



# Full wwPDB X-ray Structure Validation Report i

May 21, 2024 – 02:08 PM EDT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) i) 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 : 2.36.2  
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) : 2.36.2

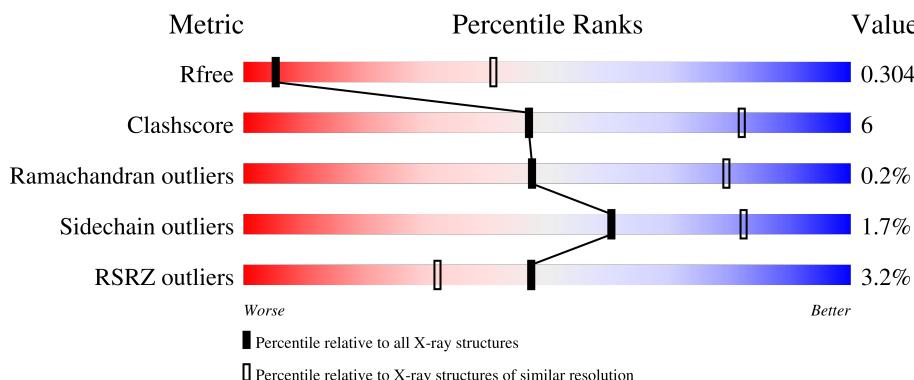
# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 Å.

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



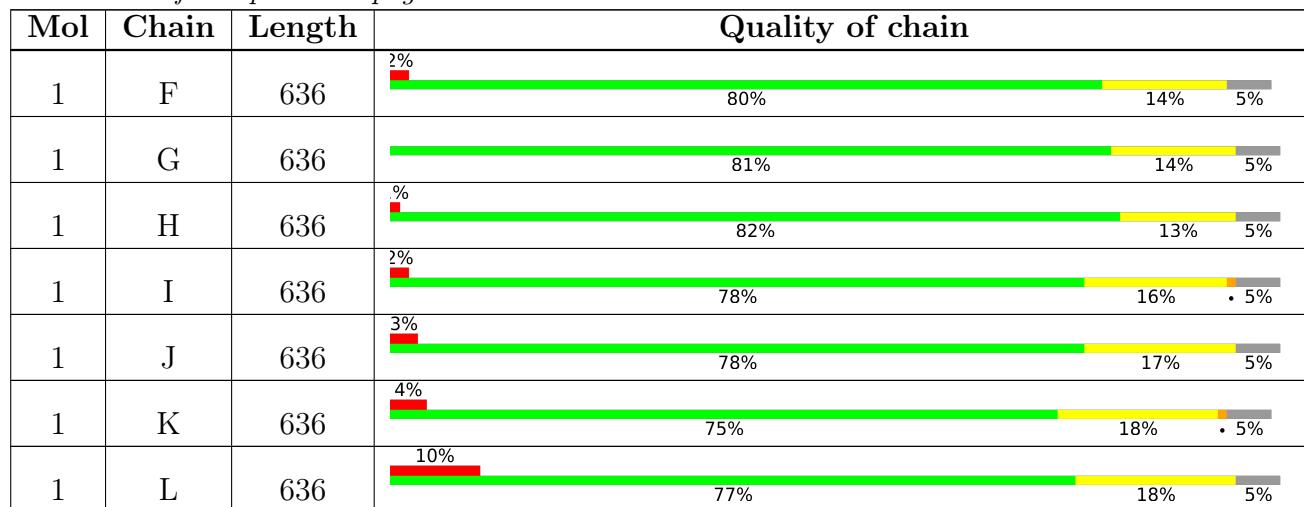
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	X4X	B	700	-	-	-	X
2	X4X	I	700	-	-	-	X

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 55530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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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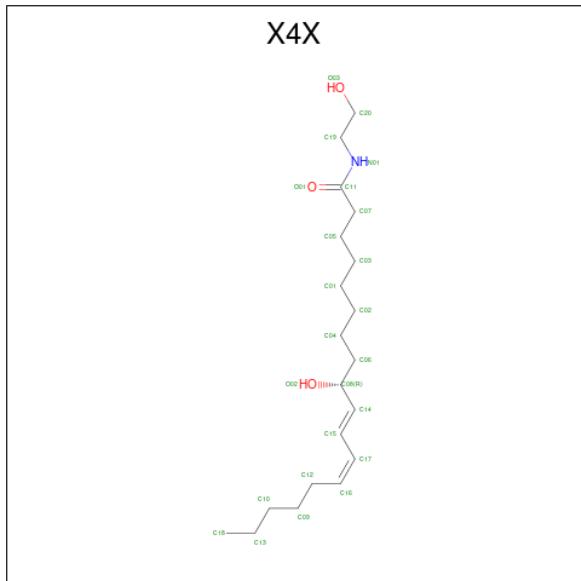
Chain	Residue	Modelled	Actual	Comment	Reference
J	636	HIS	-	expression tag	UNP Q7XJJ7
K	305	ALA	SER	engineered mutation	UNP Q7XJJ7
K	608	LYS	-	expression tag	UNP Q7XJJ7
K	609	GLY	-	expression tag	UNP Q7XJJ7
K	610	GLU	-	expression tag	UNP Q7XJJ7
K	611	PHE	-	expression tag	UNP Q7XJJ7
K	612	GLU	-	expression 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 (9R,10E,12Z)-9-hydroxy-N-(2-hydroxyethyl)octadeca-10,12-dienamide (three-letter code: X4X) (formula: C<sub>20</sub>H<sub>37</sub>NO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

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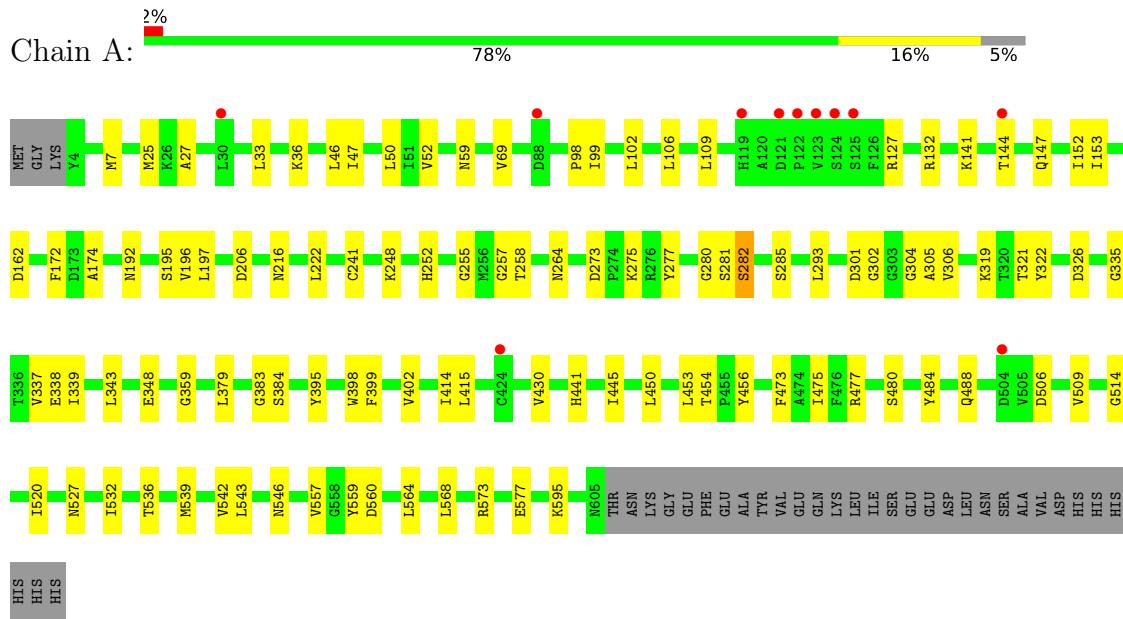
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C N O 24 20 1 3	0	0
2	F	1	Total C N O 24 20 1 3	0	0
2	G	1	Total C N O 24 20 1 3	0	0
2	H	1	Total C N O 24 20 1 3	0	0
2	I	1	Total C N O 24 20 1 3	0	0

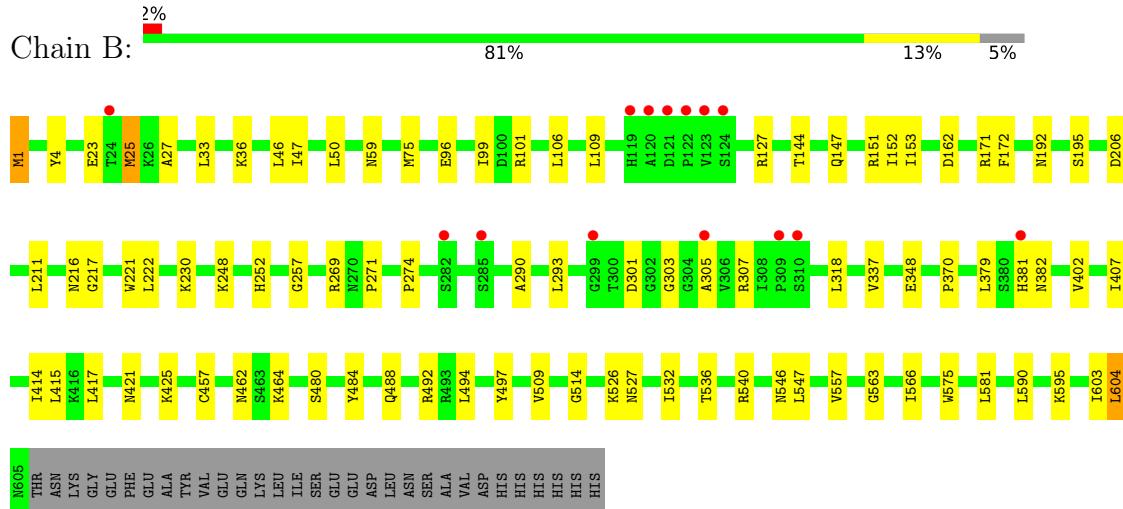
### 3 Residue-property plots

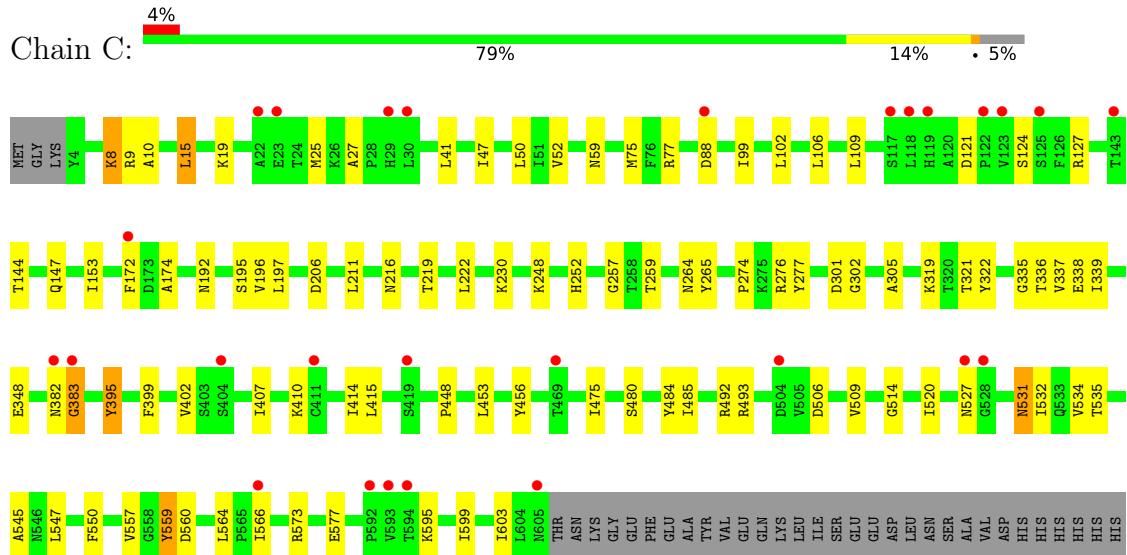
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Fatty acid amide hydrolase

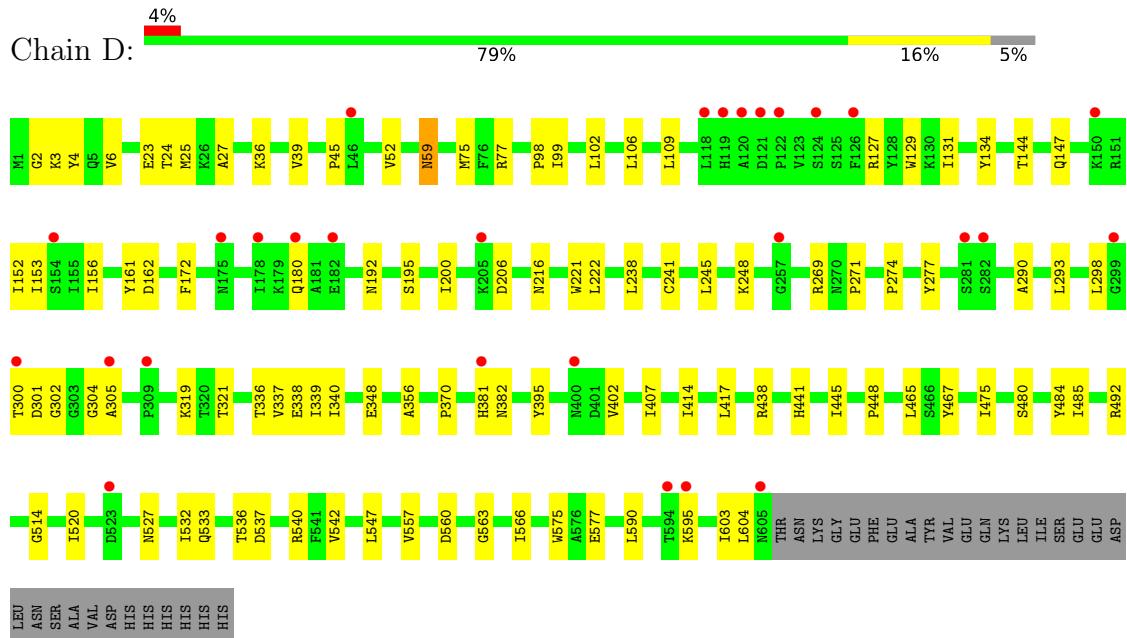


- Molecule 1: Fatty acid amide hydrolase

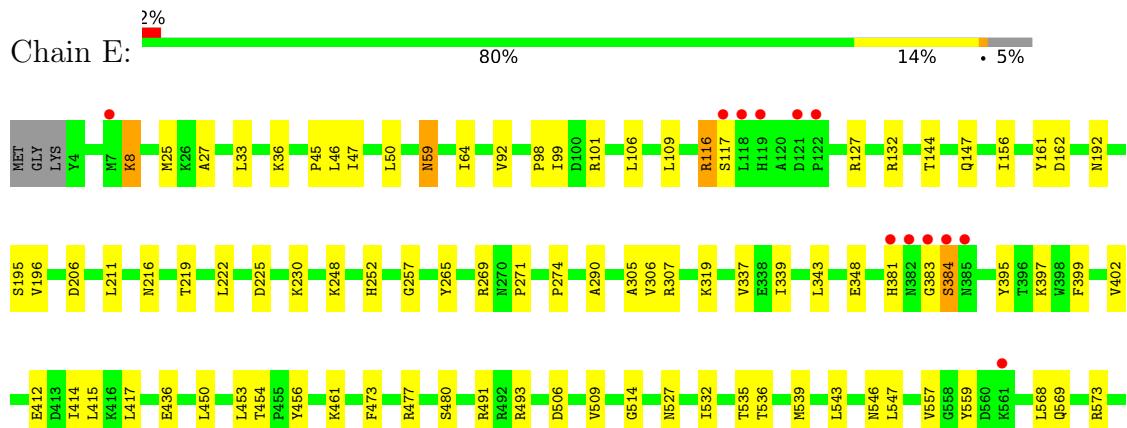


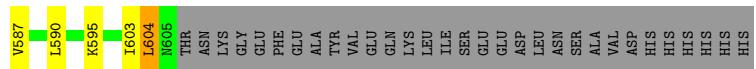


- Molecule 1: Fatty acid amide hydrolase

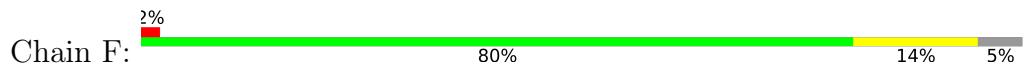


- Molecule 1: Fatty acid amide hydrolase

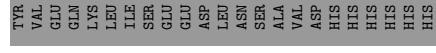
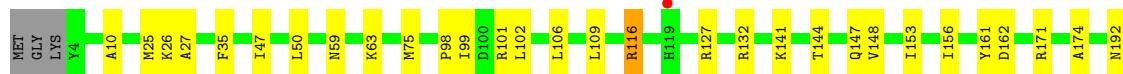
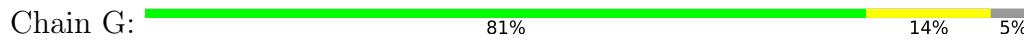




