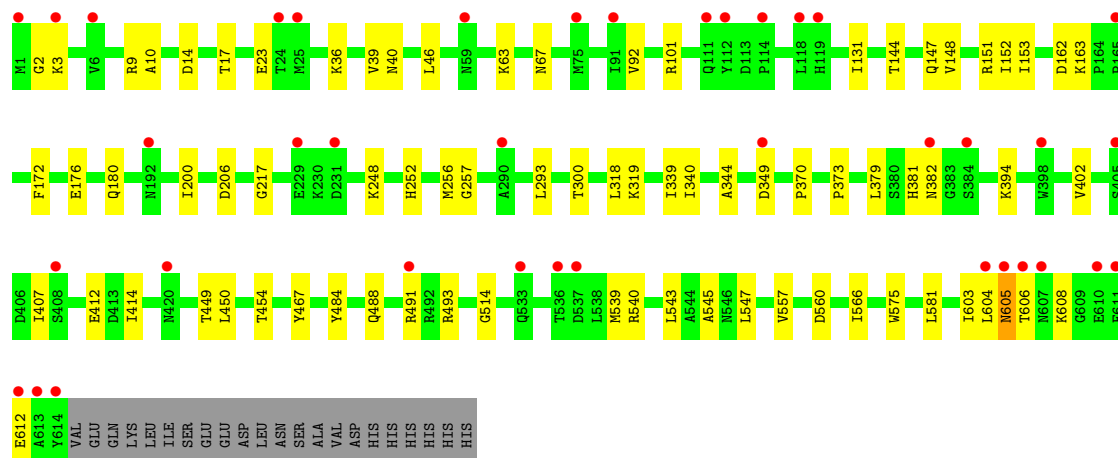
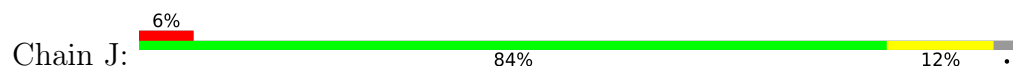




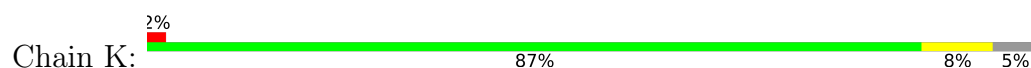
• Molecule 1: Fatty acid amide hydrolase

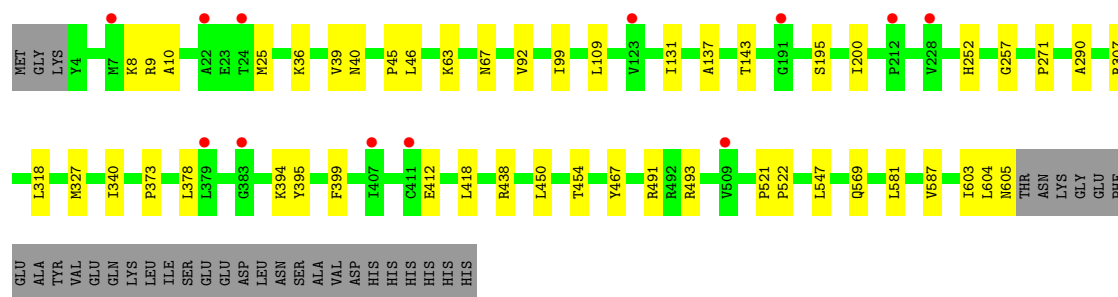


• Molecule 1: Fatty acid amide hydrolase

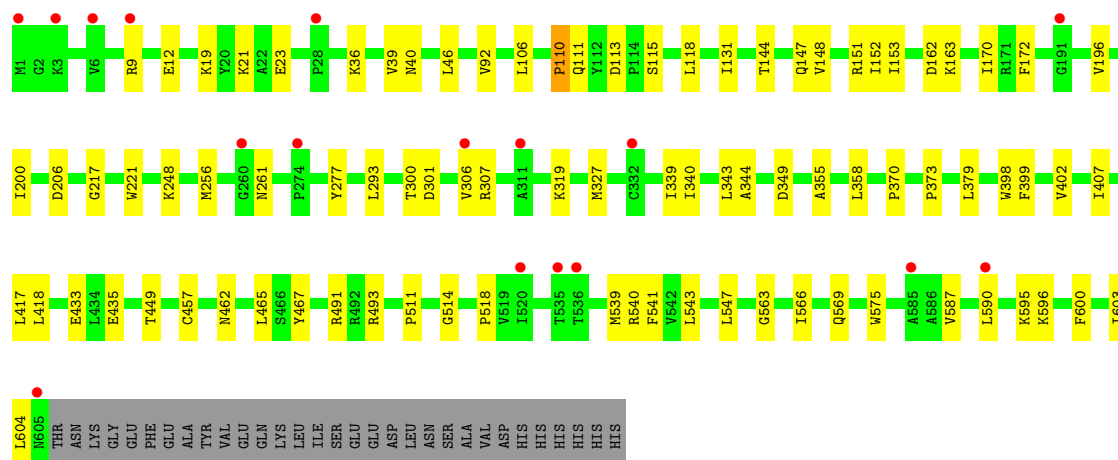
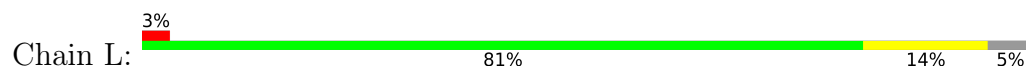


• Molecule 1: Fatty acid amide hydrolase





• 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	225.54Å 83.75Å 270.94Å 90.00° 109.57° 90.00°	Depositor
Resolution (Å)	39.82 – 3.20 39.82 – 3.20	Depositor EDS
% Data completeness (in resolution range)	88.9 (39.82-3.20) 88.8 (39.82-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.18Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.259 , 0.290 0.260 , 0.291	Depositor DCC
R_{free} test set	2013 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55639	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.52 % 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 5.0747e-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: OHN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/4704	0.26	0/6391
1	B	0.09	0/4725	0.27	1/6417 (0.0%)
1	C	0.09	0/4704	0.25	0/6391
1	D	0.10	0/4725	0.26	0/6417
1	E	0.09	0/4704	0.24	0/6391
1	F	0.09	0/4725	0.26	0/6417
1	G	0.09	0/4704	0.26	0/6391
1	H	0.09	0/4801	0.25	0/6519
1	I	0.10	0/4704	0.26	0/6391
1	J	0.11	0/4801	0.36	4/6519 (0.1%)
1	K	0.09	0/4704	0.25	0/6391
1	L	0.09	0/4725	0.26	0/6417
All	All	0.09	0/56726	0.27	5/77052 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	605	ASN	N-CA-C	-11.27	93.68	110.24
1	J	605	ASN	CB-CA-C	9.85	124.61	109.84
1	J	606	THR	CB-CA-C	8.14	122.86	110.08
1	B	358	LEU	N-CA-C	6.33	118.27	109.15
1	J	606	THR	N-CA-C	-5.66	105.40	112.93