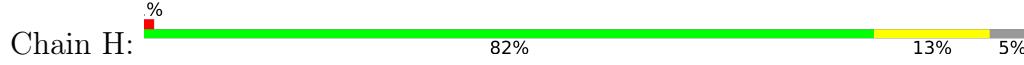
- Molecule 1: Fatty acid amide hydrolase



- Molecule 1: Fatty acid amide hydrolase



- Molecule 1: Fatty acid amide hydrolase

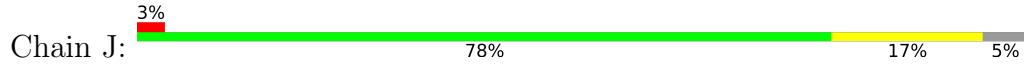




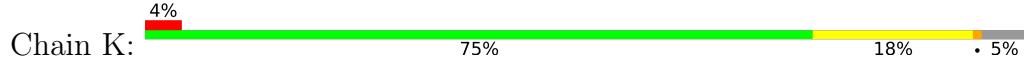
- Molecule 1: Fatty acid amide hydrolase

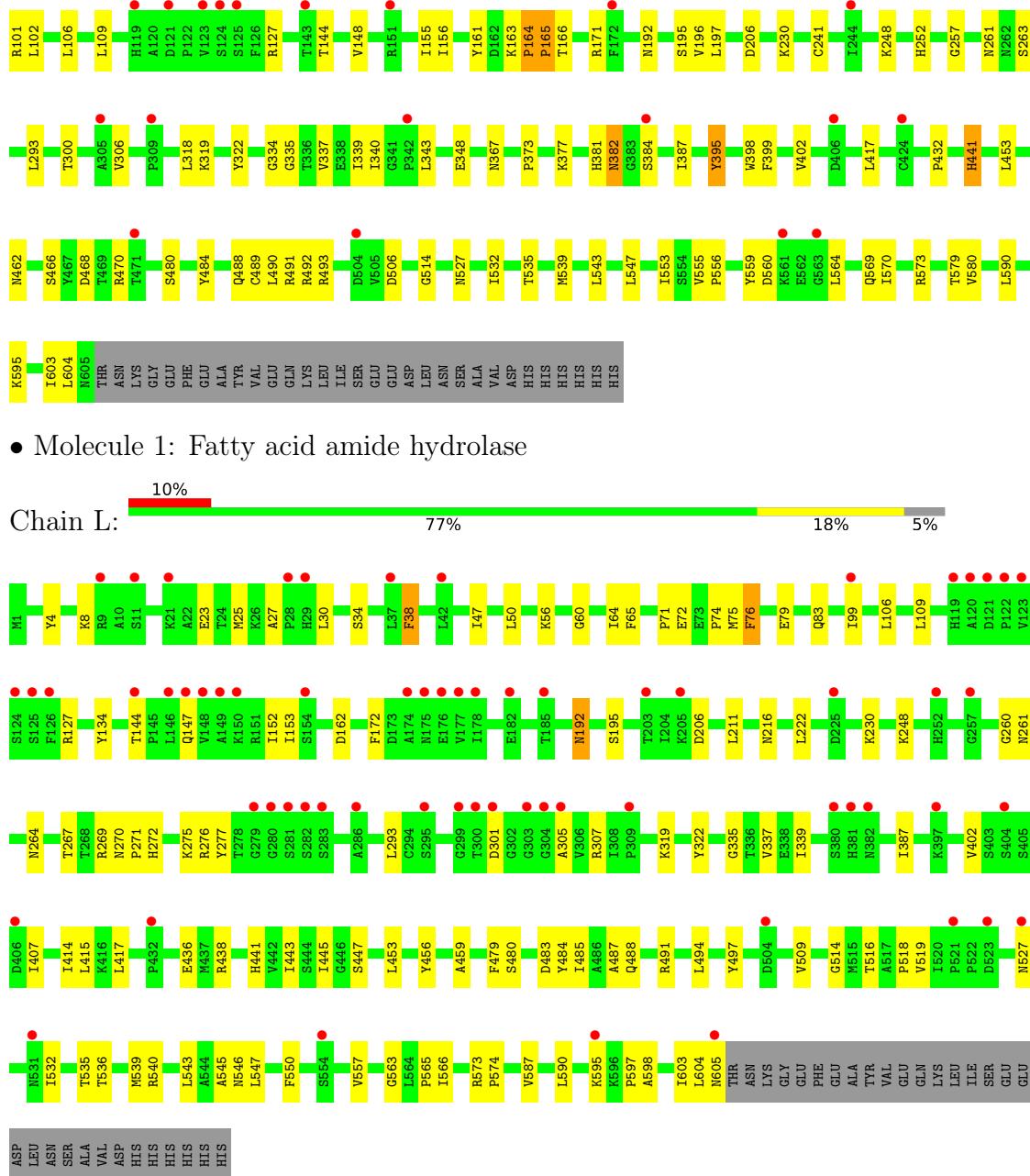


- Molecule 1: Fatty acid amide hydrolase



- Molecule 1: Fatty acid amide hydrolase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.91Å    82.91Å    271.78Å 90.00°    109.13°    90.00°	Depositor
Resolution (Å)	39.79 – 3.59 39.79 – 3.59	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.79-3.59) 96.9 (39.79-3.59)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.52 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
$R$ , $R_{free}$	0.269 , 0.305 0.269 , 0.304	Depositor DCC
$R_{free}$ test set	1982 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 30.3	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.41$ , $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	55530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5151e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: X4X

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/4704	0.41	0/6391
1	B	0.24	0/4725	0.40	0/6417
1	C	0.24	0/4704	0.46	2/6391 (0.0%)
1	D	0.24	0/4725	0.41	0/6417
1	E	0.24	0/4704	0.44	4/6391 (0.1%)
1	F	0.24	0/4725	0.41	1/6417 (0.0%)
1	G	0.24	0/4704	0.45	1/6391 (0.0%)
1	H	0.24	0/4725	0.40	0/6417
1	I	0.24	0/4704	0.44	1/6391 (0.0%)
1	J	0.24	0/4725	0.41	0/6417
1	K	0.25	0/4704	0.44	1/6391 (0.0%)
1	L	0.24	0/4725	0.42	0/6417
All	All	0.24	0/56574	0.42	10/76848 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	K	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	116	ARG	CB-CA-C	-14.58	81.24	110.40
1	I	116	ARG	CB-CA-C	-12.96	84.48	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	559	TYR	CB-CA-C	11.11	132.62	110.40
1	C	603	ILE	CB-CA-C	9.15	129.89	111.60
1	E	116	ARG	CB-CA-C	-8.78	92.84	110.40
1	E	117	SER	CB-CA-C	-6.89	97.01	110.10
1	K	263	SER	CB-CA-C	6.38	122.22	110.10
1	E	117	SER	N-CA-C	6.13	127.55	111.00
1	F	220	THR	CB-CA-C	5.37	126.11	111.60
1	E	384	SER	CB-CA-C	-5.20	100.22	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

## 5.2 Too-close contacts [\(i\)](#)

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	4605	0	4627	56	0
1	B	4626	0	4655	56	0
1	C	4605	0	4627	58	0
1	D	4626	0	4655	63	0
1	E	4605	0	4627	55	0
1	F	4626	0	4655	52	0
1	G	4605	0	4627	52	0
1	H	4626	0	4655	52	0
1	I	4605	0	4627	58	0
1	J	4626	0	4655	63	0
1	K	4605	0	4627	72	0
1	L	4626	0	4655	77	0
2	B	24	0	0	1	0
2	E	24	0	0	1	0
2	F	24	0	0	1	0
2	G	24	0	0	1	0
2	H	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	24	0	0	0	0
All	All	55530	0	55692	692	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 6.

All (692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:ARG:O	1:I:116:ARG:HG3	1.28	1.04
1:I:116:ARG:O	1:I:116:ARG:CG	2.02	1.04
1:E:116:ARG:O	1:E:116:ARG:HG3	1.59	1.01
1:G:116:ARG:O	1:G:116:ARG:HG3	1.74	0.85
1:B:221:TRP:O	1:B:221:TRP:CE3	2.38	0.76
1:E:319:LYS:HG2	1:E:339:ILE:HD11	1.69	0.74
1:J:208:ILE:O	1:J:248:LYS:NZ	2.18	0.74
1:A:282:SER:HG	1:A:285:SER:HG	1.33	0.73
1:H:319:LYS:HG2	1:H:339:ILE:HD11	1.71	0.72
1:G:319:LYS:HG2	1:G:339:ILE:HD11	1.71	0.71
1:B:221:TRP:O	1:B:221:TRP:HE3	1.72	0.71
1:D:319:LYS:HG2	1:D:339:ILE:HD11	1.74	0.69
1:D:533:GLN:NE2	1:D:537:ASP:OD2	2.24	0.69
1:F:221:TRP:CD1	1:F:464:LYS:HB3	2.27	0.69
1:L:539:MET:HB3	1:L:543:LEU:HD21	1.74	0.69
1:A:319:LYS:HG2	1:A:339:ILE:HD11	1.75	0.69
1:K:9:ARG:HH11	1:K:11:SER:H	1.41	0.68
1:I:506:ASP:OD1	1:I:573:ARG:NH2	2.25	0.68
1:C:319:LYS:HG2	1:C:339:ILE:HD11	1.77	0.67
1:I:94:GLU:OE2	1:I:360:SER:OG	2.12	0.67
1:J:171:ARG:HB2	1:J:248:LYS:HB2	1.76	0.67
1:A:402:VAL:HG12	1:A:514:GLY:HA2	1.77	0.66
1:G:25:MET:SD	1:G:59:ASN:ND2	2.67	0.66
1:I:9:ARG:O	1:I:13:VAL:HG23	1.96	0.66
1:B:301:ASP:HA	1:B:305:ALA:HB3	1.78	0.66
1:K:319:LYS:HG2	1:K:339:ILE:HD11	1.78	0.66
1:K:441:HIS:HD2	1:K:543:LEU:HD22	1.61	0.66
1:L:99:ILE:HG23	1:L:195:SER:HB3	1.78	0.66
1:D:2:GLY:HA2	1:D:6:VAL:HG22	1.78	0.65
1:D:603:ILE:HG23	1:D:604:LEU:HG	1.78	0.65
1:J:319:LYS:HG2	1:J:339:ILE:HD11	1.78	0.65
1:A:46:LEU:HD11	1:B:46:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:HA	1:C:520:ILE:HD13	1.79	0.65
1:H:25:MET:HG3	1:H:536:THR:HG21	1.78	0.65
1:D:195:SER:HG	1:D:241:CYS:HG	1.46	0.64
1:H:603:ILE:HG22	1:H:604:LEU:HG	1.79	0.64
1:C:8:LYS:HD3	1:C:493:ARG:CZ	2.28	0.64
1:D:25:MET:HA	1:D:59:ASN:HD22	1.62	0.64
1:J:25:MET:SD	1:J:59:ASN:ND2	2.70	0.64
1:J:99:ILE:HG23	1:J:195:SER:HB3	1.80	0.64
1:J:25:MET:HG3	1:J:536:THR:HG21	1.80	0.64
1:L:277:TYR:HD2	1:L:518:PRO:HG2	1.63	0.64
1:L:402:VAL:HG12	1:L:514:GLY:HA2	1.79	0.64
1:E:491:ARG:NH1	1:E:547:LEU:O	2.31	0.63
1:L:415:LEU:HD21	1:L:509:VAL:HG21	1.80	0.63
1:H:402:VAL:HG12	1:H:514:GLY:HA2	1.81	0.63
1:K:75:MET:HB2	1:K:492:ARG:HB2	1.81	0.63
1:L:30:LEU:HD12	1:L:38:PHE:HB2	1.80	0.63
1:F:402:VAL:HG12	1:F:514:GLY:HA2	1.80	0.63
1:D:99:ILE:HG23	1:D:195:SER:HB3	1.80	0.63
1:A:383:GLY:O	1:A:384:SER:HB2	1.99	0.63
1:H:206:ASP:HA	1:H:248:LYS:HE2	1.80	0.63
1:K:7:MET:HG2	1:K:69:VAL:HB	1.79	0.63
1:F:319:LYS:HG2	1:F:339:ILE:HD11	1.80	0.62
1:L:563:GLY:O	1:L:595:LYS:NZ	2.29	0.62
1:B:99:ILE:HG23	1:B:195:SER:HB3	1.80	0.62
1:J:144:THR:HG23	1:J:147:GLN:H	1.64	0.62
1:D:563:GLY:O	1:D:595:LYS:NZ	2.33	0.62
1:J:603:ILE:HG22	1:J:604:LEU:HG	1.80	0.62
1:B:153:ILE:HG12	1:B:172:PHE:HZ	1.64	0.62
1:B:307:ARG:NH2	1:B:546:ASN:OD1	2.32	0.62
1:B:269:ARG:NH1	1:H:141:LYS:O	2.30	0.61
1:B:563:GLY:O	1:B:595:LYS:NZ	2.33	0.61
1:C:480:SER:HA	1:D:480:SER:HA	1.82	0.61
1:G:206:ASP:HA	1:G:248:LYS:HE2	1.81	0.61
1:C:402:VAL:HG12	1:C:514:GLY:HA2	1.82	0.61
1:G:116:ARG:O	1:G:116:ARG:CG	2.31	0.61
1:K:539:MET:HB3	1:K:543:LEU:HD21	1.83	0.60
1:L:153:ILE:HG12	1:L:172:PHE:HZ	1.66	0.60
1:B:152:ILE:HG23	1:B:293:LEU:HD22	1.83	0.60
1:L:25:MET:HG3	1:L:536:THR:HG21	1.83	0.60
1:F:25:MET:SD	1:F:59:ASN:ND2	2.74	0.60
1:K:99:ILE:HG23	1:K:195:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:LEU:HD12	1:J:172:PHE:HD2	1.67	0.60
1:E:603:ILE:HG22	1:E:604:LEU:HG	1.84	0.60
1:J:23:GLU:HG3	1:J:540:ARG:HH21	1.67	0.60
1:G:506:ASP:OD1	1:G:573:ARG:NH2	2.29	0.60
1:B:221:TRP:CD1	1:B:464:LYS:HB3	2.37	0.59
1:H:216:ASN:HA	1:H:222:LEU:HB3	1.84	0.59
1:L:23:GLU:HG3	1:L:540:ARG:HH21	1.67	0.59
1:K:39:VAL:HG11	1:K:470:ARG:HH21	1.68	0.59
1:B:47:ILE:HA	1:B:50:LEU:HD12	1.85	0.59
1:K:480:SER:HA	1:L:480:SER:HA	1.84	0.59
1:E:25:MET:HG3	1:E:536:THR:HG21	1.84	0.59
1:B:417:LEU:HB3	1:B:590:LEU:HD13	1.84	0.59
1:D:221:TRP:O	1:D:221:TRP:CE3	2.56	0.59
1:I:72:GLU:OE2	1:I:493:ARG:NH1	2.36	0.59
1:B:402:VAL:HG12	1:B:514:GLY:HA2	1.85	0.58
1:D:144:THR:HG23	1:D:147:GLN:H	1.68	0.58
1:B:144:THR:HG23	1:B:147:GLN:H	1.66	0.58
1:C:506:ASP:OD1	1:C:573:ARG:NH2	2.32	0.58
1:H:33:LEU:HD13	1:H:33:LEU:O	2.02	0.58
1:K:4:TYR:HD2	1:L:459:ALA:HB1	1.68	0.58
1:A:506:ASP:OD1	1:A:573:ARG:NH2	2.36	0.58
1:J:402:VAL:HG12	1:J:514:GLY:HA2	1.86	0.58
1:K:441:HIS:CD2	1:K:543:LEU:HD22	2.37	0.58
1:L:271:PRO:HG2	1:L:272:HIS:HD2	1.67	0.58
1:F:2:GLY:HA2	1:F:6:VAL:HG22	1.86	0.58
1:F:206:ASP:HA	1:F:248:LYS:HE2	1.85	0.58
1:G:109:LEU:HD22	1:G:348:GLU:HG3	1.85	0.58
1:H:99:ILE:HG23	1:H:195:SER:HB3	1.85	0.58
1:L:261:ASN:ND2	1:L:277:TYR:OH	2.36	0.58
1:K:402:VAL:HG12	1:K:514:GLY:HA2	1.86	0.58
1:L:319:LYS:HG2	1:L:339:ILE:HD11	1.86	0.58
1:E:206:ASP:HA	1:E:248:LYS:HE2	1.86	0.57
1:G:603:ILE:HG22	1:G:604:LEU:N	2.19	0.57
1:K:252:HIS:NE2	1:K:468:ASP:OD2	2.35	0.57
1:L:216:ASN:HA	1:L:222:LEU:HB3	1.85	0.57
1:H:23:GLU:HA	1:H:438:ARG:HH12	1.69	0.57
1:K:28:PRO:HG2	1:K:38:PHE:HE2	1.68	0.57
1:L:491:ARG:NH1	1:L:547:LEU:O	2.37	0.57
1:A:480:SER:HA	1:B:480:SER:HA	1.86	0.57
1:E:99:ILE:HG23	1:E:195:SER:HB3	1.86	0.57
1:L:319:LYS:NZ	1:L:545:ALA:O	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:537:ASP:OD1	1:D:540:ARG:NH2	2.37	0.57
1:D:153:ILE:HG12	1:D:172:PHE:HZ	1.69	0.57
1:J:413:ASP:O	1:J:417:LEU:N	2.35	0.56
1:C:25:MET:SD	1:C:59:ASN:ND2	2.78	0.56
1:E:453:LEU:HD23	1:E:456:TYR:HD2	1.70	0.56
1:F:99:ILE:HG23	1:F:195:SER:HB3	1.86	0.56
1:G:453:LEU:HD23	1:G:456:TYR:HD2	1.69	0.56
1:F:109:LEU:HD22	1:F:348:GLU:HG3	1.87	0.56
1:J:563:GLY:O	1:J:595:LYS:NZ	2.34	0.56
1:L:83:GLN:HE22	1:L:573:ARG:HB3	1.71	0.56
1:L:443:ILE:HG13	1:L:479:PHE:CG	2.41	0.56
1:B:425:LYS:NZ	1:C:402:VAL:O	2.39	0.55
1:D:216:ASN:HA	1:D:222:LEU:HB3	1.88	0.55
1:L:414:ILE:HG13	1:L:557:VAL:HB	1.87	0.55
1:H:25:MET:HA	1:H:59:ASN:HD22	1.72	0.55
1:I:206:ASP:HA	1:I:248:LYS:HE2	1.87	0.55
1:J:206:ASP:HA	1:J:248:LYS:HE2	1.87	0.55
1:L:417:LEU:HB3	1:L:590:LEU:HD13	1.88	0.55
1:I:225:ASP:OD2	1:I:461:LYS:NZ	2.39	0.55
1:B:603:ILE:HG22	1:B:604:LEU:HG	1.88	0.55
1:E:92:VAL:HG11	1:E:101:ARG:HG2	1.88	0.55
1:E:216:ASN:HA	1:E:222:LEU:HB3	1.88	0.55
1:I:35:PHE:HE2	1:I:528:GLY:C	2.10	0.55
1:E:480:SER:HA	1:F:480:SER:HA	1.88	0.55
1:F:273:ASP:OD2	1:F:275:LYS:NZ	2.38	0.55
1:L:30:LEU:HD13	1:L:34:SER:HB2	1.88	0.55
1:I:47:ILE:HA	1:I:50:LEU:HD12	1.89	0.55
1:K:70:ILE:HD12	1:K:489:CYS:HB2	1.88	0.55
1:F:216:ASN:HA	1:F:222:LEU:HB3	1.88	0.55
1:B:25:MET:SD	1:B:59:ASN:ND2	2.80	0.55
1:D:195:SER:OG	1:D:241:CYS:SG	2.60	0.55
1:E:47:ILE:HA	1:E:50:LEU:HD12	1.88	0.55
1:G:321:THR:OG1	1:G:577:GLU:OE2	2.23	0.55
1:B:414:ILE:HG13	1:B:557:VAL:HB	1.88	0.54
1:E:25:MET:SD	1:E:59:ASN:ND2	2.80	0.54
1:K:18:VAL:HG11	1:K:432:PRO:HB3	1.89	0.54
1:G:144:THR:HG23	1:G:147:GLN:H	1.72	0.54
1:J:156:ILE:HG23	1:J:161:TYR:HB2	1.89	0.54
1:L:206:ASP:HA	1:L:248:LYS:HE2	1.89	0.54
1:D:25:MET:HG3	1:D:536:THR:HG21	1.88	0.54
1:L:441:HIS:HE2	1:L:445:ILE:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:LEU:HD22	1:H:348:GLU:HG3	1.90	0.54
1:L:603:ILE:HG23	1:L:604:LEU:HG	1.89	0.54
1:E:383:GLY:O	1:E:384:SER:HB2	2.08	0.54
1:K:367:ASN:ND2	1:L:79:GLU:OE1	2.38	0.54
1:E:417:LEU:HB3	1:E:590:LEU:HD13	1.90	0.54
1:D:301:ASP:HA	1:D:305:ALA:HB3	1.90	0.54
1:D:414:ILE:HG13	1:D:557:VAL:HB	1.89	0.54
1:B:23:GLU:OE1	1:B:540:ARG:NH2	2.41	0.53
1:J:197:LEU:HA	1:J:200:ILE:HG13	1.89	0.53
1:E:8:LYS:HD3	1:E:493:ARG:CZ	2.39	0.53
1:G:395:TYR:O	1:G:399:PHE:N	2.40	0.53
1:I:269:ARG:HB3	1:I:274:PRO:HA	1.90	0.53
1:L:76:PHE:HD1	1:L:488:GLN:HG3	1.73	0.53
1:D:417:LEU:HB3	1:D:590:LEU:HD13	1.91	0.53
1:K:506:ASP:OD1	1:K:573:ARG:NH2	2.40	0.53
1:F:7:MET:HB3	1:F:69:VAL:HB	1.90	0.53
1:B:269:ARG:HB3	1:B:274:PRO:HA	1.91	0.53
1:D:134:TYR:OH	1:D:603:ILE:HG21	2.09	0.53
1:D:152:ILE:HG23	1:D:293:LEU:HD22	1.91	0.53
1:I:480:SER:HA	1:J:480:SER:HA	1.91	0.53
1:E:506:ASP:OD1	1:E:573:ARG:NH2	2.34	0.52
1:H:152:ILE:HG23	1:H:293:LEU:HD22	1.91	0.52
1:F:152:ILE:HG23	1:F:293:LEU:HD22	1.91	0.52
1:G:491:ARG:NH1	1:G:547:LEU:O	2.43	0.52
1:B:33:LEU:HA	1:B:36:LYS:HE3	1.91	0.52
1:B:206:ASP:HA	1:B:248:LYS:HE2	1.92	0.52
1:D:52:VAL:HG13	1:D:475:ILE:HG12	1.91	0.52
1:F:319:LYS:HE2	1:F:339:ILE:HG12	1.91	0.52
1:B:25:MET:HG3	1:B:536:THR:HG21	1.92	0.52
1:B:421:ASN:HA	1:C:19:LYS:HD3	1.92	0.52
1:G:414:ILE:HG13	1:G:557:VAL:HB	1.91	0.52
1:I:112:TYR:HE2	1:I:136:TYR:HB2	1.73	0.52
1:C:15:LEU:HD23	1:C:15:LEU:H	1.74	0.52
1:C:109:LEU:HD22	1:C:348:GLU:HG3	1.91	0.52
1:E:162:ASP:OD1	1:E:162:ASP:N	2.43	0.52
1:H:33:LEU:HA	1:H:36:LYS:HE3	1.92	0.52
1:K:417:LEU:HB3	1:K:590:LEU:HD13	1.92	0.52
1:L:47:ILE:HA	1:L:50:LEU:HD12	1.91	0.52
1:L:453:LEU:HD23	1:L:456:TYR:HD2	1.74	0.52
1:B:171:ARG:HB2	1:B:248:LYS:HB2	1.90	0.51
1:E:144:THR:HG23	1:E:147:GLN:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:LEU:HD22	1:K:348:GLU:HG3	1.92	0.51
1:L:270:ASN:ND2	1:L:277:TYR:O	2.43	0.51
1:A:152:ILE:HG23	1:A:293:LEU:HD22	1.91	0.51
1:A:7:MET:HB3	1:A:69:VAL:HB	1.93	0.51
1:L:272:HIS:CE1	1:L:565:PRO:HG3	2.45	0.51
1:C:47:ILE:HA	1:C:50:LEU:HD12	1.93	0.51
1:E:109:LEU:HD22	1:E:348:GLU:HG3	1.91	0.51
1:A:206:ASP:HA	1:A:248:LYS:HE2	1.92	0.51
1:G:27:ALA:HB3	1:G:532:ILE:HB	1.92	0.51
1:I:99:ILE:HG23	1:I:195:SER:HB3	1.93	0.51
1:I:560:ASP:OD1	1:I:564:LEU:N	2.43	0.51
1:B:301:ASP:OD2	1:B:307:ARG:NH2	2.41	0.51
1:G:480:SER:HA	1:H:480:SER:HA	1.93	0.51
1:I:450:LEU:O	1:I:454:THR:OG1	2.23	0.51
1:C:206:ASP:HA	1:C:248:LYS:HE2	1.92	0.50
1:D:180:GLN:HE22	1:D:245:LEU:HB2	1.75	0.50
1:D:221:TRP:O	1:D:221:TRP:HE3	1.94	0.50
1:G:26:LYS:H	1:G:59:ASN:HD21	1.57	0.50
1:J:414:ILE:HG21	1:J:587:VAL:HG13	1.93	0.50
1:K:35:PHE:HZ	1:K:468:ASP:HA	1.76	0.50
1:A:25:MET:SD	1:A:59:ASN:ND2	2.84	0.50
1:C:99:ILE:HG23	1:C:195:SER:HB3	1.92	0.50
1:C:321:THR:OG1	1:C:577:GLU:OE2	2.19	0.50
1:D:321:THR:OG1	1:D:577:GLU:OE2	2.19	0.50
1:G:47:ILE:HA	1:G:50:LEU:HD12	1.93	0.50
1:G:102:LEU:HD11	1:G:197:LEU:HD12	1.93	0.50
1:L:75:MET:HE2	1:L:79:GLU:H	1.76	0.50
1:A:109:LEU:HD22	1:A:348:GLU:HG3	1.92	0.50
1:E:211:LEU:HD11	1:E:230:LYS:HA	1.92	0.50
1:B:96:GLU:O	1:B:101:ARG:NH1	2.44	0.50
1:B:109:LEU:HD22	1:B:348:GLU:HG3	1.93	0.50
1:K:490:LEU:HD23	1:K:493:ARG:HD3	1.92	0.50
1:C:414:ILE:HG13	1:C:557:VAL:HB	1.92	0.50
1:F:153:ILE:HG12	1:F:172:PHE:HZ	1.76	0.50
1:H:8:LYS:NZ	1:H:68:THR:HG21	2.27	0.50
1:K:9:ARG:HD2	1:K:12:GLU:H	1.77	0.50
1:H:25:MET:HA	1:H:59:ASN:ND2	2.27	0.50
1:K:603:ILE:HG22	1:K:604:LEU:H	1.77	0.50
1:L:337:VAL:HG12	1:L:547:LEU:HA	1.93	0.50
1:H:47:ILE:HA	1:H:50:LEU:HD12	1.94	0.50
1:K:559:TYR:CZ	1:K:595:LYS:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:274:PRO:HG3	1:I:599:ILE:HD11	1.94	0.50
1:K:395:TYR:O	1:K:399:PHE:N	2.43	0.50
1:L:322:TYR:OH	1:L:335:GLY:O	2.24	0.50
1:F:271:PRO:HG2	1:F:290:ALA:HB3	1.94	0.50
1:G:156:ILE:HA	1:G:161:TYR:HB2	1.94	0.50
1:H:143:THR:HG21	1:H:604:LEU:HD22	1.94	0.50
1:I:252:HIS:CE1	1:I:257:GLY:HA3	2.47	0.50
1:L:319:LYS:HE2	1:L:339:ILE:HG12	1.94	0.50
1:A:47:ILE:HA	1:A:50:LEU:HD12	1.93	0.49
1:C:216:ASN:HA	1:C:222:LEU:HB3	1.93	0.49
1:F:144:THR:HG23	1:F:147:GLN:H	1.76	0.49
1:C:27:ALA:HB3	1:C:532:ILE:HB	1.94	0.49
1:F:337:VAL:HG12	1:F:547:LEU:HA	1.94	0.49
1:H:337:VAL:HG12	1:H:547:LEU:HA	1.94	0.49
1:I:402:VAL:HG12	1:I:514:GLY:HA2	1.94	0.49
1:L:441:HIS:ND1	1:L:543:LEU:HD22	2.27	0.49
1:A:106:LEU:HD11	1:A:196:VAL:HB	1.94	0.49
1:D:337:VAL:HG12	1:D:547:LEU:HA	1.94	0.49
1:F:379:LEU:HD12	1:F:379:LEU:H	1.77	0.49
1:K:47:ILE:HG22	1:K:51:ILE:HD11	1.94	0.49
1:A:395:TYR:CZ	1:A:430:VAL:HG23	2.48	0.49
1:F:417:LEU:HB3	1:F:590:LEU:HD13	1.94	0.49
1:I:417:LEU:HB3	1:I:590:LEU:HD13	1.94	0.49
1:J:109:LEU:HD22	1:J:348:GLU:HG3	1.94	0.49
1:J:380:SER:O	1:J:380:SER:OG	2.29	0.49
1:K:88:ASP:OD1	1:K:377:LYS:NZ	2.37	0.49
1:F:395:TYR:CZ	1:F:430:VAL:HG23	2.48	0.49
1:A:395:TYR:O	1:A:399:PHE:N	2.45	0.49
1:B:106:LEU:HD23	1:B:109:LEU:HD12	1.95	0.49
1:D:221:TRP:HE1	1:D:465:LEU:HD23	1.78	0.49
1:D:402:VAL:HG12	1:D:514:GLY:HA2	1.94	0.48
1:E:395:TYR:O	1:E:399:PHE:N	2.45	0.48
1:G:171:ARG:HB2	1:G:248:LYS:HB2	1.94	0.48
1:G:305:ALA:HB2	2:G:700:X4X:N01	2.27	0.48
1:H:305:ALA:HB2	2:H:700:X4X:N01	2.28	0.48
1:E:414:ILE:HG21	1:E:587:VAL:HG13	1.96	0.48
1:E:402:VAL:HG12	1:E:514:GLY:HA2	1.95	0.48
1:E:414:ILE:HG13	1:E:557:VAL:HB	1.94	0.48
1:G:211:LEU:HD11	1:G:230:LYS:HA	1.94	0.48
1:J:151:ARG:HG2	1:J:603:ILE:HG13	1.94	0.48
1:A:52:VAL:HG13	1:A:475:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:HA	1:A:222:LEU:HB3	1.95	0.48
1:B:337:VAL:HG12	1:B:547:LEU:HA	1.95	0.48
1:B:415:LEU:HD21	1:B:509:VAL:HG21	1.95	0.48
1:G:532:ILE:HA	1:G:535:THR:OG1	2.13	0.48
1:L:550:PHE:CE1	1:L:574:PRO:HD3	2.49	0.48
1:C:41:LEU:HD22	1:C:47:ILE:HD11	1.96	0.48
1:C:75:MET:HB2	1:C:492:ARG:HB2	1.95	0.48
1:J:143:THR:HG21	1:J:604:LEU:HD22	1.94	0.48
1:L:271:PRO:HB2	1:L:597:PRO:HB3	1.95	0.48
1:L:436:GLU:OE1	1:L:436:GLU:N	2.43	0.48
1:J:252:HIS:CE1	1:J:257:GLY:HA3	2.49	0.48
1:K:553:ILE:O	1:K:569:GLN:HA	2.13	0.48
1:L:65:PHE:CE2	1:L:487:ALA:HB2	2.49	0.48
1:B:526:LYS:HA	1:B:526:LYS:HD2	1.71	0.48
1:G:252:HIS:CE1	1:G:257:GLY:HA3	2.48	0.48
1:H:33:LEU:HD13	1:H:33:LEU:C	2.34	0.48
1:I:27:ALA:HB3	1:I:532:ILE:HB	1.96	0.48
1:C:52:VAL:HG13	1:C:475:ILE:HG12	1.96	0.48
1:G:417:LEU:HB3	1:G:590:LEU:HD13	1.96	0.48
1:K:322:TYR:OH	1:K:335:GLY:O	2.26	0.48
1:K:532:ILE:HA	1:K:535:THR:OG1	2.14	0.48
1:L:443:ILE:HD11	1:L:483:ASP:HB3	1.95	0.48
1:D:106:LEU:HD23	1:D:109:LEU:HD12	1.95	0.47
1:H:10:ALA:HB2	1:H:493:ARG:CZ	2.44	0.47
1:J:25:MET:HA	1:J:59:ASN:ND2	2.29	0.47
1:B:216:ASN:HA	1:B:222:LEU:HB3	1.95	0.47
1:F:43:GLU:OE2	1:F:470:ARG:NE	2.47	0.47
1:H:536:THR:HA	1:H:539:MET:HE2	1.96	0.47
1:J:415:LEU:HD21	1:J:509:VAL:HG21	1.95	0.47
1:C:531:ASN:HB3	1:C:534:VAL:HG22	1.96	0.47
1:D:77:ARG:HG2	1:D:336:THR:HG22	1.96	0.47
1:G:162:ASP:OD1	1:G:162:ASP:N	2.47	0.47
1:G:225:ASP:OD2	1:G:461:LYS:NZ	2.39	0.47
1:H:252:HIS:CE1	1:H:257:GLY:HA3	2.49	0.47
1:I:414:ILE:HG13	1:I:557:VAL:HB	1.96	0.47
1:K:206:ASP:HA	1:K:248:LYS:HE2	1.95	0.47
1:L:270:ASN:HB2	1:L:276:ARG:O	2.14	0.47
1:D:109:LEU:HD22	1:D:348:GLU:HG3	1.97	0.47
1:E:271:PRO:HG2	1:E:290:ALA:HB3	1.96	0.47
1:K:560:ASP:OD1	1:K:564:LEU:N	2.46	0.47
1:L:443:ILE:O	1:L:447:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASP:HA	1:A:305:ALA:HB3	1.95	0.47
1:A:415:LEU:HD21	1:A:509:VAL:HG21	1.95	0.47
1:H:301:ASP:HA	1:H:305:ALA:HB3	1.95	0.47
1:I:395:TYR:O	1:I:399:PHE:N	2.43	0.47
1:E:27:ALA:HB3	1:E:532:ILE:HB	1.96	0.47
1:I:216:ASN:HA	1:I:222:LEU:HB3	1.97	0.47
1:K:384:SER:HA	1:K:387:ILE:HB	1.96	0.47
1:A:379:LEU:HD23	1:A:379:LEU:H	1.80	0.47
1:C:211:LEU:HD11	1:C:230:LYS:HA	1.95	0.47
1:E:450:LEU:O	1:E:454:THR:OG1	2.22	0.47
1:J:152:ILE:HG23	1:J:293:LEU:HD22	1.96	0.47
1:K:155:ILE:HG21	1:K:293:LEU:HD21	1.97	0.47
1:F:3:LYS:HE3	1:I:139:ARG:HD2	1.96	0.47
1:J:77:ARG:HG2	1:J:336:THR:HG22	1.97	0.47
1:K:381:HIS:HA	1:K:382:ASN:HA	1.68	0.47
1:B:252:HIS:CE1	1:B:257:GLY:HA3	2.50	0.47
1:C:106:LEU:HD11	1:C:196:VAL:HB	1.96	0.47
1:G:415:LEU:HD21	1:G:509:VAL:HG21	1.97	0.47
1:J:321:THR:OG1	1:J:577:GLU:OE2	2.24	0.47
1:L:301:ASP:HA	1:L:305:ALA:HB3	1.96	0.47
1:C:337:VAL:HG12	1:C:547:LEU:HA	1.98	0.46
1:D:129:TRP:CD1	1:D:603:ILE:HG22	2.50	0.46
1:G:219:THR:O	1:G:265:TYR:OH	2.24	0.46
1:I:20:TYR:CZ	1:I:22:ALA:HB2	2.50	0.46
1:J:192:ASN:OD1	1:J:192:ASN:N	2.48	0.46
1:K:337:VAL:HG12	1:K:547:LEU:HA	1.95	0.46
1:L:65:PHE:HE2	1:L:487:ALA:HB2	1.80	0.46