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	4605	0	4627	53	0
1	B	4626	0	4655	63	0
1	C	4605	0	4627	41	0
1	D	4626	0	4655	36	0
1	E	4605	0	4627	50	0
1	F	4626	0	4655	66	0
1	G	4605	0	4627	33	0
1	H	4700	0	4719	47	0
1	I	4605	0	4627	40	0
1	J	4700	0	4719	46	0
1	K	4605	0	4627	26	0
1	L	4626	0	4655	51	0
2	D	21	0	27	2	0
2	F	21	0	27	2	0
2	H	21	0	27	2	0
2	J	21	0	27	1	0
2	L	21	0	27	2	0
All	All	55639	0	55955	544	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 (544) 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)
2:H:700:OHN:C2	2:H:700:OHN:OAP	1.68	1.18
2:J:700:OHN:C2	2:J:700:OHN:OAP	1.68	1.15
2:L:700:OHN:OAP	2:L:700:OHN:C2	1.68	1.14
2:F:700:OHN:OAP	2:F:700:OHN:C2	1.68	1.12
2:D:700:OHN:OAP	2:D:700:OHN:C2	1.68	1.11
1:B:355:ALA:HA	1:B:358:LEU:HD23	1.46	0.97
1:A:355:ALA:HA	1:A:358:LEU:HD23	1.52	0.91
1:B:355:ALA:HA	1:B:358:LEU:CD2	2.09	0.82
1:H:137:ALA:HA	1:H:142:LEU:HD12	1.62	0.79
1:A:355:ALA:HA	1:A:358:LEU:CD2	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:LYS:HE2	1:D:339:ILE:HG12	1.69	0.74
1:F:209:ASP:OD1	1:F:226:ARG:NH2	2.21	0.73
1:A:319:LYS:HE2	1:A:339:ILE:HG12	1.71	0.71
1:B:214:PRO:HA	1:B:228:VAL:HG21	1.73	0.70
1:K:9:ARG:O	1:K:493:ARG:NH2	2.24	0.69
1:K:39:VAL:HG21	1:K:467:TYR:HB3	1.75	0.69
1:H:9:ARG:O	1:H:493:ARG:NH2	2.26	0.68
1:L:300:THR:HG22	1:L:340:ILE:HG12	1.73	0.68
1:J:9:ARG:O	1:J:493:ARG:NH2	2.25	0.68
1:D:9:ARG:O	1:D:493:ARG:NH2	2.26	0.68
1:E:319:LYS:HE2	1:E:339:ILE:HG12	1.74	0.68
1:B:319:LYS:HE2	1:B:339:ILE:HG12	1.75	0.68
1:F:156:ILE:HG23	1:F:161:TYR:HB2	1.77	0.67
1:J:539:MET:HE2	1:J:543:LEU:HD21	1.75	0.67
1:C:9:ARG:O	1:C:493:ARG:NH2	2.28	0.66
1:F:450:LEU:O	1:F:454:THR:OG1	2.13	0.65
1:H:603:ILE:HG22	1:H:604:LEU:H	1.60	0.65
1:C:36:LYS:O	1:C:40:ASN:ND2	2.30	0.65
1:F:319:LYS:HE2	1:F:339:ILE:HG12	1.79	0.65
1:A:358:LEU:HD12	1:A:358:LEU:O	1.97	0.65
1:C:319:LYS:HE2	1:C:339:ILE:HG12	1.79	0.64
1:J:491:ARG:HG3	1:J:547:LEU:HG	1.80	0.64
1:L:9:ARG:O	1:L:493:ARG:NH2	2.29	0.64
1:I:603:ILE:HG22	1:I:604:LEU:H	1.63	0.64
1:L:402:VAL:HG12	1:L:514:GLY:HA2	1.79	0.64
1:L:261:ASN:ND2	1:L:277:TYR:OH	2.30	0.63
1:D:23:GLU:HG3	1:D:540:ARG:HH21	1.64	0.63
1:B:9:ARG:O	1:B:493:ARG:NH2	2.31	0.63
1:A:402:VAL:HG12	1:A:514:GLY:HA2	1.79	0.63
1:H:402:VAL:HG12	1:H:514:GLY:HA2	1.80	0.63
1:L:148:VAL:HG13	1:L:603:ILE:HG21	1.80	0.62
1:I:25:MET:HE3	1:I:438:ARG:HE	1.64	0.62
1:C:144:THR:HG23	1:C:147:GLN:H	1.64	0.62
1:I:39:VAL:HG21	1:I:467:TYR:HB3	1.81	0.62
1:J:604:LEU:O	1:J:605:ASN:C	2.42	0.62
1:E:9:ARG:O	1:E:493:ARG:NH2	2.32	0.62
1:H:256:MET:HE3	1:H:449:THR:HG21	1.81	0.62
1:J:23:GLU:HG3	1:J:540:ARG:HH21	1.65	0.62
1:F:36:LYS:O	1:F:40:ASN:ND2	2.33	0.62
1:F:77:ARG:NH2	1:F:364:ASP:OD1	2.33	0.62
1:H:300:THR:HG22	1:H:340:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:ARG:HG2	1:L:603:ILE:HG23	1.81	0.61
1:F:381:HIS:CG	1:F:382:ASN:HA	2.35	0.61
1:A:395:TYR:HB3	1:A:398:TRP:HB3	1.83	0.61
1:D:36:LYS:O	1:D:40:ASN:ND2	2.33	0.61
1:J:319:LYS:HE2	1:J:339:ILE:HG12	1.81	0.61
1:F:206:ASP:OD2	1:F:217:GLY:N	2.33	0.61
1:I:63:LYS:HA	1:I:67:ASN:HB2	1.83	0.61
1:L:306:VAL:HG13	1:L:343:LEU:HG	1.82	0.61
1:H:151:ARG:HG2	1:H:603:ILE:HG23	1.82	0.61
1:A:36:LYS:O	1:A:40:ASN:ND2	2.34	0.60
1:G:347:LEU:O	1:G:347:LEU:HD13	2.01	0.60
1:C:46:LEU:HD13	1:D:46:LEU:HD13	1.83	0.60
1:B:92:VAL:HG13	1:B:373:PRO:HG2	1.83	0.60
1:F:173:ASP:HB3	1:F:176:GLU:HB3	1.84	0.60
1:L:256:MET:HE3	1:L:449:THR:HG21	1.82	0.60
1:E:152:ILE:HG23	1:E:293:LEU:HD22	1.83	0.59
1:J:144:THR:HG23	1:J:147:GLN:H	1.67	0.59
1:B:1:MET:HG3	1:E:107:LYS:HA	1.83	0.59
1:H:92:VAL:HG13	1:H:373:PRO:HG2	1.83	0.59
1:A:417:LEU:HB3	1:A:590:LEU:HD13	1.85	0.59
1:B:307:ARG:NH2	1:B:546:ASN:OD1	2.36	0.59
1:J:92:VAL:HG13	1:J:373:PRO:HG2	1.84	0.59
1:H:36:LYS:O	1:H:40:ASN:ND2	2.36	0.59
1:K:36:LYS:O	1:K:40:ASN:ND2	2.36	0.58
1:B:206:ASP:HA	1:B:248:LYS:HE2	1.84	0.58
1:D:206:ASP:HA	1:D:248:LYS:HE2	1.86	0.58
1:D:539:MET:HE2	1:D:543:LEU:HD21	1.85	0.58
1:B:358:LEU:O	1:B:358:LEU:HG	2.01	0.58
1:I:9:ARG:O	1:I:493:ARG:NH2	2.36	0.58
1:H:144:THR:HG23	1:H:147:GLN:H	1.67	0.58
1:D:148:VAL:HG13	1:D:603:ILE:HG21	1.86	0.58
1:H:39:VAL:HG21	1:H:467:TYR:HB3	1.86	0.58
1:B:358:LEU:O	1:B:358:LEU:CG	2.52	0.58
1:L:144:THR:HG23	1:L:147:GLN:H	1.69	0.58
1:L:23:GLU:HG3	1:L:540:ARG:HH21	1.68	0.58
1:B:99:ILE:HG23	1:B:195:SER:HB3	1.85	0.58
1:H:152:ILE:HG23	1:H:293:LEU:HD22	1.86	0.58
1:D:37:LEU:HA	1:D:40:ASN:HD22	1.69	0.57
1:K:92:VAL:HG13	1:K:373:PRO:HG2	1.86	0.57
2:L:700:OHN:O12	2:L:700:OHN:N7	2.37	0.57
1:L:327:MET:HG2	1:L:340:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:VAL:HG13	1:D:373:PRO:HG2	1.85	0.57
1:L:319:LYS:HE2	1:L:339:ILE:HG12	1.86	0.57
1:B:206:ASP:OD2	1:B:217:GLY:N	2.38	0.57
1:B:354:TYR:O	1:B:358:LEU:HD23	2.04	0.57
1:G:9:ARG:O	1:G:493:ARG:NH2	2.38	0.57
1:A:9:ARG:O	1:A:493:ARG:NH2	2.38	0.57
1:G:402:VAL:HG12	1:G:514:GLY:HA2	1.87	0.56
1:J:36:LYS:O	1:J:40:ASN:ND2	2.38	0.56
1:B:23:GLU:HG3	1:B:540:ARG:HH21	1.69	0.56
1:E:144:THR:HG23	1:E:147:GLN:H	1.70	0.56
1:F:205:LYS:NZ	1:F:281:SER:OG	2.38	0.56
1:I:131:ILE:HG23	1:I:200:ILE:HG12	1.88	0.56
1:F:307:ARG:NH1	1:F:569:GLN:OE1	2.36	0.56
1:L:539:MET:HE2	1:L:543:LEU:HD21	1.88	0.56
1:E:395:TYR:O	1:E:399:PHE:N	2.35	0.55
1:F:23:GLU:HG3	1:F:540:ARG:HH21	1.70	0.55
1:J:151:ARG:HG2	1:J:603:ILE:HG23	1.88	0.55
1:I:36:LYS:O	1:I:40:ASN:ND2	2.39	0.55
1:L:277:TYR:HD2	1:L:518:PRO:HG2	1.69	0.55
1:F:39:VAL:HG21	1:F:467:TYR:HB3	1.89	0.55
1:L:301:ASP:HB2	1:L:306:VAL:HG23	1.88	0.55
1:I:46:LEU:HD13	1:J:46:LEU:HD13	1.87	0.55
1:I:485:ILE:HD11	1:J:484:TYR:CZ	2.41	0.55
1:A:344:ALA:HB1	1:A:349:ASP:HB2	1.89	0.55
1:F:226:ARG:HH21	1:F:228:VAL:HG12	1.71	0.55
1:F:225:ASP:OD1	1:F:225:ASP:N	2.37	0.55
1:C:39:VAL:HG21	1:C:467:TYR:HB3	1.89	0.55
1:D:417:LEU:HB3	1:D:590:LEU:HD13	1.89	0.55
1:D:206:ASP:OD2	1:D:217:GLY:N	2.40	0.55
1:D:402:VAL:HG12	1:D:514:GLY:HA2	1.88	0.55
1:A:396:THR:O	1:A:400:ASN:ND2	2.40	0.54
1:B:148:VAL:HG13	1:B:603:ILE:HG21	1.88	0.54
1:L:153:ILE:HG12	1:L:172:PHE:HZ	1.72	0.54
1:J:148:VAL:HG13	1:J:603:ILE:HG21	1.88	0.54
1:K:46:LEU:HD13	1:L:46:LEU:HD13	1.88	0.54
1:A:603:ILE:HG22	1:A:604:LEU:H	1.71	0.54
1:H:1:MET:HG3	1:H:7:MET:HB2	1.88	0.54
1:E:153:ILE:HG12	1:E:172:PHE:HZ	1.72	0.54
1:G:63:LYS:HA	1:G:67:ASN:HB2	1.89	0.54
2:H:700:OHN:N7	2:H:700:OHN:O12	2.38	0.54
1:J:39:VAL:HG21	1:J:467:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:63:LYS:HA	1:K:67:ASN:HB2	1.90	0.54
1:F:417:LEU:HB3	1:F:590:LEU:HD13	1.90	0.54
1:H:176:GLU:HG3	1:H:180:GLN:HE21	1.73	0.54
1:A:206:ASP:HA	1:A:248:LYS:HE2	1.89	0.54
1:E:131:ILE:HG23	1:E:200:ILE:HG12	1.90	0.54
1:F:491:ARG:NH1	1:F:547:LEU:O	2.40	0.53
1:A:176:GLU:HG3	1:A:180:GLN:HE21	1.74	0.53
1:H:131:ILE:HG23	1:H:200:ILE:HG12	1.91	0.53
1:I:319:LYS:HE2	1:I:339:ILE:HG12	1.91	0.53
1:J:206:ASP:HA	1:J:248:LYS:HE2	1.90	0.53
1:B:417:LEU:HB3	1:B:590:LEU:HD13	1.89	0.53
1:L:92:VAL:HG13	1:L:373:PRO:HG2	1.89	0.53
1:B:450:LEU:O	1:B:454:THR:OG1	2.20	0.53
1:L:152:ILE:HG23	1:L:293:LEU:HD22	1.90	0.53
1:C:176:GLU:HG3	1:C:180:GLN:HE21	1.73	0.53
1:H:307:ARG:NH1	1:H:569:GLN:OE1	2.42	0.53
1:H:319:LYS:HE2	1:H:339:ILE:HG12	1.91	0.53
1:H:407:ILE:HG23	1:H:566:ILE:HG23	1.90	0.53
1:A:354:TYR:O	1:A:358:LEU:HD23	2.09	0.53
1:B:491:ARG:NH1	1:B:547:LEU:O	2.42	0.53
1:J:300:THR:HG22	1:J:340:ILE:HG12	1.91	0.53
1:G:9:ARG:HG2	1:G:10:ALA:H	1.74	0.53
1:F:143:THR:HG21	1:F:604:LEU:HD22	1.91	0.52
1:L:417:LEU:HB3	1:L:590:LEU:HD13	1.91	0.52
1:C:402:VAL:HG12	1:C:514:GLY:HA2	1.92	0.52
1:G:131:ILE:HG23	1:G:200:ILE:HG12	1.91	0.52
1:G:491:ARG:HG3	1:G:547:LEU:HG	1.92	0.52
1:A:355:ALA:CA	1:A:358:LEU:HD23	2.33	0.52
1:A:109:LEU:HD22	1:A:348:GLU:HG2	1.91	0.52
1:B:326:ASP:HB2	1:B:359:GLY:O	2.10	0.52
1:F:161:TYR:HH	1:F:601:TYR:HH	1.46	0.52
1:E:46:LEU:HD13	1:F:46:LEU:HD12	1.92	0.52
1:E:92:VAL:HG13	1:E:373:PRO:HG2	1.92	0.52
1:C:358:LEU:HD21	1:C:375:PHE:HE1	1.75	0.52
1:D:99:ILE:HG23	1:D:195:SER:HB3	1.92	0.52
1:D:176:GLU:HG3	1:D:180:GLN:HE21	1.74	0.52
1:F:226:ARG:HH11	1:F:331:LEU:HD23	1.73	0.52
1:B:106:LEU:HD21	1:B:196:VAL:HG11	1.93	0.51
1:E:450:LEU:O	1:E:454:THR:OG1	2.22	0.51
1:I:402:VAL:HG12	1:I:514:GLY:HA2	1.91	0.51
1:E:36:LYS:O	1:E:40:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:MET:HE3	1:F:449:THR:HG21	1.92	0.51
1:H:271:PRO:HG2	1:H:290:ALA:HB3	1.92	0.51
1:K:491:ARG:HG3	1:K:547:LEU:HG	1.92	0.51
1:G:113:ASP:OD1	1:L:19:LYS:NZ	2.43	0.51
1:L:407:ILE:HG23	1:L:566:ILE:HG23	1.91	0.51
1:E:25:MET:HE3	1:E:438:ARG:HE	1.76	0.51
1:D:414:ILE:HG13	1:D:557:VAL:HB	1.92	0.51
1:F:92:VAL:HG13	1:F:373:PRO:HG2	1.92	0.51
1:B:395:TYR:O	1:B:399:PHE:N	2.36	0.51
1:B:318:LEU:HD22	1:B:581:LEU:HD21	1.93	0.51
1:F:402:VAL:HG12	1:F:514:GLY:HA2	1.92	0.50
1:C:417:LEU:HB3	1:C:590:LEU:HD13	1.93	0.50
1:D:234:VAL:HG11	1:D:340:ILE:HG21	1.93	0.50
1:D:300:THR:HG22	1:D:340:ILE:HG12	1.93	0.50
1:B:398:TRP:HZ2	1:B:541:PHE:HA	1.76	0.50
1:B:414:ILE:HG13	1:B:557:VAL:HB	1.93	0.50
1:E:318:LEU:HD22	1:E:581:LEU:HD21	1.93	0.50
1:B:344:ALA:HB1	1:B:349:ASP:HB2	1.94	0.50
1:C:148:VAL:HG13	1:C:603:ILE:HG21	1.93	0.50
1:K:252:HIS:CE1	1:K:257:GLY:HA3	2.47	0.50
1:B:275:LYS:HG3	1:B:519:VAL:HG13	1.92	0.50
1:C:92:VAL:HG13	1:C:373:PRO:HG2	1.94	0.50
1:H:407:ILE:HA	1:H:566:ILE:HD13	1.94	0.50
1:B:131:ILE:HG23	1:B:200:ILE:HG12	1.94	0.49
1:B:395:TYR:HB3	1:B:398:TRP:HB3	1.94	0.49
1:C:152:ILE:HG23	1:C:293:LEU:HD22	1.94	0.49
1:C:364:ASP:HB3	1:C:368:LEU:HD12	1.94	0.49
1:I:144:THR:HG23	1:I:147:GLN:H	1.77	0.49
1:J:162:ASP:OD1	1:J:163:LYS:NZ	2.45	0.49
1:J:344:ALA:HB1	1:J:349:ASP:HB2	1.94	0.49
1:D:144:THR:HG23	1:D:147:GLN:H	1.77	0.49
1:G:39:VAL:HG21	1:G:467:TYR:HB3	1.94	0.49
1:H:1:MET:SD	1:H:1:MET:N	2.81	0.49
1:J:2:GLY:O	1:J:3:LYS:HD2	2.12	0.49
1:F:318:LEU:HD22	1:F:581:LEU:HD21	1.94	0.49
1:L:603:ILE:HG22	1:L:604:LEU:H	1.77	0.49
1:D:9:ARG:HG2	1:D:10:ALA:H	1.78	0.49
1:H:206:ASP:OD2	1:H:217:GLY:N	2.46	0.49
1:J:318:LEU:HD22	1:J:581:LEU:HD21	1.94	0.49
1:L:39:VAL:HG21	1:L:467:TYR:HB3	1.94	0.49
1:C:326:ASP:N	1:C:359:GLY:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:539:MET:HE2	1:F:543:LEU:HD21	1.94	0.49
1:I:225:ASP:OD2	1:I:461:LYS:NZ	2.39	0.49
1:E:307:ARG:NH2	1:E:546:ASN:OD1	2.45	0.49
1:J:394:LYS:NZ	1:J:412:GLU:OE2	2.34	0.49
1:A:391:ARG:HB2	1:A:505:VAL:HA	1.93	0.49
1:J:92:VAL:HG21	1:J:101:ARG:HG2	1.95	0.48
1:E:20:TYR:OH	1:E:401:ASP:OD2	2.21	0.48
1:I:433:GLU:OE1	1:I:493:ARG:NH2	2.31	0.48
1:H:206:ASP:HA	1:H:248:LYS:HE2	1.95	0.48
1:I:206:ASP:HA	1:I:248:LYS:HE2	1.94	0.48
1:L:433:GLU:OE1	1:L:493:ARG:NH2	2.35	0.48
1:H:300:THR:O	1:H:305:ALA:HB3	2.13	0.48
1:I:252:HIS:CE1	1:I:257:GLY:HA3	2.48	0.48
1:B:289:VAL:HG12	1:B:315:ILE:HG21	1.95	0.48
1:E:271:PRO:HG2	1:E:290:ALA:HB3	1.95	0.48
1:E:417:LEU:HB3	1:E:590:LEU:HD13	1.95	0.48
1:F:407:ILE:HG23	1:F:566:ILE:HG23	1.95	0.48
1:K:395:TYR:O	1:K:399:PHE:N	2.38	0.48
1:B:205:LYS:NZ	1:B:281:SER:OG	2.40	0.48
1:C:319:LYS:NZ	1:C:545:ALA:O	2.39	0.48
1:I:596:LYS:HE2	1:I:600:PHE:HB3	1.94	0.48
1:L:9:ARG:HG2	1:L:12:GLU:HB2	1.94	0.48
1:F:414:ILE:HG13	1:F:557:VAL:HB	1.96	0.48
1:I:395:TYR:O	1:I:399:PHE:N	2.40	0.48
1:A:109:LEU:HD23	1:A:378:LEU:HD12	1.96	0.48
1:D:152:ILE:HG23	1:D:293:LEU:HD22	1.94	0.48
1:D:132:ARG:NH2	1:D:348:GLU:OE2	2.47	0.47
1:K:327:MET:HG2	1:K:340:ILE:HG13	1.96	0.47
1:C:63:LYS:HA	1:C:67:ASN:HB2	1.96	0.47
1:H:9:ARG:HG2	1:H:10:ALA:H	1.78	0.47
1:K:131:ILE:HG23	1:K:200:ILE:HG12	1.96	0.47
1:L:491:ARG:HG3	1:L:547:LEU:HG	1.96	0.47
1:I:153:ILE:HG12	1:I:172:PHE:HZ	1.78	0.47
1:K:9:ARG:HG3	1:K:10:ALA:H	1.79	0.47
1:E:63:LYS:HA	1:E:67:ASN:HB2	1.95	0.47
1:F:162:ASP:OD1	1:F:162:ASP:N	2.45	0.47
1:J:152:ILE:HG23	1:J:293:LEU:HD22	1.97	0.47
1:A:132:ARG:NH2	1:A:348:GLU:OE2	2.35	0.47
1:A:351:PHE:HZ	1:A:375:PHE:HB3	1.79	0.47
1:E:21:LYS:NZ	1:E:435:GLU:OE1	2.33	0.47
1:H:153:ILE:HG12	1:H:172:PHE:HZ	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:LYS:HE2	1:K:493:ARG:CZ	2.45	0.47
1:K:604:LEU:O	1:K:605:ASN:ND2	2.47	0.47
1:L:36:LYS:O	1:L:40:ASN:ND2	2.48	0.47
1:L:131:ILE:HG23	1:L:200:ILE:HG12	1.97	0.47
1:A:207:ASP:OD2	1:A:300:THR:OG1	2.31	0.47
1:H:282:SER:HB3	1:H:285:SER:HB2	1.96	0.47
1:J:14:ASP:O	1:J:17:THR:HG22	2.14	0.47
1:G:485:ILE:HD11	1:H:484:TYR:CZ	2.50	0.47
1:L:457:CYS:HB3	1:L:462:ASN:HB2	1.95	0.47
1:L:596:LYS:HE2	1:L:600:PHE:HB3	1.97	0.47
1:C:9:ARG:HG2	1:C:10:ALA:H	1.80	0.47
1:E:216:ASN:HA	1:E:222:LEU:HB3	1.96	0.47
1:F:99:ILE:HG23	1:F:195:SER:HB3	1.97	0.47
1:H:394:LYS:HE3	1:H:399:PHE:CG	2.50	0.47
1:E:480:SER:HA	1:F:480:SER:HA	1.97	0.47
1:H:148:VAL:HG13	1:H:603:ILE:HG21	1.96	0.47
1:A:197:LEU:HA	1:A:200:ILE:HD12	1.96	0.46
1:J:131:ILE:HG23	1:J:200:ILE:HG12	1.97	0.46
1:B:205:LYS:HE3	1:B:282:SER:HA	1.97	0.46