1:A:559:TYR:CZ	1:A:595:LYS:HB2	2.50	0.46
1:C:545:ALA:HA	1:C:550:PHE:HB2	1.97	0.46
1:F:27:ALA:HB3	1:F:532:ILE:HB	1.96	0.46
1:F:252:HIS:CE1	1:F:257:GLY:HA3	2.50	0.46
1:H:144:THR:HG23	1:H:147:GLN:H	1.80	0.46
1:I:211:LEU:HD11	1:I:230:LYS:HA	1.97	0.46
1:I:415:LEU:HD21	1:I:509:VAL:HG21	1.97	0.46
1:J:337:VAL:HG12	1:J:547:LEU:HA	1.97	0.46
1:J:539:MET:O	1:J:543:LEU:HG	2.15	0.46
1:K:8:LYS:HD3	1:K:493:ARG:CZ	2.44	0.46
1:D:156:ILE:HG23	1:D:161:TYR:HB2	1.96	0.46
1:K:33:LEU:HA	1:K:36:LYS:HB2	1.98	0.46
1:L:83:GLN:NE2	1:L:573:ARG:HB3	2.30	0.46
1:F:560:ASP:OD1	1:F:564:LEU:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:TYR:HB3	1:G:398:TRP:HB3	1.97	0.46
1:H:27:ALA:HB3	1:H:532:ILE:HB	1.96	0.46
1:A:441:HIS:O	1:A:445:ILE:HG22	2.16	0.46
1:D:407:ILE:HA	1:D:566:ILE:HD13	1.98	0.46
1:L:484:TYR:O	1:L:488:GLN:HG2	2.16	0.46
1:C:395:TYR:O	1:C:399:PHE:N	2.48	0.46
1:C:484:TYR:CZ	1:D:485:ILE:HD11	2.50	0.46
1:H:407:ILE:HA	1:H:566:ILE:HD13	1.97	0.46
1:C:153:ILE:HG12	1:C:172:PHE:HZ	1.81	0.46
1:E:306:VAL:HG22	1:E:343:LEU:HD11	1.98	0.46
1:I:301:ASP:HA	1:I:305:ALA:HB3	1.96	0.46
1:J:8:LYS:HD3	1:J:493:ARG:CZ	2.46	0.46
1:G:402:VAL:HG12	1:G:514:GLY:HA2	1.98	0.46
1:J:216:ASN:HA	1:J:222:LEU:HB3	1.98	0.46
1:J:304:GLY:HA3	1:J:542:VAL:HG21	1.98	0.46
1:J:560:ASP:HB3	1:J:566:ILE:HD11	1.96	0.46
1:A:27:ALA:HB3	1:A:532:ILE:HB	1.97	0.46
1:H:156:ILE:HG23	1:H:161:TYR:HB2	1.98	0.46
1:I:35:PHE:CE1	1:I:530:THR:HB	2.51	0.46
1:E:559:TYR:CZ	1:E:595:LYS:HB2	2.50	0.46
1:H:153:ILE:HG12	1:H:172:PHE:HZ	1.80	0.46
1:H:414:ILE:HG21	1:H:587:VAL:HG13	1.98	0.46
1:C:302:GLY:HA3	1:C:338:GLU:HG3	1.98	0.45
1:D:23:GLU:OE1	1:D:540:ARG:NH2	2.50	0.45
1:E:45:PRO:HB2	1:E:46:LEU:HD22	1.97	0.45
1:G:603:ILE:HG22	1:G:604:LEU:H	1.80	0.45
1:H:407:ILE:HG23	1:H:566:ILE:HG23	1.97	0.45
1:I:491:ARG:NH1	1:I:547:LEU:O	2.49	0.45
1:K:41:LEU:HB3	1:K:51:ILE:HD13	1.97	0.45
1:L:276:ARG:HA	1:L:519:VAL:HA	1.99	0.45
1:A:162:ASP:OD1	1:A:162:ASP:N	2.49	0.45
1:B:407:ILE:HA	1:B:566:ILE:HD13	1.97	0.45
1:C:153:ILE:HD13	1:C:174:ALA:HB1	1.98	0.45
1:E:252:HIS:CE1	1:E:257:GLY:HA3	2.51	0.45
1:H:395:TYR:CZ	1:H:430:VAL:HG23	2.51	0.45
1:I:14:ASP:HB3	1:I:17:THR:HG22	1.97	0.45
1:L:407:ILE:HG23	1:L:566:ILE:HG23	1.98	0.45
1:C:102:LEU:HD11	1:C:197:LEU:HD12	1.98	0.45
1:D:381:HIS:HA	1:D:382:ASN:HA	1.67	0.45
1:G:216:ASN:HA	1:G:222:LEU:HB3	1.98	0.45
1:C:415:LEU:HD21	1:C:509:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LYS:HG2	1:D:467:TYR:CZ	2.52	0.45
1:H:206:ASP:OD2	1:H:217:GLY:N	2.50	0.45
1:I:532:ILE:HA	1:I:535:THR:OG1	2.16	0.45
1:K:165:PRO:HD2	1:K:166:THR:H	1.81	0.45
1:E:536:THR:HA	1:E:539:MET:HE2	1.98	0.45
1:F:221:TRP:CD1	1:F:464:LYS:CB	2.99	0.45
1:I:92:VAL:HG21	1:I:375:PHE:CE2	2.51	0.45
1:K:318:LEU:HA	1:K:553:ILE:HG13	1.99	0.45
1:C:559:TYR:CZ	1:C:595:LYS:HB2	2.51	0.45
1:F:506:ASP:OD1	1:F:573:ARG:NH2	2.45	0.45
1:L:545:ALA:HA	1:L:550:PHE:HB2	1.98	0.45
1:A:560:ASP:OD1	1:A:564:LEU:N	2.47	0.45
1:C:407:ILE:HG23	1:C:566:ILE:HG23	1.99	0.45
1:I:395:TYR:CZ	1:I:430:VAL:HG23	2.52	0.45
1:K:553:ILE:HG22	1:K:570:ILE:HB	1.99	0.45
1:E:219:THR:O	1:E:265:TYR:OH	2.25	0.45
1:F:107:LYS:O	1:F:379:LEU:HD11	2.17	0.45
1:F:532:ILE:HA	1:F:535:THR:OG1	2.17	0.45
1:K:306:VAL:HG13	1:K:343:LEU:HG	1.99	0.45
1:A:258:THR:C	1:A:280:GLY:H	2.20	0.45
1:B:381:HIS:HA	1:B:382:ASN:HA	1.58	0.45
1:C:559:TYR:O	1:C:566:ILE:HD12	2.17	0.45
1:F:414:ILE:HG21	1:F:587:VAL:HG13	1.98	0.45
1:A:153:ILE:HG12	1:A:172:PHE:HZ	1.81	0.45
1:G:10:ALA:HB2	1:G:493:ARG:CZ	2.47	0.45
1:J:453:LEU:HD23	1:J:456:TYR:HD2	1.81	0.45
1:L:75:MET:HG3	1:L:79:GLU:HG3	1.99	0.45
1:A:255:GLY:HA2	1:A:281:SER:OG	2.17	0.44
1:B:484:TYR:O	1:B:488:GLN:HG2	2.17	0.44
1:D:39:VAL:HG21	1:D:467:TYR:HD1	1.82	0.44
1:E:395:TYR:HE1	1:E:397:LYS:HE2	1.82	0.44
1:F:96:GLU:O	1:F:101:ARG:NH1	2.50	0.44
1:K:144:THR:O	1:K:148:VAL:HG23	2.17	0.44
1:L:307:ARG:NH2	1:L:546:ASN:OD1	2.46	0.44
1:I:70:ILE:HD12	1:I:489:CYS:HB2	1.98	0.44
1:J:43:GLU:OE2	1:J:470:ARG:NE	2.50	0.44
1:E:337:VAL:HB	1:E:546:ASN:HB3	2.00	0.44
1:K:9:ARG:NH1	1:K:11:SER:OG	2.51	0.44
1:A:33:LEU:HA	1:A:36:LYS:HE3	1.99	0.44
1:C:144:THR:HG23	1:C:147:GLN:H	1.83	0.44
1:F:399:PHE:CE1	1:F:511:PRO:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ILE:HA	1:E:161:TYR:HB2	1.98	0.44
1:E:491:ARG:HG3	1:E:547:LEU:HG	1.99	0.44
1:I:277:TYR:CZ	1:I:520:ILE:HG23	2.52	0.44
1:L:260:GLY:O	1:L:267:THR:HG23	2.18	0.44
1:C:219:THR:O	1:C:265:TYR:OH	2.25	0.44
1:C:559:TYR:CG	1:C:595:LYS:HD2	2.53	0.44
1:J:407:ILE:HA	1:J:566:ILE:HD13	1.99	0.44
1:L:56:LYS:HE3	1:L:56:LYS:HB3	1.68	0.44
1:A:337:VAL:HB	1:A:546:ASN:HB3	2.00	0.44
1:B:162:ASP:OD1	1:B:162:ASP:N	2.51	0.44
1:E:132:ARG:NH2	1:E:348:GLU:OE2	2.48	0.44
1:K:96:GLU:O	1:K:101:ARG:NH1	2.50	0.44
1:L:407:ILE:HA	1:L:566:ILE:HD13	2.00	0.44
1:C:560:ASP:HB3	1:C:566:ILE:HD11	2.00	0.44
1:D:27:ALA:HB3	1:D:532:ILE:HB	2.00	0.44
1:H:211:LEU:HD11	1:H:230:LYS:HA	1.99	0.44
1:I:75:MET:HE2	1:I:79:GLU:HB2	2.00	0.44
1:L:144:THR:HG23	1:L:147:GLN:H	1.83	0.44
1:A:322:TYR:OH	1:A:335:GLY:O	2.28	0.44
1:E:106:LEU:HD11	1:E:196:VAL:HB	2.00	0.44
1:E:225:ASP:OD2	1:E:461:LYS:NZ	2.43	0.44
1:J:27:ALA:HB3	1:J:532:ILE:HB	1.99	0.44
1:K:56:LYS:O	1:K:61:MET:N	2.51	0.44
1:C:274:PRO:HG3	1:C:599:ILE:HD11	1.99	0.43
1:F:407:ILE:HG23	1:F:566:ILE:HG23	2.00	0.43
1:J:407:ILE:HG23	1:J:566:ILE:HG23	2.00	0.43
1:J:417:LEU:HB3	1:J:590:LEU:HD13	1.98	0.43
1:E:415:LEU:HD21	1:E:509:VAL:HG21	1.99	0.43
1:G:148:VAL:HG13	1:G:603:ILE:HG21	1.99	0.43
1:H:2:GLY:O	1:H:3:LYS:HD2	2.18	0.43
1:A:102:LEU:HD11	1:A:197:LEU:HD12	2.00	0.43
1:A:252:HIS:CE1	1:A:257:GLY:HA3	2.53	0.43
1:A:277:TYR:CD2	1:A:520:ILE:HG12	2.53	0.43
1:B:75:MET:HB2	1:B:492:ARG:HB2	1.99	0.43
1:C:322:TYR:OH	1:C:335:GLY:O	2.28	0.43
1:D:304:GLY:HA3	1:D:542:VAL:HG21	2.00	0.43
1:F:52:VAL:HG13	1:F:475:ILE:HG12	2.00	0.43
1:G:153:ILE:HD13	1:G:174:ALA:HB1	1.99	0.43
1:I:138:TYR:HE2	1:I:199:GLY:HA3	1.83	0.43
1:J:7:MET:HB3	1:J:69:VAL:HB	2.00	0.43
1:D:206:ASP:HA	1:D:248:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ARG:HB3	1:E:274:PRO:HA	2.00	0.43
1:F:134:TYR:OH	1:F:603:ILE:HG21	2.18	0.43
1:F:306:VAL:HG13	1:F:343:LEU:HG	2.00	0.43
1:I:539:MET:HB2	1:I:539:MET:HE3	1.91	0.43
1:L:271:PRO:O	1:L:598:ALA:N	2.51	0.43
1:A:99:ILE:HG23	1:A:195:SER:HB3	2.01	0.43
1:B:370:PRO:HB3	1:B:575:TRP:CH2	2.54	0.43
1:F:162:ASP:OD1	1:F:162:ASP:N	2.51	0.43
1:I:20:TYR:CE1	1:I:22:ALA:HB2	2.54	0.43
1:J:75:MET:HB2	1:J:492:ARG:HB2	2.01	0.43
1:K:20:TYR:HH	1:K:398:TRP:HD1	1.66	0.43
1:A:153:ILE:HD13	1:A:174:ALA:HB1	2.01	0.43
1:C:301:ASP:HA	1:C:305:ALA:HB3	2.00	0.43
1:J:33:LEU:HA	1:J:36:LYS:HE3	2.00	0.43
1:K:28:PRO:HG2	1:K:38:PHE:CE2	2.50	0.43
1:C:106:LEU:HD23	1:C:109:LEU:HD12	2.00	0.43
1:E:64:ILE:HG21	1:E:436:GLU:HG3	2.00	0.43
1:F:72:GLU:OE1	1:F:493:ARG:NH1	2.50	0.43
1:I:337:VAL:HG12	1:I:547:LEU:HA	2.01	0.43
1:C:277:TYR:N	1:C:520:ILE:HD11	2.34	0.43
1:C:560:ASP:OD1	1:C:564:LEU:N	2.47	0.43
1:D:238:LEU:HD11	1:D:298:LEU:HD21	2.01	0.43
1:E:46:LEU:HD13	1:E:46:LEU:HA	1.83	0.43
1:G:101:ARG:NH2	1:G:358:LEU:O	2.51	0.43
1:J:307:ARG:NH2	1:J:546:ASN:OD1	2.52	0.43
1:A:453:LEU:HD23	1:A:456:TYR:HD2	1.83	0.43
1:E:33:LEU:HD22	1:E:36:LYS:HE3	2.01	0.43
1:L:494:LEU:HA	1:L:497:TYR:HD2	1.83	0.43
1:B:221:TRP:CD1	1:B:464:LYS:CB	3.02	0.43
1:D:277:TYR:CZ	1:D:520:ILE:HG23	2.54	0.43
1:F:42:LEU:HD23	1:F:42:LEU:HA	1.89	0.43
1:F:305:ALA:HB2	2:F:700:X4X:N01	2.34	0.43
1:I:453:LEU:HD23	1:I:456:TYR:HD2	1.84	0.43
1:J:484:TYR:O	1:J:488:GLN:HG2	2.18	0.43
1:K:27:ALA:HB1	1:K:28:PRO:HD2	2.00	0.43
1:L:60:GLY:O	1:L:64:ILE:HD12	2.19	0.43
1:L:438:ARG:HA	1:L:543:LEU:HD12	2.01	0.43
1:A:484:TYR:O	1:A:488:GLN:HG2	2.19	0.42
1:B:407:ILE:HG23	1:B:566:ILE:HG23	2.01	0.42
1:D:2:GLY:O	1:D:3:LYS:HD2	2.19	0.42
1:H:225:ASP:OD2	1:H:461:LYS:NZ	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:MET:HA	1:B:59:ASN:HD22	1.84	0.42
1:C:88:ASP:OD2	1:C:383:GLY:HA2	2.19	0.42
1:C:277:TYR:CG	1:C:520:ILE:HD11	2.54	0.42
1:E:144:THR:HG23	1:E:147:GLN:HB2	2.00	0.42
1:G:132:ARG:NH2	1:G:348:GLU:OE2	2.40	0.42
1:G:269:ARG:HB3	1:G:274:PRO:HA	2.00	0.42
1:G:395:TYR:CZ	1:G:430:VAL:HG23	2.53	0.42
1:H:484:TYR:O	1:H:488:GLN:HG2	2.18	0.42
1:K:57:LYS:HA	1:K:62:THR:HG22	2.01	0.42
1:A:98:PRO:HB2	1:A:241:CYS:SG	2.60	0.42
1:D:102:LEU:HD23	1:D:102:LEU:HA	1.88	0.42
1:G:302:GLY:HA3	1:G:338:GLU:HG3	2.01	0.42
1:L:27:ALA:HB3	1:L:532:ILE:HB	1.99	0.42
1:A:321:THR:OG1	1:A:577:GLU:OE2	2.21	0.42
1:I:173:ASP:HB3	1:I:176:GLU:HB3	2.01	0.42
1:K:102:LEU:HD11	1:K:197:LEU:HD12	2.01	0.42
1:A:273:ASP:OD2	1:A:275:LYS:NZ	2.47	0.42
1:B:27:ALA:HB3	1:B:532:ILE:HB	2.00	0.42
1:D:370:PRO:HB3	1:D:575:TRP:CH2	2.54	0.42
1:H:384:SER:O	1:H:384:SER:OG	2.31	0.42
1:H:441:HIS:O	1:H:445:ILE:HG22	2.20	0.42
1:K:106:LEU:HD11	1:K:196:VAL:HB	2.00	0.42
1:A:132:ARG:NH2	1:A:348:GLU:OE2	2.50	0.42
1:C:453:LEU:HD23	1:C:456:TYR:HD2	1.85	0.42
1:C:485:ILE:HD11	1:D:484:TYR:CZ	2.54	0.42
1:D:75:MET:HB2	1:D:492:ARG:HB2	2.01	0.42
1:E:305:ALA:HB2	2:E:700:X4X:N01	2.34	0.42
1:E:337:VAL:HG12	1:E:547:LEU:HA	2.02	0.42
1:B:526:LYS:HD3	1:H:118:LEU:HG	2.01	0.42
1:C:10:ALA:HB2	1:C:493:ARG:CZ	2.49	0.42
1:D:300:THR:HG22	1:D:340:ILE:HG12	2.01	0.42
1:D:302:GLY:HA3	1:D:338:GLU:HG3	2.01	0.42
1:H:2:GLY:HA2	1:H:6:VAL:HG12	2.01	0.42
1:A:144:THR:HG23	1:A:147:GLN:HB2	2.02	0.42
1:B:305:ALA:HB2	2:B:700:X4X:N01	2.35	0.42
1:H:272:HIS:CE1	1:H:565:PRO:HG3	2.54	0.42
1:H:532:ILE:HA	1:H:535:THR:OG1	2.20	0.42
1:I:162:ASP:OD1	1:I:162:ASP:N	2.46	0.42
1:J:536:THR:HA	1:J:539:MET:HE2	2.02	0.42
1:K:156:ILE:HG23	1:K:161:TYR:HB2	2.01	0.42
1:K:484:TYR:CZ	1:L:485:ILE:HD11	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PRO:HG2	1:B:290:ALA:HB3	2.02	0.42
1:D:271:PRO:HG2	1:D:290:ALA:HB3	2.01	0.42
1:D:441:HIS:O	1:D:445:ILE:HG22	2.20	0.42
1:H:52:VAL:HG13	1:H:475:ILE:HG12	2.00	0.42
1:J:63:LYS:HE2	1:J:63:LYS:HB3	1.84	0.42
1:K:94:GLU:CG	1:K:373:PRO:HD3	2.50	0.42
1:F:415:LEU:HD21	1:F:509:VAL:HG21	2.01	0.42
1:G:26:LYS:H	1:G:59:ASN:ND2	2.17	0.42
1:G:99:ILE:HG23	1:G:195:SER:HB3	2.00	0.42
1:I:297:ALA:O	1:I:343:LEU:N	2.46	0.42
1:I:395:TYR:HB3	1:I:398:TRP:HB3	2.02	0.42
1:J:185:THR:O	1:J:189:GLU:N	2.40	0.42
1:K:10:ALA:O	1:K:13:VAL:HG12	2.19	0.42
1:L:211:LEU:HD11	1:L:230:LYS:HA	2.02	0.42
1:B:457:CYS:HB3	1:B:462:ASN:HB2	2.02	0.41
1:E:92:VAL:CG1	1:E:101:ARG:HG2	2.50	0.41
1:G:75:MET:HB2	1:G:492:ARG:HB2	2.01	0.41
1:I:105:ALA:HB2	1:I:375:PHE:CE2	2.55	0.41
1:J:301:ASP:HA	1:J:305:ALA:HB3	2.01	0.41
1:D:24:THR:HG23	1:D:438:ARG:HH22	1.85	0.41
1:F:2:GLY:O	1:F:3:LYS:HD2	2.20	0.41
1:F:75:MET:HB2	1:F:492:ARG:HB2	2.01	0.41
1:I:327:MET:HG2	1:I:340:ILE:HG13	2.02	0.41
1:A:338:GLU:OE2	1:A:338:GLU:N	2.53	0.41
1:F:484:TYR:O	1:F:488:GLN:HG2	2.21	0.41
1:I:441:HIS:O	1:I:445:ILE:HG22	2.20	0.41
1:K:491:ARG:NH1	1:K:547:LEU:O	2.53	0.41
1:L:75:MET:CE	1:L:79:GLU:H	2.33	0.41
1:L:532:ILE:HA	1:L:535:THR:OG1	2.21	0.41
1:C:121:ASP:HB3	1:C:124:SER:OG	2.21	0.41
1:D:269:ARG:HB3	1:D:274:PRO:HA	2.01	0.41
1:E:307:ARG:NH1	1:E:569:GLN:OE1	2.51	0.41
1:E:473:PHE:O	1:E:477:ARG:HG3	2.20	0.41
1:K:163:LYS:HA	1:K:164:PRO:HD3	1.83	0.41
1:L:134:TYR:OH	1:L:603:ILE:HG21	2.20	0.41
1:B:318:LEU:HD22	1:B:581:LEU:HD21	2.01	0.41
1:C:410:LYS:O	1:C:414:ILE:HG12	2.21	0.41
1:E:539:MET:O	1:E:543:LEU:HG	2.21	0.41
1:F:453:LEU:HD23	1:F:456:TYR:HD2	1.85	0.41
1:G:26:LYS:HD2	1:G:26:LYS:HA	1.69	0.41
1:G:106:LEU:HD11	1:G:196:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2:GLY:HA2	1:J:6:VAL:HG22	2.01	0.41
1:K:334:GLY:HA3	1:L:74:PRO:HD2	2.02	0.41
1:L:106:LEU:HD23	1:L:109:LEU:HD12	2.02	0.41
1:L:414:ILE:HG21	1:L:587:VAL:HG13	2.03	0.41
1:A:306:VAL:HG13	1:A:343:LEU:HG	2.03	0.41
1:A:450:LEU:O	1:A:454:THR:OG1	2.25	0.41
1:G:473:PHE:O	1:G:477:ARG:HG3	2.21	0.41
1:I:8:LYS:HE2	1:I:70:ILE:HG22	2.03	0.41
1:J:169:LEU:HD21	1:J:288:ILE:HD12	2.03	0.41
1:A:414:ILE:HG13	1:A:557:VAL:HB	2.03	0.41
1:B:211:LEU:HD11	1:B:230:LYS:HA	2.02	0.41
1:D:162:ASP:OD1	1:D:162:ASP:N	2.49	0.41
1:F:327:MET:HG2	1:F:340:ILE:HG13	2.02	0.41
1:F:603:ILE:HG23	1:F:604:LEU:HD23	2.03	0.41
1:G:63:LYS:HB3	1:G:63:LYS:HE2	1.89	0.41
1:H:25:MET:HG2	1:H:438:ARG:CZ	2.51	0.41
1:K:86:GLU:OE1	1:K:579:THR:OG1	2.35	0.41
1:K:98:PRO:HB2	1:K:241:CYS:SG	2.61	0.41
1:K:484:TYR:O	1:K:488:GLN:HG2	2.21	0.41
1:L:443:ILE:HG13	1:L:479:PHE:CD2	2.55	0.41
1:A:536:THR:HA	1:A:539:MET:HE2	2.02	0.41
1:D:245:LEU:HD13	1:D:245:LEU:HA	1.91	0.41
1:E:98:PRO:HA	1:E:101:ARG:HB2	2.02	0.41
1:F:326:ASP:HB2	1:F:359:GLY:O	2.20	0.41
1:G:98:PRO:HB2	1:G:241:CYS:SG	2.60	0.41
1:J:151:ARG:HD3	1:J:603:ILE:HA	2.01	0.41
1:J:251:MET:HB2	1:J:281:SER:O	2.21	0.41
1:J:539:MET:HA	1:J:542:VAL:HG22	2.03	0.41
1:K:94:GLU:HG3	1:K:373:PRO:HD3	2.02	0.41
1:A:539:MET:O	1:A:543:LEU:HG	2.21	0.41
1:B:494:LEU:HA	1:B:497:TYR:HD2	1.85	0.41
1:I:27:ALA:HB1	1:I:28:PRO:HD2	2.03	0.41
1:I:144:THR:HG23	1:I:146:LEU:H	1.85	0.41
1:I:318:LEU:HD22	1:I:581:LEU:HD21	2.03	0.41
1:J:2:GLY:O	1:J:3:LYS:HD2	2.21	0.41
1:K:300:THR:HG22	1:K:340:ILE:HG12	2.03	0.41
1:L:162:ASP:OD1	1:L:162:ASP:N	2.51	0.41
1:B:25:MET:HA	1:B:59:ASN:ND2	2.36	0.40
1:C:485:ILE:HG21	1:D:448:PRO:HA	2.04	0.40
1:F:192:ASN:O	1:F:192:ASN:ND2	2.54	0.40
1:F:494:LEU:HA	1:F:497:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:VAL:HG23	1:H:68:THR:HA	2.02	0.40
1:I:484:TYR:CZ	1:J:485:ILE:HD11	2.56	0.40
1:J:395:TYR:CZ	1:J:430:VAL:HG23	2.57	0.40
1:K:453:LEU:HD23	1:K:453:LEU:HA	1.90	0.40
1:A:144:THR:HG23	1:A:147:GLN:H	1.87	0.40
1:A:302:GLY:HA3	1:A:338:GLU:HG3	2.04	0.40
1:C:252:HIS:CE1	1:C:257:GLY:HA3	2.55	0.40
1:C:259:THR:HG23	1:C:535:THR:HG22	2.02	0.40
1:D:98:PRO:HB3	1:D:356:ALA:HA	2.03	0.40
1:G:441:HIS:O	1:G:445:ILE:HG22	2.21	0.40
1:H:41:LEU:HD22	1:H:47:ILE:HD11	2.03	0.40
1:L:387:ILE:H	1:L:387:ILE:HG12	1.77	0.40
1:A:326:ASP:HB2	1:A:359:GLY:O	2.22	0.40
1:B:206:ASP:OD2	1:B:217:GLY:N	2.53	0.40
1:D:382:ASN:HA	1:D:382:ASN:HD22	1.73	0.40
1:D:560:ASP:HB3	1:D:566:ILE:HD11	2.03	0.40
1:E:532:ILE:HA	1:E:535:THR:OG1	2.21	0.40
1:F:407:ILE:HA	1:F:566:ILE:HD13	2.02	0.40
1:H:453:LEU:HD23	1:H:453:LEU:HA	1.94	0.40
1:I:92:VAL:HG21	1:I:375:PHE:CD2	2.56	0.40
1:I:221:TRP:CE3	1:I:461:LYS:HD2	2.57	0.40
1:J:99:ILE:HD13	1:J:194:ILE:HG23	2.03	0.40
1:J:169:LEU:HD11	1:J:246:LEU:HG	2.02	0.40
1:J:231:ASP:OD2	1:J:239:ARG:NH2	2.54	0.40
1:J:273:ASP:OD2	1:J:275:LYS:NZ	2.49	0.40
1:K:252:HIS:CE1	1:K:257:GLY:HA3	2.57	0.40
1:L:71:PRO:HG2	1:L:72:GLU:OE1	2.22	0.40
1:L:152:ILE:HG23	1:L:293:LEU:HD22	2.02	0.40
1:L:192:ASN:O	1:L:192:ASN:ND2	2.54	0.40
1:A:395:TYR:HB3	1:A:398:TRP:HB3	2.02	0.40
1:A:473:PHE:O	1:A:477:ARG:HG3	2.22	0.40
1:C:77:ARG:HG2	1:C:336:THR:HG22	2.03	0.40
1:D:131:ILE:HG23	1:D:200:ILE:HG13	2.02	0.40
1:G:603:ILE:CG2	1:G:604:LEU:N	2.83	0.40
1:H:276:ARG:CZ	1:H:564:LEU:HD11	2.52	0.40
1:K:570:ILE:HG22	1:K:580:VAL:HG12	2.03	0.40
1:A:304:GLY:HA3	1:A:542:VAL:HG21	2.04	0.40
1:B:1:MET:SD	1:B:1:MET:N	2.87	0.40
1:C:448:PRO:HA	1:D:485:ILE:HG21	2.03	0.40
1:H:539:MET:O	1:H:543:LEU:HG	2.21	0.40
1:I:453:LEU:HD23	1:I:453:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:421:ASN:C	1:K:19:LYS:HD3	2.42	0.40
1:K:395:TYR:HB3	1:K:398:TRP:HB3	2.04	0.40
1:K:555:VAL:HG22	1:K:556:PRO:HD2	2.03	0.40
1:L:407:ILE:HD11	1:L:516:THR:HG23	2.02	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [\(i\)](#)

#### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	600/636 (94%)	566 (94%)	33 (6%)	1 (0%)	47 79
1	B	603/636 (95%)	574 (95%)	27 (4%)	2 (0%)	41 75
1	C	600/636 (94%)	561 (94%)	38 (6%)	1 (0%)	47 79
1	D	603/636 (95%)	567 (94%)	35 (6%)	1 (0%)	47 79
1	E	600/636 (94%)	570 (95%)	29 (5%)	1 (0%)	47 79
1	F	603/636 (95%)	578 (96%)	25 (4%)	0	100 100
1	G	600/636 (94%)	564 (94%)	35 (6%)	1 (0%)	47 79
1	H	603/636 (95%)	570 (94%)	32 (5%)	1 (0%)	47 79
1	I	600/636 (94%)	562 (94%)	34 (6%)	4 (1%)	22 61
1	J	603/636 (95%)	571 (95%)	31 (5%)	1 (0%)	47 79
1	K	600/636 (94%)	565 (94%)	34 (6%)	1 (0%)	47 79
1	L	603/636 (95%)	572 (95%)	30 (5%)	1 (0%)	47 79
All	All	7218/7632 (95%)	6820 (94%)	383 (5%)	15 (0%)	47 79

All (15) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	509/539 (94%)	503 (99%)	6 (1%)	71 87
1	B	511/539 (95%)	503 (98%)	8 (2%)	62 83
1	C	509/539 (94%)	499 (98%)	10 (2%)	55 79
1	D	511/539 (95%)	505 (99%)	6 (1%)	71 87
1	E	509/539 (94%)	502 (99%)	7 (1%)	67 85
1	F	511/539 (95%)	502 (98%)	9 (2%)	59 81
1	G	509/539 (94%)	502 (99%)	7 (1%)	67 85
1	H	511/539 (95%)	505 (99%)	6 (1%)	71 87
1	I	509/539 (94%)	499 (98%)	10 (2%)	55 79
1	J	511/539 (95%)	504 (99%)	7 (1%)	67 85
1	K	509/539 (94%)	492 (97%)	17 (3%)	38 69
1	L	511/539 (95%)	501 (98%)	10 (2%)	55 79
All	All	6120/6468 (95%)	6017 (98%)	103 (2%)	60 82

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	192	ASN
1	A	264	ASN
1	A	282	SER
1	A	527	ASN
1	A	568	LEU
1	B	1	MET
1	B	4	TYR
1	B	25	MET
1	B	127	ARG
1	B	151	ARG
1	B	192	ASN
1	B	379	LEU
1	B	527	ASN
1	C	8	LYS
1	C	9	ARG
1	C	15	LEU
1	C	127	ARG
1	C	192	ASN
1	C	264	ASN
1	C	382	ASN
1	C	395	TYR
1	C	527	ASN
1	C	531	ASN
1	D	4	TYR
1	D	59	ASN
1	D	127	ARG
1	D	192	ASN
1	D	395	TYR
1	D	527	ASN
1	E	8	LYS
1	E	59	ASN
1	E	127	ARG
1	E	192	ASN
1	E	412	GLU
1	E	527	ASN
1	E	568	LEU
1	F	8	LYS
1	F	25	MET
1	F	35	PHE
1	F	66	ARG
1	F	127	ARG

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Mol	Chain	Res	Type
1	F	192	ASN
1	F	385	ASN
1	F	410	LYS
1	F	527	ASN
1	G	35	PHE
1	G	127	ARG
1	G	192	ASN
1	G	264	ASN
1	G	395	TYR
1	G	527	ASN
1	G	605	ASN
1	H	4	TYR
1	H	121	ASP
1	H	127	ARG
1	H	192	ASN
1	H	527	ASN
1	H	533	GLN
1	I	5	GLN
1	I	19	LYS
1	I	35	PHE
1	I	102	LEU
1	I	127	ARG
1	I	140	SER
1	I	192	ASN
1	I	230	LYS
1	I	395	TYR
1	I	527	ASN
1	J	4	TYR
1	J	53	ASP
1	J	127	ARG
1	J	225	ASP
1	J	382	ASN
1	J	412	GLU
1	J	527	ASN
1	K	8	LYS
1	K	9	ARG
1	K	19	LYS
1	K	25	MET
1	K	38	PHE
1	K	54	TYR
1	K	127	ARG
1	K	171	ARG

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Mol	Chain	Res	Type
1	K	192	ASN
1	K	230	LYS
1	K	261	ASN
1	K	382	ASN
1	K	395	TYR
1	K	441	HIS
1	K	462	ASN
1	K	466	SER
1	K	527	ASN
1	L	4	TYR
1	L	8	LYS
1	L	38	PHE
1	L	76	PHE
1	L	127	ARG
1	L	192	ASN
1	L	264	ASN
1	L	269	ARG
1	L	527	ASN
1	L	605	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	381	HIS
1	A	462	ASN
1	B	59	ASN
1	B	533	GLN
1	C	59	ASN
1	C	67	ASN
1	C	462	ASN
1	C	531	ASN
1	D	40	ASN
1	D	180	GLN
1	D	382	ASN
1	D	533	GLN
1	E	462	ASN
1	F	59	ASN
1	F	67	ASN
1	G	40	ASN
1	G	59	ASN
1	G	605	ASN

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Mol	Chain	Res	Type
1	H	59	ASN
1	I	59	ASN
1	J	59	ASN
1	K	29	HIS
1	K	261	ASN
1	K	262	ASN
1	L	40	ASN
1	L	83	GLN
1	L	261	ASN
1	L	272	HIS
1	L	605	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 monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	X4X	F	700	-	23,23,23	1.49	3 (13%)	24,24,24	1.18	3 (12%)
2	X4X	H	700	-	23,23,23	1.49	3 (13%)	24,24,24	1.12	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	X4X	G	700	-	23,23,23	1.49	3 (13%)	24,24,24	1.06	3 (12%)
2	X4X	I	700	-	23,23,23	1.48	3 (13%)	24,24,24	1.04	2 (8%)
2	X4X	E	700	-	23,23,23	1.49	3 (13%)	24,24,24	1.13	3 (12%)
2	X4X	B	700	-	23,23,23	1.50	3 (13%)	24,24,24	1.13	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	X4X	F	700	-	-	13/23/23/23	-
2	X4X	H	700	-	-	9/23/23/23	-
2	X4X	G	700	-	-	9/23/23/23	-
2	X4X	I	700	-	-	9/23/23/23	-
2	X4X	E	700	-	-	10/23/23/23	-
2	X4X	B	700	-	-	11/23/23/23	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	X4X	C11-N01	5.43	1.45	1.33
2	H	700	X4X	C11-N01	5.42	1.45	1.33
2	B	700	X4X	C11-N01	5.41	1.45	1.33
2	G	700	X4X	C11-N01	5.40	1.45	1.33
2	F	700	X4X	C11-N01	5.39	1.45	1.33
2	I	700	X4X	C11-N01	5.38	1.45	1.33
2	G	700	X4X	C17-C15	3.16	1.53	1.44
2	B	700	X4X	C17-C15	3.10	1.53	1.44
2	F	700	X4X	C17-C15	3.10	1.53	1.44
2	H	700	X4X	C17-C15	3.10	1.53	1.44
2	E	700	X4X	C17-C15	3.09	1.53	1.44
2	I	700	X4X	C17-C15	3.07	1.53	1.44
2	B	700	X4X	O01-C11	-2.26	1.18	1.23
2	F	700	X4X	O01-C11	-2.20	1.18	1.23
2	G	700	X4X	O01-C11	-2.17	1.18	1.23
2	I	700	X4X	O01-C11	-2.17	1.18	1.23
2	E	700	X4X	O01-C11	-2.16	1.18	1.23
2	H	700	X4X	O01-C11	-2.11	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	700	X4X	C07-C11-N01	2.66	120.91	116.42
2	B	700	X4X	C07-C11-N01	2.65	120.89	116.42
2	H	700	X4X	C07-C11-N01	2.53	120.69	116.42
2	H	700	X4X	O03-C20-C19	2.51	120.77	111.59
2	E	700	X4X	C07-C11-N01	2.51	120.64	116.42
2	F	700	X4X	O03-C20-C19	2.39	120.34	111.59
2	F	700	X4X	C08-C14-C15	-2.39	119.32	125.14
2	G	700	X4X	O03-C20-C19	2.39	120.32	111.59
2	E	700	X4X	O03-C20-C19	2.38	120.29	111.59
2	B	700	X4X	O03-C20-C19	2.34	120.14	111.59
2	G	700	X4X	C07-C11-N01	2.21	120.13	116.42
2	E	700	X4X	C08-C14-C15	-2.20	119.77	125.14
2	I	700	X4X	O03-C20-C19	2.19	119.61	111.59
2	B	700	X4X	C08-C14-C15	-2.10	120.02	125.14
2	G	700	X4X	C08-C14-C15	-2.08	120.07	125.14
2	I	700	X4X	C19-N01-C11	-2.06	119.02	122.84

There are no chirality outliers.