1:F:289:VAL:HG12	1:F:315:ILE:HG21	1.97	0.46
1:G:319:LYS:HE2	1:G:339:ILE:HG12	1.97	0.46
1:F:216:ASN:HA	1:F:222:LEU:HB3	1.96	0.46
1:G:29:HIS:NE2	1:G:529:GLU:OE1	2.46	0.46
1:J:252:HIS:CE1	1:J:257:GLY:HA3	2.50	0.46
1:C:131:ILE:HG23	1:C:200:ILE:HG12	1.96	0.46
1:F:318:LEU:HA	1:F:553:ILE:HG13	1.97	0.46
1:F:487:ALA:HA	1:F:490:LEU:HD12	1.97	0.46
1:G:252:HIS:CE1	1:G:257:GLY:HA3	2.50	0.46
1:D:131:ILE:HG23	1:D:200:ILE:HG12	1.97	0.46
1:D:207:ASP:OD2	1:D:300:THR:OG1	2.33	0.46
1:E:156:ILE:HG23	1:E:161:TYR:HB2	1.97	0.46
1:E:148:VAL:O	1:E:152:ILE:HG13	2.16	0.46
1:E:459:ALA:HB1	1:F:4:TYR:CE2	2.50	0.46
1:I:106:LEU:HD21	1:I:196:VAL:HG21	1.97	0.46
1:E:364:ASP:HB3	1:E:368:LEU:HD12	1.97	0.46
1:H:162:ASP:OD1	1:H:163:LYS:NZ	2.48	0.46
1:H:457:CYS:HB3	1:H:462:ASN:HB2	1.97	0.46
1:J:153:ILE:HG12	1:J:172:PHE:HZ	1.81	0.46
1:C:319:LYS:HG2	1:C:339:ILE:HD11	1.96	0.46
1:D:33:LEU:HA	1:D:36:LYS:HE3	1.98	0.46
1:F:407:ILE:HA	1:F:566:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:394:LYS:NZ	1:K:412:GLU:OE2	2.45	0.46
1:E:560:ASP:HB3	1:E:566:ILE:HD11	1.97	0.46
1:F:206:ASP:HA	1:F:248:LYS:HE2	1.98	0.46
1:H:137:ALA:HA	1:H:142:LEU:CD1	2.42	0.46
1:C:153:ILE:HG12	1:C:172:PHE:HZ	1.80	0.45
1:C:206:ASP:HA	1:C:248:LYS:HE2	1.97	0.45
1:J:176:GLU:HG3	1:J:180:GLN:HE21	1.81	0.45
1:J:407:ILE:HA	1:J:566:ILE:HD13	1.98	0.45
1:A:326:ASP:N	1:A:359:GLY:O	2.47	0.45
1:B:234:VAL:HG11	1:B:340:ILE:HD13	1.98	0.45
1:B:407:ILE:HG23	1:B:566:ILE:HG23	1.98	0.45
1:E:485:ILE:HD11	1:F:484:TYR:CZ	2.51	0.45
1:F:152:ILE:HG23	1:F:293:LEU:HD22	1.97	0.45
1:H:327:MET:HG2	1:H:340:ILE:HG13	1.99	0.45
1:I:132:ARG:NH2	1:I:348:GLU:OE2	2.35	0.45
1:L:118:LEU:HD23	1:L:118:LEU:HA	1.86	0.45
1:C:72:GLU:OE1	1:C:493:ARG:NH1	2.46	0.45
1:J:256:MET:HE3	1:J:449:THR:HG21	1.99	0.45
1:K:271:PRO:HG2	1:K:290:ALA:HB3	1.97	0.45
1:L:344:ALA:HB1	1:L:349:ASP:HB2	1.97	0.45
1:C:491:ARG:HG3	1:C:547:LEU:HG	1.98	0.45
1:E:270:ASN:HD22	1:E:272:HIS:H	1.62	0.45
1:F:475:ILE:HD12	2:F:700:OHN:H202	1.99	0.45
1:G:271:PRO:HG2	1:G:290:ALA:HB3	1.98	0.45
1:D:252:HIS:CE1	1:D:257:GLY:HA3	2.52	0.45
1:G:72:GLU:OE1	1:G:493:ARG:NH1	2.48	0.45
1:H:394:LYS:NZ	1:H:412:GLU:OE2	2.50	0.45
1:B:358:LEU:O	1:B:358:LEU:HD12	2.17	0.45
1:F:170:ILE:HD11	1:F:206:ASP:CG	2.42	0.45
1:F:251:MET:O	1:F:262:ASN:ND2	2.44	0.45
1:G:132:ARG:NH2	1:G:348:GLU:OE2	2.42	0.45
1:I:176:GLU:HG3	1:I:180:GLN:HE21	1.81	0.45
1:K:25:MET:HE3	1:K:438:ARG:HE	1.81	0.45
1:K:318:LEU:HD22	1:K:581:LEU:HD21	1.99	0.45
1:F:76:PHE:HD1	1:F:488:GLN:HG3	1.82	0.45
1:L:21:LYS:NZ	1:L:435:GLU:OE1	2.36	0.45
1:B:221:TRP:NE1	1:B:464:LYS:O	2.49	0.45
1:F:25:MET:HE2	1:F:438:ARG:HH21	1.82	0.45
1:B:461:LYS:HG2	1:B:464:LYS:HD2	1.99	0.44
1:G:109:LEU:HD23	1:G:378:LEU:HD12	1.99	0.44
1:I:9:ARG:HG2	1:I:10:ALA:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:271:PRO:HG2	1:I:290:ALA:HB3	1.99	0.44
1:L:206:ASP:HA	1:L:248:LYS:HE2	2.00	0.44
1:B:173:ASP:HB3	1:B:176:GLU:HB3	1.99	0.44
1:B:234:VAL:HG23	1:B:357:ILE:HB	1.99	0.44
1:F:106:LEU:HD11	1:F:196:VAL:HB	2.00	0.44
1:I:20:TYR:CE2	1:I:22:ALA:HB2	2.52	0.44
1:J:319:LYS:NZ	1:J:545:ALA:O	2.45	0.44
1:C:381:HIS:HA	1:C:382:ASN:HA	1.65	0.44
1:D:31:THR:HG22	1:D:529:GLU:HB3	2.00	0.44
1:E:206:ASP:HA	1:E:248:LYS:HE2	2.00	0.44
1:G:381:HIS:HA	1:G:382:ASN:HA	1.57	0.44
1:C:485:ILE:HD11	1:D:484:TYR:CZ	2.52	0.44
1:D:407:ILE:HA	1:D:566:ILE:HD13	2.00	0.44
1:E:381:HIS:HA	1:E:382:ASN:HA	1.61	0.44
1:E:402:VAL:HG12	1:E:514:GLY:HA2	1.99	0.44
1:F:161:TYR:OH	1:F:601:TYR:OH	2.20	0.44
1:I:92:VAL:HG13	1:I:373:PRO:HG2	1.99	0.44
1:A:55:LEU:O	1:A:59:ASN:ND2	2.51	0.44
1:A:106:LEU:HD11	1:A:196:VAL:HB	1.99	0.44
1:C:395:TYR:CZ	1:C:430:VAL:HG23	2.53	0.44
1:H:8:LYS:HE2	1:H:493:ARG:CZ	2.47	0.44
1:K:603:ILE:HG22	1:K:604:LEU:H	1.82	0.44
1:J:560:ASP:HB3	1:J:566:ILE:HD11	1.99	0.44
1:B:418:LEU:HD11	1:B:587:VAL:HG22	1.99	0.44
1:C:383:GLY:C	1:C:385:ASN:H	2.26	0.44
1:E:418:LEU:HD11	1:E:587:VAL:HG22	2.00	0.44
1:F:484:TYR:O	1:F:488:GLN:HG2	2.18	0.44
1:G:170:ILE:HD11	1:G:206:ASP:CG	2.42	0.44
1:G:515:MET:HE3	1:G:537:ASP:HB2	1.99	0.44
1:H:344:ALA:HB1	1:H:349:ASP:HB2	1.98	0.44
1:A:206:ASP:OD2	1:A:217:GLY:N	2.50	0.44
1:A:70:ILE:HD12	1:A:489:CYS:HB2	2.00	0.44
1:A:541:PHE:O	1:A:569:GLN:NE2	2.37	0.44
1:B:560:ASP:HB3	1:B:566:ILE:HD11	2.00	0.44
1:F:75:MET:O	1:F:75:MET:HG3	2.17	0.44
1:F:300:THR:HG22	1:F:340:ILE:HG12	1.99	0.44
1:L:162:ASP:OD1	1:L:163:LYS:NZ	2.50	0.44
1:L:206:ASP:OD2	1:L:217:GLY:N	2.50	0.44
1:A:476:PHE:HA	1:A:479:PHE:HD2	1.82	0.43
1:E:152:ILE:O	1:E:156:ILE:HG13	2.17	0.43
1:E:269:ARG:HB3	1:E:274:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:450:LEU:O	1:G:454:THR:OG1	2.30	0.43
1:I:560:ASP:HB3	1:I:566:ILE:HD11	1.99	0.43
1:F:14:ASP:O	1:F:17:THR:HG22	2.18	0.43
1:J:381:HIS:HA	1:J:382:ASN:HA	1.76	0.43
1:J:603:ILE:O	1:J:604:LEU:HG	2.18	0.43
1:C:25:MET:HE3	1:C:438:ARG:HE	1.83	0.43
1:I:27:ALA:HB3	1:I:532:ILE:HB	2.00	0.43
1:J:63:LYS:HA	1:J:67:ASN:HB2	2.00	0.43
1:K:307:ARG:NH1	1:K:569:GLN:OE1	2.51	0.43
1:A:337:VAL:HG21	1:A:445:ILE:HB	2.00	0.43
1:B:563:GLY:O	1:B:595:LYS:NZ	2.43	0.43
1:E:17:THR:O	1:E:17:THR:OG1	2.34	0.43
1:F:319:LYS:NZ	1:F:545:ALA:O	2.32	0.43
1:J:9:ARG:HG2	1:J:10:ALA:H	1.81	0.43
1:A:106:LEU:HD21	1:A:196:VAL:HG21	2.00	0.43
1:E:29:HIS:NE2	1:E:529:GLU:OE1	2.50	0.43
1:E:559:TYR:CZ	1:E:595:LYS:HB2	2.54	0.43
1:A:109:LEU:HD11	1:A:352:LEU:HD21	2.00	0.43
1:D:36:LYS:HG2	1:D:467:TYR:CZ	2.54	0.43
1:F:36:LYS:HG2	1:F:467:TYR:CZ	2.54	0.43
1:J:402:VAL:HG12	1:J:514:GLY:HA2	2.00	0.43
1:J:414:ILE:HG13	1:J:557:VAL:HB	2.01	0.43
1:L:110:PRO:HA	1:L:379:LEU:HD23	2.01	0.43
1:A:485:ILE:HD11	1:B:484:TYR:CZ	2.54	0.43
1:C:237:LYS:NZ	1:C:359:GLY:HA3	2.34	0.43
1:G:162:ASP:OD1	1:G:162:ASP:N	2.52	0.43
1:J:484:TYR:O	1:J:488:GLN:HG2	2.17	0.43
1:J:612:GLU:OE1	1:J:612:GLU:N	2.50	0.43
1:A:553:ILE:O	1:A:569:GLN:HA	2.19	0.43
1:B:252:HIS:CD2	1:B:257:GLY:HA3	2.53	0.43
1:C:281:SER:H	1:C:305:ALA:HB1	1.83	0.43
1:E:320:THR:H	1:E:339:ILE:HD13	1.83	0.43
1:G:31:THR:HG22	1:G:529:GLU:HB3	2.01	0.43
1:A:484:TYR:CZ	1:B:485:ILE:HD11	2.54	0.42
1:C:161:TYR:O	1:C:168:PHE:N	2.51	0.42
1:D:170:ILE:HD11	1:D:206:ASP:CG	2.44	0.42
1:I:319:LYS:HG2	1:I:339:ILE:HD11	2.00	0.42
1:L:603:ILE:HG22	1:L:604:LEU:N	2.34	0.42
1:A:144:THR:HG23	1:A:147:GLN:H	1.84	0.42
1:E:484:TYR:CZ	1:F:485:ILE:HD11	2.54	0.42
1:E:553:ILE:HD12	1:E:581:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:381:HIS:HA	1:I:382:ASN:HA	1.75	0.42
1:B:170:ILE:HD11	1:B:206:ASP:CG	2.44	0.42
1:C:8:LYS:HE3	1:C:493:ARG:NH2	2.34	0.42
1:J:370:PRO:HB3	1:J:575:TRP:CH2	2.55	0.42
1:A:237:LYS:NZ	1:A:359:GLY:HA3	2.34	0.42
1:A:370:PRO:HB3	1:A:575:TRP:CH2	2.54	0.42
1:D:106:LEU:HD11	1:D:196:VAL:HB	2.01	0.42
1:I:327:MET:HG2	1:I:340:ILE:HG13	2.00	0.42
1:K:418:LEU:HD11	1:K:587:VAL:HG22	2.02	0.42
1:B:364:ASP:HB3	1:B:368:LEU:HD12	2.02	0.42
1:C:29:HIS:NE2	1:C:529:GLU:OE1	2.50	0.42
1:G:137:ALA:HB1	1:G:143:THR:HG22	2.02	0.42
1:G:564:LEU:HA	1:G:565:PRO:HD3	1.93	0.42
1:H:417:LEU:HB3	1:H:590:LEU:HD13	2.01	0.42
1:A:63:LYS:HD3	1:A:64:ILE:HG13	2.02	0.42
1:B:399:PHE:CE2	1:B:511:PRO:HD3	2.53	0.42
1:C:354:TYR:CZ	1:C:358:LEU:HD23	2.54	0.42
1:E:140:SER:O	1:E:141:LYS:HG3	2.19	0.42
1:F:226:ARG:HH21	1:F:228:VAL:CG1	2.32	0.42
1:B:320:THR:H	1:B:339:ILE:HD13	1.85	0.42
1:C:216:ASN:HA	1:C:222:LEU:HB3	2.00	0.42
1:C:252:HIS:CE1	1:C:257:GLY:HA3	2.55	0.42
1:C:450:LEU:O	1:C:454:THR:OG1	2.30	0.42
1:H:491:ARG:HG3	1:H:547:LEU:HG	2.02	0.42
1:I:515:MET:HE3	1:I:537:ASP:HB2	2.01	0.42
1:L:110:PRO:HB2	1:L:111:GLN:H	1.71	0.42
1:F:398:TRP:CZ2	1:F:541:PHE:HA	2.55	0.42
1:G:206:ASP:HA	1:G:248:LYS:HE2	2.01	0.42
1:A:204:ILE:HD13	1:A:245:LEU:HD12	2.01	0.42
1:A:369:LYS:HE2	1:A:369:LYS:HB2	1.92	0.42
1:H:221:TRP:HZ2	1:H:465:LEU:HD21	1.85	0.42
1:J:450:LEU:O	1:J:454:THR:OG1	2.30	0.42
1:K:450:LEU:O	1:K:454:THR:OG1	2.30	0.42
1:L:106:LEU:HD21	1:L:196:VAL:HG21	2.02	0.42
1:L:370:PRO:HB3	1:L:575:TRP:CH2	2.55	0.42
1:B:43:GLU:OE1	1:B:470:ARG:NH2	2.34	0.42
1:B:206:ASP:O	1:B:215:THR:HG23	2.19	0.42
1:E:441:HIS:O	1:E:445:ILE:HG22	2.20	0.42
1:F:128:TYR:OH	1:F:290:ALA:O	2.29	0.42
1:F:169:LEU:HD21	1:F:288:ILE:HD12	2.01	0.42
1:I:347:LEU:HD12	1:I:585:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:ILE:HG23	1:K:195:SER:HB3	2.02	0.42
1:A:476:PHE:HA	1:A:479:PHE:CD2	2.55	0.41
1:D:307:ARG:NH1	1:D:569:GLN:OE1	2.52	0.41
1:E:596:LYS:HE2	1:E:600:PHE:HB3	2.02	0.41
1:H:308:ILE:HD11	1:H:542:VAL:HG21	2.02	0.41
1:H:318:LEU:HD22	1:H:581:LEU:HD21	2.02	0.41
1:B:234:VAL:HG21	1:B:340:ILE:HG21	2.02	0.41
1:A:281:SER:H	1:A:305:ALA:HB1	1.85	0.41
1:B:63:LYS:HB3	1:B:63:LYS:HE2	1.91	0.41
1:B:171:ARG:HB2	1:B:248:LYS:HB2	2.03	0.41
1:E:207:ASP:OD2	1:E:300:THR:OG1	2.27	0.41
1:H:139:ARG:NH2	1:H:195:SER:O	2.53	0.41
1:I:137:ALA:HB1	1:I:143:THR:HG22	2.02	0.41
1:A:77:ARG:NH2	1:A:364:ASP:OD1	2.53	0.41
1:I:410:LYS:HA	1:I:410:LYS:HD3	1.90	0.41
1:L:113:ASP:O	1:L:115:SER:N	2.47	0.41
1:A:216:ASN:HA	1:A:222:LEU:HB3	2.01	0.41
1:F:75:MET:HG3	1:F:491:ARG:HD2	2.02	0.41
1:F:347:LEU:HD12	1:F:585:ALA:HB2	2.03	0.41
1:J:605:ASN:HB3	1:J:608:LYS:O	2.21	0.41
1:L:399:PHE:CE2	1:L:511:PRO:HD3	2.54	0.41
1:A:561:LYS:HE2	1:A:561:LYS:HB3	1.94	0.41
1:F:272:HIS:NE2	1:F:313:CYS:O	2.50	0.41
1:H:99:ILE:HG23	1:H:195:SER:HB3	2.03	0.41
1:B:213:HIS:HD2	1:B:248:LYS:HD3	1.85	0.41
1:B:272:HIS:NE2	1:B:313:CYS:O	2.45	0.41
1:B:306:VAL:HG22	1:B:343:LEU:HD11	2.03	0.41
1:D:370:PRO:HB3	1:D:575:TRP:CH2	2.56	0.41
1:F:252:HIS:CE1	1:F:257:GLY:HA3	2.56	0.41
1:G:269:ARG:HB3	1:G:274:PRO:HA	2.03	0.41
1:H:414:ILE:HG13	1:H:557:VAL:HB	2.02	0.41
1:D:399:PHE:CE2	1:D:511:PRO:HD3	2.56	0.41
1:I:395:TYR:HB3	1:I:398:TRP:HB3	2.02	0.41
1:A:76:PHE:CD1	1:A:488:GLN:HG3	2.55	0.41
1:B:109:LEU:HD23	1:B:378:LEU:HD12	2.03	0.41
1:E:102:LEU:HD23	1:E:102:LEU:HA	1.92	0.41
1:F:203:THR:HG22	1:F:249:ALA:HB2	2.02	0.41
1:F:211:LEU:HD23	1:F:211:LEU:HA	1.94	0.41
1:G:281:SER:H	1:G:305:ALA:HB1	1.86	0.41
1:G:394:LYS:NZ	1:G:412:GLU:OE2	2.37	0.41
1:K:137:ALA:HB1	1:K:143:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:ILE:HD11	1:L:206:ASP:CG	2.46	0.41
1:L:355:ALA:HA	1:L:358:LEU:HD23	2.02	0.41
1:L:398:TRP:HZ2	1:L:541:PHE:HA	1.86	0.41
1:L:418:LEU:HD11	1:L:587:VAL:HG22	2.03	0.41
1:A:153:ILE:HG12	1:A:172:PHE:HZ	1.86	0.41
1:H:36:LYS:HG2	1:H:467:TYR:CZ	2.56	0.41
1:L:221:TRP:HZ2	1:L:465:LEU:HD21	1.86	0.41
1:A:8:LYS:HE3	1:A:493:ARG:NH2	2.37	0.40
1:G:39:VAL:HG11	1:G:467:TYR:HD1	1.87	0.40
1:G:42:LEU:HD23	1:G:42:LEU:HA	1.96	0.40
1:I:269:ARG:HB3	1:I:274:PRO:HA	2.02	0.40
1:J:319:LYS:HG2	1:J:339:ILE:HD11	2.03	0.40
1:J:379:LEU:O	1:J:379:LEU:HD12	2.21	0.40
1:K:109:LEU:HD23	1:K:378:LEU:HD12	2.03	0.40
1:B:153:ILE:HD13	1:B:172:PHE:CZ	2.55	0.40
1:C:170:ILE:HD11	1:C:206:ASP:CG	2.46	0.40
1:E:561:LYS:HE2	1:E:561:LYS:HB3	1.91	0.40
1:F:61:MET:HE2	1:F:61:MET:HB3	1.89	0.40
1:A:252:HIS:CE1	1:A:257:GLY:HA3	2.56	0.40
1:B:128:TYR:HE1	1:B:593:VAL:HG11	1.85	0.40
1:C:337:VAL:HG21	1:C:445:ILE:HB	2.03	0.40
1:D:300:THR:OG1	2:D:700:OHN:O6	2.30	0.40
1:E:188:PHE:CE1	1:E:193:PRO:HB3	2.56	0.40
1:H:603:ILE:HG22	1:H:604:LEU:N	2.33	0.40
1:I:63:LYS:HE2	1:I:63:LYS:HB3	1.89	0.40
1:K:521:PRO:HA	1:K:522:PRO:HD3	1.99	0.40
1:L:307:ARG:NH1	1:L:569:GLN:OE1	2.46	0.40
1:A:25:MET:HE3	1:A:438:ARG:HE	1.86	0.40
1:B:101:ARG:HD3	1:B:358:LEU:HD21	2.03	0.40
1:B:370:PRO:HB3	1:B:575:TRP:CH2	2.56	0.40
1:F:162:ASP:OD1	1:F:163:LYS:NZ	2.51	0.40
1:I:106:LEU:HA	1:I:109:LEU:HD12	2.04	0.40
1:J:206:ASP:OD2	1:J:217:GLY:N	2.53	0.40
1:A:418:LEU:HD11	1:A:587:VAL:HG22	2.04	0.40
1:B:215:THR:OG1	1:B:248:LYS:NZ	2.54	0.40
1:C:603:ILE:HG22	1:C:604:LEU:H	1.87	0.40
1:E:151:ARG:HH21	1:E:604:LEU:H	1.69	0.40
1:E:281:SER:H	1:E:305:ALA:HB1	1.86	0.40
1:G:77:ARG:HG2	1:G:336:THR:HG22	2.02	0.40
1:G:115:SER:HB2	1:G:116:ARG:HH21	1.85	0.40
1:I:75:MET:HE1	1:I:495:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:563:GLY:O	1:L:595:LYS:NZ	2.52	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%)	569 (95%)	29 (5%)	2 (0%)	36	68
1	B	603/636 (95%)	571 (95%)	32 (5%)	0	100	100
1	C	600/636 (94%)	574 (96%)	24 (4%)	2 (0%)	36	68
1	D	603/636 (95%)	576 (96%)	26 (4%)	1 (0%)	43	73
1	E	600/636 (94%)	572 (95%)	28 (5%)	0	100	100
1	F	603/636 (95%)	575 (95%)	27 (4%)	1 (0%)	43	73
1	G	600/636 (94%)	574 (96%)	25 (4%)	1 (0%)	43	73
1	H	612/636 (96%)	581 (95%)	29 (5%)	2 (0%)	36	68
1	I	600/636 (94%)	573 (96%)	26 (4%)	1 (0%)	43	73
1	J	612/636 (96%)	589 (96%)	23 (4%)	0	100	100
1	K	600/636 (94%)	576 (96%)	23 (4%)	1 (0%)	43	73
1	L	603/636 (95%)	568 (94%)	34 (6%)	1 (0%)	43	73
All	All	7236/7632 (95%)	6898 (95%)	326 (4%)	12 (0%)	43	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	C	45	PRO
1	D	45	PRO