All (61) torsion outliers are listed below:

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

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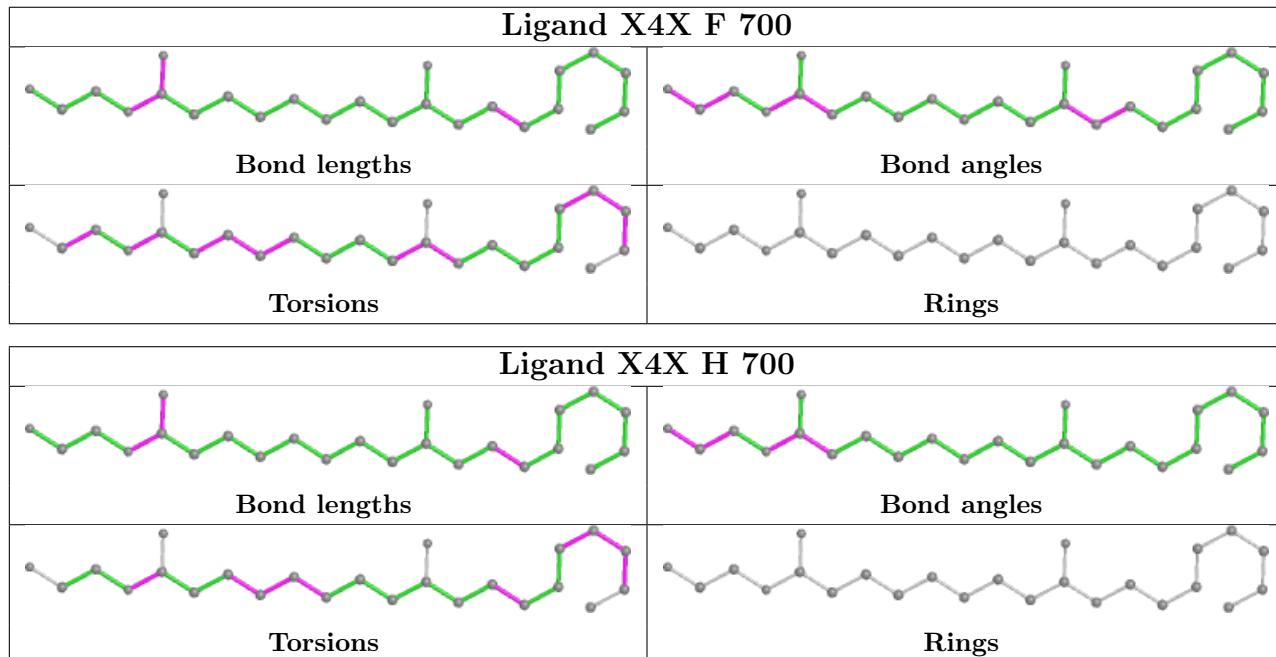
Mol	Chain	Res	Type	Atoms
2	F	700	X4X	C03-C05-C07-C11
2	I	700	X4X	C01-C03-C05-C07
2	I	700	X4X	C02-C01-C03-C05
2	G	700	X4X	C02-C01-C03-C05
2	H	700	X4X	C02-C01-C03-C05
2	H	700	X4X	C14-C15-C17-C16
2	E	700	X4X	C01-C03-C05-C07
2	B	700	X4X	C10-C09-C12-C16
2	B	700	X4X	C01-C03-C05-C07
2	E	700	X4X	O02-C08-C14-C15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

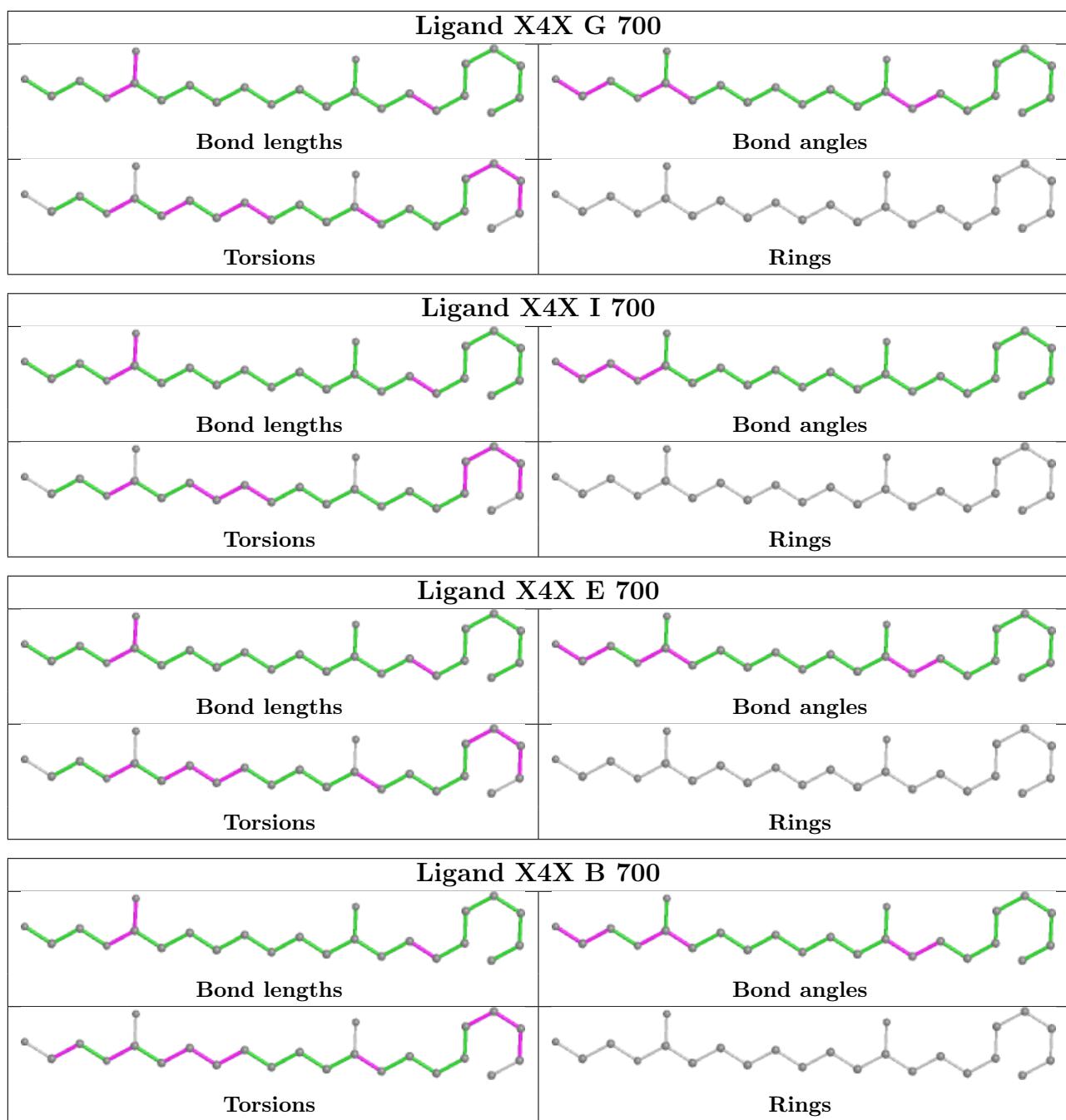
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	700	X4X	1	0
2	H	700	X4X	1	0
2	G	700	X4X	1	0
2	E	700	X4X	1	0
2	B	700	X4X	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	602/636 (94%)	-0.11	11 (1%) 68 53	63, 86, 116, 251	0
1	B	605/636 (95%)	-0.11	14 (2%) 60 44	58, 76, 113, 262	0
1	C	602/636 (94%)	0.25	27 (4%) 33 21	73, 101, 130, 250	0
1	D	605/636 (95%)	0.18	28 (4%) 32 20	64, 94, 129, 275	0
1	E	602/636 (94%)	-0.18	12 (1%) 65 49	54, 71, 100, 231	0
1	F	605/636 (95%)	-0.16	11 (1%) 68 53	54, 73, 102, 210	0
1	G	602/636 (94%)	-0.29	3 (0%) 91 83	44, 60, 89, 219	0
1	H	605/636 (95%)	-0.23	7 (1%) 79 66	49, 66, 92, 184	0
1	I	602/636 (94%)	-0.18	11 (1%) 68 53	56, 78, 109, 224	0
1	J	605/636 (95%)	0.01	21 (3%) 44 29	63, 98, 139, 253	0
1	K	602/636 (94%)	0.17	23 (3%) 40 26	74, 110, 146, 252	0
1	L	605/636 (95%)	0.59	64 (10%) 6 3	85, 137, 175, 305	0
All	All	7242/7632 (94%)	-0.01	232 (3%) 47 32	44, 85, 147, 305	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	149	ALA	8.2
1	C	22	ALA	8.0
1	J	119	HIS	7.6
1	L	282	SER	5.6
1	L	178	ILE	5.6
1	L	523	ASP	5.5
1	D	119	HIS	5.5
1	L	119	HIS	5.2
1	J	381	HIS	5.2
1	K	125	SER	5.0
1	E	119	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	125	SER	4.9
1	H	119	HIS	4.8
1	L	150	LYS	4.8
1	H	381	HIS	4.8
1	L	28	PRO	4.6
1	F	381	HIS	4.5
1	L	299	GLY	4.5
1	L	605	ASN	4.5
1	C	23	GLU	4.3
1	B	119	HIS	4.3
1	I	119	HIS	4.2
1	C	383	GLY	4.2
1	L	182	GLU	4.1
1	L	147	GLN	4.1
1	J	382	ASN	4.1
1	L	281	SER	4.0
1	I	381	HIS	4.0
1	K	119	HIS	3.9
1	F	119	HIS	3.8
1	L	283	SER	3.8
1	K	406	ASP	3.8
1	G	119	HIS	3.8
1	L	121	ASP	3.8
1	K	28	PRO	3.7
1	J	305	ALA	3.7
1	D	121	ASP	3.7
1	A	504	ASP	3.7
1	H	380	SER	3.7
1	J	121	ASP	3.7
1	C	123	VAL	3.7
1	D	182	GLU	3.6
1	L	305	ALA	3.6
1	C	117	SER	3.5
1	L	154	SER	3.5
1	L	29	HIS	3.5
1	I	384	SER	3.5
1	L	37	LEU	3.4
1	I	117	SER	3.4
1	D	175	ASN	3.4
1	D	122	PRO	3.4
1	L	124	SER	3.3
1	L	404	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	30	LEU	3.3
1	E	383	GLY	3.3
1	C	566	ILE	3.3
1	J	175	ASN	3.3
1	E	384	SER	3.3
1	K	123	VAL	3.3
1	E	118	LEU	3.2
1	L	120	ALA	3.2
1	L	176	GLU	3.2
1	H	382	ASN	3.1
1	L	304	GLY	3.1
1	A	124	SER	3.0
1	K	172	PHE	3.0
1	B	123	VAL	3.0
1	J	283	SER	2.9
1	C	605	ASN	2.9
1	L	300	THR	2.9
1	A	88	ASP	2.9
1	I	383	GLY	2.9
1	K	424	CYS	2.9
1	F	175	ASN	2.9
1	C	125	SER	2.9
1	D	605	ASN	2.9
1	L	257	GLY	2.9
1	L	205	LYS	2.9
1	L	148	VAL	2.9
1	B	121	ASP	2.8
1	I	118	LEU	2.8
1	C	382	ASN	2.8
1	D	305	ALA	2.8
1	L	99	ILE	2.8
1	J	124	SER	2.8
1	H	122	PRO	2.8
1	D	281	SER	2.8
1	L	380	SER	2.8
1	D	124	SER	2.8
1	C	594	THR	2.8
1	D	126	PHE	2.8
1	J	282	SER	2.8
1	K	384	SER	2.8
1	L	280	GLY	2.8
1	L	521	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	504	ASP	2.7
1	C	411	CYS	2.7
1	D	381	HIS	2.7
1	D	180	GLN	2.7
1	D	178	ILE	2.7
1	L	279	GLY	2.7
1	E	382	ASN	2.7
1	C	118	LEU	2.7
1	D	205	LYS	2.7
1	C	527	ASN	2.7
1	C	143	THR	2.6
1	D	300	THR	2.6
1	L	21	LYS	2.6
1	A	125	SER	2.6
1	D	594	THR	2.6
1	L	382	ASN	2.6
1	C	419	SER	2.6
1	E	117	SER	2.6
1	J	24	THR	2.6
1	L	432	PRO	2.6
1	E	121	ASP	2.6
1	B	305	ALA	2.6
1	L	381	HIS	2.6
1	L	301	ASP	2.6
1	F	24	THR	2.6
1	L	146	LEU	2.6
1	G	386	ALA	2.6
1	K	124	SER	2.6
1	C	119	HIS	2.5
1	L	286	ALA	2.5
1	D	150	LYS	2.5
1	C	528	GLY	2.5
1	K	305	ALA	2.5
1	B	124	SER	2.5
1	L	309	PRO	2.5
1	D	523	ASP	2.5
1	L	203	THR	2.5
1	C	504	ASP	2.5
1	A	123	VAL	2.5
1	L	126	PHE	2.5
1	F	150	LYS	2.5
1	F	121	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	177	VAL	2.5
1	A	122	PRO	2.5
1	C	592	PRO	2.5
1	B	381	HIS	2.5
1	F	28	PRO	2.5
1	D	257	GLY	2.5
1	J	281	SER	2.5
1	K	7	MET	2.4
1	B	282	SER	2.4
1	I	15	LEU	2.4
1	F	182	GLU	2.4
1	I	4	TYR	2.4
1	A	121	ASP	2.4
1	F	305	ALA	2.4
1	L	9	ARG	2.4
1	K	561	LYS	2.4
1	L	185	THR	2.4
1	A	144	THR	2.4
1	D	120	ALA	2.3
1	I	302	GLY	2.3
1	K	563	GLY	2.3
1	C	172	PHE	2.3
1	D	309	PRO	2.3
1	F	123	VAL	2.3
1	L	531	ASN	2.3
1	E	7	MET	2.3
1	D	299	GLY	2.3
1	K	9	ARG	2.3
1	D	118	LEU	2.3
1	J	380	SER	2.3
1	L	504	ASP	2.3
1	B	285	SER	2.3
1	H	175	ASN	2.3
1	J	605	ASN	2.2
1	B	122	PRO	2.2
1	L	122	PRO	2.2
1	C	29	HIS	2.2
1	L	595	LYS	2.2
1	B	120	ALA	2.2
1	I	594	THR	2.2
1	K	471	THR	2.2
1	C	404	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	46	LEU	2.2
1	L	175	ASN	2.2
1	L	144	THR	2.2
1	L	252	HIS	2.2
1	C	30	LEU	2.2
1	K	309	PRO	2.2
1	I	546	ASN	2.2
1	K	244	ILE	2.2
1	L	42	LEU	2.2
1	J	149	ALA	2.2
1	L	125	SER	2.2
1	K	342	PRO	2.2
1	L	397	LYS	2.2
1	C	88	ASP	2.2
1	B	310	SER	2.1
1	B	309	PRO	2.1
1	B	24	THR	2.1
1	L	303	GLY	2.1
1	L	123	VAL	2.1
1	A	119	HIS	2.1
1	L	554	SER	2.1
1	B	299	GLY	2.1
1	L	174	ALA	2.1
1	J	285	SER	2.1
1	K	34	SER	2.1
1	J	178	ILE	2.1
1	D	595	LYS	2.1
1	D	154	SER	2.1
1	L	225	ASP	2.1
1	K	151	ARG	2.1
1	L	295	SER	2.1
1	J	523	ASP	2.1
1	E	385	ASN	2.1
1	E	122	PRO	2.1
1	A	424	CYS	2.1
1	E	561	LYS	2.1
1	C	593	VAL	2.1
1	C	122	PRO	2.1
1	J	182	GLU	2.1
1	L	406	ASP	2.1
1	H	305	ALA	2.0
1	K	121	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	282	SER	2.0
1	L	527	ASN	2.0
1	J	123	VAL	2.0
1	J	257	GLY	2.0
1	D	400	ASN	2.0
1	F	149	ALA	2.0
1	G	382	ASN	2.0
1	L	11	SER	2.0
1	K	143	THR	2.0
1	C	469	THR	2.0
1	E	381	HIS	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 [\(i\)](#)