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Mol	Chain	Res	Type
1	F	45	PRO
1	H	605	ASN
1	I	45	PRO
1	K	45	PRO
1	L	110	PRO
1	A	141	LYS
1	C	141	LYS
1	H	2	GLY
1	G	603	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/539 (94%)	509 (100%)	0	100	100
1	B	511/539 (95%)	510 (100%)	1 (0%)	87	89
1	C	509/539 (94%)	509 (100%)	0	100	100
1	D	511/539 (95%)	511 (100%)	0	100	100
1	E	509/539 (94%)	509 (100%)	0	100	100
1	F	511/539 (95%)	511 (100%)	0	100	100
1	G	509/539 (94%)	509 (100%)	0	100	100
1	H	518/539 (96%)	518 (100%)	0	100	100
1	I	509/539 (94%)	509 (100%)	0	100	100
1	J	518/539 (96%)	518 (100%)	0	100	100
1	K	509/539 (94%)	509 (100%)	0	100	100
1	L	511/539 (95%)	511 (100%)	0	100	100
All	All	6134/6468 (95%)	6133 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	180	GLN
1	A	213	HIS
1	A	421	ASN
1	B	29	HIS
1	B	59	ASN
1	B	175	ASN
1	B	421	ASN
1	B	498	HIS
1	B	533	GLN
1	C	147	GLN
1	C	180	GLN
1	C	213	HIS
1	C	421	ASN
1	D	40	ASN
1	D	213	HIS
1	D	533	GLN
1	E	40	ASN
1	E	180	GLN
1	E	250	ASN
1	E	270	ASN
1	E	421	ASN
1	E	498	HIS
1	E	527	ASN
1	E	605	ASN
1	F	40	ASN
1	F	533	GLN
1	F	605	ASN
1	G	40	ASN
1	G	381	HIS
1	G	421	ASN
1	G	605	ASN
1	H	83	GLN
1	H	250	ASN
1	H	533	GLN
1	I	381	HIS
1	I	421	ASN
1	I	605	ASN
1	J	67	ASN
1	J	250	ASN
1	J	381	HIS

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Mol	Chain	Res	Type
1	J	420	ASN
1	K	421	ASN
1	K	605	ASN
1	L	261	ASN
1	L	382	ASN
1	L	400	ASN
1	L	533	GLN
1	L	546	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	OHN	J	700	-	21,21,21	4.86	7 (33%)	21,25,25	3.71	8 (38%)
2	OHN	D	700	-	21,21,21	4.89	6 (28%)	21,25,25	3.59	8 (38%)
2	OHN	F	700	-	21,21,21	4.89	7 (33%)	21,25,25	3.51	9 (42%)
2	OHN	H	700	-	21,21,21	4.86	7 (33%)	21,25,25	3.54	8 (38%)
2	OHN	L	700	-	21,21,21	4.88	7 (33%)	21,25,25	3.53	8 (38%)

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	OHN	J	700	-	-	8/17/27/27	0/1/1/1
2	OHN	D	700	-	-	5/17/27/27	0/1/1/1
2	OHN	F	700	-	-	8/17/27/27	0/1/1/1
2	OHN	H	700	-	-	9/17/27/27	0/1/1/1
2	OHN	L	700	-	-	8/17/27/27	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	OHN	OAP-C2	15.68	1.68	1.35
2	H	700	OHN	OAP-C2	15.65	1.68	1.35
2	L	700	OHN	OAP-C2	15.61	1.68	1.35
2	J	700	OHN	OAP-C2	15.54	1.68	1.35
2	F	700	OHN	OAP-C2	15.51	1.68	1.35
2	F	700	OHN	C1-C2	-11.88	1.29	1.52
2	J	700	OHN	C1-C2	-11.87	1.29	1.52
2	L	700	OHN	C1-C2	-11.87	1.29	1.52
2	H	700	OHN	C1-C2	-11.86	1.29	1.52
2	D	700	OHN	C1-C2	-11.49	1.30	1.52
2	F	700	OHN	OAP-C4	-6.68	1.29	1.46
2	L	700	OHN	OAP-C4	-6.66	1.29	1.46
2	J	700	OHN	OAP-C4	-6.66	1.29	1.46
2	D	700	OHN	OAP-C4	-6.63	1.29	1.46
2	H	700	OHN	OAP-C4	-6.57	1.30	1.46
2	D	700	OHN	C8-N7	5.98	1.46	1.34
2	F	700	OHN	C8-N7	5.83	1.46	1.34
2	L	700	OHN	C8-N7	5.68	1.46	1.34
2	J	700	OHN	C8-N7	5.62	1.45	1.34
2	H	700	OHN	C8-N7	5.46	1.45	1.34
2	D	700	OHN	C1-N7	4.94	1.56	1.45
2	F	700	OHN	C1-N7	4.68	1.55	1.45
2	L	700	OHN	C1-N7	4.42	1.55	1.45
2	J	700	OHN	C1-N7	4.30	1.54	1.45
2	H	700	OHN	C1-N7	4.27	1.54	1.45
2	J	700	OHN	C5-C4	2.47	1.57	1.51
2	L	700	OHN	C5-C4	2.47	1.57	1.51
2	F	700	OHN	C5-C4	2.44	1.57	1.51
2	H	700	OHN	C5-C4	2.42	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	OHN	C5-C4	2.38	1.57	1.51
2	H	700	OHN	O9-C8	-2.31	1.18	1.23
2	L	700	OHN	O9-C8	-2.23	1.18	1.23
2	J	700	OHN	O9-C8	-2.22	1.18	1.23
2	F	700	OHN	O9-C8	-2.22	1.18	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	700	OHN	OAP-C2-O6	-11.35	109.37	121.43
2	D	700	OHN	OAP-C2-O6	-10.78	109.98	121.43
2	L	700	OHN	OAP-C2-O6	-10.52	110.26	121.43
2	H	700	OHN	OAP-C2-O6	-10.43	110.35	121.43
2	F	700	OHN	OAP-C2-O6	-10.16	110.64	121.43
2	H	700	OHN	O12-C11-C10	-7.80	109.15	121.20
2	L	700	OHN	O12-C11-C10	-7.58	109.48	121.20
2	D	700	OHN	O12-C11-C10	-7.45	109.69	121.20
2	J	700	OHN	O12-C11-C10	-7.43	109.72	121.20
2	F	700	OHN	O12-C11-C10	-7.18	110.10	121.20
2	F	700	OHN	C4-OAP-C2	-5.39	105.52	110.35
2	J	700	OHN	C4-OAP-C2	-5.29	105.61	110.35
2	F	700	OHN	O6-C2-C1	-5.02	109.60	126.87
2	J	700	OHN	O6-C2-C1	-4.98	109.72	126.87
2	L	700	OHN	O6-C2-C1	-4.97	109.77	126.87
2	D	700	OHN	O6-C2-C1	-4.94	109.86	126.87
2	J	700	OHN	O12-C11-C13	-4.93	108.46	121.40
2	L	700	OHN	C4-OAP-C2	-4.91	105.95	110.35
2	D	700	OHN	O12-C11-C13	-4.88	108.60	121.40
2	H	700	OHN	O6-C2-C1	-4.88	110.09	126.87
2	H	700	OHN	O12-C11-C13	-4.77	108.89	121.40
2	L	700	OHN	O12-C11-C13	-4.66	109.18	121.40
2	D	700	OHN	C4-OAP-C2	-4.62	106.21	110.35
2	H	700	OHN	C4-OAP-C2	-4.54	106.28	110.35
2	F	700	OHN	O12-C11-C13	-4.52	109.53	121.40
2	F	700	OHN	C10-C11-C13	-3.27	108.23	118.03
2	D	700	OHN	C1-N7-C8	2.97	129.14	121.68
2	D	700	OHN	C5-C1-N7	-2.75	109.18	115.03
2	L	700	OHN	C10-C11-C13	-2.72	109.87	118.03
2	J	700	OHN	C10-C8-N7	2.60	120.76	116.31
2	H	700	OHN	C5-C1-N7	-2.49	109.73	115.03
2	J	700	OHN	C5-C1-N7	-2.46	109.81	115.03
2	H	700	OHN	C10-C11-C13	-2.41	110.81	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	700	OHN	C5-C1-N7	-2.37	109.99	115.03
2	F	700	OHN	C5-C1-N7	-2.36	110.00	115.03
2	H	700	OHN	C10-C8-N7	2.35	120.33	116.31
2	D	700	OHN	C10-C11-C13	-2.32	111.08	118.03
2	J	700	OHN	C10-C11-C13	-2.30	111.16	118.03
2	F	700	OHN	C10-C8-N7	2.20	120.07	116.31
2	F	700	OHN	O9-C8-C10	-2.15	118.01	121.40
2	L	700	OHN	C10-C8-N7	2.09	119.88	116.31