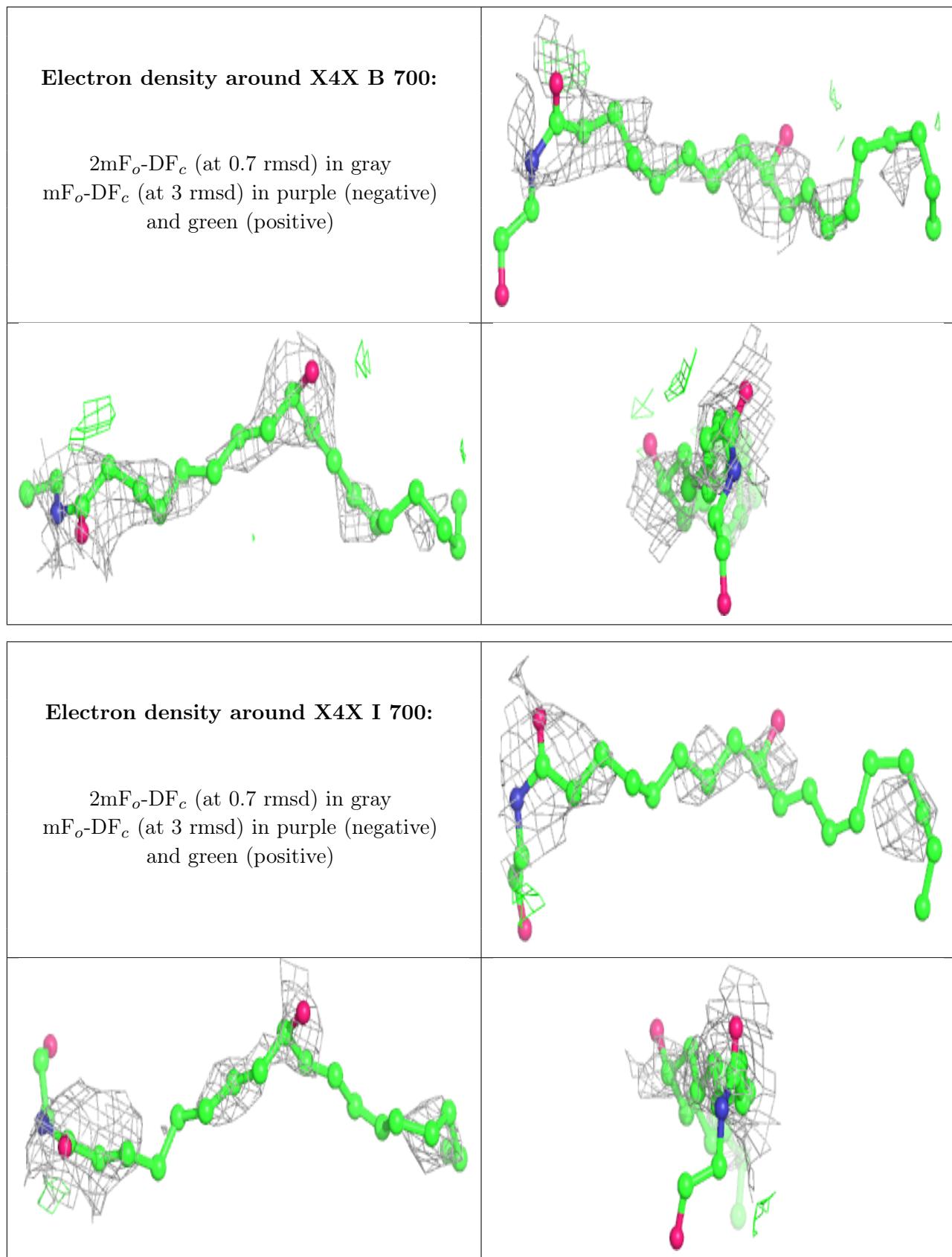
There are no monosaccharides in this entry.

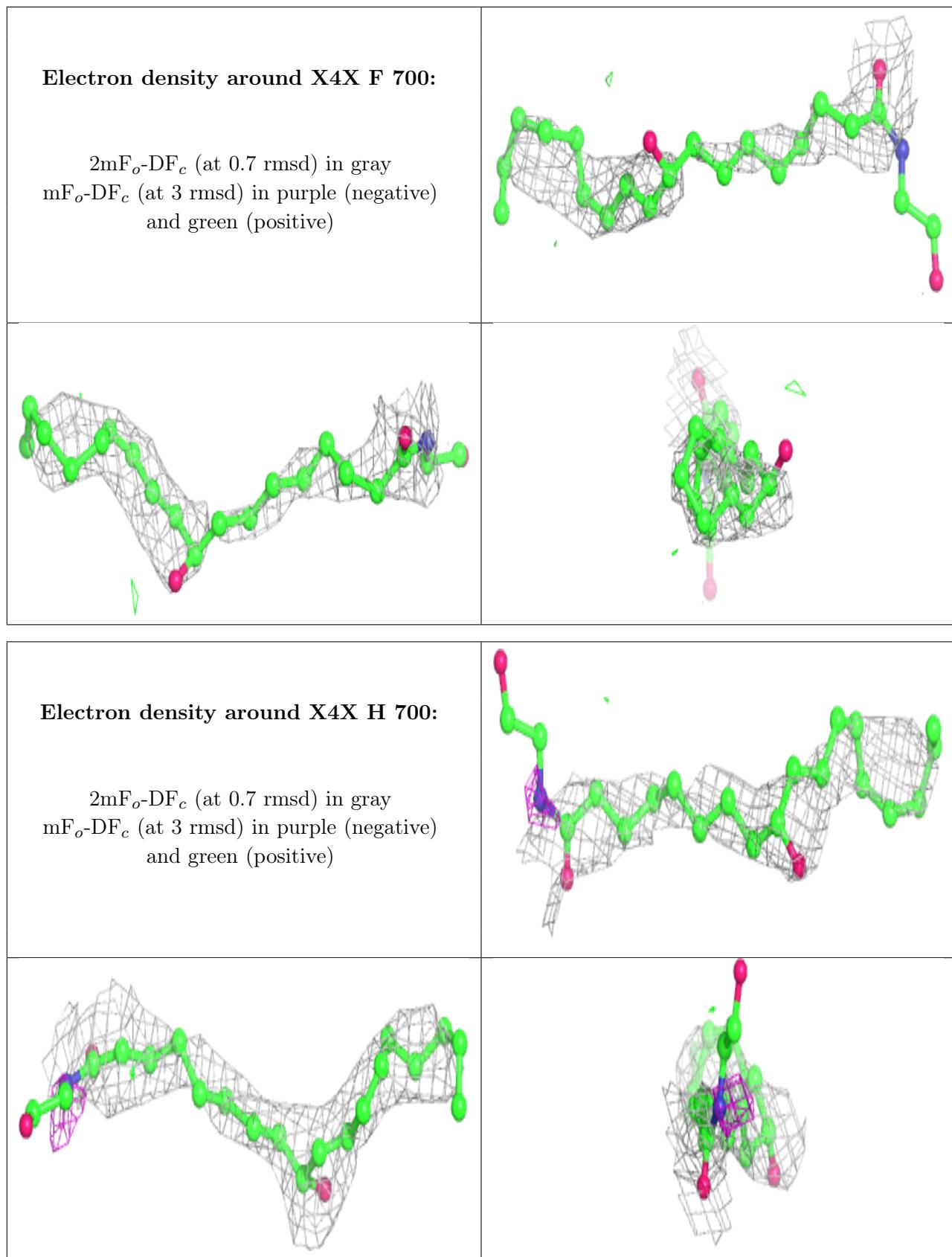
## 6.4 Ligands [\(i\)](#)

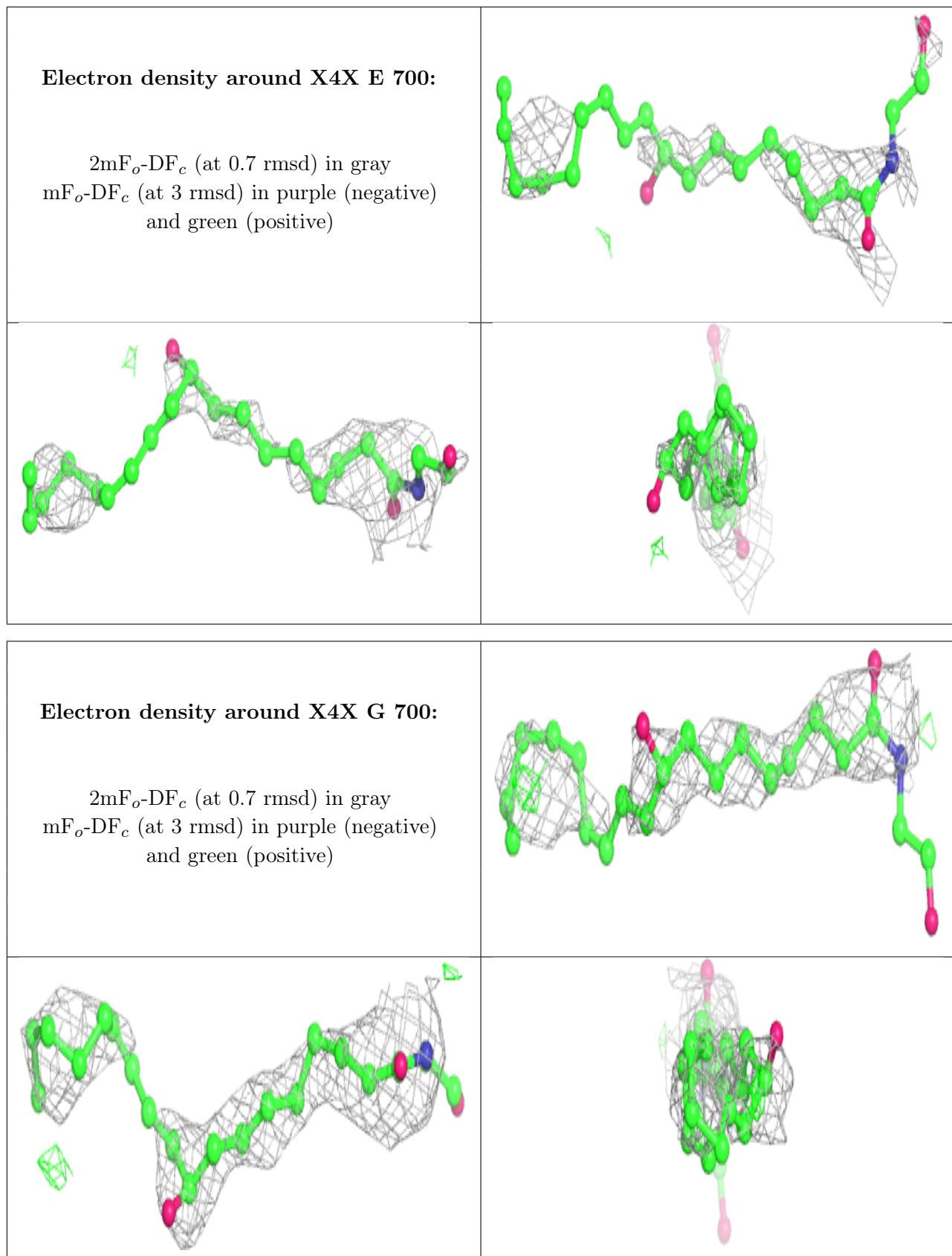
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	X4X	B	700	24/24	0.68	0.43	74,74,74,74	0
2	X4X	I	700	24/24	0.72	0.41	78,78,78,78	0
2	X4X	F	700	24/24	0.74	0.34	72,72,72,72	0
2	X4X	H	700	24/24	0.76	0.35	60,60,60,60	0
2	X4X	E	700	24/24	0.77	0.35	68,68,68,68	0
2	X4X	G	700	24/24	0.83	0.31	60,60,60,60	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.







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.