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	700	OHN	C2-C1-N7-C8
2	F	700	OHN	C11-C10-C8-O9
2	F	700	OHN	C11-C10-C8-N7
2	H	700	OHN	C11-C10-C8-O9
2	H	700	OHN	C11-C10-C8-N7
2	J	700	OHN	C11-C10-C8-O9
2	J	700	OHN	C11-C10-C8-N7
2	L	700	OHN	C11-C10-C8-O9
2	L	700	OHN	C11-C10-C8-N7
2	L	700	OHN	C5-C1-N7-C8
2	L	700	OHN	C2-C1-N7-C8
2	L	700	OHN	C11-C13-C14-C15
2	H	700	OHN	C11-C13-C14-C15
2	H	700	OHN	C13-C14-C15-C16
2	D	700	OHN	C15-C16-C17-C18
2	L	700	OHN	C13-C14-C15-C16
2	D	700	OHN	C17-C18-C19-C20
2	F	700	OHN	C13-C14-C15-C16
2	J	700	OHN	C13-C14-C15-C16
2	F	700	OHN	C17-C18-C19-C20
2	F	700	OHN	C15-C16-C17-C18
2	L	700	OHN	C17-C18-C19-C20
2	L	700	OHN	C15-C16-C17-C18
2	J	700	OHN	C15-C16-C17-C18
2	H	700	OHN	C8-C10-C11-C13
2	J	700	OHN	C8-C10-C11-C13
2	H	700	OHN	C17-C18-C19-C20
2	H	700	OHN	C15-C16-C17-C18
2	F	700	OHN	C5-C1-N7-C8

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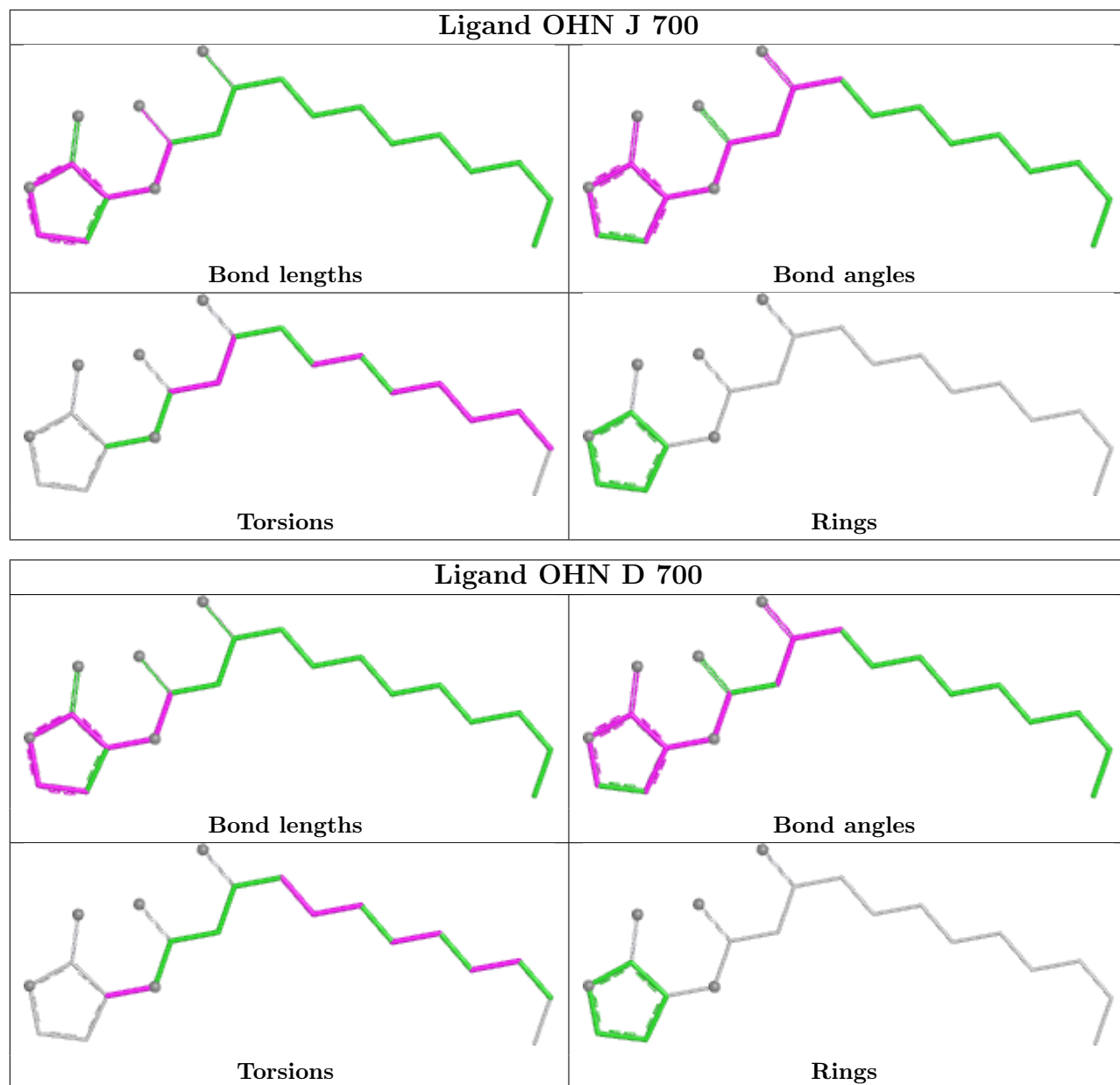
Mol	Chain	Res	Type	Atoms
2	J	700	OHN	C17-C18-C19-C20
2	H	700	OHN	C14-C15-C16-C17
2	F	700	OHN	O12-C11-C13-C14
2	H	700	OHN	O12-C11-C13-C14
2	F	700	OHN	C8-C10-C11-O12
2	J	700	OHN	C18-C19-C20-C21
2	D	700	OHN	C13-C14-C15-C16
2	J	700	OHN	C16-C17-C18-C19
2	D	700	OHN	C11-C13-C14-C15

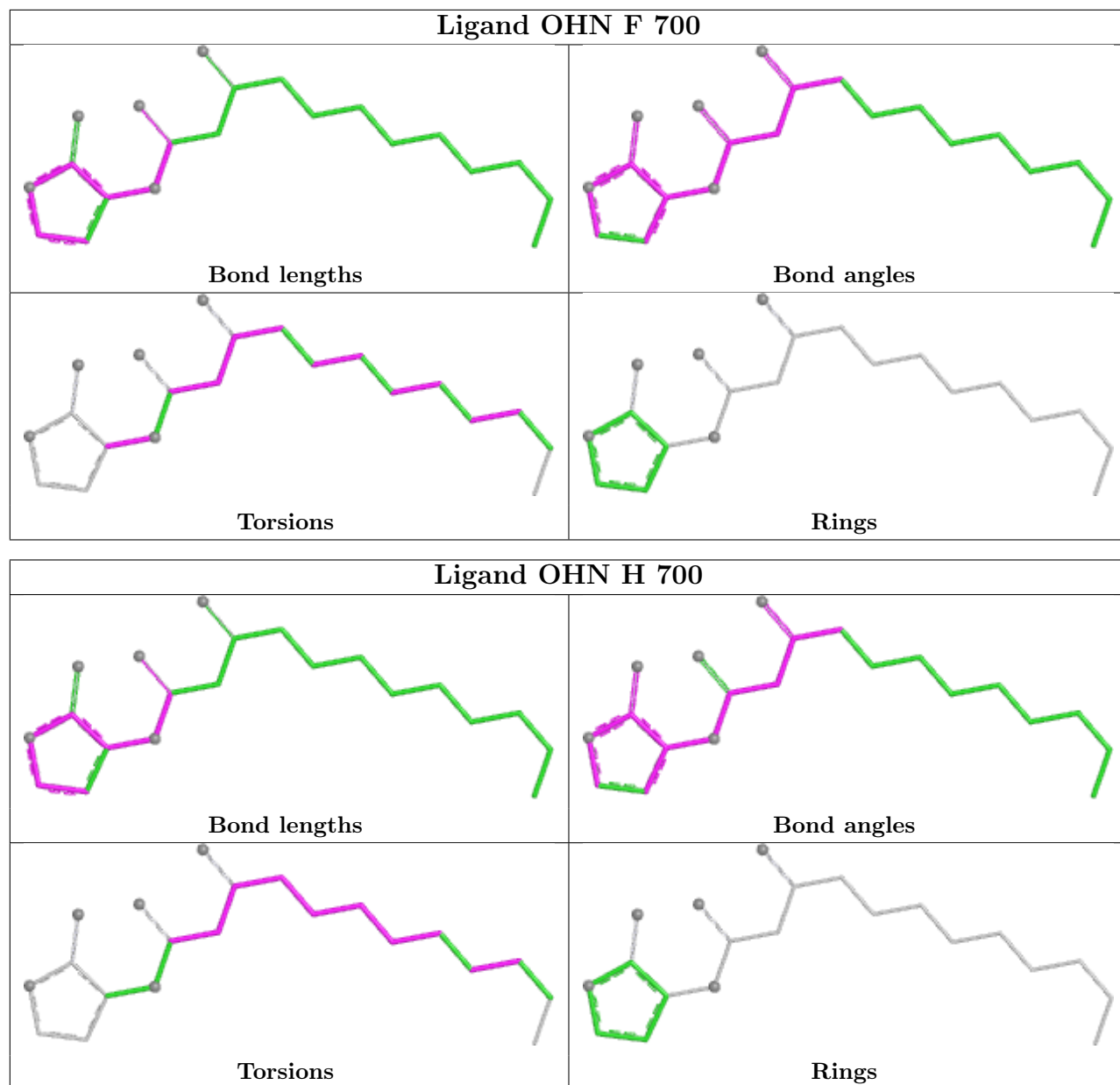
There are no ring outliers.

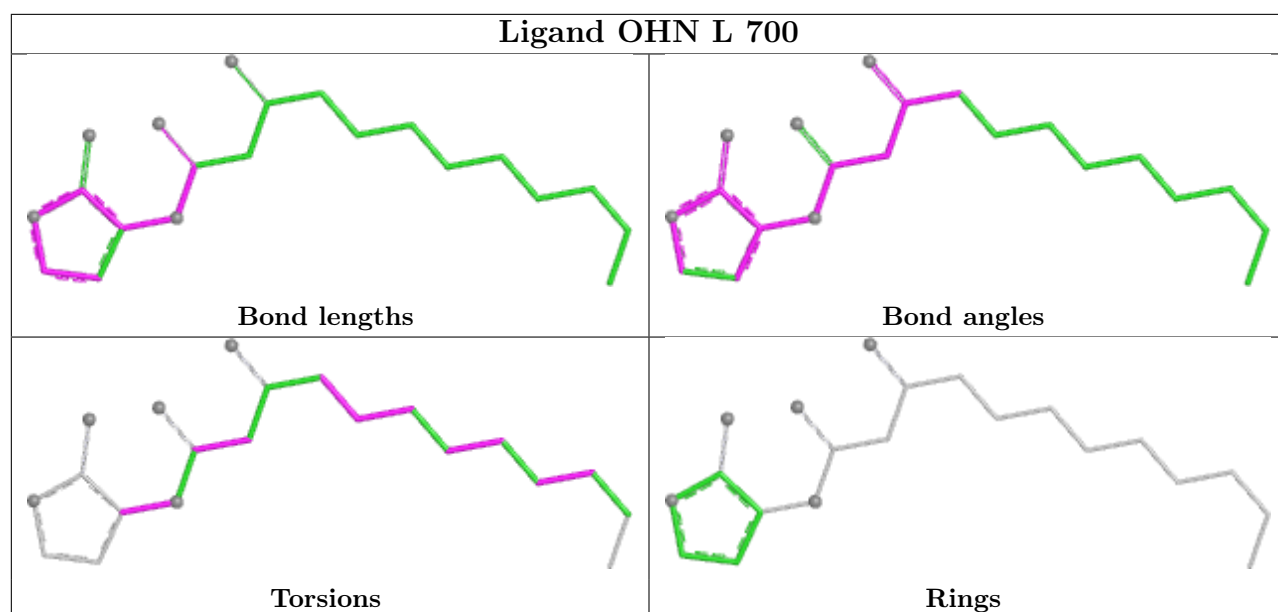
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	700	OHN	1	0
2	D	700	OHN	2	0
2	F	700	OHN	2	0
2	H	700	OHN	2	0
2	L	700	OHN	2	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%)	0.98	68 (11%) 10 7	79, 111, 146, 213	0
1	B	605/636 (95%)	1.10	85 (14%) 6 5	77, 113, 145, 230	0
1	C	602/636 (94%)	0.41	15 (2%) 58 39	53, 80, 117, 218	0
1	D	605/636 (95%)	0.21	12 (1%) 65 45	42, 61, 93, 192	0
1	E	602/636 (94%)	1.03	62 (10%) 12 8	74, 107, 142, 217	0
1	F	605/636 (95%)	1.14	92 (15%) 5 4	69, 101, 130, 224	0
1	G	602/636 (94%)	0.36	8 (1%) 75 55	49, 76, 106, 187	0
1	H	614/636 (96%)	0.39	16 (2%) 57 37	48, 69, 107, 243	0
1	I	602/636 (94%)	0.26	15 (2%) 58 39	38, 57, 86, 175	0
1	J	614/636 (96%)	0.50	38 (6%) 26 17	40, 56, 88, 199	0
1	K	602/636 (94%)	0.36	12 (1%) 65 45	49, 73, 104, 188	0
1	L	605/636 (95%)	0.37	17 (2%) 55 35	48, 76, 104, 172	0
All	All	7260/7632 (95%)	0.59	440 (6%) 27 17	38, 80, 134, 243	0

All (440) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	383	GLY	6.2
1	B	591	ALA	6.2
1	E	590	LEU	5.8
1	F	591	ALA	5.8
1	E	407	ILE	5.1
1	E	7	MET	5.0
1	J	611	PHE	5.0
1	E	302	GLY	5.0
1	A	484	TYR	4.8
1	J	111	GLN	4.8
1	J	119	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	349	ASP	4.7
1	F	247	GLY	4.4
1	B	281	SER	4.4
1	B	523	ASP	4.3
1	L	1	MET	4.2
1	E	484	TYR	4.2
1	G	7	MET	4.2
1	B	280	GLY	4.2
1	D	523	ASP	4.1
1	J	533	GLN	4.1
1	B	454	THR	4.0
1	B	232	SER	4.0
1	J	1	MET	3.9
1	F	343	LEU	3.9
1	C	407	ILE	3.8
1	A	452	SER	3.7
1	F	7	MET	3.7
1	E	604	LEU	3.7
1	K	383	GLY	3.7
1	E	411	CYS	3.7
1	B	291	ALA	3.7
1	B	152	ILE	3.7
1	B	246	LEU	3.6
1	F	214	PRO	3.6
1	A	576	ALA	3.6
1	A	538	LEU	3.5
1	I	7	MET	3.5
1	B	258	THR	3.5
1	F	268	THR	3.5
1	F	291	ALA	3.5
1	A	392	LEU	3.5
1	F	98	PRO	3.5
1	A	414	ILE	3.4
1	J	536	THR	3.4
1	A	419	SER	3.4
1	A	535	THR	3.4
1	F	280	GLY	3.4
1	J	605	ASN	3.3
1	E	374	CYS	3.3
1	B	536	THR	3.3
1	D	412	GLU	3.3
1	B	256	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	293	LEU	3.3
1	E	511	PRO	3.3
1	J	118	LEU	3.3
1	E	294	CYS	3.2
1	F	201	PHE	3.2
1	E	510	THR	3.2
1	E	591	ALA	3.2
1	B	304	GLY	3.2
1	B	7	MET	3.2
1	J	613	ALA	3.2
1	B	247	GLY	3.2
1	A	469	THR	3.2
1	B	586	ALA	3.2
1	J	398	TRP	3.2
1	F	6	VAL	3.2
1	F	235	VAL	3.2
1	A	7	MET	3.2
1	A	103	GLU	3.2
1	F	212	PRO	3.2
1	B	539	MET	3.2
1	F	152	ILE	3.2
1	I	22	ALA	3.2
1	B	332	CYS	3.1
1	B	357	ILE	3.1
1	E	387	ILE	3.1
1	K	191	GLY	3.1
1	F	400	ASN	3.1
1	E	530	THR	3.1
1	K	24	THR	3.1
1	F	260	GLY	3.1
1	H	384	SER	3.1
1	E	566	ILE	3.1
1	B	535	THR	3.1
1	A	9	ARG	3.1
1	G	383	GLY	3.1
1	I	191	GLY	3.1
1	J	606	THR	3.1
1	F	148	VAL	3.1
1	F	384	SER	3.1
1	L	306	VAL	3.1
1	B	207	ASP	3.1
1	E	196	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	283	SER	3.0
1	A	288	ILE	3.0
1	E	330	SER	3.0
1	D	591	ALA	3.0
1	E	442	VAL	3.0
1	C	535	THR	3.0
1	F	332	CYS	3.0
1	J	25	MET	3.0
1	B	245	LEU	2.9
1	J	610	GLU	2.9
1	A	311	ALA	2.9
1	K	509	VAL	2.9
1	A	170	ILE	2.9
1	C	7	MET	2.9
1	H	7	MET	2.9
1	B	6	VAL	2.9
1	D	6	VAL	2.9
1	D	384	SER	2.9
1	E	88	ASP	2.9
1	J	91	ILE	2.9
1	C	30	LEU	2.9
1	I	182	GLU	2.9
1	C	509	VAL	2.9
1	F	450	LEU	2.9
1	F	486	ALA	2.9
1	F	487	ALA	2.9
1	J	607	ASN	2.9
1	B	168	PHE	2.9
1	C	191	GLY	2.9
1	F	217	GLY	2.9
1	A	407	ILE	2.9
1	I	407	ILE	2.9
1	A	513	THR	2.9
1	J	229	GLU	2.8
1	E	30	LEU	2.8
1	B	213	HIS	2.8
1	J	114	PRO	2.8
1	A	318	LEU	2.8
1	A	499	LEU	2.8
1	E	386	ALA	2.8
1	F	444	SER	2.8
1	B	587	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	3	LYS	2.8
1	F	536	THR	2.8
1	A	218	GLY	2.8
1	A	255	GLY	2.8
1	F	216	ASN	2.8
1	J	614	TYR	2.8
1	I	411	CYS	2.8
1	F	381	HIS	2.8
1	L	536	THR	2.8
1	L	590	LEU	2.8
1	K	7	MET	2.8
1	H	271	PRO	2.8
1	B	358	LEU	2.8
1	A	315	ILE	2.7
1	J	405	SER	2.7
1	F	215	THR	2.7
1	A	20	TYR	2.7
1	F	261	ASN	2.7
1	B	356	ALA	2.7
1	E	542	VAL	2.7
1	A	590	LEU	2.7
1	I	404	SER	2.7
1	A	8	LYS	2.7
1	A	387	ILE	2.7
1	B	215	THR	2.7
1	F	535	THR	2.7
1	J	3	LYS	2.7
1	E	311	ALA	2.7
1	A	556	PRO	2.7
1	J	24	THR	2.7
1	A	544	ALA	2.7
1	E	544	ALA	2.7
1	E	136	TYR	2.7
1	K	379	LEU	2.7
1	J	192	ASN	2.7
1	B	212	PRO	2.6
1	G	24	THR	2.6
1	B	235	VAL	2.6
1	B	98	PRO	2.6
1	L	274	PRO	2.6
1	F	341	GLY	2.6
1	F	210	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	499	LEU	2.6
1	H	6	VAL	2.6
1	G	45	PRO	2.6
1	L	260	GLY	2.6
1	B	343	LEU	2.6
1	J	6	VAL	2.6
1	B	203	THR	2.6
1	B	449	THR	2.6
1	E	576	ALA	2.6
1	F	258	THR	2.6
1	F	546	ASN	2.6
1	F	312	LEU	2.6
1	G	486	ALA	2.6
1	H	536	THR	2.6
1	A	4	TYR	2.5
1	B	354	TYR	2.5
1	E	260	GLY	2.5
1	C	392	LEU	2.5
1	C	538	LEU	2.5
1	C	261	ASN	2.5
1	D	409	ASP	2.5
1	A	429	ILE	2.5
1	J	75	MET	2.5
1	F	213	HIS	2.5
1	B	465	LEU	2.5
1	E	335	GLY	2.5
1	E	6	VAL	2.5
1	J	231	ASP	2.5
1	B	156	ILE	2.5
1	H	606	THR	2.5
1	A	126	PHE	2.5
1	A	390	LEU	2.5
1	B	102	LEU	2.5
1	F	246	LEU	2.5
1	F	590	LEU	2.5
1	A	295	SER	2.5
1	E	509	VAL	2.5
1	E	22	ALA	2.5
1	A	541	PHE	2.5
1	B	169	LEU	2.5
1	F	196	VAL	2.5
1	A	310	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	411	CYS	2.5
1	F	154	SER	2.5
1	B	99	ILE	2.5
1	L	3	LYS	2.5
1	A	511	PRO	2.5
1	E	556	PRO	2.5
1	F	4	TYR	2.5
1	C	302	GLY	2.5
1	F	160	GLY	2.5
1	E	286	ALA	2.4
1	E	463	SER	2.4
1	A	80	PHE	2.4
1	D	3	LYS	2.4
1	A	510	THR	2.4
1	B	331	LEU	2.4
1	B	286	ALA	2.4
1	A	424	CYS	2.4
1	E	345	SER	2.4
1	F	331	LEU	2.4
1	F	259	THR	2.4
1	J	382	ASN	2.4
1	A	253	GLU	2.4
1	B	254	LEU	2.4
1	H	294	CYS	2.4
1	B	527	ASN	2.4
1	J	112	TYR	2.4
1	A	91	ILE	2.4
1	A	591	ALA	2.4
1	F	208	ILE	2.4
1	B	8	LYS	2.4
1	G	25	MET	2.4
1	H	3	LYS	2.4
1	L	9	ARG	2.4
1	B	253	GLU	2.4
1	C	419	SER	2.4
1	F	282	SER	2.4
1	B	446	GLY	2.4
1	D	192	ASN	2.4
1	F	314	GLY	2.4
1	A	22	ALA	2.4
1	A	599	ILE	2.4
1	B	101	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	245	LEU	2.4
1	A	285	SER	2.4
1	C	408	SER	2.4
1	E	89	VAL	2.4
1	E	323	GLY	2.3
1	F	267	THR	2.3
1	A	566	ILE	2.3
1	E	4	TYR	2.3
1	F	599	ILE	2.3
1	E	418	LEU	2.3
1	I	123	VAL	2.3
1	B	282	SER	2.3
1	E	28	PRO	2.3
1	F	285	SER	2.3
1	A	486	ALA	2.3
1	B	308	ILE	2.3
1	F	203	THR	2.3
1	F	305	ALA	2.3
1	K	411	CYS	2.3
1	H	614	TYR	2.3
1	A	483	ASP	2.3
1	B	33	LEU	2.3
1	B	538	LEU	2.3
1	J	604	LEU	2.3
1	D	229	GLU	2.3
1	F	228	VAL	2.3
1	A	11	SER	2.3
1	F	321	THR	2.3
1	B	312	LEU	2.3
1	F	525	LEU	2.3
1	L	605	ASN	2.3
1	F	231	ASP	2.3
1	A	509	VAL	2.3
1	B	3	LYS	2.3
1	B	214	PRO	2.3
1	A	471	THR	2.3
1	F	325	THR	2.3
1	F	437	MET	2.3
1	E	390	LEU	2.3
1	A	209	ASP	2.3
1	J	349	ASP	2.3
1	F	306	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	474	ALA	2.3
1	F	33	LEU	2.3
1	I	24	THR	2.3
1	B	384	SER	2.3
1	E	395	TYR	2.3
1	F	601	TYR	2.3
1	B	148	VAL	2.3
1	H	349	ASP	2.3
1	G	229	GLU	2.2
1	B	599	ILE	2.2
1	E	244	ILE	2.2
1	B	341	GLY	2.2
1	E	280	GLY	2.2
1	H	1	MET	2.2
1	F	351	PHE	2.2
1	L	535	THR	2.2
1	A	294	CYS	2.2
1	B	412	GLU	2.2
1	F	523	ASP	2.2
1	I	23	GLU	2.2
1	F	339	ILE	2.2
1	F	340	ILE	2.2
1	F	378	LEU	2.2
1	D	526	LYS	2.2
1	F	292	GLY	2.2
1	F	293	LEU	2.2
1	H	417	LEU	2.2
1	K	22	ALA	2.2
1	B	201	PHE	2.2
1	B	479	PHE	2.2
1	A	215	THR	2.2
1	A	498	HIS	2.2
1	D	4	TYR	2.2
1	B	387	ILE	2.2
1	C	429	ILE	2.2
1	J	420	ASN	2.2
1	C	358	LEU	2.2
1	F	539	MET	2.2
1	B	303	GLY	2.2
1	B	259	THR	2.2
1	B	154	SER	2.2
1	E	414	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	379	LEU	2.2
1	H	25	MET	2.2
1	B	400	ASN	2.2
1	H	605	ASN	2.2
1	L	585	ALA	2.2
1	B	518	PRO	2.2
1	F	164	PRO	2.2
1	K	212	PRO	2.2
1	E	493	ARG	2.2
1	A	6	VAL	2.1
1	K	228	VAL	2.1
1	B	475	ILE	2.1
1	F	170	ILE	2.1
1	A	415	LEU	2.1
1	F	169	LEU	2.1
1	B	330	SER	2.1
1	F	287	ALA	2.1
1	F	447	SER	2.1
1	I	140	SER	2.1
1	E	229	GLU	2.1
1	J	491	ARG	2.1
1	J	59	ASN	2.1
1	B	65	PHE	2.1
1	K	123	VAL	2.1
1	K	407	ILE	2.1
1	F	269	ARG	2.1
1	F	356	ALA	2.1
1	F	412	GLU	2.1
1	J	384	SER	2.1
1	J	408	SER	2.1
1	B	270	ASN	2.1
1	E	541	PHE	2.1
1	A	542	VAL	2.1
1	B	306	VAL	2.1
1	F	519	VAL	2.1
1	B	222	LEU	2.1
1	B	450	LEU	2.1
1	E	143	THR	2.1
1	F	454	THR	2.1
1	A	286	ALA	2.1
1	F	569	GLN	2.1
1	C	359	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	28	PRO	2.1
1	E	447	SER	2.1
1	F	172	PHE	2.1
1	F	408	SER	2.1
1	L	332	CYS	2.1
1	B	4	TYR	2.1
1	B	437	MET	2.1
1	E	27	ALA	2.1
1	H	533	GLN	2.1
1	I	190	GLN	2.1
1	A	280	GLY	2.1
1	B	2	GLY	2.1
1	B	444	SER	2.1
1	L	520	ILE	2.1
1	B	322	TYR	2.1
1	E	20	TYR	2.1
1	F	586	ALA	2.1
1	A	314	GLY	2.1
1	L	191	GLY	2.1
1	A	90	VAL	2.0
1	A	410	LYS	2.0
1	E	430	VAL	2.0
1	L	6	VAL	2.0
1	B	340	ILE	2.0
1	F	254	LEU	2.0
1	F	465	LEU	2.0
1	A	516	THR	2.0
1	F	474	ALA	2.0
1	J	290	ALA	2.0
1	L	311	ALA	2.0
1	B	292	GLY	2.0
1	I	122	PRO	2.0
1	J	165	PRO	2.0
1	J	612	GLU	2.0
1	A	256	MET	2.0
1	E	441	HIS	2.0
1	E	268	THR	2.0
1	G	591	ALA	2.0
1	H	535	THR	2.0
1	J	537	ASP	2.0
1	E	168	PHE	2.0
1	F	168	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	393	GLY	2.0
1	D	533	GLN	2.0
1	E	397	LYS	2.0
1	A	436	GLU	2.0
1	E	103	GLU	2.0
1	F	353	VAL	2.0
1	E	343	LEU	2.0
1	E	415	LEU	2.0
1	E	543	LEU	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](#)

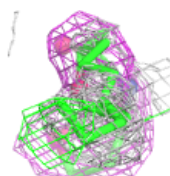
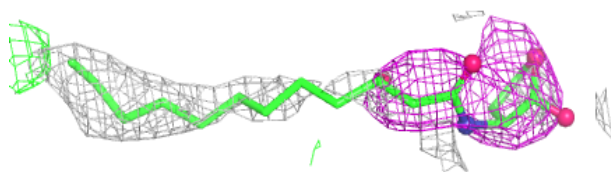
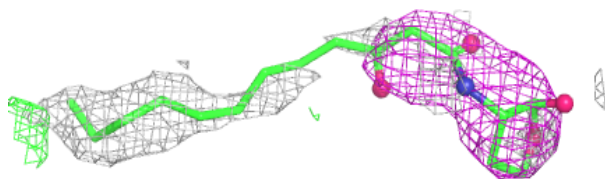
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	OHN	D	700	21/21	0.62	0.29	58,66,71,74	0
2	OHN	H	700	21/21	0.64	0.26	63,70,75,78	0
2	OHN	F	700	21/21	0.66	0.37	90,97,102,106	0
2	OHN	L	700	21/21	0.67	0.25	67,75,79,83	0
2	OHN	J	700	21/21	0.68	0.24	43,51,56,59	0

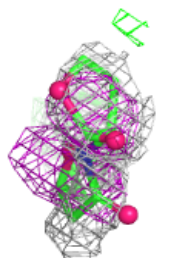
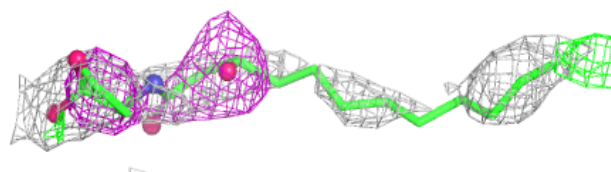
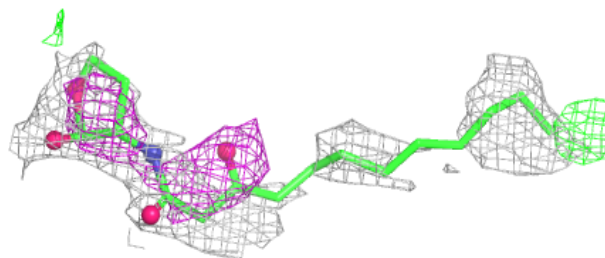
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OHN D 700:

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

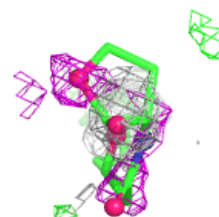
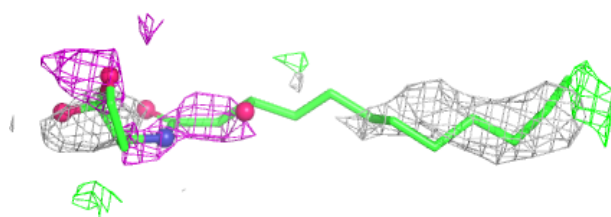
**Electron density around OHN H 700:**

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

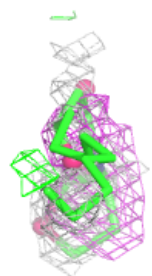
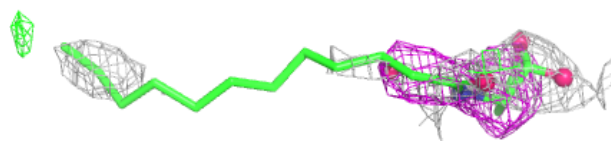
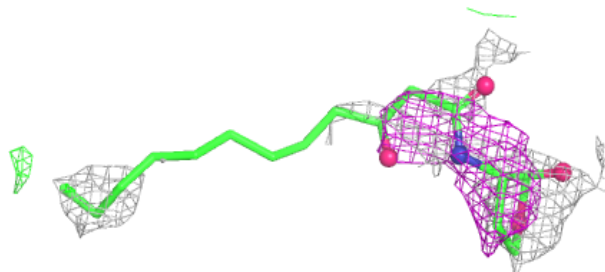


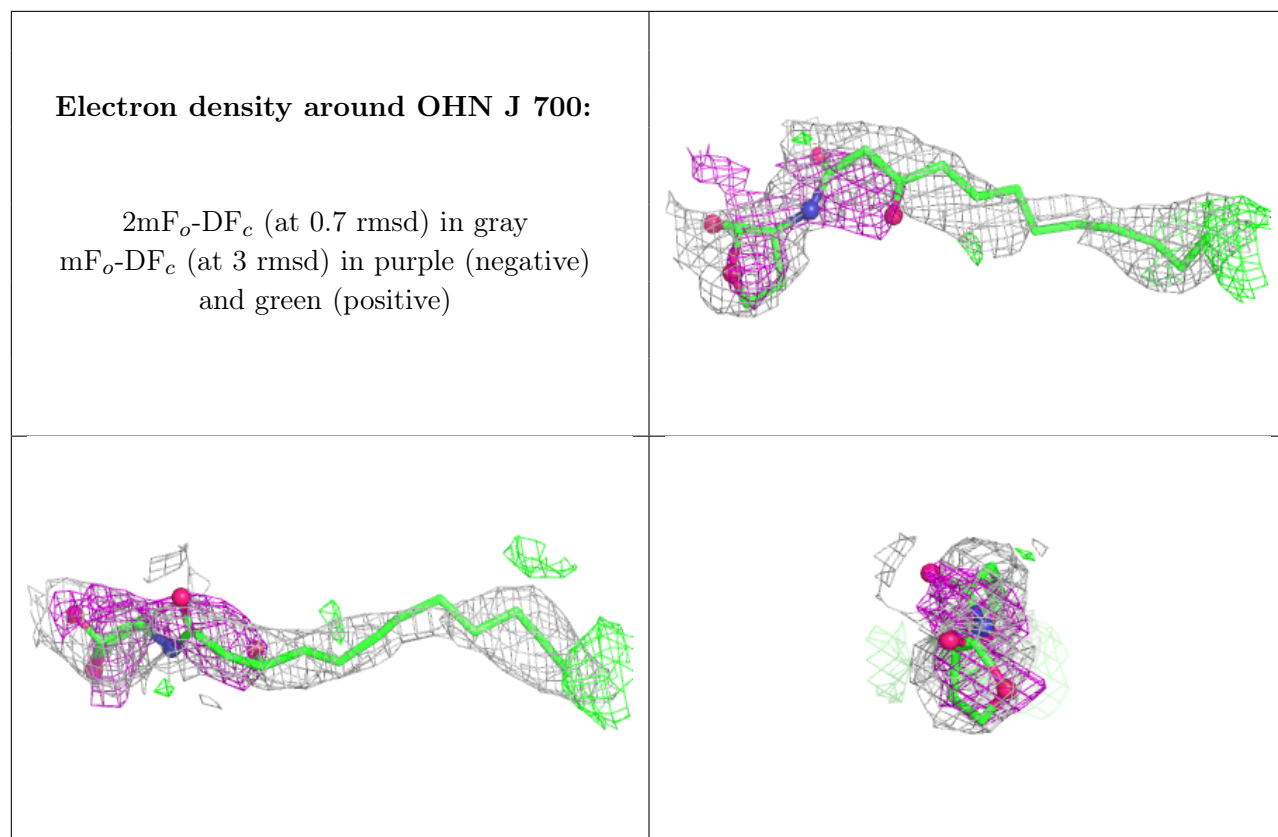
Electron density around OHN F 700:

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

**Electron density around OHN 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